data

MDPI

Supplementary Material

Prediction of retention indices and response factors of oxygenates for GC-FID by multilinear regression

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Additional materials and methods

Table S1 Comparison of the different operation conditions for the detailed hydrocarbon analysis (DHA) method.

Parameter		D 6729 -14[1]	D 6730 - 01[2]	D 6733 - 01[3]		Used
Injector settings	Temperature	250 °C	250 °C	250 °C		290
	Split ratio	175:1 – 275:1	150:1	250:1	200:1	100
	Liner	Deactivated glass	n.d.	n.d.		Quartz glass
	Injection volume	0.2 – 0.5 µL	0.1 – 0.2 µL	0.5 µL	0.3 µL	0.1 µL
Detector settings	FID temperature	300 – 350 °C	250 °C	280 °C		250 °C
Gas flows	Hydrogen	30 – 40 mL/min	30 mL/min	n.d.		34.5 mL/min
	Air	300 – 450 mL/min	300 mL/min	n.d.		400 mL/min
	Nitrogen make-up	30 mL/min	20 mL/min	n.d.		Not used
Column oven settings	Initial temperature	0 °C	5 °C	35 °C	Column oven settings	35 °C
	Initial time	15 min	10 min	10 min	15 min	13 min
	1st ramp rate	1.0 K/min	5.0 K/min	1.1 K/min	1.3 K/min	10.0 K/min
	Final temperature	50 °C	50 °C	114 °C	70 °C	45 °C
	Final time	0 min	50 min	0 min		15 min
	2nd ramp rate	2.0 K/min	1.5 K/min	1.7 K/min		1.0 K/min
	Final temperature	130 °C	200 °C	250 °C		60 °C
	Final time	0 min	5 min	5 min	20 min	5 or 120 min
	3rd ramp rate	4.0 K/min	-	-		1.9 K/min
	Final temperature	270 °C	-	-		200 °C
Column Requirements	Length	100 m	100 m	50 m		100 m
	Inside diameter	0.25 mm	0.25 mm	0.2 mm		0.25 mm
	Liquid phase	100 % dime-thylpolysiloxane	n.d.	100 % dimethylpolysiloxane		100 % dimethylpolysiloxane
	Film thickness	0.5 µm	0.5 µm	0.5 µm		0.5 µm
	Pressure	40 – 50 psig	40 psig	30 psig	27 psig	37 psig
	Flow	1.7 – 2.0 mL/min	n.d.	0.9 mL/min	0.7 mL/min	n.d.
	Linear gas velocity	24.5 cm/s	24 cm/s at 35°C	22 cm/s	21.5 cm/s	n.d.
Total analysis time		140 – 150 min	174 min	139 min	187 min	139 or 254 min

Backward regression

Table S2 Overview of the individual steps of the performed backward regression for RF and RI starting from an R^2 of 0.9341 and 0.98798.

	Eliminated factor	Response factor (RF)		Retention index (RI)	
		p-value	R^2 after elimination	p-value	R^2 after elimination
1	Categorical Aldehyde Categorical Ketone	1.0000 1.0000	0.933116	1.0000 1.0000	0,98781
2	Categorical Ether Nr. of ether groups	0.84891 0.78010	0.933025	0.73218 0.00834	0.98565
3	Aromaticity	0.93456	0.933017	0.33560	0.98544
4	Melting point	0.69950	0.923823	0.09105	0.98365
5	Boiling point	0.70051	0.923691	0.00000	0.978393
6	C-number in the ring structure	0.87947	0.923671	0.00377	0.976165
7	Interaction O-H	0.56311	0.923379	0.96903	0.976165
8	Number of Alkylgroups	0.13744	0.921445	0.08142	0.975323
9	Interaction C-H Interaction C-O	-	-	0.38956 0.29071	0.974892

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Design of experiments

Table S3 Placket-Burman design for 24 runs and 11 factors A-K on two levels; description of factors, see Table 2 of the main manuscript.

