Supporting Information to 'Taking kinetic evaluation of degradation data to the next level with nonlinear mixed-effects models'

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This document gives some additional details on the generation of synthetic data, the evaluation methods and more detailed results. It should be viewed in conjunction with the main manuscript.

Generation of synthetic data

```
sampling_times = c(0, 1, 3, 7, 14, 28, 60, 90, 120)

n_groups_sfo = 5
n_groups_biphasic = 8

trans_sd = 0.5
parent_0_mean = 100
parent_0_sd = 2

n_datasets = 100

err_twocomp = list(const = 1, prop = 0.07)
```

Simple exponential decline

```
SFO <- mkinmod(parent = mkinsub("SFO"))

sfo_mean_dt50 <- c(15, 120, 500, 800)

ds_sfo <- function(geomean_dt50) {
  mean_parms_ds <- matrix(NA, nrow = n_datasets, ncol = 2,
    dimnames = list(1:n_datasets, c("parent_0", "k_parent")))
  ds <- lapply(1:n_datasets, function(i) {
    parent_0_ds <- rnorm(n_groups_sfo, parent_0_mean, parent_0_sd)
    k_parent_ds <- rlnorm(n_groups_sfo, log(log(2)/geomean_dt50), trans_sd)
    mean_parms_ds[i, "parent_0"] <<- mean(parent_0_ds)
    mean_parms_ds[i, "k_parent"] <<- geomean(k_parent_ds)

    groups_sfo <- lapply(1:n_groups_sfo, function(j) {
      group_prediction <- mkinpredict(SFO, c(k_parent = k_parent_ds[j]),
        c(parent = parent_0_ds[j]), sampling_times)
      group <- add_err(group_prediction, sdfunc = function(value) {
        sqrt(err_twocomp$const^2 + value^2 * err_twocomp$prop^2)
        }, n = 1)[[1]]
      return(group)
    })
    names(groups_sfo) <- paste("Group", 1:n_groups_sfo)
    return(groups_sfo)
  })
  list(ds = ds, mean_parms = mean_parms_ds)
}

set.seed(123456L)
sfo_data <- lapply(sfo_mean_dt50, ds_sfo)
names(sfo_data) <- paste(sfo_mean_dt50, "days")
ds_sfo_15 <- sfo_data[["15 days"]]$ds
ds_sfo_120 <- sfo_data[["120 days"]]$ds
ds_sfo_500 <- sfo_data[["500 days"]]$ds
ds_sfo_800 <- sfo_data[["800 days"]]$ds
```

Table 1: Population parameter distributions used for the synthetic SFO datasets

Parameter	Unit	Mode				Standard deviation
		Variant 1	Variant 2	Variant 3	Variant 4	Variants 1-4
p_0	[%][a]	100	100	100	100	2
Half-life	[days]	15 days	120 days	500 days	800 days	
λ	[days^{-1}]	4.62e-02	5.78e-03	1.39e-03	8.66e-04	
log(λ days)	[-]	-3.07	-5.15	-6.58	-7.05	0.5

[a] Percent of the intended initial residue

Biphasic decline with a transformation product

```
n_datasets_biphasic = 100

DFOP_SFO <- mkinmod(
  parent = mkinsub("DFOP", "m1"),
  m1 = mkinsub("SFO"),
  unload = TRUE, overwrite = TRUE, quiet = TRUE)

mean_parms_biphasic_in <- matrix(NA, nrow = n_datasets_biphasic, ncol = 6)
colnames(mean_parms_biphasic_in) <- c("parent_0", "k_m1", "f_parent_to_m1",
  "k1", "k2", "g")

set.seed(123456L)
ds_biphasic <- lapply(1:n_datasets_biphasic, function(i) {

  parms_biphasic <- as.matrix(data.frame(
    parent_0 = rnorm(n_groups_biphasic, parent_0_mean, parent_0_sd),
    k1 = rlnorm(n_groups_biphasic, log(0.05), trans_sd),
    k2 = rlnorm(n_groups_biphasic, log(0.01), trans_sd),
    g = plogis(rnorm(n_groups_biphasic, qlogis(0.5), trans_sd)),
    f_parent_to_m1 = plogis(rnorm(n_groups_biphasic, qlogis(0.5), trans_sd)),
    k_m1 = rlnorm(n_groups_biphasic, log(0.002), trans_sd)))

  mean_parms_biphasic_in[i, "parent_0"] <<- mean(parms_biphasic[, "parent_0"])
  mean_parms_biphasic_in[i, "k_m1"] <<- geomean(parms_biphasic[, "k_m1"])
  mean_parms_biphasic_in[i, "f_parent_to_m1"] <<- plogis(mean(qlogis(parms_biphasic[, "f_paren
  mean_parms_biphasic_in[i, "k1"] <<- geomean(parms_biphasic[, "k1"])
  mean_parms_biphasic_in[i, "k2"] <<- geomean(parms_biphasic[, "k2"])
  mean_parms_biphasic_in[i, "g"] <<- plogis(mean(qlogis(parms_biphasic[, "g"])))

  ds_biphasic_mean <- lapply(1:n_groups_biphasic,
    function(i) {
      mkinpredict(DFOP_SFO, parms_biphasic[i, 2:6],
        c(parent = parms_biphasic[[i, 1]], m1 = 0), sampling_times)
    }
  )

  ds_biphasic_tmp <- lapply(ds_biphasic_mean, function(ds) {
    add_err(ds,
      sdfunc = function(value) sqrt(err_twocomp$const^2 + value^2 * err_twocomp$prop^2),
      n = 1, secondary = "m1")[[1]]
  })

  names(ds_biphasic_tmp) <- paste("Group", 1:n_groups_biphasic)
  return(ds_biphasic_tmp)

})
```

Table 2: Population parameter distributions used for the synthetic DFOP-SFO datasets

Parameter	Variable	Unit	Mode	Standard deviation
p_0	`parent_0`	[%][a]	100	2
λ_1	`k1`	[days^{-1}]	0.05	
log(λ_1 days)		[-]	-3	0.5
λ_2	`k2`	[days^{-1}]	0.01	
log(λ_2 days)		[-]	-4.61	0.5
γ_1	`g`	[-]	0.5	
logit γ_1		[-]	0	0.5
γ_2	`f_parent_to_m1`	[-]	0.5	
logit γ_2		[-]	0	0.5
λ_3	`k_m1`	[days^{-1}]	0.002	
log(λ_3 days)		[-]	-6.21	0.5

[a] Percent of the intended initial residue

Evaluation of synthetic data

Simple exponential decline

Geometric mean half-life of 15 days

Example plots for separate fits in one of the datasets are shown in Figures 1 and 2. The same separate fits combined in a single plot, together with a plot using the geometric mean half-life are shown in Figures 3 and 4. Corresponding example plots of the simultaneous evaluation of this dataset using saemix are shown in Figures 5 and 6.

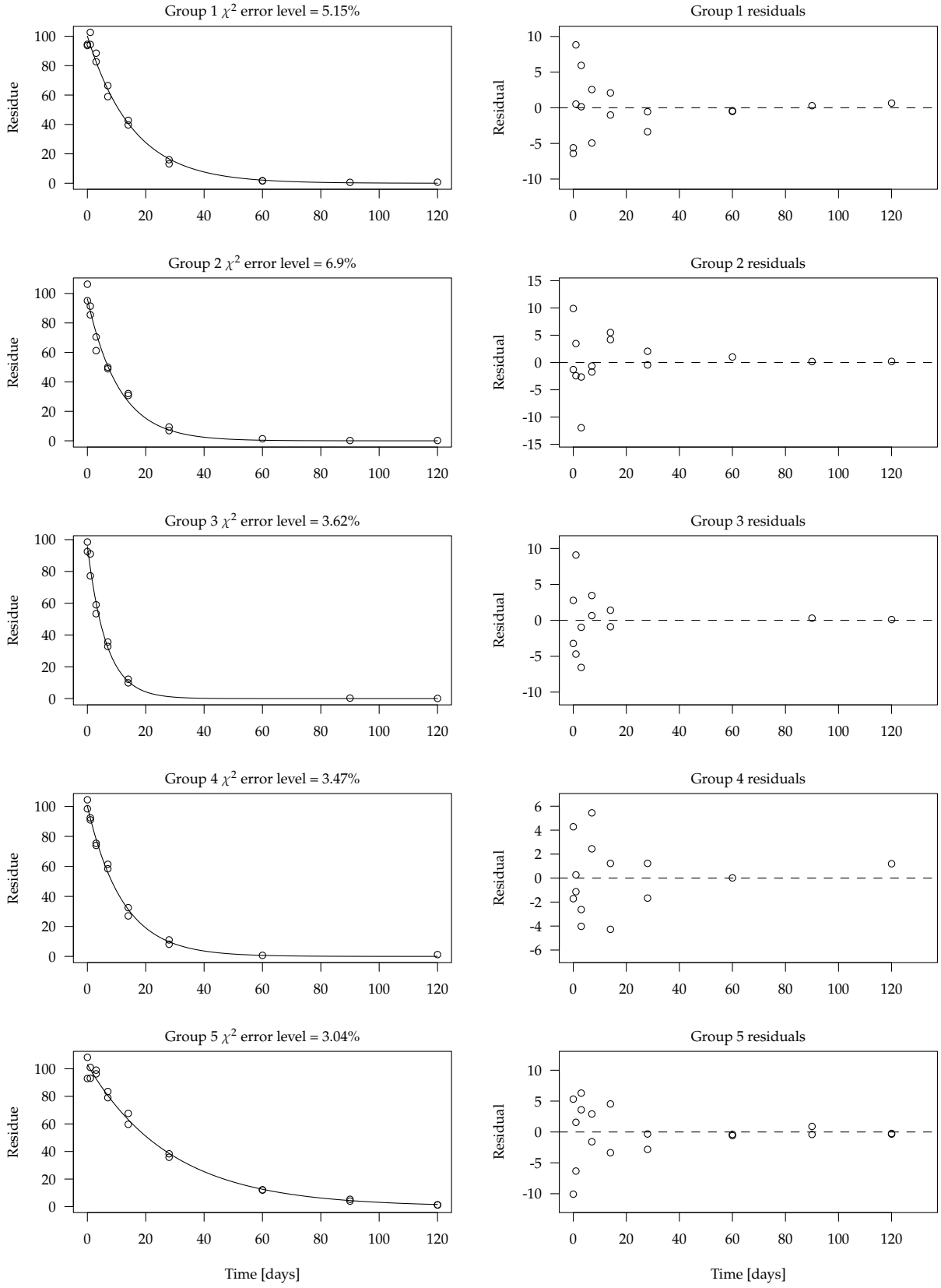

Figure 1: Separate fits to an example dataset with mean input half-life 15 days, constant variance error model

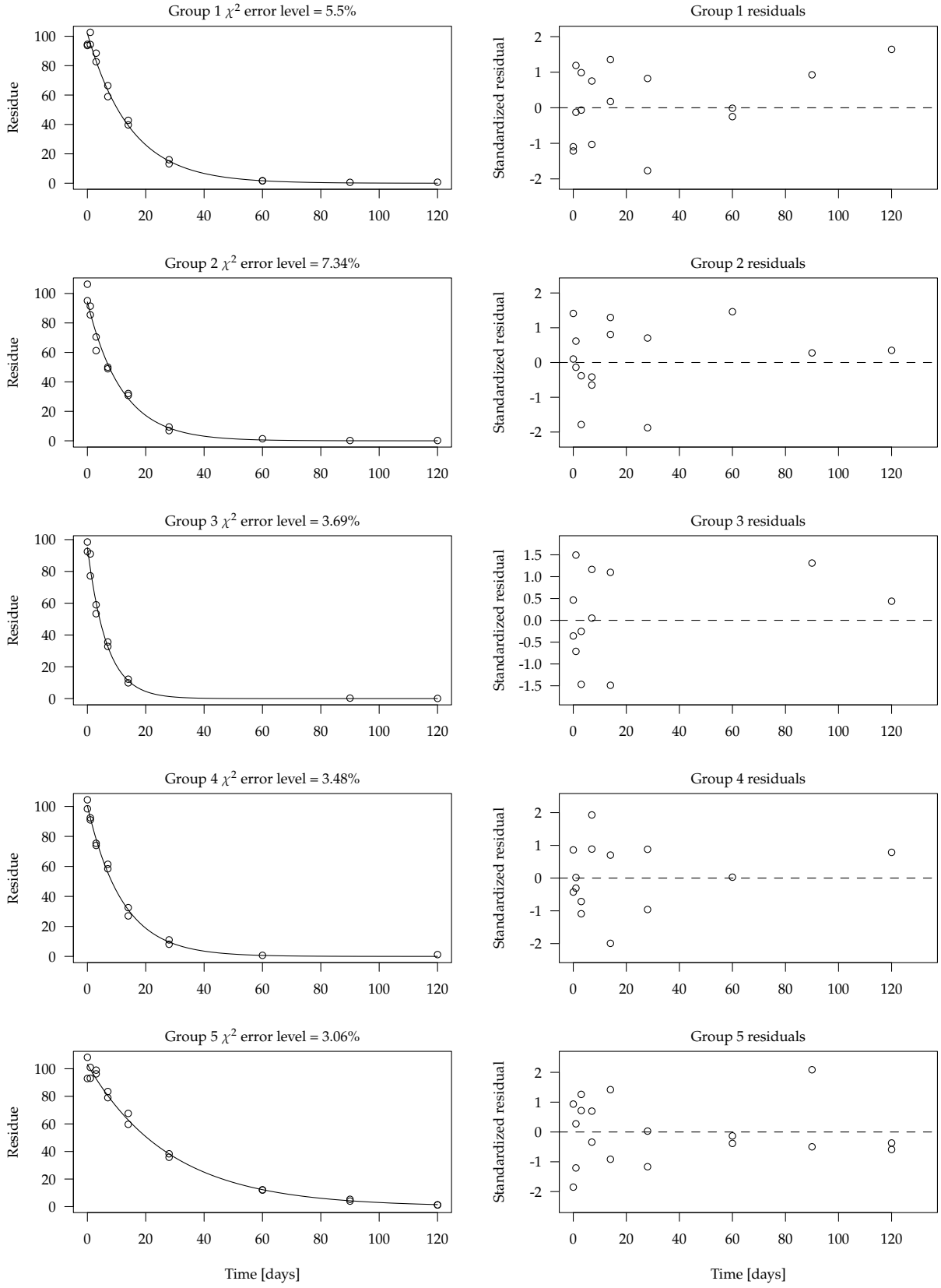

Figure 2: Separate fits to an example dataset with mean input half-life 15 days, two-component error model

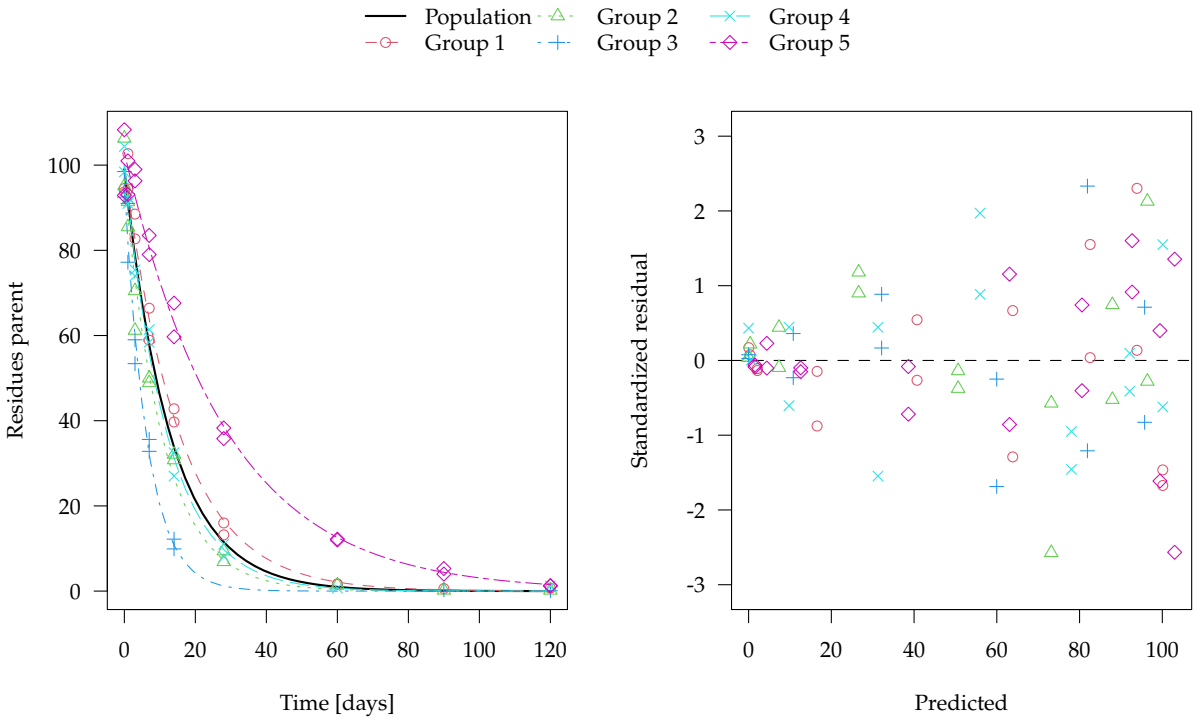

Figure 3: Combined plot of separate fits to an example dataset with mean input half-life 15 days, constant variance error model

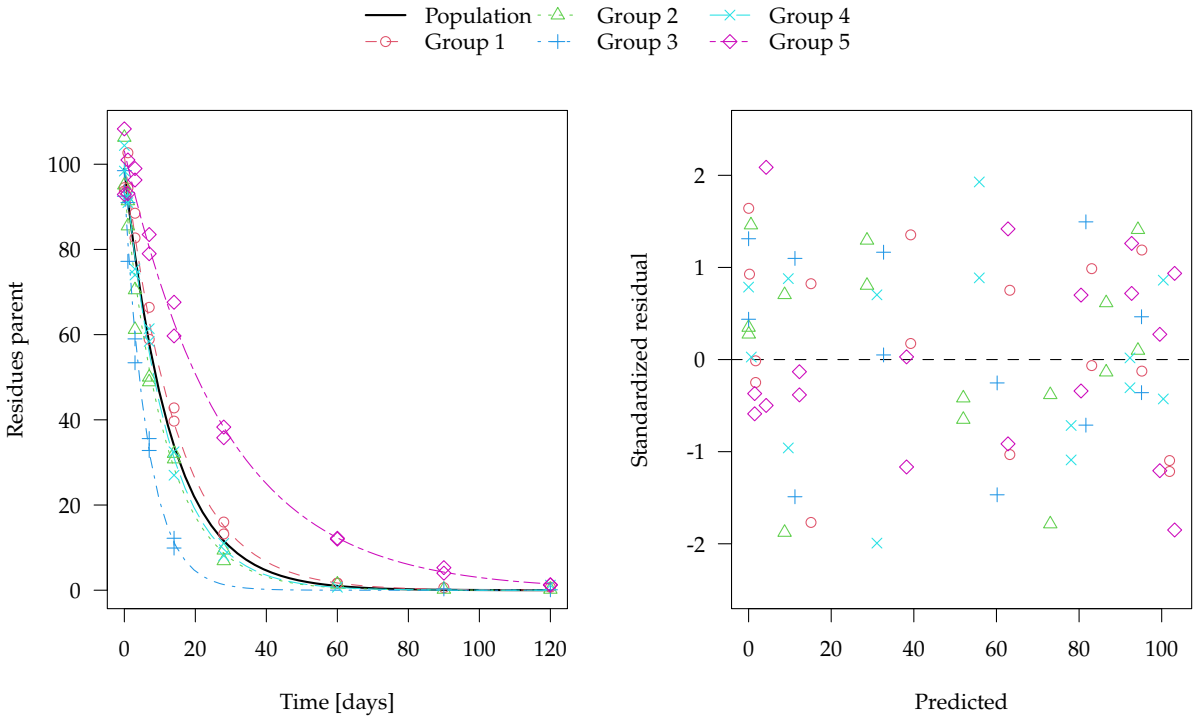

Figure 4: Combined plot of separate fits to an example dataset with mean input half-life 15 days, two-component error model

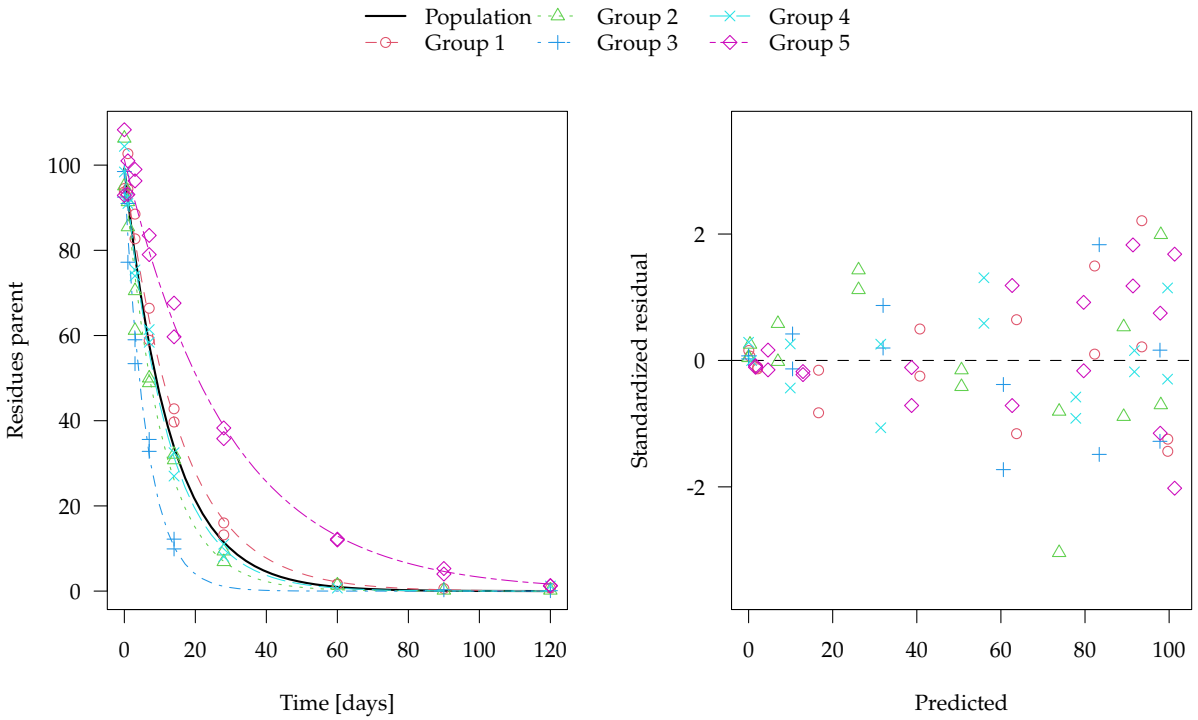

Figure 5: SFO fit with saemix to an example dataset with mean input half-life 15 days, constant variance

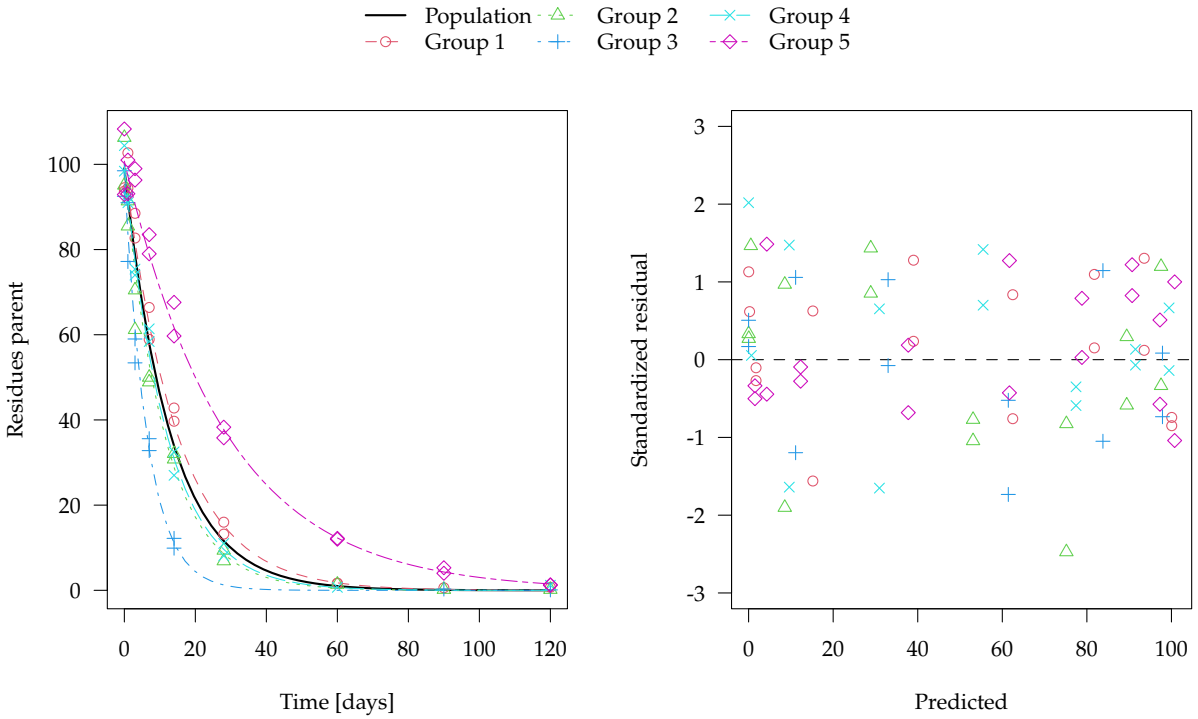

Figure 6: SFO fit with saemix to an example dataset with mean input half-life 15 days, two-component error model

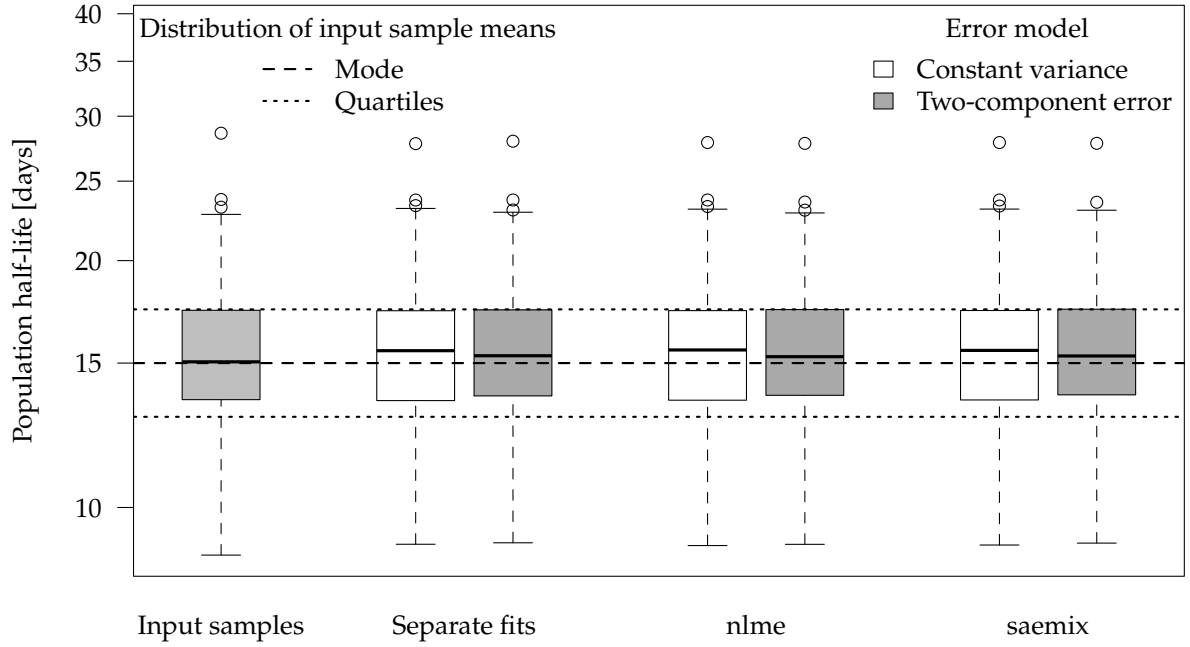

Figure 7: Boxplots of half-lives derived from 100 datasets for five groups, input 15 days

Table 3: Statistics for half-lives derived from 100 datasets with five groups, input half-life 15 days

	Input parameters		Separate fits		nlme		saemix	
	Distribution	**Sample means**	**const**	**tc**	**const**	**tc**	**const**	**tc**
Number of results			500	500	100	100	100	100
Fits with lower AIC			11	489	0	100	1	99
Minimum		8.749	9.019	9.056	8.986	9.017	9.000	9.048
25th percentile	12.90	13.555	13.524	13.691	13.549	13.705	13.566	13.724
Median	15.00	15.053	15.530	15.312	15.563	15.272	15.544	15.303
75th percentile	17.44	17.358	17.326	17.382	17.336	17.416	17.346	17.438
Maximum		28.600	27.775	27.964	27.863	27.796	27.860	27.801

Geometric mean half-life of 120 days

Example plots for separate fits in one of the synthetic datasets are shown in Figures 8 and 9. Corresponding example plots of the simultaneous evaluation of this dataset using saemix are shown in Figures 12 and 13.

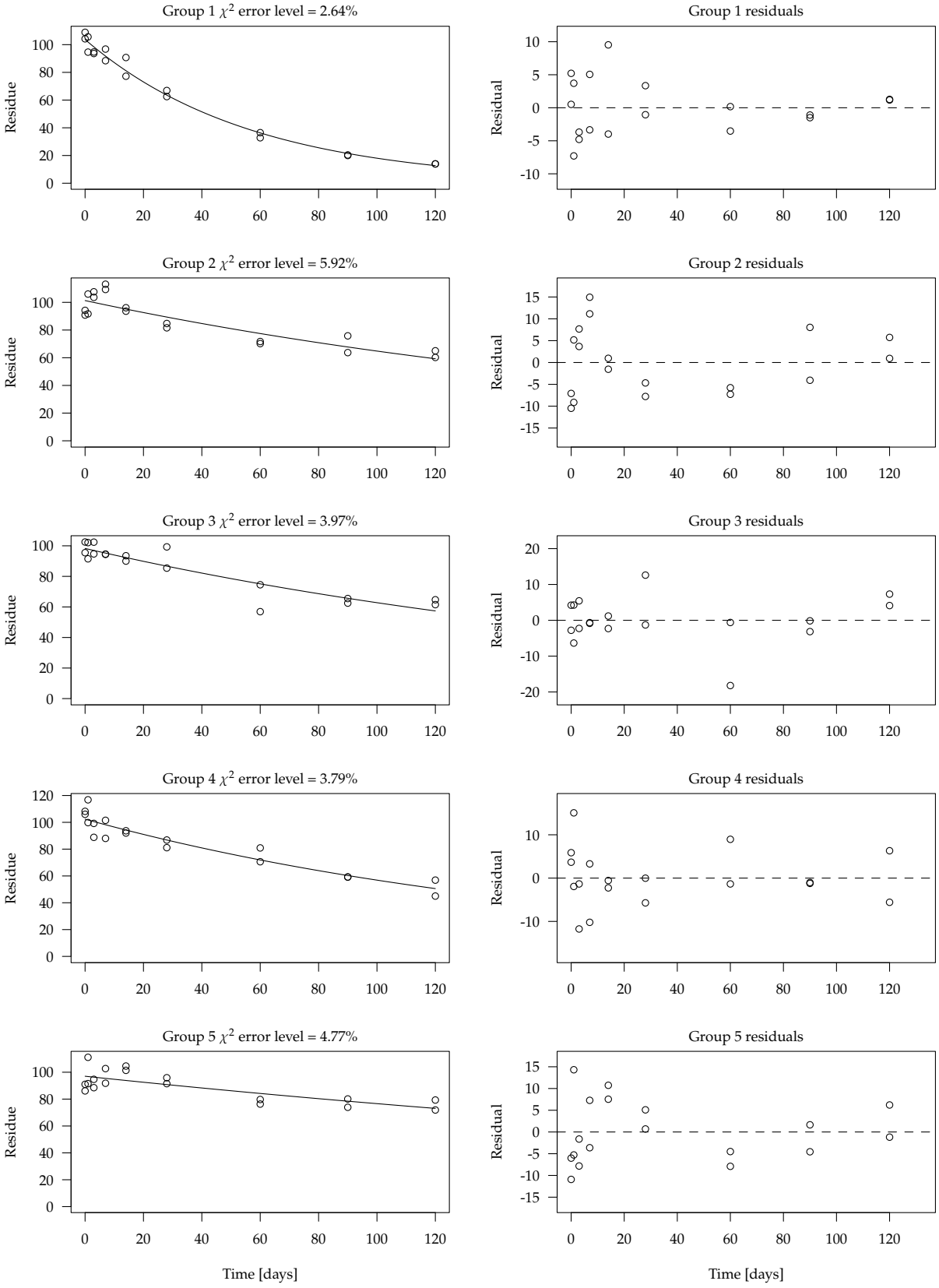

Figure 8: Separate fits to an example dataset with mean input half-life 120 days, constant variance error model

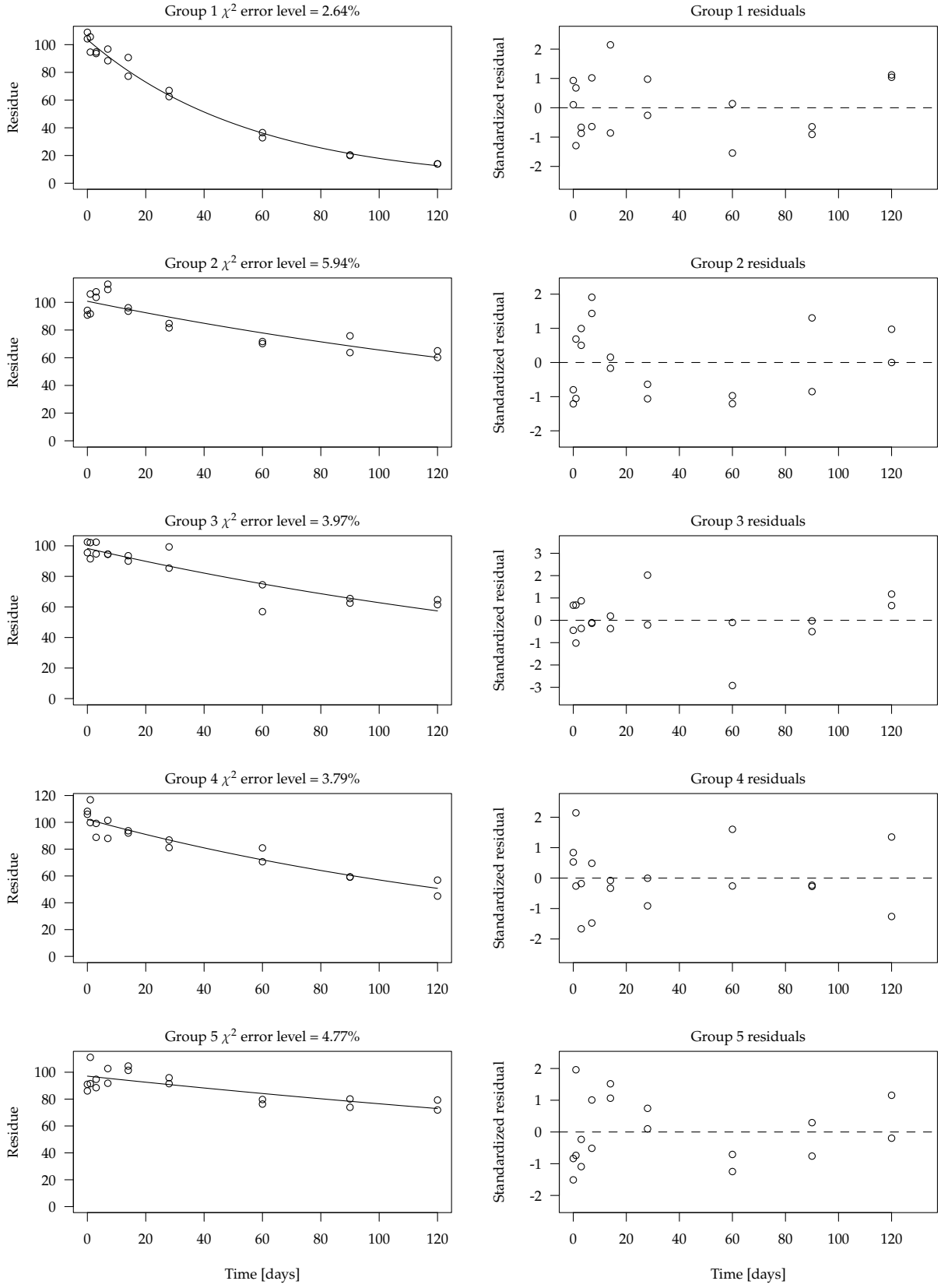

Figure 9: Separate fits to an example dataset with mean input half-life 120 days, two-component error model

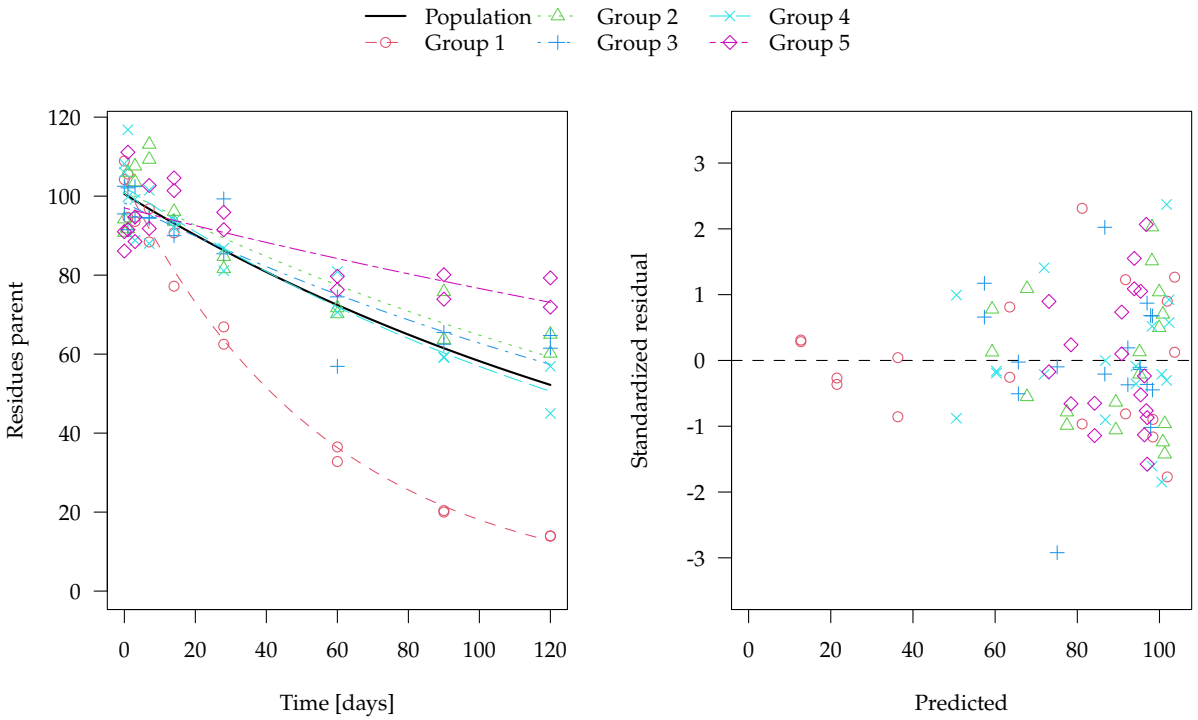

Figure 10: Combined plot of separate fits to an example dataset with mean input half-life 120 days, constant variance error model

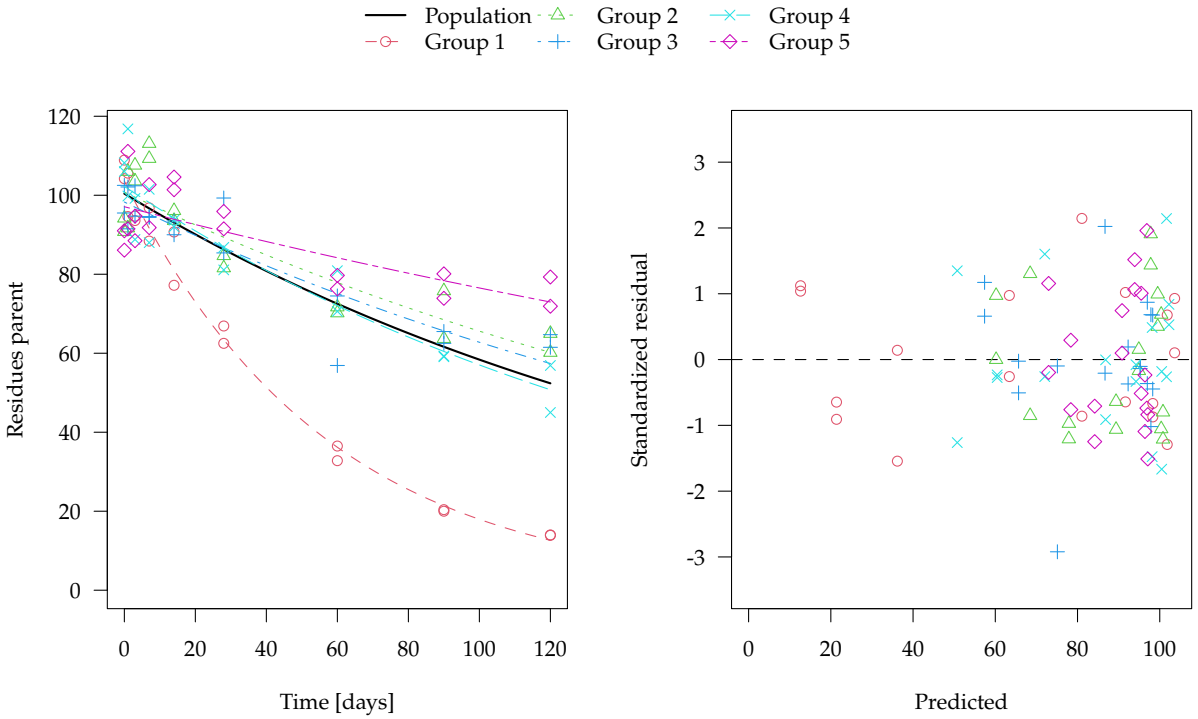

Figure 11: Combined plot of separate fits to an example dataset with mean input half-life 120 days, two-component error model

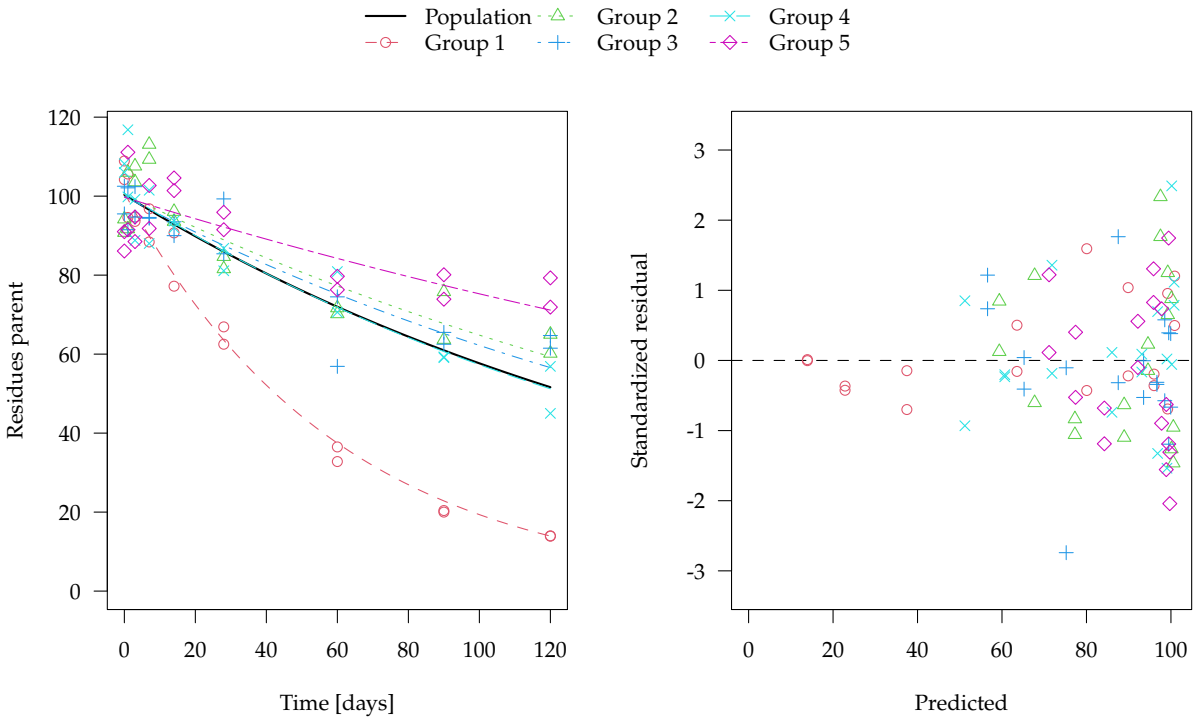

Figure 12: SFO fit with saemix to an example dataset with mean input half-life 120 days, constant variance

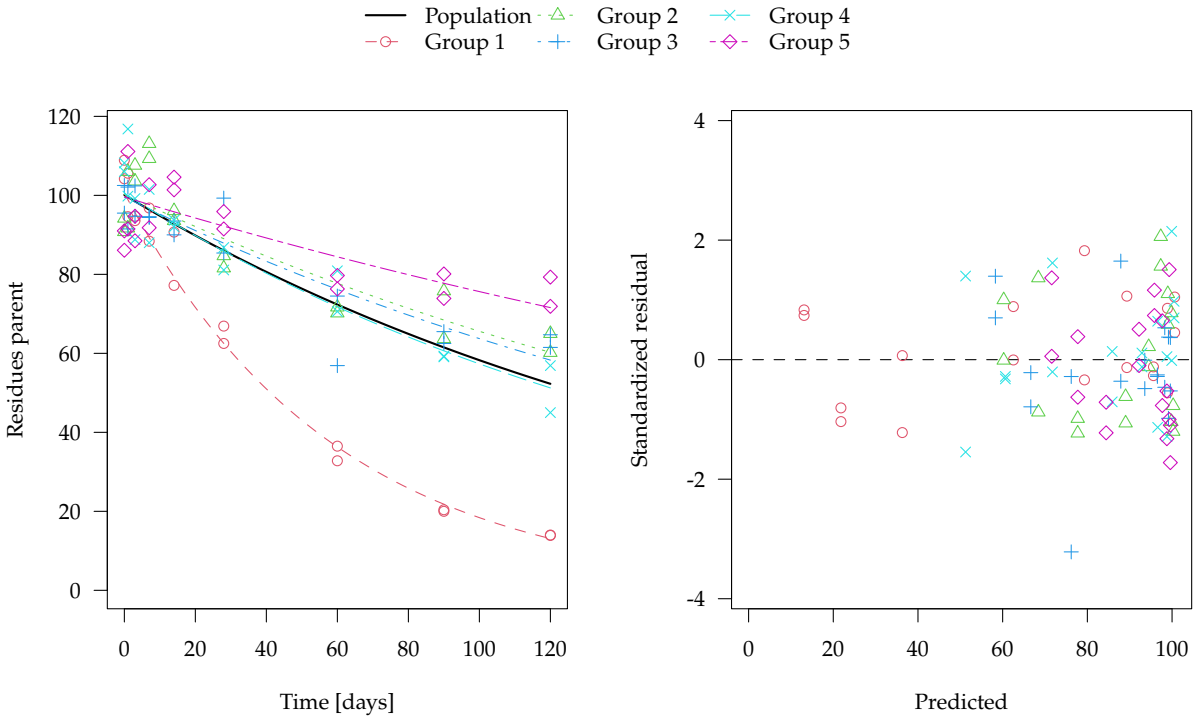

Figure 13: SFO fit with saemix to an example dataset with mean input half-life 120 days, two-component error model

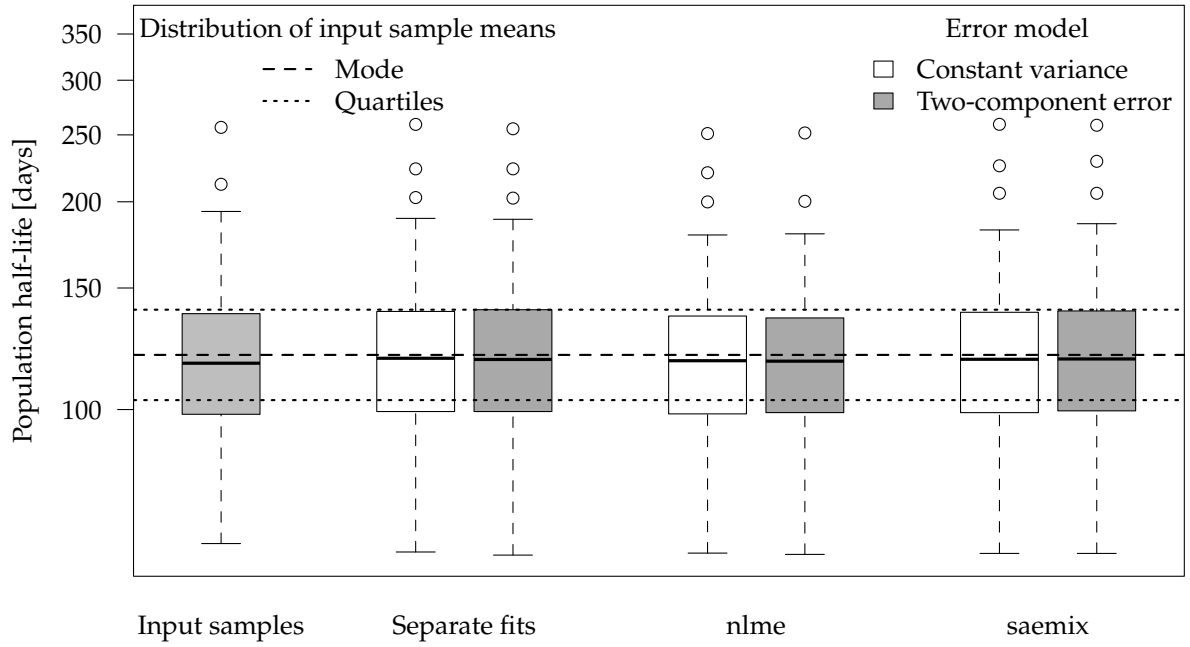

Figure 14: Boxplots of half-lives derived from 100 datasets for five groups, input 120 days

Table 4: Statistics for half-lives derived from 100 datasets with five groups, input half-life 120 days

	Input parameters		**Separate fits**		**nlme**		**saemix**	
	Distribution	**Sample means**	**const**	**tc**	**const**	**tc**	**const**	**tc**
Number of results			500	500	100	99	100	100
Fits with lower AIC			254	246	7	92	14	86
Minimum		63.95	62.18	61.53	61.95	61.68	61.88	61.88
25th percentile	103.2	98.54	99.70	99.75	98.95	98.99	99.37	100.04
Median	120.0	116.71	118.66	118.18	117.69	117.51	118.26	118.38
75th percentile	139.5	137.48	138.35	139.34	136.57	135.75	137.99	138.57
Maximum		256.33	258.88	255.12	251.11	251.59	258.96	258.15

Geometric mean half-life of 500 days

Example plots for separate fits in one of the synthetic datasets are shown in Figures 15 and 16. Corresponding example plots of the simultaneous evaluation of this dataset using saemix are shown in Figures 19 and 20.

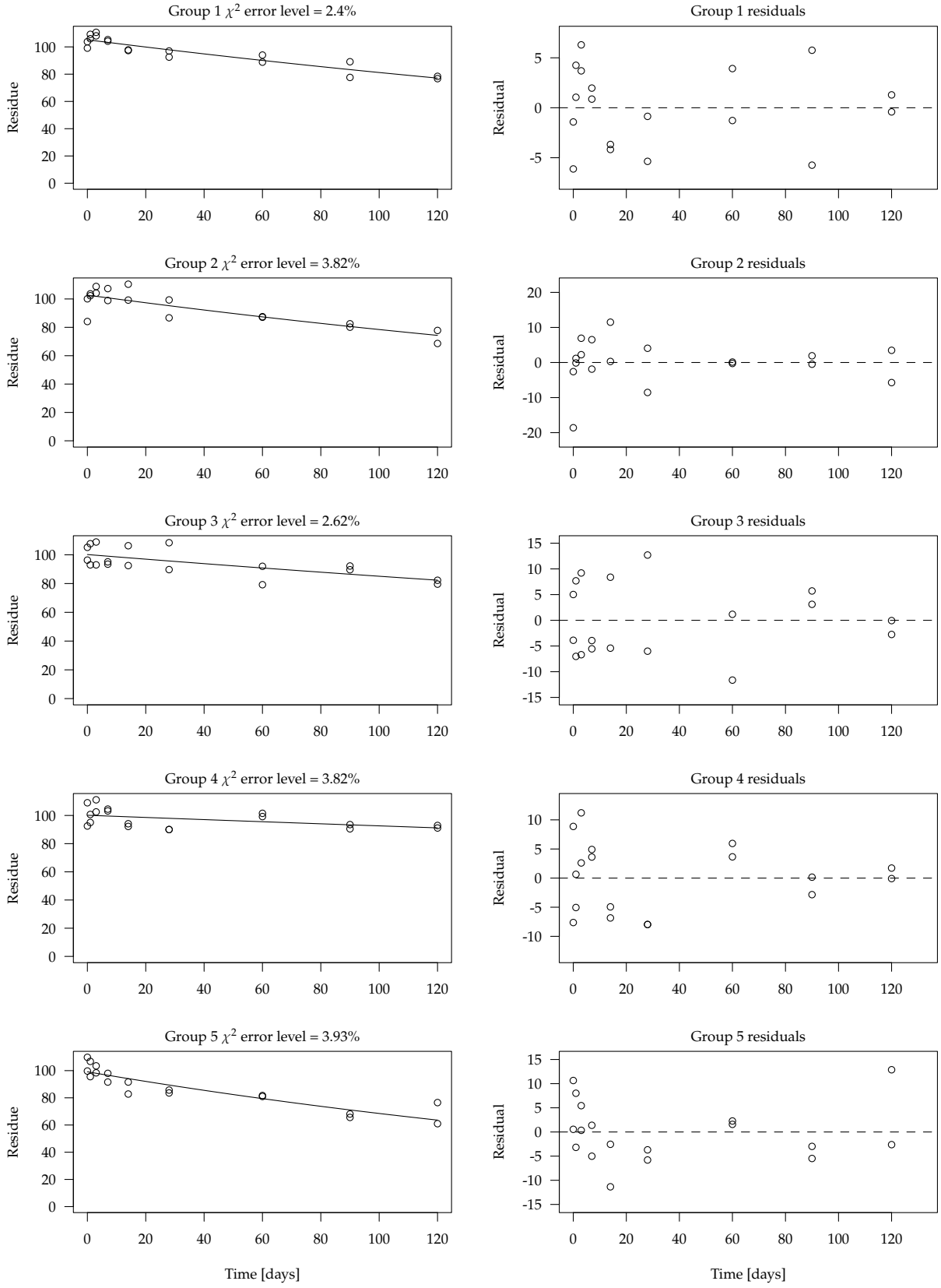

Figure 15: Separate fits to an example dataset with mean input half-life 500 days, constant variance error model

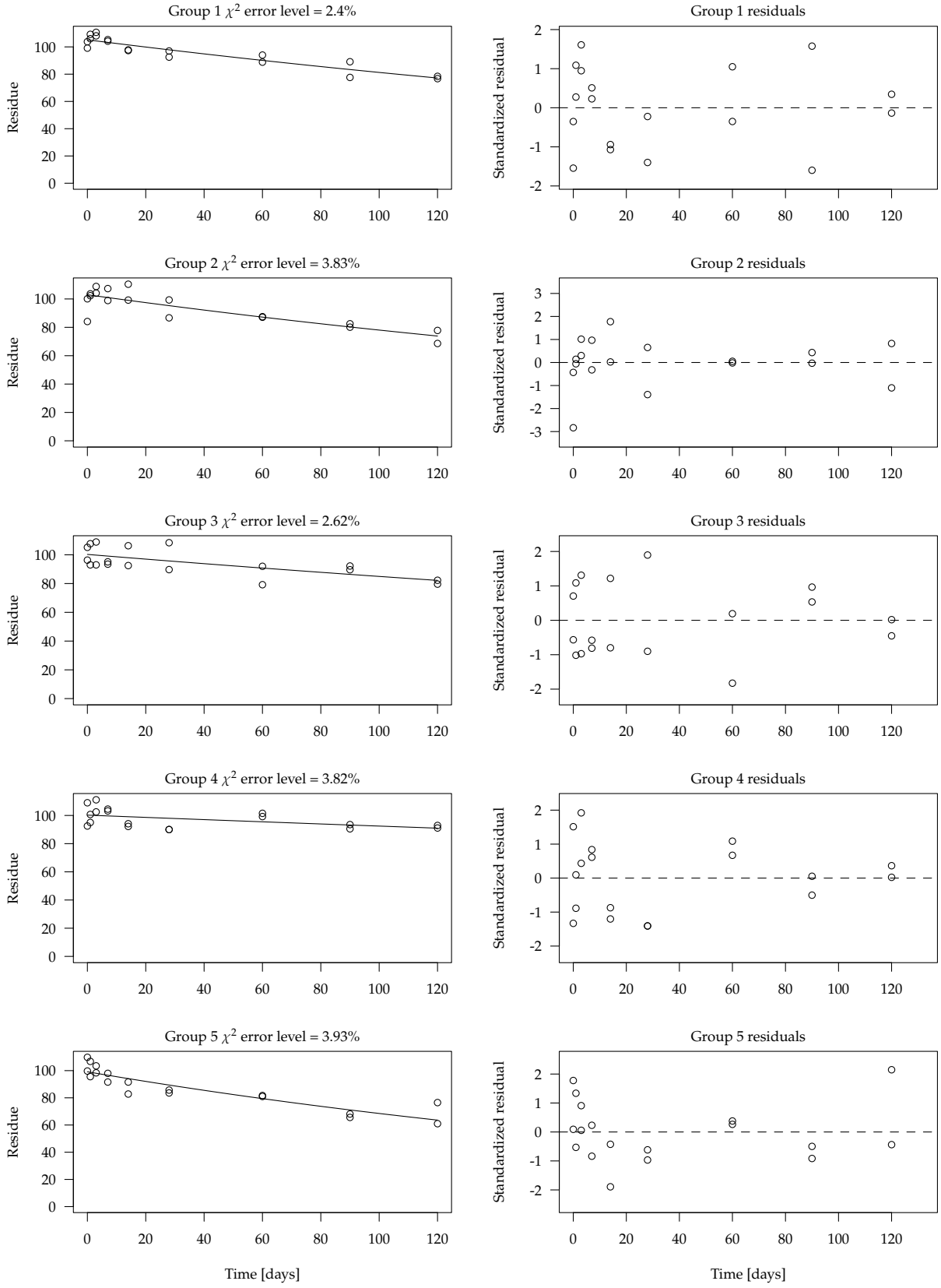

Figure 16: Separate fits to an example dataset with mean input half-life 500 days, two-component error model

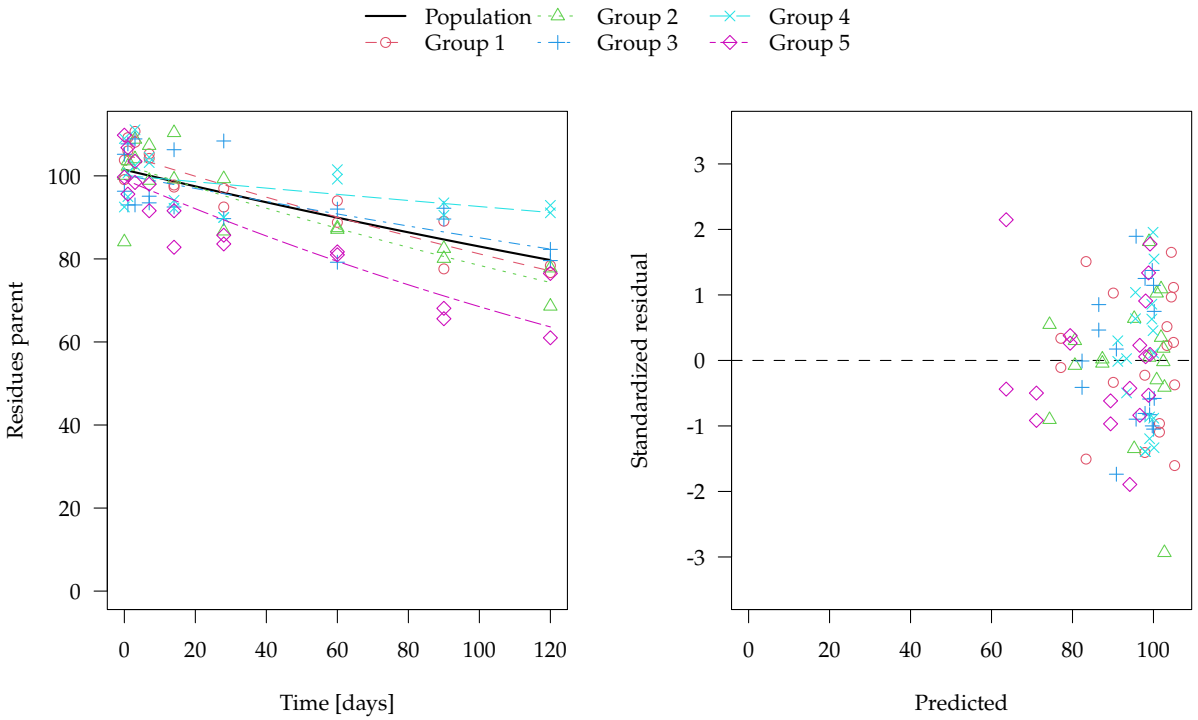

Figure 17: Combined plot of separate fits to an example dataset with mean input half-life 500 days, constant variance error model

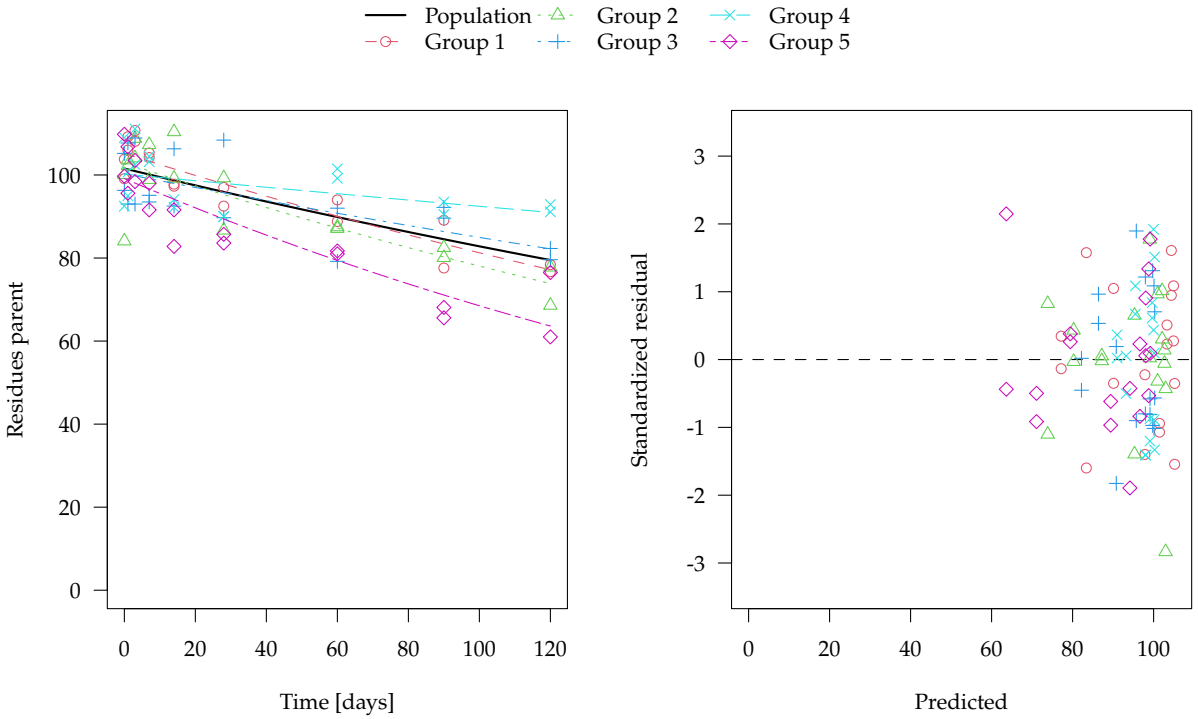

Figure 18: Combined plot of separate fits to an example dataset with mean input half-life 500 days, two-component error model

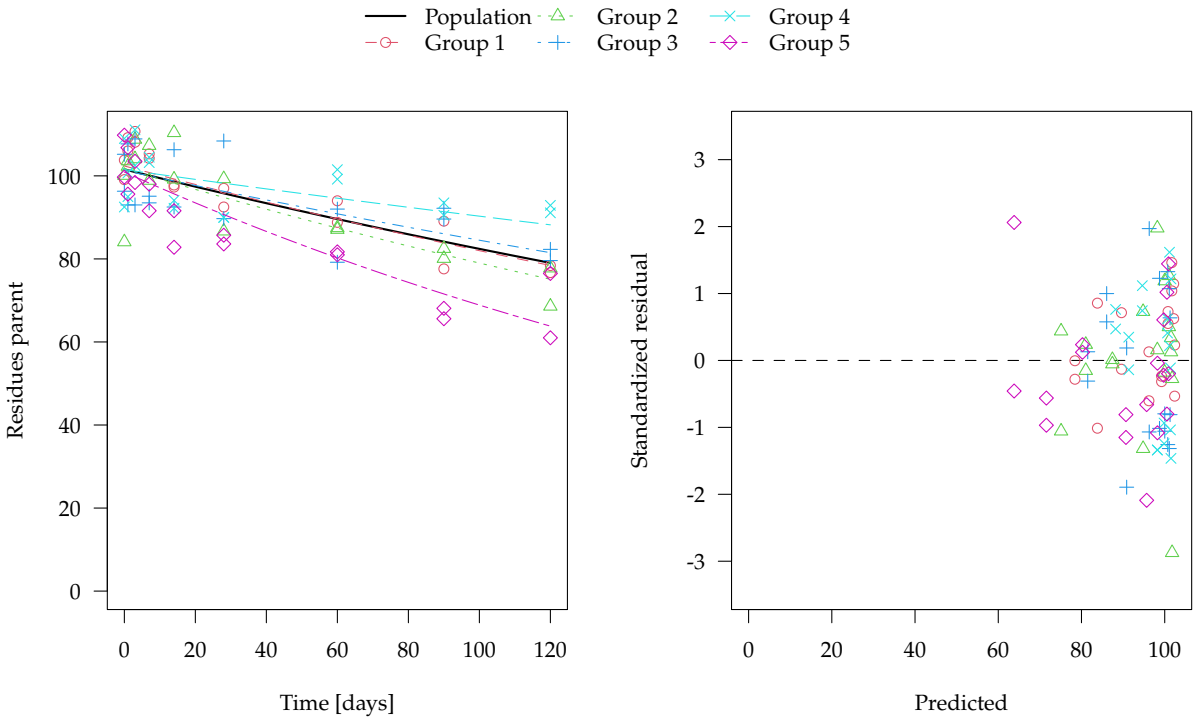

Figure 19: SFO fit with saemix to an example dataset with mean input half-life 500 days, constant variance

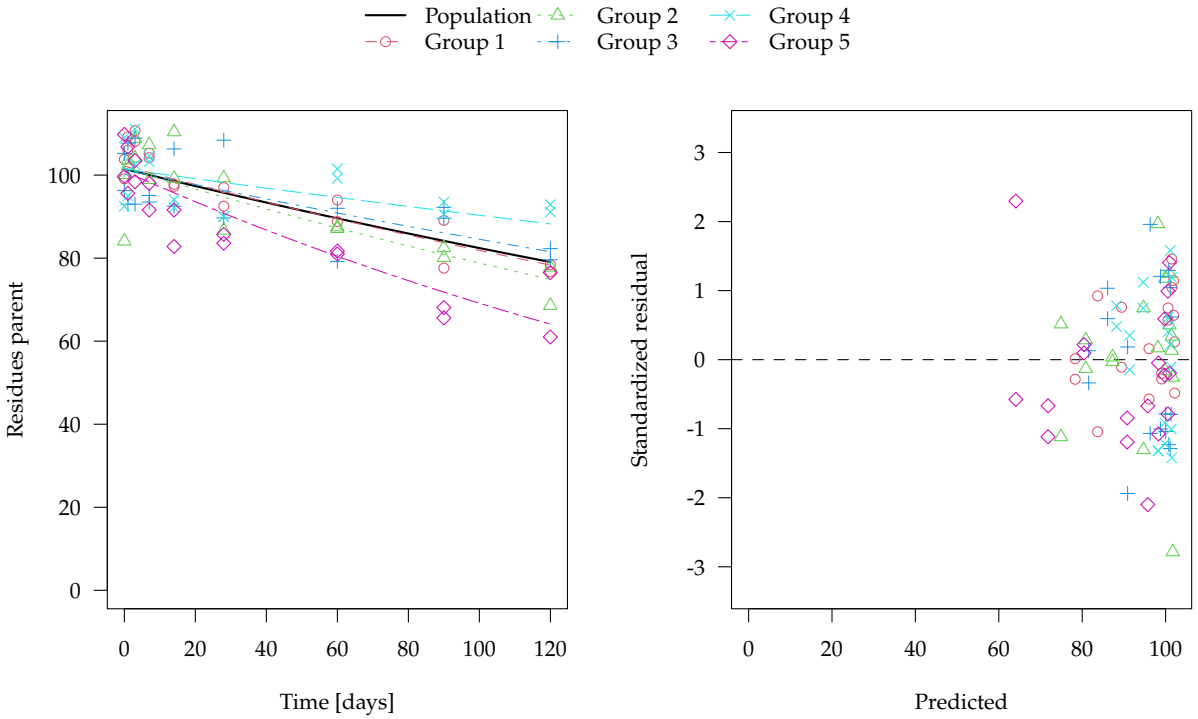

Figure 20: SFO fit with saemix to an example dataset with mean input half-life 500 days, two-component error model

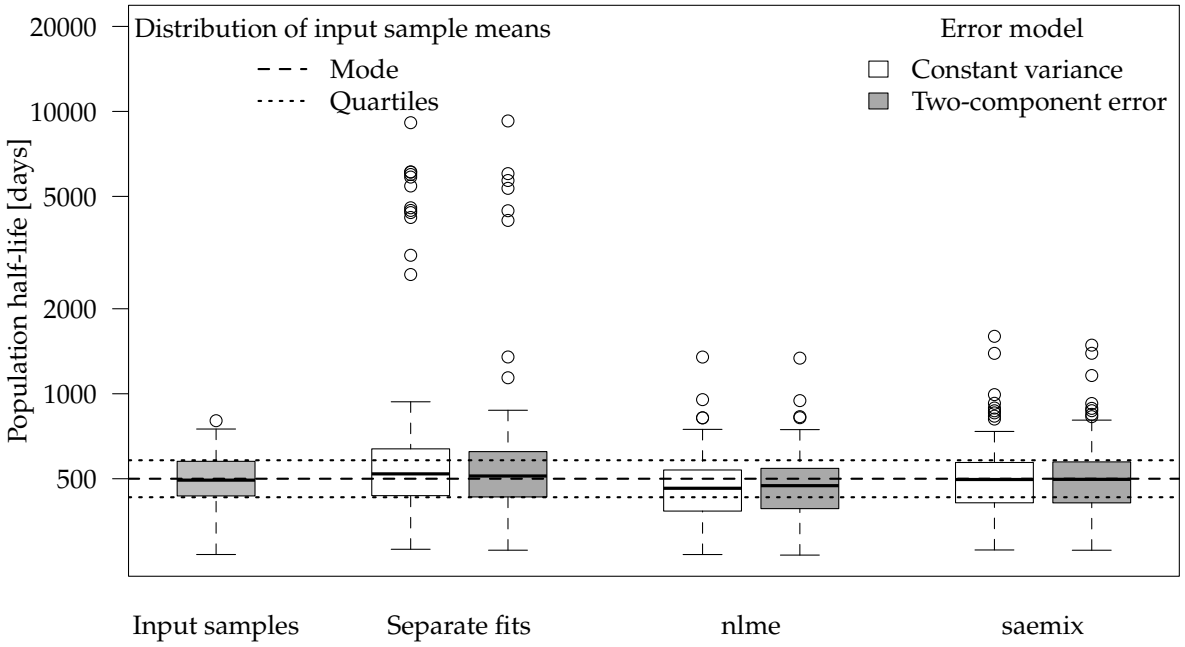

Figure 21: Boxplots of half-lives derived from 100 datasets for five groups, input 500 days

Table 5: Statistics for half-lives derived from 100 datasets with five groups, input half-life 500 days

	Input parameters		Separate fits		nlme		saemix	
	Distribution	**Sample means**	**const**	**tc**	**const**	**tc**	**const**	**tc**
Number of results			500	500	98	85	100	100
Fits with lower AIC			484	16	69	16	78	22
Minimum		269.5	281.3	279.2	269.4	268.2	279.7	279.1
25th percentile	430.0	436.3	438.3	431.5	384.6	391.8	411.6	410.8
Median	500.0	494.4	520.3	511.3	462.6	472.6	496.9	497.5
75th percentile	581.4	576.2	636.9	622.6	536.8	544.2	570.7	573.6
Maximum		802.6	76701.3	42666.4	1349.0	1337.0	1597.3	1486.4

Geometric mean half-life of 800 days

Example plots for separate fits in one of the five synthetic datasets are shown in Figures 22 and 23. Corresponding example plots of the simultaneous evaluation of this dataset using saemix are shown in Figures 26 and 27. A direct comparison of separate and simultaneous evaluations is shown in Figure 28.

