

Results

Spectrum Prediction Input Parameters:

Parent Compound Structure (InChi Format)	InChi=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5-6H3
Parent Compound Mass	204.18780076968
Spectra Type	ESI
Ion Mode	Positive
Adduct Type	[M+H] ⁺
Probability Threshold	0.001
Status	Completed

Results:

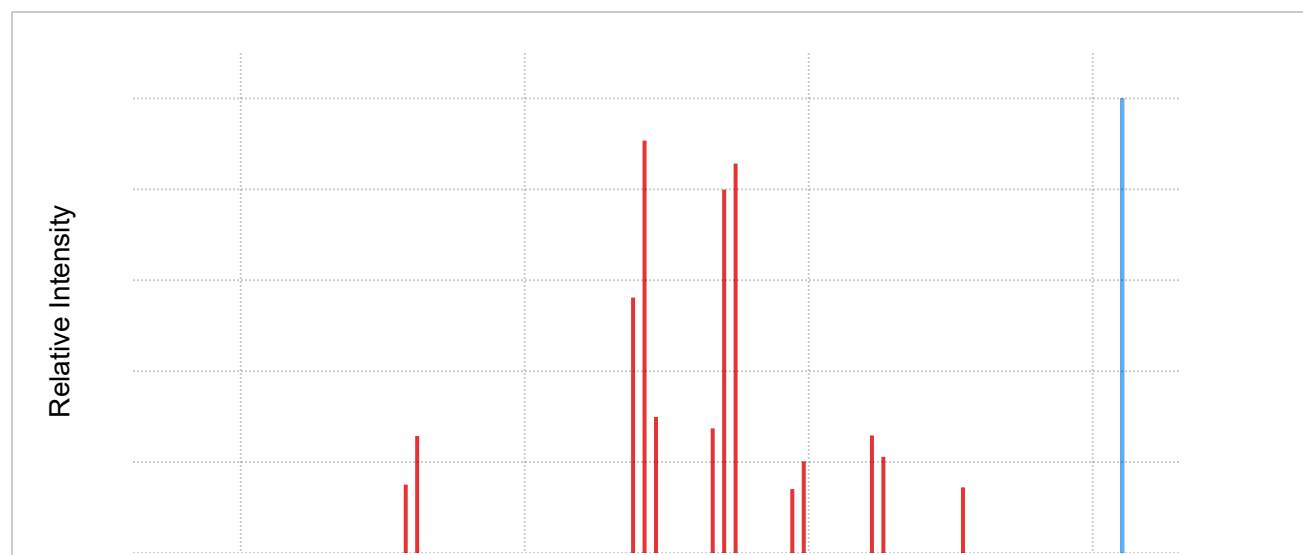
Computed Results

Computed Results:

Download [📄 \(/system/predict_queries/output_files/003/053/143/original/output.txt?1714836488\)](/system/predict_queries/output_files/003/053/143/original/output.txt?1714836488)