Nbr.	A	B	C	D	E	F	G	H	I	J	K
1	-	-	+	-	+	+	+	-	-	-	+
2	-	-	+	-	-	+	-	+	+	+	-
3	-	-	-	+	-	-	+	-	+	+	+
4	-	+	-	+	+	+	-	-	-	+	-
5	-	+	-	-	+	-	+	+	+	-	-
6	-	+	+	+	-	-	-	+	-	-	+
7	+	+	+	-	-	-	+	-	-	+	-
8	+	+	+	+	+	+	+	+	+	+	+
9	+	+	-	-	-	+	-	-	+	-	+
10	+	-	-	+	-	+	+	+	-	-	-
11	+	-	-	-	+	-	-	+	-	+	+
12	+	-	+	+	+	-	-	-	+	-	-
13	+	+	-	+	-	-	-	+	+	+	-
14	+	+	-	+	+	-	+	-	-	-	+
15	+	+	+	-	+	+	-	+	-	-	-
16	+	-	+	-	-	-	+	+	+	-	+
17	+	-	+	+	-	+	-	-	-	+	+
18	+	-	-	-	+	+	+	-	+	+	-
19	-	-	-	+	+	+	-	+	+	-	+
20	-	-	-	-	-	-	-	-	-	-	-
21	-	-	+	+	+	-	+	+	-	+	-
22	-	+	+	-	+	-	-	-	+	+	+
23	-	+	+	+	-	+	+	-	+	-	-
24	-	+	-	-	-	+	+	+	-	+	+

Database for Response factors and Retention indices

Table S4 Database of experimentally determined retention times (T_i), retention indices (RI) and response factors (RF) used in this study.

