

Results

Spectrum Prediction Input Parameters:

Parent Compound Structure (InChi Format)	InChI=1S/C21H30O2/c1-5-6-7-8-16-12-19(22)21(20(23)13-16)18-11-15(4)9-10-17(18)14(2)3/h11-13,17-18,22-23
Parent Compound Mass	314.22458020122
Spectra Type	ESI
Ion Mode	Positive
Adduct Type	[M+H] ⁺
Probability Threshold	0.001
Status	Completed

Runtime Info: [Show](#) 

Results:

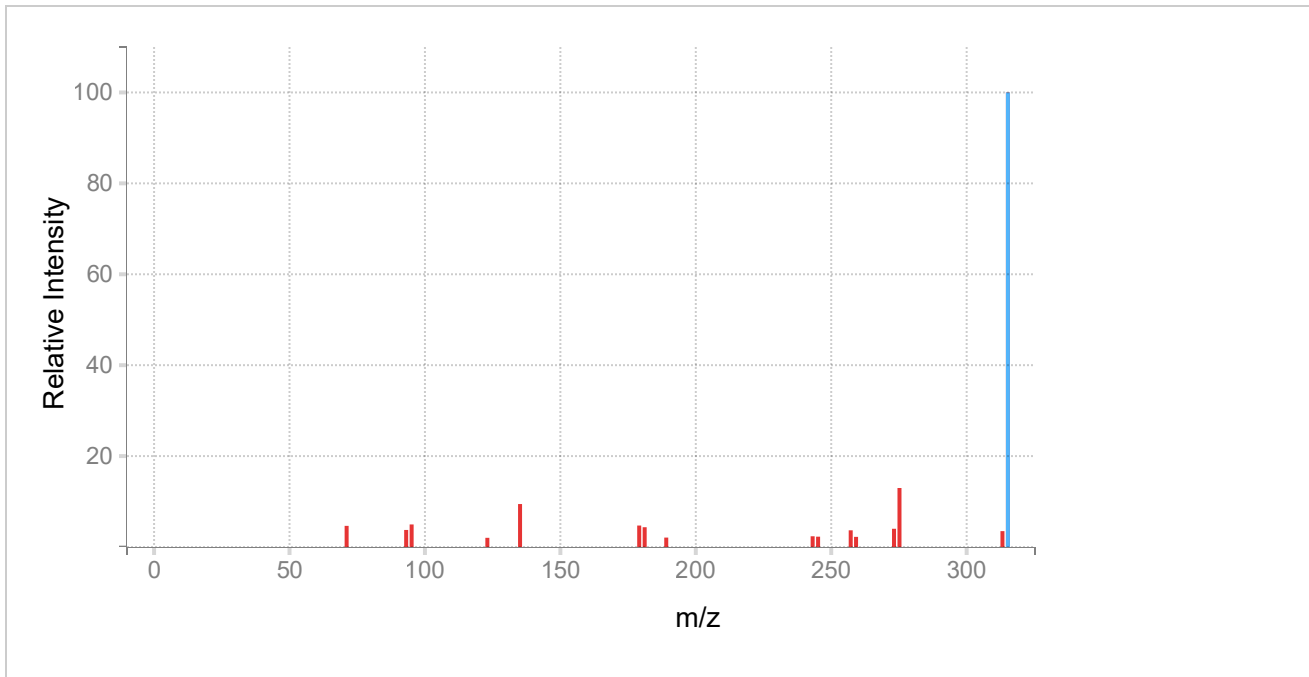
Computed Results

Computed Results:

