Results

Spectrum Prediction Input Parameters:

Parent Compound Structure (InChi Format)	InChI=1S/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h8-9H,1,4-6H2,2-3H3
Parent Compound Mass	136.12520051312
Spectra Type	ESI
Ion Mode	Positive
Adduct Type	[M+H]+
Probability Threshold	0.001
Status	**Completed**

Results:

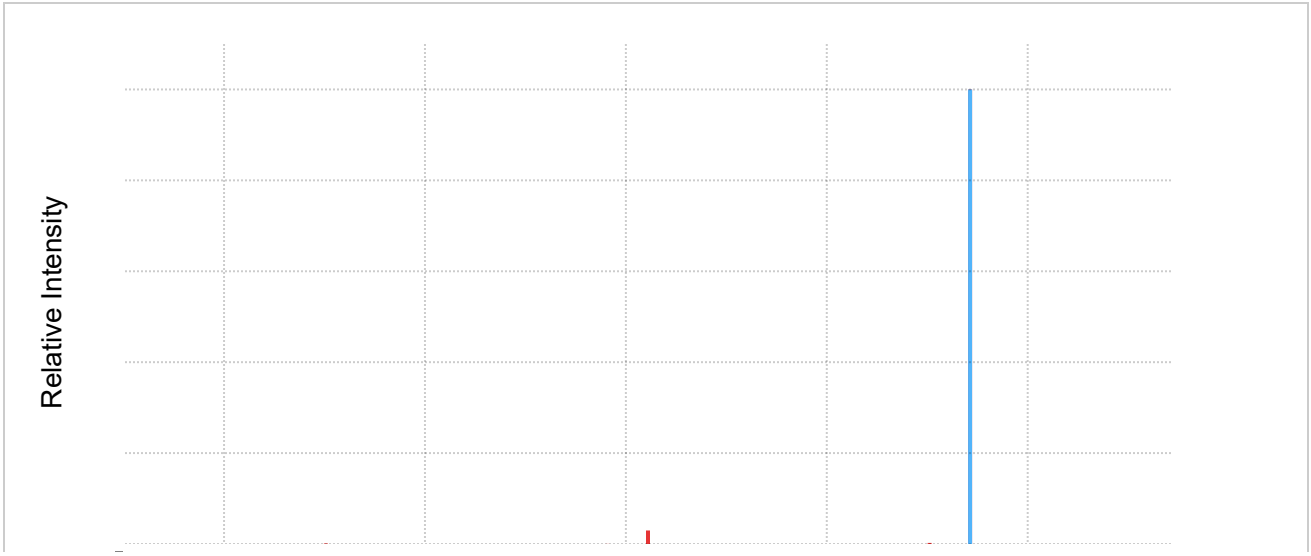
Computed Results

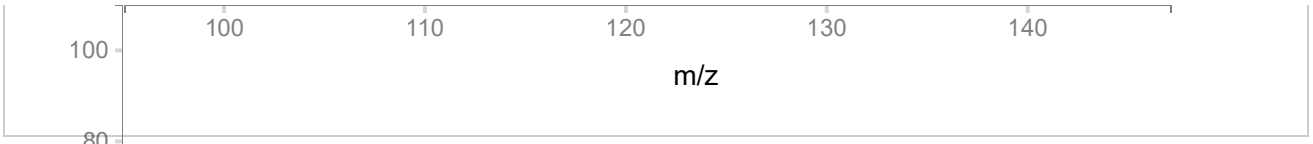
Computed Results:

Download (/system/predict_queries/output_files/003/050/693/original/output.txt?1714158560)

