

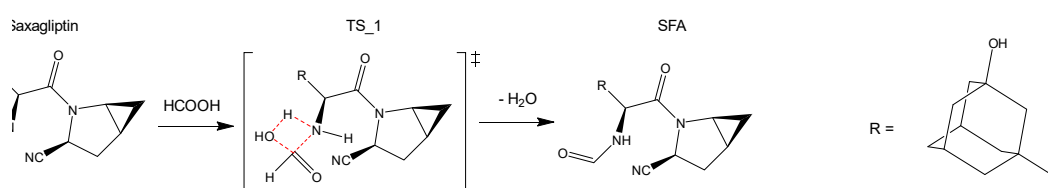
Supplementary Materials: Understanding and Kinetic Modeling of Complex Degradation Pathways in the Solid Dosage Form: The Case of Saxagliptin

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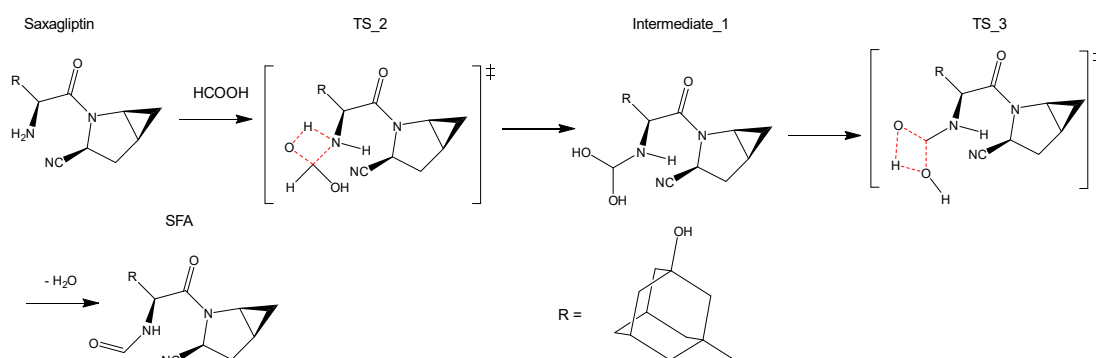
1. Studied Reaction Schemes and Mechanisms

Two parallel saxagliptin degradation reactions were evaluated: SFA formation (parallel reaction 1) and (E)SCA formation (parallel reaction 2).

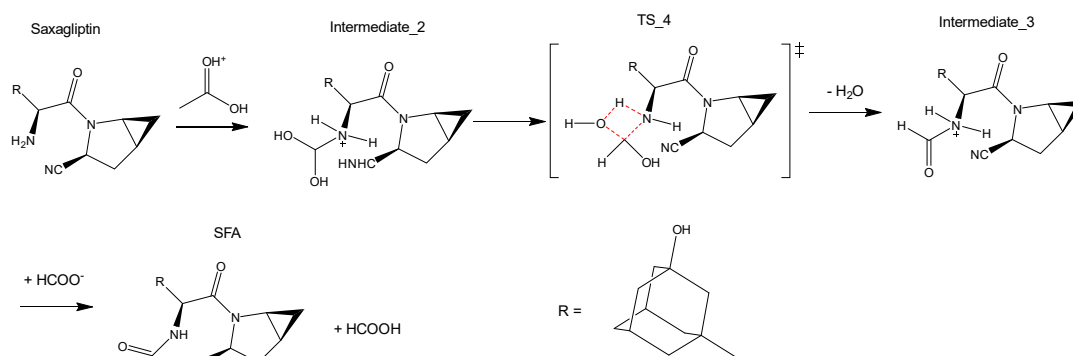
1.1. SFA Formation (Parallel Reaction 1)



Scheme S1. Reaction mechanism 1 for parallel reaction 1.

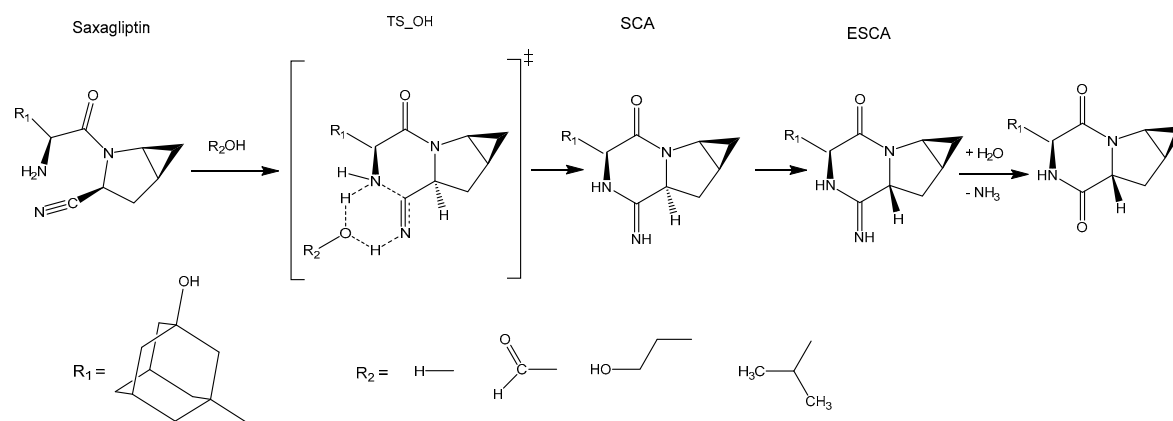
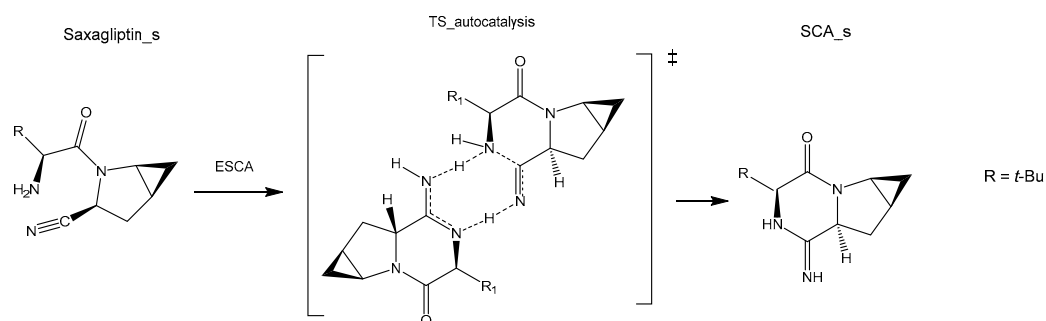
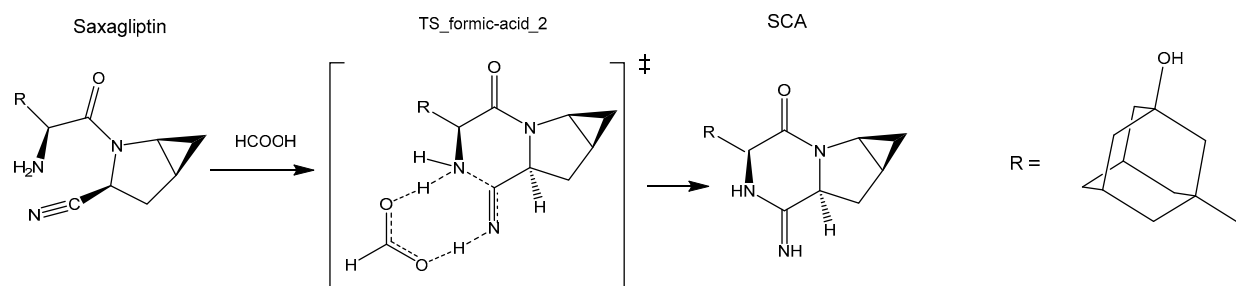


Scheme S2. Reaction mechanism 2 for parallel reaction 1.



Scheme S3. Reaction mechanism 3 for parallel reaction 1 [1]

1.2. (E)SCA Formation (Parallel Reaction 2)

**Scheme S4.** Reaction mechanism 1 for for parallel reaction 2 catalyzed by hydroxyl group [2].**Scheme S5.** Reaction mechanism 2 for parallel reaction 2 catalyzed by the ESCA [2].**Scheme S6.** Reaction mechanism 3 for parallel reaction 2 catalyzed by formic acid.

2. Analytical Methods

2.1. Saxagliptin (SAXA) Related Substances and Degradation Products Determination

SAXA was analyzed using the Acquity UPLC (Waters Corp., Milford, MA, USA), a reverse phase column, Luna C18(2)-HST, particle size 2.5 μm , dimensions 100 $\times$ 3.0 mm, from Phenomenex Inc. (Torrance, CA, USA) and a suitable UHPLC C18 3.0 mm pre-column at 25 °C. Gradient elution was used to achieve chromatographic separation with mobile phases A (buffer, pH 6) and B (buffer, pH 6 and acetonitrile, 50:50 (v/v)). The mobile phase in the gradient elution progress was: 0 min 6% B, 2 min 6% B, 11 min 50% B, 16–17.5 min 100% B and 18 min 6% B. The mobile phase flow was 0.7 mL/min. Auto-sampler temperature was set at 5 °C, the injection volume at 12 μL and run time 18 minutes. Data was recorded in photo diode array (PDA) mode and subsequently chromatograms were extracted at a wavelength of 213 nm. Solvent for sample preparation was 1.0 mL of 85% O-phosphoric acid in 1000 mL of additionally purified water. Tablet sample preparation; 2 tablets were transferred into 50 mL Erlenmeyer flask, 40 mL of solvent was added and sonicated until the tablets completely disintegrated. Dispersion was then centrifuged through Amicon Ultra-4, Ultracel® 3K ultrafilters for 15 minutes at 4000 rpm. Compounds of interest elute at 7.0 min (saxagliptin cyclic amidine epimer, ESCA), 7.7 min (saxagliptin cyclic amidine, SCA), 9.4 min (saxagliptin, SAXA) and 11.5 min (saxagliptin formyl amide, SFA). Results were first calculated as % of individual impurity against the declared dose of S (2.5 mg). For the purpose of model development, response factors for individual SAXA degradation products were applied and values were transformed into mol/g_{saxa}.

2.2. Low Molecular Weight Organic Impurities Determination

Low molecular weight organic impurities were analyzed using the Acquity UPLC (Waters Corp., Milford, MA, USA), a reverse phase column Acq UPLC HSS C18, particle size 1.8 μm , dimensions 150 $\times$ 2.1 mm from Waters Corp. (USA) at 45 °C. Gradient elution was used to achieve chromatographic separation with mobile phases A (HCl solution, pH 2.5) and B (acetonitrile and MTBE, 98:2 (v/v)). The mobile phase in the gradient elution progress was: 0–1.2 min 5% B, 6 min 19% B, 10 min 50% B, 11.5 min 55% B, 13.5–14.5 min 90% B and 15 min 5% B with equilibration time of 4 minutes. The mobile phase flow was 0.5 mL/min, autosampler temperature at 5 °C and volume of injection 4 μL . Chromatograms were recorded at a wavelength of 400 nm. Derivatization of compounds was performed at the sample preparation phase. Derivatization reagent consisted of 14.4 mg/mL EDC, 2.31 mg/mL 2-NPH and 9 $\mu\text{L/mL}$ of pyridine. Three film-coated tablets were transferred into analysis tube to which 4 mL of additionally purified water were added and sonicated until tablet disintegration. Suspension was transferred into Amicon Ultra-4, Ultracel® 3K ultrafilters and centrifuged at 5000 rpm for 1 hour. Derivatization was performed in 1.5 mL tubes in which 600 μL of sample filtrate, 200 μL of acetonitrile and 400 μL of derivatization reagent were mixed and shaken for 30 minutes at 750 rpm at 60 °C. Compounds of interest elute at 4.5 min (glycolic acid, GA), 5.3 min (formic acid, FA), 11.0 min (formaldehyde, F) and 11.9 min (acetaldehyde, A). Results are reported in ppm calculated against tablet film-coat mass. For the purpose of model development, values were transformed into mol/g_{saxa}.

3. Tables of Data

3.1. Saxagliptin (SAXA) Degradation Profile

Table S1. Data for concentration of three main SAXA degradation products ESCA, SCA and SFA and their sum (% against S, *w/w*) at temperature 60 °C.

	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum
PEG/SAXA = 0.8												
7 days	0.96	0.59	0.05	1.60	1.80	0.34	0.07	2.21	3.10	0.14	0.15	3.40
14 days	2.29	0.86	0.07	3.22	3.84	0.42	0.12	4.39	5.88	0.12	0.23	6.23
PEG/SAXA = 1.0												
7 days	0.78	0.41	0.23	1.42	1.87	0.24	0.27	2.38	3.49	0.10	0.22	3.80
14 days	2.00	0.50	0.24	2.73	3.92	0.24	0.22	4.37	6.11	0.09	0.30	6.50
PEG/SAXA = 1.2												
7 days	0.63	0.19	0.65	1.47	1.74	0.11	0.67	2.53	2.38	0.02	0.32	2.72
14 days	1.73	0.17	0.72	2.62	3.46	0.11	0.71	4.28	3.33	0.00	0.68	4.02
PEG/SAXA = 1.4												
7 days	0.46	0.06	1.36	1.89	0.95	0.02	1.87	2.84	0.80	0.00	2.82	3.62
14 days	1.35	0.05	1.69	3.09	1.85	0.00	2.23	4.08	2.07	0.00	3.28	5.35

Table S2. Data for concentration of three main SAXA degradation products ESCA, SCA and SFA and their sum (% against SAXA, *w/w*) at temperature 50 °C.

	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum
PEG/SAXA = 0.8												
14 days	0.50	0.53	0.00	1.03	1.15	0.44	0.03	1.61	2.66	0.18	0.12	2.96
30 days	1.33	0.82	0.00	2.15	2.63	0.56	0.07	3.27	4.21	0.24	0.16	4.62
45 days	2.09	1.02	0.05	3.16	3.97	0.62	0.10	4.70	5.84	0.22	0.19	6.25
60 days	3.73	1.31	0.08	5.12	6.35	0.83	0.14	7.31	9.64	0.27	0.36	10.28
PEG/SAXA = 1.0												
14 days	0.38	0.37	0.11	0.86	1.20	0.32	0.15	1.67	2.91	0.16	0.18	3.24
30 days	1.08	0.60	0.17	1.85	2.75	0.39	0.22	3.36	4.86	0.15	0.28	5.29
45 days	1.74	0.73	0.21	2.68	3.86	0.43	0.28	4.57	5.59	0.20	0.27	6.06
60 days	3.28	0.96	0.28	4.52	6.59	0.47	0.40	7.46	9.87	0.20	0.47	10.54

Table S2. *Cont.*

	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum
PEG/SAXA = 1.2												
14 days	0.27	0.19	0.60	1.06	1.11	0.16	0.58	1.85	2.24	0.04	0.25	2.53
30 days	0.87	0.27	0.71	1.86	2.42	0.16	0.69	3.27	3.46	0.03	0.38	3.87
45 days	1.60	0.29	0.77	2.66	3.74	0.16	0.82	4.72	5.36	0.07	0.41	5.84
60 days	2.76	0.30	1.05	4.12	6.21	0.19	1.09	7.49	8.30	0.06	0.57	8.93
PEG/SAXA = 1.4												
14 days	0.24	0.10	1.29	1.63	0.72	0.04	1.64	2.40	0.49	0.00	2.42	2.91
30 days	0.85	0.10	1.38	2.33	1.74	0.02	1.84	3.60	1.09	0.00	2.76	3.84
45 days	1.38	0.09	1.43	2.90	2.33	0.00	2.14	4.47	1.51	0.00	2.99	4.50
60 days	2.57	0.09	1.99	4.64	3.82	0.00	2.79	6.62	2.72	0.00	3.94	6.66

Table S3. Data for concentration of three main SAXA degradation products ESCA, SCA and SFA and their sum (% against SAXA, *w/w*) at temperature 40 °C.

	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum
PEG/SAXA = 0.8												
30 days	0.20	0.29	0.00	0.49	0.49	0.32	0.00	0.81	1.70	0.20	0.05	1.95
60 days	0.66	0.61	0.00	1.28	1.51	0.61	0.05	2.16	4.06	0.28	0.13	4.47
90 days	1.03	0.91	0.00	1.94	2.16	0.81	0.04	3.01	5.06	0.31	0.17	5.54
120 days	1.47	1.10	0.00	2.57	3.02	0.93	0.06	4.01	6.00	0.34	0.17	6.51
150 days	1.90	1.30	0.05	3.25	3.66	1.05	0.07	4.78	5.16	0.72	0.11	5.98
180 days	2.41	1.43	0.07	3.92	4.72	1.21	0.11	6.04	7.63	0.49	0.20	8.32
PEG/SAXA = 1.0												
30 days	0.16	0.21	0.06	0.44	0.47	0.26	0.09	0.81	1.87	0.17	0.08	2.12
60 days	0.56	0.44	0.08	1.08	1.29	0.42	0.24	1.96	4.34	0.21	0.18	4.74
90 days	0.84	0.69	0.07	1.60	2.24	0.61	0.11	2.96	4.87	0.27	0.21	5.35
120 days	1.18	0.81	0.08	2.07	2.65	0.56	0.23	3.44	5.64	0.31	0.21	6.16
150 days	1.62	1.00	0.11	2.72	3.68	0.74	0.13	4.55	7.53	0.30	0.26	8.09
180 days	2.08	1.14	0.15	3.37	3.88	0.74	0.35	4.97	9.18	0.28	0.35	9.81

Table S3. Cont.

	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum
PEG/SAXA = 1.2												
30 days	0.07	0.08	0.48	0.63	0.36	0.14	0.48	0.98	1.80	0.10	0.12	2.02
60 days	0.25	0.22	0.68	1.16	1.26	0.23	0.66	2.15	3.67	0.10	0.25	4.02
90 days	0.45	0.33	0.58	1.35	1.78	0.25	0.55	2.58	4.90	0.11	0.25	5.27
120 days	0.77	0.39	0.55	1.71	2.56	0.27	0.74	3.57	5.57	0.09	0.26	5.92
150 days	1.12	0.49	0.62	2.23	3.25	0.29	0.74	4.28	6.27	0.08	0.41	6.76
180 days	1.41	0.52	0.74	2.67	4.38	0.31	0.82	5.51	7.84	0.11	0.44	8.38
PEG/SAXA = 1.4												
30 days	0.06	0.07	0.96	1.09	0.34	0.06	1.10	1.51	0.30	0.00	1.95	2.25
60 days	0.33	0.15	1.41	1.89	1.09	0.06	1.56	2.72	0.72	0.00	2.72	3.44
90 days	0.58	0.18	1.24	1.99	1.73	0.06	1.34	3.13	1.26	0.00	2.37	3.63
120 days	0.94	0.19	1.24	2.37	2.30	0.06	1.50	3.85	1.43	0.00	2.58	4.01
150 days	1.32	0.22	1.33	2.87	2.88	0.08	1.59	4.55	1.92	0.00	2.87	4.79
180 days	1.68	0.20	1.39	3.27	3.73	0.07	1.66	5.46	2.25	0.00	2.77	5.02

Table S4. Data for concentration of three main SAXA degradation products ESCA, SCA and SFA and their sum (% against SAXA, *w/w*) at temperature 30 °C (continues on next page).

	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum
PEG/SAXA = 0.8												
30 days	0.04	0.07	0.00	0.11	0.07	0.10	0.00	0.17	0.31	0.13	0.00	0.44
60 days	0.11	0.16	0.00	0.27	0.23	0.21	0.00	0.43	0.93	0.23	0.00	1.17
90 days	0.17	0.27	0.00	0.43	0.35	0.33	0.00	0.68	1.36	0.30	0.00	1.67
120 days	0.21	0.34	0.00	0.55	0.48	0.39	0.00	0.86	1.57	0.35	0.00	1.92
150 days*	–	–	–	–	0.68	0.53	0.00	1.21	2.22	0.41	0.05	2.68
180 days*	0.39	0.54	0.00	0.93	–	–	–	–	–	–	–	–

Table S4. Cont.

	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum	ESCA	SCA	SFA	Sum
PEG/SAXA = 1.0												
30 days	0.04	0.06	0.00	0.10	0.07	0.08	0.05	0.20	0.48	0.13	0.00	0.61
60 days	0.10	0.14	0.00	0.24	0.23	0.18	0.00	0.41	1.02	0.20	0.05	1.27
120 days	0.20	0.28	0.00	0.48	0.40	0.26	0.08	0.73	1.89	0.27	0.06	2.23
150 days*	0.27	0.35	0.04	0.66	–	–	–	–	–	–	–	–
180 days*	–	–	–	–	0.61	0.36	0.17	1.15	2.80	0.32	0.11	3.24
PEG/SAXA = 1.2												
30 days	0.03	0.04	0.12	0.18	0.04	0.03	0.49	0.56	0.51	0.09	0.06	0.65
60 days	0.05	0.06	0.26	0.38	0.09	0.05	0.76	0.91	0.99	0.15	0.09	1.23
90 days	0.06	0.09	0.24	0.39	0.16	0.10	0.52	0.78	1.60	0.13	0.12	1.85
120 days	0.08	0.11	0.27	0.45	0.20	0.11	0.55	0.86	1.49	0.18	0.11	1.79
150 days*	–	–	–	–	0.31	0.17	0.57	1.05	2.28	0.18	0.12	2.59
180 days*	0.13	0.17	0.34	0.63	–	–	–	–	–	–	–	–
PEG/SAXA = 1.4												
30 days	0.00	0.00	0.56	0.56	0.04	0.03	0.80	0.87	0.13	0.00	1.15	1.28
60 days	0.03	0.03	0.93	0.99	0.10	0.06	1.10	1.26	0.24	0.00	1.86	2.11
90 days	0.04	0.05	0.87	0.97	0.19	0.08	0.89	1.17	0.33	0.00	1.79	2.12
120 days	0.05	0.07	0.75	0.86	0.27	0.09	0.97	1.33	0.46	0.00	1.70	2.16
150 days*	0.07	0.10	0.89	1.06	–	–	–	–	–	–	–	–
180 days*	–	–	–	–	0.56	0.12	1.08	1.76	0.72	0.00	1.99	2.71

* some results for 150 and 180 day time point are not available due to experimental issues.

3.2. PEG Degradation Profile (Low Molecular Weight or Ganic Impurities)

Table S5. Data for concentration of organic impurities A, F, GA and FA (ppm against tablet film-coat, *w/w*) at temperature 60 °C.

	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C	60 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	A	F	GA	FA	A	F	GA	FA	A	F	GA	FA
PEG/SAXA = 0.8												
7 days	0	4	234	203	0	2	240	233	0	0	250	292
14 days	0	3	231	243	0	2	246	289	0	0	272	409
PEG/SAXA = 1.0												
7 days	0	11	228	392	0	2	225	457	0	0	249	323
14 days	0	5	224	482	0	3	242	502	0	0	264	440
PEG/SAXA = 1.2												
7 days	9	19	225	756	0	3	228	924	0	1	258	391
14 days	0	6	237	977	0	1	254	1070	0	2	283	803
PEG/SAXA = 1.4												
7 days	15	69	250	1251	10	19	221	2038	31	230	238	3318
14 days	7	16	242	1464	0	6	242	2202	10	31	276	3268

Table S6. Data for concentration of organic impurities A, F, GA and FA (ppm against tablet film-coat, *w/w*) at temperature 50 °C.

	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C	50 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	A	F	GA	FA	A	F	GA	FA	A	F	GA	FA
PEG/SAXA = 0.8												
14 days	0	8	230	202	0	3	237	220	0	1	236	253
30 days	0	28	248	249	0	27	253	286	0	34	268	364
45 days	0	28	250	275	0	30	259	328	0	35	277	417
60 days	0	45	331	2780	0	40	299	480	0	38	291	548
PEG/SAXA = 1.0												
14 days	0	27	236	304	0	5	230	373	0	2	230	269
30 days	0	36	254	409	0	29	259	488	0	38	269	408
45 days	0	34	258	457	0	27	262	512	0	34	277	445
60 days	22	82	441	4163	0	30	250	433	0	26	257	550
PEG/SAXA = 1.2												
14 days	9	50	241	763	0	10	229	891	0	2	247	342
30 days	0	49	268	1141	0	29	281	1314	0	40	291	504
45 days	0	36	268	1192	0	30	282	1274	0	46	283	526
60 days	0	30	260	342	0	28	295	1399	0	39	306	625
PEG/SAXA = 1.4												
14 days	13	97	236	1154	10	52	217	1863	28	466	213	3197
30 days	0	55	296	1773	0	40	310	2628	25	209	394	4285
45 days	13	48	294	1851	0	40	301	2678	22	136	392	4097
60 days	0	38	284	1739	0	35	269	1258	0	30	252	295

Table S7. Data for concentration of organic impurities A, F, GA and FA (ppm against tablet film-coat, *w/w*) at temperature 40 °C.

	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C	40 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	A	F	GA	FA	A	F	GA	FA	A	F	GA	FA
PEG/SAXA = 0.8												
30 days	0	28	238	220	0	26	248	225	0	26	252	247
60 days	0	34	239	224	0	30	246	226	0	31	255	295
90 days	0	31	236	227	0	24	256	265	0	28	256	313
120 days	0	18	245	321	0	14	252	346	0	12	250	427
150 days	11	19	256	301	8	12	261	300	6	8	280	476
180 days	10	27	254	312	9	15	259	332	0	15	275	441
PEG/SAXA = 1.0												
30 days	0	43	249	274	0	38	254	386	0	24	255	259
60 days	0	46	241	282	0	44	255	564	0	27	256	328
90 days	0	43	253	309	0	29	244	453	0	25	252	356
120 days	0	32	285	506	0	15	291	624	0	12	291	606
150 days	8	15	270	716	12	31	268	363	7	10	273	342
180 days	11	32	261	431	0	20	272	928	9	18	288	571
PEG/SAXA = 1.2												
30 days	13	123	264	868	0	63	257	1143	0	22	248	301
60 days	18	110	265	1015	0	44	252	1153	0	28	266	410
90 days	16	85	265	1079	0	40	272	1456	0	29	275	460
120 days	12	70	323	1800	0	18	325	1924	0	13	299	715
150 days	13	52	285	1248	8	17	291	1529	7	10	292	561
180 days	15	54	276	1473	10	24	291	1577	0	17	289	618
PEG/SAXA = 1.4												
30 days	16	149	291	1437	14	107	282	2216	36	518	313	4218
60 days	17	111	295	1738	14	59	287	2372	25	309	296	4132
90 days	16	87	297	1848	0	40	287	2304	30	276	347	4007
120 days	17	71	382	2900	0	25	430	3796	21	149	553	6105
150 days	12	45	294	2115	10	28	317	2560	17	129	390	4204
180 days	11	44	324	2523	0	24	325	2771	14	94	472	4498

Table S8. Data for concentration of organic impurities A, F, GA and FA (ppm against tablet film-coat, *w/w*) at temperature 30 °C.

	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C	30 °C
	10 % RH	10 % RH	10 % RH	10 % RH	30 % RH	30 % RH	30 % RH	30 % RH	50 % RH	50 % RH	50 % RH	50 % RH
	A	F	GA	FA	A	F	GA	FA	A	F	GA	FA
PEG/SAXA = 0.8												
30 days	0	27	242	211	0	27	245	215	0	25	241	212
60 days	0	34	236	205	0	31	237	210	0	26	238	202
90 days	0	29	239	212	0	28	240	209	0	25	238	215
120 days	0	15	244	255	0	13	228	285	0	10	234	300
150 days*	–	–	–	–	9	15	248	231	7	10	263	257
180 days*	0	20	237	237	–	–	–	–	–	–	–	–
PEG/SAXA = 1.0												
30 days	0	36	241	216	0	57	241	294	0	22	242	210
60 days	0	47	242	229	0	42	240	245	0	23	244	228
90 days	0	42	236	227	0	43	241	259	0	21	240	229
120 days	0	30	221	302	0	24	224	335	0	12	232	316
150 days*	9	33	254	291	–	–	–	–	–	–	–	–
180 days*	–	–	–	–	10	42	241	515	0	16	257	338
PEG/SAXA = 1.2												
30 days	0	94	255	336	0	233	259	1273	0	27	240	232
60 days	15	152	260	450	0	221	250	1548	0	32	244	308
90 days	14	140	254	478	13	167	261	1764	0	24	246	318
120 days	15	128	266	732	12	128	281	2163	0	10	241	410
150 days*	–	–	–	–	11	123	272	1921	7	11	259	429
180 days*	16	133	273	828	–	–	–	–	–	–	–	–
PEG/SAXA = 1.4												
30 days	13	228	284	804	0	267	262	1885	26	559	293	2674
60 days	23	307	287	1251	17	230	267	2175	29	631	288	3725
90 days	25	255	293	1424	16	177	270	2293	29	531	290	3947
120 days	15	167	298	1839	14	136	314	2929	23	382	406	4964
150 days*	20	204	289	1835	–	–	–	–	–	–	–	–
180 days*	–	–	–	–	10	107	290	2999	17	339	362	4847

* some results for 150 and 180 day time point are not available due to experimental issues.

3.3. MODDE® Datasets and Statistics

Table S9. Worksheet for statistical evaluation.

Exp No	Exp Name	Run Order	Incl/Excl	Time Point	Temperature	Relative humidity	PEG/SAXA ratio	ESCA	SFA	SCA	pH	aw	F	FA	Coloration
1	N1	1	Incl	7	60	10	PEG/SAXA = 0.8	0.96	0.05	0.97	5.6	0.21	4.4	203.1	158
2	N2	2	Incl	7	60	30	PEG/SAXA = 0.8	1.80	0.07	0.55	5.53	0.31	1.5	232.7	129
3	N3	3	Incl	7	60	50	PEG/SAXA = 0.8	3.10	0.15	0.23	5.51	0.42	0.3	291.9	117
4	N4	4	Incl	14	50	10	PEG/SAXA = 0.8	0.50	0	0.87	5.59	0.22	7.6	202	197
5	N5	5	Incl	14	50	30	PEG/SAXA = 0.8	1.15	0.03	0.72	5.57	0.3	2.5	219.9	176
6	N6	6	Incl	14	50	50	PEG/SAXA = 0.8	2.66	0.12	0.3	5.54	0.43	0.8	252.6	132
7	N7	7	Incl	14	60	10	PEG/SAXA = 0.8	2.29	0.07	1.4	5.54	0.22	3.5	243.3	144
8	N8	8	Incl	14	60	30	PEG/SAXA = 0.8	3.84	0.12	0.69	5.5	0.3	1.6	289.3	133
9	N9	9	Incl	14	60	50	PEG/SAXA = 0.8	5.88	0.23	0.2	5.45	0.41	0	409.3	115
10	N10	10	Incl	30	30	10	PEG/SAXA = 0.8	0.04	0	0.12	5.74	0.2	27	211.3	212
11	N11	11	Incl	30	30	30	PEG/SAXA = 0.8	0.07	0	0.16	5.76	0.3	26.9	215.4	199
12	N12	12	Incl	30	30	50	PEG/SAXA = 0.8	0.31	0	0.22	5.73	0.43	24.6	211.7	191
13	N13	13	Incl	30	40	10	PEG/SAXA = 0.8	0.20	0	0.47	5.59	0.2	28.2	220.3	217
14	N14	14	Incl	30	40	30	PEG/SAXA = 0.8	0.49	0	0.53	5.67	0.29	26.1	224.8	195
15	N15	15	Incl	30	40	50	PEG/SAXA = 0.8	1.70	0.05	0.33	5.62	0.41	26.1	247	157
16	N16	16	Incl	30	50	10	PEG/SAXA = 0.8	1.33	0	1.35	5.67	0.21	28.1	248.6	199
17	N17	17	Incl	30	50	30	PEG/SAXA = 0.8	2.63	0.07	0.92	5.68	0.29	27.4	286.3	162
18	N18	18	Incl	30	50	50	PEG/SAXA = 0.8	4.21	0.16	0.4	5.66	0.37	34.5	364.4	125
19	N19	19	Incl	45	50	10	PEG/SAXA = 0.8	2.09	0.05	1.67	5.67	0.19	27.7	274.6	193
20	N20	20	Incl	45	50	30	PEG/SAXA = 0.8	3.97	0.1	1.02	5.66	0.27	30	328.2	155
21	N21	21	Incl	45	50	50	PEG/SAXA = 0.8	5.84	0.19	0.36	5.63	0.37	34.5	416.8	130
22	N22	22	Incl	60	30	10	PEG/SAXA = 0.8	0.11	0	0.26	5.6	0.22	33.7	205	203
23	N23	23	Incl	60	30	30	PEG/SAXA = 0.8	0.23	0	0.34	5.57	0.31	30.6	210	206
24	N24	24	Incl	60	30	50	PEG/SAXA = 0.8	0.93	0	0.38	5.56	0.42	25.6	202.3	175
25	N25	25	Incl	60	40	10	PEG/SAXA = 0.8	0.66	0	1.01	5.59	0.2	33.6	224	200
26	N26	26	Incl	60	40	30	PEG/SAXA = 0.8	1.51	0.05	0.99	5.58	0.28	30.3	226.2	178
27	N27	27	Incl	60	40	50	PEG/SAXA = 0.8	4.06	0.13	0.47	5.52	0.38	30.6	295.4	132
28	N28	28	Incl	60	50	10	PEG/SAXA = 0.8	3.73	0.08	2.16	5.6	0.2	45.5	2780	171
29	N29	29	Incl	60	50	30	PEG/SAXA = 0.8	6.35	0.14	1.36	5.55	0.27	39.8	479.9	147
30	N30	30	Incl	60	50	50	PEG/SAXA = 0.8	9.64	0.36	0.44	5.46	0.39	38.3	547.6	119
31	N31	31	Incl	90	30	10	PEG/SAXA = 0.8	0.17	0	0.44	5.71	0.19	29.2	211.5	212

Table S9. Cont.

Exp No	Exp Name	Run Order	Incl/Excl	Time Point	Temperature	Relative humidity	PEG/SAXA ratio	ESCA	SFA	SCA	pH	aw	F	FA	Coloration
32	N32	32	Incl	90	30	30	PEG/SAXA = 0.8	0.35	0	0.59	5.71	0.28	28.4	208.6	194
33	N33	33	Incl	90	30	50	PEG/SAXA = 0.8	1.36	0	0.34	5.62	0.38	25.2	215.5	167
34	N34	34	Incl	90	40	10	PEG/SAXA = 0.8	1.03	0	0.14	5.67	0.18	30.7	227.4	199
35	N35	35	Incl	90	40	30	PEG/SAXA = 0.8	2.16	0	0.53	5.63	0.26	24.3	265.4	171
36	N36	36	Incl	90	40	50	PEG/SAXA = 0.8	5.06	0.17	0.44	5.56	0.38	27.7	312.7	138
37	N37	37	Incl	120	30	10	PEG/SAXA = 0.8	0.21	0	0.18	–	0.17	15.4	255.4	–
38	N38	38	Incl	120	30	30	PEG/SAXA = 0.8	0.48	0	0.85	–	0.26	13	284.5	–
39	N39	39	Incl	120	30	50	PEG/SAXA = 0.8	1.57	0	0.42	–	0.37	9.9	300	–
40	N40	40	Incl	120	40	10	PEG/SAXA = 0.8	1.47	0	0.12	–	0.16	18.2	320.7	–
41	N41	41	Incl	120	40	30	PEG/SAXA = 0.8	3.02	0.06	0.07	–	0.24	14.1	345.9	–
42	N42	42	Incl	120	40	50	PEG/SAXA = 0.8	6.00	0.17	0.10	–	0.34	12	426.7	–
43	N43	43	Incl	150	30	30	PEG/SAXA = 0.8	0.68	0	0.13	5.75	0.28	14.6	231.1	201
44	N44	44	Incl	150	30	50	PEG/SAXA = 0.8	2.22	0.05	0.29	5.7	0.38	10.4	257.4	197
45	N45	45	Incl	150	40	10	PEG/SAXA = 0.8	1.90	0.05	0.32	5.68	0.18	18.5	300.7	197
46	N46	46	Incl	150	40	30	PEG/SAXA = 0.8	3.66	0.07	0.20	5.68	0.26	11.7	300.2	163
47	N47	47	Incl	150	40	50	PEG/SAXA = 0.8	5.16	0.11	0.82	5.62	0.32	7.6	476.1	129
48	N48	48	Incl	180	30	10	PEG/SAXA = 0.8	0.39	0	0.56	5.68	0.18	20.1	237.1	202
49	N49	49	Incl	180	40	10	PEG/SAXA = 0.8	2.41	0.07	0.24	5.63	0.18	27	311.7	189
50	N50	50	Incl	180	40	30	PEG/SAXA = 0.8	4.72	0.11	1.02	5.6	0.25	15.5	332.2	164
51	N51	51	Incl	180	40	50	PEG/SAXA = 0.8	7.63	0.2	0.62	5.57	0.33	15.4	441.3	124
52	N52	52	Incl	7	60	10	PEG/SAXA = 1.0	0.78	0.23	0.22	5.55	0.24	10.7	392.3	144
53	N53	53	Incl	7	60	30	PEG/SAXA = 1.0	1.87	0.27	0.16	5.5	0.31	1.7	456.8	136
54	N54	54	Incl	7	60	50	PEG/SAXA = 1.0	3.49	0.22	0.21	5.48	0.43	0	322.7	134
55	N55	55	Incl	14	50	10	PEG/SAXA = 1.0	0.38	0.11	0.23	5.56	0.21	26.7	303.9	184
56	N56	56	Incl	14	50	30	PEG/SAXA = 1.0	1.20	0.15	0.62	5.54	0.3	5.4	372.6	145
57	N57	57	Incl	14	50	50	PEG/SAXA = 1.0	2.91	0.18	0.60	5.51	0.42	1.7	269.4	137
58	N58	58	Incl	14	60	10	PEG/SAXA = 1.0	2.00	0.24	0.29	5.54	0.21	4.9	482.3	150
59	N59	59	Incl	14	60	30	PEG/SAXA = 1.0	3.92	0.22	1.32	5.5	0.31	2.5	502.2	134
60	N60	60	Incl	14	60	50	PEG/SAXA = 1.0	6.11	0.3	0.83	5.45	0.41	0.3	439.8	124
61	N61	61	Incl	30	30	10	PEG/SAXA = 1.0	0.04	0	0.27	5.72	0.19	35.5	215.6	222
62	N62	62	Incl	30	30	30	PEG/SAXA = 1.0	0.07	0.05	0.27	5.71	0.29	56.8	293.6	208
63	N63	63	Incl	30	30	50	PEG/SAXA = 1.0	0.48	0	0.33	5.69	0.41	22.1	209.5	194
64	N64	64	Incl	30	40	10	PEG/SAXA = 1.0	0.16	0.06	0.30	5.66	0.2	42.5	273.6	219

Table S9. Cont.