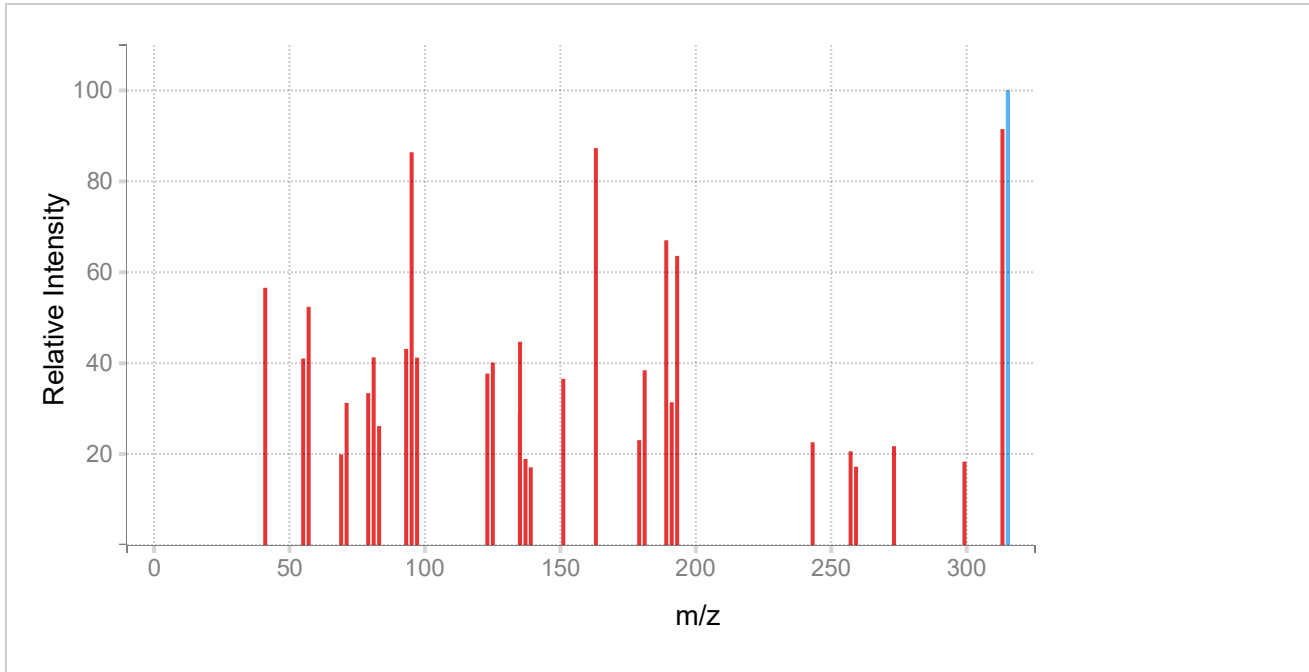
[Download](#)  (/system/predict_queries/output_files/003/050/651/original/output.txt?1714148166)

Predicted spectra are shown below. Peaks for which corresponding fragments have been found are colored red; unassigned peaks are colored blue. Hover over the peaks to see the exact mass and intensity values, along with the highest scoring assigned fragments, if found. Clicking on red spectra lines will show a list of all possible predicted fragments for that peak. A list of all possible matching fragments is shown below the spectra.