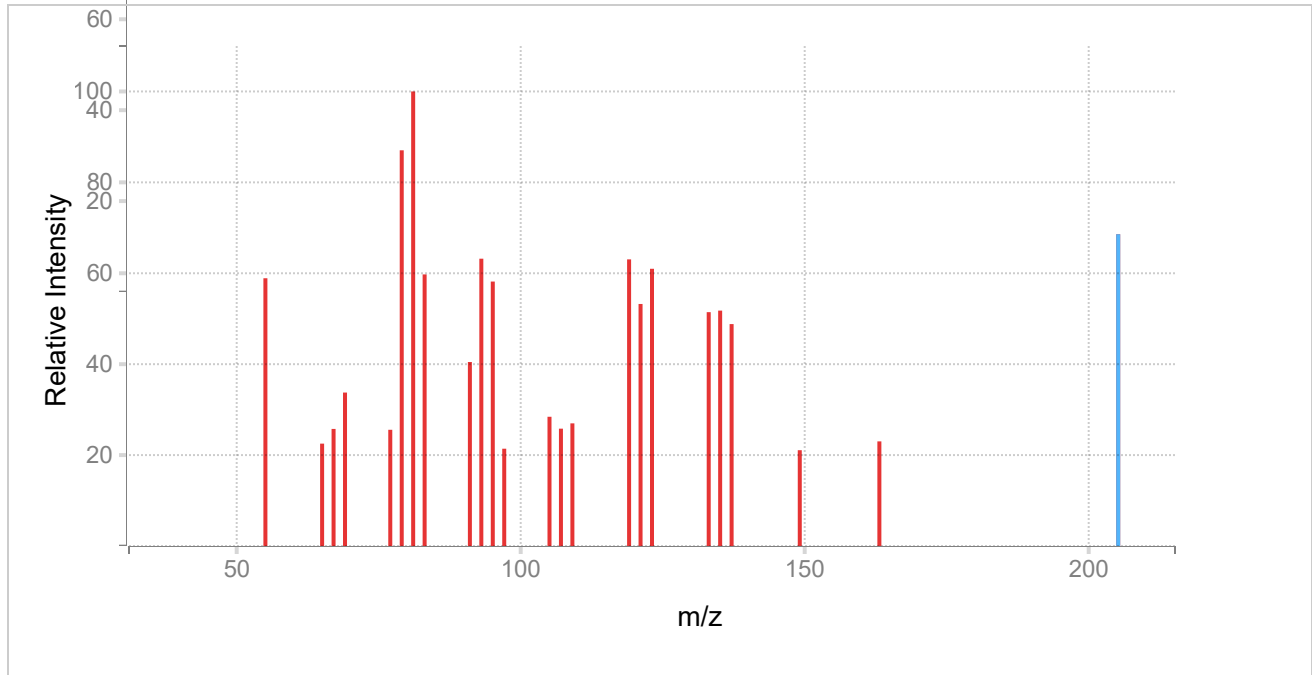
Predicted spectra are shown below. Peaks for which corresponding fragments have been found are colored red; unassigned peaks are colored blue. Hover over the peaks to see the exact mass and intensity values, along with the highest scoring assigned fragments, if found. Clicking on red spectra lines will 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]⁺

