Results

Spectrum Prediction Input Parameters:

Parent Compound Structure (InChi Format)	InChI=1S/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-2-4-6-10/h2-6,11-16,19H,7-9H2,1H3
Parent Compound Mass	303.14705815650996
Spectra Type	ESI
Ion Mode	Positive
Adduct Type	[M+H]+
Probability Threshold	0.001
Status	**Completed**

Results:

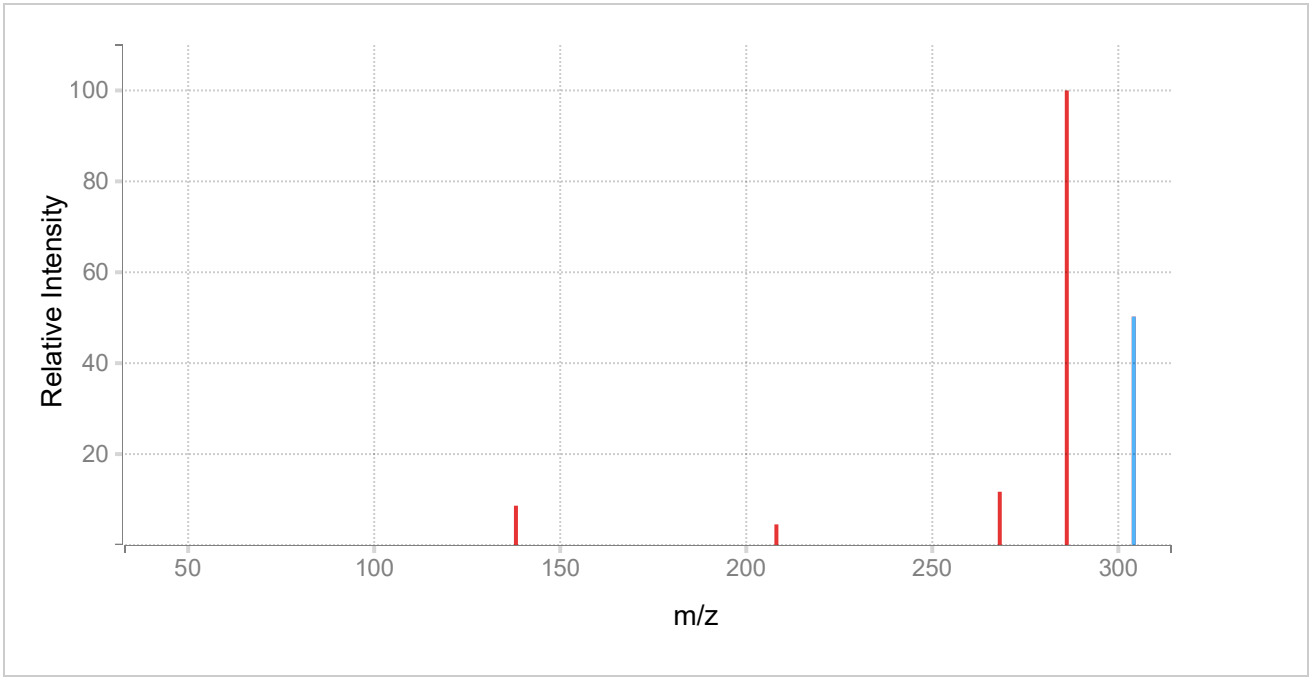
Computed Results

Computed Results:

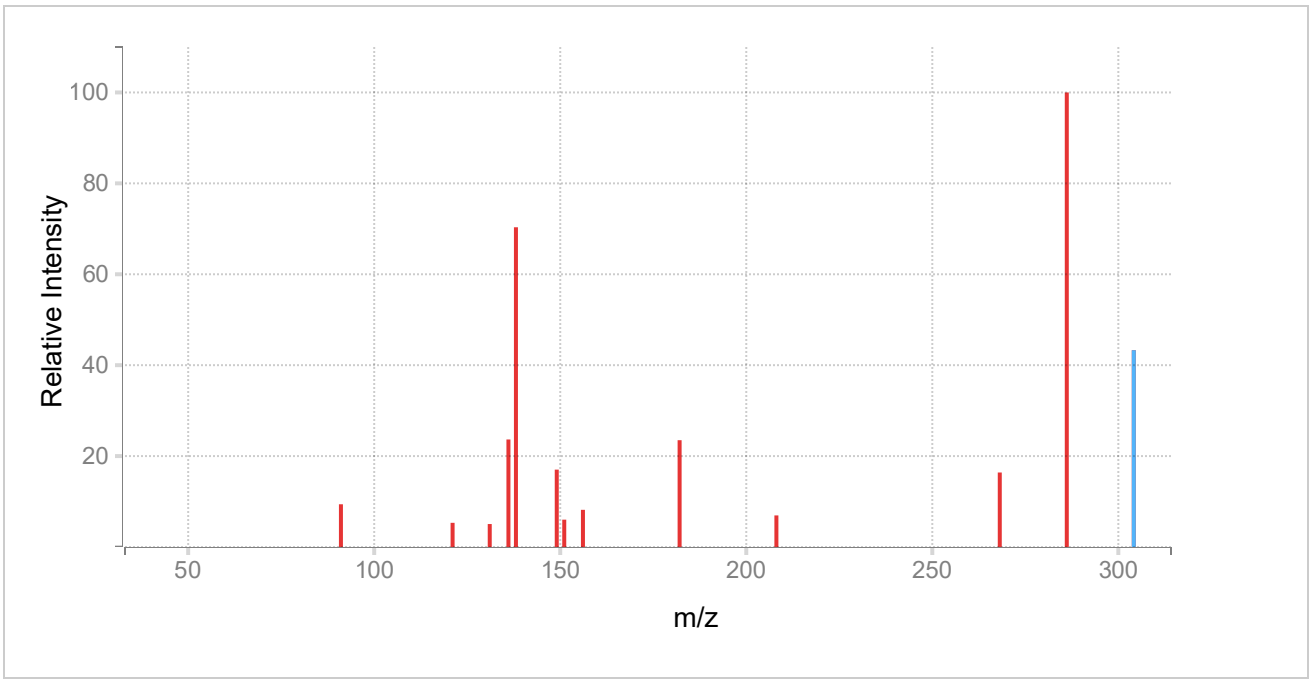
Download (/system/predict_queries/output_files/003/050/963/original/output.txt?1714245023)

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.

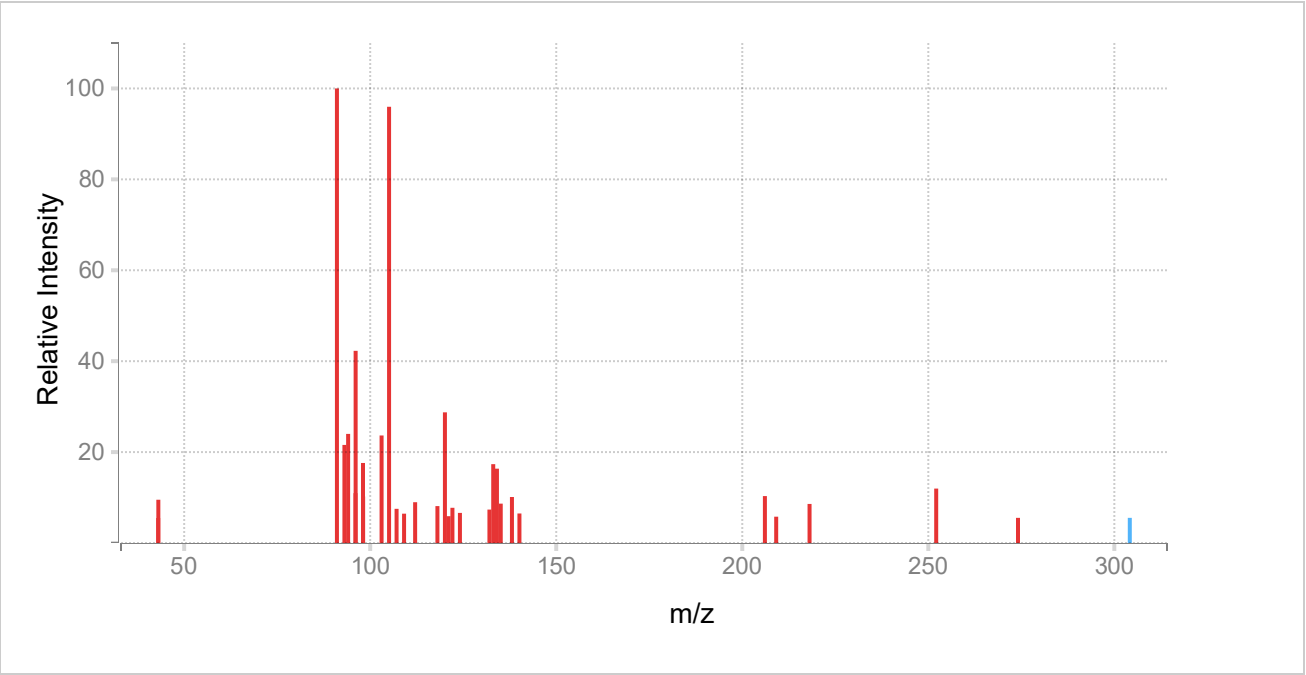
Predicted Low Energy MsMs Spectrum (10V), [M+H]+