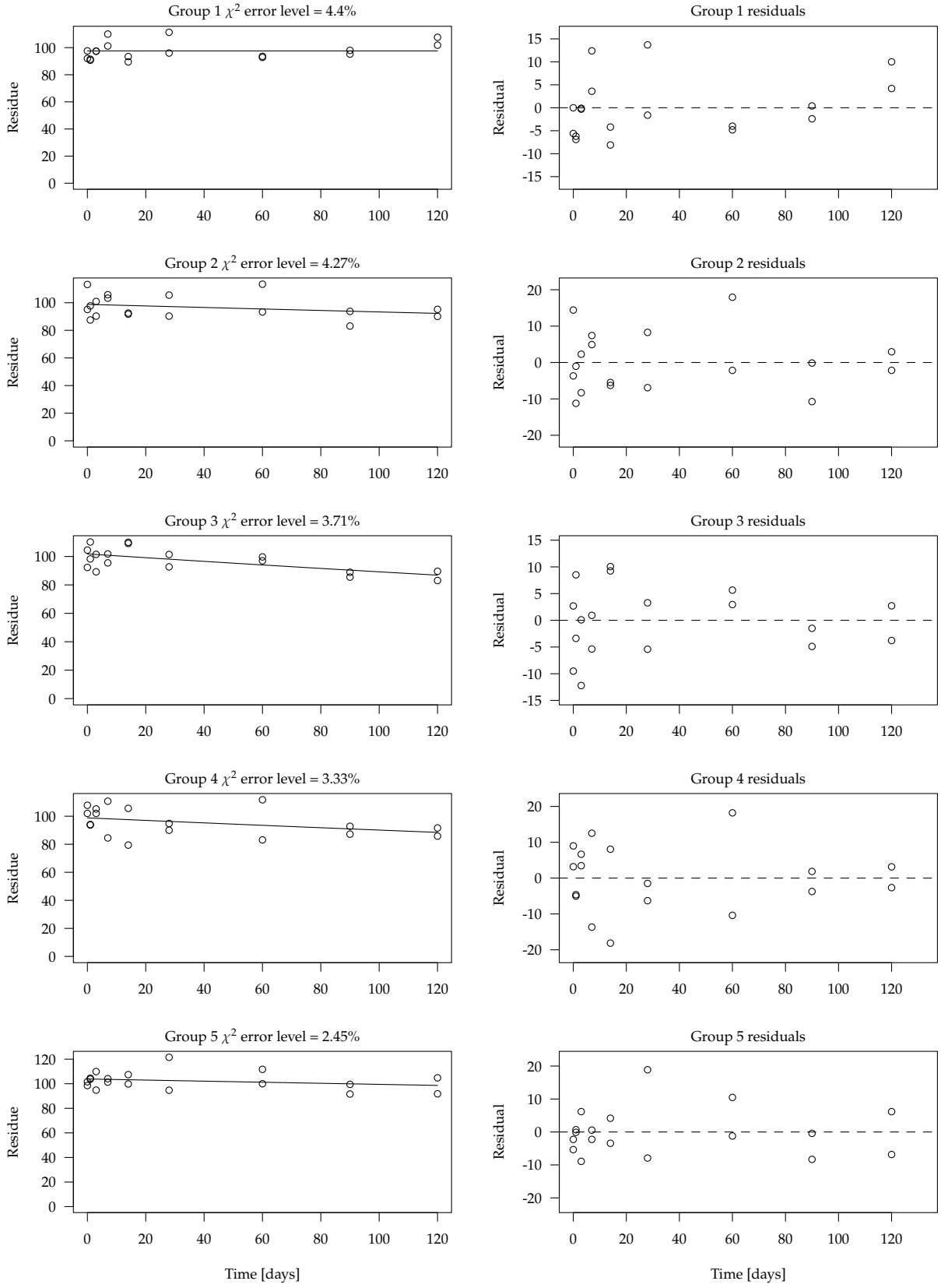

Figure 22: Separate fits to an example dataset with mean input half-life 800 days, constant variance error model

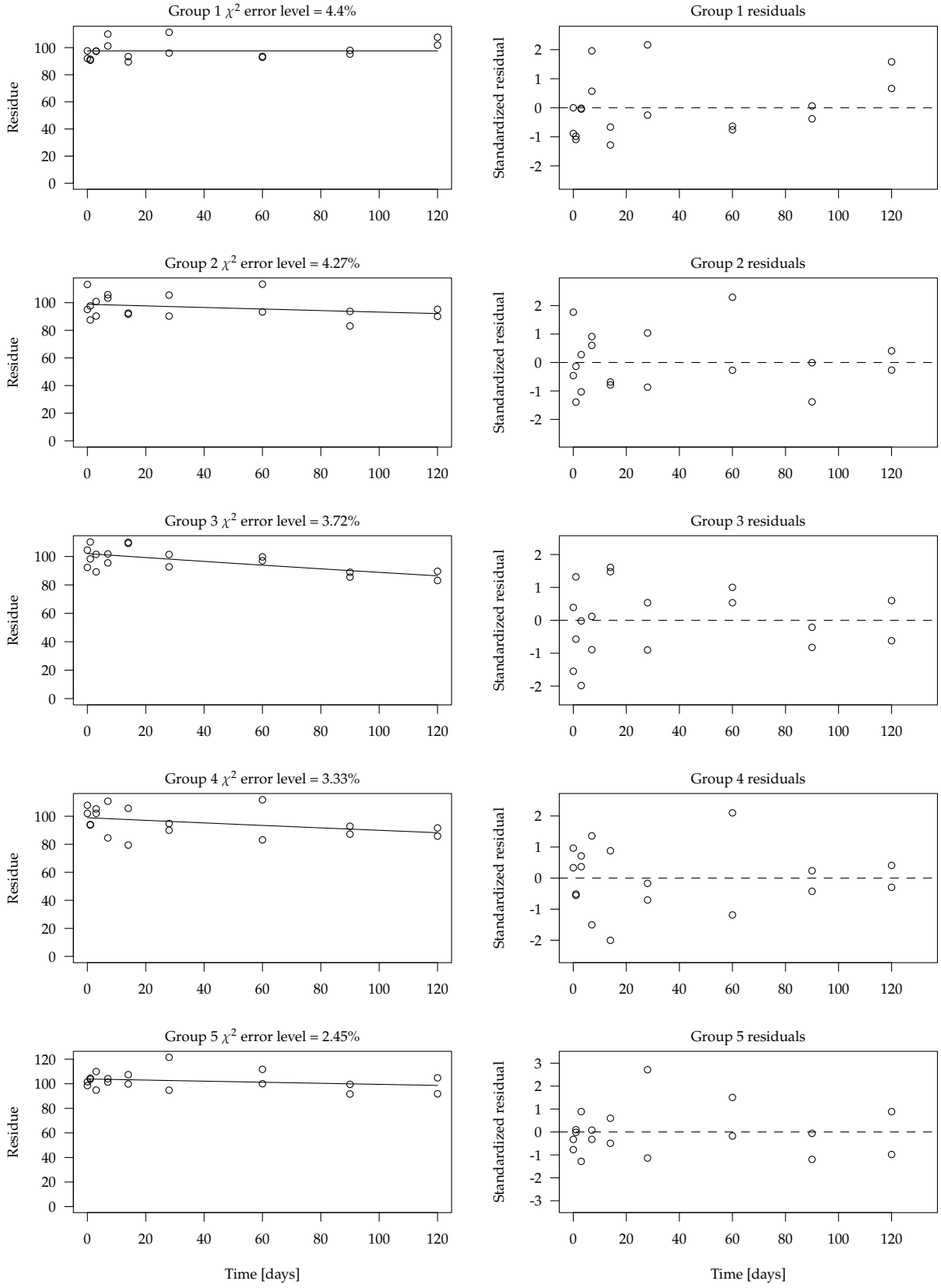

Figure 23: Separate fits to an example dataset with mean input half-life 800 days, two-component error model

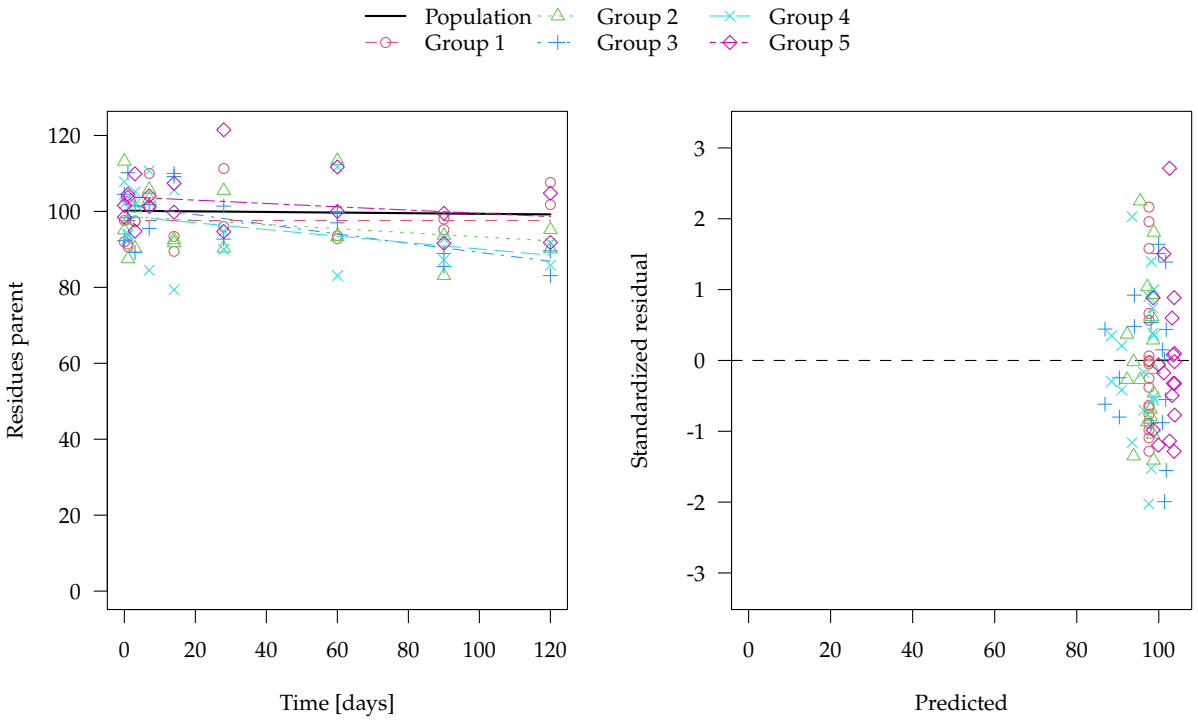

Figure 24: Combined plot of separate fits to an example dataset with mean input half-life 800 days, constant variance error model

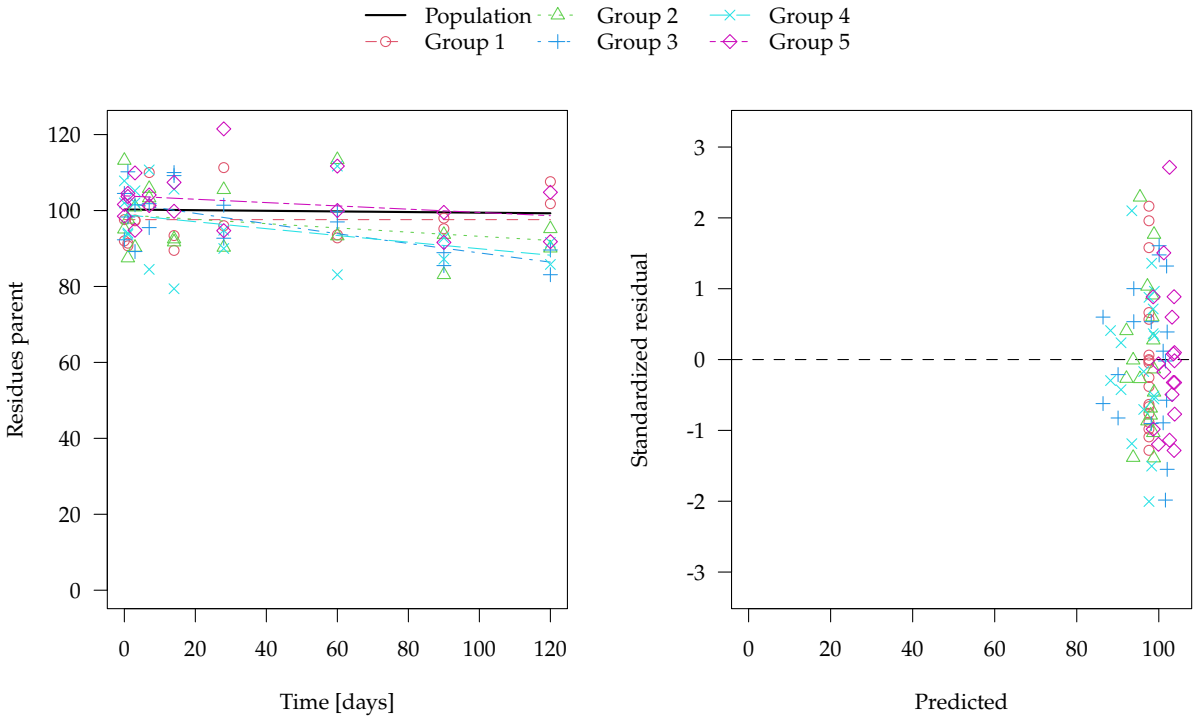

Figure 25: Combined plot of separate fits to an example dataset with mean input half-life 800 days, two-component error model

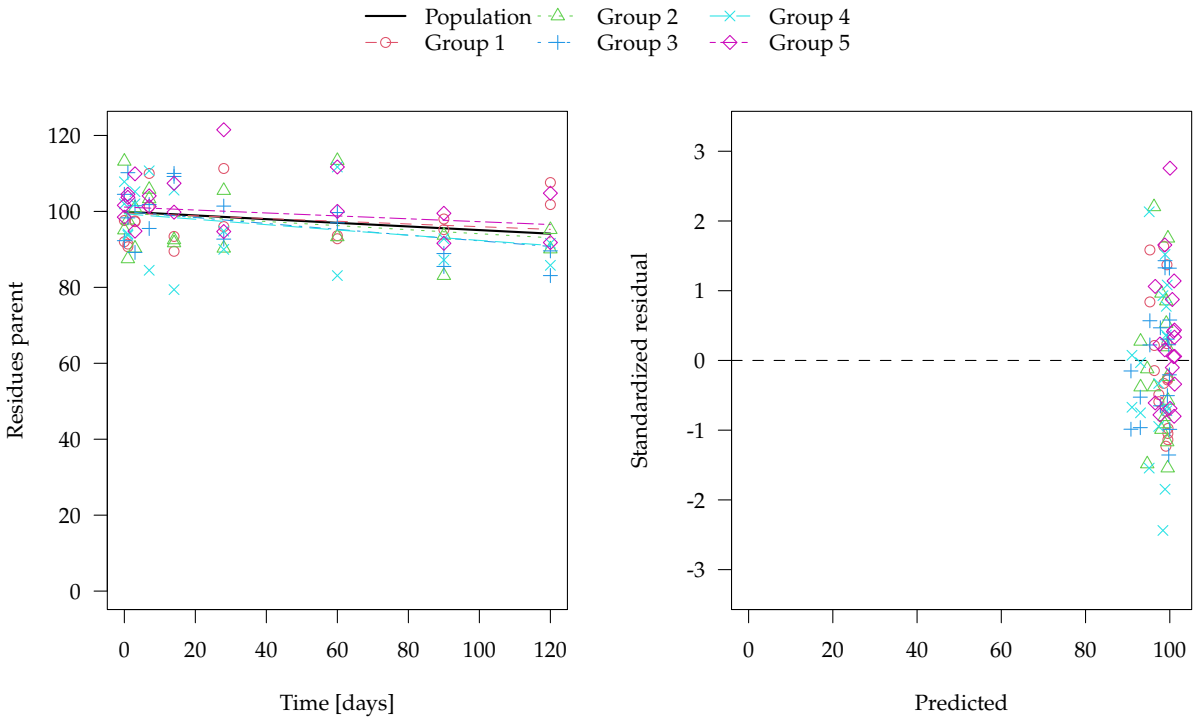

Figure 26: SFO fit with saemix to an example dataset with mean input half-life 800 days, constant variance

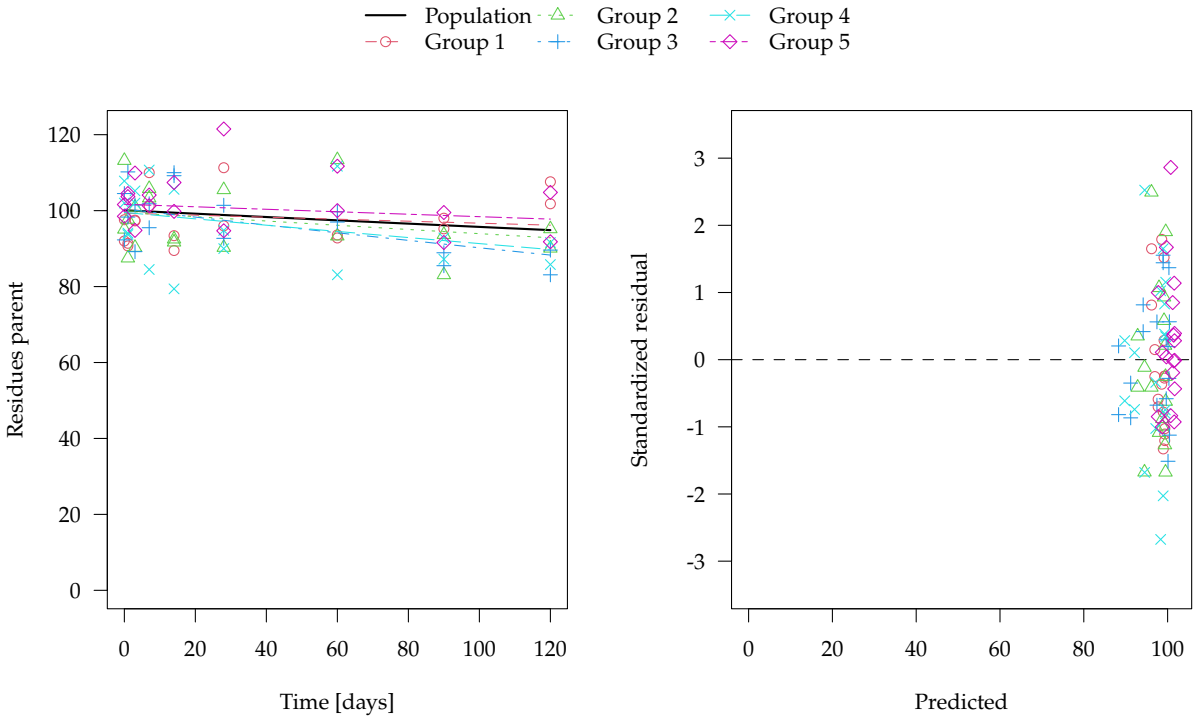

Figure 27: SFO fit with saemix to an example dataset with mean input half-life 800 days, two-component error model

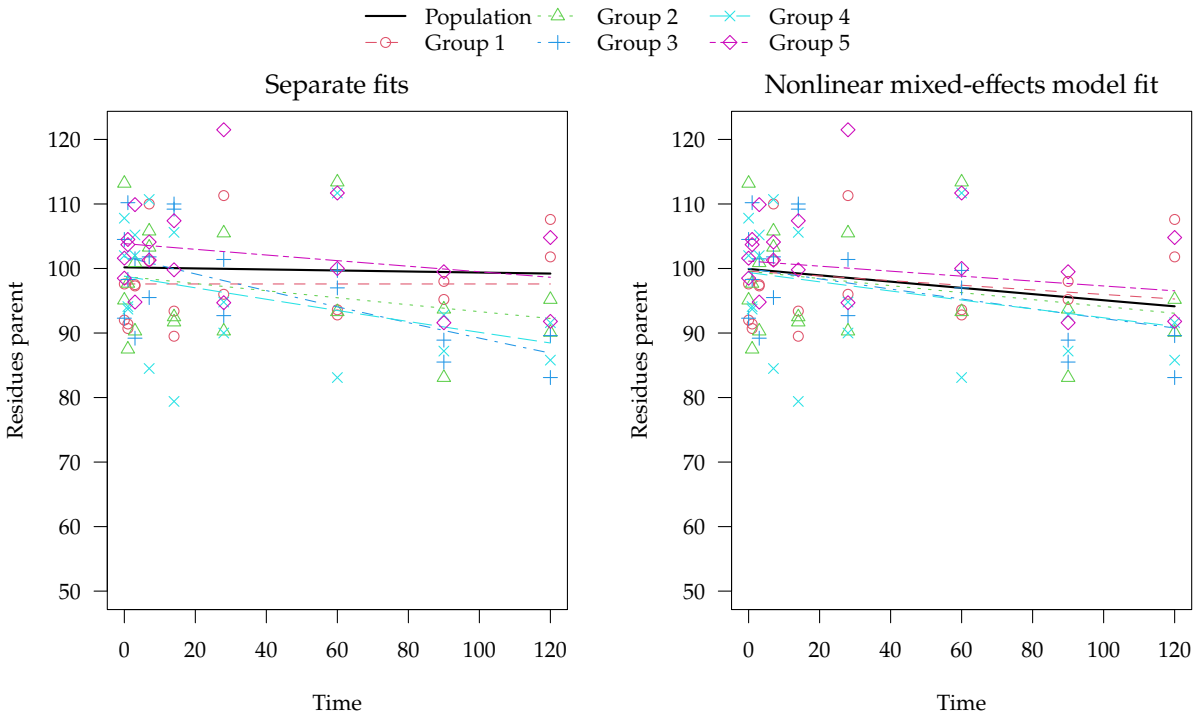

Figure 28: SFO fits with mkin and saemix to an example dataset with mean input half-life 800 days, constant variance

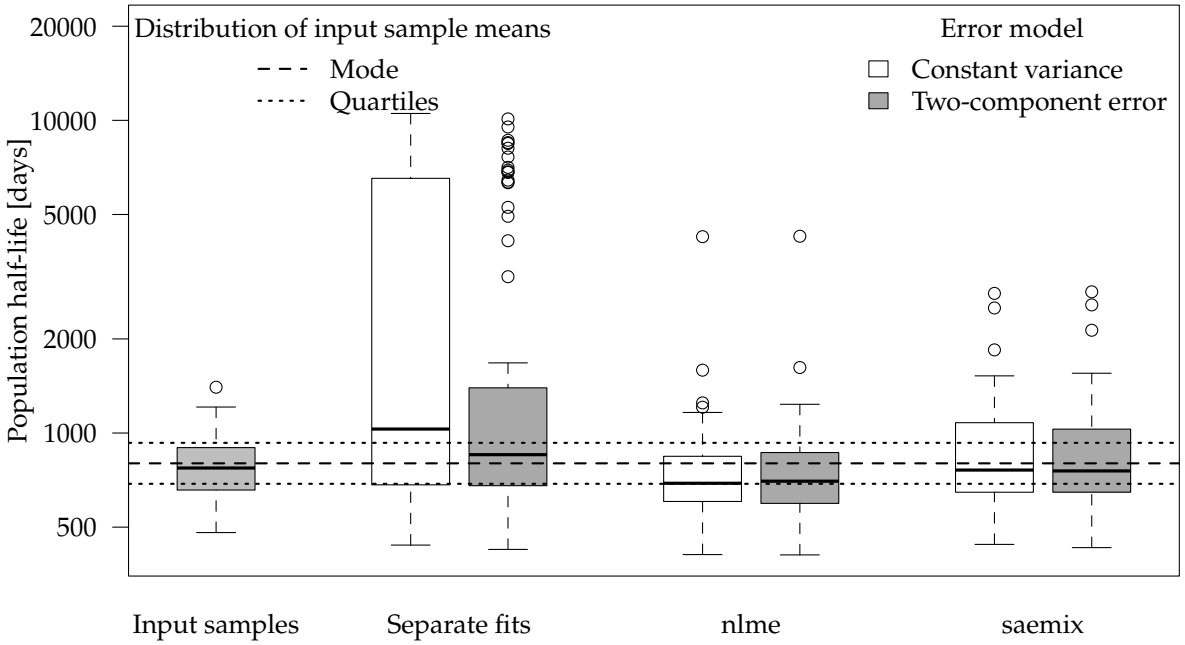

Figure 29: Boxplots for the half-lives derived from 100 datasets for five groups, half-life 800 days

Table 6: Statistics for half-lives derived from 100 datasets with five groups, input half-life 800 days

	Input parameters		Separate fits		nlme		saemix	
	Distribution	**Sample means**	**const**	**tc**	**const**	**tc**	**const**	**tc**
Number of results			500	500	94	88	100	99
Fits with lower AIC			499	1	76	11	88	11
Minimum		480.4	438.1	424.4	408.6	407.6	440.3	430.0
25th percentile	688.0	657.3	683.5	678.9	604.2	595.7	648.8	647.0
Median	800.0	772.9	1029.7	852.7	690.7	701.4	761.3	756.5
75th percentile	930.2	897.8	6483.5	1381.7	841.7	865.2	1075.9	1029.2
Maximum		1401.2	856749.0	444191.3	4246.1	4260.1	57459.9	2829.1

Biphasic decline with a metabolite

The analytical solution of the DFOP-SFO model used for the generation of the data shown in this section is given in Equation~1.

$$
\begin{aligned}
f^{(1)}(\psi, t) &= \gamma_1\, p_0\, e^{-\lambda_1 t} + (1 - \gamma_1)\; p_0\, e^{-\lambda_2 t} \\
f^{(2)}(\psi, t) &= \frac{(\gamma_2\, \gamma_1 - \gamma_2)\; \lambda_2\, p_0\, e^{-\lambda_2 t}}{\lambda_2 - \lambda_3} - \frac{\gamma_2\, \gamma_1\, \lambda_1\, p_0\, e^{-\lambda_1 t}}{\lambda_1 - \lambda_3} + \\
&\qquad \frac{((\gamma_2\, \lambda_1 + (\gamma_2\, \gamma_1 - \gamma_2)\; \lambda_3)\; \lambda_2 - \gamma_2\, \gamma_1\, \lambda_3\, \lambda_1)\; p_0\, e^{-\lambda_3 t}}{(\lambda_1 - \lambda_3)\; \lambda_2 - \lambda_3\, \lambda_1 + \lambda_3^2}
\end{aligned}
\tag{1}
$$

Here, $(p_0, 0)$ were used as the initial concentrations of parent compound and transformation product, λ_1 and λ_2 are the rate constants for the biexponential decline of the parent, γ_1 is the fraction of the parent declining with λ_1, γ_2 is the fraction of the degrading parent compound forming the transformation product (formation fraction) and λ_3 is the degradation rate constant of the transformation product.

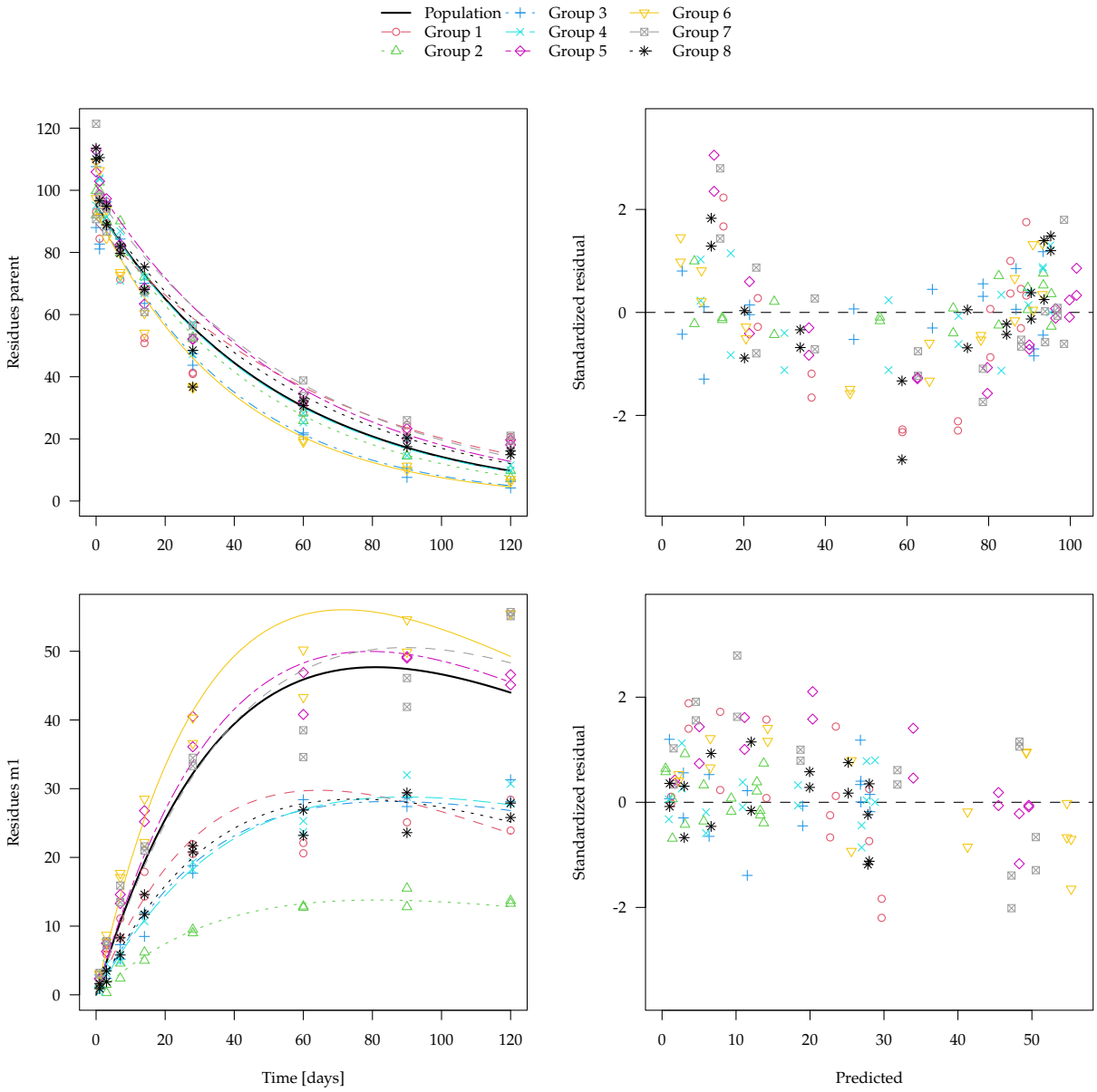

Figure 30: SFO-SFO saemix fit with two-component variance for DFOP-SFO dataset 1

Table 7: SFO-SFO population parameters for DFOP-SFO dataset 1

Evaluation	Error model	AIC	parent_0	k_parent	f_parent_to_m1	k_m1
Mean input			102	-	0.449	0.00174
Separate	const		97.9	0.0228	0.616	0.00422
	tc		94.3	0.0191	1	0.00687
saemix	const	1794.2	98	0.0229	0.548	0.00445
	tc	1689.9	95.2	0.019	0.917	0.00747

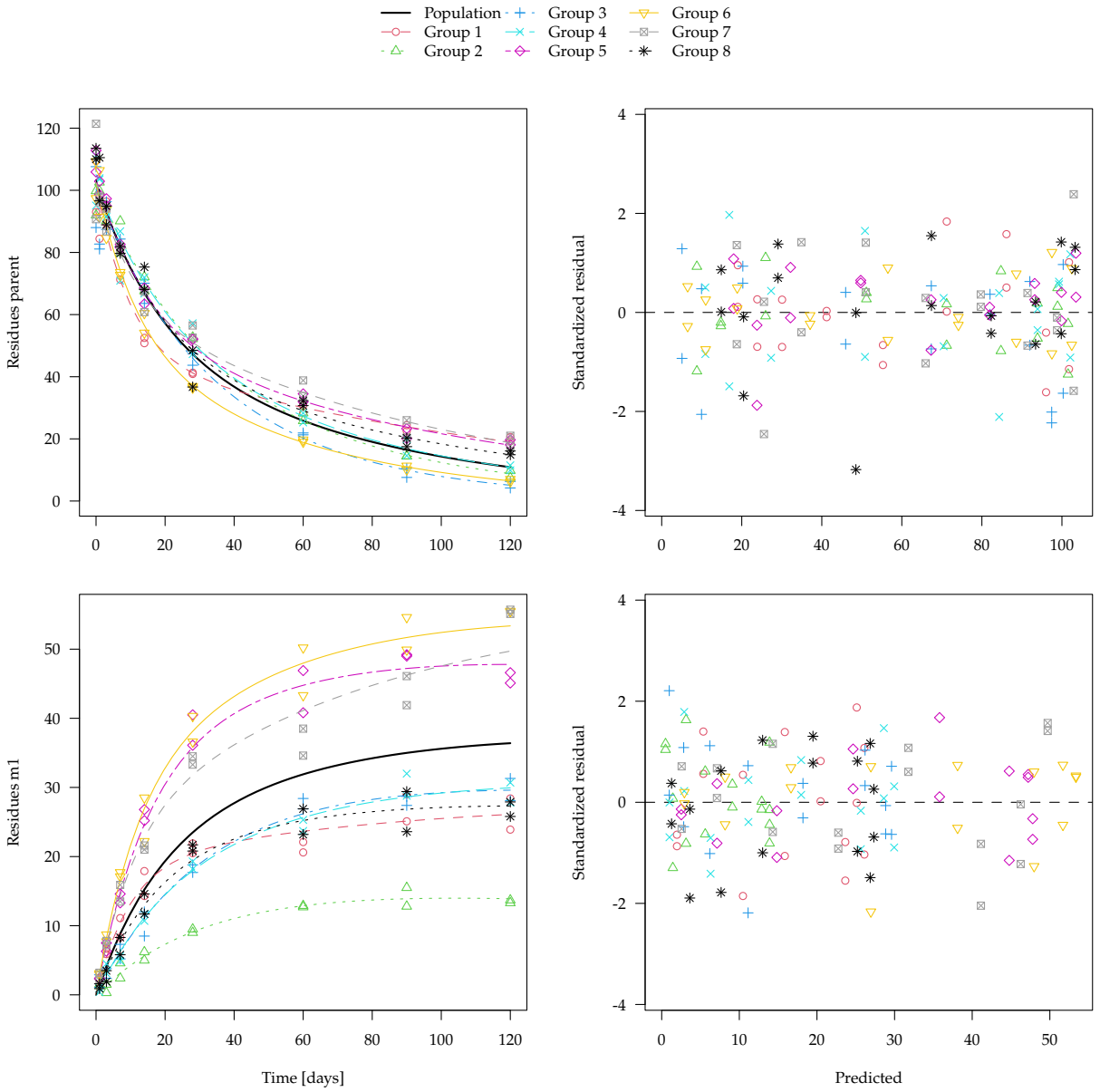

Figure 31: DFOP-SFO saemix fit with two-component variance for DFOP-SFO dataset 1

Table 8: DFOP-SFO population parameters for DFOP-SFO dataset 1

Evaluation	Error model	AIC	parent_0	k1	k2	g	f_parent_to_m1	k_m1
Mean input			102	0.0528	0.0122	0.505	0.449	0.00174
Separate	const		103	0.0598	0.0164	0.423	0.426	1.04e-05
	tc		102	0.048	0.00203	0.62	0.439	1.12e-05
saemix	const	1642.2	103	0.0564	0.0142	0.458	0.416	0.000456
	tc	1430.3	102	0.0553	0.0133	0.476	0.433	0.000952

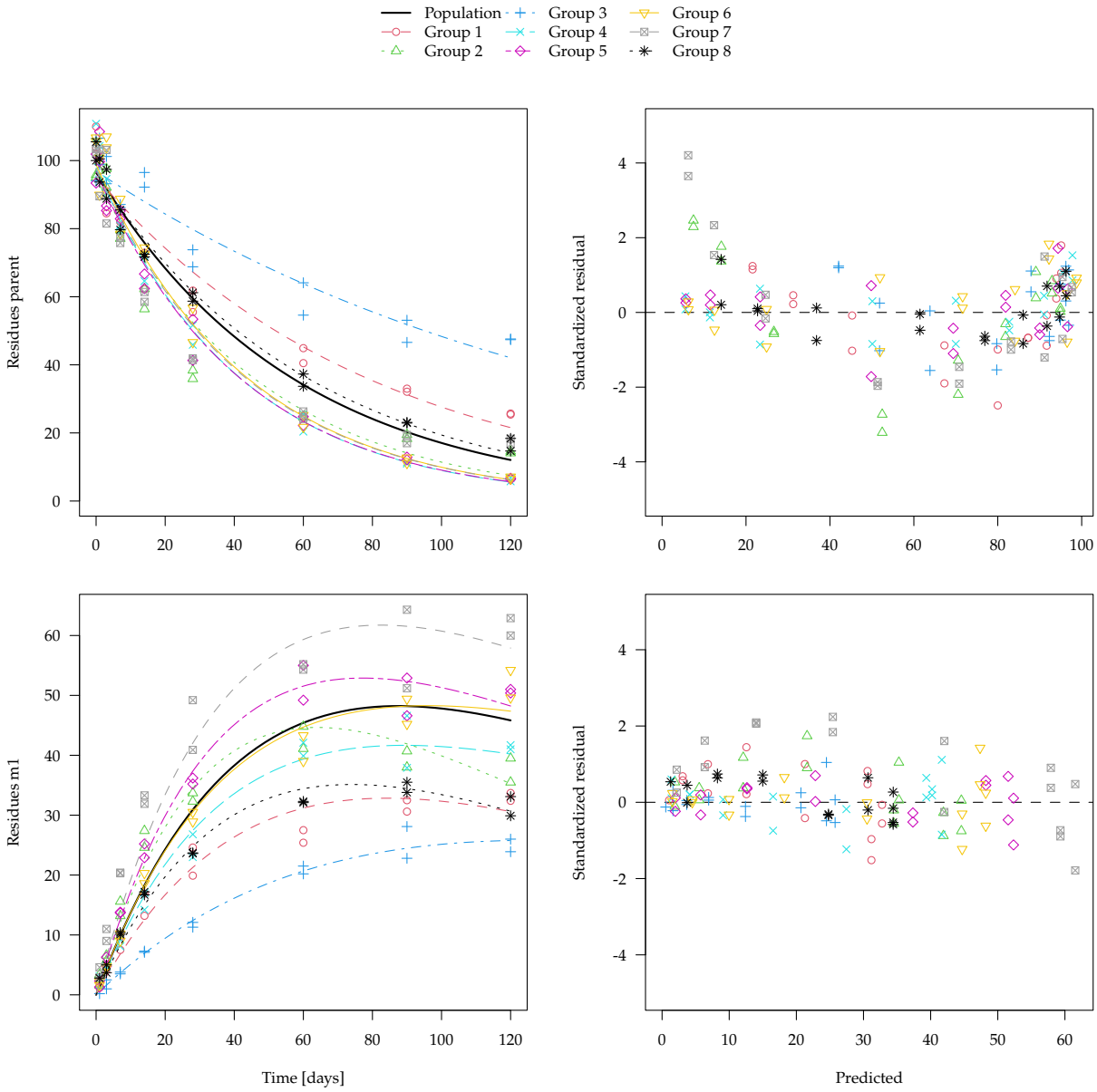

Figure 32: SFO-SFO saemix fit with two-component variance for DFOP-SFO dataset 2

Table 9: SFO-SFO population parameters for DFOP-SFO dataset 2

Evaluation	Error model	AIC	parent_0	k_parent	f_parent_to_m1	k_m1
Mean input			101	-	0.621	0.00216
Separate	const		98.7	0.0193	0.786	0.00508
	tc		97.2	0.0179	0.997	0.00663
saemix	const	1718	98.8	0.0194	0.725	0.00546
	tc	1681.4	96.7	0.0174	0.923	0.00703

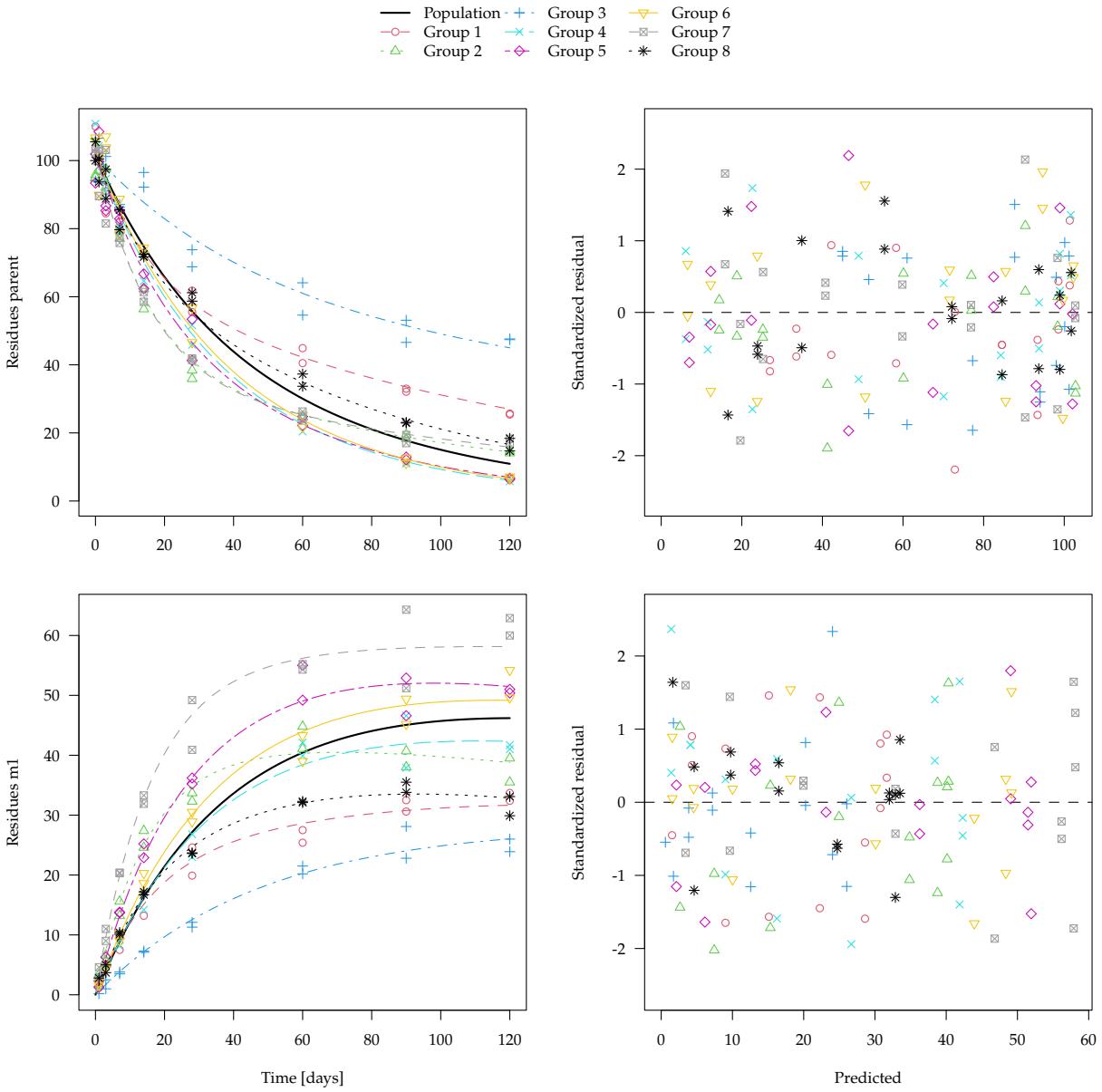

Figure 33: DFOP-SFO saemix fit with two-component variance for DFOP-SFO dataset 2

Table 10: DFOP-SFO population parameters for DFOP-SFO dataset 2

Evaluation	Error model	AIC	parent_0	k1	k2	g	f_parent_to_m1	k_m1
Mean input			101	0.046	0.00926	0.502	0.621	0.00216
Separate	const		103	0.0334	0.00229	0.549	0.581	7.93e-06
	tc		102	0.0309	0.0111	0.601	0.601	0.00153
saemix	const	1580.6	102	0.0265	0.0179	0.516	0.591	0.0019
	tc	1401.5	102	0.0314	0.0139	0.491	0.613	0.00224

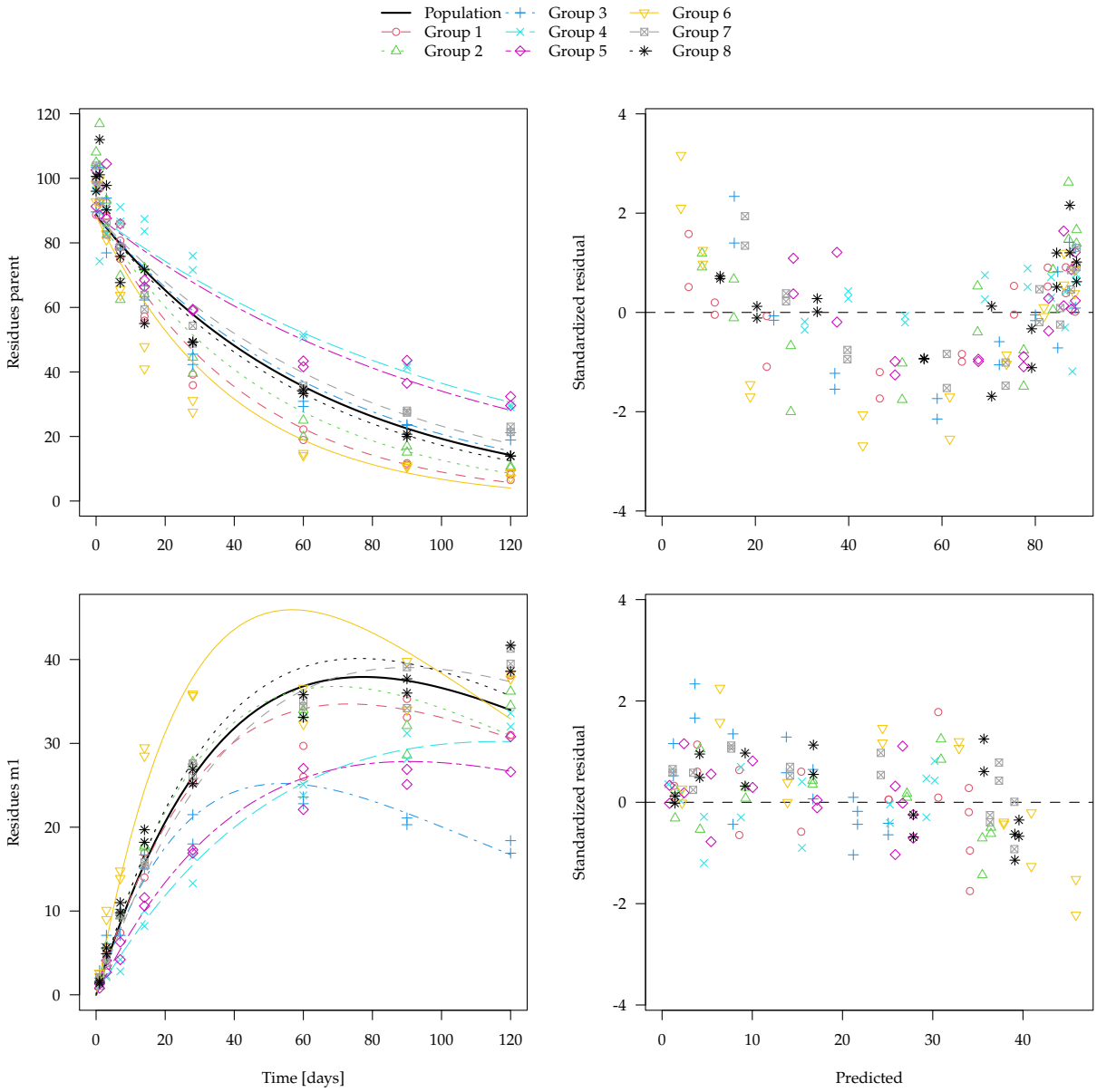

Figure 34: SFO-SFO saemix fit with two-component variance for DFOP-SFO dataset 3

Table 11: SFO-SFO population parameters for DFOP-SFO dataset 3

Evaluation	Error model	AIC	parent_0	k_parent	f_parent_to_m1	k_m1
Mean input			98.6	-	0.49	0.00166
Separate	const		94.5	0.0199	0.671	0.00608
	tc		91.4	0.0167	1	0.00923
saemix	const	1791.9	94.3	0.0199	0.607	0.00539
	tc	1664.1	88.6	0.0152	0.991	0.0108

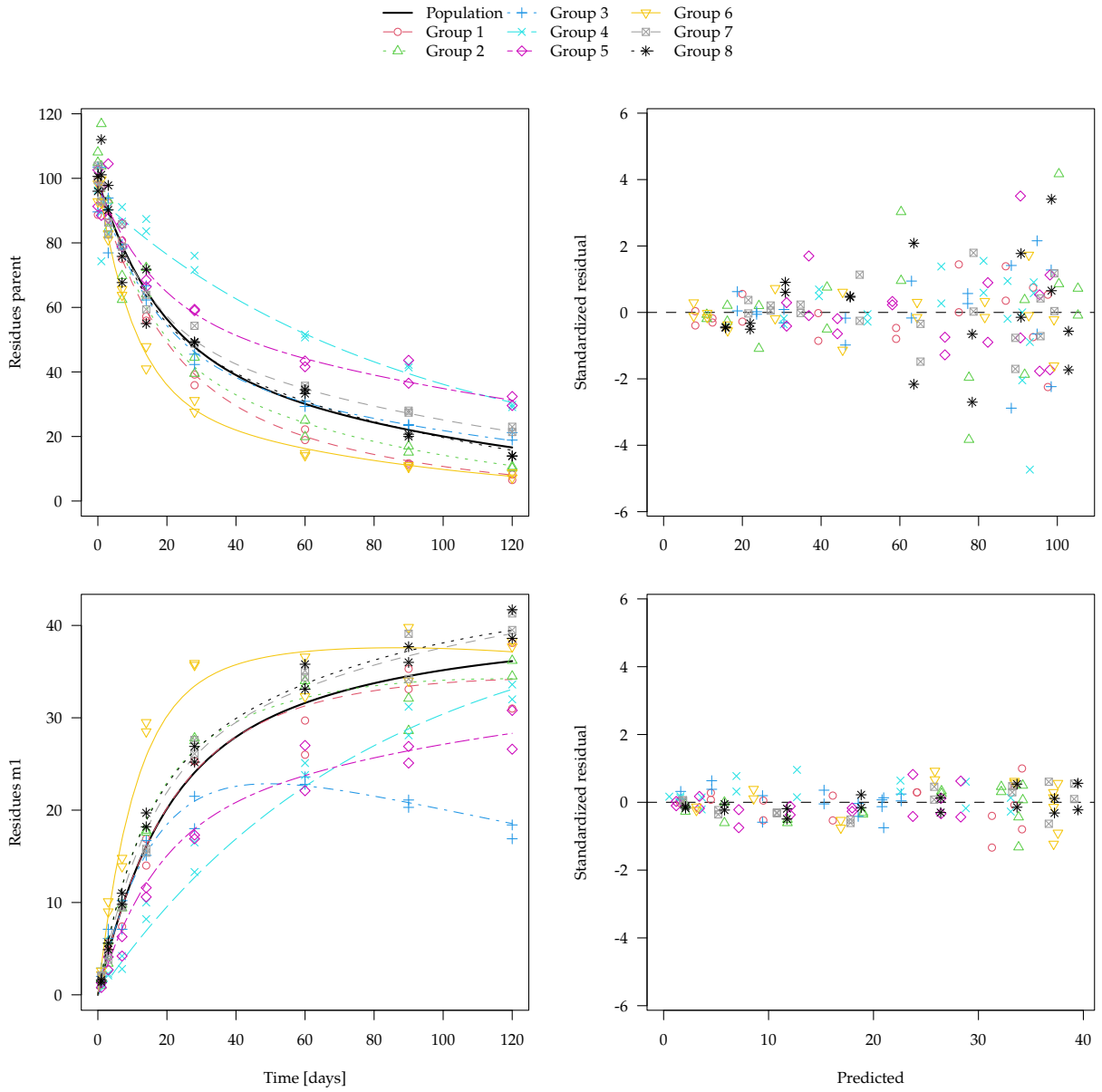

Figure 35: DFOP-SFO saemix fit with constant variance for DFOP-SFO dataset 3

Table 12: DFOP-SFO population parameters for DFOP-SFO dataset 3

Evaluation	Error model	AIC	parent_0	k1	k2	g	f_parent_to_m1	k_m1
Mean input			98.6	0.0555	0.00785	0.513	0.49	0.00166
Separate	const		99.7	0.0515	0.011	0.438	0.494	1.25e-05
	tc		98.4	0.0501	0.00872	0.499	0.509	1.63e-05
saemix	const	1636.4	99.3	0.0604	0.00921	0.496	0.474	0.000909
	tc	1409.4	98.5	0.0597	0.00882	0.48	0.489	0.00132

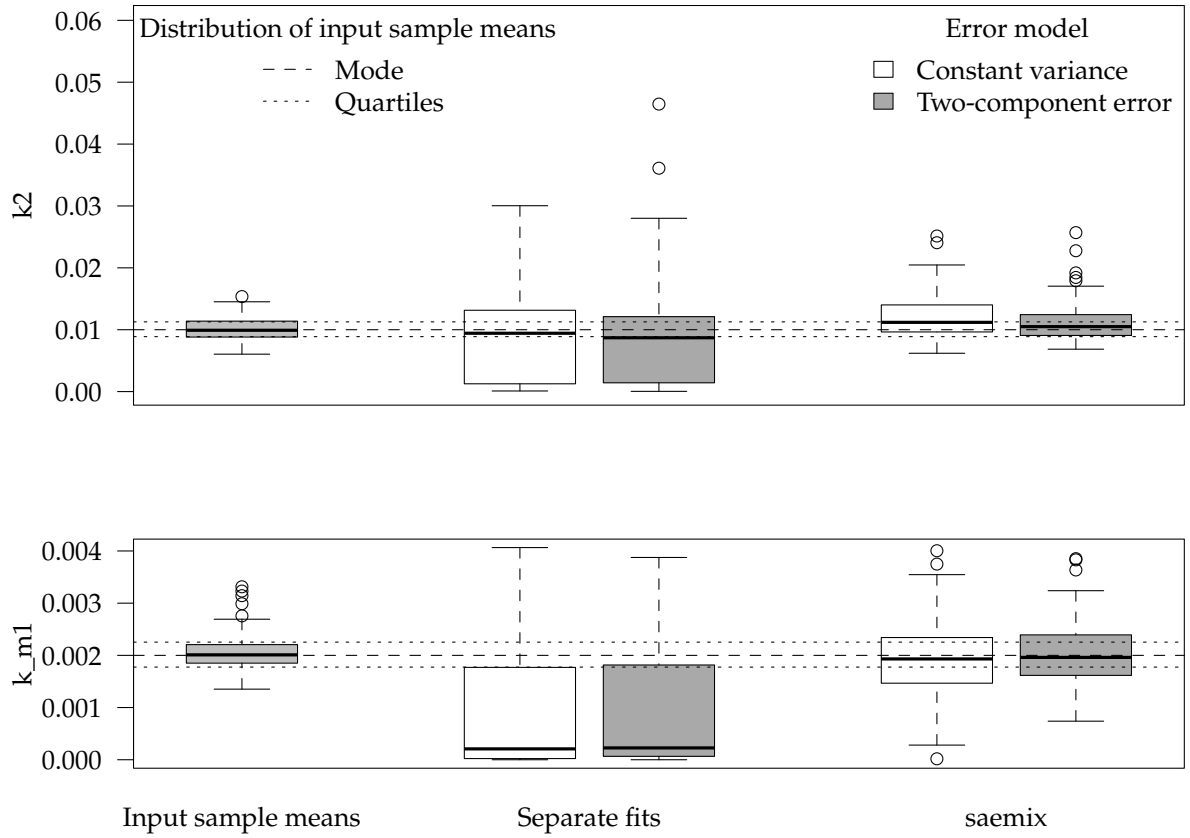

Figure 36: Selected population parameters obtained with DFOP-SFO for the biphasic datasets

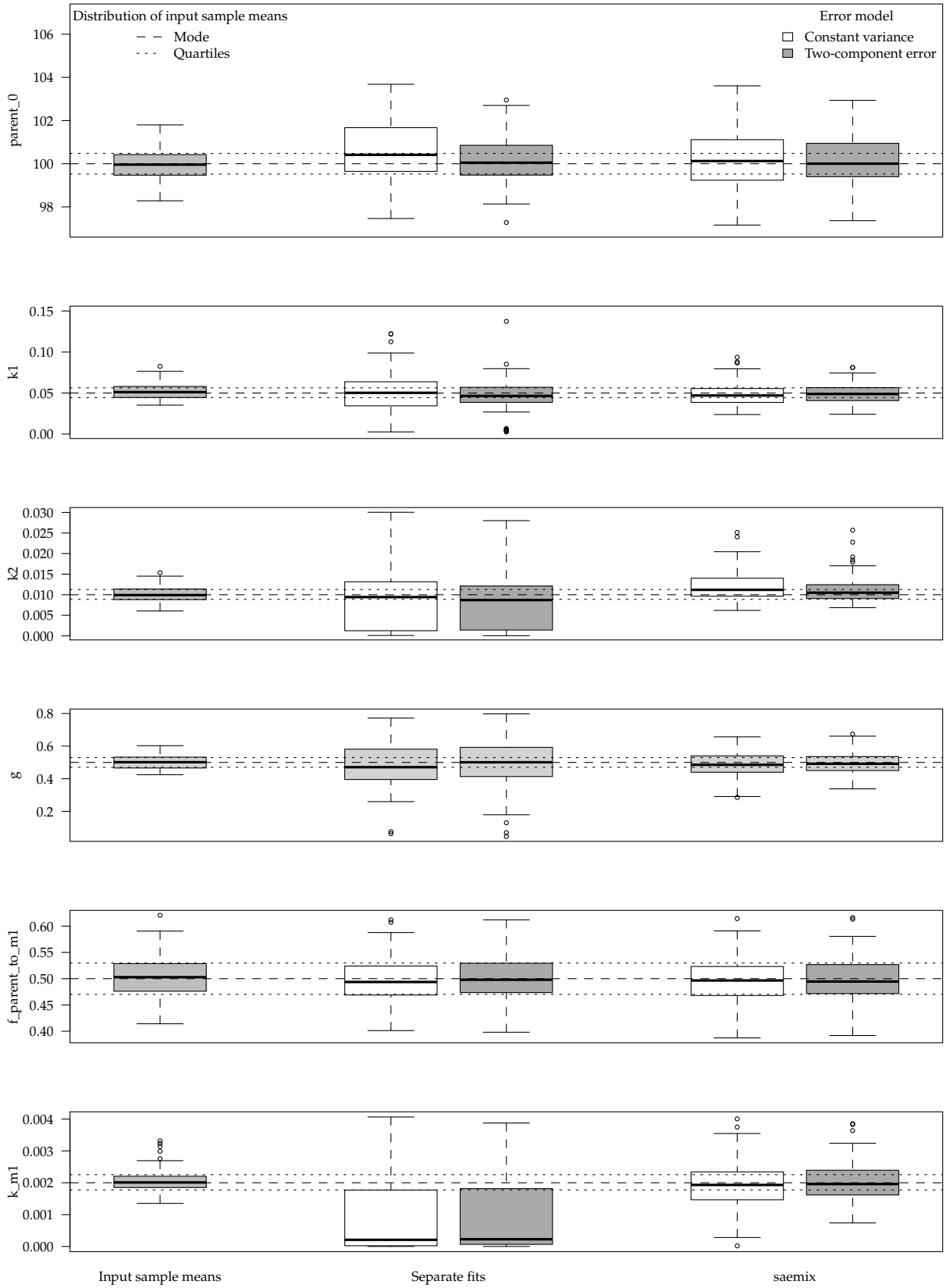

Figure 37: Population parameters obtained with DFOP-SFO for the biphasic datasets

Evaluation of experimental data

Detailed statistical summaries of the fits are given in the Appendix.

EU risk assessment of 2,4-D from 2014

In this section, the aerobic soil degradation data on 2,4-D as documented in the Review Assessment Report of the European Union pesticide risk assessment peer review 2014 are evaluated (EFSA, 2014). The data are used as available from the mkin package. The dataset in the package already contains normalisation factors for time step normalisation to reference conditions. The following code shows how the data from the package is preprocessed for this analysis as described in the main article.

```
d24_ds <- lapply(1:5, function(i) {
  subset(D24_2014$ds[[i]]$data, time <= 120, c("name", "time", "value"))
})
names(d24_ds) <- sapply(D24_2014$ds, function(ds) ds$title)
d24_ds_norm <- lapply(1:5, function(i) {
  ds_i <- subset(D24_2014$ds[[i]]$data, time <= 120, c("name", "time", "value"))
  ds_i$time <- ds_i$time * D24_2014$f_time_norm[i]
  ds_i
})
names(d24_ds_norm) <- sapply(D24_2014$ds, function(ds) ds$title)
```

The result is a list of five time step normalised datasets for the five different soils, suitable for separate analysis with `mmkin` and subsequent simultaneous analysis `nlme.mmkin` and `saem.mmkin`.

In the assessments, D24 is used as compound code for 2,4-D, as object names cannot start with numbers in R. For transformation products 2,4-dichlorophenol and 2,4-dichloroaniline, compound codes DCP and DCA are used, respectively.

Note that no pathway fits were used in the EU assessment. Instead, the decline of the metabolites from their maximum was used to derive half-lives for metabolites. This introduces considerable bias, as the datasets where no decline phase for the metabolites was found were disregarded. Therefore, pathway fits are for shown here for all data, either separately for the datasets or in a joint nonlinear mixed effects model fit.

Separate kinetic fits for the parent compound

The SFO fits to the parent data in the five datasets are shown in Figure 38. The fitted parameters are shown in Table 13. The acceptability of the SFO fits according to the FOCUS criteria is clearly confirmed for The Mississippi, Fayette, and Site E1 datasets. Residual plots in the other two datasets show repeated positive residuals towards the end of the experimental period. However, as these occur at residue levels far below 10%, the fits are acceptable based on the recommendations in the FOCUS guidance.

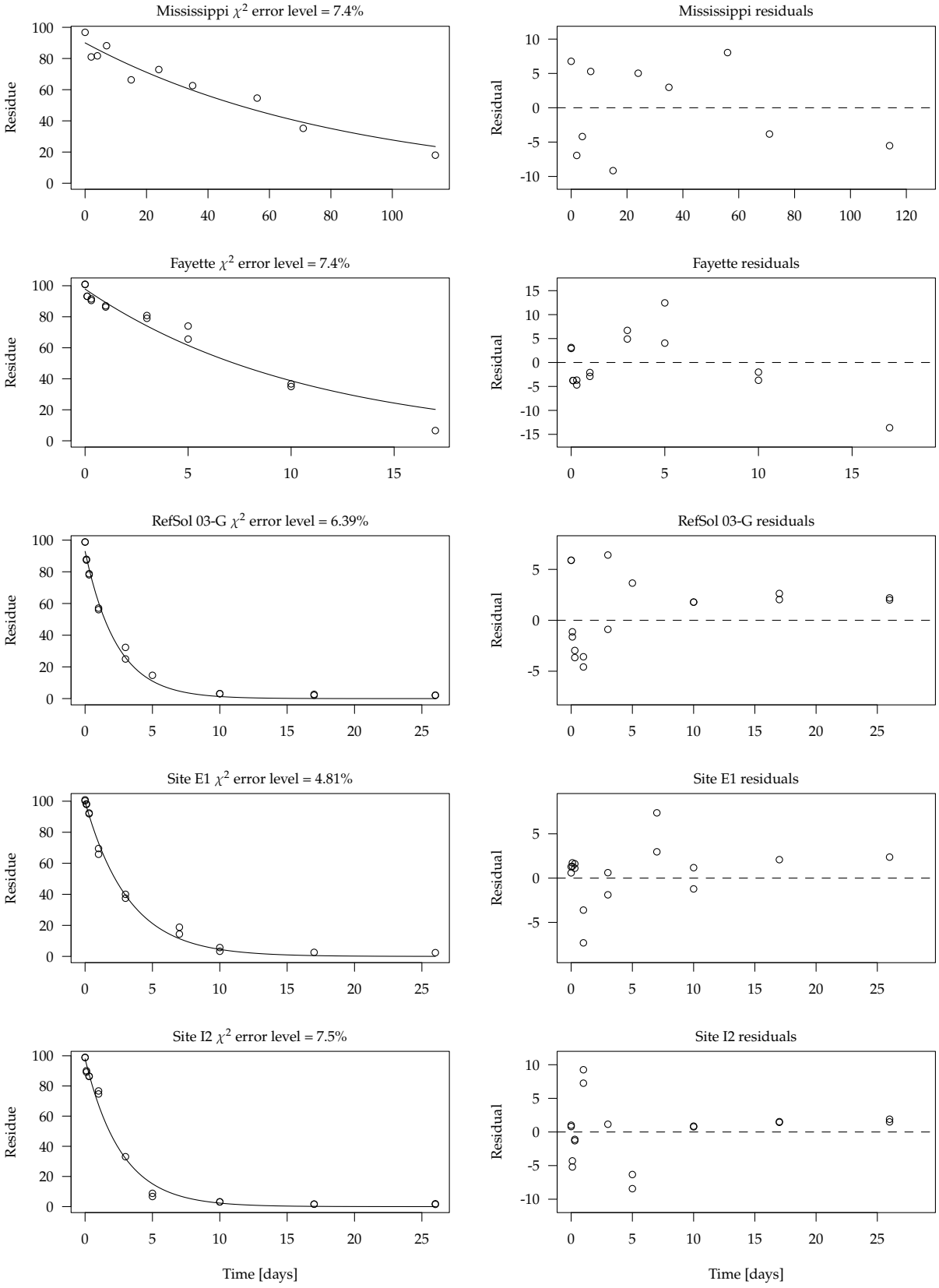

Figure 38: SFO parent kinetics in the datasets for 2,4-D

Table 13: Model parameters with confidence intervals and p-values

Dataset	Fitted parameters					
	Name	**Unit**	**Estimate**	**Pr(>t)**	**Lower**	**Upper**
Mississippi	D24_0	% AR	90.03	6.36e-09	82.86	97.21
	k_D24	d^{-1}	0.01177	2.254e-05	0.009034	0.01535
	sigma	% AR	6.059	0.001447	2.856	9.263
Fayette	D24_0	% AR	97.87	4.891e-15	93.12	102.6
	k_D24	d^{-1}	0.09275	2.222e-08	0.07745	0.1111
	sigma	% AR	5.993	7.067e-05	3.609	8.378
RefSol 03-G	D24_0	% AR	92.91	2.452e-18	89.44	96.37
	k_D24	d^{-1}	0.4259	1.77e-10	0.3706	0.4895
	sigma	% AR	3.523	2.181e-05	2.227	4.819
Site E1	D24_0	% AR	99.61	1.025e-18	96.68	102.5
	k_D24	d^{-1}	0.3093	2.184e-11	0.2773	0.345
	sigma	% AR	3.132	3.92e-05	1.936	4.328
Site I2	D24_0	% AR	97.99	8.691e-18	94	102
	k_D24	d^{-1}	0.3736	2.89e-10	0.3234	0.4316
	sigma	% AR	4.288	2.181e-05	2.71	5.865

Simultaneous kinetic fits for the parent compound

The mixed model SFO fit to the parent data as obtained by nlme and assuming constant variance is shown in Figure 39. The same fit obtained using the SAEM algorithm as implemented in saemix is shown in Figure 40. Note that the predictions for the individual datasets (coloured lines) are conditional on the population parameters that have been obtained.

Both fits look acceptable and can visually not be distinguished. An attempt to fit the FOMC model with nlme gives an error message, indicating that this fit is overparameterised. The FOMC fit can be done with saemix, but has a higher AIC (503.1 as compared to 498.7).

The residual plots do not indicate a relationship between the error and the predicted value. This is confirmed by the comparison of nlme fitted with the two error models.

```
                  Model df      AIC      BIC    logLik   Test    L.Ratio
f_d24_sfo_nlme        1  5 498.6652 510.2527 -244.3326
f_d24_sfo_nlme_tc     2  6 500.6652 514.5702 -244.3326 1 vs 2 4.8836e-06
                  p-value
f_d24_sfo_nlme
f_d24_sfo_nlme_tc  0.9982
```

This can also be confirmed by comparing the corresponding saemix fits, which shows lower values for AIC and BIC for constant variance (first row). Here we also show that the FOMC model (third row) is less preferable.

```
Likelihoods calculated by importance sampling

       AIC      BIC
1 498.7344 496.7816
2 500.7324 498.3890
3 503.1380 500.4041
```

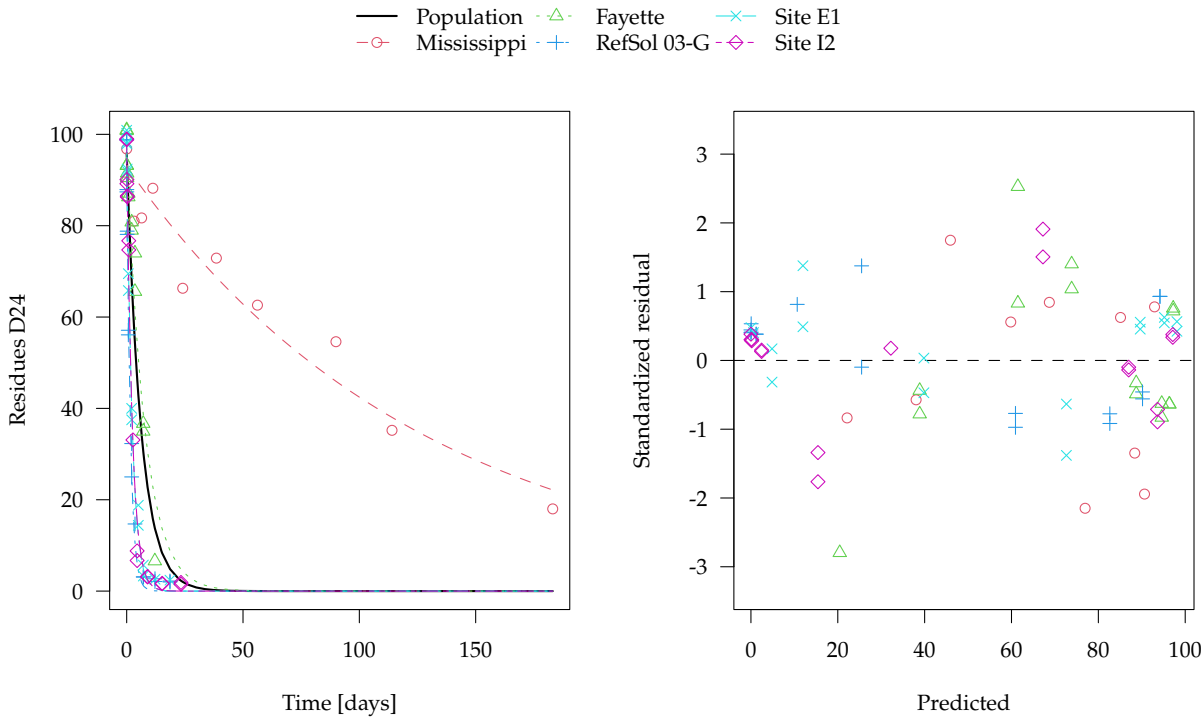

Figure 39: Mixed model SFO kinetics in the datasets for 2,4-D fitted by nlme

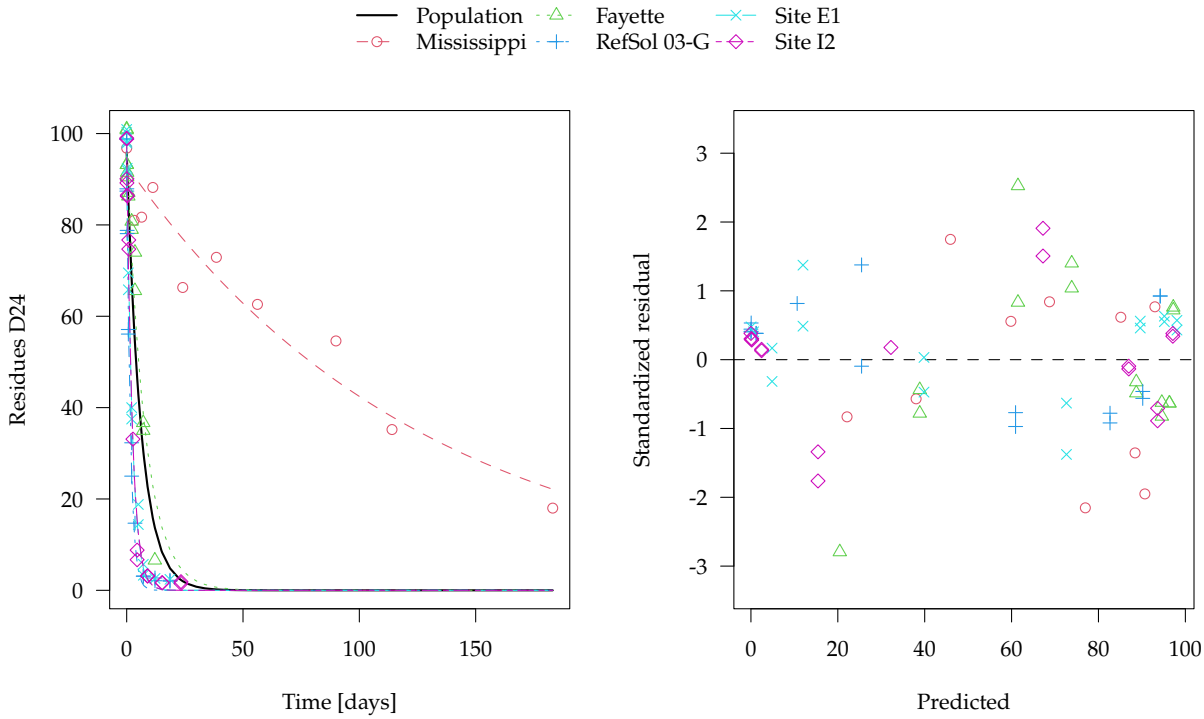

Figure 40: Mixed model SFO kinetics in the datasets for 2,4-D fitted by saemix

Separate pathway fits

In the following, the coupled fits with the linear kinetic pathway from the parent compound via DCP to DCA using SFO for all compounds to the datasets obtained at 20°C in the study by Liu and Adelfinskaya (2011) are discussed. In the fits, the error model "variance by variable", fitted by the iteratively reweighted least squares (IRLS) algorithm, is used.

Figure 41 shows the fit for the Fayette datasets.

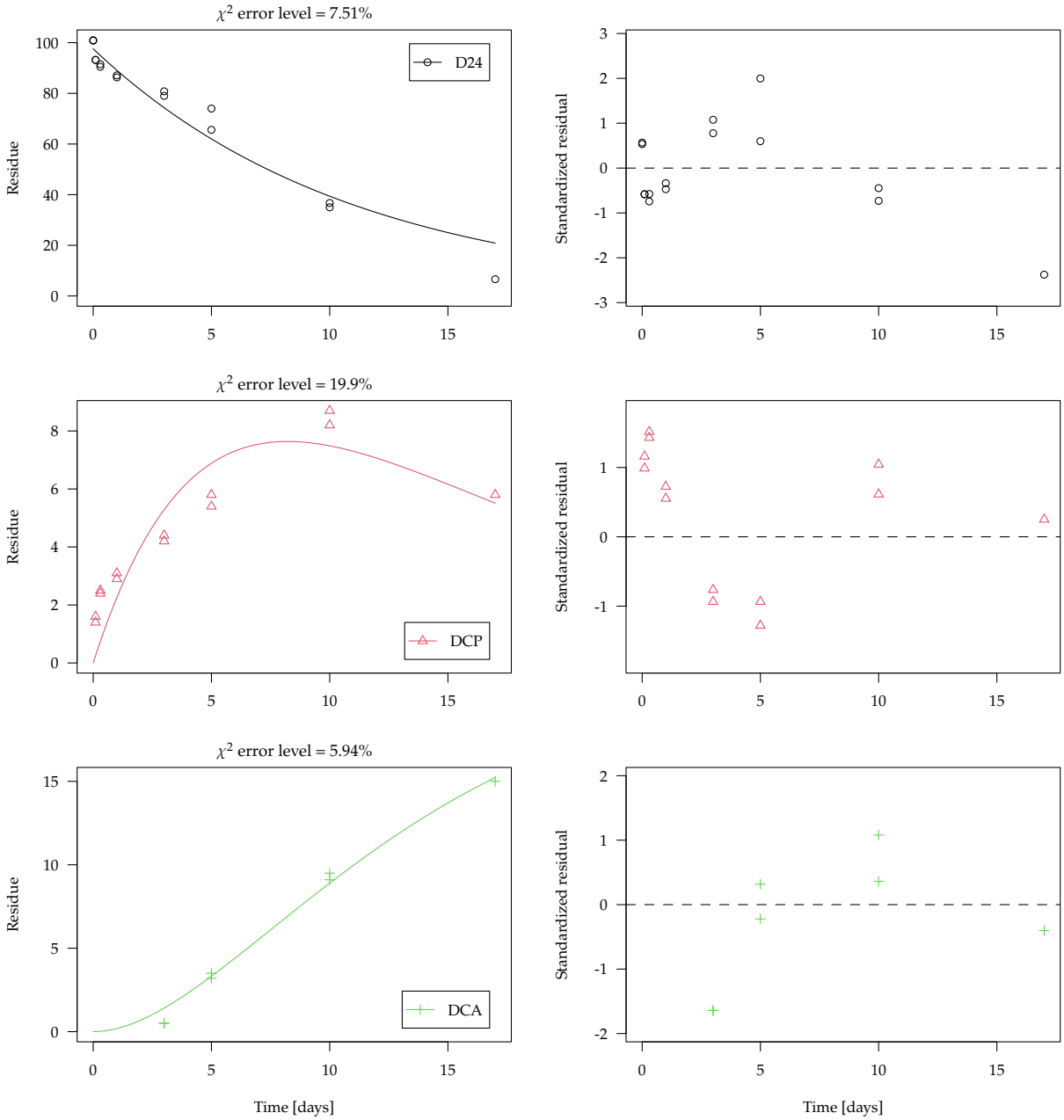

Figure 41: SFO-SFO-SFO fit for 2,4-D, Fayette

The fit looks visually acceptable and the degradation rate constant for DCP is significantly different from zero according to the t-test recommended in the FOCUS guidance, while the rate constant of

DCA is not significantly different from zero (Table 14). As the formation fraction from DCP to DCA is found to be exactly 1, the fit was repeated without a pathway from DCP to other compounds ("sink"). The acronym "SFO-SFO(ns)-SFO" is used for this model.

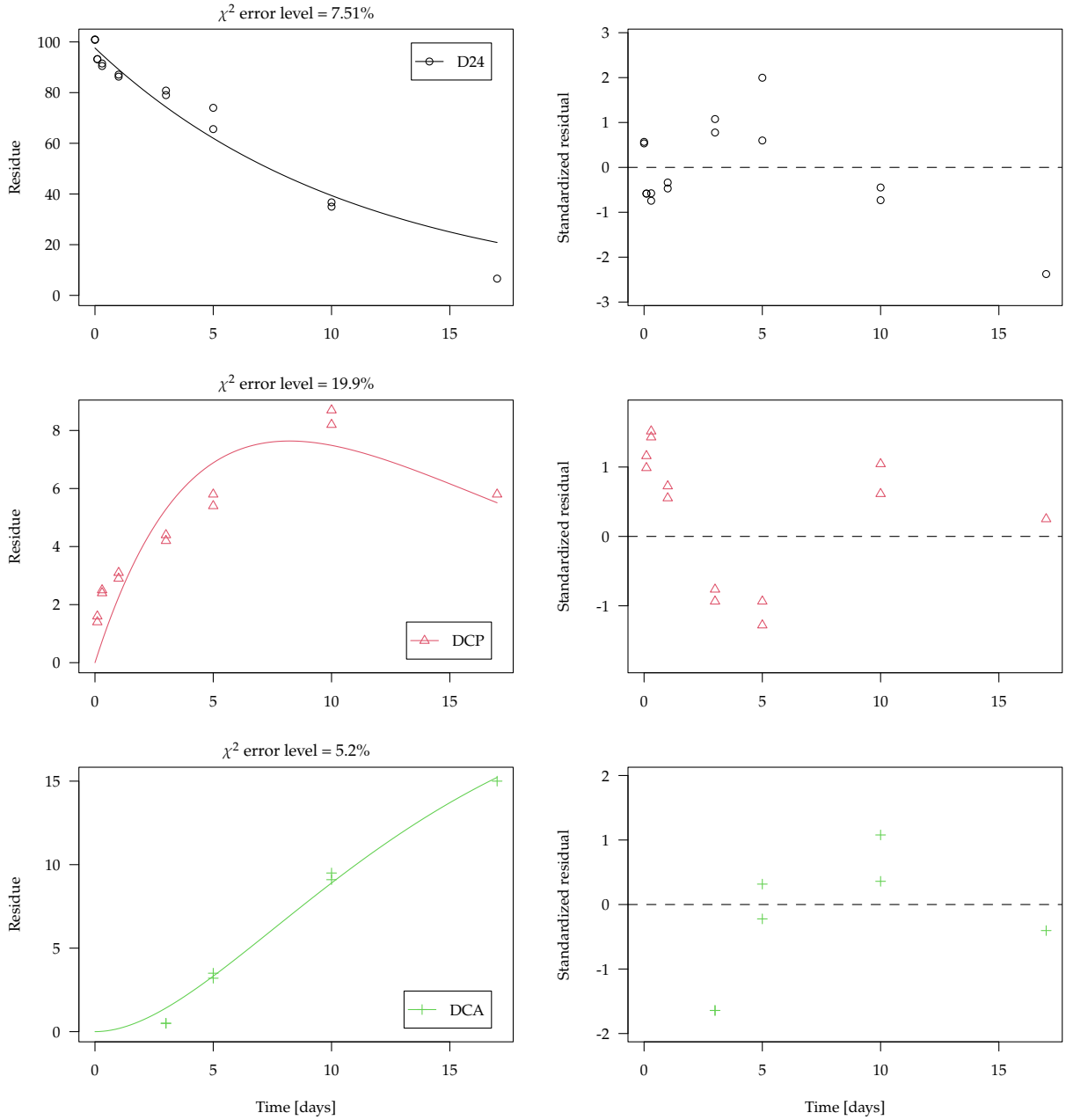

Figure 42: SFO-SFO(ns)-SFO fit for 2,4-D, Fayette

The reduction in degrees of freedom for the metabolite curves leads to a lower p-values for their rate constants. However, the p-value for the rate constant of DCA is around 0.15, and therefore expert judgement is needed according to the FOCUS guidance to specify a default value to use for this fit.

Table 14: Model parameters with confidence intervals and p-values

Model	Fitted parameters					
	Name	Unit	Estimate	Pr(>t)	Lower	Upper
SFO-SFO-SFO	D24_0	% AR	97.59	2.009e-26	93.11	102.1
	k_D24	d^{-1}	0.09072	1.914e-12	0.07663	0.1074
	k_DCP	d^{-1}	0.1589	3.474e-05	0.1353	0.1866
	k_DCA	d^{-1}	0.01166	0.2613	0.001757	0.07742
	f_D24_to_DCP	-	0.2889	2.788e-07	0.2382	0.3456
	f_DCP_to_DCA	-	1	0.0009445	0	1
	sigma_D24	% AR	6.008	5.117e-06	3.743	8.272
	sigma_DCP	% AR	1.161	3.073e-05	0.6884	1.634
	sigma_DCA	% AR	0.5565	0.0005622	0.2473	0.8657
SFO-SFO(ns)-SFO	D24_0	% AR	97.59	3.458e-27	93.12	102.1
	k_D24	d^{-1}	0.09072	8.811e-13	0.07666	0.1074
	k_DCP	d^{-1}	0.1589	2.903e-13	0.1353	0.1865
	k_DCA	d^{-1}	0.01166	0.1436	0.001763	0.07715
	f_D24_to_DCP	-	0.2889	8.264e-12	0.2383	0.3455
	sigma_D24	% AR	6.008	4.526e-06	3.747	8.268
	sigma_DCP	% AR	1.161	1.339e-05	0.6893	1.633
	sigma_DCA	% AR	0.5565	0.0004869	0.2479	0.8651

The AIC comparison shows that removing the sink improves the AIC by reducing the number of parameters in the model. The use of the two-component error model (f_d24_tc) leads to a higher AIC compared to "variance by variable" (f_d24_obs).

```
                                df      AIC
f_d24_obs[["SFO-SFO-SFO", 2]]    9 166.7987
f_d24_obs[["SFO-SFO(ns)-SFO", 2]] 8 164.7987
f_d24_tc[["SFO-SFO-SFO", 2]]     8 193.4438
f_d24_tc[["SFO-SFO(ns)-SFO", 2]] 7 191.4438
```

The likelihood ratio test confirms that the "variance by variable" error model is preferable, but does not show a significant difference between the models with and without sink (see below).

```
Likelihood ratio test

Model 1: SFO-SFO(ns)-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO(ns)-SFO with error model tc and fixed parameter(s) DCP_0, DCA_0
  #Df  LogLik Df  Chisq Pr(>Chisq)
1   8 -74.399
2   7 -88.722 -1 28.645  8.693e-08 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1


Likelihood ratio test

Model 1: SFO-SFO-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO(ns)-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
  #Df  LogLik Df Chisq Pr(>Chisq)
1   9 -74.399
2   8 -74.399 -1     0     0.9999
```

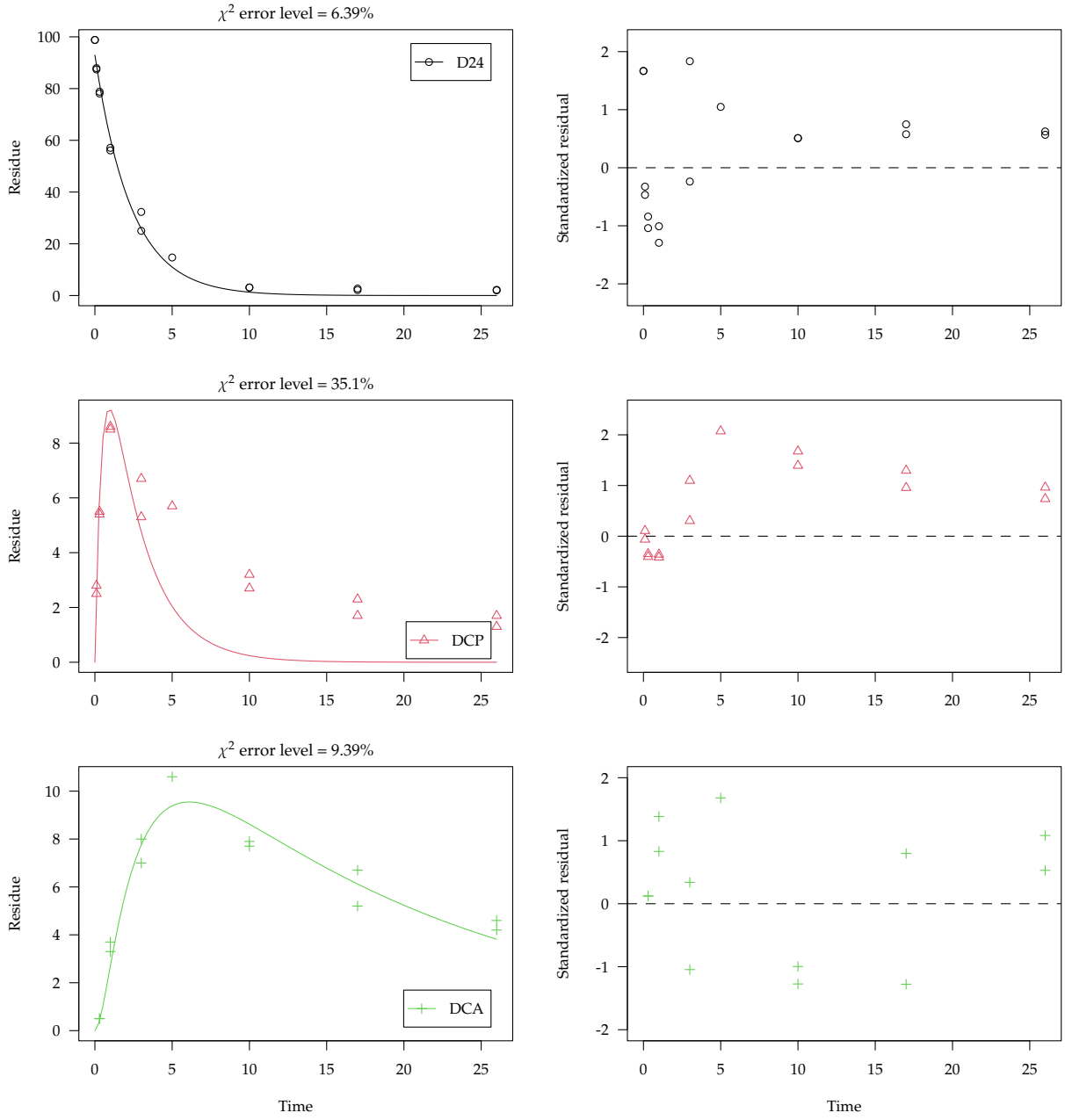

Figure 43: SFO-SFO-SFO fit for 2,4-D, RefSol 03-G

The fit for RefSol 03-G 43 looks visually acceptable for the parent and for DCA, while there are some systematic deviations in the fit for DCP, indicating biphasic behaviour for this metabolite. Parameter t-tests do not indicate problems and do not suggest to use a reduced model (Table 15).

Table 15: Model parameters with confidence intervals and p-values

Model	Fitted parameters					
	Name	Unit	Estimate	Pr(>t)	Lower	Upper
SFO-SFO-SFO	D24_0	% AR	92.93	2.134e-37	89.67	96.19
	k_D24	d^{-1}	0.4267	6.245e-18	0.3748	0.4857
	k_DCP	d^{-1}	2.148	0.00464	1.027	4.492
	k_DCA	d^{-1}	0.05274	3.346e-09	0.04029	0.06904
	f_D24_to_DCP	-	0.7482	0.0003974	0.248	0.964
	f_DCP_to_DCA	-	0.185	0.0009879	0.0972	0.3236
	sigma_D24	% AR	3.523	5.85e-07	2.298	4.748
	sigma_DCP	% AR	1.766	1.54e-05	1.014	2.517
	sigma_DCA	% AR	0.7225	5.374e-05	0.3856	1.059

The AIC comparison suggests that the model including the pathway from DCP to sink fitted assuming variance by variable is the preferred variant for this dataset.

```
                                df      AIC
f_d24_obs[["SFO-SFO-SFO", 3]]    9 197.1267
f_d24_obs[["SFO-SFO(ns)-SFO", 3]] 8 221.0217
f_d24_tc[["SFO-SFO-SFO", 3]]     8 200.7663
f_d24_tc[["SFO-SFO(ns)-SFO", 3]] 7 218.4091
```

The likelihood ratio test confirms that the "variance by variable" error model is preferable, and confirms that the model including the pathway from DCP to sink is preferable.

```
Likelihood ratio test

Model 1: SFO-SFO-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO-SFO with error model tc and fixed parameter(s) DCP_0, DCA_0
  #Df  LogLik Df  Chisq Pr(>Chisq)
1   9 -89.563
2   8 -92.383 -1 5.6396    0.01756 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1


Likelihood ratio test

Model 1: SFO-SFO-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO(ns)-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
  #Df   LogLik Df  Chisq Pr(>Chisq)
1   9  -89.563
2   8 -102.511 -1 25.895  3.605e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

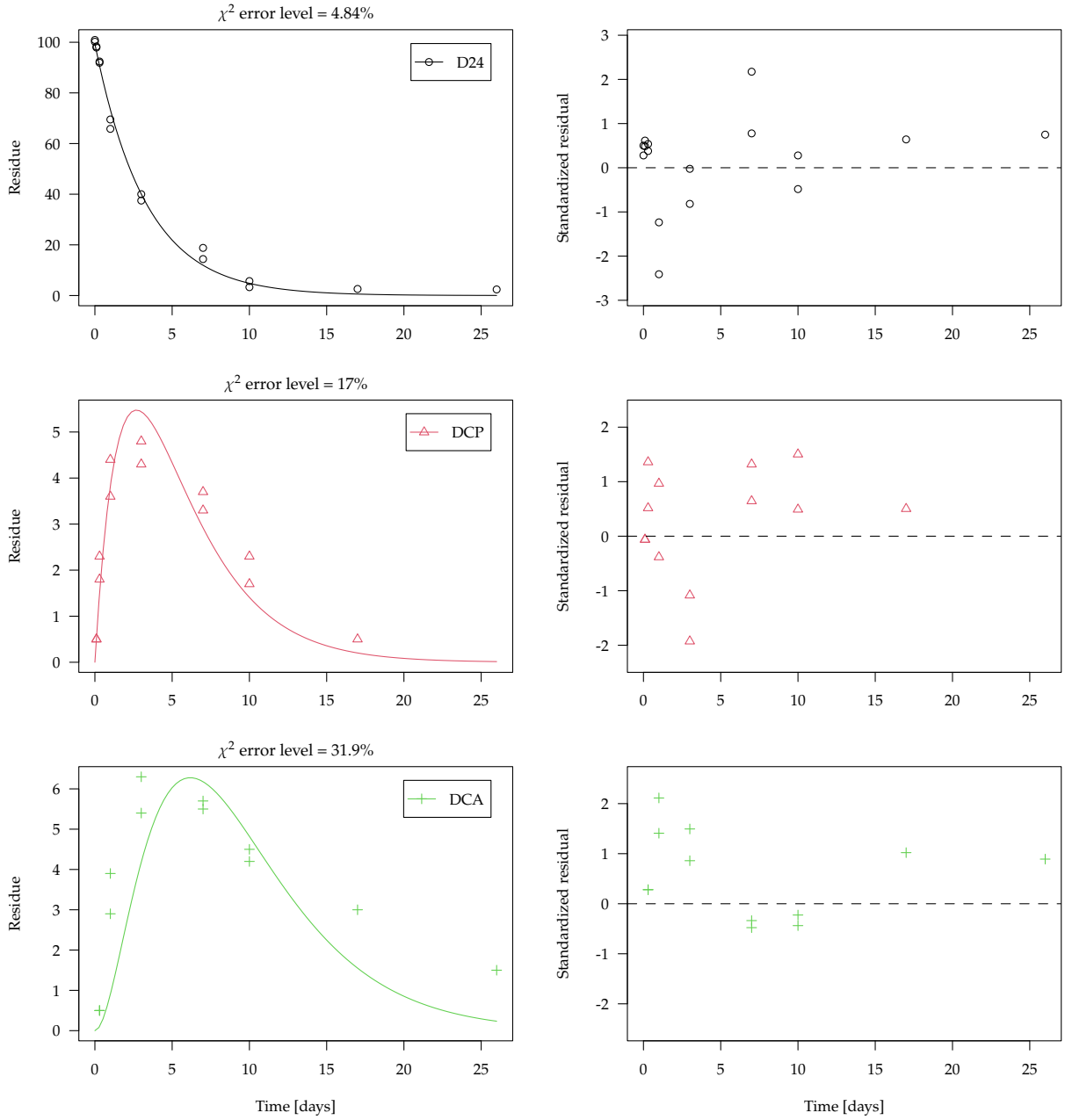

Figure 44: SFO-SFO-SFO fit for 2,4-D, Site E1

The fit for Site E1 44 looks visually acceptable for the parent and for DCP and for the most part of the DCA curve, only the last points are not found very well. As was the case for the Fayette dataset, the formation fraction from DCP to DCA is one, so the model without the pathway from DCP to sink is shown as well. Besides this possibility for improvement, the parameter statistics do not indicate problems (Table 16).

Table 16: Model parameters with confidence intervals and p-values

Model	Fitted parameters					
	Name	Unit	Estimate	Pr(>t)	Lower	Upper
SFO-SFO-SFO	D24_0	% AR	99.32	2.639e-37	96.52	102.1
	k_D24	d^{-1}	0.3025	3.343e-19	0.2716	0.337
	k_DCP	d^{-1}	0.4512	2.086e-05	0.2941	0.6921
	k_DCA	d^{-1}	0.2501	0.04773	0.1491	0.4195
	f_D24_to_DCP	-	0.1855	1.964e-07	0.1333	0.2521
	f_DCP_to_DCA	-	1	0.01212	0	1
	sigma_D24	% AR	3.151	1.809e-06	2.002	4.3
	sigma_DCP	% AR	0.5932	6.883e-05	0.3144	0.872
	sigma_DCA	% AR	1.419	0.0007881	0.7083	2.13
SFO-SFO(ns)-SFO	D24_0	% AR	99.32	3.365e-38	96.52	102.1
	k_D24	d^{-1}	0.3025	1.508e-19	0.2716	0.337
	k_DCP	d^{-1}	0.4512	1.867e-05	0.2942	0.6917
	k_DCA	d^{-1}	0.2501	0.0002008	0.1492	0.4193
	f_D24_to_DCP	-	0.1855	1.625e-07	0.1333	0.2521
	sigma_D24	% AR	3.151	1.639e-06	2.003	4.299
	sigma_DCP	% AR	0.5932	6.455e-05	0.3147	0.8716
	sigma_DCA	% AR	1.419	0.0001394	0.7091	2.129

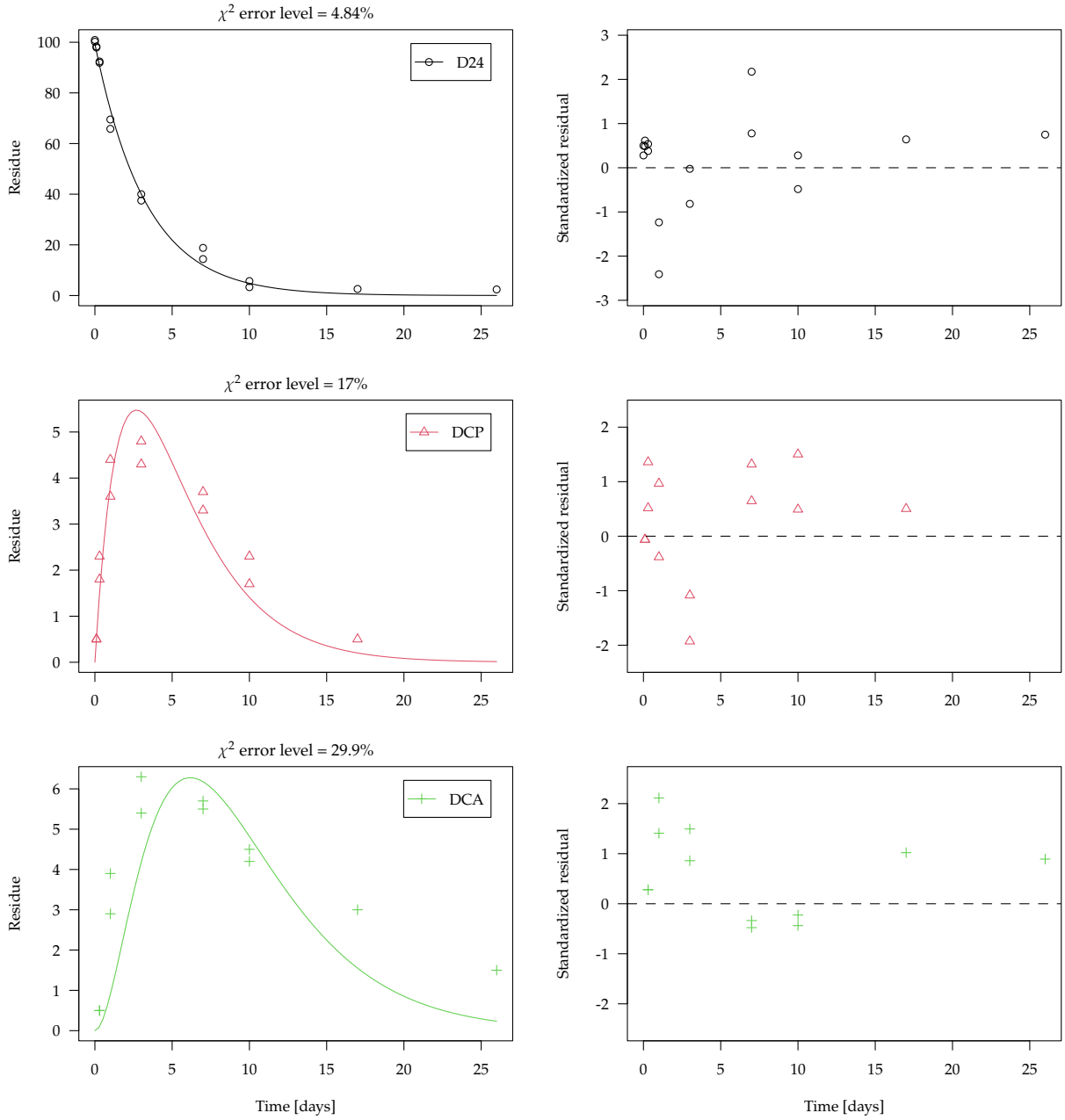

Figure 45: SFO-SFO(ns)-SFO fit for 2,4-D, Site E1

The AIC comparison suggests that the model without the pathway from DCP to sink fitted assuming variance by variable is the preferred variant for this dataset.

	df	AIC
f_d24_obs[["SFO-SFO-SFO", 4]]	9	165.9025
f_d24_obs[["SFO-SFO(ns)-SFO", 4]]	8	163.9025
f_d24_tc[["SFO-SFO-SFO", 4]]	8	181.7071
f_d24_tc[["SFO-SFO(ns)-SFO", 4]]	7	179.7071

The likelihood ratio test confirms that the "variance by variable" error model is preferable, but does not confirm that the model without the pathway from DCP to sink is preferable.