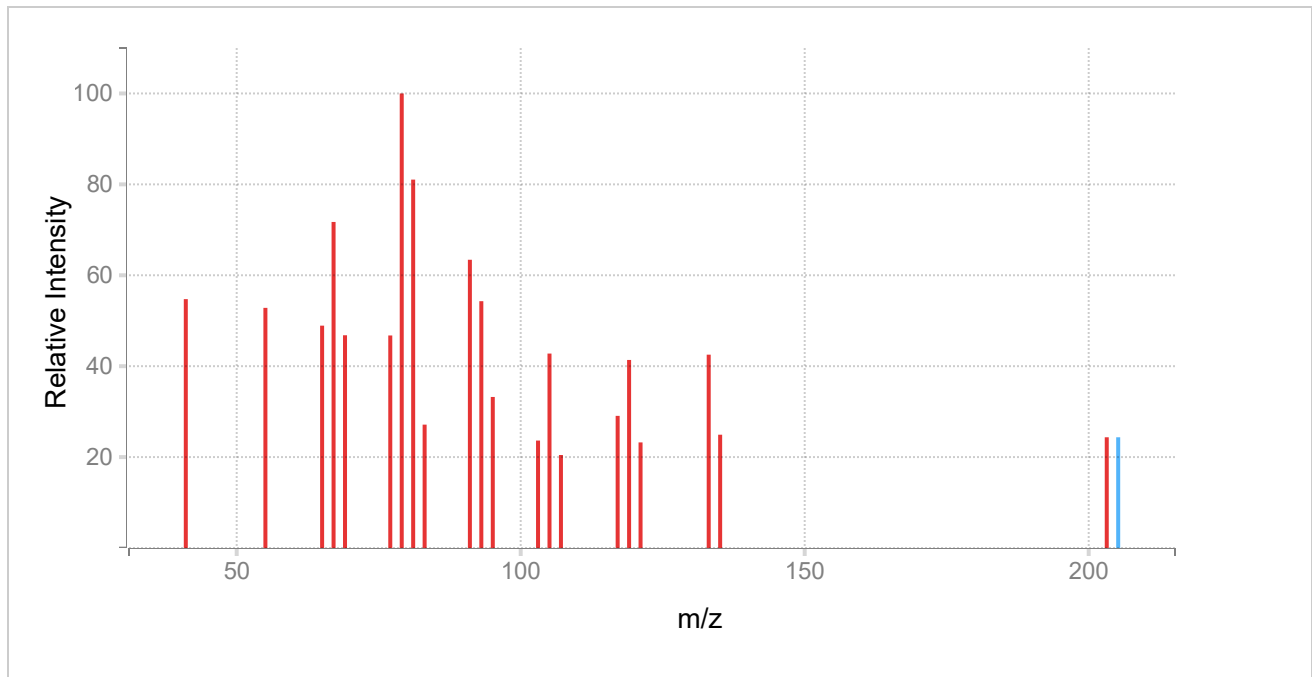




Predicted Medium Energy MsMs Spectrum (20V), [M+H]⁺



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/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5-6H3

