Results

Spectrum Prediction Input Parameters:

Parent Compound Structure (InChi Format)	InChI=1S/C17H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19/h2-16H2,1H3,(H,18,19)
Parent Compound Mass	270.2558803295
Spectra Type	ESI
Ion Mode	Positive
Adduct Type	[M+H]+
Probability Threshold	0.001
Status	**Completed**

Results:

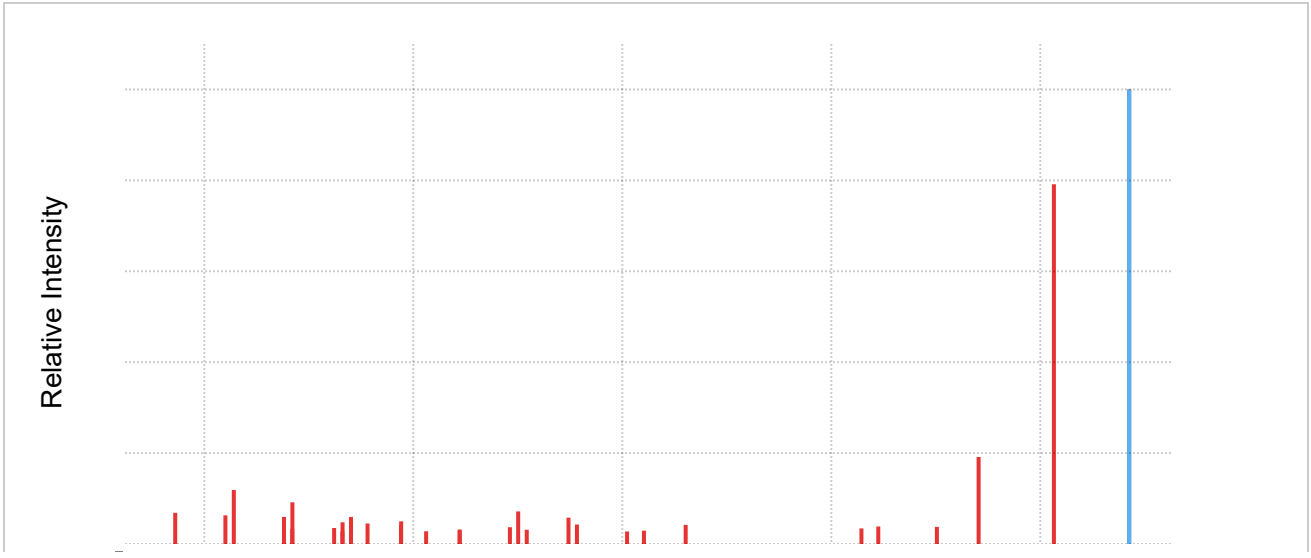
Computed Results

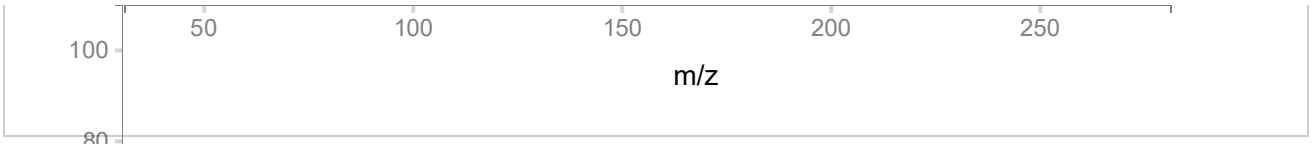
Computed Results:

Download (/system/predict_queries/output_files/003/050/939/original/output.txt?1714237854)