```
Likelihood ratio test

Model 1: SFO-SFO-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO-SFO with error model tc and fixed parameter(s) DCP_0, DCA_0
  #Df  LogLik Df  Chisq Pr(>Chisq)
1   9 -73.951
2   8 -82.854 -1 17.805  2.448e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1


Likelihood ratio test

Model 1: SFO-SFO-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO(ns)-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
  #Df  LogLik Df Chisq Pr(>Chisq)
1   9 -73.951
2   8 -73.951 -1     0     0.9999
```

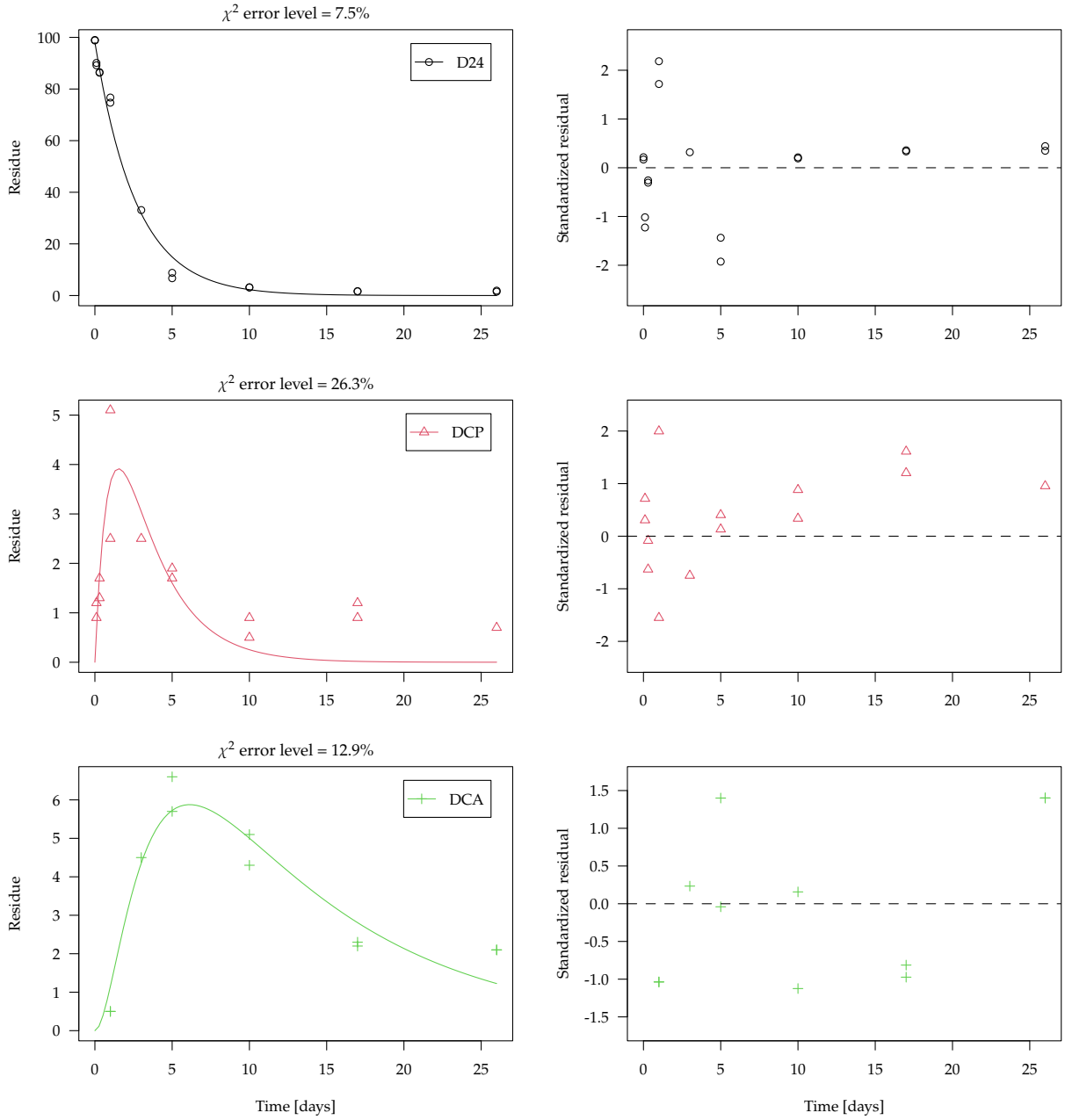

Figure 46: SFO-SFO-SFO fit for 2,4-D, Site I2

The fit for Site I2 46 looks visually acceptable for the parent and for DCA. For DCP, similar as in the case of dataset 3 (RefSol 03-G), a biphasic fit for the metabolite may be called for. Other than that, the parameter statistics do not indicate that the model would need to be simplified (Table 17).

Table 17: Model parameters with confidence intervals and p-values

Model	Fitted parameters					
	Name	Unit	Estimate	Pr(>t)	Lower	Upper
SFO-SFO-SFO	D24_0	% AR	98.08	1.039e-33	94.28	101.9
	k_D24	d^{-1}	0.3761	1.644e-16	0.3281	0.4311
	k_DCP	d^{-1}	1.041	7.164e-05	0.6486	1.672
	k_DCA	d^{-1}	0.0934	4.275e-07	0.06669	0.1308
	f_D24_to_DCP	-	0.1966	8.339e-06	0.1289	0.2881
	f_DCP_to_DCA	-	0.4933	0.000108	0.2703	0.719
	sigma_D24	% AR	4.289	8.015e-07	2.792	5.786
	sigma_DCP	% AR	0.7327	3.959e-06	0.4507	1.015
	sigma_DCA	% AR	0.6243	2.419e-05	0.3524	0.8962

The AIC comparison suggests that the model including the pathway from DCP to sink fitted assuming variance by variable is the preferred variant also for this dataset.

```
                                df      AIC
f_d24_obs[["SFO-SFO-SFO", 5]]    9 167.6242
f_d24_obs[["SFO-SFO(ns)-SFO", 5]] 8 172.2067
f_d24_tc[["SFO-SFO-SFO", 5]]     8 183.2611
f_d24_tc[["SFO-SFO(ns)-SFO", 5]] 7 183.6597
```

The likelihood ratio test confirms that the “variance by variable” error model is preferable, and that the sink from DCP to sink should be used in the model.

```
Likelihood ratio test

Model 1: SFO-SFO-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO-SFO with error model tc and fixed parameter(s) DCP_0, DCA_0
  #Df  LogLik Df  Chisq Pr(>Chisq)
1   9 -74.812
2   8 -83.631 -1 17.637  2.674e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1


Likelihood ratio test

Model 1: SFO-SFO-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
Model 2: SFO-SFO(ns)-SFO with error model obs and fixed parameter(s) DCP_0, DCA_0
  #Df  LogLik Df  Chisq Pr(>Chisq)
1   9 -74.812
2   8 -78.103 -1 6.5825     0.0103 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Simultaneous pathway fits

Fitting the SFO-SFO-SFO model with nlme is possible in several variants. The only variant that converges without adapting the control parameters is the variant without the pathway from DCP to sink and assuming constant error. When using either the variance by variable error model or the two-component error model, convergence can be obtained for the same degradation model by increasing the number of iterations in the Partial Nonlinear Least Squares step (PNLS step), and increasing the overall convergence tolerance. The same adaptations also make it possible to fit the full degradation model with two-component error.

The AIC values and the likelihood ratio tests indicate that out of the converged fits, the reduced degradation model combined with the variance by variable error model performs best (`f_d24_2_nlme_obs`).

	Model	df	AIC	BIC	logLik	Test	L.Ratio
f_d24_2_nlme_const	1	11	989.4115	1024.0977	-483.7058		
f_d24_2_nlme_obs	2	13	883.8171	924.8099	-428.9086	1 vs 2	109.59436
f_d24_nlme_tc	3	14	923.7541	967.9002	-447.8771	2 vs 3	37.93698
f_d24_2_nlme_tc	4	12	916.2860	954.1254	-446.1430	3 vs 4	3.46818

	p-value
f_d24_2_nlme_const	
f_d24_2_nlme_obs	<.0001
f_d24_nlme_tc	<.0001
f_d24_2_nlme_tc	0.1766

Plots for the reduced model assuming constant variance (Figure 47), variance by variable (Figure 48) and two-component error (Figure 49) are shown below.

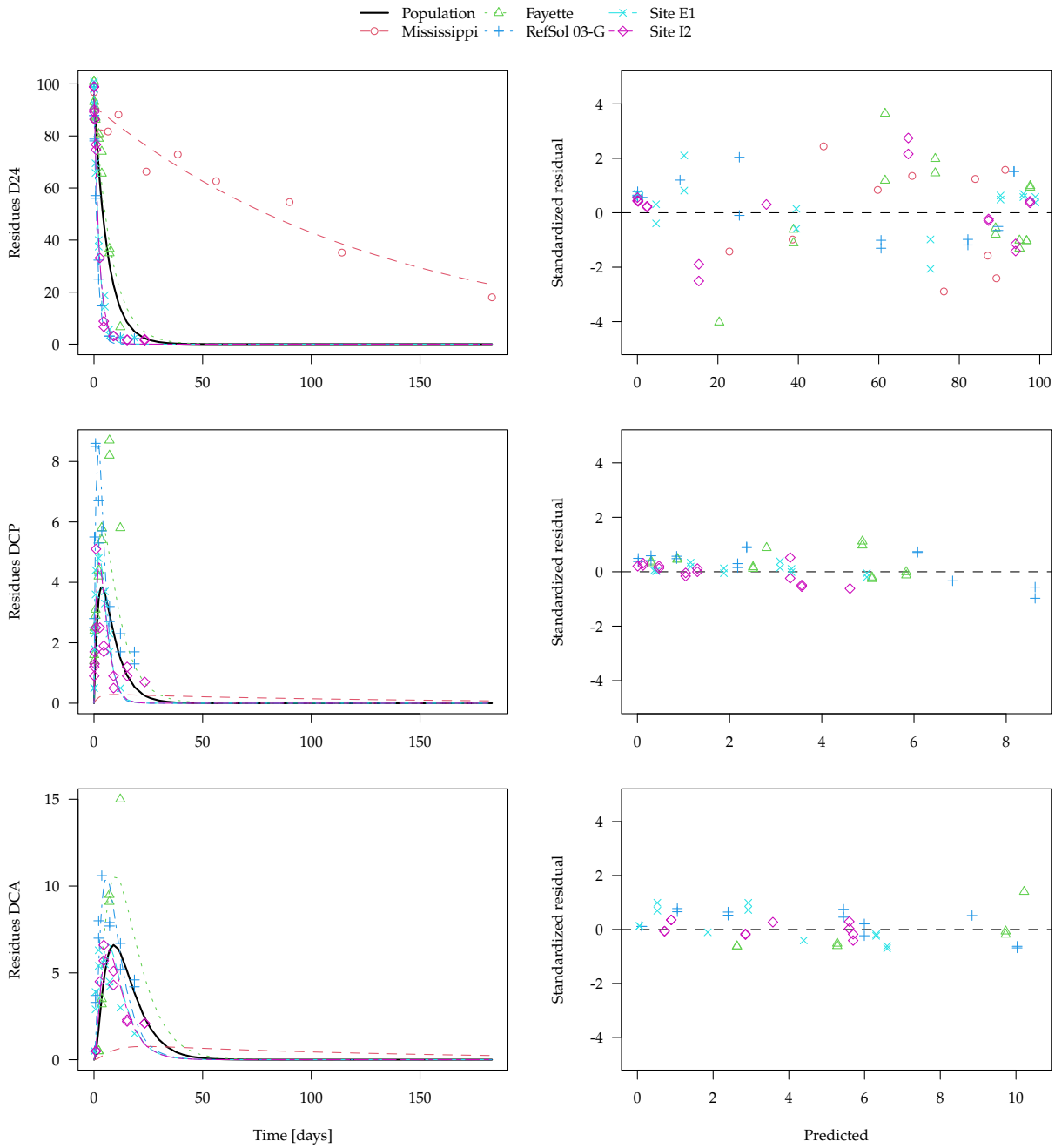

Figure 47: SFO-SFO(ns)-SFO fitted using nlme assuming constant error

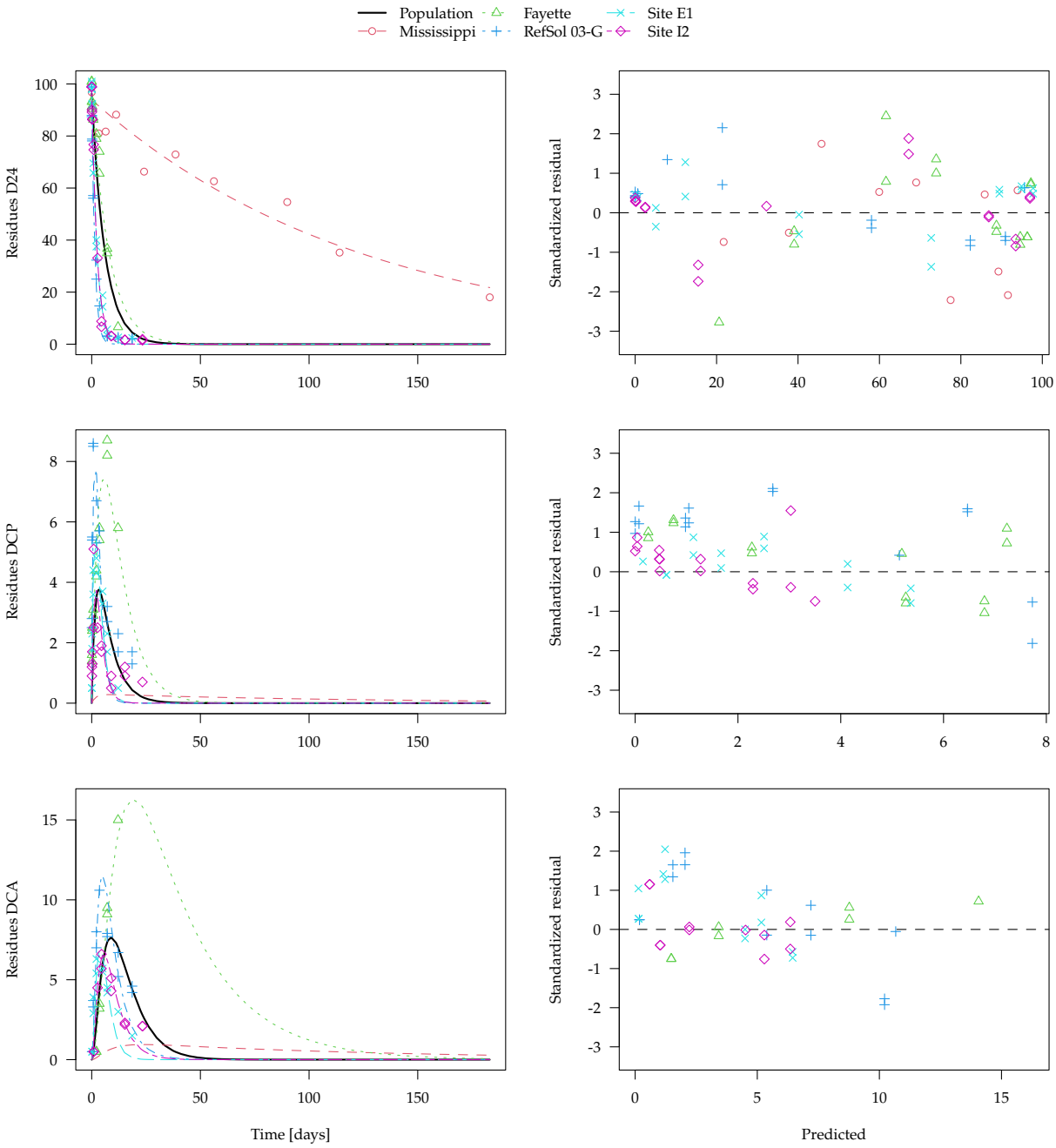

Figure 48: SFO-SFO-SFO(ns) fitted using nlme assuming variance by variable

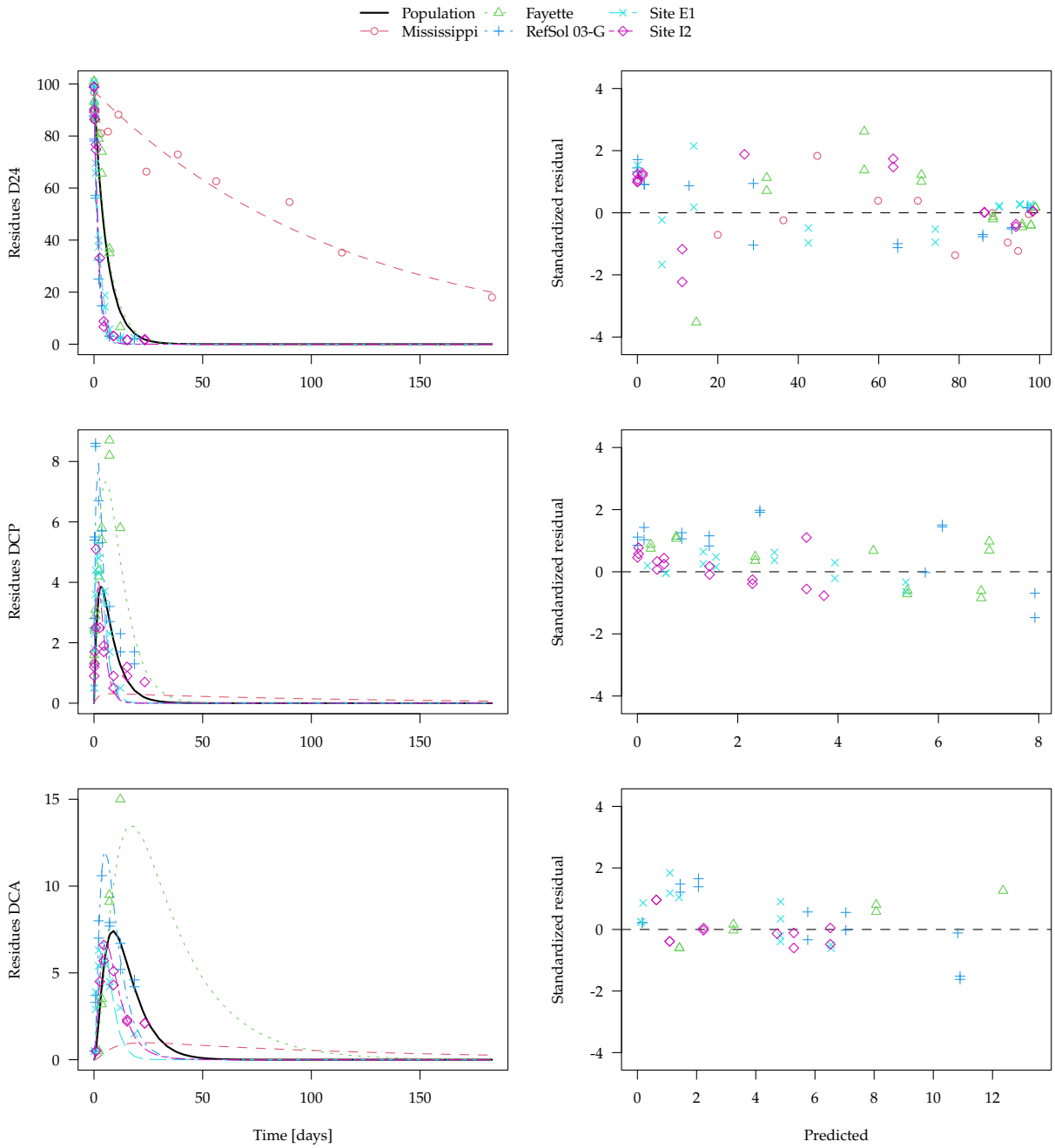

Figure 49: SFO-SFO(ns)-SFO fitted using nlme assuming two-component error

It is currently a bit time consuming to fit these degradation models using saemix, as analytical solutions have not been implemented for this degradation model. Each fit takes about 10 minutes to complete.

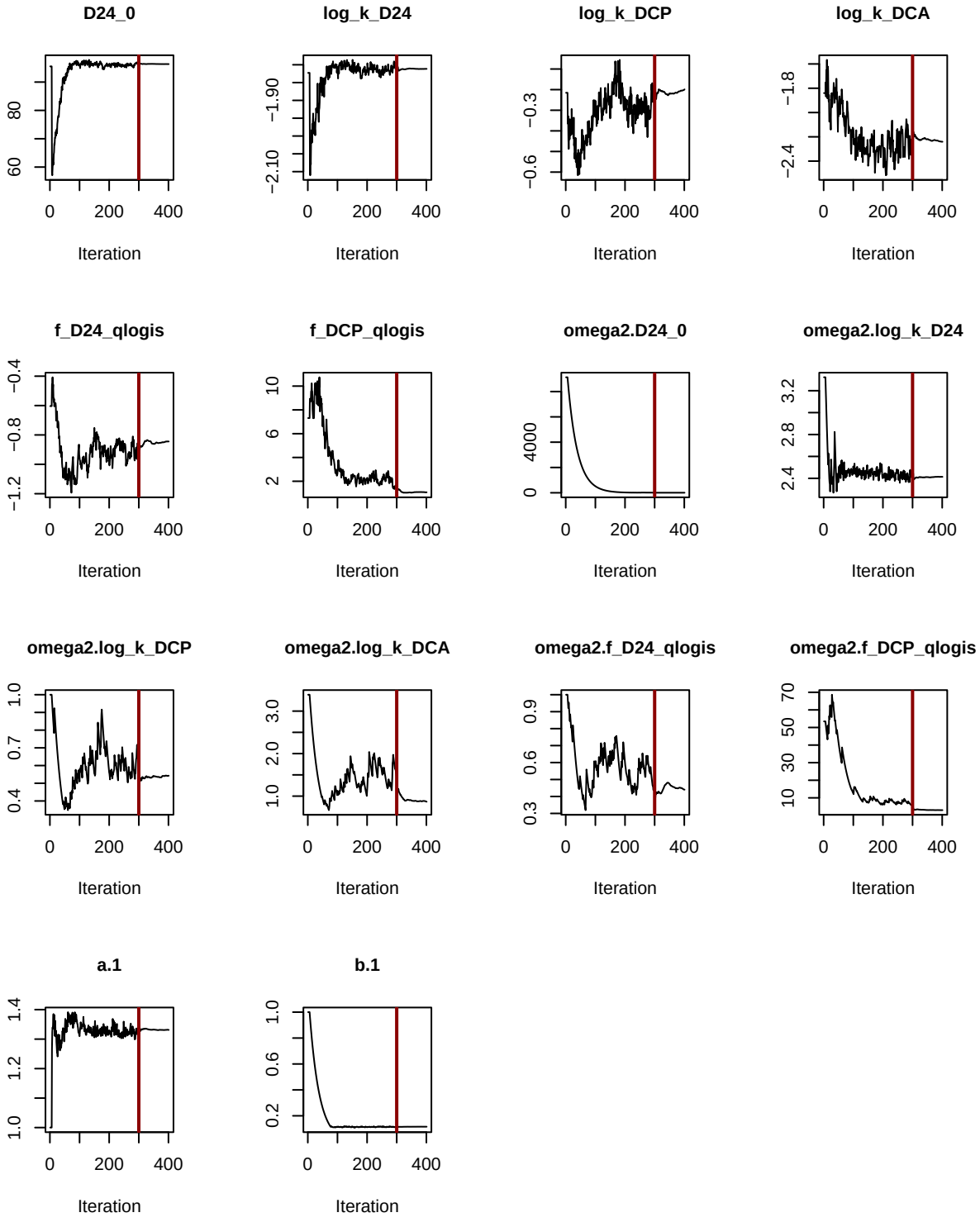

Figure 50: Convergence plot for SFO-SFO-SFO fitted using saemix assuming two-component error

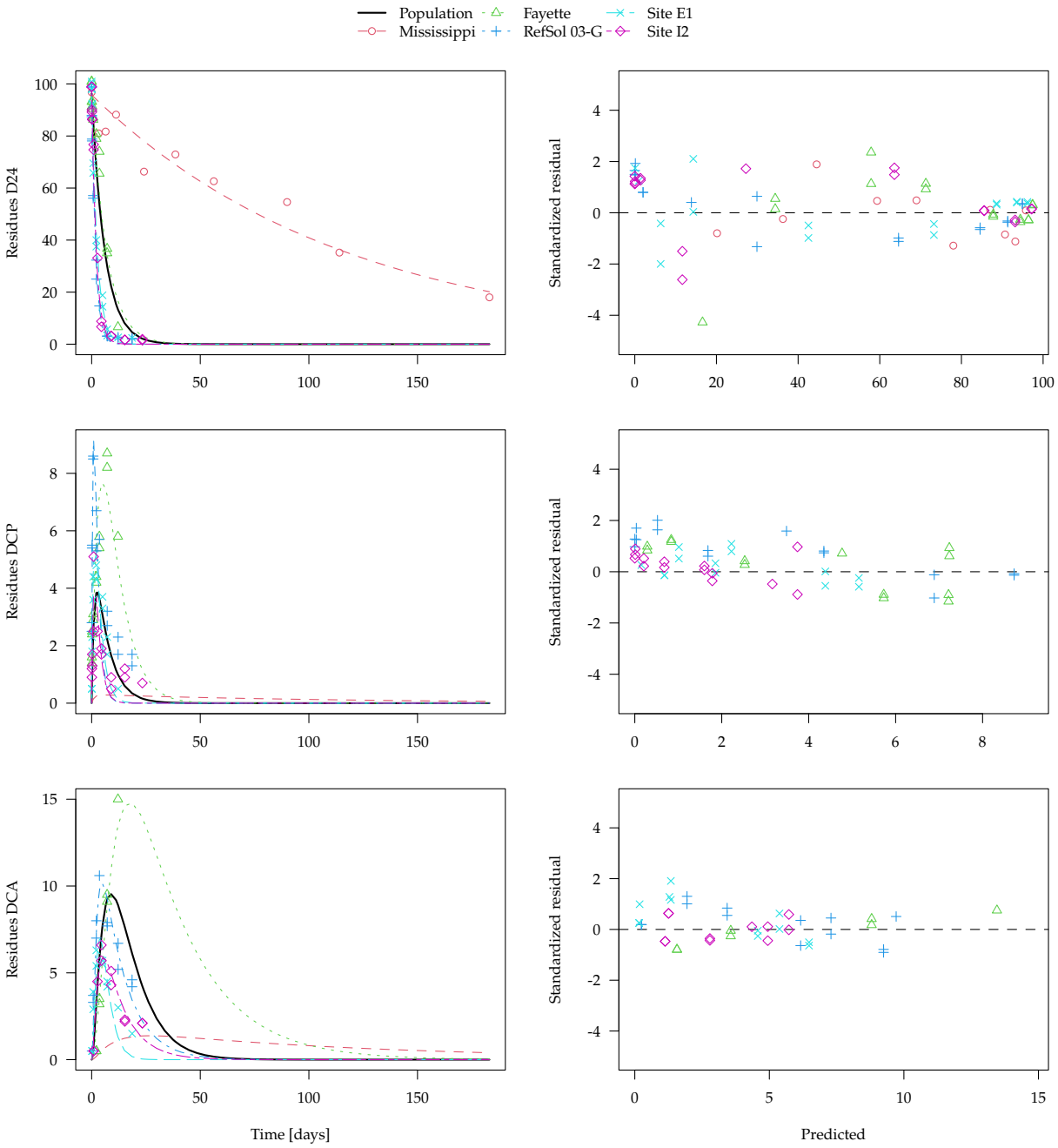

Figure 51: SFO-SFO-SFO fitted using saemix assuming two-component error

As only data for the Mississippi soil contain observations at later sampling times, the plot shown in Figure 51 is repeated below with the x axis limited to 30 normalised days.

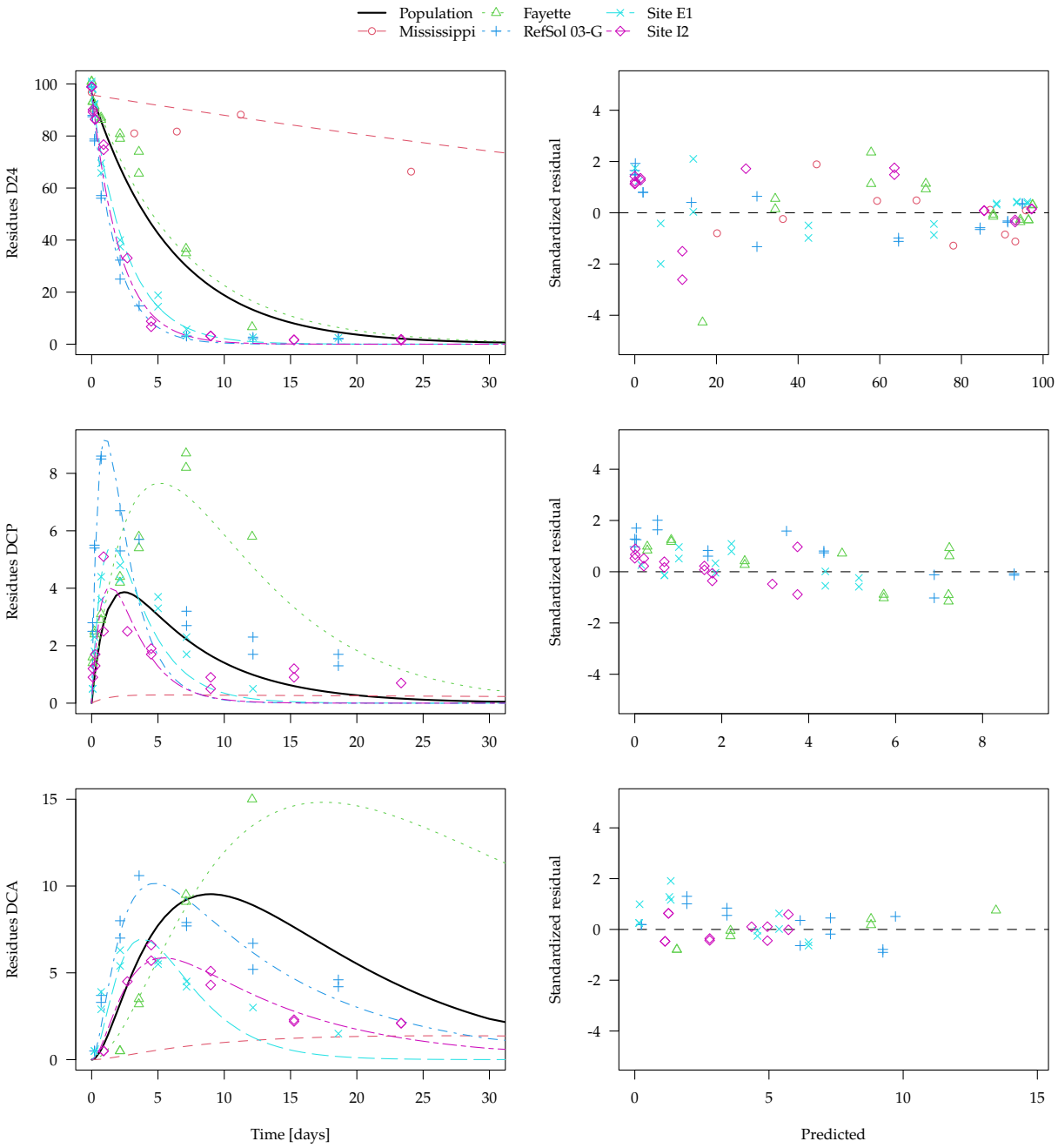

Figure 52: SFO-SFO-SFO fitted using saemix assuming two-component error

In addition to this fit with the full degradation model, saemix fits with the reduced model, without the pathway from DCP to sink, are shown. Convergence plots and summary plots for the fits using the two available error models (constant and two-component error) are shown below. As the parent data in the Mississippi soil are always fitted well, the following plots only show the first 30 normalised days.

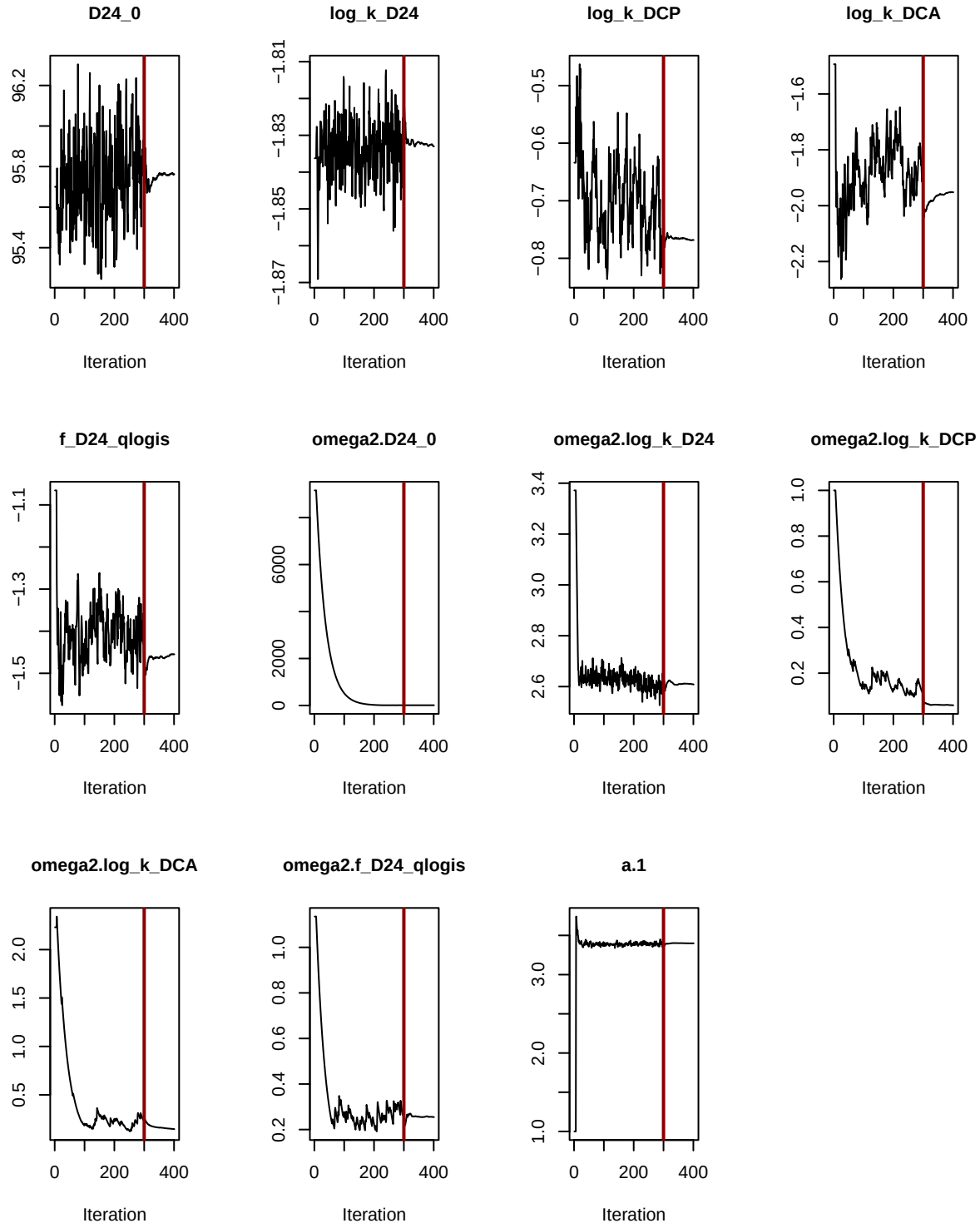

Figure 53: Convergence plot for SFO-SFO(ns)-SFO fitted using saemix assuming constant error

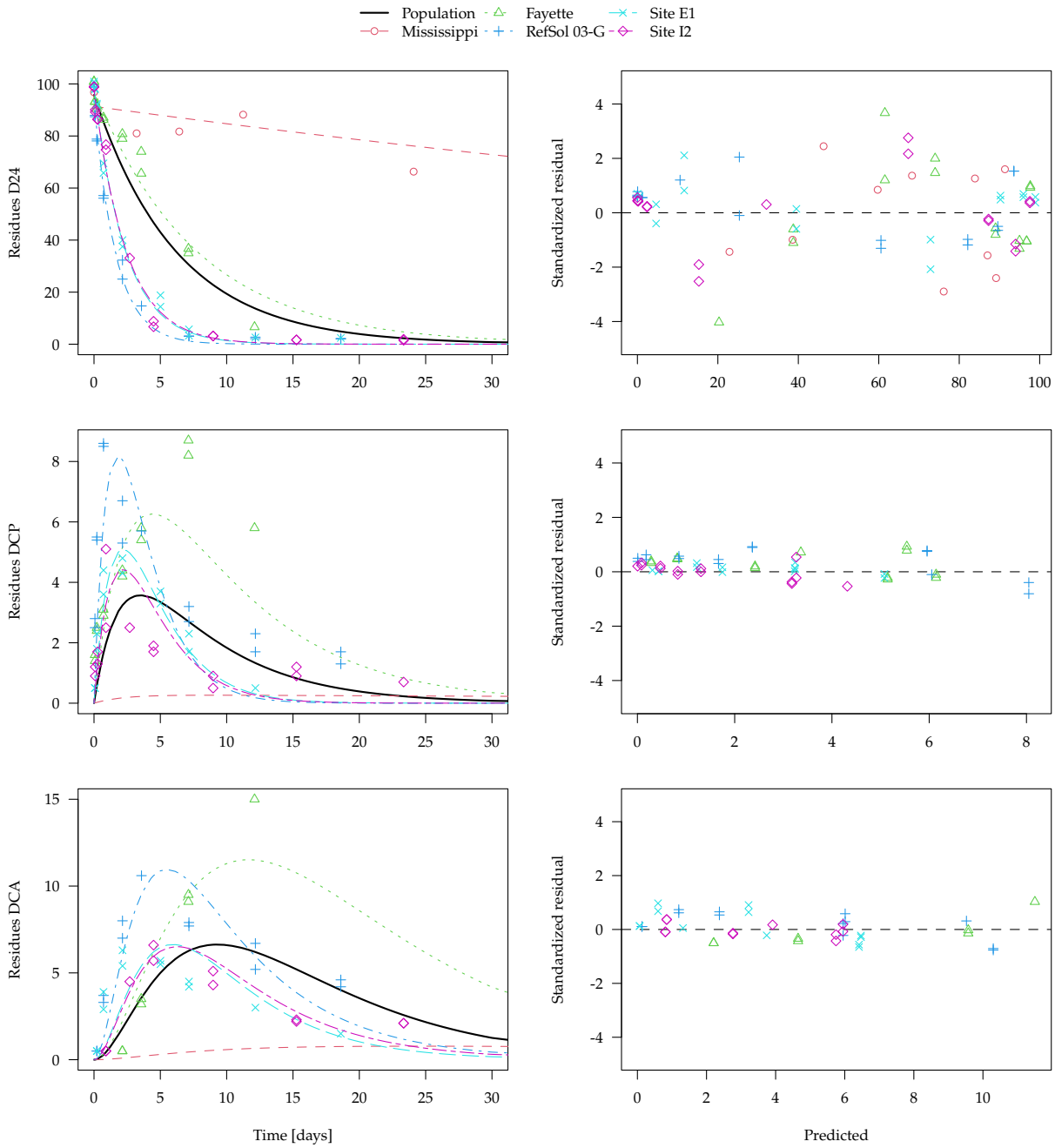

Figure 54: SFO-SFO(ns)-SFO fitted using saemix assuming constant error

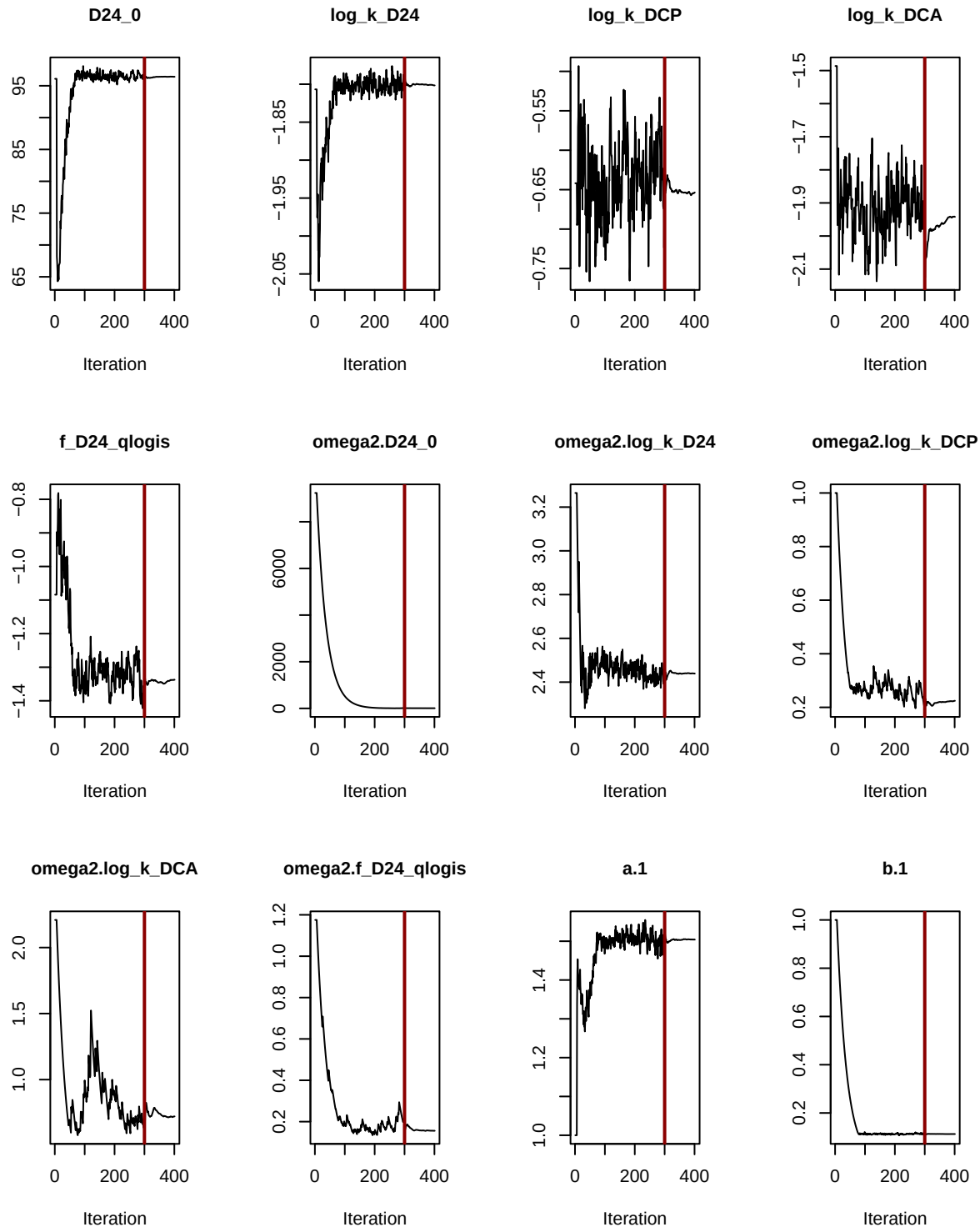

Figure 55: Convergence plot for SFO-SFO(ns)-SFO fitted using saemix assuming two-component error

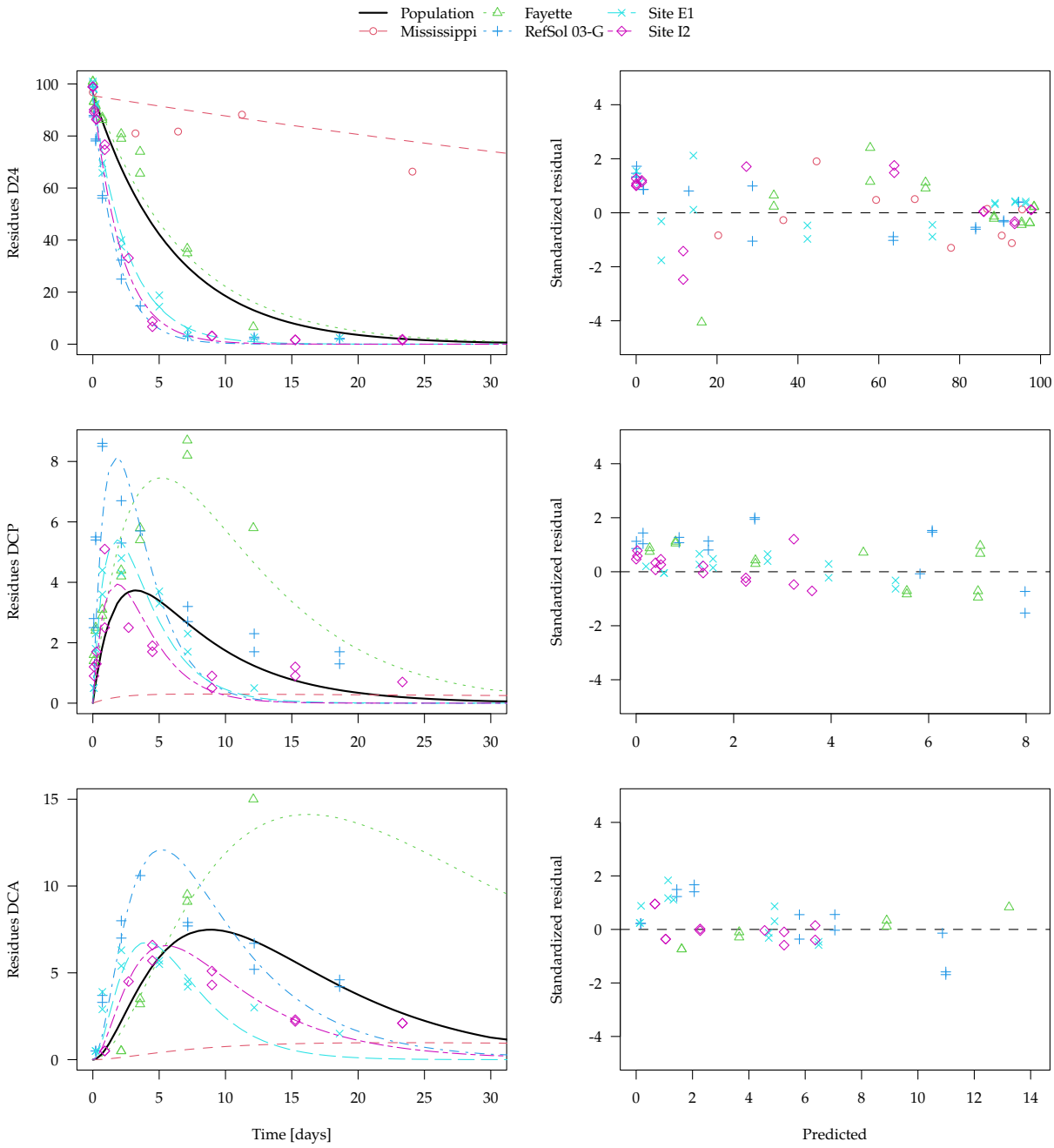

Figure 56: SFO-SFO(ns)-SFO fitted using saemix assuming two-component error

The comparison of these three saemix variants indicates that fit of the full model combined with the two-component error model (first line) is preferable over the variants with the reduced degradation model.

```
Likelihoods calculated by importance sampling

       AIC      BIC
1 907.5369 902.0690
2 989.7640 985.4678
3 913.3274 908.6406
```

Check of transformations

```
tikz output
          2


tikz output
          2
```

Endpoint comparisons

The non-normalised endpoints obtained in the separate fits are shown in Table 18, together with arithmetic mean formation fractions. Normalised DT_{50} values for modelling are shown in Table 19, together with their geometric mean values.

Table 18: Non-normalised endpoints for modelling as obtained in the separate fits to the data

Soil	2,4-D		DCP		DCA
	DT_{50} [d]	**ff to DCP** [-]	**DT_{50}** [d]	**ff to DCA** [-]	**DT_{50}** [d]
Mississippi	58.867				
Fayette	7.640	0.2889	4.3634	0.2889	59.439[a]
RefSol 03-G	1.625	0.7482	0.3227	1.0000[b]	13.142
Site E1	2.291	0.1855	1.5364	0.1855	2.772
Site I2	1.843	0.1966	0.6657	1.0000[b]	7.421
Arithmetic mean		**0.355**		**0.619**	

ff: Formation fraction
[a] Based on a non-significant rate constant
[b] Pathway from DCP to sink was negligible

Table 19: Normalised modelling DT_{50} values as obtained in the separate fits to the data

Soil	2,4-D [d]	DCP [d]	DCA [d]
Mississippi	94.555		
Fayette	5.439	3.1062	42.313[a]
RefSol 03-G	1.163	0.2309	9.405
Site E1	1.640	1.0995	1.983
Site I2	1.654	0.5976	6.662
Geometric mean	**4.39**	**0.829**	**8.52**

[a] Based on a non-significant rate constant

Table 20: Modelling endpoints derived from mixed effects models fitted to the pathway

Algorithm	**2,4-D**		**DCP**		**DCA**
	DT_{50} [d]	**ff to DCP** [-]	**DT_{50}** [d]	**ff to DCA** [-]	**DT_{50}** [d]
nlme	4.213	0.211	1.325	1.000	4.933
saemix	4.200	0.208	1.332	1.000	4.834

ff: Formation fraction

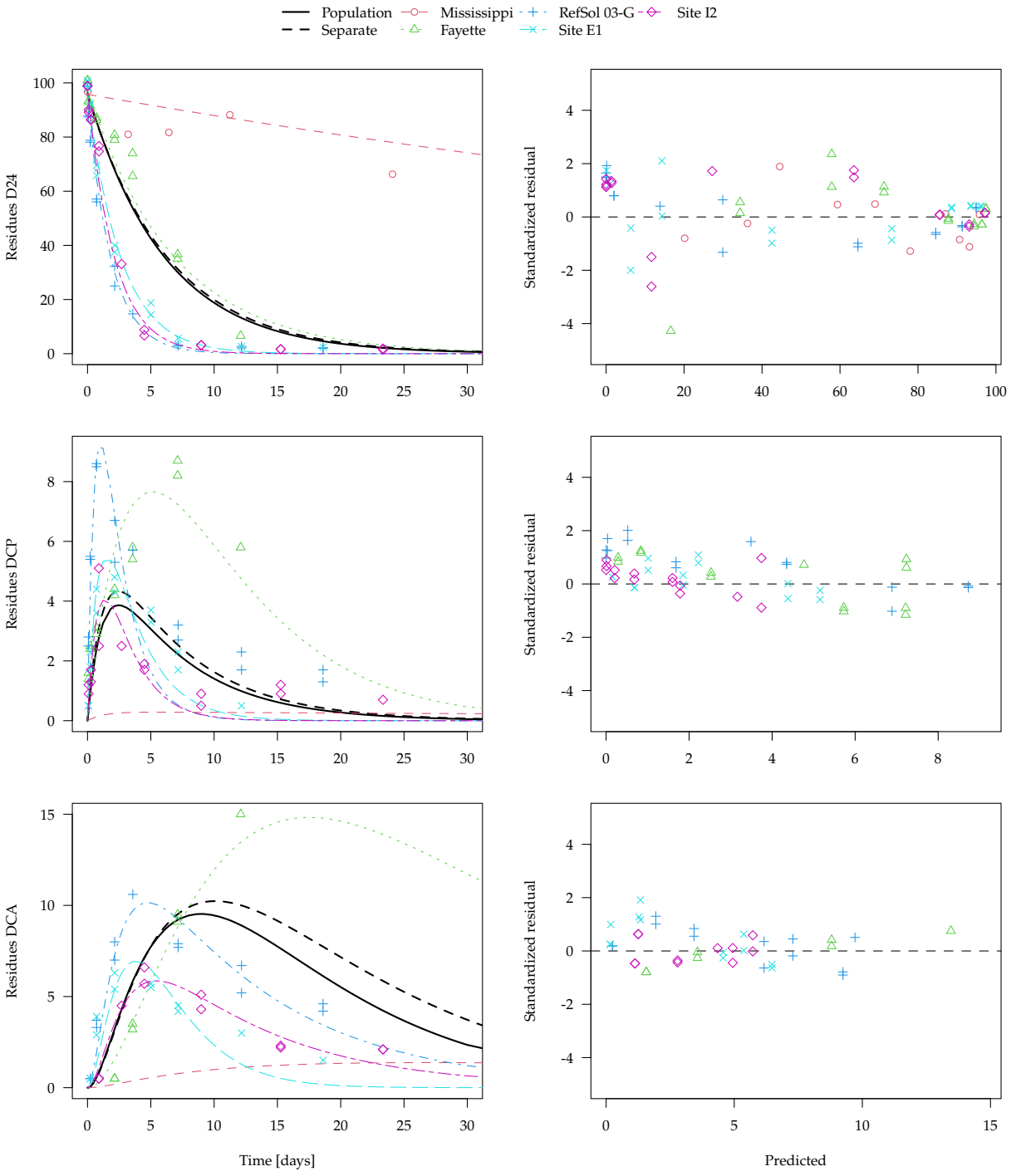

Figure 57: Overlay of degradation curves derived from separate fits and the best saemix fit, first 30 days

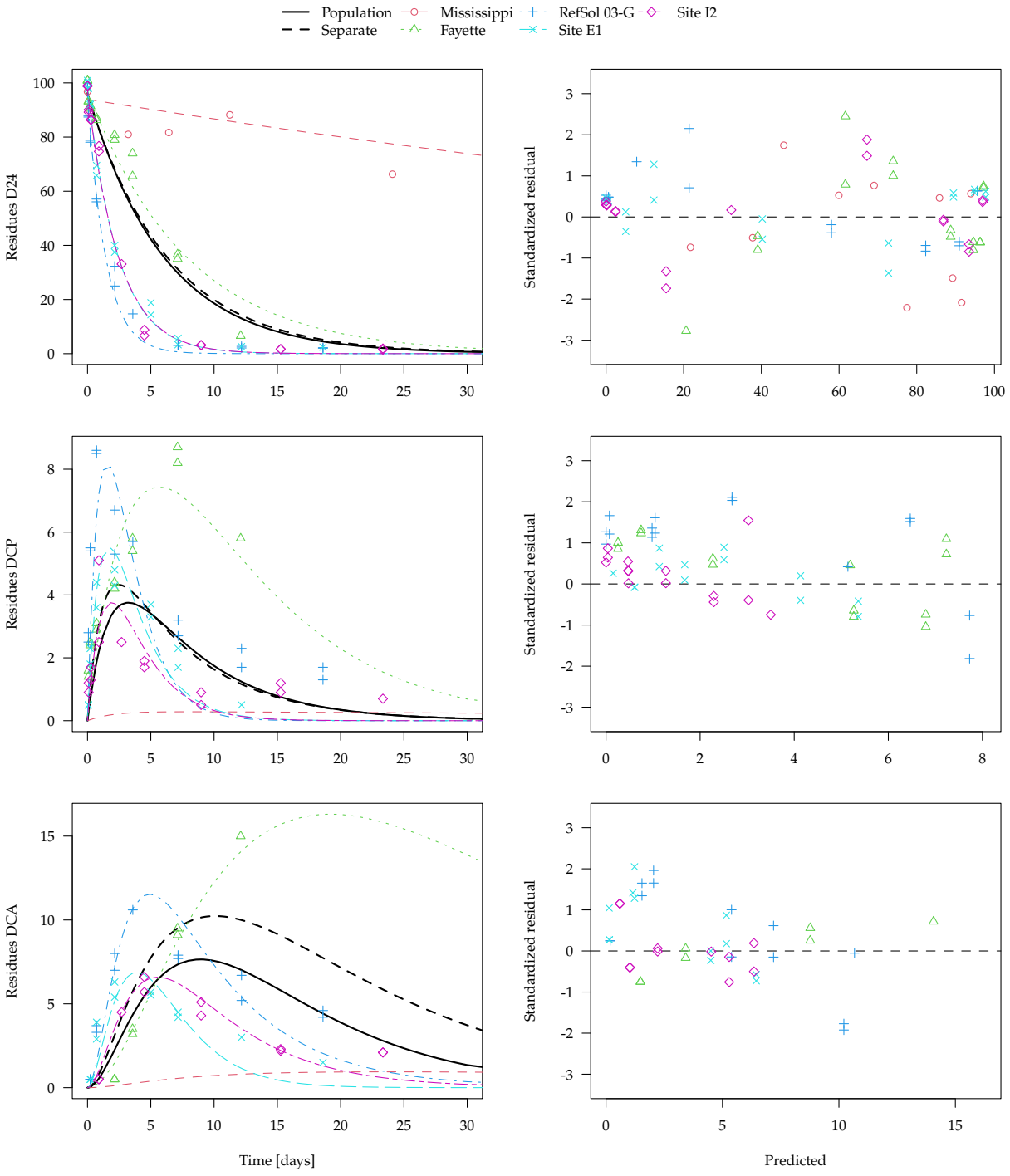

Figure 58: Overlay of degradation curves derived from separate fits and the best nlme fit, first 30 days

EU risk assessment of dimethenamid-P from 2018

In this section, the aerobic soil degradation data on dimethenamid as documented in the Review Assessment Report of the European Union pesticide risk assessment peer review for dimethenamid-P from 2018 are evaluated (EFSA, 2018).

The data are used as available from the mkin package. The dataset in the package already contains normalisation factors for time step normalisation to reference conditions. The following code shows how the data from the package is preprocessed for this analysis.

```
dmta_ds <- lapply(1:8, function(i) {
  ds_i <- dimethenamid_2018$ds[[i]]$data
  ds_i[ds_i$name == "DMTAP", "name"] <-  "DMTA"
  ds_i$time <- ds_i$time * dimethenamid_2018$f_time_norm[i]
  ds_i
})
names(dmta_ds) <- sapply(dimethenamid_2018$ds, function(ds) ds$title)
dmta_ds[["Borstel"]] <- rbind(dmta_ds[["Borstel 1"]], dmta_ds[["Borstel 2"]])
dmta_ds[["Borstel 1"]] <- NULL
dmta_ds[["Borstel 2"]] <- NULL
dmta_ds[["Elliot"]] <- rbind(dmta_ds[["Elliot 1"]], dmta_ds[["Elliot 2"]])
dmta_ds[["Elliot 1"]] <- NULL
dmta_ds[["Elliot 2"]] <- NULL
```

In the first step, the datasets are extracted from the `mkindsg` object used for storing these data in mkin. As the ratio of stereoisomers was not found to have an influence on aerobic soil degradation in the EU assessment, the acronym "DMTA" is used for both compounds, dimethenamid-P and dimethenamid. Furthermore, the data that were obtained under equivalent conditions in the Borstel and Elliot soils were merged.

The result is a list of six time step normalised datasets for the six different soils, suitable for separate analysis with `mmkin` and subsequent combined analysis with `saem.mmkin`.

Separate evaluations

Please refer to to the main article for a rationale of the degradation models used. Figures 59 shows the separate fits of the SFO-SFO3 model to these six datasets using constant variance. The visual impression of the fits appears to be acceptable, but closer inspection shows some deficiencies. First, the residual plot for the parent compound indicate some systematic deviations (a slight U shape typically found if SFO is fitted to biexponential decline data). Then, the residuals for the parent compound tend to be higher than for the transformation product, and for all compounds they tend to increase with the predicted values. Finally, the population curve derived from the mean parameters is not very accurate for M27, as the residues observed for this transformation product are overestimated at later time points.

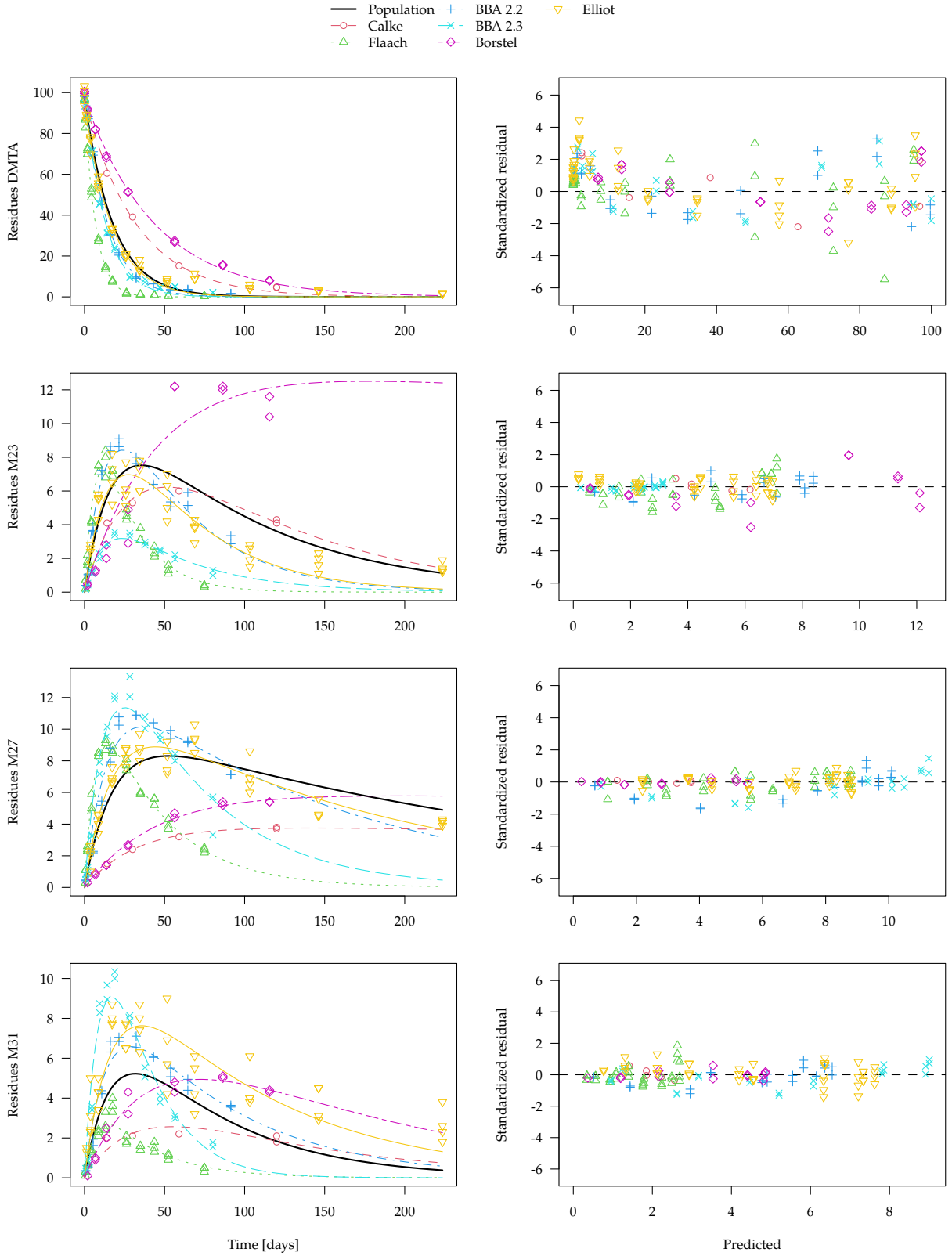

Figure 59: Separate fits of the SFO-SFO3 model to the normalised DMTA data assuming constant variance

The latter point is improved by using the additional pathway from M31 to M27 in the degradation

model, i.e. using the model that was relied on in the EU pesticide review (Figure 60).

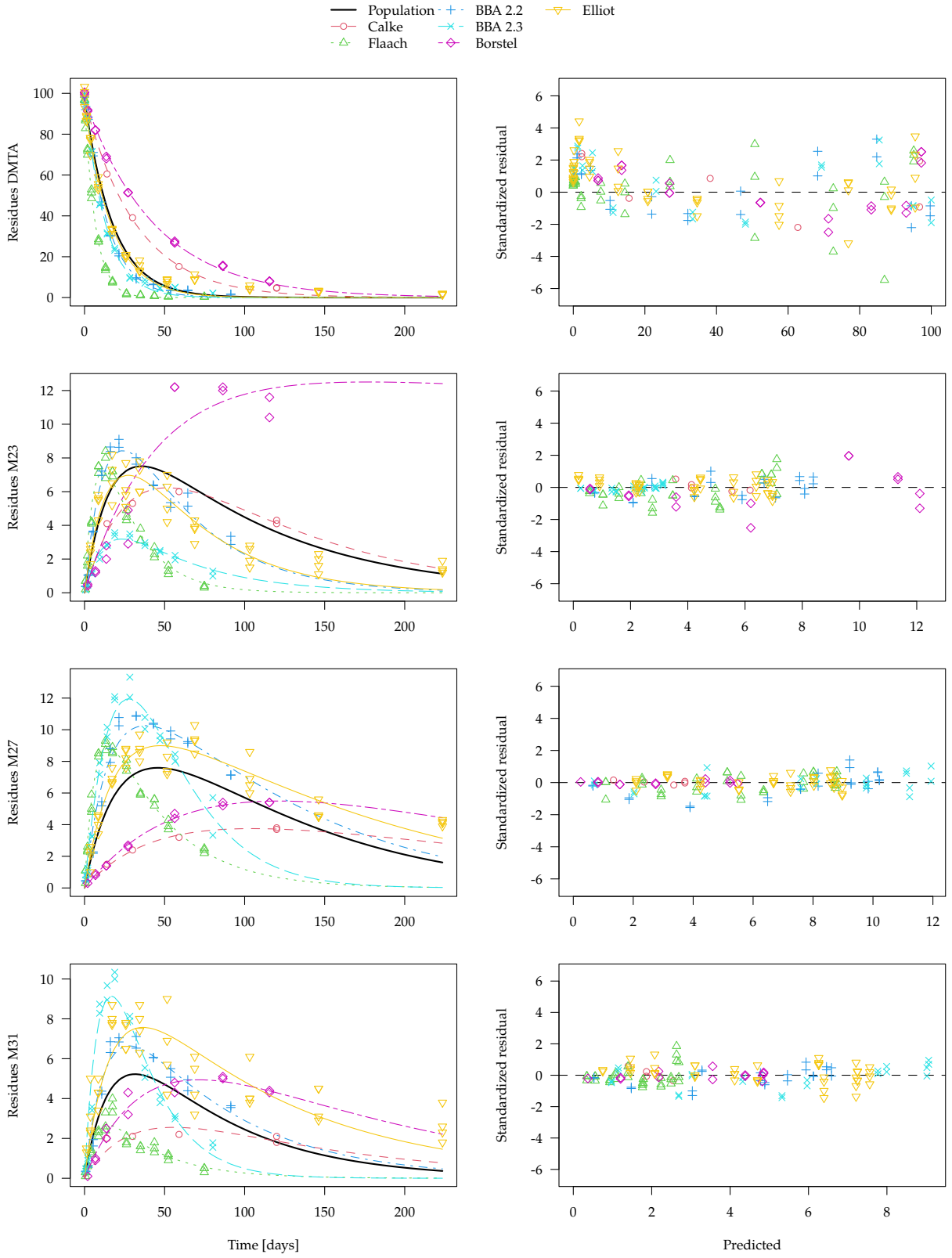

Figure 60: Separate fits of the SFO-SFO3+ model to the normalised DMTA data assuming constant variance

The slight U shape of the residual plot for the parent can be addressed by using DFOP for the parent compound, and the remaining structures in the residual plots can be addressed by using the two alternative error models. The following three tables show the AIC values for the combinations of the four degradation models with the three error models. For each soil, the lowest AIC value found across the three tables is highlighted in bold. From these values it can be concluded that the DFOP model should be used for the parent compound and either variance by variable or the two-component error model should be used.

Table 21: AIC values for the separate fits of three degradation models to data from six soils using constant variance

Soil	SFO-SFO3	SFO-SFO3+	DFOP-SFO3	DFOP-SFO3+
Calke	80.95	80.99	68.08	68.13
Flaach	318.34	318.28	319.21	301.26
BBA 2.2	291.88	290.22	283.64	281.64
BBA 2.3	332.16	325.99	313.55	304.51
Borstel	224.18	224.09	192.15	191.83
Elliot	769.51	770.04	622.3	621.08

Table 22: AIC values for the separate fits of three degradation models to data from six soils using variance by variable

Soil	SFO-SFO3	SFO-SFO3+	DFOP-SFO3	DFOP-SFO3+
Calke	43.46	46.96	**28.7**	34.02
Flaach	266.79	266.64	270.25	270.55
BBA 2.2	259.58	257.2	259.83	257.48
BBA 2.3	253.24	239.41	252.79	**238.37**
Borstel	158.95	150.78	147.48	**141.78**
Elliot	637.25	639.77	577.75	574.36

Table 23: AIC values for the separate fits of three degradation models to data from six soils using two-component error

Soil	SFO-SFO3	SFO-SFO3+	DFOP-SFO3	DFOP-SFO3+
Calke	77.81	77.87	41.84	42.25
Flaach	242.38	242.25	**240.88**	246.25
BBA 2.2	276.94	274.5	250.66	**246.68**
BBA 2.3	323.08	314.73	286.28	268.26
Borstel	198.73	198.28	194.15	193.83
Elliot	757.37	758.28	572.25	**569.81**

Figure 61 shows the separate fits of the DFOP-SFO3+ model assuming two-component error. The trends in the residual plots identified above are addressed, there is no U shape of residuals for the parent, and magnitude of the standardized residuals is comparable for the four compounds. However, the degradation curves obtained from the mean parameters are clearly wrong, because parameters k1 and k2 converged to excessively small values in one soil each, leading to geometric mean values that are much too small to be representative of the population.

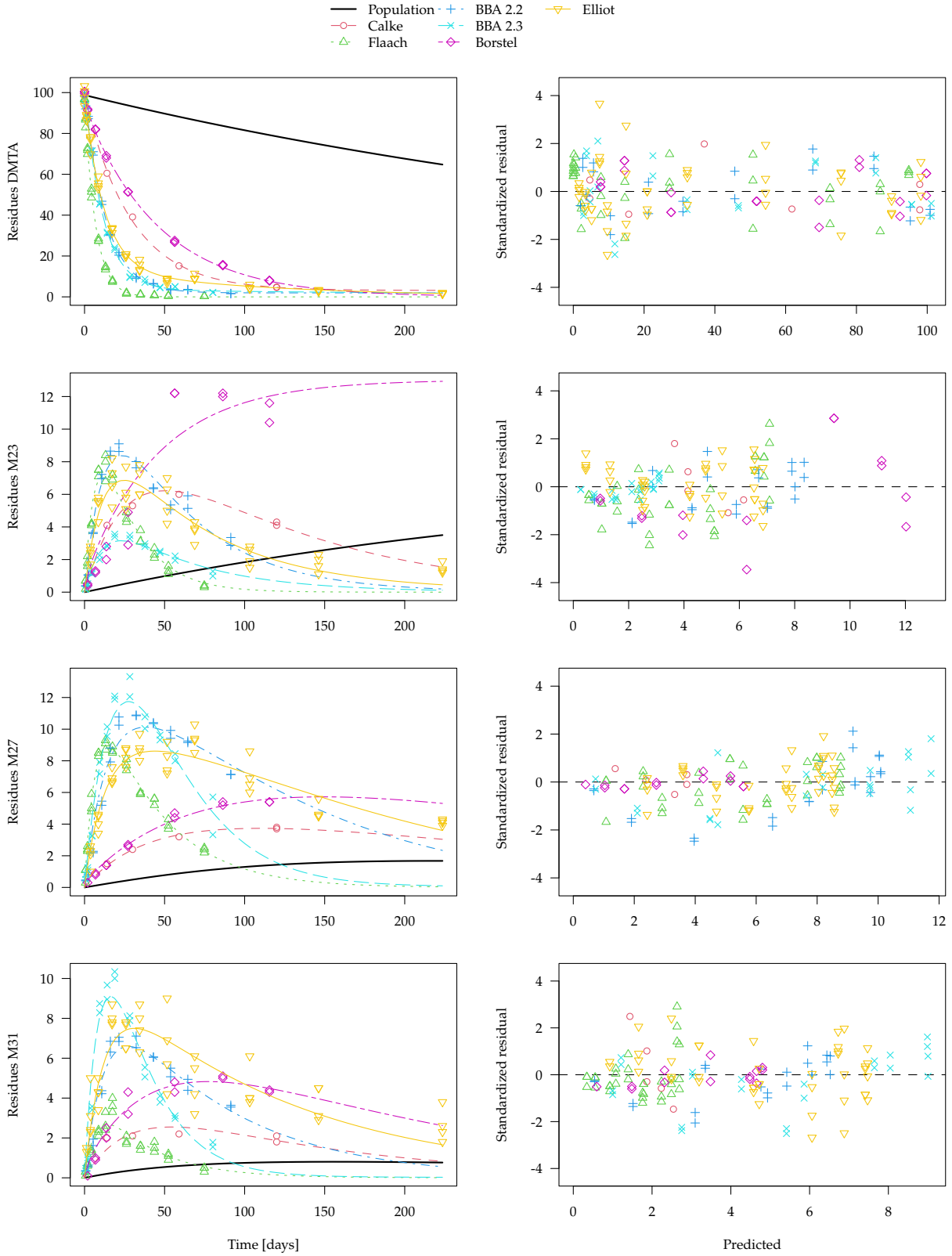

Figure 61: Separate fits of the DFOP-SFO3+ model to the normalised DMTA data assuming two-component error

This problem can be alleviated by only considering parameters in the averaging procedure that pass

the t-test for significant difference from zero (Figure 62).

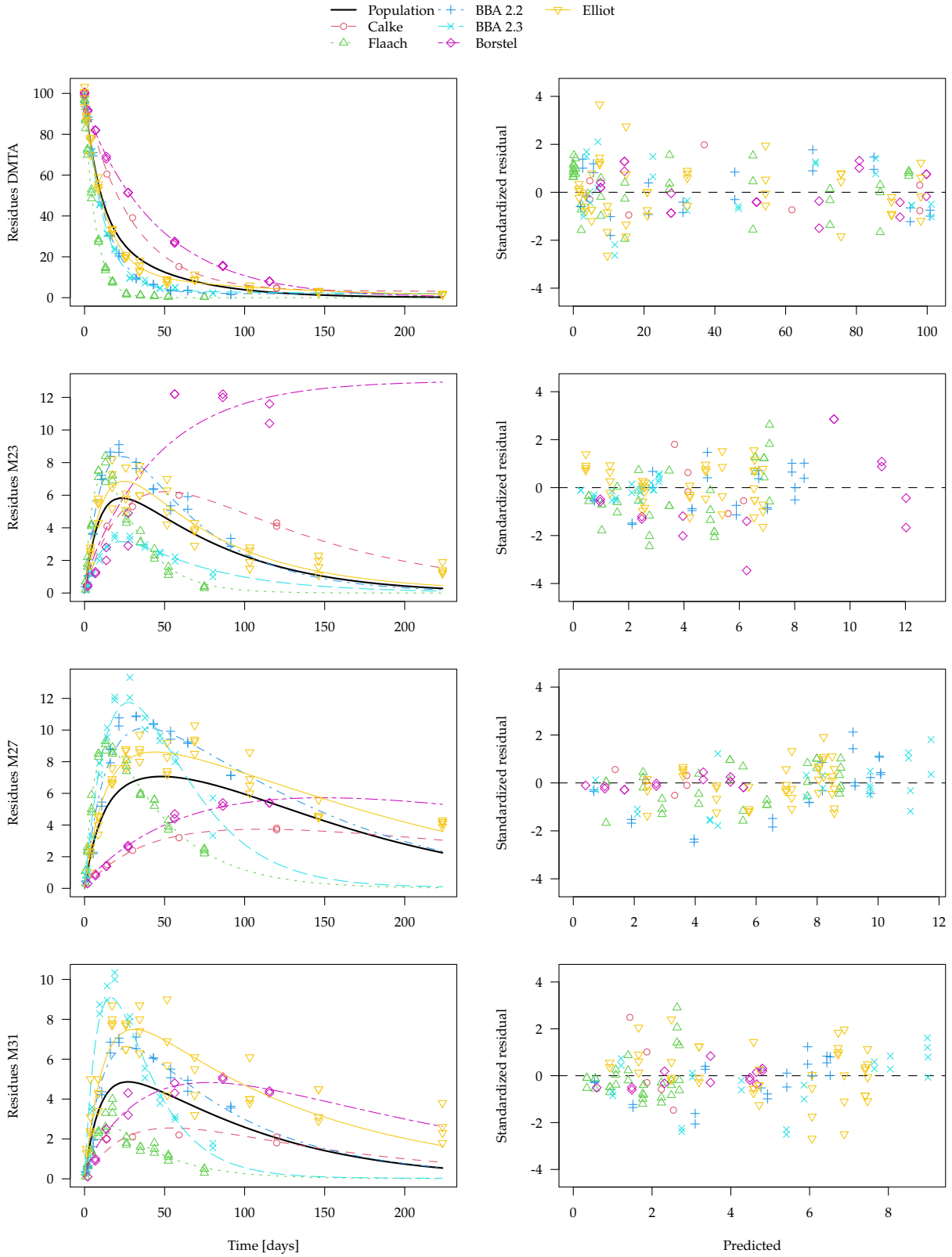

Figure 62: Separate fits of the DFOP-SFO3+ model to the normalised DMTA data assuming two-component error, average curve only considering rate constants that can be distinguished from zero

Simultaneous evaluations

The following figures show convergence plots of saemix fits and comparisons of the results obtained with the corresponding averaged results from separate fits. As no analytical solution are implemented for these degradation models, each of these fits takes more than 15 minutes to complete.