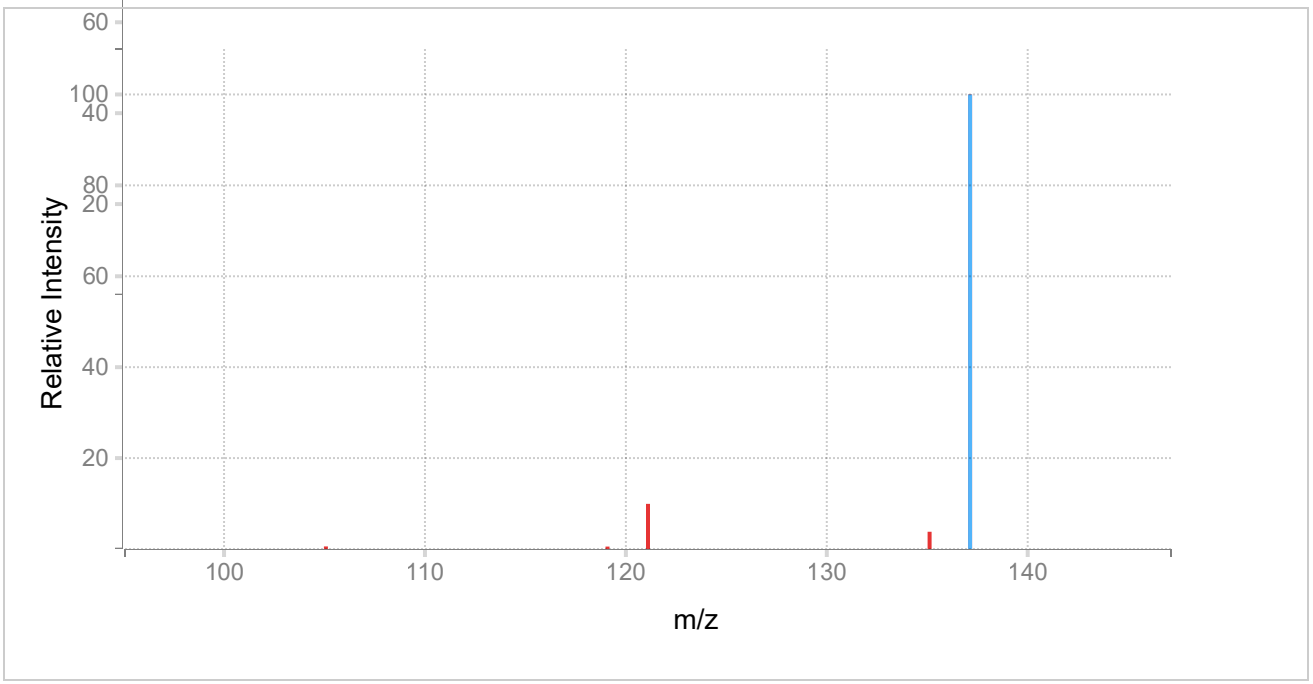
Predicted spectra are shown below. Peaks for which corresponding fragments have been found are colored red; unassigned peaks are colored blue. Hover over the peaks to see the exact mass and intensity values, along with the highest scoring assigned fragments, if found. Clicking on red spectra lines will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