Exp No	Exp Name	Run Order	Incl/Excl	Time Point	Temperature	Relative humidity	PEG/SAXA ratio	ESCA	SFA	SCA	pH	aw	F	FA	Coloration
65	N65	65	Incl	30	40	30	PEG/SAXA = 1.0	0.47	0.09	0.91	5.65	0.29	37.7	385.9	199
66	N66	66	Incl	30	40	50	PEG/SAXA = 1.0	1.87	0.08	0.81	5.64	0.41	24.1	259.5	140
67	N67	67	Incl	30	50	10	PEG/SAXA = 1.0	1.08	0.17	0.31	5.69	0.21	36.3	408.9	186
68	N68	68	Incl	30	50	30	PEG/SAXA = 1.0	2.75	0.22	0.34	5.67	0.29	28.9	487.8	156
69	N69	69	Incl	30	50	50	PEG/SAXA = 1.0	4.86	0.28	0.38	5.64	0.39	37.7	408.1	141
70	N70	70	Incl	45	50	10	PEG/SAXA = 1.0	1.74	0.21	0.35	5.67	0.19	33.8	457	170
71	N71	71	Incl	45	50	30	PEG/SAXA = 1.0	3.86	0.28	1.10	5.66	0.27	27.1	511.5	139
72	N72	72	Incl	45	50	50	PEG/SAXA = 1.0	5.59	0.27	0.93	5.61	0.38	33.8	445	120
73	N73	73	Incl	60	30	10	PEG/SAXA = 1.0	0.10	0	0.34	5.57	0.21	46.9	229.4	207
74	N74	74	Incl	60	30	30	PEG/SAXA = 1.0	0.23	0	0.52	5.57	0.3	42.1	245.1	194
75	N75	75	Incl	60	30	50	PEG/SAXA = 1.0	1.02	0.05	0.41	5.56	0.42	23.3	228.3	168
76	N76	76	Incl	60	40	10	PEG/SAXA = 1.0	0.56	0.08	1.30	5.56	0.2	46.4	281.8	192
77	N77	77	Incl	60	40	30	PEG/SAXA = 1.0	1.29	0.24	1.05	5.53	0.29	43.6	563.5	172
78	N78	78	Incl	60	40	50	PEG/SAXA = 1.0	4.34	0.18	0.72	5.49	0.4	26.7	327.6	135
79	N79	79	Incl	60	50	10	PEG/SAXA = 1.0	3.28	0.28	0.54	5.54	0.2	81.7	4162.7	165
80	N80	80	Incl	60	50	30	PEG/SAXA = 1.0	6.59	0.4	1.43	5.49	0.31	30.2	433.2	117
81	N81	81	Incl	60	50	50	PEG/SAXA = 1.0	9.87	0.47	1.21	5.45	0.38	25.9	549.7	124
82	N82	82	Incl	90	30	10	PEG/SAXA = 1.0	0.15	0	0.49	5.63	0.19	41.5	226.6	190
83	N83	83	Incl	90	30	30	PEG/SAXA = 1.0	0.35	0	0.41	5.6	0.27	42.8	258.7	200
84	N84	84	Incl	90	30	50	PEG/SAXA = 1.0	1.68	0.05	0.24	5.58	0.39	21.4	229.5	169
85	N85	85	Incl	90	40	10	PEG/SAXA = 1.0	0.84	0.07	0.10	5.63	0.18	42.9	309.2	183
86	N86	86	Incl	90	40	30	PEG/SAXA = 1.0	2.24	0.11	0.37	5.6	0.26	28.8	452.8	155
87	N87	87	Incl	90	40	50	PEG/SAXA = 1.0	4.87	0.21	0.32	5.56	0.36	25.2	355.7	133
88	N88	88	Incl	120	30	10	PEG/SAXA = 1.0	0.20	0	0.16	–	0.18	29.8	302.3	–
89	N89	89	Incl	120	30	30	PEG/SAXA = 1.0	0.40	0.08	0.50	–	0.27	24.1	334.9	–
90	N90	90	Incl	120	30	50	PEG/SAXA = 1.0	1.89	0.06	0.24	–	0.37	12.2	316.1	–
91	N91	91	Incl	120	40	10	PEG/SAXA = 1.0	1.18	0.08	0.09	–	0.16	31.5	506.2	–
92	N92	92	Incl	120	40	30	PEG/SAXA = 1.0	2.65	0.23	0.06	–	0.24	15.4	623.6	–
93	N93	93	Incl	120	40	50	PEG/SAXA = 1.0	5.64	0.21	0.08	–	0.33	11.9	606.2	–
94	N94	94	Incl	150	30	10	PEG/SAXA = 1.0	0.27	0.04	0.13	5.72	0.18	33.2	291.1	210
95	N95	95	Incl	150	40	10	PEG/SAXA = 1.0	1.62	0.11	0.21	5.66	0.18	14.8	715.5	182

Table S9. Cont.

Exp No	Exp Name	Run Order	Incl/Excl	Time Point	Temperature	Relative humidity	PEG/SAXA ratio	ESCA	SFA	SCA	pH	aw	F	FA	Coloration
96	N96	96	Incl	150	40	30	PEG/SAXA = 1.0	3.68	0.13	0.26	5.61	0.26	31.1	363.3	160
97	N97	97	Incl	150	40	50	PEG/SAXA = 1.0	7.53	0.26	0.16	5.56	0.36	10.2	341.6	122
98	N98	98	Incl	180	30	30	PEG/SAXA = 1.0	0.61	0.17	0.60	5.63	0.27	41.7	515.4	190
99	N99	99	Incl	180	30	50	PEG/SAXA = 1.0	2.80	0.11	0.38	5.62	0.38	15.6	338.2	147
100	N100	100	Incl	180	40	10	PEG/SAXA = 1.0	2.08	0.15	0.15	5.63	0.18	31.8	430.6	179
101	N101	101	Incl	180	40	30	PEG/SAXA = 1.0	3.88	0.35	0.73	5.59	0.26	19.7	928.4	148
102	N102	102	Incl	180	40	50	PEG/SAXA = 1.0	9.18	0.35	0.43	5.54	0.36	17.8	571.2	122
103	N103	103	Incl	7	60	10	PEG/SAXA = 1.2	0.63	0.65	0.20	5.44	0.21	19	755.6	149
104	N104	104	Incl	7	60	30	PEG/SAXA = 1.2	1.74	0.67	0.13	5.43	0.33	2.6	923.6	127
105	N105	105	Incl	7	60	50	PEG/SAXA = 1.2	2.38	0.32	0.18	5.47	0.44	1.4	391.2	132
106	N106	106	Incl	14	50	10	PEG/SAXA = 1.2	0.27	0.6	0.21	5.48	0.22	50.4	762.9	174
107	N107	107	Incl	14	50	30	PEG/SAXA = 1.2	1.11	0.58	0.45	5.46	0.32	9.9	891.3	150
108	N108	108	Incl	14	50	50	PEG/SAXA = 1.2	2.24	0.25	0.42	5.53	0.45	2	342	152
109	N109	109	Incl	14	60	10	PEG/SAXA = 1.2	1.73	0.72	0.21	5.46	0.21	6.2	977.4	121
110	N110	110	Incl	14	60	30	PEG/SAXA = 1.2	3.46	0.71	0.96	5.44	0.32	1.1	1070.1	124
111	N111	111	Incl	14	60	50	PEG/SAXA = 1.2	3.33	0.68	0.47	5.46	0.44	1.9	803	138
112	N112	112	Incl	30	30	10	PEG/SAXA = 1.2	0.03	0.12	0.20	5.7	0.22	93.5	335.7	211
113	N113	113	Incl	30	30	30	PEG/SAXA = 1.2	0.04	0.49	0.23	5.59	0.31	232.7	1272.8	203
114	N114	114	Incl	30	30	50	PEG/SAXA = 1.2	0.51	0.06	0.29	5.7	0.42	27	231.9	192
115	N115	115	Incl	30	40	10	PEG/SAXA = 1.2	0.07	0.48	0.24	5.61	0.2	122.9	868.5	188
116	N116	116	Incl	30	40	30	PEG/SAXA = 1.2	0.36	0.48	0.69	5.59	0.3	63.4	1142.7	192
117	N117	117	Incl	30	40	50	PEG/SAXA = 1.2	1.80	0.12	0.62	5.65	0.4	22.5	301.5	164
118	N118	118	Incl	30	50	10	PEG/SAXA = 1.2	0.87	0.71	0.27	5.59	0.2	48.9	1141.3	160
119	N119	119	Incl	30	50	30	PEG/SAXA = 1.2	2.42	0.69	0.28	5.58	0.3	28.6	1314.2	146
120	N120	120	Incl	30	50	50	PEG/SAXA = 1.2	3.46	0.38	0.26	5.61	0.42	40.4	504.1	145
121	N121	121	Incl	45	50	10	PEG/SAXA = 1.2	1.60	0.77	0.27	5.58	0.2	36.1	1192.2	155
122	N122	122	Incl	45	50	30	PEG/SAXA = 1.2	3.74	0.82	0.81	5.58	0.29	29.7	1274.1	142
123	N123	123	Incl	45	50	50	PEG/SAXA = 1.2	5.36	0.41	0.56	5.59	0.39	46	526.1	130
124	N124	124	Incl	60	30	10	PEG/SAXA = 1.2	0.05	0.26	0.31	5.52	0.21	151.6	449.8	202
125	N125	125	Incl	60	30	30	PEG/SAXA = 1.2	0.09	0.76	0.35	5.37	0.32	220.6	1547.9	192
126	N126	126	Incl	60	30	50	PEG/SAXA = 1.2	0.99	0.09	1.00	5.54	0.43	31.7	308.5	169
127	N127	127	Incl	60	40	10	PEG/SAXA = 1.2	0.25	0.68	0.74	5.45	0.23	110.5	1015.1	187
128	N128	128	Incl	60	40	30	PEG/SAXA = 1.2	1.26	0.66	0.30	5.43	0.31	43.6	1153.2	160

Table S9. Cont.

Exp No	Exp Name	Run Order	Incl/Excl	Time Point	Temperature	Relative humidity	PEG/SAXA ratio	ESCA	SFA	SCA	pH	aw	F	FA	Coloration
129	N129	129	Incl	60	40	50	PEG/SAXA = 1.2	3.67	0.25	0.37	5.48	0.41	28.3	409.9	150
130	N130	130	Incl	60	50	10	PEG/SAXA = 1.2	2.76	1.05	0.32	5.45	0.22	29.5	342	165
131	N131	131	Incl	60	50	30	PEG/SAXA = 1.2	6.21	1.09	1.14	5.41	0.3	28.2	1398.9	129
132	N132	132	Incl	60	50	50	PEG/SAXA = 1.2	8.30	0.57	0.74	5.46	0.41	38.8	625.1	139
133	N133	133	Incl	90	30	10	PEG/SAXA = 1.2	0.06	0.24	0.28	5.56	0.19	140.2	478.3	207
134	N134	134	Incl	90	30	30	PEG/SAXA = 1.2	0.16	0.52	0.19	5.46	0.3	166.6	1764.3	190
135	N135	135	Incl	90	30	50	PEG/SAXA = 1.2	1.60	0.12	0.11	5.57	0.39	24.1	318.4	166
136	N136	136	Incl	90	40	10	PEG/SAXA = 1.2	0.45	0.58	0.00	5.53	0.19	84.6	1078.5	168
137	N137	137	Incl	90	40	30	PEG/SAXA = 1.2	1.78	0.55	0.20	5.5	0.27	40	1455.7	150
138	N138	138	Incl	90	40	50	PEG/SAXA = 1.2	4.90	0.25	0.15	5.56	0.37	28.6	459.8	134
139	N139	139	Incl	120	30	10	PEG/SAXA = 1.2	0.08	0.27	0.04	–	0.18	128.3	732	–
140	N140	140	Incl	120	30	30	PEG/SAXA = 1.2	0.20	0.55	0.18	–	0.3	127.8	2163.5	–
141	N141	141	Incl	120	30	50	PEG/SAXA = 1.2	1.49	0.11	0.11	–	0.39	10	409.7	–
142	N142	142	Incl	120	40	10	PEG/SAXA = 1.2	0.77	0.55	0.00	–	0.16	69.6	1799.6	–
143	N143	143	Incl	120	40	30	PEG/SAXA = 1.2	2.56	0.74	0.04	–	0.26	18.5	1924.4	–
144	N144	144	Incl	120	40	50	PEG/SAXA = 1.2	5.57	0.26	0.03	–	0.36	12.8	715.3	–
145	N145	145	Incl	150	30	30	PEG/SAXA = 1.2	0.31	0.57	0.09	5.55	0.29	123.5	1920.6	175
146	N146	146	Incl	150	30	50	PEG/SAXA = 1.2	2.28	0.12	0.09	5.62	0.39	10.6	428.5	147
147	N147	147	Incl	150	40	10	PEG/SAXA = 1.2	1.12	0.62	0.15	5.56	0.19	52.1	1247.6	173
148	N148	148	Incl	150	40	30	PEG/SAXA = 1.2	3.25	0.74	0.10	5.51	0.28	17.4	1528.6	147
149	N149	149	Incl	150	40	50	PEG/SAXA = 1.2	6.27	0.41	0.27	5.56	0.38	10.3	561.1	132
150	N150	150	Incl	180	30	10	PEG/SAXA = 1.2	0.13	0.34	0.16	5.63	0.19	133.5	828.4	183
151	N151	151	Incl	180	40	10	PEG/SAXA = 1.2	1.41	0.74	0.00	5.52	0.19	54.4	1472.6	155
152	N152	152	Incl	180	40	30	PEG/SAXA = 1.2	4.38	0.82	0.29	5.51	0.27	23.7	1576.9	122
153	N153	153	Incl	180	40	50	PEG/SAXA = 1.2	7.84	0.44	0.16	5.53	0.37	16.6	618.3	130
154	N154	154	Incl	7	60	10	PEG/SAXA = 1.4	0.46	1.36	0.07	5.37	0.21	69.3	1250.6	179
155	N155	155	Incl	7	60	30	PEG/SAXA = 1.4	0.95	1.87	0.05	5.3	0.33	18.6	2038.1	153
156	N156	156	Incl	7	60	50	PEG/SAXA = 1.4	0.80	2.82	0.05	5.16	0.45	230.2	3317.6	185
157	N157	157	Incl	14	50	10	PEG/SAXA = 1.4	0.24	1.29	0.15	5.42	0.21	97	1154.1	199
158	N158	158	Incl	14	50	30	PEG/SAXA = 1.4	0.72	1.64	0.23	5.34	0.33	52.5	1863.2	182
159	N159	159	Incl	14	50	50	PEG/SAXA = 1.4	0.49	2.42	0.23	5.19	0.45	466	3197.2	190
160	N160	160	Incl	14	60	10	PEG/SAXA = 1.4	1.35	1.69	0.10	5.36	0.22	16.4	1464.2	156
161	N161	161	Incl	14	60	30	PEG/SAXA = 1.4	1.85	2.23	0.30	5.31	0.33	6.1	2202.1	143

Table S9. Cont.

Exp No	Exp Name	Run Order	Incl/Excl	Time Point	Temperature	Relative humidity	PEG/SAXA ratio	ESCA	SFA	SCA	pH	aw	F	FA	Coloration
162	N162	162	Incl	14	60	50	PEG/SAXA = 1.4	2.07	3.28	0.20	5.15	0.43	30.8	3267.9	164
163	N163	163	Incl	30	30	10	PEG/SAXA = 1.4	0.00	0.56	0.06	5.57	0.21	228.5	804.2	204
164	N164	164	Incl	30	30	30	PEG/SAXA = 1.4	0.04	0.8	0.09	5.48	0.32	267.4	1884.6	198
165	N165	165	Incl	30	30	50	PEG/SAXA = 1.4	0.13	1.15	0.10	5.4	0.47	558.5	2674.5	211
166	N166	166	Incl	30	40	10	PEG/SAXA = 1.4	0.06	0.96	0.13	5.51	0.2	148.7	1436.7	210
167	N167	167	Incl	30	40	30	PEG/SAXA = 1.4	0.34	1.1	0.33	5.47	0.32	106.9	2216.3	201
168	N168	168	Incl	30	40	50	PEG/SAXA = 1.4	0.30	1.95	0.25	5.29	0.46	518.3	4217.5	209
169	N169	169	Incl	30	50	10	PEG/SAXA = 1.4	0.85	1.38	0.12	5.53	0.2	55.1	1773.4	187
170	N170	170	Incl	30	50	30	PEG/SAXA = 1.4	1.74	1.84	0.10	5.43	0.32	39.6	2628.4	174
171	N171	171	Incl	30	50	50	PEG/SAXA = 1.4	1.09	2.76	0.11	5.28	0.43	209	4284.7	187
172	N172	172	Incl	45	50	10	PEG/SAXA = 1.4	1.38	1.43	0.18	5.49	0.21	47.6	1851.1	172
173	N173	173	Incl	45	50	30	PEG/SAXA = 1.4	2.33	2.14	0.39	5.43	0.31	40.1	2678.2	155
174	N174	174	Incl	45	50	50	PEG/SAXA = 1.4	1.51	2.99	0.27	5.27	0.41	135.9	4097.2	173
175	N175	175	Incl	60	30	10	PEG/SAXA = 1.4	0.03	0.93	0.09	5.38	0.21	306.8	1250.6	202
176	N176	176	Incl	60	30	30	PEG/SAXA = 1.4	0.10	1.1	0.16	5.31	0.32	230.3	2175.3	202
177	N177	177	Incl	60	30	50	PEG/SAXA = 1.4	0.24	1.86	0.18	5.17	0.44	631.3	3724.6	201
178	N178	178	Incl	60	40	10	PEG/SAXA = 1.4	0.33	1.41	0.49	5.36	0.22	110.6	1737.8	194
179	N179	179	Incl	60	40	30	PEG/SAXA = 1.4	1.09	1.56	0.29	5.29	0.32	58.9	2371.9	182
180	N180	180	Incl	60	40	50	PEG/SAXA = 1.4	0.72	2.72	0.08	5.14	0.44	309	4132	188
181	N181	181	Incl	60	50	10	PEG/SAXA = 1.4	2.57	1.99	0.16	5.34	0.2	37.8	1739.1	169
182	N182	182	Incl	60	50	30	PEG/SAXA = 1.4	3.82	2.79	0.52	5.29	0.3	35	1258.4	157
183	N183	183	Incl	60	50	50	PEG/SAXA = 1.4	2.72	3.94	0.31	5.16	0.41	29.6	295.1	182
184	N184	184	Incl	90	30	10	PEG/SAXA = 1.4	0.04	0.87	0.11	5.49	0.19	254.9	1424.4	199
185	N185	185	Incl	90	30	30	PEG/SAXA = 1.4	0.19	0.89	0.07	5.37	0.3	177.3	2292.5	186
186	N186	186	Incl	90	30	50	PEG/SAXA = 1.4	0.33	1.79	0.00	5.23	0.43	531.2	3946.7	208
187	N187	187	Incl	90	40	10	PEG/SAXA = 1.4	0.58	1.24	0.00	5.42	0.18	86.8	1847.6	168
188	N188	188	Incl	90	40	30	PEG/SAXA = 1.4	1.73	1.34	0.10	5.42	0.3	40.3	2303.5	160
189	N189	189	Incl	90	40	50	PEG/SAXA = 1.4	1.26	2.37	0.04	5.26	0.41	276.2	4006.5	173
190	N190	190	Incl	120	30	10	PEG/SAXA = 1.4	0.05	0.75	0.00	–	0.17	166.8	1838.7	–
191	N191	191	Incl	120	30	30	PEG/SAXA = 1.4	0.27	0.97	0.05	–	0.28	136.2	2928.7	–
192	N192	192	Incl	120	30	50	PEG/SAXA = 1.4	0.46	1.7	0.00	–	0.38	381.9	4964.5	–
193	N193	193	Incl	120	40	10	PEG/SAXA = 1.4	0.94	1.24	0.00	–	0.17	70.6	2899.6	–
194	N194	194	Incl	120	40	30	PEG/SAXA = 1.4	2.30	1.5	0.00	–	0.27	25.4	3796.2	–

Table S9. Cont.

Exp No	Exp Name	Run Order	Incl/Excl	Time Point	Temperature	Relative humidity	PEG/SAXA ratio	ESCA	SFA	SCA	pH	aw	F	FA	Coloration
195	N195	195	Incl	120	40	50	PEG/SAXA = 1.4	1.43	2.58	0.00	–	0.34	148.6	6104.6	–
196	N196	196	Incl	150	30	10	PEG/SAXA = 1.4	0.07	0.89	0.00	5.49	0.2	203.7	1835.3	180
197	N197	197	Incl	150	40	10	PEG/SAXA = 1.4	1.32	1.33	0.07	5.4	0.19	44.9	2114.6	165
198	N198	198	Incl	150	40	30	PEG/SAXA = 1.4	2.88	1.59	0.06	5.4	0.28	27.6	2560.1	159
199	N199	199	Incl	150	40	50	PEG/SAXA = 1.4	1.92	2.87	0.00	5.26	0.39	129	4203.5	184
200	N200	200	Incl	180	30	30	PEG/SAXA = 1.4	0.56	1.08	0.10	5.42	0.29	106.5	2999	166
201	N201	201	Incl	180	30	50	PEG/SAXA = 1.4	0.72	1.99	0.00	5.27	0.43	339.1	4847	184
202	N202	202	Incl	180	40	10	PEG/SAXA = 1.4	1.68	1.39	0.00	5.45	0.19	43.9	2522.7	163
203	N203	203	Incl	180	40	30	PEG/SAXA = 1.4	3.73	1.66	0.09	5.42	0.28	24.2	2770.7	136
204	N204	204	Incl	180	40	50	PEG/SAXA = 1.4	2.25	2.77	0.00	5.28	0.38	94.3	4497.6	164

Table S10. Factors.

Name	Abbr.	Units	Type	Settings	Transform	Precision
Time Point	TP	d	Quantitative	7 to 180	None	4.32
Temperature	T	°C	Quantitative	30 to 60	None	0.75
Relative humidity	RH	RH	Quantitative	10 to 50	None	1
PEG/SAXA ratio	ratio		Qualitative	PEG/SAXA = 0.8, PEG/SAXA = 1.0, PEG/SAXA = 1.2, PEG/SAXA = 1.4	–	–

Table S11. Responses.

Name	Abbr.	Transform	Type
ESCA	ESCA	Log (10Log(Y))	Regular
SFA	SFA	Log (10Log(Y))	Regular
SCA	CA	Log (10Log(Y))	Regular
pH	pH	None	Regular
aw	aw	None	Regular
F	F	Log (10Log(Y))	Regular
FA	FA	Log (10Log(Y))	Regular
Coloration	Color	None	Regular

Table S12. Coefficient list.

SCA~	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	−0.40	0.02	0.00	0.04
Time Point	0.33	0.03	0.00	0.05
Temperature	0.23	0.03	0.00	0.05
Relative humidity	−0.15	0.02	0.00	0.04
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	0.36	0.02	0.00	0.05
ratio(PEG/SAXA = 1.0)	0.22	0.02	0.00	0.05
ratio(PEG/SAXA = 1.2)	−0.12	0.02	0.00	0.05
ratio(PEG/SAXA = 1.4)	−0.46	0.03	0.00	0.06
N = 177 Q ² = 0.739 Cond. no. = 2.772				
DF = 170 R ² = 0.761 RSD = 0.1894				
R ² adj. = 0.753				
Confidence = 0.95				
ESCA~	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	0.53	0.02	0.00	0.04
Time Point	0.60	0.04	0.00	0.07
Temperature	0.82	0.03	0.00	0.07
Relative humidity	0.35	0.02	0.00	0.04
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	0.13	0.03	0.00	0.06
ratio(PEG/SAXA = 1.0)	0.12	0.03	0.00	0.06
ratio(PEG/SAXA = 1.2)	−0.01	0.03	0.69	0.06
ratio(PEG/SAXA = 1.4)	−0.24	0.03	0.00	0.06
N = 203 Q ² = 0.811 Cond. no. = 2.626				
DF = 196 R ² = 0.824 RSD = 0.2587				
R ² adj. = 0.819				
Confidence = 0.95				

Table S12. Cont.

SFA~	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	−0.44	0.02	0.00	0.04
Time Point	0.17	0.03	0.00	0.06
Temperature	0.32	0.03	0.00	0.06
Relative humidity	0.06	0.02	0.00	0.04
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	−0.60	0.03	0.00	0.06
ratio(PEG/SAXA = 1.0)	−0.31	0.03	0.00	0.05
ratio(PEG/SAXA = 1.2)	0.17	0.03	0.00	0.05
ratio(PEG/SAXA = 1.4)	0.75	0.03	0.00	0.05
N = 175 Q ² = 0.846 Cond. no. = 2.888				
DF = 168 R ² = 0.858 RSD = 0.2024				
R ² adj. = 0.853				
Confidence = 0.95				
pH	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	5.51	0.01	0.00	0.01
Time Point	−0.01	0.01	0.33	0.02
Temperature	−0.06	0.01	0.00	0.02
Relative humidity	−0.04	0.01	0.00	0.01
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	0.09	0.01	0.00	0.02
ratio(PEG/SAXA = 1.0)	0.07	0.01	0.00	0.02
ratio(PEG/SAXA = 1.2)	0.01	0.01	0.40	0.02
ratio(PEG/SAXA = 1.4)	−0.17	0.01	0.00	0.02
N = 180 Q ² = 0.709 Cond. no. = 2.54				
DF = 173 R ² = 0.731 RSD = 0.07068				
R ² adj. = 0.721				
Confidence = 0.95				

Table S12. Cont.

aw	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	0.29	0.00	0.00	0.00
Time Point	−0.03	0.00	0.00	0.00
Temperature	−0.00	0.00	0.06	0.00
Relative humidity	0.10	0.00	0.00	0.00
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	−0.01	0.00	0.00	0.00
ratio(PEG/SAXA = 1.0)	−0.01	0.00	0.00	0.00
ratio(PEG/SAXA = 1.2)	0.00	0.00	0.02	0.00
ratio(PEG/SAXA = 1.4)	0.01	0.00	0.00	0.00
N = 204 Q ² = 0.960 Cond. no. = 2.61				
DF = 197 R ² = 0.963 RSD = 0.01693				
R ² adj. = 0.962				
Confidence = 0.95				
F~	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	1.35	0.03	0.00	0.07
Time Point	−0.14	0.05	0.01	0.10
Temperature	−0.51	0.05	0.00	0.10
Relative humidity	−0.10	0.03	0.00	0.07
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	−0.32	0.05	0.00	0.09
ratio(PEG/SAXA = 1.0)	−0.19	0.05	0.00	0.09
ratio(PEG/SAXA = 1.2)	−0.01	0.05	0.91	0.09
ratio(PEG/SAXA = 1.4)	0.51	0.05	0.00	0.09
N = 202 Q ² = 0.541 Cond. no. = 2.609				
DF = 195 R ² = 0.573 RSD = 0.382				

Table S12. Cont.

R ² adj. =		0.560		
		Confidence =		0.95
FA~	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	2.89	0.02	0.00	0.03
Time Point	0.15	0.03	0.00	0.05
Temperature	0.12	0.03	0.00	0.05
Relative humidity	0.01	0.02	0.69	0.03
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	−0.37	0.02	0.00	0.05
ratio(PEG/SAXA = 1.0)	−0.24	0.02	0.00	0.05
ratio(PEG/SAXA = 1.2)	0.07	0.02	0.01	0.05
ratio(PEG/SAXA = 1.4)	0.54	0.02	0.00	0.05
N = 204	Q ² =	0.746	Cond. no. =	2.61
DF = 197	R ² =	0.763	RSD =	0.2054
R ² adj. =		0.755		
		Confidence =		0.95
Coloration	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	157.38	1.34	0.00	2.65
Time Point	−18.40	2.03	0.00	4.01
Temperature	−33.54	1.92	0.00	3.79
Relative humidity	−14.50	1.33	0.00	2.63
ratio DF = _____				
ratio(PEG/SAXA = 0.8)	1.18	1.88	0.53	3.72
ratio(PEG/SAXA = 1.0)	−4.63	1.88	0.01	3.72
ratio(PEG/SAXA = 1.2)	−8.75	1.88	0.00	3.72
ratio(PEG/SAXA = 1.4)	12.21	1.88	0.00	3.72
N = 180	Q ² =	0.710	Cond. no. =	2.54

Table S12. Cont.

DF = 173	R ² =	0.733	RSD =	14.6
	R ² adj. =	0.724		
			Confidence =	0.95

Table S13. Correlation matrix.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
	Time Point	Temperature	Relative humidity	ratio(PEG/SAXA = 1.0)	ratio(PEG/SAXA = 1.2)	ratio(PEG/SAXA = 1.4)	ESCA~	SFA~	SCA~	pH	aw	F~	FA~	Coloration
Time Point	1.00	-0.54	0.02	0.00	0.03	0.06	0.12	0.03	0.27	0.09	-0.17	0.19	0.19	0.00
Temperature	-0.54	1.00	-0.05	0.00	-0.04	-0.04	0.53	0.07	0.15	-0.30	0.03	-0.51	0.07	-0.59
Relative humidity	0.02	-0.05	1.00	0.00	-0.03	-0.20	0.53	-0.27	-0.16	0.03	0.96	-0.35	-0.24	-0.55
ratio(PEG/SAXA = 1.0)	0.00	0.00	0.00	1.00	0.51	0.58	-0.01	0.04	-0.13	-0.10	0.01	0.09	0.14	-0.08
ratio(PEG/SAXA = 1.2)	0.03	-0.04	-0.03	0.51	1.00	0.59	-0.11	0.45	-0.46	-0.33	0.03	0.26	0.48	-0.11
ratio(PEG/SAXA = 1.4)	0.06	-0.04	-0.20	0.58	0.59	1.00	-0.21	0.73	-0.58	-0.61	-0.15	0.42	0.72	0.06
ESCA~	0.12	0.53	0.53	-0.01	-0.11	-0.21	1.00	-0.17	0.40	-0.10	0.45	-0.54	-0.05	-0.83
SFA~	0.03	0.07	-0.27	0.04	0.45	0.73	-0.17	1.00	-0.56	-0.76	-0.22	0.37	0.86	-0.04
SCA~	0.27	0.15	-0.16	-0.13	-0.46	-0.58	0.40	-0.56	1.00	0.44	-0.29	-0.27	-0.37	-0.09
pH	0.09	-0.30	0.03	-0.10	-0.33	-0.61	-0.10	-0.76	0.44	1.00	-0.06	-0.09	-0.67	0.29
aw	-0.17	0.03	0.96	0.01	0.03	-0.15	0.45	-0.22	-0.29	-0.06	1.00	-0.37	-0.24	-0.51
F~	0.19	-0.51	-0.35	0.09	0.26	0.42	-0.54	0.37	-0.27	-0.09	-0.37	1.00	0.43	0.53
FA~	0.19	0.07	-0.24	0.14	0.48	0.72	-0.05	0.86	-0.37	-0.67	-0.24	0.43	1.00	-0.10
Coloration	0.00	-0.59	-0.55	-0.08	-0.11	0.06	-0.83	-0.04	-0.09	0.29	-0.51	0.53	-0.10	1.00

3.4. Modelling of Degradation Kinetics

Equations, experimental values, modelled values and determined rate constants for temperature of 40 °C and RH 10% used for additional model optimization are presented.

3.5. Equations

METHOD RK4

STARTTIME=0

STOPTIME=200

DT=0.1

$\text{pH08} = -570.45 * (\text{cFA08}) + 5.6703$

$\text{pH10} = -570.45 * (\text{cFA10}) + 5.6703$

$\text{pH12} = -570.45 * (\text{cFA12}) + 5.6703$

$\text{pH14} = -570.45 * (\text{cFA14}) + 5.6703$

$k1c = 1$

$k2c = 1$

$k3c = 1$

$k4c = 1$

$k5 = 1$

$k6 = 1$

$k7 = 1$

$k8 = 1$

$xS = 1$

$xPEG = 1$

$xPEGm08 = xPEG$

$xPEGm10 = xPEG * 0.125 / 0.1$

$xPEGm12 = xPEG * 0.15 / 0.1$

$xPEGm14 = xPEG * 0.175 / 0.1$

$cPEGTOT008 = 0.0181611805$

$cPEG008 = xPEGm08 * cPEGTOT008$

$d/dt(cPEG08) = -k1c * cPEG08 - k2c * cPEG08 - k3c * cPEG08$

$$\begin{aligned}d/dt(cGA08) &= k1c * cPEG08 \\d/dt(cA08) &= k2c * cPEG08 \\d/dt(cF08) &= k3c * cPEG08 - k4c * cF08 \\d/dt(cFA08) &= k4c * cF08\end{aligned}$$
$$\begin{aligned}\text{init } cPEG08 &= cPEG008 \\ \text{init } cGA08 &= 0 \\ \text{init } cA08 &= 0 \\ \text{init } cF08 &= 0 \\ \text{init } cFA08 &= 0\end{aligned}$$
$$\begin{aligned}cSTOT008 &= 0.0031704765 \\ cS008 &= xS * cSTOT008\end{aligned}$$
$$\begin{aligned}d/dt(cS08) &= -k5 * cS08 - k7 * cFA08 * cS08 + k8 * cSF08 \\d/dt(cSA08) &= k5 * cS08 - k6 * cSA08 \\d/dt(cESA08) &= k6 * cSA08 \\d/dt(cSF08) &= k7 * cFA08 * cS08 - k8 * cSF08\end{aligned}$$
$$\begin{aligned}\text{init } cS08 &= cS008 \\ \text{init } cSA08 &= 0 \\ \text{init } cESA08 &= 0 \\ \text{init } cSF08 &= 0\end{aligned}$$
$$\begin{aligned}cPEGTOT010 &= 0.0227014756 \\ cPEG010 &= xPEGm10 * cPEGTOT010\end{aligned}$$
$$\begin{aligned}d/dt(cPEG10) &= -k1c * cPEG10 - k2c * cPEG10 - k3c * cPEG10 \\d/dt(cGA10) &= k1c * cPEG10 \\d/dt(cA10) &= k2c * cPEG10 \\d/dt(cF10) &= k3c * cPEG10 - k4c * cF10 \\d/dt(cFA10) &= k4c * cF10\end{aligned}$$
$$\text{init } cPEG10 = cPEG010$$

```

init cGA10=0
init cA10=0
init cF10=0
init cFA10=0
cSTOT010=0.0031704765
cS010=xS*cSTOT010
d/dt(cS10)=-k5*((10^(pH10-14))/(10^(pH08-14)))*cS10-k7*((10^(-pH10))/(10^(-pH08)))*cFA10*cS10+k8*cSF10
d/dt(cSA10)=k5*((10^(pH10-14))/(10^(pH08-14)))*cS10-k6*((10^(pH10-14))/(10^(pH08-14)))*cSA10
d/dt(cESA10)=k6*((10^(pH10-14))/(10^(pH08-14)))*cSA10
d/dt(cSF10)=k7*((10^(-pH10))/(10^(-pH08)))*cFA10*cS10-k8*cSF10
init cS10=cS010
init cSA10=0
init cESA10=0
init cSF10=0
cPEGTOT012=0.0272417707
cPEG012=xPEGm12*cPEGTOT012
d/dt(cPEG12)=-k1c*cPEG12-k2c*cPEG12-k3c*cPEG12
d/dt(cGA12)=k1c*cPEG12
d/dt(cA12)=k2c*cPEG12
d/dt(cF12)=k3c*cPEG12-k4c*cF12
d/dt(cFA12)=k4c*cF12
init cPEG12=cPEG012
init cGA12=0
init cA12=0
init cF12=0
init cFA12=0
cSTOT012=0.0031704765
cS012=xS*cSTOT012
d/dt(cS12)=-k5*((10^(pH12-14))/(10^(pH08-14)))*cS12-k7*((10^(-pH12))/(10^(-pH08)))*cFA12*cS12+k8*cSF12
d/dt(cSA12)=k5*((10^(pH12-14))/(10^(pH08-14)))*cS12-k6*((10^(pH12-14))/(10^(pH08-14)))*cSA12
d/dt(cESA12)=k6*((10^(pH12-14))/(10^(pH08-14)))*cSA12
d/dt(cSF12)=k7*((10^(-pH12))/(10^(-pH08)))*cFA12*cS12-k8*cSF12
init cS12=cS012
init cSA12=0

```

init cESA12=0

init cSF12=0

cPEGTOT014=0.0317820658

cPEG014=xPEGm14*cPEGTOT014

$d/dt(cPEG14) = -k1c*cPEG14 - k2c*cPEG14 - k3c*cPEG14$

$d/dt(cGA14) = k1c*cPEG14$

$d/dt(cA14) = k2c*cPEG14$

$d/dt(cF14) = k3c*cPEG14 - k4c*cF14$

$d/dt(cFA14) = k4c*cF14$

init cPEG14=cPEG014

init cGA14=0

init cA14=0

init cF14=0

init cFA14=0

cSTOT014=0.0031704765

cS014=xS*cSTOT014

$d/dt(cS14) = -k5*((10^{(pH14-14)})/(10^{(pH08-14)}))*cS14 - k7*((10^{(-pH14)})/(10^{(-pH08)}))*cFA14*cS14 + k8*cSF14$

$d/dt(cSA14) = k5*((10^{(pH14-14)})/(10^{(pH08-14)}))*cS14 - k6*((10^{(pH14-14)})/(10^{(pH08-14)}))*cSA14$

$d/dt(cESA14) = k6*((10^{(pH14-14)})/(10^{(pH08-14)}))*cSA14$

$d/dt(cSF14) = k7*((10^{(-pH14)})/(10^{(-pH08)}))*cFA14*cS14 - k8*cSF14$

init cS14=cS014

init cSA14=0

init cESA14=0

init cSF14=0

Experimental data

Table S14. Imported dataset for organic impurities (values in mol/g_{saxa}).