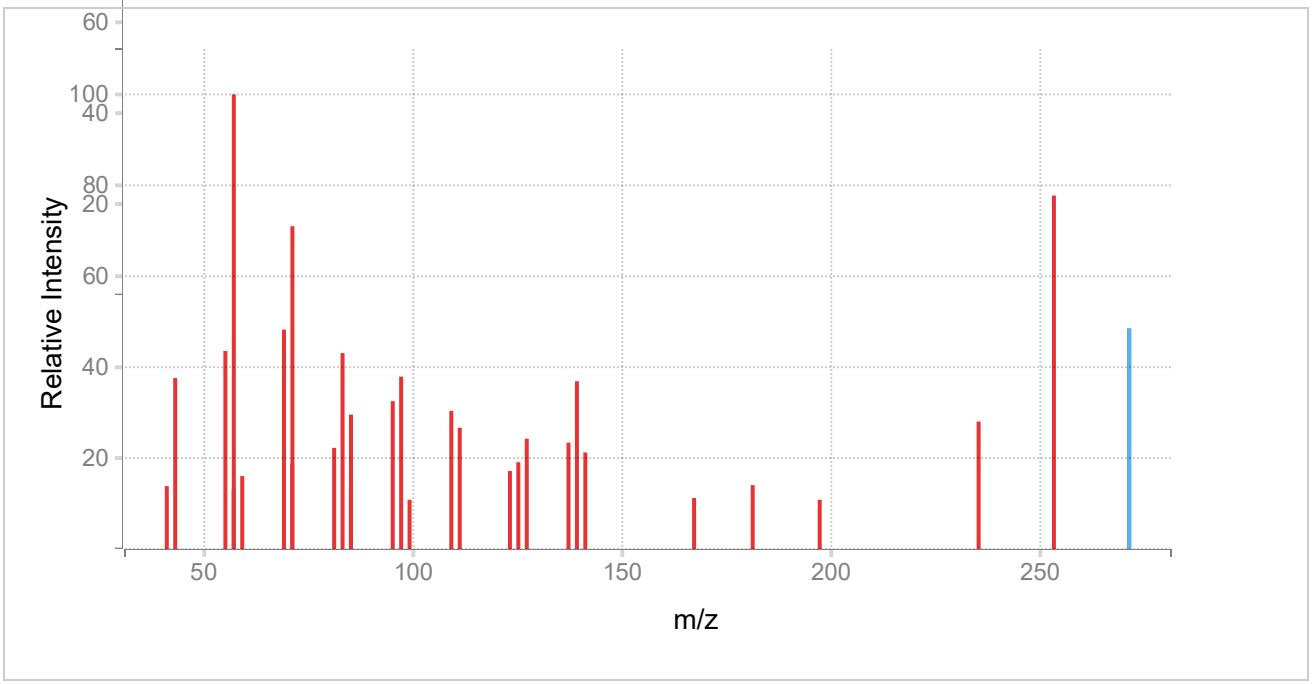
Predicted spectra are shown below. Peaks for which corresponding fragments have be en found are colored red; unassigned peaks are colored blue. Hover over the peaks to see the exact mass and intensity values, along with the highest scoring assigned frag ments, if found. Clicking on red spectra lines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

