

Environmental Science & Technology

Supporting Information

Influences of Temperature and Metal on Subcritical Hydrothermal Liquefaction of Hyperaccumulator: Implications for the Recycling of Hazardous Hyperaccumulators

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Text S1

Procedures of Modified European Community Bureau of Reference (BCR) Sequential Extraction

Modified BCR sequential extraction was carried out by using a four-stage modified procedure recommended by BCR, as listed below:¹

Step 1 (acid exchangeable fraction): 20 mL of 0.11 mol/L acetic acid were added to 0.5 g of hydrochar sample in a centrifuge tube and shaken for 16 h at room temperature. The extract was collected by centrifugation for 20 min at 5000 r/min to analyze metal content with inductively coupled plasma (ICP) technology. Residues were washed by 20 mL of deionized water, and then the supernatant was poured out.

Step 2 (easily reducible fraction): 20 mL of 0.50 mol/L hydroxylammonium chloride (pH was adjusted to 1.5) were added to the residues from step 1 in the centrifuge tube and shaken for 16 h at room temperature. The collection of the extract and residues were the same as described in Step 1.

Step 3 (oxidizable fraction): 5 mL of 8.8 mol/L hydrogen peroxide were added to the residue from step 2 in the centrifuge tube. The digestion was carried out freely at room temperature for 1 h with occasional manual shaking, followed by digestion at 85 °C for another 1 h in a water bath until the volume was reduced to about 2-3 mL. Then, another 5 mL of hydrogen peroxide were added, followed by digestion at room temperature for 1 h and at 85 °C for another 1 h. Finally, 25 mL of 1.0 mol/L ammonium acetate (pH was adjusted to 2.0) were added to the solution in

the centrifuge tube and shaken for 16 h at room temperature. The collection of the extract and residues were the same as described in Step 1.

Step 4 (residual fraction): The residue from Step 3 was digested using aqua regia to analyze metal elements content by ICP technology.

Text S2

Procedures of TCLP method

20 mL of leaching fluid (5.7 mL glacial acetic acid diluted into 1L with pH of 2.88 ± 0.05) were added to 1 g of biomass or hydrochar sample in a centrifuge tube and shaken for 16 h at room temperature. The extract was collected by centrifugation for 20 min at 5000 r/min to analyze metal content with inductively coupled plasma (ICP) technology.

References

(1) Nemati, K.; Bakar, N. K. A.; Abas, M. R.; Sobhanzadeh, E. Speciation of heavy metals by modified BCR sequential extraction procedure in different depths of sediments from Sungai Buloh, Selangor, Malaysia. *J. Hazard. Mater.* **2011**, *192*, 402-410.

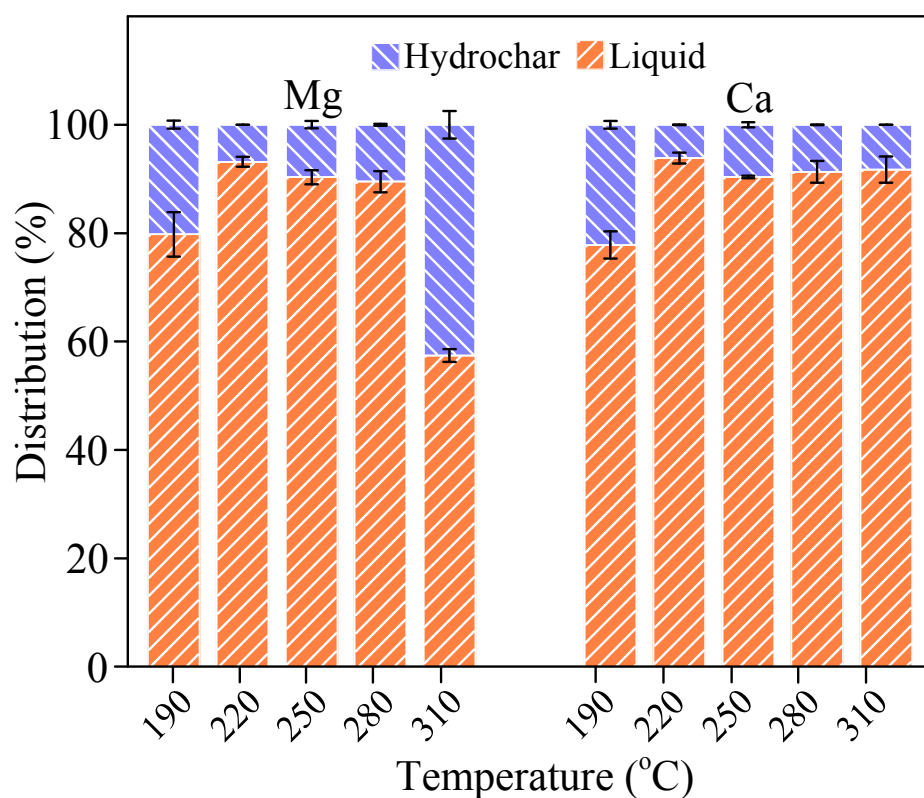


Figure S1. Distribution of Mg and Ca in hydrochar and liquid phase through HTL of *S. plumbizincicola* at various temperatures (190 - 310 °C). Experiments of metals distribution were performed in duplicate.

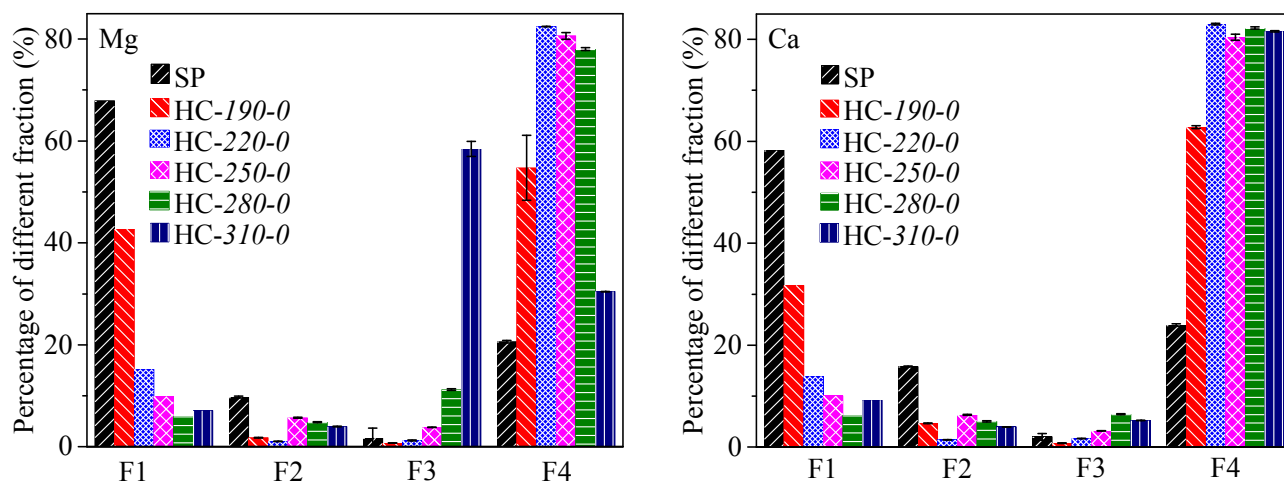


Figure S2. Percentage of different Mg and Ca fraction in *S. plumbizincicola* and hydrochar at various temperatures (190-310 °C) using modified BCR method (F1: acid exchangeable fraction; F2: easily reducible fraction; F3: oxidizable fraction; F4: residual fraction). Experiments of metals speciation distribution were performed in duplicate.

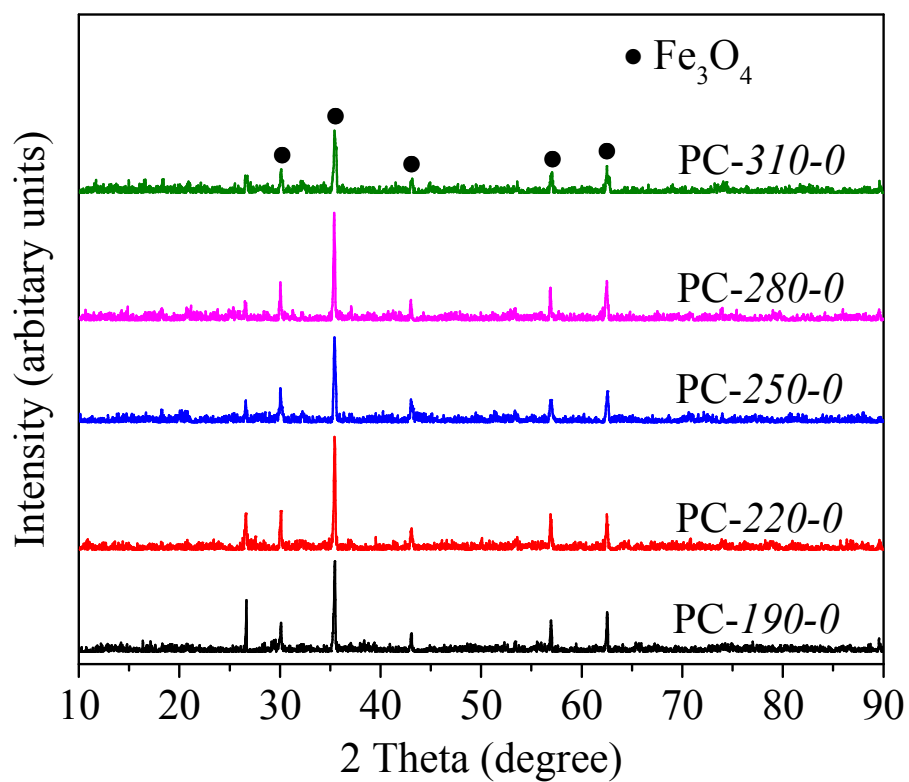


Figure S3. XRD patterns of PC samples with peak porosity from the surface area curves of different hydrochar.

Note: Based on Scherrer's equation, the crystal sizes of Fe_3O_4 were calculated as 49.8, 45.1, 36.3, 35.4 and 27.1 nm for PC-190-0, PC-220-0, PC-250-0, PC-280-0, PC-310-0 samples.

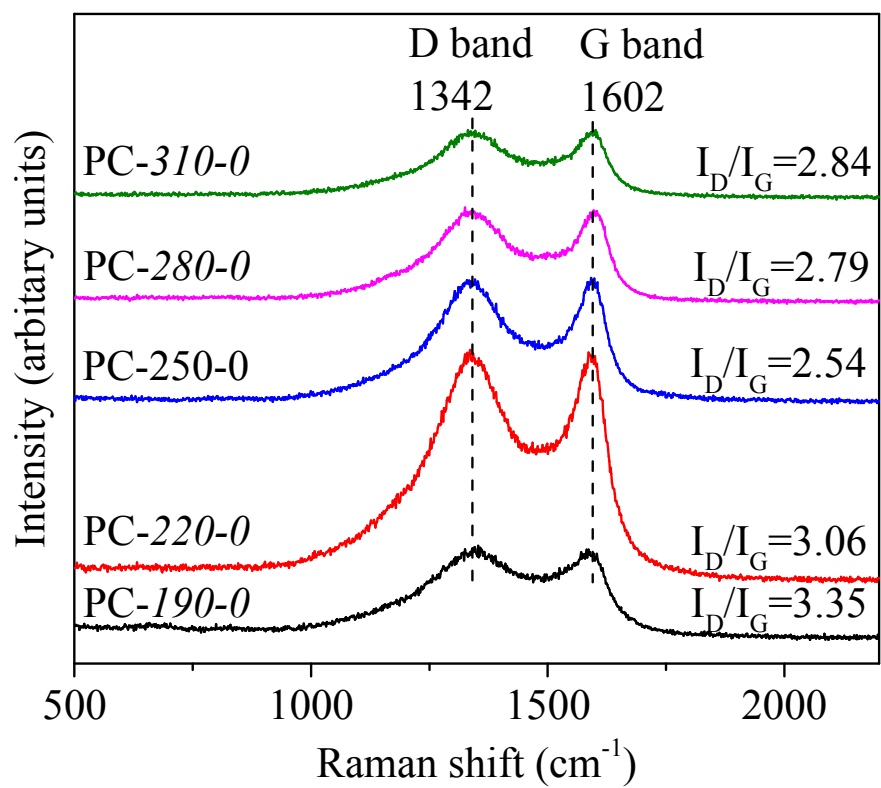


Figure S4. Raman spectra of PC samples with peak porosity.

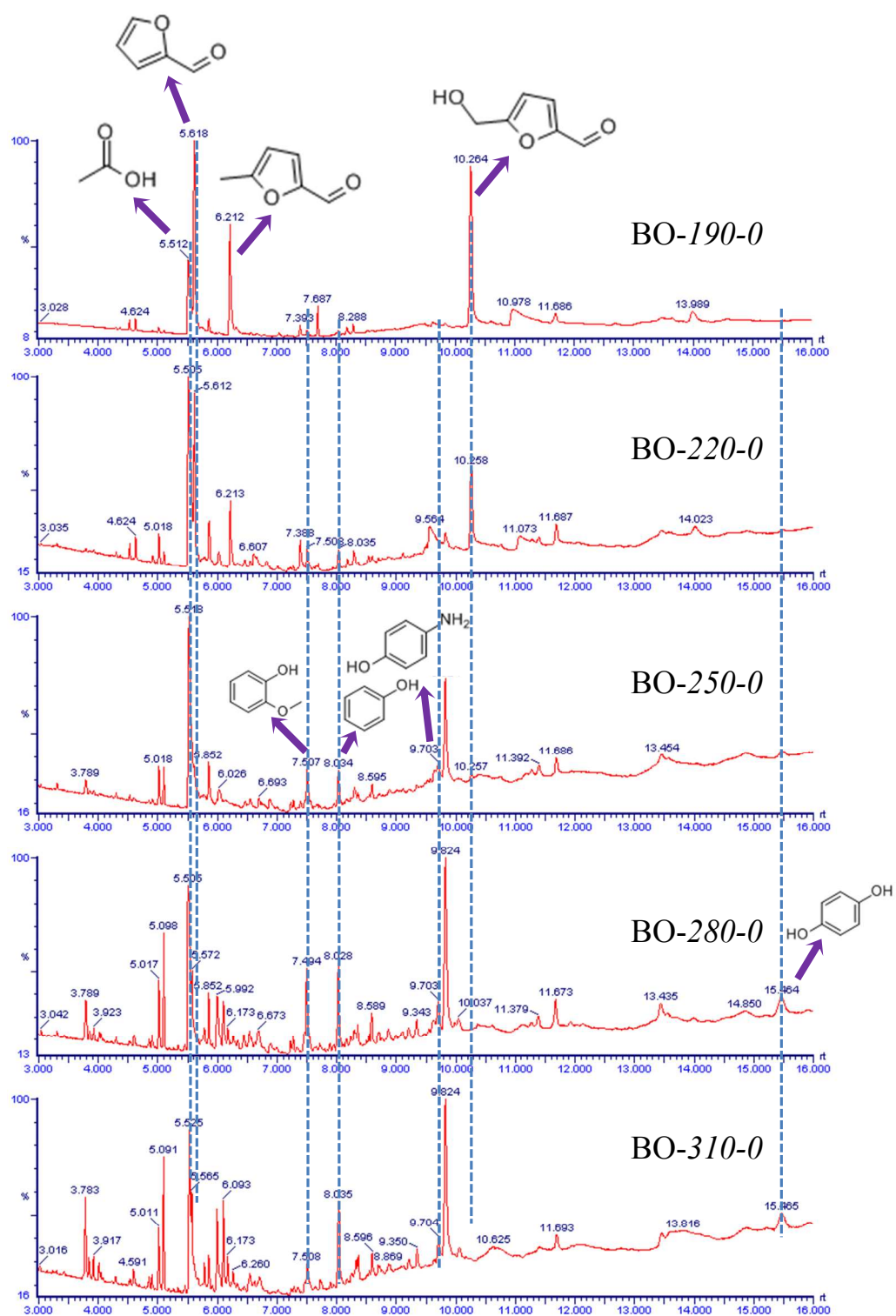


Figure S5. Total ion chromatogram (TIC) and the structure of main compounds obtained by GC-MS of bio-oils produced under different temperature of HTL.

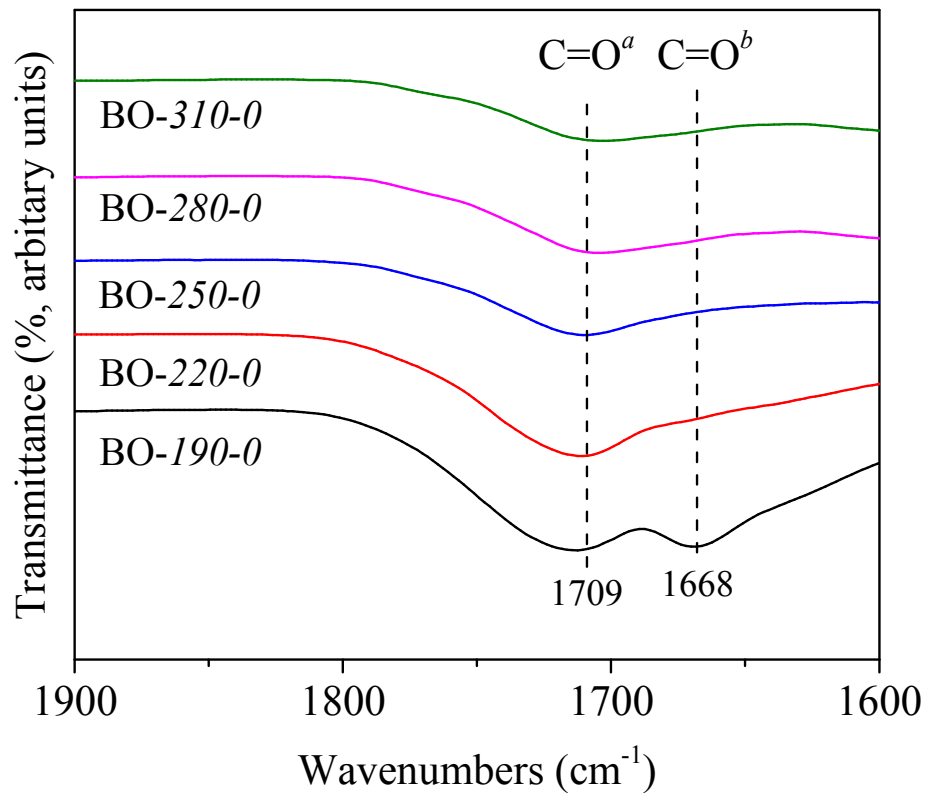


Figure S6. FTIR spectra of bio-oils derived from different temperature of HTL (C=O^a: C=O vibration in carboxylic acid, ketone, aldehydes, and esters; C=O^b: C=O vibration in carbohydrates).

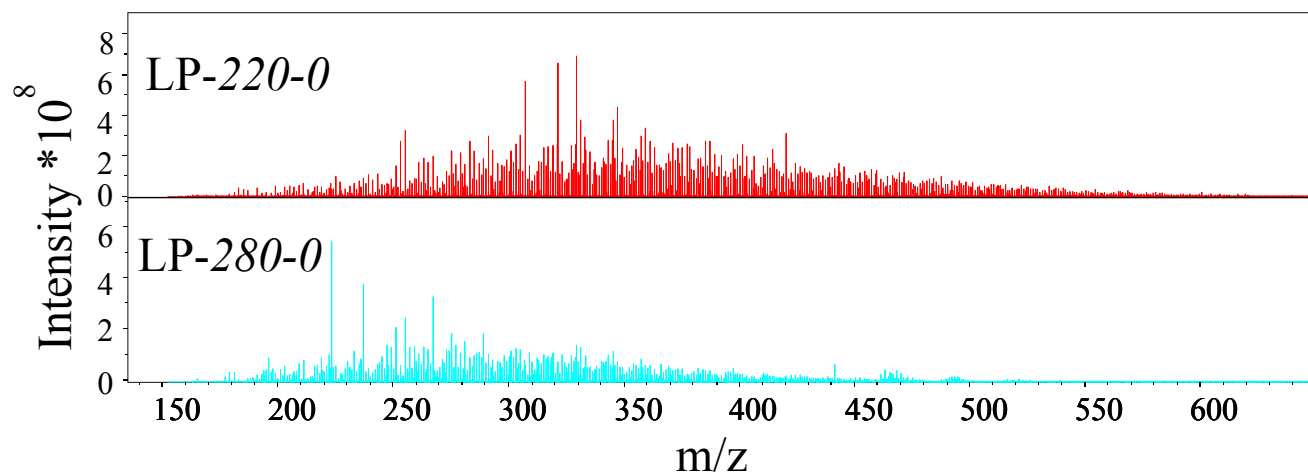


Figure S7. Broadband negative-ion ESI FT-ICR MS spectra of LP-220-0 and LP-280-0 samples analyzed at 9.4 T.

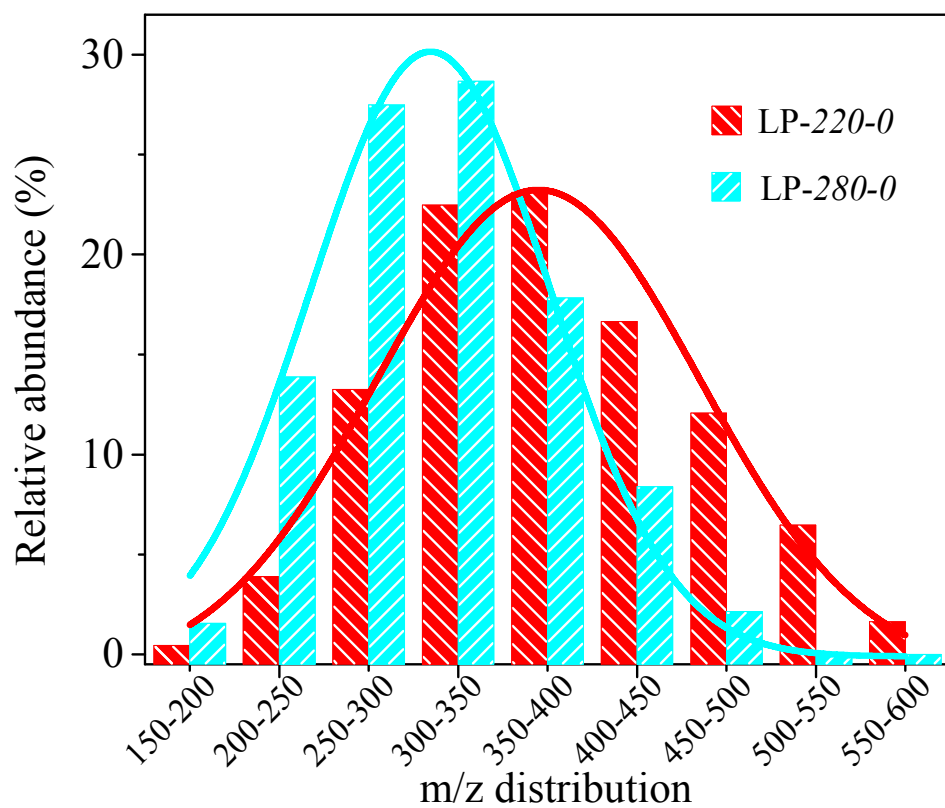


Figure S8. Mass distribution of LP-220-0 and LP-280-0 derived from negative-ion ESI FT-ICR mass spectra.

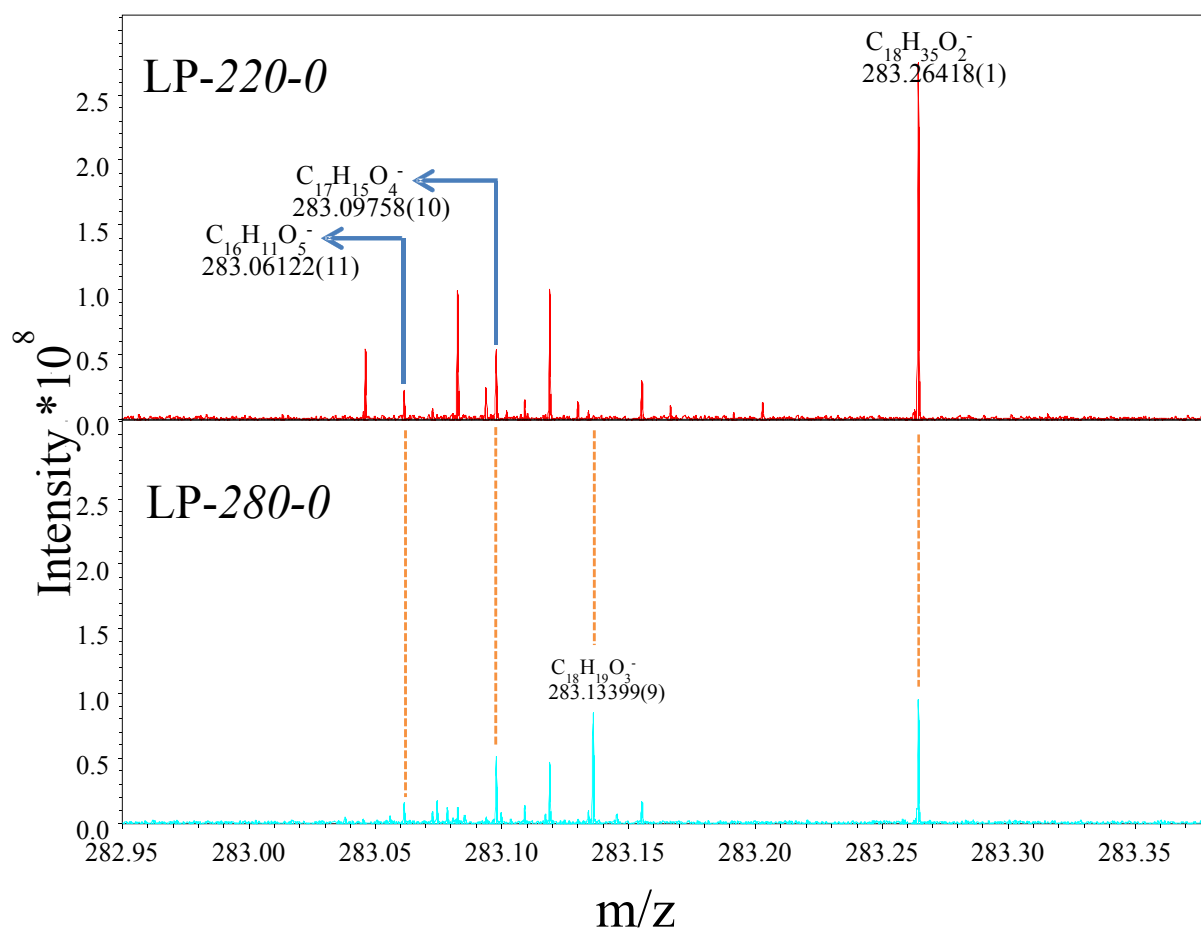


Figure S9. Mass scale-expanded segments (m/z 283) of FT-ICR MS for LP-220-0 and LP-280-0 (numbers in the brackets are the DBE values of relevant compounds).

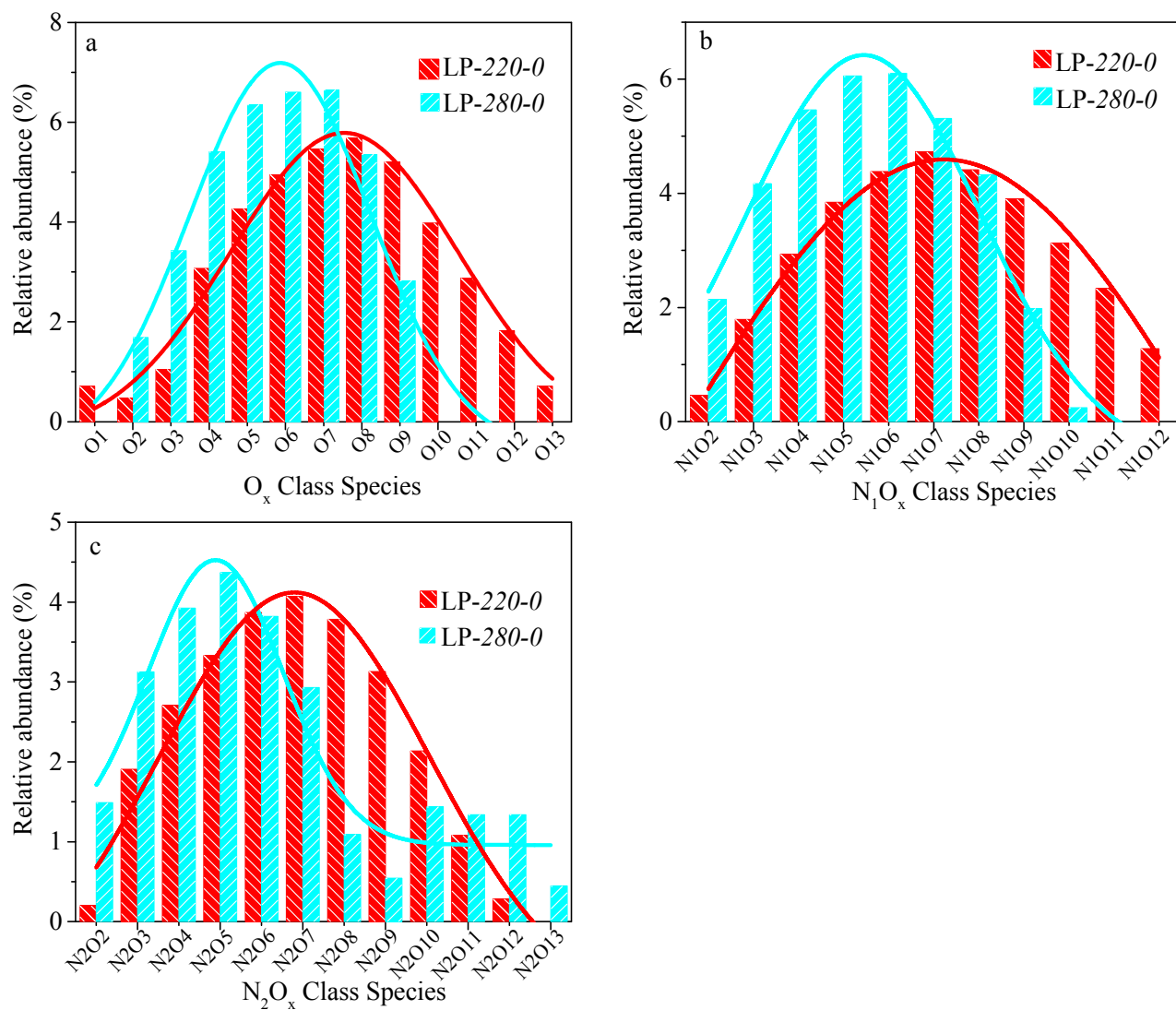


Figure S10. Relative abundance of (a) O_x class species, (b) N_1O_x class species and (c) N_2O_x class species of LP-220-0 and LP-280-0 by negative-ion ESI FT-ICR MS analysis.

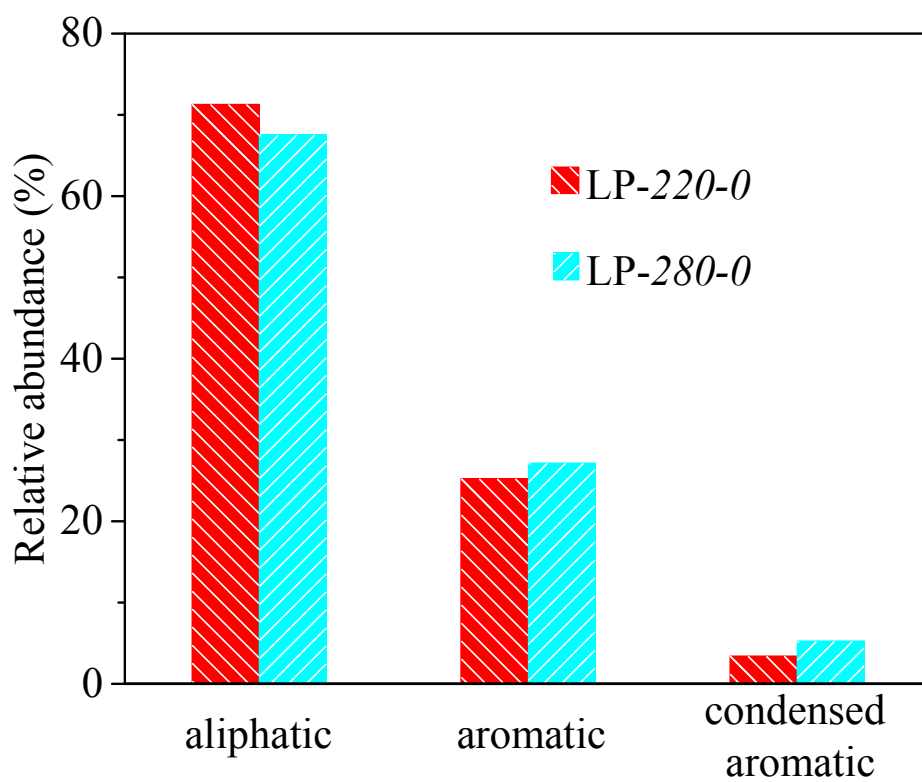


Figure S11. Classification of compounds in LP-220-0 and LP-280-0 into aliphatic, aromatic and condensed aromatic structures based on AI_{mod} values.

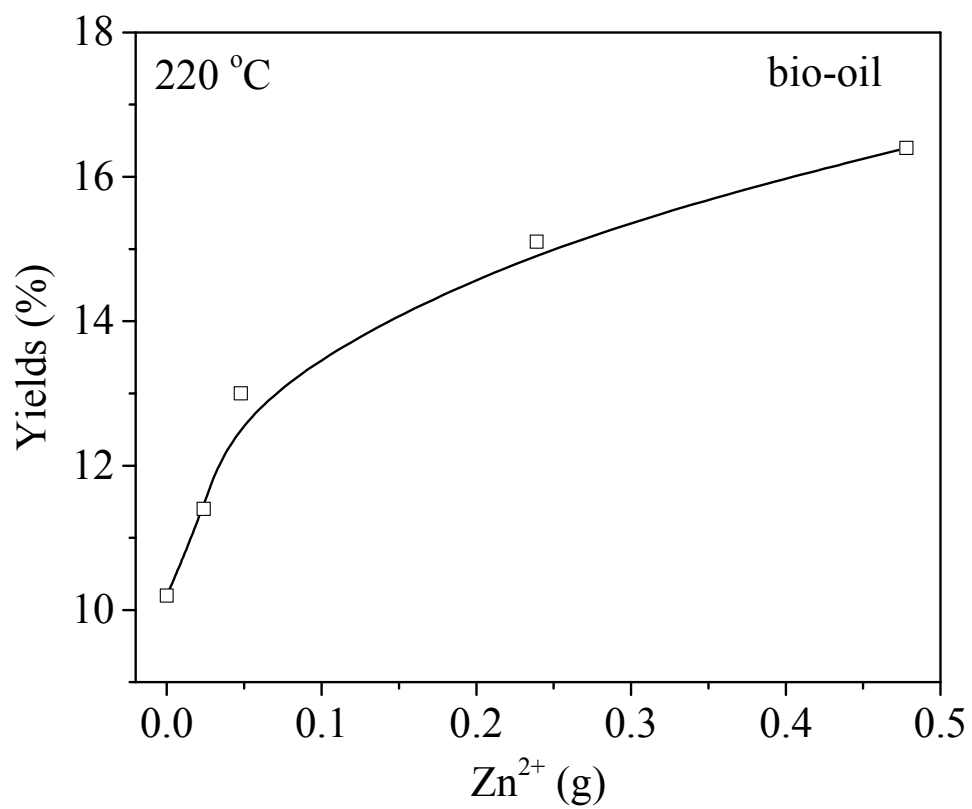


Figure S12. Effect of Zn²⁺ content on the yields of the resulting bio-oils from HTL process of *S. plumbizincicola* at 220 °C.

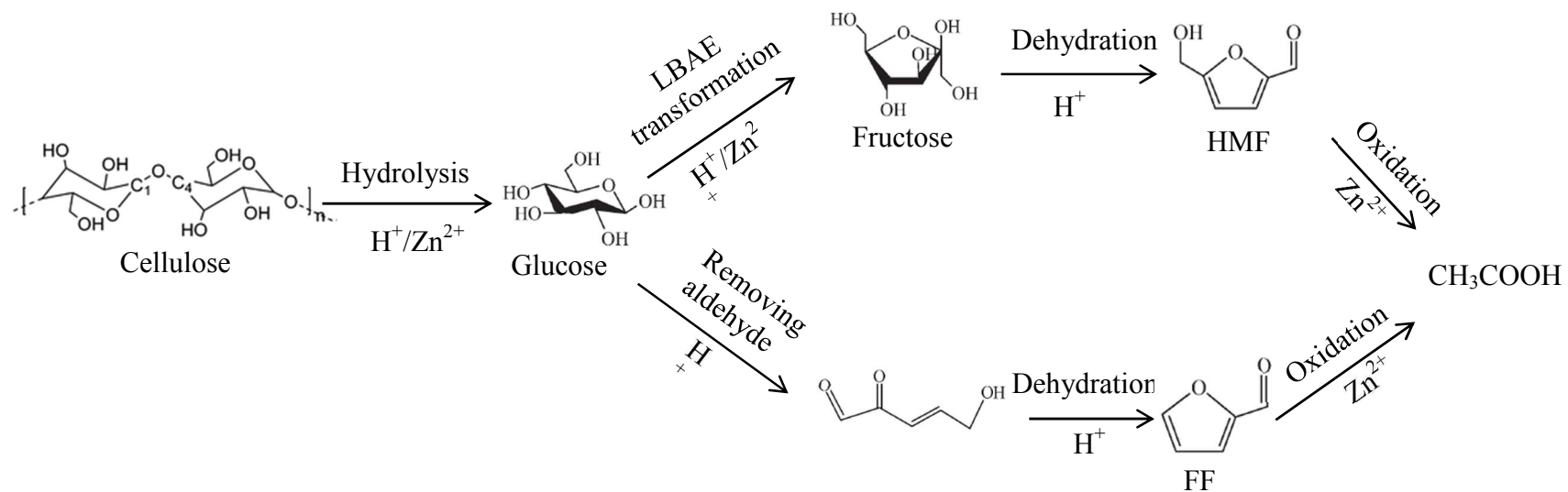


Figure S13. Proposed mechanisms for production of acetic acid from cellulose (LBAE transformation: Lobry de Bruyn-Alberda van Ekenstein transformation).

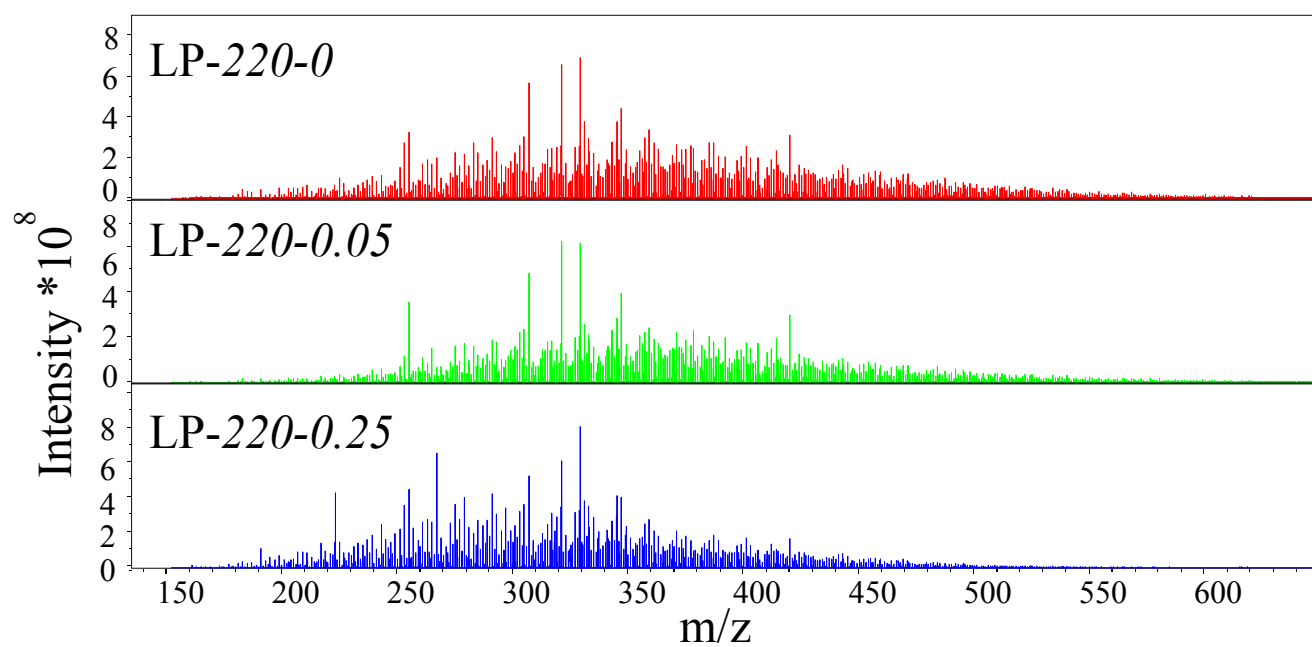


Figure S14. Broadband negative-ion ESI FT-ICR MS spectra of LP-220-0, LP-220-0.05 and LP-220-0.25 samples analyzed at 9.4 T.

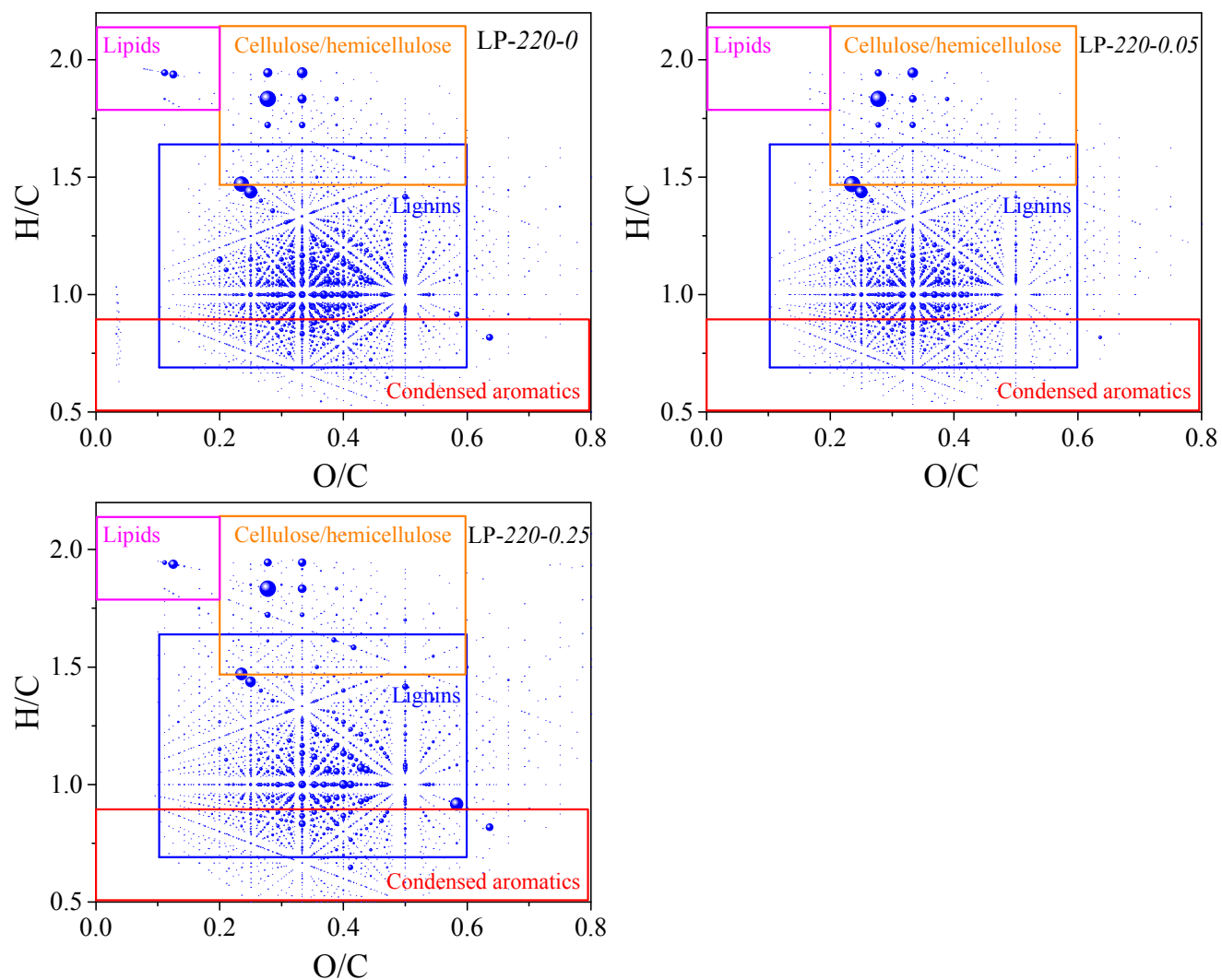


Figure S15. Van Krevelen diagram of compounds in LP-220-0, LP-220-0.05 and LP-220-0.25 (plot sizes represent relative abundance of compounds).

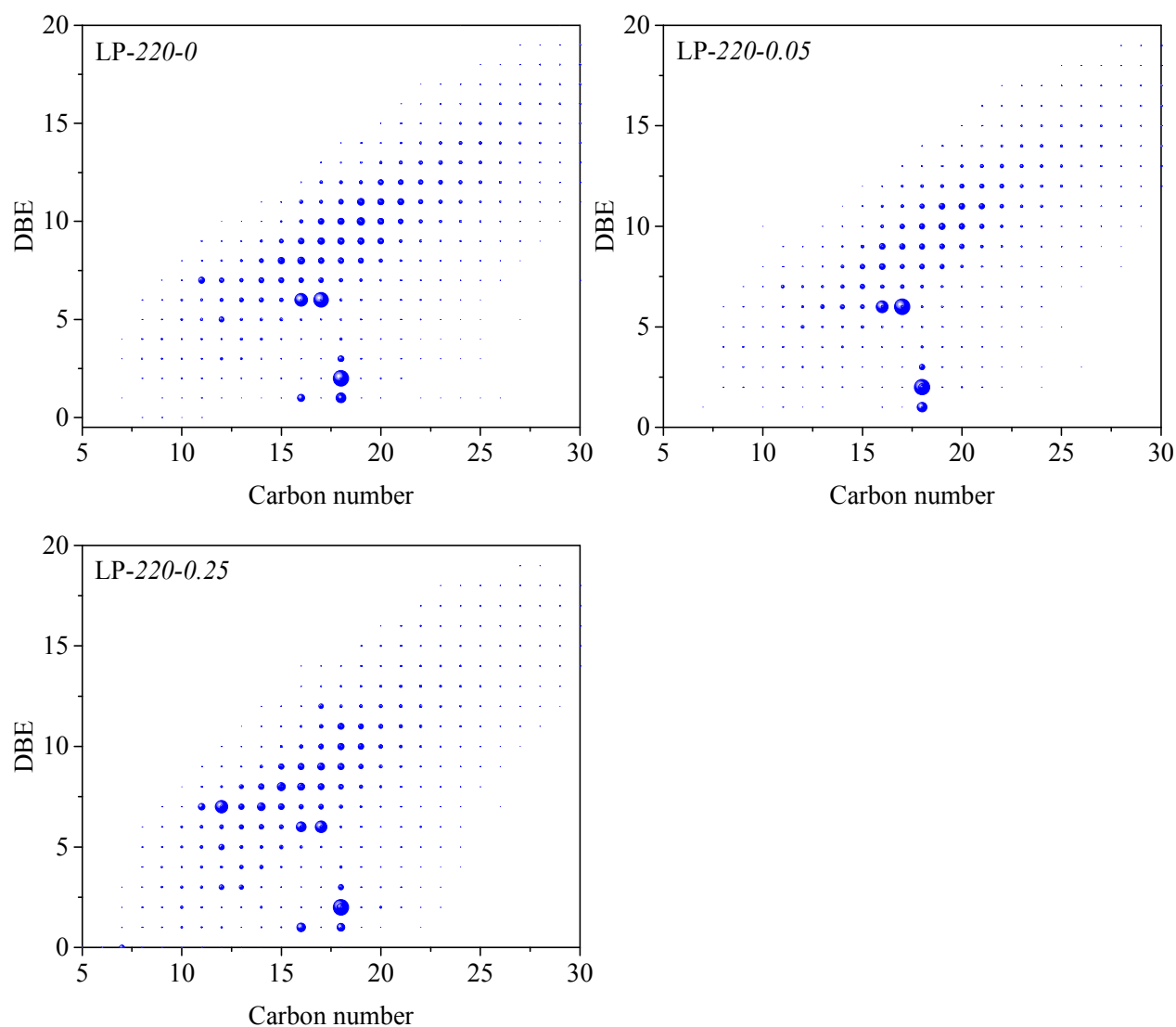


Figure S16. Plots of carbon number versus DBE for LP-220-0, LP-220-0.05 and LP-220-0.25 (plot sizes represent relative abundance of compounds).

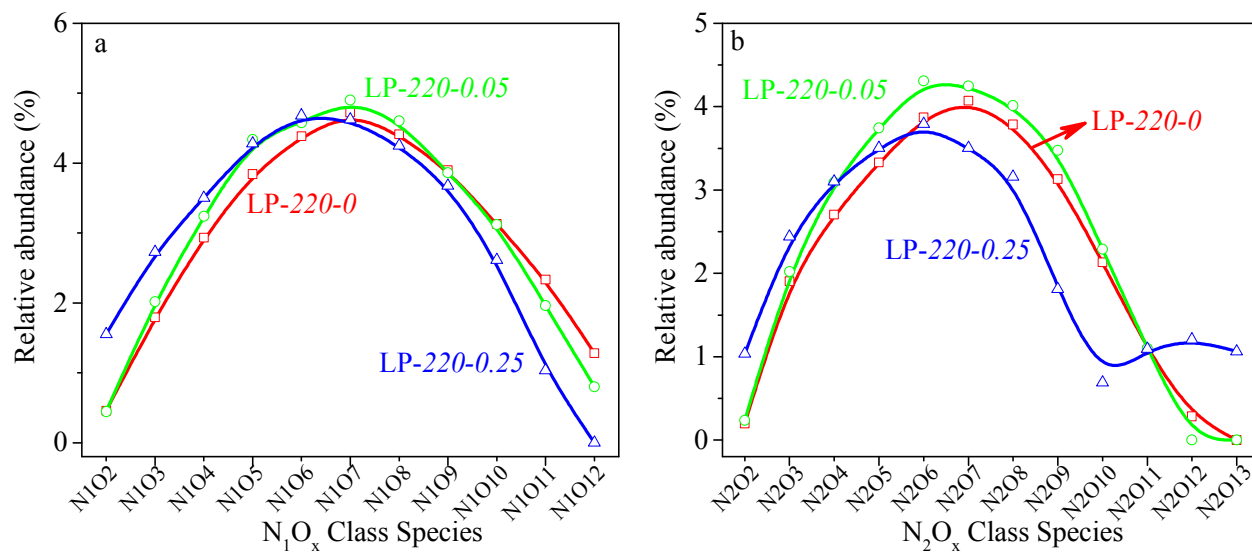


Figure S17. (a) Relative abundance of N_1O_x class species of LP-220-0, LP-220-0.05 and LP-220-0.25, (b) relative abundance of N_2O_x class species of LP-220-0, LP-220-0.05 and LP-220-0.25.

Table S1 Acetic acid concentrations and yields of the liquid phase derived from different temperatures in the HTL process

Sample	Concentration (g/L)	Yields ^a
LP-190-0	2.53	2.53
LP-220-0	2.91	2.91
LP-250-0	1.44	1.44
LP-280-0	1.63	1.63
LP-310-0	1.63	1.63

^a: Based on initial SP mass.

Table S2 Yields, ash, elemental compositions, H/C and O/C atomic ratios for hydrochar produced under different HTL temperatures

Sample	Yield (%)	Ash (%)	C (%)	H (%)	N (%)	O (%)	H/C ^a	O/C ^b
HC-190-0	45.7	8.46	51.14	9.82	1.43	37.38	2.31	0.55
HC-220-0	36.9	4.93	65.38	7.25	2.10	25.12	1.33	0.29
HC-250-0	35.8	6.78	69.33	6.97	2.28	21.23	1.21	0.23
HC-280-0	32.1	8.06	73.08	6.66	2.69	17.38	1.09	0.18
HC-310-0	29.7	9.59	73.20	6.48	2.86	17.19	1.06	0.18

^a H/C: Atomic ratio of hydrogen to carbon.

^b O/C: Atomic ratio of oxygen to carbon.

NOTE: Carbon content of hydrochar increased gradually with increasing HTL temperature, indicating a greater extent of carbonization after the HTL reaction. Decreased H/C and O/C atomic ratios indicated that hydrochar with more aromaticity and lower polarity was produced at higher HTL temperatures.

Table S3 Yields, elemental compositions, H/C and O/C atomic ratios and high heating values (HHV) for bio-oils produced under different HTL temperatures

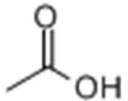
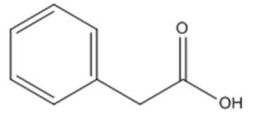
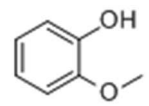
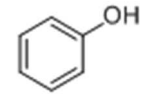
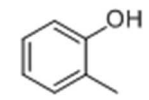
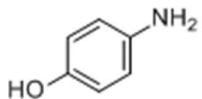
Sample	Yield (%)	C (%)	H (%)	N (%)	O (%)	H/C ^a	O/C ^b	HHV ^c (MJ/kg)
BO-190-0	12.9	38.0	6.94	0.510	54.5	2.19	1.1	13.0
BO-220-0	9.99	44.5	6.32	0.790	48.2	1.70	0.81	15.5
BO-250-0	6.85	52.0	9.00	2.21	36.7	2.08	0.53	23.9
BO-280-0	4.42	47.2	7.67	2.86	42.3	1.95	0.67	19.4
BO-310-0	5.81	46.9	7.08	2.99	43.0	1.81	0.69	18.3

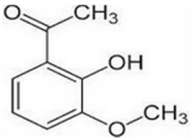
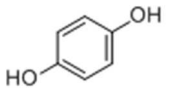
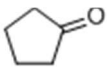
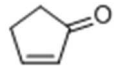
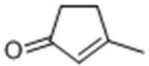
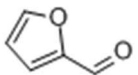
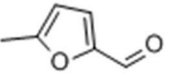
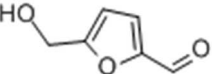
^a H/C: Atomic ratio of hydrogen to carbon.

^b O/C: Atomic ratio of oxygen to carbon.

^c HHV values were calculated with the Dulong formula: $HHV = 0.3383C + 1.422(H - O/8)$, where C, H and O are the weight percentages of carbon, hydrogen and oxygen, respectively.

Table S4 Main components and molecular structures of bio-oils obtained at various temperatures, as analyzed by GC-MS

Ret. Time (min)	Molecular structure	Components	Area (%)				
			BO-190-0	BO-220-0	BO-250-0	BO-280-0	BO-310-0
5.512		acetic acid	12.3	37.0	32.8	17.1	11.4
10.978		benzeneacetic acid	12.5	7.32	- ^a	-	-
13.989		n-hexadecanoic acid	3.40	3.08	-	-	-
Total acids			32.6	48.4	34.0	19.0	14.4
7.507		phenol, 2-methoxy-	-	1.96	5.99	6.42	2.83
8.034		phenol	-	1.97	4.06	6.42	6.95
8.355		phenol, 2-methyl-	-	1.22	1.60	-	-
9.703		phenol, 4-amino-	-	-	6.61	2.78	3.54

13.454		acetophenone,2'-Hydroxy-	-	-	1.87	2.12	1.28
15.464		hydroquinone	-	-	-	5.08	4.66
Total phenols			0.00	5.20	20.1	22.8	19.3
3.789		cyclopentanone	-	0.251	1.56	2.84	4.81
5.018		2-cyclopentenone	-	0.346	2.82	3.10	3.07
5.098		2-cyclopenten-1-one,3-methyl-	-	0.984	2.43	5.03	6.65
Total ketones			0.00	1.58	6.81	11.0	14.5
5.605		furfural	20.8	10.7	2.51	2.29	2.53
6.212		furfural, 5-methyl-	12.5	6.34	-	-	-
10.264		furfural, 5-(hydroxymethyl)-	27.2	12.2	-	-	-

Total furans

62.6

35.1

5.46

4.83

4.24

^a Below detectable level.

Table S5 Molecular formula and mass for compounds in LP-220-0, as detected by FT-ICR MS.

Molecular formula	Theoretical mass	Measured mass	Error (ppm)
C ₇ H ₁₃ O ₄	161.081932	161.08195	-0.111869
C ₉ H ₇ O ₃	163.0400674	163.04014	-0.445413
C ₈ H ₅ O ₄	165.019332	165.01938	-0.290997
C ₈ H ₇ O ₄	167.034982	167.03508	-0.586824
C ₈ H ₉ O ₄	169.050632	169.05066	-0.16575
C ₇ H ₉ O ₅	173.0455466	173.04556	-0.077552
C ₈ H ₁₃ O ₄	173.081932	173.08195	-0.104113
C ₁₀ H ₇ O ₃	175.0400674	175.03999	0.4420696
C ₁₀ H ₉ O ₃	177.0557174	177.05574	-0.127757
C ₉ H ₇ O ₄	179.034982	179.03497	0.0669137
C ₁₀ H ₁₁ O ₃	179.0713674	179.07139	-0.126319
C ₉ H ₁₀ N ₁ O ₃	180.0666164	180.06656	0.3131058
C ₈ H ₅ O ₅	181.0142466	181.01418	0.3678158
C ₉ H ₉ O ₄	181.050632	181.05068	-0.26523
C ₁₀ H ₁₃ O ₃	181.0870174	181.08702	-0.014469
C ₉ H ₁₁ O ₄	183.066282	183.06628	0.0108152
C ₈ H ₁₀ N ₁ O ₄	184.061531	184.06161	-0.429313
C ₈ H ₉ O ₅	184.0696368	184.06969	-0.288925
C ₉ H ₁₃ O ₄	185.0455466	185.04559	-0.234645
C ₇ H ₈ N ₁ O ₅	185.081932	185.082	-0.367513
C ₈ H ₁₁ O ₅	186.0407956	186.04086	-0.346269
C ₉ H ₁₅ O ₄	187.0611966	187.06129	-0.499409
C ₁₁ H ₁₀ N ₁ O ₂	187.097582	187.09769	-0.577346
C ₇ H ₉ O ₆	188.0645514	188.06421	1.8154283

$C_{11}H_9O_3$	188.0717018	188.0716	0.541176
$C_{10}H_7O_4$	189.0404612	189.04052	-0.311151
$C_{11}H_{11}O_3$	189.0557174	189.05584	-0.648592
$C_{10}H_9O_4$	191.034982	191.03498	0.0103641
$C_{10}H_{12}N_1O_3$	191.0713674	191.07138	-0.066049
$C_9H_7O_5$	192.0383368	192.03837	-0.17279
$C_{10}H_{11}O_4$	192.0747222	192.07472	0.011546
$C_9H_9O_5$	193.050632	193.0506	0.1656555
$C_{10}H_{13}O_4$	194.0822664	194.08237	-0.533898
$C_9H_{12}N_1O_4$	195.0298966	195.02995	-0.273907
$C_8H_7O_6$	195.066282	195.06633	-0.246173
$C_9H_{11}O_5$	196.0696368	196.06967	-0.169237
$C_{10}H_{15}O_4$	197.0455466	197.0456	-0.271105
$C_8H_{10}N_1O_5$	197.081932	197.08202	-0.446617
$C_{12}H_{10}N_1O_2$	198.077181	198.07722	-0.196994
$C_8H_9O_6$	199.0248112	199.02484	-0.144807
$C_9H_{13}O_5$	199.0611966	199.0612	-0.017181
$C_{10}H_{17}O_4$	199.097582	199.09755	0.1606243
$C_{11}H_8N_1O_3$	200.0564456	200.05643	0.0778775
$C_{11}H_7O_4$	200.0717018	200.07167	0.1588426
$C_8H_{11}O_6$	201.0404612	201.04046	0.005869
$C_{12}H_{11}O_3$	201.0768466	201.07688	-0.166206
$C_9H_{15}O_5$	201.113232	201.11332	-0.437664
$C_{10}H_{19}O_4$	202.0509664	202.05101	-0.215887
$C_{11}H_{10}N_1O_3$	203.034982	203.03506	-0.384269
$C_{10}H_5O_5$	203.0561112	203.05617	-0.289674

$C_{11}H_9O_4$	203.0713674	203.07142	-0.259121
$C_8H_{13}O_6$	203.0924966	203.09254	-0.213795
$C_{12}H_{13}O_3$	203.128882	203.12893	-0.236402
$C_9H_{17}O_5$	204.059466	204.05952	-0.264542
$C_{10}H_8N_1O_4$	204.0666164	204.06665	-0.164751
$C_{11}H_{12}N_1O_3$	205.0142466	205.01426	-0.065459
$C_{10}H_7O_5$	205.050632	205.05063	0.0096557
$C_{11}H_{11}O_4$	205.0699712	205.06996	0.0547018
$C_{12}H_{15}O_3$	205.0717612	205.07176	0.0057536
$C_{10}H_{10}N_1O_4$	205.0870174	205.08698	0.1822636
$C_{11}H_{14}N_1O_3$	205.1081466	205.10808	0.3246088
$C_9H_5O_6$	206.045881	206.04586	0.1018215
$C_{10}H_9O_5$	206.0539868	206.054	-0.063975
$C_{11}H_{13}O_4$	206.0822664	206.08222	0.2250553
$C_{12}H_{17}O_3$	207.0298966	207.02986	0.176689
$C_{10}H_{12}N_1O_4$	207.066282	207.06625	0.1544428
$C_{11}H_{16}N_1O_3$	207.1026674	207.10264	0.1322045
$C_9H_7O_6$	208.061531	208.06149	0.1969605
$C_{10}H_{11}O_5$	208.0696368	208.06959	0.2250098
$C_{11}H_{15}O_4$	208.0979164	208.09788	0.1748211
$C_{10}H_{14}N_1O_4$	209.0091612	209.00914	0.1013348
$C_9H_9O_6$	209.0455466	209.04553	0.0793124
$C_{10}H_{13}O_5$	209.081932	209.08192	0.0572976
$C_9H_{13}N_2O_4$	209.1183174	209.11832	-0.012529
$C_{11}H_{17}O_4$	210.0489014	210.04884	0.2923971
$C_{12}H_8N_1O_3$	210.077181	210.07716	0.0998676

$C_9H_{12}N_1O_5$	210.0852868	210.08528	0.0324521
$C_{13}H_{12}N_1O_2$	210.1135664	210.11358	-0.064823
$C_{10}H_{16}N_1O_4$	211.0248112	211.02485	-0.18396
$C_{11}H_7N_2O_3$	211.0611966	211.06118	0.0785549
$C_9H_{11}O_6$	211.097582	211.09761	-0.132735
$C_{13}H_{11}O_3$	212.0645514	212.06455	0.0066852
$C_{10}H_{15}O_5$	212.092831	212.09282	0.0517693
$C_9H_{15}N_2O_4$	213.0404612	213.04043	0.1463567
$C_{11}H_{19}O_4$	213.0768466	213.07682	0.1247433
$C_{11}H_6N_1O_4$	213.08808	213.08808	-9.43E-05
$C_{12}H_{10}N_1O_3$	213.113232	213.11318	0.2439074
$C_{13}H_{14}N_1O_2$	214.0509664	214.05099	-0.110348
$C_{12}H_9O_4$	214.0720956	214.07205	0.2129185
$C_9H_{13}O_6$	214.0873518	214.08731	0.1951535
$C_{13}H_{13}O_3$	214.108481	214.10845	0.1446925
$C_{10}H_{17}O_5$	215.0462154	215.0462	0.071519
$C_{11}H_{21}O_4$	215.0561112	215.0561	0.051986
$C_{12}H_{12}N_1O_3$	215.0713674	215.07137	-0.012182
$C_{11}H_7O_5$	215.0924966	215.09247	0.1235743
$C_{12}H_{11}O_4$	215.10373	215.10371	0.092885
$C_{11}H_{11}N_2O_3$	215.128882	215.12885	0.1486546
$C_9H_{15}O_6$	216.030231	216.03025	-0.088044
$C_{13}H_{15}O_3$	216.0666164	216.0666	0.0758095
$C_{11}H_{10}N_1O_4$	216.0958514	216.0959	-0.224818
$C_{12}H_{14}N_1O_3$	216.1030018	216.10299	0.0545106
$C_{10}H_5O_6$	217.0335858	217.03362	-0.157498

$C_{11}H_9O_5$	217.050632	217.05066	-0.129095
$C_{12}H_{13}O_4$	217.0717612	217.07179	-0.132768
$C_{11}H_{13}N_2O_3$	217.0870174	217.08703	-0.058134
$C_{10}H_8N_1O_5$	217.1081466	217.10816	-0.061813
$C_{11}H_{12}N_1O_4$	217.144532	217.14449	0.193327
$C_{12}H_{16}N_1O_3$	218.0822664	218.08233	-0.291725
$C_{10}H_7O_6$	218.1115014	218.11155	-0.222741
$C_{11}H_{11}O_5$	219.0298966	219.02993	-0.152582
$C_{12}H_{15}O_4$	219.066282	219.06635	-0.3105
$C_{11}H_{15}N_2O_3$	219.0775154	219.07759	-0.34061
$C_{10}H_{10}N_1O_5$	219.0874112	219.0875	-0.405409
$C_{11}H_{14}N_1O_4$	219.1026674	219.10273	-0.285803
$C_{10}H_9O_6$	219.112393	219.11313	-3.363662
$C_{11}H_{13}O_5$	220.061531	220.06154	-0.040989
$C_{10}H_{13}N_2O_4$	220.0696368	220.06969	-0.241661
$C_{12}H_{17}O_4$	220.0979164	220.09794	-0.107316
$C_{13}H_{21}O_3$	221.0091612	221.00904	0.5483026
$C_{10}H_{12}N_1O_5$	221.0455466	221.0455	0.2107253
$C_{14}H_{12}N_1O_2$	221.081932	221.08191	0.0994197
$C_{11}H_{16}N_1O_4$	221.0931654	221.09306	0.4766312
$C_{10}H_{11}O_6$	222.0407956	222.04082	-0.10998
$C_9H_{11}N_2O_5$	222.077181	222.07716	0.0944712
$C_{14}H_{11}O_3$	222.0852868	222.0853	-0.059357
$C_{11}H_{15}O_5$	222.1135664	222.11354	0.1187676
$C_{10}H_{15}N_2O_4$	223.0248112	223.02489	-0.353414
$C_{12}H_{19}O_4$	223.0611966	223.06123	-0.149825

$C_{14}H_{27}O_2$	223.097582	223.09762	-0.170419
$C_{12}H_6N_1O_4$	223.1088154	223.10885	-0.155171
$C_{13}H_{10}N_1O_3$	224.0564456	224.05651	-0.287517
$C_{10}H_{14}N_1O_5$	224.0645514	224.06463	-0.350713
$C_{14}H_{14}N_1O_2$	224.092831	224.0929	-0.307998
$C_{11}H_{18}N_1O_4$	224.1009368	224.10103	-0.415805
$C_9H_9O_7$	225.0404612	225.04044	0.094116
$C_{13}H_9O_4$	225.0598004	225.05971	0.4017497
$C_{10}H_{13}O_6$	225.0768466	225.07685	-0.015195
$C_{14}H_{13}O_3$	225.08808	225.08809	-0.044516
$C_{11}H_{17}O_5$	225.113232	225.11325	-0.080049
$C_{10}H_{17}N_2O_4$	225.1496174	225.14967	-0.233712
$C_{12}H_{21}O_4$	226.043816	226.0438	0.070861
$C_{11}H_{21}N_2O_3$	226.0720956	226.07203	0.290084
$C_{12}H_8N_1O_4$	226.0802014	226.08017	0.1389671
$C_{13}H_{12}N_1O_3$	226.0873518	226.08729	0.2732568
$C_{10}H_{16}N_1O_5$	226.108481	226.10839	0.4023728
$C_{14}H_{16}N_1O_2$	227.0561112	227.05616	-0.215013
$C_{12}H_7O_5$	227.0673446	227.06735	-0.02387
$C_9H_{11}O_7$	227.0713674	227.0714	-0.143656
$C_{13}H_{11}O_4$	227.0924966	227.09252	-0.10313
$C_{10}H_{15}O_6$	227.10373	227.10378	-0.220252
$C_{14}H_{15}O_3$	227.128882	227.12893	-0.211422
$C_{11}H_{19}O_5$	227.2016528	227.20165	0.0122354
$C_{12}H_{23}O_4$	228.030231	228.03015	0.3551279
$C_{12}H_{10}N_1O_4$	228.059466	228.0595	-0.149006

$C_{13}H_{14}N_1O_3$	228.0666164	228.06667	-0.235107
$C_{12}H_9O_5$	228.0877456	228.08783	-0.370121
$C_{13}H_{13}O_4$	228.0958514	228.09591	-0.256832
$C_{12}H_{13}N_2O_3$	228.1030018	228.10307	-0.299076
$C_{10}H_{17}O_6$	228.124131	228.12419	-0.258719
$C_{14}H_{17}O_3$	229.0353758	229.03524	0.5928337
$C_{11}H_{21}O_5$	229.050632	229.05057	0.2705948
$C_{12}H_{12}N_1O_4$	229.0717612	229.07173	0.1361141
$C_{13}H_{16}N_1O_3$	229.0870174	229.08699	0.1195175
$C_{11}H_7O_6$	229.1081466	229.10813	0.0723671
$C_{12}H_{11}O_5$	229.11938	229.11933	0.2181391
$C_{11}H_{11}N_2O_4$	229.144532	229.14456	-0.122281
$C_{13}H_{15}O_4$	229.1557654	229.15581	-0.194715
$C_{12}H_{15}N_2O_3$	230.045881	230.0459	-0.08268
$C_{11}H_{10}N_1O_5$	230.075116	230.07511	0.0261554
$C_{12}H_{14}N_1O_4$	230.0822664	230.08227	-0.015734
$C_{13}H_{18}N_1O_3$	230.1033956	230.10338	0.0677083
$C_{11}H_9O_6$	230.1186518	230.11879	-0.600647
$C_{12}H_{13}O_5$	231.0298966	231.02993	-0.144657
$C_{11}H_{13}N_2O_4$	231.0510258	231.05106	-0.148106
$C_{13}H_{17}O_4$	231.066282	231.06634	-0.251097
$C_{12}H_{17}N_2O_3$	231.0874112	231.08748	-0.29781
$C_{11}H_{12}N_1O_5$	231.1026674	231.10272	-0.227691
$C_{15}H_{12}N_1O_2$	231.1237966	231.12385	-0.231132
$C_{12}H_{16}N_1O_4$	231.160182	231.16024	-0.250995
$C_{11}H_{11}O_6$	232.061531	232.06149	0.1765907

$C_{12}H_{15}O_5$	232.0696368	232.06943	0.8911881
$C_{11}H_{15}N_2O_4$	232.0979164	232.09789	0.1136585
$C_9H_{19}O_7$	233.0455466	233.04559	-0.186316
$C_{13}H_{19}O_4$	233.081932	233.08196	-0.120216
$C_{15}H_{27}O_2$	233.0931654	233.0932	-0.148525
$C_{10}H_{10}N_1O_6$	233.1030612	233.10311	-0.209436
$C_{14}H_{10}N_1O_3$	233.1183174	233.11835	-0.139929
$C_{11}H_{14}N_1O_5$	233.1394466	233.13949	-0.186241
$C_{12}H_{18}N_1O_4$	234.0489014	234.04886	0.1769617
$C_{10}H_9O_7$	234.077181	234.07716	0.0896281
$C_{11}H_{13}O_6$	234.0852868	234.0853	-0.056314
$C_{10}H_{13}N_2O_5$	234.1135664	234.1136	-0.143606
$C_{15}H_{13}O_3$	235.0248112	235.02478	0.1326664
$C_{14}H_{13}N_2O_2$	235.0611966	235.06114	0.2407029
$C_{12}H_{17}O_5$	235.07243	235.07236	0.2976951
$C_{11}H_{17}N_2O_4$	235.097582	235.09753	0.2210993
$C_{13}H_{21}O_4$	235.1088154	235.10877	0.1930166
$C_{12}H_{21}N_2O_3$	236.0564456	236.0565	-0.230539
$C_{15}H_{29}O_2$	236.092831	236.09289	-0.249987
$C_{10}H_{12}N_1O_6$	236.1009368	236.10097	-0.140543
$C_{14}H_{12}N_1O_3$	236.1292164	236.12928	-0.269429
$C_{11}H_{16}N_1O_5$	237.0404612	237.04038	0.3424728
$C_{15}H_{16}N_1O_2$	237.0598004	237.05975	0.2126792
$C_{12}H_{20}N_1O_4$	237.0768466	237.07679	0.2386564
$C_{10}H_{11}O_7$	237.08808	237.08801	0.2951641
$C_{14}H_{11}O_4$	237.0961858	237.09615	0.1510682