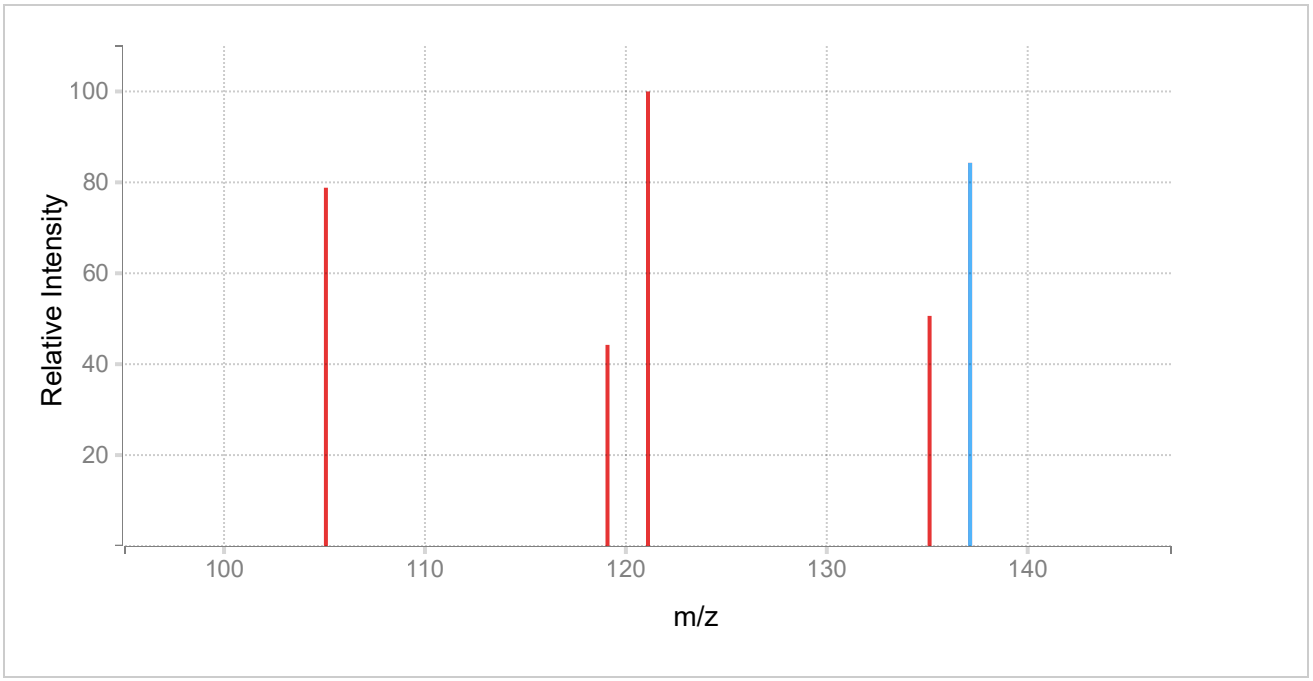




Predicted Medium Energy MsMs Spectrum (20V), [M+H]+



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/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h8-9H,1,4-6H2,2-3H3

energy0

105.0698767 0.1213183555 2 3 0.067428 0.05389

119.0855268	0.02337753444	4 6	0.019129 0.0042481
121.1011768	2.875967378	1 5	1.5966 1.2793
135.1168269	0.2308262464	7	0.23083
137.132477	96.74775971	0	96.748
137.13247651312	96.74775971		

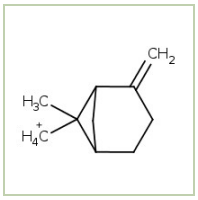
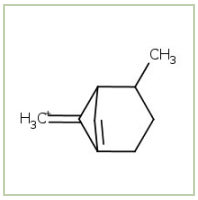
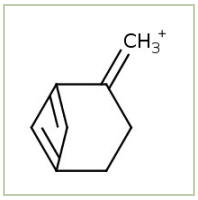
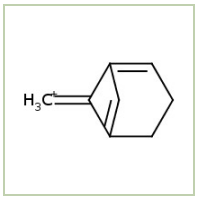
energy1

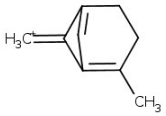
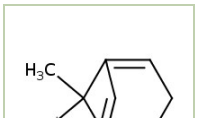
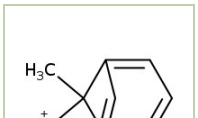
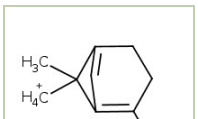
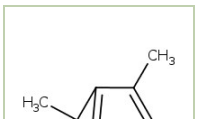
105.0698767	0.4901004511	3 2	0.42115 0.068952
119.0855268	0.4622680423	4 6	0.23705 0.22522
121.1011768	8.648256503	5 1	5.7987 2.8496
135.1168269	3.302894539	7	3.3029
137.132477	87.08605397	0	87.086
137.13247651312	87.08605397		

energy2

105.0698767	21.41197435	3 2	11.733 9.6786
119.0855268	12.01976701	6 4	6.3784 5.6414
121.1011768	27.16546056	1 5	18.554 8.6119
135.1168269	13.75226154	7	13.752
137.132477	22.89572345	0	22.896
137.13247651312	22.89572345		

Fragments Generated

Structure	ID	Mass	SMILES
	0	137.132477	C=C1CCC2CC1C2(C)[CH4+]
	1	121.1011768	CC1CCC2=CC1C2=[CH3+]
	2	105.0698767	[CH3+]=C1CCC2=CC1=C2
	3	105.0698767	[CH3+]=C1C2=CCCC1=C2

	4	119.0855268	CC1=C2C=C(CC1)C2=[CH3+]
	5	121.1011768	CC1([CH4+])C2=CCCC1=C2
	6	119.0855268	CC1([CH4+])C2=CC=CC1=C2
	7	135.1168269	CC1=C2C=C(CC1)C2(C)[CH4+]
	8	133.1011768	CC1=CC=C2C=C1C2(C)[CH4+]