Results

Spectrum Prediction Input Parameters:

Parent Compound Structure (InChi Format)	InChI=1S/C19H19N7O6/c20-19-25-15-14(17(30)26-19)23-11(8-22-15)7-21-10-3-1-9(2-4-10)16(29)24-12(18(31)32)5-6-13(27)28/h1-4,8,12,21H,5-7H2,(H,24,29)(H,27,28)(H,31,32)(H3,20,22,25,26,30)
Parent Compound Mass	441.13968136028996
Spectra Type	ESI
Ion Mode	Positive
Adduct Type	[M+H]+
Probability Threshold	0.001
Status	**Completed**

Results:

Computed Results

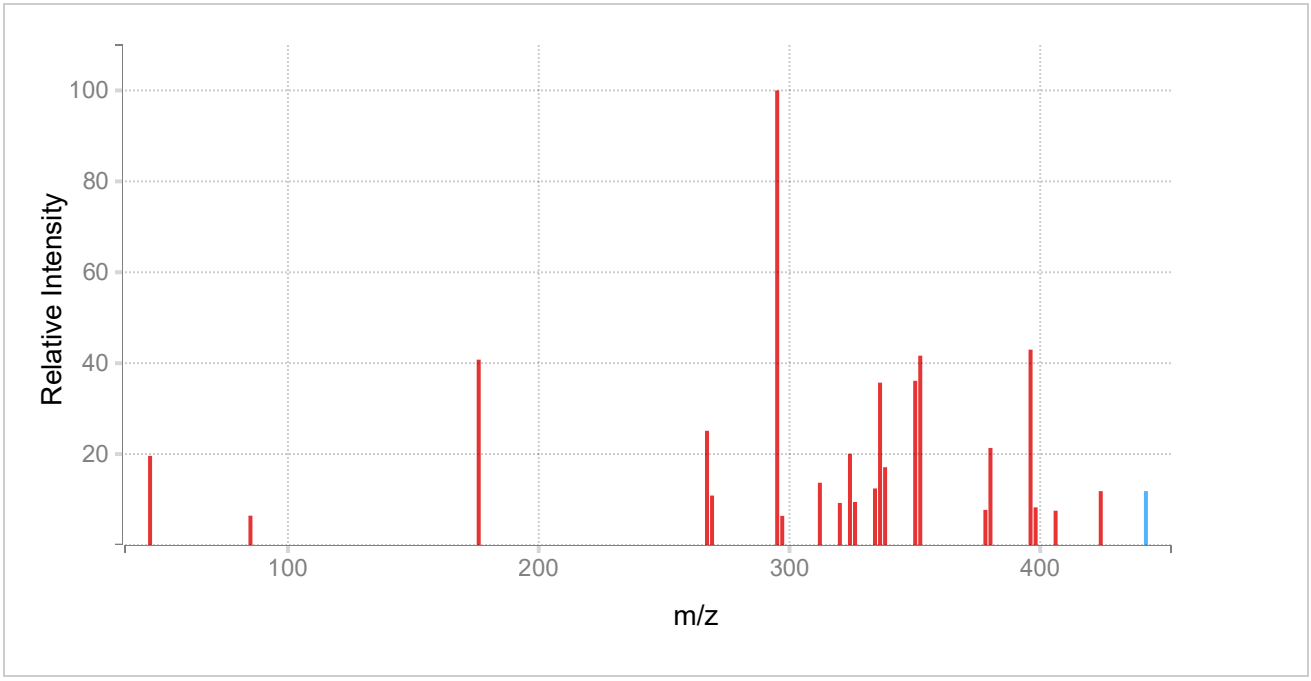
Computed Results:

Download (/system/predict_queries/output_files/003/055/011/original/output.txt?1715273288)