TimePoint (days)		GA	A	F	FA
0.8	30	0.0000288345	0.0000000000	0.0000086330	0.0000440405
	60	0.0000288906	0.0000000000	0.0000102902	0.0000447755
	90	0.0000285908	0.0000000000	0.0000094031	0.0000454649
	120	0.0000296821	0.0000000000	0.0000055805	0.0000641012
	150	0.0000309696	0.0000022343	0.0000056773	0.0000601126
	180	0.0000307233	0.0000021840	0.0000082824	0.0000623029
1	30	0.0000300946	0.0000000000	0.0000130329	0.0000546879
	60	0.0000291543	0.0000000000	0.0000142177	0.0000563260
	90	0.0000305892	0.0000000000	0.0000131391	0.0000618047
	120	0.0000345007	0.0000000000	0.0000096577	0.0001011784
	150	0.0000326029	0.0000016783	0.0000045257	0.0001430299
	180	0.0000315294	0.0000023071	0.0000097536	0.0000860655
1.2	30	0.0000319194	0.0000028043	0.0000376531	0.0001735970
	60	0.0000320094	0.0000037533	0.0000338475	0.0002029180
	90	0.0000321056	0.0000034046	0.0000259072	0.0002155883
	120	0.0000391023	0.0000025601	0.0000213116	0.0003597215
	150	0.0000344614	0.0000027292	0.0000159765	0.0002493824
	180	0.0000333889	0.0000030509	0.0000166734	0.0002943538
1.4	30	0.0000352133	0.0000033385	0.0000455659	0.0002871912
	60	0.0000356637	0.0000034776	0.0000338841	0.0003473679
	90	0.0000358764	0.0000033827	0.0000265859	0.0003693140
	120	0.0000462426	0.0000035750	0.0000216307	0.0005796135
	150	0.0000355406	0.0000025717	0.0000137465	0.0004226970
	180	0.0000392171	0.0000022911	0.0000134461	0.0005042563

Table S15. Imported dataset for saxagliptin degradation products (values in mol/g_{saxa}).

PEG/SAXA ratio	TimePoint (days)	SCA	ESCA	SFA
0.8	30	0.0000090363	0.0000063778	0.0000000000
	60	0.0000194300	0.0000210633	0.0000000000
	90	0.0000288421	0.0000326124	0.0000000000
	120	0.0000348269	0.0000467544	0.0000000000
	150	0.0000412375	0.0000601218	0.0000014596
	180	0.0000454932	0.0000765514	0.0000021721
1	30	0.0000067507	0.0000052179	0.0000017727
	60	0.0000140392	0.0000176348	0.0000022965
	90	0.0000218035	0.0000265181	0.0000021741
	120	0.0000257447	0.0000373596	0.0000023429
	150	0.0000316957	0.0000512749	0.0000030700
	180	0.0000360807	0.0000658352	0.0000044738
1.2	30	0.0000026306	0.0000022160	0.0000139546
	60	0.0000070698	0.0000080635	0.0000198998
	90	0.0000104400	0.0000142243	0.0000167838
	120	0.0000123231	0.0000245514	0.0000159019
	150	0.0000154855	0.0000356448	0.0000180762
	180	0.0000163778	0.0000447367	0.0000216494
1.4	30	0.0000020861	0.0000020375	0.0000279559
	60	0.0000046133	0.0000105469	0.0000411142
	90	0.0000056227	0.0000183767	0.0000359713
	120	0.0000060124	0.0000299248	0.0000360929
	150	0.0000069010	0.0000417796	0.0000388216
	180	0.0000061933	0.0000533430	0.0000404983

4. Modelled Data

Table S16. Modelled data for organic impurities (values in mol/g_{saxa}).

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	1.81E-06	2.83E-06	4.08E-06	5.55E-06	7.84E-06	5.29E-07	5.74E-05	1.23E-05	8.26E-07	8.97E-05	1.76E-05	1.19E-06	1.29E-04	2.40E-05	1.62E-06	1.76E-04
2	5.77E-06	9.02E-06	1.30E-05	1.77E-05	1.16E-05	7.79E-07	8.15E-05	1.81E-05	1.22E-06	1.27E-04	2.60E-05	1.75E-06	1.83E-04	3.54E-05	2.39E-06	2.50E-04
3	1.06E-05	1.65E-05	2.38E-05	3.24E-05	1.33E-05	8.97E-07	9.00E-05	2.08E-05	1.40E-06	1.41E-04	3.00E-05	2.02E-06	2.02E-04	4.08E-05	2.75E-06	2.76E-04
4	1.56E-05	2.44E-05	3.52E-05	4.79E-05	1.42E-05	9.54E-07	9.12E-05	2.21E-05	1.49E-06	1.43E-04	3.18E-05	2.15E-06	2.05E-04	4.33E-05	2.92E-06	2.79E-04
5	2.07E-05	3.23E-05	4.65E-05	6.32E-05	1.45E-05	9.80E-07	8.92E-05	2.27E-05	1.53E-06	1.39E-04	3.27E-05	2.21E-06	2.01E-04	4.45E-05	3.00E-06	2.73E-04
6	2.55E-05	3.99E-05	5.74E-05	7.81E-05	1.47E-05	9.93E-07	8.57E-05	2.30E-05	1.55E-06	1.34E-04	3.31E-05	2.23E-06	1.93E-04	4.51E-05	3.04E-06	2.63E-04
7	3.02E-05	4.71E-05	6.79E-05	9.24E-05	1.48E-05	9.99E-07	8.18E-05	2.32E-05	1.56E-06	1.28E-04	3.33E-05	2.25E-06	1.84E-04	4.54E-05	3.06E-06	2.50E-04
8	3.46E-05	5.40E-05	7.78E-05	1.06E-04	1.49E-05	1.00E-06	7.76E-05	2.32E-05	1.56E-06	1.21E-04	3.34E-05	2.25E-06	1.75E-04	4.55E-05	3.07E-06	2.38E-04
9	3.88E-05	6.06E-05	8.73E-05	1.19E-04	1.49E-05	1.00E-06	7.36E-05	2.33E-05	1.57E-06	1.15E-04	3.35E-05	2.26E-06	1.66E-04	4.56E-05	3.07E-06	2.25E-04
10	4.28E-05	6.68E-05	9.62E-05	1.31E-04	1.49E-05	1.00E-06	6.97E-05	2.33E-05	1.57E-06	1.09E-04	3.35E-05	2.26E-06	1.57E-04	4.56E-05	3.07E-06	2.13E-04
11	4.65E-05	7.27E-05	1.05E-04	1.42E-04	1.49E-05	1.00E-06	6.60E-05	2.33E-05	1.57E-06	1.03E-04	3.35E-05	2.26E-06	1.48E-04	4.56E-05	3.07E-06	2.02E-04
12	5.01E-05	7.83E-05	1.13E-04	1.53E-04	1.49E-05	1.00E-06	6.24E-05	2.33E-05	1.57E-06	9.75E-05	3.35E-05	2.26E-06	1.40E-04	4.56E-05	3.07E-06	1.91E-04
13	5.35E-05	8.35E-05	1.20E-04	1.64E-04	1.49E-05	1.00E-06	5.90E-05	2.33E-05	1.57E-06	9.23E-05	3.35E-05	2.26E-06	1.33E-04	4.56E-05	3.07E-06	1.81E-04
14	5.66E-05	8.85E-05	1.27E-04	1.73E-04	1.49E-05	1.00E-06	5.59E-05	2.33E-05	1.57E-06	8.73E-05	3.35E-05	2.26E-06	1.26E-04	4.56E-05	3.07E-06	1.71E-04
15	5.97E-05	9.32E-05	1.34E-04	1.83E-04	1.49E-05	1.00E-06	5.28E-05	2.33E-05	1.57E-06	8.26E-05	3.35E-05	2.26E-06	1.19E-04	4.56E-05	3.07E-06	1.62E-04
16	6.25E-05	9.77E-05	1.41E-04	1.91E-04	1.49E-05	1.00E-06	5.00E-05	2.33E-05	1.57E-06	7.81E-05	3.35E-05	2.26E-06	1.12E-04	4.56E-05	3.07E-06	1.53E-04
17	6.52E-05	1.02E-04	1.47E-04	2.00E-04	1.49E-05	1.00E-06	4.73E-05	2.33E-05	1.57E-06	7.39E-05	3.35E-05	2.26E-06	1.06E-04	4.56E-05	3.07E-06	1.45E-04
18	6.78E-05	1.06E-04	1.52E-04	2.08E-04	1.49E-05	1.00E-06	4.47E-05	2.33E-05	1.57E-06	6.99E-05	3.35E-05	2.26E-06	1.01E-04	4.56E-05	3.07E-06	1.37E-04
19	7.02E-05	1.10E-04	1.58E-04	2.15E-04	1.49E-05	1.00E-06	4.23E-05	2.33E-05	1.57E-06	6.61E-05	3.35E-05	2.26E-06	9.52E-05	4.56E-05	3.07E-06	1.30E-04
20	7.25E-05	1.13E-04	1.63E-04	2.22E-04	1.49E-05	1.00E-06	4.00E-05	2.33E-05	1.57E-06	6.26E-05	3.35E-05	2.26E-06	9.01E-05	4.56E-05	3.07E-06	1.23E-04
21	7.46E-05	1.17E-04	1.68E-04	2.29E-04	1.49E-05	1.00E-06	3.79E-05	2.33E-05	1.57E-06	5.92E-05	3.35E-05	2.26E-06	8.52E-05	4.56E-05	3.07E-06	1.16E-04

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
22	7.67E-05	1.20E-04	1.73E-04	2.35E-04	1.49E-05	1.00E-06	3.58E-05	2.33E-05	1.57E-06	5.60E-05	3.35E-05	2.26E-06	8.06E-05	4.56E-05	3.07E-06	1.10E-04
23	7.86E-05	1.23E-04	1.77E-04	2.41E-04	1.49E-05	1.00E-06	3.39E-05	2.33E-05	1.57E-06	5.30E-05	3.35E-05	2.26E-06	7.63E-05	4.56E-05	3.07E-06	1.04E-04
24	8.04E-05	1.26E-04	1.81E-04	2.46E-04	1.49E-05	1.00E-06	3.21E-05	2.33E-05	1.57E-06	5.01E-05	3.35E-05	2.26E-06	7.21E-05	4.56E-05	3.07E-06	9.82E-05
25	8.22E-05	1.28E-04	1.85E-04	2.52E-04	1.49E-05	1.00E-06	3.03E-05	2.33E-05	1.57E-06	4.74E-05	3.35E-05	2.26E-06	6.82E-05	4.56E-05	3.07E-06	9.29E-05
26	8.38E-05	1.31E-04	1.89E-04	2.57E-04	1.49E-05	1.00E-06	2.87E-05	2.33E-05	1.57E-06	4.48E-05	3.35E-05	2.26E-06	6.46E-05	4.56E-05	3.07E-06	8.79E-05
27	8.54E-05	1.33E-04	1.92E-04	2.61E-04	1.49E-05	1.00E-06	2.71E-05	2.33E-05	1.57E-06	4.24E-05	3.35E-05	2.26E-06	6.11E-05	4.56E-05	3.07E-06	8.31E-05
28	8.68E-05	1.36E-04	1.95E-04	2.66E-04	1.49E-05	1.00E-06	2.57E-05	2.33E-05	1.57E-06	4.01E-05	3.35E-05	2.26E-06	5.78E-05	4.56E-05	3.07E-06	7.86E-05
29	8.82E-05	1.38E-04	1.98E-04	2.70E-04	1.49E-05	1.00E-06	2.43E-05	2.33E-05	1.57E-06	3.80E-05	3.35E-05	2.26E-06	5.47E-05	4.56E-05	3.07E-06	7.44E-05
30	8.95E-05	1.40E-04	2.01E-04	2.74E-04	1.49E-05	1.00E-06	2.30E-05	2.33E-05	1.57E-06	3.59E-05	3.35E-05	2.26E-06	5.17E-05	4.56E-05	3.07E-06	7.04E-05
31	9.08E-05	1.42E-04	2.04E-04	2.78E-04	1.49E-05	1.00E-06	2.17E-05	2.33E-05	1.57E-06	3.40E-05	3.35E-05	2.26E-06	4.89E-05	4.56E-05	3.07E-06	6.66E-05
32	9.19E-05	1.44E-04	2.07E-04	2.82E-04	1.49E-05	1.00E-06	2.06E-05	2.33E-05	1.57E-06	3.21E-05	3.35E-05	2.26E-06	4.63E-05	4.56E-05	3.07E-06	6.30E-05
33	9.31E-05	1.45E-04	2.09E-04	2.85E-04	1.49E-05	1.00E-06	1.95E-05	2.33E-05	1.57E-06	3.04E-05	3.35E-05	2.26E-06	4.38E-05	4.56E-05	3.07E-06	5.96E-05
34	9.41E-05	1.47E-04	2.12E-04	2.88E-04	1.49E-05	1.00E-06	1.84E-05	2.33E-05	1.57E-06	2.88E-05	3.35E-05	2.26E-06	4.14E-05	4.56E-05	3.07E-06	5.64E-05
35	9.51E-05	1.49E-04	2.14E-04	2.91E-04	1.49E-05	1.00E-06	1.74E-05	2.33E-05	1.57E-06	2.72E-05	3.35E-05	2.26E-06	3.92E-05	4.56E-05	3.07E-06	5.33E-05
36	9.60E-05	1.50E-04	2.16E-04	2.94E-04	1.49E-05	1.00E-06	1.65E-05	2.33E-05	1.57E-06	2.57E-05	3.35E-05	2.26E-06	3.71E-05	4.56E-05	3.07E-06	5.04E-05
37	9.69E-05	1.51E-04	2.18E-04	2.97E-04	1.49E-05	1.00E-06	1.56E-05	2.33E-05	1.57E-06	2.43E-05	3.35E-05	2.26E-06	3.51E-05	4.56E-05	3.07E-06	4.77E-05
38	9.78E-05	1.53E-04	2.20E-04	2.99E-04	1.49E-05	1.00E-06	1.47E-05	2.33E-05	1.57E-06	2.30E-05	3.35E-05	2.26E-06	3.32E-05	4.56E-05	3.07E-06	4.51E-05
39	9.86E-05	1.54E-04	2.22E-04	3.02E-04	1.49E-05	1.00E-06	1.39E-05	2.33E-05	1.57E-06	2.18E-05	3.35E-05	2.26E-06	3.14E-05	4.56E-05	3.07E-06	4.27E-05
40	9.93E-05	1.55E-04	2.23E-04	3.04E-04	1.49E-05	1.00E-06	1.32E-05	2.33E-05	1.57E-06	2.06E-05	3.35E-05	2.26E-06	2.97E-05	4.56E-05	3.07E-06	4.04E-05
41	1.00E-04	1.56E-04	2.25E-04	3.06E-04	1.49E-05	1.00E-06	1.25E-05	2.33E-05	1.57E-06	1.95E-05	3.35E-05	2.26E-06	2.81E-05	4.56E-05	3.07E-06	3.82E-05
42	1.01E-04	1.57E-04	2.27E-04	3.08E-04	1.49E-05	1.00E-06	1.18E-05	2.33E-05	1.57E-06	1.84E-05	3.35E-05	2.26E-06	2.66E-05	4.56E-05	3.07E-06	3.61E-05
43	1.01E-04	1.58E-04	2.28E-04	3.10E-04	1.49E-05	1.00E-06	1.12E-05	2.33E-05	1.57E-06	1.74E-05	3.35E-05	2.26E-06	2.51E-05	4.56E-05	3.07E-06	3.42E-05
44	1.02E-04	1.59E-04	2.29E-04	3.12E-04	1.49E-05	1.00E-06	1.06E-05	2.33E-05	1.57E-06	1.65E-05	3.35E-05	2.26E-06	2.38E-05	4.56E-05	3.07E-06	3.23E-05

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
45	1.03E-04	1.60E-04	2.31E-04	3.14E-04	1.49E-05	1.00E-06	9.99E-06	2.33E-05	1.57E-06	1.56E-05	3.35E-05	2.26E-06	2.25E-05	4.56E-05	3.07E-06	3.06E-05
46	1.03E-04	1.61E-04	2.32E-04	3.16E-04	1.49E-05	1.00E-06	9.45E-06	2.33E-05	1.57E-06	1.48E-05	3.35E-05	2.26E-06	2.13E-05	4.56E-05	3.07E-06	2.89E-05
47	1.04E-04	1.62E-04	2.33E-04	3.17E-04	1.49E-05	1.00E-06	8.94E-06	2.33E-05	1.57E-06	1.40E-05	3.35E-05	2.26E-06	2.01E-05	4.56E-05	3.07E-06	2.74E-05
48	1.04E-04	1.63E-04	2.34E-04	3.19E-04	1.49E-05	1.00E-06	8.46E-06	2.33E-05	1.57E-06	1.32E-05	3.35E-05	2.26E-06	1.90E-05	4.56E-05	3.07E-06	2.59E-05
49	1.05E-04	1.63E-04	2.35E-04	3.20E-04	1.49E-05	1.00E-06	8.00E-06	2.33E-05	1.57E-06	1.25E-05	3.35E-05	2.26E-06	1.80E-05	4.56E-05	3.07E-06	2.45E-05
50	1.05E-04	1.64E-04	2.36E-04	3.21E-04	1.49E-05	1.00E-06	7.57E-06	2.33E-05	1.57E-06	1.18E-05	3.35E-05	2.26E-06	1.70E-05	4.56E-05	3.07E-06	2.32E-05
51	1.05E-04	1.65E-04	2.37E-04	3.23E-04	1.49E-05	1.00E-06	7.16E-06	2.33E-05	1.57E-06	1.12E-05	3.35E-05	2.26E-06	1.61E-05	4.56E-05	3.07E-06	2.19E-05
52	1.06E-04	1.65E-04	2.38E-04	3.24E-04	1.49E-05	1.00E-06	6.77E-06	2.33E-05	1.57E-06	1.06E-05	3.35E-05	2.26E-06	1.52E-05	4.56E-05	3.07E-06	2.07E-05
53	1.06E-04	1.66E-04	2.39E-04	3.25E-04	1.49E-05	1.00E-06	6.41E-06	2.33E-05	1.57E-06	1.00E-05	3.35E-05	2.26E-06	1.44E-05	4.56E-05	3.07E-06	1.96E-05
54	1.06E-04	1.66E-04	2.40E-04	3.26E-04	1.49E-05	1.00E-06	6.06E-06	2.33E-05	1.57E-06	9.47E-06	3.35E-05	2.26E-06	1.36E-05	4.56E-05	3.07E-06	1.86E-05
55	1.07E-04	1.67E-04	2.40E-04	3.27E-04	1.49E-05	1.00E-06	5.73E-06	2.33E-05	1.57E-06	8.96E-06	3.35E-05	2.26E-06	1.29E-05	4.56E-05	3.07E-06	1.76E-05
56	1.07E-04	1.67E-04	2.41E-04	3.28E-04	1.49E-05	1.00E-06	5.43E-06	2.33E-05	1.57E-06	8.48E-06	3.35E-05	2.26E-06	1.22E-05	4.56E-05	3.07E-06	1.66E-05
57	1.07E-04	1.68E-04	2.42E-04	3.29E-04	1.49E-05	1.00E-06	5.13E-06	2.33E-05	1.57E-06	8.02E-06	3.35E-05	2.26E-06	1.15E-05	4.56E-05	3.07E-06	1.57E-05
58	1.08E-04	1.68E-04	2.42E-04	3.30E-04	1.49E-05	1.00E-06	4.86E-06	2.33E-05	1.57E-06	7.59E-06	3.35E-05	2.26E-06	1.09E-05	4.56E-05	3.07E-06	1.49E-05
59	1.08E-04	1.69E-04	2.43E-04	3.31E-04	1.49E-05	1.00E-06	4.59E-06	2.33E-05	1.57E-06	7.18E-06	3.35E-05	2.26E-06	1.03E-05	4.56E-05	3.07E-06	1.41E-05
60	1.08E-04	1.69E-04	2.43E-04	3.31E-04	1.49E-05	1.00E-06	4.34E-06	2.33E-05	1.57E-06	6.79E-06	3.35E-05	2.26E-06	9.78E-06	4.56E-05	3.07E-06	1.33E-05
61	1.08E-04	1.69E-04	2.44E-04	3.32E-04	1.49E-05	1.00E-06	4.11E-06	2.33E-05	1.57E-06	6.42E-06	3.35E-05	2.26E-06	9.25E-06	4.56E-05	3.07E-06	1.26E-05
62	1.09E-04	1.70E-04	2.44E-04	3.33E-04	1.49E-05	1.00E-06	3.89E-06	2.33E-05	1.57E-06	6.08E-06	3.35E-05	2.26E-06	8.75E-06	4.56E-05	3.07E-06	1.19E-05
63	1.09E-04	1.70E-04	2.45E-04	3.33E-04	1.49E-05	1.00E-06	3.68E-06	2.33E-05	1.57E-06	5.75E-06	3.35E-05	2.26E-06	8.28E-06	4.56E-05	3.07E-06	1.13E-05
64	1.09E-04	1.70E-04	2.45E-04	3.34E-04	1.49E-05	1.00E-06	3.48E-06	2.33E-05	1.57E-06	5.44E-06	3.35E-05	2.26E-06	7.83E-06	4.56E-05	3.07E-06	1.07E-05
65	1.09E-04	1.71E-04	2.46E-04	3.34E-04	1.49E-05	1.00E-06	3.29E-06	2.33E-05	1.57E-06	5.14E-06	3.35E-05	2.26E-06	7.41E-06	4.56E-05	3.07E-06	1.01E-05
66	1.09E-04	1.71E-04	2.46E-04	3.35E-04	1.49E-05	1.00E-06	3.11E-06	2.33E-05	1.57E-06	4.87E-06	3.35E-05	2.26E-06	7.01E-06	4.56E-05	3.07E-06	9.54E-06
67	1.10E-04	1.71E-04	2.47E-04	3.36E-04	1.49E-05	1.00E-06	2.95E-06	2.33E-05	1.57E-06	4.60E-06	3.35E-05	2.26E-06	6.63E-06	4.56E-05	3.07E-06	9.02E-06

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
68	1.10E-04	1.71E-04	2.47E-04	3.36E-04	1.49E-05	1.00E-06	2.79E-06	2.33E-05	1.57E-06	4.35E-06	3.35E-05	2.26E-06	6.27E-06	4.56E-05	3.07E-06	8.53E-06
69	1.10E-04	1.72E-04	2.47E-04	3.37E-04	1.49E-05	1.00E-06	2.64E-06	2.33E-05	1.57E-06	4.12E-06	3.35E-05	2.26E-06	5.93E-06	4.56E-05	3.07E-06	8.07E-06
70	1.10E-04	1.72E-04	2.48E-04	3.37E-04	1.49E-05	1.00E-06	2.49E-06	2.33E-05	1.57E-06	3.90E-06	3.35E-05	2.26E-06	5.61E-06	4.56E-05	3.07E-06	7.64E-06
71	1.10E-04	1.72E-04	2.48E-04	3.37E-04	1.49E-05	1.00E-06	2.36E-06	2.33E-05	1.57E-06	3.69E-06	3.35E-05	2.26E-06	5.31E-06	4.56E-05	3.07E-06	7.22E-06
72	1.10E-04	1.72E-04	2.48E-04	3.38E-04	1.49E-05	1.00E-06	2.23E-06	2.33E-05	1.57E-06	3.49E-06	3.35E-05	2.26E-06	5.02E-06	4.56E-05	3.07E-06	6.83E-06
73	1.10E-04	1.73E-04	2.48E-04	3.38E-04	1.49E-05	1.00E-06	2.11E-06	2.33E-05	1.57E-06	3.30E-06	3.35E-05	2.26E-06	4.75E-06	4.56E-05	3.07E-06	6.47E-06
74	1.11E-04	1.73E-04	2.49E-04	3.38E-04	1.49E-05	1.00E-06	2.00E-06	2.33E-05	1.57E-06	3.12E-06	3.35E-05	2.26E-06	4.49E-06	4.56E-05	3.07E-06	6.12E-06
75	1.11E-04	1.73E-04	2.49E-04	3.39E-04	1.49E-05	1.00E-06	1.89E-06	2.33E-05	1.57E-06	2.95E-06	3.35E-05	2.26E-06	4.25E-06	4.56E-05	3.07E-06	5.79E-06
76	1.11E-04	1.73E-04	2.49E-04	3.39E-04	1.49E-05	1.00E-06	1.79E-06	2.33E-05	1.57E-06	2.79E-06	3.35E-05	2.26E-06	4.02E-06	4.56E-05	3.07E-06	5.47E-06
77	1.11E-04	1.73E-04	2.49E-04	3.39E-04	1.49E-05	1.00E-06	1.69E-06	2.33E-05	1.57E-06	2.64E-06	3.35E-05	2.26E-06	3.80E-06	4.56E-05	3.07E-06	5.18E-06
78	1.11E-04	1.73E-04	2.50E-04	3.40E-04	1.49E-05	1.00E-06	1.60E-06	2.33E-05	1.57E-06	2.50E-06	3.35E-05	2.26E-06	3.60E-06	4.56E-05	3.07E-06	4.90E-06
79	1.11E-04	1.73E-04	2.50E-04	3.40E-04	1.49E-05	1.00E-06	1.51E-06	2.33E-05	1.57E-06	2.36E-06	3.35E-05	2.26E-06	3.40E-06	4.56E-05	3.07E-06	4.63E-06
80	1.11E-04	1.74E-04	2.50E-04	3.40E-04	1.49E-05	1.00E-06	1.43E-06	2.33E-05	1.57E-06	2.24E-06	3.35E-05	2.26E-06	3.22E-06	4.56E-05	3.07E-06	4.38E-06
81	1.11E-04	1.74E-04	2.50E-04	3.40E-04	1.49E-05	1.00E-06	1.35E-06	2.33E-05	1.57E-06	2.12E-06	3.35E-05	2.26E-06	3.05E-06	4.56E-05	3.07E-06	4.15E-06
82	1.11E-04	1.74E-04	2.50E-04	3.41E-04	1.49E-05	1.00E-06	1.28E-06	2.33E-05	1.57E-06	2.00E-06	3.35E-05	2.26E-06	2.88E-06	4.56E-05	3.07E-06	3.92E-06
83	1.11E-04	1.74E-04	2.50E-04	3.41E-04	1.49E-05	1.00E-06	1.21E-06	2.33E-05	1.57E-06	1.89E-06	3.35E-05	2.26E-06	2.73E-06	4.56E-05	3.07E-06	3.71E-06
84	1.11E-04	1.74E-04	2.51E-04	3.41E-04	1.49E-05	1.00E-06	1.15E-06	2.33E-05	1.57E-06	1.79E-06	3.35E-05	2.26E-06	2.58E-06	4.56E-05	3.07E-06	3.51E-06
85	1.11E-04	1.74E-04	2.51E-04	3.41E-04	1.49E-05	1.00E-06	1.08E-06	2.33E-05	1.57E-06	1.69E-06	3.35E-05	2.26E-06	2.44E-06	4.56E-05	3.07E-06	3.32E-06
86	1.11E-04	1.74E-04	2.51E-04	3.41E-04	1.49E-05	1.00E-06	1.03E-06	2.33E-05	1.57E-06	1.60E-06	3.35E-05	2.26E-06	2.31E-06	4.56E-05	3.07E-06	3.14E-06
87	1.12E-04	1.74E-04	2.51E-04	3.42E-04	1.49E-05	1.00E-06	9.70E-07	2.33E-05	1.57E-06	1.52E-06	3.35E-05	2.26E-06	2.18E-06	4.56E-05	3.07E-06	2.97E-06
88	1.12E-04	1.74E-04	2.51E-04	3.42E-04	1.49E-05	1.00E-06	9.18E-07	2.33E-05	1.57E-06	1.43E-06	3.35E-05	2.26E-06	2.07E-06	4.56E-05	3.07E-06	2.81E-06
89	1.12E-04	1.74E-04	2.51E-04	3.42E-04	1.49E-05	1.00E-06	8.68E-07	2.33E-05	1.57E-06	1.36E-06	3.35E-05	2.26E-06	1.95E-06	4.56E-05	3.07E-06	2.66E-06
90	1.12E-04	1.75E-04	2.51E-04	3.42E-04	1.49E-05	1.00E-06	8.21E-07	2.33E-05	1.57E-06	1.28E-06	3.35E-05	2.26E-06	1.85E-06	4.56E-05	3.07E-06	2.52E-06

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
91	1.12E-04	1.75E-04	2.51E-04	3.42E-04	1.49E-05	1.00E-06	7.77E-07	2.33E-05	1.57E-06	1.21E-06	3.35E-05	2.26E-06	1.75E-06	4.56E-05	3.07E-06	2.38E-06
92	1.12E-04	1.75E-04	2.52E-04	3.42E-04	1.49E-05	1.00E-06	7.35E-07	2.33E-05	1.57E-06	1.15E-06	3.35E-05	2.26E-06	1.65E-06	4.56E-05	3.07E-06	2.25E-06
93	1.12E-04	1.75E-04	2.52E-04	3.42E-04	1.49E-05	1.00E-06	6.95E-07	2.33E-05	1.57E-06	1.09E-06	3.35E-05	2.26E-06	1.56E-06	4.56E-05	3.07E-06	2.13E-06
94	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	6.58E-07	2.33E-05	1.57E-06	1.03E-06	3.35E-05	2.26E-06	1.48E-06	4.56E-05	3.07E-06	2.01E-06
95	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	6.22E-07	2.33E-05	1.57E-06	9.72E-07	3.35E-05	2.26E-06	1.40E-06	4.56E-05	3.07E-06	1.91E-06
96	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	5.89E-07	2.33E-05	1.57E-06	9.20E-07	3.35E-05	2.26E-06	1.32E-06	4.56E-05	3.07E-06	1.80E-06
97	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	5.57E-07	2.33E-05	1.57E-06	8.70E-07	3.35E-05	2.26E-06	1.25E-06	4.56E-05	3.07E-06	1.71E-06
98	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	5.27E-07	2.33E-05	1.57E-06	8.23E-07	3.35E-05	2.26E-06	1.19E-06	4.56E-05	3.07E-06	1.61E-06
99	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	4.98E-07	2.33E-05	1.57E-06	7.79E-07	3.35E-05	2.26E-06	1.12E-06	4.56E-05	3.07E-06	1.53E-06
100	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	4.71E-07	2.33E-05	1.57E-06	7.37E-07	3.35E-05	2.26E-06	1.06E-06	4.56E-05	3.07E-06	1.44E-06
101	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	4.46E-07	2.33E-05	1.57E-06	6.97E-07	3.35E-05	2.26E-06	1.00E-06	4.56E-05	3.07E-06	1.37E-06
102	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	4.22E-07	2.33E-05	1.57E-06	6.59E-07	3.35E-05	2.26E-06	9.49E-07	4.56E-05	3.07E-06	1.29E-06
103	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	3.99E-07	2.33E-05	1.57E-06	6.24E-07	3.35E-05	2.26E-06	8.98E-07	4.56E-05	3.07E-06	1.22E-06
104	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	3.78E-07	2.33E-05	1.57E-06	5.90E-07	3.35E-05	2.26E-06	8.50E-07	4.56E-05	3.07E-06	1.16E-06
105	1.12E-04	1.75E-04	2.52E-04	3.43E-04	1.49E-05	1.00E-06	3.57E-07	2.33E-05	1.57E-06	5.58E-07	3.35E-05	2.26E-06	8.04E-07	4.56E-05	3.07E-06	1.09E-06
106	1.12E-04	1.75E-04	2.52E-04	3.44E-04	1.49E-05	1.00E-06	3.38E-07	2.33E-05	1.57E-06	5.28E-07	3.35E-05	2.26E-06	7.60E-07	4.56E-05	3.07E-06	1.03E-06
107	1.12E-04	1.75E-04	2.52E-04	3.44E-04	1.49E-05	1.00E-06	3.20E-07	2.33E-05	1.57E-06	4.99E-07	3.35E-05	2.26E-06	7.19E-07	4.56E-05	3.07E-06	9.79E-07
108	1.12E-04	1.75E-04	2.52E-04	3.44E-04	1.49E-05	1.00E-06	3.02E-07	2.33E-05	1.57E-06	4.72E-07	3.35E-05	2.26E-06	6.80E-07	4.56E-05	3.07E-06	9.26E-07
109	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.86E-07	2.33E-05	1.57E-06	4.47E-07	3.35E-05	2.26E-06	6.44E-07	4.56E-05	3.07E-06	8.76E-07
110	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.71E-07	2.33E-05	1.57E-06	4.23E-07	3.35E-05	2.26E-06	6.09E-07	4.56E-05	3.07E-06	8.29E-07
111	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.56E-07	2.33E-05	1.57E-06	4.00E-07	3.35E-05	2.26E-06	5.76E-07	4.56E-05	3.07E-06	7.84E-07
112	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.42E-07	2.33E-05	1.57E-06	3.78E-07	3.35E-05	2.26E-06	5.45E-07	4.56E-05	3.07E-06	7.42E-07
113	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.29E-07	2.33E-05	1.57E-06	3.58E-07	3.35E-05	2.26E-06	5.15E-07	4.56E-05	3.07E-06	7.02E-07

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
114	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.17E-07	2.33E-05	1.57E-06	3.39E-07	3.35E-05	2.26E-06	4.88E-07	4.56E-05	3.07E-06	6.64E-07
115	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.05E-07	2.33E-05	1.57E-06	3.20E-07	3.35E-05	2.26E-06	4.61E-07	4.56E-05	3.07E-06	6.28E-07
116	1.12E-04	1.75E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.94E-07	2.33E-05	1.57E-06	3.03E-07	3.35E-05	2.26E-06	4.36E-07	4.56E-05	3.07E-06	5.94E-07
117	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.83E-07	2.33E-05	1.57E-06	2.87E-07	3.35E-05	2.26E-06	4.13E-07	4.56E-05	3.07E-06	5.62E-07
118	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.74E-07	2.33E-05	1.57E-06	2.71E-07	3.35E-05	2.26E-06	3.91E-07	4.56E-05	3.07E-06	5.32E-07
119	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.64E-07	2.33E-05	1.57E-06	2.57E-07	3.35E-05	2.26E-06	3.69E-07	4.56E-05	3.07E-06	5.03E-07
120	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.55E-07	2.33E-05	1.57E-06	2.43E-07	3.35E-05	2.26E-06	3.49E-07	4.56E-05	3.07E-06	4.76E-07
121	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.47E-07	2.33E-05	1.57E-06	2.30E-07	3.35E-05	2.26E-06	3.31E-07	4.56E-05	3.07E-06	4.50E-07
122	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.39E-07	2.33E-05	1.57E-06	2.17E-07	3.35E-05	2.26E-06	3.13E-07	4.56E-05	3.07E-06	4.26E-07
123	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.31E-07	2.33E-05	1.57E-06	2.05E-07	3.35E-05	2.26E-06	2.96E-07	4.56E-05	3.07E-06	4.03E-07
124	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.24E-07	2.33E-05	1.57E-06	1.94E-07	3.35E-05	2.26E-06	2.80E-07	4.56E-05	3.07E-06	3.81E-07
125	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.18E-07	2.33E-05	1.57E-06	1.84E-07	3.35E-05	2.26E-06	2.65E-07	4.56E-05	3.07E-06	3.60E-07
126	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.11E-07	2.33E-05	1.57E-06	1.74E-07	3.35E-05	2.26E-06	2.50E-07	4.56E-05	3.07E-06	3.41E-07
127	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	1.05E-07	2.33E-05	1.57E-06	1.65E-07	3.35E-05	2.26E-06	2.37E-07	4.56E-05	3.07E-06	3.22E-07
128	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	9.96E-08	2.33E-05	1.57E-06	1.56E-07	3.35E-05	2.26E-06	2.24E-07	4.56E-05	3.07E-06	3.05E-07
129	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	9.42E-08	2.33E-05	1.57E-06	1.47E-07	3.35E-05	2.26E-06	2.12E-07	4.56E-05	3.07E-06	2.89E-07
130	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	8.91E-08	2.33E-05	1.57E-06	1.39E-07	3.35E-05	2.26E-06	2.01E-07	4.56E-05	3.07E-06	2.73E-07
131	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	8.43E-08	2.33E-05	1.57E-06	1.32E-07	3.35E-05	2.26E-06	1.90E-07	4.56E-05	3.07E-06	2.58E-07
132	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	7.98E-08	2.33E-05	1.57E-06	1.25E-07	3.35E-05	2.26E-06	1.79E-07	4.56E-05	3.07E-06	2.44E-07
133	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	7.55E-08	2.33E-05	1.57E-06	1.18E-07	3.35E-05	2.26E-06	1.70E-07	4.56E-05	3.07E-06	2.31E-07
134	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	7.14E-08	2.33E-05	1.57E-06	1.12E-07	3.35E-05	2.26E-06	1.61E-07	4.56E-05	3.07E-06	2.19E-07
135	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	6.75E-08	2.33E-05	1.57E-06	1.06E-07	3.35E-05	2.26E-06	1.52E-07	4.56E-05	3.07E-06	2.07E-07
136	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	6.39E-08	2.33E-05	1.57E-06	9.98E-08	3.35E-05	2.26E-06	1.44E-07	4.56E-05	3.07E-06	1.96E-07