$C_{13}H_{11}N_2O_3$	237.113232	237.11318	0.2192197
$C_{11}H_{15}O_6$	237.1244654	237.12432	0.6130953
$C_{15}H_{15}O_3$	238.043816	238.04386	-0.184766
$C_{14}H_{15}N_2O_2$	238.0720956	238.07213	-0.144578
$C_{12}H_{19}O_5$	238.0802014	238.08022	-0.078051
$C_{13}H_{23}O_4$	238.0873518	238.08735	0.0074758
$C_{12}H_{23}N_2O_3$	238.108481	238.1085	-0.07988
$C_9H_{10}N_1O_7$	238.1165868	238.11656	0.1126242
$C_{13}H_{10}N_1O_4$	239.0561112	239.05606	0.2140916
$C_{10}H_{14}N_1O_6$	239.0754504	239.07537	0.3363695
$C_{14}H_{14}N_1O_3$	239.0924966	239.09247	0.1111699
$C_{11}H_{18}N_1O_5$	239.10373	239.10371	0.0835616
$C_{13}H_9O_5$	239.1136258	239.11371	-0.352218
$C_{10}H_{13}O_7$	239.128882	239.12888	0.0082796
$C_{14}H_{13}O_4$	239.2016528	239.2015	0.6387075
$C_{13}H_{13}N_2O_3$	240.0513602	240.05135	0.0424072
$C_{11}H_{17}O_6$	240.059466	240.0595	-0.141558
$C_{15}H_{17}O_3$	240.0666164	240.06661	0.0265755
$C_{14}H_{17}N_2O_2$	240.0877456	240.08773	0.0648925
$C_{12}H_{21}O_5$	240.0958514	240.09584	0.0475548
$C_{12}H_8N_1O_5$	240.124131	240.12416	-0.120855
$C_{13}H_{12}N_1O_4$	240.1322368	240.13221	0.1116789
$C_{14}H_{16}N_1O_3$	241.0353758	241.03534	0.1484425
$C_{12}H_7O_6$	241.0717612	241.07175	0.0463758
$C_{13}H_{11}O_5$	241.0829946	241.08299	0.0189972
$C_{12}H_{11}N_2O_4$	241.0870174	241.08703	-0.052347

$C_{10}H_{15}O_7$	241.0982508	241.09832	-0.287103
$C_{14}H_{15}O_4$	241.1081466	241.10816	-0.05566
$C_{13}H_{15}N_2O_3$	241.11938	241.11938	-8.34E-05
$C_{11}H_{19}O_6$	241.144532	241.14457	-0.157665
$C_{15}H_{19}O_3$	241.1557654	241.15574	0.1052428
$C_{12}H_{23}O_5$	241.2173028	241.21738	-0.320127
$C_{12}H_{10}N_1O_5$	242.0670102	242.06703	-0.081879
$C_{13}H_{14}N_1O_4$	242.075116	242.07509	0.1074778
$C_{14}H_{18}N_1O_3$	242.0822664	242.08226	0.0263543
$C_{12}H_9O_6$	242.1033956	242.10338	0.0643523
$C_{13}H_{13}O_5$	242.1115014	242.11145	0.212372
$C_{12}H_{13}N_2O_4$	242.1186518	242.1186	0.2138617
$C_{14}H_{17}O_4$	242.139781	242.13976	0.0866438
$C_{12}H_{12}N_1O_5$	243.0510258	243.05101	0.0649242
$C_{13}H_{16}N_1O_4$	243.066282	243.06632	-0.156419
$C_{14}H_{20}N_1O_3$	243.0775154	243.07744	0.3101064
$C_{11}H_7O_7$	243.0760076	243.07744	-5.89289
$C_{12}H_{11}O_6$	243.0874112	243.08742	-0.036284
$C_{11}H_{11}N_2O_5$	243.1026674	243.10272	-0.216452
$C_{13}H_{15}O_5$	243.1139008	243.11393	-0.120191
$C_{12}H_{15}N_2O_4$	243.1237966	243.12384	-0.178593
$C_{14}H_{19}O_4$	243.1236264	243.12384	-0.878648
$C_{13}H_{19}N_2O_3$	243.160182	243.16023	-0.197483
$C_{11}H_{10}N_1O_6$	243.1714154	243.17148	-0.265739
$C_{12}H_{14}N_1O_5$	244.0462748	244.04619	0.3473927
$C_{16}H_{14}N_1O_2$	244.0543806	244.05437	0.0435055

C ₁₃ H ₁₈ N ₁ O ₄	244.061531	244.06154	-0.036958
C ₁₀ H ₅ O ₈	244.0696368	244.06962	0.0689053
C ₁₁ H ₉ O ₇	244.0826602	244.08261	0.2055857
C ₁₂ H ₁₃ O ₆	244.090766	244.09078	-0.057283
C ₁₁ H ₁₃ N ₂ O ₅	244.0979164	244.09792	-0.014831
C ₁₆ H ₁₃ O ₃	244.1190456	244.11907	-0.100034
C ₁₃ H ₁₇ O ₅	244.1271514	244.1271	0.2106185
C ₁₂ H ₁₇ N ₂ O ₄	245.0455466	245.04554	0.0268517
C ₁₄ H ₂₁ O ₄	245.0666758	245.06668	-0.01722
C ₁₃ H ₂₁ N ₂ O ₃	245.081932	245.08193	0.0080785
C ₁₆ H ₂₉ O ₂	245.0931654	245.09323	-0.263655
C ₁₁ H ₁₂ N ₁ O ₆	245.1012712	245.10132	-0.199029
C ₁₅ H ₁₂ N ₁ O ₃	245.1030612	245.10309	-0.117584
C ₁₂ H ₁₆ N ₁ O ₅	245.1183174	245.11837	-0.214672
C ₁₆ H ₁₆ N ₁ O ₂	245.1295508	245.12959	-0.159997
C ₁₃ H ₂₀ N ₁ O ₄	245.1394466	245.13948	-0.136331
C ₁₁ H ₁₁ O ₇	246.0407956	246.04082	-0.099252
C ₁₅ H ₁₁ O ₄	246.0700306	246.07015	-0.485156
C ₁₄ H ₁₁ N ₂ O ₃	246.077181	246.07721	-0.117931
C ₁₂ H ₁₅ O ₆	246.0852868	246.08524	0.1902499
C ₁₁ H ₁₅ N ₂ O ₅	246.106416	246.10647	-0.219345
C ₁₆ H ₁₅ O ₃	246.1135664	246.11359	-0.095972
C ₁₃ H ₁₉ O ₅	247.0248112	247.02479	0.08574
C ₁₂ H ₁₉ N ₂ O ₄	247.0611966	247.06116	0.1480601
C ₁₄ H ₂₃ O ₄	247.07243	247.07241	0.0808666
C ₁₃ H ₂₃ N ₂ O ₃	247.0709222	247.07241	-6.021834

$C_{16}H_{31}O_2$	247.0805358	247.08059	-0.21929
$C_{14}H_{10}N_1O_4$	247.0823258	247.08227	0.2257543
$C_{11}H_{14}N_1O_6$	247.097582	247.09758	0.0080126
$C_{15}H_{14}N_1O_3$	247.1088154	247.10891	-0.382909
$C_{12}H_{18}N_1O_5$	247.1187112	247.11872	-0.035692
$C_{16}H_{18}N_1O_2$	247.1339674	247.13388	0.353573
$C_{14}H_9O_5$	247.1550966	247.15497	0.5121476
$C_{11}H_{13}O_7$	248.0564456	248.05652	-0.300013
$C_{15}H_{13}O_4$	248.0645514	248.06462	-0.27647
$C_{14}H_{13}N_2O_3$	248.092831	248.09288	-0.197588
$C_{12}H_{17}O_6$	248.1009368	248.10103	-0.375582
$C_{11}H_{17}N_2O_5$	248.1292164	248.12926	-0.175796
$C_{16}H_{17}O_3$	249.0404612	249.04041	0.2055084
$C_{15}H_{17}N_2O_2$	249.0768466	249.07681	0.1468619
$C_{13}H_{21}O_5$	249.08808	249.08797	0.4415302
$C_{14}H_{25}O_4$	249.113232	249.11317	0.2488021
$C_{10}H_{12}N_1O_7$	250.043816	250.04385	-0.135905
$C_{14}H_{12}N_1O_4$	250.0720956	250.07217	-0.297595
$C_{11}H_{16}N_1O_6$	250.0802014	250.08025	-0.194267
$C_{15}H_{16}N_1O_3$	250.108481	250.10855	-0.275961
$C_{13}H_7O_6$	250.1448664	250.14499	-0.494194
$C_{10}H_{11}O_8$	251.0197258	251.01969	0.1425382
$C_{14}H_{11}O_5$	251.0561112	251.0561	0.0445315
$C_{13}H_{11}N_2O_4$	251.0673446	251.06736	-0.061418
$C_{11}H_{15}O_7$	251.0924966	251.09246	0.145683
$C_{15}H_{15}O_4$	251.10373	251.10368	0.1990409

$C_{14}H_{15}N_2O_3$	251.1118358	251.11176	0.301928
$C_{12}H_{19}O_6$	251.128882	251.12879	0.3662657
$C_{15}H_{19}N_2O_2$	251.1401154	251.14002	0.3797876
$C_{13}H_{23}O_5$	252.0513602	252.0514	-0.157984
$C_{13}H_{10}N_1O_5$	252.059466	252.05943	0.1428937
$C_{14}H_{14}N_1O_4$	252.0877456	252.08777	-0.096871
$C_{15}H_{18}N_1O_3$	252.0958514	252.09588	-0.113379
$C_{13}H_9O_6$	252.1030018	252.10296	0.1657255
$C_{10}H_{13}O_8$	252.1070848	252.10712	-0.139553
$C_{14}H_{13}O_5$	252.124131	252.12416	-0.115102
$C_{13}H_{13}N_2O_4$	252.9989904	252.99909	-0.393757
$C_{11}H_{17}O_7$	253.0353758	253.03543	-0.214279
$C_{15}H_{17}O_4$	253.0717612	253.0718	-0.153396
$C_{14}H_{17}N_2O_3$	253.0829946	253.08303	-0.139954
$C_{12}H_{21}O_6$	253.0870174	253.08712	-0.405474
$C_{13}H_{12}N_1O_5$	253.0911004	253.09117	-0.27493
$C_{14}H_{16}N_1O_4$	253.1081466	253.10818	-0.132039
$C_{15}H_{20}N_1O_3$	253.1079764	253.10818	-0.804479
$C_{13}H_{11}O_6$	253.11938	253.11938	-7.94E-05
$C_{12}H_{11}N_2O_5$	253.144532	253.14451	0.0868275
$C_{10}H_{15}O_8$	253.1557654	253.15577	-0.01825
$C_{14}H_{15}O_5$	253.2173028	253.21728	0.0899619
$C_{13}H_{15}N_2O_4$	254.0387306	254.03867	0.238616
$C_{15}H_{19}O_4$	254.0670102	254.06695	0.2368663
$C_{14}H_{19}N_2O_3$	254.075116	254.07504	0.2991938
$C_{12}H_{10}N_1O_6$	254.0822664	254.08223	0.1431816

C ₁₃ H ₁₄ N ₁ O ₅	254.1033956	254.10334	0.2187295
C ₁₄ H ₁₈ N ₁ O ₄	254.1115014	254.1115	0.005579
C ₁₅ H ₂₂ N ₁ O ₃	254.1186518	254.1186	0.2037627
C ₁₂ H ₉ O ₇	254.139781	254.13962	0.6334305
C ₁₃ H ₁₃ O ₆	254.2206576	254.22069	-0.127379
C ₁₂ H ₁₃ N ₂ O ₅	255.0510258	255.0511	-0.291001
C ₁₄ H ₁₇ O ₅	255.066282	255.06631	-0.109854
C ₁₃ H ₁₇ N ₂ O ₄	255.0775154	255.07756	-0.174928
C ₁₅ H ₂₁ O ₄	255.0874112	255.08748	-0.26979
C ₁₄ H ₂₁ N ₂ O ₃	255.0986446	255.09878	-0.530854
C ₁₁ H ₈ N ₁ O ₇	255.1026674	255.10277	-0.40227
C ₁₂ H ₁₂ N ₁ O ₆	255.1237966	255.12387	-0.287782
C ₁₆ H ₁₂ N ₁ O ₃	255.13503	255.1351	-0.274443
C ₁₃ H ₁₆ N ₁ O ₅	255.160182	255.16026	-0.305769
C ₁₇ H ₁₆ N ₁ O ₂	255.1714154	255.17145	-0.135674
C ₁₄ H ₂₀ N ₁ O ₄	255.2329528	255.23301	-0.224188
C ₁₂ H ₁₁ O ₇	256.061531	256.06154	-0.035226
C ₁₆ H ₁₁ O ₄	256.0826602	256.08268	-0.077397
C ₁₃ H ₁₅ O ₆	256.090766	256.09072	0.1796929
C ₁₂ H ₁₅ N ₂ O ₅	256.0979164	256.09792	-0.014136
C ₁₇ H ₁₅ O ₃	256.1190456	256.11903	0.0608307
C ₁₄ H ₁₉ O ₅	256.1271514	256.12715	0.0055351
C ₁₃ H ₁₉ N ₂ O ₄	256.1343018	256.13418	0.4754533
C ₁₅ H ₂₃ O ₄	256.2363076	256.23625	0.2248616
C ₁₄ H ₂₃ N ₂ O ₃	257.0455466	257.04555	-0.013305
C ₁₇ H ₃₁ O ₂	257.0666758	257.06664	0.1391853

C ₁₁ H ₁₀ N ₁ O ₇	257.081932	257.08188	0.202192
C ₁₅ H ₁₀ N ₁ O ₄	257.0931654	257.09311	0.2154079
C ₁₂ H ₁₄ N ₁ O ₆	257.0916576	257.09311	-5.649425
C ₁₆ H ₁₄ N ₁ O ₃	257.1012712	257.10124	0.1214218
C ₁₃ H ₁₈ N ₁ O ₅	257.1030612	257.10302	0.1601688
C ₁₇ H ₁₈ N ₁ O ₂	257.1142946	257.11431	-0.059974
C ₁₄ H ₂₂ N ₁ O ₄	257.1183174	257.11829	0.1064876
C ₁₁ H ₉ O ₈	257.1295508	257.12945	0.3919421
C ₁₅ H ₉ O ₅	257.128043	257.12945	-5.47206
C ₁₂ H ₁₃ O ₇	257.1394466	257.13941	0.1422571
C ₁₁ H ₁₃ N ₂ O ₆	257.175832	257.17585	-0.070069
C ₁₆ H ₁₃ O ₄	258.0619248	258.06197	-0.17523
C ₁₅ H ₁₃ N ₂ O ₃	258.0700306	258.07011	-0.3076
C ₁₃ H ₁₇ O ₆	258.077181	258.07725	-0.26744
C ₁₂ H ₁₇ N ₂ O ₅	258.0852868	258.08537	-0.322305
C ₁₇ H ₁₇ O ₃	258.0983102	258.09845	-0.541732
C ₁₆ H ₁₇ N ₂ O ₂	258.106416	258.10649	-0.286635
C ₁₄ H ₂₁ O ₅	258.1135664	258.11363	-0.246481
C ₁₃ H ₂₁ N ₂ O ₄	258.1428014	258.14287	-0.265676
C ₁₅ H ₂₅ O ₄	259.0248112	259.02483	-0.072658
C ₁₄ H ₂₅ N ₂ O ₃	259.0459404	259.04596	-0.07574
C ₁₆ H ₂₉ O ₃	259.0611966	259.06121	-0.051803
C ₁₇ H ₃₃ O ₂	259.07243	259.07247	-0.154475
C ₁₁ H ₁₂ N ₁ O ₇	259.0805358	259.08054	-0.016143
C ₁₅ H ₁₂ N ₁ O ₄	259.0823258	259.08232	0.0223091
C ₁₂ H ₁₆ N ₁ O ₆	259.097582	259.09756	0.0848325

$C_{16}H_{16}N_1O_3$	259.1073076	259.10753	-0.858409
$C_{13}H_{20}N_1O_5$	259.1088154	259.10881	0.0207631
$C_{11}H_{11}O_8$	259.1169212	259.1169	0.0818847
$C_{15}H_{11}O_5$	259.1187112	259.11869	0.0817382
$C_{14}H_{11}N_2O_4$	259.1452008	259.14518	0.0801863
$C_{12}H_{15}O_7$	259.143693	259.14518	-5.738207
$C_{11}H_{15}N_2O_6$	259.1550966	259.1551	-0.013197
$C_{16}H_{15}O_4$	260.0564456	260.05638	0.2521756
$C_{15}H_{15}N_2O_3$	260.0645514	260.06451	0.1592593
$C_{13}H_{19}O_6$	260.0856806	260.0857	-0.074523
$C_{12}H_{19}N_2O_5$	260.092831	260.09278	0.1960066
$C_{17}H_{19}O_3$	260.1009368	260.10089	0.1799982
$C_{16}H_{19}N_2O_2$	260.1121702	260.1121	0.2699516
$C_{14}H_{23}O_5$	260.1292164	260.12918	0.1398532
$C_{14}H_{10}N_1O_5$	261.0404612	261.04048	-0.072096
$C_{11}H_{14}N_1O_7$	261.0615904	261.06161	-0.075155
$C_{15}H_{14}N_1O_4$	261.0768466	261.07687	-0.089706
$C_{12}H_{18}N_1O_6$	261.08808	261.08811	-0.114981
$C_{16}H_{18}N_1O_3$	261.0961858	261.09623	-0.169218
$C_{14}H_9O_6$	261.0979758	261.09804	-0.245962
$C_{11}H_{13}O_8$	261.113232	261.11329	-0.222203
$C_{15}H_{13}O_5$	261.1130618	261.11329	-0.874028
$C_{14}H_{13}N_2O_4$	261.1244654	261.12452	-0.209173
$C_{12}H_{17}O_7$	261.1343612	261.13442	-0.225248
$C_{11}H_{17}N_2O_6$	262.0720956	262.07212	-0.093181
$C_{16}H_{17}O_4$	262.0802014	262.08023	-0.109059

$C_{15}H_{17}N_2O_3$	262.108481	262.1085	-0.072566
$C_{13}H_{21}O_6$	262.1165868	262.11661	-0.088443
$C_{14}H_{25}O_5$	262.1278202	262.12783	-0.037319
$C_{14}H_{12}N_1O_5$	262.1448664	262.14487	-0.01381
$C_{11}H_{16}N_1O_7$	263.0561112	263.05605	0.2325736
$C_{15}H_{16}N_1O_4$	263.0673446	263.06727	0.2835012
$C_{16}H_{20}N_1O_3$	263.0754504	263.07542	0.1156235
$C_{14}H_{11}O_6$	263.0772404	263.07718	0.229514
$C_{13}H_{11}N_2O_5$	263.0924966	263.09242	0.291076
$C_{11}H_{15}O_8$	263.10373	263.10369	0.1519549
$C_{15}H_{15}O_5$	263.1118358	263.11172	0.4401843
$C_{14}H_{15}N_2O_4$	263.128882	263.1288	0.311558
$C_{12}H_{19}O_7$	263.1287118	263.1288	-0.335274
$C_{16}H_{19}O_4$	263.1401154	263.14002	0.3624681
$C_{15}H_{19}N_2O_3$	264.0513602	264.05133	0.1142956
$C_{13}H_{23}O_6$	264.059466	264.05946	0.0227892
$C_{13}H_{10}N_1O_6$	264.0877456	264.08773	0.0589952
$C_{14}H_{14}N_1O_5$	264.124131	264.12411	0.079432
$C_{15}H_{18}N_1O_4$	264.1605164	264.16054	-0.089416
$C_{13}H_9O_7$	265.0353758	265.03545	-0.280038
$C_{14}H_{13}O_6$	265.0717612	265.07182	-0.221903
$C_{13}H_{13}N_2O_5$	265.0829946	265.08307	-0.284515
$C_{11}H_{17}O_8$	265.0911004	265.09118	-0.300207
$C_{15}H_{17}O_5$	265.1081466	265.10821	-0.239224
$C_{14}H_{17}N_2O_4$	265.11938	265.11943	-0.18867
$C_{12}H_{21}O_7$	265.1274858	265.12744	0.1728138

C ₁₆ H ₂₁ O ₄	265.144532	265.14459	-0.218824
C ₁₅ H ₂₁ N ₂ O ₃	265.1557654	265.1558	-0.130565
C ₁₃ H ₁₂ N ₁ O ₆	266.0306248	266.03067	-0.169981
C ₁₇ H ₁₂ N ₁ O ₃	266.0387306	266.03875	-0.072855
C ₁₄ H ₁₆ N ₁ O ₅	266.0670102	266.06701	0.0006761
C ₁₅ H ₂₀ N ₁ O ₄	266.075116	266.07512	-0.014967
C ₁₃ H ₁₁ O ₇	266.0822664	266.08229	-0.08877
C ₁₂ H ₁₁ N ₂ O ₆	266.1033956	266.1034	-0.01661
C ₁₄ H ₁₅ O ₆	266.1115014	266.11149	0.0429057
C ₁₃ H ₁₅ N ₂ O ₅	266.1186518	266.11859	0.2321517
C ₁₈ H ₁₅ O ₃	266.139781	266.13975	0.1164046
C ₁₅ H ₁₉ O ₅	267.0510258	267.05096	0.2463196
C ₁₄ H ₁₉ N ₂ O ₄	267.066282	267.06617	0.4192963
C ₁₆ H ₂₃ O ₄	267.0874112	267.08734	0.2665041
C ₁₈ H ₃₁ O ₂	267.0986446	267.09856	0.3166617
C ₁₂ H ₁₀ N ₁ O ₇	267.1026674	267.1026	0.2522622
C ₁₃ H ₁₄ N ₁ O ₆	267.1067504	267.1066	0.563137
C ₁₇ H ₁₄ N ₁ O ₃	267.1237966	267.12372	0.2866832
C ₁₄ H ₁₈ N ₁ O ₅	267.13503	267.13497	0.2245303
C ₁₅ H ₂₂ N ₁ O ₄	267.160182	267.16014	0.1571338
C ₁₂ H ₉ O ₈	267.1714154	267.17124	0.6564321
C ₁₆ H ₉ O ₅	267.2329528	267.23293	0.0852436
C ₁₃ H ₁₃ O ₇	268.0462748	268.04619	0.3162883
C ₁₂ H ₁₃ N ₂ O ₆	268.0543806	268.05436	0.0769161
C ₁₇ H ₁₃ O ₄	268.061531	268.0615	0.1155701
C ₁₆ H ₁₃ N ₂ O ₃	268.0826602	268.08264	0.0752749

$C_{14}H_{17}O_6$	268.090766	268.09074	0.0970481
$C_{13}H_{17}N_2O_5$	268.0979164	268.09792	-0.013503
$C_{18}H_{17}O_3$	268.1190456	268.11904	0.0208113
$C_{15}H_{21}O_5$	268.1271514	268.12712	0.1171746
$C_{14}H_{21}N_2O_4$	268.1343018	268.13425	0.1931118
$C_{15}H_{25}N_2O_3$	268.155431	268.15542	0.040946
$C_{18}H_{33}O_2$	269.0302904	269.03026	0.1129237
$C_{12}H_{12}N_1O_7$	269.0455466	269.04563	-0.310059
$C_{16}H_{12}N_1O_4$	269.0666758	269.06674	-0.238677
$C_{13}H_{16}N_1O_6$	269.0779092	269.07798	-0.263196
$C_{17}H_{16}N_1O_3$	269.081932	269.08199	-0.215622
$C_{14}H_{20}N_1O_5$	269.0931654	269.09327	-0.388788
$C_{18}H_{20}N_1O_2$	269.1012712	269.10145	-0.664368
$C_{12}H_{11}O_8$	269.1030612	269.10314	-0.292899
$C_{16}H_{11}O_5$	269.1142946	269.11447	-0.651842
$C_{15}H_{11}N_2O_4$	269.1183174	269.11847	-0.567112
$C_{13}H_{15}O_7$	269.1295508	269.12967	-0.442984
$C_{12}H_{15}N_2O_6$	269.1394466	269.13951	-0.23564
$C_{17}H_{15}O_4$	269.15068	269.15071	-0.111536
$C_{16}H_{15}N_2O_3$	269.175832	269.17591	-0.289848
$C_{14}H_{19}O_6$	269.1870654	269.18714	-0.277205
$C_{13}H_{19}N_2O_5$	269.2122174	269.21227	-0.19546
$C_{18}H_{19}O_3$	269.2486028	269.24865	-0.175377
$C_{15}H_{23}O_5$	270.0619248	270.06202	-0.352586
$C_{14}H_{23}N_2O_4$	270.077181	270.0772	-0.070425
$C_{16}H_{27}O_4$	270.0852868	270.08531	-0.085833

$C_{15}H_{27}N_2O_3$	270.0983102	270.09832	-0.036358
$C_{18}H_{35}O_2$	270.106416	270.10641	0.022279
$C_{15}H_{10}N_1O_5$	270.1135664	270.11361	-0.161488
$C_{12}H_{14}N_1O_7$	270.1346956	270.13468	0.0576746
$C_{16}H_{14}N_1O_4$	270.1428014	270.1428	0.005248
$C_{13}H_{18}N_1O_6$	271.0459404	271.04596	-0.072387
$C_{17}H_{18}N_1O_3$	271.0611966	271.06117	0.0980587
$C_{14}H_{22}N_1O_5$	271.07243	271.0724	0.1105974
$C_{15}H_9O_6$	271.0709222	271.0724	-5.451784
$C_{12}H_{13}O_8$	271.0742159	271.07432	-0.384108
$C_{16}H_{13}O_5$	271.0805358	271.08048	0.2059082
$C_{15}H_{13}N_2O_4$	271.0823258	271.08229	0.1319891
$C_{13}H_{17}O_7$	271.0935592	271.09351	0.181413
$C_{12}H_{17}N_2O_6$	271.097582	271.09753	0.1917387
$C_{17}H_{17}O_4$	271.1088154	271.10879	0.0936152
$C_{16}H_{17}N_2O_3$	271.1073076	271.10879	-5.46802
$C_{14}H_{21}O_6$	271.1187112	271.11865	0.2256572
$C_{13}H_{21}N_2O_5$	271.1299446	271.12988	0.238188
$C_{15}H_{25}O_5$	271.1339674	271.13389	0.2853936
$C_{16}H_{29}O_4$	271.1452008	271.14507	0.4823242
$C_{14}H_8N_1O_6$	271.1550966	271.15503	0.2455418
$C_{15}H_{12}N_1O_5$	272.0564456	272.05628	0.6086233
$C_{12}H_{16}N_1O_7$	272.0775748	272.07744	0.4953731
$C_{16}H_{16}N_1O_4$	272.0856806	272.08548	0.7373328
$C_{17}H_{20}N_1O_3$	272.092831	272.09275	0.2976186
$C_{14}H_7O_7$	272.1009368	272.10086	0.2823133

C ₁₅ H ₁₁ O ₆	272.1139602	272.11396	0.0006611
C ₁₄ H ₁₁ N ₂ O ₅	272.1292164	272.1292	0.0601916
C ₁₂ H ₁₅ O ₈	273.0404612	273.04046	0.0043213
C ₁₁ H ₁₅ N ₂ O ₇	273.0615904	273.06158	0.038013
C ₁₆ H ₁₅ O ₅	273.0768466	273.07682	0.0973349
C ₁₅ H ₁₅ N ₂ O ₄	273.08808	273.08808	-7.36E-05
C ₁₃ H ₁₉ O ₇	273.0979758	273.09798	-0.015453
C ₁₂ H ₁₉ N ₂ O ₆	273.1092092	273.10923	-0.076234
C ₁₇ H ₁₉ O ₄	273.113232	273.11323	0.0072494
C ₁₆ H ₁₉ N ₂ O ₃	273.1244654	273.12449	-0.090142
C ₁₄ H ₂₃ O ₆	273.1343612	273.13436	0.0043199
C ₁₅ H ₂₇ O ₅	273.1707466	273.17079	-0.158949
C ₁₆ H ₃₁ O ₄	274.0720956	274.07218	-0.308022
C ₁₄ H ₁₀ N ₁ O ₆	274.0802014	274.0803	-0.359684
C ₁₅ H ₁₄ N ₁ O ₅	274.0932248	274.09328	-0.201465
C ₁₆ H ₁₈ N ₁ O ₄	274.1013306	274.10132	0.0387364
C ₁₇ H ₂₂ N ₁ O ₃	274.108481	274.10855	-0.251798
C ₁₄ H ₉ O ₇	274.1165868	274.11664	-0.194013
C ₁₃ H ₉ N ₂ O ₆	274.1448664	274.14494	-0.268545
C ₁₁ H ₁₃ O ₉	275.0561112	275.05616	-0.177491
C ₁₅ H ₁₃ O ₆	275.0673446	275.06742	-0.274188
C ₁₄ H ₁₃ N ₂ O ₅	275.0754504	275.07553	-0.289311
C ₁₂ H ₁₇ O ₈	275.0772404	275.07724	0.0013811
C ₁₁ H ₁₇ N ₂ O ₇	275.081093	275.08099	0.374362
C ₁₆ H ₁₇ O ₅	275.0924966	275.09252	-0.085135
C ₁₅ H ₁₇ N ₂ O ₄	275.10373	275.10376	-0.109123

$C_{13}H_{21}O_7$	275.1118358	275.11187	-0.124249
$C_{17}H_{21}O_4$	275.1136258	275.11367	-0.160734
$C_{16}H_{21}N_2O_3$	275.128882	275.12891	-0.101844
$C_{14}H_{25}O_6$	275.1401154	275.14016	-0.162172
$C_{14}H_{12}N_1O_6$	275.1500112	275.15003	-0.068399
$C_{15}H_{16}N_1O_5$	276.0513602	276.05134	0.073102
$C_{16}H_{20}N_1O_4$	276.059466	276.05955	-0.304218
$C_{14}H_{11}O_7$	276.0877456	276.08772	0.0926513
$C_{13}H_{11}N_2O_6$	276.0958514	276.09583	0.0775734
$C_{15}H_{15}O_6$	276.1070848	276.10715	-0.236076
$C_{14}H_{15}N_2O_5$	276.124131	276.12411	0.07598
$C_{12}H_{19}O_8$	276.1322368	276.13223	0.02469
$C_{16}H_{19}O_5$	276.1434702	276.14351	-0.144064
$C_{15}H_{19}N_2O_4$	277.0353758	277.03533	0.1652493
$C_{13}H_{23}O_7$	277.0717612	277.07168	0.2929923
$C_{17}H_{23}O_4$	277.0829946	277.08293	0.2330706
$C_{13}H_{10}N_1O_7$	277.0911004	277.09103	0.2541319
$C_{14}H_{14}N_1O_6$	277.0928904	277.09276	0.4705278
$C_{18}H_{14}N_1O_3$	277.1081466	277.10805	0.3485278
$C_{15}H_{18}N_1O_5$	277.11938	277.11931	0.2525262
$C_{19}H_{18}N_1O_2$	277.1274858	277.12735	0.490091
$C_{16}H_{22}N_1O_4$	277.1292758	277.12919	0.3095303
$C_{13}H_9O_8$	277.144532	277.1444	0.4762133
$C_{14}H_{13}O_7$	277.1443618	277.1444	-0.137907
$C_{13}H_{13}N_2O_6$	277.1557654	277.15571	0.1998151
$C_{18}H_{13}O_4$	278.0670102	278.06692	0.32431

C ₁₁ H ₁₇ O ₉	278.075116	278.07507	0.1654866
C ₁₇ H ₁₃ N ₂ O ₃	278.0822664	278.08222	0.1667848
C ₁₅ H ₁₇ O ₆	278.1033956	278.10333	0.2358112
C ₁₄ H ₁₇ N ₂ O ₅	278.1115014	278.11146	0.1489248
C ₁₉ H ₁₇ O ₃	278.139781	278.13974	0.1473356
C ₁₆ H ₂₁ O ₅	279.0510258	279.05096	0.2357271
C ₁₅ H ₂₁ N ₂ O ₄	279.0622592	279.06233	-0.253779
C ₁₇ H ₂₅ O ₄	279.0874112	279.08738	0.1117209
C ₁₃ H ₁₂ N ₁ O ₇	279.0986446	279.09863	0.0522392
C ₁₇ H ₁₂ N ₁ O ₄	279.1026674	279.10257	0.3489035
C ₁₄ H ₁₆ N ₁ O ₆	279.1067504	279.10676	-0.034332
C ₁₈ H ₁₆ N ₁ O ₃	279.1237966	279.12377	0.0952262
C ₁₅ H ₂₀ N ₁ O ₅	279.13503	279.13501	0.0715779
C ₁₆ H ₂₄ N ₁ O ₄	279.1431358	279.14284	1.0597348
C ₁₃ H ₁₁ O ₈	279.160182	279.16016	0.0787358
C ₁₇ H ₁₁ O ₅	279.2329528	279.23301	-0.204919
C ₁₆ H ₁₁ N ₂ O ₄	280.0462748	280.04628	-0.01864
C ₁₄ H ₁₅ O ₇	280.0543806	280.05433	0.1807424
C ₁₃ H ₁₅ N ₂ O ₆	280.0826602	280.08268	-0.070765
C ₁₈ H ₁₅ O ₄	280.090766	280.09082	-0.192731
C ₁₁ H ₁₉ O ₉	280.0979164	280.09796	-0.155732
C ₁₇ H ₁₅ N ₂ O ₃	280.1190456	280.11909	-0.158576
C ₁₅ H ₁₉ O ₆	280.1271514	280.12722	-0.244826
C ₁₄ H ₁₉ N ₂ O ₅	280.1383848	280.13844	-0.196982
C ₁₉ H ₁₉ O ₃	280.155431	280.15548	-0.174975
C ₁₆ H ₂₃ O ₅	281.0302904	281.03039	-0.354482

$C_{15}H_{23}N_2O_4$	281.0455466	281.04561	-0.225658
$C_{12}H_{10}N_1O_8$	281.0666758	281.06674	-0.228487
$C_{16}H_{10}N_1O_5$	281.0779092	281.07798	-0.251959
$C_{13}H_{14}N_1O_7$	281.081932	281.08183	0.362812
$C_{17}H_{14}N_1O_4$	281.0931654	281.09322	-0.194313
$C_{14}H_{18}N_1O_6$	281.1030612	281.10314	-0.280396
$C_{18}H_{18}N_1O_3$	281.1142946	281.11436	-0.232717
$C_{15}H_{22}N_1O_5$	281.1183174	281.11838	-0.222754
$C_{16}H_9O_6$	281.1394466	281.1395	-0.190013
$C_{13}H_{13}O_8$	281.1392764	281.1395	-0.795407
$C_{12}H_{13}N_2O_7$	281.15068	281.15071	-0.106776
$C_{17}H_{13}O_5$	281.1870654	281.1871	-0.123121
$C_{16}H_{13}N_2O_4$	281.2486028	281.24864	-0.132339
$C_{14}H_{17}O_7$	282.0619248	282.06204	-0.408492
$C_{13}H_{17}N_2O_6$	282.0700306	282.07007	-0.139619
$C_{18}H_{17}O_4$	282.077181	282.07724	-0.209234
$C_{17}H_{17}N_2O_3$	282.081264	282.0813	-0.12756
$C_{15}H_{21}O_6$	282.0983102	282.09835	-0.141157
$C_{14}H_{21}N_2O_5$	282.1135664	282.11359	-0.083726
$C_{16}H_{25}O_5$	282.1346956	282.13473	-0.121999
$C_{15}H_{25}N_2O_4$	282.1428014	282.14288	-0.27852
$C_{16}H_{29}N_2O_3$	282.1499518	282.14989	0.2189612
$C_{18}H_{33}O_3$	282.2519576	282.25197	-0.04387
$C_{19}H_{37}O_2$	283.0459404	283.04596	-0.069318
$C_{12}H_{12}N_1O_8$	283.0611966	283.06122	-0.082739
$C_{16}H_{12}N_1O_5$	283.07243	283.07251	-0.282684

C ₁₃ H ₁₆ N ₁ O ₇	283.0805358	283.08054	-0.014774
C ₁₇ H ₁₆ N ₁ O ₄	283.0823258	283.08234	-0.050233
C ₁₄ H ₂₀ N ₁ O ₆	283.0821556	283.08234	-0.651472
C ₁₈ H ₂₀ N ₁ O ₃	283.0935592	283.09358	-0.073545
C ₁₅ H ₂₄ N ₁ O ₅	283.097582	283.09758	0.0069937
C ₁₂ H ₁₁ O ₉	283.1088154	283.10883	-0.051641
C ₁₆ H ₁₁ O ₆	283.1106013	283.10991	2.4417245
C ₁₅ H ₁₁ N ₂ O ₅	283.1169212	283.11701	-0.313589
C ₁₃ H ₁₅ O ₈	283.1187112	283.11871	0.0041675
C ₁₂ H ₁₅ N ₂ O ₇	283.1299446	283.12989	0.1927733
C ₁₇ H ₁₅ O ₅	283.1339674	283.134	-0.115211
C ₁₆ H ₁₅ N ₂ O ₄	283.1550966	283.15508	0.0585541
C ₁₄ H ₁₉ O ₇	283.16633	283.16635	-0.070701
C ₁₃ H ₁₉ N ₂ O ₆	283.191482	283.19134	0.5013565
C ₁₈ H ₁₉ O ₄	283.2027154	283.20272	-0.016314
C ₁₇ H ₁₉ N ₂ O ₃	283.2642528	283.26418	0.2569329
C ₁₅ H ₂₃ O ₆	284.0492952	284.04927	0.0887793
C ₁₄ H ₂₃ N ₂ O ₅	284.0564456	284.05645	-0.015561
C ₁₆ H ₂₇ O ₅	284.0775748	284.07757	0.016826
C ₁₈ H ₃₅ O ₃	284.0856806	284.08567	0.037375
C ₁₅ H ₁₀ N ₁ O ₆	284.092831	284.09279	0.1442483
C ₁₂ H ₁₄ N ₁ O ₈	284.1139602	284.11391	0.1766189
C ₁₆ H ₁₄ N ₁ O ₅	284.122066	284.12202	0.1619645
C ₁₃ H ₁₈ N ₁ O ₇	284.1292164	284.12916	0.1984305
C ₁₇ H ₁₈ N ₁ O ₄	284.1503456	284.15029	0.1956003
C ₁₄ H ₂₂ N ₁ O ₆	284.1584514	284.15841	0.1457557

$C_{18}H_{22}N_1O_3$	285.0404612	285.04045	0.0392222
$C_{15}H_9O_7$	285.0615904	285.06158	0.0364128
$C_{12}H_{13}O_9$	285.0768466	285.07679	0.1984724
$C_{16}H_{13}O_6$	285.08808	285.08804	0.140237
$C_{15}H_{13}N_2O_5$	285.0865722	285.08804	-5.148682
$C_{13}H_{17}O_8$	285.0961858	285.09613	0.1957855
$C_{12}H_{17}N_2O_7$	285.0979758	285.09791	0.2307273
$C_{17}H_{17}O_5$	285.1092092	285.10913	0.2777178
$C_{16}H_{17}N_2O_4$	285.113232	285.11316	0.2524607
$C_{14}H_{21}O_7$	285.1244654	285.12433	0.4748098
$C_{13}H_{21}N_2O_6$	285.1229576	285.12433	-4.813432
$C_{18}H_{21}O_4$	285.1343612	285.13426	0.3548499
$C_{17}H_{21}N_2O_3$	285.1455946	285.1455	0.3316899
$C_{15}H_{25}O_6$	285.1707466	285.17061	0.4789408
$C_{16}H_{29}O_5$	285.207132	285.20707	0.2173154
$C_{15}H_{12}N_1O_6$	286.0357102	286.03563	0.2803143
$C_{12}H_{16}N_1O_8$	286.0720956	286.072	0.3341112
$C_{16}H_{16}N_1O_5$	286.0932248	286.09314	0.2963366
$C_{17}H_{20}N_1O_4$	286.1013306	286.10131	0.0720643
$C_{18}H_{24}N_1O_3$	286.1062441	286.10675	-1.768301
$C_{15}H_{11}O_7$	286.108481	286.10839	0.3179909
$C_{12}H_{15}O_9$	286.112564	286.11248	0.2936526
$C_{16}H_{15}O_6$	286.1165868	286.1165	0.3034347
$C_{15}H_{15}N_2O_5$	286.1448664	286.1448	0.23198
$C_{13}H_{19}O_8$	287.0197258	287.0197	0.0898193
$C_{12}H_{19}N_2O_7$	287.0561112	287.05602	0.3176379

C ₁₇ H ₁₉ O ₅	287.0673446	287.06714	0.7126547
C ₁₆ H ₁₉ N ₂ O ₄	287.0691305	287.06906	0.2455092
C ₁₄ H ₂₃ O ₇	287.0754504	287.07545	0.001455
C ₁₃ H ₂₃ N ₂ O ₆	287.0772404	287.07717	0.2451602
C ₁₈ H ₂₃ O ₄	287.081093	287.08033	2.6577156
C ₁₇ H ₂₃ N ₂ O ₃	287.0884738	287.08843	0.1524962
C ₁₅ H ₂₇ O ₆	287.0924966	287.09242	0.266743
C ₁₆ H ₃₁ O ₅	287.10373	287.10365	0.2785749
C ₁₄ H ₁₀ N ₁ O ₇	287.1022222	287.10365	-4.973212
C ₁₅ H ₁₄ N ₁ O ₆	287.1118358	287.11182	0.0550925
C ₁₆ H ₁₈ N ₁ O ₅	287.1136258	287.11353	0.3335958
C ₁₇ H ₂₂ N ₁ O ₄	287.1134556	287.11353	-0.259201
C ₁₈ H ₂₆ N ₁ O ₃	287.1248592	287.1248	0.2061121
C ₁₅ H ₁₃ O ₇	287.128882	287.12883	0.1810333
C ₁₄ H ₁₃ N ₂ O ₆	287.1401154	287.13999	0.4366506
C ₁₉ H ₁₃ O ₄	287.1386076	287.13999	-4.81447
C ₁₆ H ₁₇ O ₆	287.1500112	287.14996	0.178234
C ₁₅ H ₁₇ N ₂ O ₅	287.1863966	287.18636	0.1273734
C ₁₇ H ₂₁ O ₅	287.222782	287.22276	0.0765256
C ₁₆ H ₂₁ N ₂ O ₄	288.0513602	288.05133	0.1047726
C ₁₄ H ₂₅ O ₇	288.0877456	288.08769	0.192927
C ₁₈ H ₂₅ O ₄	288.0958514	288.09581	0.1437636
C ₁₇ H ₂₅ N ₂ O ₃	288.1169806	288.11685	0.4533495
C ₁₄ H ₁₂ N ₁ O ₇	288.124131	288.12408	0.1769373
C ₁₅ H ₁₆ N ₁ O ₆	288.1322368	288.13224	-0.011045
C ₁₉ H ₁₆ N ₁ O ₃	288.153366	288.15333	0.1249949

$C_{16}H_{20}N_1O_5$	288.1605164	288.16046	0.1956545
$C_{17}H_{24}N_1O_4$	288.1897514	288.18979	-0.133878
$C_{18}H_{28}N_1O_3$	288.2261368	288.22605	0.3012138
$C_{14}H_{11}O_8$	289.0353758	289.03536	0.054595
$C_{15}H_{15}O_7$	289.0466092	289.0466	0.0317592
$C_{14}H_{15}N_2O_6$	289.056505	289.05637	0.4669672
$C_{19}H_{15}O_4$	289.0717612	289.07172	0.1424556
$C_{12}H_{19}O_9$	289.0829946	289.08295	0.1542114
$C_{18}H_{15}N_2O_3$	289.0814868	289.08295	-5.061618
$C_{16}H_{19}O_6$	289.0928904	289.09289	0.0013141
$C_{15}H_{19}N_2O_5$	289.1041238	289.10408	0.151433
$C_{17}H_{23}O_5$	289.1081466	289.10811	0.1265267
$C_{16}H_{23}N_2O_4$	289.11938	289.11936	0.0691061
$C_{18}H_{27}O_4$	289.1178722	289.11936	-5.146068
$C_{17}H_{27}N_2O_3$	289.1274858	289.12745	0.123882
$C_{17}H_{10}N_1O_5$	289.1292758	289.12928	-0.014596
$C_{14}H_{14}N_1O_7$	289.144532	289.1445	0.1106018
$C_{18}H_{14}N_1O_4$	289.1557654	289.15575	0.053189
$C_{15}H_{18}N_1O_6$	289.1542576	289.15575	-5.161328
$C_{19}H_{18}N_1O_3$	289.1656612	289.16568	-0.065084
$C_{16}H_{22}N_1O_5$	290.0670102	290.06698	0.1040446
$C_{14}H_{13}O_8$	290.075116	290.0751	0.0552191
$C_{13}H_{13}N_2O_7$	290.1033956	290.10338	0.0537046
$C_{18}H_{13}O_5$	290.1115014	290.11153	-0.098522
$C_{17}H_{13}N_2O_4$	290.139781	290.13979	-0.031089
$C_{15}H_{17}O_7$	290.169016	290.16909	-0.254963

C ₁₄ H ₁₇ N ₂ O ₆	291.0510258	291.05099	0.1229334
C ₁₉ H ₁₇ O ₄	291.0622592	291.06232	-0.208959
C ₁₈ H ₁₇ N ₂ O ₃	291.070365	291.07038	-0.051473
C ₁₆ H ₂₁ O ₆	291.0874112	291.08739	0.0727613
C ₁₅ H ₂₁ N ₂ O ₅	291.0986446	291.09866	-0.052972
C ₁₇ H ₂₅ O ₅	291.1067504	291.10677	-0.067268
C ₁₆ H ₂₅ N ₂ O ₄	291.1085404	291.10856	-0.067398
C ₁₈ H ₂₉ O ₄	291.1237966	291.12381	-0.046098
C ₁₇ H ₁₂ N ₁ O ₅	291.1236264	291.12381	-0.630729
C ₁₄ H ₁₆ N ₁ O ₇	291.13503	291.13506	-0.103114
C ₁₈ H ₁₆ N ₁ O ₄	291.1449258	291.14492	0.0198523
C ₁₅ H ₂₀ N ₁ O ₆	291.160182	291.16024	-0.199272
C ₁₉ H ₂₀ N ₁ O ₃	292.0462748	292.04629	-0.052115
C ₁₆ H ₂₄ N ₁ O ₅	292.0826602	292.08267	-0.033621
C ₁₇ H ₁₁ O ₆	292.0979164	292.09794	-0.080864
C ₁₆ H ₁₁ N ₂ O ₅	292.1190456	292.11907	-0.083596
C ₁₄ H ₁₅ O ₈	292.1271514	292.12716	-0.029379
C ₁₃ H ₁₅ N ₂ O ₇	292.1343018	292.13438	-0.267754
C ₁₈ H ₁₅ O ₅	292.1383848	292.13843	-0.154661
C ₁₇ H ₁₅ N ₂ O ₄	292.155431	292.15548	-0.167788
C ₁₅ H ₁₉ O ₇	293.0302904	293.03027	0.0695488
C ₁₄ H ₁₉ N ₂ O ₆	293.0666758	293.0667	-0.082644
C ₁₉ H ₁₉ O ₄	293.0779092	293.07793	-0.071039
C ₁₈ H ₁₉ N ₂ O ₃	293.081932	293.08194	-0.027365
C ₁₆ H ₂₃ O ₆	293.086015	293.08611	-0.324077
C ₁₅ H ₂₃ N ₂ O ₅	293.087805	293.0879	-0.324204

$C_{17}H_{27}O_5$	293.0931654	293.09321	-0.152239
$C_{18}H_{31}O_4$	293.1030612	293.1031	-0.132445
$C_{20}H_{39}O_2$	293.102891	293.1031	-0.713129
$C_{16}H_{10}N_1O_6$	293.1142946	293.11435	-0.189073
$C_{13}H_{14}N_1O_8$	293.1160805	293.11618	-0.339531
$C_{17}H_{14}N_1O_5$	293.1183174	293.11849	-0.588909
$C_{14}H_{18}N_1O_7$	293.1224004	293.12245	-0.169152
$C_{18}H_{18}N_1O_4$	293.1394466	293.13952	-0.250461
$C_{15}H_{22}N_1O_6$	293.15068	293.15075	-0.238854
$C_{19}H_{22}N_1O_3$	293.175832	293.17592	-0.30023
$C_{16}H_{26}N_1O_5$	294.0619248	294.0619	0.0842676
$C_{16}H_9O_7$	294.077181	294.07721	-0.098682
$C_{13}H_{13}O_9$	294.0983102	294.09838	-0.237404
$C_{24}H_9O_1$	294.1135664	294.11363	-0.216311
$C_{17}H_{13}O_6$	294.1346956	294.13478	-0.287012
$C_{16}H_{13}N_2O_5$	294.171081	294.17115	-0.234626
$C_{14}H_{17}O_8$	294.1791868	294.17935	-0.554704
$C_{13}H_{17}N_2O_7$	295.0459404	295.04598	-0.134285
$C_{18}H_{17}O_5$	295.0611966	295.06126	-0.214939
$C_{17}H_{17}N_2O_4$	295.0709222	295.07106	-0.467074
$C_{15}H_{21}O_7$	295.07243	295.07252	-0.305078
$C_{14}H_{21}N_2O_6$	295.0823258	295.08238	-0.183746
$C_{19}H_{21}O_4$	295.0935592	295.09362	-0.206104
$C_{18}H_{21}N_2O_3$	295.0953451	295.09645	-3.744288
$C_{16}H_{25}O_6$	295.097582	295.09768	-0.332162
$C_{15}H_{25}N_2O_5$	295.101665	295.10169	-0.084657

$C_{17}H_{29}O_5$	295.103455	295.10342	0.1185344
$C_{16}H_{29}N_2O_4$	295.1088154	295.10889	-0.252856
$C_{18}H_{33}O_4$	295.1187112	295.11879	-0.267079
$C_{16}H_{12}N_1O_6$	295.1299446	295.13001	-0.221665
$C_{13}H_{16}N_1O_8$	295.1339674	295.13402	-0.178292
$C_{17}H_{16}N_1O_5$	295.1380504	295.13805	0.0014153
$C_{14}H_{20}N_1O_7$	295.1550966	295.15518	-0.282631
$C_{18}H_{20}N_1O_4$	295.1549264	295.15518	-0.859278
$C_{15}H_{24}N_1O_6$	295.16633	295.16642	-0.304981
$C_{16}H_{11}O_7$	296.0411894	296.04115	0.1330217
$C_{15}H_{11}N_2O_6$	296.0564456	296.05651	-0.217594
$C_{13}H_{15}O_9$	296.0775748	296.07765	-0.254055
$C_{12}H_{15}N_2O_8$	296.0856806	296.08576	-0.268106
$C_{17}H_{15}O_6$	296.092831	296.0929	-0.233103
$C_{16}H_{15}N_2O_5$	296.1139602	296.11404	-0.269559
$C_{14}H_{19}O_8$	296.122066	296.12215	-0.283607
$C_{13}H_{19}N_2O_7$	296.1292164	296.12931	-0.316146
$C_{18}H_{19}O_5$	296.138942	296.14025	-4.416914
$C_{17}H_{19}N_2O_4$	296.1503456	296.15045	-0.352592
$C_{15}H_{23}O_7$	297.0404612	297.04052	-0.19802
$C_{14}H_{23}N_2O_6$	297.0615904	297.06166	-0.234363
$C_{19}H_{23}O_4$	297.0728238	297.07284	-0.0546
$C_{18}H_{23}N_2O_3$	297.0768466	297.07691	-0.21348
$C_{16}H_{27}O_6$	297.08808	297.08815	-0.235688
$C_{15}H_{27}N_2O_5$	297.0961858	297.09597	0.7264237
$C_{17}H_{31}O_5$	297.0979758	297.09805	-0.249817

$C_{18}H_{35}O_4$	297.0978056	297.09805	-0.822692
$C_{15}H_{10}N_1O_7$	297.1092092	297.10929	-0.272022
$C_{16}H_{14}N_1O_6$	297.113232	297.11332	-0.296251
$C_{17}H_{18}N_1O_5$	297.1244654	297.12453	-0.217485
$C_{14}H_{22}N_1O_7$	297.1325712	297.13248	0.3069933
$C_{18}H_{22}N_1O_4$	297.1343612	297.13445	-0.298922
$C_{16}H_{13}O_7$	297.1455946	297.1457	-0.354776
$C_{15}H_{13}N_2O_6$	297.1707466	297.17084	-0.314365
$C_{13}H_{17}O_9$	297.18198	297.18208	-0.336562
$C_{19}H_{13}N_2O_3$	297.2183654	297.21845	-0.284707
$C_{17}H_{17}O_6$	297.2435174	297.24356	-0.143384
$C_{16}H_{17}N_2O_5$	297.2799028	297.28009	-0.629777
$C_{14}H_{21}O_8$	298.0568394	298.05683	0.0314702
$C_{13}H_{21}N_2O_7$	298.0720956	298.07216	-0.216123
$C_{18}H_{21}O_5$	298.0802014	298.08031	-0.364272
$C_{17}H_{21}N_2O_4$	298.0932248	298.09331	-0.285884
$C_{15}H_{25}O_7$	298.0970774	298.0965	1.9368855
$C_{19}H_{25}O_4$	298.1013306	298.1014	-0.232747
$C_{18}H_{25}N_2O_3$	298.108481	298.10855	-0.231527
$C_{16}H_{29}O_6$	298.1296102	298.12973	-0.401906
$C_{17}H_{33}O_5$	298.1448664	298.14494	-0.246927
$C_{15}H_{12}N_1O_7$	298.1659956	298.16608	-0.283131
$C_{16}H_{16}N_1O_6$	299.040855	299.04102	-0.551831
$C_{17}H_{20}N_1O_5$	299.0561112	299.05617	-0.196686
$C_{18}H_{24}N_1O_4$	299.0673446	299.06741	-0.218747
$C_{15}H_{11}O_8$	299.0691305	299.06921	-0.265898

$C_{16}H_{15}O_7$	299.0754504	299.07555	-0.332967
$C_{15}H_{15}N_2O_6$	299.0772404	299.07729	-0.165911
$C_{13}H_{19}O_9$	299.0884738	299.08852	-0.154537
$C_{17}H_{19}O_6$	299.0924966	299.09257	-0.245476
$C_{16}H_{19}N_2O_5$	299.1022222	299.10285	-2.099015
$C_{14}H_{23}O_8$	299.10373	299.10381	-0.267533
$C_{18}H_{23}O_5$	299.1118358	299.11195	-0.381738
$C_{17}H_{23}N_2O_4$	299.1136258	299.11372	-0.314998
$C_{15}H_{14}N_1O_7$	299.1134556	299.11372	-0.884013
$C_{19}H_{14}N_1O_4$	299.1248592	299.12491	-0.169896
$C_{16}H_{18}N_1O_6$	299.128882	299.12897	-0.294255
$C_{20}H_{18}N_1O_3$	299.1401154	299.14021	-0.316307
$C_{17}H_{22}N_1O_5$	299.1500112	299.1501	-0.296908
$C_{18}H_{26}N_1O_4$	299.1612446	299.16132	-0.252105
$C_{15}H_{13}O_8$	299.1863966	299.1865	-0.345671
$C_{14}H_{13}N_2O_7$	299.2591674	299.25916	0.0246606
$C_{18}H_{13}N_2O_4$	300.0513602	300.05141	-0.166039
$C_{16}H_{17}O_7$	300.059466	300.0594	0.2200154
$C_{15}H_{17}N_2O_6$	300.0724894	300.07244	0.1645599
$C_{20}H_{17}O_4$	300.0877456	300.08781	-0.214671
$C_{17}H_{21}O_6$	300.1088748	300.10895	-0.250643
$C_{16}H_{21}N_2O_5$	300.124131	300.12421	-0.263291
$C_{18}H_{25}O_5$	300.1452602	300.14534	-0.265938
$C_{17}H_{25}N_2O_4$	300.153366	300.1535	-0.446379
$C_{19}H_{29}O_4$	300.1605164	300.16062	-0.345216
$C_{14}H_{12}N_1O_8$	301.0353758	301.03537	0.0192001

C ₁₈ H ₁₂ N ₁ O ₅	301.056505	301.05647	0.1161905
C ₁₅ H ₁₆ N ₁ O ₇	301.0717612	301.0718	-0.12894
C ₁₉ H ₁₆ N ₁ O ₄	301.0829946	301.08304	-0.150856
C ₁₆ H ₂₀ N ₁ O ₆	301.0847805	301.0849	-0.396971
C ₂₀ H ₂₀ N ₁ O ₃	301.0911004	301.09111	-0.031825
C ₁₇ H ₂₄ N ₁ O ₅	301.0928904	301.09295	-0.198012
C ₁₈ H ₂₈ N ₁ O ₄	301.096743	301.09612	2.0690357
C ₁₈ H ₁₁ O ₆	301.1041238	301.10419	-0.219924
C ₁₇ H ₁₁ N ₂ O ₅	301.1081466	301.1082	-0.177412
C ₁₅ H ₁₅ O ₈	301.11938	301.11946	-0.265742
C ₁₄ H ₁₅ N ₂ O ₇	301.1274858	301.12753	-0.146723
C ₁₉ H ₁₅ O ₅	301.1292758	301.12934	-0.213264
C ₁₈ H ₁₅ N ₂ O ₄	301.1405092	301.1406	-0.301587
C ₁₆ H ₁₉ O ₇	301.144532	301.14461	-0.259079
C ₁₅ H ₁₉ N ₂ O ₆	301.1557654	301.15586	-0.31419
C ₂₀ H ₁₉ O ₄	301.1656612	301.16574	-0.261717
C ₁₉ H ₁₉ N ₂ O ₃	301.2020466	301.20214	-0.310158
C ₁₇ H ₂₃ O ₆	302.0670102	302.06701	0.0005956
C ₁₆ H ₂₃ N ₂ O ₅	302.0881394	302.0882	-0.20067
C ₁₈ H ₂₇ O ₅	302.1033956	302.10342	-0.080834
C ₁₇ H ₂₇ N ₂ O ₄	302.1326306	302.13265	-0.064152
C ₁₇ H ₁₀ N ₁ O ₆	302.139781	302.13984	-0.19534
C ₁₄ H ₁₄ N ₁ O ₈	302.169016	302.16904	-0.079367
C ₁₈ H ₁₄ N ₁ O ₅	302.1761664	302.17609	0.2527661
C ₁₅ H ₁₈ N ₁ O ₇	303.0510258	303.051	0.0850679
C ₁₉ H ₁₈ N ₁ O ₄	303.0640451	303.06407	-0.082233

$C_{16}H_{22}N_1O_6$	303.070365	303.07035	0.0495519
$C_{20}H_{22}N_1O_3$	303.072155	303.07213	0.0824223
$C_{17}H_{26}N_1O_5$	303.0874112	303.0874	0.0368867
$C_{17}H_9O_7$	303.0986446	303.09867	-0.083867
$C_{14}H_{13}O_9$	303.1085404	303.10856	-0.06473
$C_{18}H_{13}O_6$	303.1197738	303.11977	0.01247
$C_{17}H_{13}N_2O_5$	303.1237966	303.12382	-0.077262
$C_{15}H_{17}O_8$	303.1236264	303.12382	-0.63875
$C_{14}H_{17}N_2O_7$	303.13503	303.13506	-0.099032
$C_{19}H_{17}O_5$	303.1431358	303.14314	-0.013796
$C_{18}H_{17}N_2O_4$	303.1449258	303.14495	-0.079896
$C_{16}H_{21}O_7$	303.1561592	303.15628	-0.398541
$C_{15}H_{21}N_2O_6$	303.160182	303.16027	-0.290342
$C_{20}H_{21}O_4$	303.1714154	303.17147	-0.180162
$C_{19}H_{21}N_2O_3$	303.1813112	303.18136	-0.161026
$C_{17}H_{25}O_6$	303.2176966	303.21774	-0.143198
$C_{18}H_{29}O_5$	304.0462748	304.04621	0.2130593
$C_{17}H_{12}N_1O_6$	304.0543806	304.05438	0.0020315
$C_{14}H_{16}N_1O_8$	304.0826602	304.08265	0.0334774
$C_{18}H_{16}N_1O_5$	304.1190456	304.11904	0.0183477
$C_{15}H_{20}N_1O_7$	304.1271514	304.12715	0.0046615
$C_{19}H_{20}N_1O_4$	304.1383848	304.1383	0.2788786
$C_{16}H_{24}N_1O_6$	304.155431	304.15546	-0.095412
$C_{17}H_{11}O_7$	304.1918164	304.19193	-0.373515
$C_{14}H_{15}O_9$	305.0666758	305.06663	0.1500652
$C_{13}H_{15}N_2O_8$	305.0779092	305.07786	0.1612044

C ₁₈ H ₁₅ O ₆	305.081932	305.08194	-0.026288
C ₁₇ H ₁₅ N ₂ O ₅	305.1030612	305.10303	0.1021946
C ₁₅ H ₁₉ O ₈	305.102891	305.10303	-0.45565
C ₁₄ H ₁₉ N ₂ O ₇	305.1142946	305.11428	0.047785
C ₁₉ H ₁₉ O ₅	305.1394466	305.13944	0.0215636
C ₁₈ H ₁₉ N ₂ O ₄	305.1392764	305.13944	-0.536214
C ₁₆ H ₂₃ O ₇	305.15068	305.15065	0.0982462
C ₁₅ H ₂₃ N ₂ O ₆	305.1605758	305.16056	0.0517102
C ₂₀ H ₂₃ O ₄	305.175832	305.17586	-0.091816
C ₁₉ H ₂₃ N ₂ O ₃	305.1870654	305.18721	-0.473874
C ₁₇ H ₂₇ O ₆	306.0619248	306.06188	0.1463099
C ₁₆ H ₂₇ N ₂ O ₅	306.0700306	306.06998	0.1653795
C ₁₈ H ₃₁ O ₅	306.0983102	306.09826	0.1639339
C ₁₆ H ₁₀ N ₁ O ₇	306.106416	306.10637	0.1503324
C ₁₃ H ₁₄ N ₁ O ₉	306.1135664	306.11354	0.0861768
C ₁₇ H ₁₄ N ₁ O ₆	306.1176494	306.1176	0.1614337
C ₁₄ H ₁₈ N ₁ O ₈	306.1346956	306.13468	0.0508923
C ₁₈ H ₁₈ N ₁ O ₅	306.1428014	306.14277	0.1026243
C ₁₅ H ₂₂ N ₁ O ₇	306.171081	306.17107	0.035862
C ₁₉ H ₂₂ N ₁ O ₄	306.2074664	306.20746	0.0208352
C ₁₆ H ₂₆ N ₁ O ₆	307.0459404	307.04585	0.294353
C ₁₆ H ₉ O ₈	307.0823258	307.08225	0.2467739
C ₁₇ H ₁₃ O ₇	307.0935592	307.09353	0.0950196
C ₁₆ H ₁₃ N ₂ O ₆	307.097582	307.0976	-0.058679
C ₁₄ H ₁₇ O ₉	307.103455	307.10331	0.4720881
C ₁₃ H ₁₇ N ₂ O ₈	307.1088154	307.1088	0.0500796

$C_{18}H_{17}O_6$	307.1187112	307.11864	0.2317667
$C_{17}H_{17}N_2O_5$	307.118541	307.11864	-0.322417
$C_{15}H_{21}O_8$	307.1299446	307.12989	0.1777095
$C_{14}H_{21}N_2O_7$	307.1380504	307.138	0.1641532
$C_{19}H_{21}O_5$	307.1550966	307.15504	0.1842063
$C_{18}H_{21}N_2O_4$	307.1549264	307.15504	-0.369911
$C_{16}H_{25}O_7$	307.16633	307.16626	0.2278241
$C_{15}H_{25}N_2O_6$	307.191482	307.19144	0.1366571
$C_{20}H_{25}O_4$	307.2027154	307.20273	-0.047591
$C_{17}H_{29}O_6$	308.0564456	308.05636	0.2778059
$C_{18}H_{33}O_5$	308.0775748	308.07749	0.2751901
$C_{16}H_{12}N_1O_7$	308.0856806	308.08559	0.2941315
$C_{17}H_{16}N_1O_6$	308.092831	308.09272	0.3602158
$C_{18}H_{20}N_1O_5$	308.1139602	308.11386	0.3251391
$C_{19}H_{24}N_1O_4$	308.122066	308.12199	0.2467129
$C_{16}H_{11}O_8$	308.1292164	308.12917	0.1505209
$C_{17}H_{15}O_7$	308.1332994	308.13326	0.1279242
$C_{16}H_{15}N_2O_6$	308.1503456	308.15032	0.0830111
$C_{14}H_{19}O_9$	308.1584514	308.15842	0.1019531
$C_{13}H_{19}N_2O_8$	308.1633649	308.16341	-0.146422
$C_{18}H_{19}O_6$	308.1696848	308.16963	0.1778815
$C_{17}H_{19}N_2O_5$	308.1948368	308.19469	0.4763795
$C_{15}H_{23}O_8$	309.0615904	309.06148	0.3571453
$C_{14}H_{23}N_2O_7$	309.0728238	309.07274	0.2710685
$C_{19}H_{23}O_5$	309.0768466	309.07675	0.3124786
$C_{18}H_{23}N_2O_4$	309.0809296	309.0808	0.4193649

$C_{16}H_{27}O_7$	309.08808	309.088	0.2587609
$C_{19}H_{27}N_2O_3$	309.0865722	309.088	-4.619483
$C_{17}H_{31}O_6$	309.0898659	309.09133	-4.736881
$C_{18}H_{35}O_5$	309.0979758	309.09788	0.3098691
$C_{16}H_{14}N_1O_7$	309.1092092	309.10907	0.4502613
$C_{20}H_{14}N_1O_4$	309.113232	309.11314	0.2975605
$C_{17}H_{18}N_1O_6$	309.1244654	309.1244	0.2115002
$C_{21}H_{18}N_1O_3$	309.1343612	309.13426	0.3273007
$C_{18}H_{22}N_1O_5$	309.1455946	309.14549	0.3382869
$C_{19}H_{26}N_1O_4$	309.1537004	309.15354	0.518893
$C_{15}H_9O_9$	309.1707466	309.17065	0.3123837
$C_{16}H_{13}O_8$	309.1705764	309.17065	-0.238121
$C_{15}H_{13}N_2O_7$	309.18198	309.18198	-6.5E-05
$C_{17}H_{17}O_7$	309.207132	309.20705	0.2651294
$C_{16}H_{17}N_2O_6$	310.0649452	310.06483	0.3715922
$C_{14}H_{21}O_9$	310.0720956	310.07204	0.1792483
$C_{20}H_{17}N_2O_3$	310.0932248	310.09313	0.3056497
$C_{18}H_{21}O_6$	310.108481	310.10839	0.2933809
$C_{17}H_{21}N_2O_5$	310.1278202	310.12783	-0.031543
$C_{15}H_{25}O_8$	310.1296102	310.12954	0.2262922
$C_{19}H_{25}O_5$	310.137716	310.13765	0.2128658
$C_{18}H_{25}N_2O_4$	310.1448664	310.14476	0.3430007
$C_{16}H_{29}O_7$	310.1659956	310.16587	0.4048797
$C_{15}H_{12}N_1O_8$	310.2104868	310.21045	0.1186862
$C_{19}H_{12}N_1O_5$	311.0561112	311.05609	0.0680903
$C_{16}H_{16}N_1O_7$	311.0673446	311.06736	-0.049572

$C_{20}H_{16}N_1O_4$	311.0754504	311.07557	-0.384416
$C_{17}H_{20}N_1O_6$	311.0772404	311.07722	0.065514
$C_{21}H_{20}N_1O_3$	311.0884738	311.08845	0.076441
$C_{18}H_{24}N_1O_5$	311.0924966	311.09247	0.0854405
$C_{19}H_{28}N_1O_4$	311.0965796	311.09656	0.0630598
$C_{16}H_{15}O_8$	311.10373	311.10367	0.1927971
$C_{15}H_{15}N_2O_7$	311.1022222	311.10367	-4.65384
$C_{20}H_{15}O_5$	311.1136258	311.11358	0.1471485
$C_8H_{19}N_2O_{12}$	311.1248592	311.12482	0.1259298
$C_{19}H_{15}N_2O_4$	311.128882	311.12885	0.1027867
$C_{17}H_{19}O_7$	311.1287118	311.12885	-0.444254
$C_{16}H_{19}N_2O_6$	311.132965	311.13289	0.2411114
$C_{21}H_{19}O_4$	311.1401154	311.14005	0.2101301
$C_{20}H_{19}N_2O_3$	311.1386076	311.14005	-4.635941
$C_{25}H_{19}O_1$	311.1500112	311.14995	0.1966251
$C_{18}H_{23}O_6$	311.1612446	311.16122	0.0789941
$C_{17}H_{23}N_2O_5$	311.1863966	311.18636	0.1175498
$C_{19}H_{27}O_5$	311.222782	311.22268	0.3276749
$C_{18}H_{27}N_2O_4$	311.2955528	311.29554	0.0410539
$C_{15}H_{14}N_1O_8$	312.0513602	312.05139	-0.095562
$C_{19}H_{14}N_1O_5$	312.059466	312.0595	-0.108897
$C_{16}H_{18}N_1O_7$	312.0724894	312.07261	-0.386513
$C_{20}H_{18}N_1O_4$	312.0877456	312.08775	-0.014163
$C_{17}H_{22}N_1O_6$	312.1088748	312.10885	0.0793951
$C_{21}H_{22}N_1O_3$	312.1127274	312.11207	2.1062259
$C_{18}H_{26}N_1O_5$	312.1169806	312.11696	0.0660576

$C_{15}H_{13}O_9$	312.1218941	312.12285	-3.062656
$C_{19}H_{13}O_6$	312.124131	312.12413	0.0031395
$C_{18}H_{13}N_2O_5$	312.1452602	312.14523	0.0966854
$C_{16}H_{17}O_8$	312.1605164	312.16053	-0.043632
$C_{15}H_{17}N_2O_7$	312.1816456	312.18174	-0.302452
$C_{20}H_{17}O_5$	313.0353758	313.03544	-0.205153
$C_{19}H_{17}N_2O_4$	313.056505	313.05663	-0.399353
$C_{17}H_{21}O_7$	313.0658882	313.06611	-0.708541
$C_{16}H_{21}N_2O_6$	313.0717612	313.07179	-0.092056
$C_{21}H_{21}O_4$	313.0829946	313.08302	-0.081193
$C_{20}H_{21}N_2O_3$	313.0911004	313.09115	-0.158364
$C_{25}H_{21}O_1$	313.0928904	313.09291	-0.062665
$C_{18}H_{25}O_6$	313.096743	313.09602	2.3091262
$C_{17}H_{25}N_2O_5$	313.1041238	313.1042	-0.243434
$C_{19}H_{29}O_5$	313.1081466	313.10817	-0.074799
$C_{18}H_{29}N_2O_4$	313.11938	313.11942	-0.127811
$C_{18}H_{12}N_1O_6$	313.1292758	313.1293	-0.077349
$C_{15}H_{16}N_1O_8$	313.1405092	313.14052	-0.034553
$C_{19}H_{16}N_1O_5$	313.144532	313.14457	-0.121414
$C_{16}H_{20}N_1O_7$	313.1557654	313.15582	-0.174418
$C_{20}H_{20}N_1O_4$	313.1656612	313.16568	-0.060096
$C_{17}H_{24}N_1O_6$	313.1768946	313.17688	0.0465548
$C_{21}H_{24}N_1O_3$	313.2020466	313.20207	-0.074776
$C_{18}H_{28}N_1O_5$	313.21328	313.21324	0.1276443
$C_{18}H_{11}O_7$	313.238432	313.23842	0.0382453
$C_{17}H_{11}N_2O_6$	314.0670102	314.06708	-0.22231

$C_{15}H_{15}O_9$	314.0881394	314.08823	-0.288518
$C_{14}H_{15}N_2O_8$	314.1033956	314.10346	-0.205092
$C_{19}H_{15}O_6$	314.1115014	314.11157	-0.218337
$C_{18}H_{15}N_2O_5$	314.1227348	314.12279	-0.175671
$C_{16}H_{19}O_8$	314.1245248	314.1246	-0.239459
$C_{15}H_{19}N_2O_7$	314.1326306	314.13268	-0.157202
$C_{20}H_{19}O_5$	314.139781	314.13983	-0.156046
$C_{19}H_{19}N_2O_4$	314.1478868	314.14783	0.1808629
$C_{17}H_{23}O_7$	314.1609102	314.16099	-0.254074
$C_{16}H_{23}N_2O_6$	315.0510258	315.05108	-0.172099
$C_{21}H_{23}O_4$	315.0622592	315.06229	-0.097822
$C_{20}H_{23}N_2O_3$	315.072155	315.07222	-0.206366
$C_{18}H_{27}O_6$	315.0833884	315.08345	-0.195568
$C_{17}H_{27}N_2O_5$	315.0874112	315.08748	-0.218416
$C_{19}H_{31}O_5$	315.0986446	315.09872	-0.239354
$C_{22}H_{43}O_2$	315.1085404	315.10859	-0.15747
$C_{17}H_{10}N_1O_7$	315.1197738	315.11989	-0.368812
$C_{18}H_{14}N_1O_6$	315.1237966	315.12387	-0.232988
$C_{15}H_{18}N_1O_8$	315.1236264	315.12387	-0.773094
$C_{19}H_{18}N_1O_5$	315.1335222	315.13433	-2.563422
$C_{16}H_{22}N_1O_7$	315.13503	315.13515	-0.380853
$C_{20}H_{22}N_1O_4$	315.1449258	315.14504	-0.362437
$C_{17}H_{26}N_1O_6$	315.1561592	315.15622	-0.192984
$C_{21}H_{26}N_1O_3$	315.160182	315.16023	-0.152367
$C_{17}H_9O_8$	315.1714154	315.17148	-0.205032
$C_{18}H_{13}O_7$	315.1813112	315.18141	-0.313534