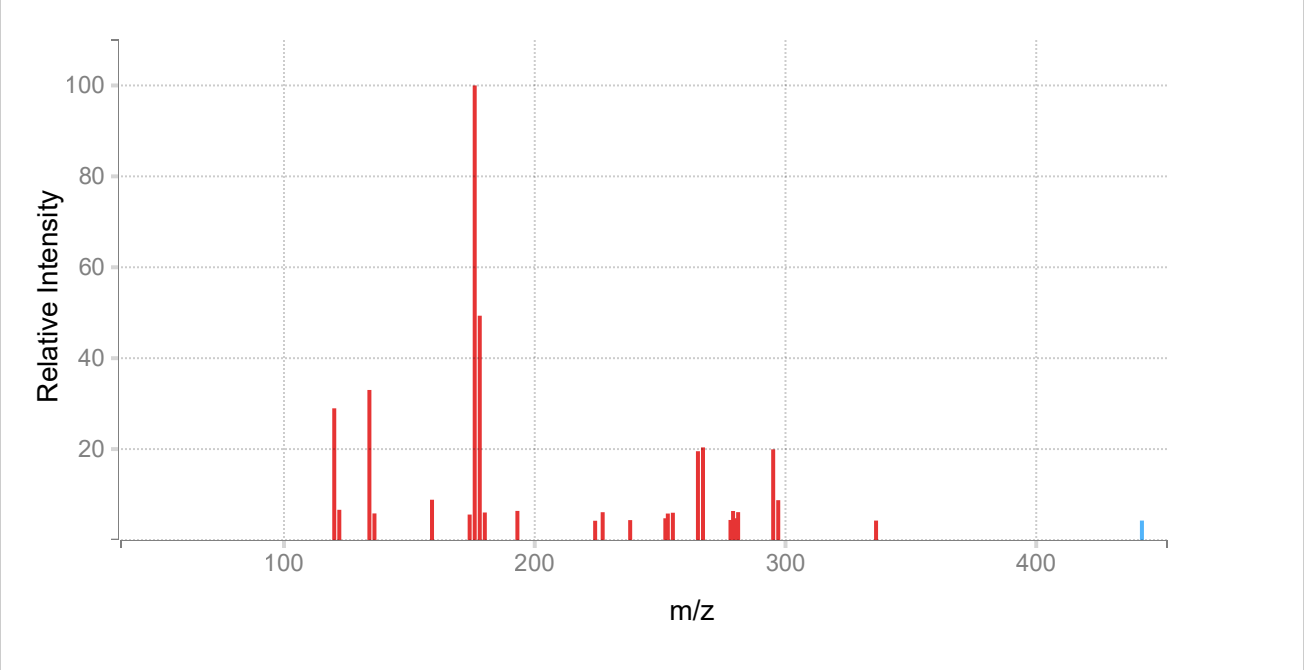
Predicted spectra are shown below. Peaks for which corresponding fragments have been found are colored red; unassigned peaks are colored blue. Hover over the peaks to see the exact mass and intensity values, along with the highest scoring assigned fragments, if found. Clicking on red spectra lines will 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/C19H19N7O6/c20-19-25-15-14(17(30)26-19)23-11(8-22-15)7-21-10-3-1-9(2-4-10)16(29)24-12(18(31)32)5-6-13(27)28/h1-4,8,12,21H,5-7H2,(H,24,29)(H,27,28)(H,31,32)(H3,20,22,25,26,30)

energy0

176.0566862	6.106299372	36 42 45 43 44	5.8459 0.13128 0.10273 0.018078 0.0083227
295.0938	22.91604108	14 157 148 160 143 152 141 154 140 142 145 139 146 104	21.588 0.49242 0.39593 0.19611 0.07656 0.05452 0.03872 0.0251 0.017813 0.014428 0.009308 0.0048204 0.0016676 0.00025261
396.1414785	3.056782848	71 31 86 90 91 88 89	2.1378 0.84908 0.033065 0.017564 0.014425 0.0032383 0.0016238
398.1571285	2.912234501	92 35	2.6504 0.26187
424.1363931	17.43376796	117 201 200	10.991 6.285 0.15812
442.1469578	29.37500971	0 218 209 217 204 213 215 207 208 205	29.18 0.072144 0.058883 0.028651 0.013668 0.010033 0.0043619 0.0032039 0.0023431 0.0019742
442.14695736028995	29.37500971		

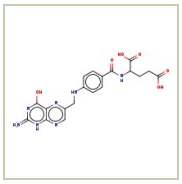
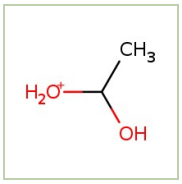
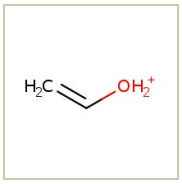
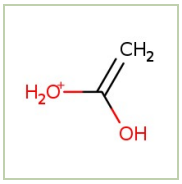
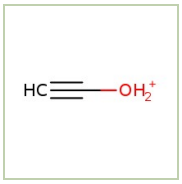
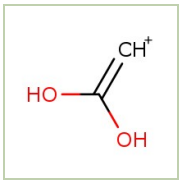
energy1

