

Supporting Information

for

Intermolecular Hydrogen Bonding Behavior of Amino Acid Radical Cations

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I. Comparison to Complexes Optimized with Implicit Water

To demonstrate the effect of implicit water solvation on the intermolecular hydrogen bonding behavior of amino acid radical cations, we re-optimized structures **4a–4d** and **7a–7d** incorporating implicit water solvation and evaluated complexation free energies using the SMD model (Figure S1). Overall, complexation free energies were found to be significantly more positive with implicit water solvation compared to the gas phase. The energy ordering of hydrogen-bonded complexes also differ compared to the gas phase. These results indicate that microsolvation environments and bulk solvation environments can significantly alter the intermolecular hydrogen-bonding behavior of amino acid radical cations.

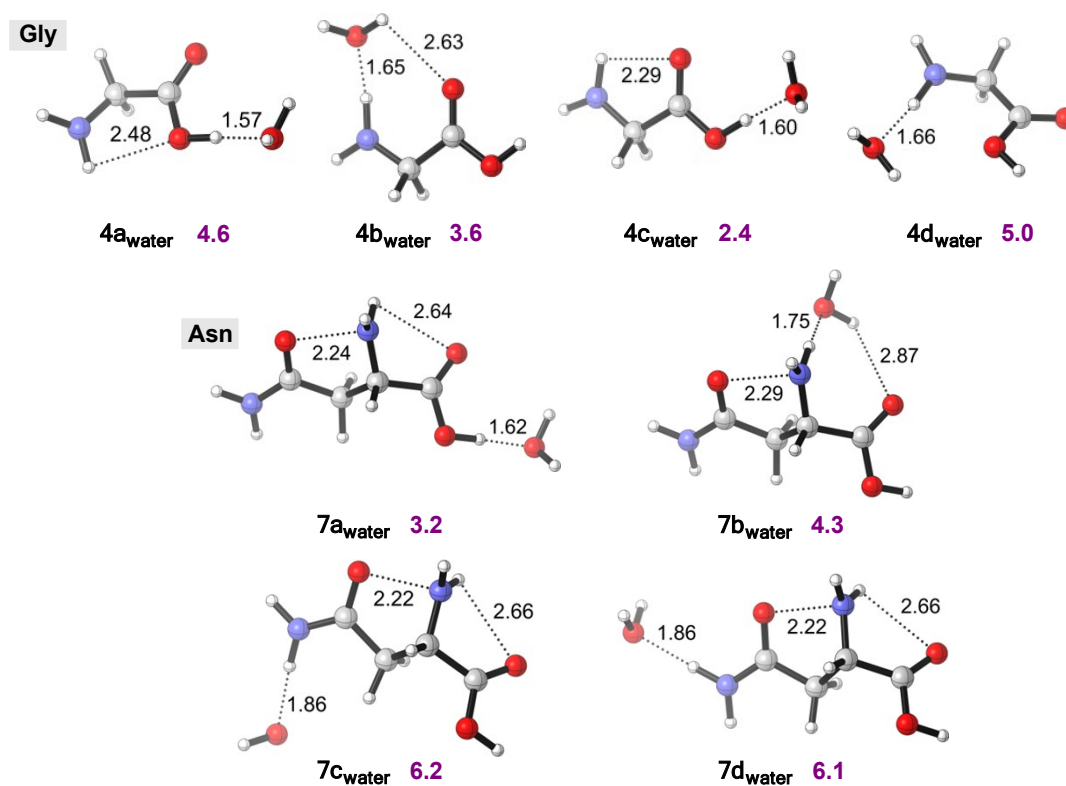


Figure S1. Computed structures and complexation free energies (in kcal/mol) for hydrogen-bonded complexes between water and amino acid radical cations at the ω B97X-D/def2-QZVPPD, SMD(H₂O)// ω B97X-D/def2-TZVPP, SMD(H₂O) level of theory. Interatomic distances are in Å.

II. Evaluation of Basis Set Superposition Error (BSSE) Energies

To evaluate the magnitude of BSSE under our chosen computational level of theory, we conducted BSSE energy calculations on representative hydrogen-bonded complex structures using the Boys-Benardi counterpoise method¹ implemented in Gaussian 16. Our calculations showed that BSSE energy corrections for these structures are generally small (<0.1 kcal/mol) and show

very low variability from structure to structure. They are therefore not expected to impact the relative favorability of hydrogen-bonded complexes examined in this study.

Table S1. BSSE energies for representative structures calculated using the counterpoise method.

Structure	BSSE Energy (kcal/mol)
4a	0.09
4b	0.09
4c	0.09
4d	0.08
8a	0.09
10a	0.08
17a	0.09

III. Calculated Energies

Table S2. Calculated energies in Hartrees.

Structure	ΔG [ω B97X-D/ def2-TZVPP]	E [ω B97X-D/ def2-QZVPPD]	$G_{\text{HFIP}} (= \Delta G + E)$
H₂O	0.004120	-76.443659	-76.439539
MeCOOH	0.035170	-229.116260	-229.081090
MeCOOH\cdot	0.032742	-228.732161	-228.699419
MeNH₂	0.041589	-95.870202	-95.828613
MeNH₂\cdot	0.037235	-95.541944	-95.504709
NH₂CH₂COOH	0.051669	-284.468698	-284.417029
NH₂CH₂COOH\cdot	0.048803	-284.136430	-284.087627
1a	0.056672	-305.576318	-305.519646
1b	0.051509	-305.217571	-305.166062
2a	0.059602	-172.325703	-172.266101
2b	0.056144	-172.017981	-171.961837
3a	0.072387	-360.923377	-360.850990
3b	0.068162	-360.610614	-360.542452
A	0.073208	-360.931112	-360.857904
B	0.099937	-400.248725	-400.148788
C	0.135204	-477.664413	-477.529209
D	0.123471	-568.971208	-568.847737
E	0.151994	-608.292986	-608.140992
F	0.147488	-625.283280	-625.135792
G	0.202811	-762.880663	-762.677852

H	0.175355	-631.300575	-631.125220
I	0.178535	-706.536420	-706.357885
J	0.104124	-475.473787	-475.369663
K	0.096613	-798.444683	-798.348070
L	0.094115	-2801.856907	-2801.762792
M	0.129650	-514.794358	-514.664708
N	0.150536	-877.079570	-876.929034
Gly I	0.048804	-284.136429	-284.087625
Gly II	0.049737	-284.137346	-284.087609
Ala	0.076138	-323.464250	-323.388112
Pro	0.110775	-400.907152	-400.796377
Asn	0.102037	-492.210149	-492.108112
Gln	0.129577	-531.539431	-531.409854
His	0.123685	-548.528551	-548.404866
Trp	0.180144	-686.150896	-685.970752
Phe	0.150613	-554.533280	-554.382667
Tyr	0.155830	-629.787985	-629.632155
Ser	0.079896	-398.696456	-398.616560
Cys	0.073251	-721.668958	-721.595707
Sel	0.073307	-2725.096372	-2725.023065
Thr	0.104664	-438.028972	-437.924308
Met	0.126760	-800.319644	-800.192884
4a	0.067314	-360.612611	-360.545297
4b	0.068266	-360.610614	-360.542348
4c	0.067001	-360.607346	-360.540345
4d	0.068437	-360.608472	-360.540035
5a	0.094245	-399.938608	-399.844363
5b	0.094786	-399.937083	-399.842297
5c	0.094628	-399.934653	-399.840025
5d	0.096083	-399.935544	-399.839461
5e	0.093799	-399.933195	-399.839396
5f	0.093389	-399.927853	-399.834464
6a	0.129964	-477.378571	-477.248607
6b	0.130452	-477.376752	-477.246300
6c	0.129810	-477.375500	-477.245690
6d	0.129195	-477.368117	-477.238922
7a	0.121352	-568.677646	-568.556294
7b	0.122996	-568.677887	-568.554891
7c	0.122058	-568.675234	-568.553176

