

# Results

## Spectrum Prediction Input Parameters:

<b>Parent Compound Structure</b> (InChi Format)	InChi=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3/t10-/m0/s1
<b>Parent Compound Mass</b>	136.12520051312
<b>Spectra Type</b>	ESI
<b>Ion Mode</b>	Positive
<b>Adduct Type</b>	[M+H] <sup>+</sup>
<b>Probability Threshold</b>	0.001
<b>Status</b>	<b>Completed</b>

## Results:

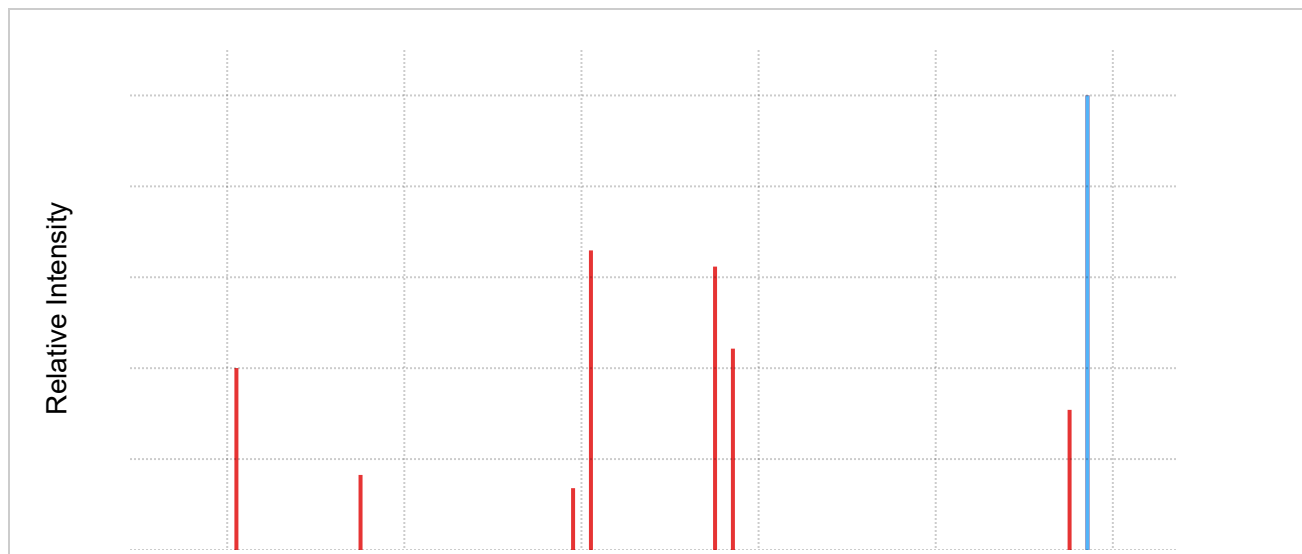
Computed Results

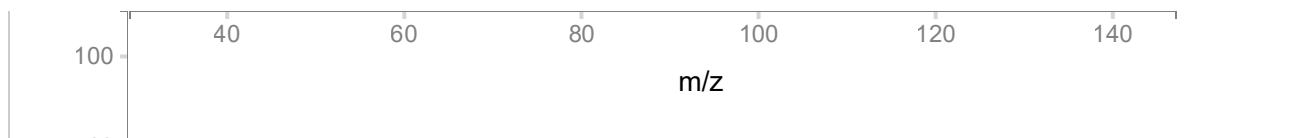
## Computed Results:

Download [📄 \(/system/predict\\_queries/output\\_files/003/053/718/original/output.txt?1715038421\)](/system/predict_queries/output_files/003/053/718/original/output.txt?1715038421)