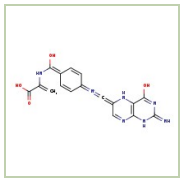
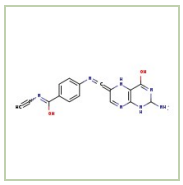
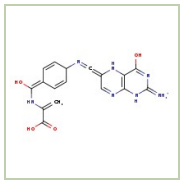
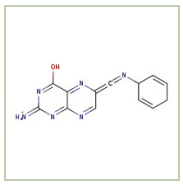
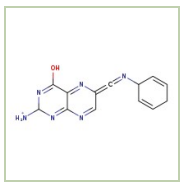
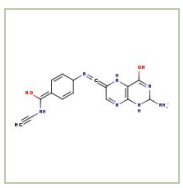
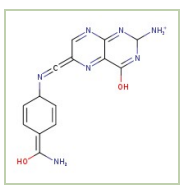
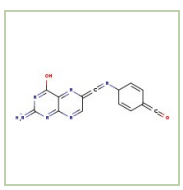
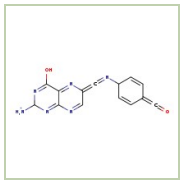
44.99710569	3.143150981	69	3.1432
85.02840582	1.034603383	114	1.0346
176.0566862	6.536677488	36 45 42 44 43	5.9958 0.19456 0.17467 0.086325 0.085301
267.0988854	4.028300933	9 149 55 110	3.4147 0.4455 0.12708 0.041031
269.1145355	1.743714522	10 61 59 60 180	1.6509 0.063761 0.014102 0.0094878 0.0054973

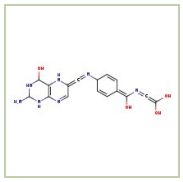
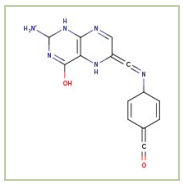
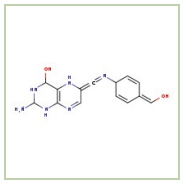
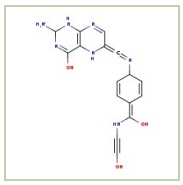
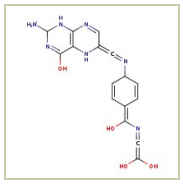
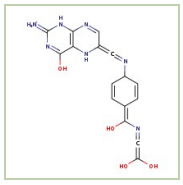
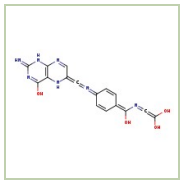
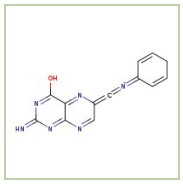
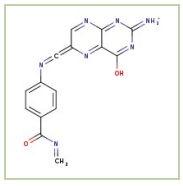
295.0938	16.03250645	14 148 160 154	13.241 0.61946 0.534 0.30615 0.30251
		152 141 140 145	0.22459 0.20524 0.20176 0.10953
		157 143 142 139	0.091431 0.08439 0.064037 0.038866
		146 104	0.0096001
297.1094501	1.026194179	16 190 171 187	0.93379 0.034189 0.010604 0.0096552
		179 169 184 172	0.0083964 0.0079505 0.005649
		177 168 188 178	0.0039605 0.0038877 0.0034728
		175	0.0026609 0.001417 0.00056118
312.1203491	2.196361823	12 108 106 102	2.0524 0.082442 0.020968 0.018234
		105 107 101	0.012267 0.0057785 0.0043073
320.089049	1.482846558	23	1.4828
324.1203491	3.216745231	74	3.2167
326.1359992	1.517434207	73	1.5174
334.104699	1.994039319	72	1.994
336.1203491	5.725113914	7	5.7251
338.1359992	2.743058292	11	2.7431
350.1359992	5.791812757	30	5.7918
352.1516492	6.677157376	33	6.6772
378.1309138	1.238684134	79 85	1.062 0.17664
380.1465639	3.423489703	38 93	1.7144 1.7091
396.1414785	6.89101195	71 31 86 91 89	5.3912 0.9803 0.19494 0.11363 0.094209
		88 90	0.077082 0.039653
398.1571285	1.327363751	35 92	0.8093 0.51806
406.1258284	1.208852653	119	1.2089
424.1363931	1.900237619	201 117 200	0.87023 0.80627 0.22373
442.14695736028995	1.900237619		
energy2			
120.0443902	6.155847258	133	6.1558
122.0600403	1.411548465	163	1.4115
134.0600403	7.014274459	162	7.0143
136.0756904	1.241873634	191	1.2419
159.0301371	1.882533326	41	1.8825
174.0410362	1.1895648	124	1.1896
176.0566862	21.25047798	45 36 43 44 42	11.323 6.4402 1.2625 1.1383 1.0863
178.0723363	10.48552676	50 49	7.1746 3.311
180.0879864	1.285470467	51	1.2855
193.0832353	1.360252987	164	1.3603
224.0930717	0.8998419099	57	0.89984
227.0927374	1.299268502	155	1.2993
238.0611029	0.9296163049	181	0.92962
252.0879864	1.014916465	161	1.0149
253.0720019	1.23654189	153 156	0.69021 0.54633
255.087652	1.274504851	182 186	0.88971 0.3848
265.0832353	4.150211348	22 128	3.8719 0.27836
267.0988854	4.329358421	55 9 149 110	1.9469 1.7246 0.37222 0.28558
278.0672509	0.9367317351	138 159 151	0.89505 0.022905 0.018776
279.0988854	1.356534803	166 165	0.99575 0.36079
280.082901	1.016843527	167 183 176 174	0.6517 0.17348 0.13989 0.03278
		189	0.019002

