Supplementary Dataset S4: Polymer Library Members

Polymer Number	*Monomer 1*	*Monomer 2*	*Mn (kDa)*	*Mw (kDa)*	*D*	*Monomer 1: Monomer 2 (mole basis)*	*BigSMILES*	*Method Key*
1	Malonyl Chloride	Bisphenol A	19.11	41.07	2.15	1:1	{[][<]C(=O)CC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
2	Terephthaloyl Chloride	2,5-hexanediol(+isomers)				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC(C)CCC(C)O[>][]}	M32
3	Terephthaloyl Chloride	1,8-octanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCCCCCCCO[>][]}	M32
4	Terephthaloyl Chloride	1,9-nonanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCCCCCCCCO[>][]}	M32
5	Terephthaloyl Chloride	1,10-decanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCCCCCCCCCO[>][]}	M32
6	Terephthaloyl Chloride	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M32
7	Terephthaloyl Chloride	2,2-Dimethyl-1,3-propanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(C)(C)CO[>][]}	M32
8	Terephthaloyl Chloride	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M32
9	Terephthaloyl Chloride	2,3-Butanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC(C)C(C)O[>][]}	M32
10	Terephthaloyl Chloride	1,4-Cyclohexanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC(CC1)CCC1O[>][]}	M32

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11	Terephthaloyl Chloride	diethylene glycol	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCOCCO[>][]}	M32
12	Terephthaloyl Chloride	triethylene glycol	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCOCCOCCO[>][]}	M32
13	Terephthaloyl Chloride	4,4′-Sulfonylbis(2-methylphenol)	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1c(C)cc(cc1)S(=O)(=O)c2ccc(c(C)c2)O[>][]}	M32
14	Terephthaloyl Chloride	2-Hydroxyethyl disulfide	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCSSCCO[>][]}	M32
15	Terephthaloyl Chloride	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M32
16	Terephthaloyl Chloride	4,4′-(alpha-Methylbenzylidene)bisphenol	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M32
17	Terephthaloyl Chloride	4,4′-Isopropylidenebis(2,6-dimethylphenol)	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1c(C)cc(cc1(C))C(C)(C)c2cc(C)c(c(C)c2)O[>][]}	M32
18	Terephthaloyl Chloride	4,4′-(9-Fluorenylidene)diphenol	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)C2(c3ccccc3c4c2ccccc4)c5ccc(cc5)O[>][]}	M32
19	Terephthaloyl Chloride	4,4′-Cyclohexylidenebisphenol	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)C2(CCCCC2)c3cc(cc3)O[>][]}	M32

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20	Terephthaloyl Chloride	(R)-(+)-1,1′-Binaphthyl-2,2′-diol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(ccc c2)c2c1c3c(cccc4)c4ccc3O[>][]}	M32
21	Phthaloyl Chloride	4,4′-Thiodiphenol	3.55	6.65	1.87	1:1	{[][<]C(=O)c(cccc1)c1C(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
23	Malonyl Chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)CC(=O)[<],[>]Oc1c(ccc2)c(ccc1)c 2O[>][]}	M32
24	Diglycolyl Chloride	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene	9.96	11.85	1.19	1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M32
25	Phthaloyl Chloride	Dianhydro-D-glucitol				1:1	{[][<]C(=O)c(cccc1)c1C(=O)[<],[>]OC(C1CO1)C(C2CO2)O[>][]}	M32
26	Phthaloyl Chloride	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)c(cccc1)c1C(=O)[<],[>]OC/C=C/C O[>][]}	M32
27	Diglycolyl Chloride	4,4′-(alpha-Methylbenzylidene)bisphenol	4.43	5.26	1.19	1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1ccc(cc1)C(C)(c 2ccccc2)c3ccc(cc3)O[>][]}	M32
28	Oxalyl Chloride	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene				1:1	{[][<]C(=O)C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c 2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M32
29	Diglycolyl Chloride	4,4′-Cyclohexylidenebisphenol	3.64	4.34	1.19	1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1ccc(cc1)C2(C CCCC2)c3cc(cc3)O[>][]}	M32
30	Phthaloyl Chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)c(cccc1)c1C(=O)[<],[>]Oc1c(ccc2) c(ccc1)c2O[>][]}	M32
31	Phthaloyl Chloride	2,7-Naphthalenediol				1:1	{[][<]C(=O)c(cccc1)c1C(=O)[<],[>]Oc1cc2c(cc 1)ccc(c2)O[>][]}	M32

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32	Phthaloyl Chloride	Bisphenol A	0.78	1.05	1.34	1:1	{[][<]C(=O)c(cccc1)c1C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
33	Sebacoyl Chloride	Bisphenol A	5.54	5.94	1.07	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
34	Diglycolyl Chloride	4,4′-(9-Fluorenylidene)diphenol	0.74	0.89	1.2	1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1ccc(cc1)C2(c3ccccc3c4c2ccccc4)c5ccc(cc5)O[>][]}	M32
35	Diglycolyl Chloride	4,4′-Thiodiphenol	5.74	6.16	1.07	1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
36	Diglycolyl Chloride	2,2′-Thiodiethanol	0.90	1.47	1.64	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCSCCO[>][]}	M32
37	Sebacoyl Chloride	4,4'-Dihydroxydiphenylmethane				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)Cc2ccc(cc2)O[>][]}	M32
38	Oxalyl Chloride	4,4′-(alpha-Methylbenzylidene)bisphenol	4.30	3.11	2.12	1:1	{[][<]C(=O)C(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M32
39	Diglycolyl Chloride	(R)-(+)-1,1′-Binaphthyl-2,2′-diol				1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1ccc(cccc2)c2c1c3c(cccc4)c4ccc3O[>][]}	M32
40	Diglycolyl Chloride	cis-2-Butene-1,4-diol	10.33	13.00	1.26	1:1	{[][<]C(=O)COC(=O)[<],[>]OC/C=C/CO[>][]}	M32
41	Diglycolyl Chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
42	Diglycolyl Chloride	2,7-Naphthalenediol				1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
43	Diglycolyl Chloride	2-Hydroxyethyl disulfide	6.28	7.80	1.24	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCSSCCO[>][]}	M32

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44	Oxalyl Chloride	4,4′-Isopropylidenedicyclohexanol, mixture of isomers	1:1	{[][<]C(=O)C(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M32
45	Oxalyl Chloride	1,4-dithiane-2,5-diol	1:1	{[][<]C(=O)C(=O)[<],[>]OC(CS1)SCC1O[>][]}	M32
46	Sebacoyl Chloride	4,4′-Thiodiphenol	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
47	Oxalyl Chloride	2,5-hexanediol(+isomers)	1:1	{[][<]C(=O)C(=O)[<],[>]OC(C)CCC(C)O[>][]}	M32
48	Oxalyl Chloride	1,8-octanediol	1:1	{[][<]C(=O)C(=O)[<],[>]OCCCCCCCCO[>][]}	M32
49	Oxalyl Chloride	1,10-decanediol	1:1	{[][<]C(=O)C(=O)[<],[>]OCCCCCCCCCCO[>][]}	M32
50	Oxalyl Chloride	2,2-diethyl-1,3-propanediol	1:1	{[][<]C(=O)C(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M32
51	Oxalyl Chloride	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)C(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M32
52	Malonyl Chloride	4,4'-Dihydroxydiphenylmethane	1:1	{[][<]C(=O)CC(=O)[<],[>]Oc1ccc(cc1)Cc2ccc(cc2)O[>][]}	M32
53	Sebacoyl Chloride	2,2′-Thiodiethanol	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCSCCO[>][]}	M32
54	Sebacoyl Chloride	1,4-dithiane-2,5-diol	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M32
55	Oxalyl Chloride	2,7-Naphthalenediol	1:1	{[][<]C(=O)C(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32

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56	Sebacoyl Chloride	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OC/C=C/CO[>][]}	M32
57	Succinyl Chloride	4,4′-(alpha-Methylbenzylidene)bisphenol				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M32
58	Succinyl Chloride	Bis(4-hydroxyphenyl) Sulfone				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32
59	Succinyl Chloride	4,4′-Cyclohexylidenebisphenol				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1ccc(cc1)C2(CCCCC2)c3cc(cc3)O[>][]}	M32
60	Succinyl Chloride	4,4′-Isopropylidenebis(2,6-dimethylphenol)				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1c(C)cc(cc1(C))C(C)(C)c2cc(C)c(c(C)c2)O[>][]}	M32
61	Succinyl Chloride	4,4′-Thiodiphenol				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
62	Sebacoyl Chloride	Resorcinol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M32
63	Succinyl Chloride	Biphenyl-2,2′-diol				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc(cccc1)c1c2c(cccc2)O[>][]}	M32
64	Succinyl Chloride	4,4′-Sulfonylbis(2-methylphenol)				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1c(C)cc(cc1)S(=O)(=O)c2ccc(c(C)c2)O[>][]}	M32
65	Succinyl Chloride	(R)-(+)-1,1′-Binaphthyl-2,2′-diol				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1ccc(cccc2)c2c1c3c(cccc4)c4ccc3O[>][]}	M32
66	Succinyl Chloride	2-Butyne-1,4-diol	10.32	20.63	2.00	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC#CCO[>][]}	M32
67	Succinyl Chloride	Dianhydro-D-glucitol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OC(C1CO1)C(C2CO2)O[>][]}	M32

