Supporting Information

A Refractive Index Study of a Diverse Set of Polymeric Materials by QSPR with quantum-chemical and additive descriptors

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Table S1

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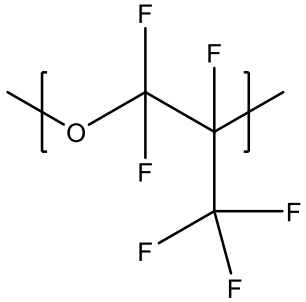
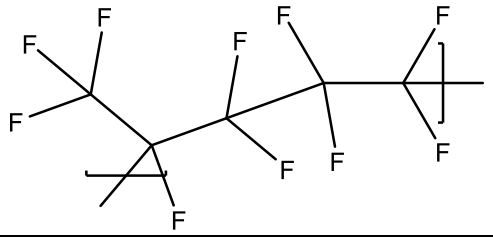
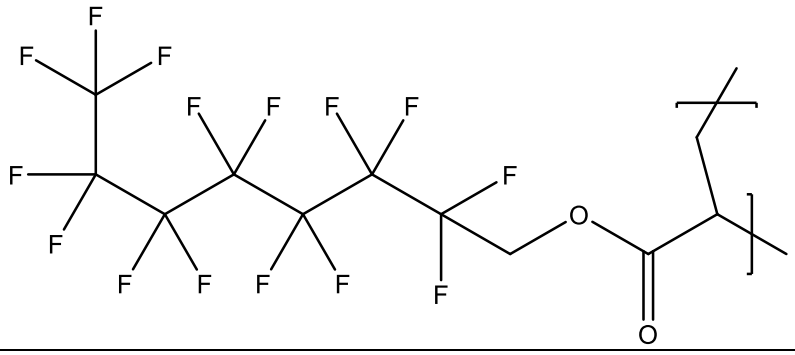
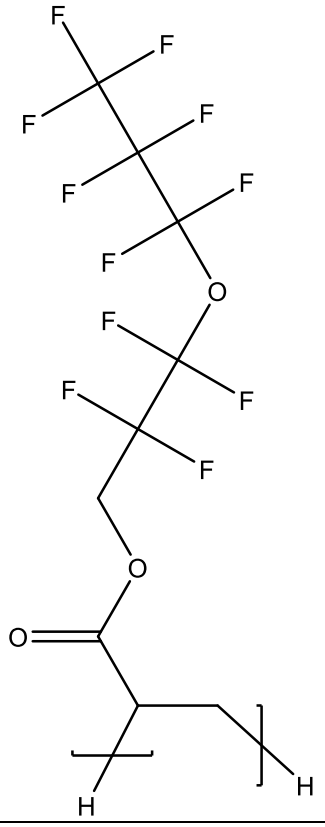
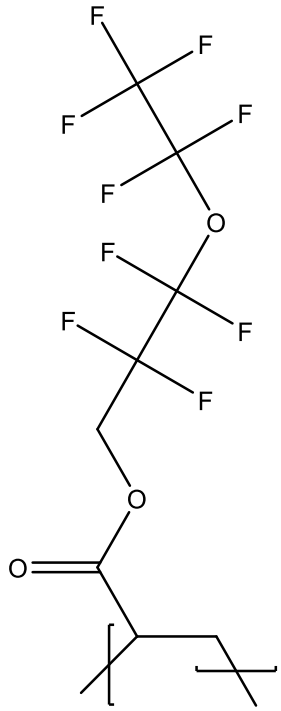
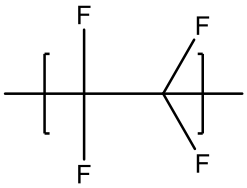
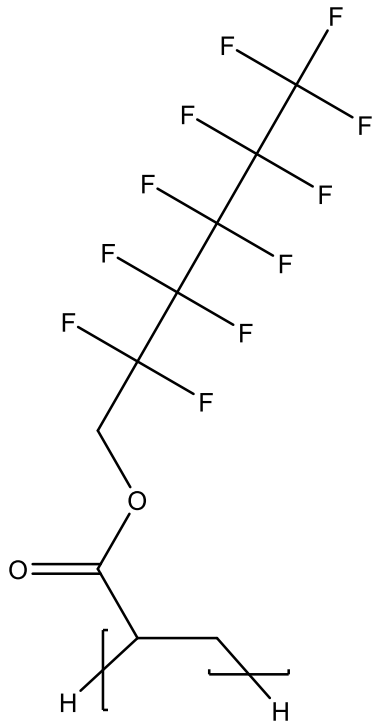
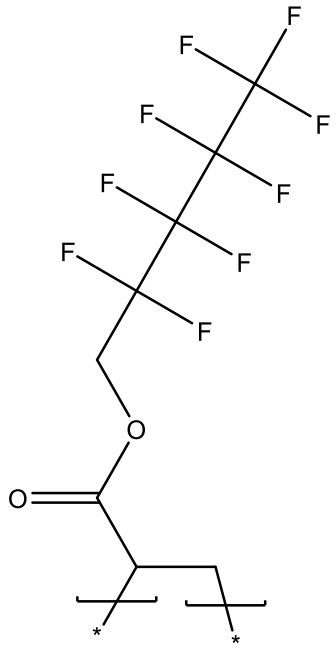
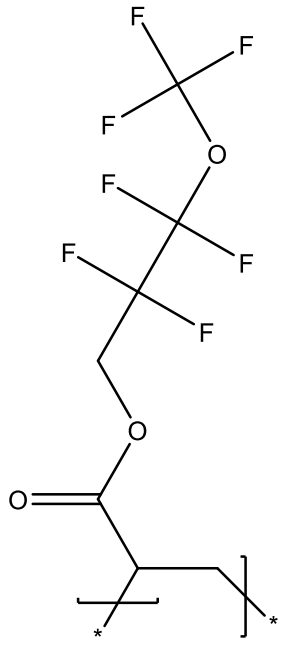
1	

2	
3	
4	

5	
6	
7	

8	
9	

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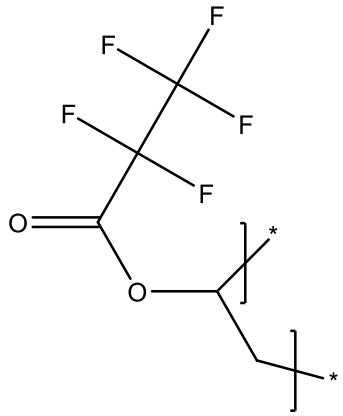

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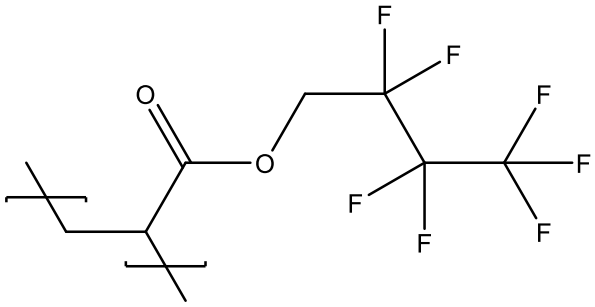

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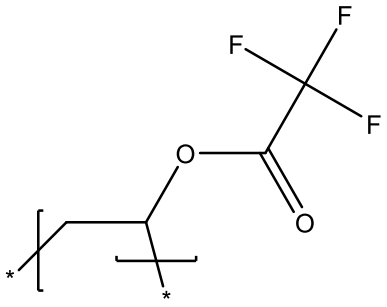

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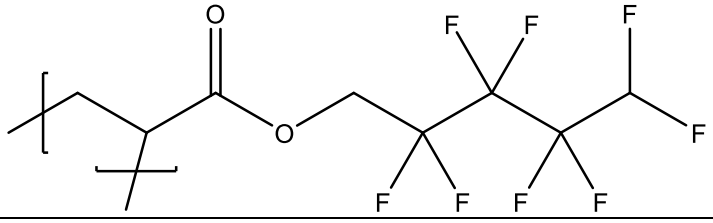

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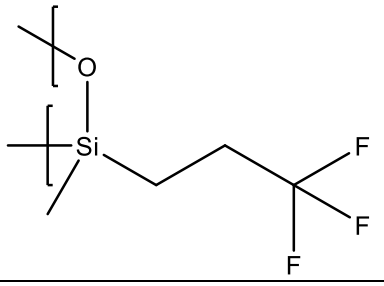
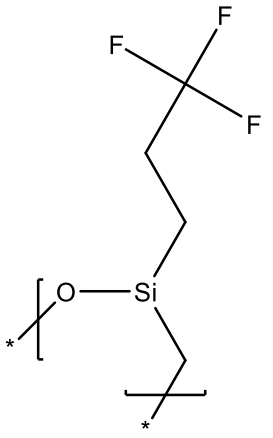
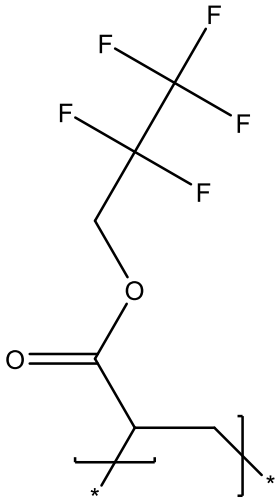
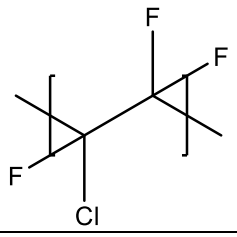
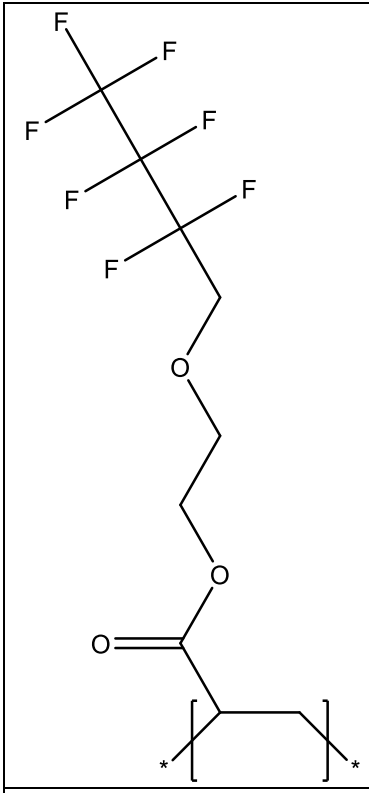
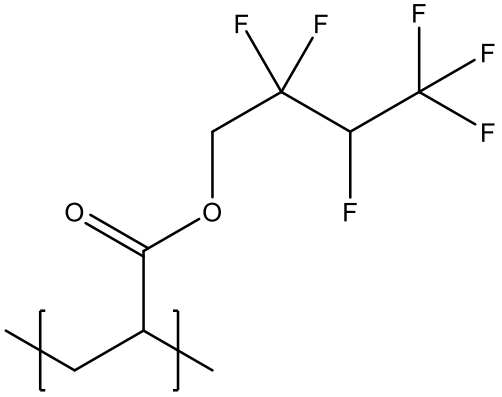
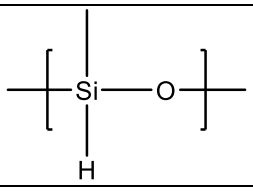
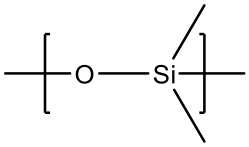


15	
16	
17	

18	
19	
20	
21	

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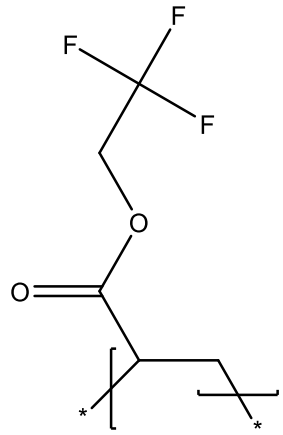

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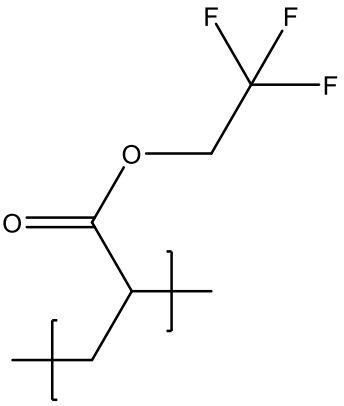

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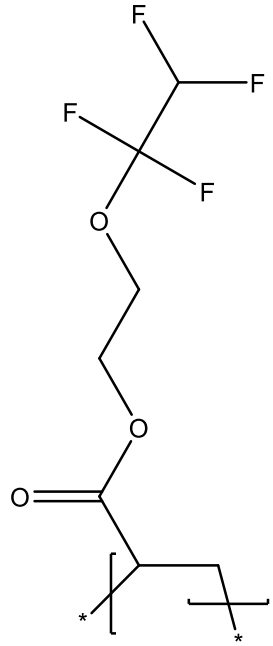
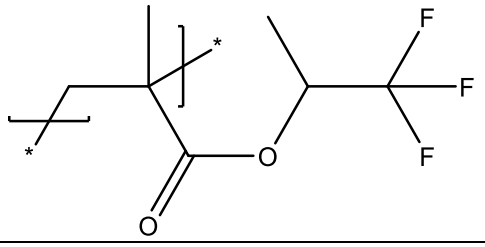
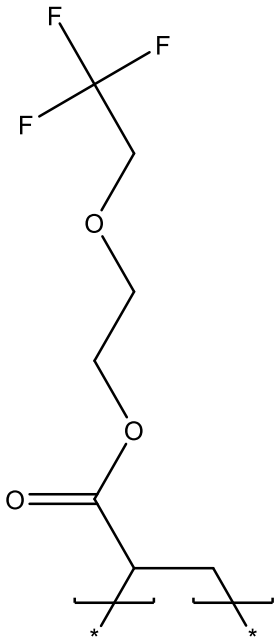
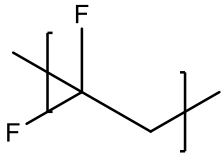
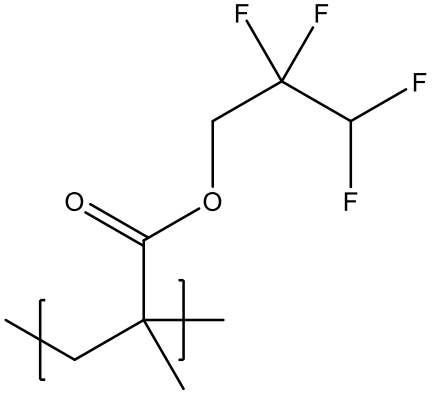
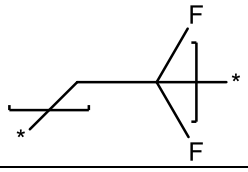
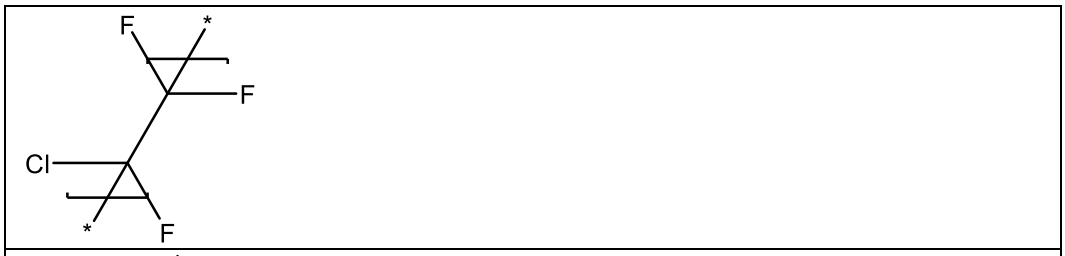
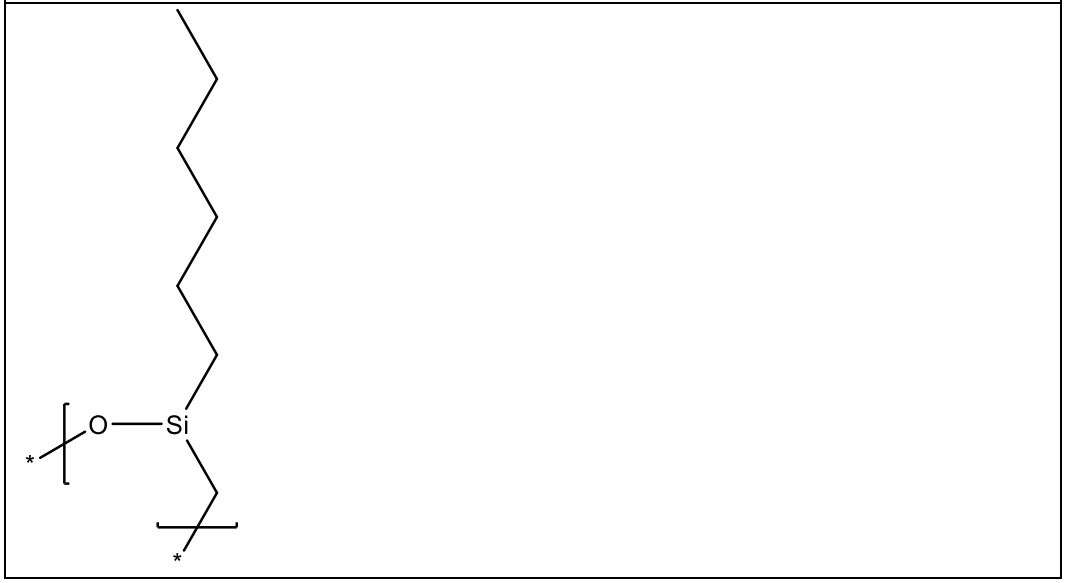
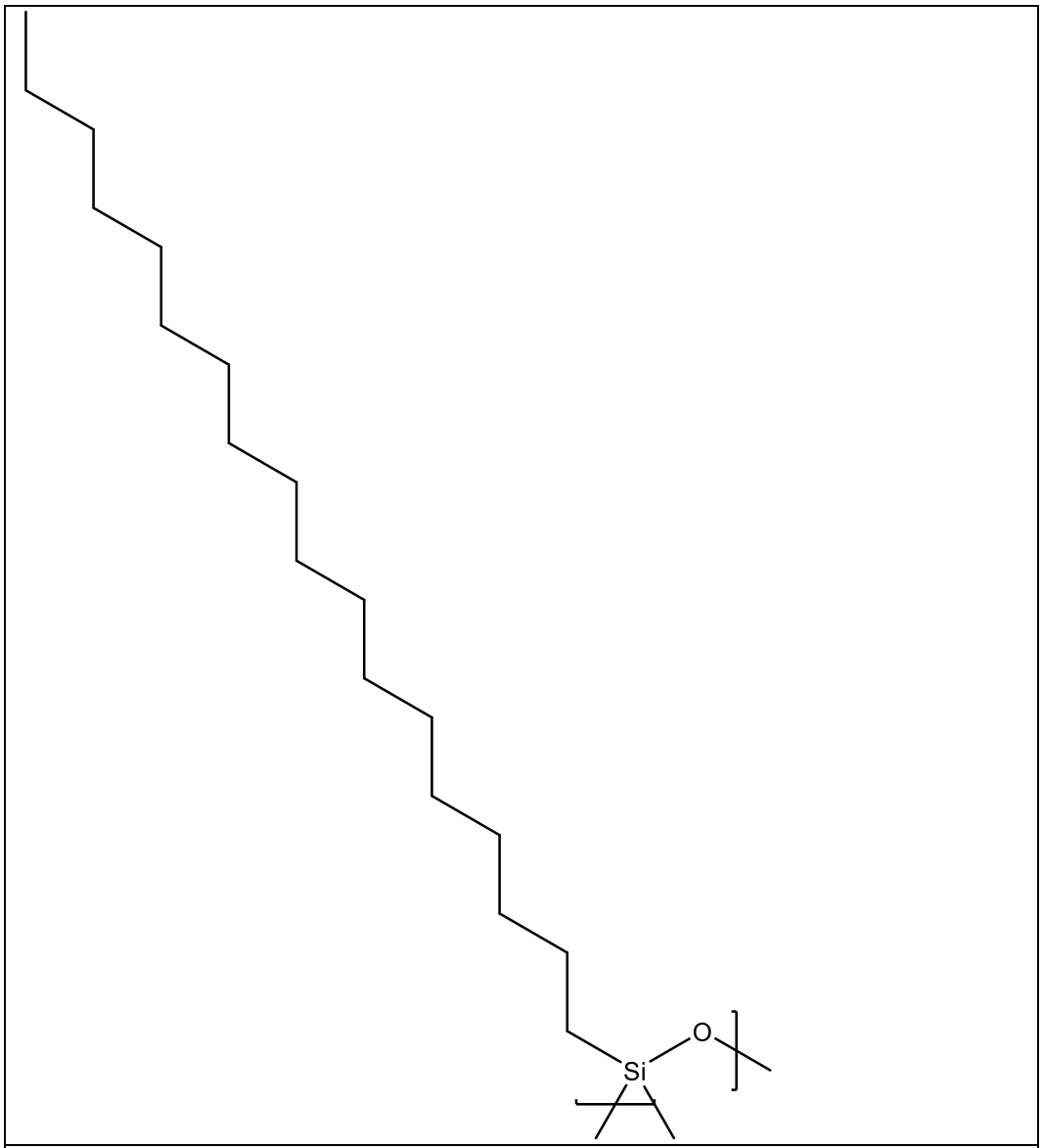


25	
26	
27	
28	
29	

30	
31	



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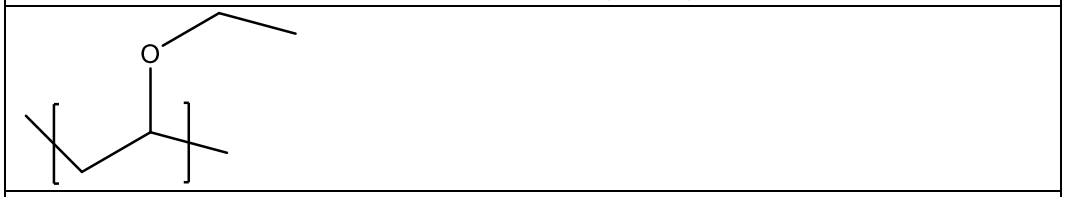