7d	0.120298	-568.672851	-568.552553
8a	0.149391	-608.006443	-607.857052
8b	0.148908	-608.002875	-607.853967
8c	0.147891	-608.000122	-607.852231
8d	0.148940	-607.998090	-607.849150
9a	0.144119	-625.001477	-624.857358
9b	0.143439	-624.999923	-624.856484
9c	0.146133	-625.000554	-624.854421
9d	0.143830	-624.997212	-624.853382
9e	0.146754	-624.999893	-624.853139
10a	0.199346	-762.619289	-762.419943
10b	0.201503	-762.612819	-762.411316
10c	0.200872	-762.611225	-762.410353
10d	0.199940	-762.603595	-762.403655
11a	0.170419	-631.000757	-630.830338
11b	0.171123	-631.000828	-630.829705
11c	0.171322	-631.000491	-630.829169
11d	0.171392	-630.998395	-630.827003
12a	0.176114	-706.258564	-706.082450
12b	0.176645	-706.250201	-706.073556
12c	0.174896	-706.245678	-706.070782
12d	0.176703	-706.244859	-706.068156
13a	0.099407	-475.166174	-475.066767
13b	0.098924	-475.164197	-475.065273
13c	0.098675	-475.163843	-475.065168
13d	0.097377	-475.160574	-475.063197
13e	0.100163	-475.162707	-475.062544
14a	0.093098	-798.137745	-798.044647
14b	0.092627	-798.134995	-798.042368
14c	0.094032	-798.134827	-798.040795
14d	0.093082	-798.130776	-798.037694
15a	0.092011	-2801.565351	-2801.473340
15b	0.092905	-2801.560249	-2801.467344
15c	0.093515	-2801.557353	-2801.463838
15d	0.090903	-2801.551927	-2801.461024
16a	0.124617	-514.497453	-514.372836
16b	0.124502	-514.494843	-514.370341
16c	0.124897	-514.494689	-514.369792
16d	0.125121	-514.488833	-514.363712

17a	0.148303	-876.790646	-876.642343
17b	0.146929	-876.783972	-876.637043
17c	0.148273	-876.784041	-876.635768
17d	0.146766	-876.780370	-876.633604
TS-Ala	0.091407	-399.922021	-399.830614
TS-Gly	0.064831	-360.587862	-360.523031
TS-Cys	0.090711	-798.115067	-798.024356
TS-Ser	0.095243	-475.141295	-475.046052
PRC-Ala	0.087904	-399.930519	-399.842615
PRC-Gly	0.063069	-360.592806	-360.529737
PRC-Cys	0.087067	-798.127317	-798.040250
PRC-Ser	0.091466	-475.148836	-475.057370

IV. Cartesian Coordinates of Calculated Structures

H₂O			
O	0.00000000	0.00000000	0.11639100
H	0.00000000	0.75856900	-0.46556500
H	0.00000000	-0.75856900	-0.46556500

MeCOOH			
C	1.38823300	-0.12182300	0.00001700
H	1.66403400	-0.70399400	-0.87873900
C	-0.09077900	0.12438900	0.00000700
O	-0.62571100	1.19768400	0.00000000
O	-0.78765300	-1.02795500	-0.00000800
H	-1.72099900	-0.79107600	0.00003500
H	1.66399500	-0.70475600	0.87826200
H	1.91515700	0.82659600	0.00036400

MeCOOH·			
C	1.35547900	-0.30251100	0.00000100
H	1.52979800	-0.90366300	-0.89704900
C	-0.08747500	0.05190000	-0.00002400
O	-0.36339900	1.26901800	-0.00000500
O	-0.98162000	-0.86011000	-0.00001800
H	-1.90019000	-0.54191700	0.00015900
H	1.53023000	-0.90166200	0.89830500
H	1.99229300	0.57964500	-0.00109300

MeNH₂			
N	0.74638400	0.00000800	-0.12041900
H	1.14816400	0.81099700	0.32737300
C	-0.70367000	0.00000300	0.01751300
H	-1.11356500	-0.87704200	-0.48394900
H	1.14825600	-0.81096500	0.32734100
H	-1.07183100	-0.00000800	1.05111900
H	-1.11369200	0.87694500	-0.48402700

MeNH₂·			
N	0.70599400	0.00000000	-0.00855200
H	1.23852100	0.86664400	0.01884700
C	-0.70120300	0.00000200	-0.01494300
H	-1.08793000	-0.91274100	-0.46677400
H	1.23851800	-0.86664600	0.01884400
H	-1.03591300	-0.00004100	1.04531600
H	-1.08793100	0.91277300	-0.46671200

NH₂CH₂COOH			
N	1.88207200	0.09970200	-0.18945900
H	1.72980900	1.04231000	0.14272500
C	0.72509700	-0.71796100	0.09799400
H	0.64300100	-1.54631300	-0.60826800
C	-0.53626700	0.10134300	0.01296100
O	-0.58424000	1.29958200	0.04431200
O	-1.62985400	-0.67167000	-0.06353900
H	-2.39314800	-0.08465400	-0.07182500
H	2.71160000	-0.26820800	0.24893800
H	0.71401500	-1.16464100	1.10272500

NH₂CH₂COOH·			
N	1.80658200	0.08814400	0.00008700

H	1.59214600	1.09625100	0.00003500
C	0.69242400	-0.77072600	-0.00008500
H	0.73780500	-1.44592600	-0.87026500
C	-0.55956400	0.10739100	-0.00001100
O	-0.45666600	1.29942600	-0.00004300
O	-1.64860700	-0.61695600	0.00007300
H	-2.43515000	-0.05356100	0.00004700
H	2.76636200	-0.24715700	0.00017200
H	0.73778400	-1.44636100	0.86974400

1a			
C	2.15647400	-0.01674300	-0.01113000
H	2.47926700	-0.59835000	-0.87397300
C	0.66093000	0.08797600	-0.00270700
O	0.05374600	1.13645200	0.00297900
O	0.06697400	-1.09920500	0.00085000
H	-0.90461000	-0.96118500	0.01152000
O	-2.45390100	-0.04368000	0.08606800
H	-1.86458100	0.72536900	0.05584300
H	-3.03288300	0.03054200	-0.67099000
H	2.48770200	-0.54709700	0.88137000
H	2.59613100	0.97479800	-0.03991800

1b			
C	2.17194700	-0.32937600	0.00002600
H	2.34387400	-0.93159500	-0.89451600
C	0.72634700	0.03843500	-0.00002100
O	0.49369200	1.27605800	-0.00008800
O	-0.18225100	-0.83057900	0.00008300
H	-1.17569600	-0.47862800	0.00012900
O	-2.50984700	0.01842500	-0.00000800
H	-3.06662900	-0.08490500	-0.77518300
H	-3.06718500	-0.08282800	0.77503300
H	2.34372100	-0.93182100	0.89444900
H	2.81939900	0.54418600	0.00016900

2a			
N	0.71015900	0.70832400	0.01842300
H	1.07332000	1.30496700	0.74780500
C	1.40049400	-0.57915900	0.00161300
H	0.95854000	-1.20891000	-0.76924600
H	0.84146600	1.19762600	-0.85574500
O	-2.04806300	-0.15143400	-0.10377800
H	-2.42552900	-0.20134200	0.77201200
H	-1.16069800	0.22679000	0.02033900
H	2.47782900	-0.51031500	-0.17979500
H	1.24550000	-1.08065200	0.95621500

2b			
N	-0.63764000	0.58543200	-0.00017900
H	-0.92232800	1.56073100	0.00056300
C	-1.62383100	-0.42238900	-0.00028600
H	-1.17290900	-1.40855800	-0.00509900
H	0.39310000	0.35828000	0.00001900
O	1.93411000	-0.13452300	-0.00011400
H	2.49897200	-0.21464100	0.77004800
H	2.50113600	-0.21439800	-0.76870100
H	-2.27812600	-0.28773600	0.87438600