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/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-2-4-6-10/h2-6,11-16,19H,7-9H2,1H3

energy0

138.0913404	4.590730777	3 83 74 79 80	4.3096 0.079582 0.079412 0.066342 0.055818
208.0968197	2.407182958	7	2.4072
268.1332052	6.221016235	25 53	6.1872 0.033787
286.1437699	53.08109095	5 32 120 52 48 50 51 39 36 176	46.659 2.329 1.7714 0.95303 0.47118 0.33359 0.32445 0.12818 0.092553 0.019073
304.1543346	26.66399472	0 175 169 153 133 143 165 134	26.143 0.22071 0.099599 0.097874 0.059018 0.021536 0.014099 0.008446
304.15433415650995	26.66399472		

energy1

91.05422664	2.254585781	101	2.2546
121.0647913	1.275833414	66 106 107 108	1.1966 0.036829 0.031876 0.010562
131.0491413	1.21176626	128	1.2118
136.0756904	5.67397261	17 72 70	5.1198 0.3509 0.2033
138.0913404	16.87218963	3 80 83 74 79	14.092 0.99057 0.95871 0.64285 0.18847
149.0597059	4.082881061	14 68	3.3181 0.7648
151.075356	1.442653809	13 129 130	1.4102 0.032298 0.00020014
156.1019051	1.961238477	26 123 125 121 122	1.852 0.042966 0.03964 0.014446 0.012206
182.0811697	5.635523083	19 94 99 95 96	4.1657 0.49441 0.46388 0.32334 0.18816
208.0968197	1.666391681	7	1.6664
268.1332052	3.931290182	25 53	3.055 0.87631

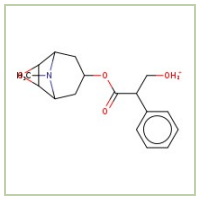
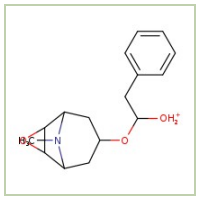
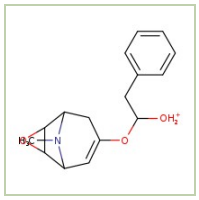
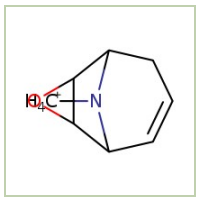
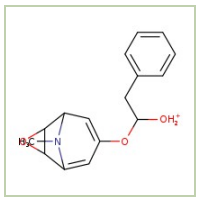
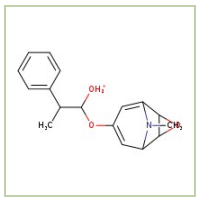
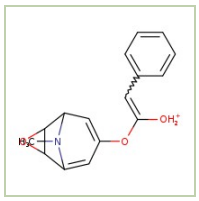
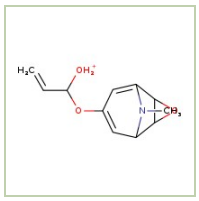
286.1437699	23.98639229	5 52 48 120 50 39 176 32 51 36	18.308 1.6477 1.0147 0.69697 0.49986 0.48153 0.44971 0.41664 0.32015 0.1512
304.1543346	10.38495694	0 153 175 169 143 133 165 134	8.7851 0.55158 0.39486 0.32236 0.11961 0.11465 0.060283 0.036526
304.15433415650995	10.38495694		