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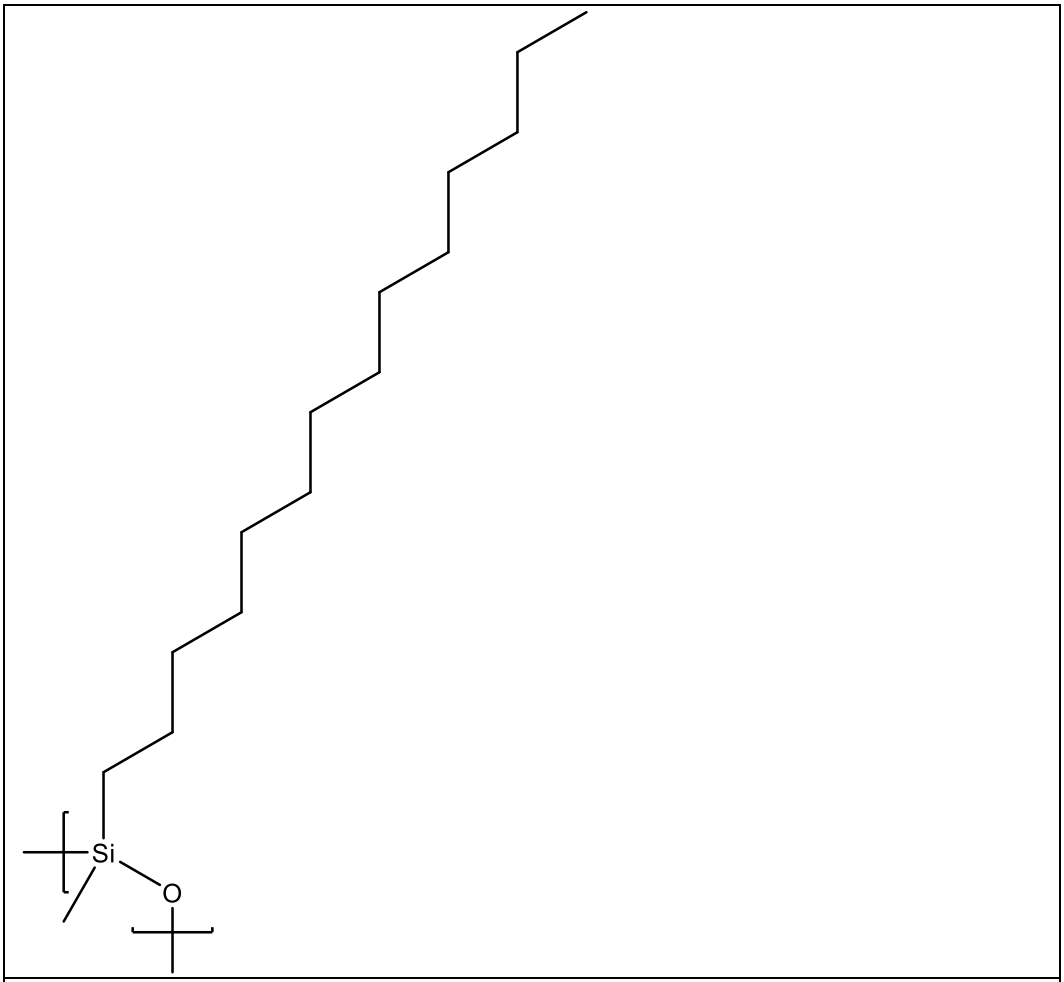

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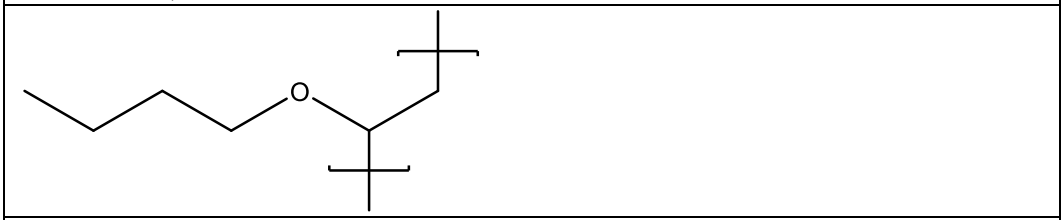

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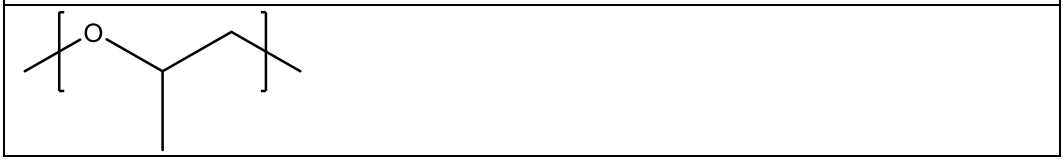

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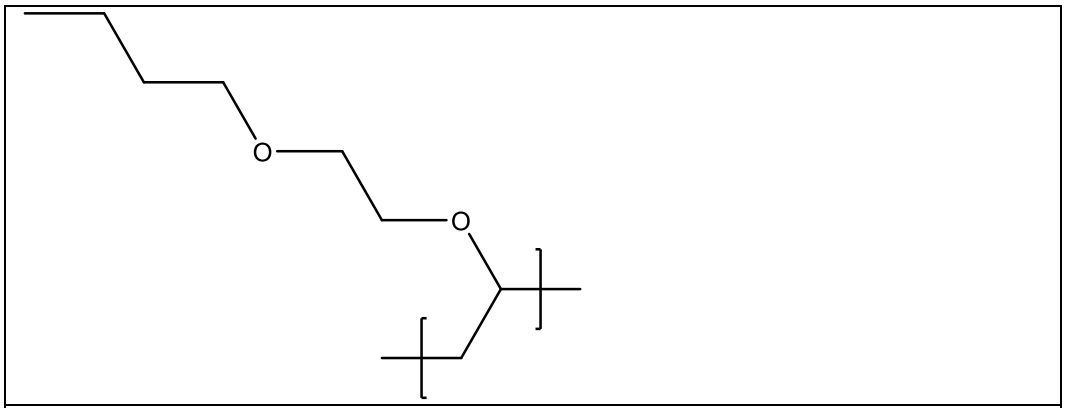

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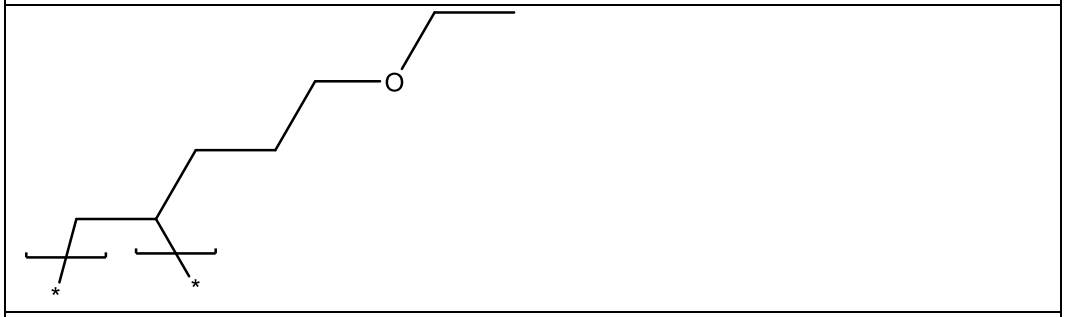

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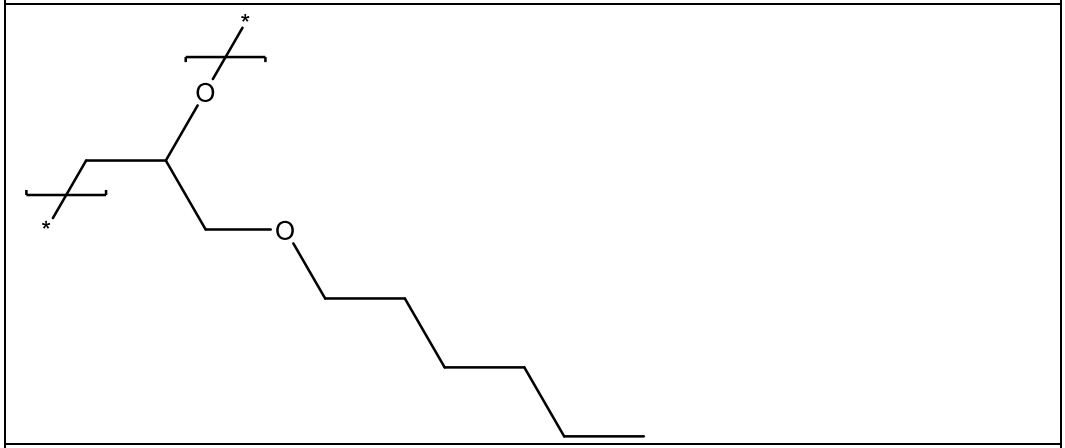

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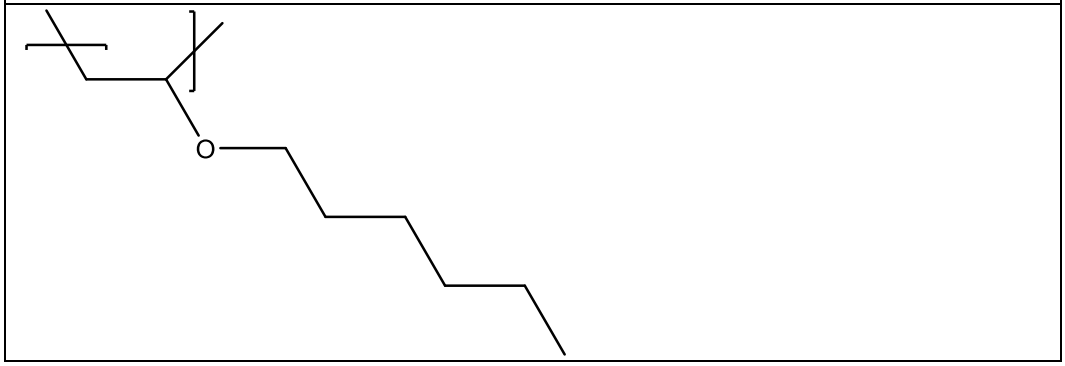

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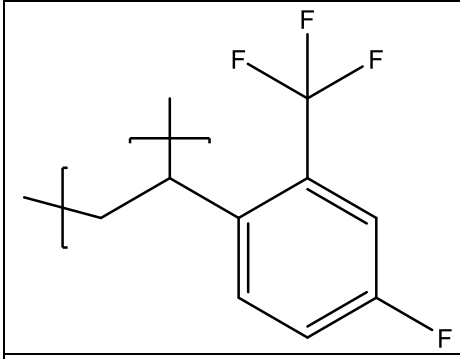

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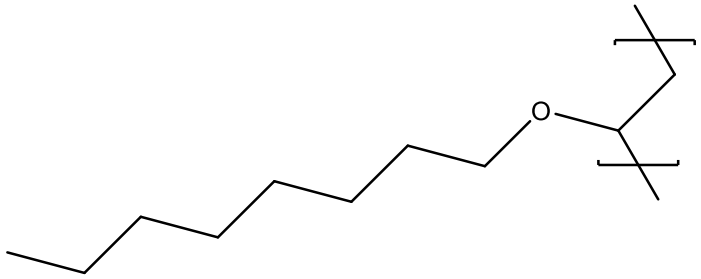

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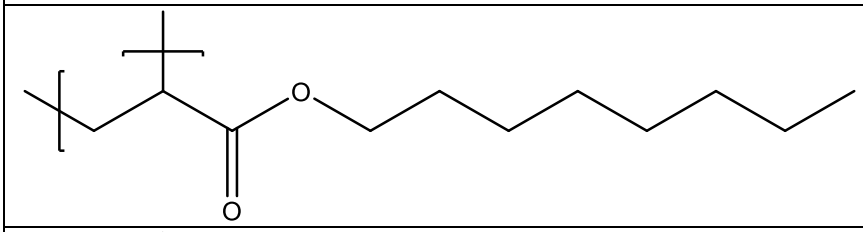

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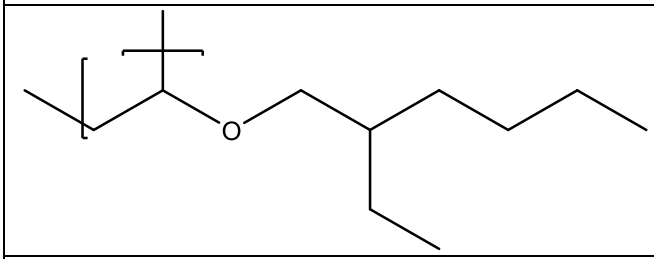

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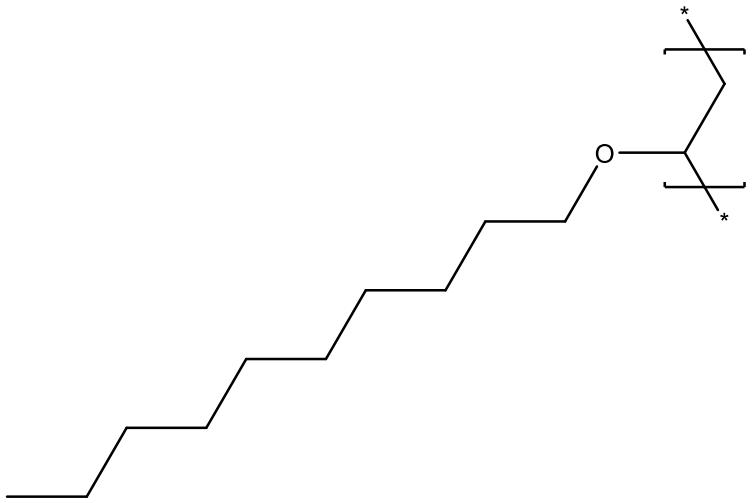

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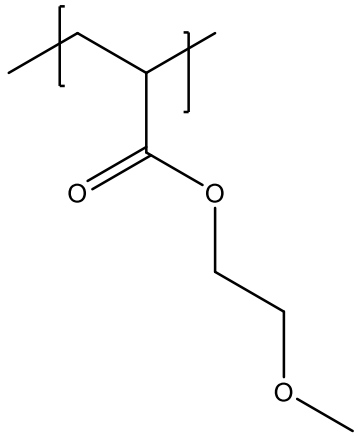

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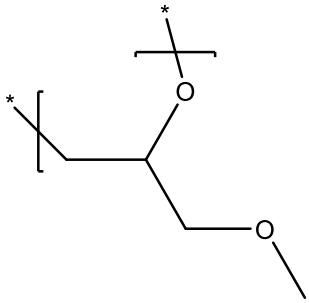

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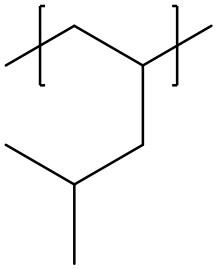

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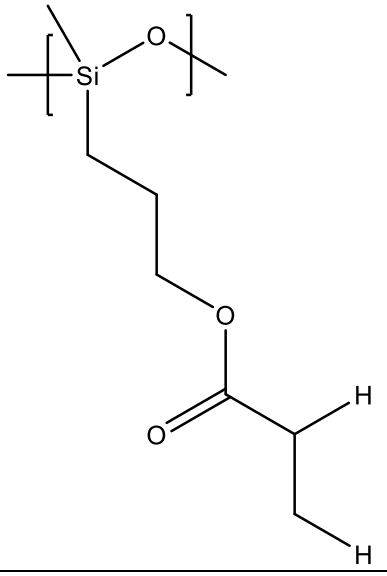

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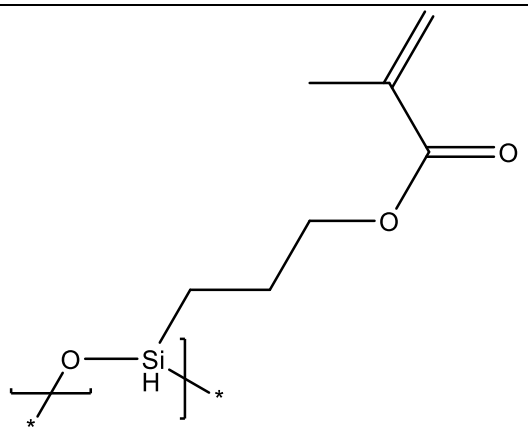

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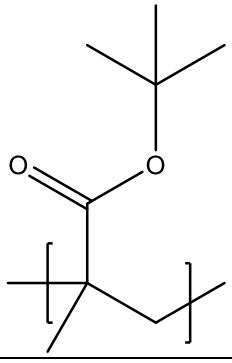

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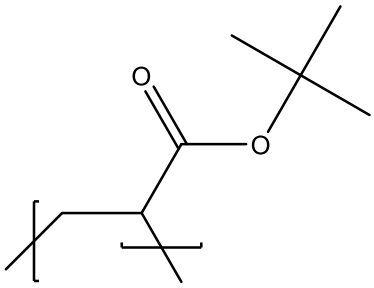

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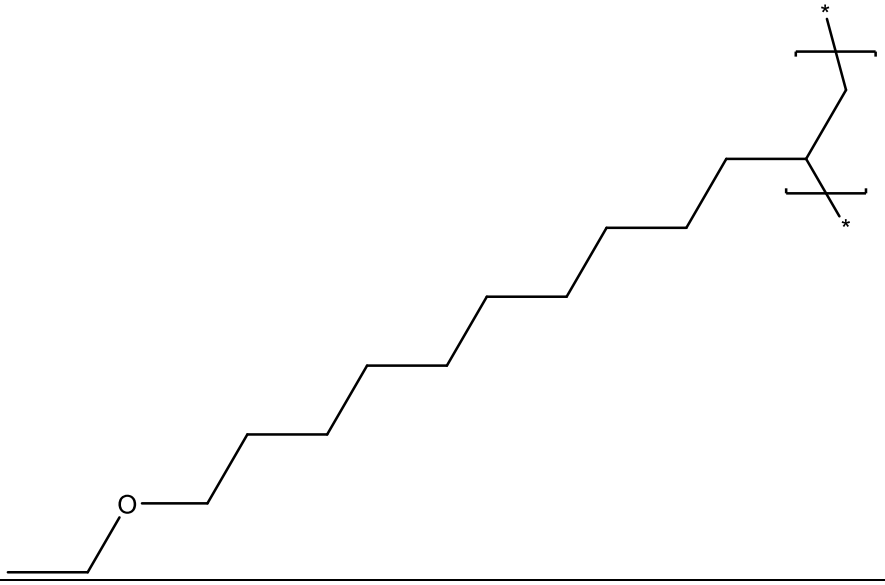

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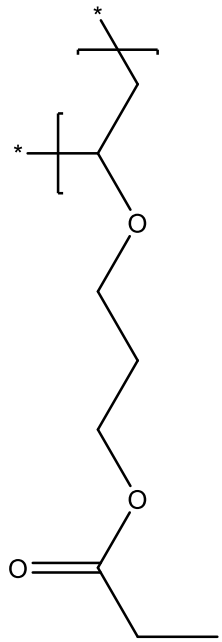

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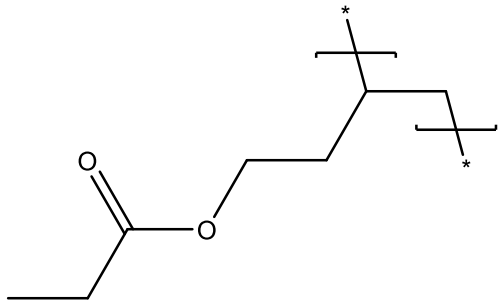

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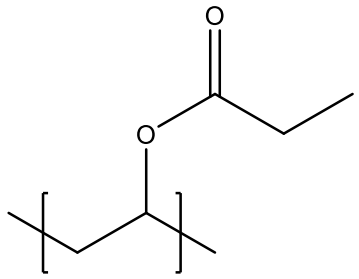

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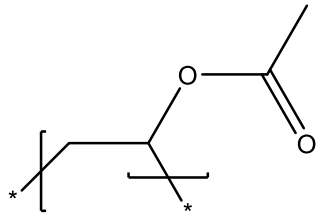

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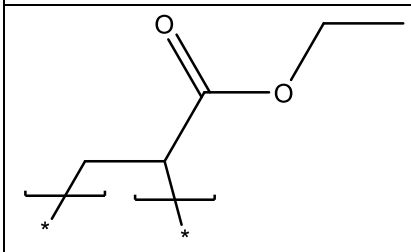

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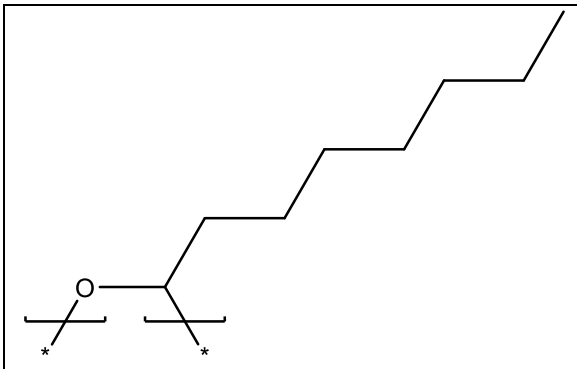

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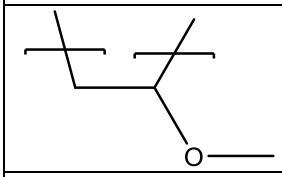

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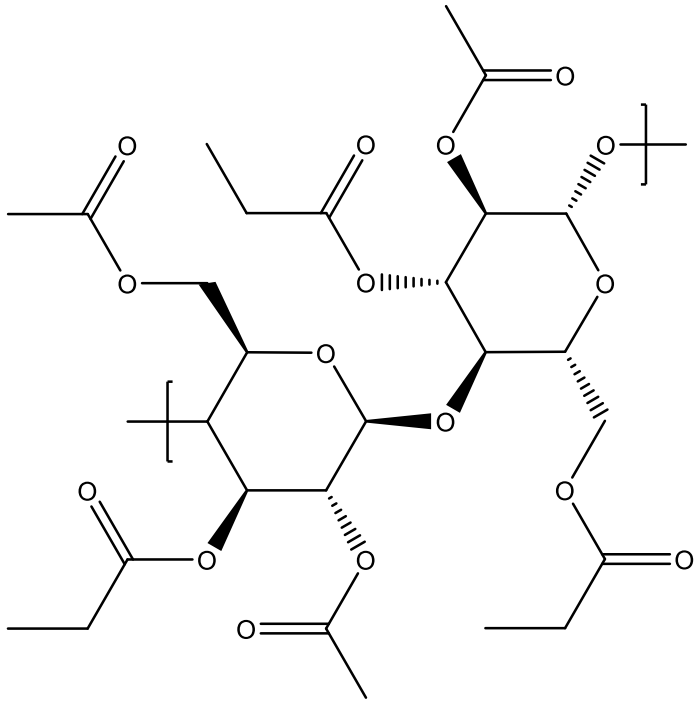

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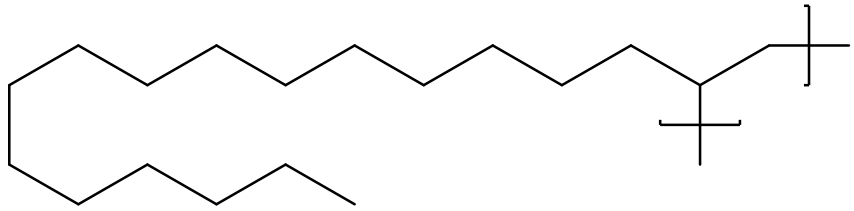

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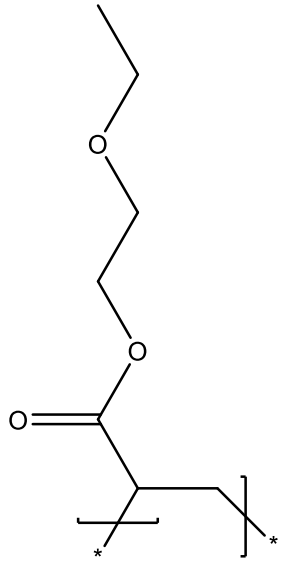

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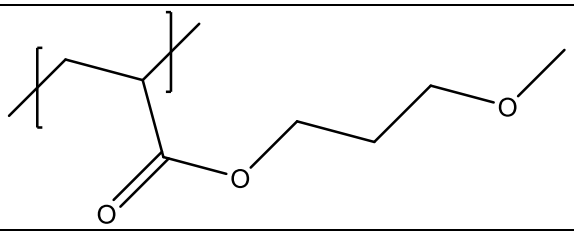

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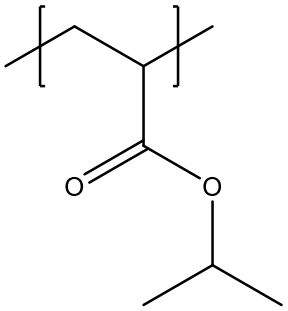

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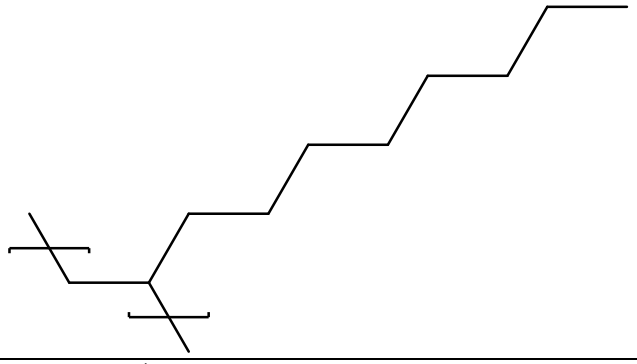

