Reaction product analysis of the most active "inactive" material in lithium ion batteries: Electrolyte decomposition – (II) Battery operation and additive impact

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Data provided in this supporting information describe the retention time on the reversed-phase stationary phase, the specific identified adduct in mass spectrometry, the calculated molecular mass of the compound and the most probable molecular formula as well as the deviation between measured signal and calculated signal based on the molecular formula. A structure suggestion is depicted in abbreviated form and the confirmation was performed *via* comparison of electrolytes (EL) containing the linear carbonate solvents dimethyl carbonate (DMC), diethyl carbonate (DEC) or ethyl methyl carbonate (EMC). All tables consider the formation of decomposition products during the cell formation process and after long-term cycling (>1000 cycles). Table S1 depicts the observation of oligo phosphates, Table S2 phosphate and carbonate products, Table S3 cyclic carbonates and Table S4 solvent decomposition products parallel to the supporting information of Part 1. Overall, 140 of 289 different compounds were identified in different electrolyte formulations and operation states of battery cells.

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Table S1: Identification results of electrochemical induced oligo phosphates in LIB electrolytes after formation and long-term cycling (>1000 cycles). Decomposition products with a molecule mass border of 638 u as well as suspected targets were considered. The target list covers 21 compounds with diphosphate (DiP), triphosphate (TriP), tetraphosphates (TetraP) and cyclic diphosphates (cycDiP) structures.

#	RT min	formed Adduct	*m/z* meas.	*m/z* calc.	m u	Dev. Δppm	Molecular formula	DBE	Group	Formation				>1000 cycles	
										EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
1	4.4	$[M+H]^+$	277.0231	277.0238	276.0160	-2.53	$C_6H_{14}O_8P_2$	1	cycDiP	0	0	0	0	0	1
2	5.1	$[M+Li]^+$	285.0469	285.0476	278.0316	-2.46	$C_6H_{16}O_8P_2$	0	DiP	0	0	0	0	0	1
3	6.0	$[M+H]^+$	291.0396	291.0394	290.0316	0.69	$C_7H_{16}O_8P_2$	1	cycDiP	0	0	0	0	0	1
4	6.0	$[M+Li]^+$	299.0606	299.0632	292.0472	-8.69	$C_7H_{18}O_8P_2$	0	DiP	0	0	0	0	0	1
5	6.5	$[M+H]^+$	305.0550	305.0550	304.0472	0.00	$C_8H_{18}O_8P_2$	1	cycDiP	0	0	0	0	0	1
6	6.9	$[M+H]^+$	307.0689	307.0706	306.0628	-5.54	$C_8H_{20}O_8P_2$	0	DiP	0	0	0	0	0	1
7	7.7	$[M+H]^+$	321.0863	321.0862	320.0784	0.31	$C_9H_{22}O_8P_2$	0	DiP	0	0	0	0	0	1
8	8.6	$[M+H]^+$	335.1016	335.1018	334.0940	-0.60	$C_{10}H_{24}O_8P_2$	0	DiP	0	0	0	0	0	1
9	5.9	$[M+Li]^+$	423.0529	423.0556	416.0396	-6.38	$C_9H_{23}O_{12}P_3$	0	TriP	0	0	0	0	0	1
10	6.6	$[M+Li]^+$	437.0681	437.0712	430.0552	-7.09	$C_{10}H_{25}O_{12}P_3$	0	TriP	0	0	0	0	0	1
11	7.2	$[M+Li]^+$	451.0829	451.0868	444.0708	-8.65	$C_{11}H_{27}O_{12}P_3$	0	TriP	0	0	0	0	0	1
12	7.9	$[M+Li]^+$	465.1004	465.1024	458.0864	-4.30	$C_{12}H_{29}O_{12}P_3$	0	TriP	0	0	0	0	0	1
13	8.5	$[M+Li]^+$	479.1145	479.1180	472.1020	-7.31	$C_{13}H_{31}O_{12}P_3$	0	TriP	0	0	0	0	0	1
14	9.1	$[M+Li]^+$	493.1312	493.1336	486.1176	-4.87	$C_{14}H_{33}O_{12}P_3$	0	TriP	0	0	0	0	0	1
15		$[M+H]^+$		555.0554	554.0476		$C_{12}H_{30}O_{16}P_4$	0	TetraP	0	0	0	0	0	0
16	6.9	$[M+Li]^+$	575.0758	575.0792	568.0632	-5.91	$C_{13}H_{32}O_{16}P_4$	0	TetraP	0	0	0	0	0	1
17	7.4	$[M+Li]^+$	589.0925	589.0948	582.0788	-3.90	$C_{14}H_{34}O_{16}P_4$	0	TetraP	0	0	0	0	0	1
18	7.9	$[M+Li]^+$	603.1089	603.1104	596.0944	-2.49	$C_{15}H_{36}O_{16}P_4$	0	TetraP	0	0	0	0	0	1
19	8.4	$[M+Li]^+$	617.1244	617.1260	610.1100	-2.59	$C_{16}H_{38}O_{16}P_4$	0	TetraP	0	0	0	0	0	1
20	9.0	$[M+Li]^+$	631.1405	631.1416	624.1256	-1.74	$C_{17}H_{40}O_{16}P_4$	0	TetraP	0	0	0	0	0	1
21	9.4	$[M+Li]^+$	645.1570	645.1572	638.1412	-0.31	$C_{18}H_{42}O_{16}P_4$	0	TetraP	0	0	0	0	0	1

Table S2: Identification results of electrochemical induced phosphate and carbonate reaction products in LIB electrolytes after formation and long-term cycling (>1000 cycles). Decomposition products with a molecule mass border of 598 u as well as suspected targets were considered. The list covers 61 different compounds with 1-3 phosphates (P) and 1-3 carbonate subunits (C). Structural isomers were considered if separation was achieved.