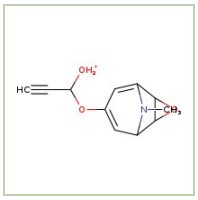
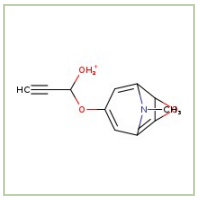
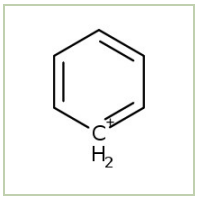
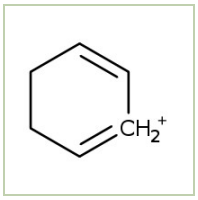
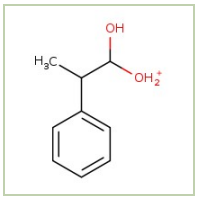
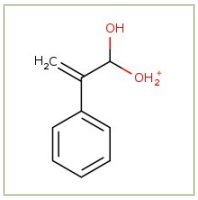
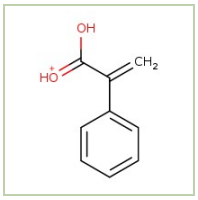
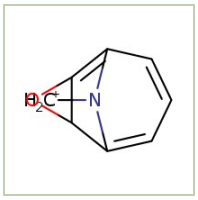
energy2

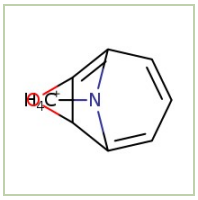
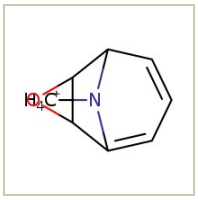
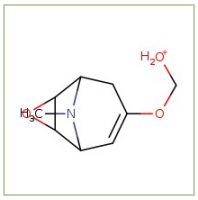
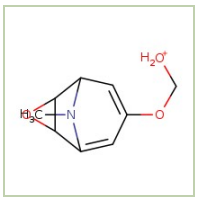
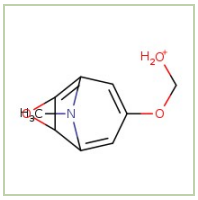
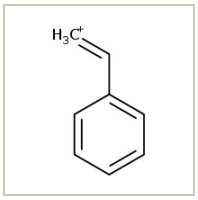
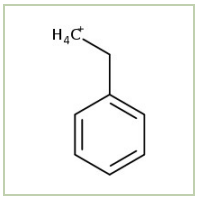
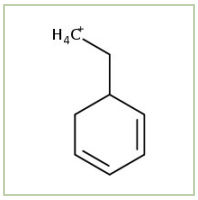
43.01784114	0.80179083	81 105	0.47263 0.32916
43.05422664	1.38913967	78	1.3891
91.05422664	14.59559009	101	14.596
93.06987671	3.149288904	103	3.1493
94.06512568	3.502918517	71 159	2.7386 0.76427
96.04439023	1.600489736	77	1.6005
96.08077574	6.170260226	82 161	5.4428 0.7275
98.0600403	2.569480104	88	2.5695
98.0964258	1.492722078	172	1.4927
103.0542266	3.452445611	104	3.4524
105.0698767	14.0071769	21	14.007
107.0855268	1.097073948	22	1.0971
109.1011768	0.9415853128	23	0.94159
112.0756904	1.309261035	124 158 76	0.79848 0.30206 0.20872
118.0651257	1.184824012	73	1.1848
120.0807757	4.195118606	84	4.1951
121.0647913	0.8605855674	66 107 108 106	0.62749 0.12117 0.083429 0.028501
122.0964258	1.130384975	92	1.1304
124.1120759	0.9663367577	177	0.96634
132.0443902	1.073044368	15	1.073
133.0647913	2.531441971	29	2.5314
134.0600403	2.386599496	16	2.3866
135.0804414	1.263750194	30	1.2638
138.0913404	1.476629049	80 83 74 3 79	0.58949 0.32318 0.30489 0.23484 0.024237
140.1069905	0.9475593985	178 86 85 90 91	0.74664 0.12427 0.036705 0.025268 0.014682
206.0811697	1.506323732	8	1.5063
209.1172208	0.8447554091	164	0.84476
218.0811697	1.254159283	47	1.2542
252.1230345	1.747176333	140	1.7472
274.1073844	0.8073303265	136 147	0.44827 0.35906
304.15433415650995	0.8073303265		