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
137	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	6.04E-08	2.33E-05	1.57E-06	9.44E-08	3.35E-05	2.26E-06	1.36E-07	4.56E-05	3.07E-06	1.85E-07
138	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	5.72E-08	2.33E-05	1.57E-06	8.93E-08	3.35E-05	2.26E-06	1.29E-07	4.56E-05	3.07E-06	1.75E-07
139	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	5.41E-08	2.33E-05	1.57E-06	8.45E-08	3.35E-05	2.26E-06	1.22E-07	4.56E-05	3.07E-06	1.66E-07
140	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	5.12E-08	2.33E-05	1.57E-06	7.99E-08	3.35E-05	2.26E-06	1.15E-07	4.56E-05	3.07E-06	1.57E-07
141	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	4.84E-08	2.33E-05	1.57E-06	7.56E-08	3.35E-05	2.26E-06	1.09E-07	4.56E-05	3.07E-06	1.48E-07
142	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	4.58E-08	2.33E-05	1.57E-06	7.15E-08	3.35E-05	2.26E-06	1.03E-07	4.56E-05	3.07E-06	1.40E-07
143	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	4.33E-08	2.33E-05	1.57E-06	6.77E-08	3.35E-05	2.26E-06	9.75E-08	4.56E-05	3.07E-06	1.33E-07
144	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	4.10E-08	2.33E-05	1.57E-06	6.40E-08	3.35E-05	2.26E-06	9.22E-08	4.56E-05	3.07E-06	1.25E-07
145	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	3.88E-08	2.33E-05	1.57E-06	6.06E-08	3.35E-05	2.26E-06	8.72E-08	4.56E-05	3.07E-06	1.19E-07
146	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	3.67E-08	2.33E-05	1.57E-06	5.73E-08	3.35E-05	2.26E-06	8.25E-08	4.56E-05	3.07E-06	1.12E-07
147	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	3.47E-08	2.33E-05	1.57E-06	5.42E-08	3.35E-05	2.26E-06	7.80E-08	4.56E-05	3.07E-06	1.06E-07
148	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	3.28E-08	2.33E-05	1.57E-06	5.13E-08	3.35E-05	2.26E-06	7.38E-08	4.56E-05	3.07E-06	1.00E-07
149	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	3.10E-08	2.33E-05	1.57E-06	4.85E-08	3.35E-05	2.26E-06	6.98E-08	4.56E-05	3.07E-06	9.51E-08
150	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.94E-08	2.33E-05	1.57E-06	4.59E-08	3.35E-05	2.26E-06	6.61E-08	4.56E-05	3.07E-06	8.99E-08
151	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.78E-08	2.33E-05	1.57E-06	4.34E-08	3.35E-05	2.26E-06	6.25E-08	4.56E-05	3.07E-06	8.51E-08
152	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.63E-08	2.33E-05	1.57E-06	4.11E-08	3.35E-05	2.26E-06	5.91E-08	4.56E-05	3.07E-06	8.05E-08
153	1.12E-04	1.76E-04	2.53E-04	3.44E-04	1.49E-05	1.00E-06	2.49E-08	2.33E-05	1.57E-06	3.88E-08	3.35E-05	2.26E-06	5.59E-08	4.56E-05	3.07E-06	7.61E-08
154	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.35E-08	2.33E-05	1.57E-06	3.67E-08	3.35E-05	2.26E-06	5.29E-08	4.56E-05	3.07E-06	7.20E-08
155	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.22E-08	2.33E-05	1.57E-06	3.48E-08	3.35E-05	2.26E-06	5.01E-08	4.56E-05	3.07E-06	6.81E-08
156	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.10E-08	2.33E-05	1.57E-06	3.29E-08	3.35E-05	2.26E-06	4.74E-08	4.56E-05	3.07E-06	6.45E-08
157	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.99E-08	2.33E-05	1.57E-06	3.11E-08	3.35E-05	2.26E-06	4.48E-08	4.56E-05	3.07E-06	6.10E-08
158	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.88E-08	2.33E-05	1.57E-06	2.94E-08	3.35E-05	2.26E-06	4.24E-08	4.56E-05	3.07E-06	5.77E-08
159	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.78E-08	2.33E-05	1.57E-06	2.78E-08	3.35E-05	2.26E-06	4.01E-08	4.56E-05	3.07E-06	5.46E-08

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
160	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.69E-08	2.33E-05	1.57E-06	2.63E-08	3.35E-05	2.26E-06	3.79E-08	4.56E-05	3.07E-06	5.16E-08
161	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.59E-08	2.33E-05	1.57E-06	2.49E-08	3.35E-05	2.26E-06	3.59E-08	4.56E-05	3.07E-06	4.88E-08
162	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.51E-08	2.33E-05	1.57E-06	2.36E-08	3.35E-05	2.26E-06	3.39E-08	4.56E-05	3.07E-06	4.62E-08
163	1.12E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.43E-08	2.33E-05	1.57E-06	2.23E-08	3.35E-05	2.26E-06	3.21E-08	4.56E-05	3.07E-06	4.37E-08
164	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.35E-08	2.33E-05	1.57E-06	2.11E-08	3.35E-05	2.26E-06	3.04E-08	4.56E-05	3.07E-06	4.13E-08
165	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.28E-08	2.33E-05	1.57E-06	2.00E-08	3.35E-05	2.26E-06	2.87E-08	4.56E-05	3.07E-06	3.91E-08
166	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.21E-08	2.33E-05	1.57E-06	1.89E-08	3.35E-05	2.26E-06	2.72E-08	4.56E-05	3.07E-06	3.70E-08
167	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.14E-08	2.33E-05	1.57E-06	1.79E-08	3.35E-05	2.26E-06	2.57E-08	4.56E-05	3.07E-06	3.50E-08
168	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.08E-08	2.33E-05	1.57E-06	1.69E-08	3.35E-05	2.26E-06	2.43E-08	4.56E-05	3.07E-06	3.31E-08
169	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.02E-08	2.33E-05	1.57E-06	1.60E-08	3.35E-05	2.26E-06	2.30E-08	4.56E-05	3.07E-06	3.13E-08
170	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	9.67E-09	2.33E-05	1.57E-06	1.51E-08	3.35E-05	2.26E-06	2.18E-08	4.56E-05	3.07E-06	2.96E-08
171	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	9.15E-09	2.33E-05	1.57E-06	1.43E-08	3.35E-05	2.26E-06	2.06E-08	4.56E-05	3.07E-06	2.80E-08
172	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	8.66E-09	2.33E-05	1.57E-06	1.35E-08	3.35E-05	2.26E-06	1.95E-08	4.56E-05	3.07E-06	2.65E-08
173	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	8.19E-09	2.33E-05	1.57E-06	1.28E-08	3.35E-05	2.26E-06	1.84E-08	4.56E-05	3.07E-06	2.51E-08
174	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	7.75E-09	2.33E-05	1.57E-06	1.21E-08	3.35E-05	2.26E-06	1.74E-08	4.56E-05	3.07E-06	2.37E-08
175	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	7.33E-09	2.33E-05	1.57E-06	1.15E-08	3.35E-05	2.26E-06	1.65E-08	4.56E-05	3.07E-06	2.24E-08
176	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	6.93E-09	2.33E-05	1.57E-06	1.08E-08	3.35E-05	2.26E-06	1.56E-08	4.56E-05	3.07E-06	2.12E-08
177	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	6.56E-09	2.33E-05	1.57E-06	1.02E-08	3.35E-05	2.26E-06	1.48E-08	4.56E-05	3.07E-06	2.01E-08
178	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	6.20E-09	2.33E-05	1.57E-06	9.69E-09	3.35E-05	2.26E-06	1.40E-08	4.56E-05	3.07E-06	1.90E-08
179	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	5.87E-09	2.33E-05	1.57E-06	9.17E-09	3.35E-05	2.26E-06	1.32E-08	4.56E-05	3.07E-06	1.80E-08
180	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	5.55E-09	2.33E-05	1.57E-06	8.68E-09	3.35E-05	2.26E-06	1.25E-08	4.56E-05	3.07E-06	1.70E-08
181	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	5.25E-09	2.33E-05	1.57E-06	8.21E-09	3.35E-05	2.26E-06	1.18E-08	4.56E-05	3.07E-06	1.61E-08
182	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	4.97E-09	2.33E-05	1.57E-06	7.76E-09	3.35E-05	2.26E-06	1.12E-08	4.56E-05	3.07E-06	1.52E-08

Table S16. Cont.

TIME (days)	cFA08:1	cFA10:1	cFA12:1	cFA14:1	cGA08:1	cA08:1	cF08:1	cGA10:1	cA10:1	cF10:1	cGA12:1	cA12:1	cF12:1	cGA14:1	cA14:1	cF14:1
183	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	4.70E-09	2.33E-05	1.57E-06	7.34E-09	3.35E-05	2.26E-06	1.06E-08	4.56E-05	3.07E-06	1.44E-08
184	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	4.45E-09	2.33E-05	1.57E-06	6.95E-09	3.35E-05	2.26E-06	1.00E-08	4.56E-05	3.07E-06	1.36E-08
185	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	4.21E-09	2.33E-05	1.57E-06	6.57E-09	3.35E-05	2.26E-06	9.46E-09	4.56E-05	3.07E-06	1.29E-08
186	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	3.98E-09	2.33E-05	1.57E-06	6.22E-09	3.35E-05	2.26E-06	8.95E-09	4.56E-05	3.07E-06	1.22E-08
187	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	3.76E-09	2.33E-05	1.57E-06	5.88E-09	3.35E-05	2.26E-06	8.47E-09	4.56E-05	3.07E-06	1.15E-08
188	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	3.56E-09	2.33E-05	1.57E-06	5.56E-09	3.35E-05	2.26E-06	8.01E-09	4.56E-05	3.07E-06	1.09E-08
189	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	3.37E-09	2.33E-05	1.57E-06	5.26E-09	3.35E-05	2.26E-06	7.58E-09	4.56E-05	3.07E-06	1.03E-08
190	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	3.19E-09	2.33E-05	1.57E-06	4.98E-09	3.35E-05	2.26E-06	7.17E-09	4.56E-05	3.07E-06	9.76E-09
191	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	3.01E-09	2.33E-05	1.57E-06	4.71E-09	3.35E-05	2.26E-06	6.78E-09	4.56E-05	3.07E-06	9.23E-09
192	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.85E-09	2.33E-05	1.57E-06	4.46E-09	3.35E-05	2.26E-06	6.42E-09	4.56E-05	3.07E-06	8.73E-09
193	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.70E-09	2.33E-05	1.57E-06	4.22E-09	3.35E-05	2.26E-06	6.07E-09	4.56E-05	3.07E-06	8.26E-09
194	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.55E-09	2.33E-05	1.57E-06	3.99E-09	3.35E-05	2.26E-06	5.74E-09	4.56E-05	3.07E-06	7.82E-09
195	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.41E-09	2.33E-05	1.57E-06	3.77E-09	3.35E-05	2.26E-06	5.43E-09	4.56E-05	3.07E-06	7.39E-09
196	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.28E-09	2.33E-05	1.57E-06	3.57E-09	3.35E-05	2.26E-06	5.14E-09	4.56E-05	3.07E-06	6.99E-09
197	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.16E-09	2.33E-05	1.57E-06	3.38E-09	3.35E-05	2.26E-06	4.86E-09	4.56E-05	3.07E-06	6.62E-09
198	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	2.04E-09	2.33E-05	1.57E-06	3.19E-09	3.35E-05	2.26E-06	4.60E-09	4.56E-05	3.07E-06	6.26E-09
199	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.93E-09	2.33E-05	1.57E-06	3.02E-09	3.35E-05	2.26E-06	4.35E-09	4.56E-05	3.07E-06	5.92E-09
200	1.13E-04	1.76E-04	2.53E-04	3.45E-04	1.49E-05	1.00E-06	1.83E-09	2.33E-05	1.57E-06	2.86E-09	3.35E-05	2.26E-06	4.12E-09	4.56E-05	3.07E-06	5.60E-09

Table S17. Modelled data for saxagliptin degradation products (values in mol/g_{saxa}).

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
0	0.00317	0	0	0	0.00317	0	0	0	0.00317	0	0	0	0.00317	0	0	0
1	0.00317	5.26E-07	6.37E-09	1.20E-09	0.00317	5.26E-07	6.37E-09	1.87E-09	0.00317	5.26E-07	6.36E-09	2.70E-09	0.00317	5.25E-07	6.35E-09	3.67E-09
2	0.003169	1.04E-06	2.53E-08	7.99E-09	0.003169	1.04E-06	2.52E-08	1.25E-08	0.003169	1.04E-06	2.51E-08	1.81E-08	0.003169	1.03E-06	2.50E-08	2.47E-08
3	0.003169	1.54E-06	5.64E-08	2.29E-08	0.003169	1.54E-06	5.61E-08	3.59E-08	0.003169	1.53E-06	5.57E-08	5.20E-08	0.003169	1.52E-06	5.52E-08	7.13E-08
4	0.003168	2.03E-06	9.95E-08	4.65E-08	0.003168	2.02E-06	9.86E-08	7.32E-08	0.003168	2.01E-06	9.75E-08	1.06E-07	0.003168	2.00E-06	9.62E-08	1.46E-07
5	0.003168	2.51E-06	1.54E-07	7.89E-08	0.003168	2.49E-06	1.52E-07	1.25E-07	0.003168	2.47E-06	1.50E-07	1.82E-07	0.003168	2.45E-06	1.47E-07	2.51E-07
6	0.003167	2.97E-06	2.20E-07	1.20E-07	0.003167	2.95E-06	2.17E-07	1.89E-07	0.003167	2.92E-06	2.13E-07	2.77E-07	0.003167	2.89E-06	2.08E-07	3.84E-07
7	0.003167	3.43E-06	2.98E-07	1.68E-07	0.003167	3.40E-06	2.92E-07	2.67E-07	0.003166	3.36E-06	2.85E-07	3.91E-07	0.003166	3.32E-06	2.77E-07	5.44E-07
8	0.003166	3.87E-06	3.86E-07	2.24E-07	0.003166	3.83E-06	3.77E-07	3.56E-07	0.003166	3.78E-06	3.67E-07	5.23E-07	0.003166	3.72E-06	3.55E-07	7.31E-07
9	0.003165	4.30E-06	4.84E-07	2.86E-07	0.003165	4.25E-06	4.72E-07	4.56E-07	0.003165	4.19E-06	4.57E-07	6.72E-07	0.003165	4.12E-06	4.41E-07	9.41E-07
10	0.003165	4.73E-06	5.93E-07	3.54E-07	0.003165	4.66E-06	5.76E-07	5.65E-07	0.003164	4.59E-06	5.56E-07	8.36E-07	0.003164	4.50E-06	5.34E-07	1.18E-06
11	0.003164	5.14E-06	7.12E-07	4.28E-07	0.003164	5.07E-06	6.90E-07	6.84E-07	0.003164	4.98E-06	6.64E-07	1.02E-06	0.003164	4.87E-06	6.34E-07	1.43E-06
12	0.003164	5.54E-06	8.41E-07	5.06E-07	0.003163	5.46E-06	8.12E-07	8.12E-07	0.003163	5.35E-06	7.79E-07	1.21E-06	0.003163	5.23E-06	7.41E-07	1.71E-06
13	0.003163	5.94E-06	9.80E-07	5.89E-07	0.003163	5.84E-06	9.43E-07	9.46E-07	0.003162	5.72E-06	9.01E-07	1.41E-06	0.003162	5.58E-06	8.54E-07	2.00E-06
14	0.003162	6.32E-06	1.13E-06	6.76E-07	0.003162	6.21E-06	1.08E-06	1.09E-06	0.003162	6.07E-06	1.03E-06	1.63E-06	0.003161	5.92E-06	9.74E-07	2.31E-06
15	0.003162	6.69E-06	1.28E-06	7.66E-07	0.003161	6.57E-06	1.23E-06	1.24E-06	0.003161	6.42E-06	1.17E-06	1.85E-06	0.00316	6.25E-06	1.10E-06	2.64E-06
16	0.003161	7.06E-06	1.45E-06	8.59E-07	0.003161	6.92E-06	1.39E-06	1.39E-06	0.00316	6.76E-06	1.31E-06	2.08E-06	0.00316	6.57E-06	1.23E-06	2.98E-06
17	0.00316	7.41E-06	1.62E-06	9.56E-07	0.00316	7.26E-06	1.55E-06	1.55E-06	0.00316	7.08E-06	1.46E-06	2.33E-06	0.003159	6.88E-06	1.37E-06	3.33E-06
18	0.00316	7.76E-06	1.81E-06	1.05E-06	0.003159	7.60E-06	1.72E-06	1.71E-06	0.003159	7.40E-06	1.62E-06	2.57E-06	0.003158	7.18E-06	1.51E-06	3.70E-06
19	0.003159	8.10E-06	2.00E-06	1.15E-06	0.003159	7.92E-06	1.90E-06	1.88E-06	0.003158	7.71E-06	1.78E-06	2.83E-06	0.003157	7.47E-06	1.65E-06	4.07E-06
20	0.003159	8.43E-06	2.20E-06	1.26E-06	0.003158	8.24E-06	2.08E-06	2.04E-06	0.003157	8.02E-06	1.95E-06	3.09E-06	0.003156	7.76E-06	1.81E-06	4.46E-06
21	0.003158	8.76E-06	2.41E-06	1.36E-06	0.003157	8.55E-06	2.27E-06	2.22E-06	0.003157	8.31E-06	2.12E-06	3.36E-06	0.003155	8.04E-06	1.96E-06	4.85E-06