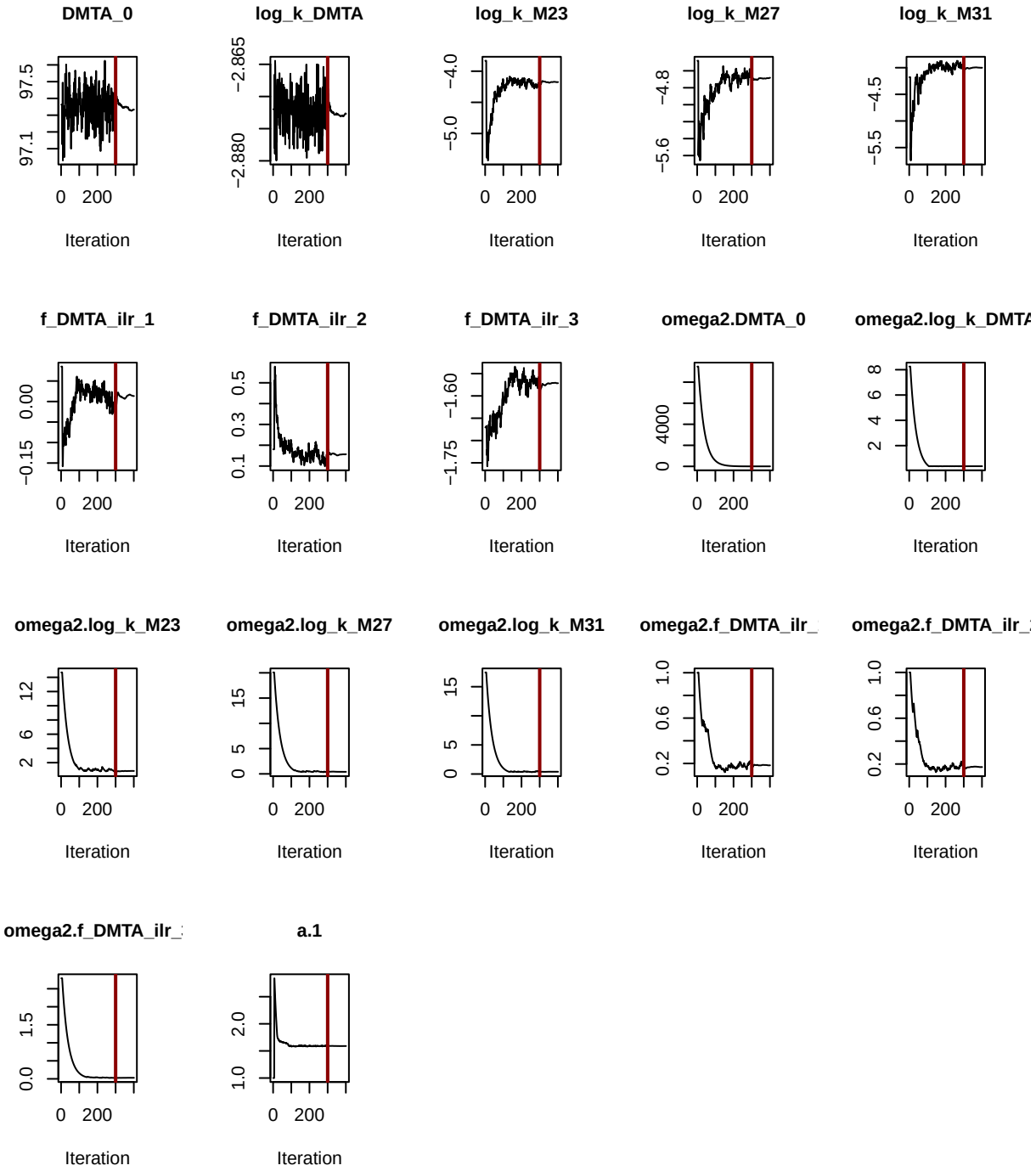

Figure 63: Convergence plot of the saemix fit of the SFO-SFO3 model with constant variance to the normalised DMTA data

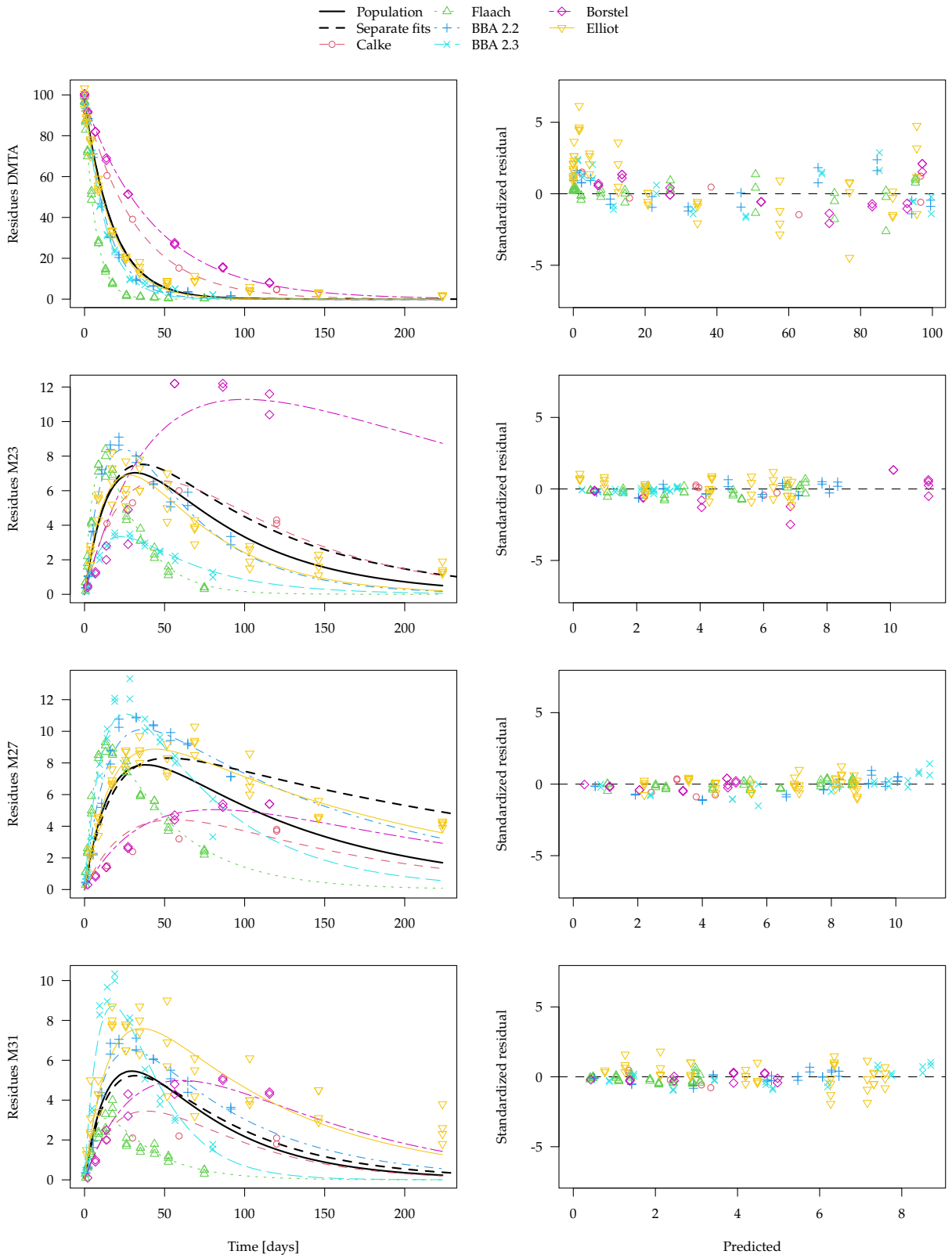

Figure 64: SFO-SFO3 model with constant variance fitted with saemix to the data for DMTA in six soils, with additional degradation curves derived from separate evaluations for comparison

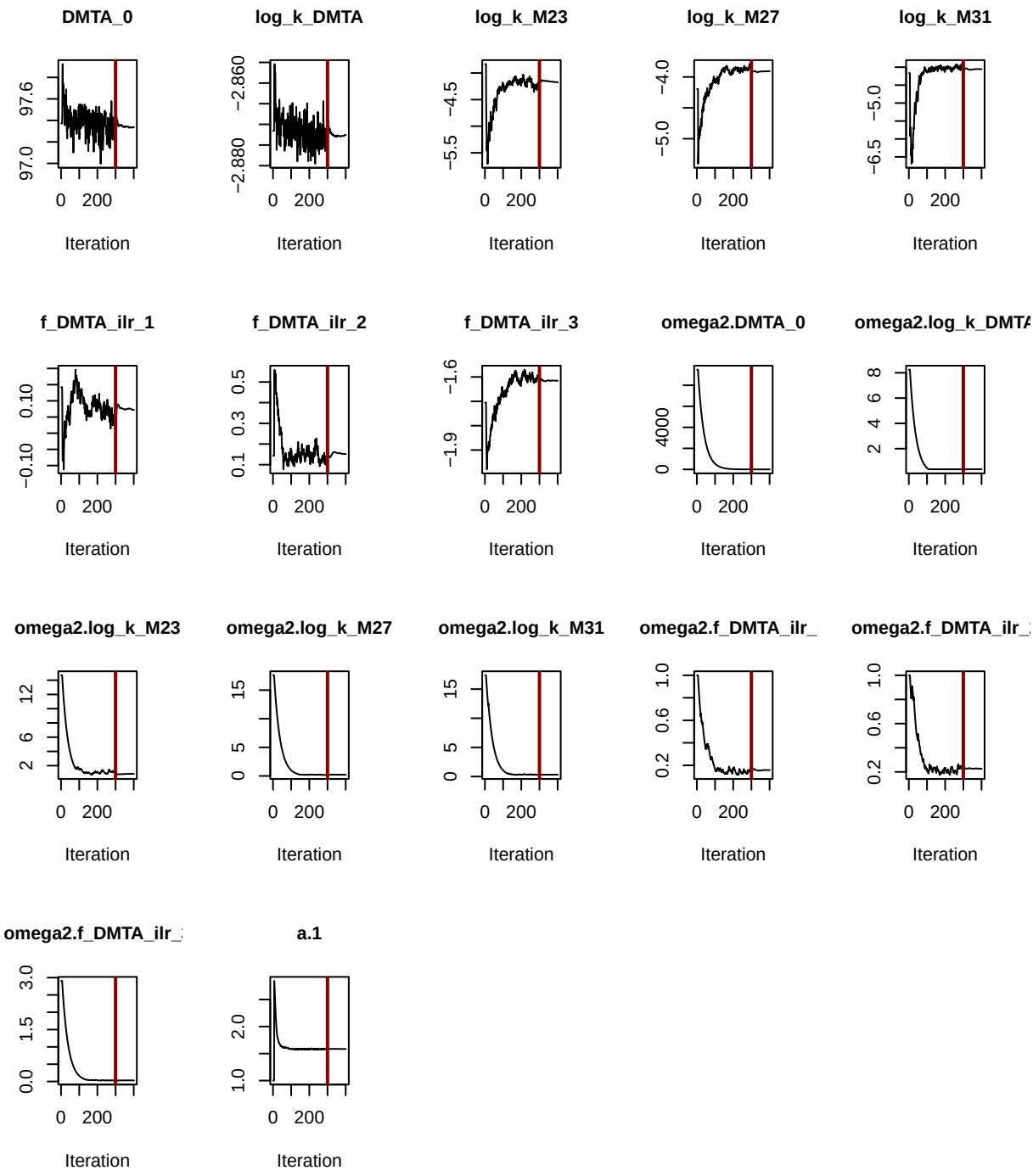

Figure 65: Convergence plot of the saemix fit of the SFO-SFO3+ model with constant variance to the normalised DMTA data

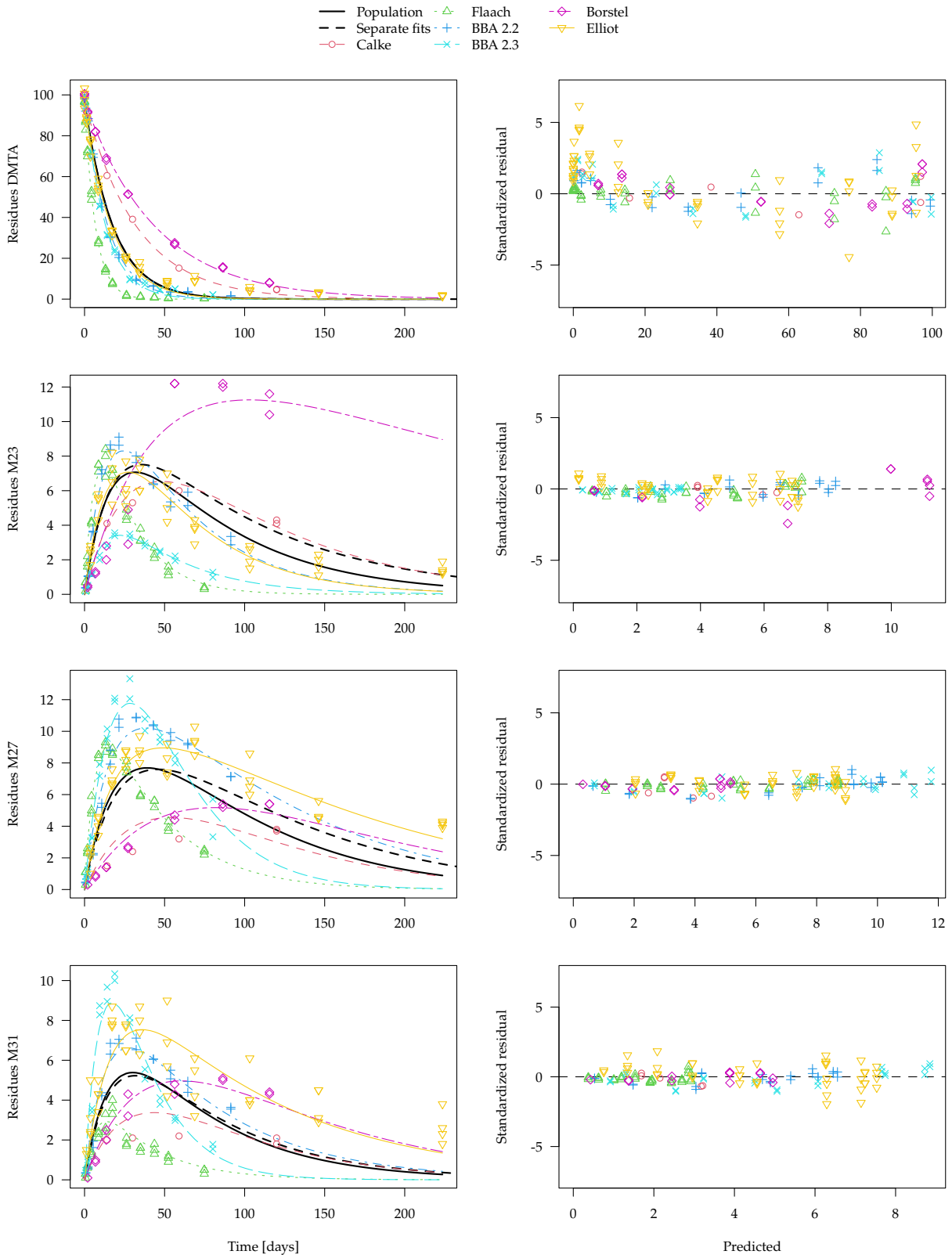

Figure 66: SFO-SFO3+ model with constant variance fitted with saemix to the data for DMTA in six soils, with additional degradation curves derived from separate evaluations for comparison

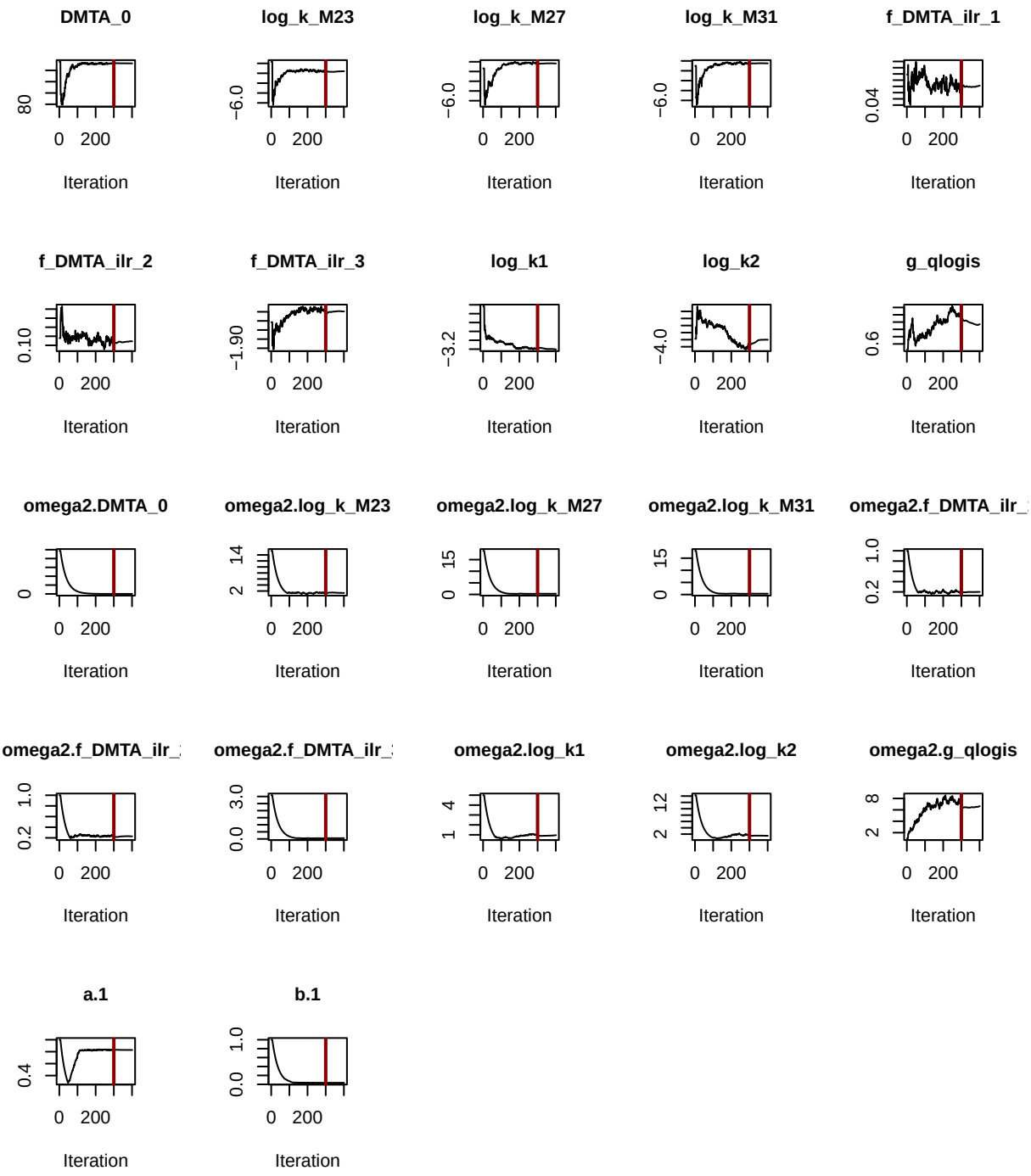

Figure 67: Convergence plot of the saemix fit of the DFOP-SFO3+ model with two-component error to the normalised DMTA data

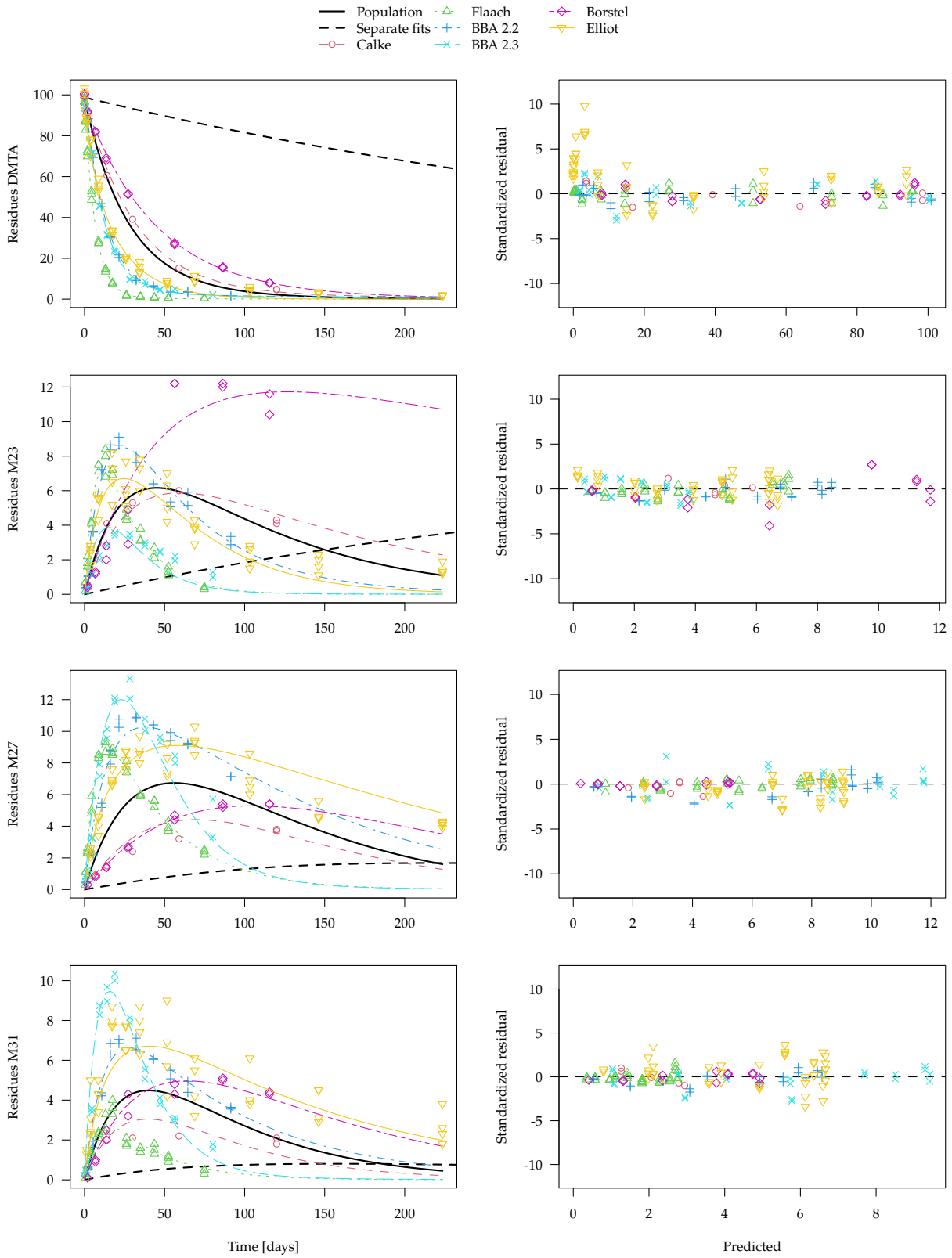

Figure 68: DFOP-SFO3+ model with two-component error fitted with saemix to the data for DMTA in six soils, with additional degradation curves derived from untested parameters from separate evaluations

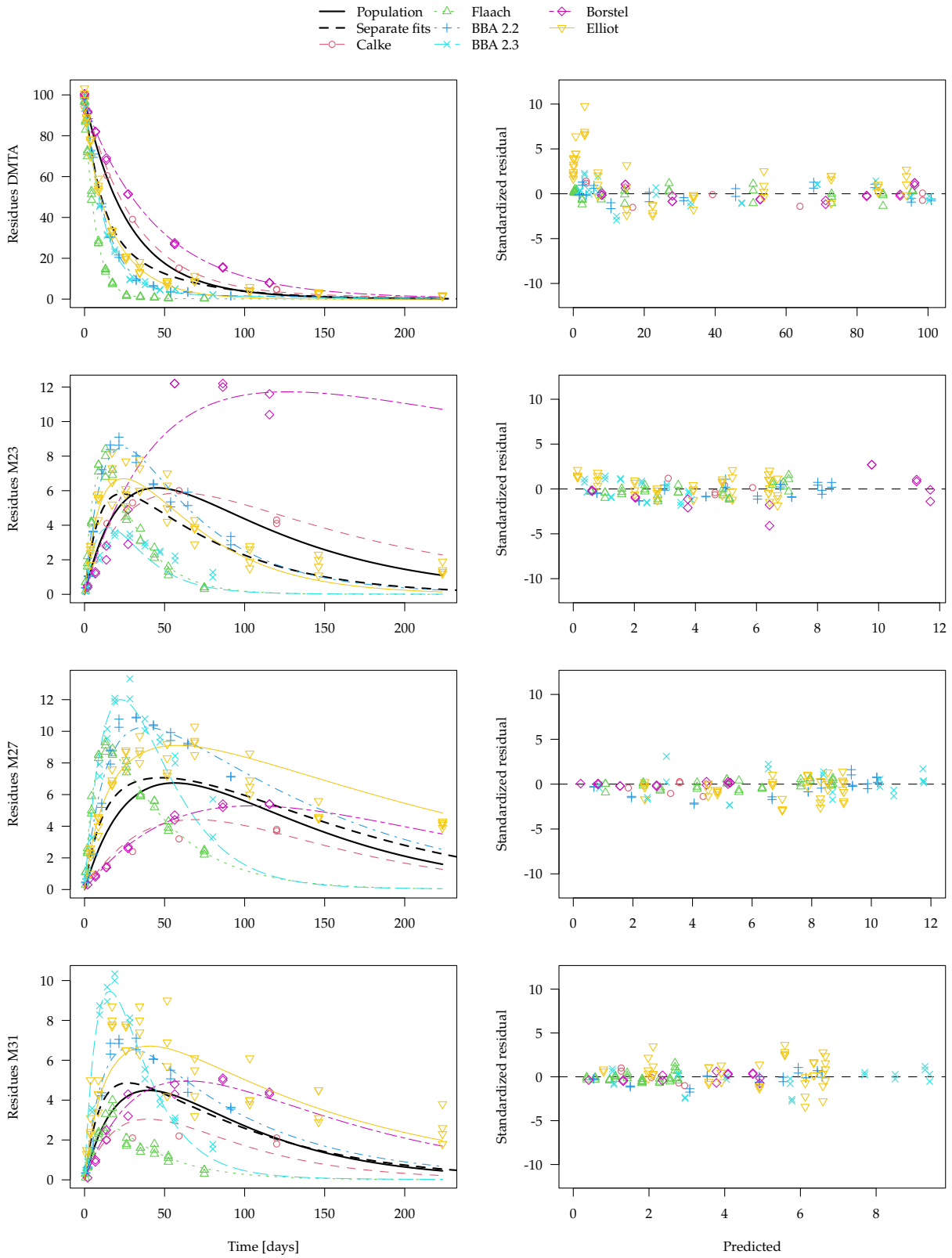

Figure 69: DFOP-SFO3+ model with two-component error fitted with saemix to the data for DMTA in six soils, with additional degradation curves derived from tested parameters from separate evaluations

The following model comparison of the three saemix fits shown above show that the DFOP-SFO3+ fit

assuming two-component error (third line) is more favorable.

```
Likelihoods calculated by importance sampling

       AIC      BIC
1 2317.586 2314.046
2 2312.859 2309.319
3 1887.286 1882.705
```

Checking all candidate combinations of degradation models and error models checked in the separate evaluations would be quite time consuming when using saemix. In addition, the variance by variable error model is not available. To check if the DFOP-SFO+ fit with two-component error is among the most favorable models, nlme fits were performed with DFOP-SFO and DFOP-SFO+, combined with variance by variable and two-component error. The comparisons of these four nlme fits indicates that DFOP-SFO+ fitted with two-component error is indeed the most favorable combination.

```
                  Model df      AIC      BIC    logLik   Test  L.Ratio p-value
f_dmta_nlme_3_obs     1 24 1927.909 2032.120 -939.9544                        
f_dmta_nlme_3_tc      2 22 1876.085 1971.612 -916.0428 1 vs 2 47.82337  <.0001
f_dmta_nlme_4_obs     3 24 1899.773 2003.984 -925.8864 2 vs 3 19.68720   1e-04
f_dmta_nlme_4_tc      4 22 1850.519 1946.046 -903.2596 3 vs 4 45.25349  <.0001
```

References

EFSA (2014). Conclusion on the peer review of the pesticide risk assessment of the active substance 2,4-D. *EFSA Journal* **12**:3812

EFSA (2018). Peer review of the pesticide risk assessment of the active substance dimethenamid-P. *EFSA Journal* **16**:5211

Appendix

Listings for separate parent only fits for 2,4-D

Listing 1: SFO fit to Mississippi data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Model predictions using solution type analytical

Fitted using 141 model solutions performed in 0.094 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0  96.8  state
k_D24   0.1 deparm

Starting values for the transformed parameters actually optimised:
             value lower upper
D24_0     96.800000  -Inf   Inf
log_k_D24 -2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC      BIC    logLik
  70.41126 71.31901 -32.20563

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error  Lower  Upper
D24_0       90.030     3.0340 82.860 97.210
log_k_D24   -4.442     0.1121 -4.707 -4.177
sigma        6.059     1.3550  2.856  9.263

Parameter correlation:
               D24_0 log_k_D24      sigma
D24_0      1.000e+00 5.737e-01 -7.934e-09
log_k_D24  5.737e-01 1.000e+00  8.152e-09
sigma     -7.934e-09 8.152e-09  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
      Estimate t value    Pr(>t)     Lower    Upper
D24_0 90.03000  29.670 6.360e-09 82.860000 97.21000
k_D24  0.01177   8.924 2.254e-05  0.009034  0.01535
sigma  6.05900   4.472 1.447e-03  2.856000  9.26300

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   7.403       2  8
D24        7.403       2  8
```

```
Estimated disappearance times:
     DT50  DT90
D24 58.87 195.6

Data:
 time variable observed predicted residual
    0      D24     96.8     90.03    6.765
    2      D24     81.0     87.94   -6.939
    4      D24     81.7     85.89   -4.193
    7      D24     88.2     82.91    5.288
   15      D24     66.3     75.46   -9.158
   24      D24     72.9     67.87    5.029
   35      D24     62.6     59.63    2.975
   56      D24     54.6     46.56    8.037
   71      D24     35.2     39.02   -3.824
  114      D24     18.0     23.52   -5.521
```

Listing 2: FOMC fit to Mississippi data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - (alpha/beta) * 1/((time/beta) + 1) * D24

Model predictions using solution type analytical

Fitted using 642 model solutions performed in 0.2 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0  96.8  state
alpha   1.0 deparm
beta   10.0 deparm

Starting values for the transformed parameters actually optimised:
              value lower upper
D24_0     96.800000  -Inf   Inf
log_alpha  0.000000  -Inf   Inf
log_beta   2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC     BIC    logLik
  72.41136 73.6217 -32.20568

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error    Lower   Upper
D24_0        90.03      3.034   82.610  97.460
log_alpha    10.50    117.400 -276.800 297.800
log_beta     14.94    117.400 -272.300 302.200
sigma         6.06      1.356    2.743   9.376

Parameter correlation:
               D24_0  log_alpha   log_beta      sigma
D24_0      1.000e+00  0.0004428 -0.0001048  5.242e-06
log_alpha  4.428e-04  1.0000000  0.9999995 -2.941e-02
log_beta  -1.048e-04  0.9999995  1.0000000 -2.941e-02
sigma      5.242e-06 -0.0294083 -0.0294083  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
       Estimate t value Pr(>t)      Lower      Upper
D24_0 9.003e+01      NA     NA  8.261e+01  9.746e+01
alpha 3.640e+04      NA     NA 6.362e-121 2.082e+129
beta  3.091e+06      NA     NA 5.387e-119 1.774e+131
sigma 6.060e+00      NA     NA  2.743e+00  9.376e+00

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   7.773       3  7
D24        7.773       3  7
```

```
Estimated disappearance times:
     DT50  DT90 DT50back
D24 58.87 195.6    58.87

Data:
 time variable observed predicted residual
    0      D24     96.8     90.03    6.765
    2      D24     81.0     87.94   -6.939
    4      D24     81.7     85.89   -4.193
    7      D24     88.2     82.91    5.288
   15      D24     66.3     75.46   -9.158
   24      D24     72.9     67.87    5.029
   35      D24     62.6     59.63    2.975
   56      D24     54.6     46.56    8.037
   71      D24     35.2     39.02   -3.824
  114      D24     18.0     23.52   -5.521
```

Listing 3: SFO fit to Fayette data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Model predictions using solution type analytical

Fitted using 136 model solutions performed in 0.071 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0 100.9  state
k_D24   0.1 deparm

Starting values for the transformed parameters actually optimised:
              value lower upper
D24_0     100.900000  -Inf   Inf
log_k_D24  -2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC      BIC    logLik
  102.2879 104.4121 -48.14397

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error  Lower   Upper
D24_0       97.870     2.1810 93.120 102.600
log_k_D24   -2.378     0.0827 -2.558  -2.198
sigma        5.993     1.0940  3.609   8.378

Parameter correlation:
               D24_0 log_k_D24      sigma
D24_0      1.000e+00 4.798e-01 -1.554e-08
log_k_D24  4.798e-01 1.000e+00  6.980e-09
sigma     -1.554e-08 6.980e-09  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
      Estimate t value    Pr(>t)    Lower    Upper
D24_0 97.87000  44.870 4.891e-15 93.12000 102.6000
k_D24  0.09275  12.090 2.222e-08  0.07745   0.1111
sigma  5.99300   5.477 7.067e-05  3.60900   8.3780

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data     7.4       2  6
D24          7.4       2  6

Estimated disappearance times:
     DT50  DT90
D24 7.473 24.83

Data:
```

time	variable	observed	predicted	residual
0.0	D24	100.8	97.87	2.932
0.0	D24	101.0	97.87	3.132
0.1	D24	93.2	96.96	-3.764
0.1	D24	93.2	96.96	-3.764
0.3	D24	90.5	95.18	-4.682
0.3	D24	91.5	95.18	-3.682
1.0	D24	86.3	89.20	-2.899
1.0	D24	87.1	89.20	-2.099
3.0	D24	79.0	74.10	4.903
3.0	D24	80.8	74.10	6.703
5.0	D24	74.0	61.55	12.449
5.0	D24	65.6	61.55	4.049
10.0	D24	35.0	38.71	-3.711
10.0	D24	36.7	38.71	-2.011
17.0	D24	6.6	20.22	-13.624

Listing 4: FOMC fit to Fayette data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:46 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - (alpha/beta) * 1/((time/beta) + 1) * D24

Model predictions using solution type analytical

Fitted using 339 model solutions performed in 0.183 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0 100.9  state
alpha   1.0 deparm
beta   10.0 deparm

Starting values for the transformed parameters actually optimised:
              value lower upper
D24_0     100.900000  -Inf   Inf
log_alpha   0.000000  -Inf   Inf
log_beta    2.302585  -Inf   Inf

Fixed parameter values:
None


Warning(s):
Optimisation did not converge:
false convergence (8)

Results:

      AIC      BIC    logLik
  104.288 107.1202 -48.14402

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error    Lower   Upper
D24_0       97.870      2.181   93.070 102.700
log_alpha   12.030    103.300 -215.400 239.500
log_beta    14.410    103.300 -213.000 241.900
sigma        5.993      1.094    3.585   8.402

Parameter correlation:
              D24_0  log_alpha   log_beta      sigma
D24_0      1.000e+00  0.0002041 -0.0001799  2.299e-05
log_alpha  2.041e-04  1.0000000  0.9999997 -1.608e-02
log_beta  -1.799e-04  0.9999997  1.0000000 -1.608e-02
sigma      2.299e-05 -0.0160814 -0.0160814  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
       Estimate t value Pr(>t)     Lower      Upper
D24_0 9.787e+01      NA     NA 9.307e+01  1.027e+02
alpha 1.677e+05      NA     NA 2.806e-94 1.003e+104
beta  1.809e+06      NA     NA 3.023e-93 1.082e+105
sigma 5.993e+00      NA     NA 3.585e+00  8.402e+00
```

```
FOCUS Chi2 error levels in percent:
          err.min n.optim df
All data   7.892       3  5
D24        7.892       3  5

Estimated disappearance times:
     DT50  DT90 DT50back
D24 7.473 24.83    7.473

Data:
 time variable observed predicted residual
  0.0      D24    100.8     97.87    2.932
  0.0      D24    101.0     97.87    3.132
  0.1      D24     93.2     96.96   -3.764
  0.1      D24     93.2     96.96   -3.764
  0.3      D24     90.5     95.18   -4.682
  0.3      D24     91.5     95.18   -3.682
  1.0      D24     86.3     89.20   -2.899
  1.0      D24     87.1     89.20   -2.099
  3.0      D24     79.0     74.10    4.903
  3.0      D24     80.8     74.10    6.703
  5.0      D24     74.0     61.55   12.449
  5.0      D24     65.6     61.55    4.049
 10.0      D24     35.0     38.71   -3.711
 10.0      D24     36.7     38.71   -2.011
 17.0      D24      6.6     20.22  -13.624
```

Listing 5: SFO fit to RefSol 03-G data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Model predictions using solution type analytical

Fitted using 135 model solutions performed in 0.038 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0  98.8  state
k_D24   0.1 deparm

Starting values for the transformed parameters actually optimised:
             value lower upper
D24_0     98.800000  -Inf   Inf
log_k_D24 -2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC      BIC    logLik
  97.05952 99.55916 -45.52976

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error   Lower   Upper
D24_0      92.9100    1.61400 89.4400 96.3700
log_k_D24  -0.8535    0.06486 -0.9927 -0.7144
sigma       3.5230    0.60420  2.2270  4.8190

Parameter correlation:
               D24_0  log_k_D24      sigma
D24_0      1.000e+00  5.067e-01 -5.652e-07
log_k_D24  5.067e-01  1.000e+00 -3.310e-07
sigma     -5.652e-07 -3.310e-07  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
      Estimate t value    Pr(>t)   Lower   Upper
D24_0  92.9100  57.560 2.452e-18 89.4400 96.3700
k_D24   0.4259  15.420 1.770e-10  0.3706  0.4895
sigma   3.5230   5.831 2.181e-05  2.2270  4.8190

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.388       2  7
D24        6.388       2  7

Estimated disappearance times:
     DT50  DT90
D24 1.627 5.406

Data:
```

time	variable	observed	predicted	residual
0.0	D24	98.8	92.905846	5.8942
0.0	D24	98.8	92.905846	5.8942
0.1	D24	87.4	89.032058	-1.6321
0.1	D24	87.9	89.032058	-1.1321
0.3	D24	78.1	81.762310	-3.6623
0.3	D24	78.8	81.762310	-2.9623
1.0	D24	57.1	60.684355	-3.5844
1.0	D24	56.1	60.684355	-4.5844
3.0	D24	25.0	25.890720	-0.8907
3.0	D24	32.3	25.890720	6.4093
5.0	D24	14.7	11.046165	3.6538
10.0	D24	3.1	1.313349	1.7867
10.0	D24	3.1	1.313349	1.7867
17.0	D24	2.7	0.066622	2.6334
17.0	D24	2.1	0.066622	2.0334
26.0	D24	2.0	0.001442	1.9986
26.0	D24	2.2	0.001442	2.1986

Listing 6: FOMC fit to RefSol 03-G data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - (alpha/beta) * 1/((time/beta) + 1) * D24

Model predictions using solution type analytical

Fitted using 229 model solutions performed in 0.068 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0  98.8  state
alpha   1.0 deparm
beta   10.0 deparm

Starting values for the transformed parameters actually optimised:
             value lower upper
D24_0     98.800000  -Inf   Inf
log_alpha  0.000000  -Inf   Inf
log_beta   2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC      BIC   logLik
  85.67721 89.01006 -38.8386

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error   Lower  Upper
D24_0       95.530     1.2830 92.7600 98.310
log_alpha    0.703     0.2083  0.2530  1.153
log_beta     1.210     0.2867  0.5907  1.829
sigma        2.377     0.4076  1.4960  3.257

Parameter correlation:
               D24_0  log_alpha   log_beta      sigma
D24_0      1.000e+00 -4.280e-01 -5.062e-01 -6.870e-08
log_alpha -4.280e-01  1.000e+00  9.858e-01  2.704e-08
log_beta  -5.062e-01  9.858e-01  1.000e+00  3.008e-08
sigma     -6.870e-08  2.704e-08  3.008e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
      Estimate t value    Pr(>t)  Lower  Upper
D24_0   95.530  74.460 8.612e-19 92.760 98.310
alpha    2.020   4.800 1.733e-04  1.288  3.168
beta     3.354   3.488 2.001e-03  1.805  6.230
sigma    2.377   5.831 2.933e-05  1.496  3.257

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   3.985       3  6
D24        3.985       3  6
```

```
Estimated disappearance times:
     DT50  DT90 DT50back
D24 1.373 7.132    2.147

Data:
 time variable observed predicted residual
  0.0      D24     98.8    95.535   3.2653
  0.0      D24     98.8    95.535   3.2653
  0.1      D24     87.4    90.030  -2.6299
  0.1      D24     87.9    90.030  -2.1299
  0.3      D24     78.1    80.353  -2.2534
  0.3      D24     78.8    80.353  -1.5534
  1.0      D24     57.1    56.395   0.7050
  1.0      D24     56.1    56.395  -0.2950
  3.0      D24     25.0    26.281  -1.2811
  3.0      D24     32.3    26.281   6.0189
  5.0      D24     14.7    15.121  -0.4209
 10.0      D24      3.1     5.863  -2.7626
 10.0      D24      3.1     5.863  -2.7626
 17.0      D24      2.7     2.502   0.1975
 17.0      D24      2.1     2.502  -0.4025
 26.0      D24      2.0     1.194   0.8055
 26.0      D24      2.2     1.194   1.0055
```

Listing 7: SFO fit to Site E1 data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Model predictions using solution type analytical

Fitted using 133 model solutions performed in 0.051 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
       value   type
D24_0 100.55  state
k_D24   0.10 deparm

Starting values for the transformed parameters actually optimised:
              value lower upper
D24_0     100.550000  -Inf   Inf
log_k_D24  -2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC      BIC    logLik
  87.94132 90.25909 -40.97066

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error  Lower   Upper
D24_0       99.610    1.35600 96.680 102.500
log_k_D24   -1.174    0.05056 -1.283  -1.064
sigma        3.132    0.55370  1.936   4.328

Parameter correlation:
              D24_0  log_k_D24      sigma
D24_0     1.000e+00  4.831e-01  2.925e-08
log_k_D24 4.831e-01  1.000e+00 -1.134e-07
sigma     2.925e-08 -1.134e-07  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
      Estimate t value    Pr(>t)   Lower   Upper
D24_0  99.6100  73.470 1.025e-18 96.6800 102.500
k_D24   0.3093  19.780 2.184e-11  0.2773   0.345
sigma   3.1320   5.657 3.920e-05  1.9360   4.328

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   4.809       2  7
D24        4.809       2  7

Estimated disappearance times:
     DT50  DT90
D24 2.241 7.445

Data:
```

time	variable	observed	predicted	residual
0.0	D24	100.2	99.60950	0.5905
0.0	D24	100.9	99.60950	1.2905
0.1	D24	97.9	96.57608	1.3239
0.1	D24	98.3	96.57608	1.7239
0.3	D24	92.4	90.78356	1.6164
0.3	D24	91.9	90.78356	1.1164
1.0	D24	65.8	73.11204	-7.3120
1.0	D24	69.5	73.11204	-3.6120
3.0	D24	37.5	39.38811	-1.8881
3.0	D24	40.0	39.38811	0.6119
7.0	D24	18.8	11.43188	7.3681
7.0	D24	14.4	11.43188	2.9681
10.0	D24	3.3	4.52045	-1.2205
10.0	D24	5.7	4.52045	1.1795
17.0	D24	2.6	0.51880	2.0812
26.0	D24	2.4	0.03208	2.3679

Listing 8: FOMC fit to Site E1 data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:45 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - (alpha/beta) * 1/((time/beta) + 1) * D24

Model predictions using solution type analytical

Fitted using 228 model solutions performed in 0.077 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
       value   type
D24_0 100.55  state
alpha   1.00 deparm
beta   10.00 deparm

Starting values for the transformed parameters actually optimised:
               value lower upper
D24_0     100.550000  -Inf   Inf
log_alpha   0.000000  -Inf   Inf
log_beta    2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC     BIC    logLik
  80.20545 83.2958 -36.10272

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error   Lower   Upper
D24_0      101.400     1.1330 98.9000 103.800
log_alpha    1.171     0.2781  0.5648   1.776
log_beta     2.117     0.3428  1.3700   2.864
sigma        2.311     0.4084  1.4210   3.200

Parameter correlation:
               D24_0  log_alpha   log_beta      sigma
D24_0      1.000e+00 -4.088e-01 -4.588e-01 -2.066e-09
log_alpha -4.088e-01  1.000e+00  9.935e-01  1.834e-09
log_beta  -4.588e-01  9.935e-01  1.000e+00  1.687e-09
sigma     -2.066e-09  1.834e-09  1.687e-09  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
      Estimate t value    Pr(>t)  Lower   Upper
D24_0  101.400  89.440 1.275e-18 98.900 103.800
alpha    3.224   3.596 1.836e-03  1.759   5.909
beta     8.309   2.917 6.450e-03  3.937  17.530
sigma    2.311   5.657 5.306e-05  1.421   3.200

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   3.397       3  6
D24        3.397       3  6
```

```
Estimated disappearance times:
     DT50  DT90 DT50back
D24 1.993 8.662    2.608

Data:
 time variable observed predicted residual
  0.0      D24    100.2   101.366 -1.16598
  0.0      D24    100.9   101.366 -0.46598
  0.1      D24     97.9    97.531  0.36937
  0.1      D24     98.3    97.531  0.76937
  0.3      D24     92.4    90.412  1.98757
  0.3      D24     91.9    90.412  1.48757
  1.0      D24     65.8    70.270 -4.46976
  1.0      D24     69.5    70.270 -0.76976
  3.0      D24     37.5    37.520 -0.02008
  3.0      D24     40.0    37.520  2.47992
  7.0      D24     18.8    14.133  4.66735
  7.0      D24     14.4    14.133  0.26735
 10.0      D24      3.3     7.937 -4.63699
 10.0      D24      5.7     7.937 -2.23699
 17.0      D24      2.6     2.795 -0.19460
 26.0      D24      2.4     1.048  1.35211
```

Listing 9: SFO fit to Site I2 data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Model predictions using solution type analytical

Fitted using 134 model solutions performed in 0.053 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0  98.9  state
k_D24   0.1 deparm

Starting values for the transformed parameters actually optimised:
              value lower upper
D24_0     98.900000  -Inf   Inf
log_k_D24 -2.302585  -Inf   Inf

Fixed parameter values:
None

Results:

       AIC      BIC    logLik
  103.7383 106.2379 -48.86913

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error  Lower    Upper
D24_0      97.9900    1.86400 94.000 102.0000
log_k_D24  -0.9846    0.06731 -1.129  -0.8402
sigma       4.2880    0.73530  2.710   5.8650

Parameter correlation:
              D24_0  log_k_D24      sigma
D24_0     1.000e+00  4.397e-01  8.666e-10
log_k_D24 4.397e-01  1.000e+00 -1.885e-09
sigma     8.666e-10 -1.885e-09  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
      Estimate t value    Pr(>t)   Lower    Upper
D24_0  97.9900  52.560 8.691e-18 94.0000 102.0000
k_D24   0.3736  14.860 2.890e-10  0.3234   0.4316
sigma   4.2880   5.831 2.181e-05  2.7100   5.8650

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   7.495       2  7
D24        7.495       2  7

Estimated disappearance times:
     DT50  DT90
D24 1.855 6.163

Data:
```

time	variable	observed	predicted	residual
0.0	D24	99.0	97.994975	1.0050
0.0	D24	98.8	97.994975	0.8050
0.1	D24	90.1	94.401574	-4.3016
0.1	D24	89.2	94.401574	-5.2016
0.3	D24	86.3	87.605242	-1.3052
0.3	D24	86.5	87.605242	-1.1052
1.0	D24	76.7	67.446295	9.2537
1.0	D24	74.7	67.446295	7.2537
3.0	D24	33.1	31.949693	1.1503
5.0	D24	8.8	15.134751	-6.3348
5.0	D24	6.7	15.134751	-8.4348
10.0	D24	3.1	2.337474	0.7625
10.0	D24	3.2	2.337474	0.8625
17.0	D24	1.6	0.171012	1.4290
17.0	D24	1.7	0.171012	1.5290
26.0	D24	1.5	0.005927	1.4941
26.0	D24	1.9	0.005927	1.8941

Listing 10: FOMC fit to Site I2 data, 2,4-D

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:17:47 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - (alpha/beta) * 1/((time/beta) + 1) * D24

Model predictions using solution type analytical

Fitted using 323 model solutions performed in 0.123 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
      value   type
D24_0  98.9  state
alpha   1.0 deparm
beta   10.0 deparm

Starting values for the transformed parameters actually optimised:
              value lower upper
D24_0     98.900000  -Inf   Inf
log_alpha  0.000000  -Inf   Inf
log_beta   2.302585  -Inf   Inf

Fixed parameter values:
None


Warning(s):
Optimisation did not converge:
false convergence (8)

Results:

       AIC      BIC    logLik
  105.7384 109.0712 -48.86918

Optimised, transformed parameters with symmetric confidence intervals:
          Estimate Std. Error    Lower   Upper
D24_0       98.000     1.8640   93.970 102.000
log_alpha   12.470   100.2000 -203.900 228.900
log_beta    13.450   100.2000 -203.000 229.900
sigma        4.288     0.7354    2.699   5.876

Parameter correlation:
               D24_0 log_alpha  log_beta      sigma
D24_0      1.0000000 -0.001986 -0.002282  0.0003748
log_alpha -0.0019865  1.000000  1.000000 -0.0127621
log_beta  -0.0022819  1.000000  1.000000 -0.0127622
sigma      0.0003748 -0.012762 -0.012762  1.0000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
       Estimate t value Pr(>t)     Lower     Upper
D24_0 9.800e+01      NA     NA 9.397e+01 1.020e+02
alpha 2.604e+05      NA     NA 2.684e-89 2.526e+99
beta  6.970e+05      NA     NA 7.180e-89 6.767e+99
sigma 4.288e+00      NA     NA 2.699e+00 5.876e+00
```

```
FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   7.922       3  6
D24        7.922       3  6

Estimated disappearance times:
     DT50  DT90 DT50back
D24 1.855 6.163    1.855

Data:
 time variable observed predicted residual
  0.0      D24     99.0 97.996874   1.0031
  0.0      D24     98.8 97.996874   0.8031
  0.1      D24     90.1 94.403232  -4.3032
  0.1      D24     89.2 94.403232  -5.2032
  0.3      D24     86.3 87.606464  -1.3065
  0.3      D24     86.5 87.606464  -1.1065
  1.0      D24     76.7 67.446394   9.2536
  1.0      D24     74.7 67.446394   7.2536
  3.0      D24     33.1 31.948647   1.1514
  5.0      D24      8.8 15.133770  -6.3338
  5.0      D24      6.7 15.133770  -8.4338
 10.0      D24      3.1  2.337157   0.7628
 10.0      D24      3.2  2.337157   0.8628
 17.0      D24      1.6  0.170976   1.4290
 17.0      D24      1.7  0.170976   1.5290
 26.0      D24      1.5  0.005925   1.4941
 26.0      D24      1.9  0.005925   1.8941
```

Listings for simultaneous fits for 2,4-D, parent only

Listing 11: SFO fit with nlme to 2,4-D data, constant variance

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:18:07 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Data:
75 observations of 1 variable(s) grouped in 5 datasets

Model predictions using solution type analytical

Fitted in 0.312 s using 2 iterations

Variance model: Constant variance

Mean of starting values for individual parameters:
    D24_0 log_k_D24
   95.683    -1.838

Fixed degradation parameter values:
None

Results:

    AIC   BIC logLik
  498.7 510.3 -244.3

Optimised, transformed parameters with symmetric confidence intervals:
           lower   est.   upper
D24_0     92.901 95.919 98.9373
log_k_D24 -3.259 -1.831 -0.4028

Correlation:
          D24_0
log_k_D24 0.016

Random effects:
 Formula: list(D24_0 ~ 1, log_k_D24 ~ 1)
 Level: ds
 Structure: Diagonal
        D24_0 log_k_D24 Residual
StdDev: 2.596     1.599    4.956


Backtransformed parameters with asymmetric confidence intervals:
         lower    est.   upper
D24_0 92.90134 95.9193 98.9373
k_D24  0.03843  0.1603  0.6684

Estimated disappearance times:
     DT50  DT90
D24 4.325 14.37
```

Listing 12: SFO fit with nlme to 2,4-D data, two-component error

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:18:08 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Data:
75 observations of 1 variable(s) grouped in 5 datasets

Model predictions using solution type analytical

Fitted in 0.446 s using 3 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
    D24_0 log_k_D24
   95.318    -1.856

Fixed degradation parameter values:
None

Results:

    AIC   BIC logLik
  500.7 514.6 -244.3

Optimised, transformed parameters with symmetric confidence intervals:
           lower   est.   upper
D24_0     92.902 95.920 98.9375
log_k_D24 -3.259 -1.831 -0.4028

Correlation:
          D24_0
log_k_D24 0.016

Random effects:
 Formula: list(D24_0 ~ 1, log_k_D24 ~ 1)
 Level: ds
 Structure: Diagonal
        D24_0 log_k_D24 Residual
StdDev: 2.596     1.599        1

Variance function:
 Structure: Constant plus proportion of variance covariate
 Formula: ~fitted(.)
 Parameter estimates:
        const          prop
 4.955596e+00 -3.170209e-07

Backtransformed parameters with asymmetric confidence intervals:
         lower    est.   upper
D24_0 92.90157 95.9195 98.9375
k_D24  0.03843  0.1603  0.6684

Estimated disappearance times:
     DT50  DT90
D24 4.325 14.37
```

Listing 13: SFO fit with saemix to 2,4-D data, constant variance

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:18:11 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Data:
75 observations of 1 variable(s) grouped in 5 datasets

Model predictions using solution type analytical

Fitted in 1.38 s using 300, 100 iterations

Variance model: Constant variance

Mean of starting values for individual parameters:
    D24_0 log_k_D24
   95.683    -1.838

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
    AIC   BIC logLik
  498.7 496.8 -244.4

Optimised parameters:
            est.  lower   upper
D24_0     95.914 92.977 98.8508
log_k_D24 -1.829 -3.234 -0.4245

Correlation:
          D24_0
log_k_D24 0.016

Random effects:
               est.   lower upper
SD.D24_0     2.552 -0.1818 5.285
SD.log_k_D24 1.600  0.6062 2.595

Variance model:
    est. lower upper
a.1 4.96 4.108 5.813

Backtransformed parameters:
         est.    lower   upper
D24_0 95.9141 92.97730 98.8508
k_D24  0.1605  0.03941  0.6541

Estimated disappearance times:
     DT50  DT90
D24 4.317 14.34
```

Listing 14: SFO fit with saemix to 2,4-D data, two-component error

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:18:16 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24

Data:
75 observations of 1 variable(s) grouped in 5 datasets

Model predictions using solution type analytical

Fitted in 3.568 s using 300, 100 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
    D24_0 log_k_D24
   95.318    -1.856

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
    AIC   BIC logLik
  500.7 498.4 -244.4

Optimised parameters:
            est.  lower   upper
D24_0     95.857 92.871 98.8421
log_k_D24 -1.831 -3.235 -0.4259

Correlation:
          D24_0
log_k_D24 0.016

Random effects:
               est.   lower upper
SD.D24_0     2.627 -0.1311 5.384
SD.log_k_D24 1.600  0.6062 2.595

Variance model:
          est.    lower   upper
a.1  4.954e+00  3.48913 6.41886
b.1 -1.926e-06 -0.02246 0.02245

Backtransformed parameters:
         est.    lower   upper
D24_0 95.8565 92.87101 98.8421
k_D24  0.1603  0.03935  0.6531

Estimated disappearance times:
     DT50  DT90
D24 4.324 14.36
```

Listing 15: FOMC fit with saemix to 2,4-D data, constant variance

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:18:19 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - (alpha/beta) * 1/((time/beta) + 1) * D24

Data:
75 observations of 1 variable(s) grouped in 5 datasets

Model predictions using solution type analytical

Fitted in 1.972 s using 300, 100 iterations

Variance model: Constant variance

Mean of starting values for individual parameters:
    D24_0 log_alpha  log_beta
    96.56      8.60     10.32

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
    AIC   BIC logLik
  503.1 500.4 -244.6

Optimised parameters:
            est.  lower  upper
D24_0     95.943   92.9  98.98
log_alpha  7.706 -130.0 145.42
log_beta   9.536 -128.2 147.29

Correlation:
          D24_0 lg_lph
log_alpha 0.184
log_beta  0.184 1.000

Random effects:
              est.     lower   upper
SD.D24_0     2.636   -0.1046   5.376
SD.log_alpha 1.510  -86.8922  89.913
SD.log_beta  1.270 -103.8801 106.421

Variance model:
     est. lower upper
a.1 4.941 4.092  5.79

Backtransformed parameters:
          est.     lower     upper
D24_0    95.94 9.290e+01 9.898e+01
alpha  2221.15 3.446e-57 1.432e+63
beta  13844.85 2.072e-56 9.253e+63

Estimated disappearance times:
     DT50  DT90 DT50back
D24 4.321 14.36    4.323
```

Listings for separate pathway fits for 2,4-D

Listing 16: SFO-SFO-SFO fit to Fayette data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:33 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 2644 model solutions performed in 2.837 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        100.9000  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
f_DCP_to_DCA   0.5000 deparm
sigma_D24      3.0000  error
sigma_DCP      3.0000  error
sigma_DCA      3.0000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
D24_0        100.900000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
f_DCP_qlogis   0.000000  -Inf   Inf
sigma_D24      3.000000     0   Inf
sigma_DCP      3.000000     0   Inf
sigma_DCA      3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  166.7987 180.7968 -74.39935

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error      Lower      Upper
D24_0         97.5900  2.177e+00  9.311e+01   102.1000
log_k_D24     -2.4000  8.210e-02 -2.569e+00    -2.2310
log_k_DCP     -1.8400  7.825e-02 -2.001e+00    -1.6790
log_k_DCA     -4.4510  9.209e-01 -6.344e+00    -2.5590
f_D24_qlogis  -0.9006  1.275e-01 -1.163e+00    -0.6386
```

```
f_DCP_qlogis  19.3600  7.821e+03 -1.606e+04 16100.0000
sigma_D24      6.0080  1.102e+00  3.743e+00     8.2720
sigma_DCP      1.1610  2.301e-01  6.884e-01     1.6340
sigma_DCA      0.5565  1.504e-01  2.473e-01     0.8657

Parameter correlation:
                 D24_0  log_k_D24  log_k_DCP  log_k_DCA f_D24_qlogis
D24_0         1.000e+00  4.778e-01 -0.1365334 -0.1557886   -0.5673655
log_k_D24     4.778e-01  1.000e+00 -0.2857601 -0.3260606   -0.7898829
log_k_DCP    -1.365e-01 -2.858e-01  1.0000000  0.5086110    0.2257435
log_k_DCA    -1.558e-01 -3.261e-01  0.5086110  1.0000000    0.6787900
f_D24_qlogis -5.674e-01 -7.899e-01  0.2257435  0.6787900    1.0000000
f_DCP_qlogis  7.531e-06  1.576e-05 -0.0002669  0.0001427   -0.0001429
sigma_D24    -4.528e-02 -9.477e-02  0.0270817  0.0309010    0.0748578
sigma_DCP     4.292e-02  8.983e-02  0.0407568  0.0624863   -0.0226949
sigma_DCA     7.417e-03  1.552e-02 -0.0948537 -0.1299843   -0.0779521
             f_DCP_qlogis  sigma_D24  sigma_DCP  sigma_DCA
D24_0           7.531e-06 -4.528e-02  4.292e-02  7.417e-03
log_k_D24       1.576e-05 -9.477e-02  8.983e-02  1.552e-02
log_k_DCP      -2.669e-04  2.708e-02  4.076e-02 -9.485e-02
log_k_DCA       1.427e-04  3.090e-02  6.249e-02 -1.300e-01
f_D24_qlogis   -1.429e-04  7.486e-02 -2.269e-02 -7.795e-02
f_DCP_qlogis    1.000e+00 -1.493e-06 -3.669e-05 -1.549e-05
sigma_D24      -1.493e-06  1.000e+00 -8.513e-03 -1.471e-03
sigma_DCP      -3.669e-05 -8.513e-03  1.000e+00 -1.477e-02
sigma_DCA      -1.549e-05 -1.471e-03 -1.477e-02  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value    Pr(>t)     Lower     Upper
D24_0        97.59000  44.710 2.009e-26 93.110000 102.10000
k_D24         0.09072  12.050 1.914e-12  0.076630   0.10740
k_DCP         0.15890   4.725 3.474e-05  0.135300   0.18660
k_DCA         0.01166   0.648 2.613e-01  0.001757   0.07742
f_D24_to_DCP  0.28890   6.582 2.788e-07  0.238200   0.34560
f_DCP_to_DCA  1.00000   3.458 9.445e-04  0.000000   1.00000
sigma_D24     6.00800   5.452 5.117e-06  3.743000   8.27200
sigma_DCP     1.16100   4.771 3.073e-05  0.688400   1.63400
sigma_DCA     0.55650   3.661 5.622e-04  0.247300   0.86570

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.278       6 13
D24        7.510       2  6
DCP       19.923       2  5
DCA        5.939       2  2

Resulting formation fractions:
                ff
D24_DCP  2.889e-01
D24_sink 7.111e-01
DCP_DCA  1.000e+00
DCP_sink 3.927e-09

Estimated disappearance times:
      DT50   DT90
D24  7.640  25.38
DCP  4.363  14.49
DCA 59.439 197.45

Data:
 time variable observed predicted residual
  0.0      D24    100.8   97.5879   3.2121
  0.0      D24    101.0   97.5879   3.4121
  0.1      D24     93.2   96.7065  -3.5065
  0.1      D24     93.2   96.7065  -3.5065
  0.3      D24     90.5   94.9677  -4.4677
```

```
 0.3      D24     91.5   94.9677  -3.4677
 1.0      D24     86.3   89.1243  -2.8243
 1.0      D24     87.1   89.1243  -2.0243
 3.0      D24     79.0   74.3355   4.6645
 3.0      D24     80.8   74.3355   6.4645
 5.0      D24     74.0   62.0007  11.9993
 5.0      D24     65.6   62.0007   3.5993
10.0      D24     35.0   39.3910  -4.3910
10.0      D24     36.7   39.3910  -2.6910
17.0      D24      6.6   20.8737 -14.2737
 0.1      DCP      1.4    0.2526   1.1474
 0.1      DCP      1.6    0.2526   1.3474
 0.3      DCP      2.5    0.7392   1.7608
 0.3      DCP      2.4    0.7392   1.6608
 1.0      DCP      2.9    2.2583   0.6417
 1.0      DCP      3.1    2.2583   0.8417
 3.0      DCP      4.4    5.2867  -0.8867
 3.0      DCP      4.2    5.2867  -1.0867
 5.0      DCP      5.8    6.8863  -1.0863
 5.0      DCP      5.4    6.8863  -1.4863
10.0      DCP      8.2    7.4871   0.7129
10.0      DCP      8.7    7.4871   1.2129
17.0      DCP      5.8    5.5086   0.2914
 3.0      DCA      0.5    1.4139  -0.9139
 3.0      DCA      0.5    1.4139  -0.9139
 5.0      DCA      3.2    3.3238  -0.1238
 5.0      DCA      3.5    3.3238   0.1762
10.0      DCA      9.5    8.8998   0.6002
10.0      DCA      9.1    8.8998   0.2002
17.0      DCA     15.0   15.2249  -0.2249
```

Listing 17: SFO-SFO(ns)-SFO fit to Fayette data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:32 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 2246 model solutions performed in 2.228 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
D24_0        100.9000  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
sigma_D24      3.0000  error
sigma_DCP      3.0000  error
sigma_DCA      3.0000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
D24_0        100.900000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
sigma_D24      3.000000     0   Inf
sigma_DCP      3.000000     0   Inf
sigma_DCA      3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  164.7987 177.2415 -74.39935

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error   Lower    Upper
D24_0         97.5900    2.17700 93.1200 102.1000
log_k_D24     -2.4000    0.08210 -2.5680  -2.2320
log_k_DCP     -1.8400    0.07825 -2.0000  -1.6790
log_k_DCA     -4.4510    0.92090 -6.3410  -2.5620
f_D24_qlogis  -0.9006    0.12750 -1.1620  -0.6391
sigma_D24      6.0080    1.10200  3.7470   8.2680
sigma_DCP      1.1610    0.23010  0.6893   1.6330
sigma_DCA      0.5565    0.15040  0.2479   0.8651
```

```
Parameter correlation:
                D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis sigma_D24
D24_0         1.000000   0.47779  -0.13653  -0.15579     -0.56737 -0.045279
log_k_D24     0.477790   1.00000  -0.28576  -0.32606     -0.78988 -0.094771
log_k_DCP    -0.136533  -0.28576   1.00000   0.50861      0.22574  0.027082
log_k_DCA    -0.155787  -0.32606   0.50861   1.00000      0.67879  0.030901
f_D24_qlogis -0.567366  -0.78988   0.22574   0.67879      1.00000  0.074858
sigma_D24    -0.045279  -0.09477   0.02708   0.03090      0.07486  1.000000
sigma_DCP     0.042920   0.08983   0.04076   0.06249     -0.02270 -0.008513
sigma_DCA     0.007417   0.01552  -0.09485  -0.12998     -0.07795 -0.001471
             sigma_DCP sigma_DCA
D24_0         0.042920  0.007417
log_k_D24     0.089831  0.015524
log_k_DCP     0.040757 -0.094855
log_k_DCA     0.062486 -0.129984
f_D24_qlogis -0.022695 -0.077952
sigma_D24    -0.008513 -0.001471
sigma_DCP     1.000000 -0.014772
sigma_DCA    -0.014772  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)     Lower     Upper
D24_0        97.59000  44.820 3.458e-27 93.120000 102.10000
k_D24         0.09072  12.180 8.811e-13  0.076660   0.10740
k_DCP         0.15890  12.780 2.903e-13  0.135300   0.18650
k_DCA         0.01166   1.086 1.436e-01  0.001763   0.07715
f_D24_to_DCP  0.28890  11.030 8.264e-12  0.238300   0.34550
sigma_D24     6.00800   5.453 4.526e-06  3.747000   8.26800
sigma_DCP     1.16100   5.048 1.339e-05  0.689300   1.63300
sigma_DCA     0.55650   3.700 4.869e-04  0.247900   0.86510

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   11.93       5 14
D24         7.51       2  6
DCP        19.92       2  5
DCA         5.20       1  3

Resulting formation fractions:
             ff
D24_DCP  0.2889
D24_sink 0.7111

Estimated disappearance times:
      DT50   DT90
D24  7.640  25.38
DCP  4.363  14.49
DCA 59.439 197.45

Data:
 time variable observed predicted residual
  0.0      D24    100.8   97.5879   3.2121
  0.0      D24    101.0   97.5879   3.4121
  0.1      D24     93.2   96.7065  -3.5065
  0.1      D24     93.2   96.7065  -3.5065
  0.3      D24     90.5   94.9677  -4.4677
  0.3      D24     91.5   94.9677  -3.4677
  1.0      D24     86.3   89.1243  -2.8243
  1.0      D24     87.1   89.1243  -2.0243
  3.0      D24     79.0   74.3355   4.6645
  3.0      D24     80.8   74.3355   6.4645
  5.0      D24     74.0   62.0007  11.9993
  5.0      D24     65.6   62.0007   3.5993
 10.0      D24     35.0   39.3910  -4.3910
 10.0      D24     36.7   39.3910  -2.6910
```

```
 17.0      D24      6.6   20.8737 -14.2737
  0.1      DCP      1.4    0.2526   1.1474
  0.1      DCP      1.6    0.2526   1.3474
  0.3      DCP      2.5    0.7392   1.7608
  0.3      DCP      2.4    0.7392   1.6608
  1.0      DCP      2.9    2.2583   0.6417
  1.0      DCP      3.1    2.2583   0.8417
  3.0      DCP      4.4    5.2867  -0.8867
  3.0      DCP      4.2    5.2867  -1.0867
  5.0      DCP      5.8    6.8863  -1.0863
  5.0      DCP      5.4    6.8863  -1.4863
 10.0      DCP      8.2    7.4871   0.7129
 10.0      DCP      8.7    7.4871   1.2129
 17.0      DCP      5.8    5.5086   0.2914
  3.0      DCA      0.5    1.4139  -0.9139
  3.0      DCA      0.5    1.4139  -0.9139
  5.0      DCA      3.2    3.3238  -0.1238
  5.0      DCA      3.5    3.3238   0.1762
 10.0      DCA      9.5    8.8998   0.6002
 10.0      DCA      9.1    8.8998   0.2002
 17.0      DCA     15.0   15.2249  -0.2249
```

Listing 18: SFO-SFO-SFO fit to Fayette data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:41 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 2542 model solutions performed in 2.555 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
D24_0        100.9000  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
f_DCP_to_DCA   0.5000 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
D24_0        100.900000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
f_DCP_qlogis   0.000000  -Inf   Inf
sigma_low      0.100000     0   Inf
rsd_high       0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC   logLik
  193.4438 205.8866 -88.7219

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error      Lower      Upper
D24_0         101.300  5.083e+00  9.083e+01   111.7000
log_k_D24      -2.192  8.970e-02 -2.376e+00    -2.0080
log_k_DCP      -1.945  1.046e-01 -2.160e+00    -1.7310
log_k_DCA     -21.020  9.477e+03 -1.947e+04 19420.0000
f_D24_qlogis   -1.190  1.459e-01 -1.490e+00    -0.8911
f_DCP_qlogis   19.360  9.047e+03 -1.854e+04 18580.0000
sigma_low       1.065  2.365e-01  5.801e-01     1.5510
rsd_high        0.142  2.668e-02  8.723e-02     0.1967
```

```
Parameter correlation:
                 D24_0  log_k_D24  log_k_DCP  log_k_DCA f_D24_qlogis
D24_0         1.000e+00  6.755e-01 -0.1178615 -3.697e-05   -0.7621514
log_k_D24     6.755e-01  1.000e+00 -0.1844587 -5.160e-05   -0.7749053
log_k_DCP    -1.179e-01 -1.845e-01  1.0000000  2.398e-04    0.1712929
log_k_DCA    -3.697e-05 -5.160e-05  0.0002398  1.000e+00    0.0001888
f_D24_qlogis -7.622e-01 -7.749e-01  0.1712929  1.888e-04    1.0000000
f_DCP_qlogis  2.682e-05  3.469e-05 -0.0002668 -1.400e-05   -0.0001786
sigma_low     5.408e-02  2.190e-02  0.0508735  1.402e-05   -0.0475623
rsd_high     -1.531e-01 -1.685e-02 -0.0450757  1.545e-05    0.0399865
             f_DCP_qlogis  sigma_low   rsd_high
D24_0           2.682e-05  5.408e-02 -1.531e-01
log_k_D24       3.469e-05  2.190e-02 -1.685e-02
log_k_DCP      -2.668e-04  5.087e-02 -4.508e-02
log_k_DCA      -1.400e-05  1.402e-05  1.545e-05
f_D24_qlogis   -1.786e-04 -4.756e-02  3.999e-02
f_DCP_qlogis    1.000e+00 -5.505e-06 -2.432e-05
sigma_low      -5.505e-06  1.000e+00 -2.921e-01
rsd_high       -2.432e-05 -2.921e-01  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate   t value    Pr(>t)    Lower    Upper
D24_0        1.013e+02 1.950e+01 9.706e-18 90.83000 111.7000
k_D24        1.117e-01 1.075e+01 1.471e-11  0.09293   0.1343
k_DCP        1.429e-01 4.099e+00 1.704e-04  0.11530   0.1771
k_DCA        7.463e-10 1.878e-08 5.000e-01  0.00000      Inf
f_D24_to_DCP 2.332e-01 5.226e+00 8.311e-06  0.18390   0.2909
f_DCP_to_DCA 1.000e+00 2.760e+00 5.131e-03  0.00000   1.0000
sigma_low    1.065e+00 4.496e+00 5.893e-05  0.58010   1.5510
rsd_high     1.420e-01 5.216e+00 8.537e-06  0.08723   0.1967

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.885       6 13
D24        7.880       2  6
DCP       20.744       2  5
DCA        6.943       2  2

Resulting formation fractions:
               ff
D24_DCP  2.332e-01
D24_sink 7.668e-01
DCP_DCA  1.000e+00
DCP_sink 3.927e-09

Estimated disappearance times:
         DT50      DT90
D24 6.205e+00 2.061e+01
DCP 4.850e+00 1.611e+01
DCA 9.288e+08 3.085e+09

Data:
 time variable observed predicted residual
  0.0      D24    100.8  101.2610 -0.46101
  0.0      D24    101.0  101.2610 -0.26101
  0.1      D24     93.2  100.1361 -6.93612
  0.1      D24     93.2  100.1361 -6.93612
  0.3      D24     90.5   97.9237 -7.42371
  0.3      D24     91.5   97.9237 -6.42371
  1.0      D24     86.3   90.5582 -4.25817
  1.0      D24     87.1   90.5582 -3.45817
  3.0      D24     79.0   72.4267  6.57333
  3.0      D24     80.8   72.4267  8.37333
  5.0      D24     74.0   57.9254 16.07456
  5.0      D24     65.6   57.9254  7.67456
```

```
 10.0      D24     35.0   33.1357  1.86427
 10.0      D24     36.7   33.1357  3.56427
 17.0      D24      6.6   15.1598 -8.55983
  0.1      DCP      1.4    0.2604  1.13958
  0.1      DCP      1.6    0.2604  1.33958
  0.3      DCP      2.5    0.7616  1.73837
  0.3      DCP      2.4    0.7616  1.63837
  1.0      DCP      2.9    2.3224  0.57761
  1.0      DCP      3.1    2.3224  0.77761
  3.0      DCP      4.4    5.4027 -1.00266
  3.0      DCP      4.2    5.4027 -1.20266
  5.0      DCP      5.8    6.9847 -1.18473
  5.0      DCP      5.4    6.9847 -1.58473
 10.0      DCP      8.2    7.4136  0.78640
 10.0      DCP      8.7    7.4136  1.28640
 17.0      DCP      5.8    5.2088  0.59117
  3.0      DCA      0.5    1.3208 -0.82077
  3.0      DCA      0.5    1.3208 -0.82077
  5.0      DCA      3.2    3.1200  0.07999
  5.0      DCA      3.5    3.1200  0.37999
 10.0      DCA      9.5    8.4715  1.02852
 10.0      DCA      9.1    8.4715  0.62852
 17.0      DCA     15.0   14.8678  0.13224
```

Listing 19: SFO-SFO(ns)-SFO fit to Fayette data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:40 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1811 model solutions performed in 1.828 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
D24_0        100.9000  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
D24_0        100.900000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
sigma_low      0.100000     0   Inf
rsd_high       0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC   logLik
  191.4438 202.3312 -88.7219

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error      Lower      Upper
D24_0         101.300  5.083e+00  9.085e+01   111.7000
log_k_D24      -2.192  8.970e-02 -2.376e+00    -2.0080
log_k_DCP      -1.945  1.046e-01 -2.160e+00    -1.7310
log_k_DCA     -20.930  9.092e+03 -1.865e+04 18600.0000
f_D24_qlogis   -1.190  1.459e-01 -1.489e+00    -0.8916
sigma_low       1.065  2.365e-01  5.809e-01     1.5500
rsd_high        0.142  2.668e-02  8.732e-02     0.1966

Parameter correlation:
                 D24_0  log_k_D24  log_k_DCP  log_k_DCA f_D24_qlogis
```

```
D24_0         1.000e+00  6.755e-01 -0.1178615 -3.853e-05   -0.7621515
log_k_D24     6.755e-01  1.000e+00 -0.1844588 -5.378e-05   -0.7749054
log_k_DCP    -1.179e-01 -1.845e-01  1.0000000  2.499e-04    0.1712929
log_k_DCA    -3.853e-05 -5.378e-05  0.0002499  1.000e+00    0.0001968
f_D24_qlogis -7.622e-01 -7.749e-01  0.1712929  1.968e-04    1.0000000
sigma_low     5.408e-02  2.190e-02  0.0508733  1.462e-05   -0.0475624
rsd_high     -1.531e-01 -1.685e-02 -0.0450755  1.611e-05    0.0399871
              sigma_low   rsd_high
D24_0         5.408e-02 -1.531e-01
log_k_D24     2.190e-02 -1.685e-02
log_k_DCP     5.087e-02 -4.508e-02
log_k_DCA     1.462e-05  1.611e-05
f_D24_qlogis -4.756e-02  3.999e-02
sigma_low     1.000e+00 -2.921e-01
rsd_high     -2.921e-01  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate   t value    Pr(>t)    Lower    Upper
D24_0        1.013e+02 1.968e+01 3.104e-18 90.85000 111.7000
k_D24        1.117e-01 1.089e+01 7.114e-12  0.09296   0.1342
k_DCP        1.429e-01 6.687e+00 1.470e-07  0.11540   0.1771
k_DCA        8.108e-10 2.690e-08 5.000e-01  0.00000      Inf
f_D24_to_DCP 2.332e-01 6.964e+00 7.137e-08  0.18400   0.2908
sigma_low    1.065e+00 4.496e+00 5.488e-05  0.58090   1.5500
rsd_high     1.420e-01 5.310e+00 5.948e-06  0.08732   0.1966

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   12.52       5 14
D24         7.88       2  6
DCP        20.74       2  5
DCA         6.08       1  3

Resulting formation fractions:
             ff
D24_DCP  0.2332
D24_sink 0.7668

Estimated disappearance times:
         DT50      DT90
D24 6.205e+00 2.061e+01
DCP 4.850e+00 1.611e+01
DCA 8.549e+08 2.840e+09

Data:
 time variable observed predicted residual
  0.0      D24    100.8  101.2610 -0.46100
  0.0      D24    101.0  101.2610 -0.26100
  0.1      D24     93.2  100.1361 -6.93612
  0.1      D24     93.2  100.1361 -6.93612
  0.3      D24     90.5   97.9237 -7.42371
  0.3      D24     91.5   97.9237 -6.42371
  1.0      D24     86.3   90.5582 -4.25817
  1.0      D24     87.1   90.5582 -3.45817
  3.0      D24     79.0   72.4267  6.57333
  3.0      D24     80.8   72.4267  8.37333
  5.0      D24     74.0   57.9254 16.07455
  5.0      D24     65.6   57.9254  7.67455
 10.0      D24     35.0   33.1357  1.86427
 10.0      D24     36.7   33.1357  3.56427
 17.0      D24      6.6   15.1598 -8.55984
  0.1      DCP      1.4    0.2604  1.13958
  0.1      DCP      1.6    0.2604  1.33958
  0.3      DCP      2.5    0.7616  1.73837
  0.3      DCP      2.4    0.7616  1.63837
  1.0      DCP      2.9    2.3224  0.57761
```

```
  1.0      DCP      3.1    2.3224  0.77761
  3.0      DCP      4.4    5.4027 -1.00266
  3.0      DCP      4.2    5.4027 -1.20266
  5.0      DCP      5.8    6.9847 -1.18473
  5.0      DCP      5.4    6.9847 -1.58473
 10.0      DCP      8.2    7.4136  0.78640
 10.0      DCP      8.7    7.4136  1.28640
 17.0      DCP      5.8    5.2088  0.59117
  3.0      DCA      0.5    1.3208 -0.82077
  3.0      DCA      0.5    1.3208 -0.82077
  5.0      DCA      3.2    3.1200  0.07999
  5.0      DCA      3.5    3.1200  0.37999
 10.0      DCA      9.5    8.4715  1.02852
 10.0      DCA      9.1    8.4715  0.62852
 17.0      DCA     15.0   14.8678  0.13224
```

Listing 20: SFO-SFO-SFO fit to RefSol 03-G data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:33 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 2842 model solutions performed in 3.003 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.8000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
f_DCP_to_DCA  0.5000 deparm
sigma_D24     3.0000  error
sigma_DCP     3.0000  error
sigma_DCA     3.0000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.800000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
f_DCP_qlogis  0.000000  -Inf   Inf
sigma_D24     3.000000     0   Inf
sigma_DCP     3.000000     0   Inf
sigma_DCA     3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  197.1267 213.3867 -89.56337

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower   Upper
D24_0         92.9300    1.60800 89.67000 96.1900
log_k_D24     -0.8518    0.06394 -0.98150 -0.7221
log_k_DCP      0.7646    0.36370  0.02694  1.5020
log_k_DCA     -2.9420    0.13280 -3.21200 -2.6730
f_D24_qlogis   1.0890    1.08400 -1.10900  3.2870
f_DCP_qlogis  -1.4830    0.36770 -2.22900 -0.7375
```

```
sigma_D24      3.5230    0.60420  2.29800  4.7480
sigma_DCP      1.7660    0.37060  1.01400  2.5170
sigma_DCA      0.7225    0.16610  0.38560  1.0590

Parameter correlation:
                D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis f_DCP_qlogis
D24_0         1.000000  0.501106 -0.062296 -0.151662    -0.205399     0.089654
log_k_D24     0.501106  1.000000 -0.124317 -0.302655    -0.315126     0.178912
log_k_DCP    -0.062296 -0.124317  1.000000 -0.423325     0.905409    -0.924105
log_k_DCA    -0.151662 -0.302655 -0.423325  1.000000    -0.310183     0.477189
f_D24_qlogis -0.205399 -0.315126  0.905409 -0.310183     1.000000    -0.973337
f_DCP_qlogis  0.089654  0.178912 -0.924105  0.477189    -0.973337     1.000000
sigma_D24     0.004614  0.009208 -0.001145 -0.002787    -0.002902     0.001647
sigma_DCP     0.061166  0.122062  0.459112 -0.258996     0.378827    -0.412617
sigma_DCA    -0.068930 -0.137555 -0.482488  0.275532    -0.396206     0.433023
             sigma_D24 sigma_DCP sigma_DCA
D24_0         0.004614  0.061166 -0.068930
log_k_D24     0.009208  0.122062 -0.137555
log_k_DCP    -0.001145  0.459112 -0.482488
log_k_DCA    -0.002787 -0.258996  0.275532
f_D24_qlogis -0.002902  0.378827 -0.396206
f_DCP_qlogis  0.001647 -0.412617  0.433023
sigma_D24     1.000000  0.001124 -0.001267
sigma_DCP     0.001124  1.000000 -0.257458
sigma_DCA    -0.001267 -0.257458  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower    Upper
D24_0        92.93000  57.770 2.134e-37 89.67000 96.19000
k_D24         0.42670  15.640 6.245e-18  0.37480  0.48570
k_DCP         2.14800   2.749 4.640e-03  1.02700  4.49200
k_DCA         0.05274   7.531 3.346e-09  0.04029  0.06904
f_D24_to_DCP  0.74820   3.663 3.974e-04  0.24800  0.96400
f_DCP_to_DCA  0.18500   3.337 9.879e-04  0.09720  0.32360
sigma_D24     3.52300   5.831 5.850e-07  2.29800  4.74800
sigma_DCP     1.76600   4.764 1.540e-05  1.01400  2.51700
sigma_DCA     0.72250   4.349 5.374e-05  0.38560  1.05900

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  11.427       6 18
D24        6.393       2  7
DCP       35.109       2  6
DCA        9.389       2  5

Resulting formation fractions:
              ff
D24_DCP  0.7482
D24_sink 0.2518
DCP_DCA  0.1850
DCP_sink 0.8150

Estimated disappearance times:
       DT50   DT90
D24  1.6246  5.397
DCP  0.3227  1.072
DCA 13.1424 43.658

Data:
 time variable observed predicted residual
  0.0      D24     98.8 9.293e+01  5.87188
  0.0      D24     98.8 9.293e+01  5.87188
  0.1      D24     87.4 8.905e+01 -1.64670
  0.1      D24     87.9 8.905e+01 -1.14670
  0.3      D24     78.1 8.176e+01 -3.66344
  0.3      D24     78.8 8.176e+01 -2.96344
```

```
  1.0      D24     57.1 6.065e+01 -3.55321
  1.0      D24     56.1 6.065e+01 -4.55321
  3.0      D24     25.0 2.584e+01 -0.83848
  3.0      D24     32.3 2.584e+01  6.46152
  5.0      D24     14.7 1.101e+01  3.69271
 10.0      D24      3.1 1.304e+00  1.79619
 10.0      D24      3.1 1.304e+00  1.79619
 17.0      D24      2.7 6.579e-02  2.63421
 17.0      D24      2.1 6.579e-02  2.03421
 26.0      D24      2.0 1.414e-03  1.99859
 26.0      D24      2.2 1.414e-03  2.19859
  0.1      DCP      2.8 2.611e+00  0.18875
  0.1      DCP      2.5 2.611e+00 -0.11125
  0.3      DCP      5.5 6.115e+00 -0.61543
  0.3      DCP      5.4 6.115e+00 -0.71543
  1.0      DCP      8.5 9.236e+00 -0.73581
  1.0      DCP      8.6 9.236e+00 -0.63581
  3.0      DCP      6.7 4.764e+00  1.93624
  3.0      DCP      5.3 4.764e+00  0.53624
  5.0      DCP      5.7 2.041e+00  3.65933
 10.0      DCP      3.2 2.418e-01  2.95824
 10.0      DCP      2.7 2.418e-01  2.45824
 17.0      DCP      2.3 1.220e-02  2.28780
 17.0      DCP      1.7 1.220e-02  1.68780
 26.0      DCP      1.3 2.622e-04  1.29974
 26.0      DCP      1.7 2.622e-04  1.69974
  0.3      DCA      0.5 4.116e-01  0.08844
  0.3      DCA      0.5 4.116e-01  0.08844
  1.0      DCA      3.3 2.700e+00  0.59961
  1.0      DCA      3.7 2.700e+00  0.99961
  3.0      DCA      8.0 7.755e+00  0.24464
  3.0      DCA      7.0 7.755e+00 -0.75536
  5.0      DCA     10.6 9.387e+00  1.21307
 10.0      DCA      7.7 8.620e+00 -0.92014
 10.0      DCA      7.9 8.620e+00 -0.72014
 17.0      DCA      5.2 6.124e+00 -0.92368
 17.0      DCA      6.7 6.124e+00  0.57632
 26.0      DCA      4.6 3.817e+00  0.78274
 26.0      DCA      4.2 3.817e+00  0.38274
```

Listing 21: SFO-SFO(ns)-SFO fit to RefSol 03-G data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:31 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1405 model solutions performed in 1.464 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.8000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
sigma_D24     3.0000  error
sigma_DCP     3.0000  error
sigma_DCA     3.0000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.800000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
sigma_D24     3.000000     0   Inf
sigma_DCP     3.000000     0   Inf
sigma_DCA     3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC     BIC    logLik
  221.0217 235.475 -102.5108

Optimised, transformed parameters with symmetric confidence intervals:
            Estimate Std. Error   Lower   Upper
D24_0         93.3600     1.6500 90.0200 96.7000
log_k_D24     -0.8176     0.0682 -0.9557 -0.6794
log_k_DCP     -0.8092     0.1814 -1.1770 -0.4417
log_k_DCA     -2.1610     0.2112 -2.5890 -1.7330
f_D24_qlogis  -1.2230     0.1606 -1.5490 -0.8980
sigma_D24      3.5550     0.6212  2.2960  4.8130
sigma_DCP      2.0220     0.3958  1.2200  2.8240
sigma_DCA      1.6530     0.3540  0.9361  2.3710
```

```
Parameter correlation:
               D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis sigma_D24
D24_0         1.00000   0.51833  -0.04392  -0.12749     -0.29327   0.09984
log_k_D24     0.51833   1.00000  -0.08473  -0.24597     -0.36481   0.19262
log_k_DCP    -0.04392  -0.08473   1.00000  -0.04777     -0.04692  -0.01632
log_k_DCA    -0.12749  -0.24597  -0.04777   1.00000      0.80824  -0.04738
f_D24_qlogis -0.29327  -0.36481  -0.04692   0.80824      1.00000  -0.07027
sigma_D24     0.09984   0.19262  -0.01632  -0.04738     -0.07027   1.00000
sigma_DCP    -0.03099  -0.05979   0.14224  -0.24893     -0.29045  -0.01152
sigma_DCA    -0.07388  -0.14254  -0.13262   0.31317      0.38139  -0.02746
             sigma_DCP sigma_DCA
D24_0         -0.03099  -0.07388
log_k_D24     -0.05979  -0.14254
log_k_DCP      0.14224  -0.13262
log_k_DCA     -0.24893   0.31317
f_D24_qlogis  -0.29045   0.38139
sigma_D24     -0.01152  -0.02746
sigma_DCP      1.00000  -0.12482
sigma_DCA     -0.12482   1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)   Lower   Upper
D24_0         93.3600  56.580 7.699e-38 90.0200 96.7000
k_D24          0.4415  14.660 2.710e-17  0.3845  0.5069
k_DCP          0.4452   5.514 1.431e-06  0.3083  0.6430
k_DCA          0.1152   4.735 1.594e-05  0.0751  0.1767
f_D24_to_DCP   0.2273   8.060 5.771e-10  0.1753  0.2895
sigma_D24      3.5550   5.722 7.477e-07  2.2960  4.8130
sigma_DCP      2.0220   5.109 5.036e-06  1.2200  2.8240
sigma_DCA      1.6530   4.671 1.942e-05  0.9361  2.3710

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   11.98       5 19
D24         6.55       2  7
DCP        35.56       2  6
DCA        20.13       1  6

Resulting formation fractions:
            ff
D24_DCP  0.2273
D24_sink 0.7727

Estimated disappearance times:
     DT50   DT90
D24 1.570  5.215
DCP 1.557  5.172
DCA 6.017 19.987