CAS	Substance	T_i [min]	RI	RF
108-95-2	Phenol	80.548 ± 0.004	966.22 ± 0.02	1.3541 ± 0.0185
95-48-7	2-Methylphenol	90.509 ± 0.009	1033.46 ± 0.08	1.2244 ± 0.007
108-39-4	3-Methylphenol	93.061 ± 0.007	1054.69 ± 0.06	1.2899 ± 0.0077
106-44-5	4-Methylphenol	92.95 ± 0.005	1053.78 ± 0.04	1.3136 ± 0.0205
526-75-0	2,3-Dimethylphenol	103.976 ± 0.008	1153.83 ± 0.08	1.1956 ± 0.0076
105-67-9	2,4-Dimethylphenol	101.074 ± 0.005	1124.27 ± 0.05	1.2473 ± 0.0164
95-87-4	2,5-Dimethylphenol	101.277 ± 0.006	1126.36 ± 0.06	1.2301 ± 0.0134
576-26-1	2,6-Dimethylphenol	96.529 ± 0.006	1082.62 ± 0.05	1.1756 ± 0.01
95-65-8	3,4-Dimethylphenol	105.379 ± 0.006	1167.82 ± 0.06	1.2535 ± 0.011
108-68-9	3,5-Dimethylphenol	103.077 ± 0.006	1144.76 ± 0.06	1.2534 ± 0.0088
697-82-5	2,3,5-Trimethylphenol	112.815 ± 0.008	1248.68 ± 0.1	1.2032 ± 0.0072
2416-94-6	2,3,6-Trimethylphenol	109.379 ± 0.007	1208.38 ± 0.08	1.1686 ± 0.0072
496-78-6	2,4,5-Trimethylphenol	112.441 ± 0.013	1244.35 ± 0.07	1.1887 ± 0.0128
527-60-6	2,4,6-Trimethylphenol	106.772 ± 0.004	1181.54 ± 0.04	1.1691 ± 0.0045
527-54-8	3,4,5-Trimethylphenol	116.48 ± 0.001	1290.33 ± 0.02	1.2142 ± 0.0037
621-34-1	3-Ethoxyphenol	114.042 ± 0.012	1262.77 ± 0.14	1.8428 ± 0.0573
120-80-9	Benzene-1,2-diol	105.443 ± 0.022	1168.46 ± 0.21	2.1456 ± 0.0859
452-86-8	4-Methyl-Benzene-1,2-diol	113.641 ± 0.022	1258.18 ± 0.26	2.0382 ± 0.0837
108-46-3	Benzene-1,3-diol	112.16 ± 0.037	1241.1 ± 0.42	2.2816 ± 0.0824
488-87-9	2,5-Dimethyl-Benzene-1,3-diol	123.742 ± 0.005	1381.72 ± 0.06	1.6187 ± 0.023
123-31-9	Benzene-1.4-diol	111.193 ± 0.062	1229.82 ± 0.73	2.2237 ± 0.0132
95-71-6	2-Methyl-Benzene-1,4-diol	117.282 ± 0.021	1299.26 ± 0.24	1.9936 ± 0.0352
608-43-5	2,3-Dimethyl-Benzene-1,4-diol	125.831 ± 0.007	1408.62 ± 0.09	1.884 ± 0.1007
654-42-2	2,6-Dimethyl-Benzene-1,4-diol	122.239 ± 0.012	1362.89 ± 0.15	2.011 ± 0.0757
90-05-1	2-Methoxyphenol	94.138 ± 0.004	1063.48 ± 0.03	1.6239 ± 0.0191
93-51-6	4-Methyl-2-Methoxyphenol	105.497 ± 0.004	1168.99 ± 0.04	1.5652 ± 0.0073
1195-09-1	5-Methyl-2-Methoxyphenol	104.837 ± 0.004	1162.44 ± 0.04	1.5658 ± 0.0099
100-66-3	Methoxybenzene	68.115 ± 0.005	894.37 ± 0.02	1.221 ± 0.0034
578-58-5	2-Methyl-1-Methoxybenzene	84.81 ± 0.003	990.16 ± 0.02	1.161 ± 0.003
100-84-5	3-Methyl-1-Methoxybenzene	86.139 ± 0.009	997.38 ± 0.05	1.2238 ± 0.007
104-93-8	4-Methyl-1-Methoxybenzene	86.205 ± 0.01	997.73 ± 0.06	1.2201 ± 0.0056
91-16-7	1,2-Dimethoxybenzene	99.887 ± 0.02	1111.93 ± 0.2	1.5449 ± 0.0096
151-10-0	1,3-Dimethoxybenzene	102.661 ± 0.009	1140.54 ± 0.09	1.6106 ± 0.0082
150-78-7	1,4-Dimethoxybenzene	102.287 ± 0.005	1136.73 ± 0.05	1.5992 ± 0.0131
4463-33-6	3-Methyl-1,2-Dimethoxybenzene	103.807 ± 0.008	1152.12 ± 0.08	1.4025 ± 0.0077
494-99-5	4-Methyl-1,2-Dimethoxybenzene	109.205 ± 0.001	1206.31 ± 0.01	1.4888 ± 0.0051
24599-58-4	2-Methyl-1,4-Dimethoxybenzene	110.753 ± 0.003	1224.65 ± 0.03	1.4806 ± 0.0059
67-56-1	Methanol	7.641 ± 0.002	315.22 ± 0.21	2.8888 ± 0.0111
64-17-5	Ethanol	8.592 ± 0.002	415.02 ± 0.13	2.0581 ± 0.0086
96-41-3	Cyclopentanol	37.578 ± 0.005	768.17 ± 0.02	1.3147 ± 0.013
18729-48-1	3-Methylcyclopentanol – Isomer	49.79 ± 0.011	823.95 ± 0.05	1.3095 ± 0.011