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
22	0.003157	9.07E-06	2.62E-06	1.47E-06	0.003157	8.86E-06	2.47E-06	2.39E-06	0.003156	8.60E-06	2.31E-06	3.63E-06	0.003155	8.31E-06	2.12E-06	5.26E-06
23	0.003157	9.38E-06	2.84E-06	1.57E-06	0.003156	9.15E-06	2.68E-06	2.57E-06	0.003155	8.88E-06	2.49E-06	3.90E-06	0.003154	8.57E-06	2.29E-06	5.66E-06
24	0.003156	9.68E-06	3.07E-06	1.68E-06	0.003155	9.44E-06	2.89E-06	2.75E-06	0.003154	9.15E-06	2.68E-06	4.18E-06	0.003153	8.83E-06	2.46E-06	6.08E-06
25	0.003155	9.97E-06	3.31E-06	1.79E-06	0.003155	9.72E-06	3.11E-06	2.93E-06	0.003154	9.42E-06	2.88E-06	4.46E-06	0.003152	9.08E-06	2.63E-06	6.50E-06
26	0.003155	1.03E-05	3.55E-06	1.89E-06	0.003154	1.00E-05	3.33E-06	3.11E-06	0.003153	9.68E-06	3.08E-06	4.74E-06	0.003151	9.33E-06	2.81E-06	6.92E-06
27	0.003154	1.05E-05	3.81E-06	2.00E-06	0.003153	1.03E-05	3.56E-06	3.29E-06	0.003152	9.94E-06	3.28E-06	5.02E-06	0.00315	9.57E-06	2.99E-06	7.34E-06
28	0.003153	1.08E-05	4.06E-06	2.11E-06	0.003153	1.05E-05	3.80E-06	3.47E-06	0.003151	1.02E-05	3.50E-06	5.31E-06	0.003149	9.80E-06	3.17E-06	7.77E-06
29	0.003153	1.11E-05	4.33E-06	2.22E-06	0.003152	1.08E-05	4.04E-06	3.65E-06	0.003151	1.04E-05	3.71E-06	5.59E-06	0.003148	1.00E-05	3.36E-06	8.20E-06
30	0.003152	1.13E-05	4.60E-06	2.33E-06	0.003151	1.10E-05	4.28E-06	3.83E-06	0.00315	1.07E-05	3.93E-06	5.88E-06	0.003148	1.03E-05	3.55E-06	8.63E-06
31	0.003152	1.16E-05	4.87E-06	2.43E-06	0.003151	1.13E-05	4.53E-06	4.01E-06	0.003149	1.09E-05	4.15E-06	6.16E-06	0.003147	1.05E-05	3.75E-06	9.06E-06
32	0.003151	1.18E-05	5.16E-06	2.54E-06	0.00315	1.15E-05	4.79E-06	4.19E-06	0.003148	1.11E-05	4.38E-06	6.45E-06	0.003146	1.07E-05	3.95E-06	9.49E-06
33	0.00315	1.21E-05	5.44E-06	2.65E-06	0.003149	1.17E-05	5.05E-06	4.37E-06	0.003148	1.13E-05	4.62E-06	6.73E-06	0.003145	1.09E-05	4.15E-06	9.92E-06
34	0.00315	1.23E-05	5.74E-06	2.75E-06	0.003149	1.20E-05	5.32E-06	4.55E-06	0.003147	1.16E-05	4.85E-06	7.01E-06	0.003144	1.11E-05	4.36E-06	1.03E-05
35	0.003149	1.25E-05	6.04E-06	2.86E-06	0.003148	1.22E-05	5.59E-06	4.72E-06	0.003146	1.18E-05	5.09E-06	7.29E-06	0.003143	1.13E-05	4.57E-06	1.08E-05
36	0.003148	1.28E-05	6.34E-06	2.96E-06	0.003147	1.24E-05	5.87E-06	4.90E-06	0.003145	1.20E-05	5.34E-06	7.57E-06	0.003142	1.15E-05	4.78E-06	1.12E-05
37	0.003148	1.30E-05	6.65E-06	3.06E-06	0.003147	1.26E-05	6.15E-06	5.07E-06	0.003144	1.22E-05	5.59E-06	7.85E-06	0.003141	1.17E-05	4.99E-06	1.16E-05
38	0.003147	1.32E-05	6.97E-06	3.17E-06	0.003146	1.28E-05	6.44E-06	5.25E-06	0.003144	1.24E-05	5.84E-06	8.12E-06	0.00314	1.19E-05	5.21E-06	1.20E-05
39	0.003147	1.34E-05	7.29E-06	3.27E-06	0.003145	1.30E-05	6.73E-06	5.42E-06	0.003143	1.26E-05	6.10E-06	8.39E-06	0.00314	1.21E-05	5.43E-06	1.25E-05
40	0.003146	1.36E-05	7.62E-06	3.37E-06	0.003145	1.32E-05	7.02E-06	5.59E-06	0.003142	1.28E-05	6.36E-06	8.66E-06	0.003139	1.22E-05	5.66E-06	1.29E-05
41	0.003145	1.38E-05	7.95E-06	3.46E-06	0.003144	1.34E-05	7.32E-06	5.75E-06	0.003141	1.29E-05	6.62E-06	8.93E-06	0.003138	1.24E-05	5.88E-06	1.33E-05
42	0.003145	1.40E-05	8.28E-06	3.56E-06	0.003143	1.36E-05	7.62E-06	5.92E-06	0.003141	1.31E-05	6.89E-06	9.19E-06	0.003137	1.26E-05	6.11E-06	1.37E-05
43	0.003144	1.42E-05	8.62E-06	3.66E-06	0.003143	1.38E-05	7.93E-06	6.08E-06	0.00314	1.33E-05	7.16E-06	9.45E-06	0.003136	1.27E-05	6.35E-06	1.41E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
44	0.003143	1.44E-05	8.97E-06	3.75E-06	0.003142	1.40E-05	8.24E-06	6.24E-06	0.003139	1.35E-05	7.43E-06	9.71E-06	0.003135	1.29E-05	6.58E-06	1.45E-05
45	0.003143	1.45E-05	9.31E-06	3.84E-06	0.003141	1.41E-05	8.55E-06	6.40E-06	0.003139	1.36E-05	7.71E-06	9.96E-06	0.003134	1.31E-05	6.82E-06	1.49E-05
46	0.003142	1.47E-05	9.67E-06	3.94E-06	0.003141	1.43E-05	8.87E-06	6.56E-06	0.003138	1.38E-05	7.99E-06	1.02E-05	0.003133	1.32E-05	7.06E-06	1.53E-05
47	0.003142	1.49E-05	1.00E-05	4.03E-06	0.00314	1.45E-05	9.19E-06	6.71E-06	0.003137	1.40E-05	8.27E-06	1.05E-05	0.003132	1.34E-05	7.30E-06	1.56E-05
48	0.003141	1.51E-05	1.04E-05	4.12E-06	0.003139	1.46E-05	9.52E-06	6.86E-06	0.003136	1.41E-05	8.56E-06	1.07E-05	0.003132	1.35E-05	7.55E-06	1.60E-05
49	0.00314	1.52E-05	1.08E-05	4.20E-06	0.003139	1.48E-05	9.85E-06	7.01E-06	0.003136	1.43E-05	8.84E-06	1.09E-05	0.003131	1.37E-05	7.79E-06	1.64E-05
50	0.00314	1.54E-05	1.11E-05	4.29E-06	0.003138	1.50E-05	1.02E-05	7.16E-06	0.003135	1.44E-05	9.14E-06	1.12E-05	0.00313	1.38E-05	8.04E-06	1.67E-05
51	0.003139	1.55E-05	1.15E-05	4.37E-06	0.003137	1.51E-05	1.05E-05	7.31E-06	0.003134	1.46E-05	9.43E-06	1.14E-05	0.003129	1.40E-05	8.30E-06	1.71E-05
52	0.003138	1.57E-05	1.19E-05	4.46E-06	0.003137	1.53E-05	1.09E-05	7.45E-06	0.003133	1.47E-05	9.73E-06	1.16E-05	0.003128	1.41E-05	8.55E-06	1.75E-05
53	0.003138	1.58E-05	1.23E-05	4.54E-06	0.003136	1.54E-05	1.12E-05	7.59E-06	0.003133	1.49E-05	1.00E-05	1.19E-05	0.003127	1.43E-05	8.81E-06	1.78E-05
54	0.003137	1.60E-05	1.26E-05	4.62E-06	0.003135	1.55E-05	1.15E-05	7.73E-06	0.003132	1.50E-05	1.03E-05	1.21E-05	0.003126	1.44E-05	9.07E-06	1.82E-05
55	0.003137	1.61E-05	1.30E-05	4.70E-06	0.003135	1.57E-05	1.19E-05	7.86E-06	0.003131	1.52E-05	1.06E-05	1.23E-05	0.003126	1.45E-05	9.33E-06	1.85E-05
56	0.003136	1.63E-05	1.34E-05	4.78E-06	0.003134	1.58E-05	1.22E-05	7.99E-06	0.003131	1.53E-05	1.09E-05	1.25E-05	0.003125	1.47E-05	9.59E-06	1.88E-05
57	0.003135	1.64E-05	1.38E-05	4.85E-06	0.003133	1.60E-05	1.26E-05	8.12E-06	0.00313	1.54E-05	1.13E-05	1.27E-05	0.003124	1.48E-05	9.86E-06	1.92E-05
58	0.003135	1.65E-05	1.42E-05	4.93E-06	0.003133	1.61E-05	1.29E-05	8.25E-06	0.003129	1.55E-05	1.16E-05	1.29E-05	0.003123	1.49E-05	1.01E-05	1.95E-05
59	0.003134	1.66E-05	1.46E-05	5.00E-06	0.003132	1.62E-05	1.33E-05	8.38E-06	0.003128	1.57E-05	1.19E-05	1.31E-05	0.003122	1.50E-05	1.04E-05	1.98E-05
60	0.003134	1.68E-05	1.50E-05	5.07E-06	0.003132	1.63E-05	1.37E-05	8.50E-06	0.003128	1.58E-05	1.22E-05	1.33E-05	0.003121	1.51E-05	1.07E-05	2.01E-05
61	0.003133	1.69E-05	1.54E-05	5.14E-06	0.003131	1.65E-05	1.40E-05	8.62E-06	0.003127	1.59E-05	1.25E-05	1.35E-05	0.003121	1.53E-05	1.09E-05	2.04E-05
62	0.003132	1.70E-05	1.58E-05	5.21E-06	0.00313	1.66E-05	1.44E-05	8.74E-06	0.003126	1.60E-05	1.28E-05	1.37E-05	0.00312	1.54E-05	1.12E-05	2.07E-05
63	0.003132	1.71E-05	1.62E-05	5.28E-06	0.00313	1.67E-05	1.48E-05	8.86E-06	0.003126	1.61E-05	1.32E-05	1.39E-05	0.003119	1.55E-05	1.15E-05	2.10E-05
64	0.003131	1.72E-05	1.66E-05	5.34E-06	0.003129	1.68E-05	1.51E-05	8.97E-06	0.003125	1.63E-05	1.35E-05	1.41E-05	0.003118	1.56E-05	1.18E-05	2.13E-05
65	0.003131	1.73E-05	1.71E-05	5.41E-06	0.003128	1.69E-05	1.55E-05	9.08E-06	0.003124	1.64E-05	1.38E-05	1.43E-05	0.003117	1.57E-05	1.21E-05	2.16E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
66	0.00313	1.74E-05	1.75E-05	5.47E-06	0.003128	1.70E-05	1.59E-05	9.19E-06	0.003124	1.65E-05	1.42E-05	1.45E-05	0.003117	1.58E-05	1.23E-05	2.18E-05
67	0.003129	1.75E-05	1.79E-05	5.54E-06	0.003127	1.71E-05	1.63E-05	9.30E-06	0.003123	1.66E-05	1.45E-05	1.46E-05	0.003116	1.59E-05	1.26E-05	2.21E-05
68	0.003129	1.76E-05	1.83E-05	5.60E-06	0.003127	1.72E-05	1.67E-05	9.41E-06	0.003122	1.67E-05	1.48E-05	1.48E-05	0.003115	1.60E-05	1.29E-05	2.24E-05
69	0.003128	1.77E-05	1.88E-05	5.66E-06	0.003126	1.73E-05	1.70E-05	9.51E-06	0.003122	1.68E-05	1.52E-05	1.50E-05	0.003114	1.61E-05	1.32E-05	2.26E-05
70	0.003128	1.78E-05	1.92E-05	5.71E-06	0.003125	1.74E-05	1.74E-05	9.61E-06	0.003121	1.69E-05	1.55E-05	1.51E-05	0.003113	1.62E-05	1.35E-05	2.29E-05
71	0.003127	1.79E-05	1.96E-05	5.77E-06	0.003125	1.75E-05	1.78E-05	9.71E-06	0.00312	1.70E-05	1.58E-05	1.53E-05	0.003113	1.63E-05	1.38E-05	2.31E-05
72	0.003127	1.80E-05	2.00E-05	5.83E-06	0.003124	1.76E-05	1.82E-05	9.80E-06	0.00312	1.71E-05	1.62E-05	1.54E-05	0.003112	1.64E-05	1.41E-05	2.34E-05
73	0.003126	1.81E-05	2.05E-05	5.88E-06	0.003124	1.77E-05	1.86E-05	9.90E-06	0.003119	1.72E-05	1.65E-05	1.56E-05	0.003111	1.65E-05	1.44E-05	2.36E-05
74	0.003125	1.82E-05	2.09E-05	5.94E-06	0.003123	1.78E-05	1.90E-05	9.99E-06	0.003118	1.73E-05	1.69E-05	1.58E-05	0.00311	1.66E-05	1.47E-05	2.39E-05
75	0.003125	1.83E-05	2.14E-05	5.99E-06	0.003122	1.79E-05	1.94E-05	1.01E-05	0.003118	1.73E-05	1.72E-05	1.59E-05	0.003109	1.67E-05	1.50E-05	2.41E-05
76	0.003124	1.84E-05	2.18E-05	6.04E-06	0.003122	1.80E-05	1.98E-05	1.02E-05	0.003117	1.74E-05	1.76E-05	1.60E-05	0.003109	1.68E-05	1.53E-05	2.43E-05
77	0.003124	1.85E-05	2.22E-05	6.09E-06	0.003121	1.80E-05	2.02E-05	1.03E-05	0.003116	1.75E-05	1.79E-05	1.62E-05	0.003108	1.69E-05	1.56E-05	2.45E-05
78	0.003123	1.85E-05	2.27E-05	6.14E-06	0.003121	1.81E-05	2.06E-05	1.03E-05	0.003116	1.76E-05	1.83E-05	1.63E-05	0.003107	1.69E-05	1.59E-05	2.47E-05
79	0.003123	1.86E-05	2.31E-05	6.19E-06	0.00312	1.82E-05	2.10E-05	1.04E-05	0.003115	1.77E-05	1.86E-05	1.65E-05	0.003106	1.70E-05	1.62E-05	2.50E-05
80	0.003122	1.87E-05	2.36E-05	6.23E-06	0.00312	1.83E-05	2.14E-05	1.05E-05	0.003115	1.78E-05	1.90E-05	1.66E-05	0.003106	1.71E-05	1.65E-05	2.52E-05
81	0.003121	1.88E-05	2.40E-05	6.28E-06	0.003119	1.84E-05	2.18E-05	1.06E-05	0.003114	1.78E-05	1.93E-05	1.67E-05	0.003105	1.72E-05	1.68E-05	2.54E-05
82	0.003121	1.88E-05	2.45E-05	6.32E-06	0.003118	1.84E-05	2.22E-05	1.07E-05	0.003113	1.79E-05	1.97E-05	1.68E-05	0.003104	1.73E-05	1.71E-05	2.56E-05
83	0.00312	1.89E-05	2.50E-05	6.37E-06	0.003118	1.85E-05	2.26E-05	1.07E-05	0.003113	1.80E-05	2.01E-05	1.70E-05	0.003103	1.73E-05	1.74E-05	2.57E-05
84	0.00312	1.90E-05	2.54E-05	6.41E-06	0.003117	1.86E-05	2.30E-05	1.08E-05	0.003112	1.81E-05	2.04E-05	1.71E-05	0.003103	1.74E-05	1.77E-05	2.59E-05
85	0.003119	1.90E-05	2.59E-05	6.45E-06	0.003117	1.86E-05	2.35E-05	1.09E-05	0.003111	1.81E-05	2.08E-05	1.72E-05	0.003102	1.75E-05	1.80E-05	2.61E-05
86	0.003119	1.91E-05	2.63E-05	6.49E-06	0.003116	1.87E-05	2.39E-05	1.09E-05	0.003111	1.82E-05	2.12E-05	1.73E-05	0.003101	1.76E-05	1.83E-05	2.63E-05
87	0.003118	1.92E-05	2.68E-05	6.53E-06	0.003115	1.88E-05	2.43E-05	1.10E-05	0.00311	1.83E-05	2.15E-05	1.74E-05	0.0031	1.76E-05	1.86E-05	2.65E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
88	0.003117	1.92E-05	2.73E-05	6.57E-06	0.003115	1.88E-05	2.47E-05	1.11E-05	0.00311	1.83E-05	2.19E-05	1.75E-05	0.0031	1.77E-05	1.90E-05	2.66E-05
89	0.003117	1.93E-05	2.77E-05	6.61E-06	0.003114	1.89E-05	2.51E-05	1.12E-05	0.003109	1.84E-05	2.23E-05	1.76E-05	0.003099	1.78E-05	1.93E-05	2.68E-05
90	0.003116	1.93E-05	2.82E-05	6.64E-06	0.003114	1.90E-05	2.55E-05	1.12E-05	0.003108	1.85E-05	2.26E-05	1.77E-05	0.003098	1.78E-05	1.96E-05	2.70E-05
91	0.003116	1.94E-05	2.86E-05	6.68E-06	0.003113	1.90E-05	2.60E-05	1.13E-05	0.003108	1.85E-05	2.30E-05	1.78E-05	0.003097	1.79E-05	1.99E-05	2.71E-05
92	0.003115	1.94E-05	2.91E-05	6.71E-06	0.003113	1.91E-05	2.64E-05	1.13E-05	0.003107	1.86E-05	2.34E-05	1.79E-05	0.003097	1.80E-05	2.02E-05	2.73E-05
93	0.003115	1.95E-05	2.96E-05	6.75E-06	0.003112	1.91E-05	2.68E-05	1.14E-05	0.003106	1.87E-05	2.37E-05	1.80E-05	0.003096	1.80E-05	2.05E-05	2.74E-05
94	0.003114	1.96E-05	3.01E-05	6.78E-06	0.003111	1.92E-05	2.72E-05	1.15E-05	0.003106	1.87E-05	2.41E-05	1.81E-05	0.003095	1.81E-05	2.09E-05	2.76E-05
95	0.003114	1.96E-05	3.05E-05	6.82E-06	0.003111	1.92E-05	2.77E-05	1.15E-05	0.003105	1.88E-05	2.45E-05	1.82E-05	0.003095	1.82E-05	2.12E-05	2.77E-05
96	0.003113	1.97E-05	3.10E-05	6.85E-06	0.00311	1.93E-05	2.81E-05	1.16E-05	0.003105	1.88E-05	2.49E-05	1.83E-05	0.003094	1.82E-05	2.15E-05	2.79E-05
97	0.003112	1.97E-05	3.15E-05	6.88E-06	0.00311	1.94E-05	2.85E-05	1.16E-05	0.003104	1.89E-05	2.53E-05	1.84E-05	0.003093	1.83E-05	2.18E-05	2.80E-05
98	0.003112	1.97E-05	3.20E-05	6.91E-06	0.003109	1.94E-05	2.90E-05	1.17E-05	0.003103	1.89E-05	2.56E-05	1.85E-05	0.003092	1.83E-05	2.22E-05	2.81E-05
99	0.003111	1.98E-05	3.24E-05	6.94E-06	0.003109	1.95E-05	2.94E-05	1.17E-05	0.003103	1.90E-05	2.60E-05	1.86E-05	0.003092	1.84E-05	2.25E-05	2.83E-05
100	0.003111	1.98E-05	3.29E-05	6.97E-06	0.003108	1.95E-05	2.98E-05	1.18E-05	0.003102	1.90E-05	2.64E-05	1.87E-05	0.003091	1.84E-05	2.28E-05	2.84E-05
101	0.00311	1.99E-05	3.34E-05	6.99E-06	0.003108	1.95E-05	3.02E-05	1.18E-05	0.003102	1.91E-05	2.68E-05	1.87E-05	0.00309	1.85E-05	2.31E-05	2.85E-05
102	0.00311	1.99E-05	3.39E-05	7.02E-06	0.003107	1.96E-05	3.07E-05	1.19E-05	0.003101	1.91E-05	2.72E-05	1.88E-05	0.00309	1.86E-05	2.35E-05	2.86E-05
103	0.003109	2.00E-05	3.43E-05	7.05E-06	0.003106	1.96E-05	3.11E-05	1.19E-05	0.0031	1.92E-05	2.75E-05	1.89E-05	0.003089	1.86E-05	2.38E-05	2.88E-05
104	0.003109	2.00E-05	3.48E-05	7.08E-06	0.003106	1.97E-05	3.16E-05	1.20E-05	0.0031	1.92E-05	2.79E-05	1.90E-05	0.003088	1.87E-05	2.41E-05	2.89E-05
105	0.003108	2.00E-05	3.53E-05	7.10E-06	0.003105	1.97E-05	3.20E-05	1.20E-05	0.003099	1.93E-05	2.83E-05	1.90E-05	0.003088	1.87E-05	2.45E-05	2.90E-05
106	0.003107	2.01E-05	3.58E-05	7.13E-06	0.003105	1.98E-05	3.24E-05	1.20E-05	0.003099	1.93E-05	2.87E-05	1.91E-05	0.003087	1.88E-05	2.48E-05	2.91E-05
107	0.003107	2.01E-05	3.63E-05	7.15E-06	0.003104	1.98E-05	3.29E-05	1.21E-05	0.003098	1.94E-05	2.91E-05	1.92E-05	0.003086	1.88E-05	2.51E-05	2.92E-05
108	0.003106	2.02E-05	3.68E-05	7.17E-06	0.003104	1.98E-05	3.33E-05	1.21E-05	0.003098	1.94E-05	2.95E-05	1.92E-05	0.003086	1.89E-05	2.55E-05	2.93E-05
109	0.003106	2.02E-05	3.73E-05	7.20E-06	0.003103	1.99E-05	3.38E-05	1.22E-05	0.003097	1.95E-05	2.99E-05	1.93E-05	0.003085	1.89E-05	2.58E-05	2.94E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
110	0.003105	2.02E-05	3.77E-05	7.22E-06	0.003103	1.99E-05	3.42E-05	1.22E-05	0.003096	1.95E-05	3.03E-05	1.94E-05	0.003084	1.89E-05	2.61E-05	2.95E-05
111	0.003105	2.03E-05	3.82E-05	7.24E-06	0.003102	2.00E-05	3.46E-05	1.22E-05	0.003096	1.95E-05	3.07E-05	1.94E-05	0.003084	1.90E-05	2.65E-05	2.96E-05
112	0.003104	2.03E-05	3.87E-05	7.26E-06	0.003102	2.00E-05	3.51E-05	1.23E-05	0.003095	1.96E-05	3.10E-05	1.95E-05	0.003083	1.90E-05	2.68E-05	2.97E-05
113	0.003104	2.03E-05	3.92E-05	7.28E-06	0.003101	2.00E-05	3.55E-05	1.23E-05	0.003095	1.96E-05	3.14E-05	1.95E-05	0.003082	1.91E-05	2.72E-05	2.98E-05
114	0.003103	2.04E-05	3.97E-05	7.30E-06	0.003101	2.01E-05	3.60E-05	1.24E-05	0.003094	1.97E-05	3.18E-05	1.96E-05	0.003082	1.91E-05	2.75E-05	2.99E-05
115	0.003103	2.04E-05	4.02E-05	7.32E-06	0.0031	2.01E-05	3.64E-05	1.24E-05	0.003094	1.97E-05	3.22E-05	1.97E-05	0.003081	1.92E-05	2.78E-05	3.00E-05
116	0.003102	2.04E-05	4.07E-05	7.34E-06	0.003099	2.01E-05	3.69E-05	1.24E-05	0.003093	1.97E-05	3.26E-05	1.97E-05	0.00308	1.92E-05	2.82E-05	3.00E-05
117	0.003102	2.04E-05	4.12E-05	7.36E-06	0.003099	2.02E-05	3.73E-05	1.25E-05	0.003092	1.98E-05	3.30E-05	1.98E-05	0.00308	1.92E-05	2.85E-05	3.01E-05
118	0.003101	2.05E-05	4.17E-05	7.38E-06	0.003098	2.02E-05	3.78E-05	1.25E-05	0.003092	1.98E-05	3.34E-05	1.98E-05	0.003079	1.93E-05	2.89E-05	3.02E-05
119	0.0031	2.05E-05	4.22E-05	7.40E-06	0.003098	2.02E-05	3.82E-05	1.25E-05	0.003091	1.98E-05	3.38E-05	1.99E-05	0.003078	1.93E-05	2.92E-05	3.03E-05
120	0.0031	2.05E-05	4.27E-05	7.41E-06	0.003097	2.03E-05	3.87E-05	1.25E-05	0.003091	1.99E-05	3.42E-05	1.99E-05	0.003078	1.94E-05	2.96E-05	3.04E-05
121	0.003099	2.05E-05	4.32E-05	7.43E-06	0.003097	2.03E-05	3.91E-05	1.26E-05	0.00309	1.99E-05	3.46E-05	2.00E-05	0.003077	1.94E-05	2.99E-05	3.04E-05
122	0.003099	2.06E-05	4.36E-05	7.45E-06	0.003096	2.03E-05	3.96E-05	1.26E-05	0.00309	1.99E-05	3.50E-05	2.00E-05	0.003076	1.94E-05	3.02E-05	3.05E-05
123	0.003098	2.06E-05	4.41E-05	7.46E-06	0.003096	2.03E-05	4.00E-05	1.26E-05	0.003089	2.00E-05	3.54E-05	2.00E-05	0.003076	1.95E-05	3.06E-05	3.06E-05
124	0.003098	2.06E-05	4.46E-05	7.48E-06	0.003095	2.04E-05	4.05E-05	1.27E-05	0.003088	2.00E-05	3.58E-05	2.01E-05	0.003075	1.95E-05	3.09E-05	3.06E-05
125	0.003097	2.06E-05	4.51E-05	7.49E-06	0.003095	2.04E-05	4.09E-05	1.27E-05	0.003088	2.00E-05	3.62E-05	2.01E-05	0.003074	1.95E-05	3.13E-05	3.07E-05
126	0.003097	2.07E-05	4.56E-05	7.51E-06	0.003094	2.04E-05	4.14E-05	1.27E-05	0.003087	2.01E-05	3.66E-05	2.02E-05	0.003074	1.96E-05	3.16E-05	3.08E-05
127	0.003096	2.07E-05	4.61E-05	7.52E-06	0.003094	2.04E-05	4.18E-05	1.27E-05	0.003087	2.01E-05	3.70E-05	2.02E-05	0.003073	1.96E-05	3.20E-05	3.08E-05
128	0.003096	2.07E-05	4.66E-05	7.53E-06	0.003093	2.05E-05	4.23E-05	1.28E-05	0.003086	2.01E-05	3.74E-05	2.03E-05	0.003072	1.96E-05	3.23E-05	3.09E-05
129	0.003095	2.07E-05	4.71E-05	7.55E-06	0.003093	2.05E-05	4.27E-05	1.28E-05	0.003086	2.01E-05	3.78E-05	2.03E-05	0.003072	1.97E-05	3.27E-05	3.10E-05
130	0.003095	2.07E-05	4.76E-05	7.56E-06	0.003092	2.05E-05	4.32E-05	1.28E-05	0.003085	2.02E-05	3.82E-05	2.03E-05	0.003071	1.97E-05	3.30E-05	3.10E-05
131	0.003094	2.08E-05	4.81E-05	7.57E-06	0.003091	2.05E-05	4.36E-05	1.28E-05	0.003085	2.02E-05	3.86E-05	2.04E-05	0.00307	1.97E-05	3.34E-05	3.11E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
132	0.003093	2.08E-05	4.86E-05	7.59E-06	0.003091	2.06E-05	4.41E-05	1.28E-05	0.003084	2.02E-05	3.90E-05	2.04E-05	0.00307	1.97E-05	3.37E-05	3.11E-05
133	0.003093	2.08E-05	4.91E-05	7.60E-06	0.00309	2.06E-05	4.45E-05	1.29E-05	0.003083	2.02E-05	3.94E-05	2.04E-05	0.003069	1.98E-05	3.41E-05	3.12E-05
134	0.003092	2.08E-05	4.96E-05	7.61E-06	0.00309	2.06E-05	4.50E-05	1.29E-05	0.003083	2.03E-05	3.99E-05	2.05E-05	0.003068	1.98E-05	3.44E-05	3.12E-05
135	0.003092	2.08E-05	5.01E-05	7.62E-06	0.003089	2.06E-05	4.55E-05	1.29E-05	0.003082	2.03E-05	4.03E-05	2.05E-05	0.003068	1.98E-05	3.48E-05	3.13E-05
136	0.003091	2.09E-05	5.06E-05	7.63E-06	0.003089	2.06E-05	4.59E-05	1.29E-05	0.003082	2.03E-05	4.07E-05	2.05E-05	0.003067	1.99E-05	3.51E-05	3.13E-05
137	0.003091	2.09E-05	5.11E-05	7.64E-06	0.003088	2.07E-05	4.64E-05	1.29E-05	0.003081	2.03E-05	4.11E-05	2.06E-05	0.003067	1.99E-05	3.55E-05	3.14E-05
138	0.00309	2.09E-05	5.17E-05	7.65E-06	0.003088	2.07E-05	4.68E-05	1.30E-05	0.003081	2.04E-05	4.15E-05	2.06E-05	0.003066	1.99E-05	3.58E-05	3.14E-05
139	0.00309	2.09E-05	5.22E-05	7.66E-06	0.003087	2.07E-05	4.73E-05	1.30E-05	0.00308	2.04E-05	4.19E-05	2.06E-05	0.003065	1.99E-05	3.62E-05	3.15E-05
140	0.003089	2.09E-05	5.27E-05	7.67E-06	0.003087	2.07E-05	4.78E-05	1.30E-05	0.00308	2.04E-05	4.23E-05	2.07E-05	0.003065	2.00E-05	3.66E-05	3.15E-05
141	0.003089	2.09E-05	5.32E-05	7.68E-06	0.003086	2.07E-05	4.82E-05	1.30E-05	0.003079	2.04E-05	4.27E-05	2.07E-05	0.003064	2.00E-05	3.69E-05	3.16E-05
142	0.003088	2.09E-05	5.37E-05	7.69E-06	0.003086	2.07E-05	4.87E-05	1.30E-05	0.003078	2.04E-05	4.31E-05	2.07E-05	0.003063	2.00E-05	3.73E-05	3.16E-05
143	0.003088	2.10E-05	5.42E-05	7.70E-06	0.003085	2.08E-05	4.91E-05	1.31E-05	0.003078	2.05E-05	4.35E-05	2.07E-05	0.003063	2.00E-05	3.76E-05	3.16E-05
144	0.003087	2.10E-05	5.47E-05	7.71E-06	0.003085	2.08E-05	4.96E-05	1.31E-05	0.003077	2.05E-05	4.39E-05	2.08E-05	0.003062	2.01E-05	3.80E-05	3.17E-05
145	0.003087	2.10E-05	5.52E-05	7.72E-06	0.003084	2.08E-05	5.01E-05	1.31E-05	0.003077	2.05E-05	4.44E-05	2.08E-05	0.003061	2.01E-05	3.83E-05	3.17E-05
146	0.003086	2.10E-05	5.57E-05	7.73E-06	0.003084	2.08E-05	5.05E-05	1.31E-05	0.003076	2.05E-05	4.48E-05	2.08E-05	0.003061	2.01E-05	3.87E-05	3.18E-05
147	0.003086	2.10E-05	5.62E-05	7.74E-06	0.003083	2.08E-05	5.10E-05	1.31E-05	0.003076	2.05E-05	4.52E-05	2.08E-05	0.00306	2.01E-05	3.91E-05	3.18E-05
148	0.003085	2.10E-05	5.67E-05	7.74E-06	0.003083	2.08E-05	5.14E-05	1.31E-05	0.003075	2.06E-05	4.56E-05	2.09E-05	0.00306	2.01E-05	3.94E-05	3.18E-05
149	0.003084	2.10E-05	5.72E-05	7.75E-06	0.003082	2.09E-05	5.19E-05	1.31E-05	0.003075	2.06E-05	4.60E-05	2.09E-05	0.003059	2.02E-05	3.98E-05	3.19E-05
150	0.003084	2.10E-05	5.77E-05	7.76E-06	0.003082	2.09E-05	5.24E-05	1.32E-05	0.003074	2.06E-05	4.64E-05	2.09E-05	0.003058	2.02E-05	4.01E-05	3.19E-05
151	0.003083	2.10E-05	5.82E-05	7.77E-06	0.003081	2.09E-05	5.28E-05	1.32E-05	0.003074	2.06E-05	4.68E-05	2.09E-05	0.003058	2.02E-05	4.05E-05	3.19E-05
152	0.003083	2.11E-05	5.87E-05	7.77E-06	0.003081	2.09E-05	5.33E-05	1.32E-05	0.003073	2.06E-05	4.72E-05	2.09E-05	0.003057	2.02E-05	4.08E-05	3.20E-05
153	0.003082	2.11E-05	5.92E-05	7.78E-06	0.00308	2.09E-05	5.38E-05	1.32E-05	0.003073	2.06E-05	4.77E-05	2.10E-05	0.003056	2.02E-05	4.12E-05	3.20E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
154	0.003082	2.11E-05	5.98E-05	7.79E-06	0.00308	2.09E-05	5.42E-05	1.32E-05	0.003072	2.07E-05	4.81E-05	2.10E-05	0.003056	2.03E-05	4.16E-05	3.20E-05
155	0.003081	2.11E-05	6.03E-05	7.79E-06	0.003079	2.09E-05	5.47E-05	1.32E-05	0.003071	2.07E-05	4.85E-05	2.10E-05	0.003055	2.03E-05	4.19E-05	3.20E-05
156	0.003081	2.11E-05	6.08E-05	7.80E-06	0.003078	2.09E-05	5.52E-05	1.32E-05	0.003071	2.07E-05	4.89E-05	2.10E-05	0.003055	2.03E-05	4.23E-05	3.21E-05
157	0.00308	2.11E-05	6.13E-05	7.81E-06	0.003078	2.09E-05	5.56E-05	1.32E-05	0.00307	2.07E-05	4.93E-05	2.10E-05	0.003054	2.03E-05	4.27E-05	3.21E-05
158	0.00308	2.11E-05	6.18E-05	7.81E-06	0.003077	2.10E-05	5.61E-05	1.32E-05	0.00307	2.07E-05	4.97E-05	2.10E-05	0.003053	2.03E-05	4.30E-05	3.21E-05
159	0.003079	2.11E-05	6.23E-05	7.82E-06	0.003077	2.10E-05	5.66E-05	1.33E-05	0.003069	2.07E-05	5.01E-05	2.11E-05	0.003053	2.03E-05	4.34E-05	3.21E-05
160	0.003079	2.11E-05	6.28E-05	7.82E-06	0.003076	2.10E-05	5.70E-05	1.33E-05	0.003069	2.07E-05	5.06E-05	2.11E-05	0.003052	2.04E-05	4.37E-05	3.22E-05
161	0.003078	2.11E-05	6.33E-05	7.83E-06	0.003076	2.10E-05	5.75E-05	1.33E-05	0.003068	2.07E-05	5.10E-05	2.11E-05	0.003052	2.04E-05	4.41E-05	3.22E-05
162	0.003078	2.11E-05	6.38E-05	7.83E-06	0.003075	2.10E-05	5.79E-05	1.33E-05	0.003068	2.08E-05	5.14E-05	2.11E-05	0.003051	2.04E-05	4.45E-05	3.22E-05
163	0.003077	2.11E-05	6.43E-05	7.84E-06	0.003075	2.10E-05	5.84E-05	1.33E-05	0.003067	2.08E-05	5.18E-05	2.11E-05	0.00305	2.04E-05	4.48E-05	3.22E-05
164	0.003077	2.12E-05	6.48E-05	7.84E-06	0.003074	2.10E-05	5.89E-05	1.33E-05	0.003067	2.08E-05	5.22E-05	2.11E-05	0.00305	2.04E-05	4.52E-05	3.23E-05
165	0.003076	2.12E-05	6.54E-05	7.85E-06	0.003074	2.10E-05	5.93E-05	1.33E-05	0.003066	2.08E-05	5.26E-05	2.11E-05	0.003049	2.04E-05	4.55E-05	3.23E-05
166	0.003076	2.12E-05	6.59E-05	7.85E-06	0.003073	2.10E-05	5.98E-05	1.33E-05	0.003066	2.08E-05	5.31E-05	2.12E-05	0.003048	2.05E-05	4.59E-05	3.23E-05
167	0.003075	2.12E-05	6.64E-05	7.86E-06	0.003073	2.10E-05	6.03E-05	1.33E-05	0.003065	2.08E-05	5.35E-05	2.12E-05	0.003048	2.05E-05	4.63E-05	3.23E-05
168	0.003075	2.12E-05	6.69E-05	7.86E-06	0.003072	2.10E-05	6.07E-05	1.33E-05	0.003065	2.08E-05	5.39E-05	2.12E-05	0.003047	2.05E-05	4.66E-05	3.23E-05
169	0.003074	2.12E-05	6.74E-05	7.86E-06	0.003072	2.11E-05	6.12E-05	1.33E-05	0.003064	2.08E-05	5.43E-05	2.12E-05	0.003047	2.05E-05	4.70E-05	3.23E-05
170	0.003074	2.12E-05	6.79E-05	7.87E-06	0.003071	2.11E-05	6.17E-05	1.33E-05	0.003063	2.08E-05	5.47E-05	2.12E-05	0.003046	2.05E-05	4.74E-05	3.24E-05
171	0.003073	2.12E-05	6.84E-05	7.87E-06	0.003071	2.11E-05	6.22E-05	1.33E-05	0.003063	2.09E-05	5.51E-05	2.12E-05	0.003045	2.05E-05	4.77E-05	3.24E-05
172	0.003072	2.12E-05	6.89E-05	7.88E-06	0.00307	2.11E-05	6.26E-05	1.34E-05	0.003062	2.09E-05	5.56E-05	2.12E-05	0.003045	2.05E-05	4.81E-05	3.24E-05
173	0.003072	2.12E-05	6.94E-05	7.88E-06	0.00307	2.11E-05	6.31E-05	1.34E-05	0.003062	2.09E-05	5.60E-05	2.12E-05	0.003044	2.05E-05	4.85E-05	3.24E-05
174	0.003071	2.12E-05	7.00E-05	7.88E-06	0.003069	2.11E-05	6.36E-05	1.34E-05	0.003061	2.09E-05	5.64E-05	2.12E-05	0.003044	2.06E-05	4.88E-05	3.24E-05
175	0.003071	2.12E-05	7.05E-05	7.89E-06	0.003069	2.11E-05	6.40E-05	1.34E-05	0.003061	2.09E-05	5.68E-05	2.13E-05	0.003043	2.06E-05	4.92E-05	3.24E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
176	0.00307	2.12E-05	7.10E-05	7.89E-06	0.003068	2.11E-05	6.45E-05	1.34E-05	0.00306	2.09E-05	5.72E-05	2.13E-05	0.003042	2.06E-05	4.96E-05	3.25E-05
177	0.00307	2.12E-05	7.15E-05	7.89E-06	0.003068	2.11E-05	6.50E-05	1.34E-05	0.00306	2.09E-05	5.77E-05	2.13E-05	0.003042	2.06E-05	4.99E-05	3.25E-05
178	0.003069	2.12E-05	7.20E-05	7.90E-06	0.003067	2.11E-05	6.54E-05	1.34E-05	0.003059	2.09E-05	5.81E-05	2.13E-05	0.003041	2.06E-05	5.03E-05	3.25E-05
179	0.003069	2.12E-05	7.25E-05	7.90E-06	0.003067	2.11E-05	6.59E-05	1.34E-05	0.003059	2.09E-05	5.85E-05	2.13E-05	0.003041	2.06E-05	5.07E-05	3.25E-05
180	0.003068	2.12E-05	7.30E-05	7.90E-06	0.003066	2.11E-05	6.64E-05	1.34E-05	0.003058	2.09E-05	5.89E-05	2.13E-05	0.00304	2.06E-05	5.10E-05	3.25E-05
181	0.003068	2.12E-05	7.35E-05	7.90E-06	0.003066	2.11E-05	6.68E-05	1.34E-05	0.003058	2.09E-05	5.93E-05	2.13E-05	0.003039	2.06E-05	5.14E-05	3.25E-05
182	0.003067	2.12E-05	7.41E-05	7.91E-06	0.003065	2.11E-05	6.73E-05	1.34E-05	0.003057	2.09E-05	5.98E-05	2.13E-05	0.003039	2.06E-05	5.18E-05	3.25E-05
183	0.003067	2.12E-05	7.46E-05	7.91E-06	0.003065	2.11E-05	6.78E-05	1.34E-05	0.003057	2.10E-05	6.02E-05	2.13E-05	0.003038	2.06E-05	5.21E-05	3.25E-05
184	0.003066	2.12E-05	7.51E-05	7.91E-06	0.003064	2.11E-05	6.82E-05	1.34E-05	0.003056	2.10E-05	6.06E-05	2.13E-05	0.003038	2.07E-05	5.25E-05	3.25E-05
185	0.003066	2.12E-05	7.56E-05	7.91E-06	0.003064	2.11E-05	6.87E-05	1.34E-05	0.003056	2.10E-05	6.10E-05	2.13E-05	0.003037	2.07E-05	5.29E-05	3.26E-05
186	0.003065	2.12E-05	7.61E-05	7.92E-06	0.003063	2.12E-05	6.92E-05	1.34E-05	0.003055	2.10E-05	6.14E-05	2.13E-05	0.003036	2.07E-05	5.32E-05	3.26E-05
187	0.003065	2.13E-05	7.66E-05	7.92E-06	0.003063	2.12E-05	6.96E-05	1.34E-05	0.003055	2.10E-05	6.19E-05	2.13E-05	0.003036	2.07E-05	5.36E-05	3.26E-05
188	0.003064	2.13E-05	7.71E-05	7.92E-06	0.003062	2.12E-05	7.01E-05	1.34E-05	0.003054	2.10E-05	6.23E-05	2.13E-05	0.003035	2.07E-05	5.40E-05	3.26E-05
189	0.003064	2.13E-05	7.76E-05	7.92E-06	0.003062	2.12E-05	7.06E-05	1.34E-05	0.003053	2.10E-05	6.27E-05	2.14E-05	0.003034	2.07E-05	5.43E-05	3.26E-05
190	0.003063	2.13E-05	7.82E-05	7.92E-06	0.003061	2.12E-05	7.11E-05	1.34E-05	0.003053	2.10E-05	6.31E-05	2.14E-05	0.003034	2.07E-05	5.47E-05	3.26E-05
191	0.003063	2.13E-05	7.87E-05	7.93E-06	0.003061	2.12E-05	7.15E-05	1.34E-05	0.003052	2.10E-05	6.35E-05	2.14E-05	0.003033	2.07E-05	5.51E-05	3.26E-05
192	0.003062	2.13E-05	7.92E-05	7.93E-06	0.00306	2.12E-05	7.20E-05	1.34E-05	0.003052	2.10E-05	6.40E-05	2.14E-05	0.003033	2.07E-05	5.54E-05	3.26E-05
193	0.003062	2.13E-05	7.97E-05	7.93E-06	0.00306	2.12E-05	7.25E-05	1.34E-05	0.003051	2.10E-05	6.44E-05	2.14E-05	0.003032	2.07E-05	5.58E-05	3.26E-05
194	0.003061	2.13E-05	8.02E-05	7.93E-06	0.003059	2.12E-05	7.29E-05	1.35E-05	0.003051	2.10E-05	6.48E-05	2.14E-05	0.003031	2.07E-05	5.62E-05	3.26E-05
195	0.003061	2.13E-05	8.07E-05	7.93E-06	0.003059	2.12E-05	7.34E-05	1.35E-05	0.00305	2.10E-05	6.52E-05	2.14E-05	0.003031	2.07E-05	5.65E-05	3.26E-05
196	0.00306	2.13E-05	8.12E-05	7.93E-06	0.003058	2.12E-05	7.39E-05	1.35E-05	0.00305	2.10E-05	6.56E-05	2.14E-05	0.00303	2.07E-05	5.69E-05	3.26E-05
197	0.00306	2.13E-05	8.17E-05	7.93E-06	0.003058	2.12E-05	7.43E-05	1.35E-05	0.003049	2.10E-05	6.61E-05	2.14E-05	0.00303	2.08E-05	5.73E-05	3.26E-05

Table S17. Cont.

TIME (days)	cSAXA08:1	cSCA08:1	cESCA08:1	cSFA08:1	cSAXA10:1	cSCA10:1	cESCA10:1	cSFA10:1	cSAXA12:1	cSCA12:1	cESCA12:1	cSFA12:1	cSAXA14:1	cSCA14:1	cESCA14:1	cSFA14:1
198	0.003059	2.13E-05	8.23E-05	7.94E-06	0.003057	2.12E-05	7.48E-05	1.35E-05	0.003049	2.10E-05	6.65E-05	2.14E-05	0.003029	2.08E-05	5.76E-05	3.26E-05
199	0.003059	2.13E-05	8.28E-05	7.94E-06	0.003057	2.12E-05	7.53E-05	1.35E-05	0.003048	2.10E-05	6.69E-05	2.14E-05	0.003028	2.08E-05	5.80E-05	3.27E-05
200	0.003058	2.13E-05	8.33E-05	7.94E-06	0.003056	2.12E-05	7.58E-05	1.35E-05	0.003048	2.10E-05	6.73E-05	2.14E-05	0.003028	2.08E-05	5.84E-05	3.27E-05

4.1. Determined Rate Constants

r_i	k_{opt}
$r_1(k_1)$	0.0867 d^{-1}
$r_2(k_2)$	0.00585 d^{-1}
$r_3(k_3)$	0.655 d^{-1}
$r_4(k_4)$	0.0555 d^{-1}
$r_5(k_5)$	$1.68\text{E}-04 \text{ L mol}^{-1} \text{ d}^{-1}$
$r_6(k_6)$	$0.0241 \text{ L mol}^{-1} \text{ d}^{-1}$
$r_7(k_7)$	$0.591 \text{ g}_{\text{SAXA}} \text{ mol}^{-2} \text{ d}^{-1}$
$r_7(k_8)$	0.025472 d^{-1}

4.2. Ab Initio Calculations

4.2.1. Structures

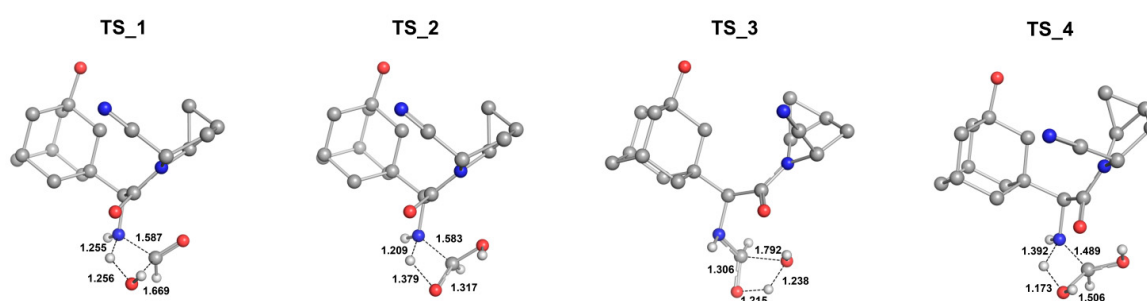


Figure S1. Structure of the transition state parallel reaction 1 in gas phase. Some hydrogen atoms are omitted for clarity.

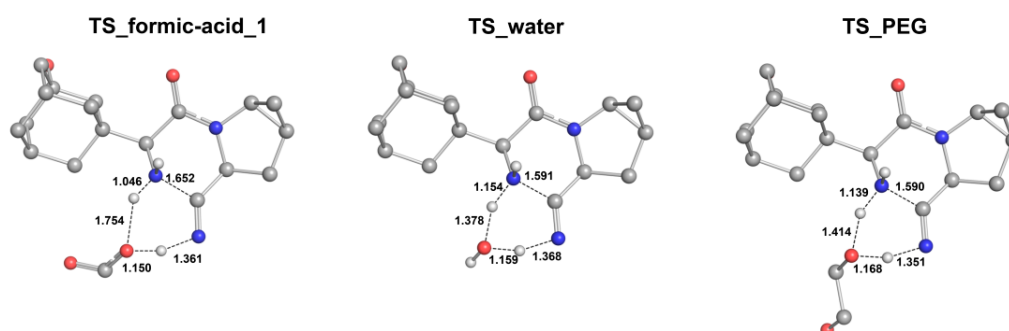


Figure S2. Structure of the transition state parallel reaction 2 in gas phase catalyzed by the hydroxyl group.

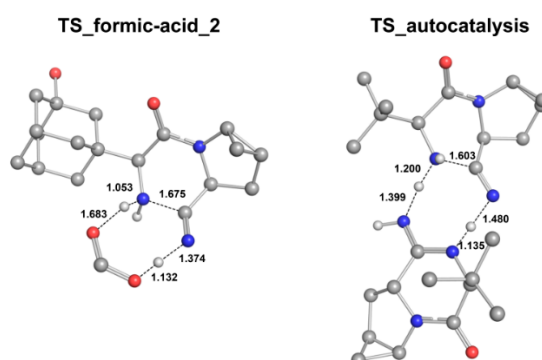


Figure S3. Structure of the transition state parallel reaction 2 in gas phase catalyzed by formic acid and ESCA.

4.2.2. Calculated Energies

Table S18. Calculated energy for the species involved in the reaction 1 in gas phase and water.

	gas phase			water		
	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm ⁻¹)	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm ⁻¹)
saxagliptin	-1014.900158	n.a.	n.a.	-1014.917957	n.a.	n.a.
formic acid	-189.664848	n.a.	n.a.	-189.676737	n.a.	n.a.
TS_1	-1204.502403	39.28	-1356	-1204.525945	43.14	-1357
TS_2	-1204.504560	37.93	-1415	-1204.531874	39.42	-1495
Intermediate_1	-1204.559858	3.23	n.a.	-1204.581799	8.09	n.a.
TS_3	-1204.506670	36.61	-1670	-1204.530424	40.33	-1670
SFA	-1128.187660	-1.57	n.a.	-1128.210647	-2.06	n.a.
H ₂ O	-76.379845		n.a.	-76.387335		n.a.

Table S19. Calculated energy for the species involved in the reaction 1 in gas phase, water and formic acid.

Structure	gas phase			water			formic acid		
	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm ⁻¹)	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm ⁻¹)	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm ⁻¹)
saxagliptin	-1014.900158	n.a.	n.a.	-1014.917957	n.a.	n.a.	-1014.917815	n.a.	n.a.
HCOOH ₂ ⁺	-189.955557	n.a.	n.a.	-190.064963	n.a.	n.a.	-190.064454	n.a.	n.a.
Intermediate_2	-1204.924983	-43.47	n.a.	-1205.009268	-16.53	n.a.	-1205.008647	-16.55	n.a.
TS_4	-1204.870810	-9.47	-1381	-1204.953494	18.47	-1413	-1204.952966	18.39	-1413
H ₂ O	-76.379845	-37.99	n.a.	-76.387335	-36.22	n.a.	-76.387284	-17.74	n.a.
Intermediate_3	-1128.536412		n.a.	-1128.623875		n.a.	-1128.623260		n.a.
HCOO ⁻	-189.105983	n.a.	n.a.	-189.211820	n.a.	n.a.	-189.211336	n.a.	n.a.
HCOOH	-189.664848	-169.84	n.a.	-189.676737	-50.19	n.a.	-189.676648	-50.73	n.a.
SFA	-1128.187660		n.a.	-1128.210647		n.a.	-1128.210516		n.a.

Table S20. Calculated energy for the species involved in the parallel reaction 2 catalyzed by the hydroxyl group in gas phase, water and formic acid.

Structure	gas phase			water			formic acid		
	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm^{-1})	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm^{-1})	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm^{-1})
saxagliptin	-1014.900158	n.a.	n.a.	-1014.917957	n.a.	n.a.	-1014.917815	n.a.	n.a.
formic acid	-189.664848	n.a.	n.a.	-189.676737	n.a.	n.a.	-189.676648	n.a.	n.a.
TS_formic_acid_1	-1204.528428	22.95	-618	/	/	/	/	/	/
TS_formic_acid_2	-1204.546003	11.92	-309	-1204.566677	17.58	-182	-1204.566543	17.52	-182
H ₂ O	-76.379845	n.a.	n.a.	-76.387335	n.a.	n.a.	/	/	/
TS_water	-1091.233322	29.29	-1146	-1091.255101	31.5	-1162	/	/	/
HOCH ₂ CH ₂ OH ¹	-230.088873	n.a.	n.a.	-230.097524	n.a.	n.a.	/	/	/
TS_PEG	-1244.942158	29.41	-1086	-1244.966634	30.65	-1070	/	/	/
SCA	-1014.912519	-7.76	n.a.	-1014.929	-6.76	n.a.	-1014.928583	-6.76	n.a.
ESCA	-1014.916325	-10.14	n.a.	-1014.934	-10.02	n.a.	-1014.933780	-10.02	n.a.

¹Ethylene glycol was used as simplified model for PEG. /: unavailable.**Table S21.** Calculated energy for the species involved in the parallel reaction 2 catalyzed by ESCA in gas phase, water and formic acid.