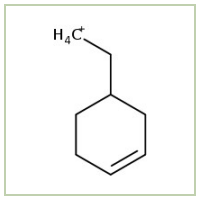
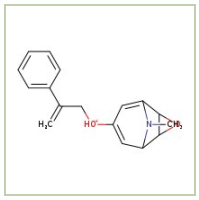
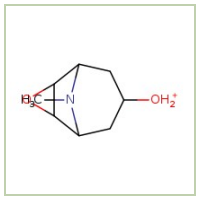
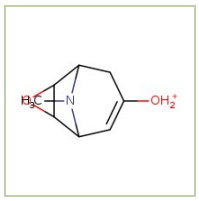
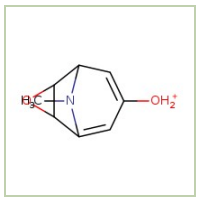
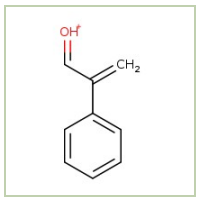
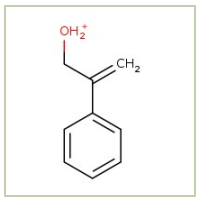
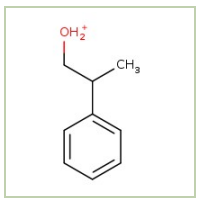
Fragments Generated

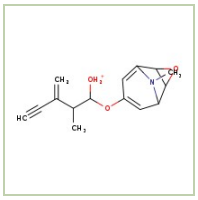
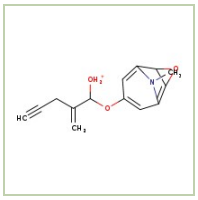
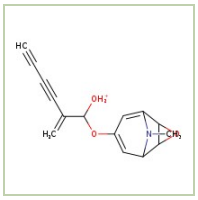
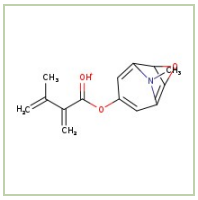
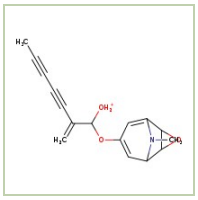
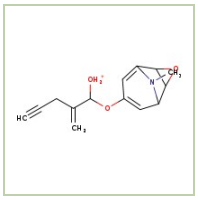
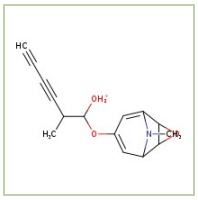
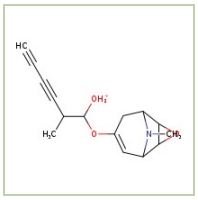
Structure	ID	Mass	SMILES

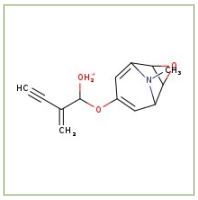
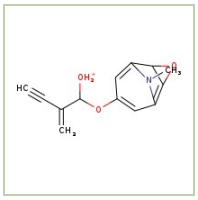
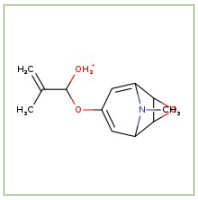
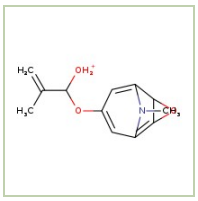
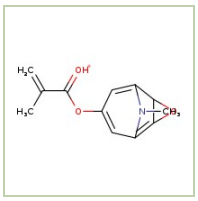
	0	304.1543346	CN1C2CC(OC(=O)C(C[OH2+])c3ccccc3)CC1C1OC12
	1	276.15942	CN1C2CC(OC([OH2+])CC3=CC=CC=C3)CC1C1OC12
	2	274.1437699	CN1C2C=C(OC([OH2+])CC3=CC=CC=C3)CC1C1OC12
	3	138.0913404	[CH4+]N1C2C=CCC1C1OC12
	4	272.1281199	CN1C2=CC(OC([OH2+])CC3=CC=CC=C3)=CC1C1OC21
	5	286.1437699	CC(C1=CC=CC=C1)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
	6	270.1124698	CN1C2=CC(OC([OH2+])=CC3=CC=CC=C3)=CC1C1OC21
	7	208.0968197	C=CC([OH2+])OC1=CC2C3OC3C(=C1)N2C

