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Electronic Supplementary Information (ESI)

First-Principle Oligopeptide Structural Optimization with Physical Prior Mean-Driven Gaussian Processes: A Test of Synergistic Impacts of the Kernel Functional and Coordinate System

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Figure S1. All-atom ball-and-stick representation of the 20 oligopeptides constructed in the testing set.

Atom color code: Red – O, yellow – S, blue – N, grey – C, white – H.

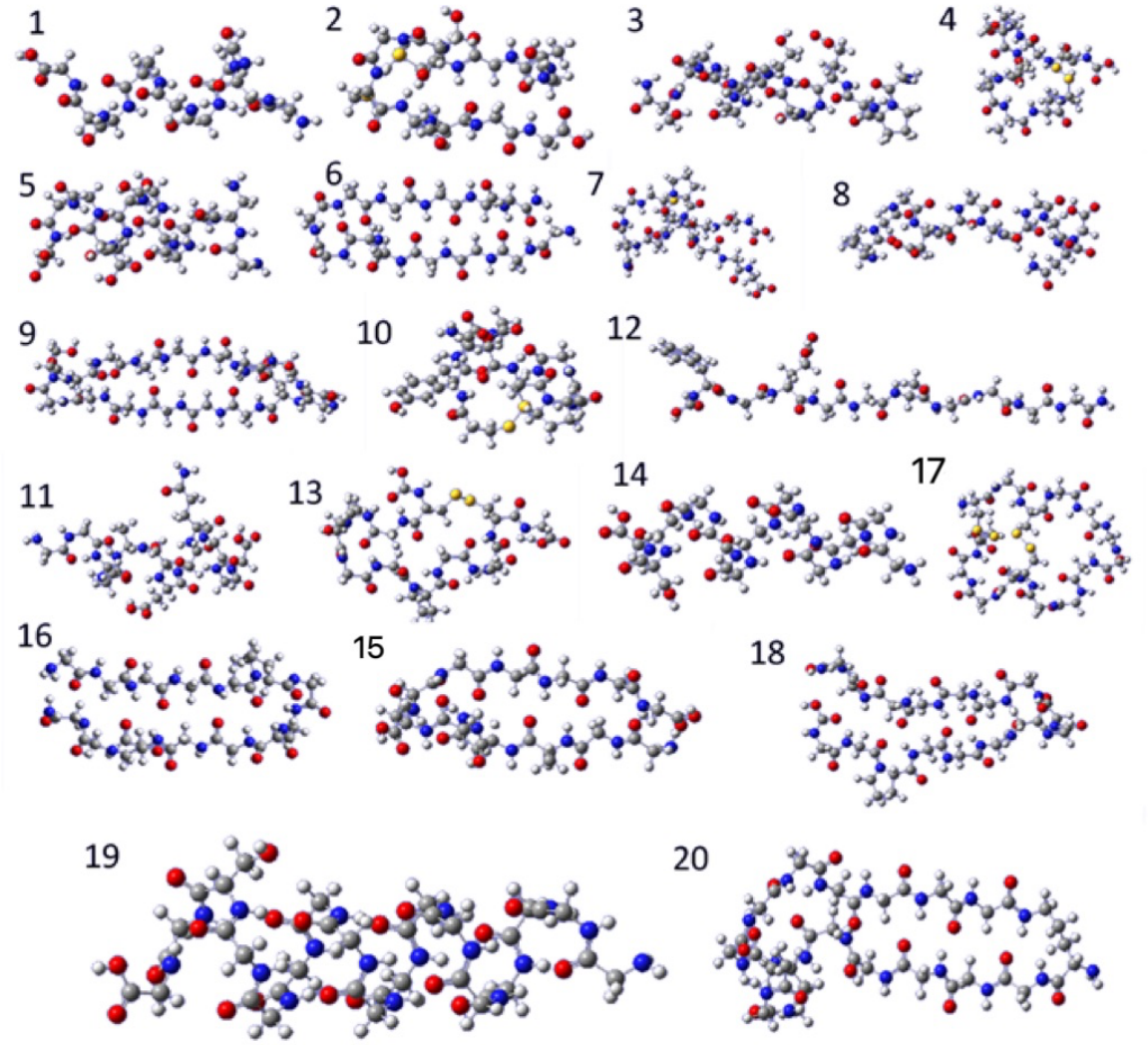

Figure S2. Structural visualization of the 20 oligopeptides optimized (which serve as the reference structures) using quantum mechanics.

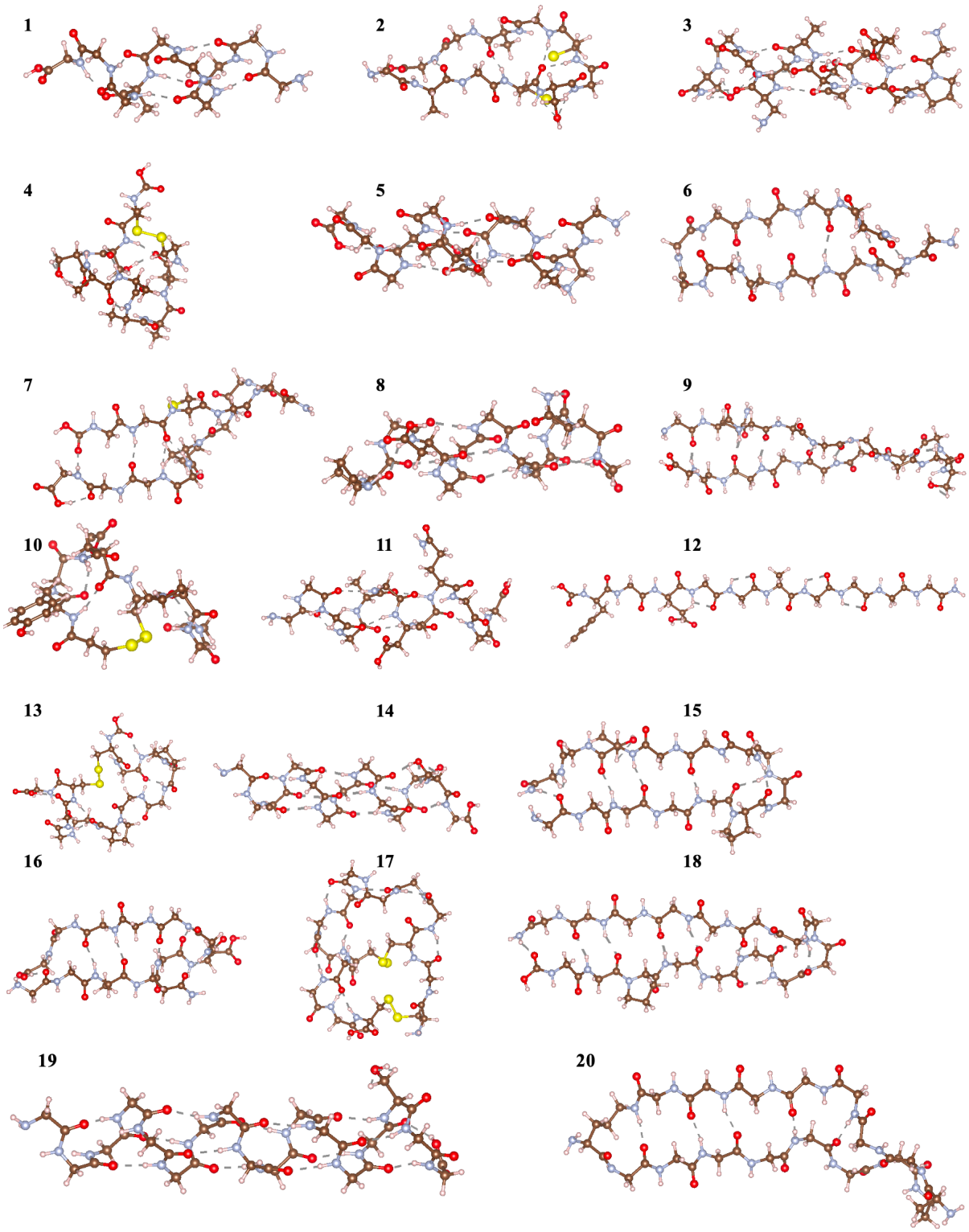

Figure S3. Structural visualization in ribbon representation of the 20 oligopeptides optimized (which serve as the reference structures) using quantum mechanics.

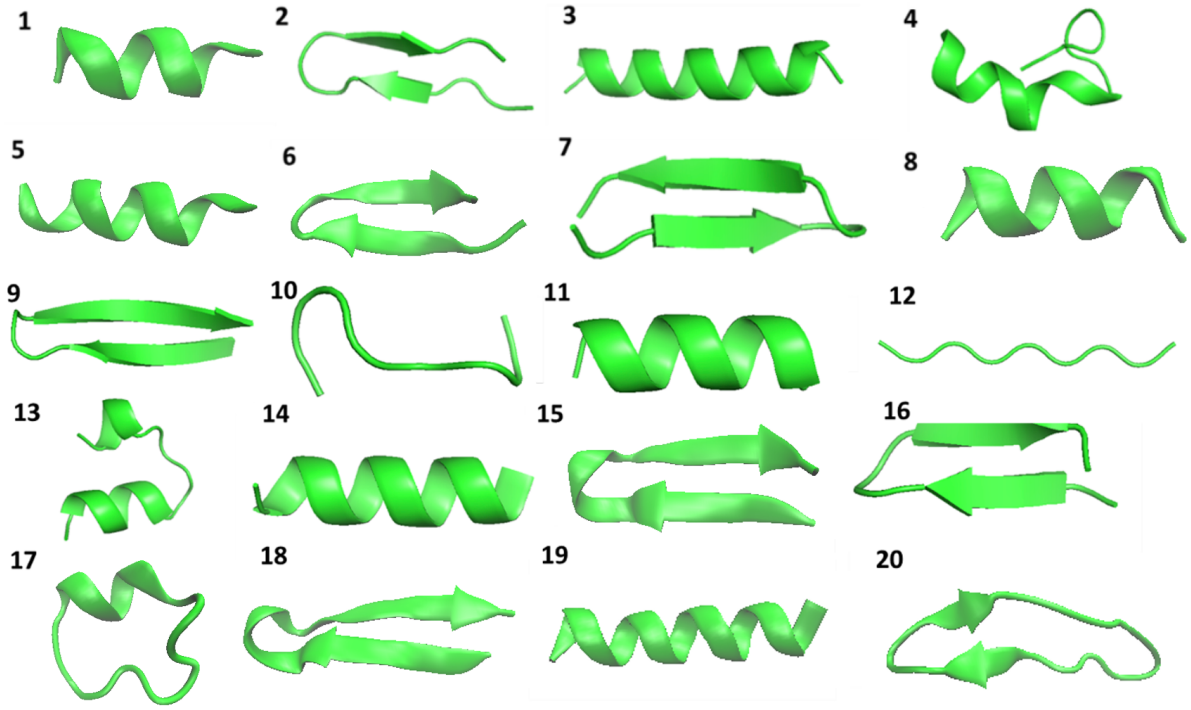

Table S2. Comparison of the quantum mechanical optimized structures in terms of the root mean squared deviations (RMSD in Å) in Cartesian coordinates.

In this table, we show four kernels, SE, RQ, M, and P, with three coordinates, ***r***, ***s***, and ***C***. The reference optimized structures are the ones optimized by the RQ kernel and ***s*** coordinates for IDs 2-5 and 7-20. For ID 1, the reference structure is optimized by the P kernel and ***s***. For ID 6, the reference structure is optimized by the SE kernel and ***s***.

	SE kernel			**RQ kernel**		**M kernel**			**P kernel**		
ID	***r***	***s***	***C***	***r***	***C***	***r***	***s***	***C***	***r***	***s***	***C***
1	0.13	0.14	0.14	0.17	0.32	0.14	0.14	0.30	0.01	Ref.	0.27
2	0.03	0.02	0.02	0.01	1.12	0.03	0.03	0.03	0.04	0.29	0.99
3	0.03	0.02	1.08	0.02	0.89	0.02	0.02	1.05	0.23	0.22	0.85
4	0.03	0.04	0.82	0.00	0.77	0.03	0.03	0.79	0.07	0.08	0.75
5	0.05	0.04	1.04	0.05	1.03	0.04	0.04	1.03	0.04	0.05	1.02
6	0.01	Ref.	0.51	Fail	0.49	0.09	0.07	0.47	Fail	Fail	0.48
7	0.02	0.04	0.86	0.25	0.87	0.02	0.02	0.86	0.03	0.03	0.78
8	0.04	0.12	0.33	0.03	0.33	0.06	0.06	0.31	0.04	0.05	0.28
9	0.04	0.04	0.37	0.06	0.35	0.06	0.05	0.34	0.03	0.06	0.32
10	0.03	0.01	0.39	0.21	0.38	0.26	0.26	0.38	0.06	0.04	0.38
11	0.01	0.02	0.58	0.01	0.53	0.03	0.03	0.53	0.04	0.05	0.49
12	0.09	0.03	0.53	0.20	0.50	0.44	0.44	0.50	0.22	0.14	0.47
13	0.03	0.03	0.46	0.00	0.42	Fail	0.21	0.35	0.06	0.07	0.35
14	0.16	0.14	1.50	0.04	1.43	0.02	0.04	1.42	0.47	0.04	1.15
15	1.29	Fail	1.00	1.28	1.03	1.29	0.34	0.97	1.29	1.28	0.99
16	0.03	0.03	0.35	0.02	0.32	0.03	0.03	0.27	0.02	0.05	0.33
17	0.01	0.01	Fail	0.00	Fail	Fail	0.01	Fail	Fail	Fail	1.52
18	0.03	Fail	1.20	0.12	1.19	0.10	0.09	1.18	0.09	0.18	1.09
19	0.04	0.03	1.19	0.01	1.17	0.13	0.12	1.19	0.63	0.65	1.20
20	0.01	0.01	1.00	0.02	0.98	0.03	0.03	0.92	Fail	Fail	0.83

[a]The entry labeled as “Ref.” means this structure was selected as a reference optimized structure. The entry labeled as “Fail” means this optimization did not finish successfully, which yielded incorrect or unphysical structures.

Procedure for generating ribbon representation from the xyz coordinate file

1. Convert the xyz file to pdb file
module load openbabel
obabel -i xyz structurename.xyz -o pdb -O structurename.pdb

2. Extract PDBname, ResName, and ResNum from structurename.gjf
For example, in gjf you have PDBName=CA,ResName=PHE,ResNum=2_A, and we need to extract CA PHE 2.

3. Modify the structurename.pdb to include missing information
before: HETATM 4 C UNL 1 1.458 6.849 6.837 1.00 0.00 C
after : HETATM 4 CA PHE 2 1.458 6.849 6.837 1.00 0.00 C

The 3rd column is atomname (same as PDB name), the 4th is the residue name, and the 5th is the residue number

4. Save the revised structurename.pdb to your PC and open it with VMD

5. To change the style:
go to tool bar --> Graphics --> Representative
in Drawing Method, select NewCartoon
in Coloring Method, select ColorID (7=green)

6. To change the background:
go to tool bar --> Graphics --> Color
under Names. select Background
under Colors, select 8 white

Table S3. Atomic Cartesian coordinates (in Å) of the initial geometries in the testing set.