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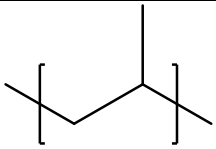

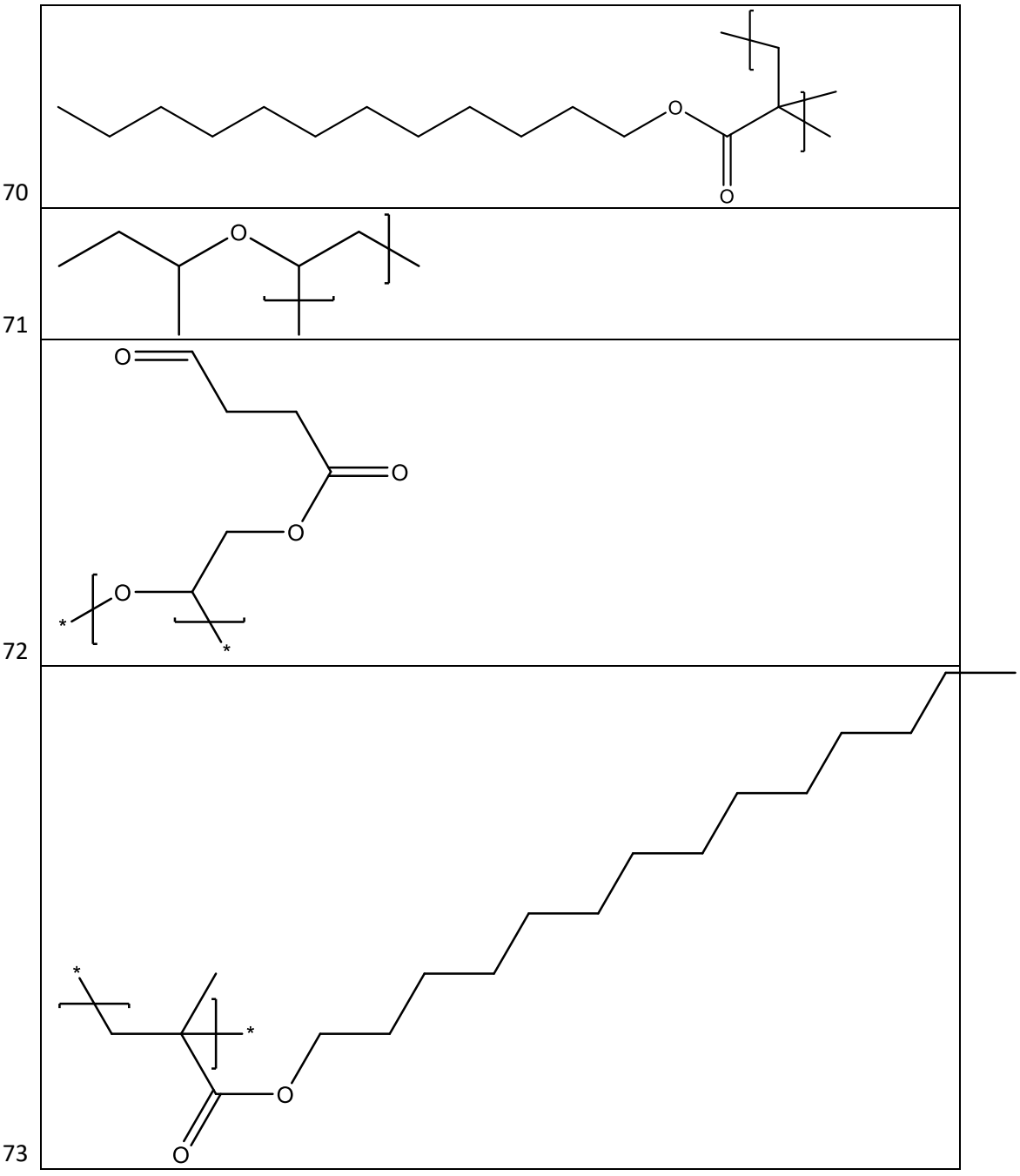
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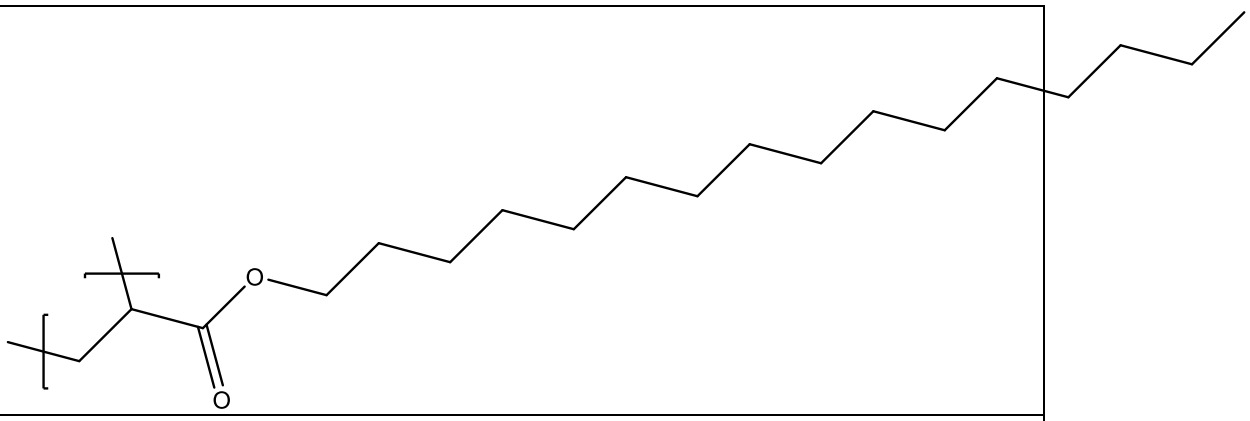

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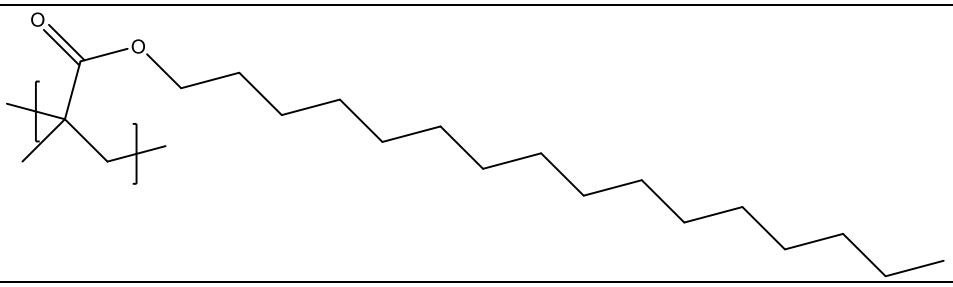

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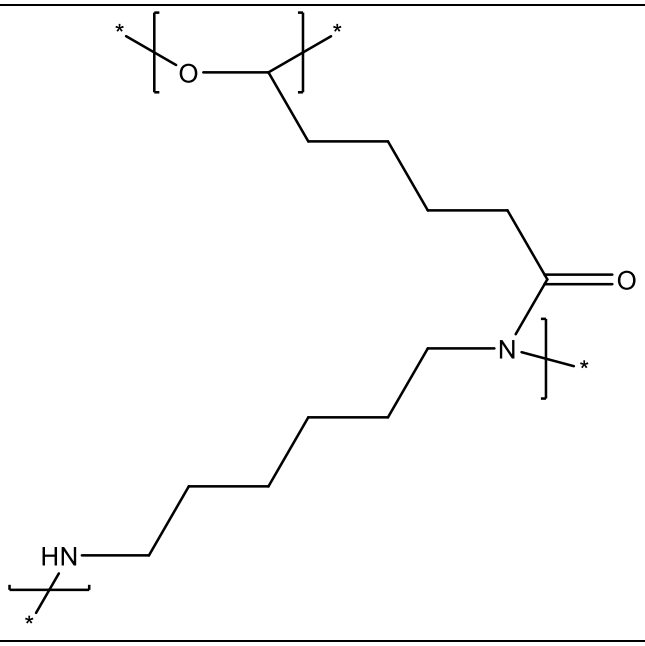
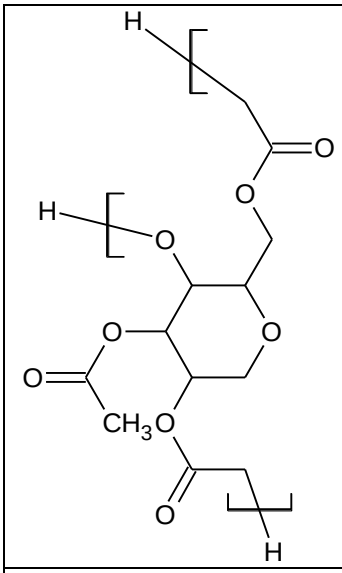
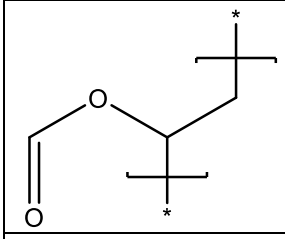
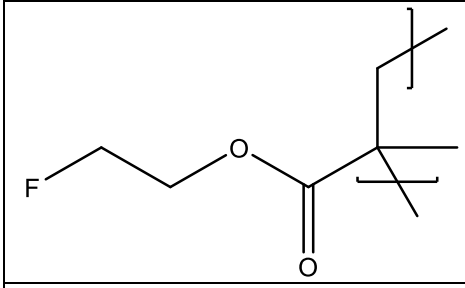
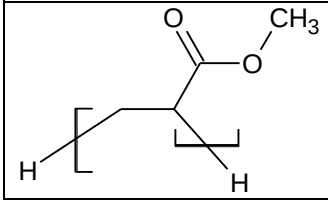


77	
78	
79	
80	

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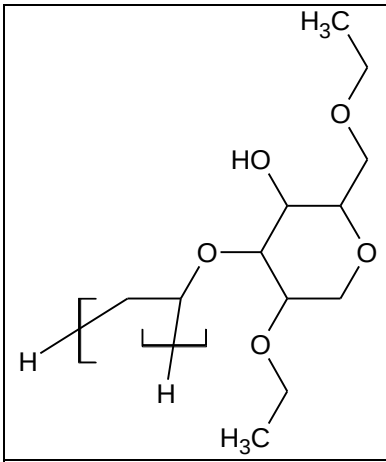

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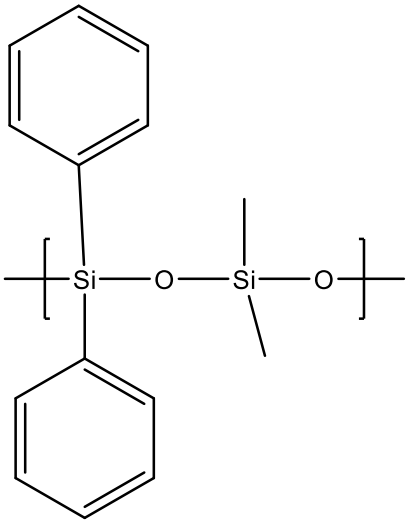

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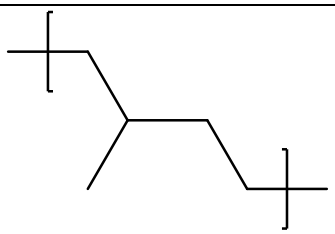

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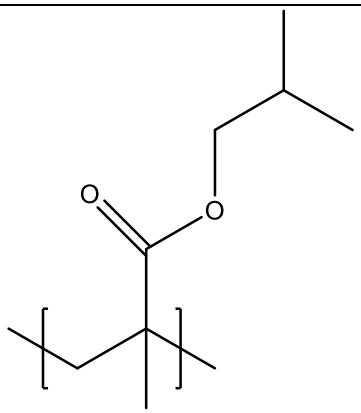
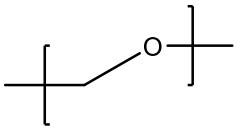
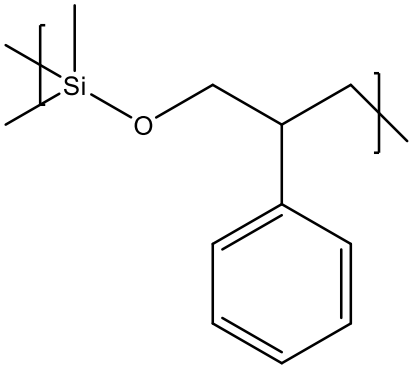
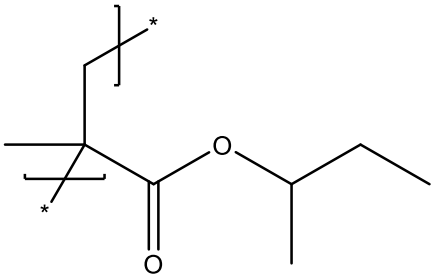
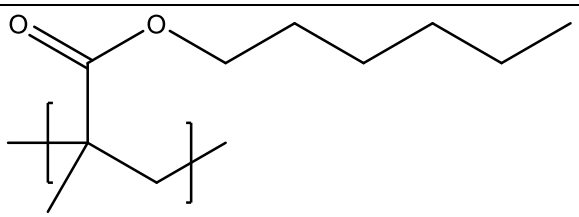
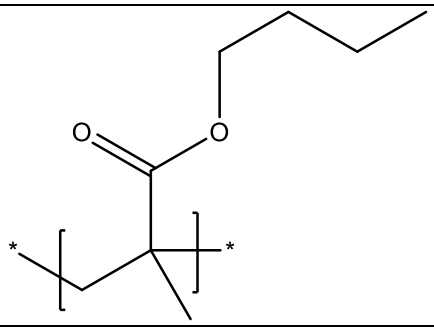


85	
86	
87	
88	
89	

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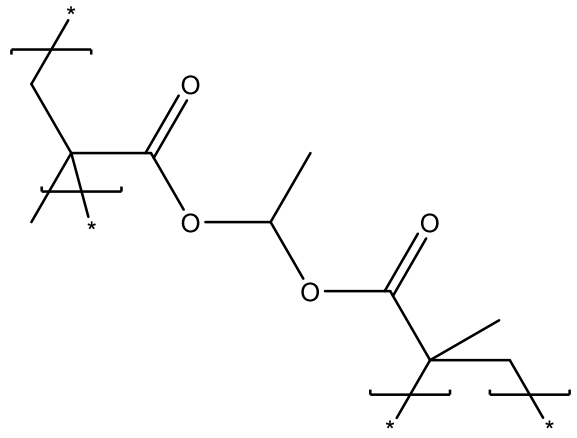

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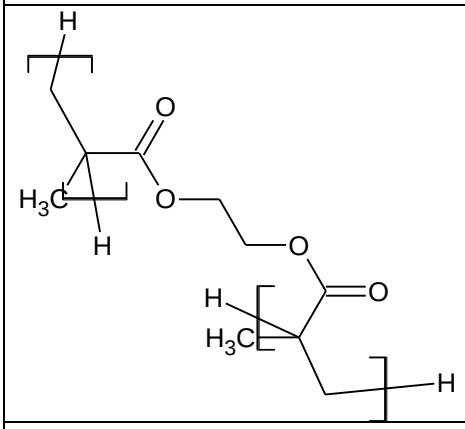

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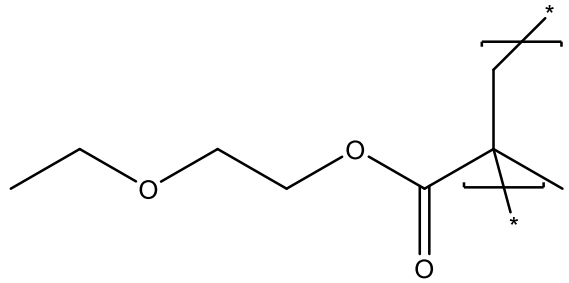

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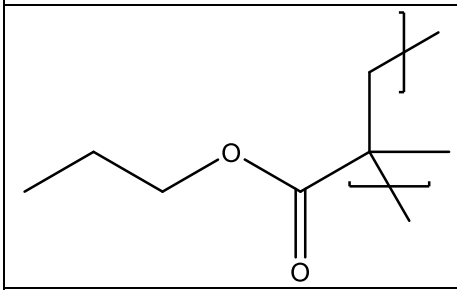

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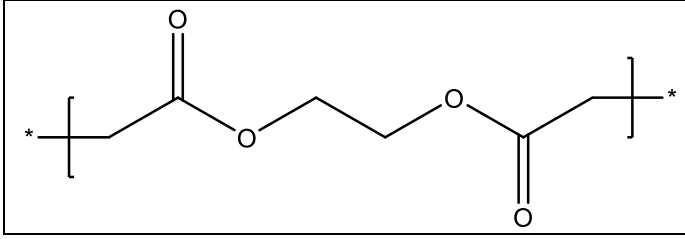
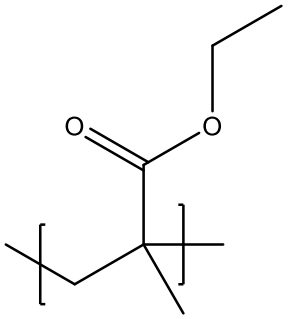
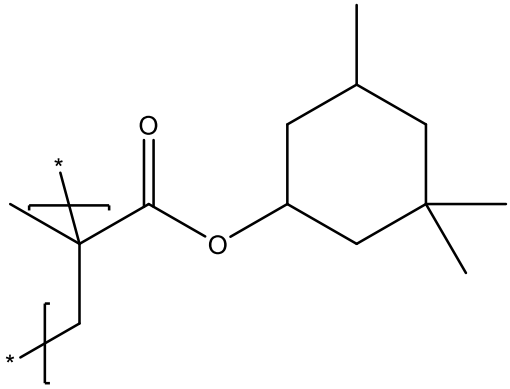
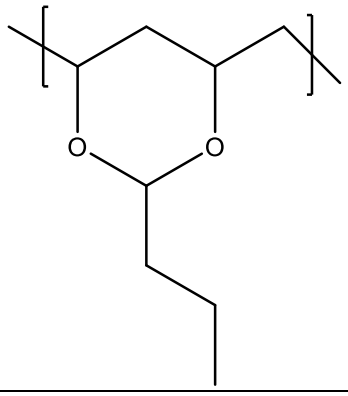
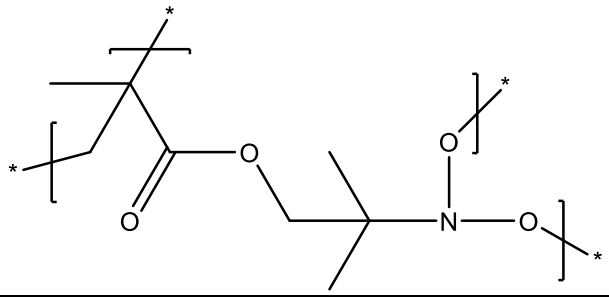
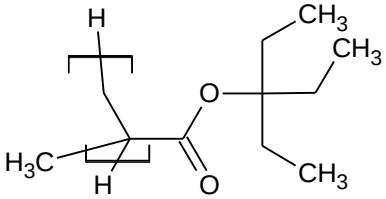


95	
96	
97	
98	
99	

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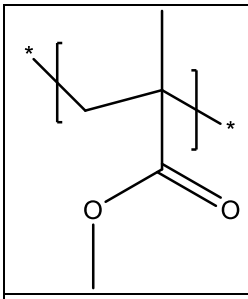

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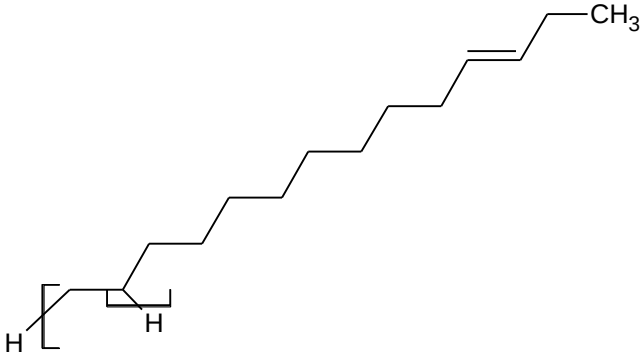

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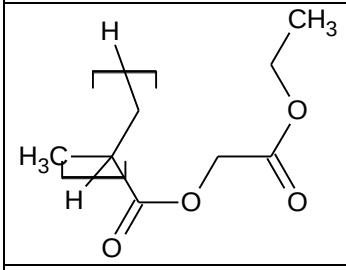

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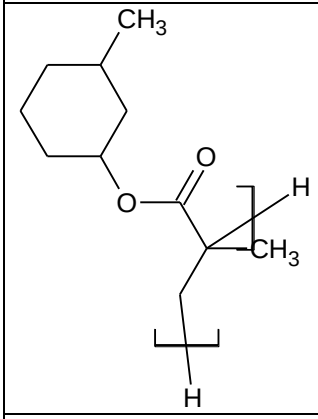

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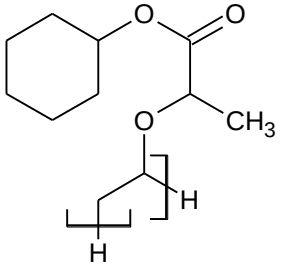

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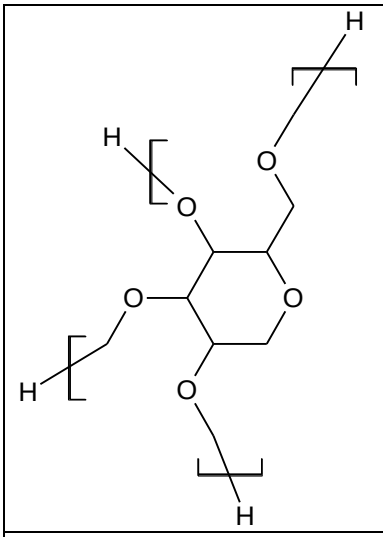

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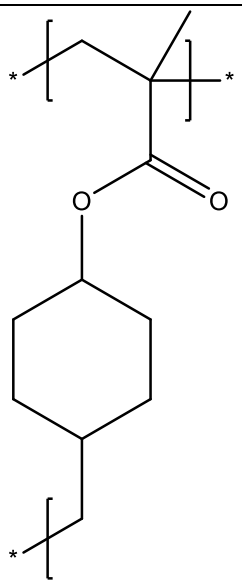

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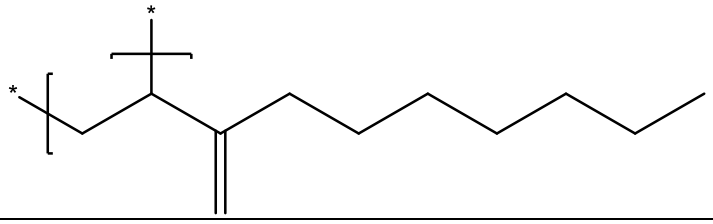