	8	206.0811697	C#CC([OH2+])OC1=CC2C3OC3C(=C1)N2C
	9	204.0655196	C#CC([OH2+])OC1=CC2=C3OC3C(=C1)N2C
	10	79.05422664	C1=CC=[CH2+]C=C1
	11	81.06987671	C1=C[CH2+]=CCC1
	12	153.0910061	CC(C1=CC=CC=C1)C(O)[OH2+]
	13	151.075356	C=C(C1=CC=CC=C1)C(O)[OH2+]
	14	149.0597059	C=C(C(O)=[OH+])C1=CC=CC=C1
	15	132.0443902	[CH2+]N1C2=CC=CC1=C1OC21

	16	134.0600403	[CH4+]N1C2=CC=CC1=C1OC21
	17	136.0756904	[CH4+]N1C2=CC=CC1C1OC21
	18	184.0968197	CN1C2C=C(OC[OH2+])CC1C1OC12
	19	182.0811697	CN1C2=CC(OC[OH2+])=CC1C1OC21
	20	180.0655196	CN1C2=CC(OC[OH2+])=CC1=C1OC21
	21	105.0698767	[CH3+]=CC1=CC=CC=C1
	22	107.0855268	[CH4+]CC1=CC=CC=C1
	23	109.1011768	[CH4+]CC1C=CC=CC1

	24	111.1168269	[CH4+]CC1CC=CCC1
	25	268.1332052	C=C(C[OH+]C1=CC2C3OC3C(=C1)N2C)C1=CC=CC=C1
	26	156.1019051	CN1C2CC([OH2+])CC1C1OC12
	27	154.086255	CN1C2C=C([OH2+])CC1C1OC12
	28	152.070605	CN1C2=CC([OH2+])=CC1C1OC21
	29	133.0647913	C=C(C=[OH+])C1=CC=CC=C1
	30	135.0804414	C=C(C[OH2+])C1=CC=CC=C1
	31	137.0960915	CC(C[OH2+])C1=CC=CC=C1
No Image	32	286.1437699	C=C=C=C(C=C)C(C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C

	33	260.1281199	C#CC(=C)C(C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
	34	244.0968197	C#CCC(=C)C([OH2+])OC1=CC2=C3OC3C(=C1)N2C
	35	256.0968197	C#CC#CC(=C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
No Image	36	286.1437699	C=C=C=C=C(C)C(C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
	37	244.0968197	C=C(C)C(=C)C(=[OH+])OC1=CC2=C3OC3C(=C1)N2C
	38	270.1124698	C=C(C#CC#CC)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
No Image	39	286.1437699	C=C=C=C=C=CC(C)C([OH2+])OC1=CC2C3OC3C(C1)N2C
	40	246.1124698	C#CCC(=C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
	41	258.1124698	C#CC#CC(C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
	42	260.1281199	C#CC#CC(C)C([OH2+])OC1=CC2C3OC3C(C1)N2C