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

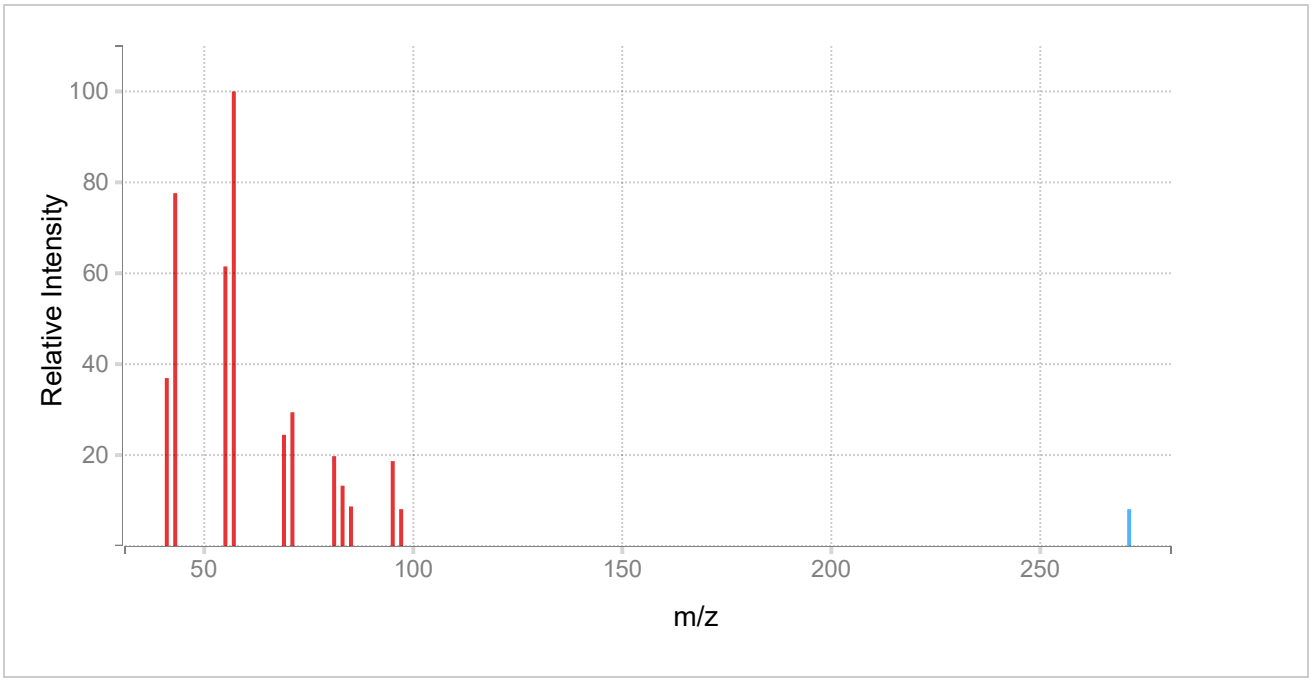




Predicted Medium Energy MsMs Spectrum (20V), [M+H]+



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/C17H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19/h2-16H2,1H3,(H,18,19)

energy0

43.05422664 1.694314627 5 1.6943

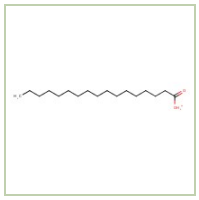
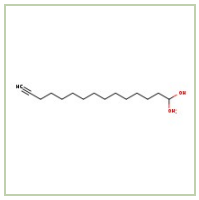
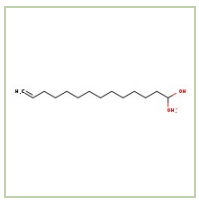
55.05422664	1.556221239	8	1.5562
57.06987671	2.934280227	9	2.9343
69.06987671	1.47245381	15	1.4725
71.04914126	0.8165982568	75	0.8166
71.08552677	2.265639644	16	2.2656
81.06987671	0.8693619676	21	0.86936
83.04914126	0.6920892319	69	0.69209
83.08552677	1.180139195	20	1.1801
85.10117684	1.469442016	22	1.4694
89.05970595	1.113549255	38	1.1135
97.06479133	1.040326132	61	1.0403
97.10117684	1.231936688	14	1.2319
103.075356	0.6899305216	66	0.68993
111.0804414	0.7181412738	112	0.71814
111.1168269	0.787138002	31	0.78714
123.1168269	0.9121951793	46	0.9122
125.0960915	1.77022053	44	1.7702
127.148127	0.7737956552	47	0.7738
137.132477	1.432282585	54	1.4323
139.148127	1.05955306	53	1.0596
151.148127	0.6799756652	113	0.67998
155.1794272	0.725300678	63	0.7253
165.1637771	1.038732387	114	1.0387
207.2107273	0.8473362209	116	0.84734
211.2420274	0.952891379	94	0.95289
225.2576775	0.9298469107	96	0.92985
235.2420274	4.726291419	117	4.7263
253.2525921	19.54774814	97	19.548
271.2631568	24.69841989	0	24.698
271.26315632949996	24.69841989		
energy1			
41.03857658	1.135173679	4	1.1352
43.05422664	3.087039046	5	3.087
55.05422664	3.577404478	8	3.5774
57.0334912	1.081098631	84	1.0811
57.06987671	8.211126814	9	8.2111
59.08552677	1.31759563	11	1.3176
69.06987671	3.962556387	15	3.9626
71.04914126	1.543665925	75	1.5437
71.08552677	5.830104549	16	5.8301
81.06987671	1.827541144	21	1.8275
83.08552677	3.538698875	20	3.5387
85.06479133	1.06832856	67	1.0683
85.10117684	2.42848964	22	2.4285
95.08552677	2.671199214	27	2.6712
97.10117684	3.114207526	14	3.1142
99.1168269	0.8904335466	28	0.89043
109.1011768	2.494097568	33	2.4941
111.1168269	2.190571867	31	2.1906

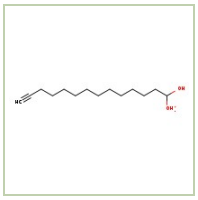
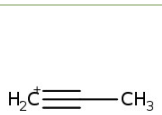
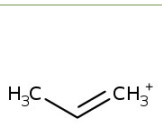
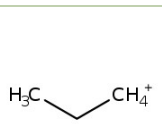
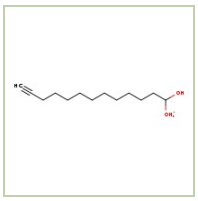
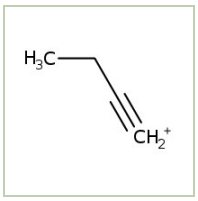
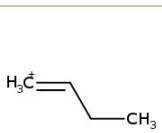
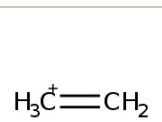
123.1168269	1.408331114	46	1.4083
125.132477	1.567572438	45	1.5676
127.148127	1.992251514	47	1.9923
137.132477	1.920396335	54	1.9204
139.148127	3.03012524	53	3.0301
141.1637771	1.743916235	55	1.7439
167.1794272	0.9207210988	70	0.92072
181.1950772	1.154777353	79	1.1548
197.2263773	0.8894419997	87	0.88944
235.2420274	2.302299333	117	2.3023
253.2525921	6.383816109	97	6.3838
271.2631568	3.983163749	0	3.9832
271.26315632949996	3.983163749		