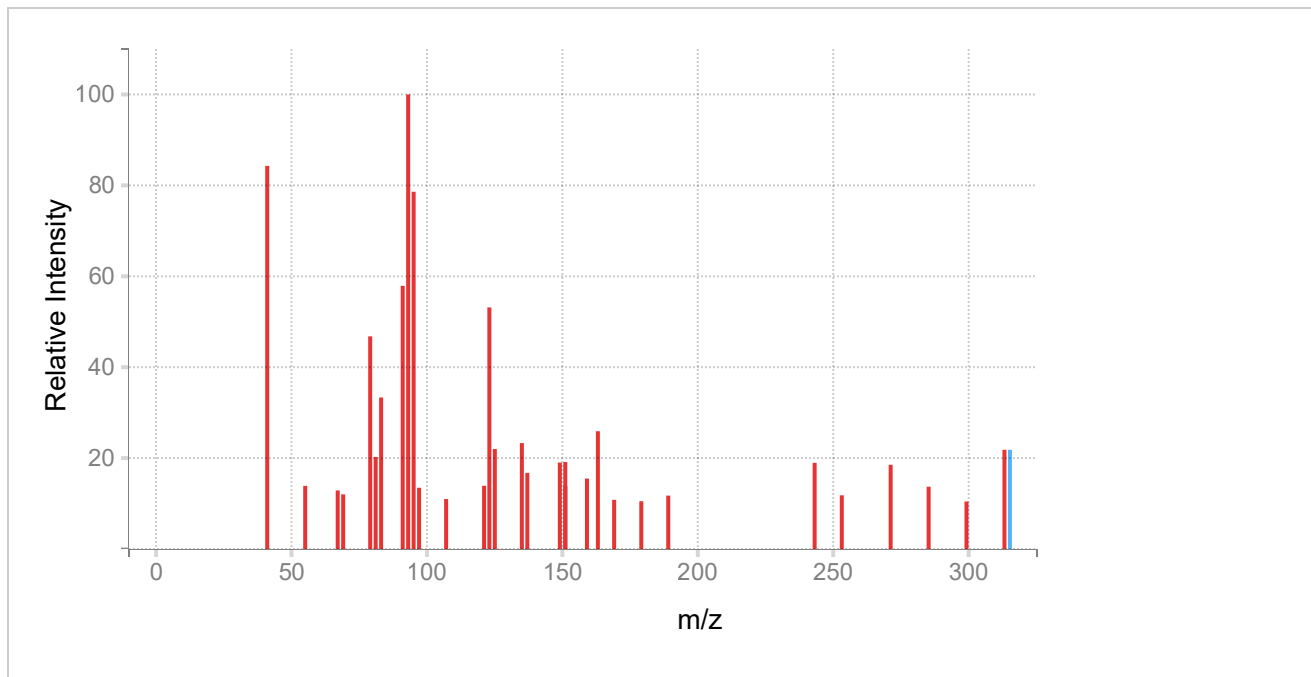
Predicted Low Energy MsMs Spectrum (10V), [M+H]⁺



Predicted Medium Energy MsMs Spectrum (20V), [M+H]⁺



Predicted High Energy MsMs Spectrum (40V), [M+H]⁺



Peak Table and Fragment Structures

Fragment IDs are shown in red. Corresponding scores for each fragment are in blue.

Spectra Peaks and Possible Matching Fragments for InChI=1S/C21H30O2/c1-5-6-7-8-16-12-19(22)21(20(23)13-16)18-11-15(4)9-10-17(18)14(2)3/h11-13,17-18,22-23H,2,5-10H2,1,3-4H3 energy0

71.08553	4.65	21 107	1.9713 0.24552
93.06988	3.75	65 72 156	1.5696 0.2151 0.0070315
95.08553	4.96	4 83 157 159	2.0319 0.33194 0.0043129 0.0005462
123.04406	2.02	28	0.96212
135.11683	9.45	74 76 82 79	2.818 0.74118 0.49672 0.45271
179.10666	4.72	9 44 43	2.0522 0.1403 0.059214
181.12231	4.35	3 38 35	1.9386 0.10732 0.031538
189.09101	2.07	136 165	0.98532 0.00094441
243.13796	2.36	143 113 115	0.82506 0.21874 0.08015
245.15361	2.27	142 116 130	0.53524 0.49712 0.04944
257.18999	3.67	6	1.7517
259.16926	2.23	124 134 176	0.74327 0.27733 0.044382
273.18491	4.01	8 128 181	1.4643 0.44711 0.0043703
275.20056	12.98	2 180	6.1929 0.0028855
313.21621	3.49	173	1.6658
315.23186	100.0	0 133 177 187 174 179 189 178 183 182	39.479 6.4239 1.2757 0.1376 0.134 0.10377 0.071936 0.037557 0.035584 0.023731
315.23185620122	100.0		

energy1

41.03858	56.59	16	3.3349
55.05423	41.02	111 158	2.4006 0.016533
57.06988	52.4	27	3.0879
69.06988	19.92	171 112	0.71612 0.45772
71.08553	31.26	21 107	1.4652 0.37682
79.05423	33.41	69 77	1.3175 0.65117