	43	232.0968197	C#CC(=C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
	44	230.0811697	C#CC(=C)C([OH2+])OC1=CC2=C3OC3C(=C1)N2C
	45	222.1124698	C=C(C)C([OH2+])OC1=CC2C3OC3C(=C1)N2C
	46	220.0968197	C=C(C)C([OH2+])OC1=CC2=C3OC3C(=C1)N2C
	47	218.0811697	C=C(C)C(=[OH+])OC1=CC2=C3OC3C(=C1)N2C
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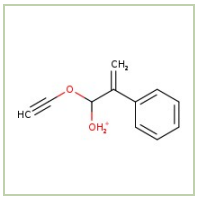	49	175.075356	C#COC([OH2+])C(=C)C1=CC=CC=C1
No Image	50	286.1437699	C=C1C2OC2C(=C=COC([OH2+])C(C)C2=CC=CC=C2)N1C
No Image	51	286.1437699	C=C(C1=CC=CC=C1)C([OH2+])OC1=CCN(C)C(C2CO2)=C1
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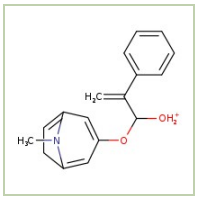
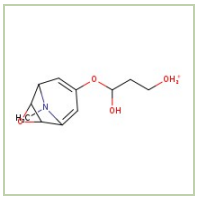
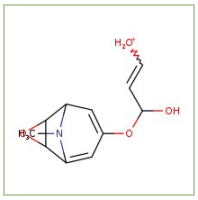
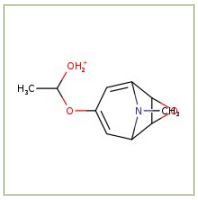
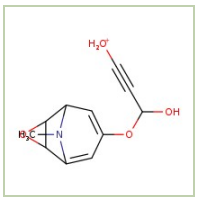
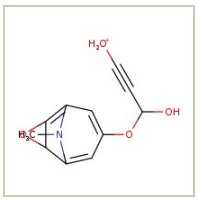
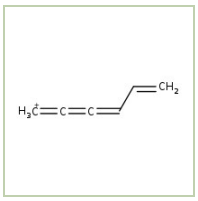
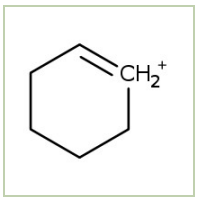
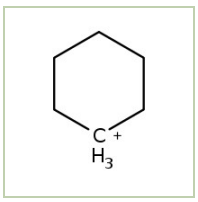
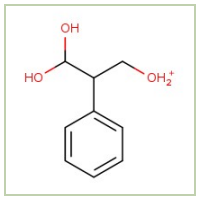
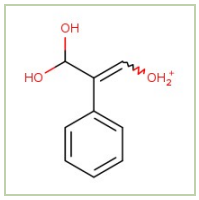
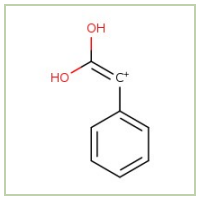
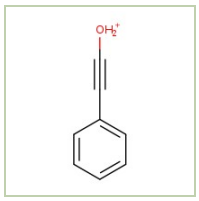
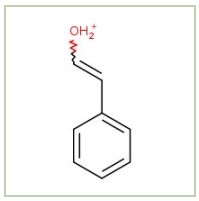
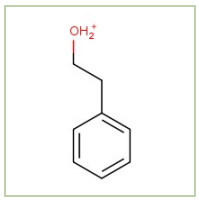
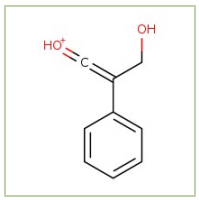
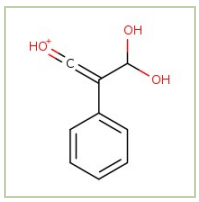
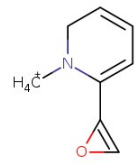
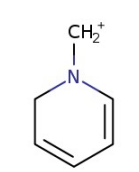
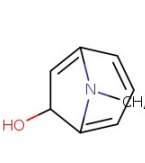
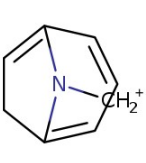
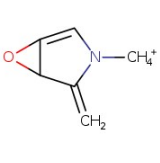
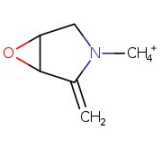
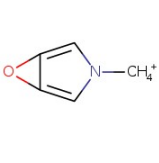
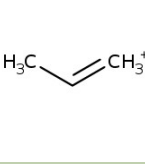
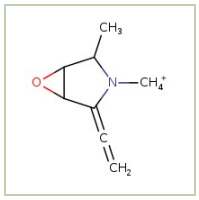
	53	268.1332052	C=C(C1=CC=CC=C1)C([OH2+])OC1=CC2=CCC(=C1)N2C

	54	226.1073844	CN1C2=CC(OC(O)CC[OH2+])=CC1C1OC21
	55	224.0917343	CN1C2=CC(OC(O)C=C[OH2+])=CC1C1OC21
	56	196.0968197	CC([OH2+])OC1=CC2C3OC3C(=C1)N2C
	57	222.0760843	CN1C2=CC(OC(O)C#C[OH2+])=CC1C1OC21
	58	220.0604342	CN1C2=CC(OC(O)C#C[OH2+])=CC1=C1OC21
	59	79.05422664	C=CC=C=C=[CH3+]
	60	83.08552677	C1=[CH2+]CCCC1
	61	85.10117684	C1CC[CH3+]CC1

	62	169.0859207	OC(O)C(C[OH2+])C1=CC=CC=C1
	63	167.0702706	OC(O)C(=C[OH2+])C1=CC=CC=C1
	64	135.0440559	OC(O)=[C+]C1=CC=CC=C1
	65	119.0491413	[OH2+]C#CC1=CC=CC=C1
	66	121.0647913	[OH2+]C=CC1=CC=CC=C1
	67	123.0804414	[OH2+]CCC1=CC=CC=C1
	68	149.0597059	OCC(=C=[OH+])C1=CC=CC=C1
	69	165.0546206	OC(O)C(=C=[OH+])C1=CC=CC=C1