energy0

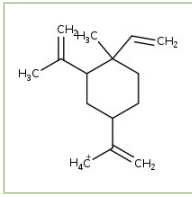
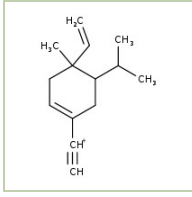
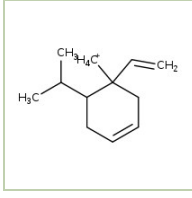
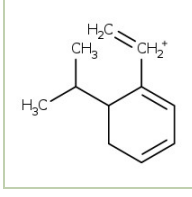
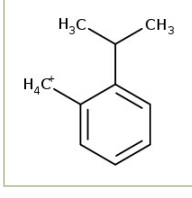
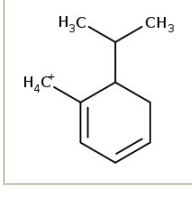
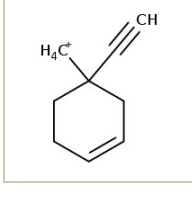
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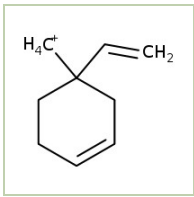
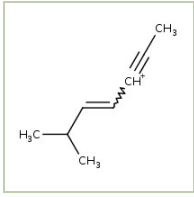
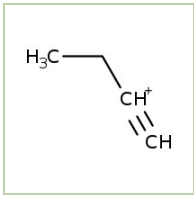
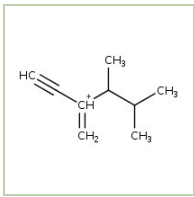
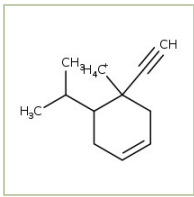
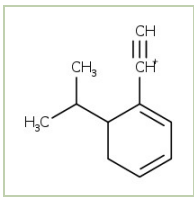
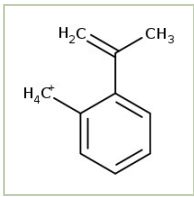
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121.1011768	12.04464685	6 59 181 64 195	10.54 0.88515 0.39514 0.21696 0.0076462
123.1168269	3.970957836	7 100 13 179 83	2.5823 0.92575 0.311 0.14283 0.0090674
133.1011768	3.639203767	45 16 91 118 72 133 137	1.4523 1.0304 0.42234 0.39337 0.28545 0.04533 0.010054
135.1168269	10.60924477	46 4 108 57 175 141	6.3276 2.8321 0.72661 0.32035 0.20582 0.19679
137.132477	11.37096475	61 5 117 71 174 140	5.4933 4.3102 0.83754 0.61367 0.06033 0.055909
147.1168269	1.8668166	88 211 138 191 40 15	1.1321 0.48034 0.11299 0.082697 0.03662 0.02206
149.132477	2.675975616	89 126 197 212 41 3	1.0002 0.45389 0.40063 0.39054 0.37156 0.059179
161.132477	3.430900356	102 28 110 104 109 62 33 32 34	3.0295 0.15856 0.15138 0.079177 0.0076538 0.0032684 0.0009963 0.00028188 8.9151e-05
163.148127	2.808165425	111 14 112 114 113 26 39 23 19 25 27	1.1945 1.0707 0.23412 0.15568 0.055516 0.05493 0.024033 0.012186 0.0034617 0.0018786 0.0011726
177.1637771	1.916337639	60 77 68 67 69 63 70	1.4994 0.17889 0.15597 0.045158 0.021418 0.012113 0.0033994
205.1950772	13.27372009	0 200 125 172 214 216 215	9.3338 1.451 0.57864 0.54306 0.52032 0.45536 0.39152
205.19507676967999	13.27372009		
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67.05422664	1.855349873	93 158	1.8113 0.044046
69.06987671	2.431796001	66	2.4318
77.03857658	1.841825815	130	1.8418
79.05422664	6.271163056	106 131	3.9544 2.3167
81.06987671	7.203892063	53 105 73 182	4.0548 2.4193 0.68697 0.042783
83.08552677	4.304126396	107 132 184	2.4019 1.1978 0.70451
91.05422664	2.915951453	54 163 207 142	2.0912 0.5688 0.14996 0.106
93.06987671	4.553226059	50 24 187 143	3.4922 0.67088 0.33321 0.056914
95.08552677	4.190967246	82 74 209 167 144	3.1695 0.64214 0.18865 0.14937 0.041334
97.10117684	1.541763198	65 94	1.3687 0.17311
105.0698767	2.048160194	165 20 183 21 134	1.0397 0.77901 0.095971 0.077867 0.055612
107.0855268	1.859449916	176 51 75 115 22 135 152	0.6605 0.49661 0.38273 0.19751 0.090004 0.017942 0.014158
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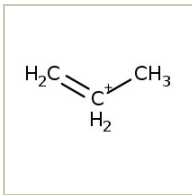
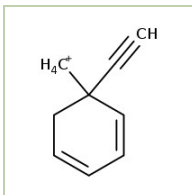
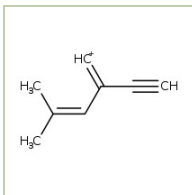
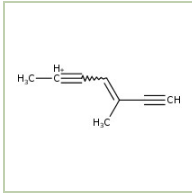
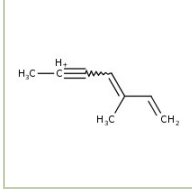
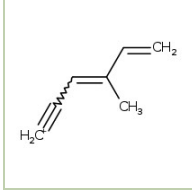
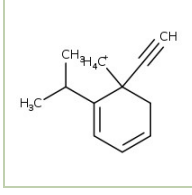
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205.1950772	4.940985652	0 125 216 172 200 214 215	1.6326 0.92802 0.7457 0.48506 0.47668 0.34817 0.32472
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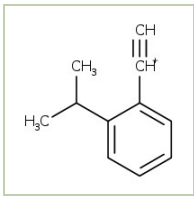
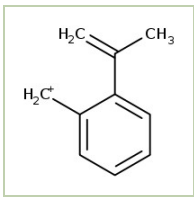
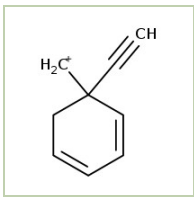
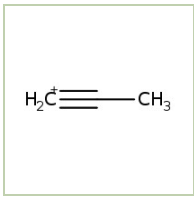
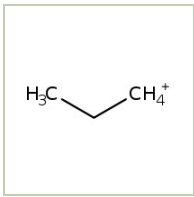
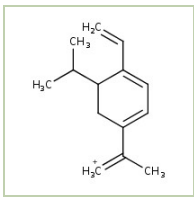
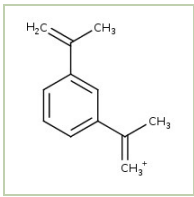
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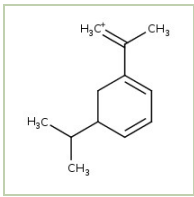
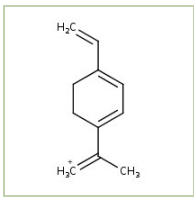
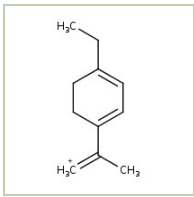
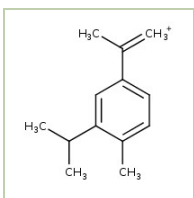
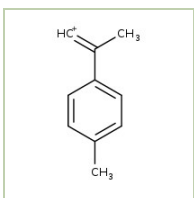
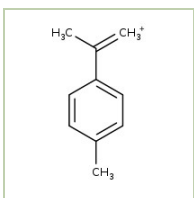
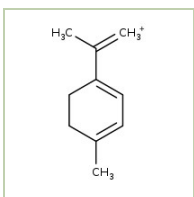
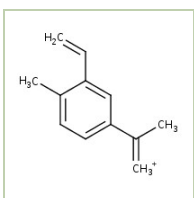
Fragments Generated