C ₁₇ H ₁₃ N ₂ O ₆	315.1925446	315.19268	-0.429642
C ₁₅ H ₁₇ O ₉	315.2176966	315.21777	-0.232919
C ₁₄ H ₁₇ N ₂ O ₈	315.254082	315.25414	-0.184042
C ₁₉ H ₁₇ O ₆	316.0462748	316.04633	-0.174722
C ₁₈ H ₁₇ N ₂ O ₅	316.0826602	316.08266	0.0005692
C ₁₆ H ₂₁ O ₈	316.1118952	316.11196	-0.204935
C ₁₅ H ₂₁ N ₂ O ₇	316.1190456	316.11905	-0.013982
C ₂₀ H ₂₁ O ₅	316.1271514	316.12715	0.0044846
C ₁₉ H ₂₁ N ₂ O ₄	316.1383848	316.13845	-0.206183
C ₁₇ H ₂₅ O ₇	316.1401748	316.1401	0.2365403
C ₁₆ H ₂₅ N ₂ O ₆	316.155431	316.15551	-0.249941
C ₂₁ H ₂₅ O ₄	317.0666758	317.06665	0.0813075
C ₁₈ H ₂₉ O ₆	317.0779092	317.07788	0.0920275
C ₁₇ H ₂₉ N ₂ O ₅	317.086015	317.08605	-0.110324
C ₁₉ H ₃₃ O ₅	317.087805	317.08779	0.0472421
C ₁₇ H ₁₂ N ₁ O ₇	317.0931654	317.09327	-0.329935
C ₁₄ H ₁₆ N ₁ O ₉	317.1030612	317.10302	0.1298628
C ₁₈ H ₁₆ N ₁ O ₆	317.102891	317.10302	-0.406871
C ₁₅ H ₂₀ N ₁ O ₈	317.1142946	317.11424	0.1721143
C ₁₉ H ₂₀ N ₁ O ₅	317.1241904	317.12421	-0.061869
C ₁₆ H ₂₄ N ₁ O ₇	317.1354238	317.13537	0.1695802
C ₂₀ H ₂₄ N ₁ O ₄	317.1394466	317.13941	0.1153433
C ₁₇ H ₂₈ N ₁ O ₆	317.15068	317.15066	0.0629981
C ₁₇ H ₁₁ O ₈	317.1605758	317.16055	0.0812834
C ₁₈ H ₁₅ O ₇	317.175832	317.17575	0.2584683
C ₁₇ H ₁₅ N ₂ O ₆	317.1870654	317.18706	0.0169613

C ₁₅ H ₁₉ O ₉	317.1969612	317.19694	0.0667721
C ₁₄ H ₁₉ N ₂ O ₈	317.2333466	317.23335	-0.010781
C ₁₉ H ₁₉ O ₆	318.0619248	318.06187	0.1722303
C ₁₈ H ₁₉ N ₂ O ₅	318.0983102	318.09824	0.2206233
C ₁₆ H ₂₃ O ₈	318.1176494	318.11761	0.1239092
C ₁₅ H ₂₃ N ₂ O ₇	318.1346956	318.13462	0.237572
C ₂₀ H ₂₃ O ₅	318.1428014	318.14276	0.1301859
C ₁₉ H ₂₃ N ₂ O ₄	318.1540348	318.15401	0.0780053
C ₁₇ H ₂₇ O ₇	318.171081	318.171	0.2545168
C ₁₆ H ₂₇ N ₂ O ₆	319.0459404	319.04588	0.1892514
C ₂₀ H ₂₇ N ₂ O ₃	319.0823258	319.08222	0.3315129
C ₁₈ H ₃₁ O ₆	319.0935592	319.09346	0.3108176
C ₁₉ H ₃₅ O ₅	319.103455	319.10324	0.6736997
C ₁₇ H ₁₄ N ₁ O ₇	319.1187112	319.1186	0.3483967
C ₁₈ H ₁₈ N ₁ O ₆	319.1299446	319.12985	0.296368
C ₁₅ H ₂₂ N ₁ O ₈	319.1398404	319.13977	0.22053
C ₁₉ H ₂₂ N ₁ O ₅	319.1550966	319.15502	0.2399457
C ₂₀ H ₂₆ N ₁ O ₄	319.16633	319.16622	0.3445849
C ₁₇ H ₁₃ O ₈	320.0775748	320.07757	0.0149336
C ₁₆ H ₁₃ N ₂ O ₇	320.0856806	320.08567	0.0331714
C ₁₄ H ₁₇ O ₁₀	320.092831	320.09287	-0.121902
C ₁₈ H ₁₇ O ₇	320.1139602	320.11391	0.1567564
C ₁₇ H ₁₇ N ₂ O ₆	320.1292164	320.12926	-0.136258
C ₁₅ H ₂₁ O ₉	320.1503456	320.1503	0.1423703
C ₁₄ H ₂₁ N ₂ O ₈	320.186731	320.18664	0.2841464
C ₁₉ H ₂₁ O ₆	321.0615904	321.06163	-0.123403

$C_{18}H_{21}N_2O_5$	321.0728238	321.07293	-0.330829
$C_{16}H_{25}O_8$	321.08808	321.0881	-0.062351
$C_{15}H_{25}N_2O_7$	321.0979758	321.09799	-0.044286
$C_{20}H_{25}O_5$	321.1092092	321.10924	-0.09598
$C_{19}H_{25}N_2O_4$	321.1109951	321.11111	-0.357888
$C_{17}H_{29}O_7$	321.113232	321.11324	-0.024976
$C_{20}H_{29}N_2O_3$	321.117315	321.11732	-0.015516
$C_{18}H_{33}O_6$	321.1343612	321.13437	-0.027465
$C_{16}H_{12}N_1O_8$	321.134191	321.13437	-0.557462
$C_{17}H_{16}N_1O_7$	321.1455946	321.1456	-0.016877
$C_{21}H_{16}N_1O_4$	321.1707466	321.17075	-0.010649
$C_{14}H_{20}N_1O_9$	321.18198	321.18194	0.1244774
$C_{18}H_{20}N_1O_6$	321.207132	321.20703	0.3174895
$C_{22}H_{20}N_1O_3$	322.0568394	322.05684	-0.001925
$C_{19}H_{24}N_1O_5$	322.0649452	322.06503	-0.263246
$C_{16}H_{11}O_9$	322.0720956	322.07226	-0.510507
$C_{17}H_{15}O_8$	322.0932248	322.09331	-0.264582
$C_{16}H_{15}N_2O_7$	322.108481	322.10856	-0.245321
$C_{21}H_{15}O_5$	322.112564	322.11257	-0.018572
$C_{20}H_{15}N_2O_4$	322.1296102	322.12968	-0.216745
$C_{18}H_{19}O_7$	322.1448664	322.14493	-0.197489
$C_{17}H_{19}N_2O_6$	322.1659956	322.16607	-0.230999
$C_{15}H_{23}O_9$	322.202381	322.20242	-0.121104
$C_{21}H_{19}N_2O_3$	323.0561112	323.05615	-0.120165
$C_{26}H_{19}O_1$	323.0673446	323.06745	-0.32631
$C_{19}H_{23}O_6$	323.0772404	323.07727	-0.091681

$C_{18}H_{23}N_2O_5$	323.0884738	323.08855	-0.235911
$C_{16}H_{27}O_8$	323.0924966	323.09256	-0.196291
$C_{20}H_{27}O_5$	323.10373	323.10379	-0.185761
$C_{19}H_{27}N_2O_4$	323.1136258	323.1137	-0.229703
$C_{17}H_{31}O_7$	323.1248592	323.12493	-0.219173
$C_{18}H_{35}O_6$	323.128882	323.12897	-0.272399
$C_{16}H_{14}N_1O_8$	323.132965	323.13303	-0.201101
$C_{20}H_{14}N_1O_5$	323.1401154	323.14016	-0.138083
$C_{17}H_{18}N_1O_7$	323.1500112	323.15009	-0.243912
$C_{21}H_{18}N_1O_4$	323.1612446	323.16133	-0.264327
$C_{18}H_{22}N_1O_6$	323.1863966	323.1865	-0.320001
$C_{19}H_{26}N_1O_5$	323.1862264	323.1865	-0.846633
$C_{16}H_{13}O_9$	323.19763	323.1977	-0.216648
$C_{20}H_{13}O_6$	324.0513602	324.05138	-0.061163
$C_{19}H_{13}N_2O_5$	324.0724894	324.07246	0.0906584
$C_{17}H_{17}O_8$	324.0805952	324.08053	0.2012391
$C_{16}H_{17}N_2O_7$	324.0877456	324.0877	0.1406406
$C_{21}H_{17}O_5$	324.0958514	324.09578	0.2203598
$C_9H_{21}N_2O_{12}$	324.1088748	324.10885	0.0764555
$C_{20}H_{17}N_2O_4$	324.1218941	324.12301	-3.442908
$C_{18}H_{21}O_7$	324.124131	324.12412	0.0338756
$C_{17}H_{21}N_2O_6$	324.1452602	324.14525	0.0314054
$C_{22}H_{21}O_4$	324.1605164	324.16049	0.0813791
$C_{21}H_{21}N_2O_3$	324.1816456	324.1817	-0.167869
$C_{26}H_{21}O_1$	324.1897514	324.18975	0.0043731
$C_{19}H_{25}O_6$	325.0353758	325.03518	0.6023341

$C_{18}H_{25}N_2O_5$	325.056505	325.05643	0.2306673
$C_{16}H_{29}O_8$	325.0717612	325.0717	0.1882043
$C_{20}H_{29}O_5$	325.0829946	325.08291	0.2601794
$C_{19}H_{29}N_2O_4$	325.0814868	325.08291	-4.378041
$C_{19}H_{12}N_1O_6$	325.0847805	325.08476	0.0629931
$C_{16}H_{16}N_1O_8$	325.0911004	325.09107	0.0935667
$C_{20}H_{16}N_1O_5$	325.0928904	325.09282	0.2164917
$C_{17}H_{20}N_1O_7$	325.1041238	325.10413	-0.019133
$C_{21}H_{20}N_1O_4$	325.1081466	325.10805	0.2970701
$C_{18}H_{24}N_1O_6$	325.11938	325.11934	0.1229699
$C_{22}H_{24}N_1O_3$	325.1292758	325.12922	0.1715622
$C_{19}H_{28}N_1O_5$	325.1405092	325.14045	0.1820133
$C_{19}H_{11}O_7$	325.144532	325.14451	0.0676004
$C_{18}H_{11}N_2O_6$	325.1557654	325.15568	0.2625815
$C_{16}H_{15}O_9$	325.1656612	325.16561	0.1573964
$C_{15}H_{15}N_2O_8$	325.2020466	325.20197	0.2354841
$C_{20}H_{15}O_6$	326.0670102	326.06695	0.184563
$C_{19}H_{15}N_2O_5$	326.0881394	326.08812	0.0594315
$C_{17}H_{19}O_8$	326.1033956	326.10331	0.2624318
$C_{16}H_{19}N_2O_7$	326.1115014	326.11145	0.1576691
$C_{21}H_{19}O_5$	326.1245248	326.1244	0.3826143
$C_{20}H_{19}N_2O_4$	326.1326306	326.13253	0.3085177
$C_{18}H_{23}O_7$	326.139781	326.13968	0.3096215
$C_{17}H_{23}N_2O_6$	326.1609102	326.16074	0.5217667
$C_{22}H_{23}O_4$	326.169016	326.16901	0.0184496
$C_{21}H_{23}N_2O_3$	326.2054014	326.20535	0.1576237

$C_{26}H_{23}O_1$	327.0510258	327.05105	-0.074056
$C_{19}H_{27}O_6$	327.072155	327.07217	-0.045923
$C_{18}H_{27}N_2O_5$	327.0833884	327.08349	-0.310686
$C_{20}H_{31}O_5$	327.0874112	327.08742	-0.026966
$C_{18}H_{10}N_1O_7$	327.0971368	327.0979	-2.333313
$C_{15}H_{14}N_1O_9$	327.0986446	327.09867	-0.077714
$C_{19}H_{14}N_1O_6$	327.1085404	327.10855	-0.02941
$C_{16}H_{18}N_1O_8$	327.1197738	327.1198	-0.080154
$C_{20}H_{18}N_1O_5$	327.1237966	327.12378	0.0506839
$C_{17}H_{22}N_1O_7$	327.13503	327.13499	0.1222122
$C_{21}H_{22}N_1O_4$	327.1431358	327.14321	-0.226758
$C_{18}H_{26}N_1O_6$	327.1449258	327.1449	0.0788027
$C_{18}H_9O_8$	327.1561592	327.15614	0.0586261
$C_{19}H_{13}O_7$	327.160182	327.16017	0.0366178
$C_{18}H_{13}N_2O_6$	327.1714154	327.1715	-0.258641
$C_{16}H_{17}O_9$	327.1813112	327.1813	0.0341704
$C_{15}H_{17}N_2O_8$	327.1925446	327.19253	0.0445606
$C_{20}H_{17}O_6$	327.2176966	327.21764	0.1729121
$C_{19}H_{17}N_2O_5$	328.0462748	328.04646	-0.564616
$C_{17}H_{21}O_8$	328.067404	328.06764	-0.719426
$C_{16}H_{21}N_2O_7$	328.0826602	328.08274	-0.243293
$C_{21}H_{21}O_5$	328.090766	328.09083	-0.195014
$C_{20}H_{21}N_2O_4$	328.1037894	328.10387	-0.245715
$C_{18}H_{25}O_7$	328.1118952	328.11193	-0.106007
$C_{17}H_{25}N_2O_6$	328.1190456	328.1191	-0.165855
$C_{19}H_{29}O_6$	328.1401748	328.14026	-0.259706

$C_{18}H_{29}N_2O_5$	328.155431	328.15548	-0.149381
$C_{20}H_{33}O_5$	328.1765602	328.17656	0.0005482
$C_{23}H_{45}O_2$	329.0302904	329.03023	0.1835086
$C_{18}H_{12}N_1O_7$	329.0666758	329.06668	-0.012824
$C_{15}H_{16}N_1O_9$	329.0779092	329.07787	0.1190596
$C_{19}H_{16}N_1O_6$	329.087805	329.08786	-0.16719
$C_{16}H_{20}N_1O_8$	329.0990384	329.09908	-0.126467
$C_{20}H_{20}N_1O_5$	329.1030612	329.1031	-0.117957
$C_{17}H_{24}N_1O_7$	329.1142946	329.11437	-0.229161
$C_{21}H_{24}N_1O_4$	329.1224004	329.12243	-0.089882
$C_{18}H_{28}N_1O_6$	329.1241904	329.12425	-0.181148
$C_{18}H_{11}O_8$	329.1354238	329.13548	-0.170811
$C_{17}H_{11}N_2O_7$	329.1394466	329.13951	-0.192685
$C_{15}H_{15}O_{10}$	329.15068	329.15076	-0.243111
$C_{19}H_{15}O_7$	329.1605758	329.16065	-0.225483
$C_{18}H_{15}N_2O_6$	329.1718092	329.17191	-0.306284
$C_{16}H_{19}O_9$	329.175832	329.17591	-0.237016
$C_{15}H_{19}N_2O_8$	329.1969612	329.19702	-0.178678
$C_{20}H_{19}O_6$	329.2333466	329.23341	-0.19263
$C_{19}H_{19}N_2O_5$	330.0619248	330.06187	0.1659686
$C_{17}H_{23}O_8$	330.0983102	330.09827	0.121721
$C_{16}H_{23}N_2O_7$	330.1176494	330.11762	0.0891128
$C_{21}H_{23}O_5$	330.1275452	330.12774	-0.590021
$C_{20}H_{23}N_2O_4$	330.1346956	330.13463	0.1986459
$C_{18}H_{27}O_7$	330.171081	330.1711	-0.057607
$C_{17}H_{27}N_2O_6$	330.2367014	330.2367	0.004293

$C_{19}H_{31}O_6$	331.0459404	331.0459	0.1219767
$C_{18}H_{31}N_2O_5$	331.0823258	331.08221	0.3497012
$C_{20}H_{35}O_5$	331.0935592	331.09344	0.3599584
$C_{21}H_{39}O_4$	331.101665	331.10156	0.3171766
$C_{17}H_{10}N_1O_8$	331.103455	331.10334	0.3472628
$C_{18}H_{14}N_1O_7$	331.1146884	331.11459	0.2971173
$C_{15}H_{18}N_1O_9$	331.1187112	331.11859	0.3659712
$C_{19}H_{18}N_1O_6$	331.118541	331.11859	-0.148044
$C_{16}H_{22}N_1O_8$	331.1299446	331.12979	0.4668255
$C_{20}H_{22}N_1O_5$	331.1284368	331.12979	-4.086693
$C_{17}H_{26}N_1O_7$	331.1380504	331.13795	0.3032503
$C_{21}H_{26}N_1O_4$	331.1398404	331.13972	0.3635319
$C_{18}H_{30}N_1O_6$	331.1510738	331.15098	0.2831937
$C_{17}H_9O_9$	331.1550966	331.15499	0.3218428
$C_{18}H_{13}O_8$	331.1549264	331.15499	-0.192116
$C_{17}H_{13}N_2O_7$	331.16633	331.1662	0.3924913
$C_{15}H_{17}O_{10}$	331.1762258	331.17616	0.1986251
$C_{19}H_{17}O_7$	331.2027154	331.20262	0.2879804
$C_{18}H_{17}N_2O_6$	331.2126112	331.21245	0.4866358
$C_{16}H_{21}O_9$	331.2489966	331.24891	0.2613741
$C_{27}H_{17}O_1$	332.0775748	332.07753	0.1348477
$C_{15}H_{21}N_2O_8$	332.092831	332.09276	0.2137351
$C_{20}H_{21}O_6$	332.1139602	332.11392	0.1209823
$C_{19}H_{21}N_2O_5$	332.122066	332.12203	0.1084472
$C_{17}H_{25}O_8$	332.1292164	332.12905	0.5009493
$C_{16}H_{25}N_2O_7$	332.1503456	332.1503	0.1372267

$C_{21}H_{25}O_5$	332.1584514	332.1584	0.1547987
$C_{20}H_{25}N_2O_4$	332.186731	332.18665	0.2437783
$C_{18}H_{29}O_7$	332.2523514	332.25228	0.2149502
$C_{22}H_{29}O_4$	333.025205	333.02529	-0.255296
$C_{19}H_{33}O_6$	333.0615904	333.06166	-0.209031
$C_{20}H_{37}O_5$	333.0728238	333.07287	-0.138769
$C_{17}H_{12}N_1O_8$	333.0809296	333.08106	-0.391443
$C_{18}H_{16}N_1O_7$	333.0979758	333.09802	-0.132754
$C_{15}H_{20}N_1O_9$	333.1092092	333.10925	-0.122543
$C_{19}H_{20}N_1O_6$	333.117315	333.11734	-0.074996
$C_{16}H_{24}N_1O_8$	333.119105	333.11914	-0.105128
$C_{20}H_{24}N_1O_5$	333.1244654	333.12446	0.0161498
$C_{21}H_{28}N_1O_4$	333.1343612	333.13439	-0.086512
$C_{17}H_{11}O_9$	333.1455946	333.14563	-0.10632
$C_{18}H_{15}O_8$	333.1537004	333.15382	-0.35894
$C_{17}H_{15}N_2O_7$	333.1554904	333.15557	-0.238988
$C_{15}H_{19}O_{10}$	333.1707466	333.17079	-0.130324
$C_{19}H_{19}O_7$	333.18198	333.18202	-0.120115
$C_{18}H_{19}N_2O_6$	333.1918758	333.19182	0.1674107
$C_{16}H_{23}O_9$	334.0568394	334.05683	0.0280788
$C_{22}H_{19}N_2O_3$	334.0720956	334.07221	-0.342501
$C_{27}H_{19}O_1$	334.0932248	334.09327	-0.135352
$C_{15}H_{23}N_2O_8$	334.1013306	334.10134	-0.028082
$C_{20}H_{23}O_6$	334.108481	334.10852	-0.116789
$C_{19}H_{23}N_2O_5$	334.112564	334.11255	0.041955
$C_{17}H_{27}O_8$	334.1296102	334.12968	-0.208961

$C_{16}H_{27}N_2O_7$	334.1448664	334.14489	-0.070688
$C_{21}H_{27}O_5$	334.1659956	334.16607	-0.222704
$C_{20}H_{27}N_2O_4$	334.202381	334.20244	-0.1766
$C_{18}H_{31}O_7$	335.0772404	335.07717	0.2100408
$C_{19}H_{35}O_6$	335.0884738	335.08836	0.3395518
$C_{17}H_{14}N_1O_8$	335.0924966	335.0924	0.2882186
$C_{21}H_{14}N_1O_5$	335.0943468	335.0944	-0.158821
$C_{18}H_{18}N_1O_7$	335.0965796	335.09654	0.1182277
$C_{22}H_{18}N_1O_4$	335.10373	335.10359	0.4177211
$C_{19}H_{22}N_1O_6$	335.1022222	335.10359	-4.0818
$C_{23}H_{22}N_1O_3$	335.1136258	335.11358	0.1366101
$C_{20}H_{26}N_1O_5$	335.1134556	335.11358	-0.371278
$C_{17}H_{13}O_9$	335.1248592	335.1248	0.1765906
$C_{18}H_{17}O_8$	335.128882	335.12885	0.0954257
$C_{17}H_{17}N_2O_7$	335.132965	335.13301	-0.134222
$C_{22}H_{17}O_5$	335.1401154	335.14014	-0.073462
$C_{10}H_{21}N_2O_{12}$	335.1441382	335.14417	-0.094945
$C_{21}H_{17}N_2O_4$	335.1500112	335.14998	0.0930327
$C_{19}H_{21}O_7$	335.1612446	335.16122	0.0733375
$C_{18}H_{21}N_2O_6$	335.1863966	335.18638	0.0494647
$C_{16}H_{25}O_9$	335.19763	335.19757	0.1789389
$C_{22}H_{21}N_2O_3$	336.0724894	336.07236	0.3849762
$C_{27}H_{21}O_1$	336.0805952	336.08052	0.2238085
$C_{15}H_{25}N_2O_8$	336.0877456	336.08766	0.2546356
$C_{20}H_{25}O_6$	336.1088748	336.10876	0.3414962
$C_{19}H_{25}N_2O_5$	336.124131	336.12401	0.3599263

$C_{17}H_{29}O_8$	336.1452602	336.14515	0.3277747
$C_{21}H_{29}O_5$	336.153366	336.15326	0.3153849
$C_{20}H_{29}N_2O_4$	336.1605164	336.16039	0.3759511
$C_{18}H_{33}O_7$	336.1645994	336.16445	0.4444778
$C_{20}H_{12}N_1O_6$	336.1816456	336.18154	0.3140561
$C_{17}H_{16}N_1O_8$	337.056505	337.05654	-0.1039
$C_{21}H_{16}N_1O_5$	337.0717612	337.07176	0.0035004
$C_{18}H_{20}N_1O_7$	337.0829946	337.0831	-0.312742
$C_{22}H_{20}N_1O_4$	337.0928904	337.09288	0.0307924
$C_{19}H_{24}N_1O_6$	337.1041238	337.10409	0.1002061
$C_{20}H_{28}N_1O_5$	337.1081466	337.10813	0.0491827
$C_{17}H_{15}O_9$	337.11938	337.11934	0.1185927
$C_{16}H_{15}N_2O_8$	337.1292758	337.12923	0.1357933
$C_{21}H_{15}O_6$	337.1291056	337.12923	-0.369058
$C_{20}H_{15}N_2O_5$	337.1405092	337.14046	0.1458736
$C_{18}H_{19}O_8$	337.144532	337.14454	-0.023788
$C_{17}H_{19}N_2O_7$	337.148615	337.14852	0.2818273
$C_{22}H_{19}O_5$	337.1557654	337.15578	-0.043363
$C_{10}H_{23}N_2O_{12}$	337.1597882	337.15973	0.1725588
$C_{21}H_{19}N_2O_4$	337.1656612	337.16562	0.1221355
$C_{19}H_{23}O_7$	337.165491	337.16562	-0.382661
$C_{18}H_{23}N_2O_6$	337.1768946	337.17684	0.1618732
$C_{23}H_{23}O_4$	337.2020466	337.20195	0.2864155
$C_{16}H_{27}O_9$	337.21328	337.21323	0.1482145
$C_{27}H_{23}O_1$	338.0670102	338.06708	-0.206527
$C_{20}H_{27}O_6$	338.0881394	338.08823	-0.268037

$C_{19}H_{27}N_2O_5$	338.0962452	338.09634	-0.280341
$C_{21}H_{31}O_5$	338.1033956	338.10349	-0.279264
$C_{18}H_{35}O_7$	338.1115014	338.11159	-0.261991
$C_{16}H_{14}N_1O_9$	338.1245248	338.12459	-0.192888
$C_{20}H_{14}N_1O_6$	338.139781	338.13983	-0.14497
$C_{17}H_{18}N_1O_8$	338.1609102	338.16095	-0.117755
$C_{21}H_{18}N_1O_5$	338.1761664	338.17625	-0.247268
$C_{18}H_{22}N_1O_7$	338.1972956	338.1973	-0.01307
$C_{22}H_{22}N_1O_4$	339.0510258	339.05096	0.1940118
$C_{19}H_{26}N_1O_6$	339.0622592	339.06229	-0.090898
$C_{20}H_{30}N_1O_5$	339.072155	339.07216	-0.014805
$C_{16}H_{13}O_{10}$	339.0833884	339.08327	0.3491174
$C_{20}H_{13}O_7$	339.0874112	339.08739	0.0624615
$C_{19}H_{13}N_2O_6$	339.0986446	339.09867	-0.074964
$C_{17}H_{17}O_9$	339.1067504	339.10681	-0.175704
$C_{16}H_{17}N_2O_8$	339.1085404	339.10852	0.0600985
$C_{21}H_{17}O_6$	339.1197738	339.11977	0.0111462
$C_{20}H_{17}N_2O_5$	339.1237966	339.1238	-0.010085
$C_{18}H_{21}O_8$	339.13503	339.13503	-5.93E-05
$C_{17}H_{21}N_2O_7$	339.1431358	339.14305	0.2530427
$C_{22}H_{21}O_5$	339.1449258	339.14495	-0.071415
$C_{21}H_{21}N_2O_4$	339.1561592	339.15613	0.0860368
$C_{19}H_{25}O_7$	339.160182	339.16023	-0.141585
$C_{18}H_{25}N_2O_6$	339.1714154	339.17147	-0.16104
$C_{27}H_{25}O_1$	339.1813112	339.18134	-0.08497
$C_{20}H_{29}O_6$	339.1925446	339.19264	-0.281315

$C_{21}H_{33}O_5$	339.2176966	339.21772	-0.069042
$C_{19}H_{12}N_1O_7$	339.3268528	339.32689	-0.109688
$C_{16}H_{16}N_1O_9$	340.0462748	340.04613	0.4257653
$C_{20}H_{16}N_1O_6$	340.0826602	340.08253	0.382789
$C_{17}H_{20}N_1O_8$	340.1037894	340.10371	0.233399
$C_{21}H_{20}N_1O_5$	340.1190456	340.11894	0.3104204
$C_{18}H_{24}N_1O_7$	340.1383848	340.13836	0.0729635
$C_{22}H_{24}N_1O_4$	340.1401748	340.14007	0.3080492
$C_{19}H_{28}N_1O_6$	340.155431	340.15535	0.2380673
$C_{20}H_{32}N_1O_5$	340.1765602	340.17649	0.2063043
$C_{19}H_{11}O_8$	340.1918164	340.19169	0.371496
$C_{16}H_{15}O_{10}$	341.0302904	341.03025	0.1184056
$C_{20}H_{15}O_7$	341.0666758	341.06665	0.0755861
$C_{19}H_{15}N_2O_6$	341.0779092	341.07787	0.1148708
$C_{17}H_{19}O_9$	341.0764014	341.07787	-4.305839
$C_{16}H_{19}N_2O_8$	341.0796951	341.07972	-0.073068
$C_{21}H_{19}O_6$	341.087805	341.08778	0.073236
$C_{20}H_{19}N_2O_5$	341.0916576	341.09101	1.898551
$C_{18}H_{23}O_8$	341.0990384	341.09906	-0.063384
$C_{17}H_{23}N_2O_7$	341.1030612	341.10298	0.2379923
$C_{22}H_{23}O_5$	341.1142946	341.11424	0.1600047
$C_{21}H_{23}N_2O_4$	341.1127868	341.11424	-4.260233
$C_{19}H_{27}O_7$	341.1160805	341.1174	-3.868249
$C_{18}H_{27}N_2O_6$	341.1224004	341.12237	0.0891695
$C_{20}H_{31}O_6$	341.1241904	341.12414	0.1476879
$C_{19}H_{31}N_2O_5$	341.1354238	341.13541	0.0403942

$C_{24}H_{47}O_2$	341.1394466	341.13938	0.1951692
$C_{19}H_{14}N_1O_7$	341.15068	341.15061	0.205129
$C_{16}H_{18}N_1O_9$	341.1605758	341.1605	0.2221238
$C_{20}H_{18}N_1O_6$	341.1718092	341.17171	0.2907037
$C_{17}H_{22}N_1O_8$	341.175832	341.1757	0.3868384
$C_{21}H_{22}N_1O_5$	341.1969612	341.19686	0.296544
$C_{18}H_{26}N_1O_7$	341.2081946	341.20812	0.2185759
$C_{22}H_{26}N_1O_4$	341.2333466	341.2332	0.4295591
$C_{19}H_{30}N_1O_6$	342.0619248	342.06199	-0.190668
$C_{19}H_{13}O_8$	342.083054	342.08309	-0.105296
$C_{18}H_{13}N_2O_7$	342.0911598	342.09113	0.087163
$C_{16}H_{17}O_{10}$	342.0983102	342.09835	-0.1164
$C_{20}H_{17}O_7$	342.1194394	342.11947	-0.089501
$C_{19}H_{17}N_2O_6$	342.1346956	342.13473	-0.100604
$C_{17}H_{21}O_9$	342.1558248	342.15588	-0.161389
$C_{16}H_{21}N_2O_8$	342.1639306	342.16394	-0.02742
$C_{21}H_{21}O_6$	342.171081	342.17112	-0.114037
$C_{20}H_{21}N_2O_5$	342.1922102	342.19218	0.0881958
$C_{18}H_{25}O_8$	343.0459404	343.04591	0.0885593
$C_{17}H_{25}N_2O_7$	343.0652796	343.0653	-0.059412
$C_{22}H_{25}O_5$	343.0823258	343.08231	0.0459945
$C_{21}H_{25}N_2O_4$	343.0935592	343.09358	-0.060683
$C_{19}H_{29}O_7$	343.0953451	343.09538	-0.101785
$C_{18}H_{29}N_2O_6$	343.103455	343.10339	0.1893886
$C_{20}H_{33}O_6$	343.1146884	343.1147	-0.033867
$C_{18}H_{12}N_1O_8$	343.1187112	343.11871	0.0034388

C ₁₉ H ₁₆ N ₁ O ₇	343.1299446	343.12997	-0.074083
C ₁₆ H ₂₀ N ₁ O ₉	343.1398404	343.13987	-0.086321
C ₂₀ H ₂₀ N ₁ O ₆	343.1510738	343.15107	0.0110153
C ₁₇ H ₂₄ N ₁ O ₈	343.1550966	343.15511	-0.039108
C ₂₁ H ₂₄ N ₁ O ₅	343.16633	343.16639	-0.174901
C ₁₈ H ₂₈ N ₁ O ₇	343.1762258	343.17627	-0.128855
C ₂₂ H ₂₈ N ₁ O ₄	343.1874592	343.18752	-0.177221
C ₁₈ H ₁₁ O ₉	343.2027154	343.20293	-0.625345
C ₁₉ H ₁₅ O ₈	343.2126112	343.21267	-0.171381
C ₁₈ H ₁₅ N ₂ O ₇	343.2489966	343.24909	-0.272164
C ₁₆ H ₁₉ O ₁₀	344.0492952	344.04924	0.1604936
C ₁₅ H ₁₉ N ₂ O ₉	344.0775748	344.07747	0.3045241
C ₂₀ H ₁₉ O ₇	344.1139602	344.11386	0.2911242
C ₁₉ H ₁₉ N ₂ O ₆	344.1350894	344.13497	0.3468984
C ₁₇ H ₂₃ O ₉	344.1503456	344.15027	0.219613
C ₁₆ H ₂₃ N ₂ O ₈	344.186731	344.18668	0.148117
C ₂₁ H ₂₃ O ₆	345.0615904	345.06154	0.1460026
C ₂₀ H ₂₃ N ₂ O ₅	345.0728238	345.07288	-0.162922
C ₁₈ H ₂₇ O ₈	345.0827196	345.0826	0.3465253
C ₁₇ H ₂₇ N ₂ O ₇	345.0979758	345.0979	0.2195895
C ₂₂ H ₂₇ O ₅	345.1092092	345.10915	0.1714817
C ₂₁ H ₂₇ N ₂ O ₄	345.119105	345.11901	0.275209
C ₁₉ H ₃₁ O ₇	345.1303384	345.13026	0.2271023
C ₂₀ H ₃₅ O ₆	345.1343612	345.13429	0.2062382
C ₁₈ H ₁₄ N ₁ O ₈	345.134191	345.13429	-0.286903
C ₁₅ H ₁₈ N ₁ O ₁₀	345.1455946	345.14553	0.1871092

C ₁₉ H ₁₈ N ₁ O ₇	345.1537004	345.15362	0.232991
C ₂₃ H ₁₈ N ₁ O ₄	345.1554904	345.15543	0.1749354
C ₁₆ H ₂₂ N ₁ O ₉	345.1667238	345.16666	0.18478
C ₂₀ H ₂₂ N ₁ O ₆	345.1707466	345.17067	0.2218609
C ₁₇ H ₂₆ N ₁ O ₈	345.1705764	345.17067	-0.271229
C ₂₁ H ₂₆ N ₁ O ₅	345.18198	345.18187	0.3186143
C ₁₈ H ₃₀ N ₁ O ₇	345.1918758	345.19176	0.3354074
C ₂₂ H ₃₀ N ₁ O ₄	345.2183654	345.21809	0.7976977
C ₁₈ H ₁₃ O ₉	345.2168576	345.21809	-3.569988
C ₁₇ H ₁₃ N ₂ O ₈	345.2282612	345.22815	0.3220475
C ₁₉ H ₁₇ O ₈	346.0568394	346.05694	-0.290762
C ₁₈ H ₁₇ N ₂ O ₇	346.0932248	346.09328	-0.159553
C ₁₁ H ₂₁ N ₂ O ₁₂	346.108481	346.10848	0.0028312
C ₁₆ H ₂₁ O ₁₀	346.112564	346.11264	-0.219531
C ₁₅ H ₂₁ N ₂ O ₉	346.114354	346.11443	-0.219639
C ₂₀ H ₂₁ O ₇	346.1296102	346.12964	-0.086153
C ₁₉ H ₂₁ N ₂ O ₆	346.1448664	346.14489	-0.068238
C ₁₇ H ₂₅ O ₉	346.1659956	346.16601	-0.041657
C ₂₈ H ₂₁ O ₁	346.231616	346.2316	0.046263
C ₂₁ H ₂₅ O ₆	347.040855	347.04077	0.24487
C ₂₀ H ₂₅ N ₂ O ₅	347.0772404	347.07718	0.1739668
C ₁₈ H ₂₉ O ₈	347.0884738	347.08846	0.0397014
C ₂₂ H ₂₉ O ₅	347.0924966	347.09246	0.1053895
C ₁₉ H ₃₃ O ₇	347.0965796	347.09658	-0.001101
C ₂₀ H ₃₇ O ₆	347.10373	347.1038	-0.201727
C ₁₈ H ₁₆ N ₁ O ₈	347.1136258	347.11359	0.1030784

$C_{22}H_{16}N_1O_5$	347.1248592	347.12485	0.0264455
$C_{19}H_{20}N_1O_7$	347.1266451	347.12671	-0.187027
$C_{23}H_{20}N_1O_4$	347.134755	347.13474	0.043153
$C_{20}H_{24}N_1O_6$	347.1401154	347.14005	0.1883386
$C_{21}H_{28}N_1O_5$	347.1441382	347.14417	-0.091663
$C_{17}H_{11}O_{10}$	347.1500112	347.14999	0.0610108
$C_{18}H_{15}O_9$	347.149841	347.14999	-0.429267
$C_{17}H_{15}N_2O_8$	347.1612446	347.16127	-0.073223
$C_{22}H_{15}O_6$	347.1711404	347.17117	-0.085318
$C_{21}H_{15}N_2O_5$	347.1863966	347.18637	0.076558
$C_{19}H_{19}O_8$	347.19763	347.19761	0.0575462
$C_{18}H_{19}N_2O_7$	347.2075258	347.20759	-0.184962
$C_{23}H_{19}O_5$	347.2325076	347.23259	-0.237363
$C_{11}H_{23}N_2O_{12}$	347.2439112	347.24394	-0.082997
$C_{16}H_{23}O_{10}$	348.0724894	348.07237	0.3429742
$C_{22}H_{19}N_2O_4$	348.0877456	348.08766	0.2458573
$C_{15}H_{23}N_2O_9$	348.1088748	348.10876	0.3297241
$C_{20}H_{23}O_7$	348.124131	348.124	0.3762448
$C_{19}H_{23}N_2O_6$	348.128214	348.12801	0.5860418
$C_{17}H_{27}O_9$	348.1452602	348.14512	0.4026477
$C_{28}H_{23}O_1$	348.153366	348.15322	0.4194063
$C_{21}H_{27}O_6$	348.1816456	348.18157	0.2170703
$C_{20}H_{27}N_2O_5$	348.247266	348.24716	0.3044323
$C_{18}H_{31}O_8$	349.056505	349.05646	0.1288614
$C_{19}H_{35}O_7$	349.0717612	349.07175	0.0320275
$C_{20}H_{39}O_6$	349.0829946	349.08289	0.2995846

C ₁₇ H ₁₄ N ₁ O ₉	349.0928904	349.09285	0.1156709
C ₂₁ H ₁₄ N ₁ O ₆	349.1041238	349.10412	0.0108274
C ₁₈ H ₁₈ N ₁ O ₈	349.1081466	349.1081	0.1334254
C ₂₂ H ₁₈ N ₁ O ₅	349.1099968	349.10998	0.0480648
C ₁₉ H ₂₂ N ₁ O ₇	349.11938	349.11929	0.2577339
C ₂₃ H ₂₂ N ₁ O ₄	349.1274858	349.12779	-0.871264
C ₂₀ H ₂₆ N ₁ O ₆	349.1292758	349.12921	0.1884113
C ₂₁ H ₃₀ N ₁ O ₅	349.1291056	349.12921	-0.299087
C ₁₇ H ₁₃ O ₁₀	349.1405092	349.14047	0.1122181
C ₂₁ H ₁₃ O ₇	349.144532	349.14449	0.1202365
C ₁₈ H ₁₇ O ₉	349.1557654	349.15574	0.0726893
C ₁₇ H ₁₇ N ₂ O ₈	349.1542576	349.15574	-4.245745
C ₂₂ H ₁₇ O ₆	349.1597882	349.15974	0.1379881
C ₂₁ H ₁₇ N ₂ O ₅	349.1656612	349.16562	0.117938
C ₁₉ H ₂₁ O ₈	349.1768946	349.17681	0.2422265
C ₁₈ H ₂₁ N ₂ O ₇	349.1867904	349.18676	0.0870019
C ₂₃ H ₂₁ O ₅	349.2020466	349.2019	0.4197567
C ₁₁ H ₂₅ N ₂ O ₁₂	349.21328	349.21316	0.343572
C ₂₂ H ₂₁ N ₂ O ₄	350.0670102	350.06714	-0.370844
C ₁₅ H ₂₅ N ₂ O ₉	350.0881394	350.08823	-0.258849
C ₂₀ H ₂₅ O ₇	350.1033956	350.10347	-0.212566
C ₁₉ H ₂₅ N ₂ O ₆	350.1245248	350.12459	-0.186277
C ₂₈ H ₂₅ O ₁	350.139781	350.13984	-0.168562
C ₂₁ H ₂₉ O ₆	350.143864	350.14392	-0.159884
C ₂₀ H ₂₉ N ₂ O ₅	350.1609102	350.16099	-0.227953
C ₁₈ H ₃₃ O ₈	350.1761664	350.17616	0.0182191

$C_{17}H_{16}N_1O_9$	350.1972956	350.19745	-0.440952
$C_{21}H_{16}N_1O_6$	351.0510258	351.0509	0.3582952
$C_{18}H_{20}N_1O_8$	351.0622592	351.06213	0.3679686
$C_{22}H_{20}N_1O_5$	351.072155	351.0721	0.1566057
$C_{19}H_{24}N_1O_7$	351.0833884	351.08331	0.2232515
$C_{23}H_{24}N_1O_4$	351.0851743	351.08521	-0.101747
$C_{20}H_{28}N_1O_6$	351.0874112	351.08734	0.2027412
$C_{21}H_{32}N_1O_5$	351.0986446	351.09867	-0.072402
$C_{20}H_{11}O_8$	351.1085404	351.10848	0.1719693
$C_{17}H_{15}O_{10}$	351.1197738	351.11973	0.1246865
$C_{21}H_{15}O_7$	351.1237966	351.12371	0.2465794
$C_{20}H_{15}N_2O_6$	351.13503	351.135	0.08538
$C_{18}H_{19}O_9$	351.1449258	351.14486	0.1873298
$C_{17}H_{19}N_2O_8$	351.1561592	351.15608	0.2254834
$C_{22}H_{19}O_6$	351.160182	351.16009	0.2619315
$C_{21}H_{19}N_2O_5$	351.164265	351.16424	0.0712422
$C_{19}H_{23}O_8$	351.1714154	351.1713	0.3285572
$C_{18}H_{23}N_2O_7$	351.1754382	351.17532	0.3365267
$C_{23}H_{23}O_5$	351.1813112	351.18125	0.1742117
$C_{22}H_{23}N_2O_4$	351.1925446	351.1925	0.1269386
$C_{20}H_{27}O_7$	351.2176966	351.21771	-0.03821
$C_{19}H_{27}N_2O_6$	352.0462748	352.04607	0.5816846
$C_{28}H_{27}O_1$	352.067404	352.06752	-0.329539
$C_{21}H_{31}O_6$	352.0755098	352.07541	0.2835122
$C_{18}H_{35}O_8$	352.0826602	352.08253	0.3697424
$C_{20}H_{14}N_1O_7$	352.090766	352.0907	0.1875019

C ₁₇ H ₁₈ N ₁ O ₉	352.1037894	352.10363	0.4526503
C ₂₁ H ₁₈ N ₁ O ₆	352.1118952	352.11178	0.327219
C ₁₈ H ₂₂ N ₁ O ₈	352.1190456	352.1189	0.4134394
C ₂₂ H ₂₂ N ₁ O ₅	352.1271514	352.12703	0.3448121
C ₁₉ H ₂₆ N ₁ O ₇	352.1287712	352.13017	-3.972468
C ₂₃ H ₂₆ N ₁ O ₄	352.1401748	352.14005	0.3543472
C ₂₀ H ₃₀ N ₁ O ₆	352.1482806	352.14814	0.3993139
C ₂₀ H ₁₃ O ₈	352.155431	352.15528	0.4287309
C ₁₇ H ₁₇ O ₁₀	352.1765602	352.1764	0.4548284
C ₁₆ H ₁₇ N ₂ O ₉	352.184666	352.1846	0.1874519
C ₂₁ H ₁₇ O ₇	353.0302904	353.03046	-0.480469
C ₂₀ H ₁₇ N ₂ O ₆	353.0666758	353.0667	-0.068599
C ₁₈ H ₂₁ O ₉	353.0779092	353.078	-0.257224
C ₁₇ H ₂₁ N ₂ O ₈	353.087805	353.08783	-0.070861
C ₂₂ H ₂₁ O ₆	353.0990384	353.09906	-0.06123
C ₂₁ H ₂₁ N ₂ O ₅	353.1030612	353.10309	-0.08162
C ₁₉ H ₂₅ O ₈	353.1142946	353.11434	-0.128627
C ₁₈ H ₂₅ N ₂ O ₇	353.1241904	353.1242	-0.027243
C ₂₃ H ₂₅ O ₅	353.1354238	353.13543	-0.017614
C ₂₂ H ₂₅ N ₂ O ₄	353.1394466	353.13945	-0.009685
C ₂₀ H ₂₉ O ₇	353.1435296	353.14361	-0.227619
C ₁₉ H ₂₉ N ₂ O ₆	353.15068	353.15067	0.0282596
C ₂₁ H ₃₃ O ₆	353.1605758	353.16055	0.0729977
C ₂₅ H ₄₉ O ₂	353.1718092	353.17183	-0.058952
C ₁₉ H ₁₂ N ₁ O ₈	353.1969612	353.19698	-0.053285
C ₂₀ H ₁₆ N ₁ O ₇	353.2081946	353.2082	-0.015345

$C_{17}H_{20}N_1O_9$	353.2333466	353.23326	0.2451068
$C_{21}H_{20}N_1O_6$	353.3425028	353.34234	0.4606859
$C_{18}H_{24}N_1O_8$	354.0619248	354.06191	0.0417438
$C_{22}H_{24}N_1O_5$	354.083054	354.08309	-0.101728
$C_{19}H_{28}N_1O_7$	354.0983102	354.09828	0.0852303
$C_{19}H_{11}O_9$	354.1194394	354.11947	-0.086468
$C_{20}H_{15}O_8$	354.1275452	354.1275	0.1276876
$C_{19}H_{15}N_2O_7$	354.1346956	354.1347	-0.012481
$C_{17}H_{19}O_{10}$	354.1428014	354.14283	-0.080708
$C_{16}H_{19}N_2O_9$	354.1558248	354.15585	-0.071212
$C_{21}H_{19}O_7$	354.1639306	354.16398	-0.139433
$C_{20}H_{19}N_2O_6$	354.171081	354.17109	-0.025468
$C_{18}H_{23}O_9$	354.1922102	354.1922	0.0287412
$C_{17}H_{23}N_2O_8$	355.0459404	355.04581	0.3672198
$C_{22}H_{23}O_6$	355.0571738	355.05707	0.2922907
$C_{21}H_{23}N_2O_5$	355.0670696	355.06696	0.3086175
$C_{19}H_{27}O_8$	355.0823258	355.08219	0.3823899
$C_{18}H_{27}N_2O_7$	355.0935592	355.09345	0.307468
$C_{23}H_{27}O_5$	355.103455	355.10334	0.3237927
$C_{22}H_{27}N_2O_4$	355.1146884	355.11455	0.3896766
$C_{20}H_{31}O_7$	355.1187112	355.11858	0.3693973
$C_{21}H_{35}O_6$	355.118541	355.11858	-0.109879
$C_{19}H_{14}N_1O_8$	355.1299446	355.1298	0.4071183
$C_{20}H_{18}N_1O_7$	355.1398404	355.13969	0.4234386
$C_{17}H_{22}N_1O_9$	355.1510738	355.15097	0.2922134
$C_{21}H_{22}N_1O_6$	355.1550966	355.15489	0.5816611

C ₁₈ H ₂₆ N ₁ O ₈	355.16633	355.1662	0.3659691
C ₂₂ H ₂₆ N ₁ O ₅	355.1762258	355.17613	0.2696687
C ₁₉ H ₃₀ N ₁ O ₇	355.1874592	355.18732	0.3918491
C ₁₉ H ₁₃ O ₉	355.2126112	355.21251	0.2848432
C ₁₈ H ₁₃ N ₂ O ₈	355.2238446	355.22376	0.2381031
C ₂₀ H ₁₇ O ₈	355.2489966	355.24893	0.1874176
C ₁₉ H ₁₇ N ₂ O ₇	355.285382	355.28533	0.1463046
C ₁₇ H ₂₁ O ₁₀	356.0411894	356.04122	-0.086002
C ₂₁ H ₂₁ O ₇	356.0775748	356.07755	0.0695913
C ₂₀ H ₂₁ N ₂ O ₆	356.098704	356.09871	-0.016906
C ₁₈ H ₂₅ O ₉	356.1139602	356.11391	0.1409097
C ₂₉ H ₂₁ O ₁	356.1350894	356.13503	0.1667342
C ₁₇ H ₂₅ N ₂ O ₈	356.1431952	356.14315	0.1269649
C ₂₂ H ₂₅ O ₆	356.1503456	356.15028	0.1841354
C ₂₁ H ₂₅ N ₂ O ₅	356.1696848	356.16962	0.1819854
C ₁₉ H ₂₉ O ₈	356.1714748	356.1714	0.2099548
C ₁₈ H ₂₉ N ₂ O ₇	356.186731	356.18662	0.3115779
C ₂₃ H ₂₉ O ₅	356.2078602	356.20763	0.6461955
C ₂₀ H ₃₃ O ₇	357.025205	357.0252	0.0139483
C ₂₁ H ₃₇ O ₆	357.0615904	357.06162	-0.082955
C ₁₈ H ₁₂ N ₁ O ₉	357.0728238	357.07286	-0.101436
C ₁₉ H ₁₆ N ₁ O ₈	357.0827196	357.0828	-0.225214
C ₁₆ H ₂₀ N ₁ O ₁₀	357.0979758	357.09803	-0.151835
C ₂₀ H ₂₀ N ₁ O ₇	357.1092092	357.10928	-0.198315
C ₁₇ H ₂₄ N ₁ O ₉	357.117315	357.11737	-0.153961
C ₂₁ H ₂₄ N ₁ O ₆	357.119105	357.11918	-0.21007

$C_{18}H_{28}N_1O_8$	357.1229576	357.12295	0.0212249
$C_{22}H_{28}N_1O_5$	357.1284882	357.12865	-0.453115
$C_{18}H_{11}O_{10}$	357.1303384	357.1304	-0.172542
$C_{19}H_{15}O_9$	357.1343612	357.13442	-0.1647
$C_{18}H_{15}N_2O_8$	357.1455946	357.14567	-0.211175
$C_{20}H_{19}O_8$	357.1554904	357.15557	-0.222928
$C_{19}H_{19}N_2O_7$	357.1667238	357.16677	-0.129408
$C_{24}H_{19}O_5$	357.1707466	357.17078	-0.093569
$C_{12}H_{23}N_2O_{12}$	357.18198	357.18201	-0.084047
$C_{17}H_{23}O_{10}$	357.1918758	357.19193	-0.151795
$C_{23}H_{19}N_2O_4$	357.207132	357.20697	0.4534621
$C_{16}H_{23}N_2O_9$	357.2282612	357.22833	-0.19265
$C_{21}H_{23}O_7$	357.2646466	357.26467	-0.065554
$C_{20}H_{23}N_2O_6$	358.0568394	358.05673	0.3054819
$C_{18}H_{27}O_9$	358.0649452	358.06477	0.4893461
$C_{29}H_{23}O_1$	358.0932248	358.09311	0.3205308
$C_{17}H_{27}N_2O_8$	358.1013306	358.10125	0.2251254
$C_{22}H_{27}O_6$	358.114354	358.11432	0.0948856
$C_{21}H_{27}N_2O_5$	358.1296102	358.12952	0.251808
$C_{19}H_{31}O_8$	358.1489494	358.14885	0.2775876
$C_{20}H_{35}O_7$	358.1507394	358.15065	0.2495594
$C_{21}H_{39}O_6$	358.1659956	358.16589	0.2947792
$C_{18}H_{14}N_1O_9$	358.202381	358.20223	0.4214933
$C_{19}H_{18}N_1O_8$	358.231616	358.23151	0.2959474
$C_{23}H_{18}N_1O_5$	359.040855	359.04084	0.041722
$C_{20}H_{22}N_1O_7$	359.0601942	359.06007	0.3459523

$C_{24}H_{22}N_1O_4$	359.0772404	359.07714	0.2795496
$C_{21}H_{26}N_1O_6$	359.0884738	359.08843	0.1219195
$C_{22}H_{30}N_1O_5$	359.0902597	359.09166	-3.899638
$C_{18}H_{13}O_{10}$	359.0965796	359.09654	0.110326
$C_{19}H_{17}O_9$	359.0983696	359.09832	0.1380677
$C_{18}H_{17}N_2O_8$	359.1136258	359.11353	0.266712
$C_{23}H_{17}O_6$	359.1248592	359.12477	0.2483256
$C_{16}H_{21}O_{11}$	359.1266451	359.12656	0.2369028
$C_{22}H_{17}N_2O_5$	359.134755	359.13468	0.2087793
$C_{20}H_{21}O_8$	359.1401154	359.13983	0.7946199
$C_{19}H_{21}N_2O_7$	359.1441382	359.14407	0.1898399
$C_{24}H_{21}O_5$	359.1459884	359.14593	0.162552
$C_{23}H_{21}N_2O_4$	359.1500112	359.14991	0.2817204
$C_{21}H_{25}O_7$	359.149841	359.14991	-0.192176
$C_{20}H_{25}N_2O_6$	359.1612446	359.16115	0.2633355
$C_{18}H_{29}O_9$	359.1693504	359.16922	0.3631092
$C_{29}H_{25}O_1$	359.1711404	359.17105	0.2516346
$C_{22}H_{29}O_6$	359.1823738	359.18223	0.4002978
$C_{21}H_{29}N_2O_5$	359.1863966	359.1863	0.2688852
$C_{19}H_{33}O_8$	359.19763	359.19746	0.4732211
$C_{20}H_{37}O_7$	359.2075258	359.2074	0.3501594
$C_{21}H_{12}N_1O_7$	359.2439112	359.24378	0.3651555
$C_{18}H_{16}N_1O_9$	360.0724894	360.07258	-0.251672
$C_{22}H_{16}N_1O_6$	360.0805952	360.08065	-0.152139
$C_{19}H_{20}N_1O_8$	360.0877456	360.08777	-0.067817
$C_{23}H_{20}N_1O_5$	360.1088748	360.10894	-0.181112

C ₁₆ H ₂₄ N ₁ O ₁₀	360.124131	360.12421	-0.219425
C ₂₀ H ₂₄ N ₁ O ₇	360.1452602	360.14532	-0.1661
C ₂₄ H ₂₄ N ₁ O ₄	360.1605164	360.16046	0.156541
C ₂₁ H ₂₈ N ₁ O ₆	360.1645994	360.1646	-0.001617
C ₁₈ H ₁₅ O ₁₀	360.1816456	360.18166	-0.040036
C ₂₂ H ₁₅ O ₇	360.2108806	360.2109	-0.053808
C ₁₉ H ₁₉ O ₉	361.056505	361.05642	0.2353645
C ₁₈ H ₁₉ N ₂ O ₈	361.0928904	361.09279	0.2779891
C ₂₃ H ₁₉ O ₆	361.1041238	361.10406	0.1766247
C ₂₂ H ₁₉ N ₂ O ₅	361.1081466	361.10808	0.1843766
C ₂₀ H ₂₃ O ₈	361.1099968	361.10987	0.3510839
C ₁₉ H ₂₃ N ₂ O ₇	361.11938	361.11949	-0.304664
C ₂₄ H ₂₃ O ₅	361.1292758	361.12918	0.2652233
C ₂₃ H ₂₃ N ₂ O ₄	361.1405092	361.14042	0.2469396
C ₂₁ H ₂₇ O ₇	361.150405	361.15044	-0.096968
C ₂₀ H ₂₇ N ₂ O ₆	361.1557654	361.15557	0.5409851
C ₁₈ H ₃₁ O ₉	361.1542576	361.15557	-3.63396
C ₂₉ H ₂₇ O ₁	361.1597882	361.15974	0.1334033
C ₂₂ H ₃₁ O ₆	361.1616384	361.16159	0.1339564
C ₂₁ H ₁₄ N ₁ O ₇	361.1656612	361.1656	0.1693957
C ₁₈ H ₁₈ N ₁ O ₉	361.165491	361.1656	-0.301856
C ₂₂ H ₁₈ N ₁ O ₆	361.1768946	361.17682	0.2064913
C ₁₉ H ₂₂ N ₁ O ₈	361.1867904	361.18659	0.5547819
C ₂₃ H ₂₂ N ₁ O ₅	361.2020466	361.20209	-0.12021
C ₂₀ H ₂₆ N ₁ O ₇	361.21328	361.21333	-0.138478
C ₂₄ H ₂₆ N ₁ O ₄	361.2231758	361.22311	0.1821032

C ₂₁ H ₃₀ N ₁ O ₆	362.0670102	362.067	0.0281161
C ₂₁ H ₁₃ O ₈	362.0881394	362.08805	0.2468457
C ₁₈ H ₁₇ O ₁₀	362.0962452	362.09614	0.2905794
C ₁₇ H ₁₇ N ₂ O ₉	362.1033956	362.10326	0.3744232
C ₂₂ H ₁₇ O ₇	362.1245248	362.1244	0.3445773
C ₂₁ H ₁₇ N ₂ O ₆	362.139781	362.13965	0.3616833
C ₁₉ H ₂₁ O ₉	362.1609102	362.16079	0.3318412
C ₁₈ H ₂₁ N ₂ O ₈	362.1972956	362.19723	0.1810613
C ₂₃ H ₂₁ O ₆	362.2265306	362.2264	0.3605967
C ₂₂ H ₂₁ N ₂ O ₅	363.072155	363.07223	-0.206626
C ₂₀ H ₂₅ O ₈	363.0833884	363.08346	-0.197255
C ₁₉ H ₂₅ N ₂ O ₇	363.0874112	363.0875	-0.244625
C ₂₄ H ₂₅ O ₅	363.0971368	363.09744	-0.835094
C ₂₃ H ₂₅ N ₂ O ₄	363.0986446	363.09878	-0.372957
C ₂₁ H ₂₉ O ₇	363.1085404	363.10858	-0.109114
C ₂₀ H ₂₉ N ₂ O ₆	363.1083702	363.10858	-0.577844
C ₁₈ H ₃₃ O ₉	363.1197738	363.11984	-0.182364
C ₂₉ H ₂₉ O ₁	363.1237966	363.12383	-0.092035
C ₂₂ H ₃₃ O ₆	363.1256468	363.12569	-0.119022
C ₂₀ H ₁₂ N ₁ O ₈	363.1278796	363.12794	-0.166284
C ₁₇ H ₁₆ N ₁ O ₁₀	363.13503	363.13509	-0.165283
C ₂₁ H ₁₆ N ₁ O ₇	363.1449258	363.14496	-0.094233
C ₁₈ H ₂₀ N ₁ O ₉	363.1447556	363.14496	-0.562916
C ₂₂ H ₂₀ N ₁ O ₆	363.1561592	363.1562	-0.112404
C ₁₉ H ₂₄ N ₁ O ₈	363.160182	363.16011	0.1982043
C ₂₃ H ₂₄ N ₁ O ₅	363.166055	363.16601	0.1238549

$C_{20}H_{28}N_1O_7$	363.1754382	363.17553	-0.252826
$C_{24}H_{28}N_1O_4$	363.1813112	363.18134	-0.079355
$C_{21}H_{32}N_1O_6$	363.1925446	363.19247	0.2053453
$C_{20}H_{11}O_9$	363.2176966	363.21772	-0.06448
$C_{21}H_{15}O_8$	363.2388258	363.23885	-0.066678
$C_{20}H_{15}N_2O_7$	364.067404	364.06732	0.2306713
$C_{18}H_{19}O_{10}$	364.0755098	364.07555	-0.110368
$C_{17}H_{19}N_2O_9$	364.0826602	364.08258	0.2202244
$C_{22}H_{19}O_7$	364.1037894	364.1037	0.2454792
$C_{21}H_{19}N_2O_6$	364.1190456	364.11895	0.2624963
$C_{19}H_{23}O_9$	364.1271514	364.1272	-0.133421
$C_{18}H_{23}N_2O_8$	364.1401748	364.14011	0.1778983
$C_{23}H_{23}O_6$	364.155431	364.15535	0.2223773
$C_{22}H_{23}N_2O_5$	364.1765602	364.17651	0.13779
$C_{20}H_{27}O_8$	364.2129456	364.21296	-0.039592
$C_{19}H_{27}N_2O_7$	364.2421806	364.2421	0.2213299
$C_{23}H_{27}N_2O_4$	365.0514196	365.05128	0.3823568
$C_{21}H_{31}O_7$	365.0666758	365.06658	0.2623628
$C_{20}H_{31}N_2O_6$	365.0779092	365.07776	0.4086248
$C_{26}H_{51}O_2$	365.087805	365.08771	0.2601563
$C_{20}H_{14}N_1O_8$	365.0990384	365.09895	0.242071
$C_{17}H_{18}N_1O_{10}$	365.1030612	365.10295	0.3045165
$C_{21}H_{18}N_1O_7$	365.1071442	365.10713	0.0389412
$C_{18}H_{22}N_1O_9$	365.1142946	365.11417	0.341208
$C_{22}H_{22}N_1O_6$	365.1127868	365.11417	-3.788473
$C_{19}H_{26}N_1O_8$	365.1241904	365.12409	0.2749199

$C_{23}H_{26}N_1O_5$	365.1354238	365.13531	0.3116101
$C_{20}H_{30}N_1O_7$	365.1394466	365.13936	0.2371146
$C_{20}H_{13}O_9$	365.15068	365.1506	0.2190326
$C_{17}H_{17}O_{11}$	365.1605758	365.16045	0.3444509
$C_{21}H_{17}O_8$	365.1718092	365.17175	0.1620604
$C_{20}H_{17}N_2O_7$	365.179915	365.17984	0.2054267
$C_{18}H_{21}O_{10}$	365.1910882	365.19098	0.2962282
$C_{17}H_{21}N_2O_9$	365.1969612	365.19686	0.2770557
$C_{22}H_{21}O_7$	365.2333466	365.23328	0.1822941
$C_{21}H_{21}N_2O_6$	366.0619248	366.062	-0.205485
$C_{19}H_{25}O_9$	366.083054	366.08312	-0.180342
$C_{30}H_{21}O_1$	366.0911598	366.09128	-0.328285
$C_{18}H_{25}N_2O_8$	366.0983102	366.09836	-0.136084
$C_{23}H_{25}O_6$	366.1194394	366.11948	-0.110948
$C_{22}H_{25}N_2O_5$	366.1346956	366.13474	-0.121322
$C_{20}H_{29}O_8$	366.1387786	366.13879	-0.031087
$C_{19}H_{29}N_2O_7$	366.1558248	366.15586	-0.096189
$C_{21}H_{33}O_7$	366.171081	366.17114	-0.161182
$C_{20}H_{16}N_1O_8$	366.1922102	366.19222	-0.026817
$C_{17}H_{20}N_1O_{10}$	366.2285956	366.22848	0.315595
$C_{21}H_{20}N_1O_7$	367.0459404	367.04581	0.3552141
$C_{18}H_{24}N_1O_9$	367.0670696	367.06698	0.2440423
$C_{22}H_{24}N_1O_6$	367.0823258	367.08224	0.2336803
$C_{19}H_{28}N_1O_8$	367.0935592	367.09355	0.025007
$C_{23}H_{28}N_1O_5$	367.101665	367.10158	0.2315917
$C_{20}H_{15}O_9$	367.103455	367.10337	0.2314876

$C_{19}H_{15}N_2O_8$	367.1146884	367.11465	0.1045447
$C_{17}H_{19}O_{11}$	367.1187112	367.11861	0.2756054
$C_{21}H_{19}O_8$	367.1299446	367.12988	0.1759047
$C_{20}H_{19}N_2O_7$	367.1284368	367.12988	-3.931104
$C_{13}H_{23}N_2O_{12}$	367.1398404	367.13973	0.3006481
$C_{18}H_{23}O_{10}$	367.1510738	367.15107	0.0102952
$C_{17}H_{23}N_2O_9$	367.1550966	367.15498	0.3175222
$C_{22}H_{23}O_7$	367.1591796	367.15889	0.7888069
$C_{21}H_{23}N_2O_6$	367.16633	367.16628	0.1361233
$C_{19}H_{27}O_9$	367.1762258	367.17617	0.1519159
$C_{18}H_{27}N_2O_8$	367.1874592	367.18739	0.1884049
$C_{23}H_{27}O_6$	367.2126112	367.21258	0.0849097
$C_{22}H_{27}N_2O_5$	367.2238446	367.22383	0.039703
$C_{20}H_{31}O_8$	367.3581528	367.35803	0.334224
$C_{24}H_{31}O_5$	368.0775748	368.07745	0.3390044
$C_{21}H_{35}O_7$	368.098704	368.0986	0.2824783
$C_{19}H_{14}N_1O_9$	368.1068098	368.10667	0.3798292
$C_{20}H_{18}N_1O_8$	368.1139602	368.11385	0.2993092
$C_{24}H_{18}N_1O_5$	368.1350894	368.13499	0.269955
$C_{17}H_{22}N_1O_{10}$	368.1431952	368.14314	0.1499897
$C_{21}H_{22}N_1O_7$	368.1503456	368.15022	0.3411104
$C_{22}H_{26}N_1O_6$	368.1600712	368.16146	-3.772327
$C_{23}H_{30}N_1O_5$	368.1714748	368.17143	0.1216278
$C_{19}H_{13}O_{10}$	368.1795806	368.17944	0.3819269
$C_{20}H_{17}O_9$	368.186731	368.18664	0.2471026
$C_{19}H_{17}N_2O_8$	368.2078602	368.20775	0.2992329

$C_{24}H_{17}O_6$	369.0615904	369.06167	-0.215737
$C_{17}H_{21}O_{11}$	369.0728238	369.07294	-0.314897
$C_{21}H_{21}O_8$	369.0746097	369.0747	-0.244725
$C_{20}H_{21}N_2O_7$	369.0827196	369.08275	-0.082421
$C_{18}H_{25}O_{10}$	369.0979758	369.09804	-0.173992
$C_{17}H_{25}N_2O_9$	369.1092092	369.10929	-0.21896
$C_{22}H_{25}O_7$	369.1109951	369.1111	-0.284256
$C_{21}H_{25}N_2O_6$	369.119105	369.11915	-0.121966
$C_{19}H_{29}O_9$	369.1303384	369.13035	-0.03148
$C_{30}H_{25}O_1$	369.1343612	369.13443	-0.186436
$C_{18}H_{29}N_2O_8$	369.1455946	369.14565	-0.150131
$C_{23}H_{29}O_6$	369.1537004	369.15381	-0.296847
$C_{22}H_{29}N_2O_5$	369.1554904	369.15555	-0.161504
$C_{20}H_{33}O_8$	369.1667238	369.16681	-0.233553
$C_{21}H_{37}O_7$	369.1707466	369.1708	-0.144703
$C_{19}H_{16}N_1O_9$	369.18198	369.18204	-0.162576
$C_{23}H_{16}N_1O_6$	369.1918758	369.19191	-0.092689
$C_{20}H_{20}N_1O_8$	369.2031092	369.20318	-0.191819
$C_{24}H_{20}N_1O_5$	369.2282612	369.22831	-0.132222
$C_{21}H_{24}N_1O_7$	370.0568394	370.05677	0.1874844
$C_{25}H_{24}N_1O_4$	370.0932248	370.09311	0.3101378
$C_{22}H_{28}N_1O_6$	370.112564	370.11254	0.064893
$C_{23}H_{32}N_1O_5$	370.114354	370.11417	0.4970893
$C_{19}H_{15}O_{10}$	370.1296102	370.12951	0.2706617
$C_{18}H_{15}N_2O_9$	370.1507394	370.15059	0.403565
$C_{23}H_{15}O_7$	370.1659956	370.16591	0.2311933

$C_{20}H_{19}O_9$	370.1871248	370.18704	0.229019
$C_{19}H_{19}N_2O_8$	370.202381	370.20237	0.0296592
$C_{24}H_{19}O_6$	371.040855	371.04075	0.2829335
$C_{17}H_{23}O_{11}$	371.0772404	371.07718	0.1627152
$C_{23}H_{19}N_2O_5$	371.0884738	371.08847	0.010186
$C_{21}H_{23}O_8$	371.0902597	371.09029	-0.08171
$C_{20}H_{23}N_2O_7$	371.0983696	371.0983	0.1874972
$C_{25}H_{23}O_5$	371.109603	371.1096	0.0080297
$C_{13}H_{27}N_2O_{12}$	371.1136258	371.11353	0.2580878
$C_{18}H_{27}O_{10}$	371.1248592	371.12478	0.2133511
$C_{24}H_{23}N_2O_4$	371.134755	371.13467	0.2289732
$C_{22}H_{27}O_7$	371.1459884	371.1459	0.2381271
$C_{21}H_{27}N_2O_6$	371.1500112	371.14993	0.2187253
$C_{19}H_{31}O_9$	371.149841	371.14993	-0.239849
$C_{30}H_{27}O_1$	371.1612446	371.16116	0.2278791
$C_{23}H_{31}O_6$	371.1597368	371.16116	-3.834522
$C_{20}H_{35}O_8$	371.1711404	371.17105	0.2434993
$C_{21}H_{39}O_7$	371.1823738	371.18245	-0.205344
$C_{18}H_{14}N_1O_{10}$	371.1863966	371.18638	0.0446673
$C_{19}H_{18}N_1O_9$	371.19763	371.19763	-5.41E-05
$C_{23}H_{18}N_1O_6$	371.2075258	371.20747	0.1502661
$C_{20}H_{22}N_1O_8$	371.2439112	371.24379	0.3264159
$C_{24}H_{22}N_1O_5$	372.0724894	372.07252	-0.082296
$C_{21}H_{26}N_1O_7$	372.0936186	372.09357	0.1305583
$C_{25}H_{26}N_1O_4$	372.1088748	372.10894	-0.175272
$C_{22}H_{30}N_1O_6$	372.124131	372.12422	-0.239222

$C_{23}H_{34}N_1O_5$	372.130004	372.13015	-0.39239
$C_{19}H_{17}O_{10}$	372.1452602	372.14532	-0.160744
$C_{18}H_{17}N_2O_9$	372.1645994	372.16468	-0.216523
$C_{23}H_{17}O_7$	372.1663894	372.1664	-0.028536
$C_{22}H_{17}N_2O_6$	372.1744952	372.17472	-0.60397
$C_{20}H_{21}O_9$	372.1816456	372.1817	-0.146219
$C_{19}H_{21}N_2O_8$	372.2027748	372.20287	-0.255829
$C_{24}H_{21}O_6$	372.218031	372.21799	0.1100965
$C_{23}H_{21}N_2O_5$	373.056505	373.05637	0.3618216
$C_{21}H_{25}O_8$	373.0677384	373.06768	0.1564861
$C_{20}H_{25}N_2O_7$	373.0758442	373.07585	-0.015499
$C_{25}H_{25}O_5$	373.0928904	373.09275	0.3762599
$C_{24}H_{25}N_2O_4$	373.1041238	373.10392	0.5461743
$C_{22}H_{29}O_7$	373.1099968	373.1101	-0.276648
$C_{21}H_{29}N_2O_6$	373.1140196	373.11374	0.7493149
$C_{19}H_{33}O_9$	373.125253	373.12516	0.2491922
$C_{30}H_{29}O_1$	373.1292758	373.12913	0.3906954
$C_{23}H_{33}O_6$	373.1291056	373.12913	-0.065447
$C_{18}H_{16}N_1O_{10}$	373.1405092	373.14041	0.2657977
$C_{22}H_{16}N_1O_7$	373.150405	373.1504	0.0133456
$C_{19}H_{20}N_1O_9$	373.1542576	373.1533	2.5661771
$C_{23}H_{20}N_1O_6$	373.1597882	373.15967	0.3167005
$C_{20}H_{24}N_1O_8$	373.1656612	373.16555	0.2979371
$C_{24}H_{24}N_1O_5$	373.1768946	373.17676	0.360633
$C_{21}H_{28}N_1O_7$	373.1753868	373.17676	-3.679825
$C_{22}H_{32}N_1O_6$	373.1867904	373.1866	0.5101464

$C_{22}H_{15}O_8$	373.2020466	373.20191	0.3659677
$C_{21}H_{15}N_2O_7$	373.2231758	373.22301	0.4441844
$C_{19}H_{19}O_{10}$	373.2595612	373.25941	0.4050262
$C_{18}H_{19}N_2O_9$	374.0598598	374.05978	0.2133822
$C_{23}H_{19}O_7$	374.0881394	374.08813	0.025074
$C_{22}H_{19}N_2O_6$	374.1033956	374.10338	0.041646
$C_{20}H_{23}O_9$	374.1245248	374.12449	0.0929634
$C_{19}H_{23}N_2O_8$	374.1326306	374.1326	0.0818365
$C_{24}H_{23}O_6$	374.139781	374.13971	0.1897149
$C_{23}H_{23}N_2O_5$	374.1609102	374.16087	0.1073867
$C_{21}H_{27}O_8$	374.169016	374.16902	-0.010643
$C_{20}H_{27}N_2O_7$	374.1972956	374.19724	0.148531
$C_{22}H_{31}O_7$	375.0357696	375.03568	0.2388569
$C_{30}H_{31}O_1$	375.072155	375.07214	0.0399387
$C_{21}H_{14}N_1O_8$	375.0833884	375.08326	0.3422703
$C_{18}H_{18}N_1O_{10}$	375.0874112	375.08728	0.3497315
$C_{22}H_{18}N_1O_7$	375.0914942	375.09144	0.1445453
$C_{19}H_{22}N_1O_9$	375.0986446	375.09854	0.2788064
$C_{23}H_{22}N_1O_6$	375.0971368	375.09854	-3.740951
$C_{20}H_{26}N_1O_8$	375.1085404	375.1085	0.1076486
$C_{24}H_{26}N_1O_5$	375.1197738	375.11974	0.090051
$C_{21}H_{30}N_1O_7$	375.1237966	375.12381	-0.035775
$C_{21}H_{13}O_9$	375.1256468	375.12583	-0.488423
$C_{22}H_{17}O_8$	375.1296696	375.12961	0.1588248
$C_{21}H_{17}N_2O_7$	375.13503	375.13492	0.2931742
$C_{19}H_{21}O_{10}$	375.140903	375.14082	0.2211966

$C_{18}H_{21}N_2O_9$	375.1449258	375.14488	0.1220326
$C_{23}H_{21}O_7$	375.1447556	375.14488	-0.331659
$C_{22}H_{21}N_2O_6$	375.1561592	375.15614	0.0511251
$C_{20}H_{25}O_9$	375.166055	375.1658	0.6796454
$C_{19}H_{25}N_2O_8$	375.1754382	375.17548	-0.111468
$C_{24}H_{25}O_6$	375.1813112	375.18131	0.0031449
$C_{23}H_{25}N_2O_5$	375.1925446	375.1926	-0.147711
$C_{21}H_{29}O_8$	375.2024404	375.20248	-0.105597
$C_{20}H_{29}N_2O_7$	375.2388258	375.23888	-0.144495
$C_{22}H_{33}O_7$	375.2752112	375.27536	-0.396563
$C_{21}H_{16}N_1O_8$	376.067404	376.06734	0.1701288
$C_{18}H_{20}N_1O_{10}$	376.0826602	376.08253	0.346147
$C_{22}H_{20}N_1O_7$	376.1037894	376.10365	0.3705889
$C_{19}H_{24}N_1O_9$	376.1190456	376.11888	0.4402327
$C_{23}H_{24}N_1O_6$	376.1401748	376.14002	0.4114953
$C_{20}H_{28}N_1O_8$	376.155431	376.15528	0.4013764
$C_{24}H_{28}N_1O_5$	376.1765602	376.17641	0.3992272
$C_{21}H_{32}N_1O_7$	376.2129456	376.21286	0.2274773
$C_{21}H_{15}O_9$	377.0514196	377.05151	-0.239808
$C_{22}H_{19}O_8$	377.0666758	377.06673	-0.143794
$C_{21}H_{19}N_2O_7$	377.087805	377.08784	-0.09287
$C_{19}H_{23}O_{10}$	377.0990384	377.09909	-0.136887
$C_{18}H_{23}N_2O_9$	377.1008243	377.10102	-0.519017
$C_{23}H_{23}O_7$	377.1030612	377.10318	-0.315087
$C_{22}H_{23}N_2O_6$	377.1142946	377.11432	-0.067407
$C_{20}H_{27}O_9$	377.1160805	377.11615	-0.184351