H	-2.28626600	-0.28118800	-0.86734000	O	0.82110600	0.94806200	-0.68563600
3a				H	1.76833100	0.80288500	-0.46957300
N	-0.62294000	1.57382500	-0.36262900	H	-2.99205900	-1.10912100	-0.20636200
H	-1.41268300	1.04075200	-0.01436800	O	3.19937700	-0.00165600	0.24782000
C	0.61432700	1.15187300	0.24847700	H	3.83430700	-0.45786800	-0.30256400
H	1.44372400	1.74916500	-0.13121900	H	2.55634200	-0.66818100	0.53190200
C	0.92173300	-0.29457500	-0.04127500	C			
O	0.12565300	-1.14545300	-0.34545100	N	1.43162000	-0.97588800	0.70446700
O	2.22028800	-0.56853400	0.12767900	C	2.37781700	-0.92312000	-0.40711800
H	2.33550800	-1.51464400	-0.01207100	C	0.63195500	0.23928700	0.69889600
H	-0.79155600	2.54900300	-0.16778900	H	1.94083400	-1.26574900	-1.35510500
O	-2.61239000	-0.70847100	0.30707600	H	3.25155100	-1.53968900	-0.19513300
H	-1.75685700	-1.04035200	0.00452300	C	2.70531600	0.55947000	-0.49513700
H	-3.19515600	-0.79986800	-0.44489700	C	1.33684700	1.20594100	-0.28521900
H	0.65282700	1.23503800	1.34657500	H	0.59749100	0.68241200	1.69855600
3b				C	-0.80645000	0.00549600	0.29131300
N	-0.79814200	1.33852800	-0.01640700	H	3.16155200	0.83974300	-1.44293400
H	-1.49607100	0.51760700	-0.02246500	H	3.38683500	0.83569700	0.31051800
C	0.60368100	1.17665100	0.00774400	H	0.79468600	1.24113900	-1.23155400
H	1.05129500	1.71726500	-0.84013800	H	1.38297000	2.22017500	0.10294400
C	1.00229600	-0.29262400	-0.00414200	O	-1.23303100	-1.05885900	-0.10517900
O	0.20565200	-1.18323000	-0.02385400	O	-1.55142400	1.09311800	0.41517100
O	2.31370700	-0.40034400	0.01089300	H	-2.46588400	0.88236300	0.12657500
H	2.57269200	-1.33131900	0.00474400	H	0.83945100	-1.79230000	0.66320000
H	-1.16834100	2.28493100	-0.02098900	O	-3.80464300	-0.10562900	-0.54522100
O	-2.56079000	-0.59449600	0.03971300	H	-3.14340600	-0.81372800	-0.54411900
H	-2.18942300	-1.47777700	-0.00516000	H	-4.52754700	-0.41033200	0.00120600
H	-3.50162900	-0.64832800	-0.12933500	D			
H	1.01406000	1.68831600	0.89255600	N	-0.08245200	2.53764400	-0.16428800
A				H	0.05261500	2.58324100	-1.16559600
N	2.58327000	-0.51517400	0.00472900	C	-0.43798800	1.18509600	0.24247500
H	2.43694300	-1.11561800	0.80415300	H	-0.69648700	1.20832300	1.30009800
C	1.63232800	0.56696500	0.00914200	C	-1.59530800	0.56831400	-0.55660500
C	0.16846000	0.16705000	0.00065600	C	0.83592200	0.36726100	0.08905400
H	1.78994400	1.20232500	0.88341900	H	-2.45356000	1.23273600	-0.47749000
H	1.79630600	1.21450400	-0.85477600	H	-1.29953500	0.49246700	-1.60415600
O	-0.21667300	-0.98146400	-0.00497100	C	-2.02439300	-0.77997800	-0.00334900
O	-0.63977600	1.21699800	0.00034700	O	1.20684900	-0.06436900	-0.98669800
H	-1.56872200	0.89951400	-0.00855800	O	-2.87687000	-0.88030300	0.85285200
H	2.45041200	-1.09669300	-0.81089000	N	-1.36883100	-1.85130400	-0.51805800
O	-2.90875800	-0.29525600	-0.08497200	H	-1.54296900	-2.75365200	-0.11407700
H	-3.47631800	-0.47532200	0.66294300	H	-0.58690600	-1.73280600	-1.13622200
H	-2.19452300	-0.94880600	-0.05142000	O	1.49998500	0.20492000	1.21169300
B				H	2.33246300	-0.28225700	1.01968900
N	-1.99723700	-1.18672100	-0.35952200	H	-0.81386500	3.18796100	0.08327200
H	-1.60284400	-1.74664600	0.38507600	O	3.55624300	-1.14734600	0.05499500
C	-1.37581100	0.12341500	-0.37142000	H	2.99476000	-0.92656700	-0.70143300
H	-1.51791000	0.57939500	-1.35290600	H	4.41339700	-0.76120500	-0.11984700
C	-1.89606100	1.09688900	0.69712900	E			
C	0.11477500	-0.04382400	-0.16770300	N	-3.02377800	-0.28964700	0.43858900
H	-1.73044000	0.68737300	1.69477500	H	-3.45788600	-1.18205300	0.24778300
H	-1.40455600	2.06739600	0.62716700	C	-1.82338800	-0.12173800	-0.36163200
H	-2.96738900	1.24694500	0.56059900	H	-2.06385600	-0.33503200	-1.40306900
O	0.60194800	-0.96565800	0.45037900	C	-1.35791400	1.33650500	-0.24997800
				C	-0.68727100	-1.04598600	0.05832900

H	-2.14391600	1.95026000	-0.68772800	C	-2.21482600	0.85890100	0.45604600
H	-1.32271200	1.59174000	0.81216600	C	-2.11751400	-1.32292500	-0.58285100
C	-0.01746300	1.65601200	-0.92900100	H	-1.69190700	2.51114000	1.67005100
O	-0.32145100	-1.14122600	1.20878900	C	-3.41877400	1.15623600	-0.17680000
H	0.07565700	1.12263900	-1.87326800	C	-3.30884500	-1.03350000	-1.21238600
H	0.01736300	2.72452900	-1.15221500	H	-1.62936200	-2.27627100	-0.74188900
C	1.22890900	1.33395600	-0.11987200	H	-3.91908300	2.10342200	-0.02224700
O	2.10045300	0.58408000	-0.52602400	C	-3.95264300	0.19647600	-1.01064900
N	1.34468800	1.97544100	1.06404200	H	-3.75838400	-1.76262900	-1.87297300
H	2.11328500	1.73372400	1.66258900	H	-4.88672800	0.39508900	-1.51903200
H	0.59181700	2.51249900	1.44888100	O	1.83375800	0.44281600	-1.44619600
O	-0.13272400	-1.68009900	-0.95718900	H	2.30220900	1.30237200	-1.52004500
H	0.72797500	-2.06798500	-0.65721600	H	3.03833300	-2.74216600	-0.78322900
H	-2.77530800	-0.28776500	1.42053500	O	3.48733500	2.58894300	-1.06582300
O	2.29039100	-2.15836300	0.07916400	H	3.63745900	2.00610700	-0.30517600
H	2.49592700	-1.23591000	-0.13589200	H	3.19341300	3.42637800	-0.71088600
H	1.94469700	-2.11483300	0.97402300				
F				H			
N	-2.71326800	-0.88487200	-1.08237600	N	2.37400300	-2.28561500	-0.03773900
H	-2.89618800	0.04814200	-1.42780400	H	2.78656500	-2.02447900	0.84855800
C	-1.40401400	-0.94783600	-0.44998100	C	1.21329200	-1.45596900	-0.30556500
H	-1.21133200	-1.98277600	-0.17158600	H	0.86726400	-1.64746400	-1.32115800
C	-0.24005400	-0.43288000	-1.31469100	C	0.03852300	-1.66885700	0.67693500
C	-1.52234000	-0.14933500	0.83564300	C	1.65699900	-0.00751500	-0.22947300
H	-0.20005500	-1.06217800	-2.20550400	H	-0.25736700	-2.71765500	0.60359200
H	-0.47156000	0.57941300	-1.65239000	H	0.41520100	-1.50404000	1.68806000
C	1.08036800	-0.44557300	-0.62014900	C	-1.14241600	-0.77647000	0.40766600
O	-1.62833200	1.05437400	0.88358500	O	2.23959100	0.43695700	0.73829300
N	1.66630500	0.69194700	-0.12779700	C	-1.32859800	0.39521900	1.13385900
C	1.93570400	-1.45699400	-0.27901600	C	-2.04394300	-1.07950400	-0.60804900
H	1.27712800	1.62585800	-0.21177700	H	-0.63277300	0.64343400	1.92626700
C	2.82200400	0.32263500	0.46973000	C	-2.38881000	1.24369100	0.85279700
N	3.01917100	-0.96875900	0.39964700	C	-3.10394300	-0.23437600	-0.89292900
H	1.83110800	-2.50883700	-0.49209900	H	-1.91451200	-1.98997400	-1.18142800
H	3.48403200	1.03464000	0.93536000	H	-2.52203000	2.14844700	1.43156100
O	-1.53708500	-0.90384200	1.92606500	C	-3.27911200	0.93187000	-0.16272100
H	-1.63568300	-0.32200900	2.68853100	H	-3.79614600	-0.48702700	-1.68531200
H	-2.76080700	-1.52146000	-1.86463500	H	-4.10787700	1.59165200	-0.38223400
O	-0.11789500	2.93045500	-0.50315400	O	1.32469800	0.70965600	-1.28397400
H	-0.19363300	3.83170800	-0.19616500	H	1.59454800	1.64175500	-1.12684800
H	-0.79197400	2.42129700	-0.02942600	H	2.11170000	-3.25973600	0.01319600
				O	2.29890400	3.03747500	-0.25042500
G				H	2.49434300	2.37477800	0.42878700
N	2.51690000	-2.58499400	0.06794600	H	1.70557800	3.66837700	0.15486300
H	3.18470100	-2.34190300	0.78885500				
C	1.55716800	-1.50742400	-0.09796900	I			
H	0.92824900	-1.72868200	-0.95965200	N	3.00350900	-2.00056200	-0.15218900
C	0.68073600	-1.40294500	1.15822100	H	3.40144400	-1.72237800	0.73572500
C	2.22983500	-0.16285900	-0.34054300	C	1.72963900	-1.33079700	-0.35107300
H	0.22449000	-2.38245000	1.30950900	H	1.37457000	-1.53748900	-1.36060800
H	1.33442200	-1.21520100	2.01268700	C	0.63289000	-1.73191900	0.66139000
C	-0.35963300	-0.33718300	1.06872300	C	1.97766600	0.16087500	-0.23948300
O	3.06444400	0.29414800	0.41512400	H	0.49969100	-2.81297400	0.57871400
C	-0.34952000	0.87447700	1.68819900	H	1.01380100	-1.52721600	1.66401100
C	-1.55138300	-0.36865800	0.26703500	O	-0.67947400	-1.02914600	0.44534900
H	0.37884700	1.28132400	2.37059100	C	2.53911700	0.64957400	0.71998500
N	-1.45812300	1.60108600	1.32583200	C	-0.99322800	0.13288000	1.13843600
				C	-1.59345500	-1.49188800	-0.49730700