Structure	gas phase			water			formic acid		
	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm^{-1})	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm^{-1})	Energy (Hartree)	ΔG_{298} (kcal/mol)	Imaginary ν (cm^{-1})
Saxagliptin_s	-707.620810	n.a.	n.a.	-707.636070	n.a.	n.a.	-707.635950	n.a.	n.a.
SCA_s	-707.634373	-8.51	n.a.	-707.647002	-6.86	n.a.	-707.646895	-6.87	n.a.
ESCA_s	-707.638442	-11.06	n.a.	-707.651746	-9.84	n.a.	-707.651631	-9.84	n.a.
TS_autocatalysis	-1415.225847	9.90	-765	-1415.249553	14.17	-776	-1415.249126	14.29	-777

4.2.3. Calculated Coordinates

Table S22. Coordinates of saxagliptin (SAXA).

in gas phase				in water				in formic acid			
O	1.312629	−2.91072	−0.20037	O	1.339106	−2.91201	−0.11407	O	1.338949	−2.91201	−0.11443
O	−1.36713	2.011005	1.292291	O	−1.32635	1.862865	1.427392	O	−1.32674	1.864144	1.426323
N	−2.2633	0.649949	−0.24928	N	−2.2759	0.648358	−0.20325	N	−2.27579	0.648404	−0.2037
N	0.358756	3.155111	−0.57124	N	0.312847	3.157438	−0.46179	N	0.313303	3.157377	−0.46262
N	−2.27692	−1.38713	2.49493	N	−2.31168	−1.50213	2.446358	N	−2.31245	−1.50118	2.446956
C	1.116611	0.813203	−0.31154	C	1.120372	0.816491	−0.28514	C	1.120407	0.816414	−0.28533
C	1.833713	−1.59703	−0.07654	C	1.856582	−1.58858	−0.05169	C	1.856473	−1.58867	−0.05168
C	3.449928	0.102126	−0.96744	C	3.414931	0.094732	−1.06278	C	3.415239	0.094668	−1.06214
C	2.793279	0.145237	1.451292	C	2.90035	0.179863	1.388631	C	2.899716	0.179707	1.389084
C	0.674834	−0.65634	−0.40094	C	0.676965	−0.6568	−0.32961	C	0.67697	−0.65685	−0.32992
C	2.277586	1.036934	−1.29889	C	2.223697	1.02278	−1.34095	C	2.224104	1.022707	−1.34075
C	1.624358	1.086003	1.118404	C	1.710788	1.110907	1.107691	C	1.710298	1.110813	1.107729
C	2.979821	−1.35649	−1.06537	C	2.941724	−1.36564	−1.11019	C	2.94203	−1.36569	−1.10976
C	2.3196	−1.31309	1.348723	C	2.425552	−1.28	1.337366	C	2.424935	−1.28016	1.337589
C	3.94182	0.382655	0.45996	C	3.988927	0.399845	0.328499	C	3.988696	0.399744	0.329373
C	−0.05316	1.761295	−0.69513	C	−0.07157	1.757142	−0.61682	C	−0.07136	1.757133	−0.6174
C	−2.35822	−0.12237	−1.46712	C	−2.39881	−0.01791	−1.48284	C	−2.39831	−0.01883	−1.48281
C	−3.67334	−0.84385	−1.43151	C	−3.71541	−0.73312	−1.48297	C	−3.71493	−0.73407	−1.48278
C	−2.38644	−1.61821	−1.32346	C	−2.43318	−1.52076	−1.44761	C	−2.43267	−1.52164	−1.44654
C	−4.38591	−0.43138	−0.15584	C	−4.41581	−0.41624	−0.17461	C	−4.41564	−0.41618	−0.17484
C	−1.27347	1.48506	0.190369	C	−1.27026	1.427857	0.27784	C	−1.27026	1.428302	0.277169
C	−3.29924	0.2569	0.704941	C	−3.32464	0.217454	0.721465	C	−3.3246	0.217909	0.72112
C	−2.72933	−0.65385	1.724492	C	−2.76155	−0.7437	1.698546	C	−2.76183	−0.74289	1.698724
H	4.263778	0.275231	−1.68083	H	4.185363	0.255113	−1.82517	H	4.185969	0.255085	−1.82423
H	3.136686	0.346944	2.472052	H	3.302774	0.398831	2.384004	H	3.301753	0.398639	2.384619
H	−0.13735	−0.8683	0.306565	H	−0.09984	−0.85622	0.421901	H	−0.09999	−0.85632	0.421407
H	0.307946	−0.89046	−1.40945	H	0.25606	−0.90121	−1.31398	H	0.256352	−0.90133	−1.3144
H	1.925705	0.843671	−2.32264	H	1.813285	0.814501	−2.3389	H	1.814053	0.814352	−2.33885
H	2.587651	2.085388	−1.25252	H	2.540429	2.070642	−1.32706	H	2.540771	2.070584	−1.32684
H	1.960233	2.127652	1.19122	H	2.044752	2.1548	1.1462	H	2.044342	2.154677	1.146369
H	0.811269	0.948166	1.839992	H	0.939788	0.979129	1.875078	H	0.939003	0.979094	1.874826

Table S22. Cont.

in gas phase				in water				in formic acid			
H	2.628318	-1.59	-2.0778	H	2.531377	-1.61113	-2.09754	H	2.532059	-1.61118	-2.09727
H	3.808259	-2.04232	-0.83674	H	3.781793	-2.04753	-0.91877	H	3.782021	-2.0476	-0.91806
H	3.143543	-1.99795	1.597265	H	3.260716	-1.9618	1.548963	H	3.260076	-1.96194	1.549432
H	1.498309	-1.50995	2.048049	H	1.646683	-1.46313	2.087994	H	1.645816	-1.46338	2.087908
H	4.790163	-0.27048	0.700963	H	4.849442	-0.24957	0.531783	H	4.849155	-0.24966	0.532953
H	4.293717	1.4185	0.537226	H	4.342968	1.437218	0.367035	H	4.342711	1.437119	0.368079
H	-1.97917	0.351152	-2.36403	H	-2.03348	0.523366	-2.34546	H	-2.03277	0.521825	-2.34573
H	-0.29265	1.56404	-1.74672	H	-0.32903	1.590079	-1.66745	H	-0.32868	1.589854	-1.66806
H	-4.26523	-0.94267	-2.33398	H	-4.31444	-0.75962	-2.38493	H	-4.31374	-0.76124	-2.38487
H	-2.0947	-2.04959	-0.37026	H	-2.13662	-2.01419	-0.52601	H	-2.13621	-2.01445	-0.52459
H	-2.08773	-2.19954	-2.18865	H	-2.14937	-2.04151	-2.35503	H	-2.14865	-2.04303	-2.35354
H	-4.84887	-1.26413	0.377735	H	-4.8706	-1.28615	0.303293	H	-4.87071	-1.28569	0.303529
H	-5.16241	0.300027	-0.39316	H	-5.1964	0.32669	-0.34837	H	-5.19607	0.326761	-0.34934
H	-3.66168	1.142289	1.232395	H	-3.68937	1.073305	1.293764	H	-3.68935	1.074063	1.292963
H	2.004899	-3.52674	0.068761	H	2.070904	-3.51752	0.063679	H	2.070329	-3.51758	0.06477
H	0.248803	3.414632	0.407983	H	0.237794	3.385297	0.528402	H	0.238323	3.385367	0.527543
H	-0.28792	3.745702	-1.0861	H	-0.37594	3.742081	-0.92827	H	-0.37534	3.742131	-0.92916

Table S23. Coordinates of SFA.

In gas phase				In water				In Formic acid			
C	-1.110813	0.377372	0.324431	C	1.114217	0.373514	-0.31621	C	1.114122	0.373535	-0.31631
C	0.020863	1.396249	0.652731	C	-0.032354	1.355641	-0.69733	C	-0.03241	1.355945	-0.69684
C	-0.502828	-1.034649	0.263007	C	0.56018	-1.064273	-0.3185	C	0.559771	-1.06413	-0.31808
C	-2.158374	0.398067	1.45441	C	2.222784	0.464034	-1.38303	C	2.222129	0.463619	-1.38374
C	-1.821357	0.675372	-1.0081	C	1.735189	0.662052	1.062769	C	1.735889	0.662223	1.062275
C	1.186833	1.198021	-0.31843	C	-1.230342	1.179781	0.238192	C	-1.23004	1.179769	0.239074
N	-0.398944	2.786662	0.699716	N	0.369422	2.754466	-0.7683	N	0.369516	2.754727	-0.76747
C	-1.578007	-2.091862	-0.00227	C	1.668462	-2.080113	-0.01936	C	1.667992	-2.08016	-0.01928
C	-3.245395	-0.657567	1.193368	C	3.337371	-0.549631	-1.08282	C	3.336666	-0.55023	-1.08394
C	-2.905887	-0.38201	-1.27237	C	2.84786	-0.355092	1.365548	C	2.848505	-0.35509	1.364638
N	2.310408	0.565289	0.141005	N	-2.306075	0.484231	-0.21585	N	-2.30625	0.484922	-0.21513
O	1.11764	1.532242	-1.49216	O	-1.219595	1.617336	1.386162	O	-1.21863	1.61623	1.387385

Table S23. Cont.

In gas phase				In water			In Formic acid				
C	-2.607898	-2.054196	1.12631	C	2.755987	-1.971	-1.08732	C	2.754986	-1.97149	-1.08783
C	-2.264806	-1.776352	-1.33547	C	2.266107	-1.776189	1.358027	C	2.266423	-1.77605	1.357717
O	-1.001696	-3.384949	-0.00525	O	1.155162	-3.403499	-0.08079	O	1.154358	-3.40341	-0.08015
C	-3.941909	-0.349642	-0.13977	C	3.943644	-0.250593	0.295668	C	3.943744	-0.25104	0.294157
C	2.609959	0.039382	1.454319	C	-2.520657	-0.175268	-1.48839	C	-2.52163	-0.17317	-1.48824
C	3.272383	0.082084	-0.85189	C	-3.347387	0.122817	0.750211	C	-3.34682	0.122261	0.751249
C	3.967858	-0.590403	1.377394	C	-3.874638	-0.81284	-1.43231	C	-3.87563	-0.81071	-1.43201
C	2.74907	-1.454316	1.567726	C	-2.640875	-1.673821	-1.44311	C	-2.64192	-1.67177	-1.44465
C	4.502361	-0.359224	-0.02483	C	-4.504973	-0.4516	-0.1002	C	-4.50509	-0.45082	-0.09911
C	2.678214	-1.04903	-1.60521	C	-2.803198	-0.865272	1.71112	C	-2.80211	-0.86739	1.710246
N	2.192998	-1.953731	-2.13693	N	-2.364203	-1.646729	2.441425	N	-2.36275	-1.65021	2.438869
H	0.357179	1.152391	1.66497	H	-0.329088	1.090426	-1.7143	H	-0.32953	1.091048	-1.7138
H	0.004372	-1.278078	1.207083	H	0.114393	-1.302831	-1.29325	H	0.113518	-1.3028	-1.2926
H	0.240219	-1.098694	-0.54306	H	-0.225783	-1.175344	0.443568	H	-0.22587	-1.17495	0.444345
H	-1.666804	0.19546	2.417096	H	1.794458	0.268135	-2.37561	H	1.793232	0.267564	-2.37605
H	-2.6122	1.395311	1.517588	H	2.634645	1.480373	-1.39675	H	2.634199	1.479874	-1.3979
H	-1.094794	0.688218	-1.82719	H	0.963053	0.623004	1.839058	H	0.964152	0.62349	1.838961
H	-2.289659	1.666194	-0.96071	H	2.16652	1.67033	1.071117	H	2.167407	1.670427	1.07015
H	-0.653185	3.168004	1.601132	H	0.508227	3.147161	-1.69082	H	0.509237	3.147481	-1.68982
H	-3.975951	-0.627973	2.009412	H	4.111119	-0.469537	-1.85387	H	4.11002	-0.47045	-1.85543
H	-3.394312	-0.159037	-2.22716	H	3.270426	-0.137441	2.352335	H	3.271642	-0.13734	2.351156
H	-2.10806	-2.305088	2.069875	H	2.320435	-2.21064	-2.06521	H	2.318892	-2.2113	-2.06543
H	-3.368757	-2.821392	0.942214	H	3.53836	-2.710627	-0.87907	H	3.537294	-2.71124	-0.87982
H	-1.520418	-1.817309	-2.14339	H	1.482124	-1.872996	2.122139	H	1.482808	-1.87244	2.122265
H	-3.018	-2.547068	-1.53722	H	3.043386	-2.516806	1.581225	H	3.043608	-2.51683	1.580682
H	-0.365414	-3.417184	-0.7325	H	0.474981	-3.484529	0.60154	H	0.476273	-3.48484	0.604202
H	-4.419979	0.636588	-0.09588	H	4.379324	0.755867	0.30302	H	4.379663	0.755323	0.30108
H	-4.730558	-1.088261	-0.32753	H	4.750674	-0.960949	0.511993	H	4.750733	-0.96153	0.510171
H	2.311188	0.652177	2.294808	H	-2.167053	0.345061	-2.36845	H	-2.16862	0.348209	-2.36792
H	3.49044	0.875256	-1.57006	H	-3.640339	1.001848	1.327861	H	-3.63916	1.000508	1.33039
H	4.659358	-0.486808	2.205132	H	-4.507544	-0.805705	-2.31105	H	-4.50911	-0.8026	-2.31035
H	2.608974	-1.892194	2.549615	H	-2.422555	-2.213823	-2.35717	H	-2.42436	-2.21075	-2.35951
H	2.389688	-2.063777	0.743941	H	-2.339206	-2.178624	-0.5294	H	-2.3396	-2.17769	-0.53179

Table S23. Cont.

In gas phase				In water				In Formic acid			
H	5.22597	0.459099	−0.00566	H	−5.249513	0.332427	−0.24883	H	−5.24951	0.333575	−0.24645
H	4.983867	−1.235654	−0.46362	H	−4.988202	−1.292832	0.40032	H	−4.98825	−1.2925	0.400734
C	−0.693289	3.62101	−0.34861	C	0.620633	3.609661	0.255084	C	0.620934	3.609724	0.25617
H	−0.454666	3.194454	−1.33269	H	0.46475	3.171392	1.2485	H	0.464378	3.171441	1.249486
O	−1.149893	4.732454	−0.18049	O	0.970726	4.767669	0.078604	O	0.971805	4.767444	0.07981

Table S24. Coordinates of TS_1.

In gas phase				In water			
O	2.35815	-2.8031	-0.6736	O	2.27813	-2.9147	-0.4122
O	-1.4458	0.94446	1.63491	O	-1.4479	0.97614	1.56621
N	-2.028	-0.4753	-0.0083	N	-2.0657	-0.4209	-0.0813
N	-1.0165	-2.7747	2.26887	N	-1.3488	-2.6365	2.39672
C	-1.8362	3.23103	-0.6506	C	-1.6714	3.31678	-0.6583
C	1.11985	0.68467	-0.1875	C	1.1429	0.64168	-0.2224
C	2.49721	-1.4331	-0.3405	C	2.45733	-1.5195	-0.2113
C	3.53606	0.76581	-0.9444	C	3.54347	0.58679	-1.0201
O	-2.6401	2.39573	-1.0605	O	-2.565	2.56369	-1.0439
C	2.9893	0.25719	1.44789	C	3.02741	0.30183	1.4166
O	-2.0009	3.69536	0.94368	O	-1.7641	3.79057	1.00861
C	1.11027	-0.821	-0.5158	C	1.08427	-0.8857	-0.421
C	2.13563	1.3729	-1.1247	C	2.15875	1.21769	-1.2334
N	-0.4061	2.6866	-0.23	N	-0.311	2.67789	-0.2781
C	1.58938	0.86716	1.26974	C	1.64168	0.9338	1.20718
C	3.48903	-0.7321	-1.2747	C	3.44912	-0.9323	-1.2202
C	2.93823	-1.2433	1.11508	C	2.93197	-1.218	1.21467
C	3.98564	0.95527	0.51162	C	4.02461	0.88772	0.40685
C	-0.3012	1.24536	-0.4519	C	-0.2646	1.23073	-0.5069
C	-2.2085	-0.8912	-1.3768	C	-2.1303	-0.9571	-1.4225
C	-3.2161	-1.9996	-1.3644	C	-3.1953	-2.0105	-1.4235
C	-1.7768	-2.2971	-1.6921	C	-1.7506	-2.4047	-1.5677
C	-3.7119	-2.1741	0.06016	C	-3.8337	-2.0353	-0.047
C	-1.3275	0.58253	0.46873	C	-1.3221	0.60173	0.40038

Table S24. Cont.

In gas phase				In water			
C	-2.7609	-1.3165	0.93436	C	-2.9057	-1.1764	0.84808
C	-1.7957	-2.1377	1.70026	C	-2.0414	-1.9962	1.72826
H	-1.6987	4.22712	-1.1019	H	-1.4897	4.31942	-1.071
H	-2.6037	3.03632	1.32439	H	-2.3766	3.14345	1.3941
H	-0.8888	3.12097	0.84448	H	-0.692	3.11985	0.8096
H	0.35375	3.2048	-0.6627	H	0.47053	3.16553	-0.7115
H	4.23489	1.27241	-1.6196	H	4.24429	1.01117	-1.7467
H	3.30448	0.38996	2.48848	H	3.36495	0.51501	2.43655
H	0.42408	-1.3588	0.14898	H	0.38947	-1.3418	0.29588
H	0.77442	-0.9906	-1.548	H	0.72603	-1.1276	-1.4304
H	1.80818	1.26904	-2.1684	H	1.80854	1.02769	-2.2563
H	2.20005	2.44682	-0.9021	H	2.25451	2.30443	-1.1131
H	1.6074	1.93506	1.52323	H	1.70061	2.01745	1.3684
H	0.88089	0.38992	1.95371	H	0.92957	0.53448	1.93704
H	3.17619	-0.8981	-2.3126	H	3.1092	-1.1724	-2.2349
H	4.48546	-1.1793	-1.1543	H	4.43399	-1.3968	-1.0784
H	3.92973	-1.6963	1.25959	H	3.91124	-1.6872	1.38055
H	2.2312	-1.7673	1.76925	H	2.22311	-1.6624	1.92432
H	4.99073	0.53777	0.64897	H	5.01913	0.45355	0.5653
H	4.04197	2.02421	0.7523	H	4.11282	1.97128	0.55221
H	-2.2414	-0.0871	-2.1017	H	-2.0237	-0.2403	-2.2259
H	-0.5566	1.03997	-1.4972	H	-0.5083	1.03841	-1.5562
H	-3.9463	-2.065	-2.1622	H	-3.8457	-2.1126	-2.2835
H	-1.159	-2.8083	-0.9581	H	-1.2452	-2.8791	-0.7305
H	-1.5468	-2.5366	-2.7243	H	-1.424	-2.7377	-2.5462
H	-3.7256	-3.2142	0.393	H	-3.96	-3.0405	0.35963
H	-4.7249	-1.7746	0.14291	H	-4.8144	-1.5586	-0.0912
H	-3.2929	-0.6863	1.65198	H	-3.459	-0.4893	1.49266
H	3.19031	-3.2438	-0.4633	H	3.13053	-3.3431	-0.2582

Table S25. Coordinates of TS_2.

In gas phase				In water			
O	2.341488	-2.79083	-0.70715	O	2.299019	-2.88689	-0.50266
O	-1.38681	0.787124	1.749763	O	-1.43712	0.875869	1.648531
C	-1.75331	3.437286	-0.4714	C	-1.63812	3.463552	-0.47251
N	-2.07886	-0.47475	0.02389	N	-2.06951	-0.44391	-0.05644
N	-0.9665	-2.91099	2.12009	N	-1.31724	-2.73946	2.339643
O	-1.99763	3.984739	0.701775	O	-1.79751	4.020432	0.733374
N	-0.43563	2.672672	-0.03994	N	-0.3426	2.671279	-0.12547
C	1.111196	0.686219	-0.14571	C	1.139185	0.6509	-0.18173
C	2.489682	-1.4242	-0.3651	C	2.471407	-1.4977	-0.25935
C	3.498552	0.784102	-0.98448	C	3.526761	0.642279	-1.01729
C	3.037376	0.251567	1.420441	C	3.052386	0.275708	1.416657
C	1.095441	-0.81517	-0.49017	C	1.090009	-0.86962	-0.42751
C	2.089602	1.3856	-1.11372	C	2.133308	1.266362	-1.19031
C	1.629869	0.856455	1.296362	C	1.658171	0.901497	1.249001
O	-2.68235	2.482008	-0.9062	O	-2.64275	2.573319	-0.86036
C	3.44708	-0.71128	-1.32579	C	3.442319	-0.87045	-1.26425
C	2.979223	-1.24609	1.07624	C	2.966643	-1.23805	1.167753
C	3.997407	0.962873	0.456715	C	4.028046	0.902632	0.410763
C	-0.32121	1.244968	-0.34681	C	-0.27875	1.236254	-0.42191
C	-2.21017	-0.88609	-1.35336	C	-2.11299	-0.95434	-1.40985
C	-3.20354	-2.00849	-1.37882	C	-3.16775	-2.01766	-1.44442
C	-1.75315	-2.28325	-1.67412	C	-1.71813	-2.39505	-1.58238
C	-3.72455	-2.20358	0.034093	C	-3.81668	-2.0795	-0.07415
C	-1.31523	0.518373	0.560842	C	-1.31404	0.551735	0.470421
C	-2.76498	-1.38885	0.935791	C	-2.89646	-1.24336	0.848735
C	-1.76691	-2.24472	1.618384	C	-2.01939	-2.08423	1.695977
H	-1.51323	4.078534	-1.33568	H	-1.43458	4.119054	-1.33133
H	-0.94361	3.132549	0.956338	H	-0.77037	3.168747	0.910607
H	0.392568	3.198128	-0.31397	H	0.477873	3.166266	-0.47297
H	-3.2543	2.372306	-0.13116	H	-3.13347	2.393813	-0.0437
H	4.171415	1.29981	-1.67873	H	4.212199	1.095751	-1.74099
H	3.387349	0.376286	2.450711	H	3.403926	0.459475	2.437558
H	0.431563	-1.36433	0.18854	H	0.409588	-1.3547	0.284656

Table S25. *Cont.*

In gas phase				In water			
H	0.730757	-0.97295	-1.51426	H	0.720185	-1.08316	-1.43887
H	1.727062	1.282669	-2.14565	H	1.76894	1.103039	-2.21284
H	2.156607	2.460257	-0.8955	H	2.221671	2.350067	-1.04127
H	1.654748	1.921387	1.56249	H	1.710549	1.979682	1.445846
H	0.945629	0.370654	1.998233	H	0.960459	0.472503	1.97594
H	3.100826	-0.87065	-2.35405	H	3.088529	-1.0812	-2.28074
H	4.448778	-1.15501	-1.24183	H	4.433032	-1.33081	-1.1525
H	3.97599	-1.69786	1.182957	H	3.952253	-1.70343	1.303476
H	2.296082	-1.77804	1.749133	H	2.273065	-1.71095	1.874153
H	5.008664	0.549627	0.555487	H	5.028714	0.473029	0.539925
H	4.056679	2.029782	0.705313	H	4.10897	1.981787	0.589027
H	-2.22769	-0.0836	-2.08045	H	-2.00299	-0.2234	-2.20001
H	-0.59313	1.103855	-1.39839	H	-0.52941	1.091337	-1.47739
H	-3.91549	-2.07718	-2.19276	H	-3.80945	-2.10711	-2.3123
H	-1.14626	-2.79911	-0.93469	H	-1.21664	-2.88418	-0.75143
H	-1.49541	-2.50269	-2.70426	H	-1.37806	-2.70174	-2.56486
H	-3.76865	-3.24955	0.344853	H	-3.94466	-3.09498	0.305486
H	-4.72836	-1.77959	0.112377	H	-4.79745	-1.60235	-0.11308
H	-3.28264	-0.81787	1.710578	H	-3.45537	-0.58722	1.519922
H	3.178888	-3.23457	-0.52582	H	3.15937	-3.31223	-0.38942

Table S26. Coordinates of Intermediate_1.

In gas phase				In water			
O	2.286211	-2.87873	-0.7626	O	2.268981	-2.93115	-0.60456
O	-1.59479	0.89553	1.6155	O	-1.507	0.808646	1.678319
N	-0.26147	2.664549	-0.02258	N	-0.25596	2.650044	0.017692
N	-2.06388	-0.50526	-0.07182	N	-2.08533	-0.47692	-0.06831
N	-1.36892	-2.84031	2.303914	N	-1.44519	-2.82762	2.303134
C	1.094028	0.601841	-0.14522	C	1.114473	0.592717	-0.13878
C	2.441808	-1.52506	-0.36715	C	2.440007	-1.55234	-0.30124
C	3.517273	0.685287	-0.8579	C	3.502342	0.617611	-0.9674
C	2.932409	0.072028	1.501449	C	3.02813	0.145014	1.447457
C	1.064183	-0.88686	-0.53157	C	1.058688	-0.91557	-0.44255
C	2.12875	1.316487	-1.03561	C	2.110336	1.248225	-1.11492
C	1.545822	0.71051	1.325997	C	1.637056	0.781288	1.300219
C	3.457215	-0.79718	-1.25417	C	3.414564	-0.88438	-1.27667
C	2.867392	-1.41012	1.100451	C	2.937886	-1.35643	1.134636
C	3.949066	0.80094	0.611532	C	4.005584	0.813267	0.470215
C	-0.29823	1.254934	-0.36972	C	-0.2836	1.239155	-0.34014
C	-2.04626	-1.04599	-1.41048	C	-2.0858	-0.97658	-1.42643
C	-1.36143	3.422866	-0.54454	C	-1.36384	3.395444	-0.51325
C	-3.11907	-2.0927	-1.47871	C	-3.1658	-2.01182	-1.51559
C	-1.67017	-2.49432	-1.54688	C	-1.72176	-2.42478	-1.59998
O	-1.26234	4.680957	0.048537	O	-1.26302	4.667361	0.05167
C	-3.82018	-2.12231	-0.13253	C	-3.86391	-2.07551	-0.16962
C	-1.37454	0.538861	0.459533	C	-1.3449	0.509837	0.49328
O	-2.63621	2.866589	-0.3144	O	-2.63313	2.837485	-0.26127
C	-2.90874	-1.30423	0.814891	C	-2.95421	-1.27684	0.79576
C	-2.05503	-2.16378	1.665526	C	-2.11793	-2.14954	1.651717
H	-0.26158	2.764848	0.991996	H	-0.2762	2.73379	1.034443
H	-1.28193	3.470086	-1.63991	H	-1.29174	3.417761	-1.60844
H	-2.08236	5.144746	-0.15655	H	-2.05135	5.157205	-0.21502
H	-2.68201	2.652861	0.631073	H	-2.70654	2.708868	0.697544
H	4.236285	1.209335	-1.49777	H	4.19262	1.096871	-1.67042
H	3.232948	0.1538	2.551824	H	3.378801	0.284338	2.475978
H	0.365054	-1.44587	0.101945	H	0.376667	-1.43017	0.247925

Table S26. *Cont.*

In gas phase				In water			
H	0.743434	-1.0125	-1.57457	H	0.690675	-1.08898	-1.46225
H	1.816612	1.241047	-2.08711	H	1.748507	1.118624	-2.1442
H	2.149738	2.379664	-0.77837	H	2.153766	2.323344	-0.91375
H	1.594351	1.766696	1.619526	H	1.702559	1.852142	1.529684
H	0.818244	0.219658	1.982609	H	0.937362	0.330717	2.013688
H	3.158052	-0.91292	-2.30303	H	3.06191	-1.05154	-2.30184
H	4.44491	-1.26582	-1.13847	H	4.403184	-1.35439	-1.18294
H	3.850936	-1.8831	1.235382	H	3.922129	-1.83081	1.248764
H	2.146251	-1.9545	1.722074	H	2.243816	-1.85658	1.821805
H	4.947596	0.366006	0.745428	H	5.005859	0.376986	0.581641
H	4.010864	1.856813	0.901543	H	4.086947	1.883463	0.696083
H	-1.87842	-0.33332	-2.20775	H	-1.91587	-0.24639	-2.2067
H	-0.53191	1.178232	-1.43931	H	-0.52788	1.168883	-1.40631
H	-3.72838	-2.18727	-2.36983	H	-3.777	-2.07653	-2.40739
H	-1.21061	-2.98573	-0.69406	H	-1.26682	-2.93742	-0.75668
H	-1.29032	-2.81754	-2.50953	H	-1.34895	-2.72682	-2.57207
H	-3.98825	-3.13059	0.251749	H	-4.03116	-3.0928	0.189624
H	-4.78643	-1.61886	-0.21388	H	-4.83007	-1.57185	-0.23407
H	-3.46499	-0.64	1.480373	H	-3.51861	-0.62147	1.462848
H	3.122846	-3.33055	-0.5978	H	3.132191	-3.35719	-0.51915

Table S27. Coordinates of TS_3.

In gas phase				In water			
O	2.443526	-2.7508	-0.78418	O	2.440836	-2.81222	-0.69318
O	-1.62625	0.836377	1.578884	O	-1.60437	0.839518	1.566172
N	-0.41052	2.639616	-0.07263	N	-0.37755	2.621461	-0.1146
N	-2.02217	-0.59944	-0.10091	N	-2.03988	-0.57805	-0.12105
N	-1.23238	-2.84665	2.320205	N	-1.3781	-2.77308	2.380398
C	1.089594	0.662414	-0.14278	C	1.106929	0.633798	-0.15211
C	2.534326	-1.39805	-0.36939	C	2.535147	-1.44285	-0.32542
C	3.515622	0.865777	-0.81433	C	3.531043	0.79823	-0.84148
C	2.920486	0.195098	1.527425	C	2.94513	0.202026	1.521078
C	1.133186	-0.8196	-0.54729	C	1.135903	-0.86071	-0.51538
C	2.102884	1.43835	-1.0062	C	2.122325	1.376497	-1.04245
C	1.507636	0.771861	1.338713	C	1.535008	0.782556	1.323185
C	3.52783	-0.61212	-1.23156	C	3.52887	-0.69115	-1.21644
C	2.929422	-1.28301	1.106599	C	2.942448	-1.28693	1.143313
C	3.917104	0.980963	0.663595	C	3.942626	0.954646	0.629535
C	-0.33311	1.229286	-0.39761	C	-0.31259	1.203863	-0.42135
C	-1.94323	-1.17315	-1.42525	C	-1.95841	-1.16147	-1.44445
C	-1.42324	3.378727	-0.62685	C	-1.39002	3.367411	-0.64268
C	-2.95722	-2.27693	-1.49015	C	-2.99745	-2.23957	-1.51645
C	-1.48842	-2.60295	-1.51466	C	-1.5384	-2.60332	-1.51126
O	-1.64691	4.581477	-0.16886	O	-1.53561	4.607921	-0.21837
C	-3.68785	-2.30967	-0.1596	C	-3.74999	-2.25132	-0.19839
C	-1.38387	0.474446	0.429507	C	-1.37427	0.471699	0.411063
O	-3.03935	2.870763	-0.04189	O	-2.97973	2.967988	0.063723
C	-2.83979	-1.42725	0.788202	C	-2.90797	-1.36975	0.755515
C	-1.95168	-2.22178	1.665929	C	-2.06257	-2.15967	1.679131
H	-0.28974	2.846418	0.914644	H	-0.183	2.8574	0.85397
H	-1.59851	3.137161	-1.68335	H	-1.63213	3.100499	-1.677
H	-2.69992	4.049556	0.121973	H	-2.56811	4.12593	0.190729
H	-2.90324	2.392352	0.792522	H	-2.81388	2.462896	0.877917
H	4.219174	1.431298	-1.43527	H	4.234921	1.338377	-1.48382
H	3.199178	0.276958	2.583534	H	3.230126	0.313133	2.572771
H	0.449775	-1.4148	0.069503	H	0.4456	-1.42944	0.120649

Table S27. Cont.

In gas phase				In water			
H	0.833769	-0.94609	-1.59638	H	0.828328	-1.01034	-1.55854
H	1.810271	1.36838	-2.06333	H	1.822228	1.282021	-2.09475
H	2.080015	2.498736	-0.73405	H	2.114155	2.443242	-0.79432
H	1.503018	1.823664	1.653546	H	1.541513	1.841634	1.611719
H	0.793752	0.236849	1.975056	H	0.82138	0.267886	1.976638
H	3.249098	-0.72638	-2.2861	H	3.240788	-0.8285	-2.26578
H	4.533994	-1.0365	-1.10787	H	4.531251	-1.12068	-1.08631
H	3.931081	-1.71174	1.253414	H	3.94036	-1.71982	1.294905
H	2.223971	-1.86772	1.709176	H	2.236166	-1.84706	1.768834
H	4.931146	0.588073	0.808319	H	4.953523	0.556909	0.7804
H	3.928733	2.034478	0.968154	H	3.962622	2.016565	0.902754
H	-1.79292	-0.47417	-2.23807	H	-1.77415	-0.47565	-2.26074
H	-0.54251	1.129904	-1.46951	H	-0.51716	1.091858	-1.49162
H	-3.53899	-2.42653	-2.39199	H	-3.56599	-2.38023	-2.42744
H	-1.02467	-3.05042	-0.64026	H	-1.1099	-3.05325	-0.62003
H	-1.06783	-2.92696	-2.46003	H	-1.10799	-2.94469	-2.44579
H	-3.8159	-3.3158	0.244971	H	-3.89808	-3.25195	0.212097
H	-4.67442	-1.85515	-0.27478	H	-4.72812	-1.78558	-0.32944
H	-3.44386	-0.78287	1.430701	H	-3.52028	-0.70454	1.367851
H	3.2947	-3.17039	-0.6088	H	3.31296	-3.20861	-0.56548

Table S28. Coordinates of HCOOH.

In gas phase				In water				In formic acid			
C	0.129858	0.360338	0	C	0.12326	0.367486	-0.000001	C	0.123121	0.367493	0
H	0.039598	1.462359	0.000001	H	0.035469	1.464785	0.000001	H	0.036408	1.464629	0.000001
O	1.172492	-0.218756	-0.000005	O	1.17076	-0.220222	-0.000006	O	1.170678	-0.220278	-0.000005
O	-1.052962	-0.279368	0.000005	O	-1.045038	-0.28181	0.000005	O	-1.044977	-0.281736	0.000005
H	-1.774981	0.360601	0.000009	H	-1.780803	0.346551	0.000009	H	-1.780743	0.346527	0.000009

Table S29. Coordinates of H₂O.

In gas phase				In water				In formic acid			
O	0	0	0.117793	O	0	0	0.119033	O	0	0	0.119023
H	0	0.76021	-0.471173	H	0	0.757444	-0.476131	H	0	0.757468	-0.476091
H	0	-0.76021	-0.471173	H	0	-0.757444	-0.476131	H	0	-0.757468	-0.476091

Table S30. Coordinates of HCOO⁻.

In gas phase				In water			
C	0	0.31016	0	C	0	0.323748	0
H	0.000649	1.456865	0	H	0.000305	1.454616	0
O	1.135822	-0.207748	0	O	1.12966	-0.212518	0
O	-1.135904	-0.20698	0	O	-1.129698	-0.21212	0

Table S31. Coordinates of HCOOH⁺.

In gas phase				In water			
C	0.00007	0.396905	-0.000076	C	0.000003	0.395295	0.000283
H	0.000034	1.490371	0.000088	H	-0.000001	1.484885	-0.000042
O	1.07207	-0.273526	0.000005	O	1.072924	-0.275841	-0.000066
H	1.893671	0.252167	0.000145	H	1.87526	0.278396	-0.000295
O	-1.072119	-0.273495	0.000006	O	-1.072926	-0.275841	-0.000067
H	-1.893727	0.25219	0.000141	H	-1.875257	0.278403	-0.000298

Table S32. Coordinates of Intermediate_2.

In gas phase				In water				In formic acid			
O	2.469636	-2.661312	-0.793752	O	2.460693	-2.761573	-0.719978	O	2.461147	-2.76046	-0.72231
O	-1.698173	1.017351	1.433986	O	-1.57868	1.010494	1.497341	O	-1.58022	1.011394	1.496116
N	-1.991846	-0.620071	-0.091125	N	-1.987263	-0.541876	-0.086566	N	-1.98715	-0.54234	-0.08687
N	-0.896217	-2.532594	2.419533	N	-1.314795	-2.640639	2.483095	N	-1.31374	-2.64012	2.48346
C	-1.872596	3.356466	-0.404485	C	-1.776429	3.350088	-0.407737	C	-1.77667	3.35042	-0.4083
C	1.076469	0.728245	-0.193817	C	1.142353	0.686824	-0.18004	C	1.141951	0.687072	-0.17992
C	2.557433	-1.315291	-0.376174	C	2.563855	-1.397842	-0.342416	C	2.563963	-1.39714	-0.34335
C	3.519879	0.958439	-0.798118	C	3.579781	0.838215	-0.827103	C	3.579822	0.839556	-0.82526
C	2.860623	0.286353	1.528162	C	2.944136	0.234407	1.521346	C	2.942694	0.233413	1.522213

Table S32. Cont.

In gas phase				In water				In formic acid			
O	-2.496808	3.567484	0.775826	O	-2.352418	3.601351	0.798162	O	-2.35309	3.601688	0.797344
C	1.15427	-0.752807	-0.59467	C	1.170932	-0.807279	-0.555708	C	1.17109	-0.80664	-0.55695
C	2.104644	1.518749	-1.033065	C	2.178492	1.430177	-1.051378	C	2.178574	1.431484	-1.04983
N	-0.503286	2.670363	-0.154454	N	-0.394829	2.680471	-0.18323	N	-0.3953	2.680605	-0.18348
C	1.441555	0.84289	1.302493	C	1.538482	0.822908	1.305825	C	1.537024	0.821793	1.306355
C	3.560643	-0.518223	-1.215816	C	3.575838	-0.647449	-1.212539	C	3.576361	-0.64574	-1.21213
C	2.901618	-1.192422	1.11205	C	2.940939	-1.252165	1.135323	C	2.940029	-1.25279	1.134785
C	3.869517	1.085905	0.691688	C	3.961262	0.986993	0.652546	C	3.960267	0.986997	0.654786
C	-0.365934	1.212981	-0.514434	C	-0.286497	1.212963	-0.489302	C	-0.28685	1.213098	-0.48971
C	-1.900586	-1.278234	-1.380501	C	-1.937227	-1.152892	-1.399578	C	-1.93602	-1.15444	-1.39934
C	-2.841418	-2.449136	-1.340464	C	-2.983576	-2.226154	-1.422055	C	-2.98198	-2.22814	-1.42159
C	-1.359977	-2.681911	-1.389699	C	-1.52768	-2.59847	-1.435317	C	-1.52598	-2.59992	-1.4338
C	-3.526212	-2.454713	0.015492	C	-3.714491	-2.200215	-0.092125	C	-3.71353	-2.20145	-0.09198
C	-1.427919	0.514425	0.3358	C	-1.353691	0.544092	0.374222	C	-1.35434	0.544213	0.373496
C	-2.733662	-1.4462	0.880327	C	-2.858453	-1.294246	0.826165	C	-2.85795	-1.29489	0.826125
C	-1.736683	-2.074843	1.771893	C	-2.007198	-2.053937	1.767367	C	-2.00635	-2.05398	1.767495
H	-1.648358	4.334128	-0.84133	H	-1.574376	4.308514	-0.88838	H	-1.57438	4.308916	-0.88877
H	-2.647412	2.708509	1.217345	H	-2.540652	2.751191	1.236842	H	-2.54065	2.751533	1.236389
H	-0.353207	2.735845	0.862372	H	-0.179015	2.826176	0.811113	H	-0.17986	2.825985	0.811016
H	0.242374	3.190632	-0.62387	H	0.310373	3.18449	-0.728845	H	0.310205	3.184582	-0.72873
H	4.228193	1.535966	-1.400226	H	4.294008	1.381568	-1.45367	H	4.29436	1.383636	-1.45084
H	3.102521	0.377026	2.591311	H	3.207705	0.339836	2.578456	H	3.205531	0.3379	2.579591
H	0.471132	-1.348177	0.017927	H	0.470078	-1.37398	0.068185	H	0.470013	-1.37402	0.066006
H	0.878747	-0.892575	-1.648163	H	0.879543	-0.950394	-1.604097	H	0.880323	-0.94888	-1.60564
H	1.844806	1.460097	-2.098862	H	1.897094	1.355239	-2.109389	H	1.897884	1.357649	-2.10813
H	2.121039	2.582558	-0.748036	H	2.218867	2.496132	-0.7907	H	2.218688	2.497183	-0.78793
H	1.422572	1.891868	1.635634	H	1.548591	1.876883	1.614976	H	1.546593	1.875485	1.61657
H	0.720188	0.290723	1.915579	H	0.813866	0.302395	1.941503	H	0.812139	0.30047	1.941053
H	3.312776	-0.637504	-2.277066	H	3.305836	-0.777264	-2.267277	H	3.30707	-0.77463	-2.26716
H	4.570069	-0.921624	-1.066889	H	4.574049	-1.080132	-1.067186	H	4.574578	-1.07834	-1.0666
H	3.903063	-1.603217	1.295015	H	3.933617	-1.689037	1.304966	H	3.932695	-1.6896	1.304668
H	2.186539	-1.7859	1.693987	H	2.219882	-1.812807	1.742786	H	2.218718	-1.81419	1.741216
H	4.882287	0.707359	0.86741	H	4.965992	0.582167	0.820224	H	4.964943	0.582186	0.822739

Table S32. Cont.