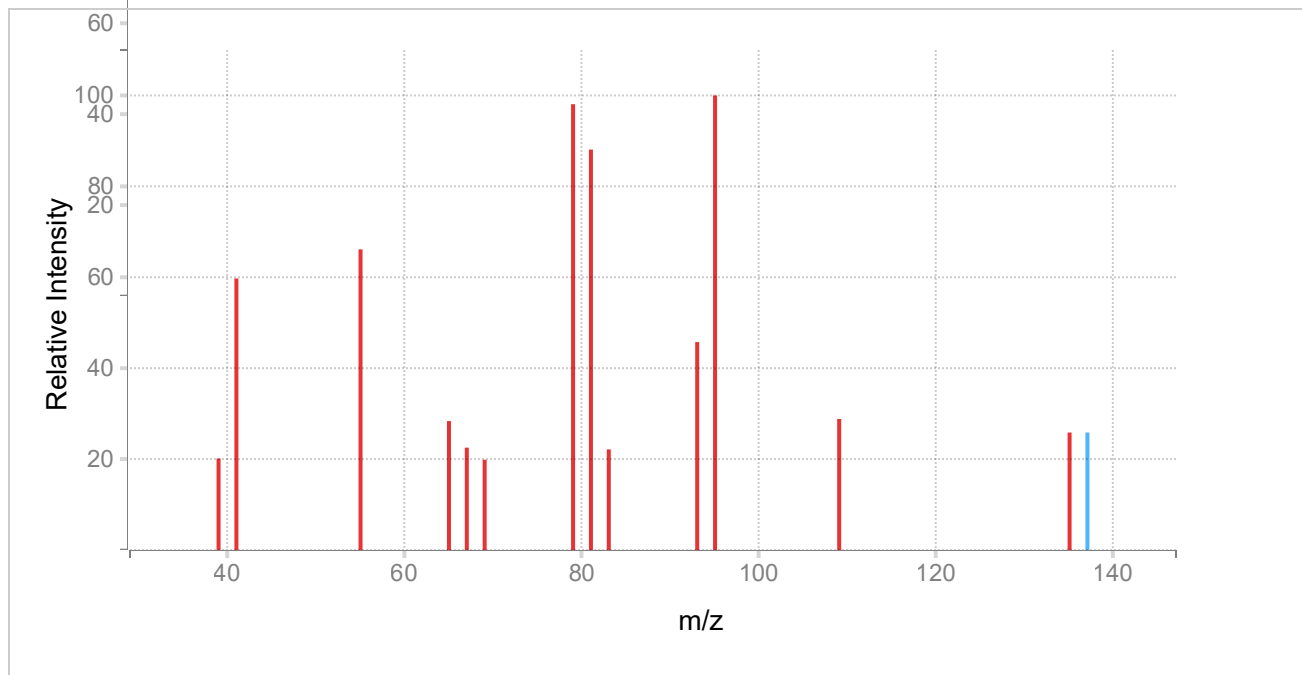
Predicted spectra are shown below. Peaks for which corresponding fragments have been found are colored red; unassigned peaks are colored blue. Hover over the peaks to see the exact mass and intensity values, along with the highest scoring assigned fragments, if found. Clicking on red spectra lines will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