H	-0.29841300	0.51932600	1.87426800	H	-0.20944700	1.26228600	1.48827000
C	-2.17617700	0.81496500	0.90195100	C	-1.13684500	0.97760600	-0.43859500
C	-2.77880900	-0.82532700	-0.74462600	C	1.22384100	0.43045500	0.15268300
H	-1.37500000	-2.39763600	-1.05096000	H	-1.93599400	1.69405400	-0.26241900
H	-2.39903300	1.72044100	1.45464900	H	-0.84749100	1.00980700	-1.48740400
C	-3.07317000	0.33705900	-0.04337700	O	1.94498100	0.56867600	-0.81065300
H	-3.48559600	-1.19199200	-1.47611500	O	1.33617900	-0.54862200	1.03016400
O	-4.24887900	0.95908800	-0.31918500	H	2.07233100	-1.13888000	0.74979400
H	-4.33016500	1.74698400	0.21758000	H	-0.23948900	3.37919500	0.24257900
O	1.50816900	0.86179300	-1.25246600	O	3.41135100	-1.74077600	-0.24860700
H	1.66991500	1.81454200	-1.07653500	H	4.31652900	-1.67165800	0.05178800
H	2.87718100	-3.00273900	-0.13649400	H	3.24734400	-0.96287700	-0.80048300
O	2.22727600	3.25928600	-0.15036300	Se	-1.83702600	-0.81293600	-0.01387100
H	2.99577300	3.74866000	-0.44039800	H	-3.01792100	-0.65619300	-0.86703300
H	2.55051800	2.58827300	0.47015600				
J				M			
N	1.42024200	1.87529500	-0.14487000	N	1.09260200	1.81537600	-0.01962000
H	1.03585200	2.19105200	0.73382300	H	0.83839200	1.87766600	0.95650800
C	1.13148400	0.48005700	-0.38836500	C	0.70519800	0.53176400	-0.55268700
H	1.40940100	0.22896500	-1.41478900	H	0.80742200	0.54854500	-1.64104600
C	1.88844600	-0.50578600	0.53327800	C	1.50070900	-0.69503900	-0.05610800
C	-0.34378400	0.17083500	-0.26910000	C	-0.76571100	0.29852200	-0.25652100
H	2.94239800	-0.22298700	0.52144900	H	1.07719100	-1.57412500	-0.55373300
H	1.52604500	-0.37914900	1.56410300	C	2.97980800	-0.60199100	-0.39057100
O	1.81431900	-1.83926100	0.11454300	O	1.28486700	-0.77588500	1.34126100
O	-0.78998800	-0.92122200	-0.57658200	O	-1.40149100	0.93122100	0.55245400
H	0.90162800	-2.02051500	-0.13043600	H	3.44271000	0.24541900	0.11614500
O	-1.07840000	1.13061900	0.25152600	H	3.49885200	-1.50546600	-0.06620800
H	-2.00626500	0.80955200	0.32870200	H	3.13184900	-0.49956600	-1.46603000
H	2.41644900	2.03818200	-0.13752500	H	1.71782700	-1.55688800	1.68187300
O	-3.39740500	-0.25397500	0.15842800	O	-1.27110000	-0.69606300	-0.97619400
H	-2.77486900	-0.90703900	-0.19052700	H	-2.20872900	-0.82105200	-0.71406800
H	-3.83742300	-0.66506100	0.90108200	H	2.08671700	1.96312700	-0.10373100
				O	-3.72344500	-0.53937100	0.21220500
K				H	-4.47175400	-0.10909200	-0.19884800
N	-0.65316800	2.37606500	0.15662200	H	-3.19936800	0.16505400	0.62400400
H	-0.36379500	2.54239200	-0.79844800				
C	-0.72466600	0.94811900	0.41543800	N			
H	-0.94187400	0.79537800	1.47253000	N	1.53448200	2.58594400	0.07957800
C	-1.77590000	0.22744100	-0.43861100	H	1.85997700	2.48362000	-0.87292700
C	0.65503100	0.37836500	0.12336400	C	0.81832300	1.39099200	0.48559800
H	-2.73509700	0.72261500	-0.29299600	H	0.67627000	1.41215600	1.56709600
H	-1.48881800	0.30223200	-1.48658400	C	-0.55525300	1.21990800	-0.19372200
S	-1.91407200	-1.52706400	0.03498300	C	1.69125100	0.19602900	0.15740400
O	1.19260800	0.53163100	-0.95233200	H	-1.12915500	2.12670600	0.01242700
H	-2.66326300	-1.90259200	-1.00696200	H	-0.40546300	1.17256200	-1.27488200
O	1.18898300	-0.27576700	1.13445500	C	-1.34321100	0.00768900	0.28259200
H	2.06849400	-0.61799800	0.85708500	O	2.30748100	0.10427600	-0.88203200
H	-1.55151000	2.81437800	0.30000000	H	-0.84074100	-0.91848900	0.00021800
O	3.45729600	-0.92112800	-0.22491100	H	-1.43397200	0.01811600	1.37064700
H	4.28225400	-0.45622600	-0.09214600	S	-2.99598300	0.02185900	-0.45130700
H	2.95305100	-0.40104800	-0.86740000	C	-3.64816700	-1.49401300	0.26702900
				H	-3.66968400	-1.43500800	1.35468000
L				H	-4.66644300	-1.61249300	-0.09810900
N	0.52540500	2.72158400	0.19885300	H	-3.06164300	-2.35857600	-0.04205100
H	0.95543200	2.78508400	-0.71469300	O	1.67695900	-0.74306100	1.08895000
C	0.06294900	1.36755600	0.43791300	H	2.22805400	-1.49680300	0.78133500
				H	0.93090200	3.39457500	0.12175500

O	3.34002300	-2.40442900	-0.28074100
H	3.25419800	-1.64302000	-0.87296300
H	3.07867900	-3.17261100	-0.78618100

H	-0.58975600	-2.19801700	0.26872000
O	1.92135100	1.21254600	-0.25604700
O	2.21501000	-1.00559200	0.00656000
H	3.12708000	-0.83144600	-0.26223900
H	-0.21666800	1.96326100	0.22552400

Amino Acid Radical Cations

Gly I

N	1.80653800	0.08806600	-0.00262200
H	2.76615900	-0.24758900	-0.00916900
C	0.69230500	-0.77064400	0.00296900
C	-0.55954600	0.10741700	0.00022400
H	0.73768800	-1.45372000	-0.86060500
H	0.73764200	-1.43838300	0.87927900
O	-0.45653500	1.29939300	0.00146200
O	-1.64860600	-0.61690800	-0.00230300
H	-2.43514500	-0.05345900	-0.00344600
H	1.59246900	1.09617800	-0.00014100

Gly II

N	1.78311200	0.13474700	-0.21557400
H	2.24076900	-0.10779900	-1.08535100
C	0.80920900	-0.67227100	0.32924800
C	-0.67161500	-0.07496100	0.01114200
H	0.83102800	-1.68575300	-0.05485900
H	0.80930800	-0.63834100	1.42451200
O	-1.55677300	-0.81897300	-0.20048300
O	-0.64693500	1.23347800	0.08361600
H	-1.53347300	1.60238500	-0.04733300
H	1.97468500	1.05362700	0.16464300

Ala

N	1.27340000	1.09239800	-0.44188300
H	1.46029300	1.57078300	0.43086600
C	0.73222300	-0.17621600	-0.44941700
H	0.75455000	-0.60275100	-1.44841200
C	1.27678300	-1.11663700	0.62990400
C	-0.86946000	-0.04386200	-0.10880900
H	1.21079000	-0.66998600	1.62140800
H	0.71376100	-2.04701800	0.61723000
H	2.31903300	-1.33249400	0.40103000
O	-1.63008200	-0.76518500	-0.64269000
O	-1.06708500	0.87901500	0.80226600
H	-2.00146800	0.91167200	1.05602900
H	1.36929800	1.63265300	-1.29165700