ID 1 Chemical Formula: $C_{21}O_{11}N_{10}H_{34}$

N	32.15300000	37.94300000	12.25200000
C	32.59400000	36.63900000	11.81100000
C	32.00200000	35.42800000	12.51400000
O	32.52100000	34.27900000	12.45400000
N	30.89500000	35.62700000	13.18800000
C	30.06700000	34.61200000	13.81400000
C	29.02500000	34.31500000	12.69500000
O	28.66500000	33.16800000	12.39500000
N	28.62800000	35.41700000	12.02700000
C	27.68600000	35.25100000	10.91200000
C	28.39600000	34.38900000	9.85000000
O	27.77000000	33.56500000	9.19100000
N	29.67400000	34.60300000	9.70300000
C	30.51200000	33.89900000	8.74800000
C	30.57800000	32.41700000	9.09800000
O	30.26100000	31.53100000	8.28000000
N	30.99300000	32.15300000	10.32700000
C	31.10400000	30.73000000	10.71500000
C	29.73400000	30.11100000	10.59500000
O	29.60200000	29.13300000	9.83300000
N	28.75300000	30.67600000	11.26900000
C	27.37500000	30.12400000	11.25700000
C	26.93800000	29.84900000	9.82700000
O	26.49000000	28.74600000	9.48900000
N	27.11000000	30.85700000	9.00200000
C	26.76000000	30.84900000	7.58600000
C	27.40800000	29.68300000	6.86800000
O	26.74300000	29.15400000	5.95000000
C	27.00300000	32.24900000	6.97100000
N	28.60300000	29.24300000	7.20800000
C	29.26000000	28.14600000	6.49600000
C	28.75900000	26.75100000	6.83100000
O	28.97400000	25.82200000	6.02300000
N	28.21600000	26.68700000	8.02400000
C	27.67600000	25.45000000	8.60200000
C	26.22800000	25.19700000	8.19700000
O	25.74100000	24.06300000	8.29900000
N	25.54700000	26.24300000	7.77600000
C	24.13800000	26.20000000	7.40500000
C	23.85800000	25.47700000	6.10400000
O	24.70449547	25.50587981	5.17331104
H	32.37066507	36.55349175	10.76806671
H	32.16079210	37.97714847	13.25138639
H	30.64118146	33.73851852	14.04257329
H	30.28383854	36.02441035	12.50349531
H	26.80053192	34.75593554	11.25223148
H	29.46130735	35.77725244	11.60769458
H	30.10252041	34.01303535	7.76605173
H	30.05869726	34.34327956	10.58875014
H	27.35311963	29.21210458	11.81634604
H	28.65709557	31.57808874	10.84824087
H	27.41819196	32.14079452	5.99079226
H	27.68416122	32.79644900	7.58842933
H	25.71249969	30.67114328	7.45946901
H	28.10214964	30.98178628	8.99378520
H	29.12955243	28.30421596	5.44583280
H	28.47571664	28.88834603	8.13429342
H	28.27502786	24.62587707	8.27506419
H	27.41676967	27.28379363	7.95280832
H	23.59614708	25.71146048	8.18770336
H	26.00671459	26.49576905	6.92466557
H	31.78686531	30.22836943	10.06157690
H	31.22222572	32.88611307	10.96731304
H	32.76832364	38.64310437	11.88974223
H	29.58756779	34.99709591	14.68964028
H	27.43565180	36.20613178	10.49975122
H	31.49865266	34.31241599	8.77044425
H	31.44808586	30.65561544	11.72543152
H	26.70600306	30.83001619	11.70296440
H	33.65696511	36.59689351	11.92603138
H	26.07457795	32.77726094	6.90876752
H	27.72988886	25.51502388	9.66866203
H	30.30675146	28.18602586	6.71419558
H	23.77943132	27.20442027	7.31857998
O	22.63169679	24.76152403	5.93319436
H	22.45574163	24.64623376	4.99652583

ID 2 Chemical Formula: $C_{27}O_{13}N_{11}S_2H_{45}$

C	15.65700000	28.59300000	12.80500000	H	12.36525689	27.06410076	21.17586833
C	14.77800000	27.54200000	13.51000000	H	7.06583573	23.43414424	21.89695430
O	13.96200000	26.92800000	12.83700000	H	8.14303167	21.31453400	21.95463234
N	15.19000000	27.13500000	14.68800000	H	8.50594972	25.35898182	22.09461269
C	14.46800000	26.17700000	15.51200000	H	10.67375667	23.71912463	22.98955898
C	14.06700000	26.85300000	16.80700000	H	8.35201508	24.07901595	26.58026469
O	14.83400000	27.56700000	17.45700000	H	10.16964772	25.02260340	24.70351875
C	15.33700000	24.91400000	15.81100000	H	12.07424628	27.14338163	28.25125708
N	12.90800000	26.43700000	17.37400000	H	11.96194690	28.99304883	28.22262018
C	12.49500000	26.98100000	18.64900000	H	14.52820058	28.19416282	27.24091148
C	12.32300000	25.94700000	19.73400000	H	9.82212568	28.10638824	27.51663410
O	11.89900000	24.77800000	19.41700000	H	10.13418229	26.81629652	25.39486935
N	12.79300000	26.19400000	20.93100000	H	10.08614922	30.59106060	23.95463708
C	12.55100000	25.36900000	22.07200000	H	10.09921280	29.22901399	22.69791182
C	11.05300000	25.45500000	22.41700000	H	9.84557132	28.24282309	24.49926795
O	10.63100000	26.53600000	22.79900000	H	15.11850395	28.42623548	23.92449540
C	13.33700000	25.81000000	23.29600000	H	15.55049448	29.91464529	24.73139507
S	13.09400000	24.77900000	24.72400000	H	14.49450850	31.23715008	23.10154454
N	10.33500000	24.33700000	22.28000000	H	12.94096091	28.82634853	23.44874146
C	8.86500000	24.44800000	22.52600000	H	14.59294797	29.60959733	19.02284196
C	8.56900000	24.52900000	23.98100000	H	15.93895483	30.68537221	21.06305770
O	7.39100000	24.81500000	24.38600000	H	18.97945856	29.22426898	18.47212583
C	8.12200000	23.27500000	21.83300000	H	16.32583129	29.03722443	17.55527056
O	8.45800000	22.05300000	22.48100000	H	15.34584622	24.27570233	14.95228129
N	9.48500000	24.32300000	24.90800000	H	15.25936411	29.57065112	12.98102269
C	9.32400000	24.44000000	26.31600000	H	11.56387748	27.49088550	18.51510594
C	9.46900000	25.87000000	26.82800000	H	8.41378837	23.22559849	20.80473980
O	8.60400000	26.29100000	27.62000000	H	10.05911651	23.82857694	26.79627654
N	10.42200000	26.63900000	26.33600000	H	16.32890532	29.47736184	23.22942090
C	10.67800000	27.96600000	26.89000000	H	14.82309664	31.31933827	18.77097494
C	10.76500000	29.07600000	25.85200000	H	18.40505740	27.70620137	17.81041330
O	10.49100000	30.24500000	26.21700000	H	16.30881629	28.92675723	10.93552443
C	11.98600000	28.05800000	27.70300000	O	19.25992761	30.36167099	16.16057516
S	13.41600000	28.12700000	26.55200000	H	19.99918237	29.97620502	15.68463569
N	10.69200000	28.77100000	24.56700000				
C	10.56800000	29.74600000	23.50900000				
C	11.89100000	30.28000000	22.94400000				
O	11.86900000	31.00500000	21.97000000				
N	12.99200000	29.82000000	23.54900000				
C	14.31800000	30.18700000	22.99700000				
C	14.35300000	29.86400000	21.53500000				
O	13.84600000	28.81900000	21.07000000				
C	15.41200000	29.44500000	23.78000000				
N	15.00300000	30.69200000	20.71100000				
C	15.17100000	30.46300000	19.31000000				
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O	17.50100000	31.04000000	19.26600000				
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C	18.24200000	28.76300000	17.84900000				
C	18.30500000	29.34200000	16.46600000				
O	17.51749422	28.93022707	15.57501837				
H	16.65639137	28.53791266	13.18326217				
H	14.74282313	28.47185407	11.02151981				
H	14.92307648	24.38533995	16.64411816				
H	16.33737278	25.21575843	16.04142604				
H	13.59798218	25.85018158	14.98175598				
H	15.18724472	27.96914979	15.23953108				
H	13.22908496	27.69051339	18.96932799				
H	13.05109633	25.46332584	17.55143186				
H	12.94801361	26.77089046	23.56110207				
H	14.36878443	25.70450796	23.03295568				
H	13.91036521	25.15406880	25.67739983				
H	12.85938173	24.37494915	21.82367840				

ID 3 Chemical Formula: $C_{36}O_{17}N_{15}H_{59}$

N	23.78900000	24.34200000	9.20000000
C	25.04200000	24.42300000	9.94300000
C	25.74800000	23.07700000	9.86400000
O	25.12400000	22.03700000	9.60300000
N	27.04300000	23.05300000	10.12500000
C	27.69200000	21.75400000	10.21300000
C	27.05100000	20.90500000	11.30400000
O	26.91100000	19.69000000	11.10800000
C	29.13700000	22.06200000	10.63100000
C	29.28600000	23.53700000	10.59200000
C	27.95300000	24.17900000	10.34000000
N	26.68900000	21.56100000	12.42200000
C	26.10700000	20.77900000	13.52700000
C	24.82100000	20.08800000	13.10200000
O	24.56800000	18.91500000	13.41400000
N	23.97200000	20.82700000	12.37200000
C	22.72100000	20.19500000	11.94100000
C	22.92900000	19.18200000	10.84800000
O	22.14900000	18.22300000	10.77100000
C	21.71500000	21.29100000	11.52200000
C	21.05900000	21.94200000	12.75700000
C	20.42000000	20.90900000	13.67200000
O	19.55000000	20.14500000	13.21100000
O	20.75300000	20.88000000	14.87300000
N	23.95600000	19.34600000	10.00200000
C	24.21900000	18.28900000	9.00900000
C	24.54300000	16.98700000	9.72800000
O	23.98400000	15.91900000	9.41900000
N	25.45700000	17.04300000	10.70900000
C	25.78900000	15.82300000	11.46800000
C	24.58200000	15.29100000	12.22300000
O	24.37200000	14.06600000	12.29900000
N	23.74900000	16.18900000	12.78000000
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C	21.61800000	14.94900000	12.63300000
O	21.07700000	13.90600000	13.01500000
C	21.87400000	16.93000000	14.19000000
O	20.74900000	16.53200000	14.95100000
N	21.38700000	15.47000000	11.42300000
C	20.48800000	14.78500000	10.49200000
C	21.06300000	13.44300000	10.07900000
O	20.35000000	12.43800000	10.08100000
C	20.22000000	15.61000000	9.21500000
N	22.34000000	13.41800000	9.70800000
C	22.93500000	12.13200000	9.29100000
C	22.84800000	11.12000000	10.43200000
O	22.49300000	9.94600000	10.23500000
N	23.17200000	11.56700000	11.64700000
C	23.15000000	10.62400000	12.76300000
C	21.74300000	10.12600000	13.07400000
O	21.52100000	8.95600000	13.39200000
C	23.74500000	11.32800000	13.98800000
N	20.74900000	11.01700000	13.00500000
C	19.38800000	10.63000000	13.31400000
C	18.83800000	9.66700000	12.26700000
O	18.21000000	8.66700000	12.60000000
N	19.05200000	9.95500000	10.99400000
C	18.51800000	9.04200000	9.96200000
C	19.21700000	7.68700000	10.04200000
O	18.57600000	6.63400000	9.95300000
N	20.54300000	7.71800000	10.20800000
C	21.27000000	6.46400000	10.29600000
C	20.85400000	5.67000000	11.52100000
O	20.77200000	4.44000000	11.46100000
C	22.77000000	6.73900000	10.22400000
O	23.18800000	7.49000000	11.33300000
N	20.57300000	6.32200000	12.65900000
H	25.66472693	25.18056615	9.51497583
H	23.46034799	25.26483460	8.99909167
H	23.10725638	23.85730493	9.74799300
H	29.78059817	21.65590276	9.87882554
H	29.24657284	21.75669657	11.65064877
H	29.90008538	23.76143008	9.74498744
H	29.59308000	23.84072267	11.57095578
H	27.65314118	24.67620784	11.23875973
H	28.02044395	24.72608495	9.42291256
H	27.61797698	21.21972740	9.28889320
H	26.81345099	20.03970651	13.84207480
H	25.95880176	22.17973647	12.13221436
H	20.93111343	20.79478731	10.98890075
H	22.28567525	22.05851773	11.04226436
H	20.25953945	22.54893479	12.38633439
H	21.85359687	22.38801031	13.31788379
H	22.32084950	19.64629002	12.76785968
H	24.46543567	21.02871288	11.52593076
H	23.35278239	18.15195907	8.39598546
H	24.76865319	19.35838967	10.58461591
H	26.13496963	15.07217959	10.78868142
H	25.05966264	17.66074120	11.38761538
H	21.49750811	17.53284800	13.39016993
H	22.57642768	17.34087018	14.88475250
H	20.41100023	17.28546747	15.44053337
H	22.88328511	15.06476852	14.31064871
H	23.36954017	16.69277802	12.00397298
H	19.92719082	14.95436674	8.42171076
H	21.11035475	16.13323074	8.93500353
H	19.56394874	14.65221135	11.01487327
H	22.27781939	15.45292466	10.96896338
H	22.40492849	11.75495960	8.44143262
H	22.84851573	13.67956519	10.52836297
H	22.99907243	12.02175386	14.31541051
H	24.70697539	11.68200676	13.68110822
H	23.72585314	9.76203541	12.49783929
H	22.46763841	12.24159975	11.86788441
H	19.36765044	10.15479869	14.27247254
H	20.71873463	11.27995359	12.04066633
H	17.46780481	8.90812558	10.11713766
H	20.04507350	9.90968776	10.88559415
H	22.92575441	7.35481594	9.36294757
H	23.25761848	5.78943965	10.29791458
H	24.13684857	7.62830895	11.28655613
H	21.02187098	5.84245437	9.46112694
H	20.67733779	8.15245007	11.09862141
H	19.59383958	6.52175191	12.69566131
H	21.68239128	20.87419487	15.11341245
H	18.68130635	9.46782410	8.99406153
H	18.77274910	11.50493765	13.34316204
N	24.00100000	10.41000000	15.16900000
H	24.59474047	9.65759152	14.88377424
H	23.13196333	10.04192344	15.49959782
H	23.96134407	12.28434173	9.02963847
H	19.43669951	16.31422271	9.40317736
H	26.56734932	16.04739175	12.16708560
H	25.04840194	18.57389132	8.39595077
H	25.89741320	21.43426092	14.34651602
H	24.83792169	24.66173636	10.96586705
H	20.82649576	5.75237603	13.44083658