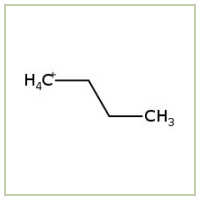
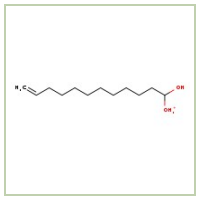
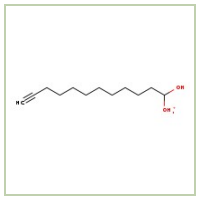
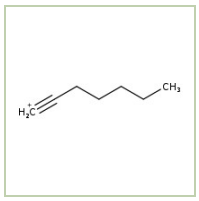
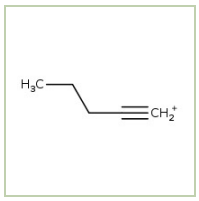
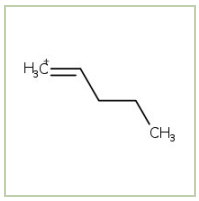
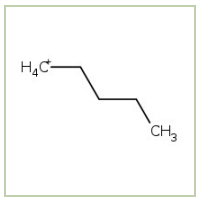
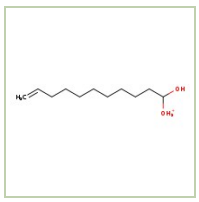
energy2

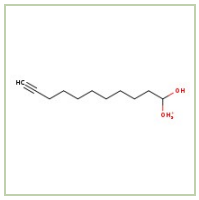
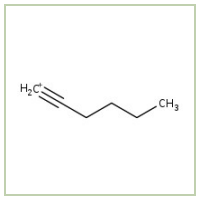
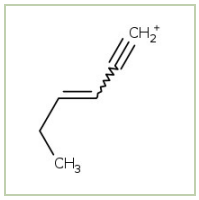
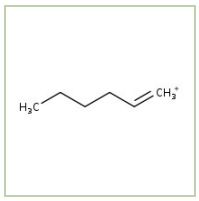
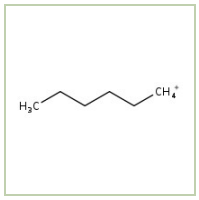
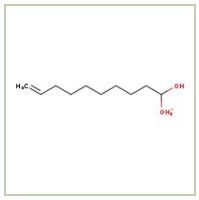
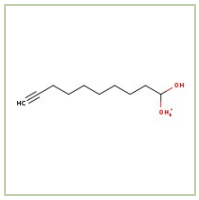
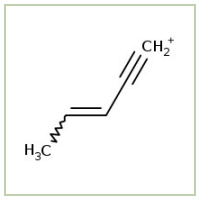
41.03857658	7.44294845	4	7.4429
43.05422664	15.63987013	5	15.64
55.05422664	12.39168404	8	12.392
57.06987671	20.14807361	9	20.148
69.06987671	4.927474489	15	4.9275
71.08552677	5.928574328	16	5.9286
81.06987671	3.98158845	21	3.9816
83.08552677	2.672735149	20	2.6727
85.10117684	1.752654905	22	1.7527
95.08552677	3.763382928	27	3.7634
97.10117684	1.633135217	14	1.6331
271.26315632949996	1.633135217		