#	RT min	formed Adduct	*m/z* meas.	*m/z* calc.	m u	Dev. Δppm	Molecular formula	DBE	Group	Formation				>1000 cycles	
										EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
1	5.4	$[M+Li]^+$	235.0541	235.0555	228.0395	-5.96	$C_6H_{13}O_7P_1$	1	1P+1C	1	0	1	0	1	1
2	6.6/6.7	$[M+Li]^+$	249.0706	249.0711	242.0551	-2.01	$C_7H_{15}O_7P_1$	1	1P+1C	0	0	2	0	2	2
3	7.6/7.8	$[M+Li]^+$	263.0871	263.0867	256.0707	1.52	$C_8H_{17}O_7P_1$	1	1P+1C	0	2	2	2	2	2
4	8.8	$[M+Li]^+$	277.1020	277.1023	270.0863	-1.08	$C_9H_{19}O_7P_1$	1	1P+1C	0	1	1	1	1	1
5	7.0	$[M+Li]^+$	323.0688	323.0714	316.0554	-8.05	$C_9H_{17}O_{10}P_1$	2	1P+2C	1	0	1	0	1	1
6	7.9/8.1	$[M+Li]^+$	337.0849	337.0870	330.0710	-6.23	$C_{10}H_{19}O_{10}P_1$	2	1P+2C	2	1	2	0	2	2
7	8.7/8.9/9.1	$[M+Li]^+$	351.1003	351.1026	344.0866	-6.55	$C_{11}H_{21}O_{10}P_1$	2	1P+2C	0	2	3	0	2	3
8	9.8/10.0	$[M+Li]^+$	365.1174	365.1182	358.1022	-2.19	$C_{12}H_{23}O_{10}P_1$	2	1P+2C	0	2	2	0	1	2
9	6.4	$[M+H]^+$	367.0569	367.0553	366.0475	4.36	$C_9H_{20}O_{11}P_2$	1	2P+1C	0	0	0	0	0	1
10	7.1/7.3	$[M+H]^+$	381.0700	381.0709	380.0631	-2.36	$C_{10}H_{22}O_{11}P_2$	1	2P+1C	0	0	0	0	0	2
11	7.9/8.0	$[M+H]^+$	395.0845	395.0865	394.0787	-5.06	$C_{11}H_{24}O_{11}P_2$	1	2P+1C	0	0	0	0	0	2
12	8.1/8.7/9.3	$[M+Li]^+$	411.0831	411.0873	404.0713	-10.22	$C_{12}H_{21}O_{13}P_1$	3	1P+3C	1	0	0	0	0	3
13	8.6/8.8	$[M+H]^+$	409.1021	409.1021	408.0943	0.00	$C_{12}H_{26}O_{11}P_2$	1	2P+1C	0	0	0	0	0	2
14	8.8/9.0/9.4	$[M+Li]^+$	425.1060	425.1029	418.0869	7.29	$C_{13}H_{23}O_{13}P_1$	3	1P+3C	1	0	1	0	0	3
15	9.3/9.5	$[M+H]^+$	423.1177	423.1177	422.1099	0.00	$C_{13}H_{28}O_{11}P_2$	1	2P+1C	0	0	0	0	0	2
16	9.6/9.8/10.0	$[M+Li]^+$	439.1153	439.1185	432.1025	-7.29	$C_{14}H_{25}O_{13}P_1$	3	1P+3C	0	2	2	0	0	3
17	10.6/10.8/11.0	$[M+Li]^+$	453.1341	453.1341	446.1181	0.00	$C_{15}H_{27}O_{13}P_1$	3	1P+3C	0	2	2	0	0	3
18		$[M+H]^+$		455.0712	454.0634		$C_{12}H_{24}O_{14}P_2$	2	2P+2C	0	0	0	0	0	0
19	8.1/8.2	$[M+H]^+$	469.0863	469.0868	468.0790	-1.07	$C_{13}H_{26}O_{14}P_2$	2	2P+2C	0	0	0	0	0	2
20	8.7/8.9	$[M+H]^+$	483.1025	483.1024	482.0946	0.21	$C_{14}H_{28}O_{14}P_2$	2	2P+2C	0	0	0	0	0	2
21	9.5/9.7	$[M+H]^+$	497.1171	497.1180	496.1102	-1.81	$C_{16}H_{30}O_{14}P_2$	2	2P+2C	0	0	0	0	0	2
22	6.8	$[M+Li]^+$	511.0746	511.0715	504.0555	6.07	$C_{12}H_{27}O_{15}P_3$	1	3P+1C	0	0	0	0	0	1
23	10.1 / 10.3	$[M+H]^+$	511.1337	511.1336	510.1258	0.20	$C_{17}H_{32}O_{14}P_2$	2	2P+2C	0	0	0	0	0	2
24	7.4 / 7.6	$[M+Li]^+$	525.0832	525.0871	518.0711	-7.43	$C_{13}H_{29}O_{15}P_3$	1	3P+1C	0	0	0	0	0	2
25	8.1 / 8.3	$[M+Li]^+$	539.1026	539.1027	532.0867	-0.19	$C_{14}H_{31}O_{15}P_3$	1	3P+1C	0	0	0	0	0	2
26		$[M+Li]^+$		549.0953	542.0793		$C_{15}H_{28}O_{17}P_2$	3	2P+3C	0	0	0	0	0	0
27	8.7 / 8.8	$[M+Li]^+$	553.1181	553.1183	546.1023	-0.36	$C_{15}H_{33}O_{15}P_3$	1	3P+1C	0	0	0	0	0	2
28	9.0 / 9.1	$[M+Li]^+$	563.1056	563.1109	556.0949	-9.41	$C_{16}H_{30}O_{17}P_2$	3	2P+3C	0	0	0	0	0	2
29	9.3 / 9.4	$[M+Li]^+$	567.1333	567.1339	560.1179	-1.06	$C_{16}H_{35}O_{15}P_3$	1	3P+1C	0	0	0	0	0	2