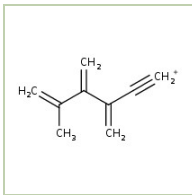
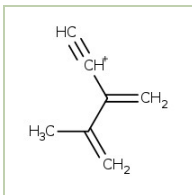
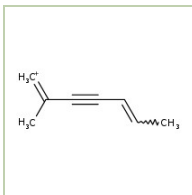
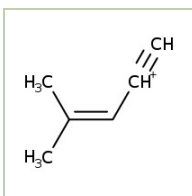
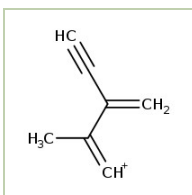
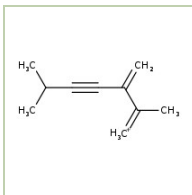
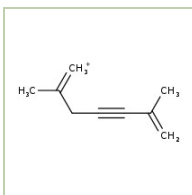
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	2	165.1637771	<chem>C=CC1([CH4+])CC=CCC1C(C)C</chem>
	3	149.132477	<chem>C=[CH2+]C1=CC=CCC1C(C)C</chem>
	4	135.1168269	<chem>CC(C)C1=CC=CC=C1[CH4+]</chem>
	5	137.132477	<chem>CC(C)C1CC=CC=C1[CH4+]</chem>
	6	121.1011768	<chem>C#CC1([CH4+])CC=CCC1</chem>

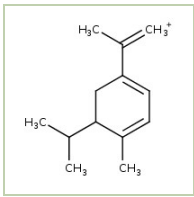
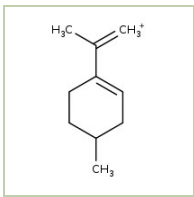
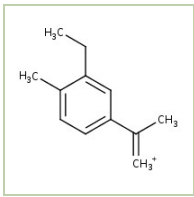
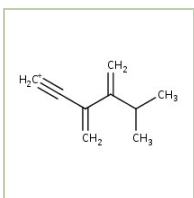
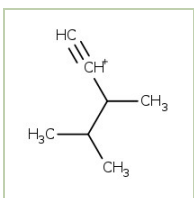
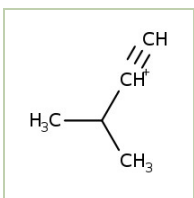
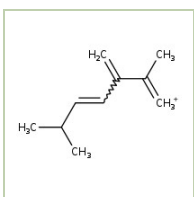
	7	123.1168269	<chem>C=CC1([CH4+])CC=CCC1</chem>
No Image	8	165.1637771	<chem>C=CC([CH4+])(C=C=CC)CC(C)C</chem>
No Image	9	165.1637771	<chem>CCC([CH4+])=C=C=CCCC(C)C</chem>
	10	109.1011768	<chem>CC#[CH+]C=CC(C)C</chem>
No Image	11	165.1637771	<chem>C=C=CCC(C(=[CH3+])CC)C(C)C</chem>
	12	55.05422664	<chem>C#[CH+]CC</chem>
	13	123.1168269	<chem>C#C[CH+](=C)C(C)C(C)C</chem>
	14	163.148127	<chem>C#CC1([CH4+])CC=CCC1C(C)C</chem>
	15	147.1168269	<chem>C#[CH+]C1=CC=CCC1C(C)C</chem>
	16	133.1011768	<chem>C=C(C)C1=CC=CC=C1[CH4+]</chem>