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68	Succinyl Chloride	cis-2-Butene-1,4-diol	1:1	{[][<]C(=O)CCC(=O)[<],[>]OC/C=C/CO[>][]}	M32
69	Succinyl Chloride	Naphthalene-1,5-diol	1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
70	Succinyl Chloride	2,7-Naphthalenediol	1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
71	Sebacoyl Chloride	Naphthalene-1,5-diol	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
72	Succinyl Chloride	2-Hydroxyethyl disulfide	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCSSCCO[>][]}	M32
73	Isophthaloyl Chloride	Bisphenol A	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
74	Isophthaloyl Chloride	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M32
75	Isophthaloyl Chloride	4,4′-(alpha-Methylbenzylidene)bisphenol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M32
76	Isophthaloyl Chloride	Bis(4-hydroxyphenyl) Sulfone	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32
77	Isophthaloyl Chloride	4,4′-Cyclohexylidenebisphenol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1ccc(cc1)C2(CCCCC2)c3cc(cc3)O[>][]}	M32
78	Isophthaloyl Chloride	4,4′-Isopropylidenebis(2,6-dimethylphenol)	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1c(C)cc(cc1(C))C(C)(C)c2cc(C)c(c(C)c2)O[>][]}	M32

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79	Sebacoyl Chloride	2,7-Naphthalenediol	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
80	Isophthaloyl Chloride	4,4′-Thiodiphenol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
81	Isophthaloyl Chloride	4,4′-Sulfonylbis(2-methylphenol)	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1c(C)cc(cc1)S(=O)(=O)c2ccc(c(C)c2)O[>][]}	M32
82	Isophthaloyl Chloride	(R)-(+)-1,1′-Binaphthyl-2,2′-diol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1ccc(ccc2)c2c1c3c(cccc4)c4ccc3O[>][]}	M32
83	Sebacoyl Chloride	2-Butyne-1,4-diol	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC#CCO[>][]}	M32
84	Isophthaloyl Chloride	Dianhydro-D-glucitol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OC(C1CO1)C(C2CO2)O[>][]}	M32
85	Isophthaloyl Chloride	cis-2-Butene-1,4-diol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OC/C=C/CO[>][]}	M32
86	Isophthaloyl Chloride	Resorcinol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1cccc(c1)O[>][]}	M32
87	Isophthaloyl Chloride	Naphthalene-1,5-diol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
88	Isophthaloyl Chloride	2,7-Naphthalenediol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
89	Terephthaloyl chloride	3-methyl-1,5-pentanediol	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCC(C)CCO[>][]}	M32

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90	Sebacoyl Chloride	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene	5.66	6.68	1.18	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M32
91	Adipoyl Chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
92	Adipoyl Chloride	2,7-Naphthalenediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
93	Adipoyl Chloride	Guaiacol glyceryl ether	6.08	7.65	1.26	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M32
94	Adipoyl Chloride	Bis(4-hydroxyphenyl) Sulfone				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32
95	Sebacoyl Chloride	4,4′-(alpha-Methylbenzylidene)bisphenol	4.69	5.49	1.17	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M32
96	Isophthaloyl Chloride	2,5-dimethyl-3-hexyne-2,5-diol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OC(C)(C)C#CC(C)(C)O[>][]}	M32
97	Sebacoyl Chloride	2,5-dimethyl-3-hexyne-2,5-diol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OC(C)(C)C#CC(C)(C)O[>][]}	M32
98	Adipoyl Chloride	2,2′-Thiodiethanol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCSCCO[>][]}	M32
99	Adipoyl Chloride	1,4-Dithiane-2,5-diol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M32
100	Adipoyl Chloride	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OC/C=C/CO[>][]}	M32
101	Adipoyl Chloride	Resorcinol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M32

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102	Adipoyl Chloride	Biphenyl-2,2′-diol	9.56	14.04	1.47	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc(cccc1)c1c2c(cccc2)O[>][]}	M32
103	Malonyl Chloride	Bis(4-hydroxyphenyl) Sulfone				1:1	{[][<]C(=O)CC(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32
104	Sebacoyl Chloride	4,4′-(9-Fluorenylidene)diphenol	4.88	5.79	1.19	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C2(c3ccccc3c4c2ccccc4)c5ccc(cc5)O[>][]}	M32
105	Adipoyl Chloride	4,4′-Sulfonylbis(2-methylphenol)				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1c(C)cc(cc1)S(=O)(=O)c2ccc(c(C)c2)O[>][]}	M32
106	Adipoyl Chloride	Bisphenol A	9.42	14.00	1.49	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
107	Adipoyl Chloride	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M32
108	Adipoyl Chloride	4,4′-Isopropylidenebis(2,6-dimethylphenol)				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1c(C)cc(cc1(C))C(C)(C)c2cc(C)c(c(C)c2)O[>][]}	M32
109	Adipoyl Chloride	4,4′-(alpha-Methylbenzylidene)bisphenol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M32
110	Adipoyl Chloride	4,4′-Cyclohexylidenebisphenol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1ccc(cc1)C2(CCCCC2)c3cc(cc3)O[>][]}	M32
111	Adipoyl Chloride	Bis(4-hydroxyphenyl) Sulfone				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32

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112	Adipoyl Chloride	2-Butyne-1,4-diol	8.64	9.54	1.10	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC#CCO[>][]}	M32
113	Adipoyl Chloride	4,4′-Thiodiphenol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
114	Sebacoyl Chloride	Dianhydro-D-glucitol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OC(C1CO1)C(C2CO2)O[>][]}	M32
115	Sebacoyl Chloride	Guaiacol glyceryl ether	6.15	8.26	1.34	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M32
116	Sebacoyl Chloride	Bis(4-hydroxyphenyl) Sulfone				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32
117	Terephthaloyl Chloride	tripropylene glycol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M32
118	Terephthaloyl Chloride	Resorcinol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1cccc(c1)O[>][]}	M32
119	Terephthaloyl Chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
120	Terephthaloyl Chloride	2,7-Naphthalenediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
121	Terephthaloyl Chloride	2-Butyne-1,4-diol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC#CCO[>][]}	M32
122	Terephthaloyl Chloride	Bisphenol A				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
123	Terephthaloyl Chloride	4,4'-Dihydroxydiphenylmethane				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)Cc2ccc(cc2)O[>][]}	M32

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124	Terephthaloyl Chloride	Bis(4-hydroxyphenyl) Sulfone				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32
125	Terephthaloyl Chloride	4,4′-Thiodiphenol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
126	Terephthaloyl Chloride	Guaiacol glyceryl ether	5.57	6.44	1.16	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M32
127	Terephthaloyl Chloride	2,2′-Thiodiethanol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCSCCO[>][]}	M32
128	Terephthaloyl Chloride	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC(CS1)SCC1O[>][]}	M32
129	Terephthaloyl Chloride	Dianhydro-D-glucitol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC(C1CO1)C(C2CO2)O[>][]}	M32
130	Malonyl Chloride	4,4′-Thiodiphenol				1:1	{[][<]C(=O)CC(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
131	Terephthaloyl Chloride	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC/C=C/CO[>][]}	M32
132	Sebacoyl Chloride	4,4′-Cyclohexylidenebisphenol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C2(CCCCC2)c3cc(cc3)O[>][]}	M32
133	Sebacoyl Chloride	(R)-(+)-1,1′-Binaphthyl-2,2′-diol	0.91	1.36	1.48	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1ccc(cccc2)c2c1c3c(cccc4)c4ccc3O[>][]}	M32

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134	Sebacoyl Chloride	4,4′-Sulfonylbis(2-methylphenol)	4.44	4.67	1.05	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]Oc1c(C)cc(cc1)S(=O)(=O)c2ccc(c(C)c2)O[>][]}	M32
135	Azelaoyl chloride	Bisphenol A	1.29	1.92	1.49	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
136	Azelaoyl chloride	4,4'-Dihydroxydiphenylmethane				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(cc1)Cc2ccc(cc2)O[>][]}	M32
137	Azelaoyl chloride	4,4′-Thiodiphenol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
138	Azelaoyl chloride	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M32
139	Azelaoyl chloride	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OC/C=C/CO[>][]}	M32
140	Azelaoyl chloride	Resorcinol	1.15	1.65	1.43	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M32
141	Azelaoyl chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
142	Azelaoyl chloride	2,7-Naphthalenediol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
143	Azelaoyl chloride	2-Butyne-1,4-diol	2.37	3.56	1.50	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC#CCO[>][]}	M32
144	Azelaoyl chloride	Guaiacol glyceryl ether	1.67	2.35	1.41	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M32

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145	Azelaoyl chloride	Bis(4-hydroxyphenyl) Sulfone				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M32
146	Azelaoyl chloride	Biphenyl-2,2′-diol	4.27	6.08	3.04	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc(cccc1)c1c2c(cccc2)O[>][]}	M32
147	Azelaoyl chloride	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene	1.52	2.53	1.67	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M32
148	Azelaoyl chloride	4,4′-(alpha-Methylbenzylidene)bisphenol	1.77	2.16	1.22	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M32
149	Azelaoyl chloride	4,4′-Isopropylidenebis(2,6-dimethylphenol)	2.02	2.35	1.17	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1c(C)cc(cc1(C))C(C)(C)c2cc(C)c(c(C)c2)O[>][]}	M32
150	Azelaoyl chloride	4,4′-(9-Fluorenylidene)diphenol	1.36	1.50	1.10	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(cc1)C2(c3ccccc3c4c2ccccc4)c5ccc(cc5)O[>][]}	M32
151	Azelaoyl chloride	(R)-(+)-1,1′-Binaphthyl-2,2′-diol	0.56	0.79	1.41	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]Oc1ccc(ccc2)c2c1c3c(cccc4)c4ccc3O[>][]}	M32
152	Suberoyl chloride	Bisphenol A				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
153	Suberoyl chloride	4,4'-Dihydroxydiphenylmethane				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]Oc1ccc(cc1)Cc2ccc(cc2)O[>][]}	M32
154	Suberoyl chloride	4,4′-Thiodiphenol				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32