#	RT min	formed Adduct	*m/z* meas.	*m/z* calc.	m u	Dev. Δppm	Molecular formula	DBE	Group	Formation EL_{DMC}	Formation EL_{DEC}	Formation EL_{EMC}	Formation EL_{EMC+VC}	>1000 cycles EL_{EMC}	>1000 cycles EL_{EMC+VC}
30	9.9	$[M+Li]^+$	581.1492	581.1495	574.1335	-0.52	$C_{17}H_{37}O_{15}P_3$	1	3P+1C	0	0	0	0	0	1
31	9.7 / 9.9	$[M+Li]^+$	577.1228	577.1265	570.1105	-6.41	$C_{17}H_{32}O_{17}P_2$	3	2P+3C	0	0	0	0	0	2
32	10.2 / 10.4	$[M+Li]^+$	591.1403	591.1421	584.1261	3.00	$C_{18}H_{34}O_{17}P_2$	3	2P+3C	0	0	0	0	0	2
33	10.9 / 11.1	$[M+Li]^+$	605.1576	605.1577	598.1417	-0.17	$C_{19}H_{36}O_{17}P_2$	3	2P+3C	0	0	0	0	0	2
							Identified species			**6**	**12**	**19**	**3**	**12**	**61**
							Unique species including structural isomers (only if separated)								**61**

Table S3: Identification results of electrochemical induced cyclic carbonates (cycC) in LIB electrolytes after formation and long-term cycling (>1000 cycles). Decomposition products with a molecule mass border of 396 u as well as suspected targets were considered. The list covers 9 identified compounds.

#	RT min	formed Adduct	*m/z* meas.	*m/z* calc.	m u	Dev. Δppm	Molecular formula	DBE	Group	Formation				>1000 cycles	
										EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
1	6.5	$[M+Li]^+$	227.0731	227.0739	220.0579	-3.52	$C_8H_{12}O_7$	3	cycC	0	1	1	1	1	0
2	4.3	$[M+Li]^+$	227.1118	227.1102	220.0942	7.05	$C_9H_{16}O_6$	2	cycC	1	1	0	1	1	0
3		$[M+H]^+$		265.0555	264.0477		$C_9H_{12}O_9$	4	cycC	0	0	0	0	0	0
4	5.6	$[M+Li]^+$	271.1002	271.1000	264.0840	0.74	$C_{10}H_{16}O_8$	3	cycC	1	1	0	1	1	0
5	5.2	$[M+H]^+$	265.1299	265.1282	264.1204	6.41	$C_{11}H_{20}O_7$	2	cycC	0	1	0	1	0	0
6	8.6	$[M+NH_4]^+$	326.1058	326.1082	308.0738	-7.35	$C_{11}H_{16}O_{10}$	4	cycC	0	1	1	1	1	0
7	6.3	$[M+NH_4]^+$	326.1445	326.1445	308.1101	0.00	$C_{12}H_{20}O_9$	3	cycC	1	1	0	1	1	0
8		$[M+NH_4]^+$		326.1808	308.1464		$C_{13}H_{24}O_8$	2	cycC	0	0	0	0	0	0
9		$[M+NH_4]^+$		414.1241	396.0897		$C_{14}H_{20}O_{13}$	5	cycC	0	0	0	0	0	0
10	8.2	$[M+NH_4]^+$	414.1614	414.1604	396.1260	2.41	$C_{15}H_{24}O_{12}$	4	cycC	0	1	0	1	1	0
11	7.6	$[M+NH_4]^+$	414.1968	414.1967	396.1623	0.24	$C_{16}H_{28}O_{11}$	3	cycC	0	1	0	1	0	0
12	7.0	$[M+NH_4]^+$	414.2335	414.2330	396.1986	0.25	$C_{17}H_{32}O_{10}$	2	cycC	0	1	0	0	0	0
							Identified species			**3**	**9**	**2**	**8**	**6**	**0**
							Unique species without structural isomers								**9**

Table S4: Identification results of electrochemical induced solvent-based decomposition products in LIB electrolytes after formation and long-term cycling (>1000 cycles), parallel to structures identified and shown in the supporting information of Part 1. Decomposition products with a molecule mass border of 602 u as well as suspected targets were considered. The list covers 50 identified compounds without structural isomers.