Data:
 time variable observed predicted residual
  0.0      D24     98.8 9.336e+01  5.44153
  0.0      D24     98.8 9.336e+01  5.44153
  0.1      D24     87.4 8.933e+01 -1.92627
  0.1      D24     87.9 8.933e+01 -1.42627
  0.3      D24     78.1 8.178e+01 -3.67679
  0.3      D24     78.8 8.178e+01 -2.97679
  1.0      D24     57.1 6.004e+01 -2.93550
  1.0      D24     56.1 6.004e+01 -3.93550
  3.0      D24     25.0 2.483e+01  0.17342
  3.0      D24     32.3 2.483e+01  7.47342
  5.0      D24     14.7 1.027e+01  4.43342
 10.0      D24      3.1 1.129e+00  1.97099
 10.0      D24      3.1 1.129e+00  1.97099
 17.0      D24      2.7 5.134e-02  2.64866
```

```
 17.0      D24      2.1 5.134e-02  2.04866
 26.0      D24      2.0 9.655e-04  1.99903
 26.0      D24      2.2 9.655e-04  2.19903
  0.1      DCP      2.8 8.964e-01  1.90356
  0.1      DCP      2.5 8.964e-01  1.60356
  0.3      DCP      5.5 2.461e+00  3.03888
  0.3      DCP      5.4 2.461e+00  2.93888
  1.0      DCP      8.5 6.015e+00  2.48516
  1.0      DCP      8.6 6.015e+00  2.58516
  3.0      DCP      6.7 7.434e+00 -0.73428
  3.0      DCP      5.3 7.434e+00 -2.13428
  5.0      DCP      5.7 5.105e+00  0.59516
 10.0      DCP      3.2 1.112e+00  2.08760
 10.0      DCP      2.7 1.112e+00  1.58760
 17.0      DCP      2.3 8.489e-02  2.21511
 17.0      DCP      1.7 8.489e-02  1.61511
 26.0      DCP      1.3 2.402e-03  1.29760
 26.0      DCP      1.7 2.402e-03  1.69760
  0.3      DCA      0.5 1.699e-01  0.33010
  0.3      DCA      0.5 1.699e-01  0.33010
  1.0      DCA      3.3 1.498e+00  1.80167
  1.0      DCA      3.7 1.498e+00  2.20167
  3.0      DCA      8.0 7.089e+00  0.91065
  3.0      DCA      7.0 7.089e+00 -0.08935
  5.0      DCA     10.6 1.063e+01 -0.03102
 10.0      DCA      7.7 1.027e+01 -2.57296
 10.0      DCA      7.9 1.027e+01 -2.37296
 17.0      DCA      5.2 5.330e+00 -0.12962
 17.0      DCA      6.7 5.330e+00  1.37038
 26.0      DCA      4.6 1.934e+00  2.66576
 26.0      DCA      4.2 1.934e+00  2.26576
```

Listing 22: SFO-SFO-SFO fit to RefSol 03-G data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:40 2021
Date of summary: Mon Jul 26 18:52:52 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1591 model solutions performed in 1.725 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.8000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
f_DCP_to_DCA  0.5000 deparm
sigma_low     0.1000  error
rsd_high      0.1000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.800000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
f_DCP_qlogis  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  200.7663 215.2196 -92.38315

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower   Upper
D24_0        89.96000     2.4760 84.94000 94.9800
log_k_D24    -0.98810     0.0507 -1.09100 -0.8854
log_k_DCP     0.46900     0.2738 -0.08575  1.0240
log_k_DCA    -2.79200     0.2202 -3.23800 -2.3460
f_D24_qlogis  0.85450     0.7429 -0.65070  2.3600
f_DCP_qlogis -1.24700     0.3395 -1.93500 -0.5588
sigma_low     1.41300     0.1806  1.04800  1.7790
rsd_high      0.06701     0.0171  0.03236  0.1017
```

```
Parameter correlation:
               D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis f_DCP_qlogis
D24_0         1.00000    0.5907  -0.11715  -0.06603     -0.31759      0.12457
log_k_D24     0.59070    1.0000  -0.19955  -0.11299     -0.40119      0.21081
log_k_DCP    -0.11715   -0.1995   1.00000  -0.22606      0.88978     -0.84960
log_k_DCA    -0.06603   -0.1130  -0.22606   1.00000     -0.16466      0.49385
f_D24_qlogis -0.31759   -0.4012   0.88978  -0.16466      1.00000     -0.88852
f_DCP_qlogis  0.12457    0.2108  -0.84960   0.49385     -0.88852      1.00000
sigma_low     0.13168    0.2301  -0.03789  -0.01804     -0.09469      0.04903
rsd_high     -0.26991   -0.3672   0.06039   0.02881      0.15102     -0.07817
             sigma_low rsd_high
D24_0          0.13168 -0.26991
log_k_D24      0.23015 -0.36723
log_k_DCP     -0.03789  0.06039
log_k_DCA     -0.01804  0.02881
f_D24_qlogis  -0.09469  0.15102
f_DCP_qlogis   0.04903 -0.07817
sigma_low      1.00000 -0.17203
rsd_high      -0.17203  1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower   Upper
D24_0        89.96000  36.330 7.554e-31 84.94000 94.9800
k_D24         0.37230  19.720 1.584e-21  0.33590  0.4126
k_DCP         1.59800   3.652 3.998e-04  0.91780  2.7840
k_DCA         0.06131   4.541 2.885e-05  0.03924  0.0958
f_D24_to_DCP  0.70150   4.510 3.170e-05  0.34280  0.9137
f_DCP_to_DCA  0.22330   3.792 2.672e-04  0.12630  0.3638
sigma_low     1.41300   7.826 1.159e-09  1.04800  1.7790
rsd_high      0.06701   3.918 1.852e-04  0.03236  0.1017

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.195       6 18
D24        7.164       2  7
DCP       29.446       2  6
DCA       11.638       2  5

Resulting formation fractions:
             ff
D24_DCP  0.7015
D24_sink 0.2985
DCP_DCA  0.2233
DCP_sink 0.7767

Estimated disappearance times:
       DT50   DT90
D24  1.8619  6.185
DCP  0.4336  1.441
DCA 11.3049 37.554

Data:
 time variable observed predicted residual
  0.0      D24     98.8 89.959393   8.8406
  0.0      D24     98.8 89.959393   8.8406
  0.1      D24     87.4 86.672008   0.7280
  0.1      D24     87.9 86.672008   1.2280
  0.3      D24     78.1 80.453239  -2.3532
  0.3      D24     78.8 80.453239  -1.6532
  1.0      D24     57.1 61.996891  -4.8969
  1.0      D24     56.1 61.996891  -5.8969
  3.0      D24     25.0 29.445349  -4.4453
  3.0      D24     32.3 29.445349   2.8547
  5.0      D24     14.7 13.985033   0.7150
 10.0      D24      3.1  2.174105   0.9259
```

```
 10.0      D24      3.1  2.174105   0.9259
 17.0      D24      2.7  0.160526   2.5395
 17.0      D24      2.1  0.160526   1.9395
 26.0      D24      2.0  0.005629   1.9944
 26.0      D24      2.2  0.005629   2.1944
  0.1      DCP      2.8  2.130205   0.6698
  0.1      DCP      2.5  2.130205   0.3698
  0.3      DCP      5.5  5.273871   0.2261
  0.3      DCP      5.4  5.273871   0.1261
  1.0      DCP      8.5  9.330000  -0.8300
  1.0      DCP      8.6  9.330000  -0.7300
  3.0      DCP      6.7  6.112982   0.5870
  3.0      DCP      5.3  6.112982  -0.8130
  5.0      DCP      5.7  2.972119   2.7279
 10.0      DCP      3.2  0.463049   2.7370
 10.0      DCP      2.7  0.463049   2.2370
 17.0      DCP      2.3  0.034189   2.2658
 17.0      DCP      1.7  0.034189   1.6658
 26.0      DCP      1.3  0.001199   1.2988
 26.0      DCP      1.7  0.001199   1.6988
  0.3      DCA      0.5  0.309436   0.1906
  0.3      DCA      0.5  0.309436   0.1906
  1.0      DCA      3.3  2.243075   1.0569
  1.0      DCA      3.7  2.243075   1.4569
  3.0      DCA      8.0  7.433461   0.5665
  3.0      DCA      7.0  7.433461  -0.4335
  5.0      DCA     10.6  9.493144   1.1069
 10.0      DCA      7.7  8.970091  -1.2701
 10.0      DCA      7.9  8.970091  -1.0701
 17.0      DCA      5.2  6.146566  -0.9466
 17.0      DCA      6.7  6.146566   0.5534
 26.0      DCA      4.6  3.561014   1.0390
 26.0      DCA      4.2  3.561014   0.6390
```

Listing 23: SFO-SFO(ns)-SFO fit to RefSol 03-G data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:41 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1308 model solutions performed in 1.316 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.8000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
sigma_low     0.1000  error
rsd_high      0.1000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.800000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  218.4091 231.0558 -102.2046

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
D24_0        91.23000    2.30800 86.56000 95.91000
log_k_D24    -0.93690    0.05327 -1.04500 -0.82900
log_k_DCP    -0.78980    0.18690 -1.16800 -0.41150
log_k_DCA    -2.03800    0.21780 -2.47900 -1.59700
f_D24_qlogis -1.06400    0.16430 -1.39600 -0.73130
sigma_low     1.93300    0.24690  1.43300  2.43300
rsd_high      0.05889    0.01939  0.01964  0.09814

Parameter correlation:
               D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis sigma_low
```

```
D24_0         1.00000   0.55065 -0.043425 -0.097570     -0.34705  0.084437
log_k_D24     0.55065   1.00000 -0.079430 -0.178190     -0.36830  0.186367
log_k_DCP    -0.04342  -0.07943  1.000000  0.208877      0.26955  0.001012
log_k_DCA    -0.09757  -0.17819  0.208877  1.000000      0.72682 -0.005355
f_D24_qlogis -0.34705  -0.36830  0.269549  0.726816      1.00000 -0.073147
sigma_low     0.08444   0.18637  0.001012 -0.005355     -0.07315  1.000000
rsd_high     -0.19005  -0.31091 -0.001720  0.008917      0.12203 -0.269874
              rsd_high
D24_0        -0.190051
log_k_D24    -0.310908
log_k_DCP    -0.001720
log_k_DCA     0.008917
f_D24_qlogis  0.122034
sigma_low    -0.269874
rsd_high      1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower    Upper
D24_0        91.23000  39.520 8.936e-33 86.56000 95.91000
k_D24         0.39190  18.770 4.028e-21  0.35180  0.43650
k_DCP         0.45390   5.351 2.204e-06  0.31100  0.66270
k_DCA         0.13030   4.592 2.355e-05  0.08383  0.20250
f_D24_to_DCP  0.25660   8.187 3.238e-10  0.19840  0.32490
sigma_low     1.93300   7.828 9.599e-10  1.43300  2.43300
rsd_high      0.05889   3.037 2.149e-03  0.01964  0.09814

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.146       5 19
D24        6.596       2  7
DCP       35.554       2  6
DCA       21.733       1  6

Resulting formation fractions:
             ff
D24_DCP  0.2566
D24_sink 0.7434

Estimated disappearance times:
     DT50   DT90
D24 1.769  5.876
DCP 1.527  5.072
DCA 5.320 17.674

Data:
 time variable observed predicted residual
  0.0      D24     98.8 91.231981  7.56802
  0.0      D24     98.8 91.231981  7.56802
  0.1      D24     87.4 87.726189 -0.32619
  0.1      D24     87.9 87.726189  0.17381
  0.3      D24     78.1 81.113582 -3.01358
  0.3      D24     78.8 81.113582 -2.31358
  1.0      D24     57.1 61.655055 -4.55506
  1.0      D24     56.1 61.655055 -5.55506
  3.0      D24     25.0 28.158652 -3.15865
  3.0      D24     32.3 28.158652  4.14135
  5.0      D24     14.7 12.860417  1.83958
 10.0      D24      3.1  1.812855  1.28715
 10.0      D24      3.1  1.812855  1.28715
 17.0      D24      2.7  0.116712  2.58329
 17.0      D24      2.1  0.116712  1.98329
 26.0      D24      2.0  0.003432  1.99657
 26.0      D24      2.2  0.003432  2.19657
  0.1      DCP      2.8  0.879222  1.92078
  0.1      DCP      2.5  0.879222  1.62078
  0.3      DCP      5.5  2.423779  3.07622
```

```
 0.3      DCP      5.4  2.423779  2.97622
 1.0      DCP      8.5  6.009952  2.49005
 1.0      DCP      8.6  6.009952  2.59005
 3.0      DCP      6.7  7.748618 -1.04862
 3.0      DCP      5.3  7.748618 -2.44862
 5.0      DCP      5.7  5.557279  0.14272
10.0      DCP      3.2  1.357656  1.84234
10.0      DCP      2.7  1.357656  1.34234
17.0      DCP      2.3  0.123204  2.17680
17.0      DCP      1.7  0.123204  1.57680
26.0      DCP      1.3  0.004450  1.29555
26.0      DCP      1.7  0.004450  1.69555
 0.3      DCA      0.5  0.169977  0.33002
 0.3      DCA      0.5  0.169977  0.33002
 1.0      DCA      3.3  1.507367  1.79263
 1.0      DCA      3.7  1.507367  2.19263
 3.0      DCA      8.0  7.222529  0.77747
 3.0      DCA      7.0  7.222529 -0.22253
 5.0      DCA     10.6 10.911196 -0.31120
10.0      DCA      7.7 10.483923 -2.78392
10.0      DCA      7.9 10.483923 -2.58392
17.0      DCA      5.2  5.133513  0.06649
17.0      DCA      6.7  5.133513  1.56649
26.0      DCA      4.6  1.654103  2.94590
26.0      DCA      4.2  1.654103  2.54590
```

Listing 24: SFO-SFO-SFO fit to Site E1 data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:34 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 2471 model solutions performed in 2.38 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
D24_0        100.5500  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
f_DCP_to_DCA   0.5000 deparm
sigma_D24      3.0000  error
sigma_DCP      3.0000  error
sigma_DCA      3.0000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
D24_0        100.550000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
f_DCP_qlogis   0.000000  -Inf   Inf
sigma_D24      3.000000     0   Inf
sigma_DCP      3.000000     0   Inf
sigma_DCA      3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  165.9025 181.3247 -73.95127

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error      Lower      Upper
D24_0         99.3200  1.377e+00  9.652e+01   102.1000
log_k_D24     -1.1960  5.300e-02 -1.304e+00    -1.0880
log_k_DCP     -0.7960  2.101e-01 -1.224e+00    -0.3680
log_k_DCA     -1.3860  2.540e-01 -1.903e+00    -0.8686
f_D24_qlogis  -1.4800  1.927e-01 -1.872e+00    -1.0870
f_DCP_qlogis  20.1100  1.076e+04 -2.189e+04 21930.0000
```

```
sigma_D24      3.1510  5.641e-01  2.002e+00     4.3000
sigma_DCP      0.5932  1.369e-01  3.144e-01     0.8720
sigma_DCA      1.4190  3.490e-01  7.083e-01     2.1300

Parameter correlation:
                 D24_0  log_k_D24  log_k_DCP  log_k_DCA f_D24_qlogis
D24_0         1.000e+00  5.017e-01 -1.814e-01 -1.743e-01   -3.204e-01
log_k_D24     5.017e-01  1.000e+00 -3.615e-01 -3.474e-01   -5.069e-01
log_k_DCP    -1.814e-01 -3.615e-01  1.000e+00  7.482e-01    9.135e-01
log_k_DCA    -1.743e-01 -3.474e-01  7.482e-01  1.000e+00    7.969e-01
f_D24_qlogis -3.204e-01 -5.069e-01  9.135e-01  7.969e-01    1.000e+00
f_DCP_qlogis  6.291e-08  9.200e-08 -3.788e-06  9.708e-05   -3.618e-06
sigma_D24    -7.958e-02 -1.586e-01  5.734e-02  5.510e-02    8.039e-02
sigma_DCP    -1.227e-03 -2.446e-03  4.854e-01  3.718e-01    4.385e-01
sigma_DCA     7.849e-02  1.564e-01 -5.490e-01 -4.313e-01   -5.237e-01
             f_DCP_qlogis  sigma_D24  sigma_DCP  sigma_DCA
D24_0           6.291e-08 -7.958e-02 -1.227e-03  7.849e-02
log_k_D24       9.200e-08 -1.586e-01 -2.446e-03  1.564e-01
log_k_DCP      -3.788e-06  5.734e-02  4.854e-01 -5.490e-01
log_k_DCA       9.708e-05  5.510e-02  3.718e-01 -4.313e-01
f_D24_qlogis   -3.618e-06  8.039e-02  4.385e-01 -5.237e-01
f_DCP_qlogis    1.000e+00 -1.561e-08 -2.195e-06 -2.928e-05
sigma_D24      -1.561e-08  1.000e+00  3.880e-04 -2.481e-02
sigma_DCP      -2.195e-06  3.880e-04  1.000e+00 -2.824e-01
sigma_DCA      -2.928e-05 -2.481e-02 -2.824e-01  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value    Pr(>t)   Lower    Upper
D24_0          99.3200  72.160 2.639e-37 96.5200 102.1000
k_D24           0.3025  18.870 3.343e-19  0.2716   0.3370
k_DCP           0.4512   4.744 2.086e-05  0.2941   0.6921
k_DCA           0.2501   1.718 4.773e-02  0.1491   0.4195
f_D24_to_DCP    0.1855   6.352 1.964e-07  0.1333   0.2521
f_DCP_to_DCA    1.0000   2.365 1.212e-02  0.0000   1.0000
sigma_D24       3.1510   5.585 1.809e-06  2.0020   4.3000
sigma_DCP       0.5932   4.329 6.883e-05  0.3144   0.8720
sigma_DCA       1.4190   3.454 7.881e-04  0.7083   2.1300

FOCUS Chi2 error levels in percent:
          err.min n.optim df
All data    8.848       6 17
D24         4.835       2  7
DCP        17.034       2  5
DCA        31.882       2  5

Resulting formation fractions:
                ff
D24_DCP  1.855e-01
D24_sink 8.145e-01
DCP_DCA  1.000e+00
DCP_sink 1.851e-09

Estimated disappearance times:
     DT50  DT90
D24 2.291 7.611
DCP 1.536 5.104
DCA 2.772 9.207

Data:
 time variable observed predicted residual
  0.0      D24    100.2  99.32303  0.87697
  0.0      D24    100.9  99.32303  1.57697
  0.1      D24     97.9  96.36330  1.53670
  0.1      D24     98.3  96.36330  1.93670
  0.3      D24     92.4  90.70580  1.69420
  0.3      D24     91.9  90.70580  1.19420
```

```
 1.0      D24     65.8  73.39508 -7.59508
 1.0      D24     69.5  73.39508 -3.89508
 3.0      D24     37.5  40.07753 -2.57753
 3.0      D24     40.0  40.07753 -0.07753
 7.0      D24     18.8  11.95003  6.84997
 7.0      D24     14.4  11.95003  2.44997
10.0      D24      3.3   4.82192 -1.52192
10.0      D24      5.7   4.82192  0.87808
17.0      D24      2.6   0.58015  2.01985
26.0      D24      2.4   0.03811  2.36189
 0.1      DCP      0.5   0.53669 -0.03669
 0.1      DCP      0.5   0.53669 -0.03669
 0.3      DCP      1.8   1.49330  0.30670
 0.3      DCP      2.3   1.49330  0.80670
 1.0      DCP      4.4   3.82673  0.57327
 1.0      DCP      3.6   3.82673 -0.22673
 3.0      DCP      4.8   5.44284 -0.64284
 3.0      DCP      4.3   5.44284 -1.14284
 7.0      DCP      3.3   2.91739  0.38261
 7.0      DCP      3.7   2.91739  0.78261
10.0      DCP      1.7   1.40855  0.29145
10.0      DCP      2.3   1.40855  0.89145
17.0      DCP      0.5   0.20151  0.29849
 0.3      DCA      0.5   0.10234  0.39766
 0.3      DCA      0.5   0.10234  0.39766
 1.0      DCA      3.9   0.90045  2.99955
 1.0      DCA      2.9   0.90045  1.99955
 3.0      DCA      6.3   4.17995  2.12005
 3.0      DCA      5.4   4.17995  1.22005
 7.0      DCA      5.7   6.17795 -0.47795
 7.0      DCA      5.5   6.17795 -0.67795
10.0      DCA      4.5   4.82056 -0.32056
10.0      DCA      4.2   4.82056 -0.62056
17.0      DCA      3.0   1.55162  1.44838
26.0      DCA      1.5   0.23461  1.26539
```

Listing 25: SFO-SFO(ns)-SFO fit to Site E1 data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:32 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1480 model solutions performed in 1.551 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
D24_0        100.5500  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
sigma_D24      3.0000  error
sigma_DCP      3.0000  error
sigma_DCA      3.0000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
D24_0        100.550000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
sigma_D24      3.000000     0   Inf
sigma_DCP      3.000000     0   Inf
sigma_DCA      3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  163.9025 177.6111 -73.95127

Optimised, transformed parameters with symmetric confidence intervals:
            Estimate Std. Error   Lower    Upper
D24_0         99.3200     1.3770 96.5200 102.1000
log_k_D24     -1.1960     0.0530 -1.3030  -1.0880
log_k_DCP     -0.7960     0.2101 -1.2230  -0.3685
log_k_DCA     -1.3860     0.2540 -1.9030  -0.8692
f_D24_qlogis  -1.4800     0.1927 -1.8720  -1.0880
sigma_D24      3.1510     0.5641  2.0030   4.2990
sigma_DCP      0.5932     0.1369  0.3147   0.8716
sigma_DCA      1.4190     0.3490  0.7091   2.1290
```

```
Parameter correlation:
                D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis sigma_D24
D24_0         1.000000  0.501734  -0.18137   -0.1743     -0.32038 -0.079579
log_k_D24     0.501734  1.000000  -0.36149   -0.3474     -0.50686 -0.158607
log_k_DCP    -0.181373 -0.361492   1.00000    0.7482      0.91351  0.057335
log_k_DCA    -0.174313 -0.347422   0.74821    1.0000      0.79688  0.055104
f_D24_qlogis -0.320380 -0.506862   0.91351    0.7969      1.00000  0.080392
sigma_D24    -0.079579 -0.158607   0.05734    0.0551      0.08039  1.000000
sigma_DCP    -0.001227 -0.002446   0.48542    0.3718      0.43854  0.000388
sigma_DCA     0.078495  0.156447  -0.54901   -0.4313     -0.52374 -0.024814
             sigma_DCP sigma_DCA
D24_0        -0.001227   0.07849
log_k_D24    -0.002446   0.15645
log_k_DCP     0.485421  -0.54901
log_k_DCA     0.371777  -0.43134
f_D24_qlogis  0.438543  -0.52374
sigma_D24     0.000388  -0.02481
sigma_DCP     1.000000  -0.28238
sigma_DCA    -0.282381   1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)   Lower    Upper
D24_0         99.3200  72.160 3.365e-38 96.5200 102.1000
k_D24          0.3025  18.870 1.508e-19  0.2716   0.3370
k_DCP          0.4512   4.760 1.867e-05  0.2942   0.6917
k_DCA          0.2501   3.938 2.008e-04  0.1492   0.4193
f_D24_to_DCP   0.1855   6.371 1.625e-07  0.1333   0.2521
sigma_D24      3.1510   5.585 1.639e-06  2.0030   4.2990
sigma_DCP      0.5932   4.334 6.455e-05  0.3147   0.8716
sigma_DCA      1.4190   4.066 1.394e-04  0.7091   2.1290

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   8.649       5 18
D24        4.835       2  7
DCP       17.034       2  5
DCA       29.895       1  6

Resulting formation fractions:
            ff
D24_DCP  0.1855
D24_sink 0.8145

Estimated disappearance times:
     DT50  DT90
D24 2.291 7.611
DCP 1.536 5.104
DCA 2.772 9.207

Data:
 time variable observed predicted residual
  0.0      D24    100.2  99.32303  0.87697
  0.0      D24    100.9  99.32303  1.57697
  0.1      D24     97.9  96.36330  1.53670
  0.1      D24     98.3  96.36330  1.93670
  0.3      D24     92.4  90.70580  1.69420
  0.3      D24     91.9  90.70580  1.19420
  1.0      D24     65.8  73.39508 -7.59508
  1.0      D24     69.5  73.39508 -3.89508
  3.0      D24     37.5  40.07753 -2.57753
  3.0      D24     40.0  40.07753 -0.07753
  7.0      D24     18.8  11.95003  6.84997
  7.0      D24     14.4  11.95003  2.44997
 10.0      D24      3.3   4.82192 -1.52192
 10.0      D24      5.7   4.82192  0.87808
```

```
 17.0      D24      2.6   0.58015  2.01985
 26.0      D24      2.4   0.03811  2.36189
  0.1      DCP      0.5   0.53669 -0.03669
  0.1      DCP      0.5   0.53669 -0.03669
  0.3      DCP      1.8   1.49330  0.30670
  0.3      DCP      2.3   1.49330  0.80670
  1.0      DCP      4.4   3.82673  0.57327
  1.0      DCP      3.6   3.82673 -0.22673
  3.0      DCP      4.8   5.44284 -0.64284
  3.0      DCP      4.3   5.44284 -1.14284
  7.0      DCP      3.3   2.91739  0.38261
  7.0      DCP      3.7   2.91739  0.78261
 10.0      DCP      1.7   1.40855  0.29145
 10.0      DCP      2.3   1.40855  0.89145
 17.0      DCP      0.5   0.20151  0.29849
  0.3      DCA      0.5   0.10234  0.39766
  0.3      DCA      0.5   0.10234  0.39766
  1.0      DCA      3.9   0.90045  2.99955
  1.0      DCA      2.9   0.90045  1.99955
  3.0      DCA      6.3   4.17995  2.12005
  3.0      DCA      5.4   4.17995  1.22005
  7.0      DCA      5.7   6.17795 -0.47795
  7.0      DCA      5.5   6.17795 -0.67795
 10.0      DCA      4.5   4.82056 -0.32056
 10.0      DCA      4.2   4.82056 -0.62056
 17.0      DCA      3.0   1.55162  1.44838
 26.0      DCA      1.5   0.23461  1.26539
```

Listing 26: SFO-SFO-SFO fit to Site E1 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:42 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 2392 model solutions performed in 2.161 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
D24_0        100.5500  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
f_DCP_to_DCA   0.5000 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
D24_0        100.550000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
f_DCP_qlogis   0.000000  -Inf   Inf
sigma_low      0.100000     0   Inf
rsd_high       0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  181.7071 195.4157 -82.85355

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error      Lower      Upper
D24_0        96.64000  2.456e+00  9.165e+01  1.016e+02
log_k_D24    -1.29700  3.538e-02 -1.369e+00 -1.225e+00
log_k_DCP    -0.40970  2.000e-01 -8.166e-01 -2.835e-03
log_k_DCA    -1.03700  2.000e-01 -1.444e+00 -6.300e-01
f_D24_qlogis -1.06100  1.983e-01 -1.464e+00 -6.573e-01
f_DCP_qlogis 20.11000  2.143e+04 -4.359e+04  4.363e+04
sigma_low     1.24500  1.937e-01  8.511e-01  1.639e+00
rsd_high      0.06861  2.143e-02  2.501e-02  1.122e-01
```

```
Parameter correlation:
                  D24_0  log_k_D24  log_k_DCP  log_k_DCA f_D24_qlogis
D24_0         1.000e+00  5.430e-01 -0.0639131 -0.0899955   -0.3032491
log_k_D24     5.430e-01  1.000e+00 -0.1184753 -0.1661780   -0.3349740
log_k_DCP    -6.391e-02 -1.185e-01  1.0000000  0.4782423    0.5810435
log_k_DCA    -9.000e-02 -1.662e-01  0.4782423  1.0000000    0.7900033
f_D24_qlogis -3.032e-01 -3.350e-01  0.5810435  0.7900033    1.0000000
f_DCP_qlogis  3.919e-07  5.131e-07 -0.0001217  0.0001376   -0.0001065
sigma_low     1.144e-01  2.403e-01 -0.0142438 -0.0319439   -0.0832671
rsd_high     -2.041e-01 -3.176e-01  0.0188444  0.0422396    0.1100059
             f_DCP_qlogis  sigma_low   rsd_high
D24_0           3.919e-07  1.144e-01 -2.041e-01
log_k_D24       5.131e-07  2.403e-01 -3.176e-01
log_k_DCP      -1.217e-04 -1.424e-02  1.884e-02
log_k_DCA       1.376e-04 -3.194e-02  4.224e-02
f_D24_qlogis   -1.065e-04 -8.327e-02  1.100e-01
f_DCP_qlogis    1.000e+00 -1.369e-05  4.815e-06
sigma_low      -1.369e-05  1.000e+00 -4.061e-01
rsd_high        4.815e-06 -4.061e-01  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value    Pr(>t)    Lower    Upper
D24_0        96.64000  39.340 1.307e-29 91.65000 101.6000
k_D24         0.27340  28.260 5.270e-25  0.25440   0.2938
k_DCP         0.66380   1.912 3.233e-02  0.44190   0.9972
k_DCA         0.35460   1.724 4.701e-02  0.23610   0.5326
f_D24_to_DCP  0.25720   2.903 3.269e-03  0.18780   0.3414
f_DCP_to_DCA  1.00000   1.275 1.057e-01  0.00000   1.0000
sigma_low     1.24500   6.206 2.635e-07  0.85110   1.6390
rsd_high      0.06861   3.188 1.566e-03  0.02501   0.1122

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  10.359       6 17
D24        5.872       2  7
DCP       20.733       2  5
DCA       28.408       2  5

Resulting formation fractions:
                ff
D24_DCP  2.572e-01
D24_sink 7.428e-01
DCP_DCA  1.000e+00
DCP_sink 1.851e-09

Estimated disappearance times:
     DT50  DT90
D24 2.535 8.421
DCP 1.044 3.469
DCA 1.955 6.494

Data:
 time variable observed predicted residual
  0.0      D24    100.2  96.64414  3.55586
  0.0      D24    100.9  96.64414  4.25586
  0.1      D24     97.9  94.03739  3.86261
  0.1      D24     98.3  94.03739  4.26261
  0.3      D24     92.4  89.03292  3.36708
  0.3      D24     91.9  89.03292  2.86708
  1.0      D24     65.8  73.52343 -7.72343
  1.0      D24     69.5  73.52343 -4.02343
  3.0      D24     37.5  42.55262 -5.05262
  3.0      D24     40.0  42.55262 -2.55262
  7.0      D24     18.8  14.25369  4.54631
  7.0      D24     14.4  14.25369  0.14631
```

```
 10.0      D24      3.3   6.27593 -2.97593
 10.0      D24      5.7   6.27593 -0.57593
 17.0      D24      2.6   0.92561  1.67439
 26.0      D24      2.4   0.07901  2.32099
  0.1      DCP      0.5   0.64849 -0.14849
  0.1      DCP      0.5   0.64849 -0.14849
  0.3      DCP      1.8   1.77231  0.02769
  0.3      DCP      2.3   1.77231  0.52769
  1.0      DCP      4.4   4.28014  0.11986
  1.0      DCP      3.6   4.28014 -0.68014
  3.0      DCP      4.8   5.28840 -0.48840
  3.0      DCP      4.3   5.28840 -0.98840
  7.0      DCP      3.3   2.40033  0.89967
  7.0      DCP      3.7   2.40033  1.29967
 10.0      DCP      1.7   1.10760  0.59240
 10.0      DCP      2.3   1.10760  1.19240
 17.0      DCP      0.5   0.16650  0.33350
  0.3      DCA      0.5   0.17845  0.32155
  0.3      DCA      0.5   0.17845  0.32155
  1.0      DCA      3.9   1.47147  2.42853
  1.0      DCA      2.9   1.47147  1.42853
  3.0      DCA      6.3   5.75039  0.54961
  3.0      DCA      5.4   5.75039 -0.35039
  7.0      DCA      5.7   6.33707 -0.63707
  7.0      DCA      5.5   6.33707 -0.83707
 10.0      DCA      4.5   4.11064  0.38936
 10.0      DCA      4.2   4.11064  0.08936
 17.0      DCA      3.0   0.93095  2.06905
 26.0      DCA      1.5   0.09860  1.40140
```

Listing 27: SFO-SFO(ns)-SFO fit to Site E1 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:40 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1436 model solutions performed in 1.477 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
D24_0        100.5500  state
k_D24          0.1000 deparm
k_DCP          0.1001 deparm
k_DCA          0.1002 deparm
f_D24_to_DCP   0.5000 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
D24_0        100.550000  -Inf   Inf
log_k_D24     -2.302585  -Inf   Inf
log_k_DCP     -2.301586  -Inf   Inf
log_k_DCA     -2.300587  -Inf   Inf
f_D24_qlogis   0.000000  -Inf   Inf
sigma_low      0.100000     0   Inf
rsd_high       0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  179.7071 191.7021 -82.85355

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower      Upper
D24_0        96.64000    2.45600 91.65000 101.600000
log_k_D24    -1.29700    0.03538 -1.36900  -1.225000
log_k_DCP    -0.40970    0.20000 -0.81620  -0.003289
log_k_DCA    -1.03700    0.20000 -1.44300  -0.630400
f_D24_qlogis -1.06100    0.19830 -1.46400  -0.657700
sigma_low     1.24500    0.19370  0.85150   1.639000
rsd_high      0.06861    0.02143  0.02506   0.112200

Parameter correlation:
               D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis sigma_low
```

```
D24_0         1.00000    0.5430  -0.06391  -0.09000     -0.30325   0.11437
log_k_D24     0.54296    1.0000  -0.11848  -0.16618     -0.33497   0.24031
log_k_DCP    -0.06391   -0.1185   1.00000   0.47824      0.58104  -0.01424
log_k_DCA    -0.09000   -0.1662   0.47824   1.00000      0.79000  -0.03194
f_D24_qlogis -0.30325   -0.3350   0.58104   0.79000      1.00000  -0.08327
sigma_low     0.11437    0.2403  -0.01424  -0.03194     -0.08327   1.00000
rsd_high     -0.20412   -0.3176   0.01884   0.04224      0.11001  -0.40613
             rsd_high
D24_0        -0.20412
log_k_D24    -0.31761
log_k_DCP     0.01884
log_k_DCA     0.04224
f_D24_qlogis  0.11001
sigma_low    -0.40613
rsd_high      1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower    Upper
D24_0        96.64000  39.350 3.052e-30 91.65000 101.6000
k_D24         0.27340  28.270 1.680e-25  0.25450   0.2938
k_DCP         0.66380   5.000 8.589e-06  0.44210   0.9967
k_DCA         0.35460   5.000 8.577e-06  0.23620   0.5324
f_D24_to_DCP  0.25720   6.787 4.169e-08  0.18790   0.3413
sigma_low     1.24500   6.429 1.202e-07  0.85150   1.6390
rsd_high      0.06861   3.202 1.480e-03  0.02506   0.1122

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  10.127       5 18
D24        5.872       2  7
DCP       20.733       2  5
DCA       26.637       1  6

Resulting formation fractions:
             ff
D24_DCP  0.2572
D24_sink 0.7428

Estimated disappearance times:
     DT50  DT90
D24 2.535 8.421
DCP 1.044 3.469
DCA 1.955 6.494

Data:
 time variable observed predicted residual
  0.0      D24    100.2  96.64414  3.55586
  0.0      D24    100.9  96.64414  4.25586
  0.1      D24     97.9  94.03739  3.86261
  0.1      D24     98.3  94.03739  4.26261
  0.3      D24     92.4  89.03292  3.36708
  0.3      D24     91.9  89.03292  2.86708
  1.0      D24     65.8  73.52343 -7.72343
  1.0      D24     69.5  73.52343 -4.02343
  3.0      D24     37.5  42.55262 -5.05262
  3.0      D24     40.0  42.55262 -2.55262
  7.0      D24     18.8  14.25369  4.54631
  7.0      D24     14.4  14.25369  0.14631
 10.0      D24      3.3   6.27593 -2.97593
 10.0      D24      5.7   6.27593 -0.57593
 17.0      D24      2.6   0.92561  1.67439
 26.0      D24      2.4   0.07901  2.32099
  0.1      DCP      0.5   0.64849 -0.14849
  0.1      DCP      0.5   0.64849 -0.14849
  0.3      DCP      1.8   1.77231  0.02769
  0.3      DCP      2.3   1.77231  0.52769
```

```
  1.0      DCP      4.4   4.28014  0.11986
  1.0      DCP      3.6   4.28014 -0.68014
  3.0      DCP      4.8   5.28840 -0.48840
  3.0      DCP      4.3   5.28840 -0.98840
  7.0      DCP      3.3   2.40033  0.89967
  7.0      DCP      3.7   2.40033  1.29967
 10.0      DCP      1.7   1.10760  0.59240
 10.0      DCP      2.3   1.10760  1.19240
 17.0      DCP      0.5   0.16650  0.33350
  0.3      DCA      0.5   0.17845  0.32155
  0.3      DCA      0.5   0.17845  0.32155
  1.0      DCA      3.9   1.47147  2.42853
  1.0      DCA      2.9   1.47147  1.42853
  3.0      DCA      6.3   5.75039  0.54961
  3.0      DCA      5.4   5.75039 -0.35039
  7.0      DCA      5.7   6.33707 -0.63707
  7.0      DCA      5.5   6.33707 -0.83707
 10.0      DCA      4.5   4.11064  0.38936
 10.0      DCA      4.2   4.11064  0.08936
 17.0      DCA      3.0   0.93095  2.06905
 26.0      DCA      1.5   0.09860  1.40140
```

Listing 28: SFO-SFO-SFO fit to Site I2 data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:34 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 3877 model solutions performed in 3.64 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.9000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
f_DCP_to_DCA  0.5000 deparm
sigma_D24     3.0000  error
sigma_DCP     3.0000  error
sigma_DCA     3.0000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.900000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
f_DCP_qlogis  0.000000  -Inf   Inf
sigma_D24     3.000000     0   Inf
sigma_DCP     3.000000     0   Inf
sigma_DCA     3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  167.6242 183.2633 -74.81212

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error   Lower    Upper
D24_0        98.08000    1.86400 94.2800 101.9000
log_k_D24    -0.97790    0.06712 -1.1140  -0.8413
log_k_DCP     0.04046    0.23270 -0.4329   0.5138
log_k_DCA    -2.37100    0.16550 -2.7080  -2.0340
f_D24_qlogis -1.40800    0.24720 -1.9110  -0.9047
f_DCP_qlogis -0.02683    0.47490 -0.9930   0.9394
```

```
sigma_D24     4.28900    0.73600  2.7920   5.7860
sigma_DCP     0.73270    0.13860  0.4507   1.0150
sigma_DCA     0.62430    0.13360  0.3524   0.8962

Parameter correlation:
               D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis f_DCP_qlogis
D24_0         1.00000   0.43764 -0.119391 -0.078526     -0.27234     0.105021
log_k_D24     0.43764   1.00000 -0.272804 -0.179428     -0.44550     0.239968
log_k_DCP    -0.11939  -0.27280  1.000000 -0.386811      0.80952    -0.829834
log_k_DCA    -0.07853  -0.17943 -0.386811  1.000000     -0.24397     0.556540
f_D24_qlogis -0.27234  -0.44550  0.809521 -0.243968      1.00000    -0.908460
f_DCP_qlogis  0.10502   0.23997 -0.829834  0.556540     -0.90846     1.000000
sigma_D24     0.01492   0.03408 -0.009298 -0.006116     -0.01518     0.008179
sigma_DCP     0.01786   0.04080 -0.023022 -0.001723     -0.02702     0.019611
sigma_DCA    -0.03856  -0.08812  0.037412  0.009514      0.04920    -0.032190
             sigma_D24 sigma_DCP sigma_DCA
D24_0         0.014919  0.017857 -0.038565
log_k_D24     0.034084  0.040803 -0.088119
log_k_DCP    -0.009298 -0.023022  0.037412
log_k_DCA    -0.006116 -0.001723  0.009514
f_D24_qlogis -0.015185 -0.027016  0.049197
f_DCP_qlogis  0.008179  0.019611 -0.032190
sigma_D24     1.000000  0.001391 -0.003003
sigma_DCP     0.001391  1.000000 -0.003767
sigma_DCA    -0.003003 -0.003767  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower    Upper
D24_0         98.0800  52.610 1.039e-33 94.28000 101.9000
k_D24          0.3761  14.900 1.644e-16  0.32810   0.4311
k_DCP          1.0410   4.298 7.164e-05  0.64860   1.6720
k_DCA          0.0934   6.041 4.275e-07  0.06669   0.1308
f_D24_to_DCP   0.1966   5.034 8.339e-06  0.12890   0.2881
f_DCP_to_DCA   0.4933   4.156 1.080e-04  0.27030   0.7190
sigma_D24      4.2890   5.828 8.015e-07  2.79200   5.7860
sigma_DCP      0.7327   5.287 3.959e-06  0.45070   1.0150
sigma_DCA      0.6243   4.672 2.419e-05  0.35240   0.8962

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.804       6 17
D24        7.504       2  7
DCP       26.259       2  6
DCA       12.900       2  4

Resulting formation fractions:
              ff
D24_DCP  0.1966
D24_sink 0.8034
DCP_DCA  0.4933
DCP_sink 0.5067

Estimated disappearance times:
      DT50   DT90
D24 1.8430  6.122
DCP 0.6657  2.211
DCA 7.4212 24.653

Data:
 time variable observed predicted residual
  0.0      D24     99.0 9.808e+01  0.92325
  0.0      D24     98.8 9.808e+01  0.72325
  0.1      D24     90.1 9.446e+01 -4.35655
  0.1      D24     89.2 9.446e+01 -5.25655
  0.3      D24     86.3 8.761e+01 -1.31211
  0.3      D24     86.5 8.761e+01 -1.11211
```

```
  1.0      D24     76.7 6.733e+01  9.36725
  1.0      D24     74.7 6.733e+01  7.36725
  3.0      D24     33.1 3.174e+01  1.36438
  5.0      D24      8.8 1.496e+01 -6.15780
  5.0      D24      6.7 1.496e+01 -8.25780
 10.0      D24      3.1 2.281e+00  0.81877
 10.0      D24      3.2 2.281e+00  0.91877
 17.0      D24      1.6 1.640e-01  1.43602
 17.0      D24      1.7 1.640e-01  1.53602
 26.0      D24      1.5 5.556e-03  1.49444
 26.0      D24      1.9 5.556e-03  1.89444
  0.1      DCP      0.9 6.757e-01  0.22430
  0.1      DCP      1.2 6.757e-01  0.52430
  0.3      DCP      1.7 1.762e+00 -0.06180
  0.3      DCP      1.3 1.762e+00 -0.46180
  1.0      DCP      2.5 3.636e+00 -1.13618
  1.0      DCP      5.1 3.636e+00  1.46382
  3.0      DCP      2.5 3.048e+00 -0.54814
  5.0      DCP      1.9 1.603e+00  0.29707
  5.0      DCP      1.7 1.603e+00  0.09707
 10.0      DCP      0.5 2.533e-01  0.24675
 10.0      DCP      0.9 2.533e-01  0.64675
 17.0      DCP      0.9 1.823e-02  0.88177
 17.0      DCP      1.2 1.823e-02  1.18177
 26.0      DCP      0.7 6.176e-04  0.69938
  1.0      DCA      0.5 1.147e+00 -0.64746
  1.0      DCA      0.5 1.147e+00 -0.64746
  3.0      DCA      4.5 4.354e+00  0.14592
  5.0      DCA      6.6 5.725e+00  0.87455
  5.0      DCA      5.7 5.725e+00 -0.02545
 10.0      DCA      5.1 5.002e+00  0.09788
 10.0      DCA      4.3 5.002e+00 -0.70212
 17.0      DCA      2.3 2.808e+00 -0.50782
 17.0      DCA      2.2 2.808e+00 -0.60782
 26.0      DCA      2.1 1.225e+00  0.87540
 26.0      DCA      2.1 1.225e+00  0.87540
```

Listing 29: SFO-SFO(ns)-SFO fit to Site I2 data, variance by variable

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:33 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1587 model solutions performed in 1.557 s

Error model: Variance unique to each observed variable

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.9000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
sigma_D24     3.0000  error
sigma_DCP     3.0000  error
sigma_DCA     3.0000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.900000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
sigma_D24     3.000000     0   Inf
sigma_DCP     3.000000     0   Inf
sigma_DCA     3.000000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  172.2067 186.1081 -78.10336

Optimised, transformed parameters with symmetric confidence intervals:
            Estimate Std. Error   Lower    Upper
D24_0         98.3800    1.88800 94.5400 102.2000
log_k_D24     -0.9532    0.06953 -1.0940  -0.8119
log_k_DCP     -0.4731    0.14330 -0.7643  -0.1818
log_k_DCA     -2.0670    0.16300 -2.3980  -1.7360
f_D24_qlogis  -1.9990    0.11750 -2.2380  -1.7610
sigma_D24      4.3150    0.74970  2.7910   5.8390
sigma_DCP      0.8468    0.16570  0.5100   1.1840
sigma_DCA      0.6939    0.15520  0.3786   1.0090
```

```
Parameter correlation:
               D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis sigma_D24
D24_0         1.00000    0.4443  -0.06860  -0.14068      -0.3516   0.07139
log_k_D24     0.44429    1.0000  -0.15440  -0.31665      -0.4562   0.16069
log_k_DCP    -0.06860   -0.1544   1.00000  -0.10310      -0.0927  -0.02481
log_k_DCA    -0.14068   -0.3167  -0.10310   1.00000       0.8205  -0.05088
f_D24_qlogis -0.35155   -0.4562  -0.09270   0.82049       1.0000  -0.07330
sigma_D24     0.07139    0.1607  -0.02481  -0.05088      -0.0733   1.00000
sigma_DCP    -0.03110   -0.0700   0.08791  -0.16990      -0.1849  -0.01125
sigma_DCA    -0.05110   -0.1150  -0.06812   0.25036       0.2940  -0.01848
             sigma_DCP sigma_DCA
D24_0         -0.03110  -0.05110
log_k_D24     -0.07000  -0.11502
log_k_DCP      0.08791  -0.06812
log_k_DCA     -0.16990   0.25036
f_D24_qlogis  -0.18492   0.29402
sigma_D24     -0.01125  -0.01848
sigma_DCP      1.00000  -0.06161
sigma_DCA     -0.06161   1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower    Upper
D24_0         98.3800  52.100 2.546e-34 94.54000 102.2000
k_D24          0.3855  14.380 2.560e-16  0.33470   0.4440
k_DCP          0.6231   6.977 2.389e-08  0.46560   0.8338
k_DCA          0.1265   6.136 2.872e-07  0.09086   0.1762
f_D24_to_DCP   0.1193   9.664 1.388e-11  0.09638   0.1467
sigma_D24      4.3150   5.755 8.957e-07  2.79100   5.8390
sigma_DCP      0.8468   5.110 6.185e-06  0.51000   1.1840
sigma_DCA      0.6939   4.472 4.104e-05  0.37860   1.0090

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.714       5 18
D24        7.583       2  7
DCP       32.617       2  6
DCA       13.568       1  5

Resulting formation fractions:
              ff
D24_DCP  0.1193
D24_sink 0.8807

Estimated disappearance times:
     DT50   DT90
D24 1.798  5.973
DCP 1.112  3.695
DCA 5.478 18.197

Data:
 time variable observed predicted residual
  0.0      D24     99.0 9.838e+01  0.62398
  0.0      D24     98.8 9.838e+01  0.42398
  0.1      D24     90.1 9.466e+01 -4.55566
  0.1      D24     89.2 9.466e+01 -5.45566
  0.3      D24     86.3 8.763e+01 -1.33171
  0.3      D24     86.5 8.763e+01 -1.13171
  1.0      D24     76.7 6.691e+01  9.79437
  1.0      D24     74.7 6.691e+01  7.79437
  3.0      D24     33.1 3.095e+01  2.15365
  5.0      D24      8.8 1.431e+01 -5.51384
  5.0      D24      6.7 1.431e+01 -7.61384
 10.0      D24      3.1 2.083e+00  1.01732
 10.0      D24      3.2 2.083e+00  1.11732
 17.0      D24      1.6 1.402e-01  1.45984
```

```
 17.0      D24      1.7 1.402e-01  1.55984
 26.0      D24      1.5 4.363e-03  1.49564
 26.0      D24      1.9 4.363e-03  1.89564
  0.1      DCP      0.9 4.301e-01  0.46991
  0.1      DCP      1.2 4.301e-01  0.76991
  0.3      DCP      1.7 1.167e+00  0.53330
  0.3      DCP      1.3 1.167e+00  0.13330
  1.0      DCP      2.5 2.738e+00 -0.23814
  1.0      DCP      5.1 2.738e+00  2.36186
  3.0      DCP      2.5 3.053e+00 -0.55264
  5.0      DCP      1.9 1.926e+00 -0.02566
  5.0      DCP      1.7 1.926e+00 -0.22566
 10.0      DCP      0.5 3.656e-01  0.13440
 10.0      DCP      0.9 3.656e-01  0.53440
 17.0      DCP      0.9 2.665e-02  0.87335
 17.0      DCP      1.2 2.665e-02  1.17335
 26.0      DCP      0.7 8.426e-04  0.69916
  1.0      DCA      0.5 9.702e-01 -0.47025
  1.0      DCA      0.5 9.702e-01 -0.47025
  3.0      DCA      4.5 4.269e+00  0.23111
  5.0      DCA      6.6 6.036e+00  0.56389
  5.0      DCA      5.7 6.036e+00 -0.33611
 10.0      DCA      5.1 5.261e+00 -0.16080
 10.0      DCA      4.3 5.261e+00 -0.96080
 17.0      DCA      2.3 2.485e+00 -0.18550
 17.0      DCA      2.2 2.485e+00 -0.28550
 26.0      DCA      2.1 8.145e-01  1.28546
 26.0      DCA      2.1 8.145e-01  1.28546
```

Listing 30: SFO-SFO-SFO fit to Site I2 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:41 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1585 model solutions performed in 1.417 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.9000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
f_DCP_to_DCA  0.5000 deparm
sigma_low     0.1000  error
rsd_high      0.1000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.900000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
f_DCP_qlogis  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  183.2611 197.1625 -83.63056

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
D24_0        99.63000    6.34600 86.73000 112.5000
log_k_D24    -0.84600    0.09454 -1.03800  -0.6539
log_k_DCP    -0.09161    0.34640 -0.79560   0.6123
log_k_DCA    -2.46900    0.28460 -3.04700  -1.8900
f_D24_qlogis -1.62300    0.36320 -2.36100  -0.8851
f_DCP_qlogis  0.14060    0.79990 -1.48500   1.7660
sigma_low     1.00000    0.16320  0.66850   1.3320
rsd_high      0.13750    0.03978  0.05669   0.2184
```

```
Parameter correlation:
               D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis f_DCP_qlogis
D24_0         1.00000   0.74432   -0.1985  -0.01707      -0.4769       0.2104
log_k_D24     0.74432   1.00000   -0.2677  -0.03197      -0.5168       0.2777
log_k_DCP    -0.19846  -0.26774    1.0000  -0.38978       0.7818      -0.8082
log_k_DCA    -0.01707  -0.03197   -0.3898   1.00000      -0.2611       0.5915
f_D24_qlogis -0.47690  -0.51684    0.7818  -0.26110       1.0000      -0.8713
f_DCP_qlogis  0.21039   0.27767   -0.8082   0.59151      -0.8713       1.0000
sigma_low     0.35330   0.46788   -0.1190   0.03394      -0.2478       0.1564
rsd_high     -0.50806  -0.56916    0.1451  -0.04139       0.3018      -0.1908
             sigma_low rsd_high
D24_0          0.35330 -0.50806
log_k_D24      0.46788 -0.56916
log_k_DCP     -0.11896  0.14505
log_k_DCA      0.03394 -0.04139
f_D24_qlogis  -0.24775  0.30176
f_DCP_qlogis   0.15643 -0.19079
sigma_low      1.00000 -0.42925
rsd_high      -0.42925  1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower    Upper
D24_0        99.63000  15.700 1.898e-17 86.73000 112.5000
k_D24         0.42910  10.580 1.358e-12  0.35410   0.5200
k_DCP         0.91250   2.887 3.358e-03  0.45130   1.8450
k_DCA         0.08469   3.513 6.366e-04  0.04749   0.1510
f_D24_to_DCP  0.16480   3.296 1.150e-03  0.08616   0.2921
f_DCP_to_DCA  0.53510   2.689 5.512e-03  0.18470   0.8540
sigma_low     1.00000   6.129 2.926e-07  0.66850   1.3320
rsd_high      0.13750   3.458 7.421e-04  0.05669   0.2184

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  14.794       6 17
D24        8.698       2  7
DCP       26.949       2  6
DCA       12.709       2  4

Resulting formation fractions:
             ff
D24_DCP  0.1648
D24_sink 0.8352
DCP_DCA  0.5351
DCP_sink 0.4649

Estimated disappearance times:
      DT50   DT90
D24 1.6152  5.366
DCP 0.7596  2.523
DCA 8.1846 27.189

Data:
 time variable observed predicted residual
  0.0      D24     99.0 9.963e+01 -0.62996
  0.0      D24     98.8 9.963e+01 -0.82996
  0.1      D24     90.1 9.544e+01 -5.34496
  0.1      D24     89.2 9.544e+01 -6.24496
  0.3      D24     86.3 8.759e+01 -1.29494
  0.3      D24     86.5 8.759e+01 -1.09494
  1.0      D24     76.7 6.487e+01 11.83354
  1.0      D24     74.7 6.487e+01  9.83354
  3.0      D24     33.1 2.750e+01  5.60329
  5.0      D24      8.8 1.166e+01 -2.85578
  5.0      D24      6.7 1.166e+01 -4.95578
 10.0      D24      3.1 1.364e+00  1.73638
```

```
 10.0      D24      3.2 1.364e+00  1.83638
 17.0      D24      1.6 6.762e-02  1.53238
 17.0      D24      1.7 6.762e-02  1.63238
 26.0      D24      1.5 1.422e-03  1.49858
 26.0      D24      1.9 1.422e-03  1.89858
  0.1      DCP      0.9 6.587e-01  0.24125
  0.1      DCP      1.2 6.587e-01  0.54125
  0.3      DCP      1.7 1.729e+00 -0.02947
  0.3      DCP      1.3 1.729e+00 -0.42947
  1.0      DCP      2.5 3.637e+00 -1.13666
  1.0      DCP      5.1 3.637e+00  1.46334
  3.0      DCP      2.5 3.079e+00 -0.57864
  5.0      DCP      1.9 1.553e+00  0.34716
  5.0      DCP      1.7 1.553e+00  0.14716
 10.0      DCP      0.5 1.979e-01  0.30212
 10.0      DCP      0.9 1.979e-01  0.70212
 17.0      DCP      0.9 9.889e-03  0.89011
 17.0      DCP      1.2 9.889e-03  1.19011
 26.0      DCP      0.7 2.079e-04  0.69979
  1.0      DCA      0.5 1.084e+00 -0.58426
  1.0      DCA      0.5 1.084e+00 -0.58426
  3.0      DCA      4.5 4.211e+00  0.28910
  5.0      DCA      6.6 5.571e+00  1.02904
  5.0      DCA      5.7 5.571e+00  0.12904
 10.0      DCA      5.1 4.890e+00  0.21030
 10.0      DCA      4.3 4.890e+00 -0.58970
 17.0      DCA      2.3 2.845e+00 -0.54459
 17.0      DCA      2.2 2.845e+00 -0.64459
 26.0      DCA      2.1 1.334e+00  0.76636
 26.0      DCA      2.1 1.334e+00  0.76636
```

Listing 31: SFO-SFO(ns)-SFO fit to Site I2 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 12:18:41 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Model predictions using solution type deSolve

Fitted using 1467 model solutions performed in 1.364 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
               value   type
D24_0        98.9000  state
k_D24         0.1000 deparm
k_DCP         0.1001 deparm
k_DCA         0.1002 deparm
f_D24_to_DCP  0.5000 deparm
sigma_low     0.1000  error
rsd_high      0.1000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
D24_0        98.900000  -Inf   Inf
log_k_D24    -2.302585  -Inf   Inf
log_k_DCP    -2.301586  -Inf   Inf
log_k_DCA    -2.300587  -Inf   Inf
f_D24_qlogis  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state


Warning(s):
Observations with value of zero were removed from the data

Results:

       AIC      BIC    logLik
  183.6597 195.8234 -84.82987

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
D24_0        101.1000    5.47500 90.00000 112.2000
log_k_D24     -0.8175    0.06878 -0.95710  -0.6779
log_k_DCP     -0.5396    0.20290 -0.95150  -0.1277
log_k_DCA     -2.1610    0.23340 -2.63500  -1.6870
f_D24_qlogis  -2.1050    0.16620 -2.44300  -1.7680
sigma_low      1.0680    0.15350  0.75620   1.3790
rsd_high       0.1303    0.03278  0.06373   0.1968

Parameter correlation:
              D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis sigma_low
```

```
D24_0         1.0000   0.65912  -0.05990 -0.109501     -0.50246  0.139785
log_k_D24     0.6591   1.00000  -0.09873 -0.176886     -0.45925  0.180166
log_k_DCP    -0.0599  -0.09873   1.00000  0.051417      0.10586  0.011204
log_k_DCA    -0.1095  -0.17689   0.05142  1.000000      0.67609  0.008297
f_D24_qlogis -0.5025  -0.45925   0.10586  0.676087      1.00000 -0.079877
sigma_low     0.1398   0.18017   0.01120  0.008297     -0.07988  1.000000
rsd_high     -0.2882  -0.24193  -0.01513 -0.010664      0.10727 -0.249670
             rsd_high
D24_0        -0.28818
log_k_D24    -0.24193
log_k_DCP    -0.01513
log_k_DCA    -0.01066
f_D24_qlogis  0.10727
sigma_low    -0.24967
rsd_high      1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value    Pr(>t)    Lower    Upper
D24_0        101.1000  18.470 6.308e-20 90.00000 112.2000
k_D24          0.4415  14.540 1.059e-16  0.38400   0.5077
k_DCP          0.5830   4.929 9.942e-06  0.38620   0.8801
k_DCA          0.1152   4.284 6.817e-05  0.07172   0.1851
f_D24_to_DCP   0.1086   6.750 4.024e-08  0.07998   0.1458
sigma_low      1.0680   6.956 2.174e-08  0.75620   1.3790
rsd_high       0.1303   3.974 1.681e-04  0.06373   0.1968

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  15.329       5 18
D24        9.205       2  7
DCP       31.504       2  6
DCA       12.887       1  5

Resulting formation fractions:
             ff
D24_DCP  0.1086
D24_sink 0.8914

Estimated disappearance times:
     DT50   DT90
D24 1.570  5.215
DCP 1.189  3.950
DCA 6.016 19.986

Data:
 time variable observed predicted residual
  0.0      D24     99.0 1.011e+02 -2.11594
  0.0      D24     98.8 1.011e+02 -2.31594
  0.1      D24     90.1 9.675e+01 -6.64842
  0.1      D24     89.2 9.675e+01 -7.54842
  0.3      D24     86.3 8.857e+01 -2.27117
  0.3      D24     86.5 8.857e+01 -2.07117
  1.0      D24     76.7 6.502e+01 11.67771
  1.0      D24     74.7 6.502e+01  9.67771
  3.0      D24     33.1 2.689e+01  6.21268
  5.0      D24      8.8 1.112e+01 -2.31816
  5.0      D24      6.7 1.112e+01 -4.41816
 10.0      D24      3.1 1.222e+00  1.87751
 10.0      D24      3.2 1.222e+00  1.97751
 17.0      D24      1.6 5.558e-02  1.54442
 17.0      D24      1.7 5.558e-02  1.64442
 26.0      D24      1.5 1.045e-03  1.49895
 26.0      D24      1.9 1.045e-03  1.89895
  0.1      DCP      0.9 4.606e-01  0.43940
  0.1      DCP      1.2 4.606e-01  0.73940
  0.3      DCP      1.7 1.247e+00  0.45268
```

```
  0.3      DCP      1.3 1.247e+00  0.05268
  1.0      DCP      2.5 2.907e+00 -0.40708
  1.0      DCP      5.1 2.907e+00  2.19292
  3.0      DCP      2.5 3.152e+00 -0.65159
  5.0      DCP      1.9 1.911e+00 -0.01073
  5.0      DCP      1.7 1.911e+00 -0.21073
 10.0      DCP      0.5 3.137e-01  0.18632
 10.0      DCP      0.9 3.137e-01  0.58632
 17.0      DCP      0.9 1.714e-02  0.88286
 17.0      DCP      1.2 1.714e-02  1.18286
 26.0      DCP      0.7 3.453e-04  0.69965
  1.0      DCA      0.5 9.712e-01 -0.47117
  1.0      DCA      0.5 9.712e-01 -0.47117
  3.0      DCA      4.5 4.254e+00  0.24646
  5.0      DCA      6.6 5.991e+00  0.60940
  5.0      DCA      5.7 5.991e+00 -0.29060
 10.0      DCA      5.1 5.236e+00 -0.13563
 10.0      DCA      4.3 5.236e+00 -0.93563
 17.0      DCA      2.3 2.580e+00 -0.28030
 17.0      DCA      2.2 2.580e+00 -0.38030
 26.0      DCA      2.1 9.254e-01  1.17456
 26.0      DCA      2.1 9.254e-01  1.17456
```

Listings for simultaneous pathway fits for 2,4-D

Listing 32: SFO-SFO-SFO fit with nlme to 2,4-D data, two-component error

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:21:13 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Data:
173 observations of 3 variable(s) grouped in 5 datasets

Model predictions using solution type deSolve

Fitted in 78.455 s using 12 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
       D24_0    log_k_D24    log_k_DCP    log_k_DCA f_D24_qlogis f_DCP_qlogis
     95.5434      -1.8227      -0.6325      -5.7005      -0.6040       7.3117

Fixed degradation parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state

Results:

    AIC   BIC logLik
  923.8 967.9 -447.9

Optimised, transformed parameters with symmetric confidence intervals:
               lower    est.    upper
D24_0        93.5213 97.3111 101.1010
log_k_D24    -3.1555 -1.7827  -0.4100
log_k_DCP    -0.8418 -0.1025   0.6367
log_k_DCA    -3.8434 -2.4736  -1.1038
f_D24_qlogis -1.1751 -0.7874  -0.3998
f_DCP_qlogis -0.9104 -0.1960   0.5184

Correlation:
             D24_0  l__D24 l__DCP l__DCA f_D24_
log_k_D24     0.024
log_k_DCP    -0.043 -0.003
log_k_DCA    -0.005  0.000 -0.047
f_D24_qlogis -0.292 -0.013  0.389 -0.076
f_DCP_qlogis  0.077  0.005 -0.379  0.209 -0.853

Random effects:
 Formula: list(D24_0 ~ 1, log_k_D24 ~ 1, log_k_DCP ~ 1, log_k_DCA ~ 1,      f_D24_qlogis ~ 1, f_DCP_qlogis ~ 1)
 Level: ds
 Structure: Diagonal
            D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis f_DCP_qlogis
StdDev: 0.0009423     1.553    0.6607     1.165    4.726e-07     2.65e-05
        Residual
StdDev:        1

Variance function:
 Structure: Constant plus proportion of variance covariate
 Formula: ~fitted(.)
 Parameter estimates:
```

```
    const      prop
1.6146751 0.1165276

Backtransformed parameters with asymmetric confidence intervals:
                lower     est.    upper
D24_0        93.52130 97.31115 101.1010
k_D24         0.04262  0.16818   0.6636
k_DCP         0.43094  0.90255   1.8903
k_DCA         0.02142  0.08428   0.3316
f_D24_to_DCP  0.23594  0.31272   0.4014
f_DCP_to_DCA  0.28692  0.45116   0.6268

Resulting formation fractions:
             ff
D24_DCP  0.3127
D24_sink 0.6873
DCP_DCA  0.4512
DCP_sink 0.5488

Estimated disappearance times:
     DT50   DT90
D24 4.122 13.691
DCP 0.768  2.551
DCA 8.225 27.321
```

Listing 33: SFO-SFO(ns)-SFO fit with nlme to 2,4-D data, constant variance

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:19:30 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Data:
173 observations of 3 variable(s) grouped in 5 datasets

Model predictions using solution type deSolve

Fitted in 1.05 s using 3 iterations

Variance model: Constant variance

Mean of starting values for individual parameters:
       D24_0    log_k_D24    log_k_DCP    log_k_DCA f_D24_qlogis
     95.7003      -1.8362      -0.9675      -2.4067      -1.0655

Fixed degradation parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state

Results:

    AIC  BIC logLik
  989.4 1024 -483.7

Optimised, transformed parameters with symmetric confidence intervals:
              lower    est.   upper
D24_0        92.757 95.8296 98.9019
log_k_D24    -3.257 -1.8313 -0.4055
log_k_DCP    -1.147 -0.8142 -0.4819
log_k_DCA    -2.339 -1.8816 -1.4237
f_D24_qlogis -2.007 -1.4061 -0.8047

Correlation:
             D24_0  l__D24 l__DCP l__DCA
log_k_D24     0.008
log_k_DCP    -0.010 -0.002
log_k_DCA    -0.014 -0.002  0.242
f_D24_qlogis -0.024 -0.003  0.128  0.335

Random effects:
 Formula: list(D24_0 ~ 1, log_k_D24 ~ 1, log_k_DCP ~ 1, log_k_DCA ~ 1,      f_D24_qlogis ~ 1)
 Level: ds
 Structure: Diagonal
        D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis Residual
StdDev: 3.139     1.614  0.004861  0.004537       0.5285    3.416


Backtransformed parameters with asymmetric confidence intervals:
               lower    est.   upper
D24_0        92.75736 95.8296 98.9019
k_D24         0.03850  0.1602  0.6666
k_DCP         0.31774  0.4430  0.6176
k_DCA         0.09638  0.1524  0.2408
f_D24_to_DCP  0.11843  0.1969  0.3090
```

```
Resulting formation fractions:
             ff
D24_DCP  0.1969
D24_sink 0.8031

Estimated disappearance times:
     DT50   DT90
D24 4.327 14.373
DCP 1.565  5.198
DCA 4.550 15.114
```

Listing 34: SFO-SFO(ns)-SFO fit with nlme to 2,4-D data, variance by variable

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:19:53 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Data:
173 observations of 3 variable(s) grouped in 5 datasets

Model predictions using solution type deSolve

Fitted in 21.734 s using 4 iterations

Variance model: Variance unique to each observed variable

Mean of starting values for individual parameters:
       D24_0    log_k_D24    log_k_DCP    log_k_DCA f_D24_qlogis
      95.736       -1.833       -1.020       -2.250       -1.121

Fixed degradation parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state

Results:

    AIC   BIC logLik
  883.8 924.8 -428.9

Optimised, transformed parameters with symmetric confidence intervals:
              lower    est.   upper
D24_0        93.642 96.2869 98.9317
log_k_D24    -3.232 -1.8047 -0.3778
log_k_DCP    -1.158 -0.6482 -0.1384
log_k_DCA    -2.938 -1.9624 -0.9865
f_D24_qlogis -1.708 -1.3208 -0.9332

Correlation:
             D24_0  l__D24 l__DCP l__DCA
log_k_D24     0.018
log_k_DCP    -0.017 -0.002
log_k_DCA    -0.022 -0.003  0.036
f_D24_qlogis -0.098 -0.009  0.035  0.085

Random effects:
 Formula: list(D24_0 ~ 1, log_k_D24 ~ 1, log_k_DCP ~ 1, log_k_DCA ~ 1,      f_D24_qlogis ~ 1)
 Level: ds
 Structure: Diagonal
        D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis Residual
StdDev: 2.026     1.614    0.4922    0.9118       0.3625    5.057

Variance function:
 Structure: Different standard deviations per stratum
 Formula: ~1 | name
 Parameter estimates:
      D24       DCP       DCA
1.0000000 0.2646706 0.2582146

Backtransformed parameters with asymmetric confidence intervals:
               lower    est.   upper
```

```
D24_0        93.64207 96.2869 98.9317
k_D24         0.03949  0.1645  0.6854
k_DCP         0.31415  0.5230  0.8707
k_DCA         0.05296  0.1405  0.3729
f_D24_to_DCP  0.15338  0.2107  0.2823

Resulting formation fractions:
             ff
D24_DCP  0.2107
D24_sink 0.7893

Estimated disappearance times:
     DT50   DT90
D24 4.213 13.995
DCP 1.325  4.403
DCA 4.933 16.386
```

Listing 35: SFO-SFO(ns)-SFO fit with nlme to 2,4-D data, two-component error

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 12:21:52 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Data:
173 observations of 3 variable(s) grouped in 5 datasets

Model predictions using solution type deSolve

Fitted in 37.657 s using 7 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
       D24_0    log_k_D24    log_k_DCP    log_k_DCA f_D24_qlogis
     96.0951      -1.8068      -0.9738      -5.5774      -1.0841

Fixed degradation parameter values:
      value  type
DCP_0     0 state
DCA_0     0 state

Results:

    AIC   BIC logLik
  916.3 954.1 -446.1

Optimised, transformed parameters with symmetric confidence intervals:
              lower    est.    upper
D24_0        93.746 97.8594 101.9725
log_k_D24    -3.143 -1.7675  -0.3921
log_k_DCP    -1.223 -0.6892  -0.1552
log_k_DCA    -2.856 -1.9334  -1.0110
f_D24_qlogis -1.753 -1.3758  -0.9987

Correlation:
             D24_0  l__D24 l__DCP l__DCA
log_k_D24     0.022
log_k_DCP    -0.019 -0.001
log_k_DCA    -0.025 -0.002  0.046
f_D24_qlogis -0.177 -0.007  0.047  0.110

Random effects:
 Formula: list(D24_0 ~ 1, log_k_D24 ~ 1, log_k_DCP ~ 1, log_k_DCA ~ 1,      f_D24_qlogis ~ 1)
 Level: ds
 Structure: Diagonal
        D24_0 log_k_D24 log_k_DCP log_k_DCA f_D24_qlogis Residual
StdDev: 1.803     1.556    0.5081    0.8317       0.3397        1

Variance function:
 Structure: Constant plus proportion of variance covariate
 Formula: ~fitted(.)
 Parameter estimates:
    const      prop
1.5195327 0.1160781

Backtransformed parameters with asymmetric confidence intervals:
               lower    est.    upper
```

```
D24_0        93.74617 97.8594 101.9725
k_D24         0.04316  0.1708   0.6756
k_DCP         0.29430  0.5020   0.8563
k_DCA         0.05752  0.1447   0.3638
f_D24_to_DCP  0.14767  0.2017   0.2692

Resulting formation fractions:
             ff
D24_DCP  0.2017
D24_sink 0.7983

Estimated disappearance times:
     DT50   DT90
D24 4.059 13.484
DCP 1.381  4.587
DCA 4.792 15.917
```

Listing 36: SFO-SFO-SFO fit with saem to 2,4-D data, two-component error

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 13:17:34 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + f_DCP_to_DCA * k_DCP * DCP - k_DCA * DCA

Data:
173 observations of 3 variable(s) grouped in 5 datasets

Model predictions using solution type deSolve

Fitted in 609.293 s using 300, 100 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
       D24_0    log_k_D24    log_k_DCP    log_k_DCA f_D24_qlogis f_DCP_qlogis
     95.5434      -1.8227      -0.2152      -1.8401      -0.6040       7.3117

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
    AIC   BIC logLik
  907.5 902.1 -439.8

Optimised parameters:
                est.   lower    upper
D24_0        96.3401 92.2207 100.4595
log_k_D24    -1.8115 -3.1745  -0.4486
log_k_DCP    -0.1987 -0.9712   0.5738
log_k_DCA    -2.2408 -3.2736  -1.2080
f_D24_qlogis -0.8446 -1.5735  -0.1157
f_DCP_qlogis  1.0715 -1.3647   3.5077

Correlation:
             D24_0  l__D24 l__DCP l__DCA f_D24_
log_k_D24     0.021
log_k_DCP    -0.026 -0.002
log_k_DCA    -0.016 -0.001 -0.024
f_D24_qlogis -0.127 -0.006  0.122 -0.015
f_DCP_qlogis  0.031  0.002 -0.169  0.139 -0.212

Random effects:
                  est.   lower upper
SD.D24_0        2.1341 -4.2764 8.545
SD.log_k_D24    1.5537  0.5896 2.518
SD.log_k_DCP    0.7366  0.1742 1.299
SD.log_k_DCA    0.9320  0.1577 1.706
SD.f_D24_qlogis 0.6635  0.1256 1.201
SD.f_DCP_qlogis 1.7360 -0.1656 3.637

Variance model:
      est.   lower  upper
a.1 1.3311 1.12223 1.5399
b.1 0.1158 0.09227 0.1394

Backtransformed parameters:
```

```
                 est.    lower    upper
D24_0        96.3401 92.22072 100.4595
k_D24         0.1634  0.04182   0.6385
k_DCP         0.8198  0.37861   1.7750
k_DCA         0.1064  0.03787   0.2988
f_D24_to_DCP  0.3006  0.17171   0.4711
f_DCP_to_DCA  0.7449  0.20348   0.9709

Resulting formation fractions:
             ff
D24_DCP  0.3006
D24_sink 0.6994
DCP_DCA  0.7449
DCP_sink 0.2551

Estimated disappearance times:
      DT50   DT90
D24 4.2420 14.092
DCP 0.8455  2.809
DCA 6.5161 21.646
```

Listing 37: SFO-SFO(ns)-SFO fit with saem to 2,4-D data, constant variance

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 13:54:57 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Data:
173 observations of 3 variable(s) grouped in 5 datasets

Model predictions using solution type deSolve

Fitted in 499.986 s using 300, 100 iterations

Variance model: Constant variance

Mean of starting values for individual parameters:
       D24_0    log_k_D24    log_k_DCP    log_k_DCA f_D24_qlogis
     95.7003      -1.8362      -0.6339      -1.4936      -1.0655

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
    AIC   BIC logLik
  989.8 985.5 -483.9

Optimised parameters:
                est.  lower   upper
D24_0        95.7626 92.671 98.8545
log_k_D24    -1.8330 -3.250 -0.4165
log_k_DCP    -0.7683 -1.195 -0.3416
log_k_DCA    -1.9522 -2.594 -1.3100
f_D24_qlogis -1.4550 -2.038 -0.8723

Correlation:
             D24_0  l__D24 l__DCP l__DCA
log_k_D24     0.007
log_k_DCP    -0.007 -0.001
log_k_DCA    -0.010 -0.002  0.165
f_D24_qlogis -0.024 -0.003  0.105  0.301

Random effects:
                  est.    lower  upper
SD.D24_0        3.1955  0.78394 5.6070
SD.log_k_D24    1.6151  0.61291 2.6173
SD.log_k_DCP    0.2440 -0.25809 0.7461
SD.log_k_DCA    0.3819 -0.27626 1.0401
SD.f_D24_qlogis 0.5044  0.06366 0.9452

Variance model:
     est. lower upper
a.1 3.399 3.018 3.781

Backtransformed parameters:
                est.    lower   upper
D24_0        95.7626 92.67063 98.8545
k_D24         0.1599  0.03879  0.6594
k_DCP         0.4638  0.30270  0.7106
```

```
k_DCA         0.1420  0.07468  0.2698
f_D24_to_DCP  0.1892  0.11530  0.2948

Resulting formation fractions:
             ff
D24_DCP  0.1892
D24_sink 0.8108

Estimated disappearance times:
     DT50   DT90
D24 4.334 14.397
DCP 1.495  4.965
DCA 4.883 16.220
```

Listing 38: SFO-SFO(ns)-SFO fit with saem to 2,4-D data, two-component error

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 14:03:27 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_D24/dt = - k_D24 * D24
d_DCP/dt = + f_D24_to_DCP * k_D24 * D24 - k_DCP * DCP
d_DCA/dt = + k_DCP * DCP - k_DCA * DCA

Data:
173 observations of 3 variable(s) grouped in 5 datasets

Model predictions using solution type deSolve

Fitted in 510.096 s using 300, 100 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
       D24_0    log_k_D24    log_k_DCP    log_k_DCA f_D24_qlogis
     96.0951      -1.8068      -0.6419      -1.4862      -1.0841

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
    AIC   BIC logLik
  913.3 908.6 -444.7

Optimised parameters:
                est.  lower    upper
D24_0        96.4208 92.034 100.8074
log_k_D24    -1.8016 -3.172  -0.4315
log_k_DCP    -0.6535 -1.153  -0.1545
log_k_DCA    -1.9422 -2.869  -1.0157
f_D24_qlogis -1.3374 -1.762  -0.9131

Correlation:
             D24_0  l__D24 l__DCP l__DCA
log_k_D24     0.019
log_k_DCP    -0.018 -0.001
log_k_DCA    -0.022 -0.002  0.045
f_D24_qlogis -0.137 -0.006  0.044  0.098

Random effects:
                  est.    lower  upper
SD.D24_0        2.8424 -2.58010 8.2648
SD.log_k_D24    1.5618  0.59263 2.5311
SD.log_k_DCP    0.4739  0.09683 0.8509
SD.log_k_DCA    0.8494  0.15353 1.5452
SD.f_D24_qlogis 0.3949  0.07589 0.7139

Variance model:
      est.   lower  upper
a.1 1.5040 1.27670 1.7313
b.1 0.1127 0.08928 0.1362

Backtransformed parameters:
                est.    lower    upper
D24_0        96.4208 92.03423 100.8074
k_D24         0.1650  0.04193   0.6496
```

```
k_DCP         0.5202  0.31582   0.8568
k_DCA         0.1434  0.05678   0.3622
f_D24_to_DCP  0.2079  0.14657   0.2864

Resulting formation fractions:
             ff
D24_DCP  0.2079
D24_sink 0.7921

Estimated disappearance times:
     DT50   DT90
D24 4.200 13.952
DCP 1.332  4.426
DCA 4.834 16.058
```

Listings for separate fits for dimethenamid

Listing 39: SFO-SFO3 fit to Calke data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:04 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1228 model solutions performed in 2.126 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        97.2500  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                value lower upper
DMTA_0       97.250000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  80.95259 90.77197 -31.47629

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower  Upper
DMTA_0        96.7300    0.69360  95.2300 98.230
log_k_DMTA    -3.4760    0.02105  -3.5210 -3.430
log_k_M23     -4.5010    0.30690  -5.1640 -3.838
log_k_M27     -7.7920   11.57000 -32.7800 17.200
log_k_M31     -4.6600    0.84700  -6.4900 -2.830
f_DMTA_ilr_1   0.7229    0.27270   0.1338  1.312
f_DMTA_ilr_2   0.3491    0.37670  -0.4647  1.163
f_DMTA_ilr_3  -2.2510    0.19640  -2.6760 -1.827
sigma          1.0120    0.15250   0.6823  1.341
```

```
Parameter correlation:
                 DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  4.272e-01 -3.149e-02 -1.254e-02 -1.221e-02
log_k_DMTA    4.272e-01  1.000e+00 -7.371e-02 -2.935e-02 -2.858e-02
log_k_M23    -3.149e-02 -7.371e-02  1.000e+00  2.163e-03  2.107e-03
log_k_M27    -1.254e-02 -2.935e-02  2.163e-03  1.000e+00  8.388e-04
log_k_M31    -1.221e-02 -2.858e-02  2.107e-03  8.388e-04  1.000e+00
f_DMTA_ilr_1 -1.942e-03 -4.545e-03  3.593e-01 -8.134e-01  1.299e-04
f_DMTA_ilr_2  3.520e-04  8.238e-04  1.499e-01  3.399e-01 -7.672e-01
f_DMTA_ilr_3 -7.554e-02 -1.012e-01  2.981e-01  5.351e-01  6.104e-01
sigma         1.187e-08  4.048e-08  4.757e-08  2.098e-08  2.754e-08
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -1.942e-03    3.520e-04   -7.554e-02  1.187e-08
log_k_DMTA     -4.545e-03    8.238e-04   -1.012e-01  4.048e-08
log_k_M23       3.593e-01    1.499e-01    2.981e-01  4.757e-08
log_k_M27      -8.134e-01    3.399e-01    5.351e-01  2.098e-08
log_k_M31       1.299e-04   -7.672e-01    6.104e-01  2.754e-08
f_DMTA_ilr_1    1.000e+00   -2.599e-01   -3.770e-01 -2.606e-08
f_DMTA_ilr_2   -2.599e-01    1.000e+00   -3.681e-01 -5.282e-10
f_DMTA_ilr_3   -3.770e-01   -3.681e-01    1.000e+00  5.837e-08
sigma          -2.606e-08   -5.282e-10    5.837e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate   t value    Pr(>t)     Lower     Upper
DMTA_0        96.730000 139.50000 2.491e-22 9.523e+01 9.823e+01
k_DMTA         0.030940  47.50000 2.910e-16 2.957e-02 3.238e-02
k_M23          0.011090   3.25800 3.113e-03 5.717e-03 2.153e-02
k_M27          0.000413   0.08646 4.662e-01 5.805e-15 2.938e+07
k_M31          0.009465   1.18100 1.294e-01 1.519e-03 5.899e-02
f_DMTA_to_M23  0.114300   5.92300 2.521e-05        NA        NA
f_DMTA_to_M27  0.041110   2.87600 6.499e-03        NA        NA
f_DMTA_to_M31  0.044690   2.38300 1.656e-02        NA        NA
sigma          1.012000   6.63300 8.148e-06 6.823e-01 1.341e+00

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   5.713       8  9
DMTA       2.809       2  3
M23        5.049       2  2
M27        2.057       2  2
M31       13.952       2  2

Resulting formation fractions:
               ff
DMTA_M23  0.11426
DMTA_M27  0.04111
DMTA_M31  0.04469
DMTA_sink 0.79994

Estimated disappearance times:
        DT50    DT90
DMTA   22.40   74.42
M23    62.48  207.54
M27  1678.29 5575.16
M31    73.23  243.27

Data:
 time variable observed predicted residual
    0     DMTA     95.8    96.728 -0.92756
    0     DMTA     98.7    96.728  1.97244
   14     DMTA     60.5    62.722 -2.22176
   30     DMTA     39.1    38.231  0.86948
   59     DMTA     15.2    15.585 -0.38505
  120     DMTA      4.8     2.360  2.43957
  120     DMTA      4.6     2.360  2.23957
   14      M23      4.1     3.579  0.52122
```

```
  30      M23      5.3     5.542 -0.24214
  59      M23      6.0     6.178 -0.17775
 120      M23      4.3     4.130  0.16957
 120      M23      4.1     4.130 -0.03043
  14      M27      1.5     1.394  0.10638
  30      M27      2.4     2.388  0.01234
  59      M27      3.2     3.284 -0.08380
 120      M27      3.8     3.737  0.06304
 120      M27      3.7     3.737 -0.03696
  14      M31      2.0     1.417  0.58343
  30      M31      2.1     2.227 -0.12687
  59      M31      2.2     2.560 -0.35953
 120      M31      1.8     1.848 -0.04820
 120      M31      2.1     1.848  0.25180
```

Listing 40: SFO-SFO3 fit to Calke data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:43 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 2753 model solutions performed in 4.608 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
DMTA_0        97.2500  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       97.250000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  77.80632 88.71674 -28.90316

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error      Lower    Upper
DMTA_0       95.42000    1.96400  91.140000 99.70000
log_k_DMTA   -3.51300    0.03850  -3.597000 -3.42900
log_k_M23    -4.46000    0.22940  -4.960000 -3.96000
log_k_M27    -7.30900    5.41000 -19.100000  4.47900
log_k_M31    -4.61600    0.61790  -5.963000 -3.27000
f_DMTA_ilr_1  0.72570    0.20430   0.280700  1.17100
```

```
f_DMTA_ilr_2  0.34850    0.28200  -0.265900  0.96290
f_DMTA_ilr_3 -2.20600    0.15600  -2.546000 -1.86600
sigma_low     0.75090    0.14490   0.435300  1.06700
rsd_high      0.02505    0.01537  -0.008431  0.05852

Parameter correlation:
               DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.000000   0.758953  -0.14064 -0.055849 -0.055235    -0.011517
log_k_DMTA    0.758953   1.000000  -0.18492 -0.073529 -0.072676    -0.014931
log_k_M23    -0.140644  -0.184924   1.00000  0.013600  0.013445     0.360924
log_k_M27    -0.055849  -0.073529   0.01360  1.000000  0.005345    -0.808469
log_k_M31    -0.055235  -0.072676   0.01344  0.005345  1.000000     0.001089
f_DMTA_ilr_1 -0.011517  -0.014931   0.36092 -0.808469  0.001089     1.000000
f_DMTA_ilr_2  0.001919   0.002516   0.14931  0.338377 -0.767062    -0.256694
f_DMTA_ilr_3 -0.298031  -0.311980   0.33570  0.525708  0.599252    -0.346511
sigma_low     0.369190   0.460012  -0.08700 -0.034111 -0.033940    -0.008076
rsd_high     -0.586697  -0.714306   0.13510  0.052968  0.052703     0.012540
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low  rsd_high
DMTA_0           0.001919      -0.2980  0.369190 -0.586697
log_k_DMTA       0.002516      -0.3120  0.460012 -0.714306
log_k_M23        0.149313       0.3357 -0.087001  0.135095
log_k_M27        0.338377       0.5257 -0.034111  0.052968
log_k_M31       -0.767062       0.5993 -0.033940  0.052703
f_DMTA_ilr_1    -0.256694      -0.3465 -0.008076  0.012540
f_DMTA_ilr_2     1.000000      -0.3490  0.001221 -0.001897
f_DMTA_ilr_3    -0.348986       1.0000 -0.147897  0.229652
sigma_low        0.001221      -0.1479  1.000000 -0.412524
rsd_high        -0.001897       0.2297 -0.412524  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value    Pr(>t)      Lower    Upper
DMTA_0        9.542e+01 48.5900 1.891e-15  9.114e+01 99.70000
k_DMTA        2.980e-02 25.9700 3.237e-12  2.740e-02  0.03241
k_M23         1.156e-02  4.3580 4.656e-04  7.015e-03  0.01906
k_M27         6.692e-04  0.1848 4.282e-01  5.081e-09 88.14000
k_M31         9.890e-03  1.6180 6.578e-02  2.573e-03  0.03801
f_DMTA_to_M23 1.193e-01  7.3670 4.326e-06         NA       NA
f_DMTA_to_M27 4.274e-02  3.8000 1.265e-03         NA       NA
f_DMTA_to_M31 4.659e-02  3.1520 4.169e-03         NA       NA
sigma_low     7.509e-01  5.1840 1.139e-04  4.353e-01  1.06700
rsd_high      2.505e-02  1.6300 6.451e-02 -8.431e-03  0.05852

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.383       8  9
DMTA       3.158       2  3
M23        5.197       2  2
M27        2.251       2  2
M31       14.133       2  2

Resulting formation fractions:
               ff
DMTA_M23  0.11928
DMTA_M27  0.04274
DMTA_M31  0.04659
DMTA_sink 0.79138

Estimated disappearance times:
        DT50    DT90
DMTA   23.26   77.27
M23    59.94  199.11
M27  1035.73 3440.62
M31    70.09  232.82

Data:
 time variable observed predicted residual
```

```
  0     DMTA     95.8    95.418  0.38211
  0     DMTA     98.7    95.418  3.28211
 14     DMTA     60.5    62.869 -2.36916
 30     DMTA     39.1    39.027  0.07339
 59     DMTA     15.2    16.445 -1.24501
120     DMTA      4.8     2.670  2.12974
120     DMTA      4.6     2.670  1.92974
 14      M23      4.1     3.564  0.53562
 30      M23      5.3     5.540 -0.23968
 59      M23      6.0     6.196 -0.19551
120      M23      4.3     4.123  0.17732
120      M23      4.1     4.123 -0.02268
 14      M27      1.5     1.384  0.11583
 30      M27      2.4     2.383  0.01742
 59      M27      3.2     3.291 -0.09129
120      M27      3.8     3.733  0.06688
120      M27      3.7     3.733 -0.03312
 14      M31      2.0     1.410  0.59050
 30      M31      2.1     2.224 -0.12430
 59      M31      2.2     2.566 -0.36587
120      M31      1.8     1.845 -0.04469
120      M31      2.1     1.845  0.25531
```