81.06988	41.28	78 89 93	1.8325 0.59074 0.0092045
83.08553	26.16	91	1.5419
93.06988	43.14	65 72 156	1.7907 0.72555 0.026221
95.08553	86.4	4 83 159 157	3.7384 1.3353 0.013762 0.0043718
97.10118	41.22	5 94	2.2576 0.17122
123.04406	37.71	28	2.2223
125.05971	40.14	29	2.3653
135.04406	29.45	161 40	1.3389 0.39673
135.11683	44.7	74 76 82 79	1.1729 0.63207 0.5126 0.31637
137.13248	18.92	85 88 95 92	0.61887 0.36741 0.094683 0.03422
139.07536	17.09	32	1.0074
151.07536	36.55	33	2.1539
163.11174	87.31	20	5.1452
179.10666	23.06	9 44 43	0.90994 0.38162 0.067375
181.12231	38.44	3 38 35	1.2415 0.96172 0.062087
189.09101	67.03	136 165	3.7856 0.16473
191.10666	31.4	141	1.8503
193.12231	63.6	135 162	3.6664 0.081913
243.13796	22.59	143 113 115	0.81611 0.41825 0.096735
257.15361	20.61	122 175 137 123	0.56624 0.30083 0.21042 0.13704
259.16926	17.22	176 134 124	0.55224 0.25407 0.20866
273.18491	21.74	8 181 128	0.91192 0.22997 0.1394
299.20056	18.32	1 18 132	0.86872 0.14314 0.067988
313.21621	91.5	173	5.3921
315.23186	100.0	0 133 177 187 179 174 183 189 182 178	2.7222 1.739 0.72783 0.18631 0.13793 0.12334 0.09941 0.076565 0.046303 0.03426
315.23185620122	100.0		

energy2

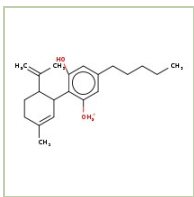
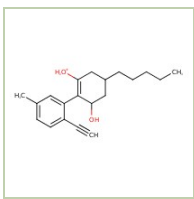
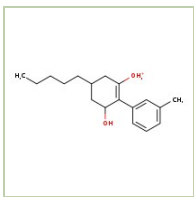
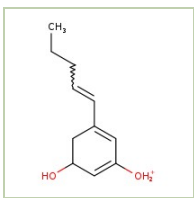
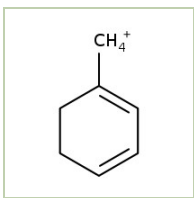
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55.05423	13.88	111 158	1.2036 0.02391
67.05423	12.88	68 155	0.74292 0.39562
69.06988	12.02	112 171	0.97335 0.089585
79.05423	46.78	69 77	2.3196 1.8166
81.06988	20.26	78 93 89	0.98882 0.54124 0.26142
83.08553	33.33	91	2.947
91.05423	57.9	62 80	4.4642 0.65543
93.06988	100.0	65 72 156	6.1905 2.33 0.32169
95.08553	78.59	4 83 157 159	3.3636 3.2003 0.24898 0.1364
97.10118	13.47	94 5	0.80127 0.38976
107.08553	10.99	70	0.97179
121.10118	13.91	86 87 168	0.82584 0.22805 0.17633
123.04406	53.14	28	4.6983
125.05971	22.0	29	1.9455
135.04406	23.3	161 40	1.305 0.75528
137.05971	16.75	31 163	0.98126 0.49974
149.05971	19.02	41 151	1.2631 0.41867
151.07536	19.14	33	1.6921
151.11174	13.86	36	1.2258
159.08044	15.5	46	1.3701