Pro

N	-0.67890500	1.05396300	0.24134900
C	-2.02272100	0.80750200	-0.17953500
C	0.08739300	-0.13305000	0.46694300
H	-2.09393400	1.14879800	-1.22490500
H	-2.71713800	1.43511400	0.38719400
C	-2.18265100	-0.70609100	-0.03422900
C	-0.75175200	-1.23319900	-0.20054100
H	0.11944300	-0.29672100	1.55807200
C	1.52825900	0.11731100	0.01778600
H	-2.86932900	-1.11123800	-0.77128600
H	-2.57096000	-0.94416200	0.95580200
H	-0.47845400	-1.31380400	-1.25297600

Asn

N	-0.13655100	1.51055500	-0.28182600
H	-0.42075800	1.92501500	0.59934100
C	-0.49651500	0.14138400	-0.51611100
H	-0.47173400	-0.05845600	-1.58496600
C	0.50425100	-0.76795100	0.21900200
C	-1.90431200	-0.10862100	0.04546200
H	0.28273400	-0.78997700	1.29009900
H	0.45455300	-1.78932600	-0.15285500
C	1.87940100	-0.15569400	0.07373900
O	-2.39119700	0.58968900	0.88235400
O	1.97915200	1.06741100	-0.09861000
N	2.94222400	-0.93452800	0.17417800
H	3.86400500	-0.52979600	0.13513700
H	2.85994500	-1.92525700	0.31786100
O	-2.43402100	-1.19610900	-0.48689300
H	-3.30599700	-1.35451000	-0.10162900
H	-0.03087200	2.14747600	-1.05680700

Gln

N	1.94633400	1.76973500	0.16064200
H	2.66633600	1.71181500	-0.56432800
C	1.26623600	0.59517200	0.48618700
H	1.05161600	0.55517600	1.55656200
C	-0.15711800	0.66188800	-0.24644600
C	2.10539300	-0.57155600	-0.03273000
H	-0.61952400	1.61687800	0.00515100
H	0.02850700	0.63617900	-1.31909800
C	-1.08688700	-0.44852400	0.20934000
O	2.94339200	-0.40055000	-0.86933200
H	-0.87737600	-1.38959300	-0.29535700
H	-0.99827700	-0.62648900	1.28307200
C	-2.53602800	0.02221800	-0.02773900
O	-2.81928500	1.19696600	0.01560200
N	-3.42643100	-0.96189600	-0.24043900
H	-4.39615700	-0.71639500	-0.34339800
H	-3.17051400	-1.93049200	-0.26300500
O	1.76712800	-1.71017100	0.53335300
H	2.31360500	-2.42609800	0.18185800
H	1.68300200	2.66899600	0.54846800

His

N	-0.50741000	1.39059500	0.45727300
H	-0.76969800	2.31111300	0.13267500
C	-1.08787600	0.32720500	-0.33999800
H	-1.06260200	0.60999200	-1.39233100
C	-0.20723000	-0.91531600	-0.12386100
C	-2.53163000	0.00926200	0.04220600
H	-0.44773200	-1.38645200	0.83193200
H	-0.35374500	-1.66878100	-0.90166500
C	1.19926400	-0.45375400	-0.10237800
O	-3.02059500	0.35288100	1.07734900

N	2.16759600	-0.93183300	0.68958900	C	3.68730500	0.06258800	0.24826300
C	1.86296000	0.56676500	-0.87807400	H	3.63699100	-2.00013400	-0.35960600
H	2.06436300	-1.65667900	1.38300300	H	4.73464500	0.03193800	0.51680400
C	3.32164700	-0.24074600	0.41439800	O	-3.06988600	1.44830300	0.01505300
N	3.13999200	0.66236700	-0.53240100	H	-3.95655000	1.59621200	-0.33854400
H	1.42123500	1.17153100	-1.65354000	H	-0.56751000	-1.74497500	1.56244800
H	4.25043400	-0.43732000	0.92819900				
O	-3.13188600	-0.72102600	-0.89269200	Tyr			
H	-4.03185800	-0.92354100	-0.60795000	N	1.50127700	-1.55422100	-0.72756700
H	-0.79459600	1.31689700	1.42742600	H	2.15915100	-2.12876000	-0.21295000
				C	1.73180400	-0.16620800	-0.42954100
Trp				H	1.42732400	0.45322800	-1.27418400
N	-3.20683000	1.61564800	0.48685700	C	0.90086100	0.26953400	0.82484800
H	-3.86577900	1.17155000	1.10719700	C	3.19863700	0.14937400	-0.12404500
C	-2.08432000	0.81193100	0.13469800	H	1.16341900	-0.40626800	1.64027400
H	-1.44557600	1.40383100	-0.52957500	H	1.17774000	1.28565500	1.10140100
C	-1.19899600	0.34196900	1.34013500	C	-0.54497300	0.18553500	0.52567900
C	-2.48091500	-0.40380900	-0.70550100	O	4.00895400	-0.68593900	0.14663500
H	-0.96268000	1.23905400	1.91338000	C	-1.25112300	1.34016600	0.08504600
H	-1.79130100	-0.31541400	1.97646200	C	-1.23595300	-1.05307500	0.62017200
C	0.05099300	-0.32012500	0.92009700	H	-0.72043500	2.27998500	0.00867400
O	-1.81933400	-1.41315400	-0.75636300	C	-2.57054400	1.27821400	-0.22864300
C	0.29338500	-1.72495000	0.92228500	C	-2.55495600	-1.13862200	0.31177800
C	1.21177700	0.26917600	0.36428500	H	-0.68925600	-1.92912600	0.93484600
H	-0.36333300	-2.51003800	1.25836000	H	-3.11352000	2.15603900	-0.55585000
N	1.48647400	-1.97398200	0.41895900	C	-3.24510400	0.02968800	-0.11754500
C	2.10787800	-0.77063800	0.04642200	H	-3.10615900	-2.06618000	0.37727900
C	1.58117500	1.59470000	0.10281400	O	-4.51055600	-0.11209900	-0.39852900
H	1.88298700	-2.89223400	0.30358000	H	-4.93296500	0.70658000	-0.68388500
C	3.33673600	-0.55244400	-0.51613000	O	3.44337600	1.46058900	-0.17139000
C	2.81863900	1.83273300	-0.46702300	H	4.37194700	1.60870700	0.04444300
H	0.91887500	2.41476600	0.34555200	H	1.64772400	-1.74836000	-1.70730500
H	4.01667500	-1.35780700	-0.75609800				
C	3.67912200	0.77951400	-0.77130100	Ser			
H	3.12735000	2.84626700	-0.67857500	N	0.40630500	1.60126800	-0.36169600
H	4.64116000	0.99443100	-1.21551700	H	-0.17525500	2.12072800	0.29097300
O	-3.59238400	-0.22988500	-1.39303600	C	0.16095900	0.27616600	-0.52276500
H	-3.75060900	-1.02147700	-1.92206000	H	0.43022400	-0.11432400	-1.50199300
H	-2.96436900	2.53138200	0.82707900	C	1.23321200	-0.64434600	0.51023300
				C	-1.23228600	-0.07720600	-0.00835700
Phe				H	1.02269200	-0.24275600	1.49785000
N	-1.32068200	-1.42135400	0.97943800	H	0.86110100	-1.65724100	0.35488900
H	-1.98843300	-2.08970800	0.61640300	O	2.50637400	-0.42146800	0.15695000
C	-1.40467600	-0.12669500	0.55834900	O	-1.81434600	0.64677100	0.74036800
H	-1.04906900	0.59882500	1.28417500	H	2.83182400	-1.06997900	-0.47352900
C	-0.40403500	0.18535200	-0.81428100	O	-1.62630300	-1.24701000	-0.47044600
C	-2.80765900	0.15295700	0.02196700	H	-2.50609100	-1.45909800	-0.13013600
H	-0.71741600	-0.56771200	-1.53213200	H	1.19426100	2.05977600	-0.79583000
H	-0.74568500	1.18047300	-1.09252600				
C	0.99757100	0.13440500	-0.44630500	Cys			
O	-3.52392800	-0.72516400	-0.35325100	N	0.46235100	1.92110000	-0.28641200
C	1.63668800	1.28409700	0.06019600	H	0.53436500	1.77400200	-1.28568900
C	1.73389500	-1.05723000	-0.57809700	C	0.50202100	0.84391800	0.54425100
H	1.07381900	2.20326500	0.16730400	H	0.85444300	1.09095100	1.54397500
C	2.97122500	1.24816300	0.39578500	C	-1.06277700	0.22474800	0.94641000
C	3.06679400	-1.08938300	-0.24219100	C	1.23236600	-0.32387500	-0.11282700
H	1.24872100	-1.94435600	-0.96624000	H	-0.82830300	-0.47125900	1.74778400
H	3.46313100	2.13501200	0.76931100	H	-1.58801600	1.10105100	1.31387800