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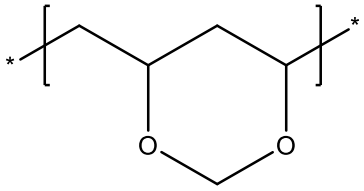
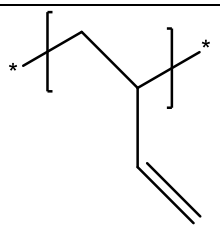
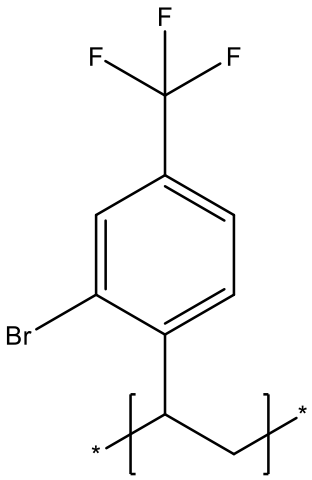
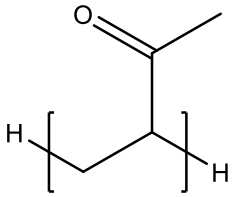
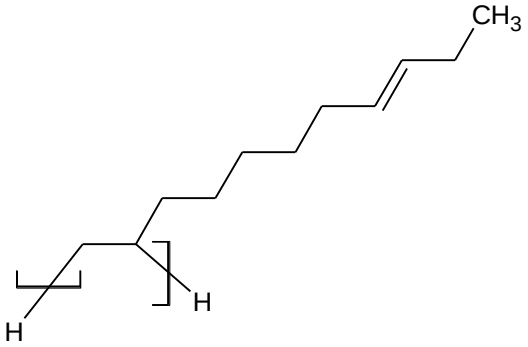
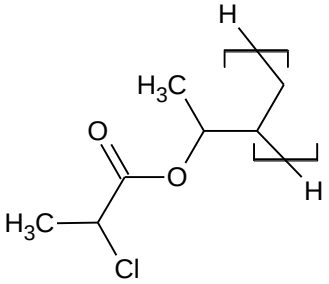
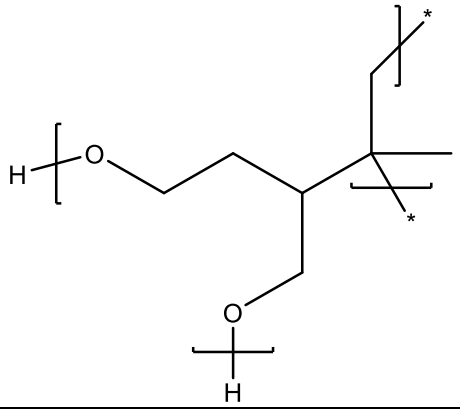
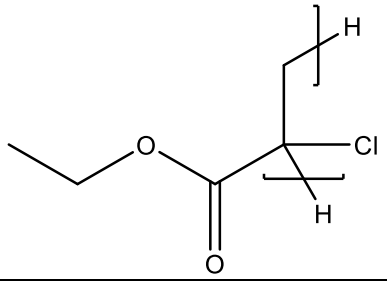
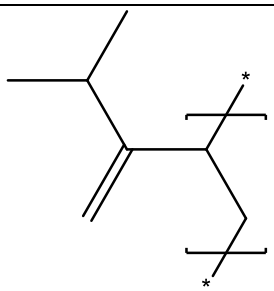
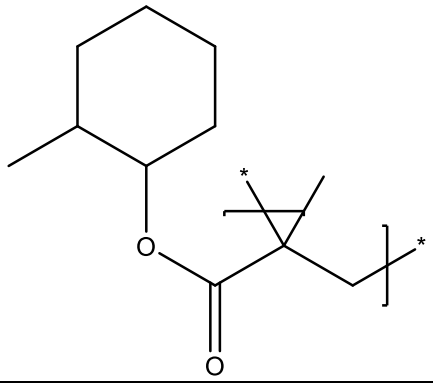
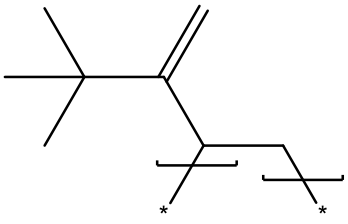
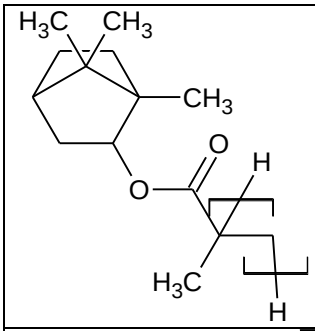
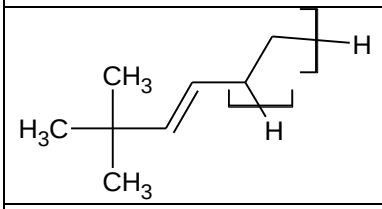
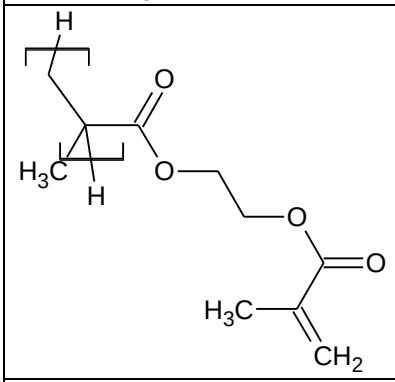
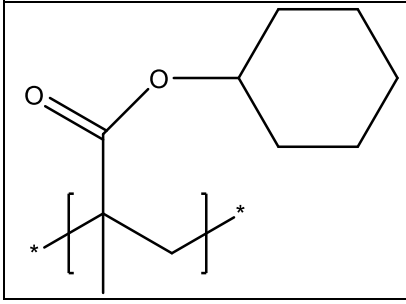


109	
110	
111	
112	
113	

114	
115	
116	
117	
118	

119	
120	
121	
122	

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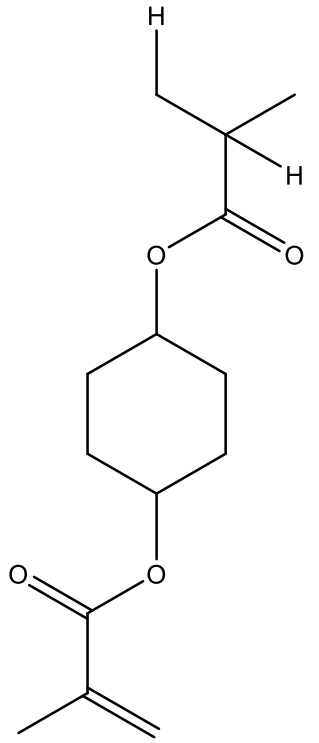

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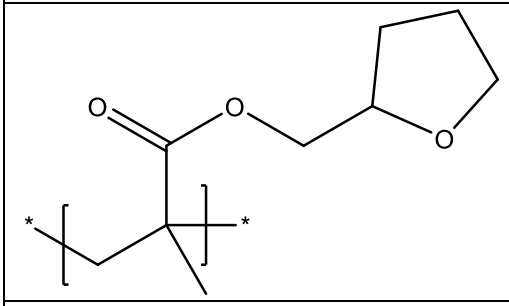

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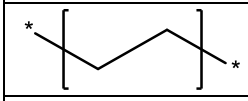

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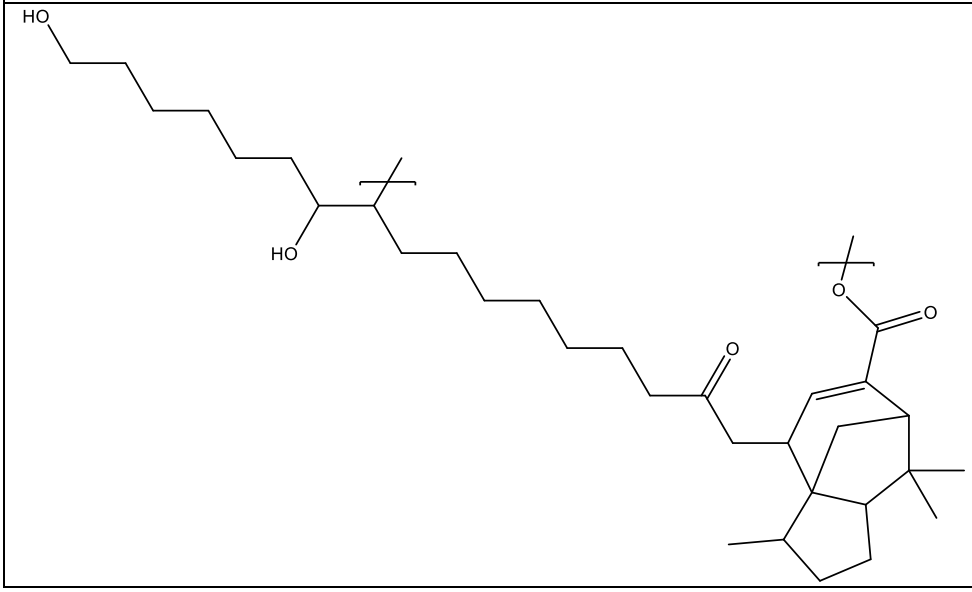
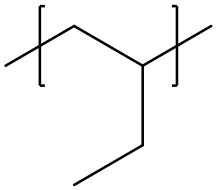
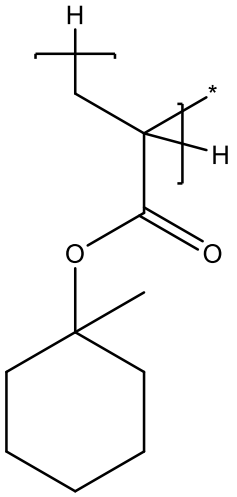
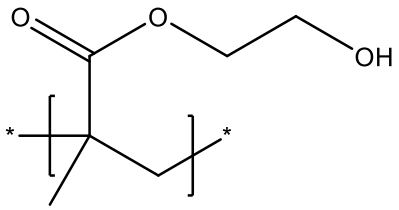
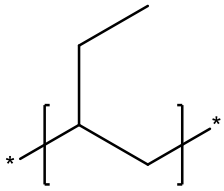
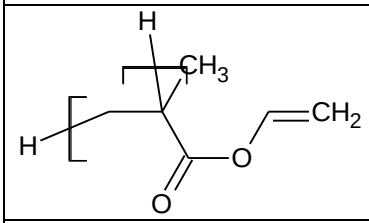
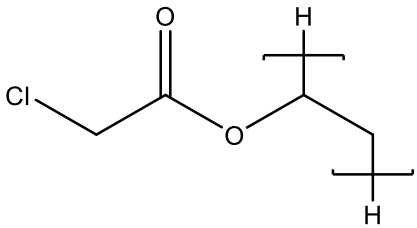
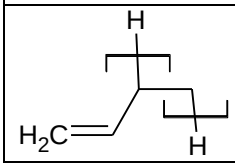
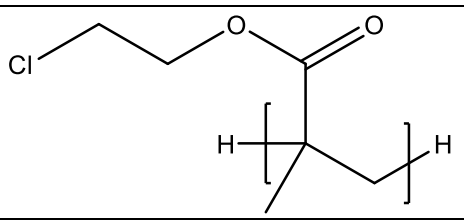
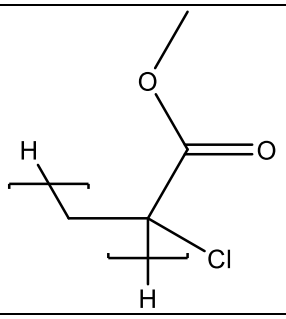
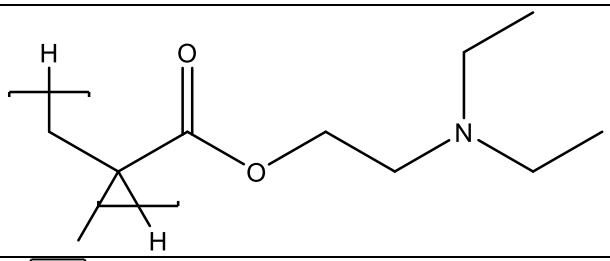
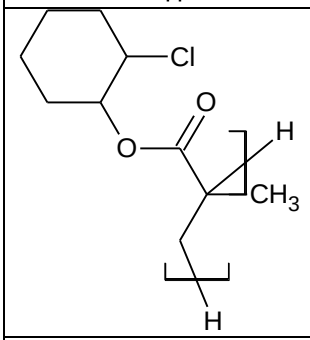
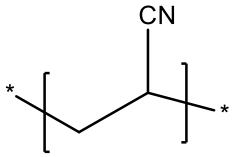
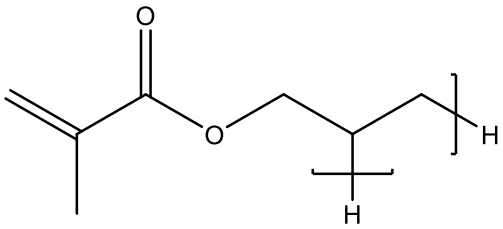
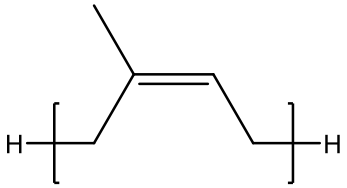


127	
128	
129	
130	
131	
132	
133	

134	
135	
136	
137	
138	
139	
140	

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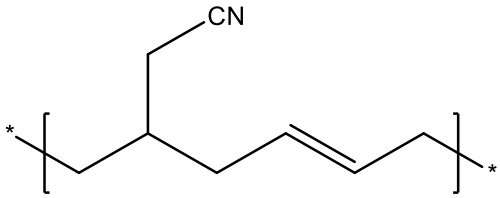

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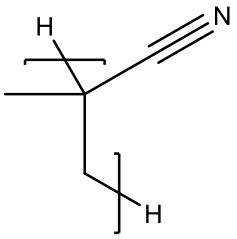

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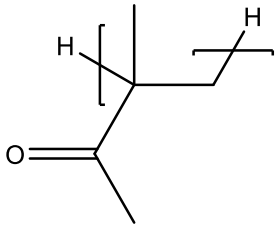

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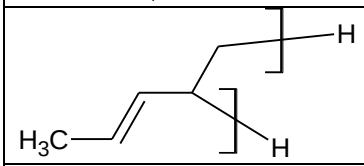

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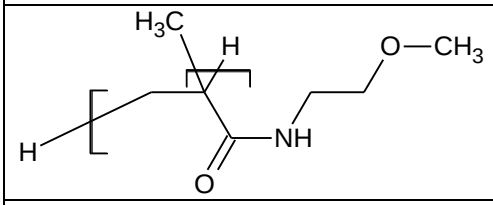

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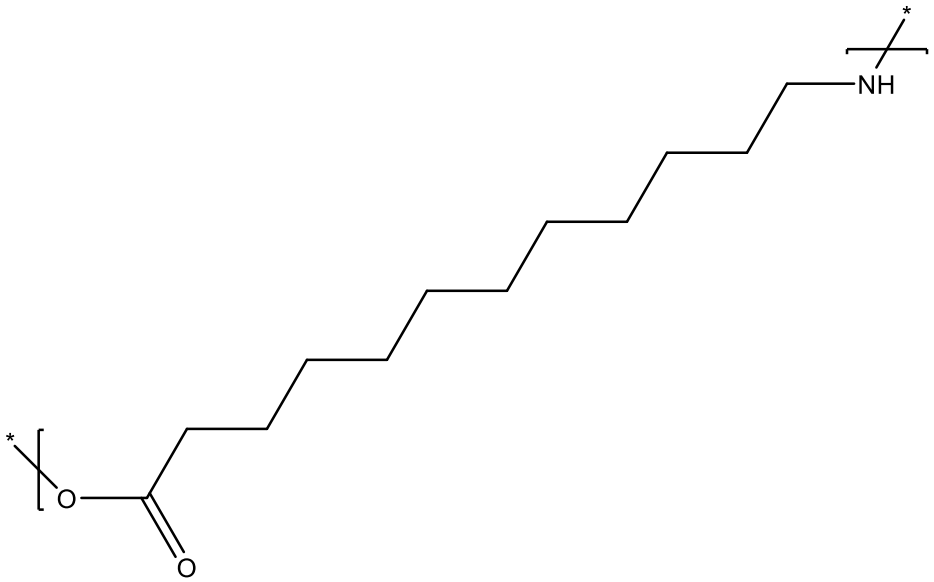
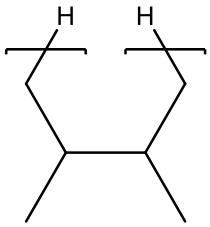
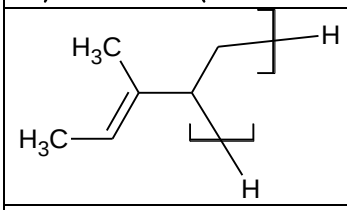
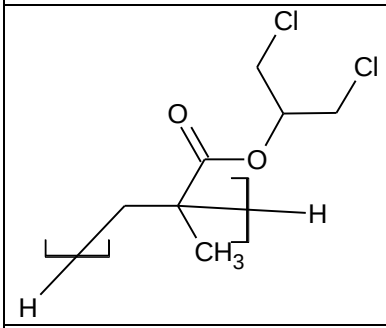
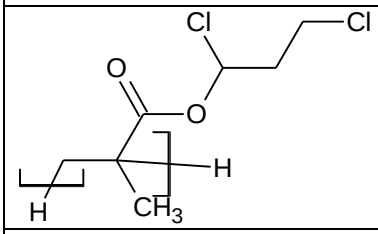
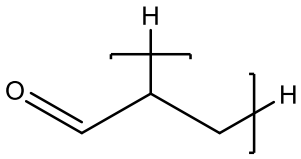
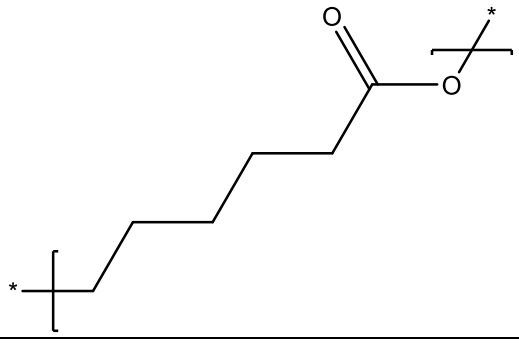
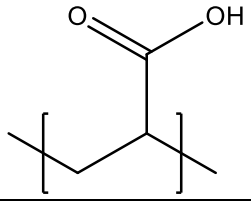


147	
148	
149	
150	
151	
152	
153	

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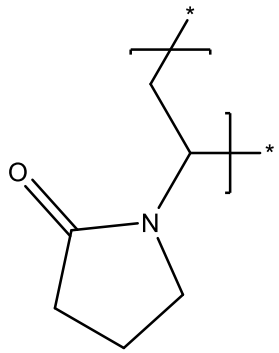

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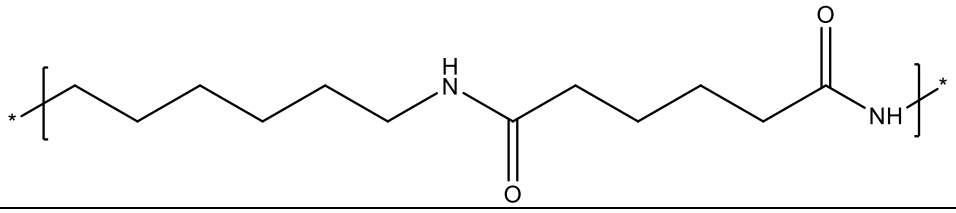

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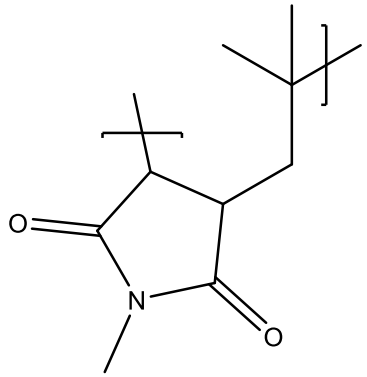

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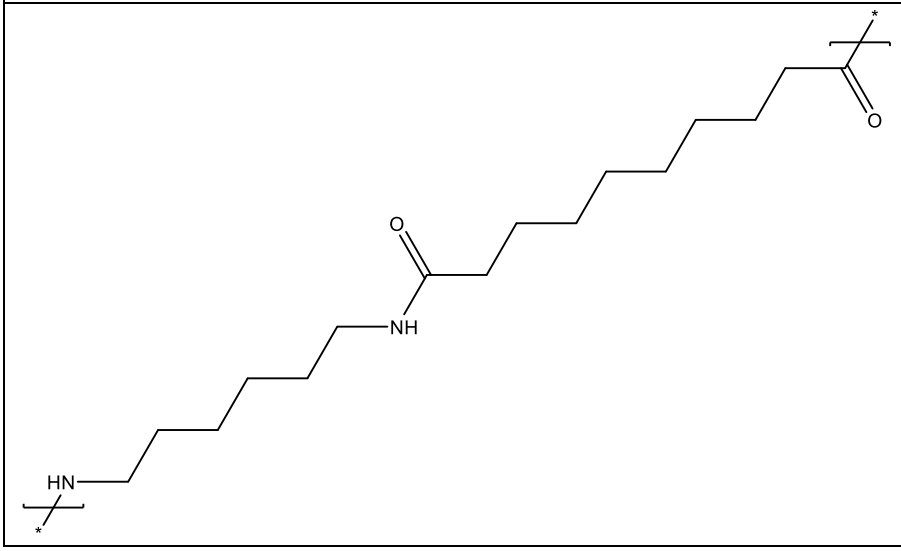

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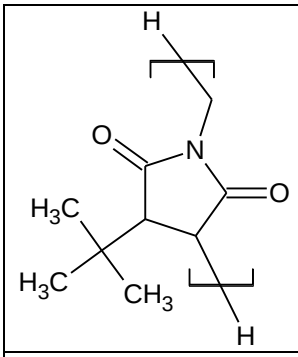

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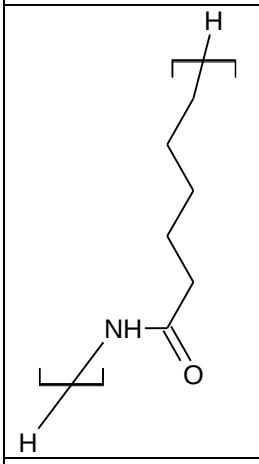

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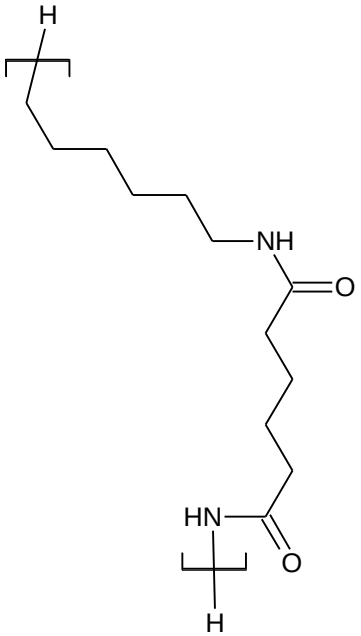

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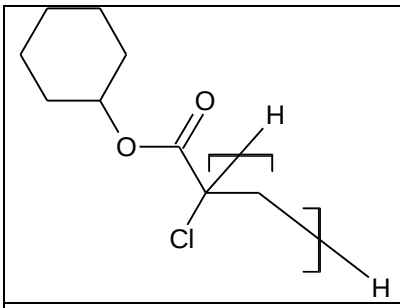

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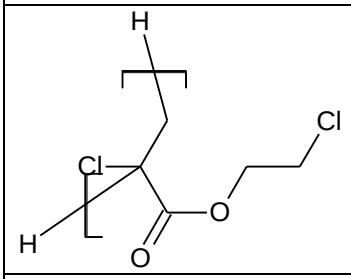