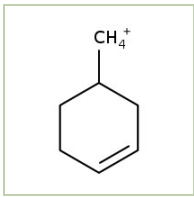
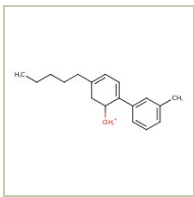
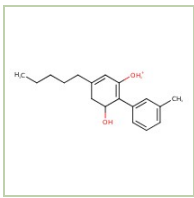
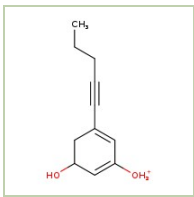
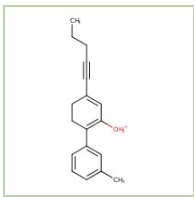
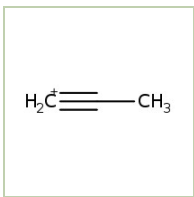
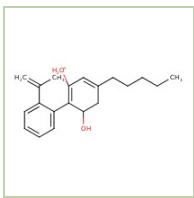
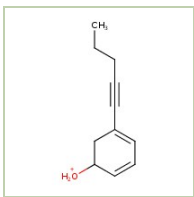
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169.12231	10.82	190	0.95653
179.14304	10.51	185	0.92972
189.09101	11.74	165 136	0.52249 0.516
243.13796	18.95	143 115 113	0.87099 0.67118 0.13358
253.15869	11.81	14	1.0447
271.20564	18.53	188	1.6384
285.22129	13.7	197	1.2109
299.20056	10.44	1 18 132	0.64971 0.13919 0.13411
313.21621	21.82	173	1.9296
315.23185620122	21.82		

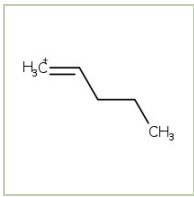
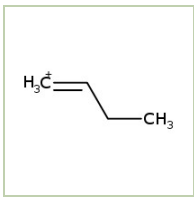
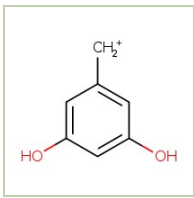
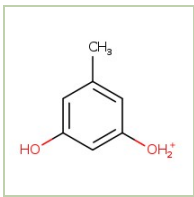
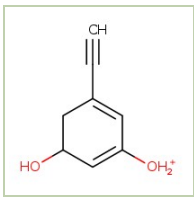
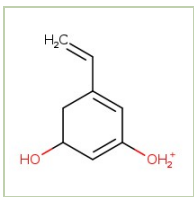
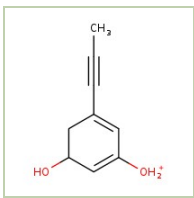
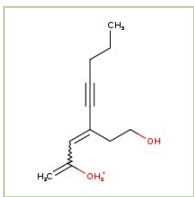
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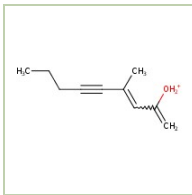
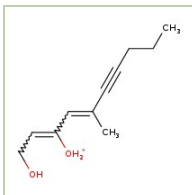
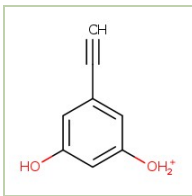
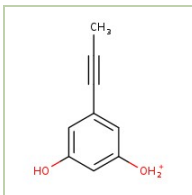
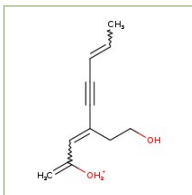
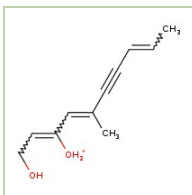
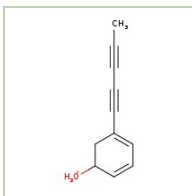
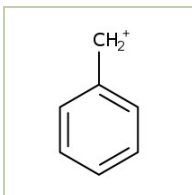
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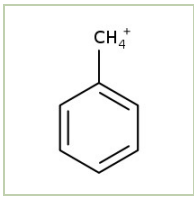
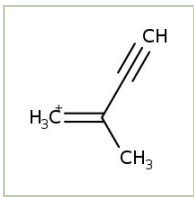
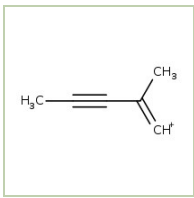
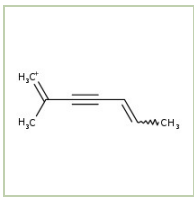
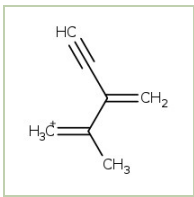
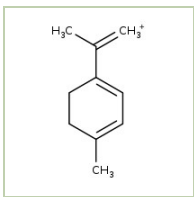
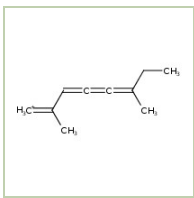
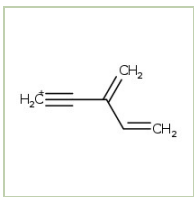
Fragments Generated