In gas phase				In water				In formic acid			
H	3.864168	2.140467	0.994251	H	3.983523	2.047316	0.930971	H	3.982221	2.047063	0.934223
H	-1.820162	-0.618989	-2.236663	H	-1.770641	-0.481535	-2.231958	H	-1.76906	-0.48372	-2.23217
H	-0.560121	1.130423	-1.585297	H	-0.490498	1.10903	-1.555107	H	-0.49039	1.109284	-1.55565
H	-3.439003	-2.692606	-2.210649	H	-3.569039	-2.383333	-2.319358	H	-3.56712	-2.38639	-2.31892
H	-0.848166	-3.04882	-0.504542	H	-1.085162	-3.026472	-0.539902	H	-1.08356	-3.0274	-0.5381
H	-0.940079	-3.033557	-2.325368	H	-1.115894	-2.965794	-2.368116	H	-1.11365	-2.96752	-2.36625
H	-3.549568	-3.440825	0.483435	H	-3.854082	-3.189262	0.347748	H	-3.85318	-3.19027	0.348401
H	-4.553345	-2.099585	-0.088857	H	-4.694639	-1.738471	-0.219871	H	-4.69371	-1.73994	-0.22045
H	-3.376157	-0.808425	1.490549	H	-3.460946	-0.600138	1.415788	H	-3.46068	-0.60087	1.415597
H	3.308923	-3.099231	-0.604489	H	3.323212	-3.17232	-0.57354	H	3.323464	-3.17147	-0.57548
O	-2.510438	2.503419	-1.282006	O	-2.449387	2.459102	-1.212158	O	-2.44935	2.459591	-1.21319
H	-3.388092	2.861964	-1.474598	H	-3.279722	2.863213	-1.501163	H	-3.28047	2.863121	-1.50078

Table S33. Coordinates of TS_4.

In gas phase				In water				In formic acid			
O	2.344187	-2.890787	-0.529863	O	2.311411	-2.968168	-0.364081	O	2.312971	-2.96734	-0.36769
O	-1.807959	1.253069	1.095345	O	-1.696562	1.178365	1.245931	O	-1.69822	1.179402	1.243825
N	-2.022422	-0.569183	-0.207146	N	-2.014441	-0.531016	-0.183919	N	-2.01413	-0.5317	-0.18438
N	-1.216076	-2.238859	2.579506	N	-1.637996	-2.401554	2.62163	N	-1.63868	-2.39891	2.623598
C	-1.504696	3.499413	-0.548331	C	-1.437079	3.479458	-0.604342	C	-1.43752	3.47943	-0.60509
C	1.065502	0.592275	-0.338269	C	1.127515	0.571961	-0.290243	C	1.127329	0.572019	-0.29028
C	2.46479	-1.515116	-0.231495	C	2.465173	-1.571682	-0.158603	C	2.465909	-1.57116	-0.16004
C	3.552757	0.669748	-0.785879	C	3.581003	0.540661	-0.898147	C	3.581548	0.542751	-0.89541
C	2.710681	0.243098	1.53753	C	2.879185	0.264852	1.494854	C	2.877131	0.2634	1.496364
O	-1.227061	3.900948	0.876439	O	-1.25652	4.091599	0.745658	O	-1.25688	4.091181	0.745204
C	1.104462	-0.920637	-0.598879	C	1.10294	-0.956409	-0.479905	C	1.103715	-0.95609	-0.48196
C	2.184512	1.261324	-1.166749	C	2.210492	1.153469	-1.226346	C	2.211103	1.155333	-1.22432
N	-0.298427	2.629028	-0.622378	N	-0.242461	2.619181	-0.424134	N	-0.24284	2.619083	-0.42541
C	1.336364	0.827194	1.161503	C	1.504575	0.875366	1.173786	C	1.502579	0.873706	1.174567
C	3.557727	-0.839711	-1.064758	C	3.523656	-0.980288	-1.09314	C	3.525163	-0.97795	-1.09254
C	2.715564	-1.267844	1.2602	C	2.822706	-1.256467	1.297503	C	2.821583	-1.2577	1.29691
C	3.80821	0.92302	0.707022	C	3.941487	0.86134	0.559629	C	3.940217	0.861659	0.563189

Table S33. *Cont.*

In gas phase			In water			In formic acid					
C	-0.330492	1.153555	-0.780934	C	-0.268838	1.165822	-0.670531	C	-0.26896	1.165585	-0.67139
C	-1.906304	-1.391706	-1.398354	C	-1.907217	-1.284491	-1.418633	C	-1.90607	-1.28625	-1.41838
C	-2.939099	-2.478241	-1.286927	C	-3.012208	-2.297935	-1.41389	C	-3.01066	-2.30016	-1.41322
C	-1.481412	-2.820258	-1.204183	C	-1.583849	-2.744271	-1.276221	C	-1.5822	-2.74576	-1.27455
C	-3.695098	-2.273202	0.014485	C	-3.829583	-2.094008	-0.152007	C	-3.82861	-2.09557	-0.1518
C	-1.447817	0.599919	0.0969	C	-1.380336	0.588185	0.202609	C	-1.38087	0.58817	0.201391
C	-2.874064	-1.22681	0.805273	C	-2.982067	-1.14906	0.733737	C	-2.98206	-1.14925	0.733394
C	-1.976695	-1.807832	1.823997	C	-2.240259	-1.854119	1.80106	C	-2.24058	-1.85268	1.801976
H	-1.363728	4.402527	-1.138864	H	-1.295616	4.255493	-1.350837	H	-1.29592	4.255876	-1.35115
H	-1.825865	3.417401	1.480993	H	-2.060447	4.133114	1.297258	H	-2.06062	4.130705	1.297222
H	-0.32463	3.185772	0.652989	H	-0.4899	3.219677	0.829546	H	-0.48987	3.219396	0.82828
H	0.379903	3.017919	-1.273542	H	0.547211	3.039282	-0.911077	H	0.546688	3.039133	-0.91263
H	4.325195	1.160918	-1.386033	H	4.329271	0.971448	-1.571148	H	4.330338	0.974842	-1.567
H	2.885129	0.421846	2.602862	H	3.131339	0.491935	2.535733	H	3.127958	0.489194	2.537836
H	0.36003	-1.432019	0.017204	H	0.367127	-1.415983	0.189905	H	0.367503	-1.41691	0.186515
H	0.892807	-1.149156	-1.651865	H	0.830347	-1.216971	-1.510275	H	0.832315	-1.21548	-1.51294
H	1.993975	1.118052	-2.239874	H	1.942235	0.952508	-2.271378	H	1.944211	0.955731	-2.26998
H	2.226479	2.341098	-0.968313	H	2.295951	2.241058	-1.107397	H	2.29602	2.242789	-1.10363
H	1.330962	1.901057	1.392941	H	1.54275	1.957567	1.341609	H	1.540042	1.955723	1.343833
H	0.555849	0.352842	1.768963	H	0.744286	0.465099	1.849581	H	0.741773	0.462173	1.849016
H	3.378252	-1.047787	-2.126021	H	3.267221	-1.232714	-2.128903	H	3.270099	-1.22914	-2.12894
H	4.535769	-1.264985	-0.806071	H	4.500923	-1.428436	-0.870914	H	4.5024	-1.42589	-0.86978
H	3.68389	-1.698352	1.547369	H	3.793112	-1.70903	1.540761	H	3.791931	-1.71007	1.540739
H	1.938932	-1.77855	1.841909	H	2.068733	-1.708597	1.953559	H	2.067092	-1.71108	1.951488
H	4.789962	0.527082	0.988898	H	4.927137	0.445647	0.799673	H	4.925789	0.446122	0.803787
H	3.825433	2.000834	0.910497	H	3.999878	1.947206	0.70124	H	3.997978	1.94736	0.706344
H	-1.712803	-0.85869	-2.320809	H	-1.634882	-0.721192	-2.301194	H	-1.63354	-0.72358	-2.30129
H	-0.494443	0.900557	-1.834718	H	-0.458257	0.969573	-1.731133	H	-0.45789	0.969059	-1.73205
H	-3.504969	-2.778113	-2.160699	H	-3.542464	-2.517031	-2.332254	H	-3.54048	-2.5203	-2.33159
H	-1.057666	-3.114687	-0.248315	H	-1.231408	-3.100355	-0.312228	H	-1.23001	-3.10089	-0.31012
H	-1.028392	-3.306478	-2.06063	H	-1.126855	-3.224502	-2.133671	H	-1.12457	-3.22656	-2.13134
H	-3.817912	-3.192191	0.590879	H	-4.064289	-3.02247	0.371505	H	-4.06283	-3.02373	0.372451
H	-4.685304	-1.862036	-0.191989	H	-4.765607	-1.590138	-0.397785	H	-4.76494	-1.59265	-0.39839

Table S33. Cont.

H	-3.499409	-0.479456	1.297525	H	-3.579694	-0.371168	1.213352	H	-3.58034	-0.37106	1.21171
H	3.154737	-3.336607	-0.253928	H	3.155687	-3.388549	-0.153674	H	3.157133	-3.38774	-0.1569
O	-2.727086	3.006132	-0.761192	O	-2.635303	2.897051	-0.764187	O	-2.63582	2.897371	-0.76522
H	-2.909719	2.280262	-0.139975	H	-2.81749	2.286163	-0.028477	H	-2.81774	2.285848	-0.02993

Table S34. Coordinates of Intermediate_3.

In gas phase				In water				In formic acid			
O	1.946267	-3.046597	-0.085228	O	2.086919	-3.067086	-0.042858	O	0.785864	-3.3649	-0.73969
O	-1.737088	1.857775	0.470484	O	-1.724141	1.840035	0.476068	O	-1.21881	1.616625	1.618345
N	-2.13428	-0.15166	-0.424965	N	-2.118308	-0.175978	-0.403801	N	-2.2579	0.599096	-0.1055
N	-2.136336	-1.13708	2.782324	N	-2.581278	-1.082357	2.845776	N	-2.60929	-1.76755	2.296918
C	-0.886522	3.070799	0.238951	C	-0.836729	3.052401	0.217299	C	1.171508	3.596119	-0.65757
C	1.143684	0.559206	-0.464044	C	1.17423	0.524411	-0.445226	C	1.107617	0.29765	-0.12319
C	2.237161	-1.667861	0.023076	C	2.316315	-1.669084	0.047198	C	1.473757	-2.18837	-0.3437
C	3.632081	0.260711	-0.762811	C	3.666567	0.285658	-0.750261	C	3.357475	-0.60634	-0.81857
C	2.644596	0.282738	1.543138	C	2.687795	0.295845	1.557455	C	2.554821	-0.9265	1.533744
C	0.986667	-0.966192	-0.508452	C	1.044457	-1.006186	-0.486668	C	0.47303	-1.04624	-0.52363
C	2.371957	0.952893	-1.310708	C	2.390133	0.944542	-1.294794	C	2.34837	0.538203	-1.00526
N	-0.187733	2.697804	-0.963057	N	-0.049933	2.665497	-0.913539	N	0.579054	2.730906	0.093913
C	1.386449	0.982376	0.997773	C	1.415259	0.964038	1.011588	C	1.544671	0.217891	1.353214
C	3.445013	-1.262648	-0.827645	C	3.513621	-1.241035	-0.806955	C	2.700736	-1.93331	-1.22432
C	2.456111	-1.239586	1.478555	C	2.534232	-1.230124	1.499228	C	1.898107	-2.25396	1.127341
C	3.857595	0.689963	0.694198	C	3.890638	0.723503	0.704289	C	3.786759	-0.67285	0.653795
C	-0.11584	1.242897	-1.08377	C	-0.080543	1.209277	-1.056441	C	0.070376	1.432263	-0.37083
C	-2.015694	-1.260936	-1.359339	C	-1.975792	-1.290774	-1.326927	C	-2.43779	0.097196	-1.45384
C	-3.247389	-2.105483	-1.188266	C	-3.247875	-2.080984	-1.25107	C	-3.84308	-0.41736	-1.54372
C	-1.915244	-2.62635	-0.74207	C	-1.977883	-2.650219	-0.691462	C	-2.68883	-1.37948	-1.58202
C	-4.138507	-1.443529	-0.151467	C	-4.195358	-1.374781	-0.299021	C	-4.52516	-0.15489	-0.21331
C	-1.386671	0.908431	-0.344828	C	-1.367969	0.88159	-0.321142	C	-1.20576	1.225192	0.452333
C	-3.255414	-0.373097	0.531522	C	-3.33084	-0.32667	0.441647	C	-3.38424	0.228175	0.759535
C	-2.659112	-0.800179	1.809118	C	-2.914663	-0.74649	1.792426	C	-2.96416	-0.88948	1.634261
H	-0.313377	3.177701	1.162213	H	-0.279265	3.157135	1.14648	H	1.310615	3.389612	-1.71534
H	0.704381	3.169575	-1.068528	H	-0.370178	3.135931	-1.754937	H	0.382134	2.915061	1.082076

Table S34. Cont.

In gas phase				In water				In formic acid			
H	4.489566	0.554725	-1.375718	H	4.517073	0.594073	-1.366923	H	4.228626	-0.41498	-1.45335
H	2.795135	0.592683	2.581756	H	2.83599	0.612482	2.594914	H	2.852464	-0.97045	2.586318
H	0.150295	-1.288486	0.120676	H	0.20929	-1.348204	0.135378	H	-0.40253	-1.26352	0.100989
H	0.80031	-1.318409	-1.532168	H	0.869617	-1.358251	-1.511947	H	0.143201	-1.02544	-1.5704
H	2.207902	0.665847	-2.357821	H	2.228772	0.643911	-2.338411	H	2.048156	0.604242	-2.05964
H	2.52341	2.040813	-1.288639	H	2.484128	2.035661	-1.27347	H	2.833268	1.484228	-0.7332
H	1.540471	2.067329	1.055941	H	1.545656	2.05159	1.046361	H	2.00891	1.163208	1.662208
H	0.519418	0.727346	1.625133	H	0.556445	0.698369	1.645546	H	0.673703	0.051897	1.996845
H	3.285056	-1.598766	-1.85884	H	3.355378	-1.580297	-1.837697	H	2.387137	-1.90977	-2.27482
H	4.344592	-1.76782	-0.4532	H	4.421925	-1.729569	-0.430069	H	3.412906	-2.76055	-1.10698
H	3.34338	-1.744392	1.881726	H	3.434576	-1.7166	1.896717	H	2.60249	-3.08462	1.267174
H	1.594382	-1.556967	2.078057	H	1.680543	-1.561249	2.103025	H	1.013458	-2.45812	1.74296
H	4.763627	0.215863	1.087034	H	4.807096	0.267057	1.096368	H	4.519253	-1.47646	0.792742
H	4.012038	1.77425	0.750256	H	4.017789	1.811389	0.753972	H	4.270124	0.266875	0.946572
H	-1.568977	-1.012458	-2.313533	H	-1.44964	-1.07038	-2.24601	H	-1.97649	0.672004	-2.24634
H	-0.190203	0.94305	-2.136443	H	-0.155633	0.932664	-2.11206	H	-0.13317	1.509939	-1.44126
H	-3.721915	-2.540446	-2.059577	H	-3.661775	-2.504179	-2.157447	H	-4.41626	-0.25508	-2.44806
H	-1.700086	-2.701281	0.320085	H	-1.856733	-2.715538	0.38625	H	-2.49447	-2.00949	-0.71837
H	-1.434462	-3.383801	-1.350552	H	-1.485173	-3.434019	-1.254471	H	-2.45118	-1.83169	-2.538
H	-4.535187	-2.144697	0.584983	H	-4.678414	-2.050136	0.40872	H	-5.09559	-1.00728	0.160099
H	-4.976809	-0.947396	-0.643983	H	-4.967333	-0.850654	-0.863211	H	-5.20053	0.696752	-0.30845
H	-3.780979	0.571258	0.691301	H	-3.827421	0.642399	0.524928	H	-3.64426	1.068464	1.406783
H	2.696819	-3.546989	0.258858	H	2.878167	-3.514888	0.284597	H	1.386507	-4.11171	-0.61606
O	-1.660545	4.159229	0.09748	O	-1.60847	4.143374	0.058361	O	1.633902	4.737941	-0.2685
H	-1.974951	4.199838	-0.818594	H	-2.132277	4.08108	-0.755212	H	1.521638	4.918875	0.681353

Table S35. Coordinates of Ethylene glycol.

In gas phase				In water			
C	-0.5736	0.49453	0.00006	C	-0.57533	0.492981	-0.00013
C	0.57357	-0.4945	-0.0017	C	0.575315	-0.4929	-0.00204
H	-0.4858	1.13562	0.88838	H	-0.49514	1.135195	0.887541
H	0.48683	-1.1372	0.88557	H	0.496376	-1.137	0.884405
H	0.48797	-1.1335	-0.8916	H	0.497919	-1.13244	-0.89179
H	-0.4891	1.13537	-0.8888	H	-0.49928	1.134539	-0.88863
O	1.76773	0.26036	0.0005	O	1.77181	0.262123	0.000823
H	2.51269	-0.3478	0.00331	H	2.513567	-0.35257	0.003236
O	-1.7677	-0.2604	0.00235	O	-1.77179	-0.26219	0.002848
H	-2.5127	0.34767	-0.0098	H	-2.51355	0.352342	-0.01112

Table S36. Coordinates of TS_formic acid1.

In gas phase			
C	1.115906	-0.311956	-0.01811
C	-0.376569	-0.157842	-0.359204
N	-2.59242	-1.109167	-0.218751
C	-3.596234	-2.139644	-0.091604
C	1.75748	-1.306064	-1.009522
C	1.824274	1.051657	-0.189849
C	-4.92324	-1.44355	-0.137632
C	1.341128	-0.810735	1.423072
C	-4.66319	0.052633	-0.311637
C	-1.26422	-1.404628	-0.189729
C	3.25982	-1.452522	-0.73202
C	3.329349	0.908836	0.078505
N	-1.04407	0.904473	0.440028
C	-2.485384	1.385527	-0.207539
C	2.848728	-0.946761	1.695952
N	-2.773559	2.566041	-0.250404
O	-0.842143	-2.531393	0.001901
O	-0.634763	3.53854	0.511963
C	3.944548	-0.098324	-0.900944

Table S36. *Cont.*

In gas phase			
C	3.455716	-1.951657	0.705348
O	3.854359	-2.331582	-1.669172
C	3.535005	0.414941	1.51853
H	-1.708154	3.296886	0.175856
H	-0.50063	1.789843	0.495069
H	-5.296734	0.496645	-1.079807
H	-3.379236	-3.079907	-0.58369
H	-5.755985	-1.896928	-0.661244
H	-4.832229	0.608205	0.615104
H	-0.450581	0.172712	-1.406158
H	1.626118	-0.949669	-2.0404
H	1.272184	-2.283505	-0.922805
H	1.658006	1.436303	-1.205769
H	-1.199689	0.580716	1.396844
H	1.434192	1.813231	0.496185
H	0.840502	-1.7738	1.56479
H	0.914282	-0.093446	2.139572
H	3.795315	1.890785	-0.049861
H	2.993819	-1.306836	2.720434
H	3.820189	0.234355	-1.938029
H	5.01884	-0.217361	-0.718372
H	2.976783	-2.934512	0.818731
H	4.528405	-2.081586	0.890407
H	3.437219	-3.196144	-1.566665
H	3.120546	1.142227	2.226992
H	4.606407	0.323361	1.733673
C	-4.446005	-2.077287	1.142524
H	-4.92564	-2.994567	1.464716
H	-4.117939	-1.419073	1.941153
C	-3.178159	0.144114	-0.721975
H	-3.107149	0.160167	-1.819307
C	0.077426	4.302588	-0.292177
H	-0.532845	4.963275	-0.938106
O	1.284556	4.30359	-0.33936

Table S37. Coordinates of TS_PEG.

In gas phase				In water			
C	1.271231	-0.389215	0.005184	C	1.231942	-0.46122	0.015893
C	-0.233612	-0.422128	-0.323601	C	-0.271159	-0.4392	-0.31851
N	-2.237262	-1.779172	-0.357724	N	-2.332703	-1.69669	-0.384
C	-3.038412	-2.978248	-0.362445	C	-3.196137	-2.85337	-0.38302
C	2.05266	-1.128188	-1.103029	C	1.979582	-1.23788	-1.09012
C	1.769626	1.073947	0.033279	C	1.781002	0.983477	0.023948
C	-4.463988	-2.530153	-0.243474	C	-4.591874	-2.33403	-0.22085
C	1.58098	-1.036168	1.370799	C	1.52596	-1.10415	1.386038
C	-4.47655	-1.00271	-0.185437	C	-4.522467	-0.80939	-0.14364
C	-0.88183	-1.823452	-0.341184	C	-0.987608	-1.80464	-0.33175
C	3.560374	-1.089468	-0.824008	C	3.488901	-1.24861	-0.81889
C	3.281889	1.120132	0.302244	C	3.295131	0.980903	0.284558
N	-1.044262	0.398726	0.611802	N	-1.056262	0.421946	0.61285
C	-2.53975	0.642075	0.129489	C	-2.495531	0.742499	0.090641
C	3.092536	-0.987173	1.644816	C	3.040661	-1.10404	1.650123
N	-3.080786	1.72478	0.332047	N	-2.965944	1.872454	0.238954
O	-0.260808	-2.873935	-0.30039	O	-0.415621	-2.88612	-0.26755
O	-0.99451	2.848477	1.043116	O	-0.870947	2.919842	1.036271
C	4.036531	0.360707	-0.795941	C	4.015271	0.184429	-0.81095
C	-0.603467	3.643129	-0.053411	C	-0.397101	3.682643	-0.04466
C	3.835462	-1.745984	0.534885	C	3.751671	-1.89921	0.544547
O	4.27589	-1.733843	-1.862268	O	4.173951	-1.93553	-1.85686
C	3.568899	0.47227	1.6648	C	3.567665	0.337735	1.652024
C	-1.393773	4.939538	-0.068773	C	-1.050142	5.054984	-0.04892
H	-2.087093	2.497166	0.823962	H	-1.985491	2.573161	0.740449
H	-0.738971	1.480375	0.795012	H	-0.675547	1.440677	0.795076
H	-5.213666	-0.572454	-0.863875	H	-5.260367	-0.33509	-0.79108
H	-2.69847	-3.779776	-1.007002	H	-2.925168	-3.658	-1.05554
H	-5.241339	-3.041339	-0.798338	H	-5.404572	-2.79603	-0.76727
H	-4.69874	-0.629564	0.818177	H	-4.685525	-0.44662	0.875196
H	-0.374277	0.030291	-1.316895	H	-0.390232	0.013842	-1.31291
H	1.865201	-0.654513	-2.076546	H	1.798861	-0.76714	-2.06594
H	1.71868	-2.168307	-1.160917	H	1.611161	-2.26661	-1.13611

Table S37. *Cont.*

In gas phase				In water			
H	-0.766175	3.124505	-1.01523	H	-0.602541	3.194457	-1.01535
H	1.539809	1.561197	-0.925287	H	1.560522	1.468243	-0.93764
H	-1.075356	-0.060352	1.524763	H	-1.136071	-0.03652	1.525119
H	1.257971	1.644627	0.818229	H	1.297167	1.578284	0.80841
H	1.228393	-2.071784	1.377022	H	1.139115	-2.12709	1.403793
H	1.058111	-0.490565	2.169905	H	1.024665	-0.53765	2.182907
H	3.605886	2.166479	0.315207	H	3.655629	2.015173	0.282935
H	3.295349	-1.458335	2.612875	H	3.233209	-1.57213	2.621326
H	3.860922	0.810909	-1.779986	H	3.844935	0.63403	-1.7967
H	5.117136	0.379404	-0.612217	H	5.097056	0.170715	-0.63142
H	3.504745	-2.79357	0.504979	H	3.388962	-2.93599	0.526888
H	4.916759	-1.742965	0.715749	H	4.833464	-1.92673	0.721953
H	3.972735	-2.649502	-1.902132	H	3.845822	-2.84447	-1.8704
H	3.054018	1.025035	2.460203	H	3.075835	0.916087	2.443552
H	4.643386	0.514029	1.880102	H	4.64418	0.343818	1.860819
H	-2.463985	4.700847	-0.158912	H	-2.140084	4.931708	-0.13496
H	-1.24004	5.452688	0.891147	H	-0.844111	5.547706	0.911562
C	-3.802401	-3.256271	0.898357	C	-3.941149	-3.10926	0.894655
H	-4.097744	-4.282117	1.087861	H	-4.286682	-4.12103	1.07419
H	-3.534445	-2.679447	1.778319	H	-3.620484	-2.55819	1.773673
C	-3.05146	-0.580172	-0.602209	C	-3.092572	-0.45875	-0.61046
H	-3.041223	-0.352306	-1.678203	H	-3.104893	-0.24048	-1.68709
H	0.466498	3.876012	0.015193	H	0.692849	3.807856	0.023756
O	-0.926625	5.702229	-1.16388	O	-0.520362	5.785894	-1.14015
H	-1.439146	6.514767	-1.210715	H	-0.925748	6.659796	-1.14142

Table S38. Coordinates of TS_water.

In gas phase				In water			
C	1.162427	0.099205	-0.085222	C	1.144494	0.101587	-0.07823
C	-0.333523	0.173616	-0.450586	C	-0.344498	0.195521	-0.4712
N	-2.489251	-0.89897	-0.211021	N	-2.506343	-0.8905	-0.32241
C	-3.433027	-1.962188	0.031147	C	-3.447296	-1.95736	-0.07741
C	1.85616	-0.947016	-0.984235	C	1.851172	-0.90094	-1.01768
C	1.834916	1.465593	-0.348288	C	1.824589	1.476819	-0.26801
C	-4.793906	-1.335833	-0.027306	C	-4.784179	-1.30166	0.090633
C	1.382976	-0.273422	1.395563	C	1.341754	-0.34118	1.385782
C	-4.615828	0.152132	-0.330555	C	-4.592202	0.204058	-0.09108
C	-1.150032	-1.104037	-0.158913	C	-1.17211	-1.08862	-0.26013
C	3.35648	-1.02541	-0.673047	C	3.345365	-0.99854	-0.68539
C	3.340519	1.390971	-0.047554	C	3.32493	1.384793	0.052026
N	-1.033957	1.291929	0.225611	N	-1.060743	1.284928	0.248809
C	-2.493742	1.585841	-0.336065	C	-2.459836	1.606228	-0.36376
C	2.888346	-0.344315	1.700765	C	2.842379	-0.43042	1.709182
N	-2.906923	2.738721	-0.405133	N	-2.818541	2.776192	-0.51866
O	-0.661808	-2.185827	0.129736	O	-0.687703	-2.18965	-0.0228
O	-0.718141	3.732019	0.193291	O	-0.64661	3.743743	0.175334
C	4.003307	0.331683	-0.936645	C	3.99975	0.367139	-0.87576
C	3.542476	-1.4039	0.801498	C	3.509031	-1.44815	0.771336
O	3.995693	-1.955229	-1.528904	O	3.994716	-1.89484	-1.57669
C	3.538554	1.018928	1.42942	C	3.49955	0.942	1.512262
H	-1.825009	3.501172	-0.059897	H	-1.751021	3.493652	-0.16316
H	-0.603051	2.359404	0.148181	H	-0.599378	2.322873	0.219732
H	-5.284888	0.492969	-1.121174	H	-5.355293	0.640773	-0.73598
H	-3.18268	-2.929507	-0.387543	H	-3.29222	-2.87927	-0.62453
H	-5.617974	-1.870539	-0.483992	H	-5.669943	-1.77208	-0.31761
H	-4.80243	0.777782	0.546724	H	-4.616047	0.73285	0.866483
H	-0.408252	0.381383	-1.528908	H	-0.396726	0.459539	-1.53694
H	1.733789	-0.675417	-2.042022	H	1.742604	-0.57608	-2.06153
H	1.398534	-1.928873	-0.83085	H	1.393004	-1.88906	-0.92007
H	1.671496	1.758849	-1.395707	H	1.674746	1.822056	-1.30069
H	-1.116943	1.085943	1.223448	H	-1.183347	1.028398	1.232336

Table S38. Cont.

In gas phase				In water			
H	1.390415	2.244942	0.281811	H	1.376886	2.226157	0.39419
H	0.907266	-1.235476	1.607825	H	0.863278	-1.3113	1.545626
H	0.923931	0.486731	2.044698	H	0.872127	0.384602	2.064249
H	3.790642	2.370169	-0.24445	H	3.779444	2.370585	-0.09322
H	3.026824	-0.618605	2.752406	H	2.964597	-0.75487	2.748221
H	3.887523	0.578153	-1.998765	H	3.898125	0.668353	-1.92543
H	5.077413	0.261921	-0.728445	H	5.070447	0.288787	-0.65129
H	3.088031	-2.387915	0.98323	H	3.053637	-2.43971	0.898987
H	4.615045	-1.488069	1.012758	H	4.578263	-1.54091	0.997092
H	3.598361	-2.820354	-1.368674	H	3.589748	-2.76481	-1.46148
H	3.090388	1.785238	2.073853	H	3.041901	1.677564	2.184887
H	4.609004	0.97892	1.664451	H	4.566136	0.887187	1.761726
C	-4.249786	-1.838937	1.283889	C	-4.105529	-1.94423	1.271692
H	-4.673243	-2.748781	1.694291	H	-4.508555	-2.88182	1.63775
H	-3.930258	-1.103413	2.015976	H	-3.676041	-1.29076	2.025267
C	-3.144787	0.290874	-0.773081	C	-3.196723	0.337894	-0.73924
H	-3.091388	0.242005	-1.870986	H	-3.305809	0.329587	-1.83203
H	-0.336775	4.209193	-0.552121	H	-0.178249	4.069569	-0.60367

Table S39. Coordinates of TS_formic_acid2.

In gas phase				In water				In formic acid			
C	1.317545	-0.185828	-0.296073	C	1.343527	-0.16644	-0.297472	C	1.34304	-0.16704	-0.29748
C	-0.144776	-0.464654	-0.698056	C	-0.123659	-0.455356	-0.678118	C	-0.12403	-0.45593	-0.67855
N	-2.221308	-1.590782	-0.138399	N	-2.179661	-1.599697	-0.101341	N	-2.18038	-1.59983	-0.10185
C	-3.151867	-2.288514	0.71557	C	-3.102789	-2.321273	0.742058	C	-3.10375	-2.32087	0.741763
C	2.139015	-1.477196	-0.490789	C	2.163005	-1.46498	-0.454435	C	2.162621	-1.46545	-0.45483
N	-0.945981	0.791369	-0.820107	N	-0.942124	0.78454	-0.791435	N	-0.94213	0.784267	-0.79264
C	1.897829	0.898492	-1.233251	C	1.919878	0.881252	-1.277353	C	1.919493	0.881152	-1.27678
C	-4.524376	-1.990329	0.204609	C	-4.471867	-2.094064	0.189783	C	-4.47288	-2.0924	0.190078
C	-2.618503	0.699205	-0.811562	C	-2.668299	0.653448	-0.835156	C	-2.66746	0.653929	-0.83441
C	1.468599	0.301714	1.162138	C	1.508553	0.372931	1.139717	C	1.507718	0.371714	1.139994
C	-4.396709	-1.114368	-1.033127	C	-4.345253	-1.254551	-1.071792	C	-4.3461	-1.25259	-1.0713

Table S39. Cont.

In gas phase				In water				In formic acid			
N	-3.276528	1.680131	-0.552164	N	-3.331319	1.635703	-0.624103	N	-3.33028	1.636098	-0.62184
C	-0.914749	-1.450314	0.204727	C	-0.881301	-1.43166	0.242355	C	-0.88195	-1.43214	0.241854
C	-1.239425	3.937409	0.636883	C	-1.413188	3.988153	0.668693	C	-1.41019	3.988836	0.667621
C	3.618809	-1.232705	-0.169552	C	3.644704	-1.21096	-0.15185	C	3.644243	-1.21147	-0.15184
C	3.38268	1.138909	-0.924041	C	3.406427	1.13225	-0.985638	C	3.405974	1.132103	-0.98468
C	2.95507	0.549163	1.471264	C	2.997196	0.627552	1.432387	C	2.996289	0.626332	1.433036
O	-2.449307	3.913405	0.22267	O	-2.556746	3.945103	0.067289	O	-2.55645	3.944629	0.07174
O	-0.430308	3.002689	0.639054	O	-0.659552	3.042248	0.878281	O	-0.65305	3.044298	0.871046
O	-0.403142	-2.081856	1.113696	O	-0.37056	-2.029082	1.181883	O	-0.37117	-2.02999	1.18102
C	-2.902879	-0.748384	-1.133743	C	-2.870271	-0.810621	-1.135366	C	-2.87081	-0.80984	-1.1353
C	4.172665	-0.162861	-1.108241	C	4.193979	-0.176396	-1.131651	C	4.193626	-0.17644	-1.13109
C	3.746148	-0.753532	1.280942	C	3.784242	-0.683359	1.280565	C	3.783461	-0.68445	1.280827
O	4.379436	-2.405452	-0.398144	O	4.402623	-2.398102	-0.33994	O	4.402279	-2.39843	-0.34032
C	3.510671	1.624355	0.527351	C	3.551531	1.665422	0.447103	C	3.550702	1.664695	0.448319
C	-4.072451	-1.410755	1.517995	C	-4.080883	-1.465485	1.500757	C	-4.08084	-1.46448	1.501047
H	-2.794731	2.90041	-0.14483	H	-2.841759	2.938832	-0.238445	H	-2.84115	2.93825	-0.2353
H	-0.709584	1.257999	-1.696301	H	-0.708474	1.279979	-1.652614	H	-0.70889	1.278344	-1.65473
H	-0.730165	1.512766	-0.083468	H	-0.776906	1.458303	-0.021785	H	-0.77545	1.459313	-0.02432
H	-0.923953	4.920311	1.022581	H	-1.14421	5.001587	1.004015	H	-1.14187	5.002023	1.004279
H	-4.702935	-1.6747	-1.919155	H	-4.584943	-1.861745	-1.946389	H	-4.58664	-1.85933	-1.94599
H	-2.82105	-3.254167	1.074371	H	-2.747867	-3.268867	1.124768	H	-2.74936	-3.26879	1.12416
H	-5.287547	-2.759537	0.210221	H	-5.198393	-2.897408	0.198196	H	-5.20009	-2.89513	0.198546
H	-4.990344	-0.198903	-0.972171	H	-4.996034	-0.377273	-1.06944	H	-4.99609	-0.37473	-1.06837
H	-0.131896	-0.916665	-1.700938	H	-0.121983	-0.911715	-1.677343	H	-0.12208	-0.91253	-1.67768
H	2.063534	-1.826635	-1.530173	H	2.073973	-1.846507	-1.480703	H	2.073883	-1.84657	-1.48129
H	1.744805	-2.263337	0.162198	H	1.777309	-2.229948	0.227384	H	1.776778	-2.2307	0.226592
H	1.775477	0.588703	-2.282761	H	1.788591	0.53522	-2.312242	H	1.788472	0.535577	-2.31188
H	-2.505345	-0.966925	-2.134892	H	-2.432502	-1.020733	-2.118685	H	-2.43353	-1.02	-2.11885
H	1.360482	1.845168	-1.090228	H	1.382583	1.832667	-1.171138	H	1.382106	1.832471	-1.17015
H	1.06526	-0.452077	1.842149	H	1.104521	-0.351338	1.851034	H	1.103674	-0.35293	1.850898
H	0.911804	1.234419	1.310939	H	0.95311	1.311797	1.25711	H	0.952187	1.310469	1.257719
H	3.769122	1.903257	-1.607183	H	3.789224	1.870953	-1.69774	H	3.788863	1.871133	-1.6964
H	3.047374	0.886582	2.50928	H	3.099355	0.999018	2.457793	H	3.098181	0.997379	2.458618

Table S39. Cont.

H	4.100832	-0.526698	-2.140483	H	4.109204	-0.571001	-2.151639	H	4.109112	-0.57066	-2.15124
H	5.235019	-0.009735	-0.885929	H	5.258088	-0.012817	-0.923099	H	5.257684	-0.01292	-0.92227
H	3.362099	-1.531212	1.955892	H	3.406818	-1.438182	1.983878	H	3.405951	-1.43957	1.983774
H	4.808084	-0.606224	1.511279	H	4.8473	-0.525297	1.499025	H	4.846477	-0.52645	1.499519
H	4.05826	-3.085431	0.207135	H	4.07348	-3.056643	0.286301	H	4.072412	-3.05761	0.284854
H	2.952527	2.559163	0.660321	H	3.004421	2.610547	0.551525	H	3.003408	2.60968	0.553051
H	4.562632	1.827794	0.761536	H	4.606691	1.86844	0.666394	H	4.605793	1.867766	0.6679
H	-4.495552	-1.830402	2.423367	H	-4.512921	-1.88301	2.402856	H	-4.51282	-1.8819	2.403222
H	-3.850694	-0.348077	1.555459	H	-3.896257	-0.395193	1.521515	H	-3.8954	-0.39434	1.521997

Table S40. Coordinates of SCA.