#	RT min	m u	Molecular formula	DBE	Group	Formation				>1000 cycles	
						EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
1	5.9	148.0732	$C_6H_{12}O_4$	1	$X_1Y_1R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
2	5.2	148.1095	$C_7H_{16}O_5$	0	$X_0Y_2R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
3	2.8	164.0680	$C_6H_{12}O_5$	1	$X_1Y_2R_{1b}R_{2a}$	0	0	0	0	0	0
4	3.2	164.1043	$C_7H_{16}O_4$	0	$X_0Y_3R_{1b}R_{2a}$	0	0	0	0	0	0
5	5.6	178.0472	$C_6H_{10}O_6$	2	$X_2Y_1R_{1b}R_{2b}$	1	0	0	0	0	0
6	4.8	178.0836	$C_7H_{14}O_5$	1	$X_1Y_2R_{1c}R_{2a}$	0	0	0	0	0	0
7	4.6	178.0836	$C_7H_{14}O_5$	1	$X_1Y_2R_{1b}R_{2b}$	0	0	0	0	0	0
8	4.4	178.1200	$C_8H_{18}O_4$	0	$X_0Y_3R_{1a}R_{2c}$	0	0	0	0	0	0
9	4.4	178.1200	$C_8H_{18}O_4$	0	$X_0Y_3R_{1b}R_{2b}$	0	0	0	0	0	0
10	7.5	192.0628	$C_7H_{12}O_6$	2	$X_2Y_1R_{1b/c}R_{2b/c}$	0	0	1	0	0	0
11	6.7	192.0993	$C_8H_{16}O_5$	1	$X_1Y_2R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
12	6.0	192.1356	$C_9H_{20}O_4$	0	$X_0Y_3R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
13	9.2	206.0785	$C_8H_{14}O_6$	2	$X_2Y_1R_{1c}R_{2c}$	0	0	1	0	0	0
14	8.2	206.1149	$C_9H_{18}O_5$	1	$X_1Y_2R_{1c}R_{2c}$	0	0	0	0	0	0
15	7.1	206.1513	$C_{10}H_{22}O_4$	0	$X_0Y_3R_{1c}R_{2c}$	0	0	0	0	0	0
16		208.0578	$C_7H_{12}O_7$	2	$X_2Y_2R_{1b}R_{2a}$	0	0	0	0	0	0
17	4.3	208.0942	$C_8H_{16}O_6$	1	$X_1Y_3R_{1b}R_{2a}$	0	0	0	0	0	0
18	4.3	208.1306	$C_9H_{20}O_5$	0	$X_0Y_4R_{1b}R_{2a}$	0	0	0	0	0	0
19	5.6	222.0734	$C_8H_{14}O_7$	2	$X_2Y_2R_{1c}R_{2a}$	0	1	1	1	0	0
20	6.4	222.0735	$C_8H_{14}O_7$	2	$X_2Y_2R_{1b}R_{2b}$	1	0	1	0	0	1
21	5.4	222.1098	$C_9H_{18}O_6$	1	$X_1Y_3R_{1c}R_{2a}$	0	1	0	0	0	0
22	5.7	222.1098	$C_9H_{18}O_6$	1	$X_1Y_3R_{1b}R_{2b}$	0	0	0	1	0	0
23	5.6	222.1462	$C_{10}H_{22}O_5$	0	$X_0Y_4R_{1c}R_{2a}$	0	0	0	0	0	0
24	5.2	222.1462	$C_{10}H_{22}O_5$	0	$X_0Y_4R_{1b}R_{2b}$	0	0	0	0	0	0
25	8.0	236.0880	$C_9H_{16}O_7$	2	$X_2Y_2R_{1b/c}R_{2b/c}$	0	0	1	0	1	1
26	7.2	236.1254	$C_{10}H_{20}O_6$	1	$X_1Y_3R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
27	6.5	236.1617	$C_{11}H_{24}O_5$	0	$X_0Y_4R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
28	9.5	250.1047	$C_{10}H_{18}O_7$	2	$X_2Y_2R_{1c}R_{2c}$	0	1	1	1	1	1
29	8.5	250.1411	$C_{11}H_{22}O_6$	1	$X_1Y_3R_{1c}R_{2c}$	0	1	0	0	1	0
30	7.5	250.1775	$C_{12}H_{26}O_5$	0	$X_0Y_4R_{1c}R_{2c}$	0	0	0	0	0	0
31	5.3	252.0840	$C_9H_{16}O_8$	2	$X_2Y_3R_{1b}R_{2a}$	0	0	0	1	0	0

#	RT min	m u	Molecular formula	DBE	Group	Formation				>1000 cycles	
						EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
32	5.2	252.1204	$C_{10}H_{20}O_7$	1	$X_1Y_4R_{1b}R_{2a}$	0	0	0	1	0	0
33	7.7	266.0633	$C_9H_{14}O_9$	3	$X_3Y_2R_{1b}R_{2b}$	1	0	1	0	1	1
34	7.4	266.0996	$C_{10}H_{18}O_8$	2	$X_2Y_3R_{1c}R_{2a}$	1	0	0	0	0	0
35	7.2	266.0996	$C_{10}H_{18}O_8$	2	$X_2Y_3R_{1b}R_{2b}$	1	0	0	0	0	0
36	6.6	266.1360	$C_{11}H_{22}O_7$	1	$X_1Y_4R_{1c}R_{2a}$	0	0	0	1	0	0
37	6.2	266.1360	$C_{11}H_{22}O_7$	1	$X_1Y_4R_{1b}R_{2b}$	0	0	0	0	0	0
38	6.1	266.1724	$C_{12}H_{26}O_6$	0	$X_0Y_5R_{1b}R_{2b}$	0	0	0	0	0	0
39	9.3	280.0789	$C_{10}H_{16}O_9$	3	$X_3Y_2R_{1b/c}R_{2b/c}$	0	0	1	1	1	1
40	8.6	280.1152	$C_{11}H_{20}O_8$	2	$X_2Y_3R_{1b/c}R_{2b/c}$	0	0	1	1	1	1
41	7.7	280.1515	$C_{12}H_{24}O_7$	1	$X_1Y_4R_{1b/c}R_{2b/c}$	0	0	1	0	0	0
42		280.1878	$C_{13}H_{28}O_6$	0	$X_0Y_5R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
43	10.5	294.0946	$C_{11}H_{18}O_9$	3	$X_3Y_2R_{1c}R_{2c}$	0	1	1	1	1	1
44	10.0	294.1309	$C_{12}H_{22}O_8$	2	$X_2Y_3R_{1c}R_{2c}$	0	1	1	1	1	1
45	8.8	294.1647	$C_{13}H_{26}O_7$	1	$X_1Y_4R_{1c}R_{2c}$	0	1	0	0	0	0
46		294.2037	$C_{14}H_{30}O_6$	0	$X_0Y_5R_{1c}R_{2c}$	0	0	0	0	0	0
47	6.2	296.0738	$C_{10}H_{16}O_{10}$	3	$X_3Y_3R_{1b}R_{2a}$	0	0	0	0	0	0
48	5.9	296.1102	$C_{11}H_{20}O_9$	2	$X_2Y_4R_{1b}R_{2a}$	0	0	0	0	0	0
49	5.8	296.1465	$C_{12}H_{24}O_8$	1	$X_1Y_5R_{1b}R_{2a}$	0	0	0	0	0	0
50	7.5	310.0894	$C_{11}H_{18}O_{10}$	3	$X_3Y_3R_{1c}R_{2a}$	0	1	0	0	0	0
51	8.3	310.0894	$C_{11}H_{18}O_{10}$	3	$X_3Y_3R_{1b}R_{2b}$	1	0	0	0	0	1
52	7.0	310.1257	$C_{12}H_{22}O_9$	2	$X_2Y_4R_{1c}R_{2a}$	0	0	0	0	0	0
53	7.7	310.1258	$C_{12}H_{22}O_9$	2	$X_2Y_4R_{1b}R_{2b}$	1	0	0	0	0	0
54	6.8	310.1620	$C_{13}H_{26}O_8$	1	$X_1Y_5R_{1c}R_{2a}$	0	0	0	0	0	0
55	7.0	310.1622	$C_{13}H_{26}O_8$	1	$X_1Y_5R_{1b}R_{2b}$	0	0	0	0	0	0
56	6.5	310.1986	$C_{14}H_{30}O_7$	0	$X_0Y_6R_{1b}R_{2b}$	0	0	0	0	0	0
57	9.6	324.1050	$C_{12}H_{20}O_{10}$	3	$X_3Y_3R_{1b/c}R_{2b/c}$	0	0	1	1	1	1
58	8.8	324.1413	$C_{13}H_{24}O_9$	2	$X_2Y_4R_{1b/c}R_{2b/c}$	0	0	0	1	1	1
59	8.1	324.1776	$C_{14}H_{28}O_8$	1	$X_1Y_5R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
60		324.2139	$C_{15}H_{32}O_7$	0	$X_0Y_6R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
61	10.8	338.1206	$C_{13}H_{22}O_{10}$	3	$X_3Y_3R_{1c}R_{2c}$	0	1	1	1	1	1
62	10.1	338.1569	$C_{14}H_{26}O_9$	2	$X_2Y_4R_{1c}R_{2c}$	0	1	0	0	1	1
63	9.1	338.1932	$C_{15}H_{30}O_8$	1	$X_1Y_5R_{1c}R_{2c}$	0	0	0	0	0	0
64	8.2	338.2295	$C_{16}H_{34}O_7$	0	$X_0Y_6R_{1c}R_{2c}$	0	0	0	0	0	0
65		340.0636	$C_{11}H_{16}O_{12}$	4	$X_4Y_3R_{1b}R_{2a}$	0	0	0	0	0	0