$C_{19}H_{27}N_2O_8$	377.1241904	377.1242	-0.025509
$C_{24}H_{27}O_6$	377.1354238	377.13544	-0.043009
$C_{23}H_{27}N_2O_5$	377.1394466	377.13948	-0.088615
$C_{21}H_{31}O_8$	377.1412968	377.14137	-0.194145
$C_{22}H_{35}O_7$	377.15068	377.15068	-5.33E-05
$C_{20}H_{14}N_1O_9$	377.156553	377.15648	0.1935003
$C_{21}H_{18}N_1O_8$	377.1605758	377.1606	-0.064217
$C_{18}H_{22}N_1O_{10}$	377.1718092	377.17185	-0.108227
$C_{22}H_{22}N_1O_7$	377.179915	377.17999	-0.198797
$C_{19}H_{26}N_1O_9$	377.1910882	377.19128	-0.508549
$C_{23}H_{26}N_1O_6$	377.1969612	377.19692	0.1091735
$C_{20}H_{30}N_1O_8$	377.2081946	377.20825	-0.146922
$C_{24}H_{30}N_1O_5$	377.2180904	377.21807	0.0540268
$C_{21}H_{34}N_1O_7$	378.083054	378.08301	0.1163234
$C_{20}H_{13}O_{10}$	378.0983102	378.09819	0.3178536
$C_{21}H_{17}O_9$	378.1194394	378.11934	0.2628267
$C_{20}H_{17}N_2O_8$	378.1346956	378.13461	0.2263212
$C_{18}H_{21}O_{11}$	378.1558248	378.15576	0.1713048
$C_{22}H_{21}O_8$	378.171081	378.17102	0.1612495
$C_{21}H_{21}N_2O_7$	378.175164	378.17509	0.1957233
$C_{19}H_{25}O_{10}$	378.1922102	378.19212	0.2384499
$C_{18}H_{25}N_2O_9$	378.2285956	378.22844	0.4113383
$C_{23}H_{25}O_7$	379.0459404	379.04589	0.1329124
$C_{22}H_{25}N_2O_6$	379.0670696	379.06704	0.0780334
$C_{20}H_{29}O_9$	379.0823258	379.08225	0.1999035
$C_{24}H_{29}O_6$	379.0935592	379.09352	0.1033515

$C_{23}H_{29}N_2O_5$	379.0920514	379.09352	-3.874046
$C_{21}H_{33}O_8$	379.103455	379.10339	0.1714041
$C_{20}H_{16}N_1O_9$	379.1146884	379.1146	0.2331218
$C_{24}H_{16}N_1O_6$	379.1187112	379.11859	0.3196358
$C_{21}H_{20}N_1O_8$	379.1299446	379.12989	0.1439609
$C_{25}H_{20}N_1O_5$	379.1398404	379.13974	0.2647569
$C_{18}H_{24}N_1O_{10}$	379.1510738	379.15101	0.1682176
$C_{22}H_{24}N_1O_7$	379.1550966	379.15502	0.2019751
$C_{19}H_{28}N_1O_9$	379.16633	379.16626	0.1845625
$C_{23}H_{28}N_1O_6$	379.1648222	379.16626	-3.792071
$C_{24}H_{32}N_1O_5$	379.1762258	379.17614	0.226227
$C_{20}H_{15}O_{10}$	379.1760556	379.17614	-0.222641
$C_{21}H_{19}O_9$	379.1874592	379.1873	0.4197921
$C_{20}H_{19}N_2O_8$	379.2067382	379.20669	0.1270544
$C_{18}H_{23}O_{11}$	379.2126112	379.21247	0.3722975
$C_{24}H_{19}N_2O_5$	379.2337404	379.2335	0.6338568
$C_{22}H_{23}O_8$	380.0775748	380.07766	-0.224218
$C_{21}H_{23}N_2O_7$	380.098704	380.09874	-0.094765
$C_{19}H_{27}O_{10}$	380.1139602	380.11401	-0.131066
$C_{18}H_{27}N_2O_9$	380.122066	380.12207	-0.010476
$C_{23}H_{27}O_7$	380.1350894	380.13513	-0.106857
$C_{22}H_{27}N_2O_6$	380.1503456	380.1504	-0.143154
$C_{20}H_{31}O_9$	380.1714748	380.17156	-0.224162
$C_{24}H_{31}O_6$	380.186731	380.18685	-0.313057
$C_{21}H_{35}O_8$	380.2078602	380.20792	-0.157335
$C_{22}H_{39}O_7$	381.0615904	381.06142	0.4471191

$C_{20}H_{18}N_1O_9$	381.0746097	381.07446	0.392779
$C_{24}H_{18}N_1O_6$	381.0827196	381.08256	0.418754
$C_{21}H_{22}N_1O_8$	381.093953	381.09386	0.2439816
$C_{25}H_{22}N_1O_5$	381.0957389	381.09571	0.0757765
$C_{22}H_{26}N_1O_7$	381.0979758	381.09783	0.382526
$C_{23}H_{30}N_1O_6$	381.1092092	381.10909	0.3127185
$C_{20}H_{17}O_{10}$	381.119105	381.11901	0.2492132
$C_{24}H_{17}O_7$	381.1303384	381.1302	0.3630776
$C_{23}H_{17}N_2O_6$	381.1343612	381.13422	0.3704203
$C_{21}H_{21}O_9$	381.1455946	381.14548	0.3006198
$C_{20}H_{21}N_2O_8$	381.1554904	381.15532	0.4470089
$C_{25}H_{21}O_6$	381.1667238	381.16662	0.272269
$C_{24}H_{21}N_2O_5$	381.1707466	381.17052	0.5944315
$C_{22}H_{25}O_8$	381.1748296	381.17474	0.2351092
$C_{21}H_{25}N_2O_7$	381.18198	381.18195	0.0786498
$C_{23}H_{29}O_7$	381.1918758	381.19178	0.2512643
$C_{22}H_{29}N_2O_6$	381.2031092	381.20282	0.758598
$C_{24}H_{33}O_6$	381.2282612	381.22816	0.265405
$C_{21}H_{37}O_8$	381.3738028	381.37366	0.3743831
$C_{22}H_{12}N_1O_8$	382.0568394	382.05687	-0.080145
$C_{19}H_{16}N_1O_{10}$	382.0932248	382.09322	0.0125098
$C_{23}H_{16}N_1O_7$	382.114354	382.11441	-0.146606
$C_{20}H_{20}N_1O_9$	382.1224598	382.12249	-0.078986
$C_{24}H_{20}N_1O_6$	382.1296102	382.12961	0.0004708
$C_{21}H_{24}N_1O_8$	382.1489494	382.14896	-0.027692
$C_{25}H_{24}N_1O_5$	382.1507394	382.15078	-0.106293

$C_{22}H_{28}N_1O_7$	382.1588452	382.15878	0.170656
$C_{23}H_{32}N_1O_6$	382.1659956	382.16598	0.0407674
$C_{19}H_{15}O_{11}$	382.1871248	382.18712	0.0125067
$C_{23}H_{15}O_8$	383.040855	383.04076	0.2479628
$C_{22}H_{15}N_2O_7$	383.0772404	383.07718	0.1576181
$C_{20}H_{19}O_{10}$	383.0884738	383.08852	-0.120651
$C_{19}H_{19}N_2O_9$	383.0965796	383.09659	-0.027101
$C_{24}H_{19}O_7$	383.0983696	383.09828	0.23383
$C_{23}H_{19}N_2O_6$	383.109603	383.10979	-0.488163
$C_{21}H_{23}O_9$	383.1136258	383.11354	0.223902
$C_{20}H_{23}N_2O_8$	383.1248592	383.12478	0.2066687
$C_{25}H_{23}O_6$	383.1266451	383.12641	0.6135781
$C_{24}H_{23}N_2O_5$	383.134755	383.13472	0.0912992
$C_{22}H_{27}O_8$	383.1459884	383.14595	0.1001704
$C_{21}H_{27}N_2O_7$	383.1500112	383.14995	0.1596761
$C_{23}H_{31}O_7$	383.149841	383.14995	-0.284536
$C_{22}H_{31}N_2O_6$	383.1612446	383.16119	0.1424463
$C_{22}H_{14}N_1O_8$	383.1693504	383.16934	0.0271882
$C_{19}H_{18}N_1O_{10}$	383.1711404	383.17111	0.0792855
$C_{23}H_{18}N_1O_7$	383.1823738	383.18242	-0.120622
$C_{20}H_{22}N_1O_9$	383.1863966	383.18629	0.2781411
$C_{24}H_{22}N_1O_6$	383.19763	383.19762	0.0260437
$C_{21}H_{26}N_1O_8$	383.2075258	383.20749	0.0933695
$C_{25}H_{26}N_1O_5$	383.2439112	383.24384	0.18573
$C_{22}H_{30}N_1O_7$	384.0724894	384.07243	0.154606
$C_{23}H_{34}N_1O_6$	384.0805952	384.08041	0.4822365

$C_{22}H_{13}O_9$	384.1088748	384.10876	0.2988213
$C_{19}H_{17}O_{11}$	384.1169806	384.11689	0.2359117
$C_{23}H_{17}O_8$	384.128214	384.12818	0.0885582
$C_{22}H_{17}N_2O_7$	384.130004	384.12987	0.3487879
$C_{20}H_{21}O_{10}$	384.1452602	384.14517	0.2347547
$C_{19}H_{21}N_2O_9$	384.153366	384.15325	0.3020088
$C_{24}H_{21}O_7$	384.1663894	384.1663	0.2326593
$C_{23}H_{21}N_2O_6$	384.1816456	384.18155	0.2487883
$C_{21}H_{25}O_9$	384.2027748	384.20269	0.2206645
$C_{20}H_{25}N_2O_8$	385.056505	385.05654	-0.090948
$C_{25}H_{25}O_6$	385.0677384	385.06776	-0.056146
$C_{24}H_{25}N_2O_5$	385.0928904	385.09294	-0.128852
$C_{22}H_{29}O_8$	385.1041238	385.10422	-0.249855
$C_{21}H_{29}N_2O_7$	385.1122296	385.11233	-0.260657
$C_{23}H_{33}O_7$	385.1140196	385.11409	-0.182855
$C_{22}H_{33}N_2O_6$	385.1292758	385.12933	-0.140784
$C_{22}H_{16}N_1O_8$	385.1405092	385.14057	-0.157917
$C_{19}H_{20}N_1O_{10}$	385.150405	385.15048	-0.194781
$C_{23}H_{20}N_1O_7$	385.1597882	385.15982	-0.082615
$C_{20}H_{24}N_1O_9$	385.1616384	385.16171	-0.185948
$C_{24}H_{24}N_1O_6$	385.1656612	385.16574	-0.204639
$C_{21}H_{28}N_1O_8$	385.165491	385.16574	-0.646528
$C_{25}H_{28}N_1O_5$	385.1768946	385.17693	-0.091958
$C_{22}H_{32}N_1O_7$	385.1867904	385.1869	-0.284589
$C_{23}H_{36}N_1O_6$	385.1980238	385.19812	-0.249794
$C_{22}H_{15}O_9$	385.2020466	385.20218	-0.346364

C ₁₉ H ₁₉ O ₁₁	385.2231758	385.22326	-0.218627
C ₁₈ H ₁₉ N ₂ O ₁₀	385.2595612	385.25961	-0.12672
C ₂₃ H ₁₉ O ₈	386.051754	386.05157	0.476568
C ₂₂ H ₁₉ N ₂ O ₇	386.0881394	386.088	0.3610054
C ₂₀ H ₂₃ O ₁₀	386.0962452	386.09606	0.479719
C ₁₉ H ₂₃ N ₂ O ₉	386.1092686	386.10919	0.2035173
C ₂₄ H ₂₃ O ₇	386.1245248	386.12437	0.4008549
C ₂₃ H ₂₃ N ₂ O ₆	386.145654	386.14552	0.3469673
C ₂₁ H ₂₇ O ₉	386.1609102	386.16079	0.3112172
C ₂₀ H ₂₇ N ₂ O ₈	386.1802494	386.18015	0.2574386
C ₂₅ H ₂₇ O ₆	386.1820394	386.18208	-0.105184
C ₂₄ H ₂₇ N ₂ O ₅	386.1972956	386.19714	0.4028508
C ₂₂ H ₃₁ O ₈	387.0357696	387.03585	-0.207785
C ₂₁ H ₃₁ N ₂ O ₇	387.072155	387.0722	-0.116309
C ₂₃ H ₃₅ O ₇	387.0833884	387.08338	0.0216488
C ₂₁ H ₁₄ N ₁ O ₉	387.0851743	387.08521	-0.092284
C ₁₈ H ₁₈ N ₁ O ₁₁	387.1085404	387.10855	-0.024851
C ₂₂ H ₁₈ N ₁ O ₈	387.1197738	387.11978	-0.016068
C ₁₉ H ₂₂ N ₁ O ₁₀	387.1215597	387.12165	-0.233317
C ₂₃ H ₂₂ N ₁ O ₇	387.1237966	387.12388	-0.215487
C ₂₀ H ₂₆ N ₁ O ₉	387.1256468	387.12577	-0.318295
C ₂₄ H ₂₆ N ₁ O ₆	387.1278796	387.12791	-0.078481
C ₂₁ H ₃₀ N ₁ O ₈	387.1296696	387.12964	0.0764082
C ₂₅ H ₃₀ N ₁ O ₅	387.13503	387.13485	0.4649021
C ₂₂ H ₃₄ N ₁ O ₇	387.1335222	387.13485	-3.429876
C ₂₁ H ₁₃ O ₁₀	387.140903	387.1409	0.0076972

C ₂₂ H ₁₇ O ₉	387.1449258	387.14494	-0.036731
C ₂₁ H ₁₇ N ₂ O ₈	387.1447556	387.14494	-0.47636
C ₁₉ H ₂₁ O ₁₁	387.1561592	387.15617	-0.027948
C ₂₃ H ₂₁ O ₈	387.164265	387.16428	-0.038698
C ₂₂ H ₂₁ N ₂ O ₇	387.166055	387.16609	-0.090452
C ₂₀ H ₂₅ O ₁₀	387.1754382	387.17544	-0.004701
C ₁₉ H ₂₅ N ₂ O ₉	387.1772884	387.17738	-0.236636
C ₂₄ H ₂₅ O ₇	387.1813112	387.18128	0.0805305
C ₂₃ H ₂₅ N ₂ O ₆	387.1925446	387.19254	0.0118285
C ₂₁ H ₂₉ O ₉	387.2024404	387.20244	0.0009811
C ₂₀ H ₂₉ N ₂ O ₈	387.2388258	387.23882	0.0149259
C ₂₅ H ₂₉ O ₆	387.2752112	387.27528	-0.177703
C ₂₄ H ₂₉ N ₂ O ₅	388.067404	388.06745	-0.118588
C ₂₂ H ₃₃ O ₈	388.0755098	388.0754	0.2829802
C ₂₃ H ₃₇ O ₇	388.1037894	388.10369	0.2560653
C ₂₁ H ₁₆ N ₁ O ₉	388.1190456	388.11896	0.2204991
C ₁₈ H ₂₀ N ₁ O ₁₁	388.1401748	388.14011	0.1668982
C ₂₂ H ₂₀ N ₁ O ₈	388.1531941	388.15376	-1.457986
C ₁₉ H ₂₄ N ₁ O ₁₀	388.155431	388.15534	0.2343904
C ₂₃ H ₂₄ N ₁ O ₇	388.1765602	388.17651	0.1292708
C ₂₀ H ₂₈ N ₁ O ₉	388.184666	388.18457	0.2473506
C ₂₄ H ₂₈ N ₁ O ₆	388.2129456	388.21289	0.1431686
C ₂₁ H ₃₂ N ₁ O ₈	389.0514196	389.05136	0.1531415
C ₂₁ H ₁₅ O ₁₀	389.087805	389.08772	0.218408
C ₂₂ H ₁₉ O ₉	389.0990384	389.09899	0.1243383
C ₂₁ H ₁₉ N ₂ O ₈	389.1030612	389.10293	0.3371341

$C_{19}H_{23}O_{11}$	389.1071442	389.1071	0.1136389
$C_{18}H_{23}N_2O_{10}$	389.1089342	389.10908	-0.374754
$C_{23}H_{23}O_8$	389.1142946	389.11433	-0.091027
$C_{22}H_{23}N_2O_7$	389.1241904	389.1241	0.2322649
$C_{20}H_{27}O_{10}$	389.1354238	389.13531	0.2923915
$C_{19}H_{27}N_2O_9$	389.1394466	389.13942	0.0683043
$C_{24}H_{27}O_7$	389.15068	389.15059	0.2312212
$C_{23}H_{27}N_2O_6$	389.1605758	389.1605	0.1947266
$C_{21}H_{31}O_9$	389.1718092	389.1717	0.2805442
$C_{22}H_{35}O_8$	389.179915	389.17982	0.2441485
$C_{21}H_{18}N_1O_9$	389.181705	389.18158	0.3211351
$C_{25}H_{18}N_1O_6$	389.1910882	389.19123	-0.364397
$C_{22}H_{22}N_1O_8$	389.1969612	389.19693	0.0801134
$C_{26}H_{22}N_1O_5$	389.2081946	389.20822	-0.065312
$C_{19}H_{26}N_1O_{10}$	389.2180904	389.21813	-0.101794
$C_{23}H_{26}N_1O_7$	389.2544758	389.25432	0.4002007
$C_{20}H_{30}N_1O_9$	390.0619248	390.0621	-0.449211
$C_{24}H_{30}N_1O_6$	390.083054	390.08304	0.0358383
$C_{21}H_{17}O_{10}$	390.0983102	390.09836	-0.127712
$C_{20}H_{17}N_2O_9$	390.1194394	390.1195	-0.155389
$C_{22}H_{21}O_9$	390.1346956	390.13479	-0.242019
$C_{21}H_{21}N_2O_8$	390.1405686	390.14041	0.4064686
$C_{19}H_{25}O_{11}$	390.1558248	390.15588	-0.141533
$C_{25}H_{21}N_2O_5$	390.1639306	390.16401	-0.203459
$C_{18}H_{25}N_2O_{10}$	390.171081	390.17121	-0.330676
$C_{23}H_{25}O_8$	390.175164	390.17537	-0.527923

$C_{22}H_{25}N_2O_7$	390.1922102	390.19224	-0.076424
$C_{20}H_{29}O_{10}$	391.0670696	391.06685	0.5614891
$C_{24}H_{29}O_7$	391.0823258	391.08218	0.3727601
$C_{23}H_{29}N_2O_6$	391.103455	391.10331	0.3706945
$C_{21}H_{33}O_9$	391.1146884	391.11452	0.4305129
$C_{23}H_{41}O_7$	391.1187112	391.11859	0.309829
$C_{20}H_{16}N_1O_{10}$	391.1299446	391.12979	0.3952137
$C_{24}H_{16}N_1O_7$	391.1398404	391.13969	0.3844658
$C_{21}H_{20}N_1O_9$	391.1510738	391.15092	0.3931471
$C_{25}H_{20}N_1O_6$	391.1550966	391.1549	0.5025625
$C_{18}H_{24}N_1O_{11}$	391.16633	391.16604	0.7413212
$C_{22}H_{24}N_1O_8$	391.1648222	391.16604	-3.113317
$C_{26}H_{24}N_1O_5$	391.1762258	391.17608	0.3726707
$C_{23}H_{28}N_1O_7$	391.1874592	391.18728	0.458041
$C_{24}H_{32}N_1O_6$	391.197355	391.1972	0.3961681
$C_{20}H_{15}O_{11}$	391.2067382	391.20663	0.2765287
$C_{21}H_{19}O_{10}$	391.2126112	391.21253	0.2075084
$C_{20}H_{19}N_2O_9$	392.0775748	392.07769	-0.293871
$C_{25}H_{19}O_7$	392.098704	392.09875	-0.117369
$C_{24}H_{19}N_2O_6$	392.1068098	392.10688	-0.178988
$C_{22}H_{23}O_9$	392.1139602	392.11402	-0.152558
$C_{21}H_{23}N_2O_8$	392.1350894	392.13517	-0.205593
$C_{26}H_{23}O_6$	392.1431952	392.14324	-0.114199
$C_{25}H_{23}N_2O_5$	392.1503456	392.15044	-0.240775
$C_{23}H_{27}O_8$	392.1714748	392.17152	-0.115307
$C_{22}H_{27}N_2O_7$	392.1795806	392.17961	-0.074921

$C_{24}H_{31}O_7$	392.186731	392.1869	-0.430968
$C_{23}H_{31}N_2O_6$	392.2078602	392.20793	-0.178018
$C_{21}H_{35}O_9$	393.0615904	393.06146	0.3317035
$C_{22}H_{39}O_8$	393.0827196	393.08256	0.4059703
$C_{23}H_{14}N_1O_8$	393.093953	393.09368	0.6944393
$C_{20}H_{18}N_1O_{10}$	393.0979758	393.09788	0.243654
$C_{24}H_{18}N_1O_7$	393.1092092	393.10906	0.3794872
$C_{21}H_{22}N_1O_9$	393.1109951	393.11084	0.3944893
$C_{25}H_{22}N_1O_6$	393.119105	393.11898	0.3179187
$C_{22}H_{26}N_1O_8$	393.1303384	393.13028	0.1485001
$C_{26}H_{26}N_1O_5$	393.1321243	393.13219	-0.167175
$C_{23}H_{30}N_1O_7$	393.1343612	393.13429	0.1810574
$C_{20}H_{17}O_{11}$	393.1455946	393.14551	0.2151363
$C_{24}H_{17}O_8$	393.1440868	393.14551	-3.620098
$C_{23}H_{17}N_2O_7$	393.1554904	393.15536	0.3316243
$C_{21}H_{21}O_{10}$	393.1667238	393.16658	0.365697
$C_{20}H_{21}N_2O_9$	393.1707466	393.17066	0.2202094
$C_{25}H_{21}O_7$	393.1748296	393.17468	0.3805373
$C_{24}H_{21}N_2O_6$	393.18198	393.18184	0.3560181
$C_{22}H_{25}O_9$	393.1918758	393.19186	0.0401328
$C_{21}H_{25}N_2O_8$	393.2031092	393.20303	0.2013715
$C_{26}H_{25}O_6$	393.213005	393.21286	0.3687058
$C_{25}H_{25}N_2O_5$	393.2223882	393.22244	-0.131783
$C_{23}H_{29}O_8$	393.2282612	393.22824	0.0538616
$C_{22}H_{29}N_2O_7$	394.0568394	394.05681	0.0745575
$C_{24}H_{33}O_7$	394.0779686	394.07777	0.5039102

$C_{23}H_{33}N_2O_6$	394.0932248	394.09321	0.0375036
$C_{23}H_{16}N_1O_8$	394.114354	394.11434	0.0354717
$C_{20}H_{20}N_1O_{10}$	394.1296102	394.12961	0.0004564
$C_{24}H_{20}N_1O_7$	394.1507394	394.15073	0.0237977
$C_{21}H_{24}N_1O_9$	394.1659956	394.16596	0.0902663
$C_{25}H_{24}N_1O_6$	394.1871248	394.18711	0.0374946
$C_{22}H_{28}N_1O_8$	394.202381	394.20238	0.0024858
$C_{26}H_{28}N_1O_5$	394.2235102	394.22361	-0.253207
$C_{23}H_{32}N_1O_7$	395.040855	395.041	-0.367102
$C_{23}H_{15}O_9$	395.0772404	395.07713	0.2793882
$C_{22}H_{15}N_2O_8$	395.0884738	395.08852	-0.116987
$C_{20}H_{19}O_{11}$	395.0983696	395.09836	0.0242469
$C_{24}H_{19}O_8$	395.109603	395.10983	-0.574575
$C_{23}H_{19}N_2O_7$	395.1136258	395.11361	0.0399376
$C_{21}H_{23}O_{10}$	395.1248592	395.12483	0.0738498
$C_{20}H_{23}N_2O_9$	395.1233514	395.12483	-3.742173
$C_{25}H_{23}O_7$	395.1266451	395.12666	-0.037765
$C_{24}H_{23}N_2O_6$	395.134755	395.13469	0.16445
$C_{22}H_{27}O_9$	395.1459884	395.14591	0.1983568
$C_{21}H_{27}N_2O_8$	395.1500112	395.14995	0.154827
$C_{26}H_{27}O_6$	395.1612446	395.16126	-0.039022
$C_{25}H_{27}N_2O_5$	395.1693504	395.16987	-1.314835
$C_{23}H_{31}O_8$	395.1711404	395.17112	0.0515723
$C_{22}H_{31}N_2O_7$	395.1823738	395.18246	-0.218178
$C_{24}H_{35}O_7$	395.19763	395.19765	-0.050658
$C_{22}H_{14}N_1O_9$	395.2075258	395.2075	0.0652313

C ₁₉ H ₁₈ N ₁ O ₁₁	395.2187592	395.21864	0.3015543
C ₂₃ H ₁₈ N ₁ O ₈	395.3894528	395.38956	-0.271176
C ₂₀ H ₂₂ N ₁ O ₁₀	396.0724894	396.07238	0.2761613
C ₂₄ H ₂₂ N ₁ O ₇	396.0936186	396.09364	-0.054078
C ₂₁ H ₂₆ N ₁ O ₉	396.1017244	396.10174	-0.039339
C ₂₅ H ₂₆ N ₁ O ₆	396.1088748	396.1088	0.1887862
C ₂₂ H ₃₀ N ₁ O ₈	396.1169806	396.1169	0.2035199
C ₂₆ H ₃₀ N ₁ O ₅	396.1186004	396.11991	-3.306131
C ₂₃ H ₃₄ N ₁ O ₇	396.130004	396.12996	0.1110239
C ₂₂ H ₁₃ O ₁₀	396.1381098	396.13804	0.1762459
C ₂₃ H ₁₇ O ₉	396.1452602	396.14518	0.2024003
C ₂₂ H ₁₇ N ₂ O ₈	396.153366	396.15328	0.2171323
C ₂₀ H ₂₁ O ₁₁	396.1663894	396.16627	0.3013378
C ₁₉ H ₂₁ N ₂ O ₁₀	396.1744952	396.17434	0.3917912
C ₂₄ H ₂₁ O ₈	396.1816456	396.18159	0.1402889
C ₂₃ H ₂₁ N ₂ O ₇	396.2027748	396.20279	-0.038415
C ₂₁ H ₂₅ O ₁₀	397.056505	397.0566	-0.239311
C ₂₀ H ₂₅ N ₂ O ₉	397.0776342	397.07756	0.1868146
C ₂₅ H ₂₅ O ₇	397.0928904	397.0929	-0.024226
C ₂₄ H ₂₅ N ₂ O ₆	397.1041238	397.10426	-0.343034
C ₂₂ H ₂₉ O ₉	397.1059097	397.10596	-0.126722
C ₂₁ H ₂₉ N ₂ O ₈	397.1140196	397.11406	-0.101785
C ₂₆ H ₂₉ O ₆	397.125253	397.12544	-0.470935
C ₂₅ H ₂₉ N ₂ O ₅	397.1292758	397.12932	-0.111349
C ₂₃ H ₃₃ O ₈	397.1405092	397.14059	-0.203505
C ₂₂ H ₃₃ N ₂ O ₇	397.150405	397.15047	-0.163717

$C_{24}H_{37}O_7$	397.1597882	397.15993	-0.357086
$C_{22}H_{16}N_1O_9$	397.1616384	397.16168	-0.104794
$C_{19}H_{20}N_1O_{11}$	397.1656612	397.16578	-0.29917
$C_{23}H_{20}N_1O_8$	397.165491	397.16578	-0.727707
$C_{20}H_{24}N_1O_{10}$	397.1768946	397.17692	-0.064002
$C_{24}H_{24}N_1O_7$	397.1867904	397.18692	-0.326345
$C_{21}H_{28}N_1O_9$	397.1980238	397.19809	-0.166718
$C_{25}H_{28}N_1O_6$	397.2231758	397.22325	-0.186847
$C_{22}H_{32}N_1O_8$	398.0881394	398.08801	0.3250032
$C_{22}H_{15}O_{10}$	398.1092686	398.1092	0.172264
$C_{23}H_{19}O_9$	398.1245248	398.12438	0.3636548
$C_{22}H_{19}N_2O_8$	398.145654	398.1456	0.1355783
$C_{20}H_{23}O_{11}$	398.1609102	398.16076	0.3771839
$C_{24}H_{23}O_8$	398.1802494	398.17929	2.409506
$C_{23}H_{23}N_2O_7$	398.1820394	398.18197	0.1742417
$C_{21}H_{27}O_{10}$	398.1972956	398.19723	0.164692
$C_{20}H_{27}N_2O_9$	399.072155	399.07227	-0.288219
$C_{25}H_{27}O_7$	399.0833884	399.08361	-0.555323
$C_{24}H_{27}N_2O_6$	399.0932842	399.09337	-0.215038
$C_{22}H_{31}O_9$	399.1085404	399.10864	-0.249607
$C_{21}H_{31}N_2O_8$	399.1197738	399.11986	-0.216026
$C_{23}H_{35}O_8$	399.1215597	399.12171	-0.376632
$C_{22}H_{18}N_1O_9$	399.1256468	399.12567	-0.058177
$C_{19}H_{22}N_1O_{11}$	399.1296696	399.12971	-0.101271
$C_{23}H_{22}N_1O_8$	399.140903	399.14098	-0.192965
$C_{27}H_{22}N_1O_5$	399.1449258	399.145	-0.185948

$C_{20}H_{26}N_1O_{10}$	399.1561592	399.15623	-0.177425
$C_{24}H_{26}N_1O_7$	399.164265	399.16437	-0.263005
$C_{21}H_{30}N_1O_9$	399.166055	399.16615	-0.238047
$C_{25}H_{30}N_1O_6$	399.1772884	399.17733	-0.104265
$C_{22}H_{17}O_{10}$	399.1813112	399.18143	-0.297659
$C_{21}H_{17}N_2O_9$	399.1925446	399.19261	-0.163881
$C_{23}H_{21}O_9$	399.2024404	399.20253	-0.224498
$C_{22}H_{21}N_2O_8$	399.2176966	399.21796	-0.659841
$C_{20}H_{25}O_{11}$	399.2388258	399.23895	-0.311142
$C_{24}H_{25}O_8$	400.067404	400.06721	0.484868
$C_{23}H_{25}N_2O_7$	400.1037894	400.10363	0.3983464
$C_{21}H_{29}O_{10}$	400.1118952	400.11178	0.2879637
$C_{20}H_{29}N_2O_9$	400.1190456	400.11908	-0.086025
$C_{25}H_{29}O_7$	400.1249186	400.12482	0.2463728
$C_{24}H_{29}N_2O_6$	400.1401748	400.14005	0.3118405
$C_{22}H_{33}O_9$	400.1482806	400.14807	0.5263491
$C_{23}H_{37}O_8$	400.1651566	400.16433	2.0655969
$C_{21}H_{16}N_1O_{10}$	400.1765602	400.17645	0.2753282
$C_{22}H_{20}N_1O_9$	400.2129456	400.21281	0.3387694
$C_{26}H_{20}N_1O_6$	401.0514196	401.05147	-0.12572
$C_{23}H_{24}N_1O_8$	401.087805	401.08785	-0.112245
$C_{20}H_{28}N_1O_{10}$	401.0990384	401.09913	-0.228423
$C_{24}H_{28}N_1O_7$	401.1008243	401.10063	0.4843623
$C_{25}H_{32}N_1O_6$	401.1030612	401.10292	0.3519791
$C_{21}H_{15}O_{11}$	401.1089342	401.10892	0.0353517
$C_{22}H_{19}O_{10}$	401.1241904	401.12422	-0.073843

$C_{21}H_{19}N_2O_9$	401.1354238	401.13551	-0.21494
$C_{26}H_{19}O_7$	401.1453196	401.14532	-0.001047
$C_{19}H_{23}O_{12}$	401.156553	401.15657	-0.042428
$C_{25}H_{19}N_2O_6$	401.1605758	401.16061	-0.085303
$C_{23}H_{23}O_9$	401.1718092	401.17182	-0.026971
$C_{22}H_{23}N_2O_8$	401.179915	401.17999	-0.186904
$C_{20}H_{27}O_{11}$	401.181705	401.18177	-0.162071
$C_{26}H_{23}N_2O_5$	401.1910882	401.19117	-0.203943
$C_{24}H_{27}O_8$	401.1929384	401.19316	-0.552403
$C_{23}H_{27}N_2O_7$	401.1969612	401.19696	0.0029409
$C_{20}H_{31}N_2O_9$	401.2081946	401.20817	0.0612647
$C_{25}H_{31}O_7$	401.2180904	401.2181	-0.023977
$C_{24}H_{31}N_2O_6$	401.2544758	401.25443	0.1140919
$C_{22}H_{35}O_9$	402.083054	402.08296	0.2337326
$C_{23}H_{39}O_8$	402.0983102	402.09822	0.2242733
$C_{21}H_{18}N_1O_{10}$	402.1194394	402.11932	0.2968767
$C_{22}H_{22}N_1O_9$	402.1346956	402.13458	0.2874159
$C_{26}H_{22}N_1O_6$	402.1558248	402.1557	0.3102775
$C_{23}H_{26}N_1O_8$	402.171081	402.17102	0.1516268
$C_{27}H_{26}N_1O_5$	402.1922102	402.19216	0.124766
$C_{20}H_{30}N_1O_{10}$	402.2285956	402.22858	0.0387339
$C_{24}H_{30}N_1O_7$	403.0670696	403.06705	0.0485773
$C_{21}H_{17}O_{11}$	403.078303	403.07856	-0.637643
$C_{25}H_{17}O_8$	403.0823258	403.08246	-0.332984
$C_{24}H_{17}N_2O_7$	403.103455	403.10345	0.0123539
$C_{22}H_{21}O_{10}$	403.1146884	403.11464	0.1200152

$C_{21}H_{21}N_2O_9$	403.1187112	403.1187	0.0277335
$C_{26}H_{21}O_7$	403.1245842	403.12463	-0.113662
$C_{25}H_{21}N_2O_6$	403.1299446	403.13003	-0.211892
$C_{23}H_{25}O_9$	403.1398404	403.13982	0.0505529
$C_{22}H_{25}N_2O_8$	403.1510738	403.15106	0.0341805
$C_{27}H_{25}O_6$	403.1550966	403.15515	-0.132505
$C_{26}H_{25}N_2O_5$	403.1569468	403.15691	0.0912297
$C_{24}H_{29}O_8$	403.1591796	403.15916	0.0486599
$C_{23}H_{29}N_2O_7$	403.1609696	403.16095	0.048566
$C_{25}H_{33}O_7$	403.1648222	403.16511	-0.713902
$C_{24}H_{33}N_2O_6$	403.16633	403.16647	-0.347301
$C_{22}H_{37}O_9$	403.1762258	403.17619	0.0887451
$C_{23}H_{41}O_8$	403.1874592	403.18743	0.072373
$C_{24}H_{16}N_1O_8$	403.195565	403.19558	-0.037159
$C_{21}H_{20}N_1O_{10}$	403.197355	403.19728	0.1859633
$C_{25}H_{20}N_1O_7$	403.2067382	403.20673	0.0202871
$C_{22}H_{24}N_1O_9$	403.2126112	403.21255	0.1517311
$C_{26}H_{24}N_1O_6$	403.2337404	403.23366	0.1993382
$C_{23}H_{28}N_1O_8$	403.2701258	403.27012	0.0143326
$C_{24}H_{32}N_1O_7$	404.0623186	404.06231	0.0212341
$C_{20}H_{15}O_{12}$	404.098704	404.09863	0.1830738
$C_{24}H_{15}O_9$	404.1068098	404.10678	0.0737867
$C_{21}H_{19}O_{11}$	404.1139602	404.11387	0.2231546
$C_{20}H_{19}N_2O_{10}$	404.1350894	404.13504	0.1221866
$C_{25}H_{19}O_8$	404.1503456	404.15028	0.1622661
$C_{24}H_{19}N_2O_7$	404.1544286	404.15447	-0.102392

$C_{22}H_{23}O_{10}$	404.1714748	404.17143	0.1107943
$C_{21}H_{23}N_2O_9$	404.186731	404.18675	-0.047058
$C_{26}H_{23}O_7$	404.2078602	404.20781	0.1241438
$C_{25}H_{23}N_2O_6$	404.2442456	404.24424	0.0138033
$C_{23}H_{27}O_9$	405.0827196	405.0826	0.2951987
$C_{22}H_{27}N_2O_8$	405.093953	405.09389	0.1554699
$C_{26}H_{27}N_2O_5$	405.0979758	405.09788	0.2364364
$C_{24}H_{31}O_8$	405.1020588	405.10211	-0.126344
$C_{23}H_{31}N_2O_7$	405.1092092	405.10905	0.3929308
$C_{25}H_{35}O_7$	405.1077014	405.10905	-3.329041
$C_{23}H_{14}N_1O_9$	405.119105	405.11904	0.160397
$C_{24}H_{18}N_1O_8$	405.1303384	405.13028	0.1441015
$C_{21}H_{22}N_1O_{10}$	405.1321243	405.13161	1.2694083
$C_{25}H_{22}N_1O_7$	405.1343612	405.13436	0.0029124
$C_{22}H_{26}N_1O_9$	405.1455946	405.14555	0.1100343
$C_{26}H_{26}N_1O_6$	405.1554904	405.15541	0.1983927
$C_{23}H_{30}N_1O_8$	405.1667238	405.16667	0.1327352
$C_{27}H_{30}N_1O_5$	405.1707466	405.1708	-0.131846
$C_{24}H_{34}N_1O_7$	405.18198	405.18188	0.2467531
$C_{23}H_{13}O_{10}$	405.1918758	405.19183	0.1129833
$C_{24}H_{17}O_9$	405.2031092	405.20314	-0.076061
$C_{23}H_{17}N_2O_8$	405.213005	405.21304	-0.086424
$C_{21}H_{21}O_{11}$	405.2223882	405.22234	0.1188974
$C_{20}H_{21}N_2O_{10}$	405.2282612	405.22814	0.2990411
$C_{25}H_{21}O_8$	406.0779686	406.07791	0.1442578
$C_{24}H_{21}N_2O_7$	406.0860744	406.08607	0.0108787

$C_{22}H_{25}O_{10}$	406.0932248	406.09319	0.0856451
$C_{21}H_{25}N_2O_9$	406.114354	406.11434	0.0344236
$C_{26}H_{25}O_7$	406.1296102	406.12958	0.074311
$C_{25}H_{25}N_2O_6$	406.1507394	406.15073	0.0230946
$C_{23}H_{29}O_9$	406.1588452	406.15884	0.0128465
$C_{22}H_{29}N_2O_8$	406.1659956	406.16602	-0.060123
$C_{26}H_{29}N_2O_5$	406.1871248	406.18711	0.0363869
$C_{24}H_{33}O_8$	406.1952306	406.19527	-0.096954
$C_{23}H_{33}N_2O_7$	406.2235102	406.22336	0.3696977
$C_{23}H_{16}N_1O_9$	407.0772404	407.07715	0.2220215
$C_{20}H_{20}N_1O_{11}$	407.0884738	407.0885	-0.064409
$C_{24}H_{20}N_1O_8$	407.0902597	407.09028	-0.04992
$C_{21}H_{24}N_1O_{10}$	407.0983696	407.09834	0.0726603
$C_{25}H_{24}N_1O_7$	407.109603	407.10961	-0.017244
$C_{22}H_{28}N_1O_9$	407.1136258	407.11359	0.0878868
$C_{26}H_{28}N_1O_6$	407.1177088	407.11793	-0.543288
$C_{23}H_{32}N_1O_8$	407.1248592	407.12483	0.0716731
$C_{24}H_{36}N_1O_7$	407.132965	407.13189	2.6404585
$C_{23}H_{15}O_{10}$	407.134755	407.13469	0.1596029
$C_{24}H_{19}O_9$	407.1459884	407.14585	0.3398778
$C_{23}H_{19}N_2O_8$	407.1500112	407.14994	0.1748248
$C_{21}H_{23}O_{11}$	407.1540942	407.1542	-0.259809
$C_{20}H_{23}N_2O_{10}$	407.1612446	407.16109	0.3796528
$C_{25}H_{23}O_8$	407.1711404	407.17107	0.1728509
$C_{24}H_{23}N_2O_7$	407.1823738	407.18206	0.7706127
$C_{22}H_{27}O_{10}$	407.2075258	407.20739	0.3334415

$C_{21}H_{27}N_2O_9$	407.2380382	407.23807	-0.078136
$C_{26}H_{27}O_7$	408.0724894	408.07253	-0.099541
$C_{25}H_{27}N_2O_6$	408.0936186	408.09358	0.0945369
$C_{23}H_{31}O_9$	408.1088748	408.10893	-0.135307
$C_{22}H_{31}N_2O_8$	408.1169806	408.11682	0.393558
$C_{24}H_{35}O_8$	408.130004	408.1299	0.2547715
$C_{23}H_{18}N_1O_9$	408.1452602	408.1454	-0.342574
$C_{20}H_{22}N_1O_{11}$	408.1663894	408.16639	-0.001519
$C_{24}H_{22}N_1O_8$	408.1744952	408.17457	-0.183212
$C_{21}H_{26}N_1O_{10}$	408.1816456	408.18178	-0.329314
$C_{25}H_{26}N_1O_7$	408.2027748	408.20285	-0.184271
$C_{22}H_{30}N_1O_9$	409.056505	409.05637	0.3299786
$C_{26}H_{30}N_1O_6$	409.0928904	409.09275	0.3431492
$C_{23}H_{34}N_1O_8$	409.1041238	409.10408	0.1070141
$C_{23}H_{17}O_{10}$	409.1122296	409.11222	0.0235087
$C_{20}H_{21}O_{12}$	409.1140196	409.11386	0.3900622
$C_{24}H_{21}O_9$	409.125253	409.12522	0.0806108
$C_{23}H_{21}N_2O_8$	409.1292758	409.12911	0.4052018
$C_{21}H_{25}O_{11}$	409.1405092	409.14035	0.3890593
$C_{25}H_{25}O_8$	409.1390014	409.14035	-3.296239
$C_{24}H_{25}N_2O_7$	409.150405	409.15026	0.3543438
$C_{22}H_{29}O_{10}$	409.1616384	409.16154	0.2404426
$C_{21}H_{29}N_2O_9$	409.1656612	409.16555	0.2717234
$C_{26}H_{29}O_7$	409.1768946	409.17673	0.4022219
$C_{25}H_{29}N_2O_6$	409.1867904	409.18662	0.4163866
$C_{23}H_{33}O_9$	409.1980238	409.19775	0.6690646

$C_{22}H_{33}N_2O_8$	409.2231758	409.22298	0.4784184
$C_{24}H_{37}O_8$	410.0881394	410.08822	-0.196592
$C_{25}H_{41}O_7$	410.1092686	410.10926	0.020921
$C_{22}H_{16}N_1O_{10}$	410.1173744	410.11746	-0.208678
$C_{23}H_{20}N_1O_9$	410.1245248	410.12462	-0.232174
$C_{27}H_{20}N_1O_6$	410.143864	410.14402	-0.380311
$C_{20}H_{24}N_1O_{11}$	410.145654	410.14577	-0.282875
$C_{24}H_{24}N_1O_8$	410.1609102	410.16101	-0.243368
$C_{21}H_{28}N_1O_{10}$	410.1820394	410.18212	-0.196547
$C_{25}H_{28}N_1O_7$	410.1972956	410.19744	-0.352075
$C_{22}H_{32}N_1O_9$	410.2184248	410.21854	-0.280875
$C_{26}H_{32}N_1O_6$	411.072155	411.07203	0.304034
$C_{22}H_{15}O_{11}$	411.0851743	411.08501	0.3996206
$C_{23}H_{19}O_{10}$	411.0914942	411.09287	-3.346657
$C_{22}H_{19}N_2O_9$	411.1085404	411.10838	0.3901157
$C_{20}H_{23}O_{12}$	411.1197738	411.11961	0.3983751
$C_{24}H_{23}O_9$	411.1278796	411.12776	0.2909501
$C_{23}H_{23}N_2O_8$	411.1296696	411.12954	0.3151801
$C_{21}H_{27}O_{11}$	411.140903	411.14064	0.6396345
$C_{20}H_{27}N_2O_{10}$	411.1449258	411.14475	0.4275376
$C_{25}H_{27}O_8$	411.1561592	411.15601	0.3628303
$C_{24}H_{27}N_2O_7$	411.1546514	411.15601	-3.304402
$C_{22}H_{31}O_{10}$	411.164265	411.16429	-0.06076
$C_{21}H_{31}N_2O_9$	411.166055	411.16583	0.5471753
$C_{26}H_{31}O_7$	411.1772884	411.17715	0.3365456
$C_{25}H_{31}N_2O_6$	411.1813112	411.18111	0.489273

$C_{23}H_{35}O_9$	411.1925446	411.1924	0.3516112
$C_{22}H_{18}N_1O_{10}$	411.2024404	411.20233	0.268432
$C_{26}H_{18}N_1O_7$	411.2388258	411.23862	0.5003903
$C_{23}H_{22}N_1O_9$	412.067404	412.06754	-0.330092
$C_{27}H_{22}N_1O_6$	412.1037894	412.1039	-0.268428
$C_{24}H_{26}N_1O_8$	412.1118952	412.11198	-0.205726
$C_{25}H_{30}N_1O_7$	412.1249186	412.12496	-0.100504
$C_{26}H_{34}N_1O_6$	412.1401748	412.14028	-0.255302
$C_{22}H_{17}O_{11}$	412.1482806	412.14836	-0.192606
$C_{23}H_{21}O_{10}$	412.161304	412.16133	-0.063131
$C_{22}H_{21}N_2O_9$	412.1694098	412.1696	-0.461418
$C_{20}H_{25}O_{12}$	412.1765602	412.17664	-0.193655
$C_{26}H_{21}N_2O_6$	412.1976894	412.19769	-0.001504
$C_{24}H_{25}O_9$	412.2129456	412.21302	-0.180538
$C_{23}H_{25}N_2O_8$	412.2340748	412.2344	-0.788921
$C_{27}H_{25}N_2O_5$	413.0514196	413.05129	0.3137137
$C_{25}H_{29}O_8$	413.087805	413.08761	0.4720059
$C_{24}H_{29}N_2O_7$	413.0990384	413.09894	0.2381509
$C_{26}H_{33}O_7$	413.1008243	413.10082	0.0103561
$C_{25}H_{33}N_2O_6$	413.1089342	413.10882	0.2763917
$C_{23}H_{37}O_9$	413.1241904	413.12402	0.4124181
$C_{25}H_{45}O_7$	413.1354238	413.13526	0.3964315
$C_{22}H_{20}N_1O_{10}$	413.1435296	413.14342	0.265326
$C_{26}H_{20}N_1O_7$	413.1453196	413.14522	0.2410288
$C_{23}H_{24}N_1O_9$	413.156553	413.15634	0.5154944
$C_{27}H_{24}N_1O_6$	413.1605758	413.16044	0.3286371

$C_{24}H_{28}N_1O_8$	413.1604056	413.16044	-0.083309
$C_{25}H_{32}N_1O_7$	413.1718092	413.17169	0.2884512
$C_{22}H_{19}O_{11}$	413.181705	413.18158	0.3024817
$C_{21}H_{19}N_2O_{10}$	413.1969612	413.19679	0.4142816
$C_{26}H_{19}O_8$	413.2081946	413.20805	0.349896
$C_{25}H_{19}N_2O_7$	413.2180904	413.21798	0.2671226
$C_{23}H_{23}O_{10}$	414.083054	414.08316	-0.256036
$C_{22}H_{23}N_2O_9$	414.0911598	414.09126	-0.241933
$C_{27}H_{23}O_7$	414.0983102	414.09837	-0.144459
$C_{26}H_{23}N_2O_6$	414.1194394	414.11949	-0.122236
$C_{24}H_{27}O_9$	414.1346956	414.13471	-0.03482
$C_{23}H_{27}N_2O_8$	414.1405686	414.14074	-0.413918
$C_{27}H_{27}N_2O_5$	414.1558248	414.1559	-0.181623
$C_{25}H_{31}O_8$	414.176954	414.17712	-0.400843
$C_{24}H_{31}N_2O_7$	414.1808066	414.18019	1.4886733
$C_{26}H_{35}O_7$	414.1922102	414.19232	-0.265143
$C_{24}H_{43}O_8$	414.2285956	414.22872	-0.300366
$C_{21}H_{18}N_1O_{11}$	415.0670696	415.06693	0.3362828
$C_{25}H_{18}N_1O_8$	415.103455	415.10329	0.3974428
$C_{22}H_{22}N_1O_{10}$	415.1146884	415.11445	0.5742507
$C_{26}H_{22}N_1O_7$	415.1245842	415.12446	0.2991389
$C_{23}H_{26}N_1O_9$	415.1299446	415.12981	0.3241874
$C_{27}H_{26}N_1O_6$	415.1398404	415.1397	0.3381509
$C_{24}H_{30}N_1O_8$	415.1510738	415.15094	0.3222439
$C_{25}H_{34}N_1O_7$	415.1591796	415.15904	0.3362992
$C_{25}H_{17}O_9$	415.1609696	415.16069	0.6734253

C ₂₂ H ₂₁ O ₁₁	415.172203	415.172	0.4889053
C ₂₆ H ₂₁ O ₈	415.1762258	415.17609	0.3270416
C ₂₅ H ₂₁ N ₂ O ₇	415.1874592	415.18728	0.4315639
C ₂₃ H ₂₅ O ₁₀	415.195565	415.19561	-0.10834
C ₂₂ H ₂₅ N ₂ O ₉	415.197355	415.19717	0.4455228
C ₂₇ H ₂₅ O ₇	415.2126112	415.21245	0.3881864
C ₂₆ H ₂₅ N ₂ O ₆	415.2337404	415.23353	0.5066542
C ₂₄ H ₂₉ O ₉	415.2701258	415.27013	-0.010162
C ₂₃ H ₂₉ N ₂ O ₈	416.098704	416.09877	-0.158665
C ₂₈ H ₂₉ O ₆	416.1068098	416.10688	-0.168664
C ₂₇ H ₂₉ N ₂ O ₅	416.1139602	416.11409	-0.311982
C ₂₅ H ₃₃ O ₈	416.1350894	416.13516	-0.169705
C ₂₄ H ₃₃ N ₂ O ₇	416.1503456	416.15053	-0.443157
C ₂₄ H ₁₆ N ₁ O ₉	416.1714748	416.17152	-0.108657
C ₂₁ H ₂₀ N ₁ O ₁₁	416.2078602	416.2079	-0.095674
C ₂₅ H ₂₀ N ₁ O ₈	417.0827196	417.08259	0.3106815
C ₂₂ H ₂₄ N ₁ O ₁₀	417.0979758	417.09783	0.34951
C ₂₆ H ₂₄ N ₁ O ₇	417.1092092	417.10902	0.45355
C ₂₃ H ₂₈ N ₁ O ₉	417.1077014	417.10902	-3.161342
C ₂₇ H ₂₈ N ₁ O ₆	417.119105	417.11897	0.3236004
C ₂₄ H ₃₂ N ₁ O ₈	417.1303384	417.13018	0.3796892
C ₂₅ H ₃₆ N ₁ O ₇	417.1343612	417.13426	0.2425595
C ₂₄ H ₁₅ O ₁₀	417.1384442	417.13832	0.2977853
C ₂₁ H ₁₉ O ₁₂	417.1455946	417.14542	0.4185107
C ₂₅ H ₁₉ O ₉	417.1554904	417.15537	0.2885732
C ₂₄ H ₁₉ N ₂ O ₈	417.1553202	417.15537	-0.119428

$C_{22}H_{23}O_{11}$	417.1667238	417.16666	0.1528883
$C_{21}H_{23}N_2O_{10}$	417.1918758	417.19174	0.3254615
$C_{26}H_{23}O_8$	417.2031092	417.20293	0.4294788
$C_{25}H_{23}N_2O_7$	417.2282612	417.22821	0.1226664
$C_{23}H_{27}O_{10}$	417.2493904	417.24909	0.7199049
$C_{22}H_{27}N_2O_9$	418.0568394	418.05683	0.0224369
$C_{27}H_{27}O_7$	418.0779686	418.07804	-0.17083
$C_{26}H_{27}N_2O_6$	418.0932248	418.0933	-0.179912
$C_{24}H_{31}O_9$	418.114354	418.11444	-0.205733
$C_{23}H_{31}N_2O_8$	418.1224598	418.12251	-0.120018
$C_{25}H_{35}O_8$	418.1296102	418.12967	-0.143066
$C_{24}H_{18}N_1O_9$	418.1507394	418.15078	-0.097142
$C_{21}H_{22}N_1O_{11}$	418.1659956	418.16604	-0.106226
$C_{25}H_{22}N_1O_8$	418.1871248	418.18716	-0.084221
$C_{22}H_{26}N_1O_{10}$	418.2235102	418.22356	-0.119123
$C_{26}H_{26}N_1O_7$	419.0619842	419.06179	0.463368
$C_{23}H_{30}N_1O_9$	419.0772404	419.07709	0.3588358
$C_{27}H_{30}N_1O_6$	419.0884738	419.08847	0.0090193
$C_{24}H_{34}N_1O_8$	419.0983696	419.09821	0.3807696
$C_{23}H_{13}O_{11}$	419.109603	419.10947	0.3172915
$C_{24}H_{17}O_{10}$	419.1136258	419.11353	0.2285297
$C_{21}H_{21}O_{12}$	419.1177088	419.11851	-1.911593
$C_{25}H_{21}O_9$	419.1248592	419.12474	0.2843542
$C_{24}H_{21}N_2O_8$	419.1266451	419.12659	0.1314116
$C_{22}H_{25}O_{11}$	419.134755	419.1346	0.3697615
$C_{21}H_{25}N_2O_{10}$	419.1459884	419.1458	0.4494374

$C_{26}H_{25}O_8$	419.1500112	419.15003	-0.044901
$C_{25}H_{25}N_2O_7$	419.1612446	419.16112	0.2972124
$C_{23}H_{29}O_{10}$	419.1711404	419.17103	0.263329
$C_{22}H_{29}N_2O_9$	419.1823738	419.18221	0.3907128
$C_{27}H_{29}O_7$	419.2075258	419.20741	0.2761876
$C_{26}H_{29}N_2O_6$	419.2187592	419.21865	0.2604366
$C_{24}H_{33}O_9$	420.0724894	420.07254	-0.120503
$C_{25}H_{37}O_8$	420.0936186	420.09365	-0.074793
$C_{23}H_{16}N_1O_{10}$	420.1088748	420.10892	-0.107639
$C_{24}H_{20}N_1O_9$	420.130004	420.13007	-0.157142
$C_{21}H_{24}N_1O_{11}$	420.1452602	420.14533	-0.166181
$C_{25}H_{24}N_1O_8$	420.1663894	420.16643	-0.096676
$C_{22}H_{28}N_1O_{10}$	420.1744952	420.17455	-0.13038
$C_{26}H_{28}N_1O_7$	420.1816456	420.18172	-0.177114
$C_{23}H_{32}N_1O_9$	420.2027748	420.20281	-0.083817
$C_{27}H_{32}N_1O_6$	420.2391602	420.23909	0.1669999
$C_{23}H_{15}O_{11}$	421.056505	421.05634	0.3918237
$C_{24}H_{19}O_{10}$	421.0776342	421.07757	0.1524182
$C_{23}H_{19}N_2O_9$	421.0928904	421.09272	0.4046136
$C_{21}H_{23}O_{12}$	421.1041238	421.1042	-0.181001
$C_{25}H_{23}O_9$	421.1122296	421.11248	-0.594574
$C_{24}H_{23}N_2O_8$	421.1140196	421.11388	0.3314539
$C_{21}H_{27}N_2O_{10}$	421.125253	421.1252	0.1258056
$C_{26}H_{27}O_8$	421.1292758	421.12918	0.2274359
$C_{25}H_{27}N_2O_7$	421.1405092	421.14035	0.3779734
$C_{23}H_{31}O_{10}$	421.1390014	421.14035	-3.202316

$C_{22}H_{31}N_2O_9$	421.148615	421.14882	-0.486722
$C_{27}H_{31}O_7$	421.150405	421.15027	0.3205028
$C_{26}H_{31}N_2O_6$	421.1616384	421.16157	0.1623602
$C_{24}H_{35}O_9$	421.1656612	421.1655	0.3826995
$C_{23}H_{35}N_2O_8$	421.1768946	421.17685	0.105846
$C_{25}H_{39}O_8$	421.1753868	421.17685	-3.474135
$C_{23}H_{18}N_1O_{10}$	421.1867904	421.18665	0.3332961
$C_{24}H_{22}N_1O_9$	421.1980238	421.19796	0.151425
$C_{21}H_{26}N_1O_{11}$	421.2231758	421.22307	0.2511255
$C_{25}H_{26}N_1O_8$	421.2344092	421.23414	0.6390264
$C_{26}H_{30}N_1O_7$	422.0881394	422.08819	-0.119928
$C_{23}H_{34}N_1O_9$	422.1092686	422.10929	-0.050745
$C_{23}H_{17}O_{11}$	422.1245248	422.12457	-0.107125
$C_{22}H_{17}N_2O_{10}$	422.1375441	422.13765	-0.250918
$C_{24}H_{21}O_{10}$	422.143864	422.14413	-0.630075
$C_{23}H_{21}N_2O_9$	422.145654	422.14575	-0.227457
$C_{21}H_{25}O_{12}$	422.1609102	422.16096	-0.118012
$C_{27}H_{21}N_2O_6$	422.1820394	422.18205	-0.025155
$C_{25}H_{25}O_9$	422.1972956	422.19734	-0.105212
$C_{24}H_{25}N_2O_8$	422.2184248	422.21842	0.0113209
$C_{21}H_{29}N_2O_{10}$	422.2548102	422.2547	0.2609323
$C_{26}H_{29}O_8$	422.257043	422.25724	-0.466499
$C_{25}H_{29}N_2O_7$	423.072155	423.0721	0.129954
$C_{23}H_{33}O_{10}$	423.0932842	423.09319	0.2225984
$C_{26}H_{33}N_2O_6$	423.1045176	423.10437	0.3488025
$C_{24}H_{37}O_9$	423.1085404	423.10839	0.3554168

$C_{23}H_{20}N_1O_{10}$	423.1197738	423.11963	0.339809
$C_{24}H_{24}N_1O_9$	423.118266	423.11963	-3.223732
$C_{28}H_{24}N_1O_6$	423.1278796	423.12802	-0.331773
$C_{25}H_{28}N_1O_8$	423.1296696	423.1295	0.4007753
$C_{22}H_{32}N_1O_{10}$	423.140903	423.14086	0.1015735
$C_{26}H_{32}N_1O_7$	423.1449258	423.14479	0.3208827
$C_{23}H_{19}O_{11}$	423.1561592	423.15605	0.2580133
$C_{22}H_{19}N_2O_{10}$	423.166055	423.16592	0.3189762
$C_{26}H_{19}N_2O_7$	423.1772884	423.17735	-0.145613
$C_{24}H_{23}O_{10}$	423.1813112	423.18122	0.215463
$C_{23}H_{23}N_2O_9$	423.1853942	423.18534	0.1281181
$C_{28}H_{23}O_7$	423.1925446	423.19236	0.4361606
$C_{27}H_{23}N_2O_6$	423.1910368	423.19236	-3.126768
$C_{25}H_{27}O_9$	423.2024404	423.20229	0.355338
$C_{24}H_{27}N_2O_8$	423.2136738	423.21358	0.22159
$C_{26}H_{31}O_8$	423.2388258	423.23865	0.4153208
$C_{25}H_{31}N_2O_7$	424.067404	424.06743	-0.061358
$C_{24}H_{39}O_9$	424.0885332	424.08857	-0.086822
$C_{22}H_{18}N_1O_{11}$	424.0923858	424.09249	-0.245749
$C_{26}H_{18}N_1O_8$	424.1037894	424.10387	-0.190095
$C_{23}H_{22}N_1O_{10}$	424.1118952	424.11199	-0.223484
$C_{27}H_{22}N_1O_7$	424.1249186	424.12497	-0.121238
$C_{24}H_{26}N_1O_9$	424.1330244	424.13313	-0.248937
$C_{28}H_{26}N_1O_6$	424.1401748	424.14021	-0.083039
$C_{25}H_{30}N_1O_8$	424.159514	424.15978	-0.627081
$C_{26}H_{34}N_1O_7$	424.161304	424.16141	-0.249952

$C_{23}H_{21}O_{11}$	424.1765602	424.17657	-0.023151
$C_{22}H_{21}N_2O_{10}$	424.1976894	424.19774	-0.119331
$C_{27}H_{21}O_8$	424.2129456	424.21289	0.1310189
$C_{26}H_{21}N_2O_7$	424.2340748	424.23429	-0.507315
$C_{24}H_{25}O_{10}$	425.0514196	425.05111	0.7283352
$C_{23}H_{25}N_2O_9$	425.087805	425.08764	0.3881078
$C_{28}H_{25}O_7$	425.0990384	425.09881	0.5372393
$C_{27}H_{25}N_2O_6$	425.1089342	425.10869	0.5743937
$C_{25}H_{29}O_9$	425.1241904	425.12403	0.3772542
$C_{24}H_{29}N_2O_8$	425.1354238	425.13524	0.4322855
$C_{26}H_{33}O_8$	425.1372097	425.13714	0.1638956
$C_{25}H_{33}N_2O_7$	425.1453196	425.14512	0.4694393
$C_{24}H_{41}O_9$	425.156553	425.15658	-0.063553
$C_{25}H_{16}N_1O_9$	425.1605758	425.16039	0.4369641
$C_{22}H_{20}N_1O_{11}$	425.1718092	425.17163	0.4214294
$C_{26}H_{20}N_1O_8$	425.181705	425.18153	0.4115415
$C_{23}H_{24}N_1O_{10}$	425.1929384	425.19283	0.2548958
$C_{27}H_{24}N_1O_7$	425.1969612	425.1969	0.143886
$C_{24}H_{28}N_1O_9$	425.2081946	425.20807	0.2929857
$C_{28}H_{28}N_1O_6$	425.2180904	425.21796	0.3066189
$C_{25}H_{32}N_1O_8$	425.2544758	425.25431	0.3898369
$C_{26}H_{36}N_1O_7$	426.083054	426.08315	-0.225355
$C_{22}H_{19}O_{12}$	426.1041832	426.10422	-0.086411
$C_{26}H_{19}O_9$	426.1194394	426.11949	-0.118793
$C_{25}H_{19}N_2O_8$	426.1405686	426.14074	-0.402262
$C_{23}H_{23}O_{11}$	426.1558248	426.15586	-0.082646

$C_{22}H_{23}N_2O_{10}$	426.176954	426.17696	-0.014126
$C_{27}H_{23}O_8$	426.1922102	426.19227	-0.140359
$C_{26}H_{23}N_2O_7$	426.2133394	426.21343	-0.212617
$C_{24}H_{27}O_{10}$	426.2214452	426.22157	-0.292764
$C_{23}H_{27}N_2O_9$	427.0670696	427.06691	0.3736647
$C_{28}H_{27}O_7$	427.103455	427.10327	0.4331033
$C_{27}H_{27}N_2O_6$	427.1146884	427.11456	0.3005748
$C_{25}H_{31}O_9$	427.1227942	427.12272	0.173762
$C_{24}H_{31}N_2O_8$	427.1245842	427.12458	0.0097861
$C_{26}H_{35}O_8$	427.1358176	427.13612	-0.708019
$C_{25}H_{18}N_1O_9$	427.1398404	427.1397	0.3286509
$C_{22}H_{22}N_1O_{11}$	427.1396702	427.1397	-0.069813
$C_{26}H_{22}N_1O_8$	427.1510738	427.15096	0.2663692
$C_{23}H_{26}N_1O_{10}$	427.149566	427.15096	-3.263541
$C_{27}H_{26}N_1O_7$	427.1609696	427.1608	0.396993
$C_{24}H_{30}N_1O_9$	427.172203	427.17209	0.2644833
$C_{28}H_{30}N_1O_6$	427.1762258	427.1761	0.294445
$C_{25}H_{34}N_1O_8$	427.1760556	427.1761	-0.103985
$C_{25}H_{17}O_{10}$	427.1874592	427.18733	0.3023963
$C_{22}H_{21}O_{12}$	427.197355	427.19711	0.5734584
$C_{21}H_{21}N_2O_{11}$	427.2337404	427.23355	0.4456106
$C_{26}H_{21}O_9$	428.098704	428.09884	-0.317731
$C_{25}H_{21}N_2O_8$	428.1139602	428.11395	0.0237785
$C_{23}H_{25}O_{11}$	428.1350894	428.13515	-0.141591
$C_{22}H_{25}N_2O_{10}$	428.1503456	428.15056	-0.500806
$C_{27}H_{25}O_8$	428.1562186	428.15631	-0.21352

$C_{26}H_{25}N_2O_7$	428.1714748	428.17154	-0.152322
$C_{24}H_{29}O_{10}$	428.1795806	428.17966	-0.185395
$C_{23}H_{29}N_2O_9$	428.192604	428.19241	0.4530202
$C_{28}H_{29}O_7$	428.1964566	428.19583	1.4633001
$C_{27}H_{29}N_2O_6$	428.2078602	428.2079	-0.092992
$C_{25}H_{33}O_9$	429.0827196	429.0826	0.2786873
$C_{24}H_{33}N_2O_8$	429.093953	429.09396	-0.01636
$C_{26}H_{37}O_8$	429.119105	429.11893	0.4077653
$C_{24}H_{16}N_1O_{10}$	429.1303384	429.13013	0.4855865
$C_{25}H_{20}N_1O_9$	429.1384442	429.13836	0.1962483
$C_{22}H_{24}N_1O_{11}$	429.1402342	429.14	0.5456955
$C_{26}H_{24}N_1O_8$	429.1455946	429.14545	0.3369017
$C_{23}H_{28}N_1O_{10}$	429.1440868	429.14545	-3.176602
$C_{27}H_{28}N_1O_7$	429.1514676	429.15147	-0.005639
$C_{24}H_{32}N_1O_9$	429.1554904	429.1553	0.4436152
$C_{28}H_{32}N_1O_6$	429.1667238	429.16658	0.3350211
$C_{24}H_{15}O_{11}$	429.1766196	429.17641	0.4883302
$C_{25}H_{19}O_{10}$	429.1918758	429.19168	0.4561594
$C_{24}H_{19}N_2O_9$	429.2031092	429.20295	0.3708731
$C_{22}H_{23}O_{12}$	429.213005	429.21288	0.2911839
$C_{21}H_{23}N_2O_{11}$	429.2857758	429.28568	0.2231145
$C_{26}H_{23}O_9$	430.0779686	430.07811	-0.328824
$C_{25}H_{23}N_2O_8$	430.0932248	430.09338	-0.360899
$C_{23}H_{27}O_{11}$	430.114354	430.11441	-0.130245
$C_{27}H_{27}O_8$	430.1296102	430.12971	-0.23207
$C_{26}H_{27}N_2O_7$	430.1354832	430.13568	-0.457577

$C_{24}H_{31}O_{10}$	430.1507394	430.1508	-0.140928
$C_{23}H_{31}N_2O_9$	430.1659956	430.16614	-0.335731
$C_{28}H_{31}O_7$	430.1871248	430.18715	-0.058626
$C_{27}H_{31}N_2O_6$	430.1952306	430.1953	-0.161281
$C_{25}H_{35}O_9$	430.2235102	430.2236	-0.208775
$C_{24}H_{35}N_2O_8$	431.0619842	431.06211	-0.291884
$C_{26}H_{39}O_8$	431.0983696	431.0982	0.3933671
$C_{24}H_{18}N_1O_{10}$	431.109603	431.10943	0.4012434
$C_{21}H_{22}N_1O_{12}$	431.1136258	431.11347	0.361343
$C_{25}H_{22}N_1O_9$	431.1248592	431.12474	0.2764394
$C_{22}H_{26}N_1O_{11}$	431.134755	431.13463	0.2898859
$C_{26}H_{26}N_1O_8$	431.1459884	431.14581	0.4137343
$C_{23}H_{30}N_1O_{10}$	431.1500112	431.15	0.0259304
$C_{27}H_{30}N_1O_7$	431.1612446	431.161	0.5672585
$C_{24}H_{34}N_1O_9$	431.1711404	431.17098	0.3719634
$C_{24}H_{17}O_{11}$	431.1709702	431.17098	-0.022775
$C_{25}H_{21}O_{10}$	431.1823738	431.18222	0.356647
$C_{24}H_{21}N_2O_9$	431.1904796	431.19051	-0.070461
$C_{22}H_{25}O_{12}$	431.2075258	431.20738	0.3380736
$C_{21}H_{25}N_2O_{11}$	431.2187592	431.21862	0.3227594
$C_{26}H_{25}O_9$	431.228655	431.22872	-0.150779
$C_{25}H_{25}N_2O_8$	431.2650404	431.26487	0.39507
$C_{23}H_{29}O_{11}$	432.0724894	432.07253	-0.094012
$C_{22}H_{29}N_2O_{10}$	432.0936186	432.09364	-0.049573
$C_{27}H_{29}O_8$	432.1017244	432.10175	-0.059204
$C_{26}H_{29}N_2O_7$	432.1088748	432.10893	-0.127792

$C_{24}H_{33}O_{10}$	432.130004	432.13009	-0.199061
$C_{23}H_{33}N_2O_9$	432.1452602	432.14534	-0.184707
$C_{28}H_{33}O_7$	432.1663894	432.16647	-0.186549
$C_{25}H_{37}O_9$	432.1816456	432.18174	-0.218473
$C_{23}H_{16}N_1O_{11}$	432.2027748	432.20283	-0.127764
$C_{24}H_{20}N_1O_{10}$	433.0776342	433.07753	0.2405571
$C_{28}H_{20}N_1O_7$	433.0928904	433.09281	0.1855951
$C_{21}H_{24}N_1O_{12}$	433.1041238	433.10415	-0.06054
$C_{25}H_{24}N_1O_9$	433.1140196	433.11389	0.299182
$C_{29}H_{24}N_1O_6$	433.125253	433.12513	0.2839361
$C_{22}H_{28}N_1O_{11}$	433.1292758	433.12912	0.3596614
$C_{26}H_{28}N_1O_8$	433.1333588	433.13327	0.2050586
$C_{27}H_{32}N_1O_7$	433.1405092	433.14041	0.2289786
$C_{23}H_{15}O_{12}$	433.1390014	433.14041	-3.25212
$C_{24}H_{19}O_{11}$	433.150405	433.15028	0.288537
$C_{25}H_{23}O_{10}$	433.1616384	433.16164	-0.00374
$C_{24}H_{23}N_2O_9$	433.1656612	433.16557	0.2104966
$C_{29}H_{23}O_7$	433.1768946	433.17684	0.1259991
$C_{26}H_{27}O_9$	433.1753868	433.17684	-3.354808
$C_{25}H_{27}N_2O_8$	433.1867904	433.18668	0.254809
$C_{22}H_{31}N_2O_{10}$	433.1980238	433.19794	0.1933986
$C_{27}H_{31}O_8$	433.2061296	433.2059	0.5300426
$C_{26}H_{31}N_2O_7$	433.2231758	433.22306	0.2672523
$C_{24}H_{35}O_{10}$	433.2344092	433.2345	-0.209633
$C_{23}H_{18}N_1O_{11}$	434.0881394	434.08806	0.1828659
$C_{27}H_{18}N_1O_8$	434.1092686	434.1092	0.1579784

$C_{24}H_{22}N_1O_{10}$	434.1245248	434.12453	-0.012024
$C_{28}H_{22}N_1O_7$	434.145654	434.14565	0.0091672
$C_{25}H_{26}N_1O_9$	434.1609102	434.16093	-0.045652
$C_{29}H_{26}N_1O_6$	434.1820394	434.18207	-0.070524
$C_{26}H_{30}N_1O_8$	434.1901452	434.1902	-0.126171
$C_{27}H_{34}N_1O_7$	434.1972956	434.19726	0.0819441
$C_{24}H_{21}O_{11}$	434.2184248	434.21846	-0.081111
$C_{23}H_{21}N_2O_{10}$	435.072155	435.07198	0.4021859
$C_{27}H_{21}N_2O_7$	435.0833884	435.08339	-0.003724
$C_{25}H_{25}O_{10}$	435.0932842	435.09319	0.2164591
$C_{24}H_{25}N_2O_9$	435.1085404	435.10847	0.1617525
$C_{28}H_{25}N_2O_6$	435.1197738	435.11973	0.1006157
$C_{26}H_{29}O_9$	435.118266	435.11973	-3.364649
$C_{25}H_{29}N_2O_8$	435.1296696	435.12953	0.3207777
$C_{27}H_{33}O_8$	435.140903	435.14074	0.3745451
$C_{26}H_{33}N_2O_7$	435.1449258	435.14483	0.2201103
$C_{23}H_{20}N_1O_{11}$	435.1561592	435.1561	0.1359969
$C_{27}H_{20}N_1O_8$	435.166055	435.16593	0.2872005
$C_{24}H_{24}N_1O_{10}$	435.1772884	435.17716	0.295006
$C_{28}H_{24}N_1O_7$	435.1813112	435.18125	0.1405849
$C_{25}H_{28}N_1O_9$	435.1925446	435.19256	-0.035433
$C_{29}H_{28}N_1O_6$	435.2024404	435.20227	0.3914957
$C_{26}H_{32}N_1O_8$	435.2136738	435.21359	0.1925029
$C_{23}H_{19}O_{12}$	435.212166	435.21359	-3.272014
$C_{27}H_{19}O_9$	435.2388258	435.23866	0.3808941
$C_{26}H_{19}N_2O_8$	436.067404	436.0674	0.0091268