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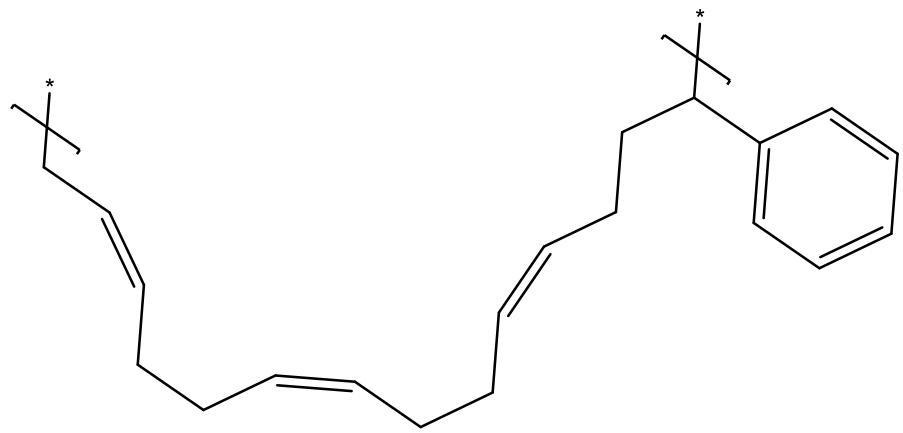

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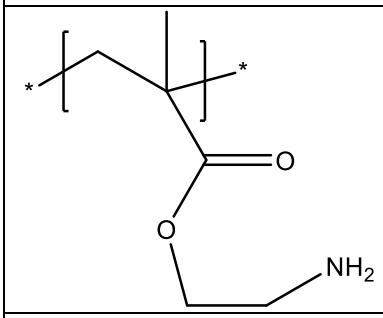

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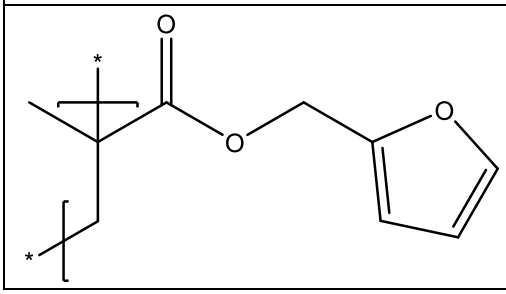

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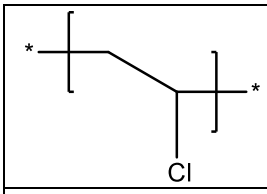

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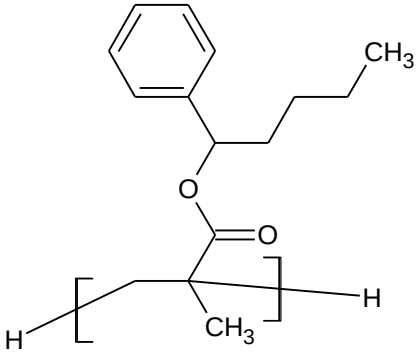

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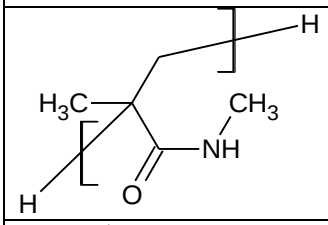

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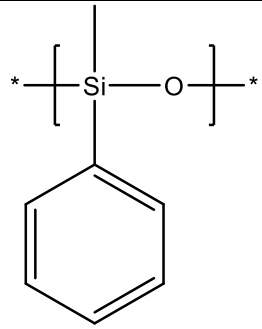

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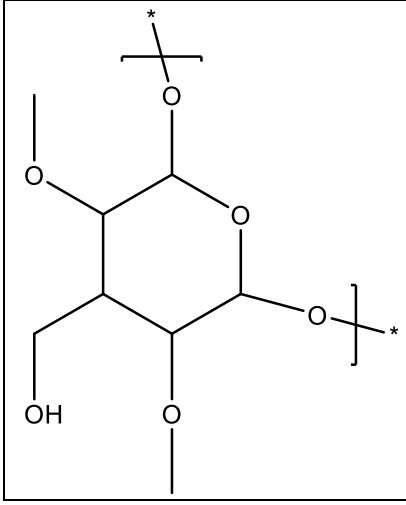

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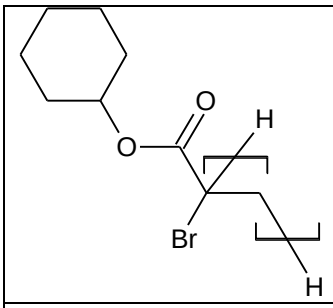

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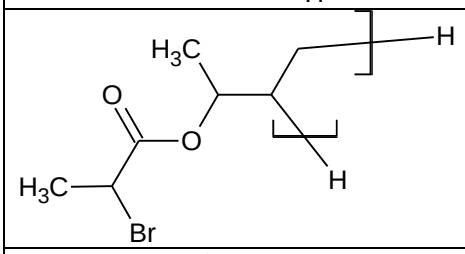

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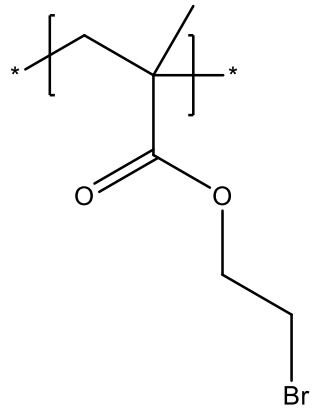

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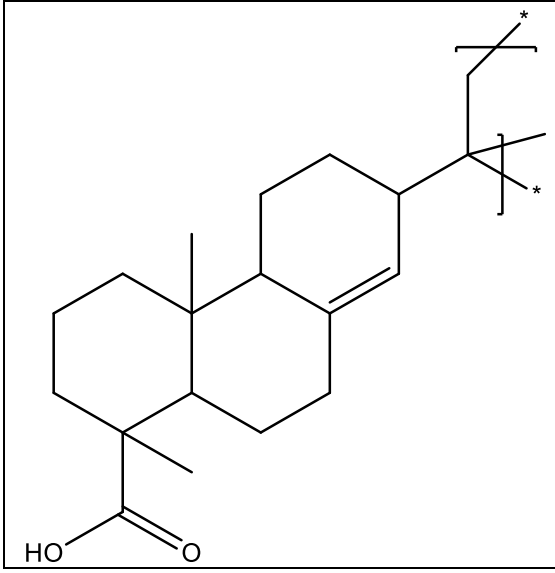
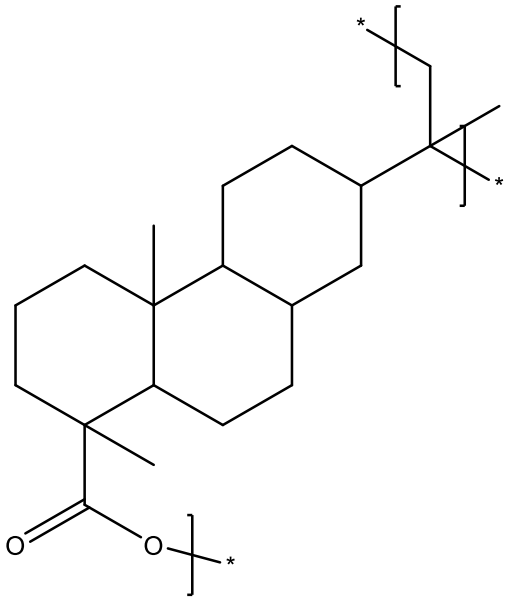
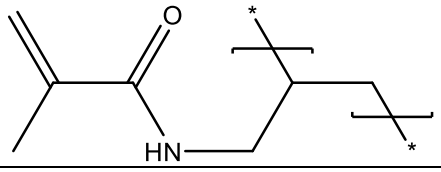
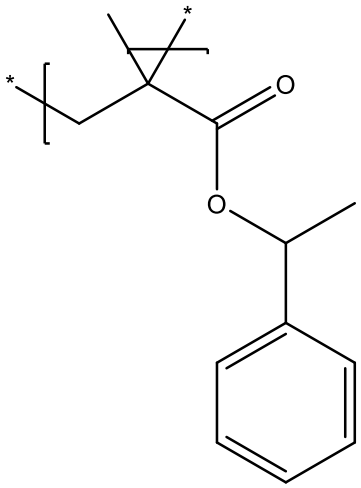
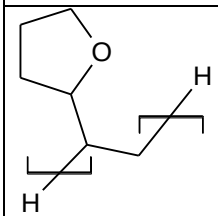
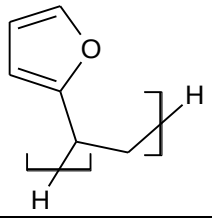


175	
176	
177	
178	
179	

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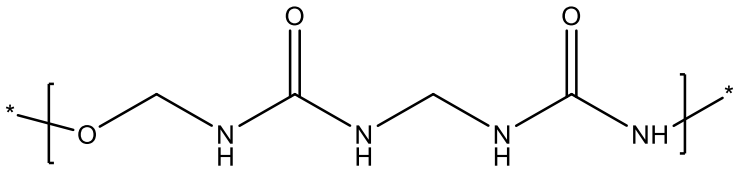

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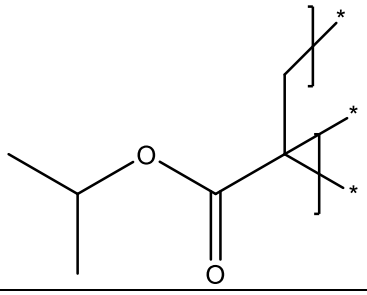

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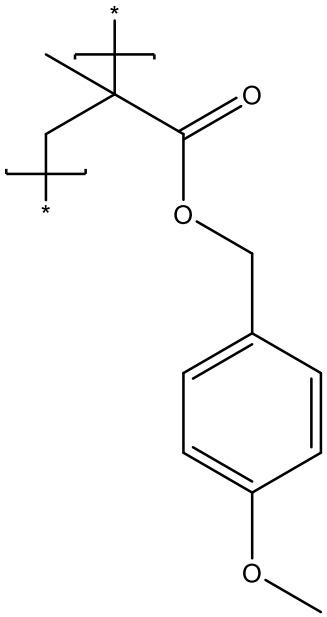

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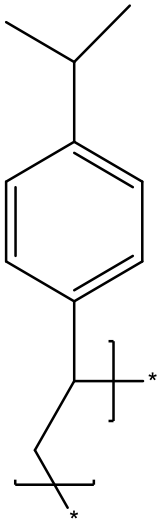
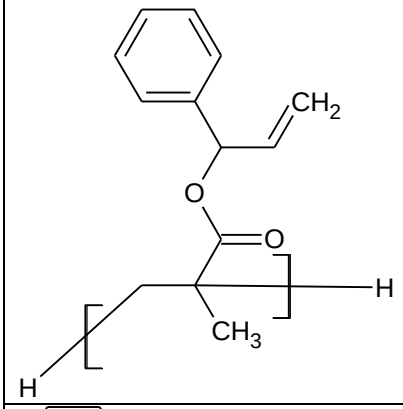
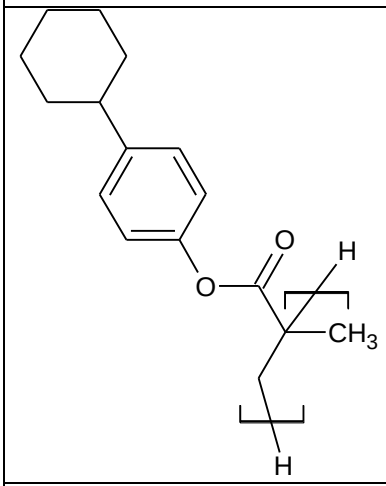
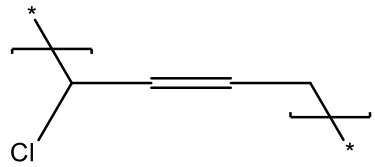
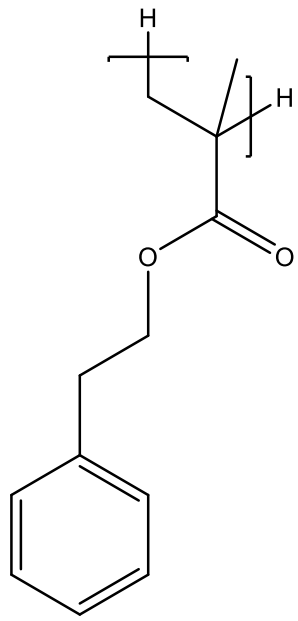
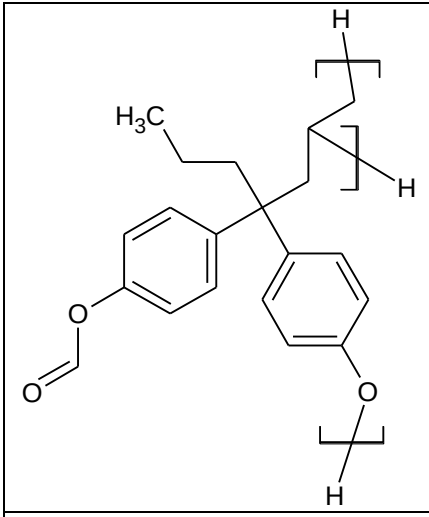
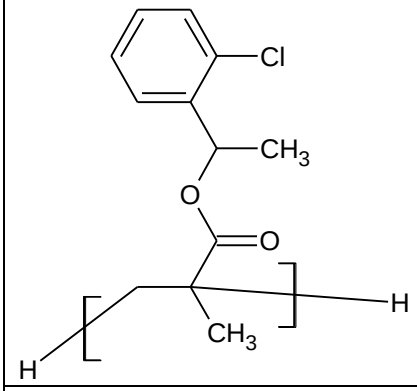
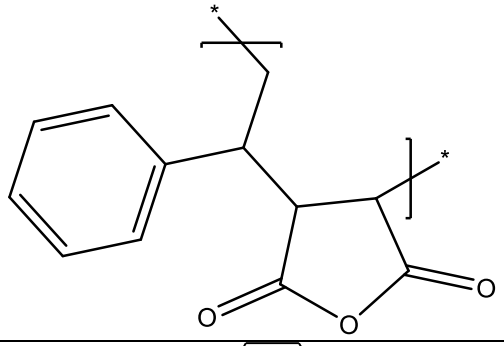
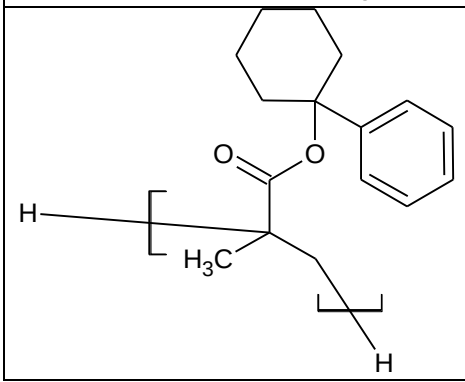
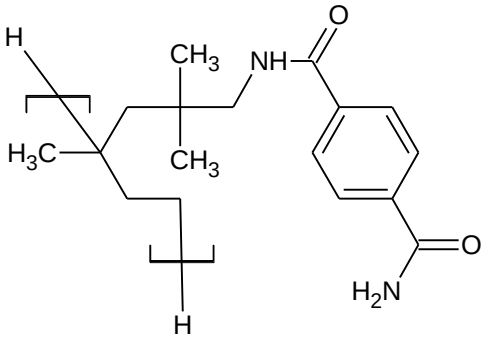
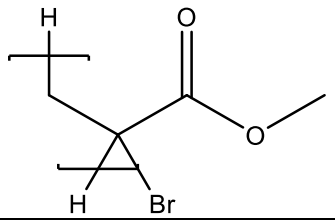
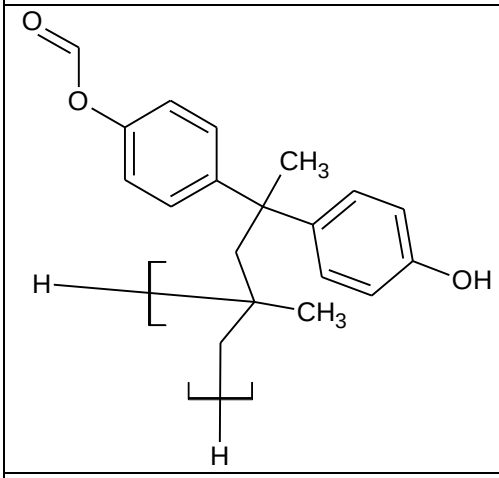
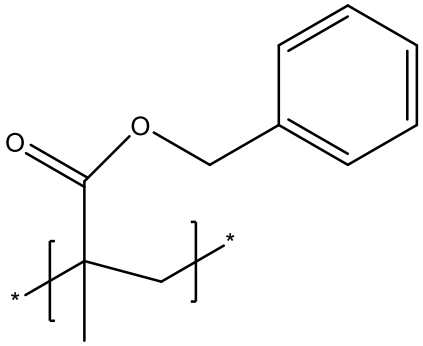


184	
185	
186	
187	

188	
189	
190	
191	

192	
193	
194	
195	

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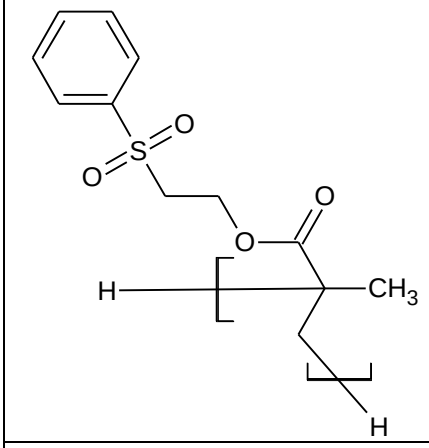

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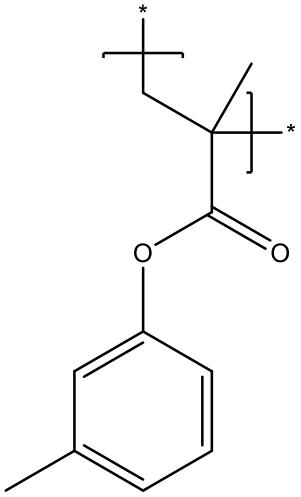

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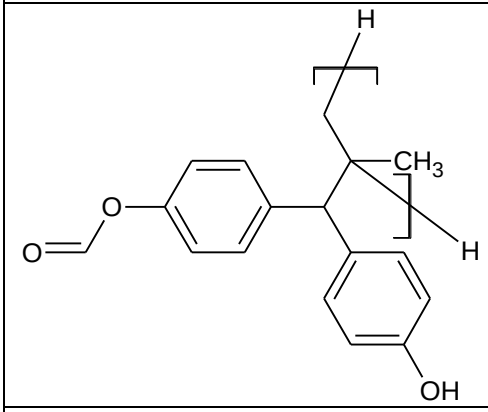

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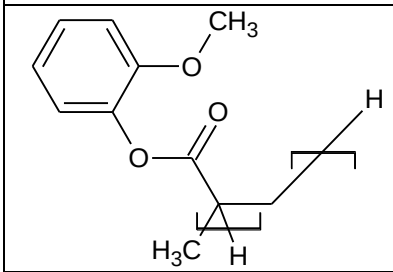

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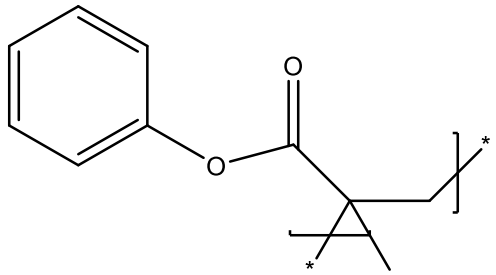

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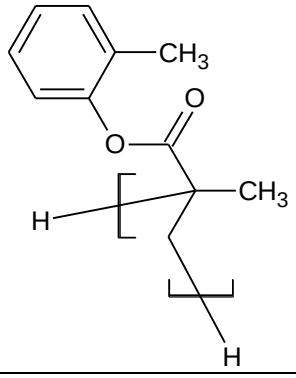

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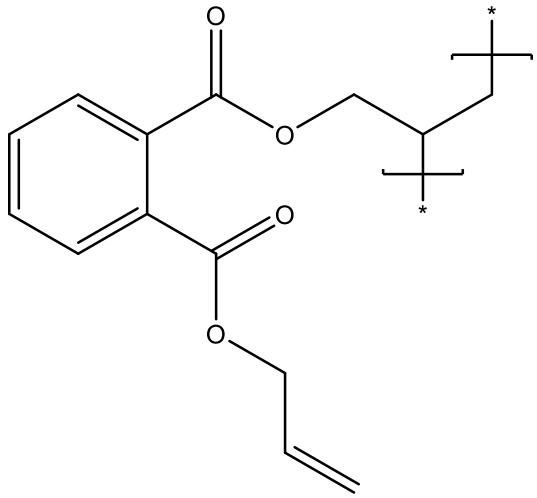

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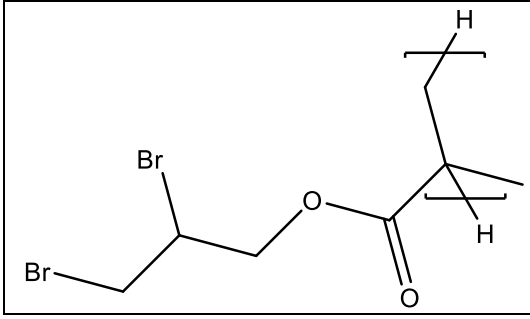

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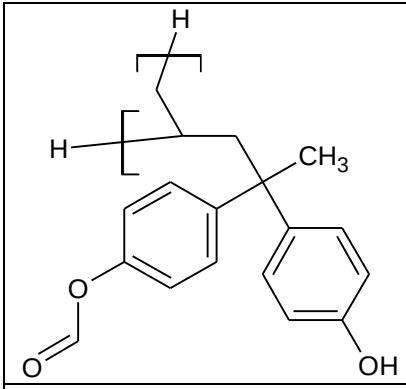

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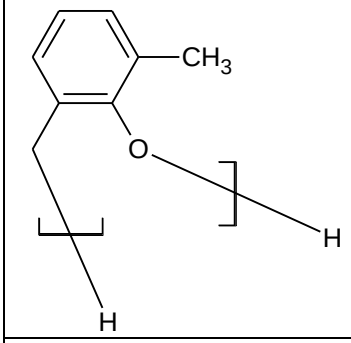