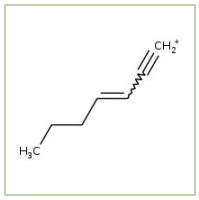
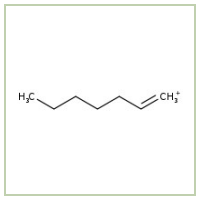
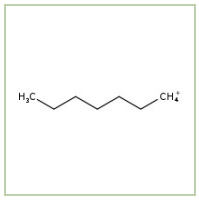
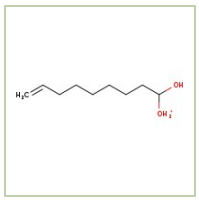
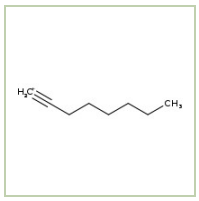
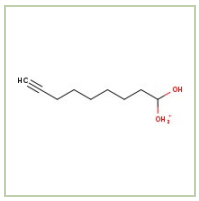
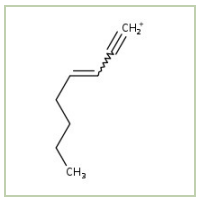
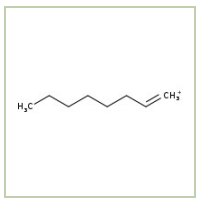
Fragments Generated

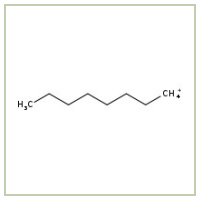
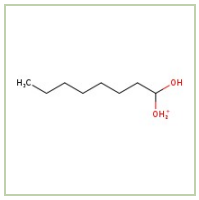
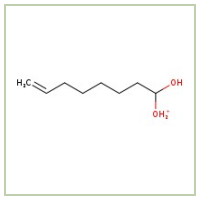
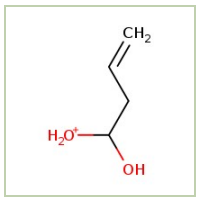
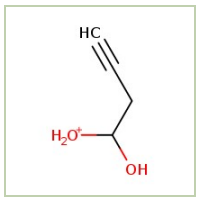
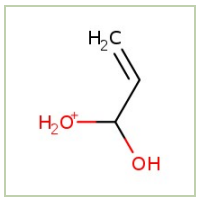
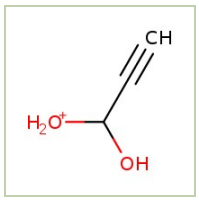
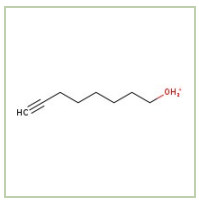
Structure	ID	Mass	SMILES
	0	271.2631568	CCCCCCCCCCCCCCCCC(=O)[OH2+]
	1	241.2162066	C#CCCCCCCCCCCCCC(O)[OH2+]
	2	229.2162066	C=CCCCCCCCCCCCC(O)[OH2+]

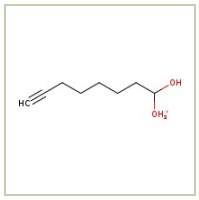
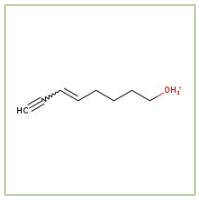
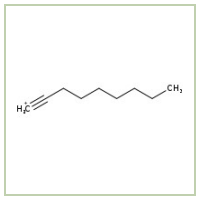
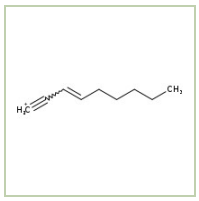
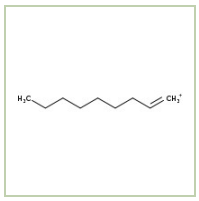
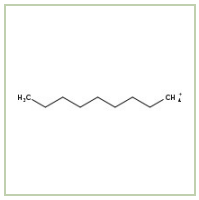
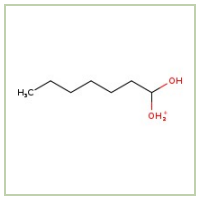
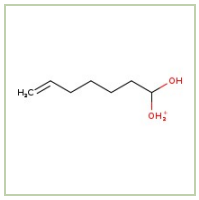
	3	227.2005565	C#CCCCCCCCCCCCC(O)[OH2+]
	4	41.03857658	[CH2+]#CC
	5	43.05422664	CC=[CH3+]
	6	45.06987671	CC[CH4+]
	7	213.1849065	C#CCCCCCCCCCCCC(O)[OH2+]
	8	55.05422664	[CH2+]#CCC
	9	57.06987671	CCC=[CH3+]
	10	29.03857658	C=[CH3+]