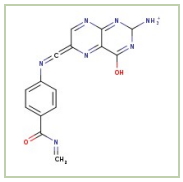
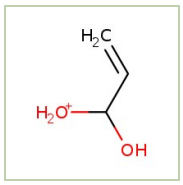
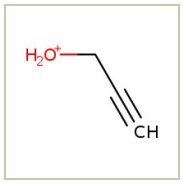
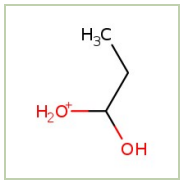
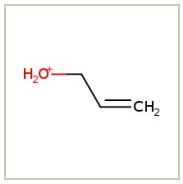
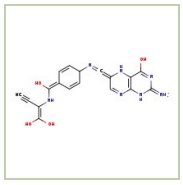
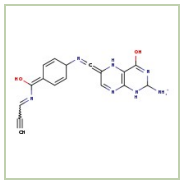
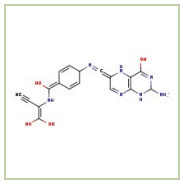
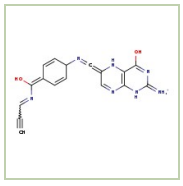
281.1145355	1.301899451	192 193	0.93193 0.36997
295.0938	4.238321363	141 14 160 146	2.1355 0.50588 0.50517 0.20133 0.13415
		140 152 143 154	0.12421 0.11295 0.112 0.10688 0.093621
		148 157 139 104	0.08944 0.060278 0.030747 0.02617
		142 145	
297.1094501	1.86152952	171 16 179 184	0.85265 0.23138 0.17612 0.11175
		187 169 188 168	0.093832 0.083562 0.067853 0.058495
		178 190 172 175	0.055935 0.049608 0.038112 0.025325
		177	0.016915
336.1203491	0.908036007	7	0.90804
442.14695736028995	0.908036007		

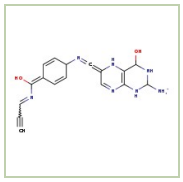
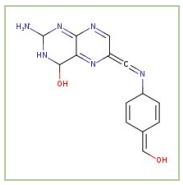
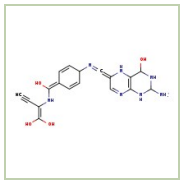
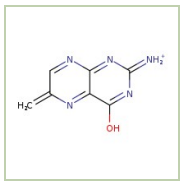
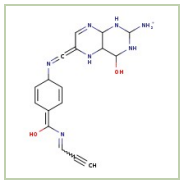
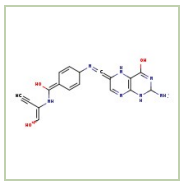
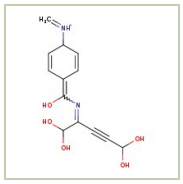
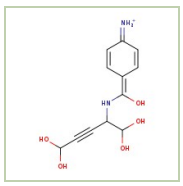
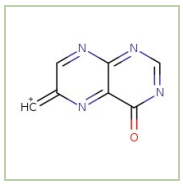
Fragments Generated