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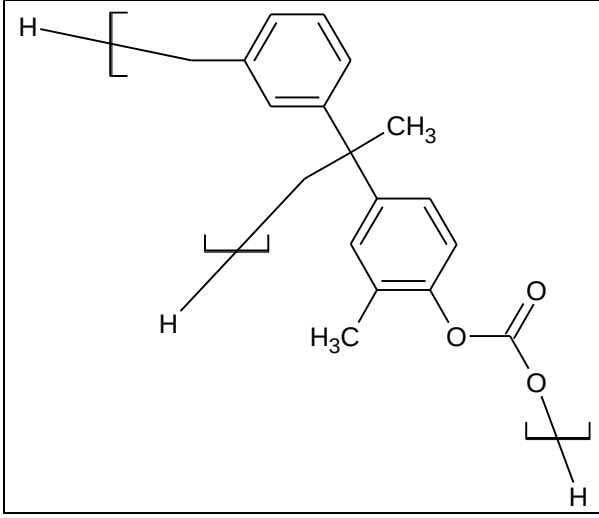
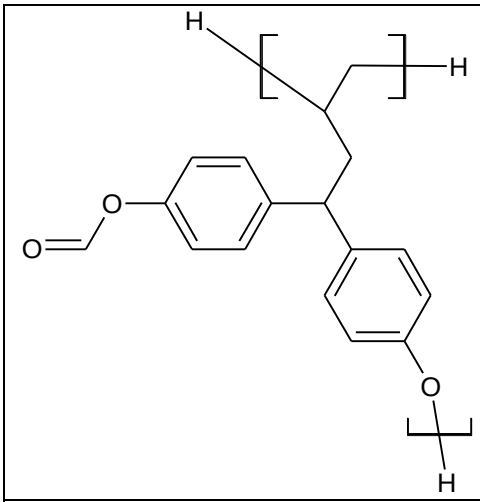
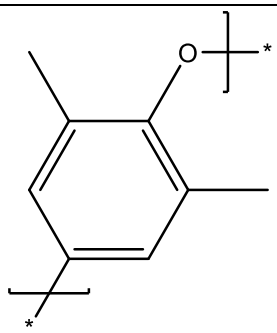
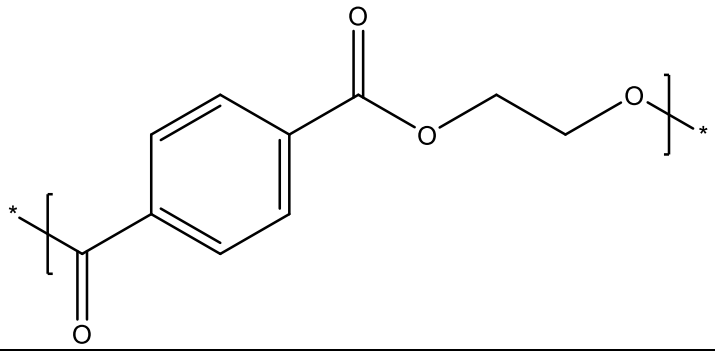
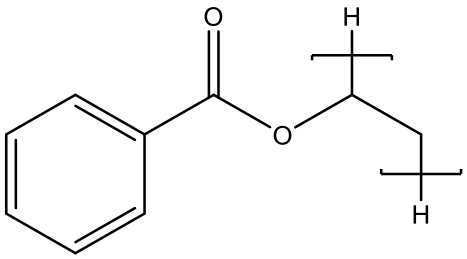
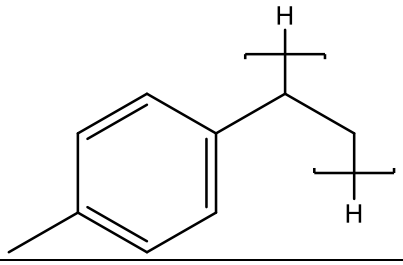


207	
208	
209	
210	
211	

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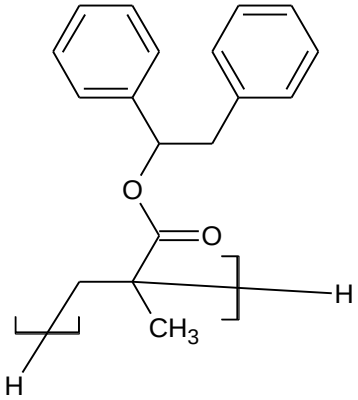

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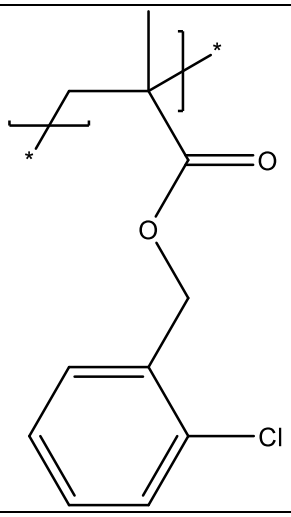

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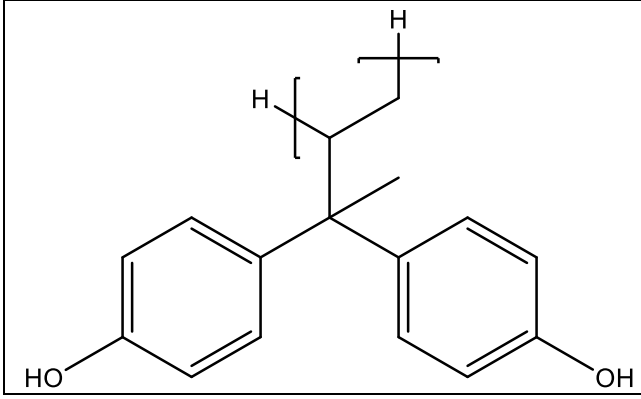
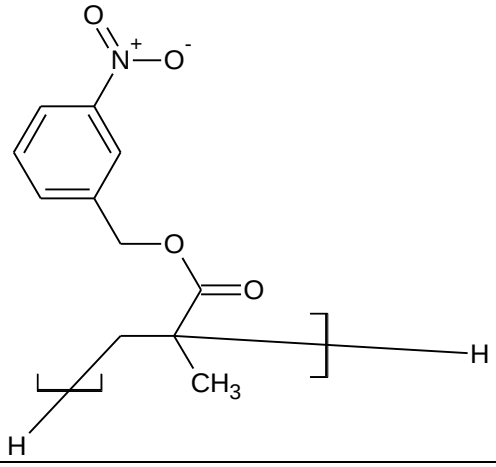
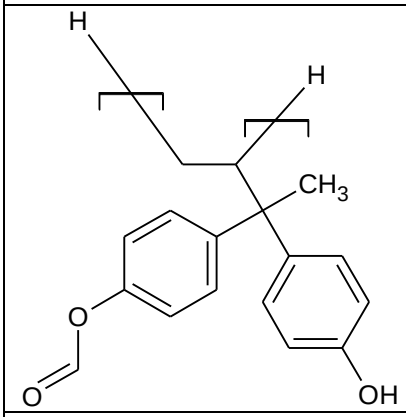
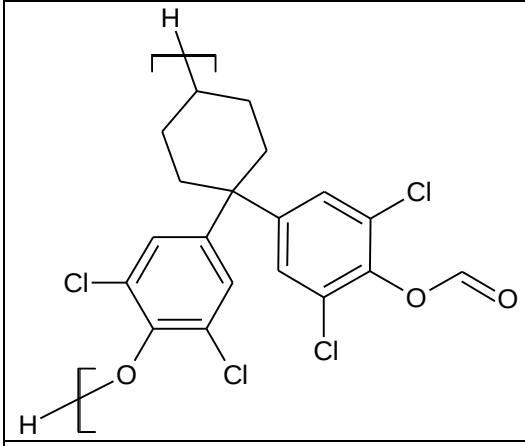
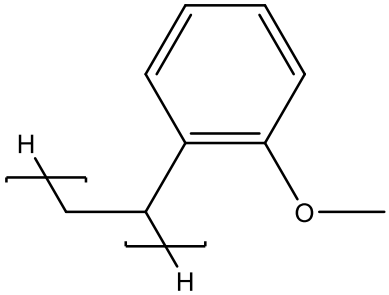
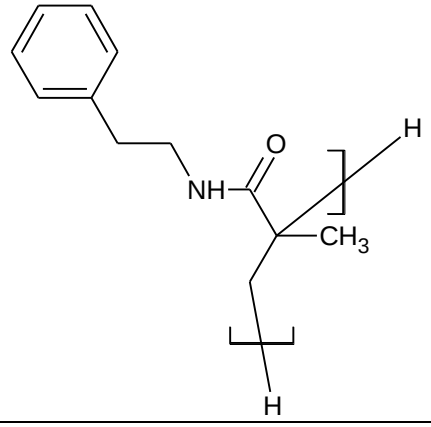
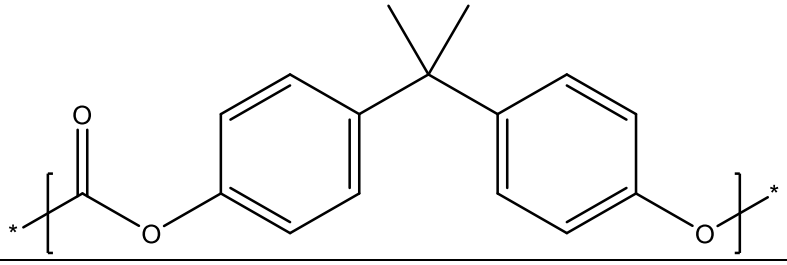
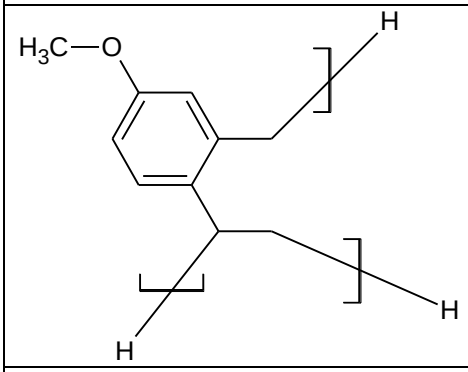
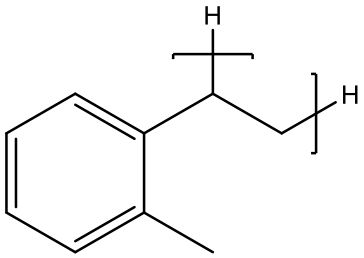
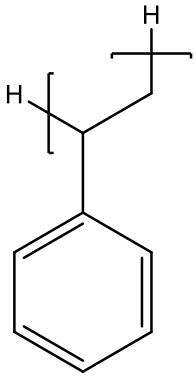


215	
216	
217	
218	

219	
220	
221	
222	
223	

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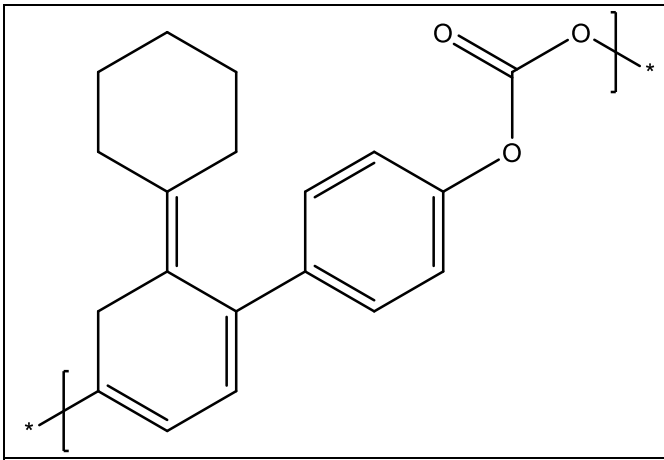

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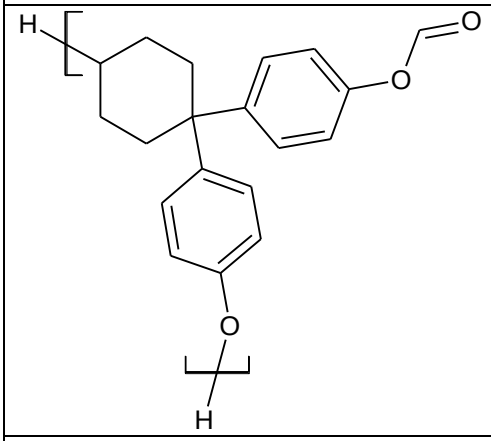

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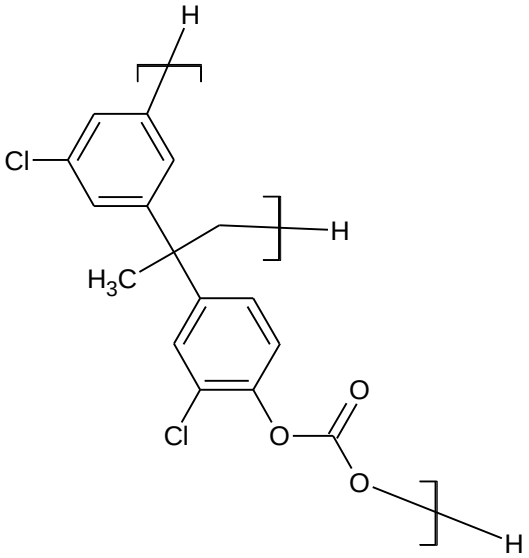

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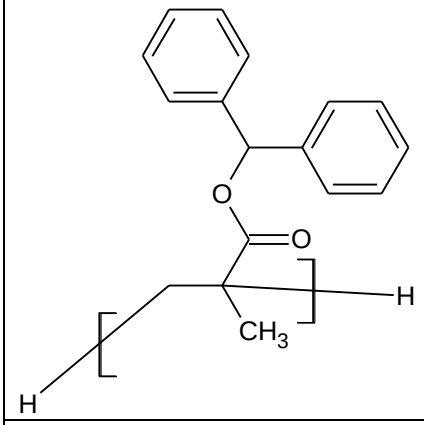

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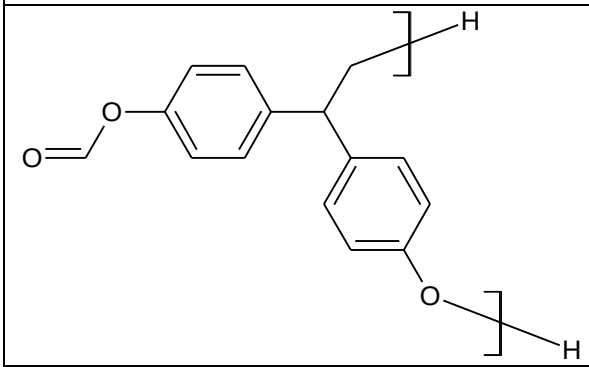

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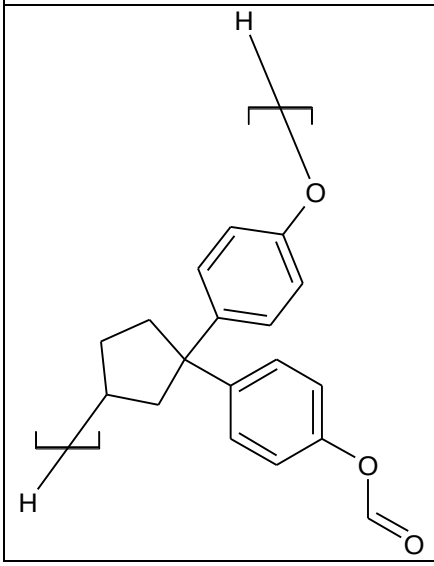

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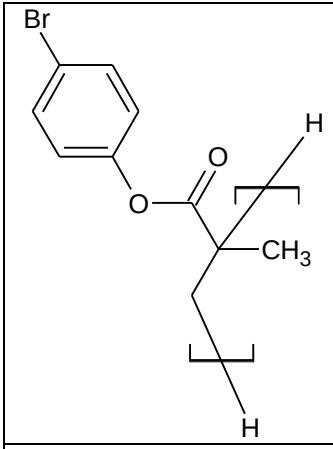

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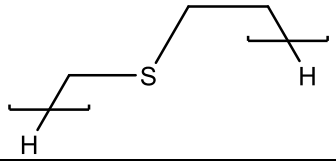

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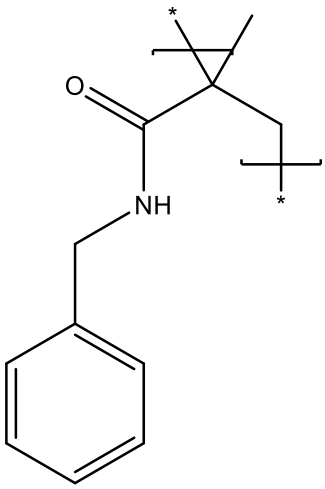

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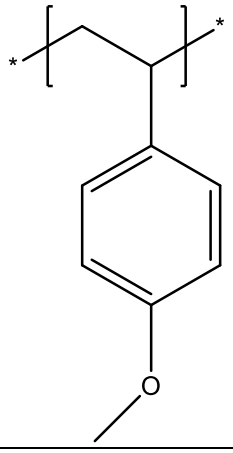
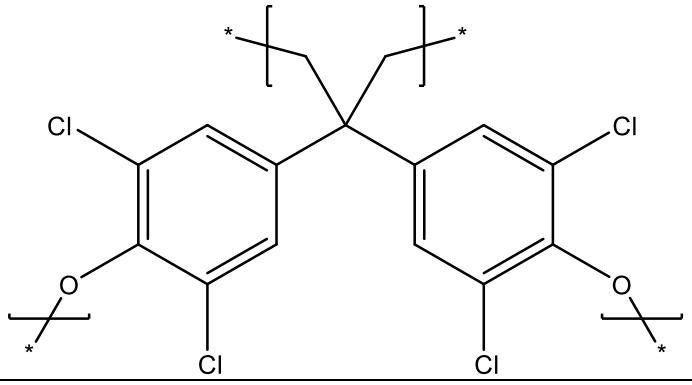
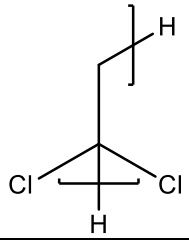
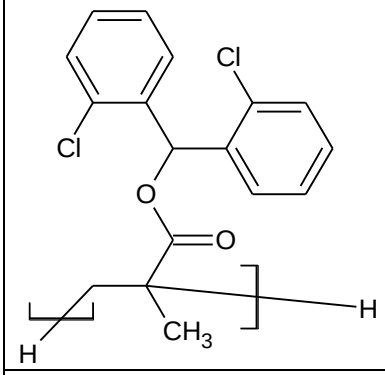
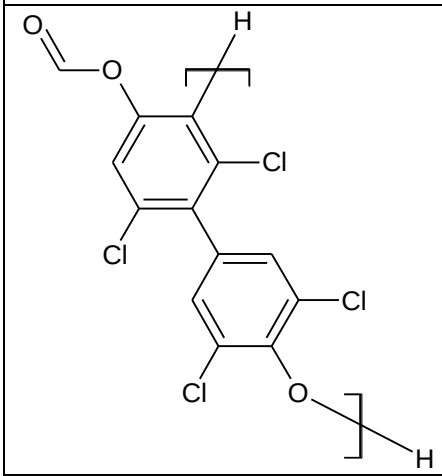
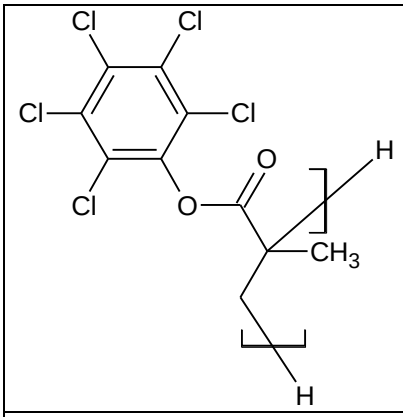
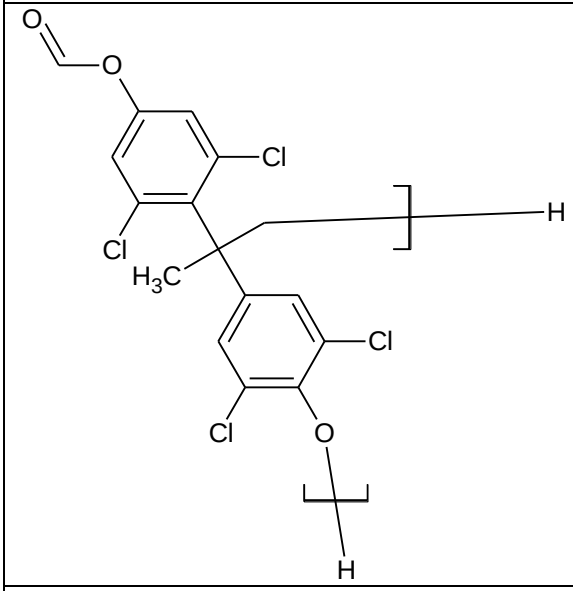
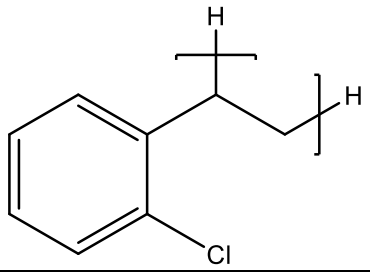
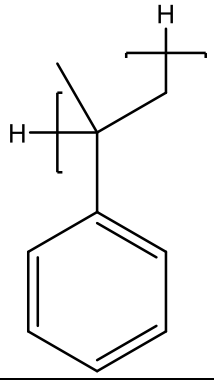


234	
235	
236	
237	

238	
239	
240	
241	

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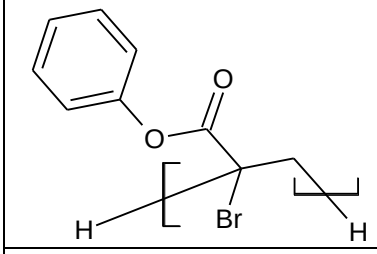

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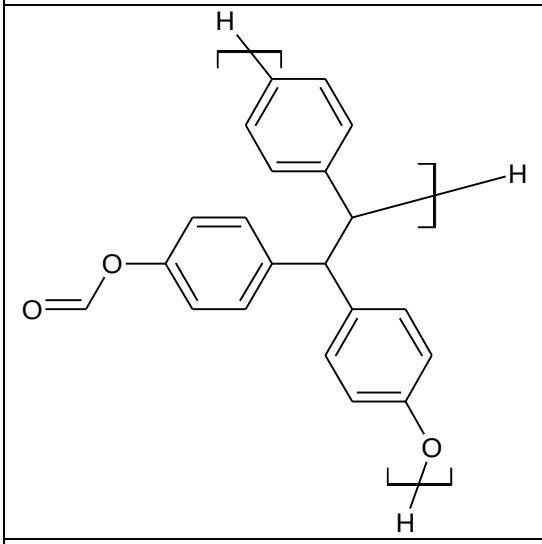

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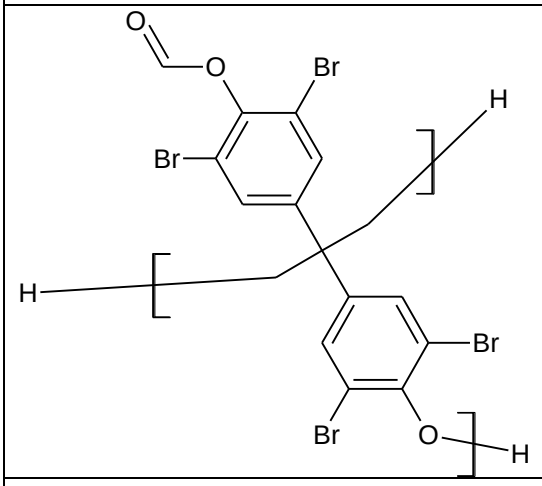

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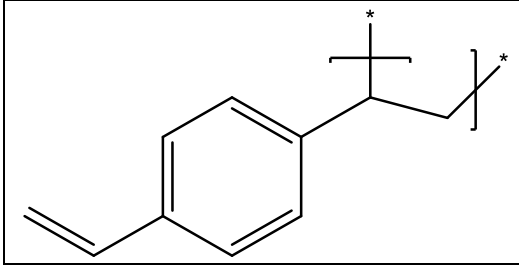
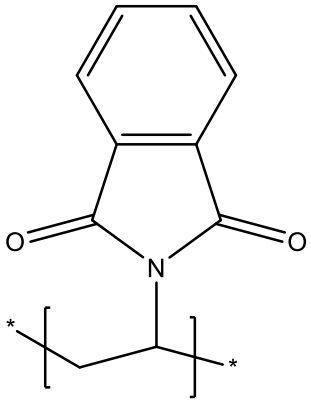
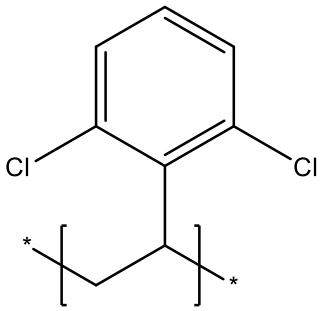
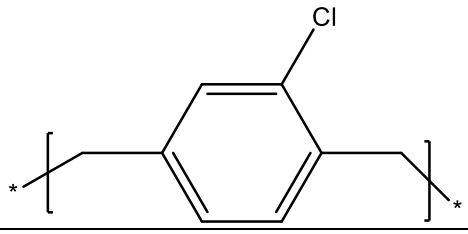
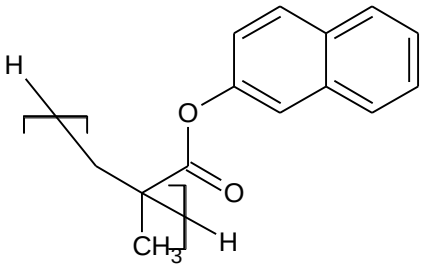
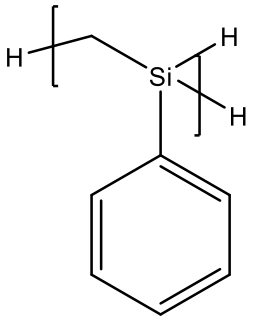