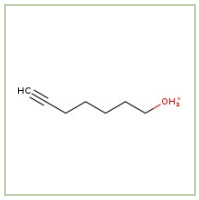
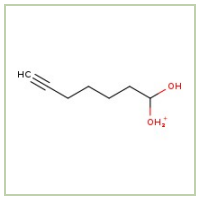
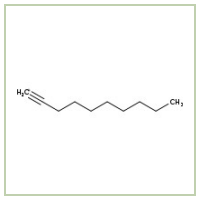
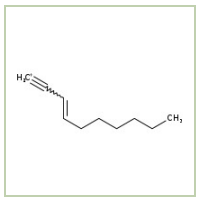
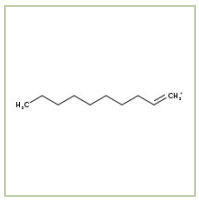
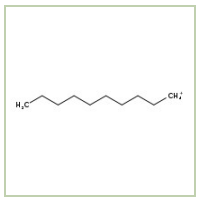
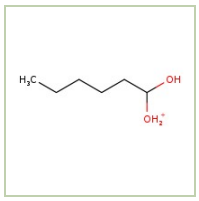
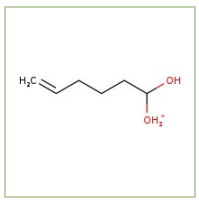
	11	59.08552677	CCC[CH4+]
	12	201.1849065	C=CCCCCCCCCCC(O)[OH2+]
	13	199.1692564	C#CCCCCCCCCCC(O)[OH2+]
	14	97.10117684	[CH2+]#CCCCCC
	15	69.06987671	[CH2+]#CCCC
	16	71.08552677	CCCC=[CH3+]
	17	73.10117684	CCCC[CH4+]
	18	187.1692564	C=CCCCCCCCCC(O)[OH2+]

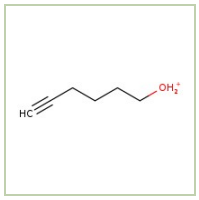
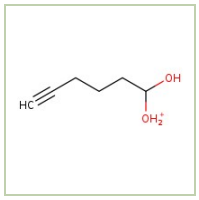
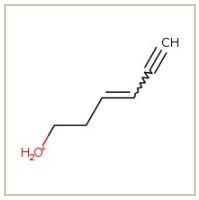
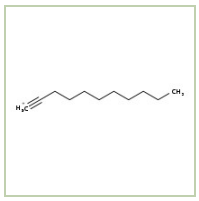
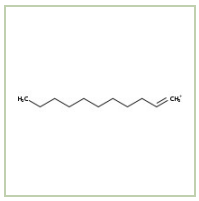
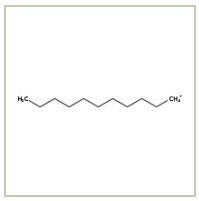
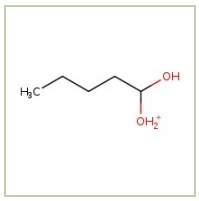
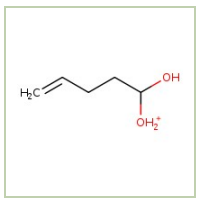
	19	185.1536063	C#CCCCCCCCCC(O)[OH2+]
	20	83.08552677	[CH2+]#CCCCC
	21	81.06987671	[CH2+]#CC=CCC
	22	85.10117684	CCCCC=[CH3+]
	23	87.1168269	CCCCC[CH4+]
	24	173.1536063	C=CCCCCCCCC(O)[OH2+]
	25	171.1379563	C#CCCCCCCCC(O)[OH2+]
	26	67.05422664	[CH2+]#CC=CC

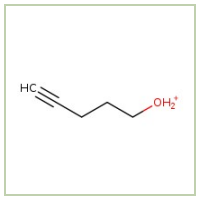
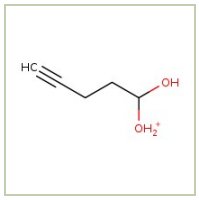
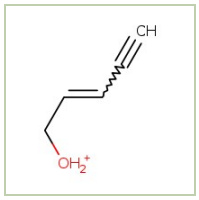
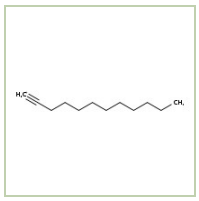
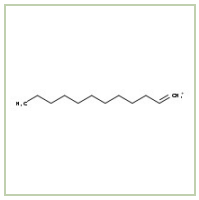
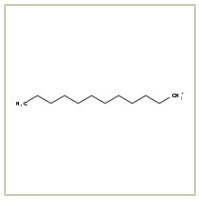
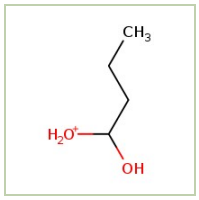
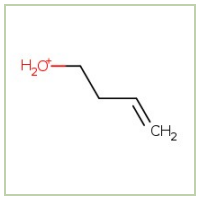
	27	95.08552677	[CH2+]#CC=CCCC
	28	99.1168269	CCCCCC=[CH3+]
	29	101.132477	CCCCCC[CH4+]
	30	159.1379563	C=CCCCCCCC(O)[OH2+]
	31	111.1168269	[CH2+]#CCCCCCC
	32	157.1223062	C#CCCCCCCC(O)[OH2+]
	33	109.1011768	[CH2+]#CC=CCCCC
	34	113.132477	CCCCCCC=[CH3+]