In gas phase				In water				In formic acid			
C	1.117437	0.265042	-0.163127	C	1.118075	0.259185	-0.153127	C	1.118087	0.259269	-0.153183
C	-0.369886	0.258572	-0.550878	C	-0.371447	0.252438	-0.533161	C	-0.37143	0.252545	-0.53323
C	1.795105	-0.987564	-0.757645	C	1.794107	-0.992449	-0.751696	C	1.794056	-0.992455	-0.751633
C	1.800924	1.504027	-0.783523	C	1.79356	1.499029	-0.781928	C	1.793673	1.499015	-0.782056
C	1.345041	0.278459	1.363783	C	1.357042	0.277209	1.371308	C	1.357021	0.277374	1.371262
C	-1.194843	-0.935594	-0.031945	C	-1.202713	-0.938237	-0.020263	C	-1.202664	-0.938141	-0.020263
N	-1.049301	1.488361	-0.12398	N	-1.050132	1.47779	-0.094295	N	-1.050082	1.477979	-0.094522
C	3.296603	-0.996496	-0.448203	C	3.297783	-0.996529	-0.452625	C	3.297728	-0.996618	-0.452544
C	3.304838	1.501713	-0.474856	C	3.299421	1.501112	-0.484054	C	3.299529	1.501027	-0.484135
C	2.851535	0.281036	1.668544	C	2.86601	0.283085	1.664229	C	2.865982	0.283164	1.664223
N	-2.502434	-0.817572	-0.390908	N	-2.505195	-0.811265	-0.375873	N	-2.505175	-0.811226	-0.375945
O	-0.765307	-1.870956	0.623986	O	-0.781065	-1.885	0.634229	O	-0.780958	-1.884821	0.634227
C	3.951992	0.239822	-1.059922	C	3.94537	0.239926	-1.072497	C	3.94541	0.23976	-1.072473
C	3.494934	-0.979739	1.072936	C	3.509479	-0.976748	1.066127	C	3.50937	-0.976754	1.06622
O	3.922907	-2.122363	-1.036736	O	3.921248	-2.128787	-1.04384	O	3.921138	-2.128897	-1.043679
C	3.507179	1.523089	1.047926	C	3.513428	1.52595	1.03685	C	3.51351	1.525939	1.036773
C	-3.536077	-1.603456	0.235697	C	-3.5488	-1.605554	0.224787	C	-3.54872	-1.605595	0.224696
C	-3.026492	0.437538	-0.95957	C	-3.021761	0.445283	-0.954063	C	-3.021813	0.445326	-0.954025
C	-4.834395	-0.912103	-0.029885	C	-4.840946	-0.90536	-0.043982	C	-4.840929	-0.905497	-0.044055
C	-4.268125	-0.930265	1.364489	C	-4.288138	-0.94231	1.356089	C	-4.288148	-0.942525	1.356016
C	-4.558323	0.316573	-0.885331	C	-4.553562	0.32485	-0.892537	C	-4.553624	0.324916	-0.892355

Table S40. Cont.

In gas phase				In water				In formic acid			
C	-2.42032	1.595934	-0.178728	C	-2.412517	1.602912	-0.17347	C	-2.41256	1.602943	-0.173434
H	-0.406232	0.213296	-1.651963	H	-0.413233	0.210535	-1.633684	H	-0.413197	0.210579	-1.633756
H	1.663215	-1.004753	-1.848112	H	1.65063	-1.010148	-1.840574	H	1.650622	-1.010245	-1.840517
H	1.328715	-1.888003	-0.344551	H	1.336743	-1.89504	-0.333994	H	1.336591	-1.89496	-0.33386
H	1.636177	1.502547	-1.86951	H	1.620778	1.493416	-1.866501	H	1.620939	1.493326	-1.866638
H	1.354313	2.428386	-0.397072	H	1.350425	2.422595	-0.391494	H	1.350531	2.422646	-0.391766
H	0.861211	-0.595769	1.809217	H	0.881609	-0.598747	1.822768	H	0.881482	-0.598493	1.822778
H	0.890287	1.172996	1.813507	H	0.902523	1.169725	1.82227	H	0.90258	1.169969	1.822176
H	-0.571493	2.049028	0.567398	H	-0.565315	2.062455	0.572823	H	-0.565376	2.062328	0.572948
H	3.763964	2.390715	-0.921523	H	3.752922	2.389596	-0.93661	H	3.753103	2.389458	-0.936732
H	2.996745	0.289525	2.75454	H	3.019929	0.293181	2.748759	H	3.019869	0.293323	2.748758
H	3.828281	0.202448	-2.14877	H	3.810875	0.205107	-2.16059	H	3.810963	0.204839	-2.160566
H	5.027343	0.216433	-0.848197	H	5.022594	0.223539	-0.867268	H	5.022626	0.223288	-0.867231
H	3.038927	-1.879211	1.509302	H	3.063849	-1.878508	1.507882	H	3.063626	-1.878436	1.508021
H	4.569046	-1.011234	1.291022	H	4.585608	-0.999272	1.276521	H	4.585489	-0.99938	1.276645
H	3.507873	-2.912432	-0.668851	H	3.520579	-2.918047	-0.655857	H	3.520319	-2.918117	-0.655792
H	3.06641	2.433478	1.473847	H	3.071475	2.434969	1.463046	H	3.071661	2.435036	1.462929
H	4.578157	1.539684	1.283683	H	4.586106	1.545034	1.264694	H	4.586186	1.544954	1.264627
H	-3.393989	-2.675927	0.208367	H	-3.418641	-2.678929	0.176902	H	-3.418401	-2.67895	0.176812
H	-2.688341	0.536259	-2.000273	H	-2.675904	0.536828	-1.991892	H	-2.676055	0.536945	-1.991891
H	-5.72877	-1.488696	-0.234992	H	-5.733002	-1.480701	-0.26066	H	-5.732951	-1.480849	-0.260851
H	-4.752611	-1.568139	2.094983	H	-4.786045	-1.584431	2.073665	H	-4.785952	-1.58477	2.073551
H	-3.854275	-0.004727	1.754431	H	-3.863215	-0.02778	1.760745	H	-3.86342	-0.027938	1.76074
H	-4.9672	0.167577	-1.887202	H	-4.953913	0.179125	-1.897621	H	-4.954101	0.17948	-1.897435
H	-4.976783	1.234507	-0.467255	H	-4.978529	1.24073	-0.477609	H	-4.978484	1.240703	-0.477106
N	-3.159003	2.507575	0.32101	N	-3.140981	2.537266	0.308662	N	-3.141066	2.537121	0.308882
H	-2.599366	3.210491	0.808531	H	-2.562516	3.22579	0.795809	H	-2.562707	3.225721	0.796043

Table S41. Coordinates of ESCA.

In gas phase				In water				In formic acid			
C	1.009901	0.343566	-0.471211	C	1.002571	0.323081	-0.481283	C	1.002602	0.323296	-0.481251
C	-0.299325	0.47298	-1.299682	C	-0.301557	0.428949	-1.323887	C	-0.301536	0.429387	-1.323794
C	1.786851	-0.918309	-0.889853	C	1.778287	-0.951438	-0.861716	C	1.778325	-0.95113	-0.861985
C	1.90355	1.570679	-0.74314	C	1.896921	1.541742	-0.788066	C	1.896986	1.542015	-0.787687
C	0.723508	0.27703	1.039665	C	0.71526	0.297104	1.030747	C	0.715224	0.296973	1.030762
C	-1.191937	-0.760379	-1.158547	C	-1.204989	-0.790548	-1.156433	C	-1.204846	-0.790257	-1.156587
N	-1.030138	1.705907	-1.028064	N	-1.037641	1.665966	-1.100665	N	-1.037618	1.666346	-1.10014
C	3.102414	-1.03015	-0.10929	C	3.094275	-1.041117	-0.078377	C	3.094269	-1.041033	-0.078599
C	3.221933	1.462523	0.038373	C	3.213998	1.454324	-0.002554	C	3.214026	1.454396	-0.002129
C	2.03896	0.166233	1.8276	C	2.031417	0.208649	1.821587	C	2.031329	0.208282	1.821647
N	-2.237874	-0.63173	-0.314375	N	-2.248024	-0.635306	-0.322099	N	-2.247868	-0.635295	-0.322109
O	-0.947493	-1.788544	-1.773414	O	-0.975431	-1.838347	-1.757132	O	-0.975129	-1.837868	-1.757434
C	3.971208	0.194564	-0.389792	C	3.963435	0.174501	-0.395371	C	3.963458	0.174661	-0.395215
C	2.791179	-1.099539	1.391699	C	2.78426	-1.068897	1.423044	C	2.784149	-1.06919	1.422808
O	3.845071	-2.158433	-0.534051	O	3.83279	-2.189582	-0.472295	O	3.832851	-2.189316	-0.472763
C	2.912563	1.396351	1.541111	C	2.905387	1.429961	1.501475	C	2.905333	1.429665	1.501877
C	-3.195569	-1.683516	-0.094158	C	-3.224924	-1.667509	-0.080358	C	-3.224504	-1.667734	-0.080396
C	-2.584602	0.567398	0.448507	C	-2.565664	0.576367	0.438573	C	-2.565791	0.576257	0.4386
C	-4.377015	-1.057399	0.58433	C	-4.388083	-1.011369	0.60063	C	-4.387841	-1.011881	0.600576
C	-3.486232	-2.006399	1.344707	C	-3.508521	-1.966561	1.365435	C	-3.508057	-1.966872	1.365386
C	-4.101231	0.43286	0.691932	C	-4.08458	0.474697	0.682263	C	-4.084684	0.474254	0.682262
H	-0.010375	0.478624	-2.357376	H	-0.002643	0.410425	-2.378056	H	-0.002677	0.411117	-2.377987
H	2.007371	-0.893876	-1.964899	H	1.998867	-0.955752	-1.937459	H	1.998949	-0.955198	-1.93771
H	1.18034	-1.814071	-0.711453	H	1.174535	-1.841707	-0.650156	H	1.1745	-1.841424	-0.65075
H	2.110352	1.640576	-1.820717	H	2.101957	1.583248	-1.86671	H	2.1021	1.583745	-1.866313
H	1.37547	2.484857	-0.444112	H	1.371056	2.464331	-0.514339	H	1.371094	2.464544	-0.513781
H	0.083346	-0.589671	1.259294	H	0.077098	-0.563565	1.277114	H	0.077001	-0.563735	1.276855
H	0.182476	1.181216	1.349111	H	0.176968	1.209489	1.318967	H	0.176921	1.209305	1.319146
H	-0.742463	2.524083	-1.544519	H	-0.714765	2.482524	-1.601062	H	-0.715014	2.482982	-1.600556
H	3.838376	2.343193	-0.173982	H	3.831443	2.327231	-0.240348	H	3.831493	2.327361	-0.239669
H	1.814733	0.113366	2.898879	H	1.80565	0.184203	2.893071	H	1.805523	0.183596	2.893121
H	4.208505	0.219902	-1.459796	H	4.198443	0.175202	-1.466695	H	4.198541	0.175574	-1.466516
H	4.916736	0.094769	0.156091	H	4.908616	0.093915	0.155094	H	4.90861	0.0939	0.155265

Table S41. Cont.

In gas phase				In water				In formic acid			
H	2.18336	-1.992439	1.595196	H	2.178724	-1.95649	1.652335	H	2.178541	-1.956815	1.651825
H	3.731924	-1.20628	1.944468	H	3.72509	-1.153639	1.980042	H	3.724936	-1.154161	1.979839
H	3.284098	-2.936572	-0.4272	H	3.290869	-2.965567	-0.276833	H	3.290528	-2.965341	-0.278637
H	2.392661	2.308696	1.859113	H	2.385412	2.350732	1.792641	H	2.385356	2.350369	1.793265
H	3.845852	1.335351	2.113763	H	3.8385	1.383759	2.075808	H	3.838418	1.383319	2.076241
H	-3.238714	-2.429489	-0.876163	H	-3.300665	-2.419558	-0.85351	H	-3.299968	-2.419822	-0.853539
H	-5.382427	-1.377617	0.337903	H	-5.399836	-1.317267	0.363224	H	-5.399529	-1.31801	0.36318
H	-3.879048	-2.994098	1.55633	H	-3.920473	-2.943714	1.588835	H	-3.919742	-2.944134	1.5888
H	-2.820298	-1.610017	2.105648	H	-2.826824	-1.574665	2.11454	H	-2.826492	-1.574807	2.114524
H	-4.63704	0.974672	-0.09073	H	-4.614929	1.004687	-0.11262	H	-4.615089	1.004205	-0.112604
H	-4.38258	0.870143	1.651593	H	-4.357473	0.930696	1.635674	H	-4.357708	0.930211	1.635653
C	-2.172081	1.829474	-0.278201	C	-2.119572	1.829659	-0.284907	C	-2.120002	1.829674	-0.28483
H	-2.053596	0.556705	1.410878	H	-2.038627	0.549041	1.401418	H	-2.038732	0.549057	1.401447
N	-2.878605	2.87857	-0.106206	N	-2.762129	2.915495	-0.063712	N	-2.763069	2.915222	-0.063896
H	-2.487807	3.676756	-0.611377	H	-2.338841	3.693221	-0.575038	H	-2.340076	3.693142	-0.575173

Table S42. Coordinates of Saxagliptin_s.

In gas phase				In water			In formic acid				
O	-0.363941	-1.787709	-0.964504	O	-0.341212	-1.785124	-0.939202	O	-0.34143	-1.785211	-0.939549
N	0.92219	0.026764	-0.663242	N	0.92815	0.042455	-0.645718	N	0.928042	0.04227	-0.64584
N	-2.481033	-0.185319	-1.879843	N	-2.440941	-0.170424	-1.906754	N	-2.441435	-0.170713	-1.906427
N	2.081849	-1.92541	1.90073	N	2.062442	-2.046242	1.809553	N	2.063007	-2.045087	1.810494
C	-2.264252	0.264869	0.54767	C	-2.274835	0.25419	0.537458	C	-2.274732	0.254297	0.537588
C	-1.262099	0.620892	1.650639	C	-1.289975	0.603072	1.658576	C	-1.289685	0.603378	1.658473
C	-3.384175	1.308664	0.518665	C	-3.393096	1.300079	0.506345	C	-3.393058	1.300114	0.50642
C	-2.862593	-1.117657	0.830667	C	-2.8796	-1.128366	0.804413	C	-2.879372	-1.128254	0.804859
C	-1.565395	0.284464	-0.84586	C	-1.551436	0.288552	-0.842652	C	-1.55162	0.288418	-0.842683
C	1.249928	1.413499	-0.426507	C	1.238525	1.434849	-0.398362	C	1.238531	1.434646	-0.398647
C	2.745705	1.513318	-0.387174	C	2.730685	1.550742	-0.337821	C	2.730727	1.550464	-0.338404
C	1.943318	1.731237	0.869119	C	1.911512	1.739529	0.91113	C	1.911779	1.739532	0.910661
C	3.302147	0.128802	-0.667196	C	3.313978	0.179988	-0.626962	C	3.313819	0.1796	-0.627446
C	-0.297435	-0.573596	-0.824017	C	-0.279495	-0.56318	-0.807941	C	-0.279693	-0.563355	-0.808107

Table S42. Cont.

In gas phase				In water				In formic acid			
C	2.096513	-0.826909	-0.495614	C	2.118643	-0.796573	-0.512258	C	2.118442	-0.796834	-0.512092
C	2.081751	-1.464595	0.840734	C	2.089096	-1.507738	0.786815	C	2.089189	-1.507284	0.78738
H	-0.4754	-0.136066	1.753498	H	-0.500197	-0.151324	1.758959	H	-0.499975	-0.151064	1.758977
H	-0.785558	1.589468	1.460856	H	-0.813617	1.573782	1.48361	H	-0.81327	1.574017	1.483226
H	-2.974837	2.319041	0.403677	H	-2.981188	2.307953	0.384458	H	-2.981231	2.308032	0.384553
H	-4.062948	1.111776	-0.31402	H	-4.077432	1.102613	-0.321829	H	-4.077295	1.102566	-0.321812
H	-3.643243	-1.358091	0.103214	H	-3.627381	-1.380691	0.04664	H	-3.627471	-1.380595	0.04741
H	-2.099708	-1.900035	0.799676	H	-2.111664	-1.906269	0.809996	H	-2.111442	-1.906163	0.810204
H	0.634195	2.146865	-0.930801	H	0.621021	2.165525	-0.903051	H	0.620983	2.165308	-0.903323
H	-1.312844	1.328126	-1.063652	H	-1.295828	1.332866	-1.044989	H	-1.29605	1.332713	-1.04524
H	3.246909	2.363003	-0.835618	H	3.222968	2.413263	-0.770009	H	3.223033	2.412874	-0.770799
H	1.950134	0.969753	1.643156	H	1.917953	0.962553	1.670434	H	1.91829	0.962738	1.67014
H	1.869795	2.750103	1.232787	H	1.816955	2.750044	1.291748	H	1.817409	2.750139	1.291094
H	4.130937	-0.153651	-0.01474	H	4.127738	-0.103251	0.043508	H	4.127785	-0.10355	0.042813
H	3.646498	0.079649	-1.703184	H	3.688564	0.151728	-1.651863	H	3.68806	0.15111	-1.652478
H	2.069204	-1.629747	-1.236099	H	2.120043	-1.562469	-1.29133	H	2.119594	-1.563128	-1.290772
H	-2.472399	-1.203742	-1.849793	H	-2.425493	-1.189036	-1.896871	H	-2.42626	-1.189326	-1.896135
H	-2.117757	0.066763	-2.794639	H	-2.047052	0.098249	-2.804966	H	-2.047756	0.097518	-2.804856
H	-3.951528	1.280891	1.454434	H	-3.958274	1.27652	1.443631	H	-3.958277	1.276537	1.443679
H	-3.320928	-1.119697	1.824741	H	-3.378159	-1.126857	1.779079	H	-3.377543	-1.126675	1.779722
H	-1.780521	0.687093	2.612258	H	-1.82083	0.654411	2.614444	H	-1.820409	0.65501	2.614395

Table S43. Coordinates of SCA_s.

In gas phase				In water				In formic acid			
C	2.629674	-0.042185	-0.027861	C	2.629674	-0.042185	-0.027861	C	2.629835	-0.048784	-0.027237
C	1.164385	0.165135	-0.463548	C	1.164385	0.165135	-0.463548	C	1.161719	0.159838	-0.452454
C	3.207921	-1.231779	-0.806361	C	3.207921	-1.231779	-0.806361	C	3.206409	-1.226881	-0.82422
C	3.437533	1.211745	-0.395772	C	3.437533	1.211745	-0.395772	C	3.433183	1.209873	-0.39104
C	2.745411	-0.307666	1.479051	C	2.745411	-0.307666	1.479051	C	2.758203	-0.324237	1.476494
C	0.212149	-1.010126	-0.164669	C	0.212149	-1.010126	-0.164669	C	0.206498	-1.01386	-0.163816
N	0.588136	1.373942	0.138645	N	0.588136	1.373942	0.138645	N	0.580641	1.351389	0.174635
N	-1.070418	-0.706008	-0.505246	N	-1.070418	-0.706008	-0.505246	N	-1.072589	-0.701429	-0.487735

Table S43. *Cont.*

In gas phase				In water				In formic acid			
O	0.53335	-2.081389	0.322482	O	0.53335	-2.081389	0.322482	O	0.523698	-2.099333	0.308747
C	-2.185685	-1.476975	-0.014304	C	-2.185685	-1.476975	-0.014304	C	-2.194255	-1.48011	-0.022269
C	-1.461073	0.667911	-0.867834	C	-1.461073	0.667911	-0.867834	C	-1.460405	0.674199	-0.85494
C	-3.406287	-0.628457	-0.167928	C	-3.406287	-0.628457	-0.167928	C	-3.410428	-0.625143	-0.167286
C	-2.866457	-0.920336	1.20648	C	-2.866457	-0.920336	1.20648	C	-2.878169	-0.940012	1.20553
C	-2.998964	0.685843	-0.819307	C	-2.998964	0.685843	-0.819307	C	-2.997844	0.693341	-0.805578
C	-0.76355	1.624948	0.08919	C	-0.76355	1.624948	0.08919	C	-0.754018	1.637092	0.090726
H	1.173577	0.29771	-1.557956	H	1.173577	0.29771	-1.557956	H	1.164284	0.303661	-1.545347
H	3.143862	-1.056175	-1.886253	H	3.143862	-1.056175	-1.886253	H	3.133728	-1.038304	-1.901038
H	2.677272	-2.153096	-0.565117	H	2.677272	-2.153096	-0.565117	H	2.68032	-2.153341	-0.592242
H	3.34059	1.443435	-1.461712	H	3.34059	1.443435	-1.461712	H	3.321564	1.45255	-1.453038
H	3.127741	2.096677	0.168151	H	3.127741	2.096677	0.168151	H	3.135215	2.08723	0.190404
H	2.199117	-1.210083	1.757132	H	2.199117	-1.210083	1.757132	H	2.218438	-1.231495	1.752443
H	2.365108	0.528628	2.077205	H	2.365108	0.528628	2.077205	H	2.376367	0.505276	2.081189
H	1.103089	1.78556	0.904029	H	1.103089	1.78556	0.904029	H	1.126822	1.832963	0.874988
H	-2.146311	-2.540446	-0.210838	H	-2.146311	-2.540446	-0.210838	H	-2.166769	-2.539006	-0.24429
H	-1.095461	0.896912	-1.878365	H	-1.095461	0.896912	-1.878365	H	-1.097606	0.894389	-1.867531
H	-4.349127	-1.075544	-0.460534	H	-4.349127	-1.075544	-0.460534	H	-4.351322	-1.069435	-0.469063
H	-3.422888	-1.611861	1.828841	H	-3.422888	-1.611861	1.828841	H	-3.442893	-1.636575	1.814585
H	-2.368919	-0.112304	1.735061	H	-2.368919	-0.112304	1.735061	H	-2.36991	-0.147132	1.747548
H	-3.401205	0.734727	-1.833762	H	-3.401205	0.734727	-1.833762	H	-3.400514	0.753511	-1.818499
H	-3.336577	1.563342	-0.263817	H	-3.336577	1.563342	-0.263817	H	-3.337122	1.565527	-0.243517
N	-1.420837	2.519232	0.71797	N	-1.420837	2.519232	0.71797	N	-1.393586	2.574047	0.68317
H	-0.806408	3.077689	1.314405	H	-0.806408	3.077689	1.314405	H	-0.760016	3.125428	1.266574
H	4.265393	-1.355762	-0.552573	H	4.265393	-1.355762	-0.552573	H	4.265279	-1.350863	-0.577051
H	3.799329	-0.436352	1.744838	H	3.799329	-0.436352	1.744838	H	3.814704	-0.451694	1.73212
H	4.496506	1.03955	-0.180996	H	4.496506	1.03955	-0.180996	H	4.494207	1.03203	-0.192156

Table S44. Coordinates of ESCA_s.

In gas phase				In water				In formic acid			
C	2.359304	-0.241626	0.345357	C	2.341604	-0.250447	0.352353	C	2.341688	-0.250391	0.352313
C	1.323642	0.087156	-0.773173	C	1.320369	0.04928	-0.789153	C	1.320407	0.049533	-0.789089
C	2.960779	-1.630273	0.102503	C	2.917686	-1.659676	0.174621	C	2.917957	-1.659487	0.174171
C	3.478809	0.80372	0.284759	C	3.482869	0.768297	0.25108	C	3.48281	0.768538	0.251375
C	1.697116	-0.193554	1.724808	C	1.677729	-0.133048	1.72707	C	1.677742	-0.133484	1.727038
C	0.188047	-0.934063	-0.827668	C	0.173327	-0.956114	-0.826645	C	0.173439	-0.955975	-0.826701
N	0.819506	1.453853	-0.704293	N	0.82127	1.418094	-0.77465	N	0.821262	1.418336	-0.774241
N	-0.982617	-0.537935	-0.281577	N	-0.98836	-0.539844	-0.290014	N	-0.988299	-0.539836	-0.289967
O	0.352689	-2.032687	-1.337679	O	0.320417	-2.069403	-1.326433	O	0.320647	-2.069155	-1.326559
C	-2.16622	-1.35703	-0.295684	C	-2.188099	-1.339035	-0.288335	C	-2.187905	-1.339196	-0.288302
C	-1.241111	0.747946	0.365446	C	-1.223022	0.756126	0.352284	C	-1.223161	0.756086	0.352302
C	-3.316098	-0.460807	0.055546	C	-3.319548	-0.420337	0.063291	C	-3.319513	-0.42065	0.063224
C	-2.862068	-1.521075	1.026292	C	-2.875994	-1.477745	1.041224	C	-2.875858	-1.477966	1.041217
C	-2.762959	0.945117	0.216705	C	-2.741106	0.977353	0.201644	C	-2.741272	0.977125	0.201605
H	1.83879	-0.030672	-1.733661	H	1.847547	-0.096058	-1.73844	H	1.847516	-0.09564	-1.738448
H	3.413947	-1.693729	-0.892299	H	3.363996	-1.779532	-0.818173	H	3.364311	-1.778993	-0.818642
H	2.206577	-2.415948	0.169574	H	2.1516	-2.428242	0.294153	H	2.151949	-2.428178	0.293342
H	3.949986	0.821087	-0.705103	H	3.959271	0.728959	-0.734846	H	3.959409	0.729391	-0.734467
H	3.105236	1.806578	0.512712	H	3.128184	1.788156	0.426416	H	3.127959	1.788323	0.426826
H	0.895666	-0.936399	1.810167	H	0.858043	-0.851952	1.842288	H	0.858178	-0.852572	1.841979
H	1.283238	0.79986	1.92796	H	1.289107	0.8769	1.894105	H	1.288937	0.876355	1.894331
H	1.398139	2.169617	-1.118578	H	1.42478	2.123413	-1.174302	H	1.424725	2.123784	-1.17371
H	-2.175241	-2.128249	-1.05413	H	-2.226779	-2.112461	-1.043128	H	-2.226346	-2.112698	-1.043031
H	-4.275676	-0.583528	-0.432663	H	-4.282798	-0.533636	-0.419301	H	-4.282735	-0.534077	-0.419398
H	-3.49588	-2.392565	1.141773	H	-3.525786	-2.335899	1.166404	H	-3.525494	-2.336236	1.166412
H	-2.334303	-1.221136	1.926909	H	-2.334444	-1.179204	1.934056	H	-2.334446	-1.179304	1.934098
H	-2.961212	1.535783	-0.6807	H	-2.93582	1.550737	-0.708027	H	-2.935981	1.550526	-0.708052
H	-3.170573	1.489898	1.070165	H	-3.138758	1.538817	1.049068	H	-3.139019	1.538586	1.048984
C	-0.40214	1.856524	-0.231061	C	-0.359224	1.847624	-0.242557	C	-0.359499	1.847704	-0.242486
H	-0.982537	0.681527	1.431559	H	-0.969841	0.684258	1.418042	H	-0.969986	0.684297	1.418073
N	-0.876905	3.041704	-0.213687	N	-0.786206	3.054269	-0.183678	N	-0.786746	3.054227	-0.183779
H	-0.212315	3.712985	-0.604302	H	-0.095838	3.697874	-0.576846	H	-0.096531	3.698014	-0.576913
H	3.741266	-1.823614	0.845379	H	3.699604	-1.827967	0.921583	H	3.699857	-1.827929	0.921121
H	2.435689	-0.410102	2.502846	H	2.412146	-0.337688	2.512066	H	2.412139	-0.338232	2.512025
H	4.255185	0.564536	1.017746	H	4.245975	0.547446	1.003476	H	4.245855	0.547706	1.003839

Table S45. Coordinates of TS_autoatalysis.

In gas phase				In water				In formic acid			
C	3.062579	-0.801969	-1.646567	C	3.100825	-0.782176	-1.633459	C	3.099126	-0.78344	-1.63341
N	4.177997	-0.48215	-0.741154	N	4.202158	-0.422233	-0.722362	N	4.201886	-0.42528	-0.72339
C	5.055704	-1.609577	-0.541954	C	5.150841	-1.497023	-0.559675	C	5.148433	-1.50198	-0.56088
C	4.593449	-2.692084	-1.463647	C	4.732834	-2.592186	-1.48645	C	4.727766	-2.5965	-1.48723
C	3.418612	-2.162001	-2.27273	C	3.521148	-2.115521	-2.273911	C	3.516574	-2.11759	-2.27407
C	4.401742	-2.842106	0.021923	C	4.580115	-2.772444	0.001023	C	4.575398	-2.77613	0.000336
C	4.10959	0.527345	0.161344	C	4.088913	0.574586	0.183552	C	4.091068	0.571851	0.182525
C	2.867572	1.420504	-0.044159	C	2.812496	1.415132	-0.021397	C	2.815768	1.414365	-0.02134
N	1.677363	0.527658	-0.020171	N	1.657121	0.475376	-0.022156	N	1.659013	0.476313	-0.01997
C	1.752928	-0.829566	-0.869434	C	1.794746	-0.868516	-0.846862	C	1.793578	-0.86766	-0.84571
N	0.841599	-1.641865	-0.83038	N	0.918205	-1.723538	-0.803457	N	0.915768	-1.72128	-0.80181
N	-1.498229	-0.682811	-0.195089	N	-1.506549	-0.752691	-0.22032	N	-1.50722	-0.75005	-0.2176
C	-1.670034	0.592566	-0.489702	C	-1.664007	0.516889	-0.573173	C	-1.66412	0.520061	-0.56836
N	-0.650293	1.364963	-0.79114	N	-0.638613	1.249795	-0.926168	N	-0.63816	1.25373	-0.91838
C	-3.071634	1.166563	-0.429373	C	-3.058874	1.100953	-0.519421	C	-3.05906	1.104167	-0.51578
N	-4.092872	0.134271	-0.542128	N	-4.085298	0.06342	-0.601211	N	-4.08546	0.066904	-0.60103
C	-3.925714	-1.189155	-0.284154	C	-3.932412	-1.229302	-0.249694	C	-3.93304	-1.2269	-0.25288
C	-2.55043	-1.5866	0.234932	C	-2.561481	-1.60792	0.297048	C	-2.56306	-1.60691	0.295152
C	-2.539078	-1.803343	1.779568	C	-2.535131	-1.701976	1.854479	C	-2.53978	-1.70557	1.85233
O	-4.815568	-2.007586	-0.453193	O	-4.828708	-2.061152	-0.365792	O	-4.82914	-2.05834	-0.37263
C	-5.279328	0.649036	-1.173767	C	-5.273804	0.566485	-1.244693	C	-5.2729	0.571289	-1.24543
C	-4.904783	1.957177	-1.80695	C	-4.897505	1.8604	-1.902808	C	-4.89544	1.866298	-1.90071
C	-3.419688	2.1601	-1.56552	C	-3.411073	2.06819	-1.674179	C	-3.40933	2.073413	-1.66944
C	-5.821151	1.930257	-0.609838	C	-5.81037	1.861102	-0.704111	C	-5.81011	1.865004	-0.70338
C	2.754842	2.614872	0.931034	C	2.632162	2.594569	0.962467	C	2.638929	2.59478	0.961971
O	4.938798	0.683216	1.045496	O	4.919228	0.759874	1.068262	O	4.922327	0.755848	1.066559
H	-0.470126	-1.129446	-0.373791	H	-0.511241	-1.185322	-0.346992	H	-0.51164	-1.18293	-0.34468
H	0.646849	1.004299	-0.409708	H	0.626542	0.923866	-0.471492	H	0.627628	0.926078	-0.46653
H	3.717012	-2.032267	-3.315735	H	3.797381	-1.96396	-3.319425	H	3.792528	-1.96656	-3.31975
H	6.091555	-1.3707	-0.33956	H	6.178377	-1.205382	-0.385102	H	6.176604	-1.21236	-0.38672
H	5.314442	-3.331023	-1.960032	H	5.483336	-3.180473	-2.000731	H	5.476761	-3.18645	-2.00182
H	2.538148	-2.808561	-2.232636	H	2.678952	-2.810785	-2.229584	H	2.67303	-2.81117	-2.22922
H	2.984886	-0.023583	-2.41787	H	2.990199	0.00098	-2.394721	H	2.989114	-0.00021	-2.39468
H	2.91877	1.831193	-1.062446	H	2.861386	1.838676	-1.033987	H	2.863932	1.83716	-1.03428
H	5.037671	-3.549642	0.541793	H	5.264852	-3.452182	0.495358	H	5.259036	-3.45709	0.494514

Table S45. Cont.

In gas phase				In water				In formic acid			
H	3.393428	-2.744106	0.413856	H	3.579	-2.72579	0.420439	H	3.574549	-2.72753	0.420148
H	1.503864	0.22026	0.93809	H	1.450868	0.183629	0.934843	H	1.454812	0.184083	0.937323
H	-0.918984	2.313916	-1.02215	H	-0.88729	2.198096	-1.184642	H	-0.8865	2.202342	-1.17598
H	-2.344896	-2.559642	-0.226473	H	-2.375552	-2.617504	-0.087684	H	-2.37618	-2.61532	-0.0922
H	-2.86297	1.891739	-2.468834	H	-2.862454	1.783356	-2.576857	H	-2.85937	1.78993	-2.57173
H	-3.161652	3.186815	-1.29099	H	-3.151628	3.098242	-1.419091	H	-3.15009	3.103019	-1.41229
H	-5.914911	-0.105701	-1.61654	H	-5.911421	-0.190129	-1.680178	H	-5.90994	-0.18454	-1.68312
H	-5.310487	2.243048	-2.769966	H	-5.307265	2.121828	-2.870676	H	-5.30367	2.129574	-2.86873
H	-5.449501	2.2721	0.351589	H	-5.434015	2.218459	0.249829	H	-5.43514	2.220626	0.25175
H	-6.869024	2.140664	-0.788654	H	-6.858171	2.067975	-0.886958	H	-6.85761	2.072376	-0.88739
H	-3.161822	1.677965	0.540632	H	-3.142269	1.632195	0.438346	H	-3.144	1.63379	0.44278
C	2.679042	2.162573	2.395622	C	2.565834	2.131344	2.423924	C	2.573178	2.132601	2.423777
H	3.570256	1.604674	2.682905	H	3.481991	1.61986	2.71961	H	3.488586	1.619406	2.718794
H	2.591327	3.043306	3.039843	H	2.425557	3.004331	3.069285	H	2.43539	3.006243	3.068792
H	1.791276	1.546777	2.586541	H	1.712469	1.466877	2.60446	H	1.718624	1.470002	2.605559
C	3.973764	3.525521	0.727648	C	3.80483	3.56712	0.771566	C	3.813386	3.564797	0.769269
H	3.873414	4.417296	1.354315	H	3.661918	4.440622	1.415192	H	3.67259	4.439351	1.411935
H	4.897498	3.011807	0.993421	H	4.754815	3.095907	1.025354	H	4.762563	3.092	1.023073
H	4.039101	3.858908	-0.314675	H	3.849797	3.919541	-0.264996	H	3.858466	3.915941	-0.26773
C	1.488552	3.415187	0.596421	C	1.331664	3.3355	0.622059	C	1.339611	3.338147	0.622411
H	1.474848	4.33854	1.183384	H	1.274153	4.255484	1.211444	H	1.284438	4.258542	1.211374
H	1.45943	3.690763	-0.464903	H	1.295472	3.610335	-0.438615	H	1.302974	3.612516	-0.43838
H	0.578956	2.855104	0.830529	H	0.446658	2.735988	0.853122	H	0.453692	2.740463	0.854605
C	-1.133917	-2.265112	2.181918	C	-1.154004	-2.220753	2.270461	C	-1.15883	-2.22372	2.269663
H	-0.382704	-1.501494	1.958608	H	-0.356228	-1.549574	1.938105	H	-0.36125	-1.55072	1.940526
H	-1.102396	-2.475967	3.255484	H	-1.099859	-2.304996	3.360177	H	-1.10672	-2.31075	3.359263
H	-0.849186	-3.174641	1.643112	H	-0.963607	-3.210634	1.841356	H	-0.96636	-3.21221	1.838329
C	-2.875896	-0.498028	2.506983	C	-2.77813	-0.327672	2.484757	C	-2.78606	-0.33344	2.486015
H	-2.139549	0.281437	2.279657	H	-1.995813	0.384468	2.199611	H	-2.00365	0.380297	2.205253
H	-3.873656	-0.133617	2.236005	H	-3.752883	0.080842	2.193243	H	-3.76033	0.074948	2.192718
H	-2.86145	-0.657592	3.589579	H	-2.76497	-0.412382	3.575586	H	-2.77606	-0.42129	3.576628
C	-3.552758	-2.888073	2.158068	C	-3.604126	-2.68863	2.335856	C	-3.60852	-2.69503	2.32846
H	-3.348288	-3.817889	1.617874	H	-3.490185	-3.66144	1.846527	H	-3.49249	-3.66611	1.836216
H	-3.483409	-3.094836	3.230968	H	-3.501982	-2.835746	3.415608	H	-3.5083	-2.84552	3.40793
H	-4.576309	-2.589933	1.922797	H	-4.613169	-2.324832	2.130015	H	-4.6176	-2.33181	2.121785

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