#	RT min	m u	Molecular formula	DBE	Group	Formation				>1000 cycles	
						EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
66	6.8	340.1000	$C_{12}H_{20}O_{11}$	3	$X_3Y_4R_{1b}R_{2a}$	0	0	0	0	0	0
67	6.5	340.1364	$C_{13}H_{24}O_{10}$	2	$X_2Y_5R_{1b}R_{2a}$	0	0	0	1	0	0
68	6.2	340.1728	$C_{14}H_{28}O_9$	1	$X_1Y_6R_{1b}R_{2a}$	0	0	0	0	0	0
69	9.2	354.0793	$C_{12}H_{18}O_{12}$	4	$X_4Y_3R_{1b}R_{2b}$	1	0	1	0	1	1
70	7.8	354.1155	$C_{13}H_{22}O_{11}$	3	$X_3Y_4R_{1c}R_{2a}$	0	0	0	0	0	0
71	8.6	354.1156	$C_{13}H_{22}O_{11}$	3	$X_3Y_4R_{1b}R_{2b}$	1	0	0	0	0	0
72	7.5	354.1518	$C_{14}H_{26}O_{10}$	2	$X_2Y_5R_{1c}R_{2a}$	0	0	0	0	0	0
73	8.0	354.1520	$C_{14}H_{26}O_{10}$	2	$X_2Y_5R_{1b}R_{2b}$	1	0	0	0	0	0
74	7.0	354.1881	$C_{15}H_{30}O_9$	1	$X_1Y_6R_{1c}R_{2a}$	0	0	0	0	0	0
75	7.4	354.1884	$C_{15}H_{30}O_9$	1	$X_1Y_6R_{1b}R_{2b}$	1	0	0	0	0	0
76		354.2244	$C_{16}H_{34}O_8$	0	$X_0Y_7R_{1b}R_{2b}$	0	0	0	0	0	0
77	6.8	354.2248	$C_{16}H_{34}O_8$	0	$X_0Y_7R_{1c}R_{2a}$	0	0	0	0	0	0
78	10.3	368.0948	$C_{13}H_{20}O_{12}$	4	$X_4Y_3R_{1b/c}R_{2b/c}$	1	0	1	0	1	1
79	9.9	368.1311	$C_{14}H_{24}O_{11}$	3	$X_3Y_4R_{1b/c}R_{2b/c}$	0	0	0	1	1	1
80	9.2	368.1674	$C_{15}H_{28}O_{10}$	2	$X_2Y_5R_{1b/c}R_{2b/c}$	0	0	0	0	1	1
81	8.4	368.2037	$C_{16}H_{32}O_9$	1	$X_1Y_6R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
82		368.2400	$C_{17}H_{36}O_8$	0	$X_0Y_7R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
83	11.3	382.1104	$C_{14}H_{22}O_{12}$	4	$X_4Y_3R_{1c}R_c$	0	1	1	0	1	1
84	11.0	382.1467	$C_{15}H_{26}O_{11}$	3	$X_3Y_4R_{1c}R_{2c}$	0	1	0	1	1	1
85	10.3	382.1830	$C_{16}H_{30}O_{10}$	2	$X_2Y_5R_{1c}R_{2c}$	0	1	0	0	0	1
86	9.3	382.2193	$C_{17}H_{34}O_9$	1	$X_1Y_6R_{1c}R_{2c}$	0	0	0	0	0	0
87		382.2556	$C_{18}H_{38}O_8$	0	$X_0Y_7R_{1c}R_{2c}$	0	0	0	0	0	0
88		384.0898	$C_{13}H_{20}O_{13}$	4	$X_4Y_4R_{1b}R_{2a}$	0	0	0	0	0	0
89	7.2	384.1262	$C_{14}H_{24}O_{12}$	3	$X_3Y_5R_{1b}R_{2a}$	0	0	0	0	0	0
90	6.9	384.1626	$C_{15}H_{28}O_{11}$	2	$X_2Y_6R_{1b}R_{2a}$	0	0	0	0	0	0
91	6.6	384.1990	$C_{16}H_{32}O_{10}$	1	$X_1Y_7R_{1b}R_{2a}$	0	0	0	0	0	0
92	8.8	398.1055	$C_{14}H_{22}O_{13}$	4	$X_4Y_4R_{1c}R_{2a}$	0	0	0	0	0	0
93	9.6	398.1055	$C_{14}H_{22}O_{13}$	4	$X_4Y_4R_{1b}R_{2b}$	1	0	0	0	0	0
94	8.3	398.1416	$C_{15}H_{26}O_{12}$	3	$X_3Y_5R_{1c}R_{2a}$	0	0	0	0	0	0
95	9.0	398.1419	$C_{15}H_{26}O_{12}$	3	$X_3Y_5R_{1b}R_{2b}$	0	0	0	0	0	0
96	7.9	398.1779	$C_{16}H_{30}O_{11}$	2	$X_2Y_6R_{1c}R_{2a}$	0	0	0	0	0	0
97	8.3	398.1782	$C_{16}H_{30}O_{11}$	2	$X_2Y_6R_{1b}R_{2b}$	0	0	0	0	0	0
98		398.2142	$C_{17}H_{34}O_{10}$	1	$X_1Y_7R_{1c}R_{2a}$	0	0	0	0	0	0
99	7.7	398.2146	$C_{17}H_{34}O_{10}$	1	$X_1Y_7R_{1b}R_{2b}$	0	0	0	0	0	0