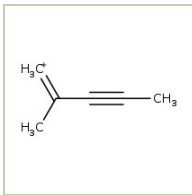
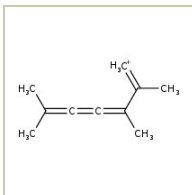
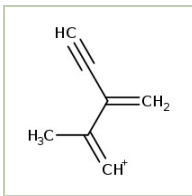
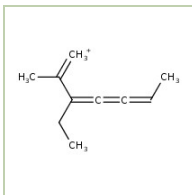
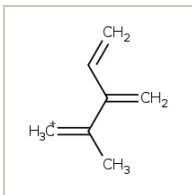
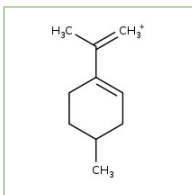
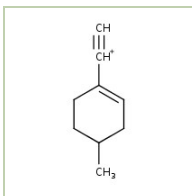
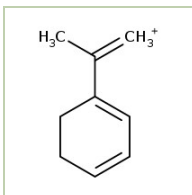
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	1	299.2005565241	<chem>C#CC1=CC=C(C)C=C1C1=C([OH2+])CC(CCCCC)CC1O</chem>
	2	275.2005565241	<chem>CCCCC1CC([OH2+])=C(C2=CC(C)=CC=C2)C(O)C1</chem>
	3	181.1223062041	<chem>CCCC=CC1=CC([OH2+])=CC(O)C1</chem>
	4	95.0855267721	<chem>[CH4+]C1=CC=CCC1</chem>

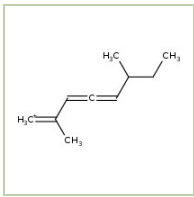
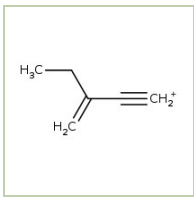
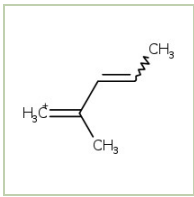
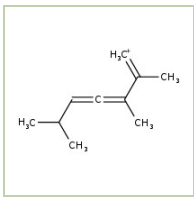
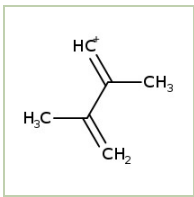
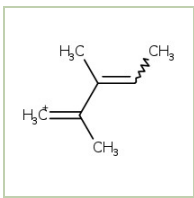
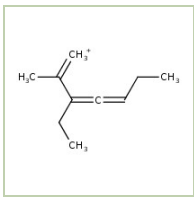
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	6	257.1899918401	CCCCC1=CC=C(C2=CC(C)=CC=C2)C([OH2+])C1
	8	273.1849064601	CCCCC1=CC([OH2+])=C(C2=CC(C)=CC=C2)C(O)C1
	9	179.1066561401	CCCC#CC1=CC([OH2+])=CC(O)C1
	14	253.1586917121	CCCC#CC1=CC([OH2+])=C(C2=CC(C)=CC=C2)CC1
	16	41.0385765801	[CH2+]#CC
	18	299.2005565241	C=C(C)C1=CC=CC=C1C1=C([OH2+])C=C(CCCCC)CC1O
	20	163.1117415201	CCCC#CC1=CC=CC([OH2+])C1