S	-1.95525600	-0.49117200	-0.35569600	H	-4.86641800	-0.23206700	-0.19510600
O	1.33483400	-0.41585800	-1.29783400	H	-3.93215900	-0.80200800	1.21939800
H	-1.42881000	-1.72401900	-0.28795300	O	2.94419600	-1.32630300	0.51689400
O	1.66454400	-1.18193800	0.79464900	H	3.75892100	-1.62852500	0.09685000
H	2.13923000	-1.90486000	0.36313000	H	1.37759800	2.34374200	0.92806200
H	0.34003800	2.85879900	0.05938100				
Sel				4a			
N	1.14627700	1.70444900	-0.78278300	N	2.26758100	-0.86241300	-0.26050000
H	0.82782200	1.26850800	-1.63665500	H	1.99245000	-1.76534200	0.10054300
C	1.06080000	0.88041200	0.39376500	C	1.81420000	0.29162500	0.31895900
H	1.73627500	1.28345600	1.14764500	C	0.18423200	0.46752000	0.03923400
C	-0.35068200	0.87019200	0.99277100	H	1.80043000	0.24381800	1.41173700
C	1.46492700	-0.55731700	0.07892300	H	2.29378100	1.18548700	-0.06116900
H	-0.37445300	0.43373800	1.98739000	O	-0.19716500	1.56162300	-0.19231900
H	-0.74072600	1.88516700	1.01264400	O	-0.41337700	-0.66240500	0.16333600
O	0.65160400	-1.38016500	-0.30715300	H	-1.42722000	-0.56324300	0.07080500
O	2.74308700	-0.79773800	0.18572400	H	2.73292500	-0.84900000	-1.15682600
H	2.95062300	-1.69895600	-0.09763600	O	-2.93009600	-0.40424500	-0.01186200
H	2.06120700	2.10244700	-0.92786000	H	-3.55906800	-1.12457800	-0.06344000
Se	-1.55558200	-0.16715800	-0.13652300	H	-3.37186100	0.39509400	-0.30054700
H	-1.80268200	-1.25861900	0.81440900				
Thr				4b			
N	-0.06570600	1.88276400	0.05631600	N	-0.79862300	1.33821000	-0.01809500
H	-0.40764800	1.96651500	1.00403100	H	-1.16886000	2.28460200	-0.02456500
C	-0.34201900	0.79429000	-0.63930300	C	0.60328000	1.17669900	0.00890100
H	-0.12188100	0.78125800	-1.69757900	C	1.00224100	-0.29246200	-0.00442400
C	1.24711600	-0.72885700	0.01649400	H	1.05302500	1.71947900	-0.83629700
C	-1.37378400	-0.10850600	-0.07117100	H	1.01093000	1.68617100	0.89638300
H	0.64783800	-1.56124800	-0.34489800	O	0.20583900	-1.18329000	-0.02550700
C	2.41822400	-0.27421600	-0.75590000	O	2.31363900	-0.39990100	0.01139100
O	1.27873900	-0.50356800	1.29809300	H	2.57286100	-1.33081400	0.00454000
O	-1.61736400	-0.13228200	1.10837400	H	-1.49666500	0.51699200	-0.02369600
H	2.74863600	0.71115200	-0.43043800	O	-2.56041700	-0.59466100	0.04211100
H	3.23782000	-0.97451900	-0.56039300	H	-2.18694200	-1.47701100	-0.00471700
H	2.22070600	-0.28697200	-1.82477200	H	-3.49959700	-0.64949400	-0.13580400
H	0.52397400	-0.88538100	1.76668600				
O	-1.91295500	-0.88821400	-0.99443700	4c			
H	-2.58270700	-1.45505100	-0.59018800	N	-2.54067100	0.35946800	-0.01527600
H	0.50862000	2.62114500	-0.31361900	H	-3.54661100	0.22038700	-0.03147900
Met				C	-1.60861000	-0.69180400	-0.00443500
N	1.01408900	1.71224500	0.23014700	C	-0.21396800	-0.05340300	0.01333000
H	1.41239700	1.96013100	-0.66887000	H	-1.78636900	-1.34700000	0.86362200
C	1.25002900	0.32452200	0.54023500	H	-1.76554200	-1.34704700	-0.87626400
H	1.28069400	0.18998500	1.62155900	O	-0.12982300	1.14919700	0.02101800
C	0.09503900	-0.52584800	-0.03790600	O	0.72349500	-0.93772300	0.01763700
C	2.56145200	-0.18779000	-0.05546200	H	1.63949800	-0.51352500	0.01442900
H	0.17656600	-0.53063900	-1.12789300	H	-2.11528600	1.30091400	-0.00636000
H	0.15140400	-1.55552300	0.30948300	O	3.05964700	0.14423900	-0.05675200
C	-1.20794100	0.14929800	0.38372500	H	3.18263400	1.08467800	0.07438600
O	3.13319400	0.36102400	-0.95048400	H	3.88528400	-0.28913900	0.16000700
H	-1.46663000	0.01021300	1.43390800				
H	-0.99796500	1.24279300	0.23421800	4d			
S	-2.55944100	-0.27120100	-0.64214100	N	0.75003300	1.05803900	-0.54260300
C	-3.97913000	-0.07028500	0.41160800	H	1.56782000	0.45782700	-0.28909500
H	-3.97778300	0.93825800	0.82714700	C	-0.37749500	1.10696400	0.26541700
				C	-1.29992400	-0.18182400	0.05634100
				H	-0.10355000	1.03669500	1.32183500
				H	-1.00758100	1.96866500	0.06749900

O	-2.44122700	-0.14747900	0.34546900	O	-3.26090500	-0.44367400	-0.24451500
O	-0.59490100	-1.19211300	-0.41829800	H	-4.01447800	0.09216500	-0.49523600
H	-1.16197600	-1.97233000	-0.50144100	H	-3.57135500	-1.34933600	-0.21208600
H	0.75476800	1.53406900	-1.43668800				
O	2.80894300	-0.46682100	0.31298900	5d			
H	2.94738900	-1.39360100	0.11449100	N	-0.72935100	1.07557500	-0.68502000
H	3.63488500	-0.13713300	0.66979100	H	-1.55653700	0.49178800	-0.33966300
				C	0.61921900	0.74327700	-0.42937500
5a				H	1.23122700	1.00548200	-1.29654500
N	1.84674500	1.16091100	-0.55267400	C	1.12790200	1.60962300	0.77328800
H	1.66708100	1.89570700	0.11747100	C	0.73451300	-0.74280300	-0.09559400
C	1.56694400	-0.14413700	-0.24463300	H	0.55468500	1.38157300	1.66882500
H	1.93910600	-0.82243600	-1.00621000	H	2.17485600	1.35491900	0.92374600
C	1.89234000	-0.57153700	1.18244500	H	1.04726900	2.66805000	0.53738700
C	-0.10861700	-0.33446700	-0.34138000	O	-0.20222700	-1.42053200	0.21125000
H	1.46962900	0.11808300	1.91186300	O	1.99156800	-1.13141900	-0.17293900
H	1.50643800	-1.57093800	1.36892700	H	2.06336200	-2.06575800	0.06191100
H	2.97591600	-0.58979300	1.29318600	H	-0.92413500	1.95962300	-1.14510300
O	-0.49604000	-1.33041900	-0.84545500	H	-2.79681100	-0.27146300	0.24938200
O	-0.70937900	0.65973800	0.20704800	O	-2.57268500	-1.17413700	0.48465300
H	-1.71898400	0.51355700	0.23335100	H	-3.74262200	-0.22383200	0.10847100
H	2.05132000	1.44479700	-1.49932200				
O	-3.21794500	0.25880500	0.32324900	5e			
H	-3.66335400	-0.44182300	-0.15457600	N	-2.11922300	-1.01536200	-0.11392900
H	-3.87145300	0.92232400	0.54670600	H	-1.56807900	-1.79663900	0.27206500
				C	-1.38285000	0.15260900	-0.38119900
5b				H	-1.54258900	0.43697000	-1.43187600
N	-0.83664400	-0.69611800	0.09949400	C	-1.89214100	1.34704800	0.48117700
H	-0.43909900	-1.54787800	0.50950100	C	0.08725800	-0.21076400	-0.11983100
C	0.09815100	0.29286200	-0.27466100	H	-1.75883500	1.12767900	1.53797100
H	-0.06738800	0.54016400	-1.33254900	H	-1.28991900	2.20906300	0.20476700
C	-0.13855800	1.59987100	0.53206400	H	-2.93851200	1.55639100	0.27038800
C	1.49122100	-0.30361000	-0.07295100	O	0.35560300	-1.30058600	0.32341300
H	0.02628900	1.42343000	1.59270900	O	0.89170100	0.75504600	-0.41929500
H	0.57061700	2.34030900	0.17038800	H	1.84919100	0.50911500	-0.22769800
H	-1.15085400	1.96227700	0.36870500	H	-3.12038400	-1.08564000	-0.26408200
O	1.64049300	-1.38201900	0.42707600	O	3.33414700	0.12786200	0.14390700
O	2.43389500	0.50636900	-0.50246100	H	3.55430500	-0.77150800	0.38807400
H	3.30263700	0.10771600	-0.36080200	H	4.12418200	0.53016500	-0.21718000
H	-1.87120000	-0.55369800	-0.00700000				
O	-3.46713600	-0.18554000	-0.20693900	5f			
H	-4.09534000	-0.07367200	0.50829300	N	0.18747100	1.27065000	-1.19006700
H	-3.98205000	-0.37103900	-0.99382300	H	-0.39341500	0.94137900	-1.96164600
				C	0.14302000	0.56522800	0.00052200
5c				H	1.02894200	-0.18174000	-0.06809400
N	-0.87563500	0.50875500	0.64215100	C	0.40051800	1.38391200	1.26039900
H	-0.66754400	0.67837000	1.61962800	C	-1.07215200	-0.37097200	-0.05656900
C	0.13692100	0.63123700	-0.30341800	H	-0.42676700	2.06960800	1.43916500
H	-0.27902600	0.55242200	-1.30434800	H	0.49193200	0.71501800	2.11096100
C	1.01763900	1.87823900	-0.12335600	H	1.32434800	1.95364700	1.16708600
C	1.12474500	-0.61791700	-0.15704600	O	-1.63996900	-0.58472300	-1.08709600
H	1.44627200	1.92040200	0.87744100	O	-1.33732900	-0.89615300	1.12043500
H	1.82175000	1.85073000	-0.85545200	H	-2.09254600	-1.49463400	1.04759000
H	0.41304900	2.76606500	-0.29503800	H	0.80749900	2.05953700	-1.32243700
O	1.66270100	-1.07175300	-1.10370700	O	2.43762200	-1.16039700	-0.18169100
O	1.25025100	-0.96990200	1.11040300	H	2.99544100	-1.32957400	0.57981600
H	1.90353400	-1.67864700	1.19318000	H	2.44136000	-1.96662200	-0.70126900
H	-1.81496700	0.13982900	0.38232700				