#	RT min	m u	Molecular formula	DBE	Group	Formation				>1000 cycles	
						EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
100	7.2	398.2510	$C_{18}H_{38}O_9$	0	$X_0Y_8R_{1b}R_{2b}$	0	0	0	0	0	0
101	10.6	412.1209	$C_{15}H_{24}O_{13}$	4	$X_4Y_4R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
102	10.1	412.1572	$C_{16}H_{28}O_{12}$	3	$X_3Y_5R_{1b/c}R_{2b/c}$	0	0	0	0	1	0
103	9.4	412.1935	$C_{17}H_{32}O_{11}$	2	$X_2Y_6R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
104		412.2298	$C_{18}H_{36}O_{10}$	1	$X_1Y_7R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
105		412.2661	$C_{19}H_{40}O_9$	0	$X_0Y_8R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
106	11.5	426.1365	$C_{16}H_{26}O_{13}$	4	$X_4Y_4R_{1c}R_{2c}$	0	1	0	0	0	0
107	11.1	426.1728	$C_{17}H_{30}O_{12}$	3	$X_3Y_5R_{1c}R_{2c}$	0	1	0	0	1	0
108	10.4	426.2091	$C_{18}H_{34}O_{11}$	2	$X_2Y_6R_{1c}R_{2c}$	0	0	0	0	0	0
109	9.5	426.2454	$C_{19}H_{38}O_{10}$	1	$X_1Y_7R_{1c}R_{2c}$	0	0	0	0	0	0
110		426.2817	$C_{20}H_{42}O_9$	0	$X_0Y_8R_{1c}R_{2c}$	0	0	0	0	0	0
111	8.0	428.1160	$C_{15}H_{24}O_{14}$	4	$X_4Y_5R_{1b}R_{2a}$	0	0	0	0	0	0
112	7.6	428.1524	$C_{16}H_{28}O_{13}$	3	$X_3Y_6R_{1b}R_{2a}$	0	0	0	0	0	0
113	7.2	428.1888	$C_{17}H_{32}O_{12}$	2	$X_2Y_7R_{1b}R_{2a}$	0	0	0	0	0	0
114	6.9	428.2252	$C_{18}H_{36}O_{11}$	1	$X_1Y_8R_{1b}R_{2a}$	0	0	0	0	0	0
115	10.2	442.0786	$C_{15}H_{22}O_{15}$	5	$X_5Y_4R_{1b}R_b$	1	0	1	0	0	0
116	9.8	442.1317	$C_{16}H_{26}O_{14}$	4	$X_4Y_5R_{1c}R_{2a}$	1	0	0	0	0	0
117		442.1317	$C_{16}H_{26}O_{14}$	4	$X_4Y_5R_{1b}R_{2b}$	0	0	0	0	0	0
118	9.3	442.1681	$C_{17}H_{30}O_{13}$	3	$X_3Y_6R_{1c}R_{2a}$	0	0	0	0	0	0
119	8.6	442.1681	$C_{17}H_{30}O_{13}$	3	$X_3Y_6R_{1b}R_{2b}$	0	0	0	0	0	0
120		442.2040	$C_{18}H_{34}O_{12}$	2	$X_2Y_7R_{1c}R_{2a}$	0	0	0	0	0	0
121	8.6	442.2045	$C_{18}H_{34}O_{12}$	2	$X_2Y_7R_{1b}R_{2b}$	0	0	0	0	0	0
122		442.2403	$C_{19}H_{38}O_{11}$	1	$X_1Y_8R_{1c}R_{2a}$	0	0	0	0	0	0
123	8.0	442.2408	$C_{19}H_{38}O_{11}$	1	$X_1Y_8R_{1b}R_{2b}$	0	0	0	0	0	0
124	7.5	442.2772	$C_{20}H_{42}O_{10}$	0	$X_0Y_9R_{1b}R_{2b}$	0	0	0	0	0	0
125	11.1	456.1107	$C_{16}H_{24}O_{15}$	5	$X_5Y_4R_{1b/c}R_{2b/c}$	0	0	1	0	0	0
126	10.9	456.1470	$C_{17}H_{28}O_{14}$	4	$X_4Y_5R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
127	10.3	456.1833	$C_{18}H_{32}O_{13}$	3	$X_3Y_6R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
128		456.2196	$C_{19}H_{36}O_{12}$	2	$X_2Y_7R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
129		456.2559	$C_{20}H_{40}O_{11}$	1	$X_1Y_8R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
130		456.2922	$C_{21}H_{44}O_{10}$	0	$X_0Y_9R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
131	12.0	470.1263	$C_{17}H_{26}O_{15}$	5	$X_5Y_4R_{1c}R_{2c}$	0	1	1	0	0	1
132	11.7	470.1626	$C_{18}H_{30}O_{14}$	4	$X_4Y_5R_{1c}R_{2c}$	0	1	0	0	0	0
133	11.3	470.1989	$C_{19}H_{34}O_{13}$	3	$X_3Y_6R_{1c}R_{2c}$	0	0	0	0	0	0