	21	71.0855267721	CCCC=[CH3+]
	27	57.0698767081	CCC=[CH3+]
	28	123.0440558841	[CH2+]C1=CC(O)=CC(O)=C1
	29	125.0597059481	CC1=CC([OH2+])=CC(O)=C1
	31	137.0597059481	C#CC1=CC([OH2+])=CC(O)=C1
	32	139.0753560121	C=CC1=CC([OH2+])=CC(O)=C1
	33	151.0753560121	CC#CC1=CC([OH2+])=CC(O)=C1
	35	181.1223062041	C=C([OH2+])C=C(C#CCCC)CCO

	36	151.1117415201	<chem>C=C([OH2+])C=C(C)C#CCCC</chem>
	38	181.1223062041	<chem>CCCC#CC(C)=CC([OH2+])=CCO</chem>
	40	135.0440558841	<chem>C#CC1=CC([OH2+])=CC(O)=C1</chem>
	41	149.0597059481	<chem>CC#CC1=CC([OH2+])=CC(O)=C1</chem>
	43	179.1066561401	<chem>C=C([OH2+])C=C(C#CC=CC)CCO</chem>
	44	179.1066561401	<chem>CC=CC#CC(C)=CC([OH2+])=CCO</chem>
	46	159.0804413921	<chem>CC#CC#CC1=CC=CC([OH2+])C1</chem>
	62	91.0542266441	<chem>[CH2+]C1=CC=CC=C1</chem>

	65	93.0698767081	[CH4+]C1=CC=CC=C1
	68	67.0542266441	C#CC(C)=[CH3+]
	69	79.0542266441	[CH+]=C(C)C#CC
	70	107.0855267721	CC=CC#CC(C)=[CH3+]
	72	93.0698767081	C#CC(=C)C(C)=[CH3+]
	74	135.1168269001	CC(=[CH3+])C1=CC=C(C)CC1
	76	135.1168269001	CCC(C)=C=C=CC(C)=[CH3+]
	77	79.0542266441	C=CC(=C)C#[CH2+]

	78	81.0698767081	<chem>CC#CC(C)=[CH3+]</chem>
	79	135.1168269001	<chem>CC(=[CH3+])C(C)=C=C(C)C</chem>
	80	91.0542266441	<chem>C#CC(=C)C(=[CH+])C</chem>
	82	135.1168269001	<chem>CC=C=C=C(CC)C(C)=[CH3+]</chem>
	83	95.0855267721	<chem>C=CC(=C)C(C)=[CH3+]</chem>
	85	137.1324769641	<chem>CC(=[CH3+])C1=CCC(C)CC1</chem>
	86	121.1011768361	<chem>C#[CH+]C1=CCC(C)CC1</chem>
	87	121.1011768361	<chem>CC(=[CH3+])C1=CC=CCC1</chem>

	88	137.1324769641	<chem>CCC(C)C=C=CC(C)=[CH3+]</chem>
	89	81.0698767081	<chem>C=C(C#[CH2+])CC</chem>
	91	83.0855267721	<chem>CC=CC(C)=[CH3+]</chem>
	92	137.1324769641	<chem>CC(=[CH3+])C(C)=C=CC(C)C</chem>
	93	81.0698767081	<chem>[CH+]=C(C)C(=C)C</chem>
	94	97.1011768361	<chem>CC=C(C)C(C)=[CH3+]</chem>
	95	137.1324769641	<chem>CCC=C=C(CC)C(C)=[CH3+]</chem>