	70	136.0756904	[CH4+]N1CC=CC=C1C1=CO1
	71	94.06512568	[CH2+]N1C=CC=CC1
	72	136.0756904	[CH4+]N1C2=CC(O)C1=CC=C2
	73	118.0651257	[CH2+]N1C2=CCC1=CC=C2
No Image	74	138.0913404	C=C=CC1C2OC2CN1[CH4+]
	75	110.0600403	C=C1C2OC2=CN1[CH4+]
	76	112.0756904	C=C1C2OC2CN1[CH4+]
	77	96.04439023	[CH4+]N1C=C2OC2=C1
	78	43.05422664	CC=[CH3+]

	79	138.0913404	C=C=C1C2OC2C(C)N1[CH4+]
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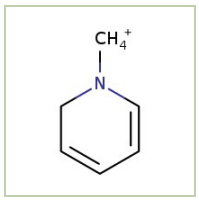
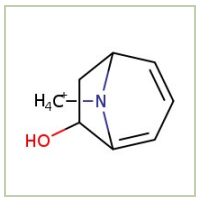
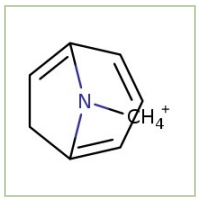
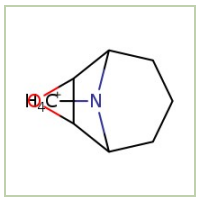
	81	43.01784114	C1=C[OH+]1
	82	96.08077574	[CH4+]N1C=CC=CC1
	83	138.0913404	[CH4+]N1C2=CC=CC1CC2O
	84	120.0807757	[CH4+]N1C2=CCC1=CC=C2
	85	140.1069905	[CH4+]N1C2CCCC1C1OC12
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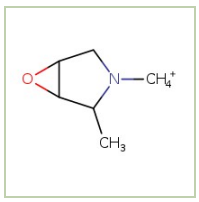
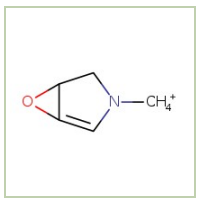
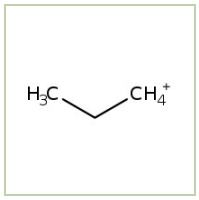
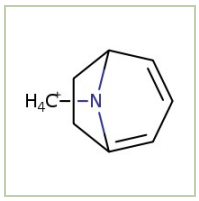
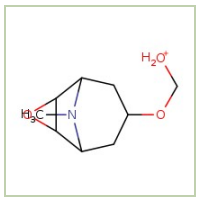
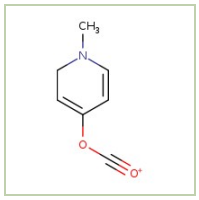
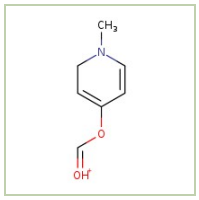
	87	114.0913404	CC1C2OC2CN1[CH4+]
	88	98.0600403	[CH4+]N1C=C2OC2C1

	89	45.06987671	CC[CH4+]
No Image	90	140.1069905	[CH4+]N1CC=CCC1C1CO1
No Image	91	140.1069905	[CH4+]N1C2C=CCC1C(O)C2
	92	122.0964258	[CH4+]N1C2=CC=CC1CC2
	93	186.1124698	CN1C2CC(OC[OH2+])CC1C1OC12
No Image	94	182.0811697	C=C(C=C1C2OC2=CN1C)OC[OH2+]
No Image	95	182.0811697	C=C1C2OC2C(=C=COC[OH2+])N1C
No Image	96	182.0811697	CN1CC=C(OC[OH2+])C=C1C1=CO1
	97	138.0549549	CN1C=CC(OC#[O+])=CC1
	98	140.070605	CN1C=CC(OC=[OH+])=CC1
No Image	99	182.0811697	CN1C2=CC(O)C1=CC(OC[OH2+])=C2

...

There are over 100 fragments, download the results (/system/predict_queries/output_files/003/050/963/original/output.txt?1714245023) to view the full list.