#	RT min	m u	Molecular formula	DBE	Group	Formation				>1000 cycles	
						EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
134	10.5	470.2352	$C_{20}H_{38}O_{12}$	2	$X_2Y_7R_{1c}R_{2c}$	0	0	0	0	0	0
135		470.2715	$C_{21}H_{42}O_{11}$	1	$X_1Y_8R_{1c}R_{2c}$	0	0	0	0	0	0
136		470.3078	$C_{22}H_{46}O_{10}$	0	$X_0Y_7R_{1c}R_{2c}$	0	0	0	0	0	0
137		472.1059	$C_{16}H_{24}O_{16}$	5	$X_5Y_5R_{1b}R_{2a}$	0	0	0	0	0	0
138	8.3	472.1422	$C_{17}H_{28}O_{15}$	4	$X_4Y_6R_{1b}R_{2a}$	0	0	0	0	0	0
139	7.9	472.1786	$C_{18}H_{32}O_{14}$	3	$X_3Y_7R_{1b}R_{2a}$	0	0	0	0	0	0
140	7.5	472.2150	$C_{19}H_{36}O_{13}$	2	$X_2Y_8R_{1b}R_{2a}$	0	0	0	0	0	0
141	7.1	472.2514	$C_{20}H_{40}O_{12}$	1	$X_1Y_9R_{1b}R_{2a}$	0	0	0	0	0	0
142	10.4	486.1215	$C_{17}H_{26}O_{16}$	5	$X_5Y_5R_{1c}R_{2a}$	0	0	0	0	0	0
143		486.1215	$C_{17}H_{26}O_{16}$	5	$X_5Y_5R_{1b}R_{2b}$	0	0	0	0	0	0
144	10.1	486.1579	$C_{18}H_{30}O_{15}$	4	$X_4Y_6R_{1c}R_{2a}$	0	0	0	0	0	0
145		486.1579	$C_{18}H_{30}O_{15}$	4	$X_4Y_6R_{1b}R_{2b}$	0	0	0	0	0	0
146	9.5	486.1943	$C_{19}H_{34}O_{14}$	3	$X_3Y_7R_{1c}R_{2c}$	0	0	0	0	0	0
147		486.1943	$C_{19}H_{34}O_{14}$	3	$X_3Y_7R_{1b}R_{2b}$	0	0	0	0	0	0
148		486.2301	$C_{20}H_{38}O_{13}$	2	$X_2Y_8R_{1c}R_{2a}$	0	0	0	0	0	0
149	8.9	486.2307	$C_{20}H_{38}O_{13}$	2	$X_2Y_8R_{1b}R_{2b}$	0	0	0	0	0	0
150	8.2	486.2643	$C_{21}H_{42}O_{12}$	1	$X_1Y_9R_{1b}R_{2b}$	0	0	0	0	0	0
151		486.2664	$C_{21}H_{42}O_{12}$	1	$X_1Y_9R_{1c}R_{2a}$	0	0	0	0	0	0
152	7.3	486.3034	$C_{22}H_{46}O_{11}$	0	$X_0Y_{10}R_{1b}R_{2b}$	0	0	0	0	0	0
153	11.4	500.1368	$C_{18}H_{28}O_{16}$	5	$X_5Y_5R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
154	11.0	500.1731	$C_{19}H_{32}O_{15}$	4	$X_4Y_6R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
155		500.2094	$C_{20}H_{36}O_{14}$	3	$X_3Y_7R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
156		500.2457	$C_{21}H_{40}O_{13}$	2	$X_2Y_8R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
157		500.2820	$C_{22}H_{44}O_{12}$	1	$X_1Y_9R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
158		500.3183	$C_{23}H_{48}O_{11}$	0	$X_0Y_{10}R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
159	12.1	514.1524	$C_{19}H_{30}O_{16}$	5	$X_5Y_5R_{1c}R_{2c}$	0	1	0	0	0	0
160	11.9	514.1887	$C_{20}H_{34}O_{15}$	4	$X_4Y_6R_{1c}R_{2c}$	0	1	0	0	0	0
161	11.4	514.2250	$C_{21}H_{38}O_{14}$	3	$X_3Y_7R_{1c}R_{2c}$	0	0	0	0	0	0
162		514.2613	$C_{22}H_{42}O_{13}$	2	$X_2Y_8R_{1c}R_{2c}$	0	0	0	0	0	0
163		514.2976	$C_{23}H_{46}O_{12}$	1	$X_1Y_9R_{1c}R_{2c}$	0	0	0	0	0	0
164		514.3339	$C_{24}H_{50}O_{11}$	0	$X_0Y_{10}R_{1c}R_{2c}$	0	0	0	0	0	0
165	10.9	530.1113	$C_{18}H_{26}O_{18}$	6	$X_6Y_5R_{1b}R_{2b}$	1	0	0	0	0	0
166	10.7	530.1477	$C_{19}H_{30}O_{17}$	5	$X_5Y_6R_{1b}R_{2b}$	0	0	0	0	0	0
167	10.5	530.1841	$C_{20}H_{34}O_{16}$	4	$X_4Y_7R_{1b}R_{2b}$	0	0	0	0	0	0