246	
247	
248	
249	
250	

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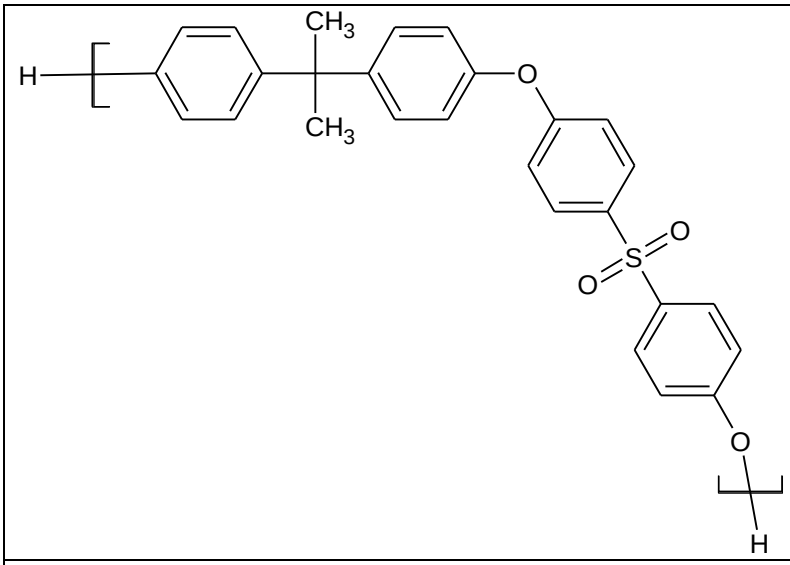

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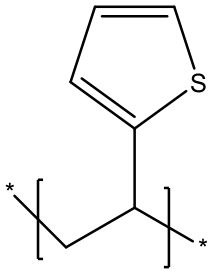

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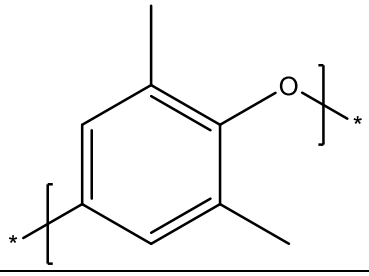

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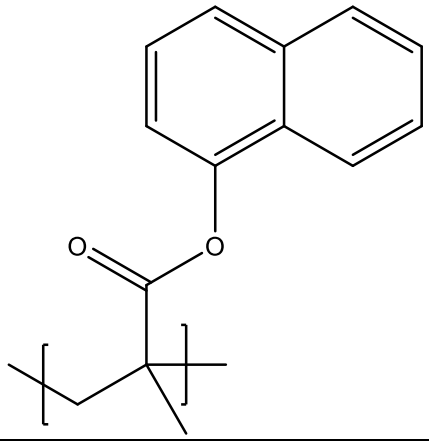
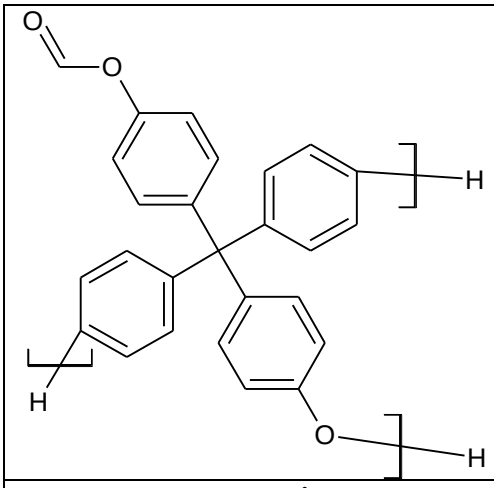
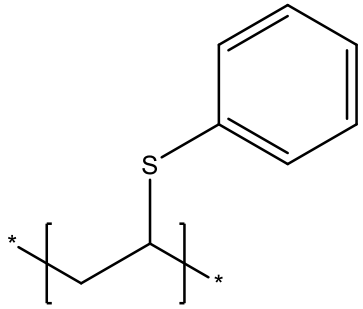
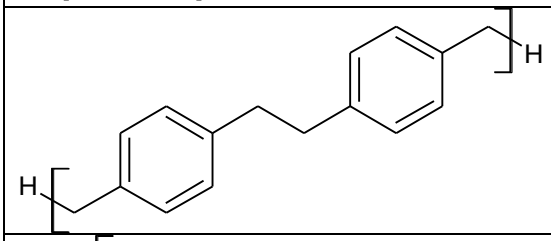
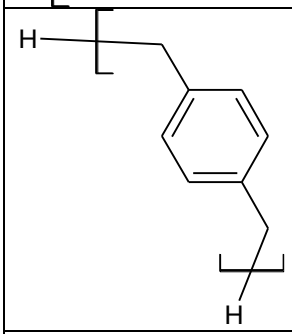
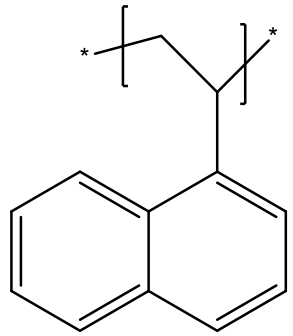


255	
256	
257	
258	
259	

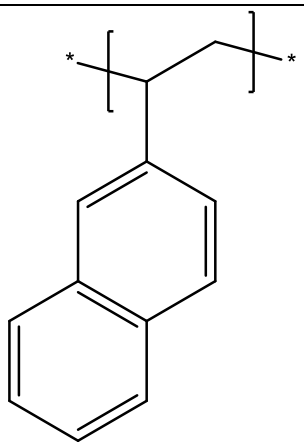
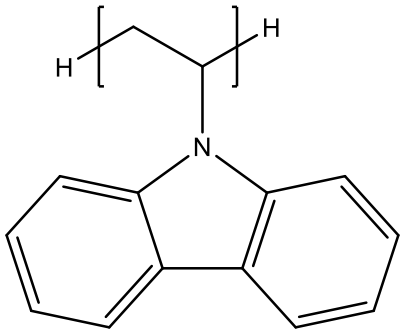
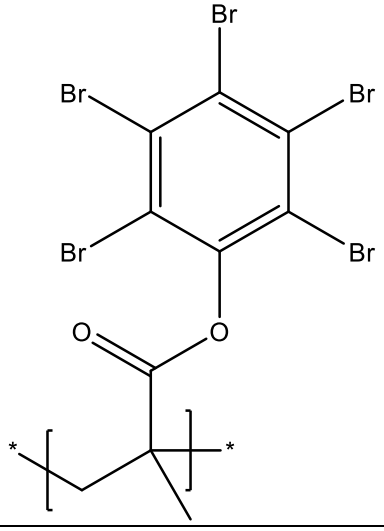
260	
261	
262	

Table S2 - Number, polymer name, Smiles notation of end-capped monomer, the experimental refractive indices before and after log transformation, predicted log transformation from 4 variable model, and which set each molecule was a part of.

#	**Polymer Name** ***Smiles END-CAPPED***	**Exp. RI**	**Exp. Log RI**	**Pred. Log RI**	**Set**
1	Poly(hexafluoropropylene oxide) *OC(F)(F)[C@H](F)C(F)(F)F*	1.31	0.117	0.115	Training
2	Poly(tetrafluoroethylene-co-hexafluoropropylene) *C(C(C(C(F)C(F)(F)F)(F)F)(F)F)(F)F*	1.34	0.126	0.112	Training
3	Poly (pentadecafluorooctyl acrylate) *C(CC)(O)OCC(C(C(C(C(C(C(CF)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F*	1.34	0.127	0.130	Training
4	Poly(tetrafluoro-3-(heptafluoropropoxy)propyl acrylate) *C(=O)(C[CH2])OC(C(COC(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F*	1.35	0.129	0.127	Training
5	Poly(tetrafluoro-3-(pentafluoroethoxy)propyl acrylate) *C(=O)(CC)OC(C(COC(C(F)(F)F)(F)F)(F)F)(F)F*	1.35	0.130	0.129	Prediction
6	Poly(tetrafluoroethylene) *C(C(F)F)(F)F*	1.35	0.130	0.119	Training
7	Poly(undecafluorohexyl acrylate) *C(=O)(CC)OC(C(C(C(C(CF)(F)F)(F)F)(F)F)(F)F)(F)F*	1.36	0.132	0.131	Training
8	Poly(nonafluoropentyl acrylate) *C(=O)(CC)OC(C(C(C(CF)(F)F)(F)F)(F)F)(F)F*	1.36	0.134	0.134	Training
9	Poly(tetrafluoro-3-(trifluoromethoxy)propyl acrylate) *CCC(=O)OCC(F)(C(F)(F)OC(F)(F)F)F*	1.36	0.134	0.133	Prediction
10	Poly(pentafluorovinyl propionate) *C(=O)(CC)OC(C(CF)(F)F)(F)F*	1.36	0.135	0.145	Training
11	Poly(heptafluorobutyl acrylate) *C(=O)(CC)OC(C(C(CF)(F)F)(F)F)(F)F*	1.37	0.136	0.139	Training
12	Poly(trifluorovinyl acetate) *C(C(OC(=O)C)F)(F)F*	1.38	0.138	0.145	Training
13	Poly(octafluoropentyl acrylate) *C(=O)(CC)OC(C(C(C(C)(F)F)(F)F)(F)F)(F)F*	1.38	0.140	0.135	Prediction
14	Poly(methyl 3,3,3-trifluoropropyl siloxane) *[SiH](O)(CCC(F)(F)F)C*	1.38	0.141	0.148	Training
15	Poly(chlorotrifluoroethylene) *C(C(F)Cl)(F)F*	1.39	0.143	0.155	Training
16	Poly(2-(heptafluorobutoxy)ethyl acrylate) *C(=O)(CC)OCCOC(C(C(CF)(F)F)(F)F)(F)F*	1.39	0.143	0.144	Training

17	Poly(2,2,3,4,4,4-hexafluorobutyl acrylate) *C(=O)(CC)OCC(C(C(F)(F)F)F)(F)F*	1.39	0.144	0.144	Prediction
18	Poly(methyl hydro siloxane) *C[SiH2]O*	1.40	0.145	0.161	Training
19	Poly(methacrylic acid), sodium salt *C(=O)(C(C)C)O*	1.43	0.155	0.172	Training
20	Poly(dimethyl siloxane) *[SiH](O)(C)C*	1.40	0.147	0.158	Training
21	Poly(trifluoroethyl acrylate) *C(=O)(CC)OC(CF)(F)F*	1.41	0.148	0.152	Training
22	Poly(2,2,2-trifluoroethyl acrylate) *C(=O)(CC)OCC(F)(F)F*	1.41	0.149	0.151	Prediction
23	Poly(2-(1,1,2,2-tetrafluoroethoxy)ethyl acrylate *C(=O)(CC)OCCOC(C(F)F)(F)F*	1.41	0.150	0.150	Training
24	Poly(trifluoroisopropyl methacrylate) *C(=O)(CC)OC(C(F)F)(C)F*	1.42	0.152	0.153	Training
25	Poly (2,2,2-trifluoro-1 -methylethyl methacrylate) *C(=O)(CC)OC(C(F)(F)F)C*	1.42	0.152	0.152	Training
26	Poly(2-trifluoroethoxyethyl acrylate) *C(=O)(CC)OCCOC(CF)(F)F*	1.42	0.152	0.156	Prediction
27	Poly(vinylidene fluoride) *C(C)(F)F*	1.42	0.152	0.136	Training
28	Poly(2,2,3,3-tetrafluoropropyl methacrylate) *C(=O)(CC)OCC(C(F)F)(F)F*	1.42	0.152	0.151	Training
29	Poly(methyl hexyl siloxane) *[SiH](O)(CCCCCC)C*	1.44	0.159	0.171	Prediction
30	Poly(methyl octadecyl siloxane) *[SiH](O)(CCCCCCCCCCCCCCCCCC)C*	1.44	0.159	0.171	Training
31	Poly(vinyl isobutyl ether) *O(CC(C)C)CC*	1.45	0.162	0.167	Training
32	Poly[oxy(methyl n-hexadecylsilylene)] *[SiH](CCCCCCCCCCCCCCCC)(C)O*	1.45	0.162	0.171	Prediction
33	Poly(ethylene oxide) *C(C)O*	1.45	0.163	0.164	Training
34	Poly(vinyl ethyl ester) *O(C(=O)C)CC*	1.45	0.163	0.164	Training
35	Poly(methyl tetradecyl siloxane) *[SiH](O)(CCCCCCCCCCCCCC)C*	1.46	0.163	0.171	Training

36	Poly(ethylene glycol mono-methyl ether) *C(CO)OC*	1.46	0.163	0.163	Prediction
37	Poly(oxyethylene) *C(CO)O*	1.46	0.163	0.176	Training
38	Poly(vinyl butyl ether) *O(CCCC)CC*	1.46	0.163	0.170	Training
39	Poly(propylene oxide) *CC(C)O*	1.46	0.163	0.158	Training
40	Poly(3-butoxypropylene oxide) *CC(COCCCC)O*	1.46	0.164	0.169	Prediction
41	Poly(methyl vinyl ether) *O(CC)C*	1.47	0.167	0.166	Training
42	Poly(vinyl pentyl ether) *O(CCCCC)CC*	1.46	0.164	0.173	Training
43	Poly(3-hexoxypropylene oxide) *CC(COCCCCCC)O*	1.46	0.164	0.171	Training
44	Poly(hexyl vinyl ether) *O(CC)CCCCCC*	1.46	0.164	0.172	Training
45	Poly(4-fluoro-2-trifluoromethylstyrene) *CCc1c(cc(cc1)F)C(F)(F)F*	1.46	0.164	0.178	Prediction
46	Poly(octyl vinyl ether) *O(CC)CCCCCCCC*	1.46	0.165	0.173	Training
47	Poly(vinyl n-octyl acrylate) *CCC(=O)OC(CCCCCCC)CC*	1.46	0.165	0.174	Training
48	Poly(vinyl 2-ethylhexyl ether) *O(CC(CCCC)CC)CC*	1.46	0.165	0.173	Training
49	Poly(vinyl decyl ether) *O(CCCCCCCCCC)CC*	1.46	0.165	0.173	Prediction
50	Poly(2-methoxyethyl acrylate) *C(=O)(CC)OCCOC*	1.46	0.165	0.168	Training
51	Poly(3-methoxypropylene oxide) *CC(COC)O*	1.46	0.165	0.160	Training
52	Poly(4-methyl-1-pentene) *CCCC(C)C*	1.46	0.165	0.168	Training
53	Poly(acryloxypropyl methyl siloxane) *[SiH](O)(C)CCCOC(=O)C=C*	1.46	0.165	0.172	Prediction
54	Poly(ethyl vinyl ether) *CCOCC*	1.45	0.161	0.165	Training

55	Poly(t-butyl methacrylate) *C(=O)(C(C)C)OC(C)(C)C*	1.46	0.165	0.161	Training
56	Poly(vinyl dodecyl ether) *O(CCCCCCCCCCCC)CC*	1.46	0.166	0.174	Training
57	Poly(3-ethoxypropyl acrylate) *C(=O)(CC)OCCCOCC*	1.47	0.166	0.170	Training
58	Poly(vinyl propionate) *C(=O)(CC)OCC*	1.47	0.166	0.171	Prediction
59	Polyoxyoctamethylene *C(CCCCCCC)O*	1.47	0.167	0.177	Training
60	Cellulose acetate propionate *O1[C@@H](C[C@@H]([C@H]([C@@H]1O[C@H]1[C@@H]([C@H]([C@@H](O[C@@H]1COC(=O)CC)O)OC(=O)CC)OC(=O)CC)OC(=O)CC)OC(=O)CC)COC(=O)CC*	1.47	0.167	0.173	Training
61	Poly(1-octadecene) *CCCCCCCCCCCCCCCCCC*	1.47	0.168	0.176	Prediction
62	Poly(2-ethoxyethyl acrylate) *C(=O)(CC)OCCOCC*	1.47	0.168	0.170	Training
63	Poly(3-methoxypropyl acrylate) *C(=O)(CC)OCCCOC*	1.47	0.168	0.171	Training
64	Poly(isopropyl acrylate) *C(=O)(CC)OC(C)C*	1.47	0.168	0.167	Training
65	Poly(1-decene) *CCCCCCCCCC*	1.47	0.168	0.177	Prediction
66	Poly(propylene) *CCC*	1.47	0.168	0.165	Training
67	Poly(dodecyl methacrylate) *C(=O)(C(C)C)OCCCCCCCCCCCC*	1.47	0.168	0.173	Training
68	Poly(vinyl sec-butyl ether) (isotactic) *O(C(CC)C)CC*	1.47	0.168	0.169	Training
69	Poly(oxyethyleneoxysuccinoyl) (poly(ethylene succinate)) *C(=O)(CCC=O)OCCO*	1.47	0.169	0.178	Prediction
70	Poly(tetradecyl acrylate) *C(=O)(CC)OCCCCCCCCCCCCCC*	1.47	0.169	0.175	Training
71	Poly(tetradecyl methacrylate) *C(=O)(C(C)C)OCCCCCCCCCCCCCC*	1.47	0.169	0.173	Training
72	Poly(hexadecyl acrylate) *C(=O)(CC)OCCCCCCCCCCCCCCCC*	1.48	0.169	0.175	Training
73	Poly(hexadecyl methacrylate) *C(=O)(C(C)C)OCCCCCCCCCCCCCCCC*	1.48	0.169	0.173	Prediction

74	Poly(vinyl formate) *C(OC=O)C*	1.48	0.169	0.170	Training
75	Ethylene/vinyl acetate copolymer-40% vinyl acetate *CCCCOC(=O)C*	1.48	0.169	0.169	Training
76	Poly(ethylene) *CC*	1.51	0.179	0.172	Training
77	Poly(2-fluoroethyl methacrylate) *C(=O)(C(C)C)OCCF*	1.48	0.169	0.167	Training
78	Poly(octyl methyl silane) *[SiH2](C)CCCCCCCC*	1.48	0.170	0.174	Prediction
79	Poly(methyl acrylate) *C(=O)(OC)CC*	1.48	0.170	0.173	Training
80	Poly(dicyanopropyl siloxane) *[SiH](CCCC#N)(CCCC#N)O*	1.48	0.170	0.174	Training
81	Poly(dimethylsiloxane-co-alpha-methyl styrene) *c1ccccc1C(C[SiH](O[Si](C)(C)C)C)C*	1.48	0.170	0.176	Training
82	Poly(ethylene-co-propylene) (EPR-rubber) *CC(CC)C*	1.48	0.170	0.170	Prediction
83	Poly(isobutyl methacrylate) *C(=O)(C(C)C)OCC(C)C*	1.48	0.170	0.168	Training
84	Poly(oxymethylene) *CO*	1.48	0.170	0.166	Training
85	Poly(sec-butyl methacrylate) *C(=O)(C(C)C)OC(CC)C*	1.48	0.170	0.169	Training
86	Poly(hexyl methacrylate) *C(=O)(C(C)C)OCCCCCC*	1.48	0.171	0.172	Training
87	Poly(butyl methacrylate) *C(=O)(CC)OCCCC*	1.48	0.171	0.174	Training
88	Poly(ethylidene dimethacrylate) *C(C)(OC(=O)C(=C)C)OC(=O)CC*	1.48	0.171	0.171	Training
89	Poly(2-ethoxyethyl methacrylate) *C(=O)(C(C)C)OCCOCC*	1.48	0.171	0.168	Prediction
90	Poly(ethylene maleate) *C(=O)(C(CC(=O)O)CC)O*	1.48	0.171	0.178	Training
91	Poly(propyl methacrylate) *C(=O)(C(C)C)OCCC*	1.48	0.171	0.171	Training
92	Poly(3,3,5-trimethylcyclohexyl methacrylate) *C(=O)(C(C)C)OC1CC(CC(C1)C)(C)C*	1.49	0.172	0.173	Training

93	Poly(ethyl methacrylate) *C(=O)(C(C)C)OCC*	1.49	0.172	0.168	Prediction
94	Poly(vinyl butyral) *C1(OC(OC(C1)CC)CCC)C*	1.49	0.172	0.177	Training
95	Poly(2-nitro-2-methylpropyl methacrylate) *C(=O)(C(C)C)OCC(C)(C)[N+](=O)[O-]*	1.49	0.172	0.166	Training
96	Poly(dimethylsiloxane-co-diphenylsiloxane) *c1ccccc1[Si](O[Si](O[Si](c1ccccc1)(O)c1ccccc1)(C)C)(O)c1ccccc1*	1.48	0.170	0.190	Prediction
97	Poly(1,1-diethylpropyl methacrylate) *C(=O)(C(C)C)OC(CC)(CC)CC*	1.49	0.173	0.173	Training
98	Poly(methyl methacrylate) *C(=O)(C(C)C)OC*	1.49	0.173	0.169	Prediction
99	Poly(2-decyl-1,3-butadiene) *C=C(CC)CCCCCCCCCC*	1.49	0.173	0.179	Training
100	Poly(2-decyl-1,4-butadiene) *C(CC)C(=C)CCCCCCCCC*	1.49	0.173	0.177	Training
101	Poly(mercaptopropyl methyl siloxane) *[Si@@H](O[SiH3])(C)CCCS*	1.49	0.173	0.173	Training
102	Poly(ethyl glycolate methacrylate) *C(=O)(COC(=O)C(C)C)OCC*	1.49	0.173	0.168	Prediction
103	Poly(3-methylcyclohexyl methacrylate) *C(=O)(C(C)C)OC1CC(CCC1)C*	1.49	0.175	0.179	Training
104	Poly(cyclohexyl alpha-ethoxyacrylate) *CC(C(=O)OC1CCCCC1)OCC*	1.50	0.175	0.179	Training
105	Poly(1-butene) *CCCC*	1.51	0.179	0.176	Training
106	Poly(4-methylcyclohexyl methacrylate) *C(=O)(C(C)C)OC1CCC(CC1)C*	1.50	0.175	0.181	Training
107	Poly(decamethylene glycol dimethacrylate) *C(OCOCOCOCOCOCOCOCOCOC(=O)C(C)C)OC(=O)C(=C)C*	1.50	0.176	0.159	Prediction
108	Poly (1,2-butadiene) *CCC=C*	1.50	0.176	0.187	Training
109	Poly(2-bromo-4-trifluoromethyl styrene) *CCc1c(cc(cc1)C(F)(F)F)Br*	1.50	0.176	0.192	Training
110	Poly(2-heptyl-1,3-butadiene) *C=C(CC)CCCCCCC*	1.50	0.176	0.179	Training
111	Poly(2-heptyl-1,4-butadiene) *CCCC(=C)CCCCCC*	1.50	0.176	0.179	Prediction