$C_{24}H_{23}O_{11}$	436.0885332	436.08828	0.58057
$C_{23}H_{23}N_2O_{10}$	436.1037894	436.10367	0.2737419
$C_{28}H_{23}O_8$	436.1249186	436.12484	0.1801775
$C_{27}H_{23}N_2O_7$	436.1401748	436.14009	0.1943868
$C_{25}H_{27}O_{10}$	436.1482806	436.14827	0.0243442
$C_{24}H_{27}N_2O_9$	436.161304	436.16124	0.1466886
$C_{29}H_{27}O_7$	436.1694098	436.1694	0.0225089
$C_{28}H_{27}N_2O_6$	436.1765602	436.17652	0.0921184
$C_{26}H_{31}O_9$	436.1862858	436.18772	-3.288091
$C_{25}H_{31}N_2O_8$	436.1976894	436.19767	0.0444292
$C_{27}H_{35}O_8$	436.2057952	436.20572	0.1724363
$C_{26}H_{35}N_2O_7$	436.2129456	436.21281	0.3108113
$C_{25}H_{43}O_9$	436.2340748	436.23399	0.194345
$C_{26}H_{18}N_1O_9$	437.0514196	437.05123	0.4337702
$C_{23}H_{22}N_1O_{11}$	437.087805	437.08775	0.1257869
$C_{27}H_{22}N_1O_8$	437.0990384	437.09904	-0.003706
$C_{24}H_{26}N_1O_{10}$	437.1071442	437.10726	-0.264883
$C_{28}H_{26}N_1O_7$	437.1089342	437.10885	0.1925833
$C_{25}H_{30}N_1O_9$	437.1201676	437.12027	-0.234307
$C_{29}H_{30}N_1O_6$	437.1241904	437.12413	0.1381299
$C_{26}H_{34}N_1O_8$	437.1354238	437.13535	0.1687804
$C_{23}H_{21}O_{12}$	437.1453196	437.14527	0.1134174
$C_{27}H_{21}O_9$	437.156553	437.15646	0.2126925
$C_{26}H_{21}N_2O_8$	437.1605758	437.16048	0.2190955
$C_{24}H_{25}O_{11}$	437.1718092	437.17168	0.29549
$C_{23}H_{25}N_2O_{10}$	437.1703014	437.17168	-3.153508

$C_{28}H_{25}O_8$	437.181705	437.18162	0.1943812
$C_{27}H_{25}N_2O_7$	437.1929384	437.19296	-0.049452
$C_{25}H_{29}O_{10}$	437.1969612	437.19673	0.5287775
$C_{24}H_{29}N_2O_9$	437.2081946	437.20799	0.4679233
$C_{28}H_{29}N_2O_6$	437.2180904	437.21801	0.1838439
$C_{26}H_{33}O_9$	437.2293238	437.22929	0.077259
$C_{25}H_{33}N_2O_8$	437.2544758	437.25446	0.0360886
$C_{25}H_{16}N_1O_{10}$	438.083054	438.08297	0.1916986
$C_{26}H_{20}N_1O_9$	438.0911598	438.09105	0.2506732
$C_{23}H_{24}N_1O_{11}$	438.1041832	438.10401	0.3952939
$C_{27}H_{24}N_1O_8$	438.1194394	438.1193	0.3181322
$C_{24}H_{28}N_1O_{10}$	438.1405686	438.14044	0.2934672
$C_{28}H_{28}N_1O_7$	438.1486744	438.14861	0.1470225
$C_{25}H_{32}N_1O_9$	438.1558248	438.15576	0.1478467
$C_{26}H_{36}N_1O_8$	438.1639306	438.16386	0.1611673
$C_{22}H_{19}O_{13}$	438.176954	438.17689	0.1460138
$C_{26}H_{19}O_{10}$	438.1922102	438.19215	0.1373368
$C_{25}H_{19}N_2O_9$	438.2133394	438.2133	0.0898647
$C_{23}H_{23}O_{12}$	439.0670696	439.06707	-0.000957
$C_{27}H_{23}O_9$	439.103455	439.10343	0.0568884
$C_{26}H_{23}N_2O_8$	439.1146884	439.1147	-0.026463
$C_{24}H_{27}O_{11}$	439.1164743	439.11655	-0.172441
$C_{23}H_{27}N_2O_{10}$	439.1227942	439.12284	-0.104259
$C_{28}H_{27}O_8$	439.1245842	439.12459	-0.013254
$C_{27}H_{27}N_2O_7$	439.1398404	439.13982	0.0464087
$C_{25}H_{31}O_{10}$	439.1396702	439.13982	-0.341167

$C_{24}H_{31}N_2O_9$	439.1510738	439.15103	0.0996921
$C_{26}H_{35}O_9$	439.1591796	439.15926	-0.183037
$C_{27}H_{39}O_8$	439.1609696	439.16093	0.0901262
$C_{25}H_{18}N_1O_{10}$	439.172203	439.17231	-0.243686
$C_{22}H_{22}N_1O_{12}$	439.1762258	439.17622	0.0131608
$C_{26}H_{22}N_1O_9$	439.1874592	439.18743	0.0664406
$C_{23}H_{26}N_1O_{11}$	439.197355	439.19728	0.1707203
$C_{27}H_{26}N_1O_8$	439.2085884	439.20865	-0.140298
$C_{24}H_{30}N_1O_{10}$	439.2337404	439.23368	0.1374664
$C_{28}H_{30}N_1O_7$	440.098704	440.09852	0.4180424
$C_{25}H_{34}N_1O_9$	440.1198332	440.11968	0.3480413
$C_{25}H_{17}O_{11}$	440.1350894	440.13498	0.2485144
$C_{24}H_{17}N_2O_{10}$	440.1431952	440.14302	0.3980925
$C_{26}H_{21}O_{10}$	440.1503456	440.1503	0.1035553
$C_{25}H_{21}N_2O_9$	440.1544286	440.15439	0.0877367
$C_{23}H_{25}O_{12}$	440.1562186	440.15616	0.1330889
$C_{27}H_{25}O_9$	440.1714748	440.17132	0.3516355
$C_{26}H_{25}N_2O_8$	440.192604	440.19266	-0.127263
$C_{24}H_{29}O_{11}$	440.2078602	440.2078	0.1367079
$C_{23}H_{29}N_2O_{10}$	441.0827196	441.08281	-0.204996
$C_{28}H_{29}O_8$	441.093953	441.09386	0.2107939
$C_{27}H_{29}N_2O_7$	441.119105	441.11916	-0.124728
$C_{25}H_{33}O_{10}$	441.1303384	441.1304	-0.139687
$C_{24}H_{33}N_2O_9$	441.1384442	441.13847	-0.058445
$C_{26}H_{37}O_9$	441.1402342	441.14018	0.1228179
$C_{25}H_{37}N_2O_8$	441.1554904	441.15551	-0.044474

$C_{25}H_{20}N_1O_{10}$	441.1667238	441.16676	-0.082101
$C_{22}H_{24}N_1O_{12}$	441.1766196	441.17667	-0.114286
$C_{26}H_{24}N_1O_9$	441.187853	441.18782	0.0747525
$C_{23}H_{28}N_1O_{11}$	441.1918758	441.19185	0.0584324
$C_{27}H_{28}N_1O_8$	441.2031092	441.2031	0.0208065
$C_{24}H_{32}N_1O_{10}$	441.2016014	441.2031	-3.396679
$C_{28}H_{32}N_1O_7$	441.213005	441.21294	0.1472756
$C_{25}H_{19}O_{11}$	441.2493904	441.24954	-0.339083
$C_{22}H_{23}O_{13}$	442.0779686	442.07786	0.2456126
$C_{26}H_{23}O_{10}$	442.0860744	442.08612	-0.103107
$C_{25}H_{23}N_2O_9$	442.114354	442.11422	0.3030435
$C_{23}H_{27}O_{12}$	442.1296102	442.12949	0.2718205
$C_{22}H_{27}N_2O_{11}$	442.1507394	442.15061	0.2926149
$C_{27}H_{27}O_9$	442.1588452	442.15865	0.4415103
$C_{26}H_{27}N_2O_8$	442.1718686	442.17161	0.584795
$C_{24}H_{31}O_{11}$	442.1871248	442.18694	0.4178772
$C_{28}H_{31}O_8$	442.2235102	442.22338	0.2943758
$C_{27}H_{31}N_2O_7$	443.0619842	443.06221	-0.509681
$C_{25}H_{35}O_{10}$	443.0983696	443.09842	-0.11379
$C_{24}H_{35}N_2O_9$	443.109603	443.10974	-0.309224
$C_{26}H_{39}O_9$	443.1136258	443.1137	-0.167497
$C_{25}H_{39}N_2O_8$	443.1194988	443.11968	-0.408964
$C_{24}H_{18}N_1O_{11}$	443.1248592	443.12504	-0.408057
$C_{25}H_{22}N_1O_{10}$	443.134755	443.13483	-0.169294
$C_{22}H_{26}N_1O_{12}$	443.1345848	443.13483	-0.553376
$C_{26}H_{26}N_1O_9$	443.1459884	443.14614	-0.342145

$C_{23}H_{30}N_1O_{11}$	443.1540942	443.15419	-0.216138
$C_{27}H_{30}N_1O_8$	443.1558842	443.15606	-0.396745
$C_{28}H_{34}N_1O_7$	443.1612446	443.16119	0.1231604
$C_{25}H_{21}O_{11}$	443.1597368	443.16119	-3.279224
$C_{24}H_{21}N_2O_{10}$	443.1711404	443.1712	-0.134531
$C_{26}H_{25}O_{10}$	443.1823738	443.18251	-0.307368
$C_{25}H_{25}N_2O_9$	443.203503	443.20376	-0.579914
$C_{22}H_{29}N_2O_{11}$	443.2075258	443.20758	-0.122336
$C_{27}H_{29}O_9$	443.2187592	443.21874	0.0432741
$C_{26}H_{29}N_2O_8$	443.228655	443.22876	-0.236943
$C_{28}H_{33}O_8$	443.2650404	443.26521	-0.382661
$C_{27}H_{33}N_2O_7$	444.0936186	444.09352	0.22198
$C_{27}H_{45}O_8$	444.1017244	444.10164	0.1900864
$C_{24}H_{20}N_1O_{11}$	444.130004	444.12982	0.4142479
$C_{28}H_{20}N_1O_8$	444.1381098	444.13786	0.5624775
$C_{25}H_{24}N_1O_{10}$	444.1452602	444.14509	0.3831627
$C_{29}H_{24}N_1O_7$	444.1663894	444.16621	0.4038574
$C_{26}H_{28}N_1O_9$	444.1816456	444.18144	0.4628284
$C_{30}H_{28}N_1O_6$	444.1857286	444.18558	0.3345846
$C_{23}H_{32}N_1O_{11}$	444.1875186	444.18771	-0.430944
$C_{27}H_{32}N_1O_8$	444.2027748	444.20259	0.415981
$C_{28}H_{36}N_1O_7$	445.0776342	445.07772	-0.192821
$C_{24}H_{19}O_{12}$	445.0928904	445.09307	-0.403556
$C_{25}H_{23}O_{11}$	445.1041238	445.10423	-0.238641
$C_{24}H_{23}N_2O_{10}$	445.1140196	445.11407	-0.113275
$C_{29}H_{23}O_8$	445.125253	445.12525	0.0066945

$C_{28}H_{23}N_2O_7$	445.1292758	445.12939	-0.2566
$C_{26}H_{27}O_{10}$	445.1333588	445.13332	0.0872047
$C_{25}H_{27}N_2O_9$	445.1405092	445.14061	-0.226491
$C_{29}H_{27}N_2O_6$	445.150405	445.15044	-0.07867
$C_{27}H_{31}O_9$	445.1502348	445.15044	-0.461013
$C_{26}H_{31}N_2O_8$	445.1616384	445.16167	-0.071031
$C_{24}H_{22}N_1O_{11}$	445.1656612	445.1659	-0.536475
$C_{28}H_{22}N_1O_8$	445.1697442	445.16989	-0.327476
$C_{25}H_{26}N_1O_{10}$	445.1768946	445.17688	0.0327508
$C_{29}H_{26}N_1O_7$	445.1867904	445.18686	-0.156384
$C_{26}H_{30}N_1O_9$	445.1980238	445.19815	-0.283515
$C_{27}H_{34}N_1O_8$	445.2231758	445.22317	0.012982
$C_{24}H_{21}O_{12}$	445.2344092	445.23443	-0.046762
$C_{28}H_{21}O_9$	445.244305	445.24446	-0.348169
$C_{27}H_{21}N_2O_8$	445.2806904	445.2807	-0.021605
$C_{25}H_{25}O_{11}$	446.0881394	446.08797	0.3797005
$C_{24}H_{25}N_2O_{10}$	446.1092686	446.10915	0.2658091
$C_{29}H_{25}O_8$	446.1245248	446.12435	0.3917738
$C_{28}H_{25}N_2O_7$	446.145654	446.14555	0.2330627
$C_{26}H_{29}O_{10}$	446.1609102	446.16082	0.2021242
$C_{25}H_{29}N_2O_9$	446.1706358	446.17184	-2.699012
$C_{29}H_{29}N_2O_6$	446.1820394	446.18186	0.402033
$C_{27}H_{33}O_9$	446.2184248	446.2183	0.2796386
$C_{26}H_{33}N_2O_8$	447.0568988	447.05673	0.3775356
$C_{28}H_{37}O_8$	447.072155	447.07233	-0.391481
$C_{27}H_{37}N_2O_7$	447.0932842	447.09328	0.0093491

$C_{27}H_{20}N_1O_9$	447.1045176	447.10464	-0.273806
$C_{24}H_{24}N_1O_{11}$	447.1085404	447.10846	0.1797772
$C_{28}H_{24}N_1O_8$	447.1197738	447.11981	-0.081008
$C_{25}H_{28}N_1O_{10}$	447.1296696	447.12964	0.0661551
$C_{29}H_{28}N_1O_7$	447.140903	447.14096	-0.127522
$C_{26}H_{32}N_1O_9$	447.1449258	447.14483	0.2142033
$C_{27}H_{19}O_{10}$	447.1561592	447.15603	0.2888921
$C_{24}H_{23}O_{12}$	447.1546514	447.15603	-3.083095
$C_{28}H_{23}O_9$	447.166055	447.16595	0.2347671
$C_{27}H_{23}N_2O_8$	447.1772884	447.17732	-0.07071
$C_{25}H_{27}O_{11}$	447.1853942	447.18524	0.344863
$C_{24}H_{27}N_2O_{10}$	447.1925446	447.19241	0.300944
$C_{29}H_{27}O_8$	447.2024404	447.20234	0.2244619
$C_{28}H_{27}N_2O_7$	447.2136738	447.2136	0.1649768
$C_{26}H_{31}O_{10}$	447.2388258	447.23885	-0.054155
$C_{25}H_{31}N_2O_9$	448.067404	448.06739	0.0312004
$C_{29}H_{31}N_2O_6$	448.1037894	448.10375	0.0878812
$C_{27}H_{35}O_9$	448.1249186	448.12486	0.1307223
$C_{26}H_{35}N_2O_8$	448.1401748	448.14011	0.1445528
$C_{26}H_{18}N_1O_{10}$	448.161304	448.16126	0.0981341
$C_{27}H_{22}N_1O_9$	448.1694098	448.16938	0.0665322
$C_{24}H_{26}N_1O_{11}$	448.1765602	448.17648	0.1789025
$C_{28}H_{26}N_1O_8$	448.1862858	448.18772	-3.200054
$C_{25}H_{30}N_1O_{10}$	448.1976894	448.19758	0.2440439
$C_{29}H_{30}N_1O_7$	448.2129456	448.21269	0.5702198
$C_{26}H_{34}N_1O_9$	448.2269244	448.22818	-2.80122

$C_{27}H_{38}N_1O_8$	448.2340748	448.23385	0.5014788
$C_{27}H_{21}O_{10}$	449.0514196	449.05123	0.4221786
$C_{24}H_{25}O_{12}$	449.087805	449.08762	0.4119014
$C_{28}H_{25}O_9$	449.0990384	449.09898	0.1299934
$C_{27}H_{25}N_2O_8$	449.1089342	449.10875	0.4101007
$C_{25}H_{29}O_{11}$	449.1201676	449.11996	0.4621923
$C_{29}H_{29}O_8$	449.1241904	449.12407	0.2680325
$C_{28}H_{29}N_2O_7$	449.1354238	449.13528	0.3201259
$C_{26}H_{33}O_{10}$	449.1453196	449.14519	0.2885033
$C_{25}H_{33}N_2O_9$	449.156553	449.15659	-0.082421
$C_{27}H_{37}O_9$	449.1605758	449.16043	0.3245608
$C_{26}H_{20}N_1O_{10}$	449.1646588	449.16479	-0.292058
$C_{23}H_{24}N_1O_{12}$	449.1718092	449.17166	0.3321221
$C_{27}H_{24}N_1O_9$	449.181705	449.18162	0.1891882
$C_{24}H_{28}N_1O_{11}$	449.1929384	449.19283	0.2412769
$C_{28}H_{28}N_1O_8$	449.2081946	449.20792	0.6112531
$C_{25}H_{32}N_1O_{10}$	449.2066868	449.20792	-2.745329
$C_{29}H_{32}N_1O_7$	449.2180904	449.21798	0.2457156
$C_{26}H_{36}N_1O_9$	449.2293238	449.22917	0.3423194
$C_{26}H_{19}O_{11}$	450.083054	450.083	0.1199332
$C_{23}H_{23}O_{13}$	450.1041832	450.10423	-0.104021
$C_{27}H_{23}O_{10}$	450.1194394	450.11947	-0.068027
$C_{26}H_{23}N_2O_9$	450.1275452	450.12761	-0.14392
$C_{24}H_{27}O_{12}$	450.1405686	450.14064	-0.158662
$C_{23}H_{27}N_2O_{11}$	450.1558248	450.15584	-0.033811
$C_{28}H_{27}O_9$	450.1655504	450.16697	-3.153551

$C_{27}H_{27}N_2O_8$	450.176954	450.17702	-0.146654
$C_{25}H_{31}O_{11}$	450.1922102	450.19224	-0.066239
$C_{24}H_{31}N_2O_{10}$	450.2133394	450.21335	-0.023589
$C_{29}H_{31}O_8$	450.2497248	450.24969	0.0772458
$C_{28}H_{31}N_2O_7$	451.0670696	451.06686	0.4646313
$C_{26}H_{35}O_{10}$	451.103455	451.10329	0.3657252
$C_{25}H_{35}N_2O_9$	451.1146884	451.11458	0.2402491
$C_{26}H_{22}N_1O_{10}$	451.1164743	451.11653	-0.12352
$C_{27}H_{26}N_1O_9$	451.1245842	451.12441	0.3861015
$C_{24}H_{30}N_1O_{11}$	451.1358176	451.13556	0.5709587
$C_{28}H_{30}N_1O_8$	451.1398404	451.13969	0.3333332
$C_{29}H_{34}N_1O_7$	451.1510738	451.15091	0.3630267
$C_{25}H_{17}O_{12}$	451.149566	451.15091	-2.979101
$C_{26}H_{21}O_{11}$	451.1609696	451.16075	0.4866997
$C_{25}H_{21}N_2O_{10}$	451.172203	451.17219	0.0287693
$C_{27}H_{25}O_{10}$	451.1762258	451.17606	0.3674394
$C_{26}H_{25}N_2O_9$	451.1874592	451.18726	0.4414571
$C_{24}H_{29}O_{12}$	451.197355	451.19709	0.5872816
$C_{23}H_{29}N_2O_{11}$	451.2085884	451.2084	0.4175007
$C_{28}H_{29}O_9$	451.2337404	451.23373	0.0230034
$C_{27}H_{29}N_2O_8$	452.098704	452.09877	-0.14603
$C_{25}H_{33}O_{11}$	452.1198332	452.11994	-0.236265
$C_{24}H_{33}N_2O_{10}$	452.1350894	452.13514	-0.111958
$C_{29}H_{33}O_8$	452.1431952	452.14325	-0.121161
$C_{28}H_{33}N_2O_7$	452.1562186	452.15623	-0.025257
$C_{26}H_{37}O_{10}$	452.1714748	452.17155	-0.166353

$C_{26}H_{41}N_2O_8$	452.1812004	452.17981	3.0748291
$C_{25}H_{20}N_1O_{11}$	452.192604	452.19262	-0.035428
$C_{26}H_{24}N_1O_{10}$	452.2078602	452.2079	-0.088057
$C_{27}H_{28}N_1O_9$	452.2289894	452.22906	-0.15616
$C_{28}H_{32}N_1O_8$	453.0827196	453.0825	0.4846353
$C_{25}H_{19}O_{12}$	453.1020588	453.1021	-0.09089
$C_{26}H_{23}O_{11}$	453.1038488	453.10383	0.0414472
$C_{25}H_{23}N_2O_{10}$	453.119105	453.119	0.2316828
$C_{27}H_{27}O_{10}$	453.1303384	453.13024	0.2171117
$C_{26}H_{27}N_2O_9$	453.1384442	453.13846	-0.034829
$C_{28}H_{31}O_9$	453.1402342	453.14016	0.1637019
$C_{27}H_{31}N_2O_8$	453.1554904	453.15536	0.2877156
$C_{29}H_{35}O_8$	453.1553202	453.15536	-0.087873
$C_{25}H_{22}N_1O_{11}$	453.1667238	453.16655	0.383479
$C_{29}H_{22}N_1O_8$	453.1766196	453.17635	0.5948672
$C_{26}H_{26}N_1O_{10}$	453.187853	453.18809	-0.523006
$C_{30}H_{26}N_1O_7$	453.1918758	453.19182	0.1230823
$C_{27}H_{30}N_1O_9$	453.2031092	453.20294	0.3732982
$C_{28}H_{34}N_1O_8$	453.213005	453.21268	0.7170578
$C_{25}H_{21}O_{12}$	453.2242384	453.22409	0.3273874
$C_{26}H_{25}O_{11}$	453.2493904	453.24916	0.5082851
$C_{25}H_{25}N_2O_{10}$	453.2857758	453.28566	0.2554236
$C_{29}H_{25}N_2O_7$	454.0779686	454.07801	-0.091218
$C_{27}H_{29}O_{10}$	454.114354	454.11435	0.0087641
$C_{26}H_{29}N_2O_9$	454.1296102	454.12952	0.1985775
$C_{28}H_{33}O_9$	454.1354832	454.1355	-0.037038

$C_{27}H_{33}N_2O_8$	454.1507394	454.15069	0.1087302
$C_{29}H_{24}N_1O_8$	454.1588452	454.15889	-0.098605
$C_{26}H_{28}N_1O_{10}$	454.1718686	454.17178	0.1950361
$C_{30}H_{28}N_1O_7$	454.1871248	454.18711	0.0325414
$C_{27}H_{32}N_1O_9$	454.208254	454.20817	0.1848929
$C_{28}H_{36}N_1O_8$	454.2235102	454.22351	0.0003961
$C_{28}H_{19}O_{10}$	455.0619842	455.06184	0.3168357
$C_{25}H_{23}O_{12}$	455.0983696	455.09828	0.1968363
$C_{24}H_{23}N_2O_{11}$	455.109603	455.10961	-0.015425
$C_{29}H_{23}O_9$	455.1177088	455.11766	0.1072639
$C_{28}H_{23}N_2O_8$	455.1194988	455.11932	0.3928197
$C_{26}H_{27}O_{11}$	455.134755	455.13462	0.2965713
$C_{25}H_{27}N_2O_{10}$	455.1459884	455.14586	0.2820631
$C_{30}H_{27}O_8$	455.1558842	455.15589	-0.012787
$C_{29}H_{27}N_2O_7$	455.1671176	455.16721	-0.203047
$C_{27}H_{31}O_{10}$	455.1711404	455.17103	0.242502
$C_{26}H_{31}N_2O_9$	455.1709702	455.17103	-0.131423
$C_{30}H_{31}N_2O_6$	455.1823738	455.18229	0.1840579
$C_{28}H_{35}O_9$	455.1922696	455.19236	-0.198642
$C_{27}H_{35}N_2O_8$	455.203503	455.20328	0.4898466
$C_{27}H_{18}N_1O_{10}$	455.2075258	455.20759	-0.141079
$C_{24}H_{22}N_1O_{12}$	455.2187592	455.21857	0.4155802
$C_{28}H_{22}N_1O_9$	455.228655	455.22846	0.428312
$C_{25}H_{26}N_1O_{11}$	456.0936186	456.09346	0.3476916
$C_{29}H_{26}N_1O_8$	456.1088748	456.10867	0.4489715
$C_{26}H_{30}N_1O_{10}$	456.130004	456.12989	0.2498847

$C_{30}H_{30}N_1O_7$	456.1381098	456.13795	0.3503713
$C_{27}H_{34}N_1O_9$	456.1452602	456.14513	0.2853913
$C_{28}H_{21}O_{10}$	456.1663894	456.16625	0.3055462
$C_{25}H_{25}O_{12}$	456.2027748	456.20265	0.2735185
$C_{29}H_{25}O_9$	456.2391602	456.23913	0.0661493
$C_{28}H_{25}N_2O_8$	457.0776342	457.07757	0.1404136
$C_{26}H_{29}O_{11}$	457.1140196	457.11401	0.0209574
$C_{25}H_{29}N_2O_{10}$	457.125253	457.12531	-0.124736
$C_{30}H_{29}O_8$	457.1333588	457.13331	0.1067909
$C_{29}H_{29}N_2O_7$	457.1351488	457.13506	0.1942093
$C_{27}H_{33}O_{10}$	457.1405092	457.14045	0.1294567
$C_{26}H_{33}N_2O_9$	457.150405	457.15037	0.0765173
$C_{27}H_{20}N_1O_{10}$	457.1616384	457.1616	0.0839526
$C_{24}H_{24}N_1O_{12}$	457.1768946	457.17673	0.3599917
$C_{28}H_{24}N_1O_9$	457.1753868	457.17673	-2.938085
$C_{25}H_{28}N_1O_{11}$	457.1867904	457.18681	-0.042915
$C_{29}H_{28}N_1O_8$	457.1980238	457.19801	0.0301399
$C_{26}H_{32}N_1O_{10}$	457.2231758	457.22329	-0.249813
$C_{30}H_{32}N_1O_7$	457.2344092	457.23438	0.0638183
$C_{27}H_{36}N_1O_9$	457.244305	457.24442	-0.251551
$C_{27}H_{19}O_{11}$	457.3170758	457.31699	0.187572
$C_{24}H_{23}O_{13}$	458.1092686	458.10913	0.302504
$C_{28}H_{23}O_{10}$	458.1173744	458.11724	0.2934132
$C_{27}H_{23}N_2O_9$	458.1245248	458.12432	0.4469962
$C_{25}H_{27}O_{12}$	458.145654	458.14551	0.3142667
$C_{24}H_{27}N_2O_{11}$	458.1537598	458.15359	0.3706566

$C_{29}H_{27}O_9$	458.1609102	458.16071	0.4369205
$C_{28}H_{27}N_2O_8$	458.1820394	458.18187	0.3696782
$C_{26}H_{31}O_{11}$	458.1901452	458.18989	0.5570126
$C_{25}H_{31}N_2O_{10}$	458.2184248	458.21821	0.4687282
$C_{30}H_{31}O_8$	459.0932842	459.09328	0.0091047
$C_{29}H_{31}N_2O_7$	459.1045176	459.10465	-0.288431
$C_{27}H_{35}O_{10}$	459.1085404	459.1086	-0.129861
$C_{26}H_{35}N_2O_9$	459.1197738	459.11984	-0.144233
$C_{27}H_{22}N_1O_{10}$	459.1296696	459.12968	-0.022695
$C_{24}H_{26}N_1O_{12}$	459.140903	459.14096	-0.124189
$C_{28}H_{26}N_1O_9$	459.1449258	459.14501	-0.183428
$C_{25}H_{30}N_1O_{11}$	459.1561592	459.15612	0.0853302
$C_{29}H_{30}N_1O_8$	459.166055	459.1661	-0.098048
$C_{26}H_{34}N_1O_{10}$	459.1772884	459.17734	-0.112419
$C_{30}H_{34}N_1O_7$	459.1925446	459.19273	-0.403796
$C_{27}H_{38}N_1O_9$	459.2024404	459.2025	-0.129834
$C_{27}H_{21}O_{11}$	459.2136738	459.21372	-0.100651
$C_{24}H_{25}O_{13}$	459.2388258	459.23872	0.2303374
$C_{28}H_{25}O_{10}$	459.2963404	459.29637	-0.06449
$C_{27}H_{25}N_2O_9$	460.0885332	460.08856	-0.058293
$C_{25}H_{29}O_{12}$	460.1037894	460.10368	0.2377288
$C_{24}H_{29}N_2O_{11}$	460.1249186	460.12484	0.1707795
$C_{29}H_{29}O_9$	460.1330244	460.13295	0.1617308
$C_{28}H_{29}N_2O_8$	460.1401748	460.14014	0.0755854
$C_{26}H_{33}O_{11}$	460.1499004	460.15117	-2.759145
$C_{25}H_{33}N_2O_{10}$	460.161304	460.1612	0.225964

$C_{30}H_{33}O_8$	460.1765602	460.17636	0.4350067
$C_{29}H_{33}N_2O_7$	460.1806432	460.18069	-0.101661
$C_{27}H_{37}O_{10}$	460.1976894	460.19754	0.3245994
$C_{26}H_{37}N_2O_9$	460.2057952	460.20577	0.0547966
$C_{26}H_{20}N_1O_{11}$	460.2340748	460.23399	0.1842104
$C_{27}H_{24}N_1O_{10}$	461.087805	461.08767	0.2927423
$C_{24}H_{28}N_1O_{12}$	461.1089342	461.10885	0.1825597
$C_{28}H_{28}N_1O_9$	461.1241904	461.1241	0.195999
$C_{25}H_{32}N_1O_{11}$	461.1354238	461.13528	0.3117954
$C_{29}H_{32}N_1O_8$	461.1453196	461.14524	0.1725701
$C_{26}H_{19}O_{12}$	461.156553	461.15658	-0.058592
$C_{27}H_{23}O_{11}$	461.1605758	461.16056	0.0342178
$C_{26}H_{23}N_2O_{10}$	461.1646588	461.16461	0.1058574
$C_{28}H_{27}O_{10}$	461.1718092	461.17175	0.1283251
$C_{27}H_{27}N_2O_9$	461.1703014	461.17175	-3.141183
$C_{24}H_{31}N_2O_{11}$	461.181705	461.18163	0.1625821
$C_{29}H_{31}O_9$	461.1815348	461.18163	-0.20647
$C_{28}H_{31}N_2O_8$	461.1929384	461.19284	0.2133161
$C_{30}H_{35}O_8$	461.1969612	461.19711	-0.322682
$C_{29}H_{35}N_2O_7$	461.2081946	461.20801	0.4002095
$C_{25}H_{18}N_1O_{12}$	461.2180904	461.21801	0.1742774
$C_{26}H_{22}N_1O_{11}$	461.2293238	461.22905	0.5935874
$C_{27}H_{26}N_1O_{10}$	462.083054	462.08302	0.0735363
$C_{24}H_{30}N_1O_{12}$	462.1041832	462.10424	-0.12296
$C_{28}H_{30}N_1O_9$	462.1194394	462.1194	0.0852158
$C_{29}H_{34}N_1O_8$	462.1405686	462.14053	0.0834809

$C_{26}H_{21}O_{12}$	462.1558248	462.15578	0.0968935
$C_{27}H_{25}O_{11}$	462.176954	462.17692	0.0735214
$C_{26}H_{25}N_2O_{10}$	462.1922102	462.19211	0.2167494
$C_{28}H_{29}O_{10}$	462.2133394	462.21316	0.388089
$C_{27}H_{29}N_2O_9$	462.2497248	462.24994	-0.465593
$C_{29}H_{33}O_9$	463.0670696	463.06688	0.4094005
$C_{28}H_{33}N_2O_8$	463.0881988	463.088	0.4292485
$C_{25}H_{20}N_1O_{12}$	463.103455	463.10332	0.2914681
$C_{26}H_{24}N_1O_{11}$	463.1146884	463.11452	0.3635814
$C_{30}H_{24}N_1O_8$	463.1245842	463.12443	0.3329124
$C_{27}H_{28}N_1O_{10}$	463.1358176	463.13578	0.0811423
$C_{28}H_{32}N_1O_9$	463.1398404	463.13972	0.2599213
$C_{29}H_{36}N_1O_8$	463.1510738	463.15088	0.4183946
$C_{26}H_{23}O_{12}$	463.149566	463.15088	-2.83714
$C_{27}H_{27}O_{11}$	463.1609696	463.1608	0.366136
$C_{26}H_{27}N_2O_{10}$	463.172203	463.17221	-0.015157
$C_{30}H_{27}N_2O_7$	463.1762258	463.176	0.48746
$C_{28}H_{31}O_{10}$	463.1803088	463.18033	-0.045732
$C_{27}H_{31}N_2O_9$	463.1874592	463.18724	0.4731991
$C_{29}H_{35}O_9$	463.1859514	463.18724	-2.782079
$C_{28}H_{35}N_2O_8$	463.197355	463.19728	0.1618746
$C_{25}H_{22}N_1O_{12}$	463.2085884	463.20833	0.5578046
$C_{29}H_{22}N_1O_9$	463.2337404	463.23366	0.1735191
$C_{26}H_{26}N_1O_{11}$	464.098704	464.09868	0.0516698
$C_{30}H_{26}N_1O_8$	464.1198332	464.11983	0.0068515
$C_{27}H_{30}N_1O_{10}$	464.1350894	464.13511	-0.044427

$C_{28}H_{34}N_1O_9$	464.144815	464.14339	3.0701192
$C_{26}H_{25}O_{12}$	464.1562186	464.15626	-0.089237
$C_{25}H_{25}N_2O_{11}$	464.1714748	464.17153	-0.118965
$C_{29}H_{25}N_2O_8$	464.192604	464.19269	-0.185311
$C_{27}H_{29}O_{11}$	464.2007098	464.20076	-0.108105
$C_{26}H_{29}N_2O_{10}$	464.2078602	464.20797	-0.236575
$C_{28}H_{33}O_{10}$	464.2289894	464.22901	-0.044418
$C_{29}H_{37}O_9$	465.0463342	465.04639	-0.120031
$C_{25}H_{24}N_1O_{12}$	465.0827196	465.08255	0.3646231
$C_{26}H_{28}N_1O_{11}$	465.1038488	465.10378	0.1478807
$C_{30}H_{28}N_1O_8$	465.119105	465.11898	0.2687052
$C_{27}H_{32}N_1O_{10}$	465.1303384	465.13016	0.3835052
$C_{28}H_{36}N_1O_9$	465.1402342	465.14002	0.4604631
$C_{25}H_{23}O_{13}$	465.1514676	465.15141	0.1237874
$C_{29}H_{23}O_{10}$	465.1554904	465.15532	0.3662859
$C_{28}H_{23}N_2O_9$	465.1595734	465.15949	0.1793314
$C_{26}H_{27}O_{12}$	465.1667238	465.1665	0.4810746
$C_{30}H_{27}O_9$	465.165216	465.1665	-2.760353
$C_{29}H_{27}N_2O_8$	465.1766196	465.17644	0.3860467
$C_{27}H_{31}O_{11}$	465.187853	465.18768	0.3718496
$C_{26}H_{31}N_2O_{10}$	465.1918758	465.19166	0.4638514
$C_{30}H_{31}N_2O_7$	465.2031092	465.20293	0.3851649
$C_{28}H_{35}O_{10}$	465.2016014	465.20293	-2.856009
$C_{27}H_{35}N_2O_9$	465.213005	465.21287	0.2901464
$C_{28}H_{39}N_2O_8$	465.2493904	465.24909	0.645632
$C_{28}H_{22}N_1O_{10}$	466.0779686	466.07788	0.1900538

$C_{29}H_{26}N_1O_9$	466.114354	466.11429	0.1372622
$C_{26}H_{30}N_1O_{11}$	466.1354832	466.13533	0.3286167
$C_{30}H_{30}N_1O_8$	466.1507394	466.15069	0.1059312
$C_{27}H_{34}N_1O_{10}$	466.1718686	466.17173	0.2972721
$C_{28}H_{21}O_{11}$	466.1871248	466.1871	0.0531544
$C_{25}H_{25}O_{13}$	466.208254	466.20823	0.051436
$C_{29}H_{25}O_{10}$	466.2235102	466.22343	0.1719774
$C_{26}H_{29}O_{12}$	467.0619842	467.06173	0.5442102
$C_{25}H_{29}N_2O_{11}$	467.0983696	467.09829	0.1703708
$C_{30}H_{29}O_9$	467.109603	467.10969	-0.186295
$C_{29}H_{29}N_2O_8$	467.1194988	467.11939	0.2328738
$C_{27}H_{33}O_{11}$	467.134755	467.13467	0.1819173
$C_{26}H_{33}N_2O_{10}$	467.1459884	467.14591	0.1677846
$C_{30}H_{33}N_2O_7$	467.1671176	467.16716	-0.090803
$C_{28}H_{37}O_{10}$	467.1711404	467.17109	0.1078404
$C_{27}H_{37}N_2O_9$	467.1823738	467.18218	0.4147843
$C_{27}H_{20}N_1O_{11}$	467.1922696	467.19219	0.1703365
$C_{28}H_{24}N_1O_{10}$	467.203503	467.20366	-0.336085
$C_{25}H_{28}N_1O_{12}$	467.2075258	467.20751	0.0337749
$C_{29}H_{28}N_1O_9$	467.2187592	467.21855	0.447713
$C_{26}H_{32}N_1O_{11}$	467.228655	467.22852	0.2888947
$C_{30}H_{32}N_1O_8$	467.2398884	467.23976	0.2747623
$C_{27}H_{36}N_1O_{10}$	467.2650404	467.26513	-0.191797
$C_{28}H_{40}N_1O_9$	468.0936186	468.09343	0.4028679
$C_{27}H_{23}N_2O_{10}$	468.130004	468.12991	0.200756
$C_{25}H_{27}O_{13}$	468.1381098	468.13791	0.4268349

C ₂₉ H ₂₇ O ₁₀	468.1511332	468.15119	-0.121371
C ₂₈ H ₂₇ N ₂ O ₉	468.1663894	468.16627	0.2549946
C ₂₆ H ₃₁ O ₁₂	468.1744952	468.17431	0.3956168
C ₃₀ H ₃₁ O ₉	468.1857286	468.1857	0.0611247
C ₂₉ H ₃₁ N ₂ O ₈	468.2027748	468.20262	0.330583
C ₂₇ H ₃₅ O ₁₁	468.223904	468.22365	0.5424326
C ₂₆ H ₃₅ N ₂ O ₁₀	469.0776342	469.07773	-0.204273
C ₂₇ H ₂₂ N ₁ O ₁₁	469.0888676	469.08858	0.6130606
C ₂₈ H ₂₆ N ₁ O ₁₀	469.1140196	469.11402	-0.000896
C ₂₉ H ₃₀ N ₁ O ₉	469.125253	469.12531	-0.121546
C ₂₆ H ₃₄ N ₁ O ₁₁	469.1333588	469.13342	-0.130416
C ₃₀ H ₃₄ N ₁ O ₈	469.1351488	469.13529	-0.301022
C ₂₇ H ₂₁ O ₁₂	469.1405092	469.14035	0.3393011
C ₂₈ H ₂₅ O ₁₁	469.1390014	469.14035	-2.874671
C ₂₇ H ₂₅ N ₂ O ₁₀	469.150405	469.15044	-0.074646
C ₂₉ H ₂₉ O ₁₀	469.1502348	469.15044	-0.437429
C ₂₈ H ₂₉ N ₂ O ₉	469.1616384	469.16162	0.0391761
C ₂₅ H ₃₃ N ₂ O ₁₁	469.1827676	469.183	-0.495372
C ₃₀ H ₃₃ O ₉	469.1867904	469.18683	-0.084444
C ₂₉ H ₃₃ N ₂ O ₈	469.1866202	469.18683	-0.4472
C ₂₇ H ₃₇ O ₁₁	469.1980238	469.1981	-0.162448
C ₂₆ H ₃₇ N ₂ O ₁₀	469.2079196	469.20793	-0.022208
C ₂₇ H ₂₄ N ₁ O ₁₁	469.2344092	469.23419	0.4671011
C ₂₈ H ₂₈ N ₁ O ₁₀	469.244305	469.24441	-0.223807
C ₂₉ H ₃₂ N ₁ O ₉	470.1092686	470.1092	0.1458808
C ₃₀ H ₃₆ N ₁ O ₈	470.145654	470.14551	0.3062453

$C_{27}H_{23}O_{12}$	470.1537598	470.15357	0.4037354
$C_{28}H_{27}O_{11}$	470.1609102	470.16072	0.4044996
$C_{27}H_{27}N_2O_{10}$	470.1820394	470.18184	0.4240483
$C_{29}H_{31}O_{10}$	470.2031686	470.20283	0.7200715
$C_{28}H_{31}N_2O_9$	470.2184248	470.21818	0.5205664
$C_{29}H_{35}N_2O_8$	471.0932842	471.09328	0.0088728
$C_{26}H_{22}N_1O_{12}$	471.1045176	471.10439	0.2708102
$C_{27}H_{26}N_1O_{11}$	471.1197738	471.11969	0.1778314
$C_{28}H_{30}N_1O_{10}$	471.1296696	471.12965	0.0415595
$C_{29}H_{34}N_1O_9$	471.140903	471.14096	-0.121026
$C_{26}H_{21}O_{13}$	471.1449258	471.14494	-0.030182
$C_{27}H_{25}O_{12}$	471.1561592	471.15598	0.3802983
$C_{26}H_{25}N_2O_{11}$	471.1546514	471.15598	-2.819924
$C_{28}H_{29}O_{11}$	471.166055	471.16602	0.0742411
$C_{27}H_{29}N_2O_{10}$	471.1772884	471.17727	0.0390085
$C_{29}H_{33}O_{10}$	471.2024404	471.20237	0.1493623
$C_{28}H_{33}N_2O_9$	471.2136738	471.21364	0.071687
$C_{30}H_{37}O_9$	471.259955	471.25995	0.0105672
$C_{26}H_{24}N_1O_{12}$	472.0885332	472.08868	-0.311001
$C_{30}H_{24}N_1O_9$	472.1037894	472.10376	0.0622319
$C_{27}H_{28}N_1O_{11}$	472.1249186	472.12481	0.2299813
$C_{28}H_{32}N_1O_{10}$	472.1401748	472.14012	0.1160247
$C_{29}H_{36}N_1O_9$	472.161304	472.16123	0.1566835
$C_{26}H_{23}O_{13}$	472.1765602	472.17653	0.0639166
$C_{30}H_{23}O_{10}$	472.1976894	472.19757	0.2528176
$C_{27}H_{27}O_{12}$	472.2340748	472.23398	0.2007053

$C_{26}H_{27}N_2O_{11}$	473.1089342	473.10882	0.2413396
$C_{30}H_{27}N_2O_8$	473.1201676	473.12005	0.2485202
$C_{28}H_{31}O_{11}$	473.1241904	473.12427	-0.168286
$C_{27}H_{31}N_2O_{10}$	473.1282734	473.12828	-0.013912
$C_{28}H_{35}N_2O_9$	473.1354238	473.13522	0.430701
$C_{29}H_{22}N_1O_{10}$	473.133916	473.13522	-2.756133
$C_{26}H_{26}N_1O_{12}$	473.1453196	473.14516	0.3372746
$C_{30}H_{26}N_1O_9$	473.156553	473.15649	0.1331058
$C_{27}H_{30}N_1O_{11}$	473.1605758	473.16072	-0.304802
$C_{28}H_{34}N_1O_{10}$	473.1718092	473.17163	0.3786783
$C_{29}H_{38}N_1O_9$	473.181705	473.18164	0.1373255
$C_{29}H_{21}O_{11}$	473.1815348	473.18164	-0.222367
$C_{26}H_{25}O_{13}$	473.1929384	473.19282	0.2501726
$C_{30}H_{25}O_{10}$	473.2010442	473.20016	1.8685878
$C_{29}H_{25}N_2O_9$	473.2180904	473.21808	0.0219347
$C_{27}H_{29}O_{12}$	473.2293238	473.22912	0.4306155
$C_{26}H_{29}N_2O_{11}$	473.275605	473.27539	0.4542383
$C_{30}H_{29}N_2O_8$	474.083054	474.08326	-0.434565
$C_{28}H_{33}O_{11}$	474.1041832	474.10423	-0.098755
$C_{27}H_{33}N_2O_{10}$	474.112289	474.11222	0.1455725
$C_{29}H_{37}O_{10}$	474.1194394	474.11951	-0.14895
$C_{28}H_{37}N_2O_9$	474.1405686	474.14063	-0.12954
$C_{29}H_{24}N_1O_{10}$	474.1558248	474.15584	-0.032099
$C_{26}H_{28}N_1O_{12}$	474.1655504	474.16698	-3.015023
$C_{30}H_{28}N_1O_9$	474.176954	474.17699	-0.075963
$C_{27}H_{32}N_1O_{11}$	474.1922102	474.19235	-0.29486

$C_{29}H_{23}O_{11}$	474.2133394	474.21338	-0.085658
$C_{28}H_{23}N_2O_{10}$	474.2497248	474.24982	-0.200781
$C_{26}H_{27}O_{13}$	475.0881988	475.08785	0.7341372
$C_{30}H_{27}O_{10}$	475.103455	475.10334	0.2420102
$C_{29}H_{27}N_2O_9$	475.1146884	475.11453	0.3333509
$C_{27}H_{31}O_{12}$	475.1131806	475.11453	-2.840208
$C_{26}H_{31}N_2O_{11}$	475.1245842	475.12442	0.3455513
$C_{30}H_{31}N_2O_8$	475.1358176	475.13582	-0.005093
$C_{28}H_{35}O_{11}$	475.1398404	475.13966	0.3796354
$C_{27}H_{35}N_2O_{10}$	475.1510738	475.15079	0.5972414
$C_{29}H_{39}O_{10}$	475.149566	475.15079	-2.576073
$C_{28}H_{39}N_2O_9$	475.1609696	475.16082	0.3147984
$C_{28}H_{22}N_1O_{11}$	475.172203	475.17207	0.2798562
$C_{29}H_{26}N_1O_{10}$	475.1762258	475.17608	0.3067912
$C_{26}H_{30}N_1O_{12}$	475.1803088	475.18027	0.0816905
$C_{30}H_{30}N_1O_9$	475.1874592	475.1872	0.5454266
$C_{27}H_{34}N_1O_{11}$	475.197355	475.1972	0.326138
$C_{29}H_{25}O_{11}$	475.2085884	475.20828	0.6489359
$C_{28}H_{25}N_2O_{10}$	475.2166942	475.21639	0.6401663
$C_{30}H_{29}O_{10}$	475.2337404	475.23361	0.274349
$C_{29}H_{29}N_2O_9$	476.098704	476.09866	0.0923756
$C_{26}H_{33}N_2O_{11}$	476.1198332	476.11977	0.1326975
$C_{30}H_{33}N_2O_8$	476.1350894	476.13502	0.1457147
$C_{28}H_{37}O_{11}$	476.1562186	476.15614	0.1650297
$C_{28}H_{24}N_1O_{11}$	476.1643244	476.16432	0.0092777
$C_{29}H_{28}N_1O_{10}$	476.1714748	476.17143	0.0940415

$C_{30}H_{32}N_1O_9$	476.1812004	476.18261	-2.96026
$C_{27}H_{36}N_1O_{11}$	476.192604	476.19256	0.0923574
$C_{28}H_{23}O_{12}$	476.2078602	476.20792	-0.125618
$C_{27}H_{23}N_2O_{11}$	476.2289894	476.22899	-0.001302
$C_{29}H_{27}O_{11}$	477.0827196	477.08265	0.1458445
$C_{28}H_{27}N_2O_{10}$	477.1038488	477.10371	0.2908799
$C_{30}H_{31}O_{10}$	477.1150822	477.11517	-0.184065
$C_{29}H_{31}N_2O_9$	477.119105	477.11902	0.1781105
$C_{26}H_{35}N_2O_{11}$	477.1303384	477.13032	0.0385218
$C_{30}H_{35}N_2O_8$	477.1288306	477.13032	-3.121631
$C_{30}H_{47}O_9$	477.1402342	477.14013	0.2183423
$C_{28}H_{26}N_1O_{11}$	477.1514676	477.15137	0.2045051
$C_{29}H_{30}N_1O_{10}$	477.1554904	477.15552	-0.062076
$C_{30}H_{34}N_1O_9$	477.1667238	477.16658	0.30132
$C_{28}H_{25}O_{12}$	477.165216	477.16658	-2.858591
$C_{27}H_{25}N_2O_{11}$	477.1766196	477.17657	0.1039026
$C_{29}H_{29}O_{11}$	477.187853	477.18771	0.2996302
$C_{28}H_{29}N_2O_{10}$	477.1918758	477.19185	0.0540242
$C_{30}H_{33}O_{10}$	477.2031092	477.20308	0.0611478
$C_{29}H_{33}N_2O_9$	477.2016014	477.20308	-3.098523
$C_{27}H_{24}N_1O_{12}$	477.213005	477.21286	0.3038054
$C_{28}H_{28}N_1O_{11}$	477.2242384	477.22414	0.2061503
$C_{29}H_{32}N_1O_{10}$	477.2493904	477.24949	-0.208738
$C_{30}H_{36}N_1O_9$	478.0779686	478.0778	0.3526201
$C_{27}H_{23}O_{13}$	478.114354	478.11429	0.1338171
$C_{28}H_{27}O_{12}$	478.1354832	478.13526	0.4667713

$C_{29}H_{31}O_{11}$	478.1507394	478.15062	0.24967
$C_{28}H_{31}N_2O_{10}$	478.160465	478.16157	-2.310982
$C_{30}H_{35}O_{10}$	478.1718686	478.17175	0.2479859
$C_{29}H_{35}N_2O_9$	478.1799744	478.17997	0.0092386
$C_{27}H_{26}N_1O_{12}$	478.1871248	478.18704	0.1772944
$C_{28}H_{30}N_1O_{11}$	478.1968504	478.19803	-2.466809
$C_{29}H_{34}N_1O_{10}$	478.208254	478.20813	0.2592592
$C_{28}H_{29}O_{12}$	478.2235102	478.22325	0.544055
$C_{27}H_{29}N_2O_{11}$	479.0619842	479.06211	-0.262638
$C_{29}H_{33}O_{11}$	479.0983696	479.09836	0.0199957
$C_{28}H_{33}N_2O_{10}$	479.109603	479.10961	-0.014652
$C_{30}H_{37}O_{10}$	479.1194988	479.11967	-0.357364
$C_{29}H_{37}N_2O_9$	479.1307322	479.13103	-0.621584
$C_{29}H_{20}N_1O_{11}$	479.134755	479.13481	-0.114832
$C_{30}H_{24}N_1O_{10}$	479.1459884	479.14611	-0.253827
$C_{27}H_{28}N_1O_{12}$	479.1558842	479.15595	-0.137367
$C_{28}H_{32}N_1O_{11}$	479.1711404	479.17124	-0.207901
$C_{29}H_{36}N_1O_{10}$	479.1823738	479.18246	-0.179932
$C_{30}H_{40}N_1O_9$	479.1922696	479.19232	-0.105219
$C_{27}H_{27}O_{13}$	479.203503	479.20346	0.0896903
$C_{30}H_{27}N_2O_9$	479.2075258	479.20778	-0.530501
$C_{28}H_{31}O_{12}$	479.2187592	479.21875	0.019156
$C_{27}H_{31}N_2O_{11}$	479.228655	479.22874	-0.17741
$C_{29}H_{35}O_{11}$	479.2398884	479.23998	-0.191178
$C_{28}H_{35}N_2O_{10}$	479.2650404	479.26523	-0.395648
$C_{29}H_{39}N_2O_9$	480.0936186	480.09355	0.1428469

$C_{29}H_{22}N_1O_{11}$	480.1017244	480.10187	-0.303232
$C_{30}H_{26}N_1O_{10}$	480.1147478	480.11461	0.2869729
$C_{27}H_{30}N_1O_{12}$	480.130004	480.12991	0.1957384
$C_{28}H_{34}N_1O_{11}$	480.1511332	480.15111	0.0482763
$C_{29}H_{21}O_{12}$	480.159239	480.15918	0.1229128
$C_{30}H_{25}O_{11}$	480.1663894	480.16629	0.2069697
$C_{29}H_{25}N_2O_{10}$	480.1875186	480.18735	0.351071
$C_{27}H_{29}O_{13}$	480.2027748	480.20269	0.1765502
$C_{30}H_{29}N_2O_9$	480.223904	480.22386	0.0915821
$C_{28}H_{33}O_{12}$	481.0776342	481.07751	0.2581286
$C_{27}H_{33}N_2O_{11}$	481.1140196	481.11392	0.2069778
$C_{29}H_{37}O_{11}$	481.125253	481.12515	0.2140397
$C_{28}H_{37}N_2O_{10}$	481.1351488	481.13523	-0.168809
$C_{29}H_{24}N_1O_{11}$	481.1463822	481.14654	-0.328008
$C_{30}H_{28}N_1O_{10}$	481.150405	481.15028	0.2597522
$C_{27}H_{32}N_1O_{12}$	481.1616384	481.16157	0.1421142
$C_{29}H_{27}N_2O_{10}$	481.1715342	481.17116	0.7776435
$C_{30}H_{31}N_2O_9$	481.1827676	481.18284	-0.150504
$C_{27}H_{35}N_2O_{11}$	481.1867904	481.18674	0.1046993
$C_{28}H_{22}N_1O_{12}$	481.1866202	481.18674	-0.24901
$C_{29}H_{26}N_1O_{11}$	481.1980238	481.19794	0.1741069
$C_{30}H_{30}N_1O_{10}$	481.2079196	481.20775	0.3524046
$C_{29}H_{25}O_{12}$	481.219153	481.21901	0.2971201
$C_{28}H_{25}N_2O_{11}$	481.2231758	481.223	0.3652773
$C_{30}H_{29}O_{11}$	481.244305	481.24426	0.0934658
$C_{29}H_{29}N_2O_{10}$	482.0728832	482.07292	-0.076379

$C_{30}H_{33}N_2O_9$	482.1092686	482.10928	-0.023688
$C_{28}H_{24}N_1O_{12}$	482.1245248	482.12441	0.2380711
$C_{29}H_{28}N_1O_{11}$	482.1303978	482.13062	-0.460913
$C_{30}H_{32}N_1O_{10}$	482.145654	482.14561	0.091217
$C_{29}H_{27}O_{12}$	482.1537598	482.15375	0.0203622
$C_{28}H_{27}N_2O_{11}$	482.1609102	482.16078	0.2699926
$C_{30}H_{31}O_{11}$	482.1667832	482.16669	0.1932524
$C_{29}H_{31}N_2O_{10}$	482.1820394	482.18203	0.019453
$C_{30}H_{35}N_2O_9$	482.2184248	482.21845	-0.0523
$C_{29}H_{30}N_1O_{11}$	483.0568988	483.05698	-0.168138
$C_{30}H_{34}N_1O_{10}$	483.0932842	483.09313	0.3191514
$C_{28}H_{25}O_{13}$	483.1296696	483.1295	0.3510029
$C_{29}H_{29}O_{12}$	483.140903	483.14075	0.3166362
$C_{30}H_{33}O_{11}$	483.1449258	483.14499	-0.132921
$C_{29}H_{33}N_2O_{10}$	483.166055	483.16593	0.2586686
$C_{30}H_{37}N_2O_9$	483.1772884	483.17717	0.245003
$C_{28}H_{28}N_1O_{12}$	483.1984176	483.19852	-0.211963
$C_{29}H_{32}N_1O_{11}$	483.2024404	483.20232	0.2491293
$C_{30}H_{36}N_1O_{10}$	483.2136738	483.21358	0.1940754
$C_{28}H_{27}O_{13}$	483.2235696	483.22348	0.1853798
$C_{29}H_{31}O_{12}$	484.0885332	484.08833	0.4197164
$C_{30}H_{35}O_{11}$	484.1037894	484.10413	-0.70361
$C_{29}H_{35}N_2O_{10}$	484.1249186	484.12483	0.1829691
$C_{28}H_{30}N_1O_{12}$	484.1330244	484.13304	-0.032186
$C_{29}H_{34}N_1O_{11}$	484.1401748	484.14016	0.0305281
$C_{30}H_{38}N_1O_{10}$	484.161304	484.16127	0.070183

$C_{28}H_{29}O_{13}$	484.1765602	484.17648	0.1656005
$C_{29}H_{33}O_{12}$	484.1976894	484.19762	0.1432884
$C_{28}H_{33}N_2O_{11}$	484.2340748	484.23404	0.0718246
$C_{30}H_{37}O_{11}$	485.1089342	485.10879	0.2972114
$C_{29}H_{37}N_2O_{10}$	485.1201676	485.11984	0.6752552
$C_{30}H_{24}N_1O_{11}$	485.1354238	485.13508	0.7086267
$C_{28}H_{32}N_1O_{12}$	485.133916	485.13508	-2.399379
$C_{29}H_{36}N_1O_{11}$	485.1453196	485.14527	0.102196
$C_{30}H_{27}N_2O_{10}$	485.156553	485.15651	0.0885898
$C_{28}H_{31}O_{13}$	485.1583389	485.1594	-2.187166
$C_{29}H_{35}O_{12}$	485.1646588	485.16442	0.4922405
$C_{28}H_{35}N_2O_{11}$	485.1718092	485.17157	0.4929798
$C_{29}H_{22}N_1O_{12}$	485.181705	485.18153	0.3606482
$C_{30}H_{26}N_1O_{11}$	485.1929384	485.19284	0.2027645
$C_{28}H_{34}N_1O_{12}$	485.2010442	485.20116	-0.238627
$C_{29}H_{38}N_1O_{11}$	485.2180904	485.21794	0.3099223
$C_{30}H_{25}O_{12}$	485.2293238	485.22932	0.0077899
$C_{30}H_{29}N_2O_{10}$	486.1041832	486.10415	0.0682568
$C_{29}H_{41}N_2O_{10}$	486.1194394	486.11925	0.3895748
$C_{29}H_{24}N_1O_{12}$	486.1405686	486.14043	0.2850614
$C_{30}H_{28}N_1O_{11}$	486.1486744	486.14859	0.1736459
$C_{30}H_{27}O_{12}$	486.1558248	486.15579	0.0715406
$C_{29}H_{27}N_2O_{11}$	486.176954	486.17687	0.1727353
$C_{30}H_{31}N_2O_{10}$	486.1850598	486.18499	0.1436031
$C_{29}H_{26}N_1O_{12}$	486.1922102	486.19223	-0.040766
$C_{30}H_{30}N_1O_{11}$	486.2133394	486.2132	0.2866641

$C_{29}H_{25}O_{13}$	487.0881988	487.08812	0.1617364
$C_{30}H_{29}O_{12}$	487.103455	487.10357	-0.236131
$C_{29}H_{28}N_1O_{12}$	487.1146884	487.1144	0.5920164
$C_{30}H_{32}N_1O_{11}$	487.1245842	487.12462	-0.073534
$C_{29}H_{27}O_{13}$	487.1358176	487.13583	-0.025496
$C_{30}H_{31}O_{12}$	487.1398404	487.13986	-0.040276
$C_{29}H_{31}N_2O_{11}$	487.1510738	487.15108	-0.012768
$C_{30}H_{35}N_2O_{10}$	487.1609696	487.16104	-0.144552
$C_{29}H_{30}N_1O_{12}$	487.172203	487.17236	-0.322309
$C_{30}H_{34}N_1O_{11}$	487.1762258	487.17658	-0.727088
$C_{29}H_{29}O_{13}$	487.1803088	487.18042	-0.228216
$C_{30}H_{33}O_{12}$	487.1874592	487.18738	0.1625245
$C_{29}H_{33}N_2O_{11}$	487.197355	487.19746	-0.21556
$C_{30}H_{37}N_2O_{10}$	487.2085884	487.20873	-0.290677
$C_{29}H_{32}N_1O_{12}$	487.2337404	487.23376	-0.040268
$C_{29}H_{31}O_{13}$	487.2449738	487.24498	-0.012766
$C_{30}H_{35}O_{12}$	487.291255	487.2912	0.1128276
$C_{29}H_{35}N_2O_{11}$	488.098704	488.09859	0.2335181
$C_{29}H_{34}N_1O_{12}$	488.1198332	488.11982	0.0270014
$C_{29}H_{37}N_2O_{11}$	488.1350894	488.13512	-0.062729
$C_{30}H_{27}N_2O_{11}$	488.1562186	488.15612	0.2019433
$C_{30}H_{26}N_1O_{12}$	488.1643244	488.1642	0.2548685
$C_{30}H_{28}N_1O_{12}$	488.1714748	488.1714	0.1531837
$C_{30}H_{30}N_1O_{12}$	488.192604	488.19247	0.2744407
$C_{30}H_{32}N_1O_{12}$	488.2007098	488.20049	0.4502609
$C_{30}H_{31}O_{13}$	488.2078602	488.20776	0.2051993

$C_{30}H_{35}N_2O_{11}$	488.2289894	488.2288	0.3878916
$C_{30}H_{34}N_1O_{12}$	489.1038488	489.10385	-0.002495
$C_{30}H_{37}N_2O_{11}$	489.119105	489.11916	-0.112488
$C_{30}H_{36}N_1O_{12}$	489.1303384	489.13023	0.2215767
$C_{30}H_{35}O_{13}$	489.1288306	489.13023	-2.861046
$C_7H_{13}O_4$	489.1402342	489.14023	0.0085454
$C_9H_7O_3$	489.1514676	489.15131	0.3221495
$C_8H_5O_4$	489.1554904	489.15546	0.0621068
$C_8H_7O_4$	489.1667238	489.16656	0.3348141
$C_8H_9O_4$	489.165216	489.16656	-2.747579
$C_7H_9O_5$	489.1766196	489.17652	0.2035664
$C_8H_{13}O_4$	489.187853	489.18769	0.3331642
$C_{10}H_7O_3$	489.2031092	489.20299	0.2436205
$C_{10}H_9O_3$	489.2016014	489.20299	-2.838544
$C_9H_7O_4$	489.213005	489.21294	0.1328254
$C_{10}H_{11}O_3$	489.2242384	489.22409	0.3032963
$C_9H_{10}N_1O_3$	490.0779686	490.078	-0.064112
$C_8H_5O_5$	490.114354	490.11433	0.0489272
$C_9H_9O_4$	490.1354832	490.13564	-0.319953
$C_{10}H_{13}O_3$	490.1507394	490.15071	0.0599405
$C_9H_{11}O_4$	490.1718686	490.17186	0.0175039
$C_8H_{10}N_1O_4$	490.1799744	490.17996	0.0294131
$C_8H_9O_5$	490.1871248	490.18715	-0.05145
$C_9H_{13}O_4$	490.208254	490.20818	0.1509152
$C_7H_8N_1O_5$	490.2446394	490.24459	0.100725
$C_8H_{11}O_5$	491.0831134	491.08315	-0.07457

$C_9H_{15}O_4$	491.0983696	491.0982	0.3453074
$C_{11}H_{10}N_1O_2$	491.109603	491.10936	0.494757
$C_7H_9O_6$	491.1194988	491.11927	0.4658335
$C_{11}H_9O_3$	491.134755	491.13462	0.2748327
$C_{10}H_7O_4$	491.1459884	491.1458	0.3835517
$C_{11}H_{11}O_3$	491.1558842	491.15569	0.3953529
$C_{10}H_9O_4$	491.1671176	491.16701	0.2190291
$C_{10}H_{12}N_1O_3$	491.1711404	491.171	0.2858065
$C_9H_7O_5$	491.1823738	491.18217	0.4148762
$C_{10}H_{11}O_4$	491.1922696	491.19218	0.1823724
$C_9H_9O_5$	491.203503	491.20331	0.3928716
$C_{10}H_{13}O_4$	491.228655	491.22845	0.41728
$C_9H_{12}N_1O_4$	491.2650404	491.26478	0.5300192
$C_8H_7O_6$	492.0936186	492.09368	-0.124814
$C_9H_{11}O_5$	492.1147478	492.11483	-0.167075
$C_{10}H_{15}O_4$	492.130004	492.13002	-0.032553
$C_8H_{10}N_1O_5$	492.1511332	492.15109	0.0877371
$C_{12}H_{10}N_1O_2$	492.1663894	492.16638	0.0190584
$C_8H_9O_6$	492.176115	492.17469	2.8952642
$C_9H_{13}O_5$	492.1875186	492.18751	0.0174322
$C_{10}H_{17}O_4$	492.2027748	492.20274	0.0706617
$C_{11}H_8N_1O_3$	492.223904	492.22389	0.0284015
$C_{11}H_7O_4$	493.0776342	493.07772	-0.17405
$C_8H_{11}O_6$	493.0888676	493.08892	-0.10631
$C_{12}H_{11}O_3$	493.1140196	493.114	0.0397066
$C_9H_{15}O_5$	493.125253	493.12516	0.1885523

$C_{10}H_{19}O_4$	493.1351488	493.13509	0.1191963
$C_{11}H_{10}N_1O_3$	493.150405	493.15031	0.1925982
$C_{10}H_5O_5$	493.1616384	493.16175	-0.226336
$C_{11}H_9O_4$	493.1715342	493.17148	0.1098602
$C_8H_{13}O_6$	493.1827676	493.1828	-0.065736
$C_{12}H_{13}O_3$	493.1867904	493.18674	0.1021518
$C_9H_{17}O_5$	493.1980238	493.19782	0.4131807
$C_{10}H_8N_1O_4$	493.2079196	493.20791	0.0194237
$C_{11}H_{12}N_1O_3$	493.219153	493.21922	-0.135883
$C_{10}H_7O_5$	493.244305	493.24417	0.2736573
$C_{11}H_{11}O_4$	493.2555384	493.25545	0.1791767
$C_{12}H_{15}O_3$	494.1092686	494.10908	0.3816563
$C_{10}H_{10}N_1O_4$	494.1173744	494.1173	0.1506073
$C_{11}H_{14}N_1O_3$	494.1303978	494.13033	0.1371701
$C_9H_5O_6$	494.145654	494.14551	0.2913714
$C_{10}H_9O_5$	494.1537598	494.15376	-0.000369
$C_{11}H_{13}O_4$	494.1667832	494.16685	-0.135218
$C_{12}H_{17}O_3$	494.1820394	494.18194	0.2010998
$C_{10}H_{12}N_1O_4$	494.2031686	494.20326	-0.184985
$C_{11}H_{16}N_1O_3$	494.2184248	494.2182	0.4548189
$C_9H_7O_6$	495.0932842	495.09328	0.0084427
$C_{10}H_{11}O_5$	495.1144134	495.11408	0.6733391
$C_{11}H_{15}O_4$	495.118266	495.11839	-0.250486
$C_{10}H_{14}N_1O_4$	495.1296696	495.12976	-0.182619
$C_9H_9O_6$	495.140903	495.141	-0.195944
$C_{10}H_{13}O_5$	495.1507988	495.15071	0.1792987

$C_9H_{13}N_2O_4$	495.1620322	495.16216	-0.258138
$C_{11}H_{17}O_4$	495.166055	495.16618	-0.252481
$C_{12}H_8N_1O_3$	495.1772884	495.17736	-0.144635
$C_9H_{12}N_1O_5$	495.1871842	495.18718	0.0084411
$C_{13}H_{12}N_1O_2$	495.2024404	495.20262	-0.362721
$C_{10}H_{16}N_1O_4$	495.2136738	495.21377	-0.1943
$C_{11}H_7N_2O_3$	495.2235696	495.22365	-0.162392
$C_9H_{11}O_6$	495.234803	495.23494	-0.276677
$C_{13}H_{11}O_3$	495.259955	495.26001	-0.111093
$C_{10}H_{15}O_5$	495.2711884	495.27145	-0.528236
$C_9H_{15}N_2O_4$	496.0885332	496.0886	-0.134694
$C_{11}H_{19}O_4$	496.1249186	496.12487	0.0979187
$C_{11}H_6N_1O_4$	496.1330244	496.13308	-0.112031
$C_{12}H_{10}N_1O_3$	496.1460478	496.14612	-0.145562
$C_{13}H_{14}N_1O_2$	496.161304	496.16122	0.1692593
$C_{12}H_9O_4$	496.1694098	496.16917	0.4833383
$C_9H_{13}O_6$	496.1824332	496.18257	-0.275746
$C_{13}H_{13}O_3$	496.1976894	496.19758	0.2204361
$C_{10}H_{17}O_5$	496.2340748	496.23407	0.0096323
$C_{11}H_{21}O_4$	497.1089342	497.10885	0.1693389
$C_{12}H_{12}N_1O_3$	497.1201676	497.12025	-0.165795
$C_{11}H_7O_5$	497.1282734	497.12809	0.3689545
$C_{12}H_{11}O_4$	497.1453196	497.14524	0.1600737
$C_{11}H_{11}N_2O_3$	497.156553	497.15649	0.1266802
$C_9H_{15}O_6$	497.1776822	497.17802	-0.679476
$C_{13}H_{15}O_3$	497.181705	497.18168	0.050243

$C_{11}H_{10}N_1O_4$	497.1929384	497.19278	0.3185482
$C_{12}H_{14}N_1O_3$	497.2010442	497.20124	-0.393769
$C_{10}H_5O_6$	497.2180904	497.21806	0.0610997
$C_{11}H_9O_5$	497.2293238	497.22897	0.7115025
$C_{12}H_{13}O_4$	497.3119904	497.3118	0.3828178
$C_{11}H_{13}N_2O_3$	498.1041832	498.10442	-0.475443
$C_{10}H_8N_1O_5$	498.1194394	498.11945	-0.02132
$C_{11}H_{12}N_1O_4$	498.1405686	498.14068	-0.223672
$C_{12}H_{16}N_1O_3$	498.1558248	498.15608	-0.51233
$C_{10}H_7O_6$	498.176954	498.17704	-0.17267
$C_{11}H_{11}O_5$	498.1922102	498.19246	-0.501453
$C_{12}H_{15}O_4$	498.1980832	498.19807	0.0264551
$C_{11}H_{15}N_2O_3$	498.2019358	498.2024	-0.931791
$C_{10}H_{10}N_1O_5$	498.2133394	498.21344	-0.201962
$C_{11}H_{14}N_1O_4$	498.2497248	498.24983	-0.211179
$C_{10}H_9O_6$	499.0881988	499.0882	-0.002445
$C_{11}H_{13}O_5$	499.1245842	499.12452	0.1285849
$C_{10}H_{13}N_2O_4$	499.1358176	499.13576	0.1153592
$C_{12}H_{17}O_4$	499.1398404	499.14005	-0.419963
$C_{13}H_{21}O_3$	499.1439234	499.1437	0.4476018
$C_{10}H_{12}N_1O_5$	499.1510738	499.15104	0.0676747
$C_{14}H_{12}N_1O_2$	499.1609696	499.16081	0.3196963
$C_{11}H_{16}N_1O_4$	499.172203	499.17211	0.1862682
$C_{10}H_{11}O_6$	499.1874592	499.18716	0.5993338
$C_9H_{11}N_2O_5$	499.197355	499.19725	0.2102974
$C_{14}H_{11}O_3$	499.2085884	499.20844	0.2972303

$C_{11}H_{15}O_5$	500.1198332	500.11984	-0.013637
$C_{10}H_{15}N_2O_4$	500.1350894	500.13508	0.0187547
$C_{12}H_{19}O_4$	500.1562186	500.15617	0.0971295
$C_{14}H_{27}O_2$	500.1643244	500.16434	-0.031154
$C_{12}H_6N_1O_4$	500.1714748	500.17134	0.2694674
$C_{13}H_{10}N_1O_3$	500.192604	500.19254	0.1279105
$C_{10}H_{14}N_1O_5$	500.2289894	500.22889	0.1986688
$C_{14}H_{14}N_1O_2$	501.1038488	501.10371	0.2769484
$C_{11}H_{18}N_1O_4$	501.119105	501.11906	0.0897589
$C_9H_9O_7$	501.1303384	501.13038	-0.083052
$C_{13}H_9O_4$	501.1402342	501.14028	-0.091432
$C_{10}H_{13}O_6$	501.1514676	501.15166	-0.383956
$C_{14}H_{13}O_3$	501.1554904	501.15567	-0.358412
$C_{11}H_{17}O_5$	501.1667238	501.16657	0.3068438
$C_{10}H_{17}N_2O_4$	501.1766196	501.17666	-0.08065
$C_{12}H_{21}O_4$	501.187853	501.1879	-0.093817
$C_{11}H_{21}N_2O_3$	501.1959588	501.19611	-0.301643
$C_{12}H_8N_1O_4$	501.2031092	501.2031	0.0183157
$C_{13}H_{12}N_1O_3$	501.213005	501.21304	-0.069871
$C_{10}H_{16}N_1O_5$	501.2242384	501.22438	-0.282548
$C_{14}H_{16}N_1O_2$	501.2493904	501.24936	0.0606084
$C_{12}H_7O_5$	501.2606238	501.26059	0.0673899
$C_9H_{11}O_7$	502.114354	502.11418	0.3464946
$C_{13}H_{11}O_4$	502.1354832	502.13533	0.3050569
$C_{10}H_{15}O_6$	502.1507394	502.1506	0.2775659
$C_{14}H_{15}O_3$	502.1718686	502.17164	0.4551826