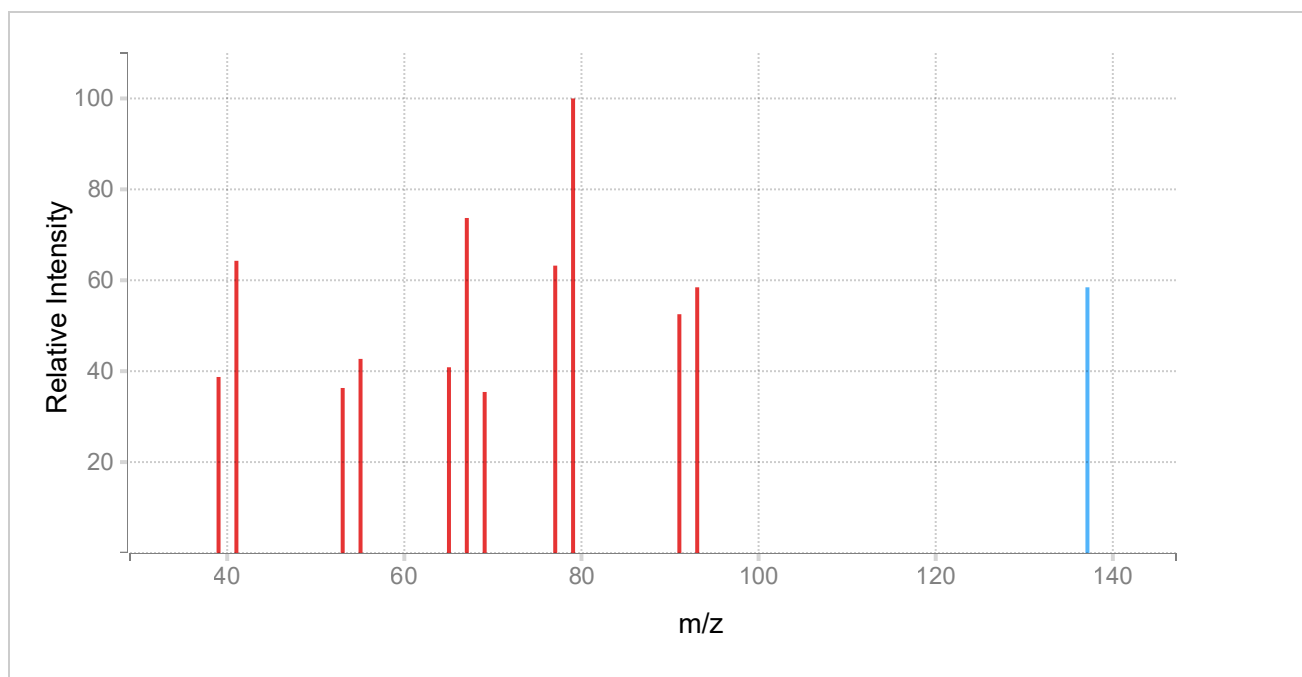




Predicted Medium Energy MsMs Spectrum (20V), [M+H]<sup>+</sup>



Predicted High Energy MsMs Spectrum (40V), [M+H]<sup>+</sup>



### 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/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3/t10-/m0/s1 energy0**

41.03857658      8.717875198    20      8.7179

55.05422664	3.596969418	9 19	2.6539 0.94305
79.05422664	2.96266908	42 5 16 21	1.2046 0.88934 0.80192 0.066805
81.06987671	14.35427144	43 39 54 7	4.7112 3.5466 3.1244 2.972
95.08552677	13.57879819	10 12 57 15	9.5952 1.9681 1.4369 0.57866
97.10117684	9.64747205	6 58 8 11 13	6.4734 1.3196 0.82286 0.5237 0.50784
135.1168269	6.714960013	52 67 61	6.6427 0.04505 0.027188
137.132477	21.77948823	0 38 53 62	15.186 3.1883 2.1117 1.2937
137.13247651312	21.77948823		

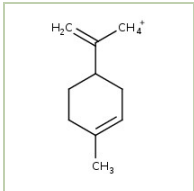
**energy1**

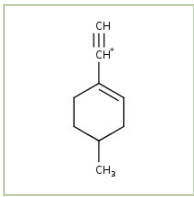
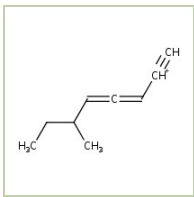
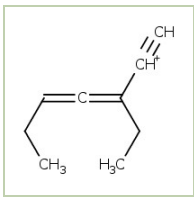
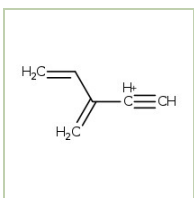
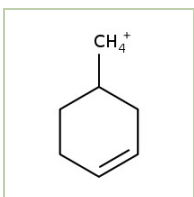
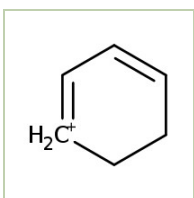
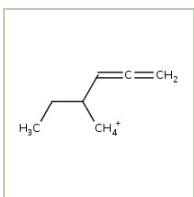
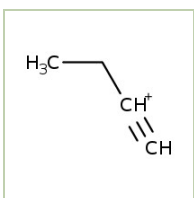
39.02292652	2.645223232	23	2.6452
41.03857658	7.848408383	20	7.8484
55.05422664	8.690363915	9 19	6.3865 2.3039
65.03857658	3.727650382	26 29	2.9147 0.81296
67.05422664	2.958243035	25 18	1.7396 1.2186
69.06987671	2.61004147	17 14	1.7624 0.84763
79.05422664	12.88613571	42 5 16 21	7.2933 4.0624 1.3287 0.20166
81.06987671	11.57478061	43 39 7 54	6.9643 3.6309 0.79971 0.17989
83.08552677	2.908379478	44	2.9084
93.06987671	6.010080093	22 31 27 55	3.6664 0.98423 0.87581 0.48365
95.08552677	13.13881053	10 57 12 15	7.9254 2.1294 1.8751 1.2088
109.1011768	3.786559858	49 65	2.6352 1.1514
135.1168269	3.396031875	52 61 67	2.9333 0.28235 0.18035
137.13247651312	3.396031875		