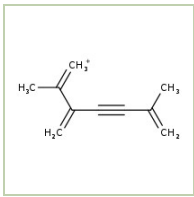
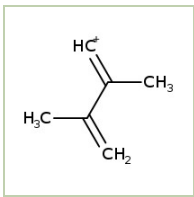
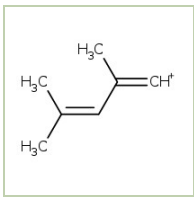
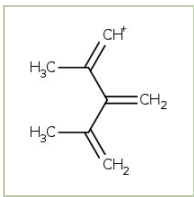
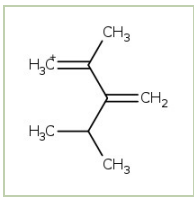
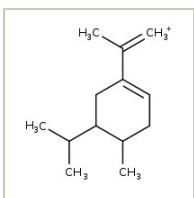
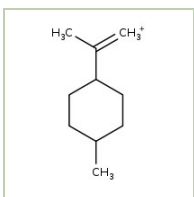
	17	43.05422664	C=[CH2+]C
	18	119.0855268	C#CC1([CH4+])C=CC=CC1
No Image	19	163.148127	C#CC([CH4+])(C=C=CC)CC(C)C
	20	105.0698767	C#CC(=[CH+])C=C(C)C
	21	105.0698767	C#CC(C)=CC#[CH+]C
	22	107.0855268	C=CC(C)=CC#[CH+]C
No Image	23	163.148127	C=CC([CH4+])=C=C=CCCC(C)C
	24	93.06987671	C=CC(C)=CC#[CH2+]
No Image	25	163.148127	C=C=CCC(C(=[CH3+])C=C)C(C)C
No Image	26	163.148127	C#CC(C)([CH4+])C(=CC=C)C(C)C
No Image	27	163.148127	C#CC([CH4+])(C=C)C(=CC)C(C)C
	28	161.132477	C#CC1([CH4+])CC=CC=C1C(C)C

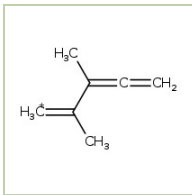
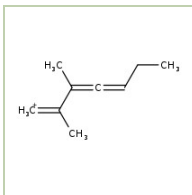
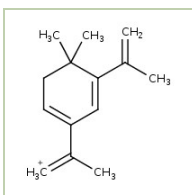
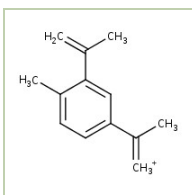
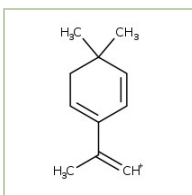
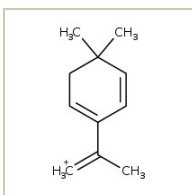
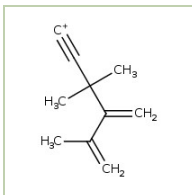
	29	145.1011768	<chem>C#[CH+]C1=CC=CC=C1C(C)C</chem>
	30	131.0855268	<chem>C=C(C)C1=CC=CC=C1[CH2+]</chem>
	31	117.0698767	<chem>C#CC1([CH2+])C=CC=CC1</chem>
No Image	32	161.132477	<chem>C#CC([CH4+])(C=C=CC)C=C(C)C</chem>
No Image	33	161.132477	<chem>C#CC([CH4+])=C=C=CCCC(C)C</chem>
No Image	34	161.132477	<chem>C#CC([CH4+])(C=C)C(=CC)C(=C)C</chem>
	35	41.03857658	<chem>[CH2+]#CC</chem>
	36	45.06987671	<chem>CC[CH4+]</chem>
	37	189.1637771	<chem>C=CC1=CC=C(C(C)=[CH3+])CC1C(C)C</chem>
	38	159.1168269	<chem>C=C(C)C1=CC(C(C)=[CH3+])=CC=C1</chem>