ID 4 Chemical Formula: $C_{27}O_{12}N_9S_2H_{45}$

C	16.35700000	-18.10300000	2.93600000
O	15.55643335	-18.96091549	2.48141819
N	17.37200000	-17.68900000	2.19700000
C	17.49200000	-18.26300000	0.86200000
C	18.87600000	-18.72800000	0.49300000
O	19.85600000	-18.33800000	1.11900000
C	16.99100000	-17.29700000	-0.21000000
S	17.04800000	-17.99700000	-1.90000000
N	18.95000000	-19.59900000	-0.50500000
C	20.23700000	-20.06300000	-0.99800000
C	20.56500000	-19.24100000	-2.24500000
O	20.29500000	-19.67500000	-3.36900000
C	20.22300000	-21.56100000	-1.33000000
O	20.44700000	-22.36400000	-0.18100000
N	21.08500000	-18.03200000	-2.00600000
C	21.49200000	-17.06300000	-3.02700000
C	21.00400000	-17.39300000	-4.40800000
O	21.63000000	-18.18300000	-5.08700000
C	23.02000000	-16.90600000	-3.02800000
O	23.69800000	-18.14000000	-2.79000000
N	19.94800000	-16.73000000	-4.86100000
C	19.36400000	-17.01700000	-6.17400000
C	19.06900000	-18.50500000	-6.36700000
O	19.91600000	-19.28400000	-6.86500000
C	20.17000000	-16.41800000	-7.33800000
N	17.88200000	-18.85500000	-5.83800000
C	17.21300000	-20.17800000	-5.79600000
C	17.88900000	-21.53600000	-5.57200000
O	17.38400000	-22.31700000	-4.76700000
C	16.14900000	-20.30800000	-6.91000000
N	19.04000000	-21.77100000	-6.19000000
C	19.77500000	-23.04400000	-6.15300000
C	19.26600000	-24.33700000	-5.48500000
O	18.06400000	-24.56400000	-5.37800000
C	21.25000000	-22.82200000	-5.83900000
N	20.20400000	-25.20500000	-5.10000000
C	19.94500000	-26.49600000	-4.46000000
C	19.12200000	-26.39100000	-3.18200000
O	18.87200000	-27.40700000	-2.52600000
C	21.30500000	-27.13900000	-4.13800000
N	18.62200000	-25.19500000	-2.87300000
C	17.90300000	-25.00300000	-1.62500000
C	17.07200000	-23.69600000	-1.50200000
O	17.25900000	-22.96500000	-0.52900000
C	18.98400000	-25.07100000	-0.52000000
N	16.18000000	-23.35200000	-2.43600000
C	15.43200000	-22.11800000	-2.16000000
C	16.13100000	-20.84900000	-2.67100000
S	15.46400000	-19.28000000	-1.98000000
H	21.05556228	-21.73083418	-1.98030486
H	19.23060523	-21.78434171	-1.66192032
H	20.62479335	-23.26767411	-0.45185538
H	20.98066495	-19.93209210	-0.23989344
H	18.54712498	-19.11712056	-1.28312848
H	23.25406633	-16.27355613	-2.19726074
H	23.28712862	-16.60694429	-4.02002217
H	24.64639094	-17.99172061	-2.80295587
H	21.02608742	-16.13717839	-2.76114324
H	21.94163483	-18.24058766	-1.53412294
H	20.08657329	-15.35144538	-7.31796926
H	19.78608443	-16.78842947	-8.26551865
H	18.41907523	-16.51525305	-6.19034551
H	20.26784016	-15.78564746	-4.93781509
H	16.06372813	-21.33331388	-7.20387100
H	16.44186814	-19.71838667	-7.75349533
H	16.87301857	-20.04835843	-4.78976658
H	17.24047498	-18.31025337	-6.37808958
H	21.46306628	-23.18177046	-4.85407971
H	21.47275367	-21.77683157	-5.89288649
H	19.54929346	-23.32723895	-7.15984271
H	19.67053947	-21.12806857	-5.75519066
H	21.84548732	-26.51040086	-3.46151158
H	21.86651725	-27.25696880	-5.04115101
H	19.36661805	-27.08767328	-5.13845195
H	20.71288990	-24.70013636	-4.40275988
H	19.58361901	-24.18539827	-0.55265929
H	19.60442174	-25.92791272	-0.68024186
H	17.15198960	-25.76147878	-1.55021148
H	17.94013663	-25.01901425	-3.58299391
H	16.87336017	-19.13520440	0.90000318
H	17.67637355	-16.47531774	-0.20883066
H	15.95601777	-17.13069667	0.00460424
H	15.29526606	-22.03054103	-1.10238251
H	15.93040325	-20.81105771	-3.72134343
H	17.14009051	-20.91351199	-2.32103638
H	18.02657941	-17.01403248	2.53750646
H	14.47098759	-22.18963193	-2.62499893
O	16.16883322	-17.57591009	4.25192913
H	15.24778882	-17.33285930	4.37110765
H	21.14890159	-28.09684920	-3.68738022
H	21.19833388	-16.69720956	-7.24067863
H	15.20498100	-19.96227592	-6.54366273
H	18.51148878	-25.14671214	0.43702707
H	21.84957011	-23.35156299	-6.54961855
H	16.03246317	-23.89509032	-3.26261103

ID 5 Chemical Formula: $C_{29}O_{16}N_{13}H_{47}$

N	23.23700000	15.68600000	76.17700000
C	23.63100000	16.43200000	77.36200000
C	22.65400000	16.20200000	78.50400000
O	23.06100000	16.08900000	79.65800000
N	21.36800000	16.12900000	78.18000000
C	20.34100000	15.92400000	79.19400000
C	20.54000000	14.59200000	79.92000000
O	20.49600000	14.53400000	81.15400000
C	18.95200000	15.97600000	78.55100000
N	20.76800000	13.52900000	79.15400000
C	20.98200000	12.21500000	79.74600000
C	22.22600000	12.22400000	80.63900000
O	22.21500000	11.65700000	81.73400000
C	21.12200000	11.12800000	78.65000000
N	23.28800000	12.88000000	80.17800000
C	24.52300000	12.95300000	80.95400000
C	24.29100000	13.63200000	82.29700000
O	24.82600000	13.19300000	83.32300000
N	23.50700000	14.70900000	82.28800000
C	23.21000000	15.44400000	83.51500000
C	22.36200000	14.57100000	84.44000000
O	22.60700000	14.50700000	85.65200000
N	21.37100000	13.88700000	83.87200000
C	20.52900000	13.00200000	84.66900000
C	21.37300000	11.90000000	85.29900000
O	21.21800000	11.57500000	86.48000000
N	22.26700000	11.31700000	84.51000000
C	23.09200000	10.23900000	85.03600000
C	23.91600000	10.73100000	86.20800000
O	24.02100000	10.06000000	87.24100000
C	24.01000000	9.68900000	83.95200000
O	23.25100000	9.15700000	82.88200000
N	24.50400000	11.91000000	86.05200000
C	25.31400000	12.46500000	87.11900000
C	24.45600000	12.70300000	88.35700000
O	24.84400000	12.33200000	89.46500000
N	23.28700000	13.30700000	88.17600000
C	22.41600000	13.57700000	89.31400000
C	21.96600000	12.32300000	90.03300000
O	21.83900000	12.32000000	91.26100000
C	21.19800000	14.40000000	88.88600000
C	21.55900000	15.84000000	88.58100000
O	22.56100000	16.32700000	89.14900000
O	20.84400000	16.48700000	87.79300000
N	21.73000000	11.25600000	89.27700000
C	21.30900000	9.99400000	89.87300000
C	22.44200000	9.38000000	90.68500000
O	22.21300000	8.82000000	91.76600000
N	23.66600000	9.48800000	90.17500000
C	24.81800000	8.96100000	90.89900000
C	24.95600000	9.71200000	92.22400000
O	25.21600000	9.12300000	93.27800000
N	24.77900000	11.02300000	92.16300000
C	24.87800000	11.85000000	93.35400000
C	23.79400000	11.47900000	94.35300000
O	24.07663635	11.36206435	95.57366101
H	24.60709298	16.11673038	77.66654486
H	22.58944229	16.22833582	75.64170487
H	18.87928339	15.09663909	77.94574246
H	18.87692963	16.94348574	78.10018319
H	20.42260056	16.70880190	79.91672217
H	21.30695554	15.31550557	77.60163992
H	22.10012160	11.17967516	78.21929382
H	20.12719463	11.98153746	80.34575247
H	21.63155116	13.73642503	78.69437597
H	24.89082138	11.96221862	81.12121153
H	22.98159131	13.82968919	80.11316050
H	20.05174276	13.56802452	85.44149062
H	21.82939503	13.27720608	83.22545118
H	24.53913295	8.86772154	84.38837141
H	24.54997234	10.52411035	83.55713221
H	23.84342495	8.81596752	82.20796029
H	22.44567980	9.45417958	85.36950728
H	22.91583172	12.04371133	84.28437187
H	26.10108541	11.78109713	87.35915291
H	23.74674547	12.55539082	85.95181886
H	20.54479733	14.42901422	89.73298551
H	20.85988303	13.97532635	87.96392126
H	23.00356698	14.14132880	90.00768440
H	22.76406451	12.67223118	87.60713533
H	20.47045970	10.16922654	90.51412855
H	22.61498176	11.04864275	88.86009442
H	24.67459754	7.91818150	91.09100340
H	23.83033667	10.47339597	90.13041030
H	25.83760306	11.70583885	93.80486531
H	23.82943641	11.12941682	91.86803484
O	22.45307230	11.26287103	93.90567329
H	24.12475894	15.70110082	84.00695045
H	22.46744825	10.84527961	93.04137546
H	23.11354610	15.02085144	81.42316319
H	23.44303089	16.08032509	88.86129702
N	17.83904513	15.89456428	79.50786973
H	17.60142897	16.81379171	79.82181158
H	17.04604565	15.47914621	79.06224697
H	20.97449699	10.16167391	79.08515140
H	20.38802889	11.29225233	77.88894312
H	25.70326980	9.09965478	90.31421607
H	21.02357772	9.31526873	89.09662510
H	25.73699654	13.39353852	86.79683522
H	22.67137796	16.33669635	83.27441837
H	25.25156829	13.50881866	80.40159266
H	24.04570772	15.48969563	75.62251247
H	24.76793338	12.87834844	93.07961919
H	23.65665895	17.47558373	77.12710723
H	19.78343301	12.56158024	84.04046177

ID 6 Chemical Formula: $C_{26}O_{13}N_{14}H_{42}$

N	3.18200000	13.40000000	15.71000000
C	2.04200000	12.51100000	15.86900000
C	1.70100000	11.79800000	14.56900000
O	1.45000000	12.43800000	13.54000000
N	1.65800000	10.47200000	14.63500000
C	1.31600000	9.65000000	13.48100000
C	-0.06400000	9.07700000	13.69300000
O	-0.42200000	8.69500000	14.81300000
N	-0.86400000	9.09100000	12.63700000
C	-2.19800000	8.54800000	12.69200000
C	-2.09300000	7.05900000	12.38700000
O	-1.49700000	6.65200000	11.39400000
N	-2.67900000	6.25200000	13.25600000
C	-2.63800000	4.80600000	13.11300000
C	-4.01000000	4.16100000	13.32900000
O	-4.95700000	4.81300000	13.77700000
N	-4.13500000	2.91100000	12.90200000
C	-5.36000000	2.16300000	13.10500000
C	-5.01000000	1.04000000	14.08600000
O	-4.06600000	0.27600000	13.84700000
N	-5.67200000	1.03400000	15.24200000
C	-5.46900000	0.00100000	16.27700000
C	-6.69200000	-0.89800000	16.15000000
O	-7.77400000	-0.56500000	16.63200000
N	-6.52200000	-1.99600000	15.41800000
C	-7.59800000	-2.93700000	15.13300000
C	-8.73400000	-2.20700000	14.41800000
O	-8.60200000	-1.85100000	13.24600000
N	-9.81300000	-1.91400000	15.13400000
C	-10.94600000	-1.22500000	14.53300000
C	-11.12400000	0.18800000	15.11200000
O	-12.22700000	0.74500000	15.11300000
N	-10.02300000	0.77400000	15.57100000
C	-10.03600000	2.10600000	16.16000000
C	-9.03800000	2.94000000	15.37900000
O	-8.05700000	2.38700000	14.87800000
N	-9.24700000	4.26200000	15.30500000
C	-8.34100000	5.16200000	14.56700000
C	-8.02800000	6.49000000	15.29300000
O	-8.89100000	7.05600000	15.98000000
N	-6.80000000	6.98000000	15.12900000
C	-6.42000000	8.22800000	15.76600000
C	-4.92600000	8.45700000	15.80400000
O	-4.15500000	7.73300000	15.18100000
N	-4.50400000	9.46300000	16.55800000
C	-3.09200000	9.79100000	16.65200000
C	-2.42100000	9.30300000	17.91000000
O	-3.06200000	9.16200000	18.95700000
N	-1.12700000	9.02400000	17.77800000
C	-0.27400000	8.57500000	18.88300000
C	1.08600000	9.21000000	18.66400000
O	1.42600000	9.56000000	17.52500000
N	1.87400000	9.41800000	19.73900000
H	2.27029471	11.78136241	16.61760572
H	3.26800000	13.98000000	16.52000000
H	3.04700000	13.97400000	14.90200000
H	1.32419505	10.25099231	12.59576496
H	0.92600000	10.28600000	15.29000000
H	-2.60974816	8.69155698	13.66911558
H	-0.39400000	8.51600000	11.96700000
H	-2.29290427	4.56486680	12.12930100
H	-3.65000000	6.47600000	13.17800000
H	-6.11376732	2.79661131	13.52365443
H	-3.44900000	2.40400000	13.42400000
H	-4.57472991	-0.55341980	16.08257857
H	-6.62700000	0.91500000	14.97000000
H	-7.22883226	-3.72254869	14.50727767
H	-5.86700000	-2.53600000	15.94700000
H	-10.78952145	-1.15197389	13.47702573
H	-9.48100000	-1.28000000	15.83200000
H	-11.01362236	2.53303211	16.07754939
H	-9.44800000	0.87500000	14.75900000
H	-7.41980853	4.64633282	14.39266228
H	-9.17500000	4.57100000	16.25300000
H	-6.72900000	8.14200000	16.78700000
H	-6.82000000	9.00600000	15.14900000
H	-6.73700000	7.17100000	14.14900000
H	-2.58815192	9.36169123	15.81132700
H	-4.75600000	9.19600000	17.48800000
H	-0.68354027	8.89825610	19.81717464
H	-0.72300000	9.89900000	17.50900000
H	-2.81655207	9.02668694	11.96182731
H	-2.98774385	10.85481153	16.60367110
H	-0.18730751	7.50860387	18.86944578
H	2.02491259	8.85457923	13.38277203
H	1.19501693	13.08299752	16.18576256
H	-1.95080022	4.40645265	13.82925301
H	-5.69792443	1.75024012	12.17745682
H	-8.78688818	5.39014599	13.62146674
H	-9.74440094	2.05429802	17.18820080
H	-11.83531625	-1.79126370	14.71565273
H	-7.96154509	-3.35191053	16.04983380
H	-5.43115319	0.44689049	17.24893070
H	2.86898312	9.39899534	19.64077879
H	1.46314814	9.59119159	20.63410079