Listing 41: SFO-SFO3 fit to Flaach data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:04 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1134 model solutions performed in 2.221 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                 value   type
DMTA_0        96.76667  state
k_DMTA         0.10000 deparm
k_M23          0.10010 deparm
k_M27          0.10020 deparm
k_M31          0.10030 deparm
f_DMTA_to_M23  0.25000 deparm
f_DMTA_to_M27  0.25000 deparm
f_DMTA_to_M31  0.25000 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       96.766667  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  318.3399 344.4874 -150.1699

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error   Lower    Upper
DMTA_0       95.10000   0.298400 94.5000 95.69000
log_k_DMTA   -1.93700   0.008114 -1.9530 -1.92100
log_k_M23    -3.07500   0.071240 -3.2160 -2.93400
log_k_M27    -3.67900   0.066370 -3.8110 -3.54800
log_k_M31    -3.52500   0.200100 -3.9210 -3.12900
f_DMTA_ilr_1 -0.03117   0.038850 -0.1081  0.04571
f_DMTA_ilr_2  0.92120   0.090880  0.7413  1.10100
f_DMTA_ilr_3 -1.76600   0.045220 -1.8550 -1.67600
sigma         0.73600   0.044790  0.6473  0.82460

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.286e-01 -4.613e-02 -4.994e-02 -1.663e-02
log_k_DMTA    5.286e-01  1.000e+00 -8.728e-02 -9.447e-02 -3.146e-02
log_k_M23    -4.613e-02 -8.728e-02  1.000e+00  8.245e-03  2.746e-03
log_k_M27    -4.994e-02 -9.447e-02  8.245e-03  1.000e+00  2.972e-03
log_k_M31    -1.663e-02 -3.146e-02  2.746e-03  2.972e-03  1.000e+00
f_DMTA_ilr_1 -9.573e-03 -1.811e-02  6.089e-01 -4.563e-01  5.698e-04
f_DMTA_ilr_2 -6.684e-04 -1.265e-03  1.500e-01  1.132e-01 -7.314e-01
f_DMTA_ilr_3 -1.516e-01 -1.687e-01  3.463e-01  2.700e-01  6.207e-01
sigma        -5.360e-07 -2.134e-06 -9.505e-08  7.486e-07  2.692e-07
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -9.573e-03   -6.684e-04   -1.516e-01 -5.360e-07
log_k_DMTA     -1.811e-02   -1.265e-03   -1.687e-01 -2.134e-06
log_k_M23       6.089e-01    1.500e-01    3.463e-01 -9.505e-08
log_k_M27      -4.563e-01    1.132e-01    2.700e-01  7.486e-07
log_k_M31       5.698e-04   -7.314e-01    6.207e-01  2.692e-07
f_DMTA_ilr_1    1.000e+00    6.975e-02    1.541e-01 -7.243e-08
f_DMTA_ilr_2    6.975e-02    1.000e+00   -6.544e-01  2.784e-07
f_DMTA_ilr_3    1.541e-01   -6.544e-01    1.000e+00  6.106e-07
sigma          -7.243e-08    2.784e-07    6.106e-07  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)    Lower    Upper
DMTA_0        95.10000 318.700 2.598e-185 94.50000 95.69000
k_DMTA         0.14410 123.200 1.642e-133  0.14180  0.14650
k_M23          0.04618  14.040  7.890e-28  0.04010  0.05317
k_M27          0.02524  15.070  2.864e-30  0.02213  0.02878
k_M31          0.02945   4.998  9.487e-07  0.01982  0.04376
f_DMTA_to_M23  0.12870  22.440  3.901e-46       NA       NA
f_DMTA_to_M27  0.13450  29.860  2.659e-59       NA       NA
f_DMTA_to_M31  0.04259   9.253  3.582e-16       NA       NA
sigma          0.73600  16.430  1.995e-33  0.64730  0.82460

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   4.706       8 37
DMTA       2.110       2 10
M23       11.577       2  9
M27        4.462       2  9
M31       19.485       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.12873
DMTA_M27  0.13453
DMTA_M31  0.04259
DMTA_sink 0.69415

Estimated disappearance times:
       DT50  DT90
DMTA  4.809 15.98
M23  15.011 49.86
M27  27.467 91.24
M31  23.537 78.19

Data:
    time variable observed predicted  residual
  0.0000     DMTA     96.5 95.095291  1.404709
  0.0000     DMTA     96.8 95.095291  1.704709
  0.0000     DMTA     97.0 95.095291  1.904709
  0.6234     DMTA     82.9 86.924158 -4.024158
  0.6234     DMTA     86.7 86.924158 -0.224158
  0.6234     DMTA     87.4 86.924158  0.475842
  1.8702     DMTA     72.8 72.627894  0.172106
  1.8702     DMTA     69.9 72.627894 -2.727894
  1.8702     DMTA     71.9 72.627894 -0.727894
```

4.3637	DMTA	51.4	50.702499	0.697501
4.3637	DMTA	52.9	50.702499	2.197501
4.3637	DMTA	48.6	50.702499	-2.102499
8.7274	DMTA	28.5	27.033340	1.466660
8.7274	DMTA	27.3	27.033340	0.266660
8.7274	DMTA	27.5	27.033340	0.466660
13.0911	DMTA	14.8	14.413520	0.386480
13.0911	DMTA	13.4	14.413520	-1.013520
13.0911	DMTA	14.4	14.413520	-0.013520
17.4548	DMTA	7.7	7.684939	0.015061
17.4548	DMTA	7.3	7.684939	-0.384939
17.4548	DMTA	8.1	7.684939	0.415061
26.1822	DMTA	2.0	2.184646	-0.184646
26.1822	DMTA	1.5	2.184646	-0.684646
26.1822	DMTA	1.9	2.184646	-0.284646
34.9096	DMTA	1.3	0.621043	0.678957
34.9096	DMTA	1.0	0.621043	0.378957
34.9096	DMTA	1.1	0.621043	0.478957
43.6370	DMTA	0.9	0.176548	0.723452
43.6370	DMTA	0.7	0.176548	0.523452
43.6370	DMTA	0.7	0.176548	0.523452
52.3644	DMTA	0.6	0.050188	0.549812
52.3644	DMTA	0.4	0.050188	0.349812
52.3644	DMTA	0.5	0.050188	0.449812
74.8063	DMTA	0.4	0.001977	0.398023
74.8063	DMTA	0.3	0.001977	0.298023
74.8063	DMTA	0.3	0.001977	0.298023
0.6234	M23	0.7	1.036647	-0.336647
0.6234	M23	0.7	1.036647	-0.336647
0.6234	M23	0.2	1.036647	-0.836647
1.8702	M23	2.2	2.765487	-0.565487
1.8702	M23	1.8	2.765487	-0.965487
1.8702	M23	1.6	2.765487	-1.165487
4.3637	M23	4.1	5.121553	-1.021553
4.3637	M23	4.2	5.121553	-0.921553
4.3637	M23	4.2	5.121553	-0.921553
8.7274	M23	7.5	6.917563	0.582437
8.7274	M23	7.1	6.917563	0.182437
8.7274	M23	7.5	6.917563	0.582437
13.0911	M23	8.4	7.111053	1.288947
13.0911	M23	6.8	7.111053	-0.311053
13.0911	M23	8.0	7.111053	0.888947
17.4548	M23	7.2	6.589565	0.610435
17.4548	M23	7.2	6.589565	0.610435
17.4548	M23	6.9	6.589565	0.310435
26.1822	M23	4.9	4.962891	-0.062891
26.1822	M23	4.3	4.962891	-0.662891
26.1822	M23	4.5	4.962891	-0.462891
34.9096	M23	3.8	3.475660	0.324340
34.9096	M23	3.1	3.475660	-0.375660
34.9096	M23	3.1	3.475660	-0.375660
43.6370	M23	2.7	2.367990	0.332010
43.6370	M23	2.3	2.367990	-0.067990
43.6370	M23	2.1	2.367990	-0.267990
52.3644	M23	1.6	1.595390	0.004610
52.3644	M23	1.1	1.595390	-0.495390
52.3644	M23	1.3	1.595390	-0.295390
74.8063	M23	0.4	0.568986	-0.168986
74.8063	M23	0.4	0.568986	-0.168986
74.8063	M23	0.3	0.568986	-0.268986
0.6234	M27	1.1	1.090548	0.009452
0.6234	M27	1.1	1.090548	0.009452
0.6234	M27	0.3	1.090548	-0.790548
1.8702	M27	2.6	2.949240	-0.349240
1.8702	M27	2.4	2.949240	-0.549240
1.8702	M27	2.3	2.949240	-0.649240
4.3637	M27	5.0	5.622774	-0.622774
4.3637	M27	5.9	5.622774	0.277226
4.3637	M27	4.8	5.622774	-0.822774

```
 8.7274      M27      8.5  8.034385  0.465615
 8.7274      M27      8.5  8.034385  0.465615
 8.7274      M27      8.3  8.034385  0.265615
13.0911      M27      9.3  8.795020  0.504980
13.0911      M27      8.7  8.795020 -0.095020
13.0911      M27      9.1  8.795020  0.304980
17.4548      M27      8.6  8.730158 -0.130158
17.4548      M27      8.5  8.730158 -0.230158
17.4548      M27      8.9  8.730158  0.169842
26.1822      M27      8.1  7.653691  0.446309
26.1822      M27      7.7  7.653691  0.046309
26.1822      M27      7.4  7.653691 -0.253691
34.9096      M27      5.9  6.325309 -0.425309
34.9096      M27      6.0  6.325309 -0.325309
34.9096      M27      5.9  6.325309 -0.425309
43.6370      M27      5.6  5.127412  0.472588
43.6370      M27      5.2  5.127412  0.072588
43.6370      M27      5.6  5.127412  0.472588
52.3644      M27      4.3  4.128757  0.171243
52.3644      M27      3.7  4.128757 -0.428757
52.3644      M27      3.9  4.128757 -0.228757
74.8063      M27      2.5  2.347799  0.152201
74.8063      M27      2.4  2.347799  0.052201
74.8063      M27      2.2  2.347799 -0.147799
 0.6234      M31      0.3  0.344759 -0.044759
 0.6234      M31      0.3  0.344759 -0.044759
 0.6234      M31      0.1  0.344759 -0.244759
 1.8702      M31      0.7  0.929790 -0.229790
 1.8702      M31      0.6  0.929790 -0.329790
 1.8702      M31      0.7  0.929790 -0.229790
 4.3637      M31      1.3  1.762253 -0.462253
 4.3637      M31      1.2  1.762253 -0.562253
 4.3637      M31      1.4  1.762253 -0.362253
 8.7274      M31      2.4  2.489326 -0.089326
 8.7274      M31      2.1  2.489326 -0.389326
 8.7274      M31      2.3  2.489326 -0.189326
13.0911      M31      3.3  2.690095  0.609905
13.0911      M31      2.4  2.690095 -0.290095
13.0911      M31      2.6  2.690095 -0.090095
17.4548      M31      4.0  2.632789  1.367211
17.4548      M31      3.6  2.632789  0.967211
17.4548      M31      3.3  2.632789  0.667211
26.1822      M31      2.1  2.237249 -0.137249
26.1822      M31      1.7  2.237249 -0.537249
26.1822      M31      1.8  2.237249 -0.437249
34.9096      M31      1.6  1.787375 -0.187375
34.9096      M31      1.6  1.787375 -0.187375
34.9096      M31      1.4  1.787375 -0.387375
43.6370      M31      1.8  1.398532  0.401468
43.6370      M31      1.5  1.398532  0.101468
43.6370      M31      1.3  1.398532 -0.098532
52.3644      M31      1.2  1.086183  0.113817
52.3644      M31      0.9  1.086183 -0.186183
52.3644      M31      1.1  1.086183  0.013817
74.8063      M31      0.5  0.562170 -0.062170
74.8063      M31      0.5  0.562170 -0.062170
74.8063      M31      0.3  0.562170 -0.262170
```

Listing 42: SFO-SFO3 fit to Flaach data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:52 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 6699 model solutions performed in 13.02 s

Error model: Two-component variance function

Error model algorithm: d_3
Three-step fitting yielded a higher likelihood than direct fitting

Starting values for parameters to be optimised:
                value   type
DMTA_0        96.76667  state
k_DMTA         0.10000 deparm
k_M23          0.10010 deparm
k_M27          0.10020 deparm
k_M31          0.10030 deparm
f_DMTA_to_M23  0.25000 deparm
f_DMTA_to_M27  0.25000 deparm
f_DMTA_to_M31  0.25000 deparm
sigma_low      0.10000  error
rsd_high       0.10000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
DMTA_0       96.766667  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state


Warning(s):
Optimisation did not converge:
iteration limit reached without convergence (10)

Results:

      AIC      BIC   logLik
  242.378 271.4308 -111.189

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
DMTA_0       94.81000   0.827100 93.17000 96.44000
```

```
log_k_DMTA   -1.94400   0.009534 -1.96300 -1.92500
log_k_M23    -3.07000   0.046680 -3.16300 -2.97800
log_k_M27    -3.67800   0.044130 -3.76500 -3.59000
log_k_M31    -3.52000   0.127000 -3.77100 -3.26800
f_DMTA_ilr_1 -0.03082   0.025970 -0.08222  0.02058
f_DMTA_ilr_2  0.91910   0.058100  0.80410  1.03400
f_DMTA_ilr_3 -1.76000   0.032920 -1.82500 -1.69500
sigma_low     0.46500   0.032860  0.39990  0.53000
rsd_high      0.02576   0.005443  0.01499  0.03653

Parameter correlation:
                DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.000e+00   0.646374 -0.099605 -0.103921 -0.037626    -0.019227
log_k_DMTA    6.464e-01   1.000000 -0.154901 -0.164913 -0.058199    -0.030508
log_k_M23    -9.961e-02  -0.154901  1.000000  0.025809  0.009014     0.601197
log_k_M27    -1.039e-01  -0.164913  0.025809  1.000000  0.009594    -0.452633
log_k_M31    -3.763e-02  -0.058199  0.009014  0.009594  1.000000     0.001775
f_DMTA_ilr_1 -1.923e-02  -0.030508  0.601197 -0.452633  0.001775     1.000000
f_DMTA_ilr_2  2.147e-06  -0.002129  0.154396  0.119230 -0.728710     0.067554
f_DMTA_ilr_3 -4.568e-01  -0.413149  0.363714  0.302509  0.563190     0.140868
sigma_low     3.595e-02   0.008066  0.002907  0.017516 -0.000633     0.003471
rsd_high     -7.918e-02  -0.011310 -0.004962 -0.033247  0.000735    -0.006067
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low  rsd_high
DMTA_0          2.147e-06    -0.456753  0.035950 -0.079178
log_k_DMTA     -2.129e-03    -0.413149  0.008066 -0.011310
log_k_M23       1.544e-01     0.363714  0.002907 -0.004962
log_k_M27       1.192e-01     0.302509  0.017516 -0.033247
log_k_M31      -7.287e-01     0.563190 -0.000633  0.000735
f_DMTA_ilr_1    6.755e-02     0.140868  0.003471 -0.006067
f_DMTA_ilr_2    1.000e+00    -0.558736  0.010102 -0.017982
f_DMTA_ilr_3   -5.587e-01     1.000000  0.005647 -0.013490
sigma_low       1.010e-02     0.005647  1.000000 -0.238404
rsd_high       -1.798e-02    -0.013490 -0.238404  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
             Estimate t value     Pr(>t)    Lower    Upper
DMTA_0        94.81000 114.600 8.799e-129 93.17000 96.44000
k_DMTA         0.14310 104.900 5.186e-124  0.14040  0.14580
k_M23          0.04641  21.420  5.839e-44  0.04232  0.05090
k_M27          0.02528  22.660  2.135e-46  0.02317  0.02759
k_M31          0.02961   7.873  7.158e-13  0.02303  0.03808
f_DMTA_to_M23  0.12920  31.210  3.745e-61       NA       NA
f_DMTA_to_M27  0.13500  39.230  1.992e-72       NA       NA
f_DMTA_to_M31  0.04286  14.310  2.091e-28       NA       NA
sigma_low      0.46500  14.150  4.957e-28  0.39990  0.53000
rsd_high       0.02576   4.733  2.941e-06  0.01499  0.03653

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   4.744       8 37
DMTA       2.148       2 10
M23       11.512       2  9
M27        4.436       2  9
M31       19.435       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.12924
DMTA_M27  0.13500
DMTA_M31  0.04286
DMTA_sink 0.69290

Estimated disappearance times:
       DT50  DT90
DMTA  4.845 16.09
M23  14.935 49.61
```

```
M27  27.415 91.07
M31  23.407 77.76

Data:
    time variable observed predicted residual
  0.0000     DMTA     96.5 94.805075  1.69492
  0.0000     DMTA     96.8 94.805075  1.99492
  0.0000     DMTA     97.0 94.805075  2.19492
  0.6234     DMTA     82.9 86.715317 -3.81532
  0.6234     DMTA     86.7 86.715317 -0.01532
  0.6234     DMTA     87.4 86.715317  0.68468
  1.8702     DMTA     72.8 72.547805  0.25219
  1.8702     DMTA     69.9 72.547805 -2.64781
  1.8702     DMTA     71.9 72.547805 -0.64781
  4.3637     DMTA     51.4 50.778656  0.62134
  4.3637     DMTA     52.9 50.778656  2.12134
  4.3637     DMTA     48.6 50.778656 -2.17866
  8.7274     DMTA     28.5 27.197615  1.30239
  8.7274     DMTA     27.3 27.197615  0.10239
  8.7274     DMTA     27.5 27.197615  0.30239
 13.0911     DMTA     14.8 14.567346  0.23265
 13.0911     DMTA     13.4 14.567346 -1.16735
 13.0911     DMTA     14.4 14.567346 -0.16735
 17.4548     DMTA      7.7  7.802433 -0.10243
 17.4548     DMTA      7.3  7.802433 -0.50243
 17.4548     DMTA      8.1  7.802433  0.29757
 26.1822     DMTA      2.0  2.238357 -0.23836
 26.1822     DMTA      1.5  2.238357 -0.73836
 26.1822     DMTA      1.9  2.238357 -0.33836
 34.9096     DMTA      1.3  0.642138  0.65786
 34.9096     DMTA      1.0  0.642138  0.35786
 34.9096     DMTA      1.1  0.642138  0.45786
 43.6370     DMTA      0.9  0.184216  0.71578
 43.6370     DMTA      0.7  0.184216  0.51578
 43.6370     DMTA      0.7  0.184216  0.51578
 52.3644     DMTA      0.6  0.052848  0.54715
 52.3644     DMTA      0.4  0.052848  0.34715
 52.3644     DMTA      0.5  0.052848  0.44715
 74.8063     DMTA      0.4  0.002131  0.39787
 74.8063     DMTA      0.3  0.002131  0.29787
 74.8063     DMTA      0.3  0.002131  0.29787
  0.6234      M23      0.7  1.030332 -0.33033
  0.6234      M23      0.7  1.030332 -0.33033
  0.6234      M23      0.2  1.030332 -0.83033
  1.8702      M23      2.2  2.749938 -0.54994
  1.8702      M23      1.8  2.749938 -0.94994
  1.8702      M23      1.6  2.749938 -1.14994
  4.3637      M23      4.1  5.097077 -0.99708
  4.3637      M23      4.2  5.097077 -0.89708
  4.3637      M23      4.2  5.097077 -0.89708
  8.7274      M23      7.5  6.892645  0.60736
  8.7274      M23      7.1  6.892645  0.20736
  8.7274      M23      7.5  6.892645  0.60736
 13.0911      M23      8.4  7.091212  1.30879
 13.0911      M23      6.8  7.091212 -0.29121
 13.0911      M23      8.0  7.091212  0.90879
 17.4548      M23      7.2  6.574324  0.62568
 17.4548      M23      7.2  6.574324  0.62568
 17.4548      M23      6.9  6.574324  0.32568
 26.1822      M23      4.9  4.951930 -0.05193
 26.1822      M23      4.3  4.951930 -0.65193
 26.1822      M23      4.5  4.951930 -0.45193
 34.9096      M23      3.8  3.465366  0.33463
 34.9096      M23      3.1  3.465366 -0.36537
 34.9096      M23      3.1  3.465366 -0.36537
 43.6370      M23      2.7  2.357870  0.34213
 43.6370      M23      2.3  2.357870 -0.05787
 43.6370      M23      2.1  2.357870 -0.25787
 52.3644      M23      1.6  1.585946  0.01405
```

```
  52.3644      M23      1.1  1.585946 -0.48595
  52.3644      M23      1.3  1.585946 -0.28595
  74.8063      M23      0.4  0.562836 -0.16284
  74.8063      M23      0.4  0.562836 -0.16284
  74.8063      M23      0.3  0.562836 -0.26284
   0.6234      M27      1.1  1.083425  0.01658
   0.6234      M27      1.1  1.083425  0.01658
   0.6234      M27      0.3  1.083425 -0.78342
   1.8702      M27      2.6  2.931700 -0.33170
   1.8702      M27      2.4  2.931700 -0.53170
   1.8702      M27      2.3  2.931700 -0.63170
   4.3637      M27      5.0  5.595354 -0.59535
   4.3637      M27      5.9  5.595354  0.30465
   4.3637      M27      4.8  5.595354 -0.79535
   8.7274      M27      8.5  8.007798  0.49220
   8.7274      M27      8.5  8.007798  0.49220
   8.7274      M27      8.3  8.007798  0.29220
  13.0911      M27      9.3  8.776495  0.52350
  13.0911      M27      8.7  8.776495 -0.07650
  13.0911      M27      9.1  8.776495  0.32350
  17.4548      M27      8.6  8.719462 -0.11946
  17.4548      M27      8.5  8.719462 -0.21946
  17.4548      M27      8.9  8.719462  0.18054
  26.1822      M27      8.1  7.651978  0.44802
  26.1822      M27      7.7  7.651978  0.04802
  26.1822      M27      7.4  7.651978 -0.25198
  34.9096      M27      5.9  6.325890 -0.42589
  34.9096      M27      6.0  6.325890 -0.32589
  34.9096      M27      5.9  6.325890 -0.42589
  43.6370      M27      5.6  5.127552  0.47245
  43.6370      M27      5.2  5.127552  0.07245
  43.6370      M27      5.6  5.127552  0.47245
  52.3644      M27      4.3  4.127815  0.17218
  52.3644      M27      3.7  4.127815 -0.42782
  52.3644      M27      3.9  4.127815 -0.22782
  74.8063      M27      2.5  2.345019  0.15498
  74.8063      M27      2.4  2.345019  0.05498
  74.8063      M27      2.2  2.345019 -0.14502
   0.6234      M31      0.3  0.343465 -0.04347
   0.6234      M31      0.3  0.343465 -0.04347
   0.6234      M31      0.1  0.343465 -0.24347
   1.8702      M31      0.7  0.926776 -0.22678
   1.8702      M31      0.6  0.926776 -0.32678
   1.8702      M31      0.7  0.926776 -0.22678
   4.3637      M31      1.3  1.758159 -0.45816
   4.3637      M31      1.2  1.758159 -0.55816
   4.3637      M31      1.4  1.758159 -0.35816
   8.7274      M31      2.4  2.486721 -0.08672
   8.7274      M31      2.1  2.486721 -0.38672
   8.7274      M31      2.3  2.486721 -0.18672
  13.0911      M31      3.3  2.689655  0.61035
  13.0911      M31      2.4  2.689655 -0.28965
  13.0911      M31      2.6  2.689655 -0.08965
  17.4548      M31      4.0  2.633761  1.36624
  17.4548      M31      3.6  2.633761  0.96624
  17.4548      M31      3.3  2.633761  0.66624
  26.1822      M31      2.1  2.238581 -0.13858
  26.1822      M31      1.7  2.238581 -0.53858
  26.1822      M31      1.8  2.238581 -0.43858
  34.9096      M31      1.6  1.787458 -0.18746
  34.9096      M31      1.6  1.787458 -0.18746
  34.9096      M31      1.4  1.787458 -0.38746
  43.6370      M31      1.8  1.397209  0.40279
  43.6370      M31      1.5  1.397209  0.10279
  43.6370      M31      1.3  1.397209 -0.09721
  52.3644      M31      1.2  1.083828  0.11617
  52.3644      M31      0.9  1.083828 -0.18383
  52.3644      M31      1.1  1.083828  0.01617
  74.8063      M31      0.5  0.558975 -0.05898
```

```
   74.8063      M31      0.5  0.558975 -0.05898
   74.8063      M31      0.3  0.558975 -0.25898
```

Listing 43: SFO-SFO3 fit to BBA 2.2 data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:04 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1165 model solutions performed in 2.136 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.4300  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.430000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  291.8813 314.3796 -136.9406

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
DMTA_0       99.70000    0.49720 98.71000 100.7000
log_k_DMTA   -2.65300    0.01259 -2.67800  -2.6280
log_k_M23    -3.81500    0.13040 -4.07500  -3.5560
log_k_M27    -4.99400    0.21610 -5.42400  -4.5640
log_k_M31    -4.30000    0.20470 -4.70800  -3.8930
f_DMTA_ilr_1  0.06628    0.06152 -0.05613   0.1887
f_DMTA_ilr_2  0.27520    0.07701  0.12200   0.4284
f_DMTA_ilr_3 -1.41600    0.05696 -1.53000  -1.3030
sigma         1.10800    0.08259  0.94370   1.2720

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.339e-01 -5.039e-02 -5.227e-02 -3.722e-02
log_k_DMTA    5.339e-01  1.000e+00 -9.438e-02 -9.790e-02 -6.971e-02
log_k_M23    -5.039e-02 -9.438e-02  1.000e+00  9.240e-03  6.579e-03
log_k_M27    -5.227e-02 -9.790e-02  9.240e-03  1.000e+00  6.825e-03
log_k_M31    -3.722e-02 -6.971e-02  6.579e-03  6.825e-03  1.000e+00
f_DMTA_ilr_1 -8.543e-03 -1.600e-02  6.402e-01 -4.984e-01  1.116e-03
f_DMTA_ilr_2 -5.308e-04 -9.943e-04  2.947e-01  2.307e-01 -7.176e-01
f_DMTA_ilr_3 -2.226e-01 -2.553e-01  4.988e-01  3.831e-01  5.210e-01
sigma         1.475e-08  2.849e-08  1.275e-08 -1.846e-08  6.835e-09
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -8.543e-03   -5.308e-04   -2.226e-01  1.475e-08
log_k_DMTA     -1.600e-02   -9.943e-04   -2.553e-01  2.849e-08
log_k_M23       6.402e-01    2.947e-01    4.988e-01  1.275e-08
log_k_M27      -4.984e-01    2.307e-01    3.831e-01 -1.846e-08
log_k_M31       1.116e-03   -7.176e-01    5.210e-01  6.835e-09
f_DMTA_ilr_1    1.000e+00    1.150e-01    1.996e-01  1.121e-08
f_DMTA_ilr_2    1.150e-01    1.000e+00   -2.137e-01 -2.089e-08
f_DMTA_ilr_3    1.996e-01   -2.137e-01    1.000e+00 -9.815e-09
sigma           1.121e-08   -2.089e-08   -9.815e-09  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)     Lower     Upper
DMTA_0        99.70000 200.500 2.665e-111 98.710000 100.70000
k_DMTA         0.07046  79.440  6.506e-79  0.068720   0.07225
k_M23          0.02203   7.667  1.693e-11  0.017000   0.02856
k_M27          0.00678   4.627  6.945e-06  0.004410   0.01042
k_M31          0.01356   4.885  2.565e-06  0.009025   0.02038
f_DMTA_to_M23  0.14350  14.330  3.252e-24        NA        NA
f_DMTA_to_M27  0.13070  18.390  5.875e-31        NA        NA
f_DMTA_to_M31  0.09775  11.840  1.169e-19        NA        NA
sigma          1.10800  13.420  1.391e-22  0.943700   1.27200

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.859       8 37
DMTA       3.514       2 10
M23        9.336       2  9
M27       10.677       2  9
M31       10.628       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.14351
DMTA_M27  0.13067
DMTA_M31  0.09775
DMTA_sink 0.62807

Estimated disappearance times:
        DT50   DT90
DMTA   9.837  32.68
M23   31.459 104.50
M27  102.236 339.62
M31   51.106 169.77

Data:
    time variable observed predicted  residual
  0.0000     DMTA    98.09   99.7020 -1.611957
  0.0000     DMTA    98.77   99.7020 -0.931957
  0.7679     DMTA    93.52   94.4508 -0.930788
  0.7679     DMTA    92.03   94.4508 -2.420788
  2.3037     DMTA    88.39   84.7636  3.626399
  2.3037     DMTA    87.18   84.7636  2.416399
  5.3752     DMTA    69.38   68.2680  1.112025
  5.3752     DMTA    71.06   68.2680  2.792025
 10.7505     DMTA    45.21   46.7445 -1.534483
```

```
 10.7505     DMTA    46.81   46.7445  0.065517
 16.1257     DMTA    30.54   32.0069 -1.466907
 16.1257     DMTA    30.07   32.0069 -1.936907
 21.5010     DMTA    21.60   21.9158 -0.315786
 21.5010     DMTA    20.41   21.9158 -1.505786
 32.2515     DMTA     9.10   10.2750 -1.175045
 32.2515     DMTA     9.70   10.2750 -0.575045
 43.0020     DMTA     6.58    4.8174  1.762625
 43.0020     DMTA     6.31    4.8174  1.492625
 53.7525     DMTA     3.47    2.2586  1.211412
 53.7525     DMTA     3.52    2.2586  1.261412
 64.5029     DMTA     3.40    1.0589  2.341078
 64.5029     DMTA     3.67    1.0589  2.611078
 91.3792     DMTA     1.62    0.1594  1.460621
 91.3792     DMTA     1.62    0.1594  1.460621
  0.7679      M23     0.36    0.7472 -0.387190
  0.7679      M23     0.40    0.7472 -0.347190
  2.3037      M23     1.03    2.0888 -1.058847
  2.3037      M23     1.07    2.0888 -1.018847
  5.3752      M23     3.60    4.2383 -0.638298
  5.3752      M23     3.66    4.2383 -0.578298
 10.7505      M23     6.97    6.6670  0.303032
 10.7505      M23     7.22    6.6670  0.553032
 16.1257      M23     8.65    7.9094  0.740578
 16.1257      M23     8.38    7.9094  0.470578
 21.5010      M23     9.10    8.3866  0.713385
 21.5010      M23     8.63    8.3866  0.243385
 32.2515      M23     7.63    8.0833 -0.453307
 32.2515      M23     8.01    8.0833 -0.073307
 43.0020      M23     6.40    7.0656 -0.665564
 43.0020      M23     6.35    7.0656 -0.715564
 53.7525      M23     5.35    5.8975 -0.547522
 53.7525      M23     5.06    5.8975 -0.837522
 64.5029      M23     5.14    4.8047  0.335276
 64.5029      M23     5.91    4.8047  1.105276
 91.3792      M23     3.35    2.7466  0.603384
 91.3792      M23     2.87    2.7466  0.123384
  0.7679      M27     0.42    0.6844 -0.264363
  0.7679      M27     0.47    0.6844 -0.214363
  2.3037      M27     0.71    1.9364 -1.226398
  2.3037      M27     0.82    1.9364 -1.116398
  5.3752      M27     2.19    4.0289 -1.838859
  5.3752      M27     2.28    4.0289 -1.748859
 10.7505      M27     5.45    6.6433 -1.193319
 10.7505      M27     5.19    6.6433 -1.453319
 16.1257      M27     8.81    8.2945  0.515528
 16.1257      M27     7.93    8.2945 -0.364472
 21.5010      M27    10.25    9.2910  0.958997
 21.5010      M27    10.77    9.2910  1.478997
 32.2515      M27    10.89   10.0982  0.791809
 32.2515      M27    10.85   10.0982  0.751809
 43.0020      M27    10.41   10.0730  0.337006
 43.0020      M27    10.35   10.0730  0.277006
 53.7525      M27     9.92    9.6859  0.234085
 53.7525      M27     9.42    9.6859 -0.265915
 64.5029      M27     9.15    9.1555 -0.005548
 64.5029      M27     9.25    9.1555  0.094452
 91.3792      M27     7.14    7.7350 -0.594976
 91.3792      M27     7.13    7.7350 -0.604976
  0.7679      M31     0.36    0.5106 -0.150632
  0.7679      M31     0.33    0.5106 -0.180632
  2.3037      M31     0.55    1.4371 -0.887092
  2.3037      M31     0.64    1.4371 -0.797092
  5.3752      M31     1.94    2.9566 -1.016647
  5.3752      M31     1.62    2.9566 -1.336647
 10.7505      M31     4.22    4.7732 -0.553242
 10.7505      M31     4.37    4.7732 -0.403242
 16.1257      M31     6.31    5.8238  0.486162
 16.1257      M31     6.85    5.8238  1.026162
```

```
  21.5010      M31     7.05    6.3635  0.686474
  21.5010      M31     6.84    6.3635  0.476474
  32.2515      M31     6.53    6.5494 -0.019369
  32.2515      M31     7.11    6.5494  0.560631
  43.0020      M31     6.06    6.1527 -0.092696
  43.0020      M31     6.05    6.1527 -0.102696
  53.7525      M31     5.50    5.5486 -0.048556
  53.7525      M31     5.07    5.5486 -0.478556
  64.5029      M31     4.94    4.9039  0.036119
  64.5029      M31     4.39    4.9039 -0.513881
  91.3792      M31     3.64    3.4756  0.164366
  91.3792      M31     3.55    3.4756  0.074366
```

Listing 44: SFO-SFO3 fit to BBA 2.2 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:45 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 3290 model solutions performed in 6.253 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.4300  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.430000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  276.9433 301.9414 -128.4716

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower     Upper
DMTA_0       99.64000    1.02000 97.61000 101.70000
log_k_DMTA   -2.64800    0.01563 -2.67900  -2.61700
log_k_M23    -3.82300    0.10840 -4.03900  -3.60700
log_k_M27    -5.00800    0.18410 -5.37400  -4.64200
log_k_M31    -4.30800    0.16990 -4.64600  -3.97000
f_DMTA_ilr_1  0.06633    0.05110 -0.03535   0.16800
```

```
f_DMTA_ilr_2  0.27450    0.06358  0.14790   0.40100
f_DMTA_ilr_3 -1.42200    0.05149 -1.52500  -1.32000
sigma_low     0.90680    0.07512  0.75730   1.05600
rsd_high      0.02305    0.00639  0.01034   0.03577

Parameter correlation:
                DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.0000000  0.6618048 -0.087913 -0.089881 -0.067224    -0.016877
log_k_DMTA    0.6618048  1.0000000 -0.135778 -0.139036 -0.102624    -0.024679
log_k_M23    -0.0879135 -0.1357783  1.000000  0.019186  0.014034     0.634297
log_k_M27    -0.0898809 -0.1390358  0.019186  1.000000  0.014378    -0.496517
log_k_M31    -0.0672241 -0.1026236  0.014034  0.014378  1.000000     0.002505
f_DMTA_ilr_1 -0.0168772 -0.0246787  0.634297 -0.496517  0.002505     1.000000
f_DMTA_ilr_2  0.0009349  0.0002647  0.292845  0.232000 -0.713510     0.110938
f_DMTA_ilr_3 -0.4368504 -0.4331884  0.488414  0.388186  0.500504     0.182923
sigma_low     0.1185122  0.1157488 -0.008654 -0.008344 -0.009363    -0.004837
rsd_high     -0.2786848 -0.2551649  0.019075  0.018399  0.020642     0.010657
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low  rsd_high
DMTA_0          0.0009349     -0.43685  0.118512 -0.278685
log_k_DMTA      0.0002647     -0.43319  0.115749 -0.255165
log_k_M23       0.2928453      0.48841 -0.008654  0.019075
log_k_M27       0.2320001      0.38819 -0.008344  0.018399
log_k_M31      -0.7135096      0.50050 -0.009363  0.020642
f_DMTA_ilr_1    0.1109380      0.18292 -0.004837  0.010657
f_DMTA_ilr_2    1.0000000     -0.19043  0.002790 -0.006149
f_DMTA_ilr_3   -0.1904340      1.00000 -0.050588  0.111522
sigma_low       0.0027898     -0.05059  1.000000 -0.178354
rsd_high       -0.0061487      0.11152 -0.178354  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value    Pr(>t)     Lower     Upper
DMTA_0        99.640000  97.640 2.869e-85 97.610000 1.017e+02
k_DMTA         0.070800  64.000 8.844e-71  0.068630 7.304e-02
k_M23          0.021860   9.221 1.616e-14  0.017620 2.713e-02
k_M27          0.006686   5.433 2.906e-07  0.004635 9.643e-03
k_M31          0.013470   5.887 4.414e-08  0.009603 1.888e-02
f_DMTA_to_M23  0.142800  16.710 4.144e-28        NA        NA
f_DMTA_to_M27  0.130100  20.960 1.556e-34        NA        NA
f_DMTA_to_M31  0.097390  14.030 1.426e-23        NA        NA
sigma_low      0.906800  12.070 5.276e-20  0.757300 1.056e+00
rsd_high       0.023050   3.608 2.682e-04  0.010340 3.577e-02

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.872       8 37
DMTA       3.520       2 10
M23        9.330       2  9
M27       10.716       2  9
M31       10.649       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.14284
DMTA_M27  0.13005
DMTA_M31  0.09739
DMTA_sink 0.62972

Estimated disappearance times:
       DT50   DT90
DMTA   9.79  32.52
M23   31.71 105.33
M27  103.68 344.41
M31   51.48 171.00

Data:
    time variable observed predicted  residual
```

```
 0.0000     DMTA    98.09   99.6371 -1.547129
 0.0000     DMTA    98.77   99.6371 -0.867129
 0.7679     DMTA    93.52   94.3648 -0.844840
 0.7679     DMTA    92.03   94.3648 -2.334840
 2.3037     DMTA    88.39   84.6424  3.747552
 2.3037     DMTA    87.18   84.6424  2.537552
 5.3752     DMTA    69.38   68.0995  1.280452
 5.3752     DMTA    71.06   68.0995  2.960452
10.7505     DMTA    45.21   46.5444 -1.334381
10.7505     DMTA    46.81   46.5444  0.265619
16.1257     DMTA    30.54   31.8119 -1.271950
16.1257     DMTA    30.07   31.8119 -1.741950
21.5010     DMTA    21.60   21.7427 -0.142692
21.5010     DMTA    20.41   21.7427 -1.332692
32.2515     DMTA     9.10   10.1569 -1.056858
32.2515     DMTA     9.70   10.1569 -0.456858
43.0020     DMTA     6.58    4.7447  1.835336
43.0020     DMTA     6.31    4.7447  1.565336
53.7525     DMTA     3.47    2.2164  1.253583
53.7525     DMTA     3.52    2.2164  1.303583
64.5029     DMTA     3.40    1.0354  2.364625
64.5029     DMTA     3.67    1.0354  2.634625
91.3792     DMTA     1.62    0.1544  1.465577
91.3792     DMTA     1.62    0.1544  1.465577
 0.7679      M23     0.36    0.7468 -0.386752
 0.7679      M23     0.40    0.7468 -0.346752
 2.3037      M23     1.03    2.0874 -1.057376
 2.3037      M23     1.07    2.0874 -1.017376
 5.3752      M23     3.60    4.2344 -0.634443
 5.3752      M23     3.66    4.2344 -0.574443
10.7505      M23     6.97    6.6591  0.310869
10.7505      M23     7.22    6.6591  0.560869
16.1257      M23     8.65    7.8989  0.751060
16.1257      M23     8.38    7.8989  0.481060
21.5010      M23     9.10    8.3752  0.724810
21.5010      M23     8.63    8.3752  0.254810
32.2515      M23     7.63    8.0742 -0.444247
32.2515      M23     8.01    8.0742 -0.064247
43.0020      M23     6.40    7.0620 -0.662008
43.0020      M23     6.35    7.0620 -0.712008
53.7525      M23     5.35    5.9001 -0.550054
53.7525      M23     5.06    5.9001 -0.840054
64.5029      M23     5.14    4.8125  0.327515
64.5029      M23     5.91    4.8125  1.097515
91.3792      M23     3.35    2.7613  0.588728
91.3792      M23     2.87    2.7613  0.108728
 0.7679      M27     0.42    0.6839 -0.263891
 0.7679      M27     0.47    0.6839 -0.213891
 2.3037      M27     0.71    1.9347 -1.224721
 2.3037      M27     0.82    1.9347 -1.114721
 5.3752      M27     2.19    4.0241 -1.834077
 5.3752      M27     2.28    4.0241 -1.744077
10.7505      M27     5.45    6.6324 -1.182390
10.7505      M27     5.19    6.6324 -1.442390
16.1257      M27     8.81    8.2781  0.531923
16.1257      M27     7.93    8.2781 -0.348077
21.5010      M27    10.25    9.2707  0.979330
21.5010      M27    10.77    9.2707  1.499330
32.2515      M27    10.89   10.0750  0.814956
32.2515      M27    10.85   10.0750  0.774956
43.0020      M27    10.41   10.0524  0.357582
43.0020      M27    10.35   10.0524  0.297582
53.7525      M27     9.92    9.6711  0.248904
53.7525      M27     9.42    9.6711 -0.251096
64.5029      M27     9.15    9.1479  0.002075
64.5029      M27     9.25    9.1479  0.102075
91.3792      M27     7.14    7.7455 -0.605458
91.3792      M27     7.13    7.7455 -0.615458
 0.7679      M31     0.36    0.5108 -0.150781
```

```
  0.7679      M31     0.33    0.5108 -0.180781
  2.3037      M31     0.55    1.4373 -0.887257
  2.3037      M31     0.64    1.4373 -0.797257
  5.3752      M31     1.94    2.9560 -1.016036
  5.3752      M31     1.62    2.9560 -1.336036
 10.7505      M31     4.22    4.7700 -0.550014
 10.7505      M31     4.37    4.7700 -0.400014
 16.1257      M31     6.31    5.8178  0.492165
 16.1257      M31     6.85    5.8178  1.032165
 21.5010      M31     7.05    6.3554  0.694588
 21.5010      M31     6.84    6.3554  0.484588
 32.2515      M31     6.53    6.5398 -0.009790
 32.2515      M31     7.11    6.5398  0.570210
 43.0020      M31     6.06    6.1447 -0.084661
 43.0020      M31     6.05    6.1447 -0.094661
 53.7525      M31     5.50    5.5437 -0.043681
 53.7525      M31     5.07    5.5437 -0.473681
 64.5029      M31     4.94    4.9027  0.037341
 64.5029      M31     4.39    4.9027 -0.512659
 91.3792      M31     3.64    3.4821  0.157904
 91.3792      M31     3.55    3.4821  0.067904
```

Listing 45: SFO-SFO3 fit to BBA 2.3 data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:04 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1141 model solutions performed in 2.091 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.3850  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.385000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  332.1562 354.6544 -157.0781

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error  Lower    Upper
DMTA_0        99.9600    0.61970 98.720 101.2000
log_k_DMTA    -2.5570    0.01577 -2.588  -2.5260
log_k_M23     -3.8930    0.44330 -4.775  -3.0110
log_k_M27     -4.0520    0.13510 -4.321  -3.7830
log_k_M31     -3.1410    0.12950 -3.399  -2.8830
f_DMTA_ilr_1  -0.8669    0.15860 -1.183  -0.5513
f_DMTA_ilr_2  -0.5641    0.11460 -0.792  -0.3361
f_DMTA_ilr_3  -1.3760    0.10060 -1.576  -1.1760
sigma          1.3860    0.10330  1.180   1.5910

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.394e-01 -1.938e-02 -6.730e-02 -6.097e-02
log_k_DMTA    5.394e-01  1.000e+00 -3.593e-02 -1.248e-01 -1.130e-01
log_k_M23    -1.938e-02 -3.593e-02  1.000e+00  4.482e-03  4.060e-03
log_k_M27    -6.730e-02 -1.248e-01  4.482e-03  1.000e+00  1.410e-02
log_k_M31    -6.097e-02 -1.130e-01  4.060e-03  1.410e-02  1.000e+00
f_DMTA_ilr_1 -6.699e-04 -1.242e-03  7.707e-01 -2.120e-01  1.404e-04
f_DMTA_ilr_2  9.792e-03  1.815e-02  6.154e-01  1.673e-01 -4.834e-01
f_DMTA_ilr_3 -1.805e-01 -2.146e-01  6.346e-01  2.859e-01  4.062e-01
sigma         2.714e-07  6.757e-09 -3.615e-08 -1.257e-08  2.445e-08
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -6.699e-04    9.792e-03   -1.805e-01  2.714e-07
log_k_DMTA     -1.242e-03    1.815e-02   -2.146e-01  6.757e-09
log_k_M23       7.707e-01    6.154e-01    6.346e-01 -3.615e-08
log_k_M27      -2.120e-01    1.673e-01    2.859e-01 -1.257e-08
log_k_M31       1.404e-04   -4.834e-01    4.062e-01  2.445e-08
f_DMTA_ilr_1    1.000e+00    6.854e-01    6.687e-01 -4.551e-09
f_DMTA_ilr_2    6.854e-01    1.000e+00    3.832e-01 -4.563e-09
f_DMTA_ilr_3    6.687e-01    3.832e-01    1.000e+00 -3.191e-08
sigma          -4.551e-09   -4.563e-09   -3.191e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)     Lower     Upper
DMTA_0        99.96000 161.300 1.175e-103 98.720000 101.20000
k_DMTA         0.07754  63.400  4.219e-71  0.075140   0.08001
k_M23          0.02039   2.256  1.339e-02  0.008441   0.04926
k_M27          0.01739   7.402  5.586e-11  0.013290   0.02276
k_M31          0.04324   7.724  1.313e-11  0.033420   0.05594
f_DMTA_to_M23  0.05135   4.614  7.294e-06        NA        NA
f_DMTA_to_M27  0.17500  16.230  1.726e-27        NA        NA
f_DMTA_to_M31  0.18920  11.630  2.973e-19        NA        NA
sigma          1.38600  13.420  1.391e-22  1.180000   1.59100

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   8.763       8 37
DMTA       4.555       2 10
M23        8.491       2  9
M27       10.561       2  9
M31       14.682       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.05135
DMTA_M27  0.17500
DMTA_M31  0.18916
DMTA_sink 0.58449

Estimated disappearance times:
      DT50   DT90
DMTA  8.94  29.70
M23  33.99 112.92
M27  39.85 132.39
M31  16.03  53.26

Data:
    time variable observed predicted residual
  0.0000     DMTA    99.33   99.9559 -0.62590
  0.0000     DMTA    97.44   99.9559 -2.51590
  0.6734     DMTA    93.73   94.8709 -1.14088
  0.6734     DMTA    93.77   94.8709 -1.10088
  2.0202     DMTA    87.84   85.4638  2.37625
  2.0202     DMTA    89.82   85.4638  4.35625
  4.7138     DMTA    71.61   69.3554  2.25465
  4.7138     DMTA    71.42   69.3554  2.06465
  9.4275     DMTA    45.60   48.1229 -2.52287
```

```
 9.4275    DMTA   45.42   48.1229 -2.70287
14.1413    DMTA   31.12   33.3905 -2.27051
14.1413    DMTA   31.68   33.3905 -1.71051
18.8550    DMTA   23.20   23.1683  0.03168
18.8550    DMTA   24.13   23.1683  0.96168
28.2825    DMTA    9.43   11.1542 -1.72418
28.2825    DMTA    9.82   11.1542 -1.33418
37.7101    DMTA    7.08    5.3701  1.70992
37.7101    DMTA    8.64    5.3701  3.26992
47.1376    DMTA    4.41    2.5854  1.82462
47.1376    DMTA    4.78    2.5854  2.19462
56.5651    DMTA    4.92    1.2447  3.67529
56.5651    DMTA    5.08    1.2447  3.83529
80.1339    DMTA    2.13    0.2002  1.92982
80.1339    DMTA    2.23    0.2002  2.02982
 0.6734     M23    0.18    0.2593 -0.07934
 0.6734     M23    0.18    0.2593 -0.07934
 2.0202     M23    0.52    0.7287 -0.20872
 2.0202     M23    0.43    0.7287 -0.29872
 4.7138     M23    1.19    1.4939 -0.30393
 4.7138     M23    1.11    1.4939 -0.38393
 9.4275     M23    2.26    2.3936 -0.13360
 9.4275     M23    1.99    2.3936 -0.40360
14.1413     M23    2.81    2.8935 -0.08349
14.1413     M23    2.83    2.8935 -0.06349
18.8550     M23    3.39    3.1274  0.26263
18.8550     M23    3.56    3.1274  0.43263
28.2825     M23    3.49    3.1352  0.35476
28.2825     M23    3.28    3.1352  0.14476
37.7101     M23    2.80    2.8540 -0.05403
37.7101     M23    2.97    2.8540  0.11597
47.1376     M23    2.42    2.4835 -0.06350
47.1376     M23    2.51    2.4835  0.02650
56.5651     M23    2.22    2.1111  0.10892
56.5651     M23    1.95    2.1111 -0.16108
80.1339     M23    1.28    1.3452 -0.06522
80.1339     M23    0.99    1.3452 -0.35522
 0.6734     M27    0.50    0.8846 -0.38464
 0.6734     M27    0.83    0.8846 -0.05464
 2.0202     M27    1.25    2.4909 -1.24095
 2.0202     M27    1.09    2.4909 -1.40095
 4.7138     M27    3.28    5.1287 -1.84866
 4.7138     M27    3.24    5.1287 -1.88866
 9.4275     M27    7.17    8.2836 -1.11355
 9.4275     M27    7.91    8.2836 -0.37355
14.1413     M27   10.15   10.1007  0.04931
14.1413     M27    9.55   10.1007 -0.55069
18.8550     M27   12.09   11.0189  1.07111
18.8550     M27   11.89   11.0189  0.87111
28.2825     M27   13.32   11.2725  2.04745
28.2825     M27   12.05   11.2725  0.77745
37.7101     M27   10.04   10.4922 -0.45220
37.7101     M27   10.78   10.4922  0.28780
47.1376     M27    9.32    9.3505 -0.03053
47.1376     M27    9.62    9.3505  0.26947
56.5651     M27    8.00    8.1507 -0.15073
56.5651     M27    8.45    8.1507  0.29927
80.1339     M27    5.71    5.5509  0.15906
80.1339     M27    3.33    5.5509 -2.22094
 0.6734     M31    0.47    0.9479 -0.47789
 0.6734     M31    0.34    0.9479 -0.60789
 2.0202     M31    1.00    2.6220 -1.62201
 2.0202     M31    0.89    2.6220 -1.73201
 4.7138     M31    3.58    5.2042 -1.62425
 4.7138     M31    3.41    5.2042 -1.79425
 9.4275     M31    8.74    7.8557  0.88430
 9.4275     M31    8.28    7.8557  0.42430
14.1413     M31    9.67    8.9128  0.75719
14.1413     M31    8.95    8.9128  0.03719
```

```
  18.8550      M31    10.34    9.0080  1.33204
  18.8550      M31    10.00    9.0080  0.99204
  28.2825      M31     7.89    7.8133  0.07674
  28.2825      M31     8.13    7.8133  0.31674
  37.7101      M31     5.06    6.0743 -1.01429
  37.7101      M31     5.54    6.0743 -0.53429
  47.1376      M31     3.79    4.4629 -0.67289
  47.1376      M31     4.11    4.4629 -0.35289
  56.5651      M31     3.11    3.1721 -0.06206
  56.5651      M31     2.98    3.1721 -0.19206
  80.1339      M31     1.78    1.2514  0.52855
  80.1339      M31     1.55    1.2514  0.29855
```

Listing 46: SFO-SFO3 fit to BBA 2.3 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:49 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 5174 model solutions performed in 9.751 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.3850  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.385000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  323.0818 348.0799 -151.5409

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error     Lower    Upper
DMTA_0       99.21000    1.42700 96.370000 102.0000
log_k_DMTA   -2.56800    0.02341 -2.614000  -2.5210
log_k_M23    -3.88200    0.37430 -4.627000  -3.1370
log_k_M27    -4.04200    0.11800 -4.277000  -3.8070
log_k_M31    -3.13300    0.11200 -3.356000  -2.9100
f_DMTA_ilr_1 -0.86560    0.13490 -1.134000  -0.5971
```

```
f_DMTA_ilr_2 -0.56460    0.09789 -0.759400  -0.3698
f_DMTA_ilr_3 -1.35700    0.09412 -1.544000  -1.1690
sigma_low     1.17100    0.10260  0.966900   1.3750
rsd_high      0.02966    0.01032  0.009112   0.0502

Parameter correlation:
               DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.000000   0.731570  -0.04615  -0.14966 -0.136270    -0.005036
log_k_DMTA    0.731570   1.000000  -0.06310  -0.20594 -0.187805    -0.005969
log_k_M23    -0.046151  -0.063096   1.00000   0.01299  0.011850     0.769448
log_k_M27    -0.149660  -0.205937   0.01299   1.00000  0.038757    -0.212810
log_k_M31    -0.136270  -0.187805   0.01185   0.03876  1.000000     0.001067
f_DMTA_ilr_1 -0.005036  -0.005969   0.76945  -0.21281  0.001067     1.000000
f_DMTA_ilr_2  0.019625   0.027781   0.61011   0.16448 -0.485013     0.676866
f_DMTA_ilr_3 -0.409744  -0.418631   0.59774   0.32623  0.430168     0.606442
sigma_low     0.254075   0.287115  -0.01809  -0.05539 -0.049710    -0.004226
rsd_high     -0.488099  -0.533088   0.03358   0.10283  0.092296     0.007844
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low  rsd_high
DMTA_0           0.019625      -0.4097  0.254075 -0.488099
log_k_DMTA       0.027781      -0.4186  0.287115 -0.533088
log_k_M23        0.610109       0.5977 -0.018086  0.033575
log_k_M27        0.164477       0.3262 -0.055385  0.102834
log_k_M31       -0.485013       0.4302 -0.049710  0.092296
f_DMTA_ilr_1     0.676866       0.6064 -0.004226  0.007844
f_DMTA_ilr_2     1.000000       0.3334  0.005353 -0.009939
f_DMTA_ilr_3     0.333399       1.0000 -0.121839  0.226215
sigma_low        0.005353      -0.1218  1.000000 -0.331063
rsd_high        -0.009939       0.2262 -0.331063  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value    Pr(>t)     Lower     Upper
DMTA_0        99.21000  69.520 1.324e-73 96.370000 102.00000
k_DMTA         0.07670  42.710 3.902e-57  0.073210   0.08036
k_M23          0.02061   2.671 4.574e-03  0.009787   0.04342
k_M27          0.01757   8.476 4.712e-13  0.013890   0.02222
k_M31          0.04360   8.927 6.119e-14  0.034890   0.05449
f_DMTA_to_M23  0.05206   5.389 3.482e-07        NA        NA
f_DMTA_to_M27  0.17710  17.130 8.602e-29        NA        NA
f_DMTA_to_M31  0.19170  12.730 3.132e-21        NA        NA
sigma_low      1.17100  11.410 9.139e-19  0.966900   1.37500
rsd_high       0.02966   2.873 2.604e-03  0.009112   0.05020

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   8.839       8 37
DMTA       4.615       2 10
M23        8.403       2  9
M27       10.473       2  9
M31       14.655       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.05206
DMTA_M27  0.17708
DMTA_M31  0.19171
DMTA_sink 0.57915

Estimated disappearance times:
       DT50   DT90
DMTA  9.037  30.02
M23  33.624 111.70
M27  39.457 131.07
M31  15.898  52.81

Data:
    time variable observed predicted residual
```

```
 0.0000    DMTA   99.33   99.2054  0.12461
 0.0000    DMTA   97.44   99.2054 -1.76539
 0.6734    DMTA   93.73   94.2116 -0.48163
 0.6734    DMTA   93.77   94.2116 -0.44163
 2.0202    DMTA   87.84   84.9656  2.87443
 2.0202    DMTA   89.82   84.9656  4.85443
 4.7138    DMTA   71.61   69.1067  2.50334
 4.7138    DMTA   71.42   69.1067  2.31334
 9.4275    DMTA   45.60   48.1398 -2.53983
 9.4275    DMTA   45.42   48.1398 -2.71983
14.1413    DMTA   31.12   33.5343 -2.41430
14.1413    DMTA   31.68   33.5343 -1.85430
18.8550    DMTA   23.20   23.3601 -0.16006
18.8550    DMTA   24.13   23.3601  0.76994
28.2825    DMTA    9.43   11.3356 -1.90556
28.2825    DMTA    9.82   11.3356 -1.51556
37.7101    DMTA    7.08    5.5006  1.57937
37.7101    DMTA    8.64    5.5006  3.13937
47.1376    DMTA    4.41    2.6692  1.74080
47.1376    DMTA    4.78    2.6692  2.11080
56.5651    DMTA    4.92    1.2952  3.62476
56.5651    DMTA    5.08    1.2952  3.78476
80.1339    DMTA    2.13    0.2125  1.91754
80.1339    DMTA    2.23    0.2125  2.01754
 0.6734     M23    0.18    0.2582 -0.07818
 0.6734     M23    0.18    0.2582 -0.07818
 2.0202     M23    0.52    0.7258 -0.20577
 2.0202     M23    0.43    0.7258 -0.29577
 4.7138     M23    1.19    1.4890 -0.29898
 4.7138     M23    1.11    1.4890 -0.37898
 9.4275     M23    2.26    2.3883 -0.12832
 9.4275     M23    1.99    2.3883 -0.39832
14.1413     M23    2.81    2.8897 -0.07970
14.1413     M23    2.83    2.8897 -0.05970
18.8550     M23    3.39    3.1254  0.26457
18.8550     M23    3.56    3.1254  0.43457
28.2825     M23    3.49    3.1358  0.35421
28.2825     M23    3.28    3.1358  0.14421
37.7101     M23    2.80    2.8548 -0.05483
37.7101     M23    2.97    2.8548  0.11517
47.1376     M23    2.42    2.4830 -0.06303
47.1376     M23    2.51    2.4830  0.02697
56.5651     M23    2.22    2.1087  0.11128
56.5651     M23    1.95    2.1087 -0.15872
80.1339     M23    1.28    1.3388 -0.05883
80.1339     M23    0.99    1.3388 -0.34883
 0.6734     M27    0.50    0.8790 -0.37903
 0.6734     M27    0.83    0.8790 -0.04903
 2.0202     M27    1.25    2.4762 -1.22620
 2.0202     M27    1.09    2.4762 -1.38620
 4.7138     M27    3.28    5.1024 -1.82239
 4.7138     M27    3.24    5.1024 -1.86239
 9.4275     M27    7.17    8.2512 -1.08123
 9.4275     M27    7.91    8.2512 -0.34123
14.1413     M27   10.15   10.0715  0.07854
14.1413     M27    9.55   10.0715 -0.52146
18.8550     M27   12.09   10.9958  1.09417
18.8550     M27   11.89   10.9958  0.89417
28.2825     M27   13.32   11.2605  2.05949
28.2825     M27   12.05   11.2605  0.78949
37.7101     M27   10.04   10.4847 -0.44469
37.7101     M27   10.78   10.4847  0.29531
47.1376     M27    9.32    9.3420 -0.02196
47.1376     M27    9.62    9.3420  0.27804
56.5651     M27    8.00    8.1381 -0.13814
56.5651     M27    8.45    8.1381  0.31186
80.1339     M27    5.71    5.5270  0.18301
80.1339     M27    3.33    5.5270 -2.19699
 0.6734     M31    0.47    0.9433 -0.47332
```

```
  0.6734      M31     0.34    0.9433 -0.60332
  2.0202      M31     1.00    2.6102 -1.61018
  2.0202      M31     0.89    2.6102 -1.72018
  4.7138      M31     3.58    5.1837 -1.60373
  4.7138      M31     3.41    5.1837 -1.77373
  9.4275      M31     8.74    7.8317  0.90829
  9.4275      M31     8.28    7.8317  0.44829
 14.1413      M31     9.67    8.8922  0.77783
 14.1413      M31     8.95    8.8922  0.05783
 18.8550      M31    10.34    8.9925  1.34755
 18.8550      M31    10.00    8.9925  1.00755
 28.2825      M31     7.89    7.8058  0.08425
 28.2825      M31     8.13    7.8058  0.32425
 37.7101      M31     5.06    6.0698 -1.00975
 37.7101      M31     5.54    6.0698 -0.52975
 47.1376      M31     3.79    4.4582 -0.66823
 47.1376      M31     4.11    4.4582 -0.34823
 56.5651      M31     3.11    3.1663 -0.05633
 56.5651      M31     2.98    3.1663 -0.18633
 80.1339      M31     1.78    1.2446  0.53537
 80.1339      M31     1.55    1.2446  0.30537
```

Listing 47: SFO-SFO3 fit to Borstel data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:07 2021
Date of summary: Mon Jul 26 18:52:53 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1435 model solutions performed in 2.154 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                 value   type
DMTA_0        100.2000  state
k_DMTA          0.1000 deparm
k_M23           0.1001 deparm
k_M27           0.1002 deparm
k_M31           0.1003 deparm
f_DMTA_to_M23   0.2500 deparm
f_DMTA_to_M27   0.2500 deparm
f_DMTA_to_M31   0.2500 deparm

Starting values for the transformed parameters actually optimised:
                  value lower upper
DMTA_0       100.200000  -Inf   Inf
log_k_DMTA    -2.302585  -Inf   Inf
log_k_M23     -2.301586  -Inf   Inf
log_k_M27     -2.300587  -Inf   Inf
log_k_M31     -2.299590  -Inf   Inf
f_DMTA_ilr_1   0.000000  -Inf   Inf
f_DMTA_ilr_2   0.000000  -Inf   Inf
f_DMTA_ilr_3   0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  224.1766 243.1745 -103.0883

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower   Upper
DMTA_0       97.21000    0.52580  96.1500 98.2600
log_k_DMTA   -3.77900    0.01477  -3.8090 -3.7490
log_k_M23    -7.75000    4.13500 -16.0500  0.5469
log_k_M27    -8.28600   16.36000 -41.1100 24.5400
log_k_M31    -4.87700    0.59520  -6.0710 -3.6830
f_DMTA_ilr_1  0.56390    0.18850   0.1857  0.9420
f_DMTA_ilr_2  0.04681    0.20900  -0.3727  0.4663
f_DMTA_ilr_3 -1.77600    0.13480  -2.0460 -1.5050
sigma         1.31100    0.11870   1.0730  1.5500

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.213e-01 -3.412e-02 -1.445e-02 -1.945e-02
log_k_DMTA    5.213e-01  1.000e+00 -6.546e-02 -2.771e-02 -3.731e-02
log_k_M23    -3.412e-02 -6.546e-02  1.000e+00  1.814e-03  2.442e-03
log_k_M27    -1.445e-02 -2.771e-02  1.814e-03  1.000e+00  1.034e-03
log_k_M31    -1.945e-02 -3.731e-02  2.442e-03  1.034e-03  1.000e+00
f_DMTA_ilr_1 -3.340e-04 -6.406e-04  3.591e-01 -8.385e-01  2.390e-05
f_DMTA_ilr_2  1.698e-03  3.257e-03  1.866e-01  4.364e-01 -7.576e-01
f_DMTA_ilr_3 -1.057e-01 -1.345e-01  3.338e-01  6.088e-01  5.747e-01
sigma        -1.353e-07 -1.197e-07  1.823e-09 -1.810e-08  4.215e-09
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -3.340e-04    1.698e-03   -1.057e-01 -1.353e-07
log_k_DMTA     -6.406e-04    3.257e-03   -1.345e-01 -1.197e-07
log_k_M23       3.591e-01    1.866e-01    3.338e-01  1.823e-09
log_k_M27      -8.385e-01    4.364e-01    6.088e-01 -1.810e-08
log_k_M31       2.390e-05   -7.576e-01    5.747e-01  4.215e-09
f_DMTA_ilr_1    1.000e+00   -3.560e-01   -4.643e-01  1.552e-08
f_DMTA_ilr_2   -3.560e-01    1.000e+00   -1.581e-01 -9.425e-09
f_DMTA_ilr_3   -4.643e-01   -1.581e-01    1.000e+00  5.301e-09
sigma           1.552e-08   -9.425e-09    5.301e-09  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate   t value    Pr(>t)     Lower     Upper
DMTA_0        9.721e+01 184.90000 2.901e-75 9.615e+01 9.826e+01
k_DMTA        2.284e-02  67.71000 1.092e-52 2.218e-02 2.353e-02
k_M23         4.309e-04   0.24190 4.049e-01 1.074e-07 1.728e+00
k_M27         2.520e-04   0.06113 4.757e-01 1.400e-18 4.538e+10
k_M31         7.618e-03   1.68000 4.945e-02 2.308e-03 2.515e-02
f_DMTA_to_M23 1.389e-01   9.34000 5.199e-13        NA        NA
f_DMTA_to_M27 6.255e-02   4.08100 7.737e-05        NA        NA
f_DMTA_to_M31 8.801e-02   4.56200 1.562e-05        NA        NA
sigma         1.311e+00  11.05000 1.501e-15 1.073e+00 1.550e+00

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.217       8 21
DMTA       2.585       2  6
M23       19.213       2  5
M27        3.918       2  5
M31        5.428       2  5

Resulting formation fractions:
               ff
DMTA_M23  0.13886
DMTA_M27  0.06255
DMTA_M31  0.08801
DMTA_sink 0.71058

Estimated disappearance times:
        DT50   DT90
DMTA   30.34  100.8
M23  1608.69 5344.0
M27  2750.24 9136.1
M31    90.98  302.2

Data:
    time variable observed predicted  residual
   0.000     DMTA    100.5   97.2083  3.291744
   0.000     DMTA    100.5   97.2083  3.291744
   0.000     DMTA     99.6   97.2083  2.391744
   1.941     DMTA     91.9   92.9918 -1.091818
   1.941     DMTA     91.3   92.9918 -1.691818
   6.795     DMTA     81.8   83.2336 -1.433603
   6.795     DMTA     82.1   83.2336 -1.133603
  13.589     DMTA     69.1   71.2679 -2.167946
  13.589     DMTA     68.0   71.2679 -3.267946
```

```
  27.178     DMTA     51.4   52.2499 -0.849884
  27.178     DMTA     51.4   52.2499 -0.849884
  27.178     DMTA     51.4   52.2499 -0.849884
  56.298     DMTA     26.8   26.8664 -0.066376
  56.298     DMTA     27.6   26.8664  0.733624
  56.298     DMTA     26.8   26.8664 -0.066376
  86.388     DMTA     15.7   13.5115  2.188498
  86.388     DMTA     15.7   13.5115  2.188498
  86.388     DMTA     15.3   13.5115  1.788498
 115.507     DMTA      7.9    6.9475  0.952519
 115.507     DMTA      7.9    6.9475  0.952519
 115.507     DMTA      8.1    6.9475  1.152519
   1.941      M23      0.4    0.5852 -0.185245
   1.941      M23      0.5    0.5852 -0.085245
   6.795      M23      1.2    1.9376 -0.737598
   6.795      M23      1.3    1.9376 -0.637598
  13.589      M23      2.8    3.5910 -0.790983
  13.589      M23      2.0    3.5910 -1.590983
  27.178      M23      2.9    6.2027 -3.302737
  27.178      M23      4.9    6.2027 -1.302737
  56.298      M23     12.2    9.6257  2.574305
  56.298      M23     12.2    9.6257  2.574305
  86.388      M23     12.2   11.3428  0.857178
  86.388      M23     12.0   11.3428  0.657178
 115.507      M23     10.4   12.1065 -1.706549
 115.507      M23     11.6   12.1065 -0.506549
   1.941      M27      0.3    0.2637  0.036307
   6.795      M27      0.8    0.8734 -0.073411
   6.795      M27      0.9    0.8734  0.026589
  13.589      M27      1.4    1.6198 -0.219767
  13.589      M27      1.4    1.6198 -0.219767
  27.178      M27      2.7    2.8018 -0.101756
  27.178      M27      2.6    2.8018 -0.201756
  56.298      M27      4.4    4.3627  0.037327
  56.298      M27      4.7    4.3627  0.337327
  86.388      M27      5.4    5.1616  0.238396
  86.388      M27      5.2    5.1616  0.038396
 115.507      M27      5.4    5.5328 -0.132803
 115.507      M27      5.4    5.5328 -0.132803
   1.941      M31      0.1    0.3683 -0.268328
   6.795      M31      1.0    1.1978 -0.197785
   6.795      M31      0.9    1.1978 -0.297785
  13.589      M31      2.0    2.1630 -0.162954
  13.589      M31      2.5    2.1630  0.337046
  27.178      M31      4.3    3.5360  0.764002
  27.178      M31      3.2    3.5360 -0.335998
  56.298      M31      4.3    4.8116 -0.511617
  56.298      M31      4.8    4.8116 -0.011617
  86.388      M31      5.0    4.8626  0.137368
  86.388      M31      5.1    4.8626  0.237368
 115.507      M31      4.3    4.4070 -0.106973
 115.507      M31      4.4    4.4070 -0.006973
```

Listing 48: SFO-SFO3 fit to Borstel data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:55 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 6215 model solutions performed in 10.568 s

Error model: Two-component variance function

Error model algorithm: d_3
Three-step fitting yielded a higher likelihood than direct fitting

Starting values for parameters to be optimised:
                 value   type
DMTA_0        100.2000  state
k_DMTA          0.1000 deparm
k_M23           0.1001 deparm
k_M27           0.1002 deparm
k_M31           0.1003 deparm
f_DMTA_to_M23   0.2500 deparm
f_DMTA_to_M27   0.2500 deparm
f_DMTA_to_M31   0.2500 deparm
sigma_low       0.1000  error
rsd_high        0.1000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
DMTA_0       100.200000  -Inf   Inf
log_k_DMTA    -2.302585  -Inf   Inf
log_k_M23     -2.301586  -Inf   Inf
log_k_M27     -2.300587  -Inf   Inf
log_k_M31     -2.299590  -Inf   Inf
f_DMTA_ilr_1   0.000000  -Inf   Inf
f_DMTA_ilr_2   0.000000  -Inf   Inf
f_DMTA_ilr_3   0.000000  -Inf   Inf
sigma_low      0.100000     0   Inf
rsd_high       0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state


Warning(s):
Optimisation did not converge:
iteration limit reached without convergence (10)

Results:

       AIC      BIC    logLik
  198.7345 219.8432 -89.36725

Optimised, transformed parameters with symmetric confidence intervals:
               Estimate Std. Error      Lower    Upper
DMTA_0        91.550000    3.69000   84.14000  98.9600
```

```
log_k_DMTA    -3.866000    0.03295   -3.93200  -3.8000
log_k_M23    -16.830000  114.00000 -245.70000 212.0000
log_k_M27     -9.881000   33.37000  -76.87000  57.1100
log_k_M31     -4.823000    0.21570   -5.25600  -4.3900
f_DMTA_ilr_1   0.522500    0.06072    0.40060   0.6444
f_DMTA_ilr_2  -0.002031    0.06457   -0.13170   0.1276
f_DMTA_ilr_3  -1.714000    0.08612   -1.88700  -1.5420
sigma_low      0.127500    0.05236    0.02237   0.2326
rsd_high       0.135200    0.01520    0.10460   0.1657

Parameter correlation:
                DMTA_0 log_k_DMTA  log_k_M23 log_k_M27  log_k_M31 f_DMTA_ilr_1
DMTA_0        1.0000000   0.693095 -0.0005559 -0.131429 -0.1352637     0.116618
log_k_DMTA    0.6930949   1.000000 -0.0006430 -0.188884 -0.2130699     0.159277
log_k_M23    -0.0005559  -0.000643  1.0000000  0.000118  0.0001844     0.002452
log_k_M27    -0.1314291  -0.188884  0.0001180  1.000000  0.0379375    -0.739236
log_k_M31    -0.1352637  -0.213070  0.0001844  0.037938  1.0000000    -0.009294
f_DMTA_ilr_1  0.1166176   0.159277  0.0024515 -0.739236 -0.0092937     1.000000
f_DMTA_ilr_2  0.0348605   0.065741  0.0012893  0.373955 -0.6731402    -0.312265
f_DMTA_ilr_3 -0.8113088  -0.753708  0.0016761  0.403102  0.4212725    -0.292497
sigma_low     0.1010415   0.091859  0.0004694 -0.027565  0.1979095     0.121734
rsd_high     -0.1335354  -0.052943  0.0011821  0.015185 -0.1142614    -0.071396
             f_DMTA_ilr_2 f_DMTA_ilr_3  sigma_low  rsd_high
DMTA_0           0.034860    -0.811309  0.1010415 -0.133535
log_k_DMTA       0.065741    -0.753708  0.0918587 -0.052943
log_k_M23        0.001289     0.001676  0.0004694  0.001182
log_k_M27        0.373955     0.403102 -0.0275646  0.015185
log_k_M31       -0.673140     0.421273  0.1979095 -0.114261
f_DMTA_ilr_1    -0.312265    -0.292497  0.1217336 -0.071396
f_DMTA_ilr_2     1.000000    -0.124931 -0.1834204  0.104747
f_DMTA_ilr_3    -0.124931     1.000000  0.0598538 -0.036004
sigma_low       -0.183420     0.059854  1.0000000 -0.378294
rsd_high         0.104747    -0.036004 -0.3782944  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
                Estimate   t value    Pr(>t)      Lower     Upper
DMTA_0        9.155e+01 2.437e+01 4.574e-30  8.414e+01 9.896e+01
k_DMTA        2.095e-02 2.965e+01 3.987e-34  1.961e-02 2.238e-02
k_M23         4.914e-08 2.504e-05 5.000e-01 1.982e-107 1.219e+92
k_M27         5.116e-05 3.129e-02 4.876e-01  4.121e-34 6.351e+24
k_M31         8.041e-03 4.625e+00 1.297e-05  5.215e-03 1.240e-02
f_DMTA_to_M23 1.393e-01 9.182e+00 1.089e-12         NA        NA
f_DMTA_to_M27 6.653e-02 1.026e+01 2.695e-14         NA        NA
f_DMTA_to_M31 9.651e-02 1.068e+01 6.566e-15         NA        NA
sigma_low     1.275e-01 2.403e+00 9.978e-03  2.237e-02 2.326e-01
rsd_high      1.352e-01 8.217e+00 3.332e-11  1.046e-01 1.657e-01

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  10.267       8 21
DMTA       4.994       2  6
M23       20.172       2  5
M27        4.560       2  5
M31        5.762       2  5

Resulting formation fractions:
               ff
DMTA_M23  0.13931
DMTA_M27  0.06653
DMTA_M31  0.09651
DMTA_sink 0.69764

Estimated disappearance times:
          DT50      DT90
DMTA 3.309e+01 1.099e+02
M23  1.411e+07 4.686e+07
```

```
M27  1.355e+04 4.501e+04
M31  8.620e+01 2.863e+02

Data:
    time variable observed predicted  residual
   0.000     DMTA    100.5   91.5481  8.951923
   0.000     DMTA    100.5   91.5481  8.951923
   0.000     DMTA     99.6   91.5481  8.051923
   1.941     DMTA     91.9   87.8997  4.000334
   1.941     DMTA     91.3   87.8997  3.400334
   6.795     DMTA     81.8   79.4021  2.397855
   6.795     DMTA     82.1   79.4021  2.697855
  13.589     DMTA     69.1   68.8676  0.232353
  13.589     DMTA     68.0   68.8676 -0.867647
  27.178     DMTA     51.4   51.8061 -0.406143
  27.178     DMTA     51.4   51.8061 -0.406143
  27.178     DMTA     51.4   51.8061 -0.406143
  56.298     DMTA     26.8   28.1482 -1.348243
  56.298     DMTA     27.6   28.1482 -0.548243
  56.298     DMTA     26.8   28.1482 -1.348243
  86.388     DMTA     15.7   14.9862  0.713841
  86.388     DMTA     15.7   14.9862  0.713841
  86.388     DMTA     15.3   14.9862  0.313841
 115.507     DMTA      7.9    8.1425 -0.242549
 115.507     DMTA      7.9    8.1425 -0.242549
 115.507     DMTA      8.1    8.1425 -0.042549
   1.941      M23      0.4    0.5083 -0.108251
   1.941      M23      0.5    0.5083 -0.008251
   6.795      M23      1.2    1.6920 -0.492021
   6.795      M23      1.3    1.6920 -0.392021
  13.589      M23      2.8    3.1596 -0.359556
  13.589      M23      2.0    3.1596 -1.159556
  27.178      M23      2.9    5.5364 -2.636351
  27.178      M23      4.9    5.5364 -0.636351
  56.298      M23     12.2    8.8321  3.367934
  56.298      M23     12.2    8.8321  3.367934
  86.388      M23     12.2   10.6656  1.534370
  86.388      M23     12.0   10.6656  1.334370
 115.507      M23     10.4   11.6190 -1.218981
 115.507      M23     11.6   11.6190 -0.018981
   1.941      M27      0.3    0.2427  0.057268
   6.795      M27      0.8    0.8080 -0.007976
   6.795      M27      0.9    0.8080  0.092024
  13.589      M27      1.4    1.5085 -0.108475
  13.589      M27      1.4    1.5085 -0.108475
  27.178      M27      2.7    2.6422  0.057812
  27.178      M27      2.6    2.6422 -0.042188
  56.298      M27      4.4    4.2110  0.188976
  56.298      M27      4.7    4.2110  0.488976
  86.388      M27      5.4    5.0795  0.320468
  86.388      M27      5.2    5.0795  0.120468
 115.507      M27      5.4    5.5269 -0.126932
 115.507      M27      5.4    5.5269 -0.126932
   1.941      M31      0.1    0.3494 -0.249370
   6.795      M31      1.0    1.1401 -0.140064
   6.795      M31      0.9    1.1401 -0.240064
  13.589      M31      2.0    2.0683 -0.068253
  13.589      M31      2.5    2.0683  0.431747
  27.178      M31      4.3    3.4100  0.889988
  27.178      M31      3.2    3.4100 -0.210012
  56.298      M31      4.3    4.7098 -0.409799
  56.298      M31      4.8    4.7098  0.090201
  86.388      M31      5.0    4.8117  0.188299
  86.388      M31      5.1    4.8117  0.288299
 115.507      M31      4.3    4.3891 -0.089109
 115.507      M31      4.4    4.3891  0.010891
```

Listing 49: SFO-SFO3 fit to Elliot data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:08 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1243 model solutions performed in 2.032 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.7000  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.700000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC     BIC    logLik
  769.5108 797.733 -375.7554

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error   Lower   Upper
DMTA_0       95.49000    0.75510 94.0000 96.9800
log_k_DMTA   -2.83000    0.02114 -2.8720 -2.7890
log_k_M23    -3.87800    0.25590 -4.3830 -3.3720
log_k_M27    -5.20000    0.22160 -5.6380 -4.7630
log_k_M31    -4.56400    0.25000 -5.0580 -4.0710
f_DMTA_ilr_1  0.05617    0.10970 -0.1604  0.2727
f_DMTA_ilr_2  0.05249    0.10690 -0.1586  0.2635
f_DMTA_ilr_3 -1.43800    0.08860 -1.6130 -1.2630
sigma         2.20600    0.11970  1.9700  2.4430

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.528e-01 -4.531e-02 -4.386e-02 -3.957e-02
log_k_DMTA    5.528e-01  1.000e+00 -8.197e-02 -7.934e-02 -7.159e-02
log_k_M23    -4.531e-02 -8.197e-02  1.000e+00  6.504e-03  5.868e-03
log_k_M27    -4.386e-02 -7.934e-02  6.504e-03  1.000e+00  5.680e-03
log_k_M31    -3.957e-02 -7.159e-02  5.868e-03  5.680e-03  1.000e+00
f_DMTA_ilr_1 -2.207e-02 -3.993e-02  7.251e-01 -3.527e-01  2.859e-03
f_DMTA_ilr_2 -5.648e-03 -1.022e-02  4.285e-01  2.116e-01 -6.388e-01
f_DMTA_ilr_3 -2.188e-01 -2.432e-01  6.056e-01  2.997e-01  4.391e-01
sigma        -7.964e-07 -1.020e-06  6.888e-07  4.219e-07 -4.683e-07
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -2.207e-02   -5.648e-03   -2.188e-01 -7.964e-07
log_k_DMTA     -3.993e-02   -1.022e-02   -2.432e-01 -1.020e-06
log_k_M23       7.251e-01    4.285e-01    6.056e-01  6.888e-07
log_k_M27      -3.527e-01    2.116e-01    2.997e-01  4.219e-07
log_k_M31       2.859e-03   -6.388e-01    4.391e-01 -4.683e-07
f_DMTA_ilr_1    1.000e+00    3.088e-01    4.377e-01  5.393e-07
f_DMTA_ilr_2    3.088e-01    1.000e+00    5.082e-02  9.261e-07
f_DMTA_ilr_3    4.377e-01    5.082e-02    1.000e+00  1.232e-06
sigma           5.393e-07    9.261e-07    1.232e-06  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)     Lower     Upper
DMTA_0        95.490000 126.500 2.417e-163 94.000000 96.980000
k_DMTA         0.058990  47.290  1.228e-96  0.056580  0.061510
k_M23          0.020700   3.907  6.855e-05  0.012480  0.034310
k_M27          0.005514   4.513  6.136e-06  0.003560  0.008541
k_M31          0.010420   4.000  4.826e-05  0.006357  0.017070
f_DMTA_to_M23  0.128600   7.316  5.710e-12        NA        NA
f_DMTA_to_M27  0.118800  12.950  4.815e-27        NA        NA
f_DMTA_to_M31  0.115900   9.368  3.211e-17        NA        NA
sigma          2.206000  18.440  7.804e-42  1.970000  2.443000

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.960       8 35
DMTA       7.787       2 10
M23       12.157       2  8
M27        6.578       2  8
M31       15.721       2  9

Resulting formation fractions:
              ff
DMTA_M23  0.1286
DMTA_M27  0.1188
DMTA_M31  0.1159
DMTA_sink 0.6368

Estimated disappearance times:
       DT50   DT90
DMTA  11.75  39.03
M23   33.49 111.26
M27  125.70 417.57
M31   66.55 221.06