112	Poly(sec-butyl alpha-chloroacrylate) *C(=O)(C(C)Cl)OC(CC)C*	1.50	0.176	0.179	Training
113	Poly(vinyl formal) *C1COCOC1C*	1.50	0.176	0.182	Training
114	Poly(vinyl methyl ketone) *C(=O)(C)CC*	1.50	0.176	0.175	Training
115	Poly(2-isopropyl-1,4-butadiene) *C/C(=C/C)/C(C)C*	1.50	0.177	0.178	Prediction
116	Poly(ethyl alpha-chloroacrylate) *C(=O)(C(C)Cl)OCC*	1.50	0.177	0.181	Training
117	Poly(2-isopropyl-1,3-butadiene) *C=C(CC)C(C)C*	1.50	0.177	0.178	Training
118	Poly(2-methylcyclohexyl methacrylate) *C(=O)(C([CH])C)OC1C(CCCC1)C*	1.50	0.177	0.181	Training
119	Poly(1,1-dimethylethylene) *C(C)(C)C*	1.51	0.178	0.158	Prediction
120	Poly(2-tert-butyl-1,3-butadiene) *C=C(CC)C(C)(C)C*	1.51	0.178	0.172	Training
121	Poly(bornyl methacrylate) *C(=O)(C(C)C)OC1CC2CCC1(C2(C)C)C*	1.51	0.178	0.183	Training
122	Poly(2-t-butyl-1,4-butadiene) *C/C(=C/C)/C(C)(C)C*	1.51	0.178	0.172	Training
123	Poly(ethylene glycol dimethacrylate) *C(=O)(OCCOC(=O)C(=C)C)C(=C)C*	1.51	0.178	0.176	Prediction
124	Poly(cyclohexyl methacrylate) *C(=O)(C(C)C)OC1CCCCC1*	1.51	0.178	0.182	Training
125	Poly(cyclohexanediol-1,4-dimethacrylate) *C1(CCC(CC1)(/C=C(/C(=O)O)\C)O)(O)CC(C(=O)O)C*	1.51	0.178	0.181	Training
126	Poly(acrylic acid) *C(=O)(CC)O*	1.53	0.185	0.177	Training
127	Gutta percha b *C/C(=C/CC/C(=C/C)/C)/C*	1.51	0.179	0.179	Training
128	Poly(tetrahydrofurfuryl methacrylate) *C(=O)(C(C)C)OCC1CCCO1*	1.51	0.179	0.179	Prediction
129	Natural rubber *C/C(=C/C)/C*	1.52	0.182	0.178	Training
130	Polyacetal *CC(OCC)OCC*	1.51	0.179	0.161	Training

131	Shellac *C1(CCC2C31CC(C2(C)C)C(=CC3CC(=O)CCCCCCCCC(O)CCCCCCO)C(=O)O)C*	1.51	0.179	0.183	Prediction
132	Poly(1-methylcyclohexyl methacrylate) *C(=O)(C(C)C)OC1(CCCCC1)C*	1.51	0.179	0.178	Training
133	Poly(2-hydroxyethyl methacrylate) *C(=O)(C(C)C)OCCO*	1.51	0.180	0.171	Training
134	Poly(vinyl methacrylate) *CC(C)C(=O)OC=C*	1.51	0.180	0.174	Training
135	Poly(vinyl chloroacetate) *C(=O)(CCl)OCC*	1.51	0.180	0.186	Prediction
136	Poly(N-butyl methacrylamide) *C(=O)(C(C)C)NCCCC*	1.51	0.180	0.171	Training
137	Terpene resin *C1CC(CC=C1C)C(C)C*	1.51	0.180	0.187	Training
138	Poly(2-chloroethyl methacrylate) *C(=O)(C(C)C)OCCCl*	1.52	0.181	0.182	Training
139	Poly(methyl alpha-chloroacrylate) *C(=O)(C(C)Cl)OC*	1.52	0.181	0.184	Prediction
140	Poly(2-diethylaminoethyl methacrylate) *C(=O)(C(C)C)OCCN(CC)CC*	1.52	0.181	0.168	Training
141	Poly(2-chlorocyclohexyl methacrylate) *C(=O)(C(C)C)OC1C(CCCC1)Cl*	1.52	0.181	0.188	Training
142	Poly(acrylonitrile) *C(#N)CC*	1.52	0.181	0.190	Training
143	Poly(allyl methacrylate) *C(=O)(C(=C)C)OCCC*	1.52	0.182	0.177	Prediction
144	Poly(butadiene-co-acrylonitrile) *C(#N)C(C)C/C=C/C*	1.52	0.182	0.188	Training
145	Poly(methacrylonitrile) *C(#N)C(C)C*	1.52	0.182	0.181	Training
146	Poly(methyl isopropenyl ketone) *C(=O)(C(C)C)C*	1.52	0.182	0.170	Prediction
147	Poly((N-2-methoxyethyl)methacrylamide) *C(=O)(C(C)C)NCCOC*	1.52	0.183	0.166	Training
148	Poly(2,3-dimethylbutadiene) [methyl rubber] *C/C(=C(/CC/C(=C(/C)\C)/C)\C)/C*	1.53	0.183	0.177	Training
149	Poly(ω-dodecanamide), Nylon 12 *C(=O)CCCCCCCCCCCN*	1.53	0.183	0.178	Training

150	Poly(1,3-dichloropropyl methacrylate) *C(=O)(C(C)C)OC(CCCl)Cl*	1.53	0.184	0.184	Prediction
151	Poly(2-chloro-1-(chloromethyl)ethyl methacrylate) *C(=O)(C(C)C)OC(CCl)CCl*	1.53	0.184	0.188	Training
152	Poly(acrolein) *C(=O)C=C*	1.53	0.184	0.198	Training
153	Poly(N-methyl-methacrylamide) *C(=O)(C(C)C)NC*	1.54	0.188	0.170	Training
154	Nylon 6 [Poly(caprolactam)] *NCCCCCC=O*	1.53	0.185	0.181	Prediction
155	Poly(1-vinyl-2-pyrrolidone) *N1(C(=O)CCC1)CC*	1.53	0.185	0.186	Training
156	Poly(hexamethylene sebacamide) *NCCCCCCNC(=O)CCCCCCCCCC(=O)NCCCCCCCNC(=O)CCCCCCCCCC(=O)NCCCCCCCNC(=O)CCCCCCCCCC=O*	1.53	0.185	0.174	Training
157	Poly(iminoadipoyliminohexamethylene) (nylon 6,6) *C(=O)CCCCC(=O)NCCCCCCN*	1.53	0.185	0.177	Training
158	Poly(N-methylmaleimide-alt-isobutene) *CC(C1C(=O)N(C(=O)C1)C)(C)C*	1.53	0.185	0.177	Prediction
159	Poly(cyclohexyl alpha-chloroacrylate) *C(=O)(C(C)Cl)OC1CCCCC1*	1.53	0.185	0.190	Training
160	Poly(2-chloroethyl alpha-chloroacrylate) *C(=O)(C(C)Cl)OCCCl*	1.53	0.186	0.191	Training
161	Poly(methyl phenyl siloxane) *[SiH](O)(c1ccccc1)C*	1.54	0.188	0.191	Training
162	Poly(butadiene-co-styrene) *C/C=C/CCCc1ccccc1*	1.54	0.186	0.202	Training
163	Poly(2-aminoethyl methacrylate) *C(=O)(C(C)C)OCCN*	1.54	0.187	0.170	Prediction
164	Poly(furfuryl methacrylate) *C(=O)(C(C)C)OCc1ccco1*	1.54	0.187	0.188	Training
165	Poly(butylmercaptyl methacrylate) *CC(C(=O)OCCCCS)C*	1.54	0.187	0.182	Training
166	Poly(vinyl chloride) *C(C)Cl*	1.54	0.187	0.190	Training
167	Poly(1-phenyl-n-amyl methacrylate) *C(=O)(C(C)C)OC(CCCC)c1ccccc1*	1.54	0.187	0.190	Prediction
168	Poly(cyclohexyl alpha-bromoacrylate)	1.54	0.188	0.197	Training

	C(=O)(C(C)Br)OC1CCCCC1				
169	Poly(sec-butyl alpha-bromoacrylate) *C(=O)(C(C)Br)OC(CC)C*	1.54	0.188	0.188	Prediction
170	Poly(2-bromoethyl methacrylate) *C(=O)(C(C)C)OCCBr*	1.54	0.188	0.192	Training
171	Poly(dihydroabietic acid) *C(=O)([C@@]1(C)[C@H]2[C@@]([C@H]3CCC(C(C)C)CC3=CC2)(CCC1)C)O*	1.54	0.189	0.189	Training
172	Poly(abietic acid) *C(=O)([C@@]1(C)[C@H]2[C@@]([C@H]3CCC(=CC3=CC2)C(C)C)(CCC1)C)O*	1.55	0.189	0.191	Training
173	Poly(ethylmercaptyl methacrylate) *CC(C(=O)OCCS)C*	1.55	0.189	0.184	Prediction
174	Poly(N-allyl methacrylamide) *C(=O)(CC)NCC*	1.55	0.190	0.172	Training
175	Poly(1-phenylethyl methacrylate) *C(=O)(C(C)C)OC(C)c1ccccc1*	1.55	0.190	0.191	Training
176	Poly(2-vinyltetrahydrofuran) *O1C(CCC1)CC*	1.55	0.190	0.189	Training
177	Poly(methyl m-chlorophenylethyl siloxane) *[SiH](O)(CCc1cc(ccc1)Cl)C*	1.55	0.190	0.186	Prediction
178	Poly(vinylfuran) *o1c(ccc1)CC*	1.55	0.190	0.203	Training
179	Poly[oxy(methyl m-chlorophenylethylsilylene)] *[SiH](C(C)c1cc(ccc1)Cl)(C)O*	1.55	0.190	0.186	Training
180	Urea-formaldehyde resin *N(C(=O)N)CO*	1.55	0.190	Not Predicted	Not Included
181	Poly(isopropyl methacrylate) *C(=O)(C(C)C)OC(C)C*	1.55	0.191	Not Predicted	Not Included
182	Poly(p-methoxybenzyl methacrylate) *C(=O)(C(C)C)OCc1ccc(cc1)OC*	1.55	0.191	0.189	Training
183	Poly(p-isopropyl styrene) *CCc1ccc(cc1)C(C)C*	1.55	0.191	0.196	Prediction
184	Poly(p,p-xylylenyl dimethacrylate) *c1(ccc(cc1)COC(=O)C(C)C)COC(=O)C(C)C*	1.56	0.192	0.184	Training
185	Poly(cyclohexyl methyl silane) *[SiH2](C)C1CCCCC1*	1.56	0.192	0.188	Training
186	Poly(1-phenylallyl methacrylate) *C(=O)(CC)OC(C)c1ccccc1*	1.56	0.192	0.195	Training
187	Poly(p-cyclohexylphenyl methacrylate) *C(=O)(C(C)C)Oc1ccc(cc1)C1CCCCC1*	1.56	0.192	0.194	Prediction

188	Poly(chloroprene) *C(=C\C)(\Cl)/C*	1.56	0.193	0.193	Training
189	Poly(2-phenylethyl methacrylate) *C(=O)(C(C)C)OCCc1ccccc1*	1.56	0.193	0.192	Training
190	Poly(methyl m-chlorophenyl siloxane) *[SiH](O[SiH3])(c1cccc(c1)Cl)C*	1.56	0.193	0.182	Training
191	Poly [4,4-heptane bis(4-phenyl)carbonate] *OC(=O)OCCCCCCCOc1ccc(cc1)c1ccc(cc1)OCCCCCCCOC(=O)O*	1.56	0.193	0.185	Prediction
192	Poly(oxycarbonyloxy-1,4-phenylene-1-propylbutylidene-1,4-phenylene) *c1(c(cccc1)C(CCC)CCC)c1ccc(cc1)OC(=O)O*	1.56	0.193	0.196	Training
193	Poly(1-(o-chlorophenyl)ethyl methacrylate) *C(=O)(C(C)C)OC(C)c1c(cccc1)Cl*	1.56	0.194	0.193	Training
194	Poly(styrene-co-maleic anhydride) *CC(C1C(=O)OC(=O)C1)c1ccccc1*	1.56	0.194	0.203	Training
195	Styrene/maleic anhydride copolymer *C1(=O)OC(=O)CC1CCc1ccccc1*	1.56	0.194	0.203	Prediction
196	Poly(1-phenylcyclohexyl methacrylate) *C(=O)(C(C)C)OC1(CCCCC1)c1ccccc1*	1.56	0.194	0.195	Training
197	Poly(2,2,2'-trimethylhexamethylene terephthalamide) *C(=O)c1ccc(cc1)C(=O)NCC(CC(CCN)C)(C)C*	1.57	0.195	0.185	Training
198	Poly(methyl α-bromoacrylate) *C(=O)(C(C)Br)OC*	1.57	0.195	0.195	Training
199	Poly(oxycarbonyloxy-1,4-phenylene-1,3-dimethylbutylidene-1,4-phenylene) *c1(c(cccc1)C(CC(C)C)C)c1ccc(cc1)OC(=O)O*	1.57	0.195	0.195	Prediction
200	Poly(benzyl methacrylate) *C(=O)(C(C)C)OCc1ccccc1*	1.57	0.195	0.195	Training
201	Poly(2-(phenylsulfonyl)ethyl methacrylate) *C(=O)(C(C)C)OCCS(=O)(=O)c1ccccc1*	1.57	0.195	0.185	Training
202	Poly(m-cresyl methacrylate) *c1(cc(ccc1)C)OC(=O)C(C)C*	1.57	0.195	0.190	Training
203	Poly(oxycarbonyloxy-1,4-phenyleneisobutylidene-1,4-phenylene) *c1(c(cccc1)CC(C)C)c1ccc(cc1)OC=O*	1.57	0.196	0.201	Prediction
204	Poly[1,1-(2-methyl propane) bis(4-phenyl)carbonate] *O(C(=O)Oc1ccccc1)c1ccc(cc1)C(C(C)C)c1cccc(OC(=O)Oc2ccccc2)c1*	1.57	0.196	0.200	Training
205	Poly(o-methoxyphenol methacrylate) *c1(c(cccc1)OC)OC(=O)C(C)C*	1.57	0.196	0.189	Training
206	Poly(phenyl methacrylate) *C(=O)(C(C)C)Oc1ccccc1*	1.57	0.196	0.195	Training

207	Poly(o-cresyl methacrylate) *c1(c(cccc1)C)OC(=O)C(C)C*	1.57	0.196	0.192	Prediction
208	Poly(diallyl phthalate) *C(=O)(c1c(C(=O)OCCC)cccc1)OCCC*	1.57	0.196	0.190	Training
209	Poly(2,3-dibromopropyl methacrylate) *C(=O)(C(C)C)OCC(CBr)Br*	1.57	0.197	0.198	Training
210	Poly(oxycarbonyloxy-1,4-phenylene-1-methyl-butylidene-1,4-phylene) *c1(c(cccc1)C(CCC)C)c1ccc(cc1)OC(=O)O*	1.57	0.197	0.198	Training
211	Poly(2,6-dimethyl-p-phenylene oxide) *c1c(c(c(cc1)C)O)C*	1.58	0.197	0.203	Prediction
212	Poly(ethylene terephthalate) *C(=O)(c1ccc(C(=O)O)cc1)OCC*	1.58	0.197	0.197	Training
213	Poly(vinyl benzoate) *C(=O)(c1ccccc1)OCC*	1.58	0.198	0.200	Training
214	Poly(4-methylstyrene) *CCc1ccc(cc1)C*	1.58	0.198	0.202	Training
215	Poly(oxycarbonyloxy-1,4-phenylenebutylidene-1,4-phenylene) *c1(c(cccc1)CCCC)c1ccc(cc1)OC=O*	1.58	0.198	0.204	Prediction
216	Poly(1,2-diphenylethyl methacrylate) *C(=O)(C(C)C)OC(Cc1ccccc1)c1ccccc1*	1.58	0.199	0.200	Training
217	Poly(o-chlorobenzyl methacrylate) *C(=O)(C(C)C)OCc1c(cccc1)Cl*	1.58	0.199	0.197	Training
218	Poly(Bisphenol B carbonate) *c1cc(ccc1O)C(C)(CC)c1ccc(cc1)OC=O*	1.58	0.199	0.201	Training
219	Poly(oxypentaerythritoloxyphthaloyl) *C(=O)c1c(C=O)c(c(cc1)O)OCC(CO)(CO)CO*	1.58	0.200	0.193	Prediction
220	Poly(m-nitrobenzyl methacrylate) *C(=O)(C(C)C)OCc1cc(ccc1)[N+](=O)[O-]*	1.58	0.200	0.190	Training
221	Poly(2-methoxystyrene) *CCc1c(cccc1)OC*	1.59	0.200	0.200	Training
222	Poly(oxycarbonyloxy-1,4-phenyleneisopropylidene-1,4-phenylene) *c1(ccccc1)C(C)(C)c1ccc(cc1)OC(=O)O*	1.59	0.200	0.201	Training
223	Poly(N-(2-phenylethyl)methacrylamide) *C(=O)(C(C)C)NCCc1ccccc1*	1.59	0.200	0.192	Prediction
224	Bisphenol-A polycarbonate *c1cc(ccc1O)C(C)(C)c1ccc(cc1)OC=O*	1.59	0.200	0.201	Training
225	Poly(Bisphenol A carbonate), PC *Oc1ccc(cc1)C(C)(C)c1ccc(cc1)OC(=O)O*	1.59	0.200	0.199	Training

226	Poly(4-methoxy-2-methylstyrene) *CCc1c(cc(cc1)OC)C*	1.59	0.201	0.195	Training
227	Poly(2-methylstyrene) *CCc1c(cccc1)C*	1.59	0.201	0.203	Prediction
228	Polystyrene *CCc1ccccc1*	1.59	0.201	0.211	Training
229	Poly(oxycarbonyloxy-1,4-phenylenecyclohexylidene-1,4-phenylene) *c1(ccccc1)C1(CCCCC1)c1ccc(cc1)OC(=O)O*	1.59	0.201	0.205	Training
230	Poly(diphenylmethyl methacrylate) *C(=O)(C(C)C)OC(c1ccccc1)c1ccccc1*	1.59	0.202	0.203	Training
231	Poly(oxycarbonyloxy-1,4-phenyleneethylidene-1,4-phenylene) *c1(ccccc1)C(C)c1ccc(cc1)OC(=O)O*	1.59	0.202	0.205	Prediction
232	Poly(2,5-dimethyl-1,4-phenylene ethylene) *C(C)c1cc(ccc1C)C*	1.60	0.203	0.199	Training
233	Poly(4-bromophenyl methacrylate) *C(=O)(C(C)C)Oc1ccc(cc1)Br*	1.60	0.203	0.205	Training
234	Poly(propylene sulfide) *CCCS*	1.60	0.203	0.195	Training
235	Poly(N-benzyl methacrylamide) *C(=O)(C(C)C)NCc1ccccc1*	1.60	0.203	0.195	Prediction
236	Poly(4-methoxystyrene) *CCc1ccc(cc1)OC*	1.60	0.203	0.200	Training
237	Poly(2,6,3',5'-tetrachloro bisphenol A carbonate) *Oc1cc(c(c(c1)Cl)C(C)(C)c1cc(c(c(c1)Cl)OC(=O)O)Cl)Cl*	1.60	0.204	0.204	Training
238	Hard Rubber (32% S) *C=C(C)C(CC)SC(C(=C)C)CC*	1.60	0.204	0.185	Training
239	Poly(vinylidene chloride) *C(=C)(Cl)Cl*	1.60	0.204	0.202	Prediction
240	Poly(o-chlorodiphenylmethyl methacrylate) *C(=O)(C(=C)C)OC(c1c(cccc1)Cl)c1ccccc1*	1.60	0.205	0.207	Training
241	Poly(oxycarbonyloxy-1,4-(2,6-dichloro)phenylene-isopropylidene-1,4-(2,6-dichloro)phenylene) *c1(cc(cc(c1)Cl)Cl)C(C)(C)c1cc(c(c(c1)Cl)OC(=O)O)Cl*	1.61	0.206	0.206	Training
242	Poly(oxycarbonyloxybis(1,4-(3,5-dichlorophenylene))) *c1(c2c(cc(cc2Cl)OC(=O)O)Cl)cc(cc(c1)Cl)Cl*	1.61	0.206	0.212	Training
243	Poly(2-chlorostyrene) *C=Cc1c(cccc1)Cl*	1.61	0.207	0.218	Prediction
244	Poly(alpha-methylstyrene) *CC(c1ccccc1)C*	1.61	0.207	0.202	Training

245	Poly(phenyl alpha-bromoacrylate) *C(=O)(C(C)Br)Oc1ccccc1*	1.61	0.207	0.208	Training
246	Poly(p-divinylbenzene) *c1(ccc(cc1)CC)CC*	1.62	0.208	0.202	Training
247	PoIy(N-vinyl phthalimide) *C1(=O)c2c(C(=O)N1CC)cccc2*	1.62	0.210	0.206	Prediction
248	Poly(2,6-dichlorostyrene) *CCc1c(cccc1Cl)Cl*	1.62	0.211	0.212	Training
249	Poly(chloro-p-xylylene) *c1cc(c(cc1C)Cl)C*	1.63	0.212	0.208	Training
250	Poly(beta-naphthyl methacrylate) *C(=O)(C(C)C)Oc1cc2c(cc1)cccc2*	1.63	0.212	0.203	Training
251	Poly(alpha-naphthyl carbinyl methacrylate) *C(=O)(C(Cc1cccc2ccccc12)C)O*	1.63	0.212	0.207	Prediction
252	Poly(phenyl methyl silane) *[SiH2](C)c1ccccc1*	1.63	0.212	0.196	Training
253	Poly(sulfone) *Oc1ccc(cc1)C(C)(C)c1ccc(cc1)Oc1ccc(cc1)S(=O)(=O)c1ccccc1*	1.63	0.213	0.203	Training
254	Poly(2-vinylthiophene) *c1(cccs1)CC*	1.64	0.214	0.219	Training
255	Poly (2,6-diphenyl-1,4-phenylene oxide) *c1(c(cc(cc1c1ccccc1)O)c1ccccc1)C*	1.64	0.215	0.216	Prediction
256	Poly[oxy(2,6-diphenyI-1,4-phenylene)] *c1c(c(c(cc1)c1ccccc1)O)c1ccccc1*	1.64	0.215	0.219	Training
257	Poly(alpha-naphthyl methacrylate) *C(=O)(C(C)C)Oc1cccc2ccccc12*	1.64	0.215	0.204	Training
258	Poly(p-phenylene ether-sulphone) *c1cc(ccc1)Oc1ccc(cc1)S(=O)=O*	1.65	0.217	0.201	Training
259	Poly(oxycarbonyloxy-1,4-phenylenediphenyl-methylene-1,4-phenylene) *c1(c(cccc1)C(c1ccccc1)c1ccccc1)c1ccc(cc1)OC(=O)O*	1.65	0.219	0.213	Prediction
260	Poly(styrene sulfide) *C(c1ccccc1)CS*	1.66	0.219	0.211	Training
261	Poly(vinyl phenyl sulfide) *S(c1ccccc1)CC*	1.66	0.219	0.214	Training
262	Poly(p-xylene) Cc1ccc(cc1)C	1.67	0.222	0.206	Training
263	Poly(p-xylylene) c1(cccc(c1)Cc1ccccc1)Cc1ccccc1	1.67	0.222	0.214	Prediction

264	Poly(2-vinylnaphthalene) c1c(ccc2ccccc12)CC	1.68	0.226	0.217	Training
265	Poly(vinylnaphthalene) c1(cccc2ccccc12)CC	1.68	0.226	0.217	Training
266	Poly(N-vinyl carbazole) n1(c2ccccc2c2ccccc12)CC	1.68	0.226	0.215	Training
267	Naphthalene-formaldehyde rubber c1c(c2c(cc1)cccc2)CO	1.70	0.229	0.220	Prediction
268	Poly(sulfides) (Thiokol) CCS(=S)S=S	1.65	0.217	0.225	Training
269	Poly(pentabromophenyl methacrylate) C(=O)(C(C)C)Oc1c(c(c(c(c1Br)Br)Br)Br)Br	1.71	0.233	Not Predicted	Not Included