CAS	Substance	T_i [min]	RI	RF
18729-48-1	3-Methylcyclopentanol – Isomer	50.081 ± 0.024	825.27 ± 0.11	1.3095 ± 0.011
108-93-0	Cyclohexanol	60.322 ± 0.008	867.07 ± 0.03	1.2755 ± 0.0036
583-59-5	cis-2-Methylcyclohexanol	72.542 ± 0.004	917.61 ± 0.03	1.2047 ± 0.0053
583-59-5	trans-2-Methylcyclohexanol	73.983 ± 0.003	926.74 ± 0.02	1.2047 ± 0.0053
24965-90-0	cis-3-Methylcyclohexanol	73.725 ± 0.002	925.12 ± 0.01	1.2999 ± 0.0064
7443-55-2	trans-3-Methylcyclohexanol	73.999 ± 0.003	926.84 ± 0.02	1.2999 ± 0.0064
589-91-3	4-Methylcyclohexanol	74.309 ± 0.004	928.79 ± 0.02	1.2777 ± 0.0052
1502-24-5	2.3-Dimethylcyclohexanol – Isomer	85.307 ± 0.04	992.87 ± 0.22	1.1809 ± 0.0066
1502-24-5	2.3-Dimethylcyclohexanol – Isomer	89.649 ± 0.003	1026.18 ± 0.03	1.1809 ± 0.0066
1502-24-5	2.3-Dimethylcyclohexanol – Isomer	90.857 ± 0.001	1036.39 ± 0.01	1.1809 ± 0.0066
69542-91-2	2.4-Dimethylcyclohexanol – Isomer	82.351 ± 0.001	976.5 ± 0.01	1.2522 ± 0.005
69542-91-2	2.4-Dimethylcyclohexanol – Isomer	86.2 ± 0.006	997.71 ± 0.03	1.2522 ± 0.005
69542-91-2	2.4-Dimethylcyclohexanol – Isomer	87.631 ± 0.007	1008.8 ± 0.06	1.2522 ± 0.005
3809-32-3	2.5-Dimethylcyclohexanol – Isomer	82.218 ± 0.01	975.75 ± 0.05	1.2007 ± 0.01
3809-32-3	2.5-Dimethylcyclohexanol – Isomer	82.58 ± 0.004	977.79 ± 0.03	1.2007 ± 0.01
3809-32-3	2.5-Dimethylcyclohexanol – Isomer	86.107 ± 0.016	997.21 ± 0.09	1.2007 ± 0.01
3809-32-3	2.5-Dimethylcyclohexanol – Isomer	87.454 ± 0min	1007.25 ± 0	1.2007 ± 0.01
5337-72-4	2.6-Dimethylcyclohexanol – Isomer	80.843 ± 0.002	967.92 ± 0.01	1.1417 ± 0.019
5337-72-4	2.6-Dimethylcyclohexanol – Isomer	81.799 ± 0.003	973.37 ± 0.02	1.1417 ± 0.019
5337-72-4	2.6-Dimethylcyclohexanol – Isomer	86.737 ± 0.004	1000.97 ± 0.03	1.1417 ± 0.019
5715-23-1	3.4-Dimethylcyclohexanol – Isomer	90.057 ± 0.005	1029.64 ± 0.04	1.2598 ± 0.0094
5715-23-1	3.4-Dimethylcyclohexanol – Isomer	90.211 ± 0.006	1030.95 ± 0.05	1.2598 ± 0.0094
5441-52-1	3.5-Dimethylcyclohexanol – Isomer	82.637 ± 0.005	978.1 ± 0.03	1.2933 ± 0.0056
5441-52-1	3.5-Dimethylcyclohexanol – Isomer	83.079 ± 0.005	980.58 ± 0.03	1.2933 ± 0.0056
931-17-9	Cyclohexane-1.2-diol – Isomer	90.113 ± 0.007	1030.11 ± 0.06	1.6845 ± 0.0182
931-17-9	Cyclohexane-1.2-diol – Isomer	90.5 ± 0.011	1033.39 ± 0.09	1.6845 ± 0.0182
504-01-8	Cyclohexane-1.3-diol – Isomer	95.16 ± 0.01	1071.71 ± 0.08	2.0963 ± 0.0508
504-01-8	Cyclohexane-1.3-diol – Isomer	95.335 ± 0.011	1073.12 ± 0.09	2.0963 ± 0.0508
556-48-9	Cyclohexane-1.4-diol – Isomer	95.071 ± 0.011	1071 ± 0.09	1.8529 ± 0.0151
556-48-9	Cyclohexane-1.4-diol – Isomer	95.484 ± 0.009	1074.31 ± 0.07	1.8529 ± 0.0151
67-64-1	Propane-2-on	9.267 ± 0.003	454.85 ± 0.16	1.8895 ± 0.009
78-93-3	Butane-2-on	13.673 ± 0.005	574.16 ± 0.09	1.5564 ± 0.005
563-80-4	3-Methylbutane-2-on	18.522 ± 0.005	637.27 ± 0.05	1.3219 ± 0.0047
120-92-3	Cyclopentanone	35.875 ± 0.01	759.73 ± 0.05	1.3439 ± 0.0062
1120-72-5	2-Methylcyclopentanone	46.9 ± 0.007	810.52 ± 0.03	1.277 ± 0.0032
1757-42-2	3-Methylcyclopentanone	47.802 ± 0.007	814.8 ± 0.03	1.3205 ± 0.0027
108-94-1	Cyclohexanone	59.153 ± 0.011	862.67 ± 0.04	1.3039 ± 0.0068
591-24-2	3-Methylcyclohexanone	72.849 ± 0.01	919.57 ± 0.06	1.2555 ± 0.0031
589-92-4	4-Methylcyclohexanone	73.903 ± 0.014	926.24 ± 0.09	1.2826 ± 0.0043
932-51-4	2,5-Dimethylcyclohexanone – Isomer	82.103 ± 0.016	975.09 ± 0.09	1.2596 ± 0.0128
932-51-4	2,5-Dimethylcyclohexanone – Isomer	84.194 ± 0.015	986.77 ± 0.09	1.2596 ± 0.0128
2816-57-1	2,6-Dimethylcyclohexanone – Isomer	82.336 ± 0.014	976.41 ± 0.08	1.1991 ± 0.0066
2816-57-1	2,6-Dimethylcyclohexanone – Isomer	83.912 ± 0.015	985.21 ± 0.08	1.1991 ± 0.0066
5465-09-8	3,4-Dimethylcyclohexanone	89.064 ± 0.013	1021.17 ± 0.11	1.3188 ± 0.0051
2320-30-1	3,5-Dimethylcyclohexanone	81.686 ± 0.012	972.73 ± 0.07	1.2869 ± 0.0055
930-68-7	2-Cyclohexene-1-on	67.708 ± 0.019	893.03 ± 0.06	1.3436 ± 0.0092
271-89-6	Benzofuran	82.601 ± 0.009	977.9 ± 0.05	1.1988 ± 0.0041
90-02-8	2-Hydroxybenzaldehyde	87.777 ± 0.008	1010.06 ± 0.07	1.5958 ± 0.0159