Data:
    time variable observed predicted residual
   0.000     DMTA     97.5 9.549e+01  2.01191
   0.000     DMTA    100.7 9.549e+01  5.21191
   0.000     DMTA     93.4 9.549e+01 -2.08809
   0.000     DMTA    103.2 9.549e+01  7.71191
   1.228     DMTA     86.4 8.881e+01 -2.41284
   1.228     DMTA     88.5 8.881e+01 -0.31284
   1.228     DMTA     89.2 8.881e+01  0.38716
   1.228     DMTA     86.6 8.881e+01 -2.21284
   3.685     DMTA     69.8 7.683e+01 -7.02965
```

3.685	DMTA	77.1	7.683e+01	0.27035
3.685	DMTA	78.2	7.683e+01	1.37035
3.685	DMTA	78.1	7.683e+01	1.27035
8.599	DMTA	59.0	5.750e+01	1.50435
8.599	DMTA	54.2	5.750e+01	-3.29565
8.599	DMTA	55.6	5.750e+01	-1.89565
8.599	DMTA	53.0	5.750e+01	-4.49565
17.199	DMTA	31.3	3.462e+01	-3.31950
17.199	DMTA	33.5	3.462e+01	-1.11950
17.199	DMTA	33.7	3.462e+01	-0.91950
17.199	DMTA	33.2	3.462e+01	-1.41950
25.798	DMTA	19.6	2.085e+01	-1.24523
25.798	DMTA	20.9	2.085e+01	0.05477
25.798	DMTA	20.9	2.085e+01	0.05477
25.798	DMTA	19.9	2.085e+01	-0.94523
34.397	DMTA	13.3	1.255e+01	0.74859
34.397	DMTA	15.8	1.255e+01	3.24859
34.397	DMTA	18.2	1.255e+01	5.64859
34.397	DMTA	12.7	1.255e+01	0.14859
51.596	DMTA	6.7	4.551e+00	2.14945
51.596	DMTA	8.7	4.551e+00	4.14945
51.596	DMTA	7.8	4.551e+00	3.24945
51.596	DMTA	9.0	4.551e+00	4.44945
68.795	DMTA	8.8	1.650e+00	7.15018
68.795	DMTA	8.7	1.650e+00	7.05018
68.795	DMTA	11.4	1.650e+00	9.75018
68.795	DMTA	9.0	1.650e+00	7.35018
103.192	DMTA	6.0	2.169e-01	5.78314
103.192	DMTA	4.4	2.169e-01	4.18314
103.192	DMTA	3.9	2.169e-01	3.68314
103.192	DMTA	4.4	2.169e-01	4.18314
146.189	DMTA	3.3	1.716e-02	3.28284
146.189	DMTA	2.8	1.716e-02	2.78284
146.189	DMTA	2.6	1.716e-02	2.58284
146.189	DMTA	3.4	1.716e-02	3.38284
223.583	DMTA	1.4	1.786e-04	1.39982
223.583	DMTA	1.8	1.786e-04	1.79982
223.583	DMTA	2.0	1.786e-04	1.99982
223.583	DMTA	1.7	1.786e-04	1.69982
3.685	M23	2.8	2.307e+00	0.49322
3.685	M23	1.7	2.307e+00	-0.60678
3.685	M23	2.6	2.307e+00	0.29322
3.685	M23	2.4	2.307e+00	0.09322
8.599	M23	4.3	4.442e+00	-0.14175
8.599	M23	5.8	4.442e+00	1.35825
8.599	M23	5.5	4.442e+00	1.05825
8.599	M23	5.6	4.442e+00	1.15825
17.199	M23	8.2	6.392e+00	1.80790
17.199	M23	5.2	6.392e+00	-1.19210
17.199	M23	7.3	6.392e+00	0.90790
17.199	M23	6.5	6.392e+00	0.10790
25.798	M23	5.1	6.960e+00	-1.86037
25.798	M23	6.1	6.960e+00	-0.86037
25.798	M23	5.8	6.960e+00	-1.16037
25.798	M23	7.7	6.960e+00	0.73963
34.397	M23	6.0	6.795e+00	-0.79526
34.397	M23	6.0	6.795e+00	-0.79526
34.397	M23	7.8	6.795e+00	1.00474
34.397	M23	7.3	6.795e+00	0.50474
51.596	M23	5.0	5.600e+00	-0.60042
51.596	M23	4.2	5.600e+00	-1.40042
51.596	M23	7.0	5.600e+00	1.39958
51.596	M23	6.3	5.600e+00	0.69958
68.795	M23	3.9	4.228e+00	-0.32782
68.795	M23	2.9	4.228e+00	-1.32782
68.795	M23	4.3	4.228e+00	0.07218
68.795	M23	3.8	4.228e+00	-0.42782
103.192	M23	1.9	2.192e+00	-0.29212
103.192	M23	1.5	2.192e+00	-0.69212

```
  103.192      M23      2.6 2.192e+00  0.40788
  103.192      M23      2.8 2.192e+00  0.60788
  146.189      M23      2.0 9.146e-01  1.08540
  146.189      M23      2.3 9.146e-01  1.38540
  146.189      M23      1.6 9.146e-01  0.68540
  146.189      M23      1.1 9.146e-01  0.18540
  223.583      M23      1.2 1.850e-01  1.01501
  223.583      M23      1.9 1.850e-01  1.71501
  223.583      M23      1.4 1.850e-01  1.21501
  223.583      M23      1.3 1.850e-01  1.11501
    3.685      M27      2.3 2.193e+00  0.10719
    3.685      M27      2.1 2.193e+00 -0.09281
    3.685      M27      1.0 2.193e+00 -1.19281
    3.685      M27      2.6 2.193e+00  0.40719
    8.599      M27      4.0 4.398e+00 -0.39810
    8.599      M27      3.4 4.398e+00 -0.99810
    8.599      M27      4.5 4.398e+00  0.10190
    8.599      M27      4.6 4.398e+00  0.20190
   17.199      M27      6.6 6.843e+00 -0.24262
   17.199      M27      6.9 6.843e+00  0.05738
   17.199      M27      7.6 6.843e+00  0.75738
   17.199      M27      6.7 6.843e+00 -0.14262
   25.798      M27      8.2 8.120e+00  0.07973
   25.798      M27      8.8 8.120e+00  0.67973
   25.798      M27      8.7 8.120e+00  0.57973
   25.798      M27      7.6 8.120e+00 -0.52027
   34.397      M27      9.7 8.704e+00  0.99568
   34.397      M27      8.8 8.704e+00  0.09568
   34.397      M27      8.0 8.704e+00 -0.70432
   34.397      M27      8.6 8.704e+00 -0.10432
   51.596      M27      8.3 8.816e+00 -0.51619
   51.596      M27      9.2 8.816e+00  0.38381
   51.596      M27      7.4 8.816e+00 -1.41619
   51.596      M27      7.2 8.816e+00 -1.61619
   68.795      M27      9.3 8.345e+00  0.95539
   68.795      M27      8.5 8.345e+00  0.15539
   68.795      M27     10.3 8.345e+00  1.95539
   68.795      M27      9.4 8.345e+00  1.05539
  103.192      M27      8.6 7.053e+00  1.54671
  103.192      M27      6.0 7.053e+00 -1.05329
  103.192      M27      6.5 7.053e+00 -0.55329
  103.192      M27      6.9 7.053e+00 -0.15329
  146.189      M27      5.6 5.585e+00  0.01536
  146.189      M27      4.5 5.585e+00 -1.08464
  146.189      M27      4.6 5.585e+00 -0.98464
  146.189      M27      4.5 5.585e+00 -1.08464
  223.583      M27      4.1 3.646e+00  0.45393
  223.583      M27      3.9 3.646e+00  0.25393
  223.583      M27      4.3 3.646e+00  0.65393
  223.583      M27      4.2 3.646e+00  0.55393
    1.228      M31      1.5 7.686e-01  0.73144
    1.228      M31      1.3 7.686e-01  0.53144
    3.685      M31      5.0 2.120e+00  2.88024
    3.685      M31      2.4 2.120e+00  0.28024
    3.685      M31      3.1 2.120e+00  0.98024
    3.685      M31      2.3 2.120e+00  0.18024
    8.599      M31      4.3 4.195e+00  0.10458
    8.599      M31      5.0 4.195e+00  0.80458
    8.599      M31      3.4 4.195e+00 -0.79542
    8.599      M31      4.3 4.195e+00  0.10458
   17.199      M31      8.0 6.362e+00  1.63787
   17.199      M31      7.7 6.362e+00  1.33787
   17.199      M31      7.8 6.362e+00  1.43787
   17.199      M31      8.7 6.362e+00  2.33787
   25.798      M31      7.8 7.338e+00  0.46189
   25.798      M31      6.5 7.338e+00 -0.83811
   25.798      M31      7.7 7.338e+00  0.36189
   25.798      M31      6.5 7.338e+00 -0.83811
   34.397      M31      8.0 7.625e+00  0.37473
```

```
  34.397      M31      7.4 7.625e+00 -0.22527
  34.397      M31      6.3 7.625e+00 -1.32527
  34.397      M31      8.7 7.625e+00  1.07473
  51.596      M31      6.9 7.211e+00 -0.31090
  51.596      M31      9.0 7.211e+00  1.78910
  51.596      M31      5.7 7.211e+00 -1.51090
  51.596      M31      4.2 7.211e+00 -3.01090
  68.795      M31      5.5 6.331e+00 -0.83142
  68.795      M31      6.1 6.331e+00 -0.23142
  68.795      M31      3.2 6.331e+00 -3.13142
  68.795      M31      4.2 6.331e+00 -2.13142
 103.192      M31      6.1 4.557e+00  1.54338
 103.192      M31      4.0 4.557e+00 -0.55662
 103.192      M31      3.8 4.557e+00 -0.75662
 103.192      M31      4.0 4.557e+00 -0.55662
 146.189      M31      3.1 2.929e+00  0.17124
 146.189      M31      2.9 2.929e+00 -0.02876
 146.189      M31      4.5 2.929e+00  1.57124
 146.189      M31      4.5 2.929e+00  1.57124
 223.583      M31      1.8 1.309e+00  0.49102
 223.583      M31      2.6 1.309e+00  1.29102
 223.583      M31      3.8 1.309e+00  2.49102
 223.583      M31      2.3 1.309e+00  0.99102
```

Listing 50: SFO-SFO3 fit to Elliot data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:56 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 3410 model solutions performed in 5.549 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.7000  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.700000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  757.3693 788.7273 -368.6847

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
DMTA_0       93.52000    1.57100 90.42000 96.62000
log_k_DMTA   -2.88300    0.03270 -2.94700 -2.81800
log_k_M23    -3.82600    0.23020 -4.28100 -3.37100
log_k_M27    -5.15800    0.19600 -5.54500 -4.77000
log_k_M31    -4.52400    0.22420 -4.96600 -4.08100
f_DMTA_ilr_1  0.06767    0.10010 -0.13000  0.26540
```

```
f_DMTA_ilr_2  0.05545    0.09727 -0.13670  0.24760
f_DMTA_ilr_3 -1.37200    0.09231 -1.55400 -1.18900
sigma_low     1.95900    0.12060  1.72100  2.19800
rsd_high      0.04209    0.01209  0.01821  0.06596

Parameter correlation:
              DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.00000    0.74504  -0.10742  -0.10323 -0.088680    -0.055278
log_k_DMTA    0.74504    1.00000  -0.14434  -0.13878 -0.120200    -0.074028
log_k_M23    -0.10742   -0.14434   1.00000   0.02003  0.017360     0.732900
log_k_M27    -0.10323   -0.13878   0.02003   1.00000  0.016698    -0.342086
log_k_M31    -0.08868   -0.12020   0.01736   0.01670  1.000000     0.008886
f_DMTA_ilr_1 -0.05528   -0.07403   0.73290  -0.34209  0.008886     1.000000
f_DMTA_ilr_2 -0.01394   -0.01855   0.43176   0.21192 -0.638078     0.312902
f_DMTA_ilr_3 -0.45868   -0.46491   0.59796   0.31410  0.434625     0.426137
sigma_low     0.25236    0.30520  -0.04360  -0.04171 -0.033409    -0.023061
rsd_high     -0.54569   -0.63206   0.09030   0.08638  0.069186     0.047761
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low rsd_high
DMTA_0          -0.013944     -0.45868  0.252360 -0.54569
log_k_DMTA      -0.018545     -0.46491  0.305199 -0.63206
log_k_M23        0.431763      0.59796 -0.043601  0.09030
log_k_M27        0.211916      0.31410 -0.041710  0.08638
log_k_M31       -0.638078      0.43463 -0.033409  0.06919
f_DMTA_ilr_1     0.312902      0.42614 -0.023061  0.04776
f_DMTA_ilr_2     1.000000      0.05545 -0.006139  0.01271
f_DMTA_ilr_3     0.055455      1.00000 -0.147119  0.30467
sigma_low       -0.006139     -0.14712  1.000000 -0.29811
rsd_high         0.012711      0.30467 -0.298106  1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)     Lower     Upper
DMTA_0        93.520000  59.530 2.187e-111 90.420000 96.620000
k_DMTA         0.055990  30.580  5.025e-69  0.052490  0.059730
k_M23          0.021800   4.343  1.241e-05  0.013840  0.034350
k_M27          0.005756   5.103  4.695e-07  0.003909  0.008476
k_M31          0.010850   4.461  7.669e-06  0.006968  0.016890
f_DMTA_to_M23  0.136200   7.743  5.205e-13        NA        NA
f_DMTA_to_M27  0.123800  13.470  2.036e-28        NA        NA
f_DMTA_to_M31  0.121300   9.913  1.169e-18        NA        NA
sigma_low      1.959000  16.240  5.657e-36  1.721000  2.198000
rsd_high       0.042090   3.482  3.214e-04  0.018210  0.065960

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  13.396       8 35
DMTA       8.052       2 10
M23       12.524       2  8
M27        6.567       2  8
M31       16.338       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.1362
DMTA_M27  0.1238
DMTA_M31  0.1213
DMTA_sink 0.6187

Estimated disappearance times:
       DT50   DT90
DMTA  12.38  41.12
M23   31.80 105.62
M27  120.42 400.03
M31   63.89 212.24

Data:
    time variable observed predicted residual
```

```
 0.000     DMTA     97.5 9.352e+01  3.97908
 0.000     DMTA    100.7 9.352e+01  7.17908
 0.000     DMTA     93.4 9.352e+01 -0.12092
 0.000     DMTA    103.2 9.352e+01  9.67908
 1.228     DMTA     86.4 8.730e+01 -0.90426
 1.228     DMTA     88.5 8.730e+01  1.19574
 1.228     DMTA     89.2 8.730e+01  1.89574
 1.228     DMTA     86.6 8.730e+01 -0.70426
 3.685     DMTA     69.8 7.608e+01 -6.28320
 3.685     DMTA     77.1 7.608e+01  1.01680
 3.685     DMTA     78.2 7.608e+01  2.11680
 3.685     DMTA     78.1 7.608e+01  2.01680
 8.599     DMTA     59.0 5.778e+01  1.21762
 8.599     DMTA     54.2 5.778e+01 -3.58238
 8.599     DMTA     55.6 5.778e+01 -2.18238
 8.599     DMTA     53.0 5.778e+01 -4.78238
17.199     DMTA     31.3 3.570e+01 -4.40114
17.199     DMTA     33.5 3.570e+01 -2.20114
17.199     DMTA     33.7 3.570e+01 -2.00114
17.199     DMTA     33.2 3.570e+01 -2.50114
25.798     DMTA     19.6 2.206e+01 -2.45813
25.798     DMTA     20.9 2.206e+01 -1.15813
25.798     DMTA     20.9 2.206e+01 -1.15813
25.798     DMTA     19.9 2.206e+01 -2.15813
34.397     DMTA     13.3 1.363e+01 -0.32873
34.397     DMTA     15.8 1.363e+01  2.17127
34.397     DMTA     18.2 1.363e+01  4.57127
34.397     DMTA     12.7 1.363e+01 -0.92873
51.596     DMTA      6.7 5.203e+00  1.49730
51.596     DMTA      8.7 5.203e+00  3.49730
51.596     DMTA      7.8 5.203e+00  2.59730
51.596     DMTA      9.0 5.203e+00  3.79730
68.795     DMTA      8.8 1.986e+00  6.81390
68.795     DMTA      8.7 1.986e+00  6.71390
68.795     DMTA     11.4 1.986e+00  9.41390
68.795     DMTA      9.0 1.986e+00  7.01390
103.192    DMTA      6.0 2.894e-01  5.71057
103.192    DMTA      4.4 2.894e-01  4.11057
103.192    DMTA      3.9 2.894e-01  3.61057
103.192    DMTA      4.4 2.894e-01  4.11057
146.189    DMTA      3.3 2.606e-02  3.27394
146.189    DMTA      2.8 2.606e-02  2.77394
146.189    DMTA      2.6 2.606e-02  2.57394
146.189    DMTA      3.4 2.606e-02  3.37394
223.583    DMTA      1.4 3.419e-04  1.39966
223.583    DMTA      1.8 3.419e-04  1.79966
223.583    DMTA      2.0 3.419e-04  1.99966
223.583    DMTA      1.7 3.419e-04  1.69966
  3.685     M23      2.8 2.279e+00  0.52100
  3.685     M23      1.7 2.279e+00 -0.57900
  3.685     M23      2.6 2.279e+00  0.32100
  3.685     M23      2.4 2.279e+00  0.12100
  8.599     M23      4.3 4.405e+00 -0.10544
  8.599     M23      5.8 4.405e+00  1.39456
  8.599     M23      5.5 4.405e+00  1.09456
  8.599     M23      5.6 4.405e+00  1.19456
 17.199     M23      8.2 6.374e+00  1.82571
 17.199     M23      5.2 6.374e+00 -1.17429
 17.199     M23      7.3 6.374e+00  0.92571
 17.199     M23      6.5 6.374e+00  0.12571
 25.798     M23      5.1 6.966e+00 -1.86640
 25.798     M23      6.1 6.966e+00 -0.86640
 25.798     M23      5.8 6.966e+00 -1.16640
 25.798     M23      7.7 6.966e+00  0.73360
 34.397     M23      6.0 6.815e+00 -0.81462
 34.397     M23      6.0 6.815e+00 -0.81462
 34.397     M23      7.8 6.815e+00  0.98538
 34.397     M23      7.3 6.815e+00  0.48538
 51.596     M23      5.0 5.613e+00 -0.61285
```

```
  51.596      M23      4.2 5.613e+00 -1.41285
  51.596      M23      7.0 5.613e+00  1.38715
  51.596      M23      6.3 5.613e+00  0.68715
  68.795      M23      3.9 4.213e+00 -0.31252
  68.795      M23      2.9 4.213e+00 -1.31252
  68.795      M23      4.3 4.213e+00  0.08748
  68.795      M23      3.8 4.213e+00 -0.41252
 103.192      M23      1.9 2.135e+00 -0.23484
 103.192      M23      1.5 2.135e+00 -0.63484
 103.192      M23      2.6 2.135e+00  0.46516
 103.192      M23      2.8 2.135e+00  0.66516
 146.189      M23      2.0 8.556e-01  1.14437
 146.189      M23      2.3 8.556e-01  1.44437
 146.189      M23      1.6 8.556e-01  0.74437
 146.189      M23      1.1 8.556e-01  0.24437
 223.583      M23      1.2 1.593e-01  1.04068
 223.583      M23      1.9 1.593e-01  1.74068
 223.583      M23      1.4 1.593e-01  1.24068
 223.583      M23      1.3 1.593e-01  1.14068
   3.685      M27      2.3 2.135e+00  0.16522
   3.685      M27      2.1 2.135e+00 -0.03478
   3.685      M27      1.0 2.135e+00 -1.13478
   3.685      M27      2.6 2.135e+00  0.46522
   8.599      M27      4.0 4.307e+00 -0.30718
   8.599      M27      3.4 4.307e+00 -0.90718
   8.599      M27      4.5 4.307e+00  0.19282
   8.599      M27      4.6 4.307e+00  0.29282
  17.199      M27      6.6 6.760e+00 -0.16039
  17.199      M27      6.9 6.760e+00  0.13961
  17.199      M27      7.6 6.760e+00  0.83961
  17.199      M27      6.7 6.760e+00 -0.06039
  25.798      M27      8.2 8.078e+00  0.12185
  25.798      M27      8.8 8.078e+00  0.72185
  25.798      M27      8.7 8.078e+00  0.62185
  25.798      M27      7.6 8.078e+00 -0.47815
  34.397      M27      9.7 8.704e+00  0.99606
  34.397      M27      8.8 8.704e+00  0.09606
  34.397      M27      8.0 8.704e+00 -0.70394
  34.397      M27      8.6 8.704e+00 -0.10394
  51.596      M27      8.3 8.869e+00 -0.56874
  51.596      M27      9.2 8.869e+00  0.33126
  51.596      M27      7.4 8.869e+00 -1.46874
  51.596      M27      7.2 8.869e+00 -1.66874
  68.795      M27      9.3 8.409e+00  0.89108
  68.795      M27      8.5 8.409e+00  0.09108
  68.795      M27     10.3 8.409e+00  1.89108
  68.795      M27      9.4 8.409e+00  0.99108
 103.192      M27      8.6 7.083e+00  1.51668
 103.192      M27      6.0 7.083e+00 -1.08332
 103.192      M27      6.5 7.083e+00 -0.58332
 103.192      M27      6.9 7.083e+00 -0.18332
 146.189      M27      5.6 5.558e+00  0.04207
 146.189      M27      4.5 5.558e+00 -1.05793
 146.189      M27      4.6 5.558e+00 -0.95793
 146.189      M27      4.5 5.558e+00 -1.05793
 223.583      M27      4.1 3.562e+00  0.53781
 223.583      M27      3.9 3.562e+00  0.33781
 223.583      M27      4.3 3.562e+00  0.73781
 223.583      M27      4.2 3.562e+00  0.63781
   1.228      M31      1.5 7.491e-01  0.75089
   1.228      M31      1.3 7.491e-01  0.55089
   3.685      M31      5.0 2.072e+00  2.92772
   3.685      M31      2.4 2.072e+00  0.32772
   3.685      M31      3.1 2.072e+00  1.02772
   3.685      M31      2.3 2.072e+00  0.22772
   8.599      M31      4.3 4.124e+00  0.17595
   8.599      M31      5.0 4.124e+00  0.87595
   8.599      M31      3.4 4.124e+00 -0.72405
   8.599      M31      4.3 4.124e+00  0.17595
```

```
  17.199      M31      8.0 6.305e+00  1.69523
  17.199      M31      7.7 6.305e+00  1.39523
  17.199      M31      7.8 6.305e+00  1.49523
  17.199      M31      8.7 6.305e+00  2.39523
  25.798      M31      7.8 7.318e+00  0.48249
  25.798      M31      6.5 7.318e+00 -0.81751
  25.798      M31      7.7 7.318e+00  0.38249
  25.798      M31      6.5 7.318e+00 -0.81751
  34.397      M31      8.0 7.638e+00  0.36158
  34.397      M31      7.4 7.638e+00 -0.23842
  34.397      M31      6.3 7.638e+00 -1.33842
  34.397      M31      8.7 7.638e+00  1.06158
  51.596      M31      6.9 7.257e+00 -0.35703
  51.596      M31      9.0 7.257e+00  1.74297
  51.596      M31      5.7 7.257e+00 -1.55703
  51.596      M31      4.2 7.257e+00 -3.05703
  68.795      M31      5.5 6.373e+00 -0.87252
  68.795      M31      6.1 6.373e+00 -0.27252
  68.795      M31      3.2 6.373e+00 -3.17252
  68.795      M31      4.2 6.373e+00 -2.17252
 103.192      M31      6.1 4.550e+00  1.55003
 103.192      M31      4.0 4.550e+00 -0.54997
 103.192      M31      3.8 4.550e+00 -0.74997
 103.192      M31      4.0 4.550e+00 -0.54997
 146.189      M31      3.1 2.877e+00  0.22282
 146.189      M31      2.9 2.877e+00  0.02282
 146.189      M31      4.5 2.877e+00  1.62282
 146.189      M31      4.5 2.877e+00  1.62282
 223.583      M31      1.8 1.244e+00  0.55581
 223.583      M31      2.6 1.244e+00  1.35581
 223.583      M31      3.8 1.244e+00  2.55581
 223.583      M31      2.3 1.244e+00  1.05581
```

Listing 51: SFO-SFO3b fit to Calke data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:04 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1081 model solutions performed in 1.778 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        97.2500  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       97.250000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  80.98565 90.80504 -31.49283

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower  Upper
DMTA_0        96.7300    0.69410 95.23000 98.230
log_k_DMTA    -3.4760    0.02107 -3.52100 -3.430
log_k_M23     -4.5010    0.30710 -5.16500 -3.838
log_k_M27     -5.0670    1.04100 -7.31700 -2.818
log_k_M31     -4.6900    0.84320 -6.51200 -2.869
f_DMTA_ilr_1   0.7710    0.32120  0.07714  1.465
f_DMTA_ilr_2   0.3324    0.42400 -0.58360  1.248
f_DMTA_ilr_3  -2.2790    0.18220 -2.67200 -1.885
sigma          1.0130    0.15270  0.68280  1.342

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  4.272e-01 -3.149e-02 -1.712e-02 -1.161e-02
log_k_DMTA    4.272e-01  1.000e+00 -7.371e-02 -4.006e-02 -2.717e-02
log_k_M23    -3.149e-02 -7.371e-02  1.000e+00  2.953e-03  2.003e-03
log_k_M27    -1.712e-02 -4.006e-02  2.953e-03  1.000e+00  6.680e-01
log_k_M31    -1.161e-02 -2.717e-02  2.003e-03  6.680e-01  1.000e+00
f_DMTA_ilr_1 -3.135e-03 -7.338e-03  3.054e-01 -3.309e-01  2.813e-01
f_DMTA_ilr_2  2.960e-04  6.928e-04  1.333e-01 -3.856e-01 -7.889e-01
f_DMTA_ilr_3 -7.930e-02 -1.044e-01  3.208e-01  7.850e-01  4.096e-01
sigma         3.833e-08  2.127e-08  1.500e-08 -1.383e-08 -5.403e-08
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -3.135e-03    2.960e-04   -7.930e-02  3.833e-08
log_k_DMTA     -7.338e-03    6.928e-04   -1.044e-01  2.127e-08
log_k_M23       3.054e-01    1.333e-01    3.208e-01  1.500e-08
log_k_M27      -3.309e-01   -3.856e-01    7.850e-01 -1.383e-08
log_k_M31       2.813e-01   -7.889e-01    4.096e-01 -5.403e-08
f_DMTA_ilr_1    1.000e+00   -5.212e-01   -3.752e-01 -2.547e-08
f_DMTA_ilr_2   -5.212e-01    1.000e+00   -1.506e-01  3.830e-08
f_DMTA_ilr_3   -3.752e-01   -1.506e-01    1.000e+00  1.746e-08
sigma          -2.547e-08    3.830e-08    1.746e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate  t value    Pr(>t)     Lower    Upper
DMTA_0        96.730000 139.4000 2.515e-22 9.523e+01 98.23000
k_DMTA         0.030940  47.4700 2.938e-16 2.957e-02  0.03238
k_M23          0.011090   3.2560 3.128e-03 5.714e-03  0.02154
k_M27          0.006298   0.9602 1.772e-01 6.639e-04  0.05975
k_M31          0.009184   1.1860 1.284e-01 1.486e-03  0.05677
f_DMTA_to_M23  0.114300   5.9190 2.539e-05        NA       NA
f_DMTA_to_M27  0.038400   2.3670 1.706e-02        NA       NA
f_DMTA_to_M31  0.044090   2.4220 1.540e-02        NA       NA
sigma          1.013000   6.6330 8.148e-06 6.828e-01  1.34200

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   5.721       8  9
DMTA       2.809       2  3
M23        5.049       2  2
M27        3.391       2  2
M31       14.017       2  2

Resulting formation fractions:
               ff
DMTA_M23  0.11426
DMTA_M27  0.03840
DMTA_M31  0.04409
DMTA_sink 0.80325

Estimated disappearance times:
       DT50   DT90
DMTA  22.40  74.41
M23   62.48 207.55
M27  110.05 365.58
M31   75.48 250.73

Data:
 time variable observed predicted residual
    0     DMTA     95.8    96.728 -0.92789
    0     DMTA     98.7    96.728  1.97211
   14     DMTA     60.5    62.721 -2.22134
   30     DMTA     39.1    38.230  0.87018
   59     DMTA     15.2    15.584 -0.38444
  120     DMTA      4.8     2.360  2.43977
  120     DMTA      4.6     2.360  2.23977
   14      M23      4.1     3.579  0.52121
   30      M23      5.3     5.542 -0.24214
```

```
 59      M23      6.0     6.178 -0.17774
120      M23      4.3     4.130  0.16957
120      M23      4.1     4.130 -0.03043
 14      M27      1.5     1.342  0.15812
 30      M27      2.4     2.365  0.03519
 59      M27      3.2     3.354 -0.15405
120      M27      3.8     3.723  0.07690
120      M27      3.7     3.723 -0.02310
 14      M31      2.0     1.400  0.59963
 30      M31      2.1     2.207 -0.10713
 59      M31      2.2     2.550 -0.35043
120      M31      1.8     1.867 -0.06655
120      M31      2.1     1.867  0.23345
```

Listing 52: SFO-SFO3b fit to Calke data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:43 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 2353 model solutions performed in 4.263 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
DMTA_0        97.2500  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       97.250000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC     BIC    logLik
  77.87317 88.7836 -28.93659

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error     Lower    Upper
DMTA_0       95.43000    1.94300 91.200000 99.67000
log_k_DMTA   -3.51300    0.03802 -3.596000 -3.43000
log_k_M23    -4.46000    0.23000 -4.961000 -3.95900
log_k_M27    -4.99400    0.73510 -6.595000 -3.39200
log_k_M31    -4.64900    0.61600 -5.991000 -3.30700
f_DMTA_ilr_1  0.77590    0.24270  0.247200  1.30500
```

```
f_DMTA_ilr_2  0.33180    0.31900 -0.363200  1.02700
f_DMTA_ilr_3 -2.23600    0.14530 -2.552000 -1.91900
sigma_low     0.75300    0.14440  0.438400  1.06800
rsd_high      0.02493    0.01514 -0.008056  0.05792

Parameter correlation:
               DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.000000   0.754553  -0.13769  -0.07567  -0.05165     -0.01590
log_k_DMTA    0.754553   1.000000  -0.18209  -0.10011  -0.06833     -0.02088
log_k_M23    -0.137689  -0.182089   1.00000   0.01824   0.01245      0.30622
log_k_M27    -0.075673  -0.100108   0.01824   1.00000   0.66510     -0.32435
log_k_M31    -0.051646  -0.068327   0.01245   0.66510   1.00000      0.28761
f_DMTA_ilr_1 -0.015899  -0.020880   0.30622  -0.32435   0.28761      1.00000
f_DMTA_ilr_2  0.001622   0.002137   0.13244  -0.38207  -0.78866     -0.52501
f_DMTA_ilr_3 -0.306291  -0.318703   0.35709   0.76633   0.40094     -0.34538
sigma_low     0.360695   0.451173  -0.08406  -0.04605  -0.03141     -0.01036
rsd_high     -0.578659  -0.706765   0.13168   0.07214   0.04921      0.01623
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low  rsd_high
DMTA_0           0.001622      -0.3063  0.360695 -0.578659
log_k_DMTA       0.002137      -0.3187  0.451173 -0.706765
log_k_M23        0.132440       0.3571 -0.084059  0.131680
log_k_M27       -0.382073       0.7663 -0.046053  0.072143
log_k_M31       -0.788663       0.4009 -0.031411  0.049207
f_DMTA_ilr_1    -0.525014      -0.3454 -0.010358  0.016226
f_DMTA_ilr_2     1.000000      -0.1342  0.001028 -0.001611
f_DMTA_ilr_3    -0.134219       1.0000 -0.148543  0.232692
sigma_low        0.001028      -0.1485  1.000000 -0.403331
rsd_high        -0.001611       0.2327 -0.403331  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value    Pr(>t)     Lower    Upper
DMTA_0        95.430000  49.120 1.661e-15 91.200000 99.67000
k_DMTA         0.029810  26.300 2.790e-12  0.027440  0.03239
k_M23          0.011560   4.348 4.737e-04  0.007004  0.01908
k_M27          0.006780   1.360 9.937e-02  0.001367  0.03364
k_M31          0.009571   1.623 6.524e-02  0.002501  0.03663
f_DMTA_to_M23  0.119200   7.363 4.348e-06        NA       NA
f_DMTA_to_M27  0.039800   3.113 4.484e-03        NA       NA
f_DMTA_to_M31  0.045880   3.203 3.795e-03        NA       NA
sigma_low      0.753000   5.215 1.082e-04  0.438400  1.06800
rsd_high       0.024930   1.647 6.277e-02 -0.008056  0.05792

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.379       8  9
DMTA       3.152       2  3
M23        5.196       2  2
M27        3.631       2  2
M31       14.205       2  2

Resulting formation fractions:
               ff
DMTA_M23  0.11923
DMTA_M27  0.03980
DMTA_M31  0.04588
DMTA_sink 0.79509

Estimated disappearance times:
       DT50   DT90
DMTA  23.25  77.24
M23   59.96 199.19
M27  102.23 339.60
M31   72.42 240.58

Data:
 time variable observed predicted residual
```

```
  0     DMTA     95.8    95.432  0.36766
  0     DMTA     98.7    95.432  3.26766
 14     DMTA     60.5    62.869 -2.36919
 30     DMTA     39.1    39.020  0.08009
 59     DMTA     15.2    16.437 -1.23705
120     DMTA      4.8     2.667  2.13278
120     DMTA      4.6     2.667  1.93278
 14      M23      4.1     3.564  0.53550
 30      M23      5.3     5.540 -0.23968
 59      M23      6.0     6.195 -0.19532
120      M23      4.3     4.123  0.17725
120      M23      4.1     4.123 -0.02275
 14      M27      1.5     1.331  0.16883
 30      M27      2.4     2.360  0.04046
 59      M27      3.2     3.364 -0.16424
120      M27      3.8     3.718  0.08158
120      M27      3.7     3.718 -0.01842
 14      M31      2.0     1.392  0.60822
 30      M31      2.1     2.203 -0.10260
 59      M31      2.2     2.556 -0.35576
120      M31      1.8     1.865 -0.06480
120      M31      2.1     1.865  0.23520
```

Listing 53: SFO-SFO3b fit to Flaach data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:04 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1126 model solutions performed in 2.121 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                 value   type
DMTA_0        96.76667  state
k_DMTA         0.10000 deparm
k_M23          0.10010 deparm
k_M27          0.10020 deparm
k_M31          0.10030 deparm
f_DMTA_to_M23  0.25000 deparm
f_DMTA_to_M27  0.25000 deparm
f_DMTA_to_M31  0.25000 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       96.766667  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  318.2829 344.4304 -150.1414

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error   Lower    Upper
DMTA_0       95.10000   0.298300 94.5100 95.69000
log_k_DMTA   -1.93700   0.008113 -1.9530 -1.92100
log_k_M23    -3.07500   0.071230 -3.2160 -2.93400
log_k_M27    -3.39200   0.066450 -3.5240 -3.26100
log_k_M31    -3.52100   0.194800 -3.9060 -3.13500
f_DMTA_ilr_1 -0.02625   0.040390 -0.1062  0.05368
f_DMTA_ilr_2  0.91680   0.092750  0.7332  1.10000
f_DMTA_ilr_3 -1.76800   0.042410 -1.8520 -1.68400
sigma         0.73580   0.044780  0.6472  0.82440

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.286e-01 -4.614e-02 -4.740e-02 -9.368e-03
log_k_DMTA    5.286e-01  1.000e+00 -8.728e-02 -8.967e-02 -1.772e-02
log_k_M23    -4.614e-02 -8.728e-02  1.000e+00  7.826e-03  1.547e-03
log_k_M27    -4.740e-02 -8.967e-02  7.826e-03  1.000e+00  5.078e-01
log_k_M31    -9.368e-03 -1.772e-02  1.547e-03  5.078e-01  1.000e+00
f_DMTA_ilr_1 -7.441e-03 -1.408e-02  5.852e-01 -2.794e-01  1.694e-01
f_DMTA_ilr_2 -6.676e-03 -1.263e-02  1.479e-01 -4.472e-01 -7.403e-01
f_DMTA_ilr_3 -1.574e-01 -1.720e-01  3.682e-01  6.626e-01  5.383e-01
sigma        -2.787e-07 -4.153e-07  7.844e-08 -9.437e-08  3.592e-07
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -7.441e-03   -6.676e-03   -1.574e-01 -2.787e-07
log_k_DMTA     -1.408e-02   -1.263e-02   -1.720e-01 -4.153e-07
log_k_M23       5.852e-01    1.479e-01    3.682e-01  7.844e-08
log_k_M27      -2.794e-01   -4.472e-01    6.626e-01 -9.437e-08
log_k_M31       1.694e-01   -7.403e-01    5.383e-01  3.592e-07
f_DMTA_ilr_1    1.000e+00   -7.649e-02    2.245e-01  3.131e-07
f_DMTA_ilr_2   -7.649e-02    1.000e+00   -5.984e-01 -1.947e-07
f_DMTA_ilr_3    2.245e-01   -5.984e-01    1.000e+00  1.334e-07
sigma           3.131e-07   -1.947e-07    1.334e-07  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)    Lower    Upper
DMTA_0        95.10000 318.800 2.532e-185 94.51000 95.69000
k_DMTA         0.14410 123.300 1.613e-133  0.14180  0.14650
k_M23          0.04617  14.040  7.764e-28  0.04010  0.05316
k_M27          0.03363  15.050  3.144e-30  0.02949  0.03836
k_M31          0.02958   5.133  5.266e-07  0.02012  0.04350
f_DMTA_to_M23  0.12870  22.440  3.813e-46       NA       NA
f_DMTA_to_M27  0.13360  27.020  1.424e-54       NA       NA
f_DMTA_to_M31  0.04267   9.401  1.571e-16       NA       NA
sigma          0.73580  16.430  1.995e-33  0.64720  0.82440

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   4.704       8 37
DMTA       2.109       2 10
M23       11.578       2  9
M27        4.440       2  9
M31       19.486       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.12872
DMTA_M27  0.13359
DMTA_M31  0.04267
DMTA_sink 0.69502

Estimated disappearance times:
       DT50  DT90
DMTA  4.809 15.98
M23  15.012 49.87
M27  20.610 68.47
M31  23.432 77.84

Data:
    time variable observed predicted  residual
  0.0000     DMTA     96.5 95.096869  1.403131
  0.0000     DMTA     96.8 95.096869  1.703131
  0.0000     DMTA     97.0 95.096869  1.903131
  0.6234     DMTA     82.9 86.924965 -4.024965
  0.6234     DMTA     86.7 86.924965 -0.224965
  0.6234     DMTA     87.4 86.924965  0.475035
  1.8702     DMTA     72.8 72.627508  0.172492
  1.8702     DMTA     69.9 72.627508 -2.727508
  1.8702     DMTA     71.9 72.627508 -0.727508
```

4.3637	DMTA	51.4	50.700749	0.699251
4.3637	DMTA	52.9	50.700749	2.199251
4.3637	DMTA	48.6	50.700749	-2.100749
8.7274	DMTA	28.5	27.031027	1.468973
8.7274	DMTA	27.3	27.031027	0.268973
8.7274	DMTA	27.5	27.031027	0.468973
13.0911	DMTA	14.8	14.411550	0.388450
13.0911	DMTA	13.4	14.411550	-1.011550
13.0911	DMTA	14.4	14.411550	-0.011550
17.4548	DMTA	7.7	7.683496	0.016504
17.4548	DMTA	7.3	7.683496	-0.383496
17.4548	DMTA	8.1	7.683496	0.416504
26.1822	DMTA	2.0	2.184013	-0.184013
26.1822	DMTA	1.5	2.184013	-0.684013
26.1822	DMTA	1.9	2.184013	-0.284013
34.9096	DMTA	1.3	0.620800	0.679200
34.9096	DMTA	1.0	0.620800	0.379200
34.9096	DMTA	1.1	0.620800	0.479200
43.6370	DMTA	0.9	0.176461	0.723539
43.6370	DMTA	0.7	0.176461	0.523539
43.6370	DMTA	0.7	0.176461	0.523539
52.3644	DMTA	0.6	0.050158	0.549842
52.3644	DMTA	0.4	0.050158	0.349842
52.3644	DMTA	0.5	0.050158	0.449842
74.8063	DMTA	0.4	0.001975	0.398025
74.8063	DMTA	0.3	0.001975	0.298025
74.8063	DMTA	0.3	0.001975	0.298025
0.6234	M23	0.7	1.036677	-0.336677
0.6234	M23	0.7	1.036677	-0.336677
0.6234	M23	0.2	1.036677	-0.836677
1.8702	M23	2.2	2.765551	-0.565551
1.8702	M23	1.8	2.765551	-0.965551
1.8702	M23	1.6	2.765551	-1.165551
4.3637	M23	4.1	5.121625	-1.021625
4.3637	M23	4.2	5.121625	-0.921625
4.3637	M23	4.2	5.121625	-0.921625
8.7274	M23	7.5	6.917574	0.582426
8.7274	M23	7.1	6.917574	0.182426
8.7274	M23	7.5	6.917574	0.582426
13.0911	M23	8.4	7.111004	1.288996
13.0911	M23	6.8	7.111004	-0.311004
13.0911	M23	8.0	7.111004	0.888996
17.4548	M23	7.2	6.589489	0.610511
17.4548	M23	7.2	6.589489	0.610511
17.4548	M23	6.9	6.589489	0.310511
26.1822	M23	4.9	4.962837	-0.062837
26.1822	M23	4.3	4.962837	-0.662837
26.1822	M23	4.5	4.962837	-0.462837
34.9096	M23	3.8	3.475659	0.324341
34.9096	M23	3.1	3.475659	-0.375659
34.9096	M23	3.1	3.475659	-0.375659
43.6370	M23	2.7	2.368028	0.331972
43.6370	M23	2.3	2.368028	-0.068028
43.6370	M23	2.1	2.368028	-0.268028
52.3644	M23	1.6	1.595449	0.004551
52.3644	M23	1.1	1.595449	-0.495449
52.3644	M23	1.3	1.595449	-0.295449
74.8063	M23	0.4	0.569042	-0.169042
74.8063	M23	0.4	0.569042	-0.169042
74.8063	M23	0.3	0.569042	-0.269042
0.6234	M27	1.1	1.083369	0.016631
0.6234	M27	1.1	1.083369	0.016631
0.6234	M27	0.3	1.083369	-0.783369
1.8702	M27	2.6	2.931742	-0.331742
1.8702	M27	2.4	2.931742	-0.531742
1.8702	M27	2.3	2.931742	-0.631742
4.3637	M27	5.0	5.596752	-0.596752
4.3637	M27	5.9	5.596752	0.303248
4.3637	M27	4.8	5.596752	-0.796752

```
 8.7274      M27      8.5  8.015213  0.484787
 8.7274      M27      8.5  8.015213  0.484787
 8.7274      M27      8.3  8.015213  0.284787
13.0911      M27      9.3  8.792315  0.507685
13.0911      M27      8.7  8.792315 -0.092315
13.0911      M27      9.1  8.792315  0.307685
17.4548      M27      8.6  8.743129 -0.143129
17.4548      M27      8.5  8.743129 -0.243129
17.4548      M27      8.9  8.743129  0.156871
26.1822      M27      8.1  7.682888  0.417112
26.1822      M27      7.7  7.682888  0.017112
26.1822      M27      7.4  7.682888 -0.282888
34.9096      M27      5.9  6.350843 -0.450843
34.9096      M27      6.0  6.350843 -0.350843
34.9096      M27      5.9  6.350843 -0.450843
43.6370      M27      5.6  5.137395  0.462605
43.6370      M27      5.2  5.137395  0.062605
43.6370      M27      5.6  5.137395  0.462605
52.3644      M27      4.3  4.118784  0.181216
52.3644      M27      3.7  4.118784 -0.418784
52.3644      M27      3.9  4.118784 -0.218784
74.8063      M27      2.5  2.294183  0.205817
74.8063      M27      2.4  2.294183  0.105817
74.8063      M27      2.2  2.294183 -0.094183
 0.6234      M31      0.3  0.345424 -0.045424
 0.6234      M31      0.3  0.345424 -0.045424
 0.6234      M31      0.1  0.345424 -0.245424
 1.8702      M31      0.7  0.931497 -0.231497
 1.8702      M31      0.6  0.931497 -0.331497
 1.8702      M31      0.7  0.931497 -0.231497
 4.3637      M31      1.3  1.765142 -0.465142
 4.3637      M31      1.2  1.765142 -0.565142
 4.3637      M31      1.4  1.765142 -0.365142
 8.7274      M31      2.4  2.492466 -0.092466
 8.7274      M31      2.1  2.492466 -0.392466
 8.7274      M31      2.3  2.492466 -0.192466
13.0911      M31      3.3  2.692365  0.607635
13.0911      M31      2.4  2.692365 -0.292365
13.0911      M31      2.6  2.692365 -0.092365
17.4548      M31      4.0  2.633819  1.366181
17.4548      M31      3.6  2.633819  0.966181
17.4548      M31      3.3  2.633819  0.666181
26.1822      M31      2.1  2.235916 -0.135916
26.1822      M31      1.7  2.235916 -0.535916
26.1822      M31      1.8  2.235916 -0.435916
34.9096      M31      1.6  1.784410 -0.184410
34.9096      M31      1.6  1.784410 -0.184410
34.9096      M31      1.4  1.784410 -0.384410
43.6370      M31      1.8  1.394666  0.405334
43.6370      M31      1.5  1.394666  0.105334
43.6370      M31      1.3  1.394666 -0.094666
52.3644      M31      1.2  1.081956  0.118044
52.3644      M31      0.9  1.081956 -0.181956
52.3644      M31      1.1  1.081956  0.018044
74.8063      M31      0.5  0.558335 -0.058335
74.8063      M31      0.5  0.558335 -0.058335
74.8063      M31      0.3  0.558335 -0.258335
```

Listing 54: SFO-SFO3b fit to Flaach data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:49 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 5109 model solutions performed in 10.478 s

Error model: Two-component variance function

Error model algorithm: d_3
Three-step fitting yielded a higher likelihood than direct fitting

Starting values for parameters to be optimised:
                value   type
DMTA_0        96.76667  state
k_DMTA         0.10000 deparm
k_M23          0.10010 deparm
k_M27          0.10020 deparm
k_M31          0.10030 deparm
f_DMTA_to_M23  0.25000 deparm
f_DMTA_to_M27  0.25000 deparm
f_DMTA_to_M31  0.25000 deparm
sigma_low      0.10000  error
rsd_high       0.10000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
DMTA_0       96.766667  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  242.2497 271.3024 -111.1248

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
DMTA_0       94.80000   0.828700 93.16000 96.44000
log_k_DMTA   -1.94400   0.009540 -1.96300 -1.92500
log_k_M23    -3.07000   0.046650 -3.16300 -2.97800
log_k_M27    -3.39000   0.043480 -3.47600 -3.30400
log_k_M31    -3.51600   0.123600 -3.76000 -3.27100
f_DMTA_ilr_1 -0.02578   0.026970 -0.07916  0.02760
```

```
f_DMTA_ilr_2  0.91450   0.059320  0.79710  1.03200
f_DMTA_ilr_3 -1.76300   0.031220 -1.82500 -1.70100
sigma_low     0.46450   0.032860  0.39950  0.52960
rsd_high      0.02582   0.005469  0.01499  0.03664

Parameter correlation:
               DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.00000   0.646262 -0.099677  -0.10111 -0.022884   -0.0152419
log_k_DMTA    0.64626   1.000000 -0.155082  -0.16007 -0.034752   -0.0237745
log_k_M23    -0.09968  -0.155082  1.000000   0.02504  0.005351    0.5775691
log_k_M27    -0.10111  -0.160073  0.025036   1.00000  0.489376   -0.2867759
log_k_M31    -0.02288  -0.034752  0.005351   0.48938  1.000000    0.1650234
f_DMTA_ilr_1 -0.01524  -0.023774  0.577569  -0.28678  0.165023    1.0000000
f_DMTA_ilr_2 -0.01218  -0.021695  0.154182  -0.41675 -0.738140   -0.0751080
f_DMTA_ilr_3 -0.47411  -0.424215  0.381369   0.62631  0.477175    0.1941824
sigma_low     0.03551   0.005975  0.002667   0.01439 -0.002995    0.0006744
rsd_high     -0.08429  -0.011213 -0.004992  -0.02699  0.005625   -0.0012437
             f_DMTA_ilr_2 f_DMTA_ilr_3  sigma_low  rsd_high
DMTA_0          -0.01218    -0.474114  0.0355078 -0.084294
log_k_DMTA      -0.02170    -0.424215  0.0059750 -0.011213
log_k_M23        0.15418     0.381369  0.0026674 -0.004992
log_k_M27       -0.41675     0.626309  0.0143864 -0.026991
log_k_M31       -0.73814     0.477175 -0.0029954  0.005625
f_DMTA_ilr_1    -0.07511     0.194182  0.0006744 -0.001244
f_DMTA_ilr_2     1.00000    -0.494450  0.0119810 -0.022489
f_DMTA_ilr_3    -0.49445     1.000000  0.0066863 -0.012528
sigma_low        0.01198     0.006686  1.0000000 -0.241054
rsd_high        -0.02249    -0.012528 -0.2410539  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value     Pr(>t)    Lower    Upper
DMTA_0        94.80000 114.400 1.128e-128 93.16000 96.44000
k_DMTA         0.14310 104.800 5.585e-124  0.14040  0.14580
k_M23          0.04640  21.440  5.423e-44  0.04231  0.05089
k_M27          0.03371  23.000  4.790e-47  0.03093  0.03674
k_M31          0.02972   8.090  2.232e-13  0.02327  0.03796
f_DMTA_to_M23  0.12920  31.220  3.580e-61       NA       NA
f_DMTA_to_M27  0.13400  36.210  1.982e-68       NA       NA
f_DMTA_to_M31  0.04294  14.570  5.169e-29       NA       NA
sigma_low      0.46450  14.140  5.440e-28  0.39950  0.52960
rsd_high       0.02582   4.721  3.097e-06  0.01499  0.03664

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   4.744       8 37
DMTA       2.148       2 10
M23       11.513       2  9
M27        4.421       2  9
M31       19.436       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.12923
DMTA_M27  0.13402
DMTA_M31  0.04294
DMTA_sink 0.69382

Estimated disappearance times:
       DT50  DT90
DMTA  4.844 16.09
M23  14.939 49.63
M27  20.563 68.31
M31  23.319 77.47

Data:
    time variable observed predicted  residual
```

```
 0.0000     DMTA     96.5 94.796944  1.703056
 0.0000     DMTA     96.8 94.796944  2.003056
 0.0000     DMTA     97.0 94.796944  2.203056
 0.6234     DMTA     82.9 86.707086 -3.807086
 0.6234     DMTA     86.7 86.707086 -0.007086
 0.6234     DMTA     87.4 86.707086  0.692914
 1.8702     DMTA     72.8 72.539592  0.260408
 1.8702     DMTA     69.9 72.539592 -2.639592
 1.8702     DMTA     71.9 72.539592 -0.639592
 4.3637     DMTA     51.4 50.771049  0.628951
 4.3637     DMTA     52.9 50.771049  2.128951
 4.3637     DMTA     48.6 50.771049 -2.171049
 8.7274     DMTA     28.5 27.191799  1.308201
 8.7274     DMTA     27.3 27.191799  0.108201
 8.7274     DMTA     27.5 27.191799  0.308201
13.0911     DMTA     14.8 14.563298  0.236702
13.0911     DMTA     13.4 14.563298 -1.163298
13.0911     DMTA     14.4 14.563298 -0.163298
17.4548     DMTA      7.7  7.799766 -0.099766
17.4548     DMTA      7.3  7.799766 -0.499766
17.4548     DMTA      8.1  7.799766  0.300234
26.1822     DMTA      2.0  2.237305 -0.237305
26.1822     DMTA      1.5  2.237305 -0.737305
26.1822     DMTA      1.9  2.237305 -0.337305
34.9096     DMTA      1.3  0.641754  0.658246
34.9096     DMTA      1.0  0.641754  0.358246
34.9096     DMTA      1.1  0.641754  0.458246
43.6370     DMTA      0.9  0.184082  0.715918
43.6370     DMTA      0.7  0.184082  0.515918
43.6370     DMTA      0.7  0.184082  0.515918
52.3644     DMTA      0.6  0.052803  0.547197
52.3644     DMTA      0.4  0.052803  0.347197
52.3644     DMTA      0.5  0.052803  0.447197
74.8063     DMTA      0.4  0.002128  0.397872
74.8063     DMTA      0.3  0.002128  0.297872
74.8063     DMTA      0.3  0.002128  0.297872
 0.6234      M23      0.7  1.030222 -0.330222
 0.6234      M23      0.7  1.030222 -0.330222
 0.6234      M23      0.2  1.030222 -0.830222
 1.8702      M23      2.2  2.749644 -0.549644
 1.8702      M23      1.8  2.749644 -0.949644
 1.8702      M23      1.6  2.749644 -1.149644
 4.3637      M23      4.1  5.096548 -0.996548
 4.3637      M23      4.2  5.096548 -0.896548
 4.3637      M23      4.2  5.096548 -0.896548
 8.7274      M23      7.5  6.892009  0.607991
 8.7274      M23      7.1  6.892009  0.207991
 8.7274      M23      7.5  6.892009  0.607991
13.0911      M23      8.4  7.090698  1.309302
13.0911      M23      6.8  7.090698 -0.290698
13.0911      M23      8.0  7.090698  0.909302
17.4548      M23      7.2  6.574027  0.625973
17.4548      M23      7.2  6.574027  0.625973
17.4548      M23      6.9  6.574027  0.325973
26.1822      M23      4.9  4.952071 -0.052071
26.1822      M23      4.3  4.952071 -0.652071
26.1822      M23      4.5  4.952071 -0.452071
34.9096      M23      3.8  3.465787  0.334213
34.9096      M23      3.1  3.465787 -0.365787
34.9096      M23      3.1  3.465787 -0.365787
43.6370      M23      2.7  2.358406  0.341594
43.6370      M23      2.3  2.358406 -0.058406
43.6370      M23      2.1  2.358406 -0.258406
52.3644      M23      1.6  1.586487  0.013513
52.3644      M23      1.1  1.586487 -0.486487
52.3644      M23      1.3  1.586487 -0.286487
74.8063      M23      0.4  0.563201 -0.163201
74.8063      M23      0.4  0.563201 -0.163201
74.8063      M23      0.3  0.563201 -0.263201
```

```
 0.6234    M27    1.1  1.075975  0.024025
 0.6234    M27    1.1  1.075975  0.024025
 0.6234    M27    0.3  1.075975 -0.775975
 1.8702    M27    2.6  2.913522 -0.313522
 1.8702    M27    2.4  2.913522 -0.513522
 1.8702    M27    2.3  2.913522 -0.613522
 4.3637    M27    5.0  5.568258 -0.568258
 4.3637    M27    5.9  5.568258  0.331742
 4.3637    M27    4.8  5.568258 -0.768258
 8.7274    M27    8.5  7.987717  0.512283
 8.7274    M27    8.5  7.987717  0.512283
 8.7274    M27    8.3  7.987717  0.312283
13.0911    M27    9.3  8.773537  0.526463
13.0911    M27    8.7  8.773537 -0.073537
13.0911    M27    9.1  8.773537  0.326463
17.4548    M27    8.6  8.732925 -0.132925
17.4548    M27    8.5  8.732925 -0.232925
17.4548    M27    8.9  8.732925  0.167075
26.1822    M27    8.1  7.682784  0.417216
26.1822    M27    7.7  7.682784  0.017216
26.1822    M27    7.4  7.682784 -0.282784
34.9096    M27    5.9  6.353444 -0.453444
34.9096    M27    6.0  6.353444 -0.353444
34.9096    M27    5.9  6.353444 -0.453444
43.6370    M27    5.6  5.139435  0.460565
43.6370    M27    5.2  5.139435  0.060565
43.6370    M27    5.6  5.139435  0.460565
52.3644    M27    4.3  4.119341  0.180659
52.3644    M27    3.7  4.119341 -0.419341
52.3644    M27    3.9  4.119341 -0.219341
74.8063    M27    2.5  2.291693  0.208307
74.8063    M27    2.4  2.291693  0.108307
74.8063    M27    2.2  2.291693 -0.091693
 0.6234    M31    0.3  0.344096 -0.044096
 0.6234    M31    0.3  0.344096 -0.044096
 0.6234    M31    0.1  0.344096 -0.244096
 1.8702    M31    0.7  0.928403 -0.228403
 1.8702    M31    0.6  0.928403 -0.328403
 1.8702    M31    0.7  0.928403 -0.228403
 4.3637    M31    1.3  1.760945 -0.460945
 4.3637    M31    1.2  1.760945 -0.560945
 4.3637    M31    1.4  1.760945 -0.360945
 8.7274    M31    2.4  2.489852 -0.089852
 8.7274    M31    2.1  2.489852 -0.389852
 8.7274    M31    2.3  2.489852 -0.189852
13.0911    M31    3.3  2.692081  0.607919
13.0911    M31    2.4  2.692081 -0.292081
13.0911    M31    2.6  2.692081 -0.092081
17.4548    M31    4.0  2.635123  1.364877
17.4548    M31    3.6  2.635123  0.964877
17.4548    M31    3.3  2.635123  0.664877
26.1822    M31    2.1  2.237867 -0.137867
26.1822    M31    1.7  2.237867 -0.537867
26.1822    M31    1.8  2.237867 -0.437867
34.9096    M31    1.6  1.785283 -0.185283
34.9096    M31    1.6  1.785283 -0.185283
34.9096    M31    1.4  1.785283 -0.385283
43.6370    M31    1.8  1.394207  0.405793
43.6370    M31    1.5  1.394207  0.105793
43.6370    M31    1.3  1.394207 -0.094207
52.3644    M31    1.2  1.080470  0.119530
52.3644    M31    0.9  1.080470 -0.180470
52.3644    M31    1.1  1.080470  0.019530
74.8063    M31    0.5  0.555863 -0.055863
74.8063    M31    0.5  0.555863 -0.055863
74.8063    M31    0.3  0.555863 -0.255863
```

Listing 55: SFO-SFO3b fit to BBA 2.2 data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:05 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1205 model solutions performed in 2.395 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.4300  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.430000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  290.2203 312.7185 -136.1101

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
DMTA_0       99.71000    0.49260 98.73000 100.7000
log_k_DMTA   -2.65300    0.01247 -2.67700  -2.6280
log_k_M23    -3.81500    0.12920 -4.07200  -3.5580
log_k_M27    -4.20600    0.14060 -4.48600  -3.9270
log_k_M31    -4.21700    0.19730 -4.61000  -3.8250
f_DMTA_ilr_1  0.09711    0.06594 -0.03410   0.2283
f_DMTA_ilr_2  0.23280    0.08461  0.06447   0.4012
f_DMTA_ilr_3 -1.42400    0.05356 -1.53100  -1.3170
sigma         1.09800    0.08183  0.93510   1.2610

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.338e-01 -5.037e-02 -6.090e-02 -3.181e-02
log_k_DMTA    5.338e-01  1.000e+00 -9.436e-02 -1.141e-01 -5.960e-02
log_k_M23    -5.037e-02 -9.436e-02  1.000e+00  1.077e-02  5.624e-03
log_k_M27    -6.090e-02 -1.141e-01  1.077e-02  1.000e+00  6.274e-01
log_k_M31    -3.181e-02 -5.960e-02  5.624e-03  6.274e-01  1.000e+00
f_DMTA_ilr_1 -9.478e-03 -1.776e-02  5.921e-01 -2.244e-01  2.219e-01
f_DMTA_ilr_2 -2.767e-03 -5.184e-03  2.661e-01 -3.965e-01 -7.594e-01
f_DMTA_ilr_3 -2.299e-01 -2.609e-01  5.239e-01  6.235e-01  3.840e-01
sigma         2.346e-07  5.874e-09 -1.248e-07  9.003e-08  5.327e-08
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -9.478e-03   -2.767e-03   -2.299e-01  2.346e-07
log_k_DMTA     -1.776e-02   -5.184e-03   -2.609e-01  5.874e-09
log_k_M23       5.921e-01    2.661e-01    5.239e-01 -1.248e-07
log_k_M27      -2.244e-01   -3.965e-01    6.235e-01  9.003e-08
log_k_M31       2.219e-01   -7.594e-01    3.840e-01  5.327e-08
f_DMTA_ilr_1    1.000e+00   -1.268e-01    2.123e-01  6.755e-09
f_DMTA_ilr_2   -1.268e-01    1.000e+00   -1.018e-01 -2.137e-07
f_DMTA_ilr_3    2.123e-01   -1.018e-01    1.000e+00 -5.712e-08
sigma           6.755e-09   -2.137e-07   -5.712e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)     Lower     Upper
DMTA_0        99.71000 202.400 1.257e-111 98.730000 100.70000
k_DMTA         0.07047  80.190  3.078e-79  0.068750   0.07224
k_M23          0.02203   7.738  1.230e-11  0.017030   0.02849
k_M27          0.01490   7.113  2.038e-10  0.011270   0.01971
k_M31          0.01474   5.068  1.244e-06  0.009952   0.02182
f_DMTA_to_M23  0.14350  14.460  1.890e-24        NA        NA
f_DMTA_to_M27  0.12510  15.500  2.939e-26        NA        NA
f_DMTA_to_M31  0.10070  11.820  1.290e-19        NA        NA
sigma          1.09800  13.420  1.391e-22  0.935100   1.26100

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.791       8 37
DMTA       3.514       2 10
M23        9.336       2  9
M27        9.988       2  9
M31       10.794       2  9

Resulting formation fractions:
              ff
DMTA_M23  0.1435
DMTA_M27  0.1251
DMTA_M31  0.1007
DMTA_sink 0.6307

Estimated disappearance times:
       DT50   DT90
DMTA  9.836  32.67
M23  31.464 104.52
M27  46.515 154.52
M31  47.036 156.25

Data:
    time variable observed predicted residual
  0.0000     DMTA    98.09   99.7055 -1.61552
  0.0000     DMTA    98.77   99.7055 -0.93552
  0.7679     DMTA    93.52   94.4533 -0.93330
  0.7679     DMTA    92.03   94.4533 -2.42330
  2.3037     DMTA    88.39   84.7643  3.62569
  2.3037     DMTA    87.18   84.7643  2.41569
  5.3752     DMTA    69.38   68.2660  1.11395
  5.3752     DMTA    71.06   68.2660  2.79395
 10.7505     DMTA    45.21   46.7402 -1.53017
```

```
 10.7505    DMTA   46.81   46.7402  0.06983
 16.1257    DMTA   30.54   32.0019 -1.46190
 16.1257    DMTA   30.07   32.0019 -1.93190
 21.5010    DMTA   21.60   21.9110 -0.31096
 21.5010    DMTA   20.41   21.9110 -1.50096
 32.2515    DMTA    9.10   10.2715 -1.17147
 32.2515    DMTA    9.70   10.2715 -0.57147
 43.0020    DMTA    6.58    4.8151  1.76492
 43.0020    DMTA    6.31    4.8151  1.49492
 53.7525    DMTA    3.47    2.2572  1.21278
 53.7525    DMTA    3.52    2.2572  1.26278
 64.5029    DMTA    3.40    1.0581  2.34185
 64.5029    DMTA    3.67    1.0581  2.61185
 91.3792    DMTA    1.62    0.1592  1.46079
 91.3792    DMTA    1.62    0.1592  1.46079
  0.7679     M23    0.36    0.7472 -0.38723
  0.7679     M23    0.40    0.7472 -0.34723
  2.3037     M23    1.03    2.0889 -1.05894
  2.3037     M23    1.07    2.0889 -1.01894
  5.3752     M23    3.60    4.2384 -0.63844
  5.3752     M23    3.66    4.2384 -0.57844
 10.7505     M23    6.97    6.6671  0.30292
 10.7505     M23    7.22    6.6671  0.55292
 16.1257     M23    8.65    7.9094  0.74055
 16.1257     M23    8.38    7.9094  0.47055
 21.5010     M23    9.10    8.3866  0.71344
 21.5010     M23    8.63    8.3866  0.24344
 32.2515     M23    7.63    8.0832 -0.45317
 32.2515     M23    8.01    8.0832 -0.07317
 43.0020     M23    6.40    7.0655 -0.66545
 43.0020     M23    6.35    7.0655 -0.71545
 53.7525     M23    5.35    5.8975 -0.54749
 53.7525     M23    5.06    5.8975 -0.83749
 64.5029     M23    5.14    4.8048  0.33521
 64.5029     M23    5.91    4.8048  1.10521
 91.3792     M23    3.35    2.7468  0.60316
 91.3792     M23    2.87    2.7468  0.12316
  0.7679     M27    0.42    0.6561 -0.23614
  0.7679     M27    0.47    0.6561 -0.18614
  2.3037     M27    0.71    1.8618 -1.15184
  2.3037     M27    0.82    1.8618 -1.04184
  5.3752     M27    2.19    3.8956 -1.70563
  5.3752     M27    2.28    3.8956 -1.61563
 10.7505     M27    5.45    6.4852 -1.03516
 10.7505     M27    5.19    6.4852 -1.29516
 16.1257     M27    8.81    8.1695  0.64049
 16.1257     M27    7.93    8.1695 -0.23951
 21.5010     M27   10.25    9.2253  1.02472
 21.5010     M27   10.77    9.2253  1.54472
 32.2515     M27   10.89   10.1575  0.73250
 32.2515     M27   10.85   10.1575  0.69250
 43.0020     M27   10.41   10.2118  0.19816
 43.0020     M27   10.35   10.2118  0.13816
 53.7525     M27    9.92    9.8408  0.07915
 53.7525     M27    9.42    9.8408 -0.42085
 64.5029     M27    9.15    9.2690 -0.11904
 64.5029     M27    9.25    9.2690 -0.01904
 91.3792     M27    7.14    7.5841 -0.44411
 91.3792     M27    7.13    7.5841 -0.45411
  0.7679     M31    0.36    0.5260 -0.16604
  0.7679     M31    0.33    0.5260 -0.19604
  2.3037     M31    0.55    1.4791 -0.92907
  2.3037     M31    0.64    1.4791 -0.83907
  5.3752     M31    1.94    3.0371 -1.09708
  5.3752     M31    1.62    3.0371 -1.41708
 10.7505     M31    4.22    4.8852 -0.66521
 10.7505     M31    4.37    4.8852 -0.51521
 16.1257     M31    6.31    5.9369  0.37310
 16.1257     M31    6.85    5.9369  0.91310
```

```
  21.5010      M31     7.05    6.4596  0.59044
  21.5010      M31     6.84    6.4596  0.38044
  32.2515      M31     6.53    6.5867 -0.05671
  32.2515      M31     7.11    6.5867  0.52329
  43.0020      M31     6.06    6.1249 -0.06493
  43.0020      M31     6.05    6.1249 -0.07493
  53.7525      M31     5.50    5.4635  0.03653
  53.7525      M31     5.07    5.4635 -0.39347
  64.5029      M31     4.94    4.7736  0.16641
  64.5029      M31     4.39    4.7736 -0.38359
  91.3792      M31     3.64    3.2829  0.35713
  91.3792      M31     3.55    3.2829  0.26713
```

Listing 56: SFO-SFO3b fit to BBA 2.2 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:49 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 4453 model solutions performed in 9.589 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.4300  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.430000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  274.5035 299.5016 -127.2518

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower     Upper
DMTA_0       99.63000   1.020000 97.60000 101.70000
log_k_DMTA   -2.64800   0.015530 -2.67900  -2.61700
log_k_M23    -3.82300   0.106800 -4.03600  -3.61100
log_k_M27    -4.21700   0.118000 -4.45100  -3.98200
log_k_M31    -4.22500   0.162700 -4.54800  -3.90100
f_DMTA_ilr_1  0.09707   0.054390 -0.01117   0.20530
```

```
f_DMTA_ilr_2  0.23220   0.069450  0.09401   0.37040
f_DMTA_ilr_3 -1.43000   0.048590 -1.52700  -1.33300
sigma_low     0.89260   0.074000  0.74530   1.04000
rsd_high      0.02311   0.006333  0.01051   0.03572

Parameter correlation:
               DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.000000   0.663964 -0.088796  -0.10700 -0.057168    -0.018759
log_k_DMTA    0.663964   1.000000 -0.136722  -0.16460 -0.087769    -0.027543
log_k_M23    -0.088796  -0.136722  1.000000   0.02285  0.012169     0.587272
log_k_M27    -0.107002  -0.164604  0.022855   1.00000  0.624487    -0.226184
log_k_M31    -0.057168  -0.087769  0.012169   0.62449  1.000000     0.220156
f_DMTA_ilr_1 -0.018759  -0.027543  0.587272  -0.22618  0.220156     1.000000
f_DMTA_ilr_2 -0.003901  -0.006483  0.264851  -0.38515 -0.755766    -0.127743
f_DMTA_ilr_3 -0.453522  -0.445934  0.508451   0.60704  0.371548     0.193222
sigma_low     0.120562   0.119787 -0.009043  -0.01125 -0.006421    -0.005047
rsd_high     -0.282207  -0.263025  0.019855   0.02470  0.014094     0.011075
             f_DMTA_ilr_2 f_DMTA_ilr_3  sigma_low  rsd_high
DMTA_0         -0.0039014     -0.45352  0.1205625 -0.282207
log_k_DMTA     -0.0064829     -0.44593  0.1197871 -0.263025
log_k_M23       0.2648512      0.50845 -0.0090430  0.019855
log_k_M27      -0.3851517      0.60704 -0.0112473  0.024697
log_k_M31      -0.7557662      0.37155 -0.0064206  0.014094
f_DMTA_ilr_1   -0.1277429      0.19322 -0.0050466  0.011075
f_DMTA_ilr_2    1.0000000     -0.08722  0.0007155 -0.001568
f_DMTA_ilr_3   -0.0872234      1.00000 -0.0528183  0.115976
sigma_low       0.0007155     -0.05282  1.0000000 -0.176589
rsd_high       -0.0015683      0.11598 -0.1765887  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value    Pr(>t)    Lower     Upper
DMTA_0        99.63000  97.680 2.785e-85 97.60000 101.70000
k_DMTA         0.07081  64.390 5.500e-71  0.06865   0.07303
k_M23          0.02186   9.363 8.518e-15  0.01767   0.02703
k_M27          0.01475   8.473 4.769e-13  0.01166   0.01865
k_M31          0.01463   6.148 1.456e-08  0.01058   0.02022
f_DMTA_to_M23  0.14280  16.940 1.705e-28       NA        NA
f_DMTA_to_M27  0.12450  18.090 2.682e-30       NA        NA
f_DMTA_to_M31  0.10030  14.090 1.101e-23       NA        NA
sigma_low      0.89260  12.060 5.475e-20  0.74530   1.04000
rsd_high       0.02311   3.650 2.332e-04  0.01051   0.03572

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.804       8 37
DMTA       3.521       2 10
M23        9.330       2  9
M27       10.029       2  9
M31       10.804       2  9

Resulting formation fractions:
              ff
DMTA_M23  0.1428
DMTA_M27  0.1245
DMTA_M31  0.1003
DMTA_sink 0.6323

Estimated disappearance times:
       DT50   DT90
DMTA  9.789  32.52
M23  31.714 105.35
M27  46.995 156.11
M31  47.378 157.39

Data:
    time variable observed predicted residual
```

```
 0.0000     DMTA    98.09   99.6346 -1.54455
 0.0000     DMTA    98.77   99.6346 -0.86455
 0.7679     DMTA    93.52   94.3620 -0.84197
 0.7679     DMTA    92.03   94.3620 -2.33197
 2.3037     DMTA    88.39   84.6391  3.75089
 2.3037     DMTA    87.18   84.6391  2.54089
 5.3752     DMTA    69.38   68.0956  1.28437
 5.3752     DMTA    71.06   68.0956  2.96437
10.7505     DMTA    45.21   46.5402 -1.33023
10.7505     DMTA    46.81   46.5402  0.26977
16.1257     DMTA    30.54   31.8081 -1.26811
16.1257     DMTA    30.07   31.8081 -1.73811
21.5010     DMTA    21.60   21.7394 -0.13938
21.5010     DMTA    20.41   21.7394 -1.32938
32.2515     DMTA     9.10   10.1547 -1.05467
32.2515     DMTA     9.70   10.1547 -0.45467
43.0020     DMTA     6.58    4.7433  1.83666
43.0020     DMTA     6.31    4.7433  1.56666
53.7525     DMTA     3.47    2.2157  1.25434
53.7525     DMTA     3.52    2.2157  1.30434
64.5029     DMTA     3.40    1.0350  2.36505
64.5029     DMTA     3.67    1.0350  2.63505
91.3792     DMTA     1.62    0.1543  1.46566
91.3792     DMTA     1.62    0.1543  1.46566
 0.7679      M23     0.36    0.7467 -0.38673
 0.7679      M23     0.40    0.7467 -0.34673
 2.3037      M23     1.03    2.0873 -1.05731
 2.3037      M23     1.07    2.0873 -1.01731
 5.3752      M23     3.60    4.2343 -0.63430
 5.3752      M23     3.66    4.2343 -0.57430
10.7505      M23     6.97    6.6589  0.31111
10.7505      M23     7.22    6.6589  0.56111
16.1257      M23     8.65    7.8987  0.75133
16.1257      M23     8.38    7.8987  0.48133
21.5010      M23     9.10    8.3749  0.72506
21.5010      M23     8.63    8.3749  0.25506
32.2515      M23     7.63    8.0741 -0.44412
32.2515      M23     8.01    8.0741 -0.06412
43.0020      M23     6.40    7.0621 -0.66205
43.0020      M23     6.35    7.0621 -0.71205
53.7525      M23     5.35    5.9003 -0.55026
53.7525      M23     5.06    5.9003 -0.84026
64.5029      M23     5.14    4.8128  0.32719
64.5029      M23     5.91    4.8128  1.09719
91.3792      M23     3.35    2.7617  0.58827
91.3792      M23     2.87    2.7617  0.10827
 0.7679      M27     0.42    0.6557 -0.23571
 0.7679      M27     0.47    0.6557 -0.18571
 2.3037      M27     0.71    1.8603 -1.15027
 2.3037      M27     0.82    1.8603 -1.04027
 5.3752      M27     2.19    3.8910 -1.70103
 5.3752      M27     2.28    3.8910 -1.61103
10.7505      M27     5.45    6.4744 -1.02442
10.7505      M27     5.19    6.4744 -1.28442
16.1257      M27     8.81    8.1532  0.65680
16.1257      M27     7.93    8.1532 -0.22320
21.5010      M27    10.25    9.2049  1.04508
21.5010      M27    10.77    9.2049  1.56508
32.2515      M27    10.89   10.1342  0.75575
32.2515      M27    10.85   10.1342  0.71575
43.0020      M27    10.41   10.1915  0.21853
43.0020      M27    10.35   10.1915  0.15853
53.7525      M27     9.92    9.8269  0.09308
53.7525      M27     9.42    9.8269 -0.40692
64.5029      M27     9.15    9.2632 -0.11320
64.5029      M27     9.25    9.2632 -0.01320
91.3792      M27     7.14    7.5984 -0.45839
91.3792      M27     7.13    7.5984 -0.46839
 0.7679      M31     0.36    0.5261 -0.16608
```

```
 0.7679     M31     0.33    0.5261 -0.19608
 2.3037     M31     0.55    1.4789 -0.92894
 2.3037     M31     0.64    1.4789 -0.83894
 5.3752     M31     1.94    3.0359 -1.09591
 5.3752     M31     1.62    3.0359 -1.41591
10.7505     M31     4.22    4.8812 -0.66122
10.7505     M31     4.37    4.8812 -0.51122
16.1257     M31     6.31    5.9302  0.37984
16.1257     M31     6.85    5.9302  0.91984
21.5010     M31     7.05    6.4509  0.59912
21.5010     M31     6.84    6.4509  0.38912
32.2515     M31     6.53    6.5771 -0.04708
32.2515     M31     7.11    6.5771  0.53292
43.0020     M31     6.06    6.1174 -0.05736
43.0020     M31     6.05    6.1174 -0.06736
53.7525     M31     5.50    5.4594  0.04056
53.7525     M31     5.07    5.4594 -0.38944
64.5029     M31     4.94    4.7734  0.16656
64.5029     M31     4.39    4.7734 -0.38344
91.3792     M31     3.64    3.2904  0.34963
91.3792     M31     3.55    3.2904  0.25963
```

Listing 57: SFO-SFO3b fit to BBA 2.3 data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:05 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1161 model solutions performed in 2.15 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.3850  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.385000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  325.9916 348.4899 -153.9958

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error   Lower    Upper
DMTA_0        99.9800    0.59900 98.7900 101.2000
log_k_DMTA    -2.5560    0.01525 -2.5860  -2.5250
log_k_M23     -3.8940    0.42860 -4.7470  -3.0410
log_k_M27     -3.2110    0.08481 -3.3800  -3.0430
log_k_M31     -3.0970    0.11660 -3.3290  -2.8650
f_DMTA_ilr_1  -0.6937    0.16720 -1.0260  -0.3610
f_DMTA_ilr_2  -0.6862    0.12750 -0.9398  -0.4326
f_DMTA_ilr_3  -1.4880    0.09144 -1.6700  -1.3060
sigma          1.3390    0.09982  1.1410   1.5380

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.392e-01 -1.937e-02 -8.364e-02 -5.282e-02
log_k_DMTA    5.392e-01  1.000e+00 -3.592e-02 -1.551e-01 -9.795e-02
log_k_M23    -1.937e-02 -3.592e-02  1.000e+00  5.571e-03  3.518e-03
log_k_M27    -8.364e-02 -1.551e-01  5.571e-03  1.000e+00  4.002e-01
log_k_M31    -5.282e-02 -9.795e-02  3.518e-03  4.002e-01  1.000e+00
f_DMTA_ilr_1 -5.198e-03 -9.639e-03  7.066e-01 -1.040e-01  2.672e-01
f_DMTA_ilr_2  6.891e-03  1.278e-02  5.345e-01 -1.725e-01 -5.885e-01
f_DMTA_ilr_3 -1.713e-01 -1.968e-01  6.657e-01  4.014e-01  5.758e-02
sigma        -4.088e-08  5.839e-08  1.180e-08  9.357e-08  1.357e-07
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -5.198e-03    6.891e-03   -1.713e-01 -4.088e-08
log_k_DMTA     -9.639e-03    1.278e-02   -1.968e-01  5.839e-08
log_k_M23       7.066e-01    5.345e-01    6.657e-01  1.180e-08
log_k_M27      -1.040e-01   -1.725e-01    4.014e-01  9.357e-08
log_k_M31       2.672e-01   -5.885e-01    5.758e-02  1.357e-07
f_DMTA_ilr_1    1.000e+00    3.043e-01    5.717e-01  2.102e-08
f_DMTA_ilr_2    3.043e-01    1.000e+00    5.838e-01 -1.064e-07
f_DMTA_ilr_3    5.717e-01    5.838e-01    1.000e+00 -1.743e-08
sigma           2.102e-08   -1.064e-07   -1.743e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)    Lower     Upper
DMTA_0        99.98000 166.900 7.313e-105 98.79000 101.20000
k_DMTA         0.07764  65.590  2.842e-72  0.07532   0.08003
k_M23          0.02036   2.333  1.106e-02  0.00868   0.04778
k_M27          0.04030  11.790  1.465e-19  0.03404   0.04771
k_M31          0.04519   8.579  2.699e-13  0.03584   0.05699
f_DMTA_to_M23  0.05130   4.776  3.916e-06       NA        NA
f_DMTA_to_M27  0.13680   8.970  4.555e-14       NA        NA
f_DMTA_to_M31  0.19410  12.730  2.567e-21       NA        NA
sigma          1.33900  13.420  1.391e-22  1.14100   1.53800

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   8.447       8 37
DMTA       4.554       2 10
M23        8.501       2  9
M27        6.783       2  9
M31       14.787       2  9

Resulting formation fractions:
              ff
DMTA_M23  0.0513
DMTA_M27  0.1368
DMTA_M31  0.1941
DMTA_sink 0.6178

Estimated disappearance times:
       DT50   DT90
DMTA  8.928  29.66
M23  34.038 113.07
M27  17.198  57.13
M31  15.338  50.95

Data:
    time variable observed predicted residual
  0.0000     DMTA    99.33   99.9838 -0.65377
  0.0000     DMTA    97.44   99.9838 -2.54377
  0.6734     DMTA    93.73   94.8908 -1.16081
  0.6734     DMTA    93.77   94.8908 -1.12081
  2.0202     DMTA    87.84   85.4700  2.37004
  2.0202     DMTA    89.82   85.4700  4.35004
  4.7138     DMTA    71.61   69.3413  2.26867
  4.7138     DMTA    71.42   69.3413  2.07867
  9.4275     DMTA    45.60   48.0900 -2.49000
```

```
 9.4275    DMTA   45.42   48.0900 -2.67000
14.1413    DMTA   31.12   33.3517 -2.23166
14.1413    DMTA   31.68   33.3517 -1.67166
18.8550    DMTA   23.20   23.1302  0.06976
18.8550    DMTA   24.13   23.1302  0.99976
28.2825    DMTA    9.43   11.1251 -1.69514
28.2825    DMTA    9.82   11.1251 -1.30514
37.7101    DMTA    7.08    5.3509  1.72905
37.7101    DMTA    8.64    5.3509  3.28905
47.1376    DMTA    4.41    2.5737  1.83631
47.1376    DMTA    4.78    2.5737  2.20631
56.5651    DMTA    4.92    1.2379  3.68211
56.5651    DMTA    5.08    1.2379  3.84211
80.1339    DMTA    2.13    0.1986  1.93139
80.1339    DMTA    2.23    0.1986  2.03139
 0.6734     M23    0.18    0.2594 -0.07945
 0.6734     M23    0.18    0.2594 -0.07945
 2.0202     M23    0.52    0.7290 -0.20899
 2.0202     M23    0.43    0.7290 -0.29899
 4.7138     M23    1.19    1.4944 -0.30436
 4.7138     M23    1.11    1.4944 -0.38436
 9.4275     M23    2.26    2.3940 -0.13396
 9.4275     M23    1.99    2.3940 -0.40396
14.1413     M23    2.81    2.8936 -0.08360
14.1413     M23    2.83    2.8936 -0.06360
18.8550     M23    3.39    3.1272  0.26277
18.8550     M23    3.56    3.1272  0.43277
28.2825     M23    3.49    3.1348  0.35520
28.2825     M23    3.28    3.1348  0.14520
37.7101     M23    2.80    2.8536 -0.05360
37.7101     M23    2.97    2.8536  0.11640
47.1376     M23    2.42    2.4833 -0.06326
47.1376     M23    2.51    2.4833  0.02674
56.5651     M23    2.22    2.1111  0.10888
56.5651     M23    1.95    2.1111 -0.16112
80.1339     M23    1.28    1.3458 -0.06585
80.1339     M23    0.99    1.3458 -0.35585
 0.6734     M27    0.50    0.7022 -0.20221
 0.6734     M27    0.83    0.7022  0.12779
 2.0202     M27    1.25    2.0295 -0.77948
 2.0202     M27    1.09    2.0295 -0.93948
 4.7138     M27    3.28    4.3820 -1.10203
 4.7138     M27    3.24    4.3820 -1.14203
 9.4275     M27    7.17    7.5899 -0.41986
 9.4275     M27    7.91    7.5899  0.32014
14.1413     M27   10.15    9.7763  0.37369
14.1413     M27    9.55    9.7763 -0.22631
18.8550     M27   12.09   11.1173  0.97271
18.8550     M27   11.89   11.1173  0.77271
28.2825     M27   13.32   11.9401  1.37992
28.2825     M27   12.05   11.9401  0.10992
37.7101     M27   10.04   11.2226 -1.18255
37.7101     M27   10.78   11.2226 -0.44255
47.1376     M27    9.32    9.7793 -0.45929
47.1376     M27    9.62    9.7793 -0.15929
56.5651     M27    8.00    8.1141 -0.11415
56.5651     M27    8.45    8.1141  0.33585
80.1339     M27    5.71    4.4628  1.24718
80.1339     M27    3.33    4.4628 -1.13282
 0.6734     M31    0.47    0.9736 -0.50365
 0.6734     M31    0.34    0.9736 -0.63365
 2.0202     M31    1.00    2.6895 -1.68949
 2.0202     M31    0.89    2.6895 -1.79949
 4.7138     M31    3.58    5.3229 -1.74290
 4.7138     M31    3.41    5.3229 -1.91290
 9.4275     M31    8.74    7.9932  0.74679
 9.4275     M31    8.28    7.9932  0.28679
14.1413     M31    9.67    9.0198  0.65018
14.1413     M31    8.95    9.0198 -0.06982
```