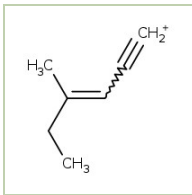
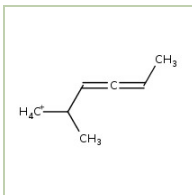
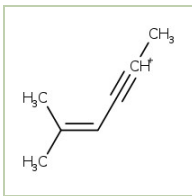
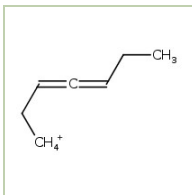
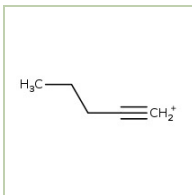
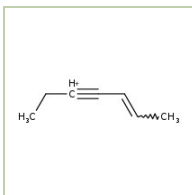
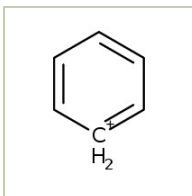
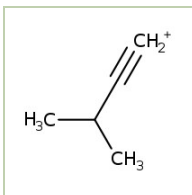
**energy2**

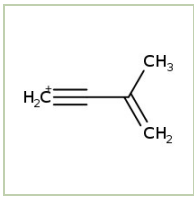
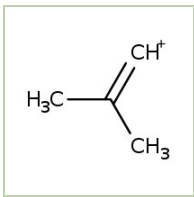
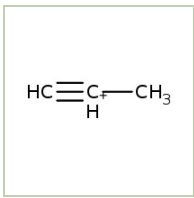
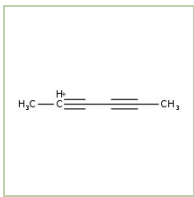
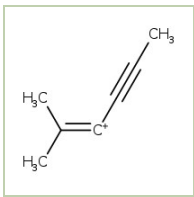
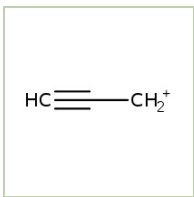
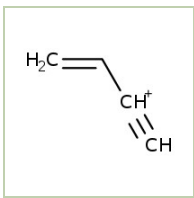
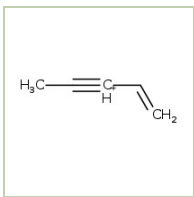
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41.03857658	8.867670952	20	8.8677
53.03857658	5.007822302	24	5.0078
55.05422664	5.890334786	9 19	5.1476 0.74273
65.03857658	5.636106115	26 29	3.028 2.6081
67.05422664	10.16688963	25 18	6.8482 3.3187
69.06987671	4.886771006	17 14	3.4462 1.4406
77.03857658	8.720750053	28	8.7208
79.05422664	13.7944486	5 42 16 21	8.8637 3.7559 0.72605 0.44885
91.05422664	7.246312541	30 33 47 56	3.4724 3.0007 0.49649 0.2768
93.06987671	8.063226041	22 31 27 55	3.3431 2.3791 1.8937 0.44728
137.13247651312	8.063226041		

**Fragments Generated**

Structure	ID	Mass	SMILES
	0	137.132477	<chem>C=C([CH4+])C1CC=C(C)CC1</chem>

	1	121.1011768	<chem>C#[CH+]C1=CCC(C)CC1</chem>
	2	121.1011768	<chem>C#[CH+]C=C=CC(C)CC</chem>
	3	121.1011768	<chem>C#[CH+]C(=C=CCC)CC</chem>
No Image	4	121.1011768	<chem>C#[CH+]C(=C)CCC(=C)C</chem>
	5	79.05422664	<chem>C#[CH+]C(=C)C=C</chem>
	6	97.10117684	<chem>[CH4+]C1CC=CCC1</chem>
	7	81.06987671	<chem>C1=CCC[CH2+]=C1</chem>
	8	97.10117684	<chem>C=C=CC([CH4+])CC</chem>
	9	55.05422664	<chem>C#[CH+]CC</chem>