ID 7 Chemical Formula: $C_{31}O_{16}N_{13}SH_{47}$

C	10.82300000	21.29900000	6.34600000	H	17.42993681	23.39364987	-0.60238222
O	11.22745620	20.33814600	7.05080163	H	16.68730424	24.71931594	0.45865800
N	11.63500000	21.86000000	5.46200000	H	14.66345339	23.24976623	-0.88538218
C	12.99300000	21.37700000	5.30500000	H	17.84044948	22.16258193	1.45025797
C	13.90900000	22.56700000	5.10300000	H	17.81713357	24.23863446	3.12405762
O	13.46000000	23.70000000	4.93200000	H	21.36204112	24.72308640	0.50620838
N	15.20400000	22.29600000	5.17100000	H	19.62629932	23.01799752	-0.24728107
C	16.20600000	23.31100000	4.92600000	H	23.75551344	23.20632016	-4.50990213
C	16.85200000	22.76100000	3.65800000	H	23.47974553	22.27774695	-2.92990091
O	17.05700000	21.55700000	3.53900000	H	26.63808275	23.49353103	-2.47951425
N	17.13800000	23.63600000	2.70500000	H	25.48663583	22.39632291	-1.79372686
C	17.75300000	23.22900000	1.44800000	H	22.30086436	24.88033168	-3.75279523
C	19.11700000	23.86500000	1.30500000	H	22.89011490	24.43083835	-1.48660492
O	19.35400000	24.97300000	1.76900000	H	18.92473653	22.83340184	-5.16947529
C	16.90000000	23.68600000	0.28000000	H	17.88753518	23.52667112	-3.79896770
S	15.29800000	22.85900000	0.19200000	H	19.83796305	24.50658475	-3.89077877
N	20.01600000	23.14400000	0.66500000	H	17.95318408	19.30256977	-2.66313275
C	21.34200000	23.65700000	0.41700000	H	18.74165891	21.68537732	-1.84858371
C	21.57300000	23.23300000	-1.00700000	H	14.79445518	18.90157465	1.01315172
O	21.34700000	22.08100000	-1.33500000	H	15.63701546	17.61048274	2.04168168
N	21.99200000	24.17600000	-1.84500000	H	14.72350269	17.25523266	-0.42576326
C	22.24000000	23.93200000	-3.26100000	H	16.24710656	16.47079096	0.27991549
C	21.10100000	23.15900000	-3.89300000	H	17.24147911	17.35675331	-1.47725451
O	21.31200000	22.22500000	-4.65700000	H	15.90611270	18.62352178	-1.69357420
C	23.56500000	23.20500000	-3.45700000	H	16.72905076	20.04507632	1.54568781
C	24.70000000	23.94500000	-2.82400000	H	19.80228216	17.67577541	3.52921408
O	24.67900000	25.16800000	-2.76100000	H	17.67011889	19.23526373	3.65537276
N	25.68900000	23.21900000	-2.32500000	H	17.85087230	18.10006595	7.55348903
N	19.88400000	23.56400000	-3.56000000	H	17.30792750	18.31660016	5.20879850
C	18.71300000	22.92900000	-4.12500000	H	13.46475102	18.49971337	7.43093859
C	18.39300000	21.53100000	-3.66000000	H	15.77223972	18.42479640	8.88730239
O	17.57400000	20.85200000	-4.27500000	H	13.24301133	20.32756831	11.45584898
N	19.03000000	21.07700000	-2.58800000	H	11.94420329	19.23533839	9.18827073
C	18.74600000	19.73600000	-2.09000000	O	11.65725295	18.54570125	12.57259999
C	18.33200000	19.81900000	-0.63700000	H	12.61005072	18.48171025	12.67099484
O	18.87500000	20.61300000	0.13100000	H	13.68866057	16.96635789	8.24733838
N	17.33600000	19.02200000	-0.24800000	H	20.37586054	19.29717643	3.79285331
C	16.90600000	19.06400000	1.15700000	H	19.62301696	19.12929312	-2.17745293
C	18.01300000	18.45000000	2.01700000	H	22.05606097	23.20249208	1.07155289
O	18.46000000	17.33800000	1.76000000	H	13.04896632	20.73138374	4.45356156
C	15.61400000	18.23200000	1.17100000	O	9.48701756	21.78540500	6.49917014
C	15.70900000	17.34600000	-0.01900000	H	8.89042623	21.25763813	5.96331483
C	16.56000000	18.06600000	-1.05600000	H	11.97088747	21.21997358	10.63680305
N	18.45600000	19.16500000	3.04100000	H	16.91143994	23.35879071	5.72910058
C	19.52900000	18.64900000	3.88000000	H	17.80887251	19.84370530	7.54333214
C	19.13700000	18.54800000	5.35400000				
O	19.92100000	18.07500000	6.18400000				
N	17.91500000	18.96300000	5.67100000				
C	17.45600000	18.96000000	7.05400000				
C	15.94500000	18.92400000	7.12200000				
O	15.27000000	19.63200000	6.38200000				
N	15.42200000	18.09400000	8.01100000				
C	13.98200000	17.99500000	8.22000000				
C	13.66700000	18.65500000	9.54600000				
O	14.24800000	18.28500000	10.57200000				
N	12.78500000	19.64600000	9.54100000				
C	12.39700000	20.25300000	10.80500000				
C	11.34900000	19.30700000	11.40200000				
O	10.21737714	19.20031998	10.86198182				
H	13.28788914	20.84102095	6.18287633				
H	11.74130842	22.80077511	5.78393277				
H	15.75410488	24.26418641	4.74676140				
H	15.35160036	21.62692884	4.44260593				

ID 8 Chemical Formula: $C_{31}O_{16}N_{13}H_{47}$

N	-11.36600000	-16.54700000	-4.68700000
C	-11.98100000	-15.40600000	-5.46600000
C	-11.18700000	-14.12100000	-5.21500000
O	-10.52200000	-13.95800000	-4.03200000
C	-13.42400000	-15.24300000	-4.90800000
C	-13.50000000	-16.00900000	-3.65900000
C	-12.23600000	-16.88200000	-3.48000000
N	-11.18000000	-13.19000000	-6.12600000
C	-10.34100000	-11.94900000	-5.91400000
C	-10.67300000	-11.23500000	-4.61000000
O	-9.72900000	-10.72000000	-3.90200000
N	-11.84200000	-11.32000000	-4.11300000
C	-12.14200000	-10.55300000	-2.85500000
C	-11.45100000	-11.17400000	-1.70400000
O	-11.17000000	-10.38000000	-0.76000000
N	-11.31900000	-12.49600000	-1.70200000
C	-10.48800000	-13.19000000	-0.72200000
C	-9.00000000	-12.98200000	-0.95800000
O	-8.23800000	-12.84000000	0.01300000
C	-10.70600000	-14.67000000	-0.63800000
C	-12.10600000	-15.02200000	-0.15200000
O	-12.57100000	-16.20800000	-0.34300000
O	-12.82100000	-14.13100000	0.44300000
N	-8.47600000	-12.78800000	-2.10500000
C	-7.02800000	-12.43800000	-2.12600000
C	-6.81000000	-10.98300000	-1.71700000
O	-5.81200000	-10.71800000	-1.15900000
N	-7.78600000	-10.07500000	-1.87700000
C	-7.67600000	-8.68200000	-1.35400000
C	-7.78900000	-8.75400000	0.18400000
O	-6.93700000	-8.09600000	0.81800000
N	-8.69800000	-9.54000000	0.77100000
C	-8.63600000	-9.64400000	2.28400000
C	-7.27100000	-10.18000000	2.71900000
O	-6.74200000	-9.79700000	3.77300000
N	-6.70400000	-11.22200000	2.13400000
C	-5.44100000	-11.78000000	2.54800000
C	-4.37400000	-10.69400000	2.39400000
O	-3.48900000	-10.54100000	3.24600000
N	-4.34700000	-9.91800000	1.28000000
C	-3.40200000	-8.88500000	1.00700000
C	-3.41100000	-7.90200000	2.18100000
O	-2.36100000	-7.53300000	2.71800000
N	-4.64200000	-7.46900000	2.58500000
C	-4.72800000	-6.47300000	3.68800000
C	-4.20700000	-7.08900000	4.97800000
O	-3.56800000	-6.40400000	5.78000000
N	-4.50500000	-8.38500000	5.27100000
C	-4.03800000	-8.94700000	6.54200000
C	-2.50600000	-9.14200000	6.40200000
O	-1.83700000	-8.94200000	7.45100000
C	-4.71600000	-10.25400000	6.85500000
C	-6.18600000	-10.10800000	7.25700000
O	-6.84100000	-11.27700000	7.24200000
N	-6.69100000	-9.03800000	7.58100000
N	-1.98700000	-9.50500000	5.26700000
C	-0.45100000	-9.67900000	5.21300000
C	0.17300000	-8.27500000	5.43000000
O	1.28547686	-8.16331145	6.00748720
H	-14.08805313	-15.70849675	-5.60603024
H	-13.55117208	-14.21113709	-4.65504508
H	-14.32382332	-16.68355171	-3.76480702
H	-13.49235122	-15.29465243	-2.86241413
H	-11.72484542	-16.54234029	-2.60349998
H	-12.53140609	-17.90700830	-3.56362556
H	-11.97861806	-15.59818981	-6.51859555
H	-10.49437722	-16.21271109	-4.32849666
H	-9.30812727	-12.22815082	-5.90180351
H	-12.12218224	-12.85594247	-6.15242347
H	-11.80651276	-9.54315280	-2.96705772
H	-11.94187991	-12.28140200	-3.85662101
H	-10.03161225	-15.02839172	0.11143748
H	-10.63708545	-15.03862059	-1.64013255
H	-10.80283745	-12.74158105	0.19707444
H	-10.87989983	-12.69696008	-2.57767465
H	-6.50262917	-13.07619119	-1.44659034
H	-8.94540819	-11.98685713	-2.47624931
H	-6.73061412	-8.26364667	-1.62990946
H	-8.55892396	-10.46097653	-1.37340228
H	-8.78934716	-8.67555384	2.71236513
H	-8.50254109	-10.46193322	0.43658267
H	-5.49913730	-12.08807107	3.57104070
H	-6.52747659	-10.90303671	1.20281693
H	-2.42548364	-9.30883499	0.89892736
H	-5.21644888	-9.42591877	1.32375747
H	-4.13826023	-5.61540632	3.43972579
H	-5.09339301	-8.28577289	2.94434162
H	-4.21506636	-10.64385824	7.71638031
H	-4.71721692	-10.80876521	5.94004968
H	-7.68603525	-8.94067929	7.60182120
H	-6.10762356	-8.26309349	7.82429371
H	-4.27442432	-8.28771736	7.35091900
H	-4.03502729	-8.91934941	4.56843587
H	-0.13144993	-10.34428245	5.98771737
H	-2.18602261	-8.75370412	4.63775878
H	-12.39590878	-13.41518039	0.92101646
H	-10.50789021	-11.27576431	-6.72874006
H	-13.19753659	-10.55846014	-2.67974963
H	-6.64528553	-12.58605708	-3.11418457
H	-8.46870604	-8.08164965	-1.74909061
H	-9.40258117	-10.30790835	2.62529020
H	-5.19581986	-12.61872145	1.93047831
H	-3.67538085	-8.37466341	0.10715586
H	-5.74757722	-6.17711242	3.82146470
H	-0.16051458	-10.06400082	4.25785991
O	-0.51610766	-7.10800999	4.97374902
H	0.07718159	-6.35382712	5.00231587

ID 9 Chemical Formula: $C_{38}O_{20}N_{18}H_{60}$

N	27.34300000	24.29400000	2.68300000
C	26.38100000	25.36100000	2.89400000
C	26.99700000	26.55700000	3.58300000
O	27.97300000	26.43900000	4.35100000
N	26.41000000	27.69400000	3.33200000
C	26.86500000	28.93400000	3.89800000
C	26.13600000	29.27200000	5.20400000
O	24.91100000	29.19100000	5.28900000
C	26.70500000	30.07500000	2.86900000
C	27.14300000	31.44900000	3.38000000
C	26.93700000	32.54500000	2.34300000
O	27.85700000	33.31400000	2.04000000
N	25.74200000	32.56800000	1.74400000
N	26.90600000	29.64700000	6.22100000
C	26.33700000	30.09700000	7.48100000
C	26.95100000	31.40700000	7.90600000
O	28.01200000	31.79400000	7.41800000
N	26.26200000	32.10700000	8.77000000
C	26.73800000	33.37500000	9.26200000
C	27.10000000	33.30500000	10.72200000
O	26.35100000	32.77200000	11.52700000
N	28.25500000	33.87400000	11.06300000
C	28.69400000	33.96400000	12.44800000
C	28.77100000	35.41600000	12.88000000
O	29.65400000	36.16400000	12.44500000
N	27.81000000	35.81300000	13.70300000
C	27.68800000	37.18500000	14.19500000
C	28.47600000	37.38700000	15.50100000
O	28.24300000	36.69700000	16.48700000
N	29.42600000	38.33400000	15.48000000
C	30.22800000	38.64800000	16.66800000
C	29.63700000	39.81400000	17.43200000
O	28.74800000	40.50000000	16.94200000
N	30.17000000	40.05900000	18.62400000
C	29.67500000	41.14100000	19.47700000
C	30.05600000	42.54000000	18.99500000
O	29.54500000	43.52900000	19.49600000
N	30.96100000	42.61900000	18.03000000
C	31.41200000	43.92300000	17.53800000
C	30.67500000	44.40900000	16.29800000
O	31.00900000	45.44200000	15.73900000
C	32.90200000	43.96600000	17.32000000
O	33.22400000	43.18700000	16.20000000
N	29.69100000	43.66800000	15.87000000
C	28.92600000	44.06400000	14.71000000
C	29.53500000	43.56800000	13.40900000
O	29.18200000	44.03200000	12.32800000
N	30.46400000	42.62900000	13.52900000
C	31.07300000	42.00200000	12.38500000
C	30.47300000	40.63600000	12.18200000
O	30.33500000	39.87000000	13.12700000
N	30.08100000	40.34400000	10.95700000
C	29.55100000	39.04900000	10.63700000
C	30.48300000	38.31400000	9.72200000
O	30.91400000	38.84800000	8.70900000
N	30.82700000	37.10500000	10.08900000
C	31.69100000	36.31200000	9.25700000
C	30.94300000	35.18100000	8.58000000
O	30.07700000	34.55800000	9.16900000
N	31.22700000	34.98700000	7.30600000
C	30.59900000	33.92700000	6.54600000
C	31.48700000	32.69500000	6.49800000
O	32.70900000	32.79800000	6.35600000
N	30.86700000	31.53500000	6.65300000
C	31.57400000	30.26800000	6.65900000
C	30.95300000	29.29300000	5.69300000
O	29.74900000	29.26800000	5.51500000
N	31.76700000	28.43000000	5.14200000
C	31.26000000	27.36200000	4.33200000
C	31.40300000	26.05900000	5.07200000
O	32.50600000	25.65700000	5.43000000
N	30.26300000	25.45700000	5.41100000
C	30.25300000	24.24700000	6.21700000
C	29.27000000	23.19800000	5.71200000
O	28.39264311	23.51314364	4.86671902
H	25.99145327	25.66923477	1.94629505
H	28.25225468	24.68717393	2.54636113
H	27.35606004	23.69397473	3.48287443
H	25.65390734	30.15508714	2.68545089
H	27.37169373	29.83771296	2.06643266
H	28.19907656	31.38464794	3.53956541
H	26.49204492	31.68474035	4.19583330
H	25.27523908	33.43934203	1.59268144
H	25.31491700	31.71386201	1.44727050
H	27.90153664	28.82273480	4.13906400
H	25.49089336	27.57949281	3.70900278
H	25.28092252	30.22415644	7.36510522
H	27.39527016	30.44734724	5.87450469
H	27.60260538	33.66407237	8.70182618
H	26.22826410	31.52635933	9.58346069
H	27.99893124	33.44469482	13.07418012
H	28.14777506	34.82731257	10.78069172
H	28.06397703	37.85734866	13.45237725
H	27.97126696	35.27728336	14.53185502
H	30.25982224	37.79007499	17.30663293
H	28.92380610	39.17871709	15.29492074
H	28.60793020	41.07638369	19.52268131
H	31.11338212	40.32085663	18.42037956
H	33.21046373	44.97697190	17.15360904
H	34.17462859	43.19606716	16.06649695
H	31.16386153	44.60610807	18.32329655
H	30.51850423	42.19521972	17.23967869
H	28.97585497	45.13217818	14.67245199
H	27.97820913	43.57545032	14.79894754
H	29.02876579	43.67790587	16.61923142
H	30.89897374	42.60073074	11.51543898
H	29.99149260	41.87937761	13.99246848
H	29.42427472	38.48654573	11.53837999
H	30.91521313	40.41033668	10.40956242
H	32.12443991	36.94028937	8.50714514
H	29.96603608	36.59673969	10.10931227
H	29.66665587	33.67072023	7.00420859
H	32.19761620	34.74636744	7.30559609
H	32.59397878	30.43448925	6.38182748
H	30.26924063	31.47308905	5.85371859
H	30.22691387	27.53783787	4.11586559
H	32.20043684	27.96912199	5.91641847
H	31.23630098	23.82508238	6.21483305
H	29.86818504	25.17195306	4.53757605
H	29.99217109	24.50614967	7.22184314
H	31.81276699	27.31500649	3.41704630
H	31.54175069	29.85331550	7.64484824
H	25.97287621	34.11076397	9.12732643
H	26.65542592	37.40208097	14.37267001
H	32.47269531	35.89994303	9.86037509
H	25.57770340	24.98983614	3.49554132
H	26.52255789	29.36018464	8.23437334
H	29.66040268	33.51462247	12.54300362
H	30.06732650	41.00285267	20.46284747
H	33.40141011	43.57663770	18.18248857
H	31.22335986	38.89623117	16.36379605
H	32.12628045	41.90814635	12.54837622
H	28.60208208	39.16456626	10.15627220
H	30.41827224	34.26918831	5.54843064
O	29.34445669	21.85540184	6.19860700
H	29.54450017	21.26158098	5.47131105