```
  18.8550      M31    10.34    9.0648  1.27518
  18.8550      M31    10.00    9.0648  0.93518
  28.2825      M31     7.89    7.7693  0.12073
  28.2825      M31     8.13    7.7693  0.36073
  37.7101      M31     5.06    5.9634 -0.90341
  37.7101      M31     5.54    5.9634 -0.42341
  47.1376      M31     3.79    4.3224 -0.53241
  47.1376      M31     4.11    4.3224 -0.21241
  56.5651      M31     3.11    3.0287  0.08133
  56.5651      M31     2.98    3.0287 -0.04867
  80.1339      M31     1.78    1.1499  0.63011
  80.1339      M31     1.55    1.1499  0.40011
```

Listing 58: SFO-SFO3b fit to BBA 2.3 data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:47 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 3631 model solutions performed in 7.531 s

Error model: Two-component variance function

Error model algorithm: d_3
Direct fitting and three-step fitting yield approximately the same likelihood

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.3850  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.385000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC     BIC    logLik
  314.7269 339.725 -147.3634

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower     Upper
DMTA_0       99.19000   1.422000 96.36000 102.00000
log_k_DMTA   -2.56800   0.023010 -2.61300  -2.52200
log_k_M23    -3.88200   0.354400 -4.58700  -3.17700
log_k_M27    -3.20500   0.073180 -3.35000  -3.05900
log_k_M31    -3.09000   0.098840 -3.28600  -2.89300
f_DMTA_ilr_1 -0.69070   0.139800 -0.96890  -0.41250
```

```
f_DMTA_ilr_2 -0.68680   0.107100 -0.90000  -0.47360
f_DMTA_ilr_3 -1.47000   0.083730 -1.63600  -1.30300
sigma_low     1.10800   0.097170  0.91490   1.30200
rsd_high      0.03014   0.009921  0.01039   0.04988

Parameter correlation:
              DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.00000    0.73392  -0.04805  -0.18158  -0.12302    -0.017220
log_k_DMTA    0.73392    1.00000  -0.06548  -0.25138  -0.16898    -0.022495
log_k_M23    -0.04805   -0.06548   1.00000   0.01646   0.01107     0.703727
log_k_M27    -0.18158   -0.25138   0.01646   1.00000   0.40905    -0.102434
log_k_M31    -0.12302   -0.16898   0.01107   0.40905   1.00000     0.270915
f_DMTA_ilr_1 -0.01722   -0.02250   0.70373  -0.10243   0.27091     1.000000
f_DMTA_ilr_2  0.01505    0.02103   0.52765  -0.16773  -0.58974     0.286887
f_DMTA_ilr_3 -0.40779   -0.40710   0.62735   0.44205   0.10524     0.518451
sigma_low     0.25118    0.29281  -0.01913  -0.06099  -0.04514    -0.009666
rsd_high     -0.48103   -0.54095   0.03535   0.11268   0.08339     0.017855
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low  rsd_high
DMTA_0           0.015052      -0.4078  0.251180 -0.481031
log_k_DMTA       0.021027      -0.4071  0.292808 -0.540951
log_k_M23        0.527647       0.6274 -0.019135  0.035351
log_k_M27       -0.167733       0.4420 -0.060989  0.112682
log_k_M31       -0.589742       0.1052 -0.045136  0.083391
f_DMTA_ilr_1     0.286887       0.5185 -0.009666  0.017855
f_DMTA_ilr_2     1.000000       0.5232  0.004508 -0.008331
f_DMTA_ilr_3     0.523246       1.0000 -0.118746  0.219378
sigma_low        0.004508      -0.1187  1.000000 -0.320319
rsd_high        -0.008331       0.2194 -0.320319  1.000000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value    Pr(>t)    Lower     Upper
DMTA_0        99.19000  69.760 1.013e-73 96.36000 102.00000
k_DMTA         0.07673  43.460 1.026e-57  0.07329   0.08032
k_M23          0.02061   2.821 3.014e-03  0.01018   0.04172
k_M27          0.04057  13.660 6.370e-23  0.03507   0.04693
k_M31          0.04552  10.120 2.852e-16  0.03739   0.05541
f_DMTA_to_M23  0.05206   5.687 1.017e-07       NA        NA
f_DMTA_to_M27  0.13830  10.300 1.265e-16       NA        NA
f_DMTA_to_M31  0.19670  14.100 1.055e-23       NA        NA
sigma_low      1.10800  11.400 9.503e-19  0.91490   1.30200
rsd_high       0.03014   3.038 1.609e-03  0.01039   0.04988

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   8.535       8 37
DMTA       4.616       2 10
M23        8.406       2  9
M27        6.752       2  9
M31       14.737       2  9

Resulting formation fractions:
               ff
DMTA_M23  0.05206
DMTA_M27  0.13826
DMTA_M31  0.19674
DMTA_sink 0.61294

Estimated disappearance times:
       DT50   DT90
DMTA  9.034  30.01
M23  33.636 111.74
M27  17.085  56.76
M31  15.227  50.58

Data:
    time variable observed predicted residual
```

0.0000	DMTA	99.33	99.1922	0.13778
0.0000	DMTA	97.44	99.1922	-1.75222
0.6734	DMTA	93.73	94.1974	-0.46743
0.6734	DMTA	93.77	94.1974	-0.42743
2.0202	DMTA	87.84	84.9497	2.89027
2.0202	DMTA	89.82	84.9497	4.87027
4.7138	DMTA	71.61	69.0888	2.52117
4.7138	DMTA	71.42	69.0888	2.33117
9.4275	DMTA	45.60	48.1214	-2.52139
9.4275	DMTA	45.42	48.1214	-2.70139
14.1413	DMTA	31.12	33.5173	-2.39725
14.1413	DMTA	31.68	33.5173	-1.83725
18.8550	DMTA	23.20	23.3453	-0.14526
18.8550	DMTA	24.13	23.3453	0.78474
28.2825	DMTA	9.43	11.3255	-1.89555
28.2825	DMTA	9.82	11.3255	-1.50555
37.7101	DMTA	7.08	5.4944	1.58561
37.7101	DMTA	8.64	5.4944	3.14561
47.1376	DMTA	4.41	2.6655	1.74449
47.1376	DMTA	4.78	2.6655	2.11449
56.5651	DMTA	4.92	1.2931	3.62687
56.5651	DMTA	5.08	1.2931	3.78687
80.1339	DMTA	2.13	0.2120	1.91802
80.1339	DMTA	2.23	0.2120	2.01802
0.6734	M23	0.18	0.2582	-0.07820
0.6734	M23	0.18	0.2582	-0.07820
2.0202	M23	0.52	0.7258	-0.20581
2.0202	M23	0.43	0.7258	-0.29581
4.7138	M23	1.19	1.4890	-0.29902
4.7138	M23	1.11	1.4890	-0.37902
9.4275	M23	2.26	2.3883	-0.12831
9.4275	M23	1.99	2.3883	-0.39831
14.1413	M23	2.81	2.8896	-0.07960
14.1413	M23	2.83	2.8896	-0.05960
18.8550	M23	3.39	3.1253	0.26474
18.8550	M23	3.56	3.1253	0.43474
28.2825	M23	3.49	3.1355	0.35446
28.2825	M23	3.28	3.1355	0.14446
37.7101	M23	2.80	2.8546	-0.05459
37.7101	M23	2.97	2.8546	0.11541
47.1376	M23	2.42	2.4829	-0.06285
47.1376	M23	2.51	2.4829	0.02715
56.5651	M23	2.22	2.1086	0.11136
56.5651	M23	1.95	2.1086	-0.15864
80.1339	M23	1.28	1.3389	-0.05893
80.1339	M23	0.99	1.3389	-0.34893
0.6734	M27	0.50	0.6961	-0.19606
0.6734	M27	0.83	0.6961	0.13394
2.0202	M27	1.25	2.0133	-0.76331
2.0202	M27	1.09	2.0133	-0.92331
4.7138	M27	3.28	4.3533	-1.07334
4.7138	M27	3.24	4.3533	-1.11334
9.4275	M27	7.17	7.5555	-0.38545
9.4275	M27	7.91	7.5555	0.35455
14.1413	M27	10.15	9.7470	0.40301
14.1413	M27	9.55	9.7470	-0.19699
18.8550	M27	12.09	11.0968	0.99315
18.8550	M27	11.89	11.0968	0.79315
28.2825	M27	13.32	11.9357	1.38432
28.2825	M27	12.05	11.9357	0.11432
37.7101	M27	10.04	11.2255	-1.18550
37.7101	M27	10.78	11.2255	-0.44550
47.1376	M27	9.32	9.7820	-0.46205
47.1376	M27	9.62	9.7820	-0.16205
56.5651	M27	8.00	8.1128	-0.11283
56.5651	M27	8.45	8.1128	0.33717
80.1339	M27	5.71	4.4507	1.25927
80.1339	M27	3.33	4.4507	-1.12073
0.6734	M31	0.47	0.9677	-0.49765

```
 0.6734      M31     0.34    0.9677 -0.62765
 2.0202      M31     1.00    2.6740 -1.67396
 2.0202      M31     0.89    2.6740 -1.78396
 4.7138      M31     3.58    5.2960 -1.71602
 4.7138      M31     3.41    5.2960 -1.88602
 9.4275      M31     8.74    7.9621  0.77795
 9.4275      M31     8.28    7.9621  0.31795
14.1413      M31     9.67    8.9938  0.67623
14.1413      M31     8.95    8.9938 -0.04377
18.8550      M31    10.34    9.0465  1.29349
18.8550      M31    10.00    9.0465  0.95349
28.2825      M31     7.89    7.7638  0.12619
28.2825      M31     8.13    7.7638  0.36619
37.7101      M31     5.06    5.9639 -0.90388
37.7101      M31     5.54    5.9639 -0.42388
47.1376      M31     3.79    4.3239 -0.53393
47.1376      M31     4.11    4.3239 -0.21393
56.5651      M31     3.11    3.0291  0.08086
56.5651      M31     2.98    3.0291 -0.04914
80.1339      M31     1.78    1.1475  0.63252
80.1339      M31     1.55    1.1475  0.40252
```

Listing 59: SFO-SFO3b fit to Borstel data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:08 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1266 model solutions performed in 2.065 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                 value   type
DMTA_0        100.2000  state
k_DMTA          0.1000 deparm
k_M23           0.1001 deparm
k_M27           0.1002 deparm
k_M31           0.1003 deparm
f_DMTA_to_M23   0.2500 deparm
f_DMTA_to_M27   0.2500 deparm
f_DMTA_to_M31   0.2500 deparm

Starting values for the transformed parameters actually optimised:
                  value lower upper
DMTA_0       100.200000  -Inf   Inf
log_k_DMTA    -2.302585  -Inf   Inf
log_k_M23     -2.301586  -Inf   Inf
log_k_M27     -2.300587  -Inf   Inf
log_k_M31     -2.299590  -Inf   Inf
f_DMTA_ilr_1   0.000000  -Inf   Inf
f_DMTA_ilr_2   0.000000  -Inf   Inf
f_DMTA_ilr_3   0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  224.0882 243.0861 -103.0441

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower   Upper
DMTA_0       97.21000    0.52540  96.1500 98.2600
log_k_DMTA   -3.77900    0.01476  -3.8090 -3.7500
log_k_M23    -7.75000    4.13200 -16.0400  0.5414
log_k_M27    -4.89100    0.77390  -6.4430 -3.3380
log_k_M31    -4.85400    0.58100  -6.0200 -3.6890
f_DMTA_ilr_1  0.61430    0.22800   0.1568  1.0720
f_DMTA_ilr_2  0.01126    0.24480  -0.4800  0.5025
f_DMTA_ilr_3 -1.79800    0.13140  -2.0620 -1.5350
sigma         1.31000    0.11860   1.0720  1.5480

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.213e-01 -3.412e-02 -2.339e-02 -1.906e-02
log_k_DMTA    5.213e-01  1.000e+00 -6.546e-02 -4.487e-02 -3.656e-02
log_k_M23    -3.412e-02 -6.546e-02  1.000e+00  2.937e-03  2.393e-03
log_k_M27    -2.339e-02 -4.487e-02  2.937e-03  1.000e+00  6.766e-01
log_k_M31    -1.906e-02 -3.656e-02  2.393e-03  6.766e-01  1.000e+00
f_DMTA_ilr_1 -2.753e-03 -5.282e-03  2.969e-01 -3.867e-01  2.581e-01
f_DMTA_ilr_2  2.439e-03  4.678e-03  1.591e-01 -2.675e-01 -7.802e-01
f_DMTA_ilr_3 -1.053e-01 -1.324e-01  3.412e-01  7.767e-01  3.573e-01
sigma         3.257e-07  2.318e-07  5.212e-07 -1.985e-07  2.651e-07
              f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -2.753e-03    2.439e-03   -1.053e-01  3.257e-07
log_k_DMTA     -5.282e-03    4.678e-03   -1.324e-01  2.318e-07
log_k_M23       2.969e-01    1.591e-01    3.412e-01  5.212e-07
log_k_M27      -3.867e-01   -2.675e-01    7.767e-01 -1.985e-07
log_k_M31       2.581e-01   -7.802e-01    3.573e-01  2.651e-07
f_DMTA_ilr_1    1.000e+00   -5.953e-01   -5.080e-01  6.345e-07
f_DMTA_ilr_2   -5.953e-01    1.000e+00    8.194e-02 -1.945e-07
f_DMTA_ilr_3   -5.080e-01    8.194e-02    1.000e+00 -2.286e-08
sigma           6.345e-07   -1.945e-07   -2.286e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
                Estimate t value    Pr(>t)     Lower    Upper
DMTA_0        9.721e+01 185.000 2.793e-75 9.615e+01 98.26000
k_DMTA        2.284e-02  67.760 1.052e-52 2.218e-02  0.02353
k_M23         4.308e-04   0.242 4.049e-01 1.080e-07  1.71800
k_M27         7.517e-03   1.292 1.010e-01 1.591e-03  0.03552
k_M31         7.794e-03   1.721 4.557e-02 2.429e-03  0.02501
f_DMTA_to_M23 1.389e-01   9.347 5.076e-13        NA       NA
f_DMTA_to_M27 5.825e-02   3.280 9.277e-04        NA       NA
f_DMTA_to_M31 8.870e-02   4.594 1.401e-05        NA       NA
sigma         1.310e+00  11.050 1.501e-15 1.072e+00  1.54800

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data   6.211       8 21
DMTA       2.585       2  6
M23       19.213       2  5
M27        2.694       2  5
M31        5.447       2  5

Resulting formation fractions:
               ff
DMTA_M23  0.13886
DMTA_M27  0.05825
DMTA_M31  0.08870
DMTA_sink 0.71419

Estimated disappearance times:
        DT50   DT90
DMTA   30.34  100.8
M23  1608.80 5344.3
M27    92.21  306.3
M31    88.93  295.4

Data:
    time variable observed predicted  residual
   0.000     DMTA    100.5   97.2083  3.291663
   0.000     DMTA    100.5   97.2083  3.291663
   0.000     DMTA     99.6   97.2083  2.391663
   1.941     DMTA     91.9   92.9919 -1.091877
   1.941     DMTA     91.3   92.9919 -1.691877
   6.795     DMTA     81.8   83.2336 -1.433617
   6.795     DMTA     82.1   83.2336 -1.133617
  13.589     DMTA     69.1   71.2679 -2.167910
  13.589     DMTA     68.0   71.2679 -3.267910
```

```
  27.178     DMTA     51.4   52.2498 -0.849788
  27.178     DMTA     51.4   52.2498 -0.849788
  27.178     DMTA     51.4   52.2498 -0.849788
  56.298     DMTA     26.8   26.8663 -0.066250
  56.298     DMTA     27.6   26.8663  0.733750
  56.298     DMTA     26.8   26.8663 -0.066250
  86.388     DMTA     15.7   13.5114  2.188601
  86.388     DMTA     15.7   13.5114  2.188601
  86.388     DMTA     15.3   13.5114  1.788601
 115.507     DMTA      7.9    6.9474  0.952591
 115.507     DMTA      7.9    6.9474  0.952591
 115.507     DMTA      8.1    6.9474  1.152591
   1.941      M23      0.4    0.5852 -0.185245
   1.941      M23      0.5    0.5852 -0.085245
   6.795      M23      1.2    1.9376 -0.737600
   6.795      M23      1.3    1.9376 -0.637600
  13.589      M23      2.8    3.5910 -0.790986
  13.589      M23      2.0    3.5910 -1.590986
  27.178      M23      2.9    6.2027 -3.302741
  27.178      M23      4.9    6.2027 -1.302741
  56.298      M23     12.2    9.6257  2.574305
  56.298      M23     12.2    9.6257  2.574305
  86.388      M23     12.2   11.3428  0.857179
  86.388      M23     12.0   11.3428  0.657179
 115.507      M23     10.4   12.1066 -1.706551
 115.507      M23     11.6   12.1066 -0.506551
   1.941      M27      0.3    0.2466  0.053384
   6.795      M27      0.8    0.8255 -0.025516
   6.795      M27      0.9    0.8255  0.074484
  13.589      M27      1.4    1.5519 -0.151905
  13.589      M27      1.4    1.5519 -0.151905
  27.178      M27      2.7    2.7468 -0.046803
  27.178      M27      2.6    2.7468 -0.146803
  56.298      M27      4.4    4.4071 -0.007133
  56.298      M27      4.7    4.4071  0.292867
  86.388      M27      5.4    5.2322  0.167789
  86.388      M27      5.2    5.2322 -0.032211
 115.507      M27      5.4    5.4875 -0.087526
 115.507      M27      5.4    5.4875 -0.087526
   1.941      M31      0.1    0.3712 -0.271168
   6.795      M31      1.0    1.2065 -0.206495
   6.795      M31      0.9    1.2065 -0.306495
  13.589      M31      2.0    2.1773 -0.177312
  13.589      M31      2.5    2.1773  0.322688
  27.178      M31      4.3    3.5548  0.745220
  27.178      M31      3.2    3.5548 -0.354780
  56.298      M31      4.3    4.8222 -0.522228
  56.298      M31      4.8    4.8222 -0.022228
  86.388      M31      5.0    4.8560  0.143983
  86.388      M31      5.1    4.8560  0.243983
 115.507      M31      4.3    4.3844 -0.084407
 115.507      M31      4.4    4.3844  0.015593
```

Listing 60: SFO-SFO3b fit to Borstel data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:51 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 3455 model solutions performed in 6.648 s

Error model: Two-component variance function

Error model algorithm: d_3
Three-step fitting yielded a higher likelihood than direct fitting

Starting values for parameters to be optimised:
                value   type
DMTA_0        100.2000  state
k_DMTA          0.1000 deparm
k_M23           0.1001 deparm
k_M27           0.1002 deparm
k_M31           0.1003 deparm
f_DMTA_to_M23   0.2500 deparm
f_DMTA_to_M27   0.2500 deparm
f_DMTA_to_M31   0.2500 deparm
sigma_low       0.1000  error
rsd_high        0.1000  error

Starting values for the transformed parameters actually optimised:
                  value lower upper
DMTA_0       100.200000  -Inf   Inf
log_k_DMTA    -2.302585  -Inf   Inf
log_k_M23     -2.301586  -Inf   Inf
log_k_M27     -2.300587  -Inf   Inf
log_k_M31     -2.299590  -Inf   Inf
f_DMTA_ilr_1   0.000000  -Inf   Inf
f_DMTA_ilr_2   0.000000  -Inf   Inf
f_DMTA_ilr_3   0.000000  -Inf   Inf
sigma_low      0.100000     0   Inf
rsd_high       0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  198.2754 219.3842 -89.13772

Optimised, transformed parameters with symmetric confidence intervals:
              Estimate Std. Error      Lower      Upper
DMTA_0        91.60000  3.661e+00  8.425e+01    98.9500
log_k_DMTA    -3.86500  3.260e-02 -3.931e+00    -3.8000
log_k_M23    -25.64000  9.308e+03 -1.871e+04 18660.0000
log_k_M27     -4.80900  2.923e-01 -5.396e+00    -4.2220
log_k_M31     -4.81100  2.107e-01 -5.234e+00    -4.3880
f_DMTA_ilr_1   0.55360  6.652e-02  4.201e-01     0.6872
```

```
f_DMTA_ilr_2  -0.02246  7.120e-02 -1.654e-01     0.1205
f_DMTA_ilr_3  -1.72900  8.344e-02 -1.897e+00    -1.5620
sigma_low      0.13070  5.356e-02  2.319e-02     0.2382
rsd_high       0.13400  1.523e-02  1.035e-01     0.1646

Parameter correlation:
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  6.927e-01 -7.025e-06 -1.770e-01 -1.274e-01
log_k_DMTA    6.927e-01  1.000e+00 -8.257e-06 -2.668e-01 -2.040e-01
log_k_M23    -7.025e-06 -8.257e-06  1.000e+00  4.112e-06  6.449e-06
log_k_M27    -1.770e-01 -2.668e-01  4.112e-06  1.000e+00  6.676e-01
log_k_M31    -1.274e-01 -2.040e-01  6.449e-06  6.676e-01  1.000e+00
f_DMTA_ilr_1  1.000e-01  1.264e-01  3.062e-05 -3.426e-01  1.875e-01
f_DMTA_ilr_2  2.891e-02  6.217e-02  8.128e-06 -2.850e-01 -7.113e-01
f_DMTA_ilr_3 -8.209e-01 -7.565e-01  2.126e-05  5.330e-01  3.465e-01
sigma_low     1.024e-01  9.153e-02  7.262e-06  1.070e-01  2.174e-01
rsd_high     -1.355e-01 -5.449e-02  1.345e-05 -6.333e-02 -1.283e-01
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3  sigma_low   rsd_high
DMTA_0          1.000e-01    2.891e-02   -8.209e-01  1.024e-01 -1.355e-01
log_k_DMTA      1.264e-01    6.217e-02   -7.565e-01  9.153e-02 -5.449e-02
log_k_M23       3.062e-05    8.128e-06    2.126e-05  7.262e-06  1.345e-05
log_k_M27      -3.426e-01   -2.850e-01    5.330e-01  1.070e-01 -6.333e-02
log_k_M31       1.875e-01   -7.113e-01    3.465e-01  2.174e-01 -1.283e-01
f_DMTA_ilr_1    1.000e+00   -4.773e-01   -2.608e-01  2.213e-01 -1.319e-01
f_DMTA_ilr_2   -4.773e-01    1.000e+00   -6.556e-02 -2.359e-01  1.385e-01
f_DMTA_ilr_3   -2.608e-01   -6.556e-02    1.000e+00  2.447e-02 -1.510e-02
sigma_low       2.213e-01   -2.359e-01    2.447e-02  1.000e+00 -3.914e-01
rsd_high       -1.319e-01    1.385e-01   -1.510e-02 -3.914e-01  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate   t value    Pr(>t)     Lower    Upper
DMTA_0        9.160e+01 2.457e+01 3.162e-30 84.250000 98.95000
k_DMTA        2.096e-02 2.994e+01 2.518e-34  0.019630  0.02238
k_M23         7.326e-12 3.751e-09 5.000e-01  0.000000      Inf
k_M27         8.154e-03 3.413e+00 6.326e-04  0.004535  0.01466
k_M31         8.136e-03 4.737e+00 8.872e-06  0.005330  0.01242
f_DMTA_to_M23 1.393e-01 9.229e+00 9.243e-13        NA       NA
f_DMTA_to_M27 6.367e-02 9.539e+00 3.142e-13        NA       NA
f_DMTA_to_M31 9.681e-02 1.078e+01 4.738e-15        NA       NA
sigma_low     1.307e-01 2.407e+00 9.879e-03  0.023190  0.23820
rsd_high      1.340e-01 8.149e+00 4.255e-11  0.103500  0.16460

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  10.191       8 21
DMTA       4.954       2  6
M23       20.147       2  5
M27        3.201       2  5
M31        5.733       2  5

Resulting formation fractions:
               ff
DMTA_M23  0.13931
DMTA_M27  0.06367
DMTA_M31  0.09681
DMTA_sink 0.70021

Estimated disappearance times:
          DT50      DT90
DMTA 3.307e+01 1.099e+02
M23  9.461e+10 3.143e+11
M27  8.500e+01 2.824e+02
M31  8.519e+01 2.830e+02

Data:
    time variable observed predicted  residual
```

```
  0.000     DMTA    100.5   91.6043  8.895733
  0.000     DMTA    100.5   91.6043  8.895733
  0.000     DMTA     99.6   91.6043  7.995733
  1.941     DMTA     91.9   87.9518  3.948207
  1.941     DMTA     91.3   87.9518  3.348207
  6.795     DMTA     81.8   79.4451  2.354889
  6.795     DMTA     82.1   79.4451  2.654889
 13.589     DMTA     69.1   68.8999  0.200090
 13.589     DMTA     68.0   68.8999 -0.899910
 27.178     DMTA     51.4   51.8229 -0.422887
 27.178     DMTA     51.4   51.8229 -0.422887
 27.178     DMTA     51.4   51.8229 -0.422887
 56.298     DMTA     26.8   28.1486 -1.348580
 56.298     DMTA     27.6   28.1486 -0.548580
 56.298     DMTA     26.8   28.1486 -1.348580
 86.388     DMTA     15.7   14.9815  0.718480
 86.388     DMTA     15.7   14.9815  0.718480
 86.388     DMTA     15.3   14.9815  0.318480
115.507     DMTA      7.9    8.1375 -0.237496
115.507     DMTA      7.9    8.1375 -0.237496
115.507     DMTA      8.1    8.1375 -0.037496
  1.941      M23      0.4    0.5088 -0.108831
  1.941      M23      0.5    0.5088 -0.008831
  6.795      M23      1.2    1.6939 -0.493909
  6.795      M23      1.3    1.6939 -0.393909
 13.589      M23      2.8    3.1630 -0.362976
 13.589      M23      2.0    3.1630 -1.162976
 27.178      M23      2.9    5.5420 -2.641999
 27.178      M23      4.9    5.5420 -0.641999
 56.298      M23     12.2    8.8401  3.359900
 56.298      M23     12.2    8.8401  3.359900
 86.388      M23     12.2   10.6744  1.525578
 86.388      M23     12.0   10.6744  1.325578
115.507      M23     10.4   11.6279 -1.227872
115.507      M23     11.6   11.6279 -0.027872
  1.941      M27      0.3    0.2335  0.066499
  6.795      M27      0.8    0.7847  0.015256
  6.795      M27      0.9    0.7847  0.115256
 13.589      M27      1.4    1.4829 -0.082890
 13.589      M27      1.4    1.4829 -0.082890
 27.178      M27      2.7    2.6481  0.051875
 27.178      M27      2.6    2.6481 -0.048125
 56.298      M27      4.4    4.3068  0.093162
 56.298      M27      4.7    4.3068  0.393162
 86.388      M27      5.4    5.1524  0.247634
 86.388      M27      5.2    5.1524  0.047634
115.507      M27      5.4    5.4183 -0.018302
115.507      M27      5.4    5.4183 -0.018302
  1.941      M31      0.1    0.3508 -0.250797
  6.795      M31      1.0    1.1444 -0.144423
  6.795      M31      0.9    1.1444 -0.244423
 13.589      M31      2.0    2.0754 -0.075391
 13.589      M31      2.5    2.0754  0.424609
 27.178      M31      4.3    3.4192  0.880847
 27.178      M31      3.2    3.4192 -0.219153
 56.298      M31      4.3    4.7141 -0.414137
 56.298      M31      4.8    4.7141  0.085863
 86.388      M31      5.0    4.8067  0.193333
 86.388      M31      5.1    4.8067  0.293333
115.507      M31      4.3    4.3756 -0.075575
115.507      M31      4.4    4.3756  0.024425
```

Listing 61: SFO-SFO3b fit to Elliot data, constant variance

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:08 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 1232 model solutions performed in 1.82 s

Error model: Constant variance

Error model algorithm: OLS

Starting values for parameters to be optimised:
                value   type
DMTA_0        98.7000  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm

Starting values for the transformed parameters actually optimised:
                 value lower upper
DMTA_0       98.700000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC     BIC    logLik
  770.0389 798.261 -376.0194

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error   Lower   Upper
DMTA_0       95.51000    0.75620 94.0100 97.0000
log_k_DMTA   -2.82900    0.02117 -2.8710 -2.7880
log_k_M23    -3.87900    0.25630 -4.3850 -3.3730
log_k_M27    -4.40000    0.16010 -4.7170 -4.0840
log_k_M31    -4.62800    0.23060 -5.0830 -4.1730
f_DMTA_ilr_1  0.09136    0.11890 -0.1434  0.3262
f_DMTA_ilr_2  0.05021    0.11440 -0.1758  0.2762
f_DMTA_ilr_3 -1.47200    0.08428 -1.6380 -1.3050
sigma         2.21000    0.11980  1.9730  2.4470

Parameter correlation:
```

```
                DMTA_0 log_k_DMTA  log_k_M23  log_k_M27  log_k_M31
DMTA_0        1.000e+00  5.524e-01 -4.524e-02 -5.351e-02 -2.663e-02
log_k_DMTA    5.524e-01  1.000e+00 -8.189e-02 -9.686e-02 -4.821e-02
log_k_M23    -4.524e-02 -8.189e-02  1.000e+00  7.933e-03  3.948e-03
log_k_M27    -5.351e-02 -9.686e-02  7.933e-03  1.000e+00  5.123e-01
log_k_M31    -2.663e-02 -4.821e-02  3.948e-03  5.123e-01  1.000e+00
f_DMTA_ilr_1 -1.828e-02 -3.310e-02  6.692e-01 -1.907e-01  2.109e-01
f_DMTA_ilr_2 -1.681e-02 -3.043e-02  4.023e-01 -2.555e-01 -6.587e-01
f_DMTA_ilr_3 -2.214e-01 -2.423e-01  6.329e-01  4.683e-01  2.196e-01
sigma        -1.165e-07 -8.492e-08  4.170e-08  8.217e-08  8.830e-08
             f_DMTA_ilr_1 f_DMTA_ilr_2 f_DMTA_ilr_3      sigma
DMTA_0         -1.828e-02   -1.681e-02   -2.214e-01 -1.165e-07
log_k_DMTA     -3.310e-02   -3.043e-02   -2.423e-01 -8.492e-08
log_k_M23       6.692e-01    4.023e-01    6.329e-01  4.170e-08
log_k_M27      -1.907e-01   -2.555e-01    4.683e-01  8.217e-08
log_k_M31       2.109e-01   -6.587e-01    2.196e-01  8.830e-08
f_DMTA_ilr_1    1.000e+00    5.863e-02    3.833e-01  2.129e-08
f_DMTA_ilr_2    5.863e-02    1.000e+00    2.394e-01 -5.488e-08
f_DMTA_ilr_3    3.833e-01    2.394e-01    1.000e+00  7.634e-08
sigma           2.129e-08   -5.488e-08    7.634e-08  1.000e+00

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
               Estimate t value     Pr(>t)     Lower    Upper
DMTA_0        95.510000 126.300 2.973e-163 94.010000 97.00000
k_DMTA         0.059050  47.240  1.471e-96  0.056630  0.06157
k_M23          0.020680   3.901  7.010e-05  0.012460  0.03430
k_M27          0.012270   6.245  1.811e-09  0.008946  0.01684
k_M31          0.009773   4.337  1.271e-05  0.006198  0.01541
f_DMTA_to_M23  0.128500   7.307  5.992e-12        NA       NA
f_DMTA_to_M27  0.112900   9.919  1.072e-18        NA       NA
f_DMTA_to_M31  0.113300  10.040  5.169e-19        NA       NA
sigma          2.210000  18.440  7.804e-42  1.973000  2.44700

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  12.989       8 35
DMTA       7.787       2 10
M23       12.150       2  8
M27        7.233       2  8
M31       15.780       2  9

Resulting formation fractions:
              ff
DMTA_M23  0.1285
DMTA_M27  0.1129
DMTA_M31  0.1133
DMTA_sink 0.6454

Estimated disappearance times:
      DT50  DT90
DMTA 11.74  39.0
M23  33.52 111.4
M27  56.47 187.6
M31  70.92 235.6

Data:
    time variable observed predicted  residual
   0.000     DMTA     97.5 9.551e+01  1.993961
   0.000     DMTA    100.7 9.551e+01  5.193961
   0.000     DMTA     93.4 9.551e+01 -2.106039
   0.000     DMTA    103.2 9.551e+01  7.693961
   1.228     DMTA     86.4 8.882e+01 -2.423676
   1.228     DMTA     88.5 8.882e+01 -0.323676
   1.228     DMTA     89.2 8.882e+01  0.376324
   1.228     DMTA     86.6 8.882e+01 -2.223676
   3.685     DMTA     69.8 7.683e+01 -7.028890
```

```
   3.685     DMTA     77.1 7.683e+01  0.271110
   3.685     DMTA     78.2 7.683e+01  1.371110
   3.685     DMTA     78.1 7.683e+01  1.271110
   8.599     DMTA     59.0 5.748e+01  1.520075
   8.599     DMTA     54.2 5.748e+01 -3.279925
   8.599     DMTA     55.6 5.748e+01 -1.879925
   8.599     DMTA     53.0 5.748e+01 -4.479925
  17.199     DMTA     31.3 3.459e+01 -3.294062
  17.199     DMTA     33.5 3.459e+01 -1.094062
  17.199     DMTA     33.7 3.459e+01 -0.894062
  17.199     DMTA     33.2 3.459e+01 -1.394062
  25.798     DMTA     19.6 2.082e+01 -1.220297
  25.798     DMTA     20.9 2.082e+01  0.079703
  25.798     DMTA     20.9 2.082e+01  0.079703
  25.798     DMTA     19.9 2.082e+01 -0.920297
  34.397     DMTA     13.3 1.253e+01  0.769388
  34.397     DMTA     15.8 1.253e+01  3.269388
  34.397     DMTA     18.2 1.253e+01  5.669388
  34.397     DMTA     12.7 1.253e+01  0.169388
  51.596     DMTA      6.7 4.539e+00  2.161180
  51.596     DMTA      8.7 4.539e+00  4.161180
  51.596     DMTA      7.8 4.539e+00  3.261180
  51.596     DMTA      9.0 4.539e+00  4.461180
  68.795     DMTA      8.8 1.644e+00  7.155955
  68.795     DMTA      8.7 1.644e+00  7.055955
  68.795     DMTA     11.4 1.644e+00  9.755955
  68.795     DMTA      9.0 1.644e+00  7.355955
 103.192     DMTA      6.0 2.157e-01  5.784298
 103.192     DMTA      4.4 2.157e-01  4.184298
 103.192     DMTA      3.9 2.157e-01  3.684298
 103.192     DMTA      4.4 2.157e-01  4.184298
 146.189     DMTA      3.3 1.703e-02  3.282967
 146.189     DMTA      2.8 1.703e-02  2.782967
 146.189     DMTA      2.6 1.703e-02  2.582967
 146.189     DMTA      3.4 1.703e-02  3.382967
 223.583     DMTA      1.4 1.765e-04  1.399824
 223.583     DMTA      1.8 1.765e-04  1.799824
 223.583     DMTA      2.0 1.765e-04  1.999824
 223.583     DMTA      1.7 1.765e-04  1.699824
   3.685      M23      2.8 2.307e+00  0.492749
   3.685      M23      1.7 2.307e+00 -0.607251
   3.685      M23      2.6 2.307e+00  0.292749
   3.685      M23      2.4 2.307e+00  0.092749
   8.599      M23      4.3 4.442e+00 -0.142332
   8.599      M23      5.8 4.442e+00  1.357668
   8.599      M23      5.5 4.442e+00  1.057668
   8.599      M23      5.6 4.442e+00  1.157668
  17.199      M23      8.2 6.392e+00  1.807703
  17.199      M23      5.2 6.392e+00 -1.192297
  17.199      M23      7.3 6.392e+00  0.907703
  17.199      M23      6.5 6.392e+00  0.107703
  25.798      M23      5.1 6.960e+00 -1.860118
  25.798      M23      6.1 6.960e+00 -0.860118
  25.798      M23      5.8 6.960e+00 -1.160118
  25.798      M23      7.7 6.960e+00  0.739882
  34.397      M23      6.0 6.795e+00 -0.794776
  34.397      M23      6.0 6.795e+00 -0.794776
  34.397      M23      7.8 6.795e+00  1.005224
  34.397      M23      7.3 6.795e+00  0.505224
  51.596      M23      5.0 5.600e+00 -0.600087
  51.596      M23      4.2 5.600e+00 -1.400087
  51.596      M23      7.0 5.600e+00  1.399913
  51.596      M23      6.3 5.600e+00  0.699913
  68.795      M23      3.9 4.228e+00 -0.328017
  68.795      M23      2.9 4.228e+00 -1.328017
  68.795      M23      4.3 4.228e+00  0.071983
  68.795      M23      3.8 4.228e+00 -0.428017
 103.192      M23      1.9 2.193e+00 -0.293104
 103.192      M23      1.5 2.193e+00 -0.693104
```

```
 103.192      M23      2.6 2.193e+00  0.406896
 103.192      M23      2.8 2.193e+00  0.606896
 146.189      M23      2.0 9.156e-01  1.084352
 146.189      M23      2.3 9.156e-01  1.384352
 146.189      M23      1.6 9.156e-01  0.684352
 146.189      M23      1.1 9.156e-01  0.184352
 223.583      M23      1.2 1.855e-01  1.014536
 223.583      M23      1.9 1.855e-01  1.714536
 223.583      M23      1.4 1.855e-01  1.214536
 223.583      M23      1.3 1.855e-01  1.114536
   3.685      M27      2.3 2.098e+00  0.201530
   3.685      M27      2.1 2.098e+00  0.001530
   3.685      M27      1.0 2.098e+00 -1.098470
   3.685      M27      2.6 2.098e+00  0.501530
   8.599      M27      4.0 4.240e+00 -0.240199
   8.599      M27      3.4 4.240e+00 -0.840199
   8.599      M27      4.5 4.240e+00  0.259801
   8.599      M27      4.6 4.240e+00  0.359801
  17.199      M27      6.6 6.682e+00 -0.082069
  17.199      M27      6.9 6.682e+00  0.217931
  17.199      M27      7.6 6.682e+00  0.917931
  17.199      M27      6.7 6.682e+00  0.017931
  25.798      M27      8.2 8.027e+00  0.172715
  25.798      M27      8.8 8.027e+00  0.772715
  25.798      M27      8.7 8.027e+00  0.672715
  25.798      M27      7.6 8.027e+00 -0.427285
  34.397      M27      9.7 8.702e+00  0.998373
  34.397      M27      8.8 8.702e+00  0.098373
  34.397      M27      8.0 8.702e+00 -0.701627
  34.397      M27      8.6 8.702e+00 -0.101627
  51.596      M27      8.3 8.974e+00 -0.673883
  51.596      M27      9.2 8.974e+00  0.226117
  51.596      M27      7.4 8.974e+00 -1.573883
  51.596      M27      7.2 8.974e+00 -1.773883
  68.795      M27      9.3 8.587e+00  0.713250
  68.795      M27      8.5 8.587e+00 -0.086750
  68.795      M27     10.3 8.587e+00  1.713250
  68.795      M27      9.4 8.587e+00  0.813250
 103.192      M27      8.6 7.251e+00  1.348953
 103.192      M27      6.0 7.251e+00 -1.251047
 103.192      M27      6.5 7.251e+00 -0.751047
 103.192      M27      6.9 7.251e+00 -0.351047
 146.189      M27      5.6 5.528e+00  0.072272
 146.189      M27      4.5 5.528e+00 -1.027728
 146.189      M27      4.6 5.528e+00 -0.927728
 146.189      M27      4.5 5.528e+00 -1.027728
 223.583      M27      4.1 3.141e+00  0.958764
 223.583      M27      3.9 3.141e+00  0.758764
 223.583      M27      4.3 3.141e+00  1.158764
 223.583      M27      4.2 3.141e+00  1.058764
   1.228      M31      1.5 7.522e-01  0.747756
   1.228      M31      1.3 7.522e-01  0.547756
   3.685      M31      5.0 2.076e+00  2.923683
   3.685      M31      2.4 2.076e+00  0.323683
   3.685      M31      3.1 2.076e+00  1.023683
   3.685      M31      2.3 2.076e+00  0.223683
   8.599      M31      4.3 4.116e+00  0.183907
   8.599      M31      5.0 4.116e+00  0.883907
   8.599      M31      3.4 4.116e+00 -0.716093
   8.599      M31      4.3 4.116e+00  0.183907
  17.199      M31      8.0 6.262e+00  1.738446
  17.199      M31      7.7 6.262e+00  1.438446
  17.199      M31      7.8 6.262e+00  1.538446
  17.199      M31      8.7 6.262e+00  2.438446
  25.798      M31      7.8 7.248e+00  0.552256
  25.798      M31      6.5 7.248e+00 -0.747744
  25.798      M31      7.7 7.248e+00  0.452256
  25.798      M31      6.5 7.248e+00 -0.747744
  34.397      M31      8.0 7.561e+00  0.439179
```

```
  34.397      M31      7.4 7.561e+00 -0.160821
  34.397      M31      6.3 7.561e+00 -1.260821
  34.397      M31      8.7 7.561e+00  1.139179
  51.596      M31      6.9 7.213e+00 -0.312546
  51.596      M31      9.0 7.213e+00  1.787454
  51.596      M31      5.7 7.213e+00 -1.512546
  51.596      M31      4.2 7.213e+00 -3.012546
  68.795      M31      5.5 6.394e+00 -0.894198
  68.795      M31      6.1 6.394e+00 -0.294198
  68.795      M31      3.2 6.394e+00 -3.194198
  68.795      M31      4.2 6.394e+00 -2.194198
 103.192      M31      6.1 4.699e+00  1.401198
 103.192      M31      4.0 4.699e+00 -0.698802
 103.192      M31      3.8 4.699e+00 -0.898802
 103.192      M31      4.0 4.699e+00 -0.698802
 146.189      M31      3.1 3.104e+00 -0.003584
 146.189      M31      2.9 3.104e+00 -0.203584
 146.189      M31      4.5 3.104e+00  1.396416
 146.189      M31      4.5 3.104e+00  1.396416
 223.583      M31      1.8 1.458e+00  0.342248
 223.583      M31      2.6 1.458e+00  1.142248
 223.583      M31      3.8 1.458e+00  2.342248
 223.583      M31      2.3 1.458e+00  0.842248
```

Listing 62: SFO-SFO3b fit to Elliot data, two-component error

```
mkin version used for fitting:    1.0.4.9000
R version used for fitting:       4.1.0
Date of fit:     Mon Jul 26 14:04:57 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Model predictions using solution type deSolve

Fitted using 4712 model solutions performed in 6.724 s

Error model: Two-component variance function

Error model algorithm: d_3
Three-step fitting yielded a higher likelihood than direct fitting

Starting values for parameters to be optimised:
               value   type
DMTA_0        98.7000  state
k_DMTA         0.1000 deparm
k_M23          0.1001 deparm
k_M27          0.1002 deparm
k_M31          0.1003 deparm
f_DMTA_to_M23  0.2500 deparm
f_DMTA_to_M27  0.2500 deparm
f_DMTA_to_M31  0.2500 deparm
sigma_low      0.1000  error
rsd_high       0.1000  error

Starting values for the transformed parameters actually optimised:
                value lower upper
DMTA_0       98.700000  -Inf   Inf
log_k_DMTA   -2.302585  -Inf   Inf
log_k_M23    -2.301586  -Inf   Inf
log_k_M27    -2.300587  -Inf   Inf
log_k_M31    -2.299590  -Inf   Inf
f_DMTA_ilr_1  0.000000  -Inf   Inf
f_DMTA_ilr_2  0.000000  -Inf   Inf
f_DMTA_ilr_3  0.000000  -Inf   Inf
sigma_low     0.100000     0   Inf
rsd_high      0.100000     0   Inf

Fixed parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

       AIC      BIC    logLik
  758.2828 789.6408 -369.1414

Optimised, transformed parameters with symmetric confidence intervals:
             Estimate Std. Error    Lower    Upper
DMTA_0       93.63000    1.53500 90.60000 96.66000
log_k_DMTA   -2.87900    0.03197 -2.94300 -2.81600
log_k_M23    -3.82900    0.23110 -4.28600 -3.37300
log_k_M27    -4.36500    0.14390 -4.64900 -4.08000
log_k_M31    -4.60400    0.20530 -5.01000 -4.19900
f_DMTA_ilr_1  0.10110    0.10860 -0.11350  0.31560
```

```
f_DMTA_ilr_2  0.05865    0.10380 -0.14640  0.26370
f_DMTA_ilr_3 -1.41100    0.08732 -1.58300 -1.23800
sigma_low     1.96900    0.12050  1.73100  2.20700
rsd_high      0.04134    0.01181  0.01801  0.06466

Parameter correlation:
               DMTA_0 log_k_DMTA log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1
DMTA_0        1.00000    0.73617  -0.10320  -0.11983  -0.05787     -0.04334
log_k_DMTA    0.73617    1.00000  -0.14034  -0.16337  -0.07951     -0.05883
log_k_M23    -0.10320   -0.14034   1.00000   0.02293   0.01117      0.67595
log_k_M27    -0.11983   -0.16337   0.02293   1.00000   0.50952     -0.18806
log_k_M31    -0.05787   -0.07951   0.01117   0.50952   1.00000      0.20949
f_DMTA_ilr_1 -0.04334   -0.05883   0.67595  -0.18806   0.20949      1.00000
f_DMTA_ilr_2 -0.03911   -0.05312   0.41085  -0.24009  -0.65198      0.06804
f_DMTA_ilr_3 -0.45254   -0.45508   0.62251   0.47259   0.22303      0.37104
sigma_low     0.23882    0.29088  -0.04039  -0.04587  -0.02066     -0.01721
rsd_high     -0.52836   -0.61509   0.08542   0.09699   0.04369      0.03639
             f_DMTA_ilr_2 f_DMTA_ilr_3 sigma_low rsd_high
DMTA_0          -0.03911      -0.4525   0.23882 -0.52836
log_k_DMTA      -0.05312      -0.4551   0.29088 -0.61509
log_k_M23        0.41085       0.6225  -0.04039  0.08542
log_k_M27       -0.24009       0.4726  -0.04587  0.09699
log_k_M31       -0.65198       0.2230  -0.02066  0.04369
f_DMTA_ilr_1     0.06804       0.3710  -0.01721  0.03639
f_DMTA_ilr_2     1.00000       0.2425  -0.01548  0.03272
f_DMTA_ilr_3     0.24250       1.0000  -0.13824  0.29231
sigma_low       -0.01548      -0.1382   1.00000 -0.28650
rsd_high         0.03272       0.2923  -0.28650  1.00000

Backtransformed parameters:
Confidence intervals for internally transformed parameters are asymmetric.
t-test (unrealistically) based on the assumption of normal distribution
for estimators of untransformed parameters.
              Estimate t value     Pr(>t)     Lower    Upper
DMTA_0        93.63000  61.010 5.147e-113 90.600000 96.66000
k_DMTA         0.05617  31.280  2.244e-70  0.052730  0.05983
k_M23          0.02173   4.326  1.331e-05  0.013770  0.03430
k_M27          0.01272   6.947  4.440e-11  0.009573  0.01690
k_M31          0.01001   4.871  1.324e-06  0.006672  0.01501
f_DMTA_to_M23  0.13570   7.738  5.356e-13        NA       NA
f_DMTA_to_M27  0.11770  10.530  2.560e-20        NA       NA
f_DMTA_to_M31  0.11760  10.750  6.413e-21        NA       NA
sigma_low      1.96900  16.340  3.130e-36  1.731000  2.20700
rsd_high       0.04134   3.500  3.017e-04  0.018010  0.06466

FOCUS Chi2 error levels in percent:
         err.min n.optim df
All data  13.386       8 35
DMTA       8.020       2 10
M23       12.502       2  8
M27        7.436       2  8
M31       16.411       2  9

Resulting formation fractions:
              ff
DMTA_M23  0.1357
DMTA_M27  0.1177
DMTA_M31  0.1176
DMTA_sink 0.6290

Estimated disappearance times:
      DT50   DT90
DMTA 12.34  40.99
M23  31.90 105.96
M27  54.49 181.02
M31  69.26 230.06

Data:
    time variable observed predicted  residual
```

```
 0.000     DMTA     97.5 9.363e+01  3.866039
 0.000     DMTA    100.7 9.363e+01  7.066039
 0.000     DMTA     93.4 9.363e+01 -0.233961
 0.000     DMTA    103.2 9.363e+01  9.566039
 1.228     DMTA     86.4 8.739e+01 -0.990889
 1.228     DMTA     88.5 8.739e+01  1.109111
 1.228     DMTA     89.2 8.739e+01  1.809111
 1.228     DMTA     86.6 8.739e+01 -0.790889
 3.685     DMTA     69.8 7.613e+01 -6.325768
 3.685     DMTA     77.1 7.613e+01  0.974232
 3.685     DMTA     78.2 7.613e+01  2.074232
 3.685     DMTA     78.1 7.613e+01  1.974232
 8.599     DMTA     59.0 5.776e+01  1.235271
 8.599     DMTA     54.2 5.776e+01 -3.564729
 8.599     DMTA     55.6 5.776e+01 -2.164729
 8.599     DMTA     53.0 5.776e+01 -4.764729
17.199     DMTA     31.3 3.564e+01 -4.336257
17.199     DMTA     33.5 3.564e+01 -2.136257
17.199     DMTA     33.7 3.564e+01 -1.936257
17.199     DMTA     33.2 3.564e+01 -2.436257
25.798     DMTA     19.6 2.198e+01 -2.384745
25.798     DMTA     20.9 2.198e+01 -1.084745
25.798     DMTA     20.9 2.198e+01 -1.084745
25.798     DMTA     19.9 2.198e+01 -2.084745
34.397     DMTA     13.3 1.356e+01 -0.262844
34.397     DMTA     15.8 1.356e+01  2.237156
34.397     DMTA     18.2 1.356e+01  4.637156
34.397     DMTA     12.7 1.356e+01 -0.862844
51.596     DMTA      6.7 5.162e+00  1.538102
51.596     DMTA      8.7 5.162e+00  3.538102
51.596     DMTA      7.8 5.162e+00  2.638102
51.596     DMTA      9.0 5.162e+00  3.838102
68.795     DMTA      8.8 1.965e+00  6.835427
68.795     DMTA      8.7 1.965e+00  6.735427
68.795     DMTA     11.4 1.965e+00  9.435427
68.795     DMTA      9.0 1.965e+00  7.035427
103.192    DMTA      6.0 2.846e-01  5.715432
103.192    DMTA      4.4 2.846e-01  4.115432
103.192    DMTA      3.9 2.846e-01  3.615432
103.192    DMTA      4.4 2.846e-01  4.115432
146.189    DMTA      3.3 2.543e-02  3.274571
146.189    DMTA      2.8 2.543e-02  2.774571
146.189    DMTA      2.6 2.543e-02  2.574571
146.189    DMTA      3.4 2.543e-02  3.374571
223.583    DMTA      1.4 3.292e-04  1.399671
223.583    DMTA      1.8 3.292e-04  1.799671
223.583    DMTA      2.0 3.292e-04  1.999671
223.583    DMTA      1.7 3.292e-04  1.699671
 3.685      M23      2.8 2.280e+00  0.519516
 3.685      M23      1.7 2.280e+00 -0.580484
 3.685      M23      2.6 2.280e+00  0.319516
 3.685      M23      2.4 2.280e+00  0.119516
 8.599      M23      4.3 4.407e+00 -0.107331
 8.599      M23      5.8 4.407e+00  1.392669
 8.599      M23      5.5 4.407e+00  1.092669
 8.599      M23      5.6 4.407e+00  1.192669
17.199      M23      8.2 6.375e+00  1.824928
17.199      M23      5.2 6.375e+00 -1.175072
17.199      M23      7.3 6.375e+00  0.924928
17.199      M23      6.5 6.375e+00  0.124928
25.798      M23      5.1 6.966e+00 -1.865827
25.798      M23      6.1 6.966e+00 -0.865827
25.798      M23      5.8 6.966e+00 -1.165827
25.798      M23      7.7 6.966e+00  0.734173
34.397      M23      6.0 6.813e+00 -0.813313
34.397      M23      6.0 6.813e+00 -0.813313
34.397      M23      7.8 6.813e+00  0.986687
34.397      M23      7.3 6.813e+00  0.486687
51.596      M23      5.0 5.612e+00 -0.612020
```

```
  51.596      M23      4.2 5.612e+00 -1.412020
  51.596      M23      7.0 5.612e+00  1.387980
  51.596      M23      6.3 5.612e+00  0.687980
  68.795      M23      3.9 4.213e+00 -0.313370
  68.795      M23      2.9 4.213e+00 -1.313370
  68.795      M23      4.3 4.213e+00  0.086630
  68.795      M23      3.8 4.213e+00 -0.413370
 103.192      M23      1.9 2.138e+00 -0.238206
 103.192      M23      1.5 2.138e+00 -0.638206
 103.192      M23      2.6 2.138e+00  0.461794
 103.192      M23      2.8 2.138e+00  0.661794
 146.189      M23      2.0 8.591e-01  1.140919
 146.189      M23      2.3 8.591e-01  1.440919
 146.189      M23      1.6 8.591e-01  0.740919
 146.189      M23      1.1 8.591e-01  0.240919
 223.583      M23      1.2 1.608e-01  1.039212
 223.583      M23      1.9 1.608e-01  1.739212
 223.583      M23      1.4 1.608e-01  1.239212
 223.583      M23      1.3 1.608e-01  1.139212
   3.685      M27      2.3 2.049e+00  0.251119
   3.685      M27      2.1 2.049e+00  0.051119
   3.685      M27      1.0 2.049e+00 -1.048881
   3.685      M27      2.6 2.049e+00  0.551119
   8.599      M27      4.0 4.163e+00 -0.163233
   8.599      M27      3.4 4.163e+00 -0.763233
   8.599      M27      4.5 4.163e+00  0.336767
   8.599      M27      4.6 4.163e+00  0.436767
  17.199      M27      6.6 6.615e+00 -0.014667
  17.199      M27      6.9 6.615e+00  0.285333
  17.199      M27      7.6 6.615e+00  0.985333
  17.199      M27      6.7 6.615e+00  0.085333
  25.798      M27      8.2 7.996e+00  0.203753
  25.798      M27      8.8 7.996e+00  0.803753
  25.798      M27      8.7 7.996e+00  0.703753
  25.798      M27      7.6 7.996e+00 -0.396247
  34.397      M27      9.7 8.708e+00  0.992431
  34.397      M27      8.8 8.708e+00  0.092431
  34.397      M27      8.0 8.708e+00 -0.707569
  34.397      M27      8.6 8.708e+00 -0.107569
  51.596      M27      8.3 9.025e+00 -0.724565
  51.596      M27      9.2 9.025e+00  0.175435
  51.596      M27      7.4 9.025e+00 -1.624565
  51.596      M27      7.2 9.025e+00 -1.824565
  68.795      M27      9.3 8.643e+00  0.656612
  68.795      M27      8.5 8.643e+00 -0.143388
  68.795      M27     10.3 8.643e+00  1.656612
  68.795      M27      9.4 8.643e+00  0.756612
 103.192      M27      8.6 7.266e+00  1.334360
 103.192      M27      6.0 7.266e+00 -1.265640
 103.192      M27      6.5 7.266e+00 -0.765640
 103.192      M27      6.9 7.266e+00 -0.365640
 146.189      M27      5.6 5.482e+00  0.118471
 146.189      M27      4.5 5.482e+00 -0.981529
 146.189      M27      4.6 5.482e+00 -0.881529
 146.189      M27      4.5 5.482e+00 -0.981529
 223.583      M27      4.1 3.048e+00  1.051763
 223.583      M27      3.9 3.048e+00  0.851763
 223.583      M27      4.3 3.048e+00  1.251763
 223.583      M27      4.2 3.048e+00  1.151763
   1.228      M31      1.5 7.297e-01  0.770323
   1.228      M31      1.3 7.297e-01  0.570323
   3.685      M31      5.0 2.020e+00  2.979725
   3.685      M31      2.4 2.020e+00  0.379725
   3.685      M31      3.1 2.020e+00  1.079725
   3.685      M31      2.3 2.020e+00  0.279725
   8.599      M31      4.3 4.028e+00  0.271927
   8.599      M31      5.0 4.028e+00  0.971927
   8.599      M31      3.4 4.028e+00 -0.628073
   8.599      M31      4.3 4.028e+00  0.271927
```

```
  17.199      M31      8.0 6.181e+00  1.819110
  17.199      M31      7.7 6.181e+00  1.519110
  17.199      M31      7.8 6.181e+00  1.619110
  17.199      M31      8.7 6.181e+00  2.519110
  25.798      M31      7.8 7.204e+00  0.595782
  25.798      M31      6.5 7.204e+00 -0.704218
  25.798      M31      7.7 7.204e+00  0.495782
  25.798      M31      6.5 7.204e+00 -0.704218
  34.397      M31      8.0 7.556e+00  0.444125
  34.397      M31      7.4 7.556e+00 -0.155875
  34.397      M31      6.3 7.556e+00 -1.255875
  34.397      M31      8.7 7.556e+00  1.144125
  51.596      M31      6.9 7.256e+00 -0.356337
  51.596      M31      9.0 7.256e+00  1.743663
  51.596      M31      5.7 7.256e+00 -1.556337
  51.596      M31      4.2 7.256e+00 -3.056337
  68.795      M31      5.5 6.450e+00 -0.949610
  68.795      M31      6.1 6.450e+00 -0.349610
  68.795      M31      3.2 6.450e+00 -3.249610
  68.795      M31      4.2 6.450e+00 -2.249610
 103.192      M31      6.1 4.730e+00  1.370377
 103.192      M31      4.0 4.730e+00 -0.729623
 103.192      M31      3.8 4.730e+00 -0.929623
 103.192      M31      4.0 4.730e+00 -0.729623
 146.189      M31      3.1 3.098e+00  0.001525
 146.189      M31      2.9 3.098e+00 -0.198475
 146.189      M31      4.5 3.098e+00  1.401525
 146.189      M31      4.5 3.098e+00  1.401525
 223.583      M31      1.8 1.430e+00  0.370323
 223.583      M31      2.6 1.430e+00  1.170323
 223.583      M31      3.8 1.430e+00  2.370323
 223.583      M31      2.3 1.430e+00  0.870323
```

Listing for the mixed effects model fits for dimethenamid

Listing 63: DFOP-SFO3 fit with nlme to dimethenamid data, variance by variable

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 15:02:51 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - ((k1 * g * exp(-k1 * time) + k2 * (1 - g) * exp(-k2 *
           time)) / (g * exp(-k1 * time) + (1 - g) * exp(-k2 * time)))
           * DMTA
d_M23/dt = + f_DMTA_to_M23 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M31 * M31

Data:
568 observations of 4 variable(s) grouped in 6 datasets

Model predictions using solution type deSolve

Fitted in 130.155 s using 15 iterations

Variance model: Variance unique to each observed variable

Mean of starting values for individual parameters:
      DMTA_0    log_k_M23    log_k_M27    log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
    98.24705     -7.23161    -12.60526     -4.24406      0.07824      0.18195
f_DMTA_ilr_3       log_k1       log_k2     g_qlogis
    -1.69698     -2.07754    -13.67191      1.93296

Fixed degradation parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

   AIC  BIC logLik
  1928 2032   -940

Optimised, transformed parameters with symmetric confidence intervals:
               lower     est.   upper
DMTA_0       96.5771 98.04219 99.5073
log_k_M23    -5.4069 -4.36954 -3.3322
log_k_M27    -5.5430 -4.85312 -4.1632
log_k_M31    -4.6289 -4.10548 -3.5820
f_DMTA_ilr_1 -0.3384  0.02432  0.3871
f_DMTA_ilr_2 -0.1979  0.16262  0.5232
f_DMTA_ilr_3 -1.8363 -1.63568 -1.4351
log_k1       -2.6925 -2.42234 -2.1522
log_k2       -4.7307 -4.18912 -3.6476
g_qlogis     -0.5776  1.65647  3.8906

Correlation:
             DMTA_0 l__M23 l__M27 l__M31 f_DMTA__1 f_DMTA__2 f_DMTA__3 log_k1
log_k_M23    -0.011
log_k_M27    -0.011  0.002
log_k_M31    -0.011  0.002  0.002
```

```
f_DMTA_ilr_1 -0.001  0.025 -0.047  0.000
f_DMTA_ilr_2  0.001  0.014  0.028 -0.068 -0.001
f_DMTA_ilr_3 -0.041  0.031  0.049  0.060  0.001    -0.022
log_k1        0.034  0.000 -0.001 -0.001  0.000     0.000    -0.007
log_k2        0.011  0.004  0.006  0.005  0.000     0.000     0.003     0.078
g_qlogis     -0.006 -0.003 -0.001  0.000  0.000     0.000     0.000    -0.077
             log_k2
log_k_M23
log_k_M27
log_k_M31
f_DMTA_ilr_1
f_DMTA_ilr_2
f_DMTA_ilr_3
log_k1
log_k2
g_qlogis     -0.113

Random effects:
 Formula: list(DMTA_0 ~ 1, log_k_M23 ~ 1, log_k_M27 ~ 1, log_k_M31 ~ 1,      f_DMTA_ilr_1 ~ 1, f_DMTA_ilr_2 ~ 1, f_DMTA_ilr_3 ~
 Level: ds
 Structure: Diagonal
        DMTA_0 log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
StdDev:  1.609     1.222    0.7834    0.6048       0.4428       0.4335
        f_DMTA_ilr_3 log_k1 log_k2 g_qlogis Residual
StdDev:       0.2385 0.2779 0.4629    2.673     1.81

Variance function:
 Structure: Different standard deviations per stratum
 Formula: ~1 | name
 Parameter estimates:
     DMTA       M23       M27       M31
1.0000000 0.4854811 0.4549994 0.4811389

Backtransformed parameters with asymmetric confidence intervals:
                  lower      est.    upper
DMTA_0        96.577107 98.042185 99.50726
k_M23          0.004486  0.012657  0.03572
k_M27          0.003915  0.007804  0.01556
k_M31          0.009765  0.016482  0.02782
f_DMTA_to_M23        NA  0.112963       NA
f_DMTA_to_M27        NA  0.109145       NA
f_DMTA_to_M31        NA  0.090985       NA
k1             0.067711  0.088714  0.11623
k2             0.008821  0.015160  0.02605
g              0.359474  0.839763  0.97998

Resulting formation fractions:
               ff
DMTA_M23  0.11296
DMTA_M27  0.10914
DMTA_M31  0.09099
DMTA_sink 0.68691

Estimated disappearance times:
       DT50  DT90 DT50back DT50_k1 DT50_k2
DMTA  9.508  43.7    13.16   7.813   45.72
M23  54.764 181.9       NA      NA      NA
M27  88.820 295.1       NA      NA      NA
M31  42.055 139.7       NA      NA      NA
```

Listing 64: DFOP-SFO3 fit with nlme to dimethenamid data, two-component error

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 15:04:44 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - ((k1 * g * exp(-k1 * time) + k2 * (1 - g) * exp(-k2 *
           time)) / (g * exp(-k1 * time) + (1 - g) * exp(-k2 * time)))
           * DMTA
d_M23/dt = + f_DMTA_to_M23 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M31 * M31

Data:
568 observations of 4 variable(s) grouped in 6 datasets

Model predictions using solution type deSolve

Fitted in 34.399 s using 4 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
      DMTA_0    log_k_M23    log_k_M27    log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
    98.72582     -7.58644    -18.75668     -4.28269      0.07539      0.18660
f_DMTA_ilr_3       log_k1       log_k2     g_qlogis
    -1.72380     -2.29259    -16.35353      2.63698

Fixed degradation parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

   AIC  BIC logLik
  1876 1972   -916

Optimised, transformed parameters with symmetric confidence intervals:
              lower     est.    upper
DMTA_0       96.1732 98.11504 100.0569
log_k_M23    -5.3553 -4.36957  -3.3838
log_k_M27    -5.5106 -4.85332  -4.1961
log_k_M31    -4.6286 -4.12125  -3.6139
f_DMTA_ilr_1 -0.3375  0.02163   0.3808
f_DMTA_ilr_2 -0.1920  0.16537   0.5227
f_DMTA_ilr_3 -1.8314 -1.64533  -1.4592
log_k1       -3.2337 -2.74966  -2.2656
log_k2       -4.9620 -4.73125  -4.5005
g_qlogis      2.0739  2.95814   3.8424

Correlation:
             DMTA_0 l__M23 l__M27 l__M31 f_DMTA__1 f_DMTA__2 f_DMTA__3 log_k1
log_k_M23    -0.013
log_k_M27    -0.015  0.001
log_k_M31    -0.014  0.002  0.001
f_DMTA_ilr_1 -0.002  0.026 -0.051  0.000
```

```
f_DMTA_ilr_2  0.001  0.015  0.030 -0.068 -0.002
f_DMTA_ilr_3 -0.075  0.035  0.057  0.065 -0.001    -0.022
log_k1        0.021 -0.003 -0.003 -0.003  0.000     0.000    -0.007
log_k2        0.053  0.000  0.002  0.000 -0.001     0.000    -0.010     0.032
g_qlogis     -0.044  0.010  0.008  0.008  0.001    -0.001     0.017    -0.022
            log_k2
log_k_M23
log_k_M27
log_k_M31
f_DMTA_ilr_1
f_DMTA_ilr_2
f_DMTA_ilr_3
log_k1
log_k2
g_qlogis     -0.240

Random effects:
 Formula: list(DMTA_0 ~ 1, log_k_M23 ~ 1, log_k_M27 ~ 1, log_k_M31 ~ 1,      f_DMTA_ilr_1 ~ 1, f_DMTA_ilr_2 ~ 1, f_DMTA_ilr_3 ~
 Level: ds
 Structure: Diagonal
        DMTA_0 log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
StdDev:  1.962     1.163    0.7431    0.5847       0.4378       0.4295
        f_DMTA_ilr_3 log_k1    log_k2 g_qlogis Residual
StdDev:       0.2186  0.602 0.0005093     1.02        1

Variance function:
 Structure: Constant plus proportion of variance covariate
 Formula: ~fitted(.)
 Parameter estimates:
      const        prop
 0.86504158 -0.03414532

Backtransformed parameters with asymmetric confidence intervals:
                  lower      est.     upper
DMTA_0        96.173151 98.115039 100.05693
k_M23          0.004723  0.012657   0.03392
k_M27          0.004044  0.007802   0.01505
k_M31          0.009769  0.016224   0.02695
f_DMTA_to_M23        NA  0.112009        NA
f_DMTA_to_M27        NA  0.108635        NA
f_DMTA_to_M31        NA  0.090085        NA
k1             0.039411  0.063950   0.10377
k2             0.006999  0.008815   0.01110
g              0.888341  0.950647   0.97901

Resulting formation fractions:
               ff
DMTA_M23  0.11201
DMTA_M27  0.10863
DMTA_M31  0.09008
DMTA_sink 0.68927

Estimated disappearance times:
      DT50   DT90 DT50back DT50_k1 DT50_k2
DMTA 11.51  41.75    12.57   10.84   78.63
M23  54.77 181.93       NA      NA      NA
M27  88.84 295.11       NA      NA      NA
M31  42.72 141.92       NA      NA      NA
```

Listing 65: DFOP-SFO3+ fit with nlme to dimethenamid data, variance by variable

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 15:04:10 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - ((k1 * g * exp(-k1 * time) + k2 * (1 - g) * exp(-k2 *
           time)) / (g * exp(-k1 * time) + (1 - g) * exp(-k2 * time)))
           * DMTA
d_M23/dt = + f_DMTA_to_M23 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M31 * M31

Data:
568 observations of 4 variable(s) grouped in 6 datasets

Model predictions using solution type deSolve

Fitted in 78.786 s using 9 iterations

Variance model: Variance unique to each observed variable

Mean of starting values for individual parameters:
      DMTA_0    log_k_M23    log_k_M27    log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
     98.3635      -7.5002      -4.3270      -4.2431       0.1393       0.1443
f_DMTA_ilr_3       log_k1       log_k2     g_qlogis
     -1.7386      -3.3253      -6.7463      -1.2510

Fixed degradation parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

   AIC  BIC logLik
  1900 2004 -925.9

Optimised, transformed parameters with symmetric confidence intervals:
              lower    est.   upper
DMTA_0       96.5656 97.9905 99.4154
log_k_M23    -4.7006 -4.1878 -3.6750
log_k_M27    -4.4915 -4.0324 -3.5733
log_k_M31    -4.5655 -4.0567 -3.5479
f_DMTA_ilr_1 -0.2640  0.1208  0.5056
f_DMTA_ilr_2 -0.2937  0.1050  0.5037
f_DMTA_ilr_3 -1.8624 -1.6671 -1.4718
log_k1       -2.5552 -2.4968 -2.4383
log_k2       -4.4230 -3.5402 -2.6573
g_qlogis     -2.9618 -0.5579  1.8459

Correlation:
             DMTA_0 l__M23 l__M27 l__M31 f_DMTA__1 f_DMTA__2 f_DMTA__3 log_k1
log_k_M23    -0.016
log_k_M27    -0.013  0.003
log_k_M31    -0.007  0.002  0.065
f_DMTA_ilr_1 -0.001  0.035 -0.016  0.025
```

```
f_DMTA_ilr_2 -0.001  0.020 -0.029 -0.068 -0.023
f_DMTA_ilr_3 -0.042  0.046  0.056  0.028 -0.004    -0.001
log_k1        0.117 -0.011 -0.009 -0.004  0.001    -0.002    -0.029
log_k2        0.007  0.003  0.004  0.004  0.001    -0.001     0.002     0.193
g_qlogis      0.032 -0.008 -0.006 -0.001 -0.001    -0.002    -0.007    -0.105
            log_k2
log_k_M23
log_k_M27
log_k_M31
f_DMTA_ilr_1
f_DMTA_ilr_2
f_DMTA_ilr_3
log_k1
log_k2
g_qlogis     -0.054

Random effects:
 Formula: list(DMTA_0 ~ 1, log_k_M23 ~ 1, log_k_M27 ~ 1, log_k_M31 ~ 1,      f_DMTA_ilr_1 ~ 1, f_DMTA_ilr_2 ~ 1, f_DMTA_ilr_3 ~
 Level: ds
 Structure: Diagonal
        DMTA_0 log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
StdDev:  1.543    0.5957    0.5421    0.5922       0.4668       0.4786
        f_DMTA_ilr_3    log_k1 log_k2 g_qlogis Residual
StdDev:       0.2334 1.232e-05  1.023    2.596    1.848

Variance function:
 Structure: Different standard deviations per stratum
 Formula: ~1 | name
 Parameter estimates:
     DMTA       M23       M27       M31
1.0000000 0.4704774 0.3971208 0.4797798

Backtransformed parameters with asymmetric confidence intervals:
                lower     est.    upper
DMTA_0        96.56558 97.99050 99.41543
k_M23          0.00909  0.01518  0.02535
k_M27          0.01120  0.01773  0.02806
k_M31          0.01041  0.01731  0.02879
f_DMTA_to_M23       NA  0.11521       NA
f_DMTA_to_M27       NA  0.09712       NA
f_DMTA_to_M31       NA  0.09301       NA
k1             0.07767  0.08235  0.08731
k2             0.01200  0.02901  0.07013
g              0.04918  0.36403  0.86365

Resulting formation fractions:
               ff
DMTA_M23  0.11521
DMTA_M27  0.09712
DMTA_M31  0.09301
DMTA_sink 0.69467

Estimated disappearance times:
      DT50  DT90 DT50back DT50_k1 DT50_k2
DMTA 15.86  64.4    19.39   8.417    23.9
M23  45.66 151.7       NA      NA      NA
M27  39.09 129.9       NA      NA      NA
M31  40.05 133.0       NA      NA      NA
```

Listing 66: DFOP-SFO3+ fit with nlme to dimethenamid data, two-component error

```
nlme version used for fitting:      3.1.152
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 15:06:27 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - ((k1 * g * exp(-k1 * time) + k2 * (1 - g) * exp(-k2 *
           time)) / (g * exp(-k1 * time) + (1 - g) * exp(-k2 * time)))
           * DMTA
d_M23/dt = + f_DMTA_to_M23 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M31 * M31

Data:
568 observations of 4 variable(s) grouped in 6 datasets

Model predictions using solution type deSolve

Fitted in 102.772 s using 12 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
      DMTA_0    log_k_M23    log_k_M27    log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
     98.7698      -7.5225      -4.3377      -4.2477       0.1380       0.1393
f_DMTA_ilr_3       log_k1       log_k2     g_qlogis
     -1.7571      -6.0086      -6.7970       0.4502

Fixed degradation parameter values:
      value  type
M23_0     0 state
M27_0     0 state
M31_0     0 state

Results:

   AIC  BIC logLik
  1851 1946 -903.3

Optimised, transformed parameters with symmetric confidence intervals:
              lower     est.    upper
DMTA_0       96.2194 98.21002 100.2006
log_k_M23    -5.3780 -4.38060  -3.3832
log_k_M27    -4.4907 -4.05041  -3.6101
log_k_M31    -4.5981 -4.09944  -3.6007
f_DMTA_ilr_1 -0.2581  0.09064   0.4394
f_DMTA_ilr_2 -0.2769  0.11667   0.5103
f_DMTA_ilr_3 -1.8702 -1.68662  -1.5030
log_k1       -3.2294 -2.74475  -2.2601
log_k2       -4.9266 -4.70760  -4.4886
g_qlogis      2.0386  2.92927   3.8199

Correlation:
             DMTA_0 l__M23 l__M27 l__M31 f_DMTA__1 f_DMTA__2 f_DMTA__3 log_k1
log_k_M23    -0.013
log_k_M27    -0.017  0.002
log_k_M31    -0.011  0.001  0.063
f_DMTA_ilr_1 -0.002  0.026 -0.026  0.024
```

```
f_DMTA_ilr_2  0.000  0.013 -0.022 -0.066 -0.026
f_DMTA_ilr_3 -0.074  0.033  0.067  0.033 -0.011     0.001
log_k1        0.021 -0.003 -0.003 -0.002  0.000     0.000    -0.007
log_k2        0.052  0.000  0.002  0.003  0.000    -0.002    -0.010     0.032
g_qlogis     -0.042  0.010  0.010  0.006  0.001     0.001     0.016    -0.021
             log_k2
log_k_M23
log_k_M27
log_k_M31
f_DMTA_ilr_1
f_DMTA_ilr_2
f_DMTA_ilr_3
log_k1
log_k2
g_qlogis     -0.232

Random effects:
 Formula: list(DMTA_0 ~ 1, log_k_M23 ~ 1, log_k_M27 ~ 1, log_k_M31 ~ 1,      f_DMTA_ilr_1 ~ 1, f_DMTA_ilr_2 ~ 1, f_DMTA_ilr_3 ~
 Level: ds
 Structure: Diagonal
        DMTA_0 log_k_M23 log_k_M27 log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
StdDev:  2.019     1.177    0.5163    0.5802       0.4201       0.4731
        f_DMTA_ilr_3 log_k1    log_k2 g_qlogis Residual
StdDev:       0.2169 0.6027 3.687e-05    1.032        1

Variance function:
 Structure: Constant plus proportion of variance covariate
 Formula: ~fitted(.)
 Parameter estimates:
      const        prop
 0.83589063 -0.03489602

Backtransformed parameters with asymmetric confidence intervals:
                  lower      est.     upper
DMTA_0        96.219417 98.210025 100.20063
k_M23          0.004617  0.012518   0.03394
k_M27          0.011213  0.017415   0.02705
k_M31          0.010070  0.016582   0.02730
f_DMTA_to_M23        NA  0.111570        NA
f_DMTA_to_M27        NA  0.098148        NA
f_DMTA_to_M31        NA  0.090710        NA
k1             0.039582  0.064264   0.10434
k2             0.007251  0.009026   0.01124
g              0.884794  0.949275   0.97854

Resulting formation fractions:
               ff
DMTA_M23  0.11157
DMTA_M27  0.09815
DMTA_M31  0.09071
DMTA_sink 0.69957

Estimated disappearance times:
      DT50   DT90 DT50back DT50_k1 DT50_k2
DMTA 11.47  41.68    12.55   10.79   76.79
M23  55.37 183.94       NA      NA      NA
M27  39.80 132.22       NA      NA      NA
M31  41.80 138.86       NA      NA      NA
```

Listing 67: SFO-SFO3 fit with saemix to dimethenamid data, constant variance

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 14:21:05 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Data:
568 observations of 4 variable(s) grouped in 6 datasets

Model predictions using solution type deSolve

Fitted in 930.764 s using 300, 100 iterations

Variance model: Constant variance

Mean of starting values for individual parameters:
      DMTA_0   log_k_DMTA    log_k_M23    log_k_M27    log_k_M31 f_DMTA_ilr_1
    97.36284     -2.87199     -3.83245     -4.48137     -4.17806      0.08517
f_DMTA_ilr_2 f_DMTA_ilr_3
     0.18013     -1.67060

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
   AIC  BIC logLik
  2318 2314  -1142

Optimised parameters:
                est.   lower   upper
DMTA_0       97.33282 95.7538 98.9119
log_k_DMTA   -2.87270 -3.3602 -2.3852
log_k_M23    -4.17451 -4.9687 -3.3804
log_k_M27    -4.68203 -5.2743 -4.0898
log_k_M31    -4.00045 -4.5787 -3.4222
f_DMTA_ilr_1  0.01341 -0.3498  0.3766
f_DMTA_ilr_2  0.15665 -0.2088  0.5221
f_DMTA_ilr_3 -1.57162 -1.7358 -1.4074

Correlation:
             DMTA_0 l__DMT l__M23 l__M27 l__M31 f_DMTA__1 f_DMTA__2
log_k_DMTA    0.006
log_k_M23    -0.004 -0.001
log_k_M27    -0.005 -0.001 -0.003
log_k_M31    -0.004 -0.001 -0.003 -0.005
f_DMTA_ilr_1 -0.001  0.000  0.070 -0.086  0.002
f_DMTA_ilr_2  0.000  0.000  0.041  0.053 -0.134  0.001
f_DMTA_ilr_3 -0.029 -0.003  0.088  0.101  0.138  0.013    -0.054

Random effects:
                  est.   lower  upper
SD.DMTA_0       1.8349 0.63764 3.0321
SD.log_k_DMTA   0.6089 0.26400 0.9537
SD.log_k_M23    0.9115 0.31716 1.5059
SD.log_k_M27    0.6361 0.17739 1.0947
SD.log_k_M31    0.6225 0.17268 1.0724
SD.f_DMTA_ilr_1 0.4285 0.16092 0.6960
```

```
SD.f_DMTA_ilr_2 0.4169 0.14367 0.6901
SD.f_DMTA_ilr_3 0.1702 0.03916 0.3012

Variance model:
    est. lower upper
a.1 1.59 1.494 1.686

Backtransformed parameters:
                 est.     lower    upper
DMTA_0        97.33282 95.753790 98.91185
k_DMTA         0.05655  0.034729  0.09207
k_M23          0.01538  0.006952  0.03404
k_M27          0.00926  0.005122  0.01674
k_M31          0.01831  0.010268  0.03264
f_DMTA_to_M23  0.11760        NA       NA
f_DMTA_to_M27  0.11539        NA       NA
f_DMTA_to_M31  0.09615        NA       NA

Resulting formation fractions:
               ff
DMTA_M23  0.11760
DMTA_M27  0.11539
DMTA_M31  0.09615
DMTA_sink 0.67087

Estimated disappearance times:
      DT50   DT90
DMTA 12.26  40.72
M23  45.06 149.69
M27  74.85 248.65
M31  37.86 125.77
```

Listing 68: SFO-SFO3+ fit with saemix to dimethenamid data, constant variance

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 14:39:14 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - k_DMTA * DMTA
d_M23/dt = + f_DMTA_to_M23 * k_DMTA * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * k_DMTA * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * k_DMTA * DMTA - k_M31 * M31

Data:
568 observations of 4 variable(s) grouped in 6 datasets

Model predictions using solution type deSolve

Fitted in 995.729 s using 300, 100 iterations

Variance model: Constant variance

Mean of starting values for individual parameters:
      DMTA_0   log_k_DMTA    log_k_M23    log_k_M27    log_k_M31 f_DMTA_ilr_1
     97.3714      -2.8716      -3.8330      -4.1947      -4.1679       0.1423
f_DMTA_ilr_2 f_DMTA_ilr_3
      0.1429      -1.7048

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
   AIC  BIC logLik
  2313 2309  -1139

Optimised parameters:
                 est.   lower   upper
DMTA_0       97.33597 95.7651 98.9068
log_k_DMTA   -2.87257 -3.3602 -2.3849
log_k_M23    -4.17445 -4.9751 -3.3738
log_k_M27    -3.90429 -4.3204 -3.4882
log_k_M31    -4.05223 -4.5861 -3.5183
f_DMTA_ilr_1  0.07194 -0.2754  0.4193
f_DMTA_ilr_2  0.15044 -0.2654  0.5663
f_DMTA_ilr_3 -1.61576 -1.7825 -1.4490

Correlation:
             DMTA_0 l__DMT l__M23 l__M27 l__M31 f_DMTA__1 f_DMTA__2
log_k_DMTA    0.006
log_k_M23    -0.004 -0.001
log_k_M27    -0.005 -0.001 -0.003
log_k_M31    -0.003 -0.001 -0.001  0.113
f_DMTA_ilr_1 -0.001  0.000  0.072 -0.051  0.050
f_DMTA_ilr_2  0.000  0.000  0.034 -0.044 -0.138 -0.047
f_DMTA_ilr_3 -0.028 -0.003  0.086  0.140  0.077 -0.008     0.000

Random effects:
                  est.   lower  upper
SD.DMTA_0       1.8249 0.63345 3.0163
SD.log_k_DMTA   0.6091 0.26410 0.9541
SD.log_k_M23    0.9209 0.32258 1.5192
SD.log_k_M27    0.4608 0.14529 0.7763
SD.log_k_M31    0.5681 0.15033 0.9858
SD.f_DMTA_ilr_1 0.3970 0.13494 0.6590
```

```
SD.f_DMTA_ilr_2 0.4767 0.16659 0.7868
SD.f_DMTA_ilr_3 0.1771 0.04554 0.3087

Variance model:
     est. lower upper
a.1 1.584 1.488 1.681

Backtransformed parameters:
                  est.     lower    upper
DMTA_0        97.33597 95.765135 98.90681
k_DMTA         0.05655  0.034728  0.09209
k_M23          0.01538  0.006908  0.03426
k_M27          0.02016  0.013294  0.03056
k_M31          0.01738  0.010192  0.02965
f_DMTA_to_M23  0.11809        NA       NA
f_DMTA_to_M27  0.10667        NA       NA
f_DMTA_to_M31  0.09335        NA       NA

Resulting formation fractions:
               ff
DMTA_M23  0.11809
DMTA_M27  0.10667
DMTA_M31  0.09335
DMTA_sink 0.68190

Estimated disappearance times:
      DT50   DT90
DMTA 12.26  40.72
M23  45.06 149.68
M27  34.39 114.24
M31  39.87 132.46
```

Listing 69: DFOP-SFO3+ fit with saemix to dimethenamid data, two-component error

```
saemix version used for fitting:      3.1.9000
mkin version used for pre-fitting:  1.0.4.9000
R version used for fitting:         4.1.0
Date of fit:     Mon Jul 26 15:00:23 2021
Date of summary: Mon Jul 26 18:52:54 2021

Equations:
d_DMTA/dt = - ((k1 * g * exp(-k1 * time) + k2 * (1 - g) * exp(-k2 *
           time)) / (g * exp(-k1 * time) + (1 - g) * exp(-k2 * time)))
           * DMTA
d_M23/dt = + f_DMTA_to_M23 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M23 * M23
d_M27/dt = + f_DMTA_to_M27 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M27 * M27 + k_M31 * M31
d_M31/dt = + f_DMTA_to_M31 * ((k1 * g * exp(-k1 * time) + k2 * (1 - g)
           * exp(-k2 * time)) / (g * exp(-k1 * time) + (1 - g) *
           exp(-k2 * time))) * DMTA - k_M31 * M31

Data:
568 observations of 4 variable(s) grouped in 6 datasets

Model predictions using solution type deSolve

Fitted in 1260.253 s using 300, 100 iterations

Variance model: Two-component variance function

Mean of starting values for individual parameters:
      DMTA_0    log_k_M23    log_k_M27    log_k_M31 f_DMTA_ilr_1 f_DMTA_ilr_2
     98.7698      -3.9216      -4.3377      -4.2477       0.1380       0.1393
f_DMTA_ilr_3       log_k1       log_k2     g_qlogis
     -1.7571      -2.2341      -3.7763       0.4502

Fixed degradation parameter values:
None

Results:

Likelihood computed by importance sampling
   AIC  BIC logLik
  1887 1883 -921.6

Optimised parameters:
               est.   lower    upper
DMTA_0       98.0792 95.9861 100.1722
log_k_M23    -4.3979 -5.3950  -3.4008
log_k_M27    -4.0880 -4.5663  -3.6096
log_k_M31    -4.1245 -4.6470  -3.6020
f_DMTA_ilr_1  0.1026 -0.2727   0.4778
f_DMTA_ilr_2  0.1220 -0.2809   0.5250
f_DMTA_ilr_3 -1.6982 -1.8943  -1.5021
log_k1       -3.2061 -4.0255  -2.3866
log_k2       -3.8016 -4.9281  -2.6751
g_qlogis      1.1415 -2.5388   4.8219

Correlation:
             DMTA_0 l__M23 l__M27 l__M31 f_DMTA__1 f_DMTA__2 f_DMTA__3 log_k1
log_k_M23    -0.019
log_k_M27    -0.024  0.004
log_k_M31    -0.016  0.003  0.085
f_DMTA_ilr_1 -0.003  0.043 -0.034  0.032
f_DMTA_ilr_2 -0.001  0.023 -0.028 -0.088 -0.030
f_DMTA_ilr_3 -0.079  0.053  0.089  0.044 -0.004     0.008
```

```
log_k1        0.011 -0.003  0.001  0.002 -0.001    -0.003     0.000
log_k2        0.032  0.001 -0.005 -0.003  0.001     0.000    -0.014     0.027
g_qlogis     -0.056  0.006  0.009  0.004  0.001     0.002     0.022    -0.112
             log_k2
log_k_M23
log_k_M27
log_k_M31
f_DMTA_ilr_1
f_DMTA_ilr_2
f_DMTA_ilr_3
log_k1
log_k2
g_qlogis     -0.345

Random effects:
                  est.    lower  upper
SD.DMTA_0       2.1889  0.45331 3.9245
SD.log_k_M23    1.1651  0.42863 1.9015
SD.log_k_M27    0.5506  0.19389 0.9073
SD.log_k_M31    0.5969  0.20331 0.9905
SD.f_DMTA_ilr_1 0.4470  0.17115 0.7229
SD.f_DMTA_ilr_2 0.4783  0.18263 0.7740
SD.f_DMTA_ilr_3 0.2278  0.08192 0.3737
SD.log_k1       0.9785  0.38444 1.5725
SD.log_k2       1.2164  0.40211 2.0307
SD.g_qlogis     2.5805 -0.30634 5.4673

Variance model:
       est.   lower   upper
a.1 0.82828 0.76311 0.89345
b.1 0.03577 0.02993 0.04161

Backtransformed parameters:
                  est.     lower     upper
DMTA_0        98.07919 95.986142 100.17224
k_M23          0.01230  0.004539   0.03335
k_M27          0.01677  0.010396   0.02706
k_M31          0.01617  0.009590   0.02727
f_DMTA_to_M23  0.11169        NA        NA
f_DMTA_to_M27  0.09661        NA        NA
f_DMTA_to_M31  0.08946        NA        NA
k1             0.04052  0.017854   0.09194
k2             0.02234  0.007240   0.06890
g              0.75796  0.073179   0.99201

Resulting formation fractions:
               ff
DMTA_M23  0.11169
DMTA_M27  0.09661
DMTA_M31  0.08946
DMTA_sink 0.70225

Estimated disappearance times:
      DT50   DT90 DT50back DT50_k1 DT50_k2
DMTA 19.53  68.39    20.59   17.11   31.03
M23  56.34 187.15       NA      NA      NA
M27  41.32 137.27       NA      NA      NA
M31  42.86 142.38       NA      NA      NA
```