6a				O	-1.18788200	1.37036000	0.00158200
N	-0.27623300	0.92701900	0.19540300	O	-1.58289400	-0.83219400	-0.25047400
C	-1.53531700	1.45141000	-0.23212100	H	-2.54064600	-0.61356300	-0.04217600
C	-0.31734700	-0.48121700	0.46123600	H	0.99759100	1.96630500	-0.15356400
H	-1.41698400	1.71974300	-1.29410700	O	-4.03014600	-0.21635000	0.36122500
H	-1.74928400	2.38756600	0.28976000	H	-4.25088700	0.71488100	0.39860300
C	-2.52481200	0.30657300	-0.02193300	H	-4.82260500	-0.68819100	0.10488500
C	-1.64723700	-0.94111100	-0.15685000				
H	-0.35396800	-0.59908400	1.55682500	6d			
C	0.96327800	-1.16636200	-0.00899500	N	-0.38848600	-0.83544600	-0.95057200
H	-3.33624100	0.33206900	-0.74301700	C	-1.61457300	-1.45211900	-0.53912900
H	-2.95791700	0.36899100	0.97627200	C	0.18360900	0.02084500	0.02704100
H	-1.49328900	-1.20216600	-1.20439000	H	-1.41268100	-2.52930300	-0.44155600
H	-2.04681900	-1.81090500	0.35424100	H	-2.37027800	-1.35051800	-1.32235900
O	1.92027900	-0.57868200	-0.42175100	C	-1.92681900	-0.78043000	0.79912800
O	0.84785500	-2.47508900	0.12013400	C	-0.54548400	-0.36699600	1.32186600
H	1.66288400	-2.90367400	-0.17152300	H	-0.13118700	1.05743200	-0.24267900
O	0.61314100	1.49228700	0.22100700	C	1.70177200	-0.03225900	-0.07450600
O	2.01321500	2.29351600	0.07391400	H	-2.45248400	-1.44981700	1.47331000
H	2.71671600	1.70404300	-0.20511100	H	-2.54635600	0.09922300	0.62990500
H	2.41321600	3.08828600	0.42583500	H	-0.03186000	-1.19985700	1.80333600
				H	-0.58210600	0.46285300	2.01985000
6b				O	2.25945500	-0.52781400	-1.00993700
N	1.19190900	-1.13777200	-0.41334700	O	2.26639500	0.54982100	0.96588400
C	2.24056800	-1.05898500	0.57156800	H	3.22734600	0.52158200	0.87010000
C	0.73503700	0.11379200	-0.87226000	H	0.13512400	-1.07277000	-1.79166800
H	3.16538000	-1.41380900	0.09576000	O	-1.38859300	2.56663700	-0.50502400
H	2.02892400	-1.73375600	1.40242900	H	-1.51911600	3.22819200	0.17557400
C	2.29830500	0.43264400	0.90927400	H	-1.48607900	3.03770700	-1.33359800
C	1.76811600	1.10809800	-0.36077200				
H	0.56661400	0.09676400	-1.95423300	7a			
C	-0.73162700	0.35474800	-0.29558500	N	-0.76348000	1.62488300	0.21365100
H	3.30369500	0.74954600	1.16844900	H	-0.46072000	2.01763000	-0.67190800
H	1.64711900	0.64388900	1.75713400	C	-0.20326500	0.35992200	0.58751500
H	2.55576600	1.22504900	-1.10426300	H	-0.26959400	0.23866000	1.66602000
H	1.31834500	2.07853500	-0.17361600	C	-0.98146400	-0.75981300	-0.12540200
O	-1.05197900	1.42569800	0.10540700	C	1.26504100	0.30728800	0.12219600
O	-1.43720400	-0.73810700	-0.38368900	H	-0.67433500	-0.82549900	-1.17333200
H	-2.38046600	-0.57685800	-0.06775000	H	-0.78957100	-1.72510600	0.33835900
H	0.74494700	-2.00598700	-0.68424100	C	-2.44656300	-0.38621900	-0.12807600
O	-3.82129000	-0.27760500	0.50247900	O	1.65810900	1.02533900	-0.75771600
H	-4.62859300	-0.70731200	0.21887300	O	-2.76643400	0.80844100	-0.08430400
H	-4.04370300	0.62666800	0.72797300	N	-3.35049400	-1.34861000	-0.21846000
				H	-4.32740700	-1.11140000	-0.27880600
6c				H	-3.08848000	-2.31712700	-0.25874800
N	1.42183200	1.03861800	-0.17620300	O	1.93005500	-0.61445400	0.75798100
C	2.69507900	0.69398200	0.37812100	H	2.86684700	-0.66903100	0.40817400
C	0.62013600	-0.08315600	-0.54095300	H	-1.05905600	2.28259800	0.91836400
H	2.66411500	0.96939900	1.44370700	O	4.32127200	-0.71943200	-0.28075000
H	3.48094800	1.30830100	-0.07032500	H	5.14296100	-0.94874500	0.15345800
C	2.79229400	-0.81596300	0.15581600	H	4.51066500	-0.00210800	-0.88700900
C	1.32628000	-1.26736000	0.13156700				
H	0.67295800	-0.18086200	-1.63941700	7b			
C	-0.84990900	0.23722900	-0.21921300	N	0.12507300	0.71287700	1.19953600
H	3.37137500	-1.30171300	0.93543600	H	0.28866100	1.56595100	0.63536500
H	3.27607200	-1.01837900	-0.79951800	C	0.35528200	-0.55997000	0.58796300
H	0.93408100	-1.39847200	1.14035900	H	0.20226700	-1.34838900	1.32178300
H	1.16826500	-2.19095500	-0.41526600	C	-0.63373500	-0.71664200	-0.57676500