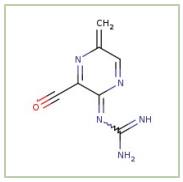
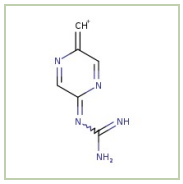
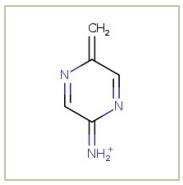
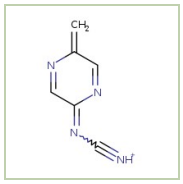
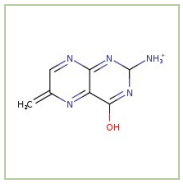
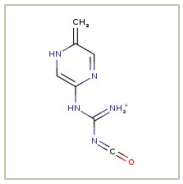
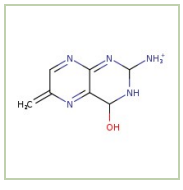
Structure	ID	Mass	SMILES
	0	442.14695 78	[NH2+]=c1nc(O)c2nc(CNc3ccc(C(=O)NC(CCC(=O)O)C(=O)O)cc3) cnc2[nH]1
	1	63.044055 88	CC(O)[OH2+]
	2	45.033491 2	C=C[OH2+]
	3	61.028405 82	C=C(O)[OH2+]
	4	43.017841 14	C#C[OH2+]
	5	59.012755 76	[CH+]=C(O)O

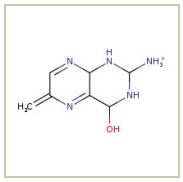
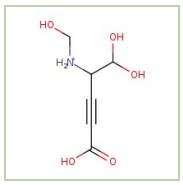
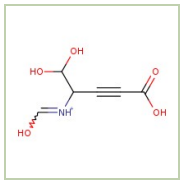
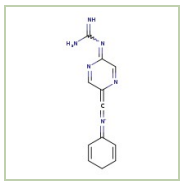
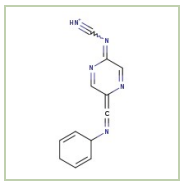
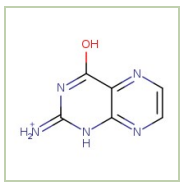
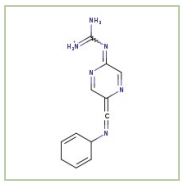
	6	380.1101783	C=C(NC(O)=C1C=CC(=[N+]=C=C2C=NC3=C(N2)C(O)=NC(=N)N3)C=C1)C(=O)O
	7	336.1203491	C#CN=C(O)C1=CC=C(N=C=C2C=NC3=C(N2)C(O)=NC([NH3+])N3)C=C1
	8	382.1258284	C=C(NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC(=[NH2+])N3)C=C1)C(=O)O
	9	267.0988854	[NH2+]=C1N=C(O)C2=NC(=C=NC3C=CCC=C3)C=NC2=N1
	10	269.1145355	[NH3+]C1N=C(O)C2=NC(=C=NC3C=CCC=C3)C=NC2=N1
	11	338.1359992	C#CNC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC([NH3+])N3)C=C1
	12	312.1203491	NC(O)=C1C=CC(N=C=C2C=NC3=NC([NH3+])N=C(O)C3=N2)C=C1
	13	293.0781499	[NH2+]=C1N=C(O)C2=NC(=C=NC3C=CC(=C=O)C=C3)C=NC2=N1
	14	295.0938	[NH3+]C1N=C(O)C2=NC(=C=NC3C=CC(=C=O)C=C3)C=NC2=N1