$C_{11}H_{19}O_5$	502.1799744	502.17966	0.6261056
$C_{12}H_{23}O_4$	502.1871248	502.18695	0.3480374
$C_{12}H_{10}N_1O_4$	502.208254	502.20812	0.2667816
$C_{13}H_{14}N_1O_3$	503.0983696	503.0984	-0.060466
$C_{12}H_9O_5$	503.1194988	503.11961	-0.221061
$C_{13}H_{13}O_4$	503.134755	503.13463	0.2484024
$C_{12}H_{13}N_2O_3$	503.1459884	503.1461	-0.221844
$C_{10}H_{17}O_6$	503.1558842	503.15581	0.1474293
$C_{14}H_{17}O_3$	503.1671176	503.16711	0.0150644
$C_{11}H_{21}O_5$	503.1711404	503.17115	-0.019119
$C_{12}H_{12}N_1O_4$	503.1823738	503.18227	0.2062471
$C_{13}H_{16}N_1O_3$	503.1922696	503.19225	0.0389114
$C_{11}H_7O_6$	503.203503	503.20351	-0.013951
$C_{12}H_{11}O_5$	503.2187592	503.21863	0.2567072
$C_{11}H_{11}N_2O_4$	503.228655	503.22867	-0.029847
$C_{13}H_{15}O_4$	503.2398884	503.23976	0.2551068
$C_{12}H_{15}N_2O_3$	504.0936186	504.09366	-0.082167
$C_{11}H_{10}N_1O_5$	504.130004	504.12998	0.0475669
$C_{12}H_{14}N_1O_4$	504.1511332	504.15119	-0.112704
$C_{13}H_{18}N_1O_3$	504.159239	504.15943	-0.378813
$C_{11}H_9O_6$	504.1663894	504.16637	0.0384395
$C_{12}H_{13}O_5$	504.1875186	504.18748	0.076519
$C_{11}H_{13}N_2O_4$	504.1956244	504.19548	0.2864319
$C_{13}H_{17}O_4$	504.2027748	504.20283	-0.10952
$C_{12}H_{17}N_2O_3$	504.223904	504.22372	0.3648774
$C_{11}H_{12}N_1O_5$	504.2602894	504.26024	0.0979254

$C_{15}H_{12}N_1O_2$	505.1140196	505.11403	-0.020629
$C_{12}H_{16}N_1O_4$	505.1351488	505.13492	0.4529083
$C_{11}H_{11}O_6$	505.150405	505.15011	0.5839447
$C_{12}H_{15}O_5$	505.1616384	505.16126	0.7490274
$C_{11}H_{15}N_2O_4$	505.1715342	505.17124	0.5823367
$C_9H_{19}O_7$	505.1697442	505.17124	-2.96095
$C_{13}H_{19}O_4$	505.1867904	505.18667	0.2382879
$C_{15}H_{27}O_2$	505.1980238	505.19779	0.462749
$C_{10}H_{10}N_1O_6$	505.196516	505.19779	-2.521831
$C_{14}H_{10}N_1O_3$	505.2079196	505.20778	0.2762821
$C_{11}H_{14}N_1O_5$	505.219153	505.21894	0.4215594
$C_{12}H_{18}N_1O_4$	505.244305	505.24429	0.0296488
$C_{10}H_9O_7$	506.1092686	506.10924	0.0564698
$C_{11}H_{13}O_6$	506.1303978	506.13055	-0.300753
$C_{10}H_{13}N_2O_5$	506.145654	506.14565	0.0078632
$C_{15}H_{13}O_3$	506.1667832	506.16675	0.0655513
$C_{14}H_{13}N_2O_2$	506.1820394	506.18206	-0.040737
$C_{12}H_{17}O_5$	506.2031686	506.20316	0.0169495
$C_{11}H_{17}N_2O_4$	506.2184248	506.21851	-0.168346
$C_{13}H_{21}O_4$	506.239554	506.23948	0.1461362
$C_{12}H_{21}N_2O_3$	507.0932842	507.09318	0.2054452
$C_{15}H_{29}O_2$	507.1144134	507.11447	-0.111652
$C_{10}H_{12}N_1O_6$	507.1296696	507.12966	0.0188904
$C_{14}H_{12}N_1O_3$	507.140903	507.14092	-0.033561
$C_{11}H_{16}N_1O_5$	507.1507988	507.15075	0.0961842
$C_{15}H_{16}N_1O_2$	507.1620322	507.16169	0.6746954

$C_{12}H_{20}N_1O_4$	507.166055	507.16603	0.0492539
$C_{10}H_{11}O_7$	507.1772884	507.17731	-0.042628
$C_{14}H_{11}O_4$	507.1871842	507.18721	-0.050908
$C_{13}H_{11}N_2O_3$	507.1984176	507.19848	-0.123068
$C_{11}H_{15}O_6$	507.2024404	507.20251	-0.137263
$C_{15}H_{15}O_3$	507.2136738	507.21366	0.0271678
$C_{14}H_{15}N_2O_2$	507.2235696	507.22355	0.0386021
$C_{12}H_{19}O_5$	507.234803	507.23495	-0.289846
$C_{13}H_{23}O_4$	508.1249186	508.12477	0.2924082
$C_{12}H_{23}N_2O_3$	508.161304	508.16107	0.4604442
$C_9H_{10}N_1O_7$	508.1694098	508.16923	0.3538538
$C_{13}H_{10}N_1O_4$	508.1824332	508.18238	0.1046473
$C_{10}H_{14}N_1O_6$	508.1976894	508.19747	0.4316822
$C_{14}H_{14}N_1O_3$	508.2340748	508.23402	0.1077848
$C_{11}H_{18}N_1O_5$	509.0725488	509.0729	-0.689922
$C_{13}H_9O_5$	509.1089342	509.10897	-0.070358
$C_{10}H_{13}O_7$	509.1201676	509.12036	-0.377946
$C_{14}H_{13}O_4$	509.1453196	509.14535	-0.059747
$C_{13}H_{13}N_2O_3$	509.156553	509.15662	-0.13163
$C_{11}H_{17}O_6$	509.1646588	509.16473	-0.139802
$C_{15}H_{17}O_3$	509.1664488	509.16659	-0.277355
$C_{14}H_{17}N_2O_2$	509.1776822	509.17793	-0.486707
$C_{12}H_{21}O_5$	509.181705	509.18174	-0.068777
$C_{12}H_8N_1O_5$	509.1929384	509.19294	-0.003182
$C_{13}H_{12}N_1O_4$	509.2028342	509.20283	0.0082087
$C_{14}H_{16}N_1O_3$	509.2140676	509.21429	-0.436791

$C_{12}H_7O_6$	509.2180904	509.21813	-0.077806
$C_{13}H_{11}O_5$	509.2293238	509.22928	0.0859729
$C_{12}H_{11}N_2O_4$	509.2392196	509.239	0.431192
$C_{10}H_{15}O_7$	509.2868384	509.28684	-0.003181
$C_{14}H_{15}O_4$	510.1041832	510.10411	0.1434607
$C_{13}H_{15}N_2O_3$	510.1405686	510.14048	0.1736382
$C_{11}H_{19}O_6$	510.1486744	510.14875	-0.148157
$C_{15}H_{19}O_3$	510.176954	510.17679	0.3214177
$C_{12}H_{23}O_5$	510.1850598	510.18515	-0.176764
$C_{12}H_{10}N_1O_5$	510.2133394	510.21329	0.0967828
$C_{13}H_{14}N_1O_4$	511.0881988	511.08811	0.1737076
$C_{14}H_{18}N_1O_3$	511.1245842	511.1244	0.3603425
$C_{12}H_9O_6$	511.1358176	511.13564	0.3474221
$C_{13}H_{13}O_5$	511.1439234	511.1438	0.2414539
$C_{12}H_{13}N_2O_4$	511.1609696	511.16082	0.2926278
$C_{14}H_{17}O_4$	511.172203	511.17214	0.1232068
$C_{12}H_{12}N_1O_5$	511.197355	511.19728	0.1466751
$C_{13}H_{16}N_1O_4$	511.2085884	511.20822	0.7206059
$C_{14}H_{20}N_1O_3$	511.2337404	511.23388	-0.273104
$C_{11}H_7O_7$	512.1198332	512.1198	0.0647893
$C_{12}H_{11}O_6$	512.1350894	512.13528	-0.372207
$C_{11}H_{11}N_2O_5$	512.1562186	512.1561	0.2315307
$C_{13}H_{15}O_5$	512.1714748	512.1716	-0.244489
$C_{12}H_{15}N_2O_4$	512.192604	512.19262	-0.031277
$C_{14}H_{19}O_4$	512.2289894	512.22907	-0.157391
$C_{13}H_{19}N_2O_3$	513.1038488	513.10373	0.2314929

$C_{11}H_{10}N_1O_6$	513.1402342	513.14011	0.2419999
$C_{12}H_{14}N_1O_5$	513.1514676	513.15141	0.1122084
$C_{16}H_{14}N_1O_2$	513.1667238	513.16646	0.5140238
$C_{13}H_{18}N_1O_4$	513.165216	513.16646	-2.42421
$C_{10}H_5O_8$	513.1766196	513.17654	0.1550731
$C_{11}H_9O_7$	513.187853	513.18784	0.0252927
$C_{12}H_{13}O_6$	513.213005	513.21295	0.1071288
$C_{11}H_{13}N_2O_5$	513.2242384	513.22422	0.0358126
$C_{16}H_{13}O_3$	514.1507394	514.15055	0.3683354
$C_{13}H_{17}O_5$	514.1718686	514.17172	0.2889693
$C_{12}H_{17}N_2O_4$	514.1871248	514.18682	0.5927412
$C_{14}H_{21}O_4$	514.208254	514.20825	0.0077399
$C_{13}H_{21}N_2O_3$	514.2446394	514.24452	0.2321461
$C_{16}H_{29}O_2$	515.0983696	515.0985	-0.253195
$C_{11}H_{12}N_1O_6$	515.1194988	515.11949	0.0170444
$C_{15}H_{12}N_1O_3$	515.1307322	515.13033	0.7807337
$C_{12}H_{16}N_1O_5$	515.134755	515.13475	0.0096672
$C_{16}H_{16}N_1O_2$	515.1459884	515.14597	0.035679
$C_{13}H_{20}N_1O_4$	515.1558842	515.15593	-0.088944
$C_{11}H_{11}O_7$	515.1671176	515.16724	-0.237632
$C_{15}H_{11}O_4$	515.1711404	515.17117	-0.057496
$C_{14}H_{11}N_2O_3$	515.1823738	515.18235	0.0461582
$C_{12}H_{15}O_6$	515.180866	515.18235	-2.880581
$C_{11}H_{15}N_2O_5$	515.1922696	515.1923	-0.059046
$C_{16}H_{15}O_3$	515.203503	515.2036	-0.188314
$C_{13}H_{19}O_5$	515.2187592	515.21904	-0.54505

$C_{12}H_{19}N_2O_4$	515.228655	515.22883	-0.339694
$C_{14}H_{23}O_4$	515.2398884	515.23997	-0.158412
$C_{13}H_{23}N_2O_3$	516.0936186	516.09334	0.5397856
$C_{16}H_{31}O_2$	516.1147478	516.11466	0.1700783
$C_{14}H_{10}N_1O_4$	516.130004	516.12985	0.2983355
$C_{11}H_{14}N_1O_6$	516.1511332	516.15113	0.0061608
$C_{15}H_{14}N_1O_3$	516.1663894	516.16639	-0.001201
$C_{12}H_{18}N_1O_5$	516.1875186	516.18745	0.1328585
$C_{16}H_{18}N_1O_2$	516.1956244	516.19527	0.6865957
$C_{14}H_9O_5$	516.2027748	516.20262	0.2998432
$C_{11}H_{13}O_7$	516.223904	516.22388	0.0464525
$C_{15}H_{13}O_4$	517.1140196	517.11383	0.3666114
$C_{14}H_{13}N_2O_3$	517.1351488	517.13509	0.1136645
$C_{12}H_{17}O_6$	517.150405	517.15029	0.2223336
$C_{11}H_{17}N_2O_5$	517.1616384	517.16171	-0.138487
$C_{16}H_{17}O_3$	517.1715342	517.17136	0.3367933
$C_{15}H_{17}N_2O_2$	517.1827676	517.18293	-0.314048
$C_{13}H_{21}O_5$	517.1867904	517.18672	0.1360822
$C_{14}H_{25}O_4$	517.1980238	517.19799	0.0653133
$C_{10}H_{12}N_1O_7$	517.2079196	517.20768	0.4632178
$C_{14}H_{12}N_1O_4$	517.219153	517.21904	0.2184372
$C_{11}H_{16}N_1O_6$	518.1092686	518.10934	-0.137848
$C_{15}H_{16}N_1O_3$	518.1303978	518.13065	-0.486789
$C_{13}H_7O_6$	518.145654	518.14566	-0.011619
$C_{10}H_{11}O_8$	518.1667832	518.16684	-0.109656
$C_{14}H_{11}O_5$	518.1820394	518.18212	-0.155583

$C_{13}H_{11}N_2O_4$	518.2031686	518.20335	-0.350095
$C_{11}H_{15}O_7$	518.2184248	518.21877	-0.666167
$C_{15}H_{15}O_4$	518.239554	518.23964	-0.165985
$C_{14}H_{15}N_2O_3$	519.0932842	519.09316	0.2392246
$C_{12}H_{19}O_6$	519.1144134	519.11435	0.1220924
$C_{15}H_{19}N_2O_2$	519.1296696	519.12964	0.0569798
$C_{13}H_{23}O_5$	519.140903	519.14076	0.2754164
$C_{13}H_{10}N_1O_5$	519.1507988	519.15078	0.0361743
$C_{14}H_{14}N_1O_4$	519.1620322	519.1623	-0.51587
$C_{15}H_{18}N_1O_3$	519.166055	519.16603	0.0481154
$C_{13}H_9O_6$	519.1772884	519.17725	0.0739245
$C_{10}H_{13}O_8$	519.1871842	519.18704	0.2777031
$C_{14}H_{13}O_5$	519.1984176	519.19864	-0.428391
$C_{13}H_{13}N_2O_4$	519.2024404	519.20262	-0.345954
$C_{11}H_{17}O_7$	519.2136738	519.21351	0.3154383
$C_{15}H_{17}O_4$	519.2235696	519.22333	0.4614195
$C_{14}H_{17}N_2O_3$	519.234803	519.23468	0.2368483
$C_{12}H_{21}O_6$	520.1249186	520.12487	0.0934004
$C_{13}H_{12}N_1O_5$	520.1460478	520.14619	-0.273423
$C_{14}H_{16}N_1O_4$	520.161304	520.16116	0.2767986
$C_{15}H_{20}N_1O_3$	520.1824332	520.1823	0.2560254
$C_{13}H_{11}O_6$	520.1976894	520.19751	0.3448303
$C_{12}H_{11}N_2O_5$	520.2188186	520.21849	0.6316186
$C_{10}H_{15}O_8$	520.2340748	520.23412	-0.086923
$C_{14}H_{15}O_5$	520.255204	520.25482	0.7380607
$C_{13}H_{15}N_2O_4$	521.1089342	521.10905	-0.222257

$C_{15}H_{19}O_4$	521.1300634	521.13017	-0.204594
$C_{14}H_{19}N_2O_3$	521.1453196	521.14538	-0.115937
$C_{12}H_{10}N_1O_6$	521.156553	521.15667	-0.224539
$C_{13}H_{14}N_1O_5$	521.1664488	521.16621	0.4581644
$C_{14}H_{18}N_1O_4$	521.1776822	521.17781	-0.245252
$C_{15}H_{22}N_1O_3$	521.181705	521.18177	-0.124755
$C_{12}H_9O_7$	521.1929384	521.19307	-0.252536
$C_{13}H_{13}O_6$	521.2028342	521.20284	-0.011167
$C_{12}H_{13}N_2O_5$	521.2140676	521.21435	-0.54185
$C_{14}H_{17}O_5$	521.2180904	521.21806	0.0582864
$C_{13}H_{17}N_2O_4$	521.2293238	521.22918	0.2758477
$C_{15}H_{21}O_4$	521.2392196	521.23928	-0.115916
$C_{14}H_{21}N_2O_3$	521.250453	521.25038	0.1400093
$C_{11}H_8N_1O_7$	522.1041832	522.10408	0.1976232
$C_{12}H_{12}N_1O_6$	522.1405686	522.14055	0.0355841
$C_{16}H_{12}N_1O_3$	522.1486744	522.14847	0.3914933
$C_{13}H_{16}N_1O_5$	522.1616978	522.16202	-0.617089
$C_{17}H_{16}N_1O_2$	522.176954	522.17688	0.1416759
$C_{14}H_{20}N_1O_4$	522.1850598	522.18536	-0.574858
$C_{12}H_{11}O_7$	522.1980832	522.19808	0.0060895
$C_{16}H_{11}O_4$	522.2133394	522.21337	-0.058635
$C_{13}H_{15}O_6$	523.0881988	523.08779	0.7814741
$C_{12}H_{15}N_2O_5$	523.1245842	523.12433	0.4858879
$C_{17}H_{15}O_3$	523.1358176	523.13559	0.4350302
$C_{14}H_{19}O_5$	523.1609696	523.16063	0.6490926
$C_{13}H_{19}N_2O_4$	523.172203	523.17203	0.3306366

$C_{15}H_{23}O_4$	523.1933322	523.19314	0.367321
$C_{14}H_{23}N_2O_3$	523.197355	523.19713	0.4300096
$C_{17}H_{31}O_2$	523.2085884	523.20831	0.5320629
$C_{11}H_{10}N_1O_7$	523.2337404	523.23383	-0.171281
$C_{15}H_{10}N_1O_4$	523.2449738	523.24461	0.6952382
$C_{12}H_{14}N_1O_6$	524.0834478	524.08323	0.4155443
$C_{16}H_{14}N_1O_3$	524.1198332	524.11983	0.0060671
$C_{13}H_{18}N_1O_5$	524.1562186	524.15621	0.016369
$C_{17}H_{18}N_1O_2$	524.1643244	524.16426	0.122896
$C_{14}H_{22}N_1O_4$	524.1773478	524.17717	0.3391598
$C_{11}H_9O_8$	524.192604	524.19258	0.0457464
$C_{15}H_9O_5$	524.2289894	524.22894	0.0941953
$C_{12}H_{13}O_7$	525.1038488	525.10385	-0.002324
$C_{11}H_{13}N_2O_6$	525.1402342	525.14021	0.0460447
$C_{16}H_{13}O_4$	525.1514676	525.15142	0.0906022
$C_{15}H_{13}N_2O_3$	525.1595734	525.15954	0.0636334
$C_{13}H_{17}O_6$	525.1766196	525.17662	-0.0008
$C_{12}H_{17}N_2O_5$	525.187853	525.18789	-0.070489
$C_{17}H_{17}O_3$	525.213005	525.21287	0.2570003
$C_{16}H_{17}N_2O_2$	525.2242384	525.22414	0.1873103
$C_{14}H_{21}O_5$	526.0990978	526.09942	-0.61247
$C_{13}H_{21}N_2O_4$	526.1354832	526.13552	-0.069982
$C_{15}H_{25}O_4$	526.143589	526.14294	1.2335372
$C_{14}H_{25}N_2O_3$	526.1507394	526.15056	0.3409287
$C_{16}H_{29}O_3$	526.1718686	526.17175	0.2253634
$C_{17}H_{33}O_2$	526.1799744	526.17974	0.4455086

$C_{11}H_{12}N_1O_7$	526.208254	526.20812	0.2546138
$C_{15}H_{12}N_1O_4$	526.2446394	526.24446	0.3408679
$C_{12}H_{16}N_1O_6$	527.1194988	527.11952	-0.040257
$C_{16}H_{16}N_1O_3$	527.1558842	527.15579	0.1786566
$C_{13}H_{20}N_1O_5$	527.1671176	527.16702	0.1851024
$C_{11}H_{11}O_8$	527.1752234	527.17515	0.1392662
$C_{15}H_{11}O_5$	527.1823738	527.1823	0.1399514
$C_{14}H_{11}N_2O_4$	527.180866	527.1823	-2.720167
$C_{12}H_{15}O_7$	527.1922696	527.19212	0.2837293
$C_{11}H_{15}N_2O_6$	527.203503	527.20337	0.2522364
$C_{16}H_{15}O_4$	527.228655	527.22862	0.0663467
$C_{15}H_{15}N_2O_3$	527.2398884	527.2399	-0.022039
$C_{13}H_{19}O_6$	528.1147478	528.11492	-0.326104
$C_{12}H_{19}N_2O_5$	528.130004	528.13002	-0.030334
$C_{17}H_{19}O_3$	528.1511332	528.15117	-0.069715
$C_{16}H_{19}N_2O_2$	528.1663894	528.16627	0.2260271
$C_{14}H_{23}O_5$	528.1875186	528.18757	-0.097352
$C_{14}H_{10}N_1O_5$	528.1956244	528.19563	-0.010569
$C_{11}H_{14}N_1O_7$	528.223904	528.22375	0.291505
$C_{15}H_{14}N_1O_4$	529.1351488	529.13485	0.5646571
$C_{12}H_{18}N_1O_6$	529.1463822	529.14598	0.7600541
$C_{16}H_{18}N_1O_3$	529.1616384	529.16158	0.1103253
$C_{14}H_9O_6$	529.1601306	529.16158	-2.739095
$C_{11}H_{13}O_8$	529.1715342	529.17139	0.2724634
$C_{15}H_{13}O_5$	529.1827676	529.18254	0.4300592
$C_{14}H_{13}N_2O_4$	529.1908734	529.1908	0.1387358

$C_{12}H_{17}O_7$	529.196516	529.19755	-1.953944
$C_{11}H_{17}N_2O_6$	529.2079196	529.20781	0.207064
$C_{16}H_{17}O_4$	529.244305	529.24409	0.4062016
$C_{15}H_{17}N_2O_3$	530.1303978	530.13041	-0.023051
$C_{13}H_{21}O_6$	530.1667832	530.16679	-0.012864
$C_{14}H_{25}O_5$	530.174889	530.17499	-0.19047
$C_{14}H_{12}N_1O_5$	530.1820394	530.18205	-0.020031
$C_{11}H_{16}N_1O_7$	530.2031686	530.20299	0.3368141
$C_{15}H_{16}N_1O_4$	530.239554	530.23921	0.6487255
$C_{16}H_{20}N_1O_3$	531.1144134	531.11452	-0.200748
$C_{14}H_{11}O_6$	531.1296696	531.12954	0.2439704
$C_{13}H_{11}N_2O_5$	531.140903	531.14098	-0.145009
$C_{11}H_{15}O_8$	531.1507988	531.15095	-0.284703
$C_{15}H_{15}O_5$	531.166055	531.16617	-0.216543
$C_{14}H_{15}N_2O_4$	531.1772884	531.17721	0.1475588
$C_{12}H_{19}O_7$	531.1871842	531.18725	-0.123911
$C_{16}H_{19}O_4$	531.1984176	531.19852	-0.192809
$C_{15}H_{19}N_2O_3$	531.2136738	531.21372	-0.087008
$C_{13}H_{23}O_6$	531.2235696	531.22368	-0.20786
$C_{13}H_{10}N_1O_6$	531.234803	531.2349	-0.182631
$C_{14}H_{14}N_1O_5$	531.2711884	531.27154	-0.661847
$C_{15}H_{18}N_1O_4$	532.1249186	532.1248	0.2228422
$C_{13}H_9O_7$	532.161304	532.16123	0.1390178
$C_{14}H_{13}O_6$	532.1824332	532.18241	0.0435563
$C_{13}H_{13}N_2O_5$	532.1976894	532.19752	0.318265
$C_{11}H_{17}O_8$	532.2188186	532.21862	0.373117

$C_{15}H_{17}O_5$	533.1089342	533.10873	0.3829985
$C_{14}H_{17}N_2O_4$	533.1300634	533.12986	0.3814827
$C_{12}H_{21}O_7$	533.1453196	533.14532	-0.000788
$C_{16}H_{21}O_4$	533.1664488	533.16628	0.3165614
$C_{15}H_{21}N_2O_3$	533.1776822	533.17767	0.022844
$C_{13}H_{12}N_1O_6$	533.181705	533.18175	-0.084437
$C_{17}H_{12}N_1O_3$	533.1929384	533.19292	0.0344714
$C_{14}H_{16}N_1O_5$	533.2028342	533.20265	0.3454218
$C_{15}H_{20}N_1O_4$	533.2140676	533.21413	-0.117064
$C_{13}H_{11}O_7$	533.2293238	533.22914	0.3446545
$C_{12}H_{11}N_2O_6$	533.2392196	533.23888	0.6368247
$C_{14}H_{15}O_6$	533.250453	533.25003	0.7932106
$C_{13}H_{15}N_2O_5$	534.1041832	534.10419	-0.012769
$C_{18}H_{15}O_3$	534.1405686	534.1406	-0.058824
$C_{15}H_{19}O_5$	534.1616978	534.16203	-0.621947
$C_{14}H_{19}N_2O_4$	534.176954	534.17705	-0.179753
$C_{16}H_{23}O_4$	534.1980832	534.1982	-0.218683
$C_{18}H_{31}O_2$	534.2133394	534.21343	-0.169633
$C_{12}H_{10}N_1O_7$	534.2344686	534.23459	-0.227279
$C_{13}H_{14}N_1O_6$	534.270854	534.27097	-0.217156
$C_{17}H_{14}N_1O_3$	535.1358176	535.13588	-0.116643
$C_{14}H_{18}N_1O_5$	535.1457134	535.14538	0.6229703
$C_{15}H_{22}N_1O_4$	535.1609696	535.16088	0.1673887
$C_{12}H_9O_8$	535.172203	535.17202	0.3419085
$C_{16}H_9O_5$	535.1820988	535.18195	0.2779986
$C_{13}H_{13}O_7$	535.197355	535.19749	-0.252281

$C_{12}H_{13}N_2O_6$	535.2085884	535.20872	-0.245923
$C_{17}H_{13}O_4$	535.2184842	535.21808	0.7551681
$C_{16}H_{13}N_2O_3$	535.2297176	535.22936	0.6680868
$C_{14}H_{17}O_6$	536.1198332	536.11967	0.3043721
$C_{13}H_{17}N_2O_5$	536.1562186	536.15615	0.1279103
$C_{18}H_{17}O_3$	536.192604	536.1925	0.1939227
$C_{15}H_{21}O_5$	536.2137332	536.21381	-0.143264
$C_{14}H_{21}N_2O_4$	536.2289894	536.229	-0.019805
$C_{15}H_{25}N_2O_3$	537.1038488	537.10369	0.2956223
$C_{18}H_{33}O_2$	537.1402342	537.14032	-0.159772
$C_{12}H_{12}N_1O_7$	537.1514676	537.1515	-0.060356
$C_{16}H_{12}N_1O_4$	537.1766196	537.1767	-0.149709
$C_{13}H_{16}N_1O_6$	537.187853	537.18802	-0.310916
$C_{17}H_{16}N_1O_3$	537.2089822	537.20886	0.2274346
$C_{14}H_{20}N_1O_5$	537.213005	537.21307	-0.121032
$C_{18}H_{20}N_1O_2$	537.2242384	537.22442	-0.338071
$C_{12}H_{11}O_8$	537.2341342	537.2339	0.4358991
$C_{16}H_{11}O_5$	537.2453676	537.24504	0.6097398
$C_{15}H_{11}N_2O_4$	538.1354832	538.13536	0.2289013
$C_{13}H_{15}O_7$	538.1718686	538.17166	0.3875712
$C_{12}H_{15}N_2O_6$	538.208254	538.20819	0.1188757
$C_{17}H_{15}O_4$	538.2446394	538.24451	0.2403738
$C_{16}H_{15}N_2O_3$	539.1194988	539.11938	0.220322
$C_{14}H_{19}O_6$	539.1558842	539.15586	0.0448477
$C_{13}H_{19}N_2O_5$	539.1671176	539.16691	0.385001
$C_{18}H_{19}O_3$	539.1922696	539.192	0.4999699

$C_{15}H_{23}O_5$	539.203503	539.20325	0.4691733
$C_{14}H_{23}N_2O_4$	539.2398884	539.2398	0.1638972
$C_{16}H_{27}O_4$	540.1147478	540.11489	-0.263315
$C_{15}H_{27}N_2O_3$	540.1511332	540.15112	0.0244004
$C_{18}H_{35}O_2$	540.176115	540.17759	-2.730628
$C_{15}H_{10}N_1O_5$	540.1875186	540.18747	0.0899315
$C_{12}H_{14}N_1O_7$	540.223904	540.22379	0.2109864
$C_{16}H_{14}N_1O_4$	541.0987634	541.09865	0.2095364
$C_{13}H_{18}N_1O_6$	541.1351488	541.13497	0.3303794
$C_{17}H_{18}N_1O_3$	541.1463822	541.14669	-0.56883
$C_{14}H_{22}N_1O_5$	541.1715342	541.17149	0.0816375
$C_{15}H_9O_6$	541.1827676	541.18269	0.1433525
$C_{12}H_{13}O_8$	541.2079196	541.2078	0.22095
$C_{16}H_{13}O_5$	541.219153	541.21892	0.4304724
$C_{15}H_{13}N_2O_4$	541.244305	541.24431	-0.009275
$C_{13}H_{17}O_7$	542.1303978	542.1307	-0.557468
$C_{12}H_{17}N_2O_6$	542.145654	542.14556	0.1733481
$C_{17}H_{17}O_4$	542.1667832	542.16656	0.4116444
$C_{16}H_{17}N_2O_3$	542.2031686	542.20306	0.2002569
$C_{14}H_{21}O_6$	542.239554	542.23983	-0.509037
$C_{13}H_{21}N_2O_5$	543.1144134	543.11407	0.6322423
$C_{15}H_{25}O_5$	543.1296696	543.12974	-0.129656
$C_{16}H_{29}O_4$	543.1507988	543.15078	0.0345758
$C_{14}H_8N_1O_6$	543.1620322	543.16188	0.280174
$C_{15}H_{12}N_1O_5$	543.1772884	543.17726	0.052248
$C_{12}H_{16}N_1O_7$	543.1871842	543.18721	-0.047534

C ₁₆ H ₁₆ N ₁ O ₄	543.1984176	543.19849	-0.133322
C ₁₇ H ₂₀ N ₁ O ₃	543.234803	543.23467	0.2447927
C ₁₄ H ₇ O ₇	544.1249186	544.125	-0.149635
C ₁₅ H ₁₁ O ₆	544.1460478	544.14623	-0.334874
C ₁₄ H ₁₁ N ₂ O ₅	544.161304	544.1614	-0.176455
C ₁₂ H ₁₅ O ₈	544.1824332	544.18264	-0.380057
C ₁₁ H ₁₅ N ₂ O ₇	544.2188186	544.21891	-0.167984
C ₁₆ H ₁₅ O ₅	544.255204	544.25557	-0.672516
C ₁₅ H ₁₅ N ₂ O ₄	545.1089342	545.10898	-0.084057
C ₁₃ H ₁₉ O ₇	545.1300634	545.12998	0.1529541
C ₁₂ H ₁₉ N ₂ O ₆	545.1453196	545.14546	-0.257583
C ₁₇ H ₁₉ O ₄	545.156553	545.15649	0.1155263
C ₁₆ H ₁₉ N ₂ O ₃	545.1664488	545.16635	0.1811922
C ₁₄ H ₂₃ O ₆	545.1776822	545.17742	0.4809073
C ₁₅ H ₂₇ O ₅	545.1929384	545.19269	0.4555817
C ₁₆ H ₃₁ O ₄	545.2028342	545.20263	0.3745026
C ₁₄ H ₁₀ N ₁ O ₆	545.2140676	545.21388	0.3440482
C ₁₅ H ₁₄ N ₁ O ₅	545.2392196	545.23899	0.4210627
C ₁₆ H ₁₈ N ₁ O ₄	545.250453	545.25013	0.5923515
C ₁₇ H ₂₂ N ₁ O ₃	546.1405686	546.14048	0.1621925
C ₁₄ H ₉ O ₇	546.1616978	546.16169	0.0142447
C ₁₃ H ₉ N ₂ O ₆	546.176954	546.1768	0.2819231
C ₁₁ H ₁₃ O ₉	546.1980832	546.19782	0.4818397
C ₁₅ H ₁₃ O ₆	547.1245842	547.12445	0.2452456
C ₁₄ H ₁₃ N ₂ O ₅	547.1358176	547.13578	0.0686848
C ₁₂ H ₁₇ O ₈	547.1457134	547.14569	0.0427307

$C_{11}H_{17}N_2O_7$	547.1609696	547.16115	-0.329739
$C_{16}H_{17}O_5$	547.172203	547.17228	-0.14076
$C_{15}H_{17}N_2O_4$	547.1820988	547.18212	-0.038781
$C_{13}H_{21}O_7$	547.1933322	547.19299	0.6253364
$C_{17}H_{21}O_4$	547.2085884	547.2087	-0.203981
$C_{16}H_{21}N_2O_3$	547.2184842	547.21832	0.3000262
$C_{14}H_{25}O_6$	547.2297176	547.22983	-0.205435
$C_{14}H_{12}N_1O_6$	547.2548696	547.25467	0.3646928
$C_{15}H_{16}N_1O_5$	547.266103	547.26611	-0.012828
$C_{16}H_{20}N_1O_4$	548.1198332	548.11975	0.151755
$C_{14}H_{11}O_7$	548.1562186	548.15604	0.3257829
$C_{13}H_{11}N_2O_6$	548.1773478	548.17739	-0.077019
$C_{15}H_{15}O_6$	548.192604	548.19242	0.3356118
$C_{14}H_{15}N_2O_5$	548.2137332	548.21387	-0.249574
$C_{12}H_{19}O_8$	549.1402342	549.13997	0.4810791
$C_{16}H_{19}O_5$	549.1514676	549.15121	0.4690507
$C_{15}H_{19}N_2O_4$	549.1766196	549.17652	0.1813258
$C_{13}H_{23}O_7$	549.187853	549.18768	0.314974
$C_{17}H_{23}O_4$	549.2089822	549.2092	-0.396607
$C_{13}H_{10}N_1O_7$	549.2242384	549.22425	-0.021157
$C_{14}H_{14}N_1O_6$	549.2341342	549.23373	0.7358973
$C_{18}H_{14}N_1O_3$	550.1354832	550.13541	0.1330216
$C_{15}H_{18}N_1O_5$	550.1718686	550.17173	0.2518847
$C_{19}H_{18}N_1O_2$	550.208254	550.20818	0.134458
$C_{16}H_{22}N_1O_4$	550.2293832	550.22906	0.5873549
$C_{13}H_9O_8$	551.1194988	551.11952	-0.038504

$C_{14}H_{13}O_7$	551.1307322	551.13068	0.0946779
$C_{13}H_{13}N_2O_6$	551.1558842	551.15591	-0.046847
$C_{18}H_{13}O_4$	551.1671176	551.16693	0.3403322
$C_{11}H_{17}O_9$	551.1922696	551.19232	-0.091475
$C_{17}H_{13}N_2O_3$	551.203503	551.20338	0.2231116
$C_{15}H_{17}O_6$	551.2246322	551.22463	0.0039546
$C_{14}H_{17}N_2O_5$	551.2398884	551.23981	0.1421884
$C_{19}H_{17}O_3$	551.322555	551.32262	-0.117935
$C_{16}H_{21}O_5$	552.1511332	552.15114	-0.012352
$C_{15}H_{21}N_2O_4$	552.1875186	552.1875	0.0336478
$C_{17}H_{25}O_4$	552.223904	552.22369	0.3874876
$C_{13}H_{12}N_1O_7$	553.1351488	553.13527	-0.219151
$C_{17}H_{12}N_1O_4$	553.1463822	553.14602	0.6547632
$C_{14}H_{16}N_1O_6$	553.1715342	553.17168	-0.263607
$C_{18}H_{16}N_1O_3$	553.1827676	553.18265	0.2125516
$C_{15}H_{20}N_1O_5$	553.2079196	553.20768	0.4330739
$C_{16}H_{24}N_1O_4$	553.219153	553.21906	0.1680706
$C_{13}H_{11}O_8$	554.1303978	554.13038	0.0320861
$C_{17}H_{11}O_5$	554.1667832	554.16668	0.1861893
$C_{16}H_{11}N_2O_4$	554.2031686	554.2033	-0.237133
$C_{14}H_{15}O_7$	554.239554	554.23959	-0.06499
$C_{13}H_{15}N_2O_6$	555.1144134	555.11414	0.4924749
$C_{18}H_{15}O_4$	555.1507988	555.15063	0.3040253
$C_{11}H_{19}O_9$	555.1871842	555.18695	0.4218035
$C_{17}H_{15}N_2O_3$	555.1984176	555.19834	0.1397336
$C_{15}H_{19}O_6$	555.2235696	555.22374	-0.30694

$C_{14}H_{19}N_2O_5$	555.234803	555.23494	-0.246779
$C_{19}H_{19}O_3$	556.1460478	556.14604	0.013989
$C_{16}H_{23}O_5$	556.1824332	556.18226	0.3113725
$C_{15}H_{23}N_2O_4$	556.2188186	556.21884	-0.03851
$C_{12}H_{10}N_1O_8$	557.1664488	557.16625	0.3567693
$C_{16}H_{10}N_1O_5$	557.1776822	557.17767	0.02186
$C_{13}H_{14}N_1O_7$	557.2028342	557.20275	0.1510759
$C_{17}H_{14}N_1O_4$	557.2140676	557.21393	0.2469067
$C_{14}H_{18}N_1O_6$	557.2392196	557.23904	0.3222672
$C_{18}H_{18}N_1O_3$	557.250453	557.25067	-0.389448
$C_{15}H_{22}N_1O_5$	558.1041832	558.10442	-0.42433
$C_{16}H_9O_6$	558.1405686	558.14073	-0.28921
$C_{13}H_{13}O_8$	558.1616978	558.16196	-0.469792
$C_{12}H_{13}N_2O_7$	558.1980832	558.19802	0.1131854
$C_{17}H_{13}O_5$	558.2344686	558.23444	0.0511969
$C_{16}H_{13}N_2O_4$	558.270854	558.27104	-0.333208
$C_{14}H_{17}O_7$	559.1457134	559.14597	-0.45895
$C_{13}H_{17}N_2O_6$	559.172203	559.17224	-0.066205
$C_{18}H_{17}O_4$	559.1820988	559.18189	0.3733666
$C_{17}H_{17}N_2O_3$	559.1933322	559.19349	-0.282228
$C_{15}H_{21}O_6$	559.2184842	559.21856	-0.135582
$C_{14}H_{21}N_2O_5$	559.2297176	559.22955	0.299662
$C_{16}H_{25}O_5$	559.266103	559.26632	-0.388044
$C_{15}H_{25}N_2O_4$	560.1198332	560.11988	-0.083589
$C_{16}H_{29}N_2O_3$	560.1562186	560.15624	-0.03824
$C_{18}H_{33}O_3$	560.1773478	560.17773	-0.68232

$C_{19}H_{37}O_2$	560.2137332	560.21351	0.3983835
$C_{12}H_{12}N_1O_8$	561.1038488	561.10362	0.4077318
$C_{16}H_{12}N_1O_5$	561.1402342	561.1403	-0.117297
$C_{13}H_{16}N_1O_7$	561.1514676	561.15144	0.0491488
$C_{17}H_{16}N_1O_4$	561.1613634	561.1614	-0.065258
$C_{14}H_{20}N_1O_6$	561.187853	561.18805	-0.351077
$C_{18}H_{20}N_1O_3$	561.1977488	561.19786	-0.198183
$C_{15}H_{24}N_1O_5$	561.2089822	561.20886	0.2177084
$C_{12}H_{11}O_9$	561.2341342	561.23408	0.0965371
$C_{16}H_{11}O_6$	561.2453676	561.24535	0.031323
$C_{15}H_{11}N_2O_5$	562.1354832	562.1354	0.1479713
$C_{13}H_{15}O_8$	562.1718686	562.17162	0.4421778
$C_{12}H_{15}N_2O_7$	562.1929978	562.19278	0.3873757
$C_{17}H_{15}O_5$	563.1671176	563.16695	0.2975669
$C_{16}H_{15}N_2O_4$	563.203503	563.2036	-0.172265
$C_{14}H_{19}O_7$	563.2246322	563.22435	0.5010077
$C_{13}H_{19}N_2O_6$	564.1147478	564.1144	0.6165056
$C_{18}H_{19}O_4$	564.1511332	564.15105	0.1474426
$C_{17}H_{19}N_2O_3$	564.1875186	564.18724	0.4937718
$C_{15}H_{23}O_6$	565.1351488	565.13519	-0.072938
$C_{14}H_{23}N_2O_5$	565.1463822	565.14664	-0.456201
$C_{16}H_{27}O_5$	565.1715342	565.17153	0.0073958
$C_{18}H_{35}O_3$	565.1827676	565.18264	0.2257321
$C_{15}H_{10}N_1O_6$	565.219153	565.21939	-0.419342
$C_{12}H_{14}N_1O_8$	566.1303978	566.13071	-0.551499
$C_{16}H_{14}N_1O_5$	566.1667832	566.16657	0.376532

$C_{13}H_{18}N_1O_7$	566.2031686	566.20317	-0.002508
$C_{17}H_{18}N_1O_4$	567.1507988	567.15094	-0.248999
$C_{14}H_{22}N_1O_6$	567.1620322	567.162	0.0567385
$C_{18}H_{22}N_1O_3$	567.1871842	567.18691	0.4834028
$C_{15}H_9O_7$	567.1984176	567.19824	0.3130825
$C_{12}H_{13}O_9$	567.234803	567.2344	0.7104287
$C_{16}H_{13}O_6$	568.1824332	568.18232	0.1991964
$C_{15}H_{13}N_2O_5$	568.2188186	568.21871	0.1910882
$C_{13}H_{17}O_8$	569.1300634	569.13008	-0.029203
$C_{12}H_{17}N_2O_7$	569.1664488	569.16642	0.050565
$C_{17}H_{17}O_5$	569.2028342	569.20276	0.1303224
$C_{16}H_{17}N_2O_4$	569.2140676	569.21383	0.4173823
$C_{14}H_{21}O_7$	569.250453	569.25035	0.1809044
$C_{13}H_{21}N_2O_6$	570.1616978	570.16127	0.7502782
$C_{18}H_{21}O_4$	570.1980832	570.19774	0.6018608
$C_{17}H_{21}N_2O_3$	570.2344686	570.23434	0.225486
$C_{15}H_{25}O_6$	571.1457134	571.14571	0.0059178
$C_{16}H_{29}O_5$	571.1820988	571.18174	0.6281358
$C_{15}H_{12}N_1O_6$	571.2184842	571.21824	0.427472
$C_{12}H_{16}N_1O_8$	571.2297176	571.2295	0.3808974
$C_{16}H_{16}N_1O_5$	572.1773478	572.17746	-0.196128
$C_{17}H_{20}N_1O_4$	572.2137332	572.21384	-0.186679
$C_{18}H_{24}N_1O_3$	572.2501186	572.25042	-0.526728
$C_{15}H_{11}O_7$	573.1613634	573.1612	0.2850504
$C_{12}H_{15}O_9$	573.1977488	573.19771	0.0676554
$C_{16}H_{15}O_6$	573.2089822	573.20881	0.3003789

$C_{15}H_{15}N_2O_5$	573.2341342	573.23418	-0.079933
$C_{13}H_{19}O_8$	573.2453676	573.24548	-0.196112
$C_{12}H_{19}N_2O_7$	574.1354832	574.1355	-0.029296
$C_{17}H_{19}O_5$	574.1929978	574.19309	-0.160608
$C_{16}H_{19}N_2O_4$	574.2293832	574.22912	0.4583184
$C_{14}H_{23}O_7$	575.1671176	575.16705	0.1174961
$C_{13}H_{23}N_2O_6$	575.1770134	575.17682	0.3362094
$C_{18}H_{23}O_4$	575.2133988	575.21335	0.0848031
$C_{17}H_{23}N_2O_3$	575.2246322	575.22421	0.7339392
$C_{15}H_{27}O_6$	576.1147478	576.11501	-0.455153
$C_{16}H_{31}O_5$	576.1511332	576.15099	0.248511
$C_{14}H_{10}N_1O_7$	576.2086478	576.20868	-0.055917
$C_{15}H_{14}N_1O_6$	576.2450332	576.24506	-0.046543
$C_{16}H_{18}N_1O_5$	577.1351488	577.13508	0.1191747
$C_{17}H_{22}N_1O_4$	577.1827676	577.18279	-0.038844
$C_{18}H_{26}N_1O_3$	577.2766676	577.27642	0.4288756
$C_{15}H_{13}O_7$	578.1303978	578.13031	0.1518341
$C_{14}H_{13}N_2O_6$	578.1667832	578.16672	0.1092763
$C_{19}H_{13}O_4$	579.1507988	579.15075	0.0842266
$C_{16}H_{17}O_6$	579.1620322	579.16235	-0.548759
$C_{15}H_{17}N_2O_5$	579.1984176	579.19814	0.4792484
$C_{17}H_{21}O_5$	580.1460478	580.14612	-0.124486
$C_{16}H_{21}N_2O_4$	580.1824332	580.18261	-0.304766
$C_{14}H_{25}O_7$	581.1300634	581.13013	-0.114639
$C_{18}H_{25}O_4$	581.1664488	581.16672	-0.466682
$C_{17}H_{25}N_2O_3$	582.1616978	582.16192	-0.381715

$C_{14}H_{12}N_1O_7$	582.1980832	582.19791	0.2974587
$C_{15}H_{16}N_1O_6$	583.1457134	583.14576	-0.079946
$C_{19}H_{16}N_1O_3$	583.1820988	583.18235	-0.430775
$C_{16}H_{20}N_1O_5$	583.1933322	583.19344	-0.184879
$C_{17}H_{24}N_1O_4$	583.2297176	583.23006	-0.58711
$C_{18}H_{28}N_1O_3$	584.1773478	584.17723	0.2016167
$C_{14}H_{11}O_8$	584.2137332	584.21379	-0.097259
$C_{15}H_{15}O_7$	585.1613634	585.16138	-0.028403
$C_{14}H_{15}N_2O_6$	585.1977488	585.19775	-0.002085
$C_{19}H_{15}O_4$	585.2089822	585.20875	0.396747
$C_{12}H_{19}O_9$	585.2453676	585.2451	0.4572098
$C_{18}H_{15}N_2O_3$	586.1929978	586.19319	-0.327913
$C_{16}H_{19}O_6$	587.1770134	587.17721	-0.334857
$C_{15}H_{19}N_2O_5$	587.2133988	587.21341	-0.019107
$C_{17}H_{23}O_5$	587.2246322	587.22463	0.0037122
$C_{16}H_{23}N_2O_4$	588.2086478	588.20841	0.4042441
$C_{18}H_{27}O_4$	589.2402822	589.24055	-0.454518
$C_{17}H_{27}N_2O_3$	591.1620322	591.16199	0.0713508
$C_{17}H_{10}N_1O_5$	592.1460478	592.14591	0.2326789
$C_{14}H_{14}N_1O_7$	594.1616978	594.16153	0.2823809
$C_{18}H_{14}N_1O_4$	596.1773478	596.17755	-0.339195
$C_{15}H_{18}N_1O_6$	598.1929978	598.19328	-0.471788
$C_{19}H_{18}N_1O_3$	599.1770134	599.17729	-0.461667
$C_{16}H_{22}N_1O_5$	599.2246322	599.22454	0.153832
$C_{14}H_{13}O_8$	600.2086478	600.20857	0.1295881
$C_{13}H_{13}N_2O_7$	601.2402822	601.24075	-0.778092

$\text{C}_{18}\text{H}_{13}\text{O}_5$	602.2242978	602.22448	-0.302578
$\text{C}_{17}\text{H}_{13}\text{N}_2\text{O}_4$	603.2083134	603.20874	-0.707252

Table S6 Molecular formula and mass for compounds in LP-280-0, as detected by FT-ICR MS.

Molecular formula	Theoretical mass	Measured mass	Error (ppm)
C ₁₀ H ₉ O ₂	161.0608028	161.06083	-0.169005
C ₇ H ₁₃ O ₄	161.081932	161.08197	-0.23603
C ₉ H ₇ O ₃	163.0400674	163.04014	-0.445413
C ₉ H ₉ O ₃	165.0557174	165.05577	-0.318802
C ₉ H ₁₁ O ₃	167.0713674	167.07139	-0.135392
C ₈ H ₉ O ₄	169.050632	169.05065	-0.106596
C ₈ H ₁₃ O ₄	173.081932	173.08194	-0.046337
C ₁₀ H ₈ N ₁ O ₂	174.0560518	174.05606	-0.047227
C ₁₁ H ₁₁ O ₂	175.0764528	175.07646	-0.04124
C ₁₀ H ₁₀ N ₁ O ₂	176.0717018	176.07175	-0.273866
C ₁₀ H ₉ O ₃	177.0557174	177.0558	-0.466633
C ₁₁ H ₁₃ O ₂	177.0921028	177.09218	-0.436045
C ₁₀ H ₁₂ N ₁ O ₂	178.0873518	178.08743	-0.439223
C ₉ H ₇ O ₄	179.034982	179.03499	-0.044796
C ₁₀ H ₁₁ O ₃	179.0713674	179.07139	-0.126319
C ₁₁ H ₁₅ O ₂	179.1077528	179.10781	-0.319473
C ₉ H ₁₀ N ₁ O ₃	180.0666164	180.06661	0.0354308
C ₉ H ₉ O ₄	181.050632	181.05066	-0.154764
C ₁₀ H ₁₃ O ₃	181.0870174	181.08704	-0.124913
C ₁₁ H ₁₇ O ₂	181.1234028	181.1234	0.0153481
C ₉ H ₁₂ N ₁ O ₃	182.0822664	182.08232	-0.294483
C ₉ H ₁₁ O ₄	183.066282	183.06629	-0.04381
C ₁₀ H ₁₅ O ₃	183.1026674	183.10269	-0.123538
C ₁₀ H ₁₇ O ₃	185.1183174	185.11839	-0.39229

$C_8H_{11}O_5$	187.0611966	187.06127	-0.392492
$C_{12}H_{11}O_2$	187.0764528	187.07654	-0.466227
$C_9H_{15}O_4$	187.097582	187.09767	-0.47045
$C_{11}H_{10}N_1O_2$	188.0717018	188.07171	-0.043707
$C_{11}H_9O_3$	189.0557174	189.05578	-0.331226
$C_{12}H_{13}O_2$	189.0921028	189.09218	-0.408373
$C_{10}H_8N_1O_3$	190.0509664	190.05098	-0.071666
$C_{11}H_{12}N_1O_2$	190.0873518	190.08734	0.061971
$C_{10}H_7O_4$	191.034982	191.03499	-0.041982
$C_{11}H_{11}O_3$	191.0713674	191.07139	-0.118386
$C_{12}H_{15}O_2$	191.1077528	191.10777	-0.090107
$C_{10}H_{10}N_1O_3$	192.0666164	192.06669	-0.383305
$C_{11}H_{14}N_1O_2$	192.1030018	192.10302	-0.094845
$C_{10}H_9O_4$	193.050632	193.05061	0.1138556
$C_{11}H_{13}O_3$	193.0870174	193.08701	0.0382206
$C_{12}H_{17}O_2$	193.1234028	193.12337	0.1697355
$C_{10}H_{12}N_1O_3$	194.0822664	194.08234	-0.379324
$C_9H_7O_5$	195.0298966	195.02996	-0.325181
$C_{10}H_{11}O_4$	195.066282	195.06629	-0.041115
$C_{11}H_{15}O_3$	195.1026674	195.10268	-0.064684
$C_{12}H_{19}O_2$	195.1390528	195.13905	0.0142457
$C_9H_{10}N_1O_4$	196.061531	196.0615	0.1580111
$C_{10}H_{14}N_1O_3$	196.0979164	196.09791	0.0325343
$C_9H_9O_5$	197.0455466	197.04557	-0.118856
$C_{10}H_{13}O_4$	197.081932	197.08199	-0.294396
$C_{11}H_{17}O_3$	197.1183174	197.11841	-0.469871

$C_{12}H_8N_1O_2$	198.0560518	198.05609	-0.192976
$C_9H_{12}N_1O_4$	198.077181	198.07726	-0.398936
$C_{10}H_{16}N_1O_3$	198.1135664	198.11353	0.1836315
$C_{12}H_7O_3$	199.0400674	199.04011	-0.214128
$C_9H_{11}O_5$	199.0611966	199.06118	0.0832905
$C_{13}H_{11}O_2$	199.0764528	199.07645	0.013964
$C_{10}H_{15}O_4$	199.097582	199.09755	0.1606243
$C_{11}H_{19}O_3$	199.1339674	199.13396	0.03706
$C_{12}H_{23}O_2$	199.1703528	199.17035	0.0139574
$C_8H_{10}N_1O_5$	200.0564456	200.05644	0.0278916
$C_{12}H_{10}N_1O_2$	200.0717018	200.07169	0.0588784
$C_9H_{14}N_1O_4$	200.092831	200.09284	-0.04508
$C_{12}H_9O_3$	201.0557174	201.05574	-0.112507
$C_{11}H_9N_2O_2$	201.0669508	201.06685	0.5012256
$C_9H_{13}O_5$	201.0768466	201.07687	-0.116473
$C_{13}H_{13}O_2$	201.0921028	201.09213	-0.135361
$C_{10}H_{17}O_4$	201.113232	201.11329	-0.288495
$C_{11}H_8N_1O_3$	202.0509664	202.05103	-0.314872
$C_{12}H_{12}N_1O_2$	202.0873518	202.08741	-0.288094
$C_{11}H_7O_4$	203.034982	203.03509	-0.532027
$C_{12}H_{11}O_3$	203.0713674	203.07142	-0.259121
$C_{11}H_{11}N_2O_2$	203.0826008	203.08267	-0.340847
$C_9H_{15}O_5$	203.0924966	203.09254	-0.213795
$C_{13}H_{15}O_2$	203.1077528	203.10778	-0.134018
$C_{10}H_{19}O_4$	203.128882	203.12884	0.2066663
$C_{11}H_{10}N_1O_3$	204.0666164	204.06664	-0.115747

$C_{12}H_{14}N_1O_2$	204.1030018	204.10301	-0.040274
$C_{11}H_9O_4$	205.050632	205.05065	-0.087881
$C_{10}H_9N_2O_3$	205.0618654	205.06189	-0.120062
$C_{12}H_{13}O_3$	205.0870174	205.08701	0.0359842
$C_{10}H_8N_1O_4$	206.045881	206.04589	-0.043777
$C_{11}H_{12}N_1O_3$	206.0822664	206.08223	0.176531
$C_{12}H_{16}N_1O_2$	206.1186518	206.11861	0.2026983
$C_{10}H_7O_5$	207.0298966	207.02985	0.2249912
$C_{11}H_{11}O_4$	207.066282	207.06624	0.2027365
$C_{12}H_{15}O_3$	207.1026674	207.10266	0.035634
$C_{13}H_{19}O_2$	207.1390528	207.1391	-0.227963
$C_{10}H_{10}N_1O_4$	208.061531	208.06151	0.1008351
$C_{11}H_{14}N_1O_3$	208.0979164	208.09791	0.0306582
$C_{10}H_9O_5$	209.0455466	209.04552	0.1271488
$C_{11}H_{13}O_4$	209.081932	209.08192	0.0572976
$C_{12}H_{17}O_3$	209.1183174	209.11834	-0.108169
$C_{10}H_{12}N_1O_4$	210.077181	210.07716	0.0998676
$C_{11}H_{16}N_1O_3$	210.1135664	210.11356	0.0303641
$C_{10}H_{11}O_5$	211.0611966	211.06118	0.0785549
$C_{11}H_{15}O_4$	211.097582	211.09757	0.0567505
$C_{13}H_{10}N_1O_2$	212.0717018	212.07166	0.1970084
$C_{10}H_{14}N_1O_4$	212.092831	212.09285	-0.089678
$C_{11}H_{18}N_1O_3$	212.1292164	212.12921	0.0300755
$C_{13}H_9O_3$	213.0557174	213.05567	0.2223827
$C_{10}H_{13}O_5$	213.0768466	213.07683	0.0778118
$C_{14}H_{13}O_2$	213.0921028	213.09207	0.1538297

$C_{11}H_{17}O_4$	213.113232	213.11323	0.0092904
$C_{12}H_8N_1O_3$	214.0509664	214.05097	-0.016912
$C_9H_{12}N_1O_5$	214.0720956	214.07207	0.119492
$C_{13}H_{12}N_1O_2$	214.0873518	214.08732	0.1484436
$C_{11}H_{20}N_1O_3$	214.1448664	214.14485	0.0764898
$C_{12}H_7O_4$	215.034982	215.035	-0.083801
$C_{13}H_{11}O_3$	215.0713674	215.07134	0.1273061
$C_{12}H_{11}N_2O_2$	215.0826008	215.08258	0.0966136
$C_{10}H_{15}O_5$	215.0924966	215.09246	0.1700659
$C_{14}H_{15}O_2$	215.1077528	215.10773	0.1058999
$C_{11}H_{19}O_4$	215.128882	215.12885	0.1486546
$C_{11}H_6N_1O_4$	216.030231	216.03023	0.0045359
$C_{12}H_{10}N_1O_3$	216.0666164	216.06663	-0.063037
$C_{13}H_{14}N_1O_2$	216.1030018	216.103	0.0082364
$C_{12}H_9O_4$	217.050632	217.05069	-0.267311
$C_9H_{13}O_6$	217.0717612	217.07179	-0.132768
$C_{13}H_{13}O_3$	217.0870174	217.08704	-0.104198
$C_{12}H_{13}N_2O_2$	217.0982508	217.09828	-0.134594
$C_{10}H_{17}O_5$	217.1081466	217.10814	0.030307
$C_{14}H_{17}O_2$	217.1234028	217.12337	0.1509736
$C_{11}H_{21}O_4$	217.144532	217.14453	0.0091179
$C_{11}H_8N_1O_4$	218.045881	218.04594	-0.270677
$C_{12}H_{12}N_1O_3$	218.0822664	218.08231	-0.200017
$C_{13}H_{16}N_1O_2$	218.1186518	218.11868	-0.12938
$C_{11}H_7O_5$	219.0298966	219.02987	0.1213528
$C_{12}H_{11}O_4$	219.066282	219.06634	-0.264852

$C_{11}H_{11}N_2O_3$	219.0775154	219.0776	-0.386256
$C_{13}H_{15}O_3$	219.1026674	219.10274	-0.331443
$C_{12}H_{15}N_2O_2$	219.1139008	219.11399	-0.407186
$C_{11}H_{10}N_1O_4$	220.061531	220.06153	0.0044528
$C_{12}H_{14}N_1O_3$	220.0979164	220.09793	-0.061882
$C_{13}H_{18}N_1O_2$	220.1343018	220.13437	-0.309902
$C_{11}H_9O_5$	221.0455466	221.04549	0.2559649
$C_{12}H_{13}O_4$	221.081932	221.08189	0.1898839
$C_{13}H_{17}O_3$	221.1183174	221.11831	0.0333753
$C_{11}H_{12}N_1O_4$	222.077181	222.07715	0.1395006
$C_{12}H_{16}N_1O_3$	222.1135664	222.11352	0.2088116
$C_{11}H_{11}O_5$	223.0611966	223.06123	-0.149825
$C_{12}H_{15}O_4$	223.097582	223.0976	-0.080772
$C_{13}H_{19}O_3$	223.1339674	223.13398	-0.056558
$C_{10}H_{10}N_1O_5$	224.0564456	224.05647	-0.108991
$C_{14}H_{10}N_1O_2$	224.0717018	224.07179	-0.393714
$C_{11}H_{14}N_1O_4$	224.092831	224.09289	-0.263373
$C_{12}H_{18}N_1O_3$	224.1292164	224.12927	-0.239237
$C_{11}H_{13}O_5$	225.0768466	225.07684	0.029234
$C_{12}H_{17}O_4$	225.113232	225.11323	0.0087951
$C_{11}H_{17}N_2O_3$	225.1244654	225.12442	0.2015769
$C_{13}H_{21}O_3$	225.1496174	225.14962	-0.011637
$C_{14}H_{25}O_2$	225.1860028	225.18605	-0.209694
$C_{13}H_8N_1O_3$	226.0509664	226.05098	-0.060252
$C_{10}H_{12}N_1O_5$	226.0720956	226.072	0.422785
$C_{14}H_{12}N_1O_2$	226.0873518	226.08731	0.1847954

$C_{11}H_{16}N_1O_4$	226.108481	226.10846	0.0927869
$C_{13}H_7O_4$	227.034982	227.03505	-0.299602
$C_{12}H_7N_2O_3$	227.0462154	227.04623	-0.064393
$C_{10}H_{11}O_6$	227.0561112	227.0562	-0.391181
$C_{14}H_{11}O_3$	227.0713674	227.07139	-0.099617
$C_{13}H_{11}N_2O_2$	227.0826008	227.08264	-0.172713
$C_{11}H_{15}O_5$	227.0924966	227.09253	-0.147165
$C_{15}H_{15}O_2$	227.1077528	227.1078	-0.207919
$C_{12}H_{19}O_4$	227.128882	227.12892	-0.167394
$C_{14}H_{27}O_2$	227.2016528	227.20163	0.1002629
$C_{12}H_6N_1O_4$	228.030231	228.03028	-0.214972
$C_{13}H_{10}N_1O_3$	228.0666164	228.06662	-0.015873
$C_{10}H_{14}N_1O_5$	228.0877456	228.08778	-0.150907
$C_{14}H_{14}N_1O_2$	228.1030018	228.10305	-0.211396
$C_{11}H_{18}N_1O_4$	228.124131	228.12418	-0.214883
$C_{12}H_{22}N_1O_3$	228.1605164	228.16057	-0.23501
$C_{13}H_9O_4$	229.050632	229.0506	0.1396193
$C_{12}H_9N_2O_3$	229.0618654	229.06181	0.2417683
$C_{10}H_{13}O_6$	229.0717612	229.07174	0.0924597
$C_{14}H_{13}O_3$	229.0870174	229.08698	0.163169
$C_{13}H_{13}N_2O_2$	229.0982508	229.09821	0.1780018
$C_{11}H_{17}O_5$	229.1081466	229.1081	0.2033097
$C_{15}H_{17}O_2$	229.1234028	229.12338	0.099422
$C_{12}H_{21}O_4$	229.144532	229.1445	0.1395621
$C_{11}H_{21}N_2O_3$	229.1557654	229.15575	0.0671155
$C_{12}H_8N_1O_4$	230.045881	230.04594	-0.256558

$C_{13}H_{12}N_1O_3$	230.0822664	230.08228	-0.059197
$C_{10}H_{16}N_1O_5$	230.1033956	230.10344	-0.193044
$C_{14}H_{16}N_1O_2$	230.1186518	230.11863	0.0946464
$C_{12}H_7O_5$	231.0298966	231.02992	-0.101373
$C_{11}H_7N_2O_4$	231.04113	231.04119	-0.259781
$C_{13}H_{11}O_4$	231.066282	231.06632	-0.164542
$C_{12}H_{11}N_2O_3$	231.0775154	231.07759	-0.322922
$C_{10}H_{15}O_6$	231.0874112	231.08748	-0.29781
$C_{14}H_{15}O_3$	231.1026674	231.10273	-0.270962
$C_{13}H_{15}N_2O_2$	231.1139008	231.11396	-0.256238
$C_{11}H_{19}O_5$	231.1237966	231.12386	-0.274399
$C_{15}H_{19}O_2$	231.1390528	231.13904	0.055291
$C_{12}H_{23}O_4$	231.160182	231.16022	-0.164475
$C_{12}H_{10}N_1O_4$	232.061531	232.06148	0.2196827
$C_{13}H_{14}N_1O_3$	232.0979164	232.09788	0.1567438
$C_{14}H_{18}N_1O_2$	232.1343018	232.13427	0.1369031
$C_{12}H_9O_5$	233.0455466	233.0456	-0.229226
$C_{13}H_{13}O_4$	233.081932	233.08195	-0.077312
$C_{12}H_{13}N_2O_3$	233.0931654	233.09318	-0.062722
$C_{14}H_{17}O_3$	233.1183174	233.11832	-0.011239
$C_{13}H_{17}N_2O_2$	233.1295508	233.12952	0.1320292
$C_{15}H_{21}O_2$	233.1547028	233.15467	0.1405929
$C_{12}H_{12}N_1O_4$	234.077181	234.07719	-0.038535
$C_{13}H_{16}N_1O_3$	234.1135664	234.11361	-0.18632
$C_{14}H_{20}N_1O_2$	234.1499518	234.15002	-0.291352
$C_{12}H_{11}O_5$	235.0611966	235.06117	0.1130765

C ₁₁ H ₁₁ N ₂ O ₄	235.07243	235.07244	-0.042626
C ₁₃ H ₁₅ O ₄	235.097582	235.09753	0.2210993
C ₁₂ H ₁₅ N ₂ O ₃	235.1088154	235.10871	0.4482176
C ₁₄ H ₁₉ O ₃	235.1339674	235.13392	0.2015017
C ₁₁ H ₁₀ N ₁ O ₅	236.0564456	236.05649	-0.188176
C ₁₂ H ₁₄ N ₁ O ₄	236.092831	236.0929	-0.292343
C ₁₃ H ₁₈ N ₁ O ₃	236.1292164	236.12928	-0.269429
C ₁₂ H ₁₃ O ₅	237.0768466	237.0768	0.196476
C ₁₁ H ₁₃ N ₂ O ₄	237.08808	237.08807	0.0420936
C ₁₃ H ₁₇ O ₄	237.113232	237.11321	0.0926979
C ₁₂ H ₁₇ N ₂ O ₃	237.1244654	237.12437	0.4022356
C ₁₄ H ₂₁ O ₃	237.1496174	237.1496	0.0732866
C ₁₁ H ₁₂ N ₁ O ₅	238.0720956	238.07214	-0.186583
C ₁₅ H ₁₂ N ₁ O ₂	238.0873518	238.08742	-0.286534
C ₁₂ H ₁₆ N ₁ O ₄	238.108481	238.10851	-0.121878
C ₁₃ H ₂₀ N ₁ O ₃	238.1448664	238.14486	0.02679
C ₁₁ H ₁₁ O ₆	239.0561112	239.05606	0.2140916
C ₁₅ H ₁₁ O ₃	239.0713674	239.07134	0.1145261
C ₁₄ H ₁₁ N ₂ O ₂	239.0826008	239.08262	-0.080391
C ₁₂ H ₁₅ O ₅	239.0924966	239.0925	-0.014305
C ₁₃ H ₁₉ O ₄	239.128882	239.1289	-0.075357
C ₁₄ H ₂₃ O ₃	239.1652674	239.16526	0.0308569
C ₁₅ H ₂₇ O ₂	239.2016528	239.20167	-0.07199
C ₁₄ H ₁₀ N ₁ O ₃	240.0666164	240.06663	-0.056735
C ₁₁ H ₁₄ N ₁ O ₅	240.0877456	240.08776	-0.060062
C ₁₅ H ₁₄ N ₁ O ₂	240.1030018	240.10301	-0.034236

$C_{12}H_{18}N_1O_4$	240.124131	240.12413	0.0040808
$C_{14}H_9O_4$	241.050632	241.05062	0.0496987
$C_{13}H_9N_2O_3$	241.0618654	241.06185	0.0638006
$C_{11}H_{13}O_6$	241.0717612	241.07175	0.0463758
$C_{10}H_{13}N_2O_5$	241.0829946	241.08289	0.4337921
$C_{15}H_{13}O_3$	241.0870174	241.08703	-0.052347
$C_{14}H_{13}N_2O_2$	241.0982508	241.09823	0.0861885
$C_{12}H_{17}O_5$	241.1081466	241.10817	-0.097135
$C_{16}H_{17}O_2$	241.1234028	241.12342	-0.071416
$C_{13}H_{21}O_4$	241.144532	241.14458	-0.199134
$C_{12}H_{21}N_2O_3$	241.1557654	241.15583	-0.26796
$C_{14}H_{25}O_3$	241.1809174	241.18091	0.030599
$C_{15}H_{29}O_2$	241.2173028	241.21737	-0.27867
$C_{13}H_8N_1O_4$	242.045881	242.04589	-0.037266
$C_{14}H_{12}N_1O_3$	242.0822664	242.08225	0.0676625
$C_{11}H_{16}N_1O_5$	242.1033956	242.10336	0.1469616
$C_{15}H_{16}N_1O_2$	242.1186518	242.11861	0.1725596
$C_{12}H_{20}N_1O_4$	242.139781	242.13968	0.4170314
$C_{13}H_{24}N_1O_3$	242.1761664	242.17613	0.1502208
$C_{13}H_7O_5$	243.0298966	243.0299	-0.014073
$C_{14}H_{11}O_4$	243.066282	243.06628	0.0081455
$C_{13}H_{11}N_2O_3$	243.0775154	243.07753	-0.060146
$C_{11}H_{15}O_6$	243.0874112	243.08744	-0.118559
$C_{15}H_{15}O_3$	243.1026674	243.10269	-0.093048
$C_{14}H_{15}N_2O_2$	243.1139008	243.11393	-0.120191
$C_{12}H_{19}O_5$	243.1237966	243.12383	-0.137461

$C_{13}H_{23}O_4$	243.160182	243.16022	-0.156358
$C_{12}H_{23}N_2O_3$	243.1714154	243.17156	-0.594725
$C_{13}H_{10}N_1O_4$	244.061531	244.06153	0.004015
$C_{10}H_{14}N_1O_6$	244.0826602	244.0827	-0.163142
$C_{14}H_{14}N_1O_3$	244.0979164	244.0979	0.0671038
$C_{11}H_{18}N_1O_5$	244.1190456	244.11905	-0.018106
$C_{15}H_{18}N_1O_2$	244.1343018	244.13427	0.1301738
$C_{13}H_9O_5$	245.0455466	245.04552	0.1084692
$C_{12}H_9N_2O_4$	245.05678	245.05676	0.0815317
$C_{10}H_{13}O_7$	245.0666758	245.06667	0.023585
$C_{14}H_{13}O_4$	245.081932	245.08194	-0.032724
$C_{13}H_{13}N_2O_3$	245.0931654	245.09318	-0.059651
$C_{11}H_{17}O_6$	245.1030612	245.10307	-0.035985
$C_{15}H_{17}O_3$	245.1183174	245.11834	-0.092282
$C_{14}H_{17}N_2O_2$	245.1295508	245.12957	-0.078408
$C_{12}H_{21}O_5$	245.1394466	245.13947	-0.095538
$C_{13}H_{25}O_4$	245.175832	245.17589	-0.236647
$C_{12}H_8N_1O_5$	246.0407956	246.04086	-0.261827
$C_{13}H_{12}N_1O_4$	246.077181	246.07719	-0.036656
$C_{14}H_{16}N_1O_3$	246.1135664	246.11356	0.0259226
$C_{15}H_{20}N_1O_2$	246.1499518	246.14994	0.0478566
$C_{13}H_{11}O_5$	247.0611966	247.06117	0.1075843
$C_{12}H_{11}N_2O_4$	247.07243	247.07237	0.2427624
$C_{10}H_{15}O_7$	247.0823258	247.08229	0.1448096
$C_{14}H_{15}O_4$	247.097582	247.09755	0.1294221
$C_{13}H_{15}N_2O_3$	247.1088154	247.10879	0.1027074

$C_{11}H_{19}O_6$	247.1187112	247.11869	0.0857074
$C_{15}H_{19}O_3$	247.1339674	247.13396	0.0298619
$C_{12}H_{10}N_1O_5$	248.0564456	248.05652	-0.300013
$C_{13}H_{14}N_1O_4$	248.092831	248.09286	-0.116973
$C_{14}H_{18}N_1O_3$	248.1292164	248.12924	-0.095193
$C_{15}H_{22}N_1O_2$	248.1656018	248.16562	-0.073419
$C_{13}H_{13}O_5$	249.0768466	249.07678	0.2673067
$C_{12}H_{13}N_2O_4$	249.08808	249.08808	-8.07E-05
$C_{14}H_{17}O_4$	249.113232	249.11318	0.2086597
$C_{13}H_{17}N_2O_3$	249.1244654	249.12442	0.1821575
$C_{15}H_{21}O_3$	249.1496174	249.14956	0.230303
$C_{12}H_{12}N_1O_5$	250.0720956	250.07216	-0.257606
$C_{13}H_{16}N_1O_4$	250.108481	250.10854	-0.235978
$C_{14}H_{20}N_1O_3$	250.1448664	250.14492	-0.214356
$C_{12}H_{11}O_6$	251.0561112	251.0561	0.0445315
$C_{16}H_{11}O_3$	251.0713674	251.07134	0.1090523
$C_{13}H_{15}O_5$	251.0924966	251.09243	0.2651609
$C_{12}H_{15}N_2O_4$	251.10373	251.10367	0.238865
$C_{14}H_{19}O_4$	251.128882	251.12882	0.2468051
$C_{13}H_{19}N_2O_3$	251.1401154	251.14003	0.3399692
$C_{15}H_{23}O_3$	251.1652674	251.16515	0.4673413
$C_{15}H_{10}N_1O_3$	252.0666164	252.06659	0.1046545
$C_{12}H_{14}N_1O_5$	252.0877456	252.08776	-0.057203
$C_{16}H_{14}N_1O_2$	252.1030018	252.10302	-0.072272
$C_{13}H_{18}N_1O_4$	252.124131	252.12414	-0.035776
$C_{14}H_{22}N_1O_3$	252.1605164	252.16033	0.739132

$C_{11}H_9O_7$	253.0353758	253.03545	-0.293319
$C_{15}H_9O_4$	253.050632	253.05066	-0.110729
$C_{12}H_{13}O_6$	253.0717612	253.07178	-0.074367
$C_{11}H_{13}N_2O_5$	253.0829946	253.08303	-0.139954
$C_{16}H_{13}O_3$	253.0870174	253.08699	0.1081837
$C_{15}H_{13}N_2O_2$	253.0982508	253.09829	-0.15496
$C_{13}H_{17}O_5$	253.1081466	253.10816	-0.053021
$C_{14}H_{21}O_4$	253.144532	253.14454	-0.031682
$C_{16}H_{29}O_2$	253.2173028	253.21726	0.1689454
$C_{14}H_8N_1O_4$	254.045881	254.04584	0.1613091
$C_{11}H_{12}N_1O_6$	254.0670102	254.06706	-0.19609
$C_{15}H_{12}N_1O_3$	254.0822664	254.0822	0.2612536
$C_{12}H_{16}N_1O_5$	254.1033956	254.10334	0.2187295
$C_{16}H_{16}N_1O_2$	254.1186518	254.11859	0.2431144
$C_{13}H_{20}N_1O_4$	254.139781	254.13973	0.2005979
$C_{14}H_7O_5$	255.0298966	255.02993	-0.131044
$C_{15}H_{11}O_4$	255.066282	255.06631	-0.109854
$C_{14}H_{11}N_2O_3$	255.0775154	255.07757	-0.214131
$C_{12}H_{15}O_6$	255.0874112	255.08747	-0.230588
$C_{16}H_{15}O_3$	255.1026674	255.10273	-0.24547
$C_{15}H_{15}N_2O_2$	255.1139008	255.11397	-0.27133
$C_{13}H_{19}O_5$	255.1237966	255.12385	-0.209389
$C_{14}H_{23}O_4$	255.160182	255.16028	-0.384151
$C_{16}H_{31}O_2$	255.2329528	255.23297	-0.067468
$C_{14}H_{10}N_1O_4$	256.061531	256.06154	-0.035226
$C_{11}H_{14}N_1O_6$	256.0826602	256.08263	0.1178522