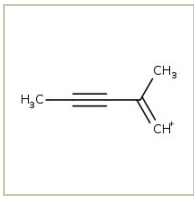
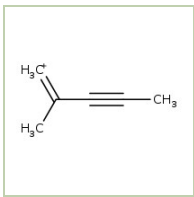
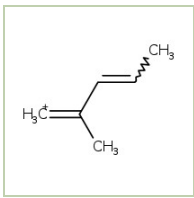
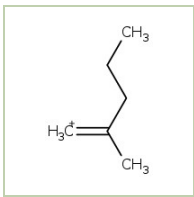
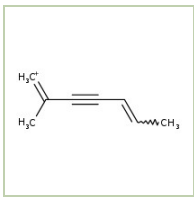
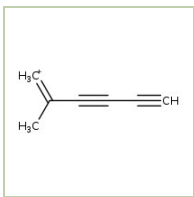
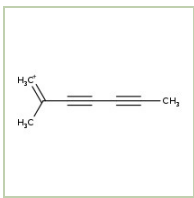
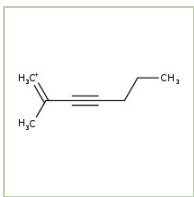
	10	95.08552677	[CH2+]#CC=C(C)CC
	11	97.10117684	CC=C=CC(C)[CH4+]
	12	95.08552677	C[CH+]#CC=C(C)C
	13	97.10117684	CCC=C=CC[CH4+]
	14	69.06987671	[CH2+]#CCCC
	15	95.08552677	CC=CC#[CH+]CC
	16	79.05422664	C1=CC=[CH2+]C=C1
	17	69.06987671	[CH2+]#CC(C)C

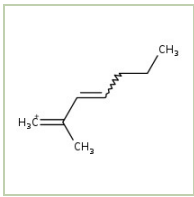
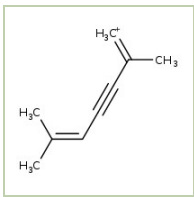
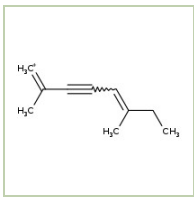
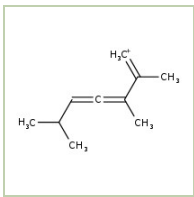
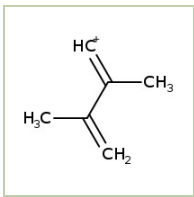
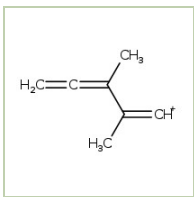
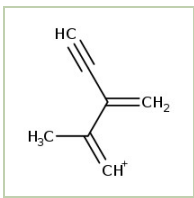
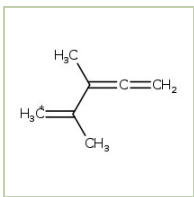
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	19	55.05422664	<chem>[CH+]=C(C)C</chem>
	20	41.03857658	<chem>C#[CH+]C</chem>
	21	79.05422664	<chem>CC#CC#[CH+]C</chem>
	22	93.06987671	<chem>CC#C[C+]=C(C)C</chem>
	23	39.02292652	<chem>C#C[CH2+]</chem>
	24	53.03857658	<chem>C#[CH+]C=C</chem>
	25	67.05422664	<chem>C=C[CH+]#CC</chem>