CAS	Substance	T_i [min]	RI	RF
71-41-0	Pentanol	35.231 ± 0.006	756.43 ± 0.03	1.2783 ± 0.0188
71-36-3	Butanol	19.503 ± 0.001	646.99 ± 0.01	1.3568 ± 0.0193
71-23-8	Propane-1-ol	11.968 ± 0.003	541.57 ± 0.06	1.5881 ± 0.0054
67-63-0	Propane-2-ol	9.578 ± 0.002	472.22 ± 0.1	1.8426 ± 0.0027
488-17-5	3-Methyl-1,2-Dihydroxybenzene	111.132 ± 0.011	1229.09 ± 0.13	1.8067 ± 0.0396
101-84-8	Phenoxybenzen	123.947 ± 0.003	1384.27 ± 0.04	1.094 ± 0.0028
14786-82-4	4-Methoxy-3-Methylphenol	114.179 ± 0.003	1264.33 ± 0.03	1.9013 ± 0.0104
134108-92-2	(1S,2S)-(+)-2-Methoxycyclohexanol	86.507 ± 0.004	999.36 ± 0.02	1.737 ± 0.0096
931-56-6	Methoxycyclohexane	57.942 ± 0.01	858.03 ± 0.04	1.1442 ± 0.0789
3637-61-4	Cyclopentanemethanol	65.945 ± 0.006	887.1 ± 0.02	1.2598 ± 0.0115

Table S5 Database of substances used for calibration and their producers including purity.