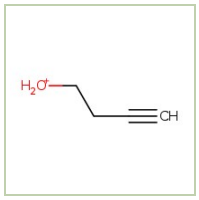
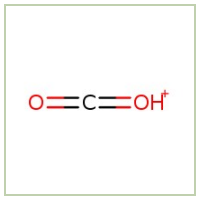
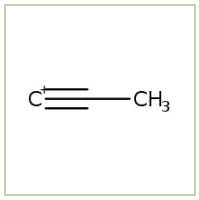
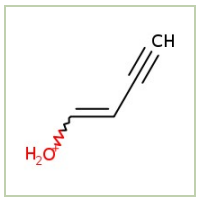
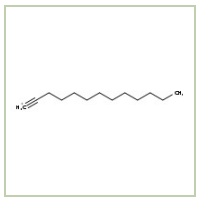
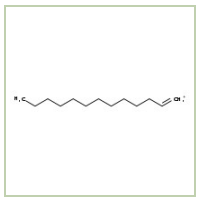
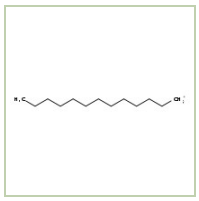
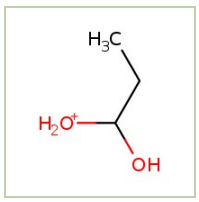
	35	115.148127	CCCCCCC[CH4+]
	36	147.1379563	CCCCCCCC(O)[OH2+]
	37	145.1223062	C=CCCCCCC(O)[OH2+]
	38	89.05970595	C=CCC(O)[OH2+]
	39	87.04405588	C#CCC(O)[OH2+]
	40	75.04405588	C=CC(O)[OH2+]
	41	73.02840582	C#CC(O)[OH2+]
	42	127.1117415	C#CCCCCCC[OH2+]

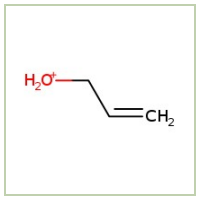
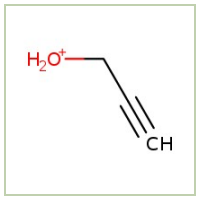
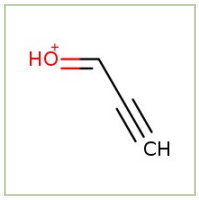
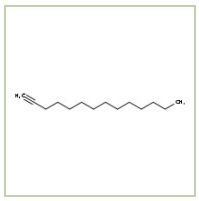
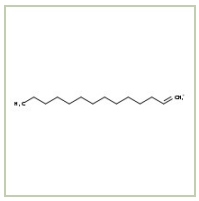
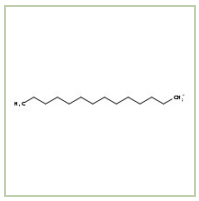
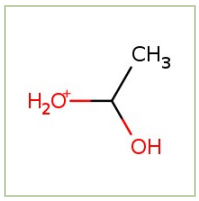
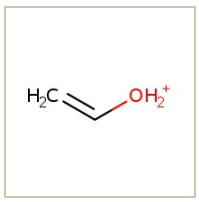
	43	143.1066561	C#CCCCCCC(O)[OH2+]
	44	125.0960915	C#CC=CCCCC[OH2+]
	45	125.132477	[CH2+]#CCCCCCCC
	46	123.1168269	[CH2+]#CC=CCCCCC
	47	127.148127	CCCCCCCC=[CH3+]
	48	129.1637771	CCCCCCCC[CH4+]
	49	133.1223062	CCCCCCC(O)[OH2+]
	50	131.1066561	C=CCCCCC(O)[OH2+]