C ₁₅ H ₁₄ N ₁ O ₃	256.0979164	256.09792	-0.014136
C ₁₂ H ₁₈ N ₁ O ₅	256.1190456	256.11904	0.0217864
C ₁₆ H ₁₈ N ₁ O ₂	256.1343018	256.13428	0.0850331
C ₁₄ H ₉ O ₅	257.0455466	257.04548	0.2590199
C ₁₁ H ₁₃ O ₇	257.0666758	257.06663	0.1780857
C ₁₅ H ₁₃ O ₄	257.081932	257.08187	0.2410901
C ₁₄ H ₁₃ N ₂ O ₃	257.0931654	257.09311	0.2154079
C ₁₂ H ₁₇ O ₆	257.1030612	257.10302	0.1601688
C ₁₆ H ₁₇ O ₃	257.1183174	257.11829	0.1064876
C ₁₅ H ₁₇ N ₂ O ₂	257.1295508	257.12955	0.0030331
C ₁₃ H ₂₁ O ₅	257.1394466	257.1394	0.1811465
C ₁₄ H ₂₅ O ₄	257.175832	257.17583	0.0076986
C ₁₄ H ₁₂ N ₁ O ₄	258.077181	258.07725	-0.26744
C ₁₁ H ₁₆ N ₁ O ₆	258.0983102	258.09838	-0.270517
C ₁₅ H ₁₆ N ₁ O ₃	258.1135664	258.11364	-0.285224
C ₁₆ H ₂₀ N ₁ O ₂	258.1499518	258.15002	-0.264265
C ₁₄ H ₁₁ O ₅	259.0611966	259.06121	-0.051803
C ₁₃ H ₁₁ N ₂ O ₄	259.07243	259.07241	0.0771209
C ₁₁ H ₁₅ O ₇	259.0823258	259.08232	0.0223091
C ₁₅ H ₁₅ O ₄	259.097582	259.09755	0.123428
C ₁₄ H ₁₅ N ₂ O ₃	259.1088154	259.1088	0.0593569
C ₁₂ H ₁₉ O ₆	259.1187112	259.1187	0.0431459
C ₁₆ H ₁₉ O ₃	259.1339674	259.13393	0.1442493
C ₁₅ H ₁₉ N ₂ O ₂	259.1452008	259.14519	0.0415979
C ₁₃ H ₂₃ O ₅	259.1550966	259.15498	0.4498461
C ₁₃ H ₁₀ N ₁ O ₅	260.0564456	260.05634	0.4059884

C ₁₄ H ₁₄ N ₁ O ₄	260.092831	260.09277	0.2344544
C ₁₅ H ₁₈ N ₁ O ₃	260.1292164	260.12917	0.1782956
C ₁₆ H ₂₂ N ₁ O ₂	260.1656018	260.16556	0.1605896
C ₁₃ H ₉ O ₆	261.0404612	261.04045	0.0428282
C ₁₄ H ₁₃ O ₅	261.0768466	261.07688	-0.128009
C ₁₃ H ₁₃ N ₂ O ₄	261.08808	261.08814	-0.229884
C ₁₁ H ₁₇ O ₇	261.0979758	261.09802	-0.169362
C ₁₅ H ₁₇ O ₄	261.113232	261.11328	-0.183905
C ₁₄ H ₁₇ N ₂ O ₃	261.1244654	261.12453	-0.247469
C ₁₂ H ₂₁ O ₆	261.1343612	261.1344	-0.148659
C ₁₆ H ₂₁ O ₃	261.1496174	261.14965	-0.12491
C ₁₃ H ₁₂ N ₁ O ₅	262.0720956	262.07213	-0.131338
C ₁₄ H ₁₆ N ₁ O ₄	262.108481	262.10849	-0.034414
C ₁₅ H ₂₀ N ₁ O ₃	262.1448664	262.14487	-0.01381
C ₁₃ H ₁₁ O ₆	263.0561112	263.05608	0.1185295
C ₁₄ H ₁₅ O ₅	263.0924966	263.0924	0.3670948
C ₁₃ H ₁₅ N ₂ O ₄	263.10373	263.10367	0.2279705
C ₁₅ H ₁₉ O ₄	263.128882	263.1288	0.311558
C ₁₄ H ₁₉ N ₂ O ₃	263.1401154	263.14006	0.2104578
C ₁₆ H ₂₃ O ₃	263.1652674	263.16519	0.2940354
C ₁₂ H ₁₀ N ₁ O ₆	264.0513602	264.05136	0.0006813
C ₁₃ H ₁₄ N ₁ O ₅	264.0877456	264.08772	0.0968614
C ₁₇ H ₁₄ N ₁ O ₂	264.1030018	264.10301	-0.031125
C ₁₄ H ₁₈ N ₁ O ₄	264.124131	264.12414	-0.034151
C ₁₅ H ₂₂ N ₁ O ₃	264.1605164	264.1605	0.0620074
C ₁₃ H ₁₃ O ₆	265.0717612	265.07182	-0.221903

$C_{12}H_{13}N_2O_5$	265.0829946	265.08302	-0.095895
$C_{16}H_{13}N_2O_2$	265.0982508	265.09828	-0.110224
$C_{14}H_{17}O_5$	265.1081466	265.1082	-0.201503
$C_{13}H_{17}N_2O_4$	265.11938	265.11945	-0.264108
$C_{15}H_{21}O_4$	265.144532	265.14459	-0.218824
$C_{14}H_{21}N_2O_3$	265.1557654	265.1558	-0.130565
$C_{16}H_{25}O_3$	265.1809174	265.18095	-0.123011
$C_{12}H_{12}N_1O_6$	266.0670102	266.06706	-0.187246
$C_{16}H_{12}N_1O_3$	266.0822664	266.08227	-0.013605
$C_{13}H_{16}N_1O_5$	266.1033956	266.1034	-0.01661
$C_{17}H_{16}N_1O_2$	266.1186518	266.11866	-0.030889
$C_{14}H_{20}N_1O_4$	266.139781	266.13974	0.1539789
$C_{12}H_{11}O_7$	267.0510258	267.05092	0.3961037
$C_{16}H_{11}O_4$	267.066282	267.06623	0.194633
$C_{13}H_{15}O_6$	267.0874112	267.08732	0.341386
$C_{12}H_{15}N_2O_5$	267.0986446	267.09859	0.2043436
$C_{17}H_{15}O_3$	267.1026674	267.10263	0.1399458
$C_{16}H_{15}N_2O_2$	267.1139008	267.11382	0.3024174
$C_{14}H_{19}O_5$	267.1237966	267.12372	0.2866832
$C_{13}H_{19}N_2O_4$	267.13503	267.13494	0.336833
$C_{15}H_{23}O_4$	267.160182	267.16012	0.2319953
$C_{16}H_{27}O_3$	267.1965674	267.19642	0.5515786
$C_{17}H_{31}O_2$	267.2329528	267.23291	0.1600847
$C_{15}H_{10}N_1O_4$	268.061531	268.06149	0.152875
$C_{12}H_{14}N_1O_6$	268.0826602	268.08266	0.0006711
$C_{16}H_{14}N_1O_3$	268.0979164	268.09789	0.0983965

$C_{13}H_{18}N_1O_5$	268.1190456	268.11903	0.0581081
$C_{17}H_{18}N_1O_2$	268.1343018	268.13427	0.1185223
$C_{14}H_{22}N_1O_4$	268.155431	268.15545	-0.070929
$C_{15}H_9O_5$	269.0455466	269.04557	-0.087049
$C_{12}H_{13}O_7$	269.0666758	269.06672	-0.164346
$C_{11}H_{13}N_2O_6$	269.0779092	269.078	-0.337523
$C_{16}H_{13}O_4$	269.081932	269.08199	-0.215622
$C_{15}H_{13}N_2O_3$	269.0931654	269.09325	-0.314464
$C_{13}H_{17}O_6$	269.1030612	269.10313	-0.255739
$C_{17}H_{17}O_3$	269.1183174	269.11839	-0.269845
$C_{16}H_{17}N_2O_2$	269.1295508	269.12954	0.0400547
$C_{14}H_{21}O_5$	269.1394466	269.13952	-0.272796
$C_{15}H_{25}O_4$	269.175832	269.17584	-0.029795
$C_{16}H_{29}O_3$	269.2122174	269.21219	0.1017038
$C_{17}H_{33}O_2$	269.2486028	269.24863	-0.101097
$C_{14}H_8N_1O_5$	270.0407956	270.04086	-0.238557
$C_{11}H_{12}N_1O_7$	270.0619248	270.06203	-0.389615
$C_{15}H_{12}N_1O_4$	270.077181	270.07719	-0.033398
$C_{12}H_{16}N_1O_6$	270.0983102	270.09835	-0.147428
$C_{16}H_{16}N_1O_3$	270.1135664	270.11358	-0.050424
$C_{13}H_{20}N_1O_5$	270.1346956	270.13472	-0.0904
$C_{17}H_{20}N_1O_2$	270.1499518	270.14995	0.0065886
$C_{15}H_{11}O_5$	271.0611966	271.06115	0.1718427
$C_{14}H_{11}N_2O_4$	271.07243	271.07241	0.0737069
$C_{12}H_{15}O_7$	271.0823258	271.08222	0.3902132
$C_{16}H_{15}O_4$	271.097582	271.09752	0.2286258

$C_{15}H_{15}N_2O_3$	271.1088154	271.10877	0.1673863
$C_{13}H_{19}O_6$	271.1187112	271.11864	0.2625415
$C_{17}H_{19}O_3$	271.1339674	271.13389	0.2853936
$C_{16}H_{19}N_2O_2$	271.1452008	271.14511	0.3348018
$C_{14}H_{23}O_5$	271.1550966	271.155	0.3561795
$C_{14}H_{10}N_1O_5$	272.0564456	272.05636	0.3145667
$C_{11}H_{14}N_1O_7$	272.0775748	272.07743	0.5321273
$C_{15}H_{14}N_1O_4$	272.092831	272.09275	0.2976186
$C_{12}H_{18}N_1O_6$	272.1139602	272.11391	0.1844077
$C_{16}H_{18}N_1O_3$	272.1292164	272.12914	0.2806751
$C_{13}H_{22}N_1O_5$	272.1503456	272.15034	0.020503
$C_{17}H_{22}N_1O_2$	272.1656018	272.16546	0.5209325
$C_{14}H_9O_6$	273.0404612	273.04043	0.1141952
$C_{13}H_9N_2O_5$	273.0516946	273.05172	-0.093096
$C_{11}H_{13}O_8$	273.0615904	273.06159	0.0013913
$C_{15}H_{13}O_5$	273.0768466	273.07683	0.0607151
$C_{14}H_{13}N_2O_4$	273.08808	273.08803	0.1830175
$C_{12}H_{17}O_7$	273.0979758	273.09794	0.1310149
$C_{16}H_{17}O_4$	273.113232	273.11322	0.0438642
$C_{15}H_{17}N_2O_3$	273.1244654	273.12444	0.0929243
$C_{13}H_{21}O_6$	273.1343612	273.13437	-0.032292
$C_{17}H_{21}O_3$	273.1496174	273.14965	-0.119422
$C_{16}H_{21}N_2O_2$	273.1608508	273.16088	-0.10697
$C_{14}H_{25}O_5$	273.1707466	273.17069	0.2071228
$C_{15}H_{29}O_4$	273.207132	273.20723	-0.358776
$C_{10}H_{12}N_1O_8$	274.0568394	274.05691	-0.257684

C ₁₄ H ₁₂ N ₁ O ₅	274.0720956	274.07217	-0.271535
C ₁₅ H ₁₆ N ₁ O ₄	274.108481	274.10854	-0.215317
C ₁₆ H ₂₀ N ₁ O ₃	274.1448664	274.14493	-0.232067
C ₁₄ H ₁₁ O ₆	275.0561112	275.05615	-0.141135
C ₁₃ H ₁₁ N ₂ O ₅	275.0673446	275.06736	-0.056059
C ₆ H ₁₅ N ₂ O ₁₀	275.0732176	275.07325	-0.11786
C ₁₅ H ₁₅ O ₅	275.0924966	275.09253	-0.121487
C ₁₄ H ₁₅ N ₂ O ₄	275.10373	275.10379	-0.218173
C ₁₂ H ₁₉ O ₇	275.1136258	275.11369	-0.233431
C ₁₆ H ₁₉ O ₄	275.128882	275.1289	-0.065497
C ₁₅ H ₁₉ N ₂ O ₃	275.1401154	275.14014	-0.089482
C ₁₇ H ₂₃ O ₃	275.1652674	275.16532	-0.191231
C ₁₄ H ₁₄ N ₁ O ₅	276.0877456	276.08773	0.056431
C ₁₅ H ₁₈ N ₁ O ₄	276.124131	276.12411	0.07598
C ₁₆ H ₂₂ N ₁ O ₃	276.1605164	276.16048	0.1317346
C ₁₄ H ₁₃ O ₆	277.0717612	277.07169	0.2569006
C ₁₃ H ₁₃ N ₂ O ₅	277.0829946	277.08289	0.3774317
C ₁₈ H ₁₃ O ₃	277.0870174	277.08701	0.0266339
C ₁₅ H ₁₇ O ₅	277.1081466	277.10806	0.3124408
C ₁₄ H ₁₇ N ₂ O ₄	277.11938	277.11928	0.3607828
C ₁₆ H ₂₁ O ₄	277.144532	277.14445	0.295802
C ₁₅ H ₂₁ N ₂ O ₃	277.1557654	277.15565	0.4162998
C ₁₃ H ₁₂ N ₁ O ₆	278.0670102	278.06696	0.1804597
C ₁₇ H ₁₂ N ₁ O ₃	278.0822664	278.08218	0.3106271
C ₁₄ H ₁₆ N ₁ O ₅	278.1033956	278.10334	0.1998534
C ₁₈ H ₁₆ N ₁ O ₂	278.1186518	278.1186	0.1861792

$C_{15}H_{20}N_1O_4$	278.139781	278.13974	0.1473356
$C_{16}H_{24}N_1O_3$	278.1761664	278.17609	0.2745738
$C_{13}H_{11}O_7$	279.0510258	279.05098	0.1640557
$C_{16}H_{11}N_2O_3$	279.0775154	279.07743	0.3059361
$C_{14}H_{15}O_6$	279.0874112	279.08738	0.1117209
$C_{13}H_{15}N_2O_5$	279.0986446	279.09861	0.1238985
$C_{18}H_{15}O_3$	279.1026674	279.10272	-0.188533
$C_{17}H_{15}N_2O_2$	279.1139008	279.11388	0.0744495
$C_{15}H_{19}O_5$	279.1237966	279.12378	0.0593998
$C_{14}H_{19}N_2O_4$	279.13503	279.13502	0.0357529
$C_{16}H_{23}O_4$	279.160182	279.1602	-0.064551
$C_{15}H_{23}N_2O_3$	279.1714154	279.17147	-0.195651
$C_{18}H_{31}O_2$	279.2329528	279.23302	-0.240731
$C_{16}H_{10}N_1O_4$	280.061531	280.06155	-0.067914
$C_{13}H_{14}N_1O_6$	280.0826602	280.08266	0.0006423
$C_{17}H_{14}N_1O_3$	280.0979164	280.09797	-0.191433
$C_{14}H_{18}N_1O_5$	280.1190456	280.11909	-0.158576
$C_{18}H_{18}N_1O_2$	280.1343018	280.13436	-0.207829
$C_{15}H_{22}N_1O_4$	280.155431	280.15548	-0.174975
$C_{13}H_{13}O_7$	281.0666758	281.06677	-0.335223
$C_{12}H_{13}N_2O_6$	281.0779092	281.07798	-0.251959
$C_{17}H_{13}O_4$	281.081932	281.08201	-0.277571
$C_{16}H_{13}N_2O_3$	281.0931654	281.09323	-0.229889
$C_{14}H_{17}O_6$	281.1030612	281.10314	-0.280396
$C_{13}H_{17}N_2O_5$	281.1142946	281.11435	-0.197144
$C_{18}H_{17}O_3$	281.1183174	281.11844	-0.436187

$C_{17}H_{17}N_2O_2$	281.1295508	281.1296	-0.17508
$C_{15}H_{21}O_5$	281.1394466	281.13952	-0.261152
$C_{14}H_{21}N_2O_4$	281.15068	281.15073	-0.177912
$C_{16}H_{25}O_4$	281.175832	281.17588	-0.170783
$C_{18}H_{33}O_2$	281.2486028	281.24865	-0.167895
$C_{15}H_8N_1O_5$	282.0407956	282.04088	-0.299319
$C_{12}H_{12}N_1O_7$	282.0619248	282.06203	-0.373039
$C_{16}H_{12}N_1O_4$	282.077181	282.07726	-0.280136
$C_{13}H_{16}N_1O_6$	282.0983102	282.09839	-0.282951
$C_{17}H_{16}N_1O_3$	282.1135664	282.11362	-0.190066
$C_{14}H_{20}N_1O_5$	282.1346956	282.13474	-0.157443
$C_{18}H_{20}N_1O_2$	282.1499518	282.15001	-0.206345
$C_{16}H_{11}O_5$	283.0611966	283.06124	-0.153395
$C_{15}H_{11}N_2O_4$	283.07243	283.07246	-0.106051
$C_{13}H_{15}O_7$	283.0823258	283.08235	-0.085559
$C_{12}H_{15}N_2O_6$	283.0935592	283.09364	-0.285489
$C_{17}H_{15}O_4$	283.097582	283.09761	-0.098977
$C_{16}H_{15}N_2O_3$	283.1088154	283.10887	-0.19293
$C_{14}H_{19}O_6$	283.1187112	283.11872	-0.031153
$C_{13}H_{19}N_2O_5$	283.1299446	283.1299	0.1574539
$C_{18}H_{19}O_3$	283.1339674	283.13399	-0.079892
$C_{17}H_{19}N_2O_2$	283.1452008	283.14521	-0.032563
$C_{15}H_{23}O_5$	283.1550966	283.15509	0.0232378
$C_{18}H_{35}O_2$	283.2642528	283.2642	0.1863274
$C_{15}H_{10}N_1O_5$	284.0564456	284.05645	-0.015561
$C_{12}H_{14}N_1O_7$	284.0775748	284.07759	-0.053577

C ₁₆ H ₁₄ N ₁ O ₄	284.092831	284.09281	0.0738487
C ₁₃ H ₁₈ N ₁ O ₆	284.1139602	284.11394	0.0710275
C ₁₇ H ₁₈ N ₁ O ₃	284.1292164	284.12919	0.0928447
C ₁₄ H ₂₂ N ₁ O ₅	284.1503456	284.15033	0.0548298
C ₁₅ H ₉ O ₆	285.0404612	285.04045	0.0392222
C ₁₆ H ₁₃ O ₅	285.0768466	285.0768	0.1633942
C ₁₅ H ₁₃ N ₂ O ₄	285.08808	285.08801	0.2454676
C ₁₃ H ₁₇ O ₇	285.0979758	285.09791	0.2307273
C ₁₂ H ₁₇ N ₂ O ₆	285.1092092	285.10915	0.2075692
C ₁₇ H ₁₇ O ₄	285.113232	285.11316	0.2524607
C ₁₆ H ₁₇ N ₂ O ₃	285.1244654	285.12439	0.2643754
C ₁₄ H ₂₁ O ₆	285.1343612	285.13429	0.2496363
C ₁₈ H ₂₁ O ₃	285.1496174	285.14956	0.2012273
C ₁₇ H ₂₁ N ₂ O ₂	285.1608508	285.16076	0.3183463
C ₁₅ H ₂₅ O ₅	285.1707466	285.17069	0.1984071
C ₁₆ H ₂₉ O ₄	285.207132	285.20705	0.2874399
C ₁₅ H ₁₂ N ₁ O ₅	286.0720956	286.07201	0.299155
C ₁₂ H ₁₆ N ₁ O ₇	286.0932248	286.09312	0.3662439
C ₁₆ H ₁₆ N ₁ O ₄	286.108481	286.10839	0.3179909
C ₁₃ H ₂₀ N ₁ O ₆	286.1296102	286.12951	0.3501207
C ₁₇ H ₂₀ N ₁ O ₃	286.1448664	286.14479	0.2669274
C ₁₄ H ₂₄ N ₁ O ₅	286.1659956	286.16597	0.0893883
C ₁₅ H ₁₁ O ₆	287.0561112	287.05605	0.2131287
C ₁₄ H ₁₁ N ₂ O ₅	287.0673446	287.06719	0.5384796
C ₁₂ H ₁₅ O ₈	287.0772404	287.07729	-0.172846
C ₁₆ H ₁₅ O ₅	287.0924966	287.09242	0.266743

C ₁₅ H ₁₅ N ₂ O ₄	287.10373	287.10366	0.2437443
C ₁₃ H ₁₉ O ₇	287.1136258	287.11356	0.2291076
C ₁₇ H ₁₉ O ₄	287.128882	287.12881	0.2506885
C ₁₆ H ₁₉ N ₂ O ₃	287.1401154	287.14006	0.1928672
C ₁₄ H ₂₃ O ₆	287.1500112	287.14994	0.247884
C ₁₅ H ₂₇ O ₅	287.1863966	287.18641	-0.04673
C ₁₆ H ₃₁ O ₄	287.222782	287.22272	0.2157903
C ₁₄ H ₁₀ N ₁ O ₆	288.0513602	288.05127	0.3130688
C ₁₁ H ₁₄ N ₁ O ₈	288.0724894	288.07248	0.0325609
C ₁₅ H ₁₄ N ₁ O ₅	288.0877456	288.08767	0.2623503
C ₁₆ H ₁₈ N ₁ O ₄	288.124131	288.12408	0.1769373
C ₁₇ H ₂₂ N ₁ O ₃	288.1605164	288.16049	0.0915459
C ₁₄ H ₉ O ₇	289.0353758	289.03529	0.2967799
C ₁₅ H ₁₃ O ₆	289.0717612	289.07169	0.2462361
C ₁₄ H ₁₃ N ₂ O ₅	289.0829946	289.08298	0.050435
C ₁₂ H ₁₇ O ₈	289.0928904	289.09286	0.105087
C ₁₆ H ₁₇ O ₅	289.1081466	289.1081	0.1611158
C ₁₅ H ₁₇ N ₂ O ₄	289.11938	289.11934	0.1382816
C ₁₃ H ₂₁ O ₇	289.1292758	289.12929	-0.049182
C ₁₇ H ₂₁ O ₄	289.144532	289.1445	0.1106018
C ₁₄ H ₂₅ O ₆	289.1656612	289.16561	0.1769916
C ₁₈ H ₂₅ O ₃	289.1809174	289.18085	0.2330026
C ₁₄ H ₁₂ N ₁ O ₆	290.0670102	290.067	0.035095
C ₁₅ H ₁₆ N ₁ O ₅	290.1033956	290.10337	0.0881751
C ₁₆ H ₂₀ N ₁ O ₄	290.139781	290.13976	0.0723096
C ₁₇ H ₂₄ N ₁ O ₃	290.1761664	290.17619	-0.081399

C ₁₄ H ₁₁ O ₇	291.0510258	291.05098	0.1572917
C ₁₅ H ₁₅ O ₆	291.0874112	291.08741	0.0040534
C ₁₄ H ₁₅ N ₂ O ₅	291.0986446	291.09862	0.0844384
C ₁₆ H ₁₉ O ₅	291.1237966	291.12379	0.0226017
C ₁₅ H ₁₉ N ₂ O ₄	291.13503	291.13506	-0.103114
C ₁₇ H ₂₃ O ₄	291.160182	291.1602	-0.061891
C ₁₄ H ₁₄ N ₁ O ₆	292.0826602	292.08266	0.0006159
C ₁₈ H ₁₄ N ₁ O ₃	292.0979164	292.09794	-0.080864
C ₁₅ H ₁₈ N ₁ O ₅	292.1190456	292.11907	-0.083596
C ₁₉ H ₁₈ N ₁ O ₂	292.1343018	292.13429	0.0403236
C ₁₆ H ₂₂ N ₁ O ₄	292.155431	292.15547	-0.133559
C ₁₇ H ₂₆ N ₁ O ₃	292.1918164	292.19188	-0.217734
C ₁₄ H ₁₃ O ₇	293.0666758	293.06668	-0.0144
C ₁₃ H ₁₃ N ₂ O ₆	293.0779092	293.07803	-0.412246
C ₁₈ H ₁₃ O ₄	293.081932	293.08192	0.0408756
C ₁₇ H ₁₃ N ₂ O ₃	293.0931654	293.09322	-0.186357
C ₁₅ H ₁₇ O ₆	293.1030612	293.10311	-0.166563
C ₁₄ H ₁₇ N ₂ O ₅	293.1142946	293.11437	-0.257306
C ₁₉ H ₁₇ O ₃	293.1183174	293.11835	-0.111286
C ₁₈ H ₁₇ N ₂ O ₂	293.1295508	293.12958	-0.099683
C ₁₆ H ₂₁ O ₅	293.1394466	293.13952	-0.250461
C ₁₅ H ₂₁ N ₂ O ₄	293.15068	293.15078	-0.34119
C ₁₇ H ₂₅ O ₄	293.175832	293.17592	-0.30023
C ₁₈ H ₂₉ O ₃	293.2122174	293.21228	-0.213566
C ₁₃ H ₁₂ N ₁ O ₇	294.0619248	294.06193	-0.017752
C ₁₇ H ₁₂ N ₁ O ₄	294.077181	294.07723	-0.166691

C ₁₄ H ₁₆ N ₁ O ₆	294.0983102	294.0984	-0.305408
C ₁₈ H ₁₆ N ₁ O ₃	294.1135664	294.11362	-0.182311
C ₁₅ H ₂₀ N ₁ O ₅	294.1346956	294.13479	-0.32101
C ₁₉ H ₂₀ N ₁ O ₂	294.1499518	294.15005	-0.333912
C ₁₆ H ₂₄ N ₁ O ₄	294.171081	294.17114	-0.200632
C ₁₇ H ₁₁ O ₅	295.0611966	295.06129	-0.316613
C ₁₆ H ₁₁ N ₂ O ₄	295.07243	295.07241	0.0677118
C ₁₄ H ₁₅ O ₇	295.0823258	295.08237	-0.149857
C ₁₃ H ₁₅ N ₂ O ₆	295.0935592	295.09361	-0.172217
C ₁₈ H ₁₅ O ₄	295.097582	295.09766	-0.264387
C ₁₇ H ₁₅ N ₂ O ₃	295.1088154	295.1089	-0.286742
C ₁₅ H ₁₉ O ₆	295.1187112	295.11879	-0.267079
C ₁₄ H ₁₉ N ₂ O ₅	295.1299446	295.13001	-0.221665
C ₁₉ H ₁₉ O ₃	295.1339674	295.13406	-0.313824
C ₁₈ H ₁₉ N ₂ O ₂	295.1452008	295.14533	-0.437819
C ₁₆ H ₂₃ O ₅	295.1550966	295.15517	-0.248751
C ₁₅ H ₂₃ N ₂ O ₄	295.16633	295.16643	-0.33886
C ₁₇ H ₂₇ O ₄	295.191482	295.19159	-0.365932
C ₁₈ H ₃₁ O ₃	295.2278674	295.22806	-0.652446
C ₁₆ H ₁₀ N ₁ O ₅	296.0564456	296.05649	-0.150039
C ₁₃ H ₁₄ N ₁ O ₇	296.0775748	296.07767	-0.321605
C ₁₇ H ₁₄ N ₁ O ₄	296.092831	296.09289	-0.19933
C ₁₄ H ₁₈ N ₁ O ₆	296.1139602	296.11403	-0.235788
C ₁₈ H ₁₈ N ₁ O ₃	296.1292164	296.12931	-0.316146
C ₁₅ H ₂₂ N ₁ O ₅	296.1503456	296.15045	-0.352592
C ₁₃ H ₁₃ O ₈	297.0615904	297.06171	-0.402678

$C_{17}H_{13}O_5$	297.0768466	297.07692	-0.247142
$C_{16}H_{13}N_2O_4$	297.08808	297.08818	-0.336668
$C_{14}H_{17}O_7$	297.0979758	297.09807	-0.317135
$C_{13}H_{17}N_2O_6$	297.1092092	297.10931	-0.339337
$C_{18}H_{17}O_4$	297.113232	297.11329	-0.195279
$C_{17}H_{17}N_2O_3$	297.1244654	297.12451	-0.150173
$C_{15}H_{21}O_6$	297.1343612	297.13444	-0.265268
$C_{19}H_{21}O_3$	297.1496174	297.14971	-0.311695
$C_{16}H_{25}O_5$	297.1707466	297.17082	-0.247064
$C_{17}H_{29}O_4$	297.207132	297.20718	-0.161571
$C_{18}H_{33}O_3$	297.2435174	297.24356	-0.143384
$C_{16}H_{12}N_1O_5$	298.0720956	298.07214	-0.149025
$C_{13}H_{16}N_1O_7$	298.0932248	298.09329	-0.218791
$C_{17}H_{16}N_1O_4$	298.108481	298.10856	-0.265072
$C_{14}H_{20}N_1O_6$	298.1296102	298.12971	-0.334821
$C_{18}H_{20}N_1O_3$	298.1448664	298.14494	-0.246927
$C_{15}H_{24}N_1O_5$	298.1659956	298.16601	-0.048363
$C_{16}H_{11}O_6$	299.0561112	299.05618	-0.230124
$C_{15}H_{11}N_2O_5$	299.0673446	299.06736	-0.051561
$C_8H_{15}N_2O_{10}$	299.0732176	299.07333	-0.375895
$C_{13}H_{15}O_8$	299.0772404	299.07734	-0.333092
$C_{17}H_{15}O_5$	299.0924966	299.09256	-0.212042
$C_{16}H_{15}N_2O_4$	299.10373	299.10382	-0.300966
$C_{14}H_{19}O_7$	299.1136258	299.11372	-0.314998
$C_{13}H_{19}N_2O_6$	299.1248592	299.12495	-0.303619
$C_{18}H_{19}O_4$	299.128882	299.12894	-0.193964

C ₁₇ H ₁₉ N ₂ O ₃	299.1401154	299.14019	-0.249449
C ₁₅ H ₂₃ O ₆	299.1500112	299.15009	-0.26348
C ₁₆ H ₂₇ O ₅	299.1863966	299.18646	-0.211975
C ₁₂ H ₁₄ N ₁ O ₈	300.0724894	300.07263	-0.46862
C ₁₆ H ₁₄ N ₁ O ₅	300.0877456	300.08779	-0.148024
C ₁₃ H ₁₈ N ₁ O ₇	300.1088748	300.10901	-0.45057
C ₁₇ H ₁₈ N ₁ O ₄	300.124131	300.1242	-0.229972
C ₁₄ H ₂₂ N ₁ O ₆	300.1452602	300.14538	-0.399207
C ₁₈ H ₂₂ N ₁ O ₃	300.1605164	300.16058	-0.211954
C ₁₆ H ₁₃ O ₆	301.0717612	301.0718	-0.12894
C ₁₅ H ₁₃ N ₂ O ₅	301.0829946	301.08304	-0.150856
C ₈ H ₁₇ N ₂ O ₁₀	301.0888676	301.08891	-0.140889
C ₁₃ H ₁₇ O ₈	301.0928904	301.09291	-0.065163
C ₁₂ H ₁₇ N ₂ O ₇	301.1041238	301.10411	0.0457646
C ₁₇ H ₁₇ O ₅	301.1081466	301.10818	-0.11099
C ₁₆ H ₁₇ N ₂ O ₄	301.11938	301.11946	-0.265742
C ₁₄ H ₂₁ O ₇	301.1292758	301.12936	-0.279681
C ₁₈ H ₂₁ O ₄	301.144532	301.14461	-0.259079
C ₁₇ H ₂₁ N ₂ O ₃	301.1557654	301.15587	-0.347395
C ₁₅ H ₂₅ O ₆	301.1656612	301.16574	-0.261717
C ₁₅ H ₁₂ N ₁ O ₆	302.0670102	302.06702	-0.03251
C ₁₆ H ₁₆ N ₁ O ₅	302.1033956	302.10341	-0.047732
C ₁₇ H ₂₀ N ₁ O ₄	302.139781	302.13985	-0.228438
C ₁₈ H ₂₄ N ₁ O ₃	302.1761664	302.17623	-0.21054
C ₁₅ H ₁₁ O ₇	303.0510258	303.05106	-0.112919
C ₁₆ H ₁₅ O ₆	303.0874112	303.08741	0.0038929

$C_{15}H_{15}N_2O_5$	303.0986446	303.09868	-0.11686
$C_8H_{19}N_2O_{10}$	303.1045176	303.10458	-0.205936
$C_{13}H_{19}O_8$	303.1085404	303.10852	0.0672363
$C_{17}H_{19}O_5$	303.1237966	303.12381	-0.044273
$C_{16}H_{19}N_2O_4$	303.13503	303.13504	-0.033055
$C_{14}H_{23}O_7$	303.1449258	303.14502	-0.310809
$C_{18}H_{23}O_4$	303.160182	303.16022	-0.125413
$C_{17}H_{23}N_2O_3$	303.1714154	303.17152	-0.345086
$C_{15}H_{27}O_6$	303.1813112	303.18137	-0.19401
$C_{15}H_{14}N_1O_6$	304.0826602	304.08263	0.099249
$C_{16}H_{18}N_1O_5$	304.1190456	304.11904	0.0183477
$C_{17}H_{22}N_1O_4$	304.155431	304.15543	0.0032217
$C_{18}H_{26}N_1O_3$	304.1918164	304.19185	-0.110523
$C_{14}H_9O_8$	305.0302904	305.03047	-0.58886
$C_{15}H_{13}O_7$	305.0666758	305.06663	0.1500652
$C_{16}H_{17}O_6$	305.1030612	305.10302	0.1349705
$C_{15}H_{17}N_2O_5$	305.1142946	305.11423	0.2116581
$C_{17}H_{21}O_5$	305.1394466	305.13944	0.0215636
$C_{16}H_{21}N_2O_4$	305.15068	305.15059	0.2948704
$C_{18}H_{25}O_4$	305.175832	305.17587	-0.124584
$C_{14}H_{12}N_1O_7$	306.0619248	306.06192	0.0156174
$C_{18}H_{12}N_1O_4$	306.077181	306.07706	0.3952595
$C_{15}H_{16}N_1O_6$	306.0983102	306.09825	0.1966032
$C_{19}H_{16}N_1O_3$	306.1135664	306.11347	0.3148501
$C_{16}H_{20}N_1O_5$	306.1346956	306.13466	0.116223
$C_{17}H_{24}N_1O_4$	306.171081	306.17108	0.0032005

$C_{18}H_{28}N_1O_3$	306.2074664	306.20747	-0.011822
$C_{17}H_{11}N_2O_4$	307.07243	307.07227	0.5209843
$C_{15}H_{15}O_7$	307.0823258	307.08225	0.2467739
$C_{14}H_{15}N_2O_6$	307.0935592	307.0935	0.1927097
$C_{19}H_{15}O_4$	307.097582	307.09756	0.071573
$C_{18}H_{15}N_2O_3$	307.1088154	307.10868	0.4408206
$C_{16}H_{19}O_6$	307.1187112	307.11866	0.1666453
$C_{15}H_{19}N_2O_5$	307.1299446	307.12993	0.0474714
$C_{19}H_{19}N_2O_2$	307.1452008	307.14509	0.360676
$C_{17}H_{23}O_5$	307.1550966	307.15506	0.1190926
$C_{16}H_{23}N_2O_4$	307.16633	307.16633	-6.54E-05
$C_{18}H_{27}O_4$	307.191482	307.19144	0.1366571
$C_{17}H_{10}N_1O_5$	308.0564456	308.05624	0.6673449
$C_{14}H_{14}N_1O_7$	308.0775748	308.07749	0.2751901
$C_{18}H_{14}N_1O_4$	308.092831	308.09277	0.197927
$C_{15}H_{18}N_1O_6$	308.1139602	308.11387	0.2926836
$C_{19}H_{18}N_1O_3$	308.1292164	308.12919	0.0856131
$C_{16}H_{22}N_1O_5$	308.1503456	308.15025	0.3101729
$C_{17}H_{26}N_1O_4$	308.186731	308.18659	0.4574496
$C_{14}H_{13}O_8$	309.0615904	309.06148	0.3571453
$C_{18}H_{13}O_5$	309.0768466	309.07675	0.3124786
$C_{17}H_{13}N_2O_4$	309.08808	309.08795	0.4205271
$C_{15}H_{17}O_7$	309.0979758	309.09788	0.3098691
$C_{14}H_{17}N_2O_6$	309.1092092	309.10922	-0.035004
$C_{19}H_{17}O_4$	309.113232	309.11318	0.1681581
$C_{18}H_{17}N_2O_3$	309.1244654	309.12439	0.2438497

$C_{16}H_{21}O_6$	309.1343612	309.13427	0.2949523
$C_{15}H_{21}N_2O_5$	309.1455946	309.14555	0.1442036
$C_{19}H_{21}N_2O_2$	309.1608508	309.16072	0.4230157
$C_{17}H_{25}O_5$	309.1707466	309.17065	0.3123837
$C_{18}H_{29}O_4$	309.207132	309.20704	0.2974702
$C_{17}H_{12}N_1O_5$	310.0720956	310.07204	0.1792483
$C_{14}H_{16}N_1O_7$	310.0932248	310.09316	0.2089046
$C_{18}H_{16}N_1O_4$	310.108481	310.10839	0.2933809
$C_{15}H_{20}N_1O_6$	310.1296102	310.12953	0.2585367
$C_{19}H_{20}N_1O_3$	310.1448664	310.14476	0.3430007
$C_{16}H_{24}N_1O_5$	310.1659956	310.1659	0.3081572
$C_{17}H_{11}O_6$	311.0561112	311.05613	-0.060504
$C_9H_{15}N_2O_{10}$	311.0732176	311.07316	0.1851008
$C_{14}H_{15}O_8$	311.0772404	311.07719	0.161953
$C_{13}H_{15}N_2O_7$	311.0884738	311.0885	-0.084285
$C_{18}H_{15}O_5$	311.0924966	311.09246	0.1175853
$C_{17}H_{15}N_2O_4$	311.10373	311.10368	0.1606535
$C_{15}H_{19}O_7$	311.1136258	311.11357	0.1792911
$C_{14}H_{19}N_2O_6$	311.1248592	311.12481	0.1580713
$C_{19}H_{19}O_4$	311.128882	311.12883	0.1670687
$C_{18}H_{19}N_2O_3$	311.1401154	311.14008	0.1137105
$C_{16}H_{23}O_6$	311.1500112	311.14994	0.2287639
$C_{17}H_{27}O_5$	311.1863966	311.18633	0.213955
$C_{18}H_{31}O_4$	311.222782	311.22269	0.2955436
$C_{13}H_{14}N_1O_8$	312.0724894	312.07249	-0.001987
$C_{17}H_{14}N_1O_5$	312.0877456	312.08775	-0.014163

C ₁₄ H ₁₈ N ₁ O ₇	312.1088748	312.10891	-0.112846
C ₁₈ H ₁₈ N ₁ O ₄	312.124131	312.12412	0.035178
C ₁₅ H ₂₂ N ₁ O ₆	312.1452602	312.14526	0.0005763
C ₁₉ H ₂₂ N ₁ O ₃	312.1605164	312.1605	0.0524727
C ₁₇ H ₁₃ O ₆	313.0717612	313.07182	-0.187881
C ₁₆ H ₁₃ N ₂ O ₅	313.0829946	313.08311	-0.368657
C ₉ H ₁₇ N ₂ O ₁₀	313.0888676	313.08896	-0.295188
C ₁₄ H ₁₇ O ₈	313.0928904	313.09297	-0.254302
C ₁₃ H ₁₇ N ₂ O ₇	313.1041238	313.10409	0.1078871
C ₁₈ H ₁₇ O ₅	313.1081466	313.10818	-0.106737
C ₁₇ H ₁₇ N ₂ O ₄	313.11938	313.11942	-0.127811
C ₁₅ H ₂₁ O ₇	313.1292758	313.12929	-0.045413
C ₁₉ H ₂₁ O ₄	313.144532	313.14455	-0.057546
C ₁₈ H ₂₁ N ₂ O ₃	313.1557654	313.15581	-0.142485
C ₁₆ H ₂₅ O ₆	313.1656612	313.16568	-0.060096
C ₁₇ H ₂₉ O ₅	313.2020466	313.20211	-0.202489
C ₁₈ H ₃₃ O ₄	313.238432	313.23843	0.0063207
C ₁₆ H ₁₂ N ₁ O ₆	314.0670102	314.06707	-0.190469
C ₁₃ H ₁₆ N ₁ O ₈	314.0881394	314.0883	-0.511385
C ₁₇ H ₁₆ N ₁ O ₅	314.1033956	314.10346	-0.205092
C ₁₄ H ₂₀ N ₁ O ₇	314.1245248	314.12464	-0.366798
C ₁₈ H ₂₀ N ₁ O ₄	314.139781	314.13986	-0.251544
C ₁₉ H ₂₄ N ₁ O ₃	314.1761664	314.17624	-0.234327
C ₁₆ H ₁₁ O ₇	315.0510258	315.05106	-0.108618
C ₁₇ H ₁₅ O ₆	315.0874112	315.0875	-0.28189
C ₁₆ H ₁₅ N ₂ O ₅	315.0986446	315.09871	-0.207618

C ₉ H ₁₉ N ₂ O ₁₀	315.1045176	315.10461	-0.2933
C ₁₄ H ₁₉ O ₈	315.1085404	315.10863	-0.28441
C ₁₈ H ₁₉ O ₅	315.1237966	315.12388	-0.264722
C ₁₇ H ₁₉ N ₂ O ₄	315.13503	315.13514	-0.349121
C ₁₅ H ₂₃ O ₇	315.1449258	315.14506	-0.4259
C ₁₉ H ₂₃ O ₄	315.160182	315.16033	-0.469666
C ₁₈ H ₂₃ N ₂ O ₃	315.1714154	315.17145	-0.109845
C ₁₆ H ₂₇ O ₆	315.1813112	315.18142	-0.345262
C ₁₇ H ₃₁ O ₅	315.2176966	315.21779	-0.296367
C ₁₆ H ₁₄ N ₁ O ₆	316.0826602	316.08265	0.0322064
C ₁₃ H ₁₈ N ₁ O ₈	316.1037894	316.1039	-0.349949
C ₁₇ H ₁₈ N ₁ O ₅	316.1190456	316.11905	-0.013982
C ₁₈ H ₂₂ N ₁ O ₄	316.155431	316.15548	-0.155051
C ₁₆ H ₁₃ O ₇	317.0666758	317.0666	0.239003
C ₁₅ H ₁₃ N ₂ O ₆	317.0779092	317.07785	0.1866415
C ₁₇ H ₁₇ O ₆	317.1030612	317.10299	0.2244693
C ₁₆ H ₁₇ N ₂ O ₅	317.1142946	317.11424	0.1721143
C ₉ H ₂₁ N ₂ O ₁₀	317.1201676	317.12017	-0.007631
C ₁₄ H ₂₁ O ₈	317.1241904	317.1241	0.2849984
C ₁₈ H ₂₁ O ₅	317.1394466	317.1394	0.1468751
C ₁₇ H ₂₁ N ₂ O ₄	317.15068	317.15061	0.2206519
C ₁₉ H ₂₅ O ₄	317.175832	317.17569	0.4476378
C ₁₈ H ₂₅ N ₂ O ₃	317.1870654	317.18687	0.6159769
C ₁₉ H ₁₂ N ₁ O ₄	318.077181	318.07706	0.3803476
C ₁₆ H ₁₆ N ₁ O ₆	318.0983102	318.09822	0.2834969
C ₁₇ H ₂₀ N ₁ O ₅	318.1346956	318.13459	0.3318717

$C_{18}H_{24}N_1O_4$	318.171081	318.17101	0.2230872
$C_{16}H_{15}O_7$	319.0823258	319.08223	0.300173
$C_{15}H_{15}N_2O_6$	319.0935592	319.09351	0.1541238
$C_{20}H_{15}O_4$	319.097582	319.09746	0.3822652
$C_8H_{19}N_2O_{11}$	319.0994322	319.09937	0.1948606
$C_{17}H_{19}O_6$	319.1187112	319.11859	0.379733
$C_{16}H_{19}N_2O_5$	319.1299446	319.12981	0.4217088
$C_{18}H_{23}O_5$	319.1550966	319.155	0.3026112
$C_{17}H_{23}N_2O_4$	319.16633	319.16618	0.4699114
$C_{18}H_{10}N_1O_5$	320.0564456	320.0564	0.1424121
$C_{15}H_{14}N_1O_7$	320.0775748	320.07753	0.1399033
$C_{19}H_{14}N_1O_4$	320.092831	320.0928	0.0967841
$C_{16}H_{18}N_1O_6$	320.1139602	320.11391	0.1567564
$C_{20}H_{18}N_1O_3$	320.1292164	320.12914	0.2385908
$C_{17}H_{22}N_1O_5$	320.1503456	320.15031	0.111135
$C_{18}H_{26}N_1O_4$	320.186731	320.18666	0.2216828
$C_{15}H_{13}O_8$	321.0615904	321.06159	0.0011833
$C_{14}H_{13}N_2O_7$	321.0728238	321.07293	-0.330829
$C_{19}H_{13}O_5$	321.0768466	321.0769	-0.166378
$C_{18}H_{13}N_2O_4$	321.08808	321.08818	-0.311504
$C_{16}H_{17}O_7$	321.0979758	321.098	-0.075429
$C_{15}H_{17}N_2O_6$	321.1092092	321.10918	0.0908722
$C_{20}H_{17}O_4$	321.113232	321.11327	-0.118401
$C_{19}H_{17}N_2O_3$	321.1244654	321.12449	-0.076668
$C_{17}H_{21}O_6$	321.1343612	321.13438	-0.058605
$C_{16}H_{21}N_2O_5$	321.1455946	321.14558	0.0453997

$C_{18}H_{25}O_5$	321.1707466	321.17076	-0.041785
$C_{17}H_{25}N_2O_4$	321.18198	321.18195	0.0933424
$C_{18}H_{12}N_1O_5$	322.0720956	322.07219	-0.293164
$C_{15}H_{16}N_1O_7$	322.0932248	322.09333	-0.326676
$C_{19}H_{16}N_1O_4$	322.108481	322.10858	-0.307412
$C_{16}H_{20}N_1O_6$	322.1296102	322.1297	-0.278832
$C_{20}H_{20}N_1O_3$	322.1448664	322.14494	-0.228531
$C_{17}H_{24}N_1O_5$	322.1659956	322.16607	-0.230999
$C_{18}H_{28}N_1O_4$	322.202381	322.2024	-0.059032
$C_{17}H_{11}N_2O_5$	323.0673446	323.06729	0.1689428
$C_{15}H_{15}O_8$	323.0772404	323.07723	0.0321282
$C_{19}H_{15}O_5$	323.0924966	323.09251	-0.041536
$C_{18}H_{15}N_2O_4$	323.10373	323.1038	-0.216711
$C_{16}H_{19}O_7$	323.1136258	323.11366	-0.105907
$C_{15}H_{19}N_2O_6$	323.1248592	323.12498	-0.373911
$C_{20}H_{19}O_4$	323.128882	323.12899	-0.334294
$C_{19}H_{19}N_2O_3$	323.1401154	323.14022	-0.323761
$C_{17}H_{23}O_6$	323.1500112	323.15006	-0.151076
$C_{18}H_{27}O_5$	323.1863966	323.18647	-0.227176
$C_{17}H_{27}N_2O_4$	323.19763	323.1978	-0.526056
$C_{14}H_{14}N_1O_8$	324.0724894	324.07249	-0.001913
$C_{18}H_{14}N_1O_5$	324.0877456	324.08768	0.2023523
$C_{15}H_{18}N_1O_7$	324.1088748	324.10889	-0.04696
$C_{19}H_{18}N_1O_4$	324.124131	324.1241	0.0955804
$C_{16}H_{22}N_1O_6$	324.1452602	324.14525	0.0314054
$C_{20}H_{22}N_1O_3$	324.1605164	324.16048	0.112228

$C_{17}H_{26}N_1O_5$	324.1816456	324.18163	0.0480592
$C_{18}H_{13}O_6$	325.0717612	325.07165	0.3420165
$C_{17}H_{13}N_2O_5$	325.0829946	325.08288	0.3524635
$C_{10}H_{17}N_2O_{10}$	325.0888676	325.08875	0.3616854
$C_{15}H_{17}O_8$	325.0928904	325.09278	0.3395334
$C_{14}H_{17}N_2O_7$	325.1041238	325.10406	0.196183
$C_{19}H_{17}O_5$	325.1081466	325.10804	0.3278291
$C_{18}H_{17}N_2O_4$	325.11938	325.11928	0.3075175
$C_{16}H_{21}O_7$	325.1292758	325.12919	0.2638332
$C_{15}H_{21}N_2O_6$	325.1405092	325.14044	0.2127692
$C_{20}H_{21}O_4$	325.144532	325.14445	0.2521337
$C_{19}H_{21}N_2O_3$	325.1557654	325.15567	0.293336
$C_{17}H_{25}O_6$	325.1656612	325.16555	0.3419177
$C_{18}H_{29}O_5$	325.2020466	325.20195	0.2969843
$C_{17}H_{12}N_1O_6$	326.0670102	326.06692	0.2765686
$C_{14}H_{16}N_1O_8$	326.0881394	326.0881	0.1207646
$C_{18}H_{16}N_1O_5$	326.1033956	326.10328	0.3544272
$C_{15}H_{20}N_1O_7$	326.1245248	326.12445	0.2292986
$C_{19}H_{20}N_1O_4$	326.139781	326.13966	0.3709449
$C_{16}H_{24}N_1O_6$	326.1609102	326.16071	0.6137458
$C_{20}H_{24}N_1O_3$	326.1761664	326.17603	0.4181173
$C_{17}H_{11}O_7$	327.0510258	327.05104	-0.04348
$C_{18}H_{15}O_6$	327.0874112	327.08741	0.0036073
$C_{17}H_{15}N_2O_5$	327.0986446	327.09865	-0.01657
$C_{10}H_{19}N_2O_{10}$	327.1045176	327.10454	-0.068541
$C_{15}H_{19}O_8$	327.1085404	327.10852	0.0623032

$C_{19}H_{19}O_5$	327.1237966	327.12378	0.0506839
$C_{18}H_{19}N_2O_4$	327.13503	327.13503	-6.14E-05
$C_{16}H_{23}O_7$	327.1449258	327.14493	-0.0129
$C_{15}H_{23}N_2O_6$	327.1561592	327.15623	-0.216472
$C_{20}H_{23}O_4$	327.160182	327.16014	0.128316
$C_{19}H_{23}N_2O_3$	327.1714154	327.17138	0.1081387
$C_{17}H_{27}O_6$	327.1813112	327.18132	-0.026958
$C_{18}H_{31}O_5$	327.2176966	327.21765	0.1423514
$C_{17}H_{14}N_1O_6$	328.0826602	328.08276	-0.304253
$C_{14}H_{18}N_1O_8$	328.1037894	328.10384	-0.154281
$C_{18}H_{18}N_1O_5$	328.1190456	328.11911	-0.196331
$C_{15}H_{22}N_1O_7$	328.1401748	328.14019	-0.046383
$C_{19}H_{22}N_1O_4$	328.155431	328.15546	-0.088434
$C_{20}H_{26}N_1O_3$	328.1918164	328.19188	-0.19385
$C_{17}H_{13}O_7$	329.0666758	329.06668	-0.012824
$C_{18}H_{17}O_6$	329.1030612	329.10309	-0.087572
$C_{17}H_{17}N_2O_5$	329.1142946	329.11438	-0.259545
$C_{10}H_{21}N_2O_{10}$	329.1201676	329.12026	-0.28081
$C_{15}H_{21}O_8$	329.1241904	329.12423	-0.12038
$C_{14}H_{21}N_2O_7$	329.1354238	329.13546	-0.110046
$C_{19}H_{21}O_5$	329.1394466	329.13949	-0.13192
$C_{18}H_{21}N_2O_4$	329.15068	329.15073	-0.151967
$C_{16}H_{25}O_7$	329.1605758	329.16064	-0.195103
$C_{20}H_{25}O_4$	329.175832	329.1759	-0.206638
$C_{19}H_{25}N_2O_3$	329.1870654	329.18711	-0.135546
$C_{17}H_{29}O_6$	329.1969612	329.19707	-0.330562

$C_{18}H_{33}O_5$	329.2333466	329.23341	-0.19263
$C_{16}H_{12}N_1O_7$	330.0619248	330.06176	0.4992393
$C_{13}H_{16}N_1O_9$	330.083054	330.08307	-0.048534
$C_{17}H_{16}N_1O_6$	330.0983102	330.09822	0.273191
$C_{14}H_{20}N_1O_8$	330.1194394	330.11934	0.3010423
$C_{18}H_{20}N_1O_5$	330.1346956	330.13462	0.2289366
$C_{15}H_{24}N_1O_7$	330.1558248	330.15578	0.1356326
$C_{19}H_{24}N_1O_4$	330.171081	330.17102	0.1846918
$C_{17}H_{15}O_7$	331.0823258	331.08219	0.4101092
$C_{16}H_{15}N_2O_6$	331.0935592	331.09343	0.3901613
$C_9H_{19}N_2O_{11}$	331.0994322	331.0993	0.3992151
$C_{18}H_{19}O_6$	331.1187112	331.11857	0.4263725
$C_{17}H_{19}N_2O_5$	331.1299446	331.12982	0.3762266
$C_{10}H_{23}N_2O_{10}$	331.1358176	331.1357	0.3550806
$C_{15}H_{23}O_8$	331.1398404	331.13972	0.3635319
$C_{19}H_{23}O_5$	331.1550966	331.15496	0.4124348
$C_{18}H_{23}N_2O_4$	331.16633	331.16623	0.3019024
$C_{16}H_{27}O_7$	331.1762258	331.17621	0.047648
$C_{18}H_{35}O_5$	331.2489966	331.24889	0.3217516
$C_{16}H_{14}N_1O_7$	332.0775748	332.07757	0.0143939
$C_{20}H_{14}N_1O_4$	332.092831	332.09272	0.3341834
$C_{17}H_{18}N_1O_6$	332.1139602	332.11391	0.1510924
$C_{21}H_{18}N_1O_3$	332.1292164	332.12916	0.1697529
$C_{18}H_{22}N_1O_5$	332.1503456	332.15028	0.1974404
$C_{19}H_{26}N_1O_4$	332.186731	332.18664	0.2738818
$C_{16}H_{13}O_8$	333.0615904	333.06148	0.3314099

$C_{15}H_{13}N_2O_7$	333.0728238	333.07295	-0.378956
$C_{17}H_{17}O_7$	333.0979758	333.09803	-0.162775
$C_{16}H_{17}N_2O_6$	333.1092092	333.1092	0.0275582
$C_{21}H_{17}O_4$	333.113232	333.11327	-0.114136
$C_9H_{21}N_2O_{11}$	333.1150822	333.11515	-0.203594
$C_{20}H_{17}N_2O_3$	333.1244654	333.12457	-0.314057
$C_{18}H_{21}O_6$	333.1343612	333.13439	-0.086512
$C_{17}H_{21}N_2O_5$	333.1455946	333.14562	-0.076303
$C_{19}H_{25}O_5$	333.1707466	333.17075	-0.010265
$C_{18}H_{25}N_2O_4$	333.18198	333.18192	0.1800214
$C_{19}H_{12}N_1O_5$	334.0720956	334.07213	-0.103032
$C_{16}H_{16}N_1O_7$	334.0932248	334.09323	-0.015625
$C_{20}H_{16}N_1O_4$	334.108481	334.10852	-0.116789
$C_{17}H_{20}N_1O_6$	334.1296102	334.12967	-0.179033
$C_{21}H_{20}N_1O_3$	334.1448664	334.14496	-0.280178
$C_{18}H_{24}N_1O_5$	334.1659956	334.16606	-0.192779
$C_{19}H_{28}N_1O_4$	334.202381	334.20246	-0.236444
$C_{18}H_{11}N_2O_5$	335.0673446	335.06732	0.0733581
$C_{16}H_{15}O_8$	335.0772404	335.07717	0.2100408
$C_{15}H_{15}N_2O_7$	335.0884738	335.0884	0.2201804
$C_{20}H_{15}O_5$	335.0924966	335.09242	0.2285336
$C_{19}H_{15}N_2O_4$	335.10373	335.10371	0.059623
$C_{17}H_{19}O_7$	335.1136258	335.11356	0.1962913
$C_{16}H_{19}N_2O_6$	335.1248592	335.1248	0.1765906
$C_{21}H_{19}O_4$	335.128882	335.12883	0.1551042
$C_{20}H_{19}N_2O_3$	335.1401154	335.13999	0.3741119

$C_{18}H_{23}O_6$	335.1500112	335.14993	0.2422196
$C_{17}H_{23}N_2O_5$	335.1612446	335.16108	0.4910469
$C_{19}H_{27}O_5$	335.1863966	335.18634	0.1688013
$C_{15}H_{14}N_1O_8$	336.0724894	336.07233	0.4742426
$C_{19}H_{14}N_1O_5$	336.0877456	336.08757	0.5224228
$C_{16}H_{18}N_1O_7$	336.1088748	336.10871	0.4902575
$C_{20}H_{18}N_1O_4$	336.124131	336.12397	0.4789299
$C_{17}H_{22}N_1O_6$	336.1452602	336.14512	0.4170218
$C_{21}H_{22}N_1O_3$	336.1605164	336.16046	0.1677172
$C_{18}H_{26}N_1O_5$	336.1816456	336.18153	0.3438019
$C_{19}H_{13}O_6$	337.0717612	337.07174	0.062835
$C_{18}H_{13}N_2O_5$	337.0829946	337.08301	-0.045746
$C_{11}H_{17}N_2O_{10}$	337.0888676	337.08873	0.4081413
$C_{16}H_{17}O_8$	337.0928904	337.09287	0.0604578
$C_{20}H_{17}O_5$	337.1081466	337.10816	-0.039809
$C_{19}H_{17}N_2O_4$	337.11938	337.11937	0.0296035
$C_{17}H_{21}O_7$	337.1292758	337.12924	0.1061311
$C_{16}H_{21}N_2O_6$	337.1405092	337.14049	0.0568899
$C_{21}H_{21}O_4$	337.144532	337.14453	0.0058726
$C_{20}H_{21}N_2O_3$	337.1557654	337.1558	-0.102683
$C_{18}H_{25}O_6$	337.1656612	337.16565	0.0331585
$C_{19}H_{29}O_5$	337.2020466	337.20194	0.3160713
$C_{18}H_{12}N_1O_6$	338.0670102	338.06718	-0.502327
$C_{15}H_{16}N_1O_8$	338.0881394	338.08826	-0.356771
$C_{19}H_{16}N_1O_5$	338.1033956	338.10347	-0.22011
$C_{16}H_{20}N_1O_7$	338.1245248	338.12462	-0.281613

$C_{20}H_{20}N_1O_4$	338.139781	338.13985	-0.204117
$C_{17}H_{24}N_1O_6$	338.1609102	338.16097	-0.176898
$C_{21}H_{24}N_1O_3$	338.1761664	338.17616	0.0188656
$C_{18}H_{28}N_1O_5$	338.1972956	338.19733	-0.101775
$C_{19}H_{15}O_6$	339.0874112	339.08739	0.0624615
$C_{18}H_{15}N_2O_5$	339.0986446	339.09862	0.072486
$C_{11}H_{19}N_2O_{10}$	339.1045176	339.10446	0.1697999
$C_{16}H_{19}O_8$	339.1085404	339.10851	0.0895875
$C_{15}H_{19}N_2O_7$	339.1197738	339.11963	0.4239797
$C_{20}H_{19}O_5$	339.1237966	339.12377	0.0783782
$C_{19}H_{19}N_2O_4$	339.13503	339.13502	0.0294275
$C_{17}H_{23}O_7$	339.1449258	339.14494	-0.041929
$C_{21}H_{23}O_4$	339.160182	339.16013	0.1532606
$C_{20}H_{23}N_2O_3$	339.1714154	339.17138	0.1043127
$C_{18}H_{27}O_6$	339.1813112	339.18133	-0.055487
$C_{17}H_{27}N_2O_5$	339.1925446	339.19253	0.0429841
$C_{19}H_{31}O_5$	339.2176966	339.21766	0.1078361
$C_{18}H_{14}N_1O_6$	340.0826602	340.08252	0.4121936
$C_{15}H_{18}N_1O_8$	340.1037894	340.10373	0.1745935
$C_{19}H_{18}N_1O_5$	340.1190456	340.11892	0.3692234
$C_{16}H_{22}N_1O_7$	340.1401748	340.14001	0.484447
$C_{20}H_{22}N_1O_4$	340.155431	340.15532	0.3262623
$C_{21}H_{26}N_1O_3$	340.1918164	340.19178	0.1069394
$C_{18}H_{13}O_7$	341.0666758	341.06661	0.1928652
$C_{17}H_{13}N_2O_6$	341.0779092	341.07789	0.0562332
$C_{19}H_{17}O_6$	341.1030612	341.10298	0.2379923

$C_{18}H_{17}N_2O_5$	341.1142946	341.11421	0.2479518
$C_{11}H_{21}N_2O_{10}$	341.1201676	341.12013	0.1101662
$C_{16}H_{21}O_8$	341.1241904	341.12412	0.2063175
$C_{15}H_{21}N_2O_7$	341.1354238	341.13551	-0.252744
$C_{20}H_{21}O_5$	341.1394466	341.13939	0.1658556
$C_{19}H_{21}N_2O_4$	341.15068	341.1506	0.2344416
$C_{17}H_{25}O_7$	341.1605758	341.16052	0.1635004
$C_{21}H_{25}O_4$	341.175832	341.17569	0.4161488
$C_{18}H_{29}O_6$	341.1969612	341.19686	0.296544
$C_{19}H_{33}O_5$	341.2333466	341.23314	0.6053919
$C_{17}H_{12}N_1O_7$	342.0619248	342.06203	-0.307605
$C_{18}H_{16}N_1O_6$	342.0983102	342.09838	-0.204094
$C_{15}H_{20}N_1O_8$	342.1194394	342.11953	-0.264879
$C_{19}H_{20}N_1O_5$	342.1346956	342.13475	-0.15906
$C_{16}H_{24}N_1O_7$	342.1558248	342.15593	-0.307521
$C_{20}H_{24}N_1O_4$	342.171081	342.1711	-0.055587
$C_{18}H_{15}O_7$	343.0823258	343.08228	0.1334371
$C_{17}H_{15}N_2O_6$	343.0935592	343.09362	-0.17727
$C_{10}H_{19}N_2O_{11}$	343.0994322	343.09943	0.0063536
$C_{19}H_{19}O_6$	343.1187112	343.11871	0.0034388
$C_{18}H_{19}N_2O_5$	343.1299446	343.12995	-0.015796
$C_{11}H_{23}N_2O_{10}$	343.1358176	343.13582	-0.007053
$C_{16}H_{23}O_8$	343.1398404	343.13991	-0.202891
$C_{15}H_{23}N_2O_7$	343.1510738	343.1509	0.5064239
$C_{20}H_{23}O_5$	343.1550966	343.15512	-0.068249
$C_{19}H_{23}N_2O_4$	343.16633	343.16638	-0.145761

$C_{17}H_{27}O_7$	343.1762258	343.17628	-0.157995
$C_{20}H_{27}N_2O_3$	343.2027154	343.20277	-0.159148
$C_{18}H_{31}O_6$	343.2126112	343.21266	-0.142244
$C_{19}H_{35}O_5$	343.2489966	343.24903	-0.097364
$C_{17}H_{14}N_1O_7$	344.0775748	344.07748	0.2754608
$C_{14}H_{18}N_1O_9$	344.098704	344.09873	-0.075618
$C_{18}H_{18}N_1O_6$	344.1139602	344.11383	0.3783046
$C_{19}H_{22}N_1O_5$	344.1503456	344.15023	0.3358413
$C_{20}H_{26}N_1O_4$	344.186731	344.18666	0.206225
$C_{17}H_{13}O_8$	345.0615904	345.06146	0.3778453
$C_{18}H_{17}O_7$	345.0979758	345.09791	0.1906122
$C_{17}H_{17}N_2O_6$	345.1092092	345.10916	0.1425053
$C_{10}H_{21}N_2O_{11}$	345.1150822	345.11509	-0.022659
$C_{19}H_{21}O_6$	345.1343612	345.13427	0.2641867
$C_{18}H_{21}N_2O_5$	345.1455946	345.14555	0.1291626
$C_{11}H_{25}N_2O_{10}$	345.1514676	345.15141	0.166825
$C_{16}H_{25}O_8$	345.1554904	345.15554	-0.143762
$C_{20}H_{25}O_5$	345.1707466	345.17066	0.2508321
$C_{19}H_{25}N_2O_4$	345.18198	345.18187	0.3186143
$C_{18}H_{33}O_6$	345.2282612	345.22814	0.3510138
$C_{17}H_{16}N_1O_7$	346.0932248	346.09329	-0.188447
$C_{21}H_{16}N_1O_4$	346.108481	346.10861	-0.372774
$C_{14}H_{20}N_1O_9$	346.114354	346.11437	-0.046286
$C_{18}H_{20}N_1O_6$	346.1296102	346.12965	-0.115044
$C_{22}H_{20}N_1O_3$	346.1448664	346.14506	-0.559361
$C_{19}H_{24}N_1O_5$	346.1659956	346.16603	-0.099432

$C_{20}H_{28}N_1O_4$	346.202381	346.20241	-0.083824
$C_{17}H_{15}O_8$	347.0772404	347.0772	0.1163427
$C_{16}H_{15}N_2O_7$	347.0884738	347.08841	0.1837569
$C_{21}H_{15}O_5$	347.0924966	347.09247	0.0765787
$C_{20}H_{15}N_2O_4$	347.10373	347.10363	0.2880404
$C_{18}H_{19}O_7$	347.1136258	347.11359	0.1030784
$C_{17}H_{19}N_2O_6$	347.1248592	347.12487	-0.031171
$C_{10}H_{23}N_2O_{11}$	347.1307322	347.13073	0.0062798
$C_{21}H_{19}N_2O_3$	347.1401154	347.14013	-0.042116
$C_{19}H_{23}O_6$	347.1500112	347.15001	0.0033988
$C_{18}H_{23}N_2O_5$	347.1612446	347.16121	0.0996076
$C_{20}H_{27}O_5$	347.1863966	347.18641	-0.038654
$C_{18}H_{35}O_6$	347.2439112	347.24395	-0.111795
$C_{16}H_{14}N_1O_8$	348.0724894	348.07246	0.0844074
$C_{20}H_{14}N_1O_5$	348.0877456	348.08761	0.3894992
$C_{17}H_{18}N_1O_7$	348.1088748	348.10873	0.4159041
$C_{21}H_{18}N_1O_4$	348.124131	348.124	0.3762448
$C_{18}H_{22}N_1O_6$	348.1452602	348.14511	0.4313714
$C_{22}H_{22}N_1O_3$	348.1605164	348.16046	0.1619365
$C_{19}H_{26}N_1O_5$	348.1816456	348.18154	0.3032322
$C_{20}H_{30}N_1O_4$	348.218031	348.21777	0.7494727
$C_{20}H_{13}O_6$	349.0717612	349.07172	0.1179697
$C_{19}H_{13}N_2O_5$	349.0829946	349.08315	-0.445224
$C_{17}H_{17}O_8$	349.0928904	349.09286	0.0870253
$C_{16}H_{17}N_2O_7$	349.1041238	349.10412	0.0108274
$C_{21}H_{17}O_5$	349.1081466	349.10811	0.104781

C ₉ H ₂₁ N ₂ O ₁₂	349.1099968	349.11006	-0.181089
C ₂₀ H ₁₇ N ₂ O ₄	349.11938	349.11935	0.0858729
C ₁₈ H ₂₁ O ₇	349.1292758	349.12922	0.1597686
C ₁₇ H ₂₁ N ₂ O ₆	349.1405092	349.14048	0.0835764
C ₂₂ H ₂₁ O ₄	349.144532	349.14449	0.1202365
C ₂₁ H ₂₁ N ₂ O ₃	349.1557654	349.1557	0.1872514
C ₁₉ H ₂₅ O ₆	349.1656612	349.16562	0.117938
C ₁₈ H ₂₅ N ₂ O ₅	349.1768946	349.17683	0.184949
C ₂₀ H ₂₉ O ₅	349.2020466	349.20198	0.190663
C ₁₉ H ₁₂ N ₁ O ₆	350.0670102	350.06711	-0.285146
C ₁₆ H ₁₆ N ₁ O ₈	350.0881394	350.08825	-0.315978
C ₂₀ H ₁₆ N ₁ O ₅	350.1033956	350.10344	-0.126877
C ₁₇ H ₂₀ N ₁ O ₇	350.1245248	350.12459	-0.186277
C ₂₁ H ₂₀ N ₁ O ₄	350.139781	350.13988	-0.282802
C ₁₈ H ₂₄ N ₁ O ₆	350.1609102	350.16097	-0.170836
C ₂₂ H ₂₄ N ₁ O ₃	350.1761664	350.17617	-0.010338
C ₁₉ H ₂₈ N ₁ O ₅	350.1972956	350.19739	-0.26962
C ₂₀ H ₁₅ O ₆	351.0874112	351.08732	0.2597071
C ₁₉ H ₁₅ N ₂ O ₅	351.0986446	351.09863	0.0415265
C ₁₂ H ₁₉ N ₂ O ₁₀	351.1045176	351.10452	-0.006893
C ₁₇ H ₁₉ O ₈	351.1085404	351.10844	0.2858942
C ₁₆ H ₁₉ N ₂ O ₇	351.1197738	351.11972	0.1531668
C ₂₁ H ₁₉ O ₅	351.1237966	351.12372	0.2180994
C ₂₀ H ₁₉ N ₂ O ₄	351.13503	351.13496	0.1992963
C ₁₈ H ₂₃ O ₇	351.1449258	351.14485	0.215808
C ₁₇ H ₂₃ N ₂ O ₆	351.1561592	351.15615	0.0261419

C ₂₁ H ₂₃ N ₂ O ₃	351.1714154	351.17133	0.2431288
C ₁₉ H ₂₇ O ₆	351.1813112	351.18126	0.1457364
C ₁₈ H ₂₇ N ₂ O ₅	351.1925446	351.19252	0.0699898
C ₁₉ H ₁₄ N ₁ O ₆	352.0826602	352.08254	0.34134
C ₁₆ H ₁₈ N ₁ O ₈	352.1037894	352.10369	0.282246
C ₂₀ H ₁₈ N ₁ O ₅	352.1190456	352.1189	0.4134394
C ₁₇ H ₂₂ N ₁ O ₇	352.1401748	352.14006	0.3259495
C ₂₁ H ₂₂ N ₁ O ₄	352.155431	352.15526	0.485524
C ₁₈ H ₂₆ N ₁ O ₆	352.1765602	352.1765	0.1708799
C ₁₉ H ₁₃ O ₇	353.0666758	353.06659	0.2429567
C ₁₆ H ₁₇ O ₉	353.087805	353.08778	0.070747
C ₂₀ H ₁₇ O ₆	353.1030612	353.10309	-0.08162
C ₁₉ H ₁₇ N ₂ O ₅	353.1142946	353.11433	-0.100308
C ₁₂ H ₂₁ N ₂ O ₁₀	353.1201676	353.12018	-0.035172
C ₁₇ H ₂₁ O ₈	353.1241904	353.12421	-0.055561
C ₁₆ H ₂₁ N ₂ O ₇	353.1354238	353.13548	-0.159203
C ₂₁ H ₂₁ O ₅	353.1394466	353.13945	-0.009685
C ₂₀ H ₂₁ N ₂ O ₄	353.15068	353.15067	0.0282596
C ₁₈ H ₂₅ O ₇	353.1605758	353.16055	0.0729977
C ₂₂ H ₂₅ O ₄	353.175832	353.17586	-0.079338
C ₂₁ H ₂₅ N ₂ O ₃	353.1870654	353.18707	-0.013081
C ₁₉ H ₂₉ O ₆	353.1969612	353.19698	-0.053285
C ₁₅ H ₁₆ N ₁ O ₉	354.083054	354.08302	0.0959659
C ₁₉ H ₁₆ N ₁ O ₆	354.0983102	354.09827	0.113471
C ₁₆ H ₂₀ N ₁ O ₈	354.1194394	354.11935	0.2524004
C ₂₀ H ₂₀ N ₁ O ₅	354.1346956	354.1347	-0.012481