CAS	Substance	Producer	Purity
108-95-2	Phenol	TCI	> 99,5
95-48-7	2-Methylphenol	TCI	> 99
108-39-4	3-Methylphenol	Thermo Fisher Scientific	99
106-44-5	4-Methylphenol	Thermo Fisher Scientific	> 99
526-75-0	2,3-Dimethylphenol	TCI	> 98
105-67-9	2,4-Dimethylphenol	Thermo Fisher Scientific	99
95-87-4	2,5-Dimethylphenol	Thermo Fisher Scientific	> 99
576-26-1	2,6-Dimethylphenol	Thermo Fisher Scientific	99
95-65-8	3,4-Dimethylphenol	Thermo Fisher Scientific	99
108-68-9	3,5-Dimethylphenol	Thermo Fisher Scientific	> 99
697-82-5	2,3,5-Trimethylphenol	Thermo Fisher Scientific	> 98
2416-94-6	2,3,6-Trimethylphenol	TCI	> 98
496-78-6	2,4,5-Trimethylphenol	Thermo Fisher Scientific	99
527-60-6	2,4,6-Trimethylphenol	Thermo Fisher Scientific	99
527-54-8	3,4,5-Trimethylphenol	Thermo Fisher Scientific	97
621-34-1	3-Ethoxyphenol	Thermo Fisher Scientific	98
120-80-9	Benzene-1,2-diol	Thermo Fisher Scientific	> 99
452-86-8	4-Methyl-Benzene-1,2-diol	Thermo Fisher Scientific	98
108-46-3	Benzene-1,3-diol	TCI	> 99
488-87-9	2,5-Dimethyl-Benzene-1,3-diol	Thermo Fisher Scientific	95
123-31-9	Benzene-1,4-diol	Thermo Fisher Scientific	99,5
95-71-6	2-Methyl-Benzene-1,4-diol	Thermo Fisher Scientific	99
608-43-5	2,3-Dimethyl-Benzene-1,4-diol	TCI	> 98
654-42-2	2,6-Dimethyl-Benzene-1,4-diol	TCI	> 98
90-05-1	2-Methoxyphenol	Thermo Fisher Scientific	> 99
93-51-6	4-Methyl-2-Methoxyphenol	Thermo Fisher Scientific	99
1195-09-1	5-Methyl-2-Methoxyphenol	TCI	> 98
100-66-3	Methoxybenzene	TCI	> 99

CAS	Substance	Producer	Purity
578-58-5	2-Methyl-1-Methoxybenzene	Thermo Fisher Scientific	99
100-84-5	3-Methyl-1-Methoxybenzene	Thermo Fisher Scientific	99
104-93-8	4-Methyl-1-Methoxybenzene	Thermo Fisher Scientific	99
91-16-7	1,2-Dimethoxybenzene	Thermo Fisher Scientific	> 99
151-10-0	1,3-Dimethoxybenzene	TCI	> 99
150-78-7	1,4-Dimethoxybenzene	TCI	> 99
4463-33-6	3-Methyl-1,2-Dimethoxybenzene	Thermo Fisher Scientific	> 98
494-99-5	4-Methyl-1,2-Dimethoxybenzene	TCI	> 99
24599-58-4	2-Methyl-1,4-Dimethoxybenzene	TCI	> 98
67-56-1	Methanol	Thermo Fisher Scientific	> 99,9
64-17-5	Ethanol	Thermo Fisher Scientific	> 99,9
96-41-3	Cyclopentanol	TCI	> 99
18729-48-1	3-Methylcyclopentanol – Isomer	Sigma Aldrich	99
18729-48-1	3-Methylcyclopentanol – Isomer	Sigma Aldrich	99
108-93-0	Cyclohexanol	Thermo Fisher Scientific	99
583-59-5	cis-2-Methylcyclohexanol	Thermo Fisher Scientific	99
583-59-5	trans-2-Methylcyclohexanol	Thermo Fisher Scientific	99
24965-90-0	cis-3-Methylcyclohexanol	TCI	> 98
7443-55-2	trans-3-Methylcyclohexanol	TCI	> 98
589-91-3	4-Methylcyclohexanol	Thermo Fisher Scientific	99
1502-24-5	2,3-Dimethylcyclohexanol – Isomer	TCI	> 98
1502-24-5	2,3-Dimethylcyclohexanol – Isomer	TCI	> 98
1502-24-5	2,3-Dimethylcyclohexanol – Isomer	TCI	> 98
69542-91-2	2,4-Dimethylcyclohexanol – Isomer	Sigma Aldrich	> 99
69542-91-2	2,4-Dimethylcyclohexanol – Isomer	Sigma Aldrich	> 99
69542-91-2	2,4-Dimethylcyclohexanol – Isomer	Sigma Aldrich	> 99
3809-32-3	2,5-Dimethylcyclohexanol – Isomer	TCI	> 99
3809-32-3	2,5-Dimethylcyclohexanol – Isomer	TCI	> 99
3809-32-3	2,5-Dimethylcyclohexanol – Isomer	TCI	> 99
3809-32-3	2,5-Dimethylcyclohexanol – Isomer	TCI	> 99
5337-72-4	2,6-Dimethylcyclohexanol – Isomer	Thermo Fisher Scientific	99
5337-72-4	2,6-Dimethylcyclohexanol – Isomer	Thermo Fisher Scientific	99
5337-72-4	2,6-Dimethylcyclohexanol – Isomer	Thermo Fisher Scientific	99
5715-23-1	3,4-Dimethylcyclohexanol – Isomer	TCI	> 97
5715-23-1	3,4-Dimethylcyclohexanol – Isomer	TCI	> 97
5441-52-1	3,5-Dimethylcyclohexanol – Isomer	TCI	> 98
5441-52-1	3,5-Dimethylcyclohexanol – Isomer	TCI	> 98
931-17-9	Cyclohexane-1,2-diol – Isomer	Thermo Fisher Scientific	98
931-17-9	Cyclohexane-1,2-diol – Isomer	Thermo Fisher Scientific	98
504-01-8	Cyclohexane-1,3-diol – Isomer	Thermo Fisher Scientific	98