ID 10 Chemical Formula: $C_{32}O_{12}N_9S_2H_{43}$

C	19.39200000	5.71400000	9.14700000
C	18.13100000	5.09100000	8.58700000
O	17.48800000	4.19100000	9.06000000
C	20.53000000	4.82100000	9.16900000
S	22.10300000	5.59300000	8.46000000
H	19.19100000	6.03400000	10.15900000
H	19.64400000	6.57200000	8.54100000
H	20.71757752	4.53021287	10.18150063
N	17.72700000	5.79500000	7.44700000
C	16.45500000	5.56900000	6.78100000
C	16.76900000	5.45000000	5.29700000
O	17.83700000	5.72300000	4.79000000
C	15.49600000	6.75200000	6.97500000
C	15.33300000	7.20800000	8.40200000
C	16.18900000	8.13500000	8.98100000
C	14.30800000	6.70300000	9.19100000
C	16.02100000	8.57900000	10.28600000
C	14.10700000	7.17800000	10.47900000
C	14.95200000	8.12500000	11.06000000
O	14.71000000	8.55100000	12.29900000
H	18.39300000	6.54400000	7.04300000
H	15.97900000	4.68800000	7.18600000
H	15.86800000	7.58500000	6.39700000
H	14.52500000	6.46100000	6.60300000
H	17.01200000	8.52300000	8.39900000
H	13.66100000	5.93200000	8.79900000
H	16.72400000	9.28300000	10.70600000
H	13.27000000	6.80400000	11.05000000
N	15.69200000	4.94600000	4.55100000
C	15.78700000	4.85500000	3.10300000
C	16.16100000	6.20400000	2.51800000
O	15.40600000	7.17500000	2.59400000
H	14.79100000	4.62600000	5.05400000
H	16.53488468	4.13582998	2.84153683
N	17.34600000	6.20600000	1.79900000
C	17.86300000	7.43700000	1.12400000
C	18.08600000	8.62000000	2.04200000
O	18.18000000	9.78000000	1.69400000
H	17.91400000	5.29000000	1.72300000
H	18.79276079	7.19701888	0.65192593
C	18.72600000	9.27000000	4.36400000
C	19.53500000	8.60500000	5.44000000
O	19.11700000	8.25900000	6.52300000
C	17.50400000	9.94100000	4.95100000
C	17.76900000	10.81400000	6.18500000
O	18.96300000	11.32600000	6.32200000
N	16.84200000	11.03000000	7.11200000
H	19.34600000	10.01600000	3.88700000
H	17.06600000	10.56700000	4.18700000
H	16.80100000	9.17100000	5.23100000
H	17.16200000	11.71600000	7.82300000
H	15.81000000	10.85500000	7.23700000
N	20.78300000	8.28600000	4.97400000
C	21.69900000	7.57100000	5.84800000
C	23.06100000	8.12100000	5.49900000
O	23.78100000	7.72000000	4.63000000
C	21.67000000	6.08200000	5.54500000
S	22.77900000	5.14900000	6.68200000
H	24.94600000	9.95500000	4.99300000
H	25.75900000	11.29500000	7.24900000
H	24.43200000	11.88000000	6.24500000
H	24.34000000	10.21600000	8.72800000
H	23.38100000	11.63500000	8.30800000
H	22.34900000	9.15900000	8.15100000
H	21.91600000	10.39200000	6.96700000
N	25.75900000	7.74500000	7.15300000
C	26.83200000	6.87500000	7.52600000
C	27.41000000	6.09600000	6.38300000
O	28.59500000	5.80200000	6.30300000
H	24.74700000	7.49500000	7.43400000
H	27.61044948	7.46365644	7.96463425
N	26.50400000	5.58900000	5.45800000
C	27.02500000	4.76000000	4.39200000
C	25.79400000	4.18800000	3.73700000
O	24.61600000	4.36000000	4.02500000
H	25.44900000	5.80600000	5.53300000
H	27.59300000	5.35100000	3.69000000
H	27.64900000	3.97300000	4.78900000
N	26.12800000	3.29900000	2.68600000
H	26.62595737	3.79551649	1.97500785
H	15.54191874	8.70676769	12.75204264
H	26.70239897	2.56215727	3.04255100
O	18.29700000	8.28300000	3.39200000
H	14.84330332	4.54551550	2.70480920
H	17.16363231	7.72508468	0.36716973
H	26.47109644	6.18504626	8.25990221
H	20.29069394	3.94724025	8.59963500

H	21.08100000	8.56100000	3.97300000
H	21.44300000	7.69600000	6.89000000
H	20.66000000	5.71900000	5.66100000
H	21.99500000	5.92400000	4.52700000
N	23.53700000	9.12900000	6.37200000
C	24.82500000	9.78100000	6.05200000
C	26.00600000	8.92200000	6.42600000
O	27.14000000	9.22400000	6.11600000
C	24.78600000	11.05500000	6.84600000
C	23.82000000	10.72400000	7.92900000
C	22.73300000	9.83200000	7.39800000

ID 11 Chemical Formula: $C_{30}O_{16}N_{13}H_{47}$

N	-8.49400000	-12.78600000	-1.98200000	H	0.75000000	-3.45000000	4.30700000
C	-7.10200000	-12.38300000	-2.13900000	H	-2.38400000	-3.50400000	3.12600000
C	-6.87400000	-10.97800000	-1.65200000	H	-2.37600000	-2.20600000	2.39600000
O	-5.83300000	-10.72200000	-1.05900000	N	-0.81900000	-5.82400000	7.26800000
H	-6.48008892	-13.05116644	-1.58071672	C	-0.81500000	-5.54200000	8.70100000
N	-7.79300000	-10.05100000	-1.84900000	C	0.23700000	-6.37200000	9.40800000
C	-7.72800000	-8.68700000	-1.31400000	O	0.98200000	-5.88800000	10.26900000
C	-7.74200000	-8.73400000	0.20300000	H	-1.52400000	-6.14200000	6.89200000
O	-6.95100000	-8.08000000	0.87200000	H	-0.60666463	-4.50384643	8.85505695
H	-8.47700000	-10.26100000	-2.32500000	N	0.35000000	-7.64000000	9.11400000
H	-6.82692843	-8.21610413	-1.64750727	C	1.31400000	-8.56100000	9.68800000
N	-8.60900000	-9.56100000	0.79900000	C	2.73100000	-8.06800000	9.43400000
C	-8.65500000	-9.68300000	2.24500000	O	3.54100000	-7.98200000	10.34100000
C	-7.31200000	-10.19100000	2.79500000	H	-0.19400000	-7.95700000	8.52800000
O	-6.80000000	-9.70400000	3.81900000	H	1.14867180	-8.63430131	10.74260585
H	-9.14900000	-10.02700000	0.31700000	N	3.03900000	-7.74400000	8.18600000
H	-8.87042421	-8.72583138	2.67199021	C	4.37800000	-7.27700000	7.82400000
N	-6.72600000	-11.17100000	2.14100000	C	4.70200000	-5.96300000	8.48900000
C	-5.45900000	-11.73300000	2.52900000	O	5.86114218	-5.75001417	8.93013150
C	-4.35400000	-10.67900000	2.38600000	H	2.43800000	-7.80900000	7.57500000
O	-3.54300000	-10.52700000	3.29100000	H	5.09731387	-8.00890586	8.12698740
H	-7.11900000	-11.49100000	1.44600000	O	3.69205239	-4.95892171	8.61835467
H	-5.51116455	-12.05682249	3.54748802	H	4.08460721	-4.15147102	8.95824303
N	-4.33000000	-9.96000000	1.28700000	H	-6.39158778	-12.11023317	7.28119780
C	-3.39600000	-8.87600000	1.06000000	H	-8.86664788	-12.37951036	-1.14779395
C	-3.44600000	-7.88300000	2.21200000	H	-8.54750608	-13.78263140	-1.91984739
O	-2.40600000	-7.49200000	2.74000000	H	-9.42859775	-10.37097769	2.51543155
C	-3.77500000	-8.23300000	-0.28800000	H	-5.23468729	-12.57001930	1.90131974
H	-4.89900000	-10.14300000	0.66900000	H	-6.83639110	-12.44112614	-3.17387838
H	-2.49000000	-9.24400000	0.99500000	H	-8.57167354	-8.12771860	-1.66087069
H	-3.54913655	-8.91232803	-1.08323527	H	-3.21744488	-7.32955753	-0.42150657
H	-4.82160584	-8.01059882	-0.29534377	H	-0.34102089	-10.03214123	4.22646943
N	-4.64800000	-7.45400000	2.62100000	H	-5.76506829	-6.21650854	3.86232035
C	-4.74100000	-6.49700000	3.73000000	H	-1.77741575	-5.77232342	9.10794845
C	-4.22200000	-7.07700000	5.01900000	H	1.18999878	-9.52593372	9.24254897
O	-3.59600000	-6.38500000	5.80300000	H	4.43016199	-7.15379949	6.76239708
H	-5.36200000	-7.73900000	2.23600000				
H	-4.17013204	-5.62550291	3.48606848				
N	-4.52800000	-8.34000000	5.29500000				
C	-4.04600000	-8.97200000	6.53100000				
C	-2.55400000	-9.17500000	6.50500000				
O	-1.89200000	-9.03300000	7.55200000				
C	-4.77500000	-10.29800000	6.77500000				
C	-6.21800000	-10.18300000	7.26000000				
O	-6.65200000	-9.09800000	7.63200000				
O	-6.86300000	-11.27400000	7.27200000				
H	-5.01200000	-8.79100000	4.74600000				
H	-4.25400000	-8.37300000	7.27700000				
H	-4.77100000	-10.80500000	5.94800000				
H	-4.27300000	-10.80700000	7.43000000				
N	-1.99500000	-9.49900000	5.35100000				
C	-0.55700000	-9.65700000	5.20500000				
C	0.14900000	-8.32700000	5.39800000				
O	1.18800000	-8.26000000	6.02100000				
H	-2.49900000	-9.61900000	4.66500000				
H	-0.20278155	-10.35358152	5.93589225				
N	-0.40600000	-7.23500000	4.87100000				

C	0.15300000	-5.91500000	5.07100000
C	0.26200000	-5.59100000	6.55400000
O	1.31800000	-5.13300000	7.00000000
C	-0.72800000	-4.85600000	4.35600000
C	-0.20500000	-3.44100000	4.47400000
C	-0.85800000	-2.43700000	3.52100000
O	-0.31100000	-1.37300000	3.27700000
N	-2.00600000	-2.75300000	2.94800000
H	-1.11900000	-7.31800000	4.39800000
H	1.05100000	-5.89300000	4.67800000
H	-0.79300000	-5.08700000	3.41600000
H	-1.62200000	-4.89000000	4.73000000
H	-0.34000000	-3.13600000	5.38500000

ID 12 Chemical Formula: $C_{32}O_{14}N_{11}H_{45}$

C	1.49600000	7.79900000	4.92400000	O	3.68400000	7.24600000	29.03300000
O	0.25800000	7.84300000	4.98100000	H	3.31000000	7.25900000	26.44400000
N	2.22300000	7.32600000	5.91400000	H	0.68825220	6.91795727	27.83266952
C	1.62100000	6.82100000	7.14400000	N	1.68600000	7.57600000	29.98200000
C	2.38400000	7.30000000	8.35600000	C	2.24900000	8.11400000	31.21700000
O	3.64500000	7.27000000	8.40800000	C	1.53700000	7.55400000	32.42500000
C	1.62500000	5.23700000	7.20500000	O	0.30100000	7.47400000	32.48000000
C	1.12300000	4.35300000	6.01100000	H	0.66300000	7.50300000	29.89000000
C	1.67400000	3.07600000	5.78900000	H	3.28651870	7.85795218	31.27080018
C	-0.05200000	4.73100000	5.34900000	N	2.30700000	7.15500000	33.41500000
C	0.95500000	2.17100000	5.00300000	C	1.75600000	6.59200000	34.64500000
C	-0.73600000	3.84300000	4.54300000	C	2.46700000	7.14400000	35.85700000
C	-0.24400000	2.56200000	4.39500000	O	3.72500000	7.23900000	35.91000000
H	3.24900000	7.31100000	5.81800000	H	3.32900000	7.24200000	33.31900000
H	0.58500000	7.20300000	7.21900000	H	0.71566206	6.83433992	34.70719592
H	2.63100000	4.90600000	7.51500000	N	1.69700000	7.51800000	36.85700000
H	1.01500000	5.03600000	8.09000000	C	2.24600000	8.07000000	38.09200000
H	2.62000000	2.74200000	6.27500000	C	1.54800000	7.49200000	39.30000000
H	-0.55700000	5.66600000	5.52100000	O	0.29100000	7.37900000	39.35600000
H	1.28900000	1.14600000	4.95800000	H	0.67600000	7.42000000	36.76400000
H	-1.65400000	4.22200000	4.07200000	H	3.28964576	7.84024073	38.14598344
H	-0.86100000	1.88900000	3.82900000	N	2.32700000	7.11200000	40.29000000
N	1.65500000	7.74900000	9.35600000	H	3.20961581	6.81590290	39.92487558
C	2.25700000	8.24300000	10.59100000	H	1.89745524	6.35334131	40.77982475
C	1.50600000	7.73800000	11.79900000	O	2.22016485	8.58199784	3.97142473
O	0.24500000	7.75100000	11.85700000	H	1.82883588	8.47124644	3.10182956
H	0.62900000	7.75300000	9.26500000	H	2.23783479	9.31282279	10.58755054
H	3.27247125	7.91002361	10.64433730	H	2.11985128	9.13253163	38.08839039
N	2.24500000	7.28300000	12.78900000	H	1.86857655	5.52811239	34.62577298
C	1.65400000	6.76300000	14.01900000	H	2.14975155	9.17938094	31.21336798
C	2.40500000	7.26000000	15.23200000	H	1.74648267	5.63777474	20.87464628
O	3.62900000	7.26200000	15.28200000	H	2.20899513	9.27000458	17.46242712
C	1.74200000	5.29000000	13.58800000	H	1.80702001	5.58255761	27.75070694
C	2.05200000	4.30100000	14.65600000				
C	2.02400000	2.88900000	14.19100000				
O	2.47700000	2.06000000	14.90500000				
O	1.63100000	2.68400000	12.89700000				
H	3.27000000	7.29400000	12.69300000				
H	0.61300000	7.12800000	14.09500000				
H	0.77000000	5.06900000	13.06600000				
H	2.53400000	5.05000000	12.81300000				
H	3.06000000	4.53000000	15.02900000				
H	1.44000000	4.42900000	15.55500000				
H	2.42600000	2.34900000	12.49600000				
N	1.66600000	7.69200000	16.23100000				
C	2.25500000	8.20100000	17.46600000				
C	1.51600000	7.67700000	18.67500000				
O	0.28100000	7.64900000	18.72600000				
H	0.64000000	7.66900000	16.14000000				
H	3.27849984	7.89363548	17.51962031				
N	2.26600000	7.24000000	19.66400000				
C	1.68800000	6.70600000	20.89400000				
C	2.42600000	7.22100000	22.10700000				
O	3.66100000	7.26400000	22.15300000				
H	3.29000000	7.27700000	19.56900000				
H	0.66123609	7.00057072	20.95632151				
N	1.67600000	7.63400000	23.10600000				

C	2.25200000	8.15700000	24.34200000
C	1.52600000	7.61500000	25.55000000
O	0.29200000	7.55600000	25.60100000
C	2.50600000	9.66900000	24.49300000
H	0.65100000	7.58600000	23.01500000
H	3.30300000	7.82000000	24.41200000
H	3.36000000	9.92700000	25.10100000
H	1.56000000	10.10900000	24.90800000
H	2.74400000	10.10800000	23.51000000
N	2.28600000	7.19700000	26.54000000
C	1.72200000	6.64900000	27.77000000
C	2.44700000	7.18200000	28.98200000