C ₁₇ H ₂₄ N ₁ O ₇	354.1558248	354.15591	-0.240629
C ₂₁ H ₂₄ N ₁ O ₄	354.171081	354.17112	-0.110173
C ₁₈ H ₂₈ N ₁ O ₆	354.1922102	354.19226	-0.140658
C ₁₉ H ₁₅ O ₇	355.0823258	355.0822	0.3542274
C ₁₈ H ₁₅ N ₂ O ₆	355.0935592	355.09346	0.2793064
C ₁₁ H ₁₉ N ₂ O ₁₁	355.0994322	355.09942	0.0343
C ₂₀ H ₁₉ O ₆	355.1187112	355.11857	0.3975569
C ₁₉ H ₁₉ N ₂ O ₅	355.1299446	355.12982	0.3508009
C ₁₂ H ₂₃ N ₂ O ₁₀	355.1358176	355.13565	0.4718755
C ₁₇ H ₂₃ O ₈	355.1398404	355.13966	0.5079123
C ₂₁ H ₂₃ O ₅	355.1550966	355.15497	0.3564074
C ₂₀ H ₂₃ N ₂ O ₄	355.16633	355.16619	0.3941249
C ₁₈ H ₂₇ O ₇	355.1762258	355.17609	0.3822888
C ₁₉ H ₃₁ O ₆	355.2126112	355.21247	0.3974518
C ₁₈ H ₁₄ N ₁ O ₇	356.0775748	356.07753	0.1257588
C ₁₅ H ₁₈ N ₁ O ₉	356.098704	356.09877	-0.185398
C ₁₉ H ₁₈ N ₁ O ₆	356.1139602	356.11392	0.1128288
C ₁₆ H ₂₂ N ₁ O ₈	356.1350894	356.13506	0.0824965
C ₂₀ H ₂₂ N ₁ O ₅	356.1503456	356.15027	0.2122135
C ₂₁ H ₂₆ N ₁ O ₄	356.186731	356.18667	0.1712021
C ₁₈ H ₁₃ O ₈	357.0615904	357.06162	-0.082955
C ₁₉ H ₁₇ O ₇	357.0979758	357.09801	-0.095828
C ₁₈ H ₁₇ N ₂ O ₆	357.1092092	357.10932	-0.310326
C ₁₁ H ₂₁ N ₂ O ₁₁	357.1150822	357.11517	-0.245915
C ₁₆ H ₂₁ O ₉	357.119105	357.11899	0.3219651
C ₂₀ H ₂₁ O ₆	357.1343612	357.13444	-0.220702

$C_{19}H_{21}N_2O_5$	357.1455946	357.14567	-0.211175
$C_{12}H_{25}N_2O_{10}$	357.1514676	357.15159	-0.342768
$C_{17}H_{25}O_8$	357.1554904	357.15554	-0.138931
$C_{21}H_{25}O_5$	357.1707466	357.17082	-0.20556
$C_{20}H_{25}N_2O_4$	357.18198	357.18213	-0.42001
$C_{18}H_{29}O_7$	357.1918758	357.19196	-0.235784
$C_{19}H_{33}O_6$	357.2282612	357.22838	-0.332617
$C_{18}H_{16}N_1O_7$	358.0932248	358.09313	0.2646794
$C_{19}H_{20}N_1O_6$	358.1296102	358.12949	0.3355766
$C_{20}H_{24}N_1O_5$	358.1659956	358.16591	0.2389392
$C_{21}H_{28}N_1O_4$	358.202381	358.20234	0.1144043
$C_{18}H_{15}O_8$	359.0772404	359.0772	0.1124546
$C_{17}H_{15}N_2O_7$	359.0884738	359.08848	-0.017322
$C_{19}H_{19}O_7$	359.1136258	359.11355	0.2110193
$C_{18}H_{19}N_2O_6$	359.1248592	359.1248	0.1647892
$C_{11}H_{23}N_2O_{11}$	359.1307322	359.13066	0.200985
$C_{16}H_{23}O_9$	359.134755	359.13461	0.4036922
$C_{20}H_{23}O_6$	359.1500112	359.14991	0.2817204
$C_{19}H_{23}N_2O_5$	359.1612446	359.16113	0.3190208
$C_{12}H_{27}N_2O_{10}$	359.1671176	359.16702	0.2716838
$C_{17}H_{27}O_8$	359.1711404	359.17122	-0.221677
$C_{21}H_{27}O_5$	359.1863966	359.18634	0.1575224
$C_{20}H_{27}N_2O_4$	359.19763	359.19746	0.4732211
$C_{18}H_{31}O_7$	359.2075258	359.20747	0.155286
$C_{17}H_{14}N_1O_8$	360.0724894	360.0725	-0.029494
$C_{18}H_{18}N_1O_7$	360.1088748	360.10899	-0.319959

C ₂₂ H ₁₈ N ₁ O ₄	360.124131	360.12427	-0.386034
C ₁₅ H ₂₂ N ₁ O ₉	360.130004	360.1301	-0.266626
C ₁₉ H ₂₂ N ₁ O ₆	360.1452602	360.14535	-0.2494
C ₂₀ H ₂₆ N ₁ O ₅	360.1816456	360.18169	-0.123327
C ₁₈ H ₁₇ O ₈	361.0928904	361.09278	0.3056828
C ₁₇ H ₁₇ N ₂ O ₇	361.1041238	361.10404	0.2320104
C ₂₂ H ₁₇ O ₅	361.1081466	361.108	0.4059169
C ₁₀ H ₂₁ N ₂ O ₁₂	361.1099968	361.10998	0.0464676
C ₂₁ H ₁₇ N ₂ O ₄	361.11938	361.11935	0.0830194
C ₁₉ H ₂₁ O ₇	361.1292758	361.12918	0.2652233
C ₁₈ H ₂₁ N ₂ O ₆	361.1405092	361.14047	0.1084894
C ₁₁ H ₂₅ N ₂ O ₁₁	361.1463822	361.14633	0.1444841
C ₂₂ H ₂₁ N ₂ O ₃	361.1557654	361.15574	0.0702741
C ₂₀ H ₂₅ O ₆	361.1656612	361.16558	0.2247719
C ₁₉ H ₂₅ N ₂ O ₅	361.1768946	361.17688	0.0403678
C ₁₈ H ₃₃ O ₇	361.2231758	361.22311	0.1821032
C ₁₇ H ₁₆ N ₁ O ₈	362.0881394	362.0881	0.1087578
C ₂₁ H ₁₆ N ₁ O ₅	362.1033956	362.10331	0.2363411
C ₁₈ H ₂₀ N ₁ O ₇	362.1245248	362.1244	0.3445773
C ₂₂ H ₂₀ N ₁ O ₄	362.139781	362.13971	0.1960014
C ₁₉ H ₂₄ N ₁ O ₆	362.1609102	362.16081	0.2766171
C ₂₀ H ₂₈ N ₁ O ₅	362.1972956	362.19718	0.3191076
C ₂₁ H ₁₅ O ₆	363.0874112	363.08745	-0.106917
C ₂₀ H ₁₅ N ₂ O ₅	363.0986446	363.09889	-0.675905
C ₁₈ H ₁₉ O ₈	363.1085404	363.10861	-0.191734
C ₁₇ H ₁₉ N ₂ O ₇	363.1197738	363.11983	-0.154825

$C_{22}H_{19}O_5$	363.1237966	363.1239	-0.284807
$C_{10}H_{23}N_2O_{12}$	363.1256468	363.12573	-0.229177
$C_{21}H_{19}N_2O_4$	363.13503	363.1351	-0.192821
$C_{19}H_{23}O_7$	363.1449258	363.14503	-0.286993
$C_{18}H_{23}N_2O_6$	363.1561592	363.15628	-0.332695
$C_{20}H_{27}O_6$	363.1813112	363.18137	-0.161958
$C_{20}H_{14}N_1O_6$	364.0826602	364.08252	0.3850222
$C_{17}H_{18}N_1O_8$	364.1037894	364.10372	0.1905498
$C_{21}H_{18}N_1O_5$	364.1190456	364.11898	0.1801057
$C_{18}H_{22}N_1O_7$	364.1401748	364.14006	0.315208
$C_{22}H_{22}N_1O_4$	364.155431	364.15536	0.1949165
$C_{19}H_{26}N_1O_6$	364.1765602	364.17654	0.0554124
$C_{21}H_{17}O_6$	365.1030612	365.10299	0.1949584
$C_{20}H_{17}N_2O_5$	365.1142946	365.11426	0.0947098
$C_{18}H_{21}O_8$	365.1241904	365.12407	0.3296958
$C_{17}H_{21}N_2O_7$	365.1354238	365.13544	-0.044422
$C_{22}H_{21}O_5$	365.1394466	365.13929	0.4288222
$C_{21}H_{21}N_2O_4$	365.15068	365.15055	0.3559624
$C_{19}H_{25}O_7$	365.1605758	365.16046	0.3170657
$C_{20}H_{29}O_6$	365.1969612	365.19676	0.5508805
$C_{16}H_{16}N_1O_9$	366.083054	366.0831	-0.125709
$C_{20}H_{16}N_1O_6$	366.0983102	366.09839	-0.218029
$C_{17}H_{20}N_1O_8$	366.1194394	366.11954	-0.274829
$C_{21}H_{20}N_1O_5$	366.1346956	366.13478	-0.230571
$C_{18}H_{24}N_1O_7$	366.1558248	366.15586	-0.096189
$C_{22}H_{24}N_1O_4$	366.171081	366.17113	-0.133872

$C_{19}H_{28}N_1O_6$	366.1922102	366.19224	-0.081433
$C_{20}H_{15}O_7$	367.0823258	367.08219	0.3698895
$C_{19}H_{15}N_2O_6$	367.0935592	367.09342	0.3791401
$C_{12}H_{19}N_2O_{11}$	367.0994322	367.09943	0.0059382
$C_{17}H_{19}O_9$	367.103455	367.10351	-0.149876
$C_{16}H_{19}N_2O_8$	367.1146884	367.11446	0.6220942
$C_{21}H_{19}O_6$	367.1187112	367.11864	0.193888
$C_{20}H_{19}N_2O_5$	367.1299446	367.12987	0.2031431
$C_{13}H_{23}N_2O_{10}$	367.1358176	367.1359	-0.224495
$C_{18}H_{23}O_8$	367.1398404	367.13972	0.3278857
$C_{17}H_{23}N_2O_7$	367.1510738	367.15104	0.0920055
$C_{22}H_{23}O_5$	367.1550966	367.15498	0.3175222
$C_{21}H_{23}N_2O_4$	367.16633	367.16628	0.1361233
$C_{19}H_{27}O_7$	367.1762258	367.17614	0.2336205
$C_{20}H_{31}O_6$	367.2126112	367.21263	-0.051251
$C_{19}H_{14}N_1O_7$	368.0775748	368.07747	0.284668
$C_{16}H_{18}N_1O_9$	368.098704	368.09871	-0.016355
$C_{20}H_{18}N_1O_6$	368.1139602	368.11391	0.1363162
$C_{17}H_{22}N_1O_8$	368.1350894	368.13491	0.4872665
$C_{21}H_{22}N_1O_5$	368.1503456	368.15027	0.2052963
$C_{18}H_{26}N_1O_7$	368.1714748	368.17139	0.2302729
$C_{22}H_{26}N_1O_4$	368.186731	368.18666	0.1927823
$C_{20}H_{17}O_7$	369.0979758	369.09806	-0.228178
$C_{19}H_{17}N_2O_6$	369.1092092	369.10928	-0.191868
$C_{12}H_{21}N_2O_{11}$	369.1150822	369.1152	-0.319196
$C_{17}H_{21}O_9$	369.119105	369.11917	-0.176149

$C_{21}H_{21}O_6$	369.1343612	369.13445	-0.240617
$C_{20}H_{21}N_2O_5$	369.1455946	369.14574	-0.393937
$C_{13}H_{25}N_2O_{10}$	369.1514676	369.15163	-0.439982
$C_{18}H_{25}O_8$	369.1554904	369.15561	-0.324037
$C_{22}H_{25}O_5$	369.1707466	369.17083	-0.225966
$C_{21}H_{25}N_2O_4$	369.18198	369.18205	-0.189663
$C_{19}H_{29}O_7$	369.1918758	369.19192	-0.119775
$C_{19}H_{16}N_1O_7$	370.0932248	370.09311	0.3101378
$C_{16}H_{20}N_1O_9$	370.114354	370.11427	0.2269026
$C_{20}H_{20}N_1O_6$	370.1296102	370.1295	0.2976792
$C_{17}H_{24}N_1O_8$	370.1507394	370.15053	0.5656612
$C_{21}H_{24}N_1O_5$	370.1659956	370.1659	0.2582082
$C_{19}H_{15}O_8$	371.0772404	371.07725	-0.025925
$C_{20}H_{19}O_7$	371.1136258	371.11358	0.1233582
$C_{19}H_{19}N_2O_6$	371.1248592	371.12482	0.1055707
$C_{12}H_{23}N_2O_{11}$	371.1307322	371.13071	0.059763
$C_{17}H_{23}O_9$	371.134755	371.13473	0.0673068
$C_{21}H_{23}O_6$	371.1500112	371.14994	0.191782
$C_{20}H_{23}N_2O_5$	371.1612446	371.1612	0.1201093
$C_{13}H_{27}N_2O_{10}$	371.1671176	371.1672	-0.222057
$C_{22}H_{27}O_5$	371.1863966	371.18641	-0.036155
$C_{19}H_{31}O_7$	371.2075258	371.20747	0.1502661
$C_{20}H_{35}O_6$	371.2439112	371.24388	0.0839876
$C_{18}H_{14}N_1O_8$	372.0724894	372.07269	-0.539196
$C_{19}H_{18}N_1O_7$	372.1088748	372.10893	-0.148398
$C_{20}H_{22}N_1O_6$	372.1452602	372.14533	-0.187615

$C_{21}H_{26}N_1O_5$	372.1816456	372.18176	-0.307431
$C_{19}H_{17}O_8$	373.0928904	373.09269	0.5370778
$C_{18}H_{17}N_2O_7$	373.1041238	373.104	0.331757
$C_{11}H_{21}N_2O_{12}$	373.1099968	373.10994	0.1521801
$C_{22}H_{17}N_2O_4$	373.11938	373.11914	0.6431719
$C_{20}H_{21}O_7$	373.1292758	373.12913	0.3906954
$C_{19}H_{21}N_2O_6$	373.1405092	373.14035	0.4265951
$C_{12}H_{25}N_2O_{11}$	373.1463822	373.14625	0.3542307
$C_{23}H_{21}N_2O_3$	373.1557654	373.15556	0.5503865
$C_{21}H_{25}O_6$	373.1656612	373.16556	0.2711394
$C_{20}H_{25}N_2O_5$	373.1768946	373.17678	0.3070391
$C_{19}H_{33}O_7$	373.2231758	373.22301	0.4441844
$C_{18}H_{16}N_1O_8$	374.0881394	374.08822	-0.215511
$C_{19}H_{20}N_1O_7$	374.1245248	374.12454	-0.040682
$C_{23}H_{20}N_1O_4$	374.139781	374.13991	-0.344845
$C_{20}H_{24}N_1O_6$	374.1609102	374.16088	0.0806602
$C_{21}H_{28}N_1O_5$	374.1972956	374.19724	0.148531
$C_{18}H_{15}O_9$	375.072155	375.07232	-0.439969
$C_{21}H_{15}N_2O_5$	375.0986446	375.09868	-0.094429
$C_{19}H_{19}O_8$	375.1085404	375.10856	-0.052305
$C_{18}H_{19}N_2O_7$	375.1197738	375.11971	0.1700254
$C_{23}H_{19}O_5$	375.1237966	375.12394	-0.382327
$C_{11}H_{23}N_2O_{12}$	375.1256468	375.12561	0.0980469
$C_{22}H_{19}N_2O_4$	375.13503	375.13505	-0.053368
$C_{20}H_{23}O_7$	375.1449258	375.14491	0.0420635
$C_{19}H_{23}N_2O_6$	375.1561592	375.15614	0.0511251

C ₁₂ H ₂₇ N ₂ O ₁₁	375.1620322	375.16204	-0.020845
C ₂₁ H ₂₇ O ₆	375.1813112	375.18135	-0.10347
C ₂₀ H ₂₇ N ₂ O ₅	375.1925446	375.19275	-0.547506
C ₁₈ H ₃₁ O ₈	375.2024404	375.20256	-0.318815
C ₂₁ H ₁₄ N ₁ O ₆	376.0826602	376.08241	0.6652258
C ₁₈ H ₁₈ N ₁ O ₈	376.1037894	376.10359	0.5301194
C ₂₂ H ₁₈ N ₁ O ₅	376.1190456	376.11886	0.4934073
C ₁₉ H ₂₂ N ₁ O ₇	376.1401748	376.14002	0.4114953
C ₂₃ H ₂₂ N ₁ O ₄	376.155431	376.15526	0.4545459
C ₂₀ H ₂₆ N ₁ O ₆	376.1765602	376.17642	0.3726439
C ₁₈ H ₁₇ O ₉	377.087805	377.0878	0.0132062
C ₂₂ H ₁₇ O ₆	377.1030612	377.10316	-0.262051
C ₂₁ H ₁₇ N ₂ O ₅	377.1142946	377.11441	-0.306061
C ₁₉ H ₂₁ O ₈	377.1241904	377.12422	-0.078542
C ₁₈ H ₂₁ N ₂ O ₇	377.1354238	377.13545	-0.069524
C ₂₃ H ₂₁ O ₅	377.1394466	377.13958	-0.353769
C ₁₁ H ₂₅ N ₂ O ₁₂	377.1412968	377.14137	-0.194145
C ₂₂ H ₂₁ N ₂ O ₄	377.15068	377.15078	-0.265199
C ₂₀ H ₂₅ O ₇	377.1605758	377.16067	-0.249814
C ₁₉ H ₂₅ N ₂ O ₆	377.1718092	377.1719	-0.240792
C ₂₁ H ₂₉ O ₆	377.1969612	377.197	-0.102917
C ₁₇ H ₁₆ N ₁ O ₉	378.083054	378.08298	0.195671
C ₂₁ H ₁₆ N ₁ O ₆	378.0983102	378.09822	0.2385091
C ₁₈ H ₂₀ N ₁ O ₈	378.1194394	378.11937	0.1834867
C ₂₂ H ₂₀ N ₁ O ₅	378.1346956	378.13465	0.1205388
C ₁₉ H ₂₄ N ₁ O ₇	378.1558248	378.15579	0.0919724

$C_{23}H_{24}N_1O_4$	378.171081	378.17097	0.2934648
$C_{20}H_{28}N_1O_6$	378.1922102	378.19224	-0.078849
$C_{21}H_{15}O_7$	379.0823258	379.08224	0.226283
$C_{18}H_{19}O_9$	379.103455	379.10336	0.2505382
$C_{17}H_{19}N_2O_8$	379.1146884	379.11471	-0.057028
$C_{22}H_{19}O_6$	379.1187112	379.11862	0.2405049
$C_{21}H_{19}N_2O_5$	379.1299446	379.12992	0.0648324
$C_{19}H_{23}O_8$	379.1398404	379.13978	0.159255
$C_{18}H_{23}N_2O_7$	379.1510738	379.15118	-0.280152
$C_{23}H_{23}O_5$	379.1550966	379.15505	0.1228518
$C_{22}H_{23}N_2O_4$	379.16633	379.16613	0.52742
$C_{20}H_{27}O_7$	379.1762258	379.17618	0.1207352
$C_{20}H_{14}N_1O_7$	380.0775748	380.07749	0.2230595
$C_{17}H_{18}N_1O_9$	380.098704	380.09872	-0.042147
$C_{21}H_{18}N_1O_6$	380.1139602	380.11402	-0.157374
$C_{18}H_{22}N_1O_8$	380.1350894	380.13518	-0.238389
$C_{22}H_{22}N_1O_5$	380.1503456	380.15043	-0.22207
$C_{19}H_{26}N_1O_7$	380.1714748	380.17148	-0.013731
$C_{23}H_{26}N_1O_4$	380.186731	380.18685	-0.313057
$C_{20}H_{30}N_1O_6$	380.2078602	380.20793	-0.183637
$C_{21}H_{17}O_7$	381.0979758	381.0978	0.461246
$C_{20}H_{17}N_2O_6$	381.1092092	381.10909	0.3127185
$C_{13}H_{21}N_2O_{11}$	381.1150822	381.1149	0.4780181
$C_{18}H_{21}O_9$	381.119105	381.11901	0.2492132
$C_{22}H_{21}O_6$	381.1343612	381.13424	0.3179454
$C_{21}H_{21}N_2O_5$	381.1455946	381.14546	0.3530932

C ₁₄ H ₂₅ N ₂ O ₁₀	381.1514676	381.1514	0.1773046
C ₁₉ H ₂₅ O ₈	381.1554904	381.15532	0.4470089
C ₂₂ H ₂₅ N ₂ O ₄	381.18198	381.18178	0.524631
C ₂₀ H ₂₉ O ₇	381.1918758	381.19163	0.6447669
C ₂₀ H ₁₆ N ₁ O ₇	382.0932248	382.09329	-0.170692
C ₁₇ H ₂₀ N ₁ O ₉	382.114354	382.11447	-0.303627
C ₂₁ H ₂₀ N ₁ O ₆	382.1296102	382.12966	-0.130375
C ₂₂ H ₂₄ N ₁ O ₅	382.1659956	382.16601	-0.037733
C ₂₃ H ₂₈ N ₁ O ₄	382.202381	382.20237	0.028728
C ₂₀ H ₁₅ O ₈	383.0772404	383.07719	0.1315137
C ₂₁ H ₁₉ O ₇	383.1136258	383.1136	0.0672905
C ₂₀ H ₁₉ N ₂ O ₆	383.1248592	383.12478	0.2066687
C ₁₃ H ₂₃ N ₂ O ₁₁	383.1307322	383.13071	0.0578912
C ₁₈ H ₂₃ O ₉	383.134755	383.13476	-0.013103
C ₂₂ H ₂₃ O ₆	383.1500112	383.14993	0.211875
C ₂₁ H ₂₃ N ₂ O ₅	383.1612446	383.16119	0.1424463
C ₁₄ H ₂₇ N ₂ O ₁₀	383.1671176	383.16702	0.2546667
C ₁₉ H ₂₇ O ₈	383.1711404	383.17112	0.0531875
C ₂₃ H ₂₇ O ₅	383.1863966	383.18641	-0.035022
C ₂₂ H ₂₇ N ₂ O ₄	383.19763	383.19765	-0.052245
C ₂₀ H ₁₈ N ₁ O ₇	384.1088748	384.10879	0.2207184
C ₁₇ H ₂₂ N ₁ O ₉	384.130004	384.12991	0.2446565
C ₂₁ H ₂₂ N ₁ O ₆	384.1452602	384.14519	0.182691
C ₂₂ H ₂₆ N ₁ O ₅	384.1816456	384.18151	0.3529057
C ₂₀ H ₁₇ O ₈	385.0928904	385.09301	-0.310627
C ₁₉ H ₁₇ N ₂ O ₇	385.1041238	385.10415	-0.068086

$C_{12}H_{21}N_2O_{12}$	385.1099968	385.11001	-0.034328
$C_{21}H_{21}O_7$	385.1292758	385.12935	-0.192715
$C_{20}H_{21}N_2O_6$	385.1405092	385.14055	-0.105988
$C_{13}H_{25}N_2O_{11}$	385.1463822	385.14654	-0.409767
$C_{18}H_{25}O_9$	385.150405	385.15062	-0.558276
$C_{22}H_{25}O_6$	385.1656612	385.16573	-0.178677
$C_{21}H_{25}N_2O_5$	385.1768946	385.17705	-0.403503
$C_{20}H_{33}O_7$	385.2231758	385.22332	-0.374381
$C_{19}H_{16}N_1O_8$	386.0881394	386.08796	0.4646087
$C_{20}H_{20}N_1O_7$	386.1245248	386.12434	0.47855
$C_{21}H_{24}N_1O_6$	386.1609102	386.16075	0.4148009
$C_{22}H_{28}N_1O_5$	386.1972956	386.19721	0.2215963
$C_{19}H_{15}O_9$	387.072155	387.07222	-0.167979
$C_{20}H_{19}O_8$	387.1085404	387.10857	-0.076516
$C_{19}H_{19}N_2O_7$	387.1197738	387.11976	0.035596
$C_{12}H_{23}N_2O_{12}$	387.1256468	387.12569	-0.111644
$C_{23}H_{19}N_2O_4$	387.13503	387.13488	0.3874098
$C_{21}H_{23}O_7$	387.1449258	387.14498	-0.140051
$C_{20}H_{23}N_2O_6$	387.1561592	387.15621	-0.131265
$C_{13}H_{27}N_2O_{11}$	387.1620322	387.16213	-0.252659
$C_{22}H_{27}O_6$	387.1813112	387.18137	-0.151919
$C_{21}H_{27}N_2O_5$	387.1925446	387.1927	-0.401403
$C_{19}H_{31}O_8$	387.2024404	387.20229	0.3883754
$C_{19}H_{18}N_1O_8$	388.1037894	388.10373	0.1530001
$C_{23}H_{18}N_1O_5$	388.1190456	388.11905	-0.011389
$C_{20}H_{22}N_1O_7$	388.1401748	388.14017	0.0123149

$C_{24}H_{22}N_1O_4$	388.155431	388.15535	0.2086275
$C_{21}H_{26}N_1O_6$	388.1765602	388.17655	0.0262249
$C_{19}H_{17}O_9$	389.087805	389.08777	0.0899023
$C_{18}H_{17}N_2O_8$	389.0990384	389.09897	0.1757391
$C_{22}H_{17}N_2O_5$	389.1142946	389.11425	0.1145676
$C_{20}H_{21}O_8$	389.1241904	389.12417	0.0523738
$C_{19}H_{21}N_2O_7$	389.1354238	389.1354	0.0611096
$C_{12}H_{25}N_2O_{12}$	389.1412968	389.14133	-0.085368
$C_{23}H_{21}N_2O_4$	389.15068	389.15046	0.5652821
$C_{21}H_{25}O_7$	389.1605758	389.16053	0.1176376
$C_{20}H_{25}N_2O_6$	389.1718092	389.1717	0.2805442
$C_{13}H_{29}N_2O_{11}$	389.1776822	389.17754	0.3653342
$C_{22}H_{29}O_6$	389.1969612	389.19691	0.1315013
$C_{19}H_{33}O_8$	389.2180904	389.21796	0.334979
$C_{22}H_{16}N_1O_6$	390.0983102	390.09834	-0.076443
$C_{19}H_{20}N_1O_8$	390.1194394	390.11948	-0.104122
$C_{23}H_{20}N_1O_5$	390.1346956	390.13482	-0.318916
$C_{20}H_{24}N_1O_7$	390.1558248	390.15592	-0.244057
$C_{24}H_{24}N_1O_4$	390.171081	390.17115	-0.176897
$C_{21}H_{28}N_1O_6$	390.1922102	390.19229	-0.204566
$C_{22}H_{15}O_7$	391.0823258	391.0821	0.5773206
$C_{21}H_{15}N_2O_6$	391.0935592	391.09343	0.3303043
$C_{19}H_{19}O_9$	391.103455	391.1033	0.3962632
$C_{23}H_{19}O_6$	391.1187112	391.11859	0.309829
$C_{22}H_{19}N_2O_5$	391.1299446	391.1298	0.3696467
$C_{20}H_{23}O_8$	391.1398404	391.13967	0.4355984

$C_{19}H_{23}N_2O_7$	391.1510738	391.15092	0.3931471
$C_{12}H_{27}N_2O_{12}$	391.1569468	391.15669	0.6564626
$C_{21}H_{27}O_7$	391.1762258	391.17605	0.4493624
$C_{20}H_{27}N_2O_6$	391.1874592	391.18736	0.2535355
$C_{21}H_{14}N_1O_7$	392.0775748	392.07764	-0.166345
$C_{18}H_{18}N_1O_9$	392.098704	392.09879	-0.219384
$C_{22}H_{18}N_1O_6$	392.1139602	392.11408	-0.305575
$C_{19}H_{22}N_1O_8$	392.1350894	392.13523	-0.358601
$C_{23}H_{22}N_1O_5$	392.1503456	392.15048	-0.342777
$C_{20}H_{26}N_1O_7$	392.1714748	392.17157	-0.242802
$C_{24}H_{26}N_1O_4$	392.186731	392.1868	-0.175988
$C_{21}H_{30}N_1O_6$	392.2078602	392.20776	0.2554255
$C_{22}H_{17}O_7$	393.0979758	393.09791	0.1673372
$C_{21}H_{17}N_2O_6$	393.1092092	393.10912	0.2268578
$C_{19}H_{21}O_9$	393.119105	393.11896	0.3687938
$C_{18}H_{21}N_2O_8$	393.1303384	393.13015	0.4791792
$C_{23}H_{21}O_6$	393.1343612	393.13424	0.3082404
$C_{22}H_{21}N_2O_5$	393.1455946	393.14546	0.3423157
$C_{20}H_{25}O_8$	393.1554904	393.15542	0.1790129
$C_{24}H_{25}O_5$	393.1707466	393.1706	0.3728149
$C_{23}H_{25}N_2O_4$	393.18198	393.18178	0.5086192
$C_{21}H_{29}O_7$	393.1918758	393.19171	0.421626
$C_{21}H_{16}N_1O_7$	394.0932248	394.09334	-0.292368
$C_{18}H_{20}N_1O_9$	394.114354	394.11434	0.0354717
$C_{22}H_{20}N_1O_6$	394.1296102	394.12961	0.0004564
$C_{19}H_{24}N_1O_8$	394.1507394	394.15065	0.2267658

$C_{23}H_{24}N_1O_5$	394.1659956	394.16599	0.0141562
$C_{20}H_{28}N_1O_7$	394.1871248	394.1871	0.0628633
$C_{24}H_{28}N_1O_4$	394.202381	394.2023	0.2054272
$C_{21}H_{15}O_8$	395.0772404	395.07715	0.2287651
$C_{17}H_{19}N_2O_9$	395.109603	395.10965	-0.119005
$C_{22}H_{19}O_7$	395.1136258	395.1136	0.0652468
$C_{21}H_{19}N_2O_6$	395.1248592	395.12483	0.0738498
$C_{14}H_{23}N_2O_{11}$	395.1307322	395.13068	0.1320573
$C_{19}H_{23}O_9$	395.134755	395.1348	-0.113936
$C_{23}H_{23}O_6$	395.1500112	395.14997	0.1042133
$C_{22}H_{23}N_2O_5$	395.1612446	395.16117	0.1887328
$C_{20}H_{27}O_8$	395.1711404	395.17117	-0.074955
$C_{24}H_{27}O_5$	395.1863966	395.1864	-0.008654
$C_{21}H_{31}O_7$	395.2075258	395.20745	0.1917471
$C_{22}H_{35}O_6$	395.2439112	395.24383	0.2053919
$C_{20}H_{14}N_1O_8$	396.0724894	396.07246	0.0741781
$C_{21}H_{18}N_1O_7$	396.1088748	396.10884	0.0878039
$C_{18}H_{22}N_1O_9$	396.130004	396.12995	0.1362681
$C_{22}H_{22}N_1O_6$	396.1452602	396.14521	0.1266705
$C_{19}H_{26}N_1O_8$	396.1663894	396.16613	0.6547246
$C_{23}H_{26}N_1O_5$	396.1816456	396.18158	0.1655299
$C_{24}H_{30}N_1O_4$	396.218031	396.21795	0.2043822
$C_{21}H_{17}O_8$	397.0928904	397.09291	-0.049409
$C_{20}H_{17}N_2O_7$	397.1041238	397.10438	-0.645221
$C_{22}H_{21}O_7$	397.1292758	397.12931	-0.086169
$C_{21}H_{21}N_2O_6$	397.1405092	397.14061	-0.253865

$C_{14}H_{25}N_2O_{11}$	397.1463822	397.1465	-0.296667
$C_{23}H_{25}O_6$	397.1656612	397.16572	-0.1481
$C_{22}H_{25}N_2O_5$	397.1768946	397.17696	-0.164713
$C_{20}H_{29}O_8$	397.1867904	397.18691	-0.301168
$C_{20}H_{16}N_1O_8$	398.0881394	398.08789	0.6264439
$C_{21}H_{20}N_1O_7$	398.1245248	398.12434	0.4641259
$C_{22}H_{24}N_1O_6$	398.1609102	398.16071	0.5027613
$C_{23}H_{28}N_1O_5$	398.1972956	398.19706	0.591616
$C_{21}H_{19}O_8$	399.1085404	399.10862	-0.199495
$C_{20}H_{19}N_2O_7$	399.1197738	399.11987	-0.241081
$C_{13}H_{23}N_2O_{12}$	399.1256468	399.12571	-0.158396
$C_{22}H_{23}O_7$	399.1449258	399.14502	-0.236055
$C_{21}H_{23}N_2O_6$	399.1561592	399.15623	-0.177425
$C_{14}H_{27}N_2O_{11}$	399.1620322	399.16208	-0.119801
$C_{23}H_{27}O_6$	399.1813112	399.18144	-0.322711
$C_{22}H_{27}N_2O_5$	399.1925446	399.19266	-0.289134
$C_{21}H_{35}O_7$	399.2388258	399.23893	-0.261047
$C_{22}H_{39}O_6$	399.2752112	399.27543	-0.548043
$C_{20}H_{18}N_1O_8$	400.1037894	400.1036	0.4733269
$C_{21}H_{22}N_1O_7$	400.1401748	400.14003	0.361823
$C_{22}H_{26}N_1O_6$	400.1765602	400.17645	0.2753282
$C_{23}H_{30}N_1O_5$	400.2129456	400.21296	-0.036031
$C_{20}H_{17}O_9$	401.087805	401.08788	-0.187042
$C_{19}H_{17}N_2O_8$	401.0990384	401.0991	-0.153628
$C_{23}H_{17}N_2O_5$	401.1142946	401.11435	-0.138165
$C_{21}H_{21}O_8$	401.1241904	401.12429	-0.248352

$C_{20}H_{21}N_2O_7$	401.1354238	401.13563	-0.514091
$C_{13}H_{25}N_2O_{12}$	401.1412968	401.14141	-0.282245
$C_{24}H_{21}N_2O_4$	401.15068	401.15067	0.0248782
$C_{22}H_{25}O_7$	401.1605758	401.16064	-0.160086
$C_{21}H_{25}N_2O_6$	401.1718092	401.17194	-0.326095
$C_{14}H_{29}N_2O_{11}$	401.1776822	401.17779	-0.268759
$C_{23}H_{29}O_6$	401.1969612	401.19705	-0.221388
$C_{20}H_{33}O_8$	401.2180904	401.21805	0.1006433
$C_{23}H_{16}N_1O_6$	402.0983102	402.09828	0.075056
$C_{20}H_{20}N_1O_8$	402.1194394	402.11936	0.1974038
$C_{24}H_{20}N_1O_5$	402.1346956	402.13466	0.0884776
$C_{21}H_{24}N_1O_7$	402.1558248	402.15576	0.1610816
$C_{22}H_{28}N_1O_6$	402.1922102	402.1921	0.2739484
$C_{20}H_{19}O_9$	403.103455	403.10344	0.0371614
$C_{19}H_{19}N_2O_8$	403.1146884	403.115	-0.773031
$C_{24}H_{19}O_6$	403.1187112	403.1187	0.0277335
$C_{23}H_{19}N_2O_5$	403.1299446	403.12997	-0.063057
$C_{21}H_{23}O_8$	403.1398404	403.13987	-0.073474
$C_{20}H_{23}N_2O_7$	403.1510738	403.15112	-0.114647
$C_{13}H_{27}N_2O_{12}$	403.1569468	403.15697	-0.057596
$C_{24}H_{23}N_2O_4$	403.16633	403.16633	-4.99E-05
$C_{22}H_{27}O_7$	403.1762258	403.17625	-0.060073
$C_{21}H_{27}N_2O_6$	403.1874592	403.18756	-0.250058
$C_{19}H_{18}N_1O_9$	404.098704	404.09877	-0.163376
$C_{23}H_{18}N_1O_6$	404.1139602	404.11389	0.1736636
$C_{20}H_{22}N_1O_8$	404.1350894	404.13503	0.1469308

$C_{24}H_{22}N_1O_5$	404.1503456	404.15034	0.0138065
$C_{21}H_{26}N_1O_7$	404.1714748	404.17139	0.2097622
$C_{25}H_{26}N_1O_4$	404.186731	404.18685	-0.294468
$C_{22}H_{30}N_1O_6$	404.2078602	404.20778	0.198363
$C_{18}H_{17}N_2O_9$	405.093953	405.09384	0.278898
$C_{23}H_{17}O_7$	405.0979758	405.09801	-0.084474
$C_{22}H_{17}N_2O_6$	405.1092092	405.10909	0.294192
$C_{20}H_{21}O_9$	405.119105	405.11895	0.3825539
$C_{19}H_{21}N_2O_8$	405.1303384	405.13033	0.0206845
$C_{24}H_{21}O_6$	405.1343612	405.1344	-0.09582
$C_{23}H_{21}N_2O_5$	405.1455946	405.14553	0.1593992
$C_{21}H_{25}O_8$	405.1554904	405.15546	0.0749833
$C_{20}H_{25}N_2O_7$	405.1667238	405.16671	0.0340104
$C_{25}H_{25}O_5$	405.1707466	405.17082	-0.181208
$C_{13}H_{29}N_2O_{12}$	405.1725968	405.17248	0.2882226
$C_{24}H_{25}N_2O_4$	405.18198	405.18182	0.3948347
$C_{22}H_{29}O_7$	405.1918758	405.19174	0.3351003
$C_{22}H_{16}N_1O_7$	406.0932248	406.09322	0.0117705
$C_{19}H_{20}N_1O_9$	406.114354	406.11417	0.4530249
$C_{23}H_{20}N_1O_6$	406.1296102	406.12961	0.000443
$C_{20}H_{24}N_1O_8$	406.1507394	406.15074	-0.001527
$C_{24}H_{24}N_1O_5$	406.1659956	406.16598	0.0383585
$C_{21}H_{28}N_1O_7$	406.1871248	406.18701	0.2825789
$C_{23}H_{19}O_7$	407.1136258	407.11358	0.1124499
$C_{22}H_{19}N_2O_6$	407.1248592	407.12488	-0.051139
$C_{20}H_{23}O_9$	407.134755	407.13458	0.4297837

$C_{19}H_{23}N_2O_8$	407.1459884	407.14615	-0.396959
$C_{24}H_{23}O_6$	407.1500112	407.14983	0.4449954
$C_{23}H_{23}N_2O_5$	407.1612446	407.16094	0.7480572
$C_{21}H_{27}O_8$	407.1711404	407.17105	0.2219703
$C_{22}H_{18}N_1O_7$	408.1088748	408.10902	-0.355837
$C_{23}H_{22}N_1O_6$	408.1452602	408.14541	-0.367075
$C_{24}H_{26}N_1O_5$	408.1816456	408.18173	-0.20682
$C_{22}H_{17}O_8$	409.0928904	409.09273	0.3920379
$C_{21}H_{17}N_2O_7$	409.1041238	409.10409	0.0825704
$C_{18}H_{21}N_2O_9$	409.125253	409.1251	0.3739195
$C_{23}H_{21}O_7$	409.1292758	409.12914	0.3318753
$C_{22}H_{21}N_2O_6$	409.1405092	409.14042	0.2179689
$C_{15}H_{25}N_2O_{11}$	409.1463822	409.1462	0.4452683
$C_{20}H_{25}O_9$	409.150405	409.15027	0.3299029
$C_{24}H_{25}O_6$	409.1656612	409.16551	0.3694834
$C_{23}H_{25}N_2O_5$	409.1768946	409.1767	0.4755398
$C_{21}H_{16}N_1O_8$	410.0881394	410.08817	-0.074667
$C_{18}H_{20}N_1O_{10}$	410.1092686	410.10931	-0.100998
$C_{22}H_{20}N_1O_7$	410.1245248	410.12463	-0.256556
$C_{19}H_{24}N_1O_9$	410.145654	410.14577	-0.282875
$C_{23}H_{24}N_1O_6$	410.1609102	410.16101	-0.243368
$C_{20}H_{28}N_1O_8$	410.1820394	410.18191	0.3154207
$C_{24}H_{28}N_1O_5$	410.1972956	410.19742	-0.303318
$C_{21}H_{32}N_1O_7$	410.2184248	410.21847	-0.110234
$C_{22}H_{19}O_8$	411.1085404	411.1083	0.5847115
$C_{21}H_{19}N_2O_7$	411.1197738	411.1197	0.1794608

$C_{14}H_{23}N_2O_{12}$	411.1256468	411.12539	0.6245777
$C_{23}H_{23}O_7$	411.1449258	411.14468	0.5977938
$C_{22}H_{23}N_2O_6$	411.1561592	411.15594	0.5330819
$C_{24}H_{27}O_6$	411.1813112	411.18126	0.1244704
$C_{23}H_{27}N_2O_5$	411.1925446	411.19243	0.2786527
$C_{21}H_{18}N_1O_8$	412.1037894	412.1039	-0.268428
$C_{18}H_{22}N_1O_{10}$	412.1249186	412.12522	-0.73138
$C_{22}H_{22}N_1O_7$	412.1401748	412.14031	-0.328092
$C_{23}H_{26}N_1O_6$	412.1765602	412.17671	-0.363485
$C_{21}H_{17}O_9$	413.087805	413.08775	0.1330949
$C_{22}H_{21}O_8$	413.1241904	413.12398	0.5092413
$C_{21}H_{21}N_2O_7$	413.1354238	413.13527	0.3722264
$C_{14}H_{25}N_2O_{12}$	413.1412968	413.14118	0.2826633
$C_{23}H_{25}O_7$	413.1605758	413.16033	0.5948774
$C_{22}H_{25}N_2O_6$	413.1718092	413.17166	0.3610602
$C_{24}H_{29}O_6$	413.1969612	413.19685	0.2690724
$C_{23}H_{29}N_2O_5$	413.2081946	413.20792	0.6645074
$C_{21}H_{20}N_1O_8$	414.1194394	414.11953	-0.218826
$C_{18}H_{24}N_1O_{10}$	414.1405686	414.1404	0.4070596
$C_{22}H_{24}N_1O_7$	414.1558248	414.15592	-0.229914
$C_{23}H_{28}N_1O_6$	414.1922102	414.19235	-0.337573
$C_{24}H_{32}N_1O_5$	414.2285956	414.2285	0.2307419
$C_{21}H_{19}O_9$	415.103455	415.10328	0.4215332
$C_{20}H_{19}N_2O_8$	415.1146884	415.11465	0.0924561
$C_{24}H_{19}N_2O_5$	415.1299446	415.12971	0.5650758
$C_{22}H_{23}O_8$	415.1398404	415.13969	0.3622391

$C_{21}H_{23}N_2O_7$	415.1510738	415.15098	0.2258934
$C_{14}H_{27}N_2O_{12}$	415.1569468	415.15681	0.3294655
$C_{23}H_{27}O_7$	415.1762258	415.17602	0.4956447
$C_{22}H_{27}N_2O_6$	415.1874592	415.1875	-0.098317
$C_{15}H_{31}N_2O_{11}$	415.1933322	415.1931	0.5592091
$C_{24}H_{31}O_6$	415.2126112	415.21229	0.7735312
$C_{20}H_{18}N_1O_9$	416.098704	416.09888	-0.423025
$C_{24}H_{18}N_1O_6$	416.1139602	416.11411	-0.360046
$C_{21}H_{22}N_1O_8$	416.1350894	416.13517	-0.193735
$C_{25}H_{22}N_1O_5$	416.1503456	416.15052	-0.419128
$C_{22}H_{26}N_1O_7$	416.1714748	416.17154	-0.156714
$C_{23}H_{30}N_1O_6$	416.2078602	416.2078	0.144591
$C_{21}H_{21}O_9$	417.119105	417.11888	0.5393661
$C_{13}H_{25}N_2O_{13}$	417.1362114	417.13622	-0.020665
$C_{24}H_{21}N_2O_5$	417.1455946	417.14552	0.1787863
$C_{22}H_{25}O_8$	417.1554904	417.15537	0.2885732
$C_{21}H_{25}N_2O_7$	417.1667238	417.16656	0.3926006
$C_{14}H_{29}N_2O_{12}$	417.1725968	417.17254	0.1361065
$C_{25}H_{25}N_2O_4$	417.18198	417.18206	-0.191811
$C_{23}H_{29}O_7$	417.1918758	417.19174	0.3254615
$C_{23}H_{16}N_1O_7$	418.0932248	418.09335	-0.299503
$C_{20}H_{20}N_1O_9$	418.114354	418.11436	-0.014398
$C_{24}H_{20}N_1O_6$	418.1296102	418.12965	-0.095234
$C_{21}H_{24}N_1O_8$	418.1507394	418.15079	-0.121057
$C_{25}H_{24}N_1O_5$	418.1659956	418.1661	-0.24971
$C_{22}H_{28}N_1O_7$	418.1871248	418.18719	-0.155959

$C_{23}H_{32}N_1O_6$	418.2235102	418.22345	0.1438941
$C_{19}H_{19}N_2O_9$	419.109603	419.10959	0.0309702
$C_{24}H_{19}O_7$	419.1136258	419.11345	0.4194087
$C_{23}H_{19}N_2O_6$	419.1248592	419.12494	-0.192831
$C_{21}H_{23}O_9$	419.134755	419.13454	0.5129136
$C_{20}H_{23}N_2O_8$	419.1459884	419.14588	0.2585732
$C_{25}H_{23}O_6$	419.1500112	419.15002	-0.021043
$C_{13}H_{27}N_2O_{13}$	419.1518614	419.15161	0.5997347
$C_{24}H_{23}N_2O_5$	419.1612446	419.16107	0.4164982
$C_{22}H_{27}O_8$	419.1711404	419.17087	0.6450346
$C_{21}H_{27}N_2O_7$	419.1823738	419.18227	0.247577
$C_{14}H_{31}N_2O_{12}$	419.1882468	419.18809	0.3740083
$C_{23}H_{31}O_7$	419.2075258	419.20737	0.3716057
$C_{23}H_{18}N_1O_7$	420.1088748	420.10891	-0.083836
$C_{20}H_{22}N_1O_9$	420.130004	420.13022	-0.514174
$C_{24}H_{22}N_1O_6$	420.1452602	420.14532	-0.14238
$C_{21}H_{26}N_1O_8$	420.1663894	420.16649	-0.239477
$C_{25}H_{26}N_1O_5$	420.1816456	420.18166	-0.034319
$C_{22}H_{30}N_1O_7$	420.2027748	420.20305	-0.65497
$C_{19}H_{21}N_2O_9$	421.125253	421.12521	0.1020597
$C_{24}H_{21}O_7$	421.1292758	421.12904	0.5598753
$C_{23}H_{21}N_2O_6$	421.1405092	421.14039	0.2829932
$C_{21}H_{25}O_9$	421.150405	421.15026	0.3442473
$C_{25}H_{25}O_6$	421.1656612	421.16538	0.667623
$C_{24}H_{25}N_2O_5$	421.1768946	421.17671	0.4382479
$C_{22}H_{29}O_8$	421.1867904	421.18661	0.4282658

$C_{22}H_{16}N_1O_8$	422.0881394	422.08843	-0.688529
$C_{19}H_{20}N_1O_{10}$	422.1092686	422.10934	-0.169198
$C_{23}H_{20}N_1O_7$	422.1245248	422.12458	-0.130815
$C_{20}H_{24}N_1O_9$	422.145654	422.14594	-0.677539
$C_{24}H_{24}N_1O_6$	422.1609102	422.16098	-0.165387
$C_{25}H_{28}N_1O_5$	422.1972956	422.19741	-0.271011
$C_{23}H_{19}O_8$	423.1085404	423.10832	0.520859
$C_{22}H_{19}N_2O_7$	423.1197738	423.11985	-0.180138
$C_{24}H_{23}O_7$	423.1449258	423.14479	0.3208827
$C_{23}H_{23}N_2O_6$	423.1561592	423.15594	0.5179646
$C_{16}H_{27}N_2O_{11}$	423.1620322	423.16184	0.454152
$C_{25}H_{27}O_6$	423.1813112	423.18119	0.2863546
$C_{24}H_{27}N_2O_5$	423.1925446	423.19234	0.4834204
$C_{22}H_{31}O_8$	423.2024404	423.20247	-0.06999
$C_{23}H_{35}O_7$	423.2388258	423.23858	0.5807121
$C_{22}H_{18}N_1O_8$	424.1037894	424.104	-0.496624
$C_{19}H_{22}N_1O_{10}$	424.1249186	424.12505	-0.309862
$C_{23}H_{22}N_1O_7$	424.1401748	424.14026	-0.200924
$C_{20}H_{26}N_1O_9$	424.161304	424.16128	0.0565349
$C_{24}H_{26}N_1O_6$	424.1765602	424.1766	-0.093876
$C_{25}H_{30}N_1O_5$	424.2129456	424.21304	-0.222577
$C_{23}H_{21}O_8$	425.1241904	425.12396	0.541912
$C_{22}H_{21}N_2O_7$	425.1354238	425.13528	0.3381979
$C_{24}H_{25}O_7$	425.1605758	425.16037	0.4840051
$C_{23}H_{25}N_2O_6$	425.1718092	425.17171	0.2332702
$C_{25}H_{29}O_6$	425.1969612	425.19686	0.2379601

$C_{23}H_{37}O_7$	425.2544758	425.25426	0.5074136
$C_{21}H_{16}N_1O_9$	426.083054	426.08277	0.6664895
$C_{22}H_{20}N_1O_8$	426.1194394	426.11954	-0.236131
$C_{23}H_{24}N_1O_7$	426.1558248	426.15588	-0.129577
$C_{20}H_{28}N_1O_9$	426.176954	426.17703	-0.178377
$C_{24}H_{28}N_1O_6$	426.1922102	426.19235	-0.328068
$C_{22}H_{19}O_9$	427.103455	427.10322	0.5501709
$C_{21}H_{19}N_2O_8$	427.1146884	427.11463	0.1366844
$C_{23}H_{23}O_8$	427.1398404	427.13961	0.5393547
$C_{22}H_{23}N_2O_7$	427.1510738	427.15093	0.336602
$C_{15}H_{27}N_2O_{12}$	427.1569468	427.15683	0.2733887
$C_{24}H_{27}O_7$	427.1762258	427.17606	0.3880832
$C_{23}H_{27}N_2O_6$	427.1874592	427.18719	0.6301213
$C_{25}H_{31}O_6$	427.2126112	427.21227	0.7986185
$C_{22}H_{35}O_8$	427.2337404	427.23369	0.1179212
$C_{21}H_{18}N_1O_9$	428.098704	428.0985	0.4764787
$C_{25}H_{18}N_1O_6$	428.1139602	428.11382	0.3274359
$C_{22}H_{22}N_1O_8$	428.1350894	428.13513	-0.094877
$C_{26}H_{22}N_1O_5$	428.1503456	428.15015	0.4568019
$C_{23}H_{26}N_1O_7$	428.1714748	428.17156	-0.199033
$C_{24}H_{30}N_1O_6$	428.2078602	428.2079	-0.092992
$C_{22}H_{21}O_9$	429.119105	429.11893	0.4077653
$C_{21}H_{21}N_2O_8$	429.1303384	429.1301	0.5554953
$C_{14}H_{25}N_2O_{13}$	429.1362114	429.13589	0.7488995
$C_{25}H_{21}N_2O_5$	429.1455946	429.14568	-0.199047
$C_{23}H_{25}O_8$	429.1554904	429.15527	0.5135199

$C_{22}H_{25}N_2O_7$	429.1667238	429.16657	0.358322
$C_{15}H_{29}N_2O_{12}$	429.1725968	429.17238	0.5051112
$C_{24}H_{29}O_7$	429.1918758	429.19167	0.479459
$C_{24}H_{16}N_1O_7$	430.0932248	430.09331	-0.198143
$C_{21}H_{20}N_1O_9$	430.114354	430.11464	-0.664986
$C_{25}H_{20}N_1O_6$	430.1296102	430.12966	-0.115826
$C_{22}H_{24}N_1O_8$	430.1507394	430.15083	-0.210671
$C_{26}H_{24}N_1O_5$	430.1659956	430.16597	0.0594652
$C_{23}H_{28}N_1O_7$	430.1871248	430.18719	-0.151609
$C_{24}H_{32}N_1O_6$	430.2235102	430.22361	-0.232019
$C_{20}H_{19}N_2O_9$	431.109603	431.10943	0.4012434
$C_{25}H_{19}O_7$	431.1136258	431.11379	-0.380921
$C_{24}H_{19}N_2O_6$	431.1248592	431.1246	0.6011713
$C_{22}H_{23}O_9$	431.134755	431.13447	0.6609996
$C_{21}H_{23}N_2O_8$	431.1459884	431.1459	0.2049883
$C_{14}H_{27}N_2O_{13}$	431.1518614	431.15183	0.0727815
$C_{23}H_{27}O_8$	431.1711404	431.17091	0.534312
$C_{15}H_{31}N_2O_{12}$	431.1882468	431.18819	0.1316824
$C_{24}H_{31}O_7$	431.2075258	431.20725	0.6395526
$C_{24}H_{18}N_1O_7$	432.1088748	432.10893	-0.127792
$C_{21}H_{22}N_1O_9$	432.130004	432.13011	-0.245343
$C_{25}H_{22}N_1O_6$	432.1452602	432.14529	-0.069005
$C_{22}H_{26}N_1O_8$	432.1663894	432.1665	-0.255966
$C_{26}H_{26}N_1O_5$	432.1816456	432.18184	-0.449857
$C_{23}H_{30}N_1O_7$	432.2027748	432.20297	-0.451686
$C_{20}H_{21}N_2O_9$	433.125253	433.12491	0.7918723

$C_{25}H_{21}O_7$	433.1292758	433.12915	0.2903981
$C_{24}H_{21}N_2O_6$	433.1405092	433.1404	0.2520658
$C_{22}H_{25}O_9$	433.150405	433.1503	0.2423636
$C_{26}H_{25}O_6$	433.1656612	433.16557	0.2104966
$C_{25}H_{25}N_2O_5$	433.1768946	433.17679	0.2414254
$C_{23}H_{29}O_8$	433.1867904	433.18663	0.3702327
$C_{24}H_{33}O_7$	433.2231758	433.22295	0.521163
$C_{24}H_{20}N_1O_7$	434.1245248	434.12453	-0.012024
$C_{21}H_{24}N_1O_9$	434.145654	434.14564	0.0322009
$C_{25}H_{24}N_1O_6$	434.1609102	434.16083	0.1846778
$C_{22}H_{28}N_1O_8$	434.1820394	434.18195	0.2058581
$C_{26}H_{28}N_1O_5$	434.1972956	434.19727	0.0589131
$C_{24}H_{19}O_8$	435.1085404	435.10835	0.4375458
$C_{23}H_{19}N_2O_7$	435.1197738	435.11978	-0.014295
$C_{25}H_{23}O_7$	435.1449258	435.14472	0.4728997
$C_{24}H_{23}N_2O_6$	435.1561592	435.15604	0.2738785
$C_{22}H_{27}O_9$	435.166055	435.16586	0.4480586
$C_{26}H_{27}O_6$	435.1813112	435.1814	-0.204099
$C_{25}H_{27}N_2O_5$	435.1925446	435.1924	0.3322205
$C_{23}H_{31}O_8$	435.2024404	435.20224	0.4604292
$C_{23}H_{18}N_1O_8$	436.1037894	436.10375	0.0902994
$C_{24}H_{22}N_1O_7$	436.1401748	436.14008	0.2173152
$C_{21}H_{26}N_1O_9$	436.161304	436.16141	-0.243075
$C_{25}H_{26}N_1O_6$	436.1765602	436.17639	0.3901629
$C_{26}H_{30}N_1O_5$	436.2129456	436.21291	0.0815654
$C_{24}H_{21}O_8$	437.1241904	437.12407	0.2753906

$C_{25}H_{25}O_7$	437.1605758	437.1605	0.1733457
$C_{24}H_{25}N_2O_6$	437.1718092	437.17162	0.4327358
$C_{22}H_{29}O_9$	437.181705	437.18181	-0.240221
$C_{26}H_{29}O_6$	437.1969612	437.19679	0.3915395
$C_{25}H_{29}N_2O_5$	437.2081946	437.208	0.4450509
$C_{23}H_{20}N_1O_8$	438.1194394	438.11914	0.6833294
$C_{24}H_{24}N_1O_7$	438.1558248	438.15567	0.3532531
$C_{25}H_{28}N_1O_6$	438.1922102	438.192	0.4796523
$C_{23}H_{19}O_9$	439.103455	439.10355	-0.216396
$C_{24}H_{23}O_8$	439.1398404	439.13976	0.1830394
$C_{16}H_{27}N_2O_{12}$	439.1569468	439.15706	-0.257812
$C_{25}H_{27}O_7$	439.1762258	439.17619	0.0814705
$C_{24}H_{27}N_2O_6$	439.1874592	439.1875	-0.092945
$C_{23}H_{22}N_1O_8$	440.1350894	440.13488	0.4757174
$C_{24}H_{26}N_1O_7$	440.1714748	440.17135	0.2834802
$C_{25}H_{30}N_1O_6$	440.2078602	440.20768	0.4093064
$C_{23}H_{21}O_9$	441.119105	441.11934	-0.532782
$C_{22}H_{21}N_2O_8$	441.1303384	441.13045	-0.253032
$C_{24}H_{25}O_8$	441.1554904	441.15553	-0.08981
$C_{23}H_{25}N_2O_7$	441.1667238	441.16664	0.1899053
$C_{16}H_{29}N_2O_{12}$	441.1725968	441.17246	0.3100372
$C_{25}H_{29}O_7$	441.1918758	441.1919	-0.054897
$C_{24}H_{29}N_2O_6$	441.2031092	441.20308	0.0661371
$C_{23}H_{24}N_1O_8$	442.1507394	442.15045	0.6544825
$C_{24}H_{28}N_1O_7$	442.1871248	442.18688	0.5535663
$C_{25}H_{32}N_1O_6$	442.2235102	442.22331	0.4526668

$C_{21}H_{19}N_2O_9$	443.109603	443.10969	-0.196385
$C_{23}H_{23}O_9$	443.134755	443.13471	0.1015039
$C_{22}H_{23}N_2O_8$	443.1459884	443.14611	-0.274447
$C_{15}H_{27}N_2O_{13}$	443.1518614	443.15183	0.0708107
$C_{24}H_{27}O_8$	443.1711404	443.17119	-0.111966
$C_{23}H_{27}N_2O_7$	443.1823738	443.18221	0.3695542
$C_{16}H_{31}N_2O_{12}$	443.1882468	443.18832	-0.165212
$C_{25}H_{31}O_7$	443.2075258	443.20756	-0.07721
$C_{26}H_{22}N_1O_6$	444.1452602	444.145	0.5857991
$C_{23}H_{26}N_1O_8$	444.1663894	444.16612	0.6064842
$C_{21}H_{21}N_2O_9$	445.125253	445.12534	-0.195496
$C_{26}H_{21}O_7$	445.1292758	445.12933	-0.121808
$C_{25}H_{21}N_2O_6$	445.1405092	445.14084	-0.743181
$C_{23}H_{25}O_9$	445.150405	445.15057	-0.370706
$C_{27}H_{25}O_6$	445.1656612	445.16566	0.0026505
$C_{15}H_{29}N_2O_{13}$	445.1675114	445.16738	0.2951246
$C_{26}H_{25}N_2O_5$	445.1768946	445.17693	-0.079564
$C_{24}H_{29}O_8$	445.1867904	445.18681	-0.044072
$C_{23}H_{29}N_2O_7$	445.1980238	445.19801	0.0309523
$C_{16}H_{33}N_2O_{12}$	445.2038968	445.2038	0.2173833
$C_{25}H_{20}N_1O_7$	446.1245248	446.12465	-0.280684
$C_{22}H_{24}N_1O_9$	446.145654	446.14549	0.3675479
$C_{26}H_{24}N_1O_6$	446.1609102	446.16084	0.1572973
$C_{23}H_{28}N_1O_8$	446.1820394	446.18215	-0.247926
$C_{24}H_{32}N_1O_7$	446.2184248	446.21823	0.4365125
$C_{24}H_{19}N_2O_7$	447.1197738	447.11988	-0.237565

$C_{26}H_{23}O_7$	447.1449258	447.14506	-0.300171
$C_{25}H_{23}N_2O_6$	447.1561592	447.15614	0.0428931
$C_{23}H_{27}O_9$	447.166055	447.16608	-0.055953
$C_{15}H_{31}N_2O_{13}$	447.1831614	447.18334	-0.399434
$C_{26}H_{27}N_2O_5$	447.1925446	447.19236	0.4127526
$C_{24}H_{31}O_8$	447.2024404	447.20243	0.0232107
$C_{24}H_{18}N_1O_8$	448.1037894	448.10371	0.1771462
$C_{25}H_{22}N_1O_7$	448.1401748	448.14007	0.2338105
$C_{26}H_{26}N_1O_6$	448.1765602	448.17648	0.1789025
$C_{23}H_{30}N_1O_8$	448.1976894	448.19769	-0.001384
$C_{25}H_{21}O_8$	449.1241904	449.12392	0.6020159
$C_{24}H_{21}N_2O_7$	449.1354238	449.13514	0.6318359
$C_{26}H_{25}O_7$	449.1605758	449.16055	0.0573957
$C_{25}H_{25}N_2O_6$	449.1718092	449.17159	0.4879645
$C_{23}H_{29}O_9$	449.181705	449.18153	0.3895526
$C_{24}H_{20}N_1O_8$	450.1194394	450.11947	-0.068027
$C_{25}H_{24}N_1O_7$	450.1558248	450.15585	-0.056025
$C_{26}H_{28}N_1O_6$	450.1922102	450.19215	0.133676
$C_{25}H_{23}O_8$	451.1398404	451.13969	0.3333332
$C_{24}H_{23}N_2O_7$	451.1510738	451.15094	0.2965302
$C_{17}H_{27}N_2O_{12}$	451.1569468	451.15703	-0.184459
$C_{26}H_{27}O_7$	451.1762258	451.17606	0.3674394
$C_{25}H_{27}N_2O_6$	451.1874592	451.18728	0.3971296
$C_{24}H_{22}N_1O_8$	452.1350894	452.13514	-0.111958
$C_{25}H_{26}N_1O_7$	452.1714748	452.17151	-0.077891
$C_{26}H_{30}N_1O_6$	452.2078602	452.20787	-0.021716

$C_{24}H_{21}O_9$	453.119105	453.11884	0.5847908
$C_{25}H_{25}O_8$	453.1554904	453.15532	0.3759855
$C_{24}H_{25}N_2O_7$	453.1667238	453.1666	0.2731443
$C_{26}H_{29}O_7$	453.1918758	453.19166	0.4761336
$C_{23}H_{20}N_1O_9$	454.114354	454.11433	0.0528059
$C_{24}H_{24}N_1O_8$	454.1507394	454.15073	0.0206537
$C_{25}H_{28}N_1O_7$	454.1871248	454.18714	-0.033511
$C_{26}H_{32}N_1O_6$	454.2235102	454.22346	0.110474
$C_{24}H_{23}O_9$	455.134755	455.13466	0.2086852
$C_{23}H_{23}N_2O_8$	455.1459884	455.14592	0.1502373
$C_{16}H_{27}N_2O_{13}$	455.1518614	455.15185	0.0250024
$C_{25}H_{27}O_8$	455.1711404	455.17104	0.2205322
$C_{24}H_{27}N_2O_7$	455.1823738	455.18203	0.7552575
$C_{26}H_{31}O_7$	455.2075258	455.20756	-0.075175
$C_{23}H_{22}N_1O_9$	456.130004	456.12986	0.3156554
$C_{27}H_{22}N_1O_6$	456.1452602	456.14505	0.4607741
$C_{24}H_{26}N_1O_8$	456.1663894	456.16623	0.3493898
$C_{25}H_{30}N_1O_7$	456.2027748	456.20261	0.3611988
$C_{24}H_{25}O_9$	457.150405	457.15044	-0.076605
$C_{25}H_{29}O_8$	457.1867904	457.18681	-0.042915
$C_{24}H_{29}N_2O_7$	457.1980238	457.19793	0.2051188
$C_{26}H_{20}N_1O_7$	458.1245248	458.12445	0.1632305
$C_{23}H_{24}N_1O_9$	458.145654	458.14545	0.4452294
$C_{24}H_{28}N_1O_8$	458.1820394	458.18193	0.2387259
$C_{22}H_{23}N_2O_9$	459.140903	459.14104	-0.298427
$C_{26}H_{23}N_2O_6$	459.1561592	459.15618	-0.045344

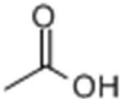
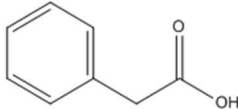
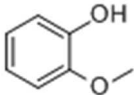
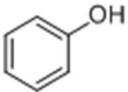
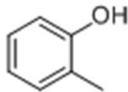
$C_{24}H_{27}O_9$	459.166055	459.16618	-0.272276
$C_{23}H_{27}N_2O_8$	459.1772884	459.17732	-0.068863
$C_{16}H_{31}N_2O_{13}$	459.1831614	459.18322	-0.127662
$C_{25}H_{31}O_8$	459.2024404	459.20252	-0.173388
$C_{26}H_{22}N_1O_7$	460.1401748	460.14004	0.2929105
$C_{27}H_{26}N_1O_6$	460.1765602	460.17645	0.2394296
$C_{24}H_{30}N_1O_8$	460.1976894	460.1975	0.4115186
$C_{26}H_{21}O_8$	461.1241904	461.12423	-0.085921
$C_{22}H_{25}N_2O_9$	461.156553	461.15648	0.1582541
$C_{27}H_{25}O_7$	461.1605758	461.16049	0.1860087
$C_{26}H_{25}N_2O_6$	461.1718092	461.1716	0.4535834
$C_{24}H_{29}O_9$	461.181705	461.18154	0.357733
$C_{25}H_{33}O_8$	461.2180904	461.21816	-0.150948
$C_{25}H_{20}N_1O_8$	462.1194394	462.11941	0.0635764
$C_{26}H_{24}N_1O_7$	462.1558248	462.15575	0.1618067
$C_{23}H_{28}N_1O_9$	462.176954	462.17676	0.4197092
$C_{27}H_{28}N_1O_6$	462.1922102	462.19206	0.3249295
$C_{26}H_{23}O_8$	463.1398404	463.13965	0.4110635
$C_{25}H_{23}N_2O_7$	463.1510738	463.15102	0.1161174
$C_{27}H_{27}O_7$	463.1762258	463.17609	0.2931495
$C_{26}H_{27}N_2O_6$	463.1874592	463.18721	0.5379677
$C_{24}H_{31}O_9$	463.197355	463.19726	0.2050528
$C_{25}H_{22}N_1O_8$	464.1350894	464.13513	-0.087518
$C_{26}H_{26}N_1O_7$	464.1714748	464.1715	-0.054334
$C_{27}H_{30}N_1O_6$	464.2078602	464.20771	0.3235186
$C_{26}H_{25}O_8$	465.1554904	465.15529	0.4307805

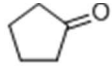
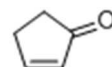
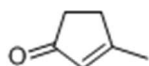
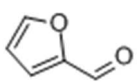
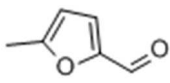
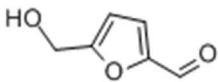
$C_{25}H_{25}N_2O_7$	465.1667238	465.16638	0.7390466
$C_{27}H_{29}O_7$	465.1918758	465.19161	0.5713339
$C_{25}H_{24}N_1O_8$	466.1507394	466.15077	-0.065687
$C_{26}H_{28}N_1O_7$	466.1871248	466.18706	0.1389569
$C_{25}H_{23}O_9$	467.134755	467.13464	0.2461386
$C_{24}H_{23}N_2O_8$	467.1459884	467.14594	0.1035648
$C_{26}H_{27}O_8$	467.1711404	467.17105	0.1934621
$C_{25}H_{26}N_1O_8$	468.1663894	468.16619	0.425874
$C_{26}H_{30}N_1O_7$	468.2027748	468.20256	0.4587327
$C_{25}H_{25}O_9$	469.150405	469.1503	0.223766
$C_{24}H_{25}N_2O_8$	469.1616384	469.16148	0.3375807
$C_{26}H_{29}O_8$	469.1867904	469.18663	0.3418253
$C_{25}H_{29}N_2O_7$	469.1980238	469.19809	-0.141135
$C_{24}H_{24}N_1O_9$	470.145654	470.14533	0.6891054
$C_{25}H_{28}N_1O_8$	470.1820394	470.18185	0.40278
$C_{26}H_{32}N_1O_7$	470.2184248	470.21812	0.6481666
$C_{27}H_{23}N_2O_6$	471.1561592	471.15624	-0.171536
$C_{25}H_{27}O_9$	471.166055	471.16608	-0.053103
$C_{26}H_{31}O_8$	471.2024404	471.20243	0.0220285
$C_{24}H_{26}N_1O_9$	472.161304	472.16103	0.5802676
$C_{28}H_{26}N_1O_6$	472.1765602	472.1764	0.3392373
$C_{25}H_{30}N_1O_8$	472.1976894	472.19755	0.2951728
$C_{28}H_{25}O_7$	473.1605758	473.16026	0.6673842
$C_{25}H_{29}O_9$	473.181705	473.18154	0.3486608
$C_{27}H_{24}N_1O_7$	474.1558248	474.15585	-0.053189
$C_{28}H_{28}N_1O_6$	474.1922102	474.19214	0.1479988

$C_{27}H_{23}O_8$	475.1398404	475.13979	0.1060317
$C_{27}H_{27}N_2O_6$	475.1874592	475.1871	0.7558699
$C_{26}H_{22}N_1O_8$	476.1350894	476.13535	-0.547366
$C_{27}H_{26}N_1O_7$	476.1714748	476.17146	0.031039
$C_{28}H_{30}N_1O_6$	476.2078602	476.20822	-0.755595
$C_{26}H_{21}O_9$	477.119105	477.11922	-0.241072
$C_{27}H_{25}O_8$	477.1554904	477.15567	-0.376439
$C_{26}H_{25}N_2O_7$	477.1667238	477.16684	-0.243563
$C_{26}H_{24}N_1O_8$	478.1507394	478.15048	0.5424647
$C_{26}H_{23}O_9$	479.134755	479.13482	-0.135703
$C_{25}H_{23}N_2O_8$	479.1459884	479.14624	-0.525143
$C_{27}H_{27}O_8$	479.1711404	479.17124	-0.207901
$C_{26}H_{27}N_2O_7$	479.1823738	479.18261	-0.492965
$C_{26}H_{26}N_1O_8$	480.1663894	480.16616	0.4777092
$C_{27}H_{30}N_1O_7$	480.2027748	480.20296	-0.385712
$C_{26}H_{25}O_9$	481.150405	481.15022	0.3844534
$C_{27}H_{29}O_8$	481.1867904	481.18682	-0.061556
$C_{25}H_{24}N_1O_9$	482.145654	482.1458	-0.302855
$C_{26}H_{28}N_1O_8$	482.1820394	482.18211	-0.146459
$C_{25}H_{27}N_2O_8$	483.1772884	483.17692	0.7624115
$C_{25}H_{43}N_2O_7$	483.3075738	483.30734	0.4837083
$C_{26}H_{30}N_1O_8$	484.1976894	484.19761	0.1639411
$C_{26}H_{29}O_9$	485.181705	485.18145	0.5255349
$C_{26}H_{31}O_9$	487.197355	487.19746	-0.21556
$C_{28}H_{26}N_1O_7$	488.1714748	488.17129	0.3785143
$C_{27}H_{24}N_1O_8$	490.1507394	490.15076	-0.042069

$C_{28}H_{28}N_1O_7$	490.1871248	490.18711	0.0301515
$C_{27}H_{23}O_9$	491.134755	491.13476	-0.010221
$C_{27}H_{26}N_1O_8$	492.1663894	492.16627	0.24256
$C_{28}H_{30}N_1O_7$	492.2027748	492.20254	0.4769983
$C_{28}H_{29}O_8$	493.1867904	493.1867	0.1832569
$C_{26}H_{24}N_1O_9$	494.145654	494.1455	0.3116083
$C_{27}H_{28}N_1O_8$	494.1820394	494.18188	0.3225125
$C_{27}H_{27}O_9$	495.166055	495.16606	-0.010138
$C_{26}H_{27}N_2O_8$	495.1772884	495.17721	0.1582865
$C_{27}H_{30}N_1O_8$	496.1976894	496.19784	-0.303549
$C_{27}H_{29}O_9$	497.181705	497.18185	-0.291684
$C_{28}H_{26}N_1O_8$	504.1663894	504.16645	-0.120238
$C_{28}H_{28}N_1O_8$	506.1820394	506.18207	-0.060492

Table S7 Main components and molecular structures of bio-oils obtained at different Zn²⁺ contents, as analyzed by GC-MS

Ret. Time (min)	Molecular structure	Components	Area (%)				
			BO-220 -0	BO-220-0.0 25	BO-220-0. 05	BO-220-0. 25	BO-220-0 .5
5.512		acetic acid	37.0	42.2	40.3	50.7	48.6
10.978		benzeneacetic acid	7.32	6.84	7.86	8.62	8.67
13.989		n-hexadecanoic acid	3.08	3.59	3.53	5.03	5.17
Total acids			48.4	52.6	51.7	64.4	62.4
7.507		phenol, 2-methoxy-	1.96	0.941	0.470	0.878	0.615
8.034		phenol	1.97	0.574	0.233	0.452	0.357
8.355		phenol, 2-methyl-	1.22	0.957	0.867	0.931	0.805
Total phenols			5.20	2.47	1.57	2.26	1.78

3.789		cyclopentanone ^a	0.251	0.133	0.307	0.420	0.514
5.018		2-cyclopentenone	0.346	0.200	0.218	0.189	0.237
5.098		2-cyclopenten-1-one,3-methyl-	0.984	0.774	0.971	0.916	1.126
Total ketones			1.58	1.11	1.50	1.52	1.88
5.605		furfural	10.7	12.1	13.9	8.52	7.30
6.212		furfural, 5-methyl-	6.34	5.67	5.87	3.54	2.34
10.264		furfural, 5-(hydroxymethyl)-	12.2	14.3	14.5	10.4	9.87
Total furans			35.1	36.1	38.2	24.1	20.5

^a Below detectable level.

Table S8 Molecular formula, mass and intensity for compounds with DBE values of 1 and two O in LP-220-0, LP-220-0.05 and LP-220-0.25, as detected by FT-ICR MS.

Molecular formula	Theoretical mass	Measured mass	Error (ppm)	Intensity		
				LP-220-0	LP-220-0.05	LP-220-0.25
C ₁₄ H ₂₇ O ₂	227.2016528	227.20165	0.0122354	13525094	30561476	52410395
C ₁₅ H ₂₉ O ₂	241.2173028	241.21738	-0.320127	26136937	40651430	55365360
C ₁₇ H ₃₃ O ₂	269.2486028	269.24865	-0.175377	23257283	28453679	32885864
C ₁₈ H ₃₅ O ₂	283.2642528	283.26418	0.2569329	275647970	287741074	300720619