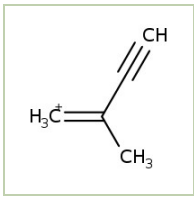
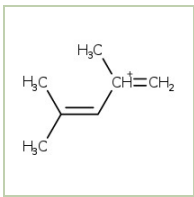
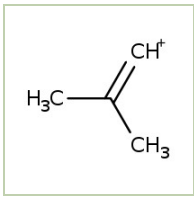
	39	163.148127	<chem>CC(=[CH3+])C1=CC=CC(C(C)C)C1</chem>
	40	147.1168269	<chem>C=CC1=CC=C(C(C)=[CH3+])CC1</chem>
	41	149.132477	<chem>CCC1=CC=C(C(C)=[CH3+])CC1</chem>
No Image	42	189.1637771	<chem>C=CC(=C=C=CC(C)=[CH3+])C(C)C(C)C</chem>
	43	175.148127	<chem>CC(=[CH3+])C1=CC=C(C(C)C(C)C)=C1</chem>
	44	131.0855268	<chem>[CH+]=C(C)C1=CC=C(C)C=C1</chem>
	45	133.1011768	<chem>CC(=[CH3+])C1=CC=C(C)C=C1</chem>
	46	135.1168269	<chem>CC(=[CH3+])C1=CC=C(C)CC1</chem>
	47	159.1168269	<chem>C=CC1=CC(C(C)=[CH3+])=CC=C1C</chem>
No Image	48	175.148127	<chem>C=C(C(C)=C=C=CC(C)=[CH3+])C(C)C</chem>

	49	119.0855268	<chem>C=C(C)C(=C)C(=C)C#[CH2+]</chem>
	50	93.06987671	<chem>C#[CH+]C(=C)C(=C)C</chem>
	51	107.0855268	<chem>CC=CC#CC(C)=[CH3+]</chem>
No Image	52	175.148127	<chem>CC(=[CH3+])C(C)=C=C=C(C)C=C(C)C</chem>
	53	81.06987671	<chem>C#[CH+]C=C(C)C</chem>
	54	91.05422664	<chem>C#CC(=C)C(=[CH+])C</chem>
No Image	55	175.148127	<chem>C=C=C=C=C(CCC(C)C)C(C)=[CH3+]</chem>
No Image	56	175.148127	<chem>C=C(C)C(=CC(=C)C(C)=[CH3+])C(=C)C</chem>
	57	135.1168269	<chem>C=C(C#CC(C)C)C(C)=[CH3+]</chem>
No Image	58	175.148127	<chem>C=C=C(C)C(=CCC(C)=[CH3+])C(=C)C</chem>
	59	121.1011768	<chem>C=C(C)C#CCC(C)=[CH3+]</chem>