ID 13 Chemical Formula: $C_{33}O_{15}N_{12}S_2H_{48}$

C	7.34500000	40.86600000	51.77900000	H	12.42878233	38.96440567	52.13444284
O	8.36100000	40.39500000	51.25900000	H	10.52130643	38.11042109	51.69878918
N	7.10500000	40.71900000	53.08500000	H	10.55209084	39.17162779	50.17971293
C	8.00200000	40.06600000	54.01800000	H	12.83687166	36.41987104	49.04718603
C	8.25600000	38.63100000	53.55800000	H	12.44168864	32.98240098	51.64626886
O	9.38100000	38.11800000	53.64000000	H	10.59036139	32.93817646	51.57325107
C	7.39200000	40.10600000	55.43200000	H	10.87139512	34.62525664	50.49134514
S	8.33300000	39.13600000	56.61000000	H	12.18138847	34.24589840	55.92396183
N	7.25500000	37.94400000	53.00400000	H	10.44757068	34.93903710	53.77625493
C	7.37800000	36.55800000	52.57600000	H	9.54495305	30.58327663	58.94968473
C	8.13300000	36.40500000	51.27600000	H	9.50397304	32.28995800	59.67097480
O	8.66200000	35.32900000	51.00700000	H	11.58533709	30.88204291	58.15383592
N	8.19900000	37.41200000	50.41300000	H	11.68042241	31.90441318	59.69669620
C	8.79200000	37.27200000	49.08400000	H	11.51235342	33.79728869	58.55946349
C	10.22000000	36.68300000	49.11400000	H	12.30118055	32.76524275	57.23759626
O	10.50600000	35.73600000	48.38400000	H	8.97954559	31.41315558	56.84338252
N	11.12100000	37.20800000	49.95000000	H	5.25143598	33.66685827	56.97386457
C	12.47900000	36.63200000	50.03300000	H	6.73988022	31.39389141	57.77539041
C	12.57400000	35.29400000	50.74400000	H	4.27177682	32.74763043	61.58951032
O	13.66700000	34.71600000	50.80300000	H	6.58307052	32.44550243	59.93842937
C	13.28500000	37.68800000	50.80200000	H	7.78608011	35.68907972	62.72215029
C	12.38100000	38.78900000	51.08000000	H	7.00958132	34.37537716	60.34342672
C	10.98700000	38.40000000	50.78000000	H	2.29581130	37.77014174	60.03127593
N	11.48700000	34.73300000	51.27200000	H	4.81180465	36.58529149	60.72846499
C	11.49400000	33.41300000	51.89400000	O	4.34452399	37.84659986	62.77264066
C	11.43400000	33.42500000	53.40800000	H	8.94109663	40.57797957	54.04757078
O	11.44300000	32.35900000	54.04000000	H	6.43423448	39.63497878	55.35634142
N	11.33200000	34.57400000	54.06700000	H	7.46403633	41.12241275	55.75852089
C	11.27900000	34.64700000	55.51200000	H	6.93763586	38.47127921	58.87136662
C	10.07400000	33.82800000	56.01500000	H	5.45583776	37.91157576	56.97814531
O	9.00300000	33.88100000	55.41200000	H	5.75482898	36.14873876	57.46570041
N	10.25700000	33.06100000	57.08600000	H	5.16546087	38.00834369	62.30200114
C	9.21000000	32.16500000	57.56900000	H	7.27079651	35.72431161	59.14064928
C	7.86500000	32.85500000	57.81700000	H	6.24648092	41.08504848	53.44410095
O	7.83100000	33.93800000	58.40800000	H	8.82807025	38.23598847	48.62104733
C	9.79400000	31.62200000	58.88700000	H	8.90107482	35.41432982	61.40545177
C	11.26100000	31.72400000	58.72900000	H	6.39736364	36.14759765	52.45425338
C	11.48200000	32.95600000	57.89900000	H	4.70017176	32.05313231	57.30984989
N	6.75000000	32.29600000	57.34400000	O	6.38518920	41.56607538	50.98303663
C	5.40700000	32.80600000	57.59000000	H	6.69678239	42.45873719	50.81670987
C	5.15300000	33.19300000	59.03200000	H	2.51463699	36.34034846	61.01497825
O	4.49500000	34.20100000	59.28200000	H	11.16980161	35.66736161	55.81504770
N	5.58700000	32.40100000	60.01500000	H	5.73633291	31.90671621	62.03054723
C	5.32800000	32.69100000	61.42800000				
C	5.96300000	34.00200000	61.81900000				
O	5.37000000	34.80900000	62.56900000				
N	7.16500000	34.29500000	61.32800000				
C	7.86900000	35.51300000	61.67000000				
C	7.26100000	36.68300000	60.91100000				
O	7.00100000	37.73700000	61.48300000				
N	6.99400000	36.56000000	59.61500000				
C	6.31100000	37.60400000	58.86400000				
C	4.98800000	37.95500000	59.50400000				
O	4.59800000	39.14400000	59.52800000				
C	6.08100000	37.16700000	57.42500000				
S	7.62700000	37.17200000	56.49500000				
N	4.23700000	36.98600000	60.01500000				

C	2.95900000	37.26100000	60.69900000					
C	3.23800000	38.14100000	61.91600000					
O	2.49410377	39.12503088	62.16474122					
H	7.88967667	36.00729762	53.33745511					
H	7.06838073	38.43894751	52.15535389					
H	8.16877141	36.63117949	48.49592246					
H	8.78619419	38.08090943	50.86881045					
H	14.04108713	38.05589019	50.14026814					
H	13.56021516	37.25668955	51.74174886					
H	12.63357269	39.57164001	50.39546976					

ID 14 Chemical Formula: $C_{27}O_{15}N_{13}H_{43}$

N	-23.56000000	7.85100000	3.45600000	H	-15.22418687	1.47166599	12.05921442
C	-22.44100000	8.06600000	4.35500000	H	-16.80188548	0.64171085	9.82370748
C	-22.57400000	7.20400000	5.61200000	H	-16.67509763	-3.11649464	12.03233614
O	-21.57700000	6.70500000	6.13800000	H	-16.26619694	-1.07724519	10.08225307
N	-23.80900000	7.02400000	6.08200000	H	-13.14386030	-3.98398229	8.78644098
C	-24.04700000	6.17400000	7.25300000	H	-14.53705557	-1.66007861	9.71989288
C	-23.51300000	4.75100000	6.98500000	H	-11.23036815	0.53592126	13.19080766
O	-22.79900000	4.15500000	7.80800000	H	-12.87184627	0.37947613	12.34477308
N	-23.82000000	4.23400000	5.80600000	H	-11.42574009	2.12124425	11.65854464
C	-23.35500000	2.88300000	5.44900000	H	-10.46101564	-1.14415381	11.52912165
C	-21.83600000	2.81400000	5.33500000	H	-13.22500052	-1.69083221	11.30719624
O	-21.18600000	1.86400000	5.79900000	H	-12.53072663	-3.16238153	15.44233211
N	-21.25400000	3.81400000	4.67200000	H	-12.95067064	-3.06638960	12.60567746
C	-19.82100000	3.88100000	4.52600000	H	-15.11022039	2.57438277	7.84921418
C	-19.15900000	3.84400000	5.90400000	H	-18.27665258	-0.29074456	5.69018764
O	-18.23700000	3.08100000	6.10900000	H	-22.41103726	9.09745269	4.63803282
N	-19.66800000	4.65500000	6.84300000	H	-25.09751750	6.12786193	7.45095017
C	-19.09700000	4.68400000	8.20200000	H	-23.78710787	2.60315798	4.51098548
C	-19.24400000	3.32700000	8.89200000	H	-19.55628679	4.79058397	4.02852245
O	-18.32900000	2.88300000	9.59400000	H	-12.95349416	-2.34930597	8.21366289
N	-20.38400000	2.68000000	8.68700000	H	-13.73154889	-4.02540153	14.52103906
C	-20.59600000	1.32300000	9.22000000	H	-17.20692632	-3.18914573	10.36864266
C	-19.52900000	0.35900000	8.66900000	H	-16.95314008	1.23717310	12.10357866
O	-18.92800000	-0.42600000	9.41500000	H	-21.56697556	0.97770708	8.93211242
N	-19.27000000	0.43700000	7.36400000	H	-19.60463468	5.42790539	8.77976448
C	-18.27200000	-0.44500000	6.74900000	O	-11.57416238	-5.28221164	12.94497209
C	-16.85400000	-0.17300000	7.28900000	H	-11.17675335	-6.15414637	13.00324634
O	-16.08400000	-1.09000000	7.56500000	H	-23.39484023	7.56872591	2.51241580
N	-16.51600000	1.10500000	7.41700000				
C	-15.20900000	1.51300000	7.94200000				
C	-15.05400000	1.12100000	9.41900000				
O	-13.97700000	0.64300000	9.83500000				
N	-16.12700000	1.28000000					
10.19400000							
C	-16.04500000	0.94500000	11.61900000				
C	-15.83800000	-0.54700000					
11.80000000							
O	-15.00500000	-0.98500000					
12.62800000							
N	-16.57400000	-1.31700000					
11.00300000							
C	-16.48500000	-2.77000000					
11.03800000							
C	-15.07200000	-3.19800000					
10.60500000							
O	-14.42900000	-4.00100000					
11.28100000							
N	-14.56400000	-2.63700000	9.50800000				
C	-13.19200000	-2.95200000	9.06500000				
C	-12.16600000	-2.68500000					
10.16800000							
O	-11.25000000	-3.47900000					
10.39300000							
N	-12.34900000	-1.55300000					
10.84500000							
C	-11.46000000	-1.11100000					
11.91100000							

C -11.49300000 -2.03500000 13.12400000 O -10.45500000 -2.22400000 13.77200000 C -11.80400000 0.31900000 12.31400000 O -11.37700000 1.22500000 11.31800000 N -12.66900000 -2.58900000 13.43800000 C -12.74200000 -3.61900000 14.49800000 C -11.74800000 -4.74800000 14.26000000 O -11.07963391 -5.21078759 15.22056492 H -21.53173972 7.81353676 3.85061121 H -24.49567843 7.97285686 3.78159107 H -23.54346431 6.58857271 8.10122243 H -24.29189408 6.56166425 5.33832066 H -23.67888299 2.19388993 6.20074937 H -23.37111230 4.83538623 5.14506548 H -19.48313047 3.04733007 3.94657043 H -21.48457384 4.62834075 5.20462074 H -18.05878947 4.93553388 8.14076607 H -20.60286930 4.32522868 6.97441641 H -20.53192816 1.34847984 10.28777600 H -20.42541606 2.56349089 7.69467428 H -18.53319481 -1.46219611 6.95391303 H -18.89846486 1.35701139 7.23933773 H -14.43861203 1.03823449 7.37103583 H -17.16830294 1.46273142 8.08522834	

ID 15 Chemical Formula: $C_{33}O_{15}N_{15}H_{53}$

N 59.22700000 4.06400000 19.38600000 C 59.91300000 3.63600000 20.60900000 C 61.17100000 4.43000000 20.72400000 O 61.99400000 4.36900000 19.81300000 N 61.31800000 5.19100000 21.81400000 C 62.47000000 6.09900000 22.00100000 C 63.32400000 5.59100000 23.17500000 O 62.79000000 5.33100000 24.27400000 N 64.63600000 5.46000000 22.96400000 C 65.51700000 4.99200000 24.03000000 C 66.30800000 6.18200000 24.47600000 O 67.08100000 6.78900000 23.67000000 N 66.08900000 6.54000000 25.74700000 C 66.72600000 7.73500000 26.31100000 C 67.75400000 7.30500000 27.34100000 O 67.50500000 6.35100000 28.08900000 N 68.90400000 7.96300000 27.36100000 C 69.87300000 7.77000000 28.41800000 C 70.00200000 9.15900000 29.04800000 O 70.75500000 9.98600000 28.54000000 N 69.24200000 9.45000000 30.13200000 C 69.11300000 10.88200000 30.57100000 C 70.34200000 11.59600000 31.15800000 O 70.39000000 12.83800000 31.09600000 C 67.94800000 10.86400000 31.58200000 C 67.18300000 9.59400000 31.24500000 C 68.26500000 8.58900000 30.82200000 N 71.31600000 10.85700000 31.72000000 C 72.54900000 11.50900000 32.21400000 C 73.32800000 12.04400000 31.02300000	H 67.20865008 8.28601733 25.53104565 H 66.46261735 5.78397919 26.28444080 H 69.51109408 7.06365733 29.13563789 H 68.63431085 8.92181496 27.45011581 H 67.31267457 11.69755253 31.36647325 H 68.36391996 10.74736729 32.56093176 H 66.57300811 9.79699837 30.38966290 H 66.73584245 9.23249862 32.14736737 H 68.72582853 8.20031232 31.70600167 H 67.83952640 7.92100287 30.10251960 H 68.95980697 11.47203036 29.69162746 H 72.29161167 12.31648727 32.86715814 H 71.62877983 10.25536462 30.98501452 H 74.89160790 12.05607191 28.93278233 H 72.24055702 11.44017601 29.64499906 H 71.51107761 14.69274098 27.38637886 H 70.03191246 13.72173153 27.93766019 H 71.81940924 13.13707526 29.09761905 H 70.60748994 12.34071130 23.68240776 H 70.17090443 11.60565131 26.28866823 H 67.43353072 9.15329213 23.36130752 H 69.49924999 10.28266194 22.47151040 H 68.00841634 5.41541309 20.57080369 H 69.61123877 5.15543933 18.40630499 H 67.92402906 4.70207578 18.37712356 H 68.42323557 6.25215402 17.74378560 H 70.30361323 5.92523104 20.34607579 H 67.78168312 8.05042005 19.12663606 H 66.41526183 8.11495838 21.34716028 H 63.76590207 6.26572846 18.55470221 H 66.46820802 6.18830842 17.83974260 H 65.75024603 2.38113723 17.80529808 H 63.43139317 3.87109378 18.36821912 H 62.44390713 3.19903097 17.43099667 H 62.03647804 1.71472818 17.97644460 H 64.16708164 6.71434053 16.90848386 H 66.72988070 10.53633465 22.55281588

O	74.04500000	13.05800000	31.13800000	H	71.36622178	10.84321478	24.12482360
N	73.20300000	11.33200000	29.89400000	H	74.03624101	10.80343149	28.07028376
C	73.92400000	11.67900000	28.67500000	H	73.14585203	10.79539295	32.74261388
C	73.17000000	12.73300000	27.89200000	H	70.81137259	7.45144101	28.01441970
O	73.78400000	13.44600000	27.08100000	H	65.98519500	8.34939018	26.77858171
N	71.85700000	12.82900000	28.14700000	H	66.17321299	4.23327679	23.65767809
C	70.97700000	13.76700000	27.43800000	H	62.11694501	7.08600060	22.21566718
C	70.71200000	13.35200000	25.99600000	H	64.67163883	1.95429327	19.10952094
O	70.38900000	14.19500000	25.16600000	H	60.14609624	2.59345351	20.54847753
N	70.85000000	12.05600000	25.70900000				
C	70.58400000	11.52800000	24.37800000				
C	69.22000000	10.79200000	24.22600000				
O	68.61000000	10.34200000	25.21700000				
N	68.75000000	10.70700000	22.98000000				
C	67.59400000	9.90900000	22.62100000				
C	67.85800000	9.26700000	21.29300000				
O	68.44500000	9.88800000	20.36700000				
N	67.39300000	8.03300000	21.15400000				
C	67.44900000	7.34900000	19.86300000				
C	66.08500000	6.80600000	19.54500000				
O	65.34400000	6.38600000	20.46200000				
C	68.41100000	6.15800000	19.91400000				
O	69.66500000	6.64200000	20.35000000				
C	68.60800000	5.51600000	18.49800000				
N	65.76800000	6.77400000	18.24800000				
C	64.50400000	6.19800000	17.78300000				
C	64.77800000	4.73100000	17.45000000				
O	65.31200000	4.40800000	16.39000000				
N	64.43100000	3.84400000	18.36100000				
C	64.74900000	2.46600000	18.17300000				
C	63.79600000	1.83700000	17.17900000				
O	64.21900000	0.98500000	16.42600000				
N	62.49500000	2.21800000	17.24400000				
H	59.28888734	3.81980057	21.45847086				
H	59.71134292	3.70384958	18.58868976				
H	59.21262913	5.06301759	19.34407943				
H	63.06103833	6.11607902	21.10921415				
H	61.41014420	4.52949635	22.55825961				
H	64.93749158	4.60993196	24.84430584				
H	64.95031264	6.38994674	22.77319481				