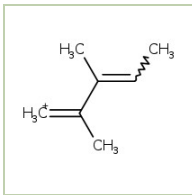
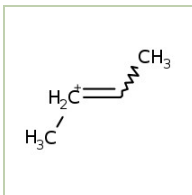
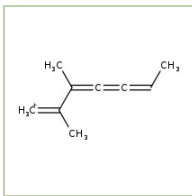
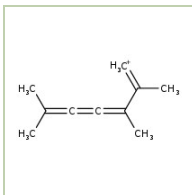
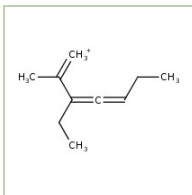
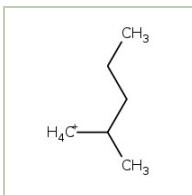
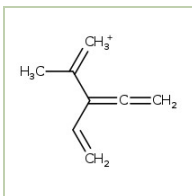
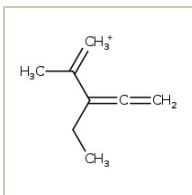
	26	65.03857658	[CH2+]#CC#CC
	27	93.06987671	C=C=C=C([CH4+])C=C
	28	77.03857658	C#CC(=C)C#[CH2+]
	29	65.03857658	C#CC(=[CH+])C
	30	91.05422664	C#CC(C)=CC#[CH2+]
	31	93.06987671	CCC=C=C=C=[CH3+]
	32	51.02292652	C#C[CH+]#C
	33	91.05422664	C=C[CH+]#CC#CC

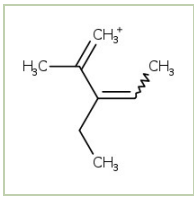
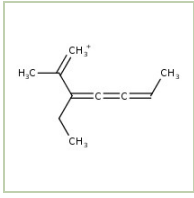
	34	43.05422664	CC=[CH3+]
	35	45.06987671	CC[CH4+]
	36	121.1011768	CC(=[CH3+])C1=CC=CCC1
	37	121.1011768	C=C=C=CCCC(C)=[CH3+]
	38	137.132477	CCC(C)C=C=CC(C)=[CH3+]
	39	81.06987671	C=C(C#[CH2+])CC
	40	63.02292652	[C+]#CC#CC
	41	71.08552677	CCC(C)=[CH3+]



	42	79.05422664	<chem>[CH+]=C(C)C#CC</chem>
	43	81.06987671	<chem>CC#CC(C)=[CH3+]</chem>
	44	83.08552677	<chem>CC=CC(C)=[CH3+]</chem>
	45	85.10117684	<chem>CCCC(C)=[CH3+]</chem>
	46	107.0855268	<chem>CC=CC#CC(C)=[CH3+]</chem>
	47	91.05422664	<chem>C#CC#CC(C)=[CH3+]</chem>
	48	105.0698767	<chem>CC#CC#CC(C)=[CH3+]</chem>
	49	109.1011768	<chem>CCCC#CC(C)=[CH3+]</chem>

	50	111.1168269	<chem>CCCC=CC(C)=[CH3+]</chem>
	51	121.1011768	<chem>CC(=[CH3+])C#CC=C(C)C</chem>
	52	135.1168269	<chem>CCC(C)=CC#CC(C)=[CH3+]</chem>
	53	137.132477	<chem>CC(=[CH3+])C(C)=C=CC(C)C</chem>
	54	81.06987671	<chem>[CH+]=C(C)C(=C)C</chem>
	55	93.06987671	<chem>[CH+]=C(C)C(C)=C=C</chem>
	56	91.05422664	<chem>C#CC(=C)C(=[CH+])C</chem>
	57	95.08552677	<chem>C=C=C(C)C(C)=[CH3+]</chem>

	58	97.10117684	<chem>CC=C(C)C(C)=[CH3+]</chem>
	59	57.06987671	<chem>CC=[CH2+]C</chem>
	60	121.1011768	<chem>CC=C=C=C(C)C(C)=[CH3+]</chem>
	61	135.1168269	<chem>CC(=[CH3+])C(C)=C=C=C(C)C</chem>
	62	137.132477	<chem>CCC=C=C(CC)C(C)=[CH3+]</chem>
	63	87.1168269	<chem>CCCC(C)[CH4+]</chem>
	64	107.0855268	<chem>C=C=C(C=C)C(C)=[CH3+]</chem>
	65	109.1011768	<chem>C=C=C(CC)C(C)=[CH3+]</chem>

	66	111.1168269	<chem>CC=C(CC)C(C)=[CH3+]</chem>
	67	135.1168269	<chem>CC=C=C=C(CC)C(C)=[CH3+]</chem>