CAS	Substance	Producer	Purity
504-01-8	Cyclohexane-1,3-diol – Isomer	Thermo Fisher Scientific	98
556-48-9	Cyclohexane-1,4-diol – Isomer	TCI	> 99
556-48-9	Cyclohexane-1,4-diol – Isomer	TCI	> 99
67-64-1	Propane-2-on	Thermo Fisher Scientific	> 99
78-93-3	Butane-2-on	Thermo Fisher Scientific	> 99
563-80-4	3-Methylbutane-2-on	TCI	> 99
120-92-3	Cyclopentanone	TCI	> 99
1120-72-5	2-Methylcyclopentanone	Thermo Fisher Scientific	99
1757-42-2	3-Methylcyclopentanone	Thermo Fisher Scientific	99
108-94-1	Cyclohexanone	Thermo Fisher Scientific	99,8
591-24-2	3-Methylcyclohexanone	TCI	> 97
589-92-4	4-Methylcyclohexanone	TCI	> 98
932-51-4	2,5-Dimethylcyclohexanone – Isomer	TCI	> 95
932-51-4	2,5-Dimethylcyclohexanone – Isomer	TCI	> 95
2816-57-1	2,6-Dimethylcyclohexanone – Isomer	Thermo Fisher Scientific	99
2816-57-1	2,6-Dimethylcyclohexanone – Isomer	Thermo Fisher Scientific	99
5465-09-8	3,4-Dimethylcyclohexanone	TCI	> 98
2320-30-1	3,5-Dimethylcyclohexanone	TCI	> 98
930-68-7	2-Cyclohexene-1-on	Sigma Aldrich	> 98
271-89-6	Benzofuran	Thermo Fisher Scientific	99,5
90-02-8	2-Hydroxybenzaldehyde	TCI	> 98
71-41-0	Pentanol	Thermo Fisher Scientific	99
71-36-3	Butanol	TCI	99
71-23-8	Propane-1-ol	TCI	> 99
67-63-0	Propane-2-ol	TCI	> 99
488-17-5	3-Methyl-1,2-Dihydroxybenzene	Sigma Aldrich	99
101-84-8	Phenoxybenzen	TCI	99
14786-82-4	4-Methoxy-3-Methylphenol	AOB Chem USA	97
134108-92-2	(1S,2S)-(+)-2-Methoxycyclohexanol	Thermo Fisher Scientific	99
931-56-6	Methoxycyclohexane	TCI	> 99
3637-61-4	Cyclopentanemethanol	TCI	98

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