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155	Malonyl Chloride	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M32
156	Suberoyl chloride	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M32
157	Suberoyl chloride	Resorcinol	1.34	2.45	1.83	1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M32
158	Suberoyl chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
159	Suberoyl chloride	2,7-Naphthalenediol				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M32
160	Dimethylmalonyl chloride	Bisphenol A				1:1	{[][<]C(=O)C(C)(C)C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M32
161	Dimethylmalonyl chloride	Biphenyl-2,2′-diol				1:1	{[][<]C(=O)C(C)(C)C(=O)[<],[>]Oc(cccc1)c1c2c(cccc2)O[>][]}	M32
162	Dimethylmalonyl chloride	4,4′-Thiodiphenol				1:1	{[][<]C(=O)C(C)(C)C(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M32
163	Dimethylmalonyl chloride	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)C(C)(C)C(=O)[<],[>]OC/C=C/CO[>][]}	M32
164	Dimethylmalonyl chloride	Naphthalene-1,5-diol				1:1	{[][<]C(=O)C(C)(C)C(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M32
165	Terephthaloyl Chloride	Biphenyl-2,2′-diol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc(cccc1)c1c2c(cccc2)O[>][]}	M32
166	Terephthaloyl Chloride	1,3-Propanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCCO[>][]}	M32
167	Terephthaloyl Chloride	1,5-pentanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCCCCO[>][]}	M32

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168	Dimethylcarbonate	1,3-Bis[2-(4-hydroxyphenyl)-2-propyl]benzene				1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)C(C)(C)c3ccc(cc3)O[>][]}	M27
169	Dimethylcarbonate	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)[<],[>]OC/C=C/CO[>][]}	M27
170	Dimethylcarbonate	1,3-Propanediol				1:1	{[][<]C(=O)[<],[>]OCCCO[>][]}	M27
171	Dimethylcarbonate	1,5-pentanediol	10.49	14.15	1.35	1:1	{[][<]C(=O)[<],[>]OCCCCCO[>][]}	M27
172	Dimethylcarbonate	1,8-octanediol	1.65	2.87	1.74	1:1	{[][<]C(=O)[<],[>]OCCCCCCCCO[>][]}	M28
173	Dimethylcarbonate	1,9-nonanediol	1.92	3.19	1.66	1:1	{[][<]C(=O)[<],[>]OCCCCCCCCCO[>][]}	M27
174	Dimethylcarbonate	1,10-decanediol	1.82	2.92	1.61	1:1	{[][<]C(=O)[<],[>]OCCCCCCCCCCO[>][]}	M27
175	Dimethylcarbonate	4,4′-(alpha-Methylbenzylidene)bisphenol	2.16	2.19	1.01	1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)C(C)(c2ccccc2)c3ccc(cc3)O[>][]}	M28
176	Dimethylcarbonate	2,2-diethyl-1,3-propanediol	1.13	1.83	1.61	1:1	{[][<]C(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M27
177	Dimethylcarbonate	2,2-Dimethyl-1,3-propanediol	3.31	6.30	1.90	1:1	{[][<]C(=O)[<],[>]OCC(C)(C)CO[>][]}	M28
178	Dimethylcarbonate	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane				1:1	{[][<]C(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M28
179	Dimethylcarbonate	1,4-cyclohexanediol				1:1	{[][<]C(=O)[<],[>]OC(CC1)CCC1O[>][]}	M27
180	Dimethylcarbonate	diethylene glycol				1:1	{[][<]C(=O)[<],[>]OCCOCCO[>][]}	M28
181	Dimethylcarbonate	4,4′-Sulfonylbis(2-methylphenol)				1:1	{[][<]C(=O)[<],[>]Oc1c(C)cc(cc1)S(=O)(=O)c2ccc(c(C)c2)O[>][]}	M29
182	Dimethylcarbonate	2-Hydroxyethyl disulfide				1:1	{[][<]C(=O)[<],[>]OCCSSCCO[>][]}	M29

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183	Dimethylcarbonate	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M27
184	Dimethylcarbonate	dipropylene glycol	4.52	5.04	1.12	1:1	{[][<]C(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M27
185	Dimethylcarbonate	Naphthalene-1,5-diol				1:1	{[][<]C(=O)[<],[>]Oc1c(ccc2)c(ccc1)c2O[>][]}	M27
186	Dimethylcarbonate	2,7-Naphthalenediol				1:1	{[][<]C(=O)[<],[>]Oc1cc2c(cc1)ccc(c2)O[>][]}	M27
187	Dimethylcarbonate	2-Butyne-1,4-diol				1:1	{[][<]C(=O)[<],[>]OCC#CCO[>][]}	M27
188	Dimethylcarbonate	Bisphenol A				1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M29
189	Dimethylcarbonate	4,4'-Dihydroxydiphenylmethane				1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)Cc2ccc(cc2)O[>][]}	M29
191	Dimethylcarbonate	4,4′-(9-Fluorenylidene)diphenol	2.14	2.16	1.01	1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)C2(c3ccccc3c4c2ccccc4)c5ccc(cc5)O[>][]}	M27
192	Dimethylcarbonate	1,4-Butanediol	1.67	2.76	1.66	1:1	{[][<]C(=O)[<],[>]OCCCCO[>][]}	M29
193	Dimethylcarbonate	1,6-Hexanediol	3.68	7.70	2.09	1:1	{[][<]C(=O)[<],[>]OCCCCCCO[>][]}	M29
194	Dimethylcarbonate	2-Methyl-1,3-propanediol	2.00	3.04	1.52	1:1	{[][<]C(=O)[<],[>]OCC(C)CO[>][]}	M29
195	Dimethylcarbonate	2-Butyl-2-ethyl-1,3-propanediol	2.28	3.54	1.55	1:1	{[][<]C(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M29
196	dimethylcarbonate	1,5-hexadiene-3,5-diol				1:1	{[][<]C(=O)[<],[>]OC(C=C)C(C=C)O[>][]}	M30
197	Dimethylcarbonate	4,4′-Cyclohexylidenebisphenol	1.84	1.88	1.02	1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)C2(CCCCC2)c3cc(cc3)O[>][]}	M27

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198	Dimethylcarbonate	(R)-(+)-1,1′-Binaphthyl-2,2′-diol				1:1	{[][<]C(=O)[<],[>]Oc1ccc(cccc2)c2c1c3c(cccc4)c4ccc3O[>][]}	M28
199	Dimethylcarbonate	4,4′-Thiodiphenol	2.55	2.56	1.01	1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)Sc2ccc(cc2)O[>][]}	M27
200	Dimethylcarbonate	Guaiacol glyceryl ether				1:1	{[][<]C(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M28
201	Dimethylcarbonate	2,2′-Thiodiethanol				1:1	{[][<]C(=O)[<],[>]OCCSCCO[>][]}	M28
202	Diglycolic acid	ethylene glycol				1:1	{[][<]C(=O)COC(=O)[<],[>]OCCO[>][]}	M25
203	Diglycolic acid	1,10-decanediol	7.88	27.97	3.55	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M25
204	Diglycolic acid	1,2-Propanediol	6.50	11.68	1.80	1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(C)O[>][]}	M25
205	Diglycolic acid	1,3-Propanediol	14.56	19.47	1.34	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCO[>][]}	M25
206	Diglycolic acid	1,4-Butanediol				1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCCO[>][]}	M25
207	Diglycolic acid	1,5-pentanediol	5.19	10.20	1.97	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCCCO[>][]}	M25
208	Diglycolic acid	1,6-Hexanediol	9.96	22.53	2.26	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCCCCO[>][]}	M25
209	Diglycolic acid	3-methyl-1,5-pentanediol	7.92	21.51	2.72	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
210	Diglycolic acid	1,7-heptanediol	10.24	28.59	2.79	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCCCCCO[>][]}	M25
211	Diglycolic acid	1,8-octanediol	4.88	14.40	2.95	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCCCCCCO[>][]}	M25
212	Diglycolic acid	1,9-nonanediol	9.55	32.64	3.42	1:1	{[][<]C(=O)COC(=O)[<],[>]OCCCCCCCCCO[>][]}	M25

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213	2,2′-Thiodiacetic acid	3-methyl-1,5-pentanediol	8.67	27.38	3.16	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
214	2,2′-Thiodiacetic acid	1,10-decanediol	5.36	16.70	3.12	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCCCCCCCCCCO[>][]}	M25
215	[(Carboxymethyl)(methyl)amino]acetic acid	1,4-Butanediol	5.31	10.99	2.07	1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCCCCO[>][]}	M25
216	[(Carboxymethyl)(methyl)amino]acetic acid	1,6-Hexanediol	4.50	8.75	1.95	1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCCCCCCCO[>][]}	M25
217	[(Carboxymethyl)(methyl)amino]acetic acid	3-methyl-1,5-pentanediol	3.53	6.05	1.72	1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
218	[(Carboxymethyl)(methyl)amino]acetic acid	1,10-decanediol	3.30	5.52	1.68	1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCCCCCCCCCCCO[>][]}	M25
219	2,2′-Thiodiacetic acid	ethylene glycol	3.05	5.06	1.66	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCO[>][]}	M25
220	2,2′-Thiodiacetic acid	1,4-Butanediol	8.76	21.37	2.44	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCCCO[>][]}	M25
221	2,2′-Thiodiacetic acid	1,6-Hexanediol	11.35	31.59	2.78	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCCCCCO[>][]}	M25
222	Adipic acid	2,2-Diethyl-1,3-propanediol	7.79	14.79	1.90	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M25
223	Adipic acid	1,2-Propanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(C)O[>][]}	M25
224	Adipic acid	2-Methyl-1,3-propanediol	9.47	17.96	1.90	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(C)CO[>][]}	M25
225	Adipic acid	2-Butyl-2-ethyl-1,3-propanediol	12.23	24.49	2.00	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M25