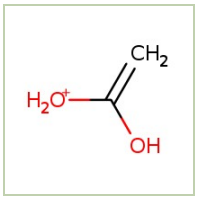
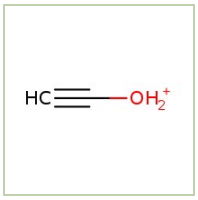
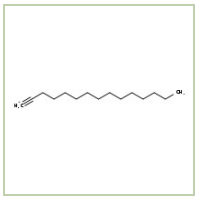
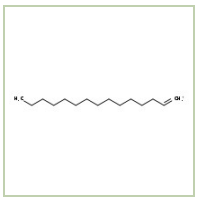
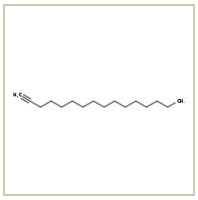
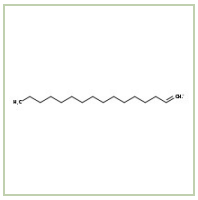
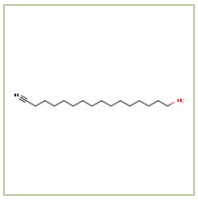
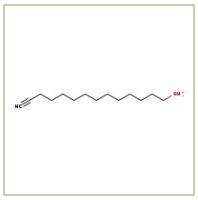
	51	113.0960915	C#CCCCCC[OH2+]
	52	129.0910061	C#CCCCCC(O)[OH2+]
	53	139.148127	[CH2+]#CCCCCCCCC
	54	137.132477	[CH2+]#CC=CCCCCCC
	55	141.1637771	CCCCCCCCC=[CH3+]
	56	143.1794272	CCCCCCCCC[CH4+]
	57	119.1066561	CCCCCC(O)[OH2+]
	58	117.0910061	C=CCCCC(O)[OH2+]

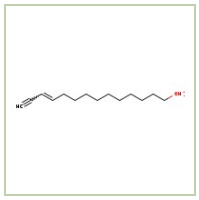
	59	99.08044139	C#CCCCC[OH2+]
	60	115.075356	C#CCCCC(O)[OH2+]
	61	97.06479133	C#CC=CCC[OH2+]
	62	153.1637771	[CH2+]#CCCCCCCCCC
	63	155.1794272	CCCCCCCCCC=[CH3+]
	64	157.1950772	CCCCCCCCCC[CH4+]
	65	105.0910061	CCCCC(O)[OH2+]
	66	103.075356	C=CCCC(O)[OH2+]

	67	85.06479133	C#CCCC[OH2+]
	68	101.0597059	C#CCCC(O)[OH2+]
	69	83.04914126	C#CC=CC[OH2+]
	70	167.1794272	[CH2+]#CCCCCCCCCCC
	71	169.1950772	CCCCCCCCCCC=[CH3+]
	72	171.2107273	CCCCCCCCCCC[CH4+]
	73	91.07535601	CCCC(O)[OH2+]
	74	73.06479133	C=CCC[OH2+]

	75	71.04914126	C#CCC[OH2+]
	76	44.99710569	O=C=[OH+]
	77	39.02292652	[C+]#CC
	78	69.0334912	C#CC=C[OH2+]
	79	181.1950772	[CH2+]#CCCCCCCCCCCC
	80	183.2107273	CCCCCCCCCCCC=[CH3+]
	81	185.2263773	CCCCCCCCCCCC[CH4+]
	82	77.05970595	CCC(O)[OH2+]

	83	59.04914126	C=CC[OH2+]
	84	57.0334912	C#CC[OH2+]
	85	55.01784114	C#CC=[OH+]
	86	195.2107273	[CH2+]#CCCCCCCCCCCCC
	87	197.2263773	CCCCCCCCCCCCC=[CH3+]
	88	199.2420274	CCCCCCCCCCCCC[CH4+]
	89	63.04405588	CC(O)[OH2+]
	90	45.0334912	C=C[OH2+]

	91	61.02840582	C=C(O)[OH2+]
	92	43.01784114	C#C[OH2+]
	93	209.2263773	[CH2+]#CCCCCCCCCCCCCC
	94	211.2420274	CCCCCCCCCCCCCC=[CH3+]
	95	223.2420274	[CH2+]#CCCCCCCCCCCCCCC
	96	225.2576775	CCCCCCCCCCCCCCC=[CH3+]
	97	253.2525921	C#CCCCCCCCCCCCCCCC[OH2+]
	98	211.2056419	C#CCCCCCCCCCCCC[OH2+]

	99	209.1899918	C#CC=CCCCCCCCCC[OH2+]

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There are over 100 fragments, download the results (/system/predict_queries/output_files/003/050/939/original/output.txt?1714237854) to view the full list.