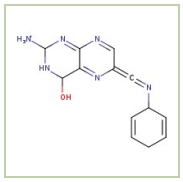
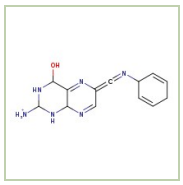
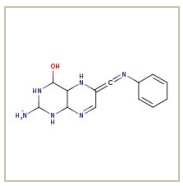
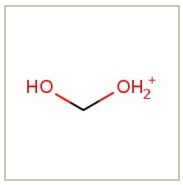
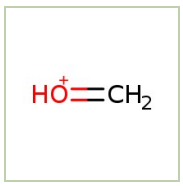
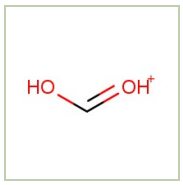
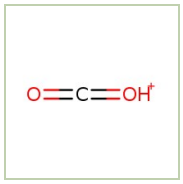
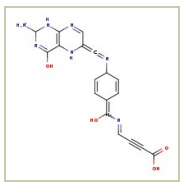
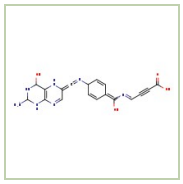
	15	372.1414785	[NH3+]C1NC2=C(NC(=C=NC3C=CC(=C(O)N=C=C(O)O)C=C3)C=N2)C(O)N1
	16	297.1094501	[NH3+]C1N=C(O)C2=C(N=CC(=C=NC3C=CC(=C=O)C=C3)N2)N1
	17	301.1407502	[NH3+]C1NC2=C(NC(=C=NC3C=CC(=CO)C=C3)C=N2)C(O)N1
	18	354.1309138	[NH3+]C1N=C(O)C2=C(N=CC(=C=NC3C=CC(=C(O)NC#CO)C=C3)N2)N1
	19	370.1258284	[NH3+]C1N=C(O)C2=C(N=CC(=C=NC3C=CC(=C(O)N=C=C(O)O)C=C3)N2)N1
	20	368.1101783	[NH2+]=C1N=C(O)C2=C(N=CC(=C=NC3C=CC(=C(O)N=C=C(O)O)C=C3)N2)N1
	21	366.0945283	N=C1N=C(O)C2=C(N=CC(=C=[N+]=C3C=CC(=C(O)N=C=C(O)O)C=C3)N2)N1
	22	265.0832353	N=C1N=C(O)C2=NC(=C=[N+]=C3C=CCC=C3)C=NC2=N1
	23	320.0890449	C=NC(=O)C1=CC=C(N=C=C2C=NC3=NC(=[NH2+])N=C(O)C3=N2)C=C1

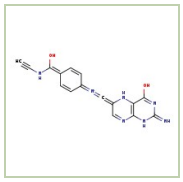
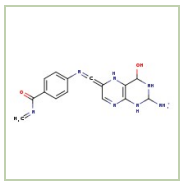
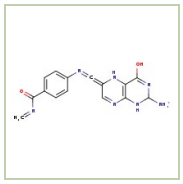
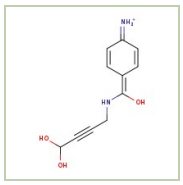
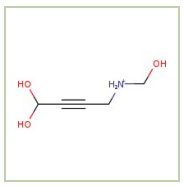
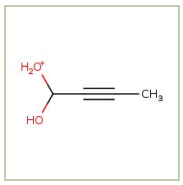
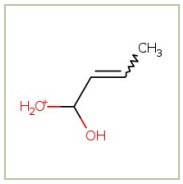
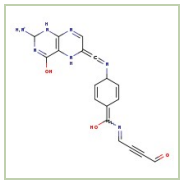
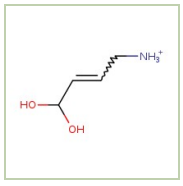
	24	322.104699	C=NC(=O)C1=CC=C(N=C=C2C=NC3=NC([NH3+])N=C(O)C3=N2)C=C1
	25	75.04405588	C=CC(O)[OH2+]
	26	57.0334912	C#CC[OH2+]
	27	77.05970595	CCC(O)[OH2+]
	28	59.04914126	C=CC[OH2+]
	29	394.1258284	C#CC(NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC(=[NH2+])N3)C=C1)=C(O)O
	30	350.1359992	C#CC=NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC([NH3+])N3)C=C1
	31	396.1414785	C#CC(NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC([NH3+])N3)C=C1)=C(O)O
	32	348.1203491	C#CC=NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC(=[NH2+])N3)C=C1