ID 16 Chemical Formula: $C_{29}O_{16}N_{13}H_{45}$

C	21.08000000	3.46200000	26.84200000	H	31.85806487	2.92308142	31.73266648
C	22.50800000	3.96500000	26.73500000	H	31.98355858	5.24560744	30.25060594
O	23.40900000	3.17000000	26.47500000	H	36.55449987	3.41279858	31.36071237
N	22.74300000	5.26100000	26.91300000	H	35.87808457	2.68595209	32.92559464
C	24.11200000	5.75800000	26.80100000	H	35.32887110	5.02322956	33.53324184
C	24.72400000	5.78500000	28.18300000	H	33.89824269	3.36339110	32.71314391
O	24.14200000	6.35600000	29.12200000	H	36.33621649	8.13256674	30.85027386
N	25.87600000	5.12800000	28.30600000	H	34.69733162	8.86158178	31.31642130
C	26.55300000	4.95700000	29.59600000	H	34.66035325	7.14024199	32.43248361
C	27.91900000	5.61500000	29.57100000	H	34.19805824	7.85705692	26.94537862
O	28.50600000	5.80000000	28.49900000	H	33.54105991	6.88185371	29.35165145
C	26.68600000	3.47400000	29.94100000	H	29.84929256	7.03598131	27.01324215
N	28.39800000	5.98900000	30.75400000	H	32.27485078	7.17283383	25.51823254
C	29.78000000	6.35800000	30.94900000	H	29.48752894	3.69428471	24.11823618
C	30.54900000	5.11400000	31.41000000	H	28.46984301	5.39746821	25.72489743
O	30.41300000	4.68400000	32.56400000	H	25.20264955	3.13671891	24.27123145
C	29.87500000	7.47000000	31.99300000	H	27.72676091	1.90951292	23.92096115

C	31.28800000	7.74400000	32.43300000	H	24.56757375	-0.90613335	25.94016527
O	32.23800000	7.43100000	31.73200000	H	23.84778921	1.48058476	25.03551228
N	31.43400000	8.35600000	33.61600000	O	21.75205164	1.03263811	25.85842904
N	31.33000000	4.53100000	30.50000000	H	39.47857458	3.17596030	32.94453984
C	32.17900000	3.36800000	30.81400000	H	22.31076267	1.81288308	25.83274296
C	33.61600000	3.85900000	30.95300000	H	24.10428216	6.74623179	26.39083129
O	34.34300000	3.96400000	29.95400000	H	30.01342230	7.96253585	25.54344318
N	33.99400000	4.20900000	32.18800000	H	25.59963647	2.16214362	22.87555619
C	35.34700000	4.67400000	32.52200000	H	32.11667348	2.65024501	30.02289749
C	35.80400000	5.89500000	31.68600000	H	34.57632945	6.15787876	26.96622555
O	36.94600000	5.96700000	31.20900000	H	29.67680871	2.89753589	25.65875409
C	36.33000000	3.50300000	32.40300000	H	24.15396829	0.08827324	27.31799325
C	37.65800000	3.75700000	33.09500000	N	20.61910381	3.09941815	25.49403520
O	37.82500000	4.73900000	33.86200000	H	19.85310572	2.46042838	25.56431309
O	38.55600000	2.91900000	32.87800000	H	20.32288260	3.92297093	25.01028546
N	34.90700000	6.85600000	31.50600000	H	20.45475064	4.23249587	27.24237402
C	35.26700000	8.09500000	30.83400000				
C	34.87700000	8.15500000	29.36900000				
O	35.04300000	9.19800000	28.71000000				
N	34.39300000	7.03200000	28.85000000				
C	33.99500000	6.92600000	27.43200000				
C	32.50400000	6.59200000	27.26300000				
O	31.99000000	5.67200000	27.91200000				
N	31.82000000	7.34500000	26.39200000				
C	30.39100000	7.12700000	26.09500000				
C	30.20600000	5.85900000	25.27500000				
O	30.82100000	5.71200000	24.22300000				
N	29.36200000	4.94800000	25.77000000				
C	29.13600000	3.65300000	25.12800000				
C	27.66300000	3.30500000	25.12900000				
O	26.95200000	3.54200000	26.11500000				
N	27.21000000	2.76100000	24.01000000				
C	25.83500000	2.35700000	23.90100000				
C	25.61800000	1.09000000	24.72400000				
O	26.38100000	0.13200000	24.62700000				
N	24.61000000	1.14000000	25.58600000				
C	24.05100000	-0.02500000	26.25900000				
C	22.57100000	-0.13900000	25.89700000				
O	22.07271564	-1.26393432	25.63279168				
H	21.04658522	2.60251713	27.47845318				
H	24.68031714	5.10924999	26.16772355				
H	22.48690525	5.43652427	27.86358230				
H	27.33895621	3.36039438	30.78102497				
H	25.72241117	3.07603225	30.18186975				
H	27.08974313	2.94735613	29.10163255				
H	25.96018895	5.42986630	30.35089902				
H	26.52042999	5.66972253	27.76632724				
H	29.36125084	7.10710087	32.85860153				
H	29.53912260	8.36165939	31.50614283				
H	32.05548273	7.97703062	34.30166860				
H	30.92148197	9.19171908	33.81322800				
H	30.20325679	6.72273374	30.03646343				
H	28.28217792	5.17819569	31.32774351				

ID 17 Chemical Formula: $C_{34}O_{16}N_{15}S_4H_{51}$

N	23.51600000	13.17200000	5.10000000	H	23.10890085	17.92537958	3.44781235
C	23.65400000	13.91900000	3.81100000	H	23.47760073	15.76704869	2.15171508
C	23.54800000	15.43800000	3.96200000	H	25.36862098	22.59722358	-1.83919390
O	23.05100000	15.96400000	4.97000000	H	23.16896854	20.96530549	-2.55241537
C	22.63000000	13.42100000	2.77000000	H	21.61793293	24.83822064	-2.92730814
S	20.90900000	13.24000000	3.33000000	H	22.18556967	22.59568382	-1.91728860
N	24.00400000	16.12700000	2.92200000	H	18.56542498	23.45322181	0.03093296
C	23.86900000	17.56600000	2.78600000	H	19.54438495	25.26147757	-1.94025296
				H	15.63815835	24.92186701	-3.46230107
				H	18.16572460	23.79590096	-3.02316994
				H	16.45789467	20.86865997	-5.52109425
				H	16.88284755	22.17424895	-3.12068761
				H	13.62216966	20.72850651	-1.94617515
				H	14.48696474	20.05188168	-4.55735191
				H	12.85814019	16.03069798	-2.04936208
				H	14.42348098	17.71222190	-3.73540201

C	23.46900000	17.84700000	1.32400000
O	23.25100000	16.89400000	0.54800000
N	23.26300000	19.11400000	0.96400000
C	23.04400000	19.49400000	-0.44900000
C	23.72200000	20.82700000	-0.78900000
O	23.91900000	21.68000000	0.07900000
C	21.53100000	19.60700000	-0.84600000
S	20.36700000	18.23800000	-0.53400000
N	24.04700000	20.99900000	-2.07500000
C	24.67400000	22.23900000	-2.57000000
C	23.62700000	23.31300000	-2.83300000
O	23.96500000	24.46800000	-3.07200000
N	22.35700000	22.91000000	-2.85100000
C	21.28200000	23.84000000	-3.11600000
C	20.09900000	23.51600000	-2.19900000
O	19.58500000	22.40300000	-2.23500000
N	19.72400000	24.47300000	-1.35200000
C	18.52300000	24.35400000	-0.54500000
C	17.32400000	24.31400000	-1.45900000
O	16.22300000	24.04400000	-0.98900000
N	17.56900000	24.55500000	-2.76300000
C	16.57300000	24.58600000	-3.86000000
C	16.35700000	23.23300000	-4.53400000
O	15.61600000	23.15500000	-5.50700000
N	17.09800000	22.22400000	-4.09600000
C	16.92200000	20.87400000	-4.55700000
C	16.01600000	20.21900000	-3.53400000
O	16.47800000	19.55400000	-2.60700000
N	14.71700000	20.50100000	-3.69400000
C	13.64200000	20.06200000	-2.78300000
C	13.76000000	18.62700000	-2.24800000
O	13.96400000	18.41800000	-1.04900000
N	13.61800000	17.62000000	-3.15000000
C	13.61400000	16.19800000	-2.78800000
C	14.97300000	15.73300000	-2.22600000
O	15.04300000	14.76800000	-1.45900000
N	16.03700000	16.42800000	-2.61400000
C	17.38700000	16.23400000	-2.06700000

H	17.87158369	17.99353636	1.61932974
H	16.00727497	17.77663011	-0.52904469
H	13.47515925	16.02108427	2.60304922
H	15.46166148	15.98122979	0.54324802
H	15.23861545	11.67795956	1.88047231
H	16.18351146	14.33892651	1.55133598
H	24.24410241	13.45058235	5.72630564
H	22.62717891	13.37634003	5.51017340
H	24.64643519	13.71377674	3.46769866
H	22.94744072	12.43114612	2.51638478
H	22.60137638	14.18257083	2.01894038
H	23.48156282	18.69470844	-1.00986699
H	21.54554840	19.70153399	-1.91171650
H	21.16048182	20.40930486	-0.24273954
H	17.74493014	15.24451647	-2.26118642
H	17.98414189	18.20887912	-2.37513768
H	18.29480958	17.02783653	-3.76916924
H	18.45589105	13.17331535	4.91451228
H	19.41321013	15.28921100	5.38649888
H	18.25082156	16.05263822	4.16145533
H	17.10471212	14.48228973	2.71399576
H	23.25633514	19.82544365	1.66671155
H	15.91154936	17.12462013	-3.32038696
H	16.67729970	12.09545399	0.98121447
H	12.71024983	20.14804601	-3.30197755
H	13.38276812	15.61969561	-3.65805508
H	16.90158783	25.28646761	-4.59910430
H	13.17642681	15.43603663	0.99947191
H	18.44640532	25.19600174	0.11079443
H	17.86459946	20.36907313	-4.59514591
H	16.54444313	19.07799968	1.27822732
H	20.97697136	23.75238435	-4.13785176
H	24.80112238	18.04250617	3.00733627
H	25.19768688	22.02899639	-3.47914825
O	15.54359382	14.60302875	5.46347375
H	15.01765263	14.48971266	6.25854942

C 17.32300000 16.47900000 -0.57100000 O 17.55300000 15.58900000 0.25000000 C 18.33800000 17.26200000 -2.72600000 S 20.11400000 17.28300000 -2.34800000 N 16.95300000 17.70100000 -0.21300000 C 16.89500000 18.07100000 1.18900000 C 15.92100000 17.11400000 1.93600000 O 16.09000000 16.88100000 3.14300000 N 14.95300000 16.53200000 1.20500000 C 13.93100000 15.57100000 1.74600000 C 14.44700000 14.18100000 2.15700000 O 13.96500000 13.57400000 3.14500000 N 15.43500000 13.68700000 1.43000000 C 16.01700000 12.40300000 1.76500000 C 16.80100000 12.52300000 3.07500000 O 16.96200000 11.54100000 3.81900000 N 17.24000000 13.74600000 3.37700000 C 17.91100000 14.05200000 4.63900000 C 16.92200000 14.37200000 5.76600000 O 17.32324983 14.43134307 6.95723782 C 18.87200000 15.23600000 4.46500000 S 20.14600000 15.11700000 3.18200000	

ID 18 Chemical Formula: $C_{36}O_{18}N_{17}H_{55}$

C	3.15700000	26.88400000	20.93500000	H	2.77265604	29.20506142	20.03335766
O	3.02861753	27.71603382	21.87031183	H	1.91161522	26.62585625	19.61712119
N	2.73500000	27.18200000	19.73000000	H	-1.64225128	28.69843230	20.13550861
C	2.31700000	28.48700000	19.38400000	H	0.43563251	30.28390154	19.80676168
C	0.80200000	28.49900000	19.56600000	H	-3.20210812	31.24026539	16.83982629
O	0.13900000	27.76200000	18.89800000	H	-4.76903460	32.14155885	17.24861905
N	0.26100000	29.44300000	20.31900000	H	-4.78392130	29.56142487	17.19381196
C	-1.13500000	29.51000000	20.61400000	H	-5.37847195	30.43591996	18.71580666
C	-1.68300000	30.82900000	20.09700000	H	-3.84306877	29.09779961	19.69670749
O	-1.21800000	31.90800000	20.48400000	H	-2.80603032	29.04445098	18.16164880
N	-2.72800000	30.80300000	19.27200000	H	-2.68089969	32.79138186	18.64675970
C	-3.36900000	31.98100000	18.76800000	H	-6.47759797	33.92957362	20.47034253
C	-4.44000000	32.56300000	19.70000000	H	-4.94728233	33.77750926	18.46950839
O	-4.96300000	31.95400000	20.72200000	H	-7.35303133	35.85925457	16.57027328
C	-3.98000000	31.47800000	17.53500000	H	-8.14286618	34.94213362	19.07716422
C	-4.58900000	30.19200000	18.03600000	H	-10.69819182	38.68112446	17.48358238
C	-3.43900000	29.58500000	18.83400000	H	-9.28661040	37.18442156	15.81833456
N	-4.69900000	33.79700000	19.43800000	H	-11.66386583	37.56125783	13.23683099
C	-5.74600000	34.57300000	20.02800000	H	-12.43034976	38.73490988	15.72621544
C	-6.36800000	35.37000000	18.88800000	H	-14.69917984	41.34562111	13.30112222
O	-5.84300000	36.39800000	18.48800000	H	-12.67661957	40.14972531	14.91350371
N	-7.46300000	34.87400000	18.34700000	H	-10.85051243	43.83177920	12.47442447
C	-8.10900000	35.47200000	17.22100000	H	-11.22062544	41.31296067	13.65250140

C	-9.08100000	36.59300000	17.53500000	H	-9.42746525	39.03567227	11.25425902
O	-9.77200000	36.57300000	18.55900000	H	-10.71554328	40.94301562	11.42115353
N	-9.07000000	37.61400000	16.69500000	H	-5.25767180	39.74547877	12.63639407
C	-9.96000000	38.78500000	16.71600000	H	-7.75480309	39.04965723	13.04394040
C	-10.60400000	38.77600000	15.36400000	H	-5.21911257	37.15524649	16.35890726
O	-10.01100000	39.26100000		H	-4.17158592	38.90339974	14.79419414
14.42800000				H	-1.15716563	37.96260175	17.90731365
N	-11.78300000	38.13900000		H	-3.31361303	36.30859028	17.63874671
15.25100000				H	-0.20679942	33.77935461	18.80136845
C	-12.40900000	37.90600000	13.92300000	H	0.27224134	36.43903068	19.21020216
C	-13.00900000	39.16200000	13.40500000	H	2.47241919	34.15185206	22.28044683
O	-12.94500000	39.44200000		H	1.37785721	32.70655382	20.36649374
12.24500000				H	4.17831213	30.16710141	21.44569740
N	-13.44500000	40.02900000		H	4.09099244	32.43983456	23.00361182
14.28500000				H	4.41069668	28.75653693	22.86508542
C	-13.80400000	41.39700000	13.88500000	H	-9.15117654	40.28500123	10.06349306
C	-12.78200000	42.15700000	13.09700000	H	5.63911273	31.13717062	21.46128803
O	-13.11000000	42.70700000		H	2.56826142	28.69736411	18.36541537
12.04500000				H	-1.28139907	29.45071189	21.67227796
N	-11.54700000	42.25800000		H	1.23676252	34.29951005	17.97733715
13.63300000				H	-4.35145892	36.13863780	15.23059727
C	-10.43400000	42.99800000	13.00000000	H	-8.64193442	34.70608641	16.69730421
C	-9.56500000	42.23100000	12.03700000	H	1.12478941	33.23763906	22.93237350
O	-8.66700000	42.80200000	11.53900000	H	-5.34326213	35.23611900	20.76486864
N	-9.82600000	40.94100000	11.87800000	H	-2.14371761	37.76399230	19.34140748
C	-9.06400000	40.03000000	11.09900000	H	-13.17273373	37.16264235	14.01802731
C	-7.56000000	40.11200000	11.53400000	H	-14.01750245	41.95482078	14.77277963
O	-6.69900000	40.36500000	10.70700000	H	-9.39504169	39.68281447	16.85618305
N	-7.34000000	39.93800000	12.84700000	H	-5.76548311	40.69715610	14.01408551
C	-5.97700000	39.83000000	13.42400000	H	-9.80610696	43.37697901	13.77911824
C	-5.92600000	38.60500000	14.28900000	O	3.76316857	25.61347559	21.18645058
O	-6.97900000	38.01700000	14.68700000	H	3.94403099	25.17400606	20.35233109
N	-4.71200000	38.10100000	14.54100000	H	3.49344352	29.52460839	23.97656171
C	-4.42900000	37.12500000	15.63800000				
C	-3.11300000	37.50900000	16.30400000				
O	-2.23700000	38.08700000	15.64900000				
N	-3.05700000	37.27300000	17.57500000				
C	-1.89400000	37.35200000	18.38600000				
C	-1.38000000	35.98300000	18.55000000				
O	-2.12300000	35.03500000	18.78700000				
N	-0.07600000	35.83900000	18.49000000				
C	0.55400000	34.53100000	18.76800000				
C	1.31600000	34.52800000	20.10100000				
O	2.01900000	35.50400000	20.46000000				
N	1.11200000	33.50000000	20.91400000				
C	1.81200000	33.32600000	22.11700000				
C	2.61000000	32.04200000	21.96600000				
O	2.04000000	30.96600000	21.80800000				
N	3.93200000	32.11300000	22.07200000				
C	4.72200000	30.92500000	21.97000000				
C	5.00200000	30.48100000	23.36100000				
O	5.71800000	31.12700000	24.14500000				
N	4.42900000	29.35100000	23.66900000				