#	RT min	m u	Molecular formula	DBE	Group	Formation				>1000 cycles	
						EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
168	9.6	530.2205	$C_{21}H_{38}O_{15}$	3	$X_3Y_8R_{1b}R_{2b}$	0	0	0	0	0	0
169	9.0	530.2569	$C_{22}H_{42}O_{14}$	2	$X_2Y_9R_{1b}R_{2b}$	0	0	0	0	0	0
170	8.5	530.2933	$C_{23}H_{46}O_{13}$	1	$X_1Y_{10}R_{1b}R_{2b}$	0	0	0	0	0	0
171		530.3297	$C_{24}H_{50}O_{12}$	0	$X_0Y_{11}R_{1b}R_{2b}$	0	0	0	0	0	0
172		544.1266	$C_{19}H_{28}O_{18}$	6	$X_6Y_5R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
173	11.6	544.1629	$C_{20}H_{32}O_{17}$	5	$X_5Y_6R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
174	11.2	544.1992	$C_{21}H_{36}O_{16}$	4	$X_4Y_7R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
175		544.2355	$C_{22}H_{40}O_{15}$	3	$X_3Y_8R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
176		544.2718	$C_{23}H_{44}O_{14}$	2	$X_2Y_9R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
177		544.3081	$C_{24}H_{48}O_{13}$	1	$X_1Y_{10}R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
178		544.3444	$C_{25}H_{52}O_{12}$	0	$X_0Y_{11}R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
179		558.1422	$C_{20}H_{30}O_{18}$	6	$X_6Y_5R_{1c}R_{2c}$	0	0	0	0	0	0
180	12.4	558.1785	$C_{21}H_{34}O_{17}$	5	$X_5Y_6R_{1c}R_{2c}$	0	1	0	0	0	0
181	12.0	558.2148	$C_{22}H_{38}O_{16}$	4	$X_4Y_7R_{1c}R_{2c}$	0	0	0	0	0	0
182	11.5	558.2511	$C_{23}H_{42}O_{15}$	3	$X_3Y_8R_{1c}R_{2c}$	0	0	0	0	0	0
183		558.2874	$C_{24}H_{46}O_{14}$	2	$X_2Y_9R_{1c}R_{2c}$	0	0	0	0	0	0
184		558.3237	$C_{25}H_{50}O_{13}$	1	$X_1Y_{10}R_{1c}R_{2c}$	0	0	0	0	0	0
185		558.3600	$C_{26}H_{54}O_{12}$	0	$X_0Y_{11}R_{1c}R_{2c}$	0	0	0	0	0	0
186		574.1376	$C_{20}H_{30}O_{19}$	6	$X_6Y_6R_{1b}R_{2b}$	0	0	0	0	0	0
187	11.0	574.1739	$C_{21}H_{34}O_{18}$	5	$X_5Y_7R_{1b}R_{2b}$	0	0	0	0	0	0
188	10.5	574.2103	$C_{22}H_{38}O_{17}$	4	$X_4Y_8R_{1b}R_{2b}$	0	0	0	0	0	0
189	9.3	574.2467	$C_{23}H_{42}O_{16}$	3	$X_3Y_9R_{1b}R_{2a}$	0	0	0	0	0	0
190	9.3	574.2831	$C_{24}H_{46}O_{15}$	2	$X_2Y_{10}R_{1b}R_{2a}$	0	0	0	0	0	0
191		574.3195	$C_{25}H_{50}O_{14}$	1	$X_1Y_{11}R_{1b}R_{2a}$	0	0	0	0	0	0
192		574.3559	$C_{26}H_{54}O_{13}$	0	$X_0Y_{12}R_{1b}R_{2a}$	0	0	0	0	0	0
193		588.1527	$C_{21}H_{32}O_{19}$	6	$X_6Y_6R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
194		588.1890	$C_{22}H_{36}O_{18}$	5	$X_5Y_7R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
195		588.2253	$C_{23}H_{40}O_{17}$	4	$X_4Y_8R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
196		588.2616	$C_{24}H_{44}O_{16}$	3	$X_3Y_9R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
197		588.2979	$C_{25}H_{48}O_{15}$	2	$X_2Y_{10}R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
198		588.3342	$C_{26}H_{52}O_{14}$	1	$X_1Y_{11}R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
199		588.3705	$C_{27}H_{56}O_{13}$	0	$X_0Y_{12}R_{1b/c}R_{2b/c}$	0	0	0	0	0	0
200		602.1683	$C_{22}H_{34}O_{19}$	6	$X_6Y_6R_{1c}R_{2c}$	0	0	0	0	0	0
201	12.5	602.2046	$C_{23}H_{38}O_{18}$	5	$X_5Y_7R_{1c}R_{2c}$	0	0	0	0	0	0

#	RT min	m u	Molecular formula	DBE	Group	Formation				>1000 cycles	
						EL_{DMC}	EL_{DEC}	EL_{EMC}	EL_{EMC+VC}	EL_{EMC}	EL_{EMC+VC}
202	12.0	602.2409	$C_{24}H_{42}O_{17}$	4	$X_4Y_8R_{1c}R_{2c}$	0	0	0	0	0	0
203		602.2772	$C_{25}H_{46}O_{16}$	3	$X_3Y_9R_{1c}R_{2c}$	0	0	0	0	0	0
204		602.3135	$C_{26}H_{50}O_{15}$	2	$X_2Y_{10}R_{1c}R_{2c}$	0	0	0	0	0	0
205		602.3498	$C_{27}H_{54}O_{14}$	1	$X_1Y_{11}R_{1c}R_{2c}$	0	0	0	0	0	0
206		602.3861	$C_{28}H_{58}O_{13}$	0	$X_0Y_{12}R_{1c}R_{2c}$	0	0	0	0	0	0
			Identified species			**16**	**20**	**20**	**16**	**20**	**21**
			Unique species without structural isomers								**50**

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