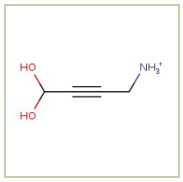
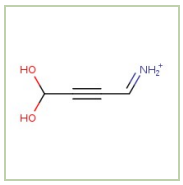
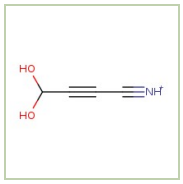
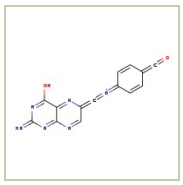
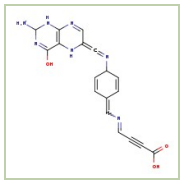
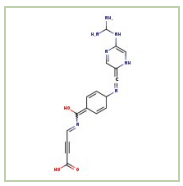
	33	352.1516492	C#CC=NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)NC([NH3+])N3)C=C1
	34	299.1251001	[NH3+]C1N=C2N=CC(=C=NC3C=CC(=CO)C=C3)N=C2C(O)N1
	35	398.1571285	C#CC(NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)NC([NH3+])N3)C=C1)=C(O)O
	36	176.0566862	C=C1C=NC2=NC(=[NH2+])N=C(O)C2=N1
	37	354.1672993	C#CC=NC(O)=C1C=CC(N=C=C2C=NC3NC([NH3+])NC(O)C3N2)C=C1
	38	380.1465639	C#CC(=CO)NC(O)=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC([NH3+])N3)C=C1
	39	279.097548	C=[NH+]C1C=CC(=C(O)N=C(C#CC(O)O)C(O)O)C=C1
	40	267.097548	[NH2+]=C1C=CC(=C(O)NC(C#CC(O)O)C(O)O)C=C1
	41	159.0301371	[CH+]=C1C=NC2=NC=NC(=O)C2=N1

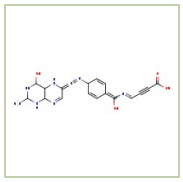
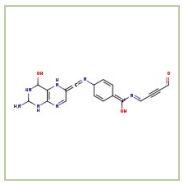
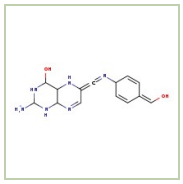
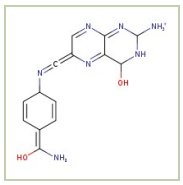
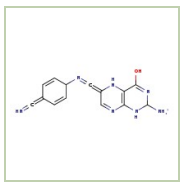
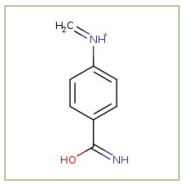
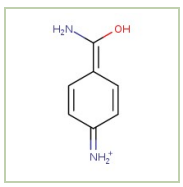
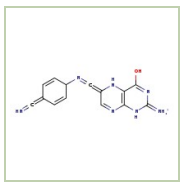
	42	176.0566862	C=C1C=NC(=NC(=N)N)C(C#[O+])=N1
No Image	43	176.0566862	[CH+]=C1C=NC(NC#N)=C(C(=N)O)N1
No Image	44	176.0566862	[CH+]=C1C=NC(N)=C(C(O)=NC#N)N1
No Image	45	176.0566862	[CH+]=C1C=NC(NC(=N)N=C=O)=CN1
	46	148.0617716	[CH+]=C1C=NC(=NC(=N)N)C=N1
	47	108.0556236	C=C1C=NC(=[NH2+])C=N1
	48	133.0508726	C=C1C=NC(=NC#[NH+])C=N1
	49	178.0723363	C=C1C=NC2=NC([NH3+])N=C(O)C2=N1
	50	178.0723363	C=C1C=NC(NC(=[NH2+])N=C=O)=CN1
	51	180.0879864	C=C1C=NC2=NC([NH3+])NC(O)C2=N1

	52	182.1036364	C=C1C=NC2NC([NH3+])NC(O)C2=N1
	53	176.0553488	O=C(O)C#CC([NH2+]CO)C(O)O
	54	174.0396988	O=C(O)C#CC([NH+]=CO)C(O)O
No Image	55	267.0988854	N=C(N=C=O)NC1=CNC(=C=[N+]=C2C=CCC=C2)C=N1
	56	239.1039708	N=C(N)N=C1C=NC(=C=[N+]=C2C=CCC=C2)C=N1
	57	224.0930717	[NH+]#CN=C1C=NC(=C=NC2C=CCC=C2)C=N1
	58	164.0566862	[NH2+]=C1N=C(O)C2=NC=CN=C2N1
No Image	59	269.1145355	N=C(N)NC1=C(C=O)NC(=C=[N+]=C2C=CCC=C2)C=N1
No Image	60	269.1145355	N=C(O)C1=C(NC#[NH+])N=CC(=C=NC2C=CCC=C2)N1
No Image	61	269.1145355	[NH2+]=C(N=C=O)NC1=CNC(=C=NC2C=CCC=C2)C=N1
	62	241.1196208	NC(=[NH2+])N=C1C=NC(=C=NC2C=CCC=C2)C=N1