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226	Adipic acid	2,2,4-Trimethyl-1,3-pentanediol	7.06	16.39	2.32	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M25
227	Adipic acid	2,2-Dimethyl-1,3-propanediol	6.02	11.83	1.96	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M25
228	Adipic acid	cis-2-Butene-1,4-diol	9.66	18.83	1.95	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OC/C=C/CO[>][]}	M25
229	Adipic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers	6.53	14.56	2.23	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M25
230	Adipic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	6.91	13.18	1.91	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M25
231	Adipic acid	2-Butyne-1,4-diol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC#CCO[>][]}	M25
232	Adipic acid	2,3-Butanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OC(C)C(C)O[>][]}	M25
233	Succinic acid	Resorcinol				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M25
234	Adipic acid	1,4-Cyclohexanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M25
235	Adipic acid	Resorcinol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M25
236	Succinic acid	2,3-Butanediol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OC(C)C(C)O[>][]}	M25
237	Succinic acid	1,4-Cyclohexanediol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M25
238	Succinic acid	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OC/C=C/CO[>][]}	M25
239	Succinic acid	2,2-Diethyl-1,3-propanediol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M25

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240	Suberic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M25
241	Succinic acid	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(C)CO[>][]}	M25
242	Succinic acid	2-Butyl-2-ethyl-1,3-propanediol	20.47	32.80	1.60	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M25
243	Succinic acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M25
244	Succinic acid	2,2-Dimethyl-1,3-propanediol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M25
245	Succinic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M25
246	Succinic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)CCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M25
247	Succinic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M25
248	Succinic acid	Bisphenol A				1:1	{[][<]C(=O)CCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M25
249	[(Carboxymethyl)(methyl)amino]acetic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M25
250	2,2′-Thiodiacetic acid	2,3-Butanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OC(C)C(C)O[>][]}	M25
251	2,2′-Thiodiacetic acid	Bisphenol A				1:1	{[][<]C(=O)CSCC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M25

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252	[(Carboxymethyl)(methyl)amino]acetic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M25
253	[(Carboxymethyl)(methyl)amino]acetic acid	2-Butyl-2-ethyl-1,3-propanediol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M25
254	[(Carboxymethyl)(methyl)amino]acetic acid	Resorcinol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M25
255	[(Carboxymethyl)(methyl)amino]acetic acid	2,3-Butanediol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OC(C)C(C)O[>][]}	M25
256	2,2′-Thiodiacetic acid	1,4-Cyclohexanedimethanol	26.76	40.97	2.22	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M25
257	2,2′-Thiodiacetic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M25
258	2,2′-Thiodiacetic acid	2-Butyl-2-ethyl-1,3-propanediol	26.76	50.57	1.89	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M25
259	2,2′-Thiodiacetic acid	Resorcinol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M25
260	Diglycolic acid	2,2-Diethyl-1,3-propanediol	12.91	19.18	1.49	1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M25
261	Diglycolic acid	Bisphenol A	10.80	18.57	1.72	1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M25
262	Diglycolic acid	Resorcinol				1:1	{[][<]C(=O)COC(=O)[<],[>]Oc1cccc(c1)O[>][]}	M25
263	Diglycolic acid	2-Methyl-1,3-propanediol	20.45	29.38	1.44	1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(C)CO[>][]}	M25

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264	Diglycolic acid	2-Butyl-2-ethyl-1,3-propanediol	14.84	23.83	1.61	1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M25
265	Diglycolic acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M25
266	Diglycolic acid	2,2-Dimethyl-1,3-propanediol	16.45	26.42	1.61	1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(C)(C)CO[>][]}	M25
267	Diglycolic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M25
268	Diglycolic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers	8.29	14.89	1.80	1:1	{[][<]C(=O)COC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M25
269	Diglycolic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane				1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M25
270	Diglycolic acid	Dianhydro-D-glucitol				1:1	{[][<]C(=O)COC(=O)[<],[>]OC(C1CO1)C(C2CO2)O[>][]}	M25
271	Terephthaloyl Chloride	ethylene glycol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCO[>][]}	M31
272	Terephthaloyl Chloride	1,4-Butanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCCCCO[>][]}	M31
273	Terephthaloyl Chloride	cis-2-Butene-1,4-diol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC/C=C/CO[>][]}	M31
274	Terephthaloyl Chloride	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(C)CO[>][]}	M31
275	Terephthaloyl Chloride	2-Butyl-2-ethyl-1,3-propanediol				1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M31

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276	Terephthaloyl Chloride	1,4-Cyclohexanedimethanol	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M31
277	Terephthaloyl Chloride	4,4′-Isopropylidenedicyclohexanol, mixture of isomers	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M31
278	Terephthaloyl Chloride	Bisphenol A	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O[>][]}	M31
279	1,4-Cyclohexanedicarboxylic acid	ethylene glycol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCO[>][]}	M25
280	1,4-Cyclohexanedicarboxylic acid	2,2-Dimethyl-1,3-propanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(C)(C)CO[>][]}	M25
281	1,4-Cyclohexanedicarboxylic acid	2-Methyl-1,3-propanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(C)CO[>][]}	M25
282	1,4-Cyclohexanedicarboxylic acid	1,4-Butanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCCO[>][]}	M25
283	1,4-Cyclohexanedicarboxylic acid	3-methyl-1,5-pentanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCC(C)CCO[>][]}	M25
284	1,4-Cyclohexanedicarboxylic acid	1,10-decanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCCCCCCCCO[>][]}	M25
285	1,4-Cyclohexanedicarboxylic acid	2-Butyl-2-ethyl-1,3-propanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M25
286	1,4-Cyclohexanedicarboxylic acid	1,4-Cyclohexanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OC(CC1)CCC1O[>][]}	M25

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287	1,4-Cyclohexanedicarboxylic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M25
288	1,4-Cyclohexanedicarboxylic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M25
289	1,4-Cyclohexanedicarboxylic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M25
290	azelaic acid	ethylene glycol	8.89	19.11	2.15	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCO[>][]}	M25
291	pimelic acid	3-methyl-1,5-pentanediol	16.32	62.65	3.84	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
292	azelaic acid	1,3-Propanediol	9.44	26.33	2.79	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCCO[>][]}	M25
293	azelaic acid	1,4-Butanediol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCCCO[>][]}	M25
294	azelaic acid	1,5-pentanediol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCCCCO[>][]}	M25
295	azelaic acid	3-methyl-1,5-pentanediol	8.02	42.88	5.35	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
296	azelaic acid	1,10-decanediol	15.75	137.4	8.72	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCCCCCCCCCCO[>][]}	M25
297	pimelic acid	ethylene glycol	11.41	59.09	5.18	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCO[>][]}	M25
298	pimelic acid	1,3-Propanediol	8.13	12.47	1.53	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCCO[>][]}	M25
299	pimelic acid	1,4-Butanediol	11.70	37.81	3.23	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCCCO[>][]}	M25

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300	Succinic acid	ethylene glycol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCO[>][]}	M25
302	Succinic acid	1,10-decanediol	17.90	49.25	2.75	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M25
303	Succinic acid	1,3-Propanediol	5.35	8.50	1.59	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCO[>][]}	M25
304	Succinic acid	1,4-Butanediol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCCO[>][]}	M25
305	Succinic acid	1,5-pentanediol	12.13	52.16	4.30	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCCCO[>][]}	M25
306	Succinic acid	1,6-Hexanediol	13.67	38.96	2.85	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCCCCO[>][]}	M25
307	Succinic acid	2,5-hexanediol(+isomers)				1:1	{[][<]C(=O)CCC(=O)[<],[>]OC(C)CCC(C)O[>][]}	M25
308	Succinic acid	3-methyl-1,5-pentanediol	7.35	27.46	3.74	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
309	Succinic acid	1,7-heptanediol	14.85	45.93	3.09	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCCCCCO[>][]}	M25
310	Succinic acid	1,8-octanediol	14.14	40.09	2.84	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCCCCCCO[>][]}	M25
311	glutaric acid	ethylene glycol	5.60	9.44	1.68	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCO[>][]}	M25
312	glutaric acid	1,10-decanediol	13.96	37.78	2.71	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M25
313	azelaic acid	1,8-octanediol	14.67	60.83	4.15	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCCCCCCCO[>][]}	M25
314	glutaric acid	1,3-Propanediol	6.41	11.98	1.87	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCO[>][]}	M25
315	glutaric acid	1,4-Butanediol	4.58	13.20	2.88	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCCO[>][]}	M25
316	glutaric acid	1,5-pentanediol	6.57	20.15	3.07	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCCCO[>][]}	M25

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317	glutaric acid	1,6-Hexanediol	12.71	33.62	2.65	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCCCCO[>][]}	M25
318	glutaric acid	3-methyl-1,5-pentanediol	5.64	15.50	2.75	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
319	glutaric acid	1,7-heptanediol	9.66	32.56	3.37	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCCCCCO[>][]}	M25
320	glutaric acid	1,8-octanediol	9.80	49.39	5.04	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCCCCCCO[>][]}	M25
321	glutaric acid	1,9-nonanediol	14.95	58.88	3.94	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCCCCCCCCO[>][]}	M25
322	Adipic acid	ethylene glycol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCO[>][]}	M25
323	Adipic acid	1,10-decanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M25
324	azelaic acid	1,9-nonanediol	25.36	102.9	4.06	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCCCCCCCCO[>][]}	M25
325	Adipic acid	1,3-Propanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCO[>][]}	M25
326	Adipic acid	1,4-Butanediol	3.60	7.86	2.19	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCCO[>][]}	M25
327	Adipic acid	1,5-pentanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCCCO[>][]}	M25
328	Adipic acid	1,6-Hexanediol	8.25	44.50	5.39	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCCCCO[>][]}	M25
329	Adipic acid	3-methyl-1,5-pentanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
330	Adipic acid	1,7-heptanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCCCCCO[>][]}	M25