ID 19 Chemical Formula: $C_{35}O_{19}N_{17}H_{55}$

N	-16.07700000	4.33600000	0.60300000	N	-15.58100000	22.61900000	1.60600000
C	-16.05000000	5.24100000	1.75200000	C	-14.64900000	23.69000000	1.29400000
C	-14.99800000	6.33600000	1.59200000	C	-15.21200000	24.63600000	0.23500000
O	-15.27200000	7.51800000	1.85300000	O	-15.16100000	25.85300000	0.39500000
H	-16.50127085	3.47075032	0.87009032	H	-15.32300000	21.84700000	1.32900000
H	-17.01238381	5.69635815	1.85861311	H	-14.44513040	24.24576991	2.18532317
N	-13.78400000	5.96700000	1.16800000	N	-15.76600000	24.09700000	-0.85100000
C	-12.72900000	6.97500000	1.07700000	C	-16.26400000	24.97500000	-1.91000000
C	-13.07800000	8.03500000	0.04600000	C	-17.50200000	25.73100000	-1.45300000
O	-12.72500000	9.20800000	0.21700000	O	-17.68400000	26.89800000	-1.81500000
H	-13.55400000	5.17200000	0.93700000	H	-15.86300000	23.25500000	-0.99700000
H	-12.60502358	7.44113191	2.03211826	H	-15.50041814	25.67719036	-2.17224308
N	-13.77200000	7.64400000	-1.02900000	N	-18.33800000	25.10800000	-0.61500000
C	-14.21400000	8.60300000	-2.03100000	C	-19.53100000	25.79400000	-0.14100000
C	-15.33100000	9.48800000	-1.49200000	C	-19.16600000	26.98400000	0.72700000
O	-15.40200000	10.68000000	-	O	-19.81100000	28.04500000	0.65300000
1.84300000				C	-20.42000000	24.82200000	0.64100000
H	-13.99800000	6.83200000	-1.19900000	O	-20.80800000	23.71900000	-0.16700000

H	-13.38635242	9.21813731	-2.31649183
N	-16.19900000	8.93100000	-0.64600000
C	-17.24000000	9.73900000	-0.02700000
C	-16.63400000	10.79800000	0.88300000
O	-17.11300000	11.93900000	0.92900000
H	-16.20600000	8.10100000	-0.41700000
H	-17.81417792	10.21902349	-0.79172032
N	-15.54500000	10.45300000	1.57200000
C	-14.88000000	11.42700000	2.43800000
C	-14.19800000	12.52500000	1.62300000
O	-14.21300000	13.69800000	2.02400000
H	-15.17500000	9.67700000	1.55800000
H	-15.60615606	11.87218212	3.08561892
N	-13.57600000	12.16600000	0.49500000
C	-12.97400000	13.18100000	-0.37800000
C	-14.03800000	14.14500000	-0.88300000
O	-13.82600000	15.36800000	-0.92500000
H	-13.48800000	11.35700000	0.21500000
H	-12.23519433	13.72629653	0.17128851
N	-15.19300000	13.60500000	-1.28200000
C	-16.28400000	14.43200000	-1.78000000
C	-16.82800000	15.31600000	-0.67700000
O	-17.07300000	16.50400000	-0.89200000
H	-15.36900000	12.76300000	-1.27300000
H	-15.92476423	15.04598558	-2.57929429
N	-17.03600000	14.74500000	0.51700000
C	-17.46600000	15.53400000	1.66400000
C	-16.56500000	16.74200000	1.87900000
O	-17.04900000	17.86600000	2.03100000
H	-16.93500000	13.90800000	0.68500000
H	-18.46851369	15.87043451	1.50066563
N	-15.24400000	16.52100000	1.87700000
C	-14.29200000	17.60300000	2.10400000
C	-14.39400000	18.66100000	1.02300000
O	-14.43300000	19.86400000	1.30900000
H	-14.87600000	15.75500000	1.74600000
H	-14.49265299	18.05249116	3.05405057
N	-14.44000000	18.23600000	-0.24700000
C	-14.60100000	19.18700000	-1.35000000
C	-15.85300000	20.04300000	-1.19100000
O	-15.82800000	21.26000000	-1.39100000
H	-14.38100000	17.41500000	-0.49400000
H	-13.74451330	19.82744304	-1.38410635
N	-16.98100000	19.41300000	-0.87500000
H	-18.23700000	24.30900000	-0.31600000
H	-20.03400000	26.11400000	-0.90600000
H	-19.92600000	24.49200000	1.40800000
H	-21.21600000	25.29100000	0.93600000
H	-20.98100000	23.98000000	-0.94600000
N	-18.13600000	26.82500000	1.55800000
C	-17.66900000	27.93900000	2.38000000
C	-17.02900000	29.02700000	1.53000000
O	-17.32700000	30.21500000	1.69000000
H	-17.69500000	26.09400000	1.66400000
H	-18.49992371	28.35384326	2.91138579
N	-16.15000000	28.64200000	0.60300000
C	-15.50000000	29.63000000	-0.25500000
C	-16.52400000	30.41900000	-1.05700000
O	-16.45800000	31.64900000	-1.13500000
H	-15.91500000	27.82800000	0.45200000
H	-14.93518253	30.30520736	0.35325673
H	-13.73669512	23.26409922	0.93177309
H	-14.83810126	29.12767868	-0.92913897
H	-16.94928498	27.57649258	3.08391666
H	-16.50932230	24.38557478	-2.76865877
H	-16.98266349	21.09978791	3.45868826
H	-19.03586391	19.47060537	-0.61774270
H	-14.66599298	18.64418664	-2.26979866
H	-13.30015753	17.20159490	2.10873810
H	-17.44164313	14.91960673	2.53968696
H	-17.06715398	13.80064997	-2.14464637
H	-12.50940817	12.69870870	-1.21253552
H	-14.14483510	10.92354110	3.03042021
H	-17.88135211	9.10525865	0.54914179
H	-15.83254813	4.67621074	2.63439887
H	-14.56999062	8.07345618	-2.88992609
H	-16.60575027	4.75216501	-0.13674985
H	-11.81233939	6.49990077	0.79608355
O	-17.53952007	29.67156865	-1.73151122
H	-17.91420685	30.20412890	-2.43691139

C -18.22900000 20.15600000 -0.77300000 C -18.17400000 21.13600000 0.38700000 O -18.59100000 22.29400000 0.25400000 H -17.05100000 18.57000000 -0.71800000 H -18.39398241 20.69493333 -1.68252277 N -17.66500000 20.69300000 1.53800000 C -17.50400000 21.60400000 2.67200000 C -16.71200000 22.84200000 2.25500000 O -17.10600000 23.98500000 2.52800000 H -17.41000000 19.88600000 1.68800000 H -18.46900788 21.90410068 3.02356702	

ID 20 Chemical Formula: $C_{38}O_{16}N_{18}H_{62}$

N 9.44000000 -7.08400000 -30.74000000 C 8.74100000 -7.78500000 -29.67300000 C 8.10600000 -6.78600000 -28.72400000 O 8.61600000 -5.67300000 -28.55200000 N 7.02500000 -7.18400000 -28.06200000 C 6.54200000 -6.42600000 -26.91600000 C 7.12000000 -7.00100000 -25.62900000 O 7.16200000 -8.22000000 -25.45100000 N 7.58100000 -6.12300000 -24.74800000 C 8.00400000 -6.53300000 -23.42800000 C 6.87400000 -6.16900000 -22.48400000 O 6.41200000 -5.03700000 -22.47900000 N 6.40400000 -7.12900000 -21.70500000 C 5.39000000 -6.80800000 -20.70000000 C 6.05600000 -6.69200000 -19.28500000 O 6.76400000 -7.63800000 -18.85300000 N 5.89400000 -5.56000000 -18.61500000 C 6.52400000 -5.39800000 -17.31200000 C 5.64400000 -6.06500000 -16.27200000 O 4.48900000 -5.68400000 -16.09500000 N 6.17300000 -7.08300000 -15.59700000 C 5.41400000 -7.85000000 -14.61200000 C 5.96100000 -7.56200000 -13.22400000 O 7.17700000 -7.61500000 -13.00000000 N 5.06100000 -7.28200000 -12.29100000 C 5.43300000 -7.04400000 -10.91400000	O 7.59800000 -5.86100000 -31.39100000 H 6.84296071 -5.40392439 -27.01440781 H 7.27958054 -8.07337244 -27.68225612 H 8.17314598 -7.58936056 -23.40820107 H 6.80493504 -5.51549172 -24.57871658 H 4.92423814 -5.87778602 -20.95033547 H 7.48913351 -5.85993340 -17.31790297 H 4.91278231 -5.51745581 -18.42684625 H 4.38302334 -7.56703414 -14.65578873 H 6.90539383 -6.66211851 -15.06178225 H -0.68962681 -7.80563222 -12.23994525 H 1.78436376 -8.35199984 -11.49700310 H 2.22751369 -6.54009053 -15.36884003 H -0.12181756 -5.95720742 -13.95993606 H 1.67139174 -2.24864972 -14.54375954 H 2.82983835 -4.15185449 -16.04898044 H 4.76246102 -1.37722109 -18.02746978 H 3.02082257 -0.99325572 -18.53142028 H 2.34853039 -2.69569393 -17.39654661 H 4.94595242 -3.56251463 -21.68841218 H 5.08117891 -1.51115242 -20.43017453 H 6.81855111 -0.68240210 -24.58496804 H 5.73189224 -3.03983161 -23.97456744 H 6.89987190 -3.23031733 -28.16400303 H 7.83909757 -1.12624515 -26.76721863 H 10.16472710 -6.58237691 -30.26761784 H 7.97923621 -8.40594976 -30.09612802 H 6.47231707 -7.25913487 -10.77821698 H -0.12136514 -10.61349034 -8.38318135 H 1.27687356 -11.35365792 -7.97852450 H 1.93549459 -9.40188601 -8.95922221 H 2.91259915 -10.07500183 -11.13927964 H 2.09385179 -11.70682776 -10.82069388 H 4.50446525 -11.56762193 -10.38441962 H 3.41617210 -11.97738708 -8.94136365 H 5.13053674 -10.58286395 -8.22445447 H 3.58790131 -9.57945214 -8.44386430 H 9.26643438 -5.62581494 -34.41477918 H 7.94251365 -5.20850588 -33.55468982 H 10.60470105 -5.69380321 -32.63988913 H 8.98515246 -3.55892300 -31.37803932 H 10.41922376 -3.27283170 -32.51658720 H 11.85371428 -3.71354327 -30.97871262 H 10.67937792 -4.82940858 -30.07844669 H 10.52113402 -1.88964001 -30.20442414 H 11.23824380 -2.88160477 -28.81285687 H 6.02588245 -9.45386198 -10.09141814 H 4.09566558 -7.23399215 -12.54756325 H 8.88536015 -3.88400255 -28.87444519 H -0.05706499 -6.37610792 -11.44627383 H 8.09596896 -1.79566480 -24.17087759 H 8.89661405 -6.01243501 -23.15023707 H 6.73877549 -8.06629164 -21.80200388

C 4.59500000 -7.96600000 -10.02800000 O 3.48000000 -7.62200000 -9.64400000 N 0.69700000 -11.06400000 -8.74000000 C 1.46000000 -10.10100000 -9.61500000 C 2.55100000 -10.81200000 -10.45300000 C 3.77400000 -11.27100000 -9.66100000 C 4.40100000 -10.13300000 -8.86500000 N 5.13200000 -9.19700000 -9.72400000 C 0.50200000 -9.36800000 -10.57400000 O -0.56700000 -9.86400000 -10.91400000 N 0.94300000 -8.14200000 -10.99900000 C 0.19800000 -7.30100000 -11.92000000 C 1.09900000 -7.04400000 -13.10100000 O 2.33200000 -7.16300000 -12.98700000 N 0.49400000 -6.69700000 -14.23100000 C 1.23200000 -6.14800000 -15.35800000 C 1.27000000 -4.63600000 -15.16900000 O 0.22000000 -3.99400000 -15.05500000 N 2.47600000 -4.06200000 -15.11800000 C 2.62700000 -2.64700000 -14.81400000 C 3.17600000 -1.85000000 -15.98300000 O 3.52800000 -0.68100000 -15.81600000 N 3.28600000 -2.45000000 -17.15000000 C 3.77800000 -1.70800000 -18.28500000 C 3.92900000 -2.60200000 -19.48800000 O 3.79700000 -3.83100000 -19.41600000 N 4.20200000 -1.95200000 -20.61100000 C 4.40900000 -2.65400000 -21.86500000 C 5.22200000 -1.74100000 -22.77400000 O 5.02800000 -0.52600000 -22.77400000 N 6.21100000 -2.32800000 -23.46100000 C 7.07500000 -1.71600000 -24.48100000 C 6.90600000 -2.40500000 -25.81200000 O 6.76600000 -3.62500000 -25.87600000 N 6.97500000 -1.61700000 -26.87900000 C 7.05100000 -2.17200000 -28.20900000 C 8.42800000 -1.87800000 -28.79800000 O 8.79200000 -0.73000000 -29.01700000 N 8.91100000 -5.01300000 -33.70900000	H 4.65086175 -7.58146663 -20.68199934 H 3.46512887 -2.87207574 -22.31936799 H 0.73376270 -6.38945163 -16.27362039 H 5.23893189 -6.02320371 -10.65863262 H 5.50728239 -8.89476159 -14.82335659 H 3.29237457 -2.54218645 -13.98262114 H 6.62357790 -4.35682885 -17.08628586 H 5.47393716 -6.47938653 -26.88006059 H 9.43619372 -8.39400414 -29.13381576 H 6.29658243 -1.72893524 -28.82499330

C 9.66400000 -5.22100000 -32.44900000 C 9.92800000 -3.87000000 -31.77700000 C 10.87500000 -3.91300000 -30.59500000 C 10.55000000 -2.79000000 -29.62700000 N 9.22400000 -2.96300000 -29.06700000 C 8.79200000 -6.09000000 -31.53800000	