	63	271.1301855	[NH3+]C1N=C2N=CC(=C=NC3C=CCC=C3)N=C2C(O)N1
	64	273.1458356	[NH3+]C1NC(O)C2=NC(=C=NC3C=CCC=C3)C=NC2N1
	65	275.1614856	[NH3+]C1NC(O)C2NC(=C=NC3C=CCC=C3)C=NC2N1
	66	49.02840582	OC[OH2+]
	67	31.01784114	C=[OH+]
	68	47.01275576	OC=[OH+]
	69	44.99710569	O=C=[OH+]
	70	394.1258284	[NH3+]C1N=C(O)C2=C(N=CC(=C=NC3C=CC(=C(O)N=CC#CC(=O)O)C=C3)N2)N1
	71	396.1414785	[NH3+]C1NC2=C(NC(=C=NC3C=CC(=C(O)N=CC#CC(=O)O)C=C3)C=N2)C(O)N1

	72	334.104699	C#CNC(O)=C1C=CC(=[N+]=C=C2C=NC3=C(N2)C(O)=NC(=N)N3)C=C1
	73	326.1359992	C=NC(=O)C1=CC=C(N=C=C2C=NC3=C(N2)C(O)NC([NH3+])N3)C=C1
	74	324.1203491	C=NC(=O)C1=CC=C(N=C=C2C=NC3=C(N2)C(O)=NC([NH3+])N3)C=C1
	75	221.0920687	[NH2+]=C1C=CC(=C(O)NCC#CC(O)O)C=C1
	76	132.0655196	OC[NH2+]CC#CC(O)O
	77	87.04405588	CC#CC(O)[OH2+]
	78	89.05970595	CC=CC(O)[OH2+]
	79	378.1309138	[NH3+]C1N=C(O)C2=C(N=CC(=C=NC3C=CC(=C(O)N=CC#CC=O)C=C3)N2)N1
	80	104.070605	[NH3+]CC=CC(O)O

	81	102.0549549	[NH3+]CC#CC(O)O
	82	100.0393049	[NH2+]=CC#CC(O)O
	83	98.02365479	[NH+]#CC#CC(O)O
	84	291.0624999	N=C1N=C(O)C2=NC(=C=[N+]=C3C=CC(=C=O)C=C3)C=NC2=N1
	85	378.1309138	[NH3+]C1N=C(O)C2=C(N=CC(=C=NC3C=CC(=CN=CC#CC(=O)O)C=C3)N2)N1
No Image	86	396.1414785	NC([NH3+])NC1=C(C=O)NC(=C=NC2C=CC(=C(O)N=CC#CC(=O)O)C=C2)C=N1
	87	368.1465639	NC([NH3+])NC1=CNC(=C=NC2C=CC(=C(O)N=CC#CC(=O)O)C=C2)C=N1
No Image	88	396.1414785	N=C(O)C1=C(NC[NH3+])N=CC(=C=NC2C=CC(=C(O)N=CC#CC(=O)O)C=C2)N1
No Image	89	396.1414785	NC1=C(C(O)=NC[NH3+])NC(=C=NC2C=CC(=C(O)N=CC#CC(=O)O)C=C2)C=N1
No Image	90	396.1414785	NC([NH3+])N=C(O)C1=CN=CC(=C=NC2C=CC(=C(O)N=CC#CC(=O)O)C=C2)N1
No Image	91	396.1414785	[NH3+]C(N=CO)NC1=CNC(=C=NC2C=CC(=C(O)N=CC#CC(=O)O)C=C2)C=N1

	92	398.1571285	[NH3+]C1NC(O)C2NC(=C=NC3C=CC(=C(O)N=CC#CC(=O)O)C=C3)C=NC2N1
	93	380.1465639	[NH3+]C1NC2=C(NC(=C=NC3C=CC(=C(O)N=CC#CC=O)C=C3)C=N2)C(O)N1
	94	303.1564003	[NH3+]C1NC(O)C2NC(=C=NC3C=CC(=CO)C=C3)C=NC2N1
	95	314.1359992	NC(O)=C1C=CC(N=C=C2C=NC3=NC([NH3+])NC(O)C3=N2)C=C1
	96	296.1254345	N=C=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC([NH3+])N3)C=C1
	97	149.0709393	C=[NH+]C1=CC=C(C(=N)O)C=C1
	98	137.0709393	NC(O)=C1C=CC(=[NH2+])C=C1
	99	294.1097844	N=C=C1C=CC(N=C=C2C=NC3=C(N2)C(O)=NC(=[NH2+])N3)C=C1

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There are over 100 fragments, download the results (/system/predict_queries/output_files/003/055/011/original/output.txt?1715273288) to view the full list.