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331	Adipic acid	1,8-octanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCCCCCCO[>][]}	M25
332	Adipic acid	1,9-nonanediol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCCCCCCCCO[>][]}	M25
333	isophthalic acid	ethylene glycol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCO[>][]}	M25
334	isophthalic acid	1,10-decanediol	4.09	9.09	2.22	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCCCCCCCCO[>][]}	M25
335	isophthalic acid	1,2-Propanediol	6.00	12.80	2.13	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(C)O[>][]}	M25
336	isophthalic acid	1,3-Propanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCO[>][]}	M25
337	isophthalic acid	1,4-Butanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCCO[>][]}	M25
338	isophthalic acid	1,5-pentanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCCCO[>][]}	M25
339	isophthalic acid	1,6-Hexanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCCCCO[>][]}	M25
340	isophthalic acid	3-methyl-1,5-pentanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCC(C)CCO[>][]}	M25
341	isophthalic acid	1,7-heptanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCCCCCO[>][]}	M25
342	isophthalic acid	1,8-octanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCCCCCCO[>][]}	M25
343	isophthalic acid	1,9-nonanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCCCCCCCCO[>][]}	M25

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344	Terephthaloyl Chloride	1,2-propanediol	7.56	19.29	2.55	1:1	{[][<]C(=O)c1ccc(cc1)C(=O)[<],[>]OCC(C)O[>][]}	M31
345	1,4-Cyclohexanedicarboxylic acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M1
346	isophthalic acid	1,2-propanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(C)O[>][]}	M18
347	[(Carboxymethyl)(methyl)amino]acetic acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M11
348	2,6-Naphthalenedicarboxylic Acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M11
349	2,6-Naphthalenedicarboxylic Acid	1,4-Butanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCCCO[>][]}	M12
350	2,2′-Thiodiacetic acid	1,5-pentanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCCCCO[>][]}	M12
351	1,4-Cyclohexanedicarboxylic acid	1,5-pentanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCCCO[>][]}	M12
352	[(Carboxymethyl)(methyl)amino]acetic acid	1,5-pentanediol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCCCCCO[>][]}	M12
353	2,6-Naphthalenedicarboxylic Acid	1,5-pentanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCCCCO[>][]}	M12
354	1,4-Cyclohexanedicarboxylic acid	1,6-Hexanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCCCCO[>][]}	M12
355	2,6-Naphthalenedicarboxylic Acid	1,6-Hexanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCCCCCO[>][]}	M12

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356	isophthalic acid	2,3-Butanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OC(C)C(C)O[>][]}	M18
357	1,4-Cyclohexanedicarboxylic acid	1,7-heptanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCCCCCCO[>][]}	M12
358	2,6-Naphthalenedicarboxylic Acid	1,7-heptanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCCCCCCCO[>][]}	M12
359	1,4-Cyclohexanedicarboxylic acid	1,8-octanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCCCCCCCO[>][]}	M12
360	[(Carboxymethyl)(methyl)amino]acetic acid	1,8-octanediol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCCCCCCCCCO[>][]}	M12
361	2,6-Naphthalenedicarboxylic Acid	1,8-octanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCCCCCCCO[>][]}	M12
362	glutaric acid	1,4-Cyclohexanedimethanol	6.73	9.01	1.34	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M12
363	2,6-Naphthalenedicarboxylic Acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M12
364	2,2′-Thiodiacetic acid	1,9-nonanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCCCCCCCCO[>][]}	M12
365	1,4-Cyclohexanedicarboxylic acid	1,9-nonanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCCCCCCCO[>][]}	M12
366	isophthalic acid	1,4-cyclohexanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OC(CC1)CCC1O[>][]}	M18

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367	2,6-Naphthalenedicarboxylic Acid	1,9-nonanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCCCCCCCCO[>][]}	M12
368	pimelic acid	1,10-decanediol	6.07	10.76	1.77	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M12
369	Sebacic Acid	2-Methyl-1,3-propanediol	2.51	4.27	1.70	1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OCC(C)CO[>][]}	M8
370	Sebacic Acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M8
371	Sebacic Acid	2,2,4-Trimethyl-1,3-pentanediol	2.59	4.10	1.58	1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M8
372	Sebacic Acid	1,4-Butanediol				1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OCCCCO[>][]}	M20
373	Sebacic Acid	1,5-pentanediol	4.04	7.60	1.88	1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OCCCCCO[>][]}	M8
374	pimelic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M13
375	glutaric acid	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(C)CO[>][]}	M3
376	azelaic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers	6.98	8.54	1.22	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M13

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377	pimelic acid	2,2,4-Trimethyl-1,3-pentanediol	6.81	8.13	1.20	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M13
378	azelaic acid	2,2,4-Trimethyl-1,3-pentanediol	6.78	8.14	1.20	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M13
379	pimelic acid	1,6-Hexanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCCCCCO[>][]}	M13
380	azelaic acid	1,6-Hexanediol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCCCCCO[>][]}	M13
381	Sebacic Acid	1,6-Hexanediol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCCCCCO[>][]}	M13
382	Sebacic Acid	1,7-heptanediol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCCCCCCO[>][]}	M13
383	pimelic acid	1,8-octanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCCCCCCO[>][]}	M13
384	pimelic acid	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(C)CO[>][]}	M3
385	Sebacic Acid	1,8-octanediol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCCCCCCCO[>][]}	M13
386	pimelic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M13
387	azelaic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M13
388	Sebacic Acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M13

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389	pimelic acid	1,9-nonanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCCCCCCCCO[>][]}	M13
390	Sebacic Acid	1,9-nonanediol				1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M13
391	Sebacic Acid	1,10-decanediol				1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M13
392	pimelic acid	diethylene glycol	1.97	2.81	1.42	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCOCCO[>][]}	M14
393	azelaic acid	diethylene glycol	1.84	2.91	1.58	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCOCCO[>][]}	M14
394	Sebacic Acid	diethylene glycol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCOCCO[>][]}	M14
395	2,2′-Thiodiacetic acid	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(C)CO[>][]}	M3
396	1,4-Cyclohexanedicarboxylic acid	diethylene glycol	1.38	2.54	1.85	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCOCCO[>][]}	M14
397	2,6-Naphthalenedicarboxylic Acid	diethylene glycol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCOCCO[>][]}	M14
398	glutaric acid	diethylene glycol	1.76	3.18	1.81	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCOCCO[>][]}	M14
399	2,2′-Thiodiacetic acid	diethylene glycol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCOCCO[>][]}	M20
400	isophthalic acid	diethylene glycol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCOCCO[>][]}	M14

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401	Suberic acid	diethylene glycol				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]OCCOCCO[>][]}	M14
402	Adipic acid	diethylene glycol	7.18	8.82	1.23	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCOCCO[>][]}	M14
403	azelaic acid	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(C)CO[>][]}	M3
404	azelaic acid	triethylene glycol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCOCCOCCO[>][]}	M14
405	Sebacic Acid	triethylene glycol	1.79	3.51	1.96	1:1	{[][<]C(=O)CCCCCCCCCC(=O)[<],[>]OCCOCCOCCO[>][]}	M14
406	1,4-Cyclohexanedicarboxylic acid	triethylene glycol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCOCCOCCO[>][]}	M20
407	2,6-Naphthalenedicarboxylic Acid	triethylene glycol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCOCCOCCO[>][]}	M14
408	2,2′-Thiodiacetic acid	triethylene glycol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCOCCOCCO[>][]}	M14
409	1,4-Cyclohexanedicarboxylic acid	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(C)CO[>][]}	M3
410	Suberic acid	triethylene glycol	1.35	2.42	1.80	1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]OCCOCCOCCO[>][]}	M14
411	Adipic acid	triethylene glycol	7.44	9.31	1.25	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCOCCOCCO[>][]}	M14
412	pimelic acid	tripropylene glycol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15

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413	azelaic acid	tripropylene glycol	1.47	2.55	1.73	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15
414	Sebacic Acid	tripropylene glycol	1.73	2.98	1.72	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15
415	1,4-Cyclohexanedicarboxylic acid	tripropylene glycol	0.89	1.68	1.89	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15
416	glutaric acid	tripropylene glycol	0.88	1.67	1.89	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15
417	2,2′-Thiodiacetic acid	tripropylene glycol	1.01	1.58	1.57	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15
418	Suberic acid	tripropylene glycol				1:1	{[][<]C(=O)CCCCCCC(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15
419	Succinic acid	tripropylene glycol	0.95	1.68	1.76	1:1	{[][<]C(=O)CCC(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M15
420	azelaic acid	dipropylene glycol	1.41	2.51	1.78	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M15
421	Sebacic Acid	dipropylene glycol	1.46	2.59	1.78	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M15
422	1,4-Cyclohexanedicarboxylic acid	dipropylene glycol	0.76	1.32	1.74	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M15
423	2,6-Naphthalenedicarboxylic Acid	dipropylene glycol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M15

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424	glutaric acid	dipropylene glycol	0.88	1.61	1.84	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M15
425	2,2′-Thiodiacetic acid	dipropylene glycol	1.06	1.78	1.68	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M15
426	diglycolic acid	dipropylene glycol	0.58	0.67	1.15	1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M15
427	adipic acid	dipropylene glycol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(C)OCC(C)O[>][]}	M21
428	isophthalic acid	2,2-Diethyl-1,3-propanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M18
429	azelaic acid	2,2′-Thiodiethanol	1.19	1.96	1.64	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCCSCCO[>][]}	M16
430	Sebacic Acid	2,2′-Thiodiethanol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCSCCO[>][]}	M16
431	1,4-Cyclohexanedicarboxylic acid	2,2′-Thiodiethanol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCSCCO[>][]}	M16
432	glutaric acid	2,2′-Thiodiethanol	1.62	2.80	1.72	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCCSCCO[>][]}	M16
433	2,2′-Thiodiacetic acid	2,2′-Thiodiethanol	0.92	1.74	1.89	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCSCCO[>][]}	M16
434	2,2′-[ethylenebis(oxy)] bisacetic acid	2,2′-Thiodiethanol				1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCCSCCO[>][]}	M16
435	diglycolic acid	2,2′-Thiodiethanol				1:1	{[][<]C(=O)COC(=O)[<],[>]OCCSCCO[>][]}	M21