	60	177.1637771	<chem>CC(=[CH3+])C1=CC=C(C)C(C(C)C)C1</chem>
	61	137.132477	<chem>CC(=[CH3+])C1=CCC(C)CC1</chem>
	62	161.132477	<chem>CCC1=CC(C(C)=[CH3+])=CC=C1C</chem>
No Image	63	177.1637771	<chem>CC(=[CH3+])C=C=C=C(C)C(C)C(C)C</chem>
	64	121.1011768	<chem>C=C(C#[CH2+])C(=C)C(C)C</chem>
	65	97.10117684	<chem>C#[CH+]C(C)C(C)C</chem>
	66	69.06987671	<chem>C#[CH+]C(C)C</chem>
No Image	67	177.1637771	<chem>CC(=[CH3+])C(C)=C=C=C(C)CC(C)C</chem>
No Image	68	177.1637771	<chem>CC=C=C=C(CCC(C)C)C(C)=[CH3+]</chem>
No Image	69	177.1637771	<chem>C=C=C(CC(C=C)C(C)C)C(C)=[CH3+]</chem>
No Image	70	177.1637771	<chem>C=C(C)C(=CC(=C)C(C)=[CH3+])C(C)C</chem>
	71	137.132477	<chem>C=C(C=CC(C)C)C(C)=[CH3+]</chem>

	72	133.1011768	<chem>C=C(C)C#CC(=C)C(C)=[CH3+]</chem>
	73	81.06987671	<chem>[CH+]=C(C)C(=C)C</chem>
	74	95.08552677	<chem>[CH+]=C(C)C=C(C)C</chem>
	75	107.0855268	<chem>[CH+]=C(C)C(=C)C(=C)C</chem>
	76	111.1168269	<chem>C=C(C(C)=[CH3+])C(C)C</chem>
No Image	77	177.1637771	<chem>C=C=C(C)C(=CCC(C)=[CH3+])C(C)C</chem>
	78	179.1794272	<chem>CC(=[CH3+])C1=CCC(C)C(C)C1</chem>
	79	139.148127	<chem>CC(=[CH3+])C1CCC(C)CC1</chem>
No Image	80	179.1794272	<chem>CC(=[CH3+])C=C=CC(C)C(C)C(C)C</chem>
No Image	81	179.1794272	<chem>CC(=[CH3+])C(C)=C=CC(C)CC(C)C</chem>

	82	95.08552677	<chem>C=C=C(C)C(C)=[CH3+]</chem>
	83	123.1168269	<chem>CCC=C=C(C)C(C)=[CH3+]</chem>
No Image	84	179.1794272	<chem>CCC=C=C(CCC(C)C)C(C)=[CH3+]</chem>
No Image	85	179.1794272	<chem>C=C=C(C)C(CCC(C)=[CH3+])C(C)C</chem>
	86	189.1637771	<chem>C=C(C)C1=CC(C(C)=[CH3+])=CCC1(C)C</chem>
	87	173.132477	<chem>C=C(C)C1=CC(C(C)=[CH3+])=CC=C1C</chem>
	88	147.1168269	<chem>[CH+]=C(C)C1=CCC(C)(C)C=C1</chem>
	89	149.132477	<chem>CC(=[CH3+])C1=CCC(C)(C)C=C1</chem>
No Image	90	189.1637771	<chem>C=C(C)C(=C)C(C)(C)C=C=CC(C)=[CH3+]</chem>
	91	133.1011768	<chem>[C+]#CC(C)(C)C(=C)C(=C)C</chem>
No Image	92	189.1637771	<chem>[CH+]=C(C)C(C)=C=CC(C)(C)C=C(C)C</chem>

	93	67.05422664	C#CC(C)=[CH3+]
	94	97.10117684	C=[CH+](C)C=C(C)C
No Image	95	189.1637771	CC(=[CH3+])C(=C=C=C(C)C)C=CC(C)C
No Image	96	189.1637771	C=C=C(C=C(C(=C)C)C(C)C)C(C)=[CH3+]
No Image	97	189.1637771	[CH+]=C(C)C(=C)C=C(C(=C)C)C(C)(C)C
	98	55.05422664	[CH+]=C(C)C
No Image	99	189.1637771	C=CC(C)(C)C(=C=CC(C)=[CH3+])C(=C)C

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