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436	isophthalic acid	2,2′-Thiodiethanol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCCSCCO[>][]}	M16
437	Adipic acid	2,2′-Thiodiethanol	1.86	3.22	1.73	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCCSCCO[>][]}	M16
438	glutaric acid	1,4-Cyclohexanediol				1:1	{[][<]C(=O)CCCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M3
439	Succinic acid	2,2′-Thiodiethanol	0.81	1.41	1.74	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCSCCO[>][]}	M16
440	azelaic acid	Guaiacol glyceryl ether				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
441	Sebacic Acid	Guaiacol glyceryl ether				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
442	1,4-Cyclohexanedicarboxylic acid	Guaiacol glyceryl ether				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
443	glutaric acid	Guaiacol glyceryl ether	5.28	5.84	1.11	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
444	2,2′-Thiodiacetic acid	Guaiacol glyceryl ether				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
445	2,2′-[ethylenebis(oxy)] bisacetic acid	Guaiacol glyceryl ether				1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
446	Diglycolic acid	Guaiacol glyceryl ether				1:1	{[][<]C(=O)COC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
447	Adipic acid	Guaiacol glyceryl ether	4.83	5.13	1.06	1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16

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448	pimelic acid	1,4-Cyclohexanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M3
449	Succinic acid	Guaiacol glyceryl ether	4.63	4.82	1.04	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCC(COC(CCCC1)C1OC)O[>][]}	M16
450	azelaic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M17
451	1,4-Cyclohexanedicarboxylic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OC(CS1)SCC1O[>][]}	M21
452	glutaric acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CCCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M17
453	2,2′-Thiodiacetic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M17
454	2,2′-[ethylenebis(oxy)] bisacetic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M17
455	Diglycolic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)COC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M17
456	isophthalic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OC(CS1)SCC1O[>][]}	M17
457	adipic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CCCCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M21
458	pimelic acid	3-methyl-1,5-pentanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCC(C)CCO[>][]}	M3
459	Succinic acid	1,4-dithiane-2,5-diol				1:1	{[][<]C(=O)CCC(=O)[<],[>]OC(CS1)SCC1O[>][]}	M17

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460	quinoline-2,4-dicarboxylic acid	tripropylene glycol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OC(C)COC(C)COC(C)CO[>][]}	M22
461	quinoline-2,4-dicarboxylic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M22
462	quinoline-2,4-dicarboxylic acid	1,4-Cyclohexanediol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OC(CC1)CCC1O[>][]}	M22
463	quinoline-2,4-dicarboxylic acid	2,2,4-Trimethyl-1,3-pentanediol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M22
464	quinoline-2,4-dicarboxylic acid	2,2-Dimethyl-1,3-propanediol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(C)(C)CO[>][]}	M22
465	quinoline-2,4-dicarboxylic acid	2-Methyl-1,3-propanediol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(C)CO[>][]}	M22
466	quinoline-2,4-dicarboxylic acid	1,2-Propanediol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(C)O[>][]}	M22
467	quinoline-2,4-dicarboxylic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M22
468	quinoline-2,4-dicarboxylic acid	2,2-Diethyl-1,3-propanediol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M22
469	2,2′-Thiodiacetic acid	1,4-Cyclohexanediol	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M4
470	quinoline-2,4-dicarboxylic acid	2-Butyl-2-ethyl-1,3-propanediol	1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M22

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471	quinoline-2,4-dicarboxylic acid	1,10-decanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCCCCCCCCO[>][]}	M22
472	quinoline-2,4-dicarboxylic acid	1,9-nonanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCCCCCCCO[>][]}	M23
473	quinoline-2,4-dicarboxylic acid	1,8-octanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCCCCCCO[>][]}	M23
474	quinoline-2,4-dicarboxylic acid	1,6-Hexanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCCCCO[>][]}	M23
475	quinoline-2,4-dicarboxylic acid	1,5-pentanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCCCO[>][]}	M23
476	quinoline-2,4-dicarboxylic acid	1,3-Propanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCCO[>][]}	M23
477	quinoline-2,4-dicarboxylic acid	ethylene glycol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCO[>][]}	M23
478	azelaic acid	1,4-Cyclohexanediol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M4
479	quinoline-2,4-dicarboxylic acid	2,2-Diethyl-1,3-propanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M23
480	quinoline-2,4-dicarboxylic acid	triethylene glycol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCOCCOCCO[>][]}	M23
481	quinoline-2,4-dicarboxylic acid	3-methyl-1,5-pentanediol				1:1	{[][<]C(=O)c1nc2ccccc2c(c1)C(=O)[<],[>]OCCC(C)CCO[>][]}	M23
482	2,5-furandicarboxylic acid	1,5-pentanediol	12.00	17.57	1.47	1:1	{[][<]O=C(O)c1oc(C(=O)O)cc1[<],[>]OCCCCCO[>][]}	M24

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483	2,5-furandicarboxylic acid	1,4-butanediol				1:1	{[][<]O=C(O)c1oc(C(=O)O)cc1[<],[>]OCCCCO[>][]}	M24
484	2,5-furandicarboxylic acid	1,6-hexanediol				1:1	{[][<]O=C(O)c1oc(C(=O)O)cc1[<],[>]OCCCCCCO[>][]}	M24
485	2,5-furandicarboxylic acid	ethylene glycol				1:1	{[][<]O=C(O)c1oc(C(=O)O)cc1[<],[>]OCCO[>][]}	M24
486	2,5-furandicarboxylic acid	1,3-Propanediol				1:1	{[][<]O=C(O)c1oc(C(=O)O)cc1[<],[>]OCCCO[>][]}	M24
487	2,5-furandicarboxylic acid	2-Methyl-1,3-propanediol				1:1	{[][<]O=C(O)c1oc(C(=O)O)cc1[<],[>]OCC(C)CO[>][]}	M24
488	Sebacic Acid	1,4-Cyclohexanediol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M4
489	2,5-furandicarboxylic acid	1,4-Cyclohexanediol				1:1	{[][<]O=C(O)c1oc(C(=O)O)cc1[<],[>]OC(CC1)CCC1O[>][]}	M24
490	Diglycolic acid	1,4-cyclohexanediol				1:1	{[][<]C(=O)COC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M18
491	[(Carboxymethyl)(methyl)amino]acetic acid	1,4-Cyclohexanediol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M4
492	glutaric acid	2,2-Diethyl-1,3-propanediol	13.74	20.19	1.47	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M4
493	pimelic acid	2,2-Diethyl-1,3-propanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M4
494	2,2′-Thiodiacetic acid	2,2-Diethyl-1,3-propanediol	11.04	17.95	1.63	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M4

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495	Sebacic Acid	2,2-Diethyl-1,3-propanediol	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M4
496	1,4-Cyclohexanedicarboxylic acid	2,2-Diethyl-1,3-propanediol	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M4
497	[(Carboxymethyl)(methyl)amino]acetic acid	2,2-Diethyl-1,3-propanediol	1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M18
498	glutaric acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M5
499	pimelic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M5
500	isophthalic acid	2-Butyl-2-ethyl-1,3-propanediol	1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M2
501	2,2′-Thiodiacetic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M5
502	azelaic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M5
503	Sebacic Acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M5
504	[(Carboxymethyl)(methyl)amino]acetic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M19

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505	2,6-Naphthalenedicarboxylic Acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M19
506	2,2′-[ethylenebis(oxy)] bisacetic acid	2-Methyl-1,3-propanediol				1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCC(C)CO[>][]}	M6
507	isophthalic acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M2
508	2,2′-[ethylenebis(oxy)] bisacetic acid	3-methyl-1,5-pentanediol	13.17	19.98	1.52	1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCCC(C)CCO[>][]}	M6
509	2,2′-[ethylenebis(oxy)] bisacetic acid	1,4-Cyclohexanediol	6.32	8.57	1.36	1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OC(CC1)CCC1O[>][]}	M6
510	2,2′-[ethylenebis(oxy)] bisacetic acid	2,2-Diethyl-1,3-propanediol				1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M6
511	2,2′-[ethylenebis(oxy)] bisacetic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane	7.31	10.36	1.42	1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M6
512	1,4-Cyclohexanedicarboxylic acid	2,3-Butanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OC(C)C(C)O[>][]}	M6
513	Diglycolic acid	2,3-Butanediol				1:1	{[][<]C(=O)COC(=O)[<],[>]OC(C)C(C)O[>][]}	M6
514	glutaric acid	2-Butyl-2-ethyl-1,3-propanediol				1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M7
515	pimelic acid	2-Butyl-2-ethyl-1,3-propanediol	5.94	7.83	1.32	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M7

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516	azelaic acid	2-Butyl-2-ethyl-1,3-propanediol	5.21	6.53	1.26	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M7
517	isophthalic acid	2,2-Dimethyl-1,3-propanediol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(C)(C)CO[>][]}	M2
518	Sebacic Acid	2-Butyl-2-ethyl-1,3-propanediol	5.70	7.75	1.36	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M7
519	2,2′-[ethylenebis(oxy)] bisacetic acid	2-Butyl-2-ethyl-1,3-propanediol	7.42	10.86	1.46	1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M7
520	2,6-Naphthalenedicarboxylic Acid	2-Butyl-2-ethyl-1,3-propanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCC(CC)(CCCC)CO[>][]}	M19
521	2,2′-Thiodiacetic acid	2,2-Dimethyl-1,3-propanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M19
522	2,2′-[ethylenebis(oxy)] bisacetic acid	2,2-Dimethyl-1,3-propanediol	7.77	11.28	1.45	1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M19
523	[(Carboxymethyl)(methyl)amino]acetic acid	2,2-Dimethyl-1,3-propanediol				1:1	{[][<]C(=O)CN(C)CC(=O)[<],[>]OCC(C)(C)CO[>][]}	M19
524	2,2′-Thiodiacetic acid	1,3-Propanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCCCO[>][]}	M7
525	1,4-Cyclohexanedicarboxylic acid	1,3-Propanediol				1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCCCO[>][]}	M7
526	Sebacic Acid	3-methyl-1,5-pentanediol	5.16	6.68	1.30	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCC(C)CCO[>][]}	M8

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527	isophthalic acid	1,4-Cyclohexanedimethanol				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(CC1)CCC1CO[>][]}	M18
528	azelaic acid	2,2-Diethyl-1,3-propanediol	8.78	10.80	1.23	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(CC)(CC)CO[>][]}	M9
529	azelaic acid	2,3-Butanediol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OC(C)C(C)O[>][]}	M9
530	Sebacic Acid	2,3-Butanediol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OC(C)C(C)O[>][]}	M8
531	glutaric acid	1,2-Propanediol				1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(C)O[>][]}	M9
532	pimelic acid	1,2-Propanediol				1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(C)O[>][]}	M9
533	2,2′-Thiodiacetic acid	1,2-Propanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(C)O[>][]}	M9
534	azelaic acid	1,2-Propanediol				1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(C)O[>][]}	M9
535	Sebacic Acid	1,2-Propanediol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(C)O[>][]}	M8
536	Sebacic Acid	ethylene glycol				1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCO[>][]}	M8
537	2,6-Naphthalenedicarboxylic Acid	ethylene glycol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCO[>][]}	M19
538	glutaric acid	2,2-Dimethyl-1,3-propanediol	16.56	25.53	1.54	1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M10
539	pimelic acid	2,2-Dimethyl-1,3-propanediol	8.20	11.95	1.46	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M10

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540	azelaic acid	2,2-Dimethyl-1,3-propanediol	7.46	11.21	1.50	1:1	{[][<]C(=O)CCCCCCCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M10
541	Sebacic Acid	2,2-Dimethyl-1,3-propanediol	9.92	14.92	1.50	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCC(C)(C)CO[>][]}	M8
542	Sebacic Acid	1,3-Propanediol	4.85	8.31	1.71	1:1	{[][<]C(=O)CCCCCCCCC(=O)[<],[>]OCCCO[>][]}	M8
543	2,2′-[ethylenebis(oxy)] bisacetic acid	1,3-Propanediol				1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCCCO[>][]}	M10
544	2,6-Naphthalenedicarboxylic Acid	1,3-Propanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCCCO[>][]}	M19
545	isophthalic acid	4,8-Bis(hydroxymethyl)tricyclo[5.2.1.02,6]decane				1:1	{[][<]C(=O)c(ccc1)cc1C(=O)[<],[>]OCC(CC(C1)C2C3)C1C2CC3CO[>][]}	M2
546	glutaric acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)CCCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M10
547	1,4-Cyclohexanedicarboxylic acid	1,2-Propanediol	0.92	1.66	1.81	1:1	{[][<]C(=O)C(CC1)CCC1C(=O)[<],[>]OCC(C)O[>][]}	M11
548	2,6-Naphthalenedicarboxylic Acid	1,2-Propanediol				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OCC(C)O[>][]}	M11
549	2,2′-[ethylenebis(oxy)] bisacetic acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers	1.40	3.09	2.21	1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M11

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550	2,6-Naphthalenedicarboxylic Acid	4,4′-Isopropylidenedicyclohexanol, mixture of isomers				1:1	{[][<]C(=O)c(ccc1c2)cc1ccc2C(=O)[<],[>]OC(CC1)CCC1C(C)(C)C(CC2)CCC2O[>][]}	M11
551	glutaric acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)CCCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M11
552	2,2′-Thiodiacetic acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)CSCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M11
553	2,2′-[ethylenebis(oxy)] bisacetic acid	2,2,4-Trimethyl-1,3-pentanediol				1:1	{[][<]C(=O)COCCOCC(=O)[<],[>]OCC(C)(C)C(C(C)C)O[>][]}	M11
554	e-caprolactone		8.02	13.56	1.69	NA	{[][<]OCCCCCC(=O)[>][]}	M33
555	undecanoic d-lactone	e-decalactone				NR	{[][<]OC(CCCCCC)CCCC(=O)[>],[<]OC(CCCCCC)CCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
556	d-nonalactone	e-decalactone				NR	{[][<]OC(CCCC)CCCC(=O)[>],[<]OC(CCCC)CCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
557	pentadecanolide	e-decalactone				1.8:1	{[][<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
558	b-butyrolactone	e-decalactone	14.91	26.11	1.75	1.1:1	{[][<]OC(C)CC(=O)[>],[<]OC(C)CC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36

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559	5-dodecanolide	e-decalactone				NR	{[][<]OC(CCCCCCC)CCCC(=O)[>],[<]OC(CCCCCCC)CCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
560	16-hexadecanolide	e-decalactone				2.7:1	{[][<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
561	e-decalactone	e-caprolactone				2:1	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OCCCCCC(=O)[>][]}	M36
562	e-decalactone	delta-valerolactone				2.4:1	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OCCCCC(=O)[>][]}	M36
563	glycolide	e-caprolactone				2:1	{[][<]OCC(=O)OCC(=O)[>],[<]OCC(=O)OCC(=O)[>],[<]OCCCCCC(=O)[>][]}	M34
564	e-caprolactone	e-decalactone				1.9:1	{[][<]OCCCCCC(=O)[>],[<]OCCCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
565	delta-valerolactone	e-decalactone	86.27	138.0	1.60	1.75:1	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
566	e-caprolactone	massoia lactone				1:1	{[][<]OCCCCCC(=O)[>],[<]OCCCCCC(=O)[>],[<]OC(CCCCC)CC=CC(O)[>][]}	M36

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567	e-caprolactone	pentadecanolide				6.6:1	{[][<]OCCCCCC(=O)[>],[<]OCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>][]}	M36
568	e-caprolactone	b-butyrolactone				4.1:1	{[][<]OCCCCCC(=O)[>],[<]OCCCCCC(=O)[>],[<]OC(C)CC(=O)[>][]}	M36
569	e-caprolactone	glycolide				1:1	{[][<]OCCCCCC(=O)[>],[<]OCCCCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M34
570	pentadecanolide	e-caprolactone				1:1.1	{[][<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCC(=O)[>][]}	M36
571	b-butyrolactone	e-caprolactone				1:0.9	{[][<]OC(C)CC(=O)[>],[<]OC(C)CC(=O)[>],[<]OCCCCCC(=O)[>][]}	M36
572	beta-propiolactone					NR	{[][<]OCCC(=O)[>],[<]OCCC(=O)[>],[<]OCCC(=O)[>][]}	M33
573	pentadecanolide	massoia lactone				2:1	{[][<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OC(CCCCC)CC=CC(O)[>][]}	M36
574	16-hexadecanolide	massoia lactone				1.7:1	{[][<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OC(CCCCC)CC=CC(O)[>][]}	M36
575	delta-valerolactone		2.49	3.78	1.52	NR	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>][]}	M33

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576	delta-valerolactone	massoia lactone				2.4:1	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OC(CCCCC)CC=CC(O)[>][]}	M36
577	e-caprolactone	beta-propiolactone				0.25:1	{[][<]OCCCCCC(=O)[>],[<]OCCCCCC(=O)[>],[<]OCCC(=O)[>][]}	M33
578	beta-propiolactone	e-caprolactone				1:0.2	{[][<]OCCC(=O)[>],[<]OCCC(=O)[>],[<]OCCCCCC(=O)[>][]}	M33
579	e-caprolactone	delta-valerolactone	7.81	9.43	1.21	NR	{[][<]OCCCCCC(=O)[>],[<]OCCCCCC(=O)[>],[<]OCCCCC(=O)[>][]}	M33
580	pentadecanolide	b-butyrolactone				2.8:1	{[][<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>],[<]OC(C)CC(=O)[>][]}	M36
581	delta-valerolactone	e-caprolactone				NR	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OCCCCCC(=O)[>][]}	M33
582	b-butyrolactone	pentadecanolide				1.3:1	{[][<]OC(C)CC(=O)[>],[<]OC(C)CC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>][]}	M36
583	pentadecanolide	delta-valerolactone				NR	{[][<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCC(=O)[>][]}	M36
584	delta-valerolactone	pentadecanolide				NR	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OCCCCCCCCCCCCCC(=O)[>][]}	M36

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585	b-butyrolactone	delta-valerolactone	31.17	56.14	1.30	1.3:1	{[][<]OC(C)CC(=O)[>],[<]OC(C)CC(=O)[>],[<]OCCCCC(=O)[>][]}	M36
586	beta-propiolactone	delta-valerolactone				2.3:1	{[][<]OCCC(=O)[>],[<]OCCC(=O)[>],[<]OCCCCC(=O)[>][]}	M33
587	delta-valerolactone	b-butyrolactone	43.82	68.79	2.42	2.9:1	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OC(C)CC(=O)[>][]}	M36
588	delta-valerolactone	beta-propiolactone				1.3:1	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OCCC(=O)[>][]}	M33
589	beta-propiolactone	glycolide				Insoluble	{[][<]OCCC(=O)[>],[<]OCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M34
590	glycolide	beta-propiolactone				1.5:1	{[][<]OCC(=O)OCC(=O)[>],[<]OCC(=O)OCC(=O)[>],[<]OCCC(=O)[>][]}	M34
591	beta-propiolactone	lactide				Insoluble	{[][<]OCCC(=O)[>],[<]OCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M33
592	lactide	beta-propiolactone				Insoluble	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OCCC(=O)[>][]}	M33
593	delta-valerolactone	glycolide				Insoluble	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M34
594	glycolide	delta-valerolactone				Insoluble	{[][<]OCC(=O)OCC(=O)[>],[<]OCC(=O)OCC(=O)[>],[<]OCCCCC(=O)[>][]}	M34

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595	delta-valerolactone	lactide	6.80	9.25	1.36	Insoluble	{[][<]OCCCCC(=O)[>],[<]OCCCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M33
596	lactide	delta-valerolactone	27.72	36.89	1.33	1.3:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OCCCCC(=O)[>][]}	M33
597	e-decalactone					NA	{[][<]OC(CCCC)CCCCC(=O)[>][]}	M35
598	pentadecanolide					NA	{[][<]OCCCCCCCCCCCCCCC(=O)[>][]}	M35
599	16-hexadecanolide					NA	{[][<]OCCCCCCCCCCCCCCCC(=O)[>][]}	M35
600	coumarin					NA	{[][<]Oc(cccc1)c1C=CC(=O)[>][]}	M35
601	b-butyrolactone					NA	{[][<]OC(C)CC(=O)[>][]}	M35
602	lactide	undecanoic d-lactone				6.5:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(CCCCCC)CCCC(=O)[>][]}	M36
603	lactide	d-nonalactone	11.45	20.10	1.76	1.9:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(CCCC)CCCC(=O)[>][]}	M36
604	lactide	pentadecanolide	5.90	29.14	4.94	4:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>][]}	M36
605	5-dodecanolide					NA	{[][<]OC(CCCCCCC)CCCC(=O)[>][]}	M36

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606	lactide	b-butyrolactone				5:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)CC(=O)[>][]}	M36
607	lactide	5-dodecanolide	22.07	46.87	2.12	Insoluble	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(CCCCCCCC)CCCC(=O)[>][]}	M36
608	lactide	16-hexadecanolide				8:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OCCCCCCCCCCCCCCCCC(=O)[>][]}	M36
609	lactide	coumarin	9.44	30.94	3.28	1.5:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36
610	e-decalactone	lactide	12.46	34.22	2.75	2:1	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M36
611	massoia lactone	lactide	11.91	19.43	1.63	2:1	{[][<]OC(CCCCC)CC=CC(O)[>],[<]OC(CCCCC)CC=CC(O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M36
612	undecanoic d-lactone	lactide	29.03	38.09	1.31	1:2.5	{[][<]OC(CCCCCC)CCCC(=O)[>],[<]OC(CCCCCC)CCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M36

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613	d-nonalactone	lactide	14.07	20.59	1.46	1:2.9	{[][<]OC(CCCC)CCCC(=O)[>],[<]OC(CCCC)CCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M36
614	pentadecanolide	lactide	12.31	17.80	1.45	1.8:1	{[][<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M36
616	5-dodecanolide	lactide	12.84	20.87	1.63	2.8:1	{[][<]OC(CCCCCCC)CCCC(=O)[>],[<]OC(CCCCCCC)CCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M36
617	16-hexadecanolide	lactide				0.45:1	{[][<]OCCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M36
618	glycolide	e-decalactone				1:0	{[][<]OCC(=O)OCC(=O)[>],[<]OCC(=O)OCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
619	glycolide	massoia lactone				Insoluble	{[][<]OCC(=O)OCC(=O)[>],[<]OCC(=O)OCC(=O)[>],[<]OC(CCCCC)CC=CC(O)[>][]}	M36
620	glycolide	undecanoic d-lactone				1:0	{[][<]OCC(=O)OCC(=O)[>],[<]OCC(=O)OCC(=O)[>],[<]OC(CCCCCC)CCCC(=O)[>][]}	M36

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621	glycolide	d-nonalactone				1:0	{[][<]OCC(=O)OCC(=O)[>], [<]OCC(=O)OCC(=O)[>],[<]OC(CCCC)CCCC(=O)[>][]}	M36
622	glycolide	pentadecanolide				Insoluble	{[][<]OCC(=O)OCC(=O)[>], [<]OCC(=O)OCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>][]}	M36
623	glycolide	b-butyrolactone	5.70	7.50	1.32	1:0	{[][<]OCC(=O)OCC(=O)[>], [<]OCC(=O)OCC(=O)[>],[<]OC(C)CC(=O)[>][]}	M36
624	glycolide	5-dodecanolide				Insoluble	{[][<]OCC(=O)OCC(=O)[>], [<]OCC(=O)OCC(=O)[>],[<]OC(CCCCCCC)CCCC(=O)[>][]}	M36
625	glycolide					NA	{[][<]OCC(=O)OCC(=O)[>][]}	M34
626	glycolide	16-hexadecanolide				Insoluble	{[][<]OCC(=O)OCC(=O)[>], [<]OCC(=O)OCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>][]}	M36
627	glycolide	coumarin				0.8:1	{[][<]OCC(=O)OCC(=O)[>], [<]OCC(=O)OCC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36
628	e-decalactone	glycolide				Insoluble	{[][<]OC(CCCC)CCCCC(=O)[>], [<]OC(CCCC)CCCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36

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629	massoia lactone	glycolide		0.8:1	{[][<]OC(CCCCC)CC=CC(O)[>],[<]OC(CCCCC)CC=CC(O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36
630	undecanoic d-lactone	glycolide		Insoluble	{[][<]OC(CCCCCC)CCCC(=O)[>],[<]OC(CCCCCC)CCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36
631	d-nonalactone	glycolide		Insoluble	{[][<]OC(CCCC)CCCC(=O)[>],[<]OC(CCCC)CCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36
632	pentadecanolide	glycolide		Insoluble	{[][<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36
633	b-butyrolactone	glycolide		0:1	{[][<]OC(C)CC(=O)[>],[<]OC(C)CC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36
634	5-dodecanolide	glycolide		Insoluble	{[][<]OC(CCCCCCC)CCCC(=O)[>],[<]OC(CCCCCCC)CCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36
635	16-hexadecanolide	glycolide		Insoluble	{[][<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36

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636	glycolide	lactide	3:1	{[][<]OCC(=O)OCC(=O)[>], [<]OCC(=O)OCC(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>][]}	M34
637	coumarin	glycolide	1:0	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M36
638	coumarin	e-decalactone	2.6:1	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>][]}	M36
639	coumarin	massoia lactone	2:1	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OC(CCCCC)CC=CC(O)[>][]}	M36
640	coumarin	undecanoic d-lactone	3.2:1	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OC(CCCCCC)CCCC(=O)[>][]}	M36
641	coumarin	d-nonalactone	2.2:1	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OC(CCCC)CCCC(=O)[>][]}	M36
642	coumarin	pentadecanolide	2.1:1	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>][]}	M36

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643	coumarin	b-butyrolactone	10:1	{[][<]Oc(cccc1)c1C=CC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>],[<]OC(C)CC(=O)[>][]}	M36
644	coumarin	5-dodecanolide	10:1	{[][<]Oc(cccc1)c1C=CC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>],[<]OC(CCCCCCC)CCCC(=O)[>][]}	M36
645	e-decalactone	coumarin	0.8:1	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36
646	lactide	glycolide	1.5:1	{[][<]OC(C)C(=O)OC(C)C(=O)[>],[<]OC(C)C(=O)OC(C)C(=O)[>],[<]OCC(=O)OCC(=O)[>][]}	M34
647	pentadecanolide	coumarin	2:1	{[][<]OCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36
648	b-butyrolactone	coumarin	0.2:1	{[][<]OC(C)CC(=O)[>],[<]OC(C)CC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36
649	16-hexadecanolide	coumarin	1:0	{[][<]OCCCCCCCCCCCCCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36

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650	coumarin	e-caprolactone				2:1	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OCCCCCC(=O)[>][]}	M36
651	coumarin	delta-valerolactone				3.3:1	{[][<]Oc(cccc1)c1C=CC(=O)[>], [<]Oc(cccc1)c1C=CC(=O)[>],[<]OCCCCC(=O)[>][]}	M36
652	lactide	e-caprolactone				1:0	{[][<]OC(C)C(=O)OC(C)C(=O)[>], [<]OC(C)C(=O)OC(C)C(=O)[>],[<]OCCCCCC(=O)[>][]}	M33
653	e-caprolactone	coumarin				3.25:1	{[][<]OCCCCCC(=O)[>], [<]OCCCCCC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36
654	delta-valerolactone	coumarin				1.6:1	{[][<]OCCCCC(=O)[>], [<]OCCCCC(=O)[>],[<]Oc(cccc1)c1C=CC(=O)[>][]}	M36
655	e-decalactone	massoia lactone	9.82	15.79	1.61	2.1:1	{[][<]OC(CCCC)CCCCC(=O)[>], [<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCCC)CC=CC(O)[>][]}	M36
656	e-decalactone	undecanoic d-lactone	12.97	19.54	1.51	NR	{[][<]OC(CCCC)CCCCC(=O)[>], [<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCCCC)CCCC(=O)[>][]}	M36

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657	e-decalactone	d-nonalactone	20.23	31.10	1.54	NR	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCC(=O)[>][]}	M36
658	e-decalactone	pentadecanolide	23.44	44.05	1.88	2.9:1	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OCCCCCCCCCCCCCCC(=O)[>][]}	M36
659	e-decalactone	b-butyrolactone	19.18	28.78	1.50	3.2:1	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OC(C)CC(=O)[>][]}	M36
660	e-decalactone	5-dodecanolide	19.63	30.55	1.56	NR	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCCCCC)CCCC(=O)[>][]}	M36
661	e-decalactone	16-hexadecanolide	21.40	41.60	1.94	2.8:1	{[][<]OC(CCCC)CCCCC(=O)[>],[<]OC(CCCC)CCCCC(=O)[>],[<]OCCCCCCCCCCCCCCCC(=O)[>][]}	M36
*301**	Succinic acid	1,9-nonanediol	12.74	44.30	3.48	1:1	{[][<]C(=O)CCC(=O)[<],[>]OCCCCCCCCCCO[>][]}	M25
*662**	pimelic acid	1,5-pentanediol	10.85	29.55	2.72	1:1	{[][<]C(=O)CCCCCC(=O)[<],[>]OCCC(C)CCO[>][]}	M25
*190**	Dimethylcarbonate	Bis(4-hydroxyphenyl) Sulfone	2.48	2.48	1.00	1:1	{[][<]C(=O)[<],[>]Oc1ccc(cc1)S(=O)(=O)c2ccc(cc2)O[>][]}	M29

*indicates polymers with molecular weight confirmed by GPC, but clear on clear-zone assay test