C	1.79020100	-0.64576100	0.04084900	H	5.40750200	0.07643600	-0.74676000
H	-0.36371300	-0.03786900	-1.39076600				
H	-0.63181300	-1.73432900	-0.96209400	8a			
C	-1.99130700	-0.27906800	-0.06927600	N	0.60596600	1.79574500	-0.59689500
O	2.44528600	0.30566200	-0.26629200	H	0.26948300	1.55741100	-1.52572700
O	-2.05200000	0.51701900	0.87206000	C	-0.16304000	1.32026100	0.50876400
N	-3.07544200	-0.74352900	-0.67402400	H	-0.57257700	2.17812700	1.05199000
H	-3.98373600	-0.42500700	-0.37865400	C	0.68868000	0.50471900	1.50078800
H	-3.01939900	-1.39466500	-1.43597900	C	-1.32601000	0.51418500	-0.07375200
O	2.15827700	-1.91150600	-0.07390000	H	1.49726400	1.13577000	1.87121600
H	3.04805000	-1.95537700	-0.44750700	H	0.04541000	0.27416900	2.34753500
H	0.06880100	0.79081000	2.20324000	C	1.24317100	-0.79692800	0.94019200
O	0.67629800	2.58897200	-0.70243200	O	-1.43897800	0.35111300	-1.26300000
H	1.60425200	2.44451100	-0.90179200	H	1.71238000	-1.35610200	1.74991100
H	0.49367200	3.51639400	-0.85429000	H	0.43806500	-1.43063500	0.55711500
				C	2.25135000	-0.62924200	-0.17432500
7c				O	2.28684300	0.37827000	-0.89274900
N	1.27711700	-1.60467800	-0.17292600	N	3.10865800	-1.62378700	-0.37398800
H	1.68363800	-1.78776700	0.73724500	H	3.76841900	-1.56673500	-1.13192500
C	0.99926400	-0.23588500	-0.50465100	H	3.11443500	-2.44116000	0.20881100
H	0.92309400	-0.13666800	-1.58515800	O	-2.11441500	0.05105200	0.85573600
C	-0.32556200	0.16863000	0.16194500	H	-2.86428900	-0.46497900	0.44375700
C	2.12462300	0.65517700	0.03471300	H	1.29909800	2.51928200	-0.49063300
H	-0.17433500	0.32778800	1.23357200	O	-3.98325000	-1.33606900	-0.34140100
H	-0.73203900	1.08776800	-0.25406300	H	-3.97988400	-1.20163500	-1.29019900
C	-1.27910000	-0.99712700	0.03119900	H	-4.89667600	-1.44011200	-0.07435500
O	2.84314000	0.31449800	0.92594400				
O	-0.81069500	-2.14886000	-0.04341800	8b			
N	-2.57264500	-0.76135500	0.03898600	N	-0.52671600	0.74617900	1.21949700
H	-3.21227900	-1.53848600	0.00492300	H	-0.84647800	1.53699500	0.61963100
H	-2.93298400	0.19245200	0.08547400	C	-0.84519500	-0.61958400	0.95516300
O	2.13784600	1.82565900	-0.58274600	H	-1.48687400	-0.98692000	1.76404900
H	2.83447900	2.37853700	-0.20571000	C	0.41469700	-1.51423000	0.93978200
H	1.51886000	-2.25966300	-0.89996200	C	-1.62996600	-0.71615200	-0.34684100
O	-3.25841900	1.99296700	0.10297500	H	0.92583700	-1.40222000	1.89656500
H	-3.69444300	2.42872900	-0.63035000	H	0.06915400	-2.54438900	0.88061100
H	-3.55561700	2.45066100	0.89033400	C	1.37716500	-1.25079900	-0.20967000
				O	-1.80135100	0.19864800	-1.09973100
7d				H	2.14865300	-2.02124000	-0.20033200
N	-0.83181000	1.50742800	-0.28738000	H	0.87050900	-1.33951100	-1.17492700
H	-1.11966800	1.92821300	0.58855200	C	2.04656800	0.10655900	-0.17310100
C	-1.20706200	0.14007200	-0.51041200	O	1.56451800	1.06365700	0.43769800
H	-1.18480100	-0.06911100	-1.57768800	N	3.18732600	0.23330400	-0.84772300
C	-0.20911900	-0.76680200	0.22818800	H	3.64904000	1.12676900	-0.87489300
C	-2.61455100	-0.10024800	0.04891500	H	3.60969400	-0.54107400	-1.32645400
H	-0.42176700	-0.76812500	1.30117900	O	-2.07407400	-1.95134100	-0.53192600
H	-0.26931000	-1.79399900	-0.12515200	H	-2.57814600	-1.98921500	-1.35413700
C	1.17188500	-0.17140500	0.06002200	H	-0.11537900	0.97929100	2.11088900
O	-3.11025300	0.61087200	0.87047800	O	-1.45681400	2.91698300	-0.14409300
O	1.27077200	1.05826900	-0.11927400	H	-1.09151100	3.79665300	-0.23377400
N	2.22640300	-0.95008400	0.14537200	H	-1.81661100	2.67013200	-0.99723300
H	3.17757400	-0.56527000	0.09309900				
H	2.11626400	-1.93725000	0.29550200	8c			
O	-3.14397200	-1.19918100	-0.46424600	N	0.85443300	-1.25051300	1.11156100
H	-4.01594100	-1.34763100	-0.07585800	H	0.81445800	-1.98739100	0.41668000
H	-0.75558800	2.13905900	-1.06911000	C	1.74513600	-0.15831500	0.86401300
O	4.87123300	-0.03812000	0.03747100	H	2.53643900	-0.15514100	1.61987400
H	5.35441700	0.37185000	0.75458800	C	1.01822900	1.19803600	0.93751000

C	2.38759300	-0.40431400	-0.49718400
H	0.61152800	1.31869100	1.94207900
H	1.77028600	1.97283000	0.80131000
C	-0.07647600	1.38288100	-0.10369000
O	2.09183900	-1.32961500	-1.19780900
H	-0.42287300	2.41552600	-0.06881600
H	0.31282600	1.22414300	-1.11361300
C	-1.27475800	0.47249400	0.05790300
O	-1.18307800	-0.64536700	0.60240900
N	-2.43308800	0.88994500	-0.41279500
H	-3.26790500	0.29797900	-0.37498800
H	-2.51143700	1.79900100	-0.83254900
O	3.28183900	0.52762100	-0.78626900
H	3.68360500	0.33013200	-1.64154900
H	0.53611900	-1.45470100	2.04467700
O	-4.84221900	-0.59068500	-0.42259500
H	-5.10308100	-1.23804700	-1.07703300
H	-5.49477100	-0.63938400	0.27536200

8d

N	-1.28240800	1.61040300	0.01659300
H	-2.27975500	1.83315800	0.03978300
C	-0.93402500	0.24915100	-0.07386100
H	-0.28640200	0.15005000	-0.95806700
C	-0.04982300	-0.17436500	1.15369300
C	-2.21148600	-0.56237900	-0.23780900
H	0.42668200	0.72037800	1.55086000
H	-0.71418300	-0.55980400	1.92589600
C	1.01072800	-1.20339900	0.80044200
O	-3.29459500	-0.05457800	-0.20421100
H	1.47387500	-1.55223800	1.72522000
H	0.56726300	-2.08085800	0.32634600
C	2.09612500	-0.64191000	-0.10582900
O	2.03237100	0.49344300	-0.56542600
N	3.11055800	-1.46453800	-0.38510400
H	3.85215200	-1.14127000	-0.98262200
H	3.16882800	-2.39115600	-0.00471200
O	-1.95752700	-1.84850900	-0.40750300
H	-2.78902200	-2.33019000	-0.50665800
H	-0.49502700	2.32713200	0.01807300
O	0.96010500	2.91611500	0.01929100
H	1.32312900	3.75123200	-0.27276900
H	1.56347700	2.19814800	-0.23878800

9a

N	-0.02690900	1.84776000	0.08318500
H	0.43466900	2.13909800	-0.77394300
C	0.44019300	0.51310300	0.43781400
H	0.29023000	0.35573900	1.50668900
C	-0.35072200	-0.57581200	-0.32327300
C	1.92949400	0.31161500	0.13272200
H	-0.13872700	-0.48782900	-1.39835300
H	-0.01795200	-1.56978000	-0.02727000
C	-1.81036900	-0.46702700	-0.16185900
O	2.54649500	1.08808600	-0.54772200
N	-2.44924800	0.69528900	-0.01841400
C	-2.87025400	-1.46394800	-0.14843300
H	-1.88051800	1.56317200	0.02186000

C	-3.78276700	0.42996400	0.07768300
N	-4.04090200	-0.88018500	-0.00235400
H	-2.74851800	-2.53301200	-0.24108900
H	-4.52711000	1.20139500	0.20338100
O	2.39354600	-0.79383800	0.66630900
H	3.35019200	-0.90843200	0.41456700
H	0.27349000	2.51198200	0.78533600
O	4.87454600	-0.93230000	-0.19768900
H	5.05569000	-0.09723700	-0.63267800
H	5.67782200	-1.19809600	0.24946600

9b

N	-0.14533800	1.63006400	0.34347300
H	-0.44250400	1.65645200	1.31243700
C	-0.45092500	0.32830600	-0.25337700
H	-0.30329500	0.42940500	-1.33226100
C	0.49735800	-0.76107700	0.26369900
C	-1.90180100	-0.13635800	-0.07162700
H	0.32665300	-0.92327900	1.33726600
H	0.26911200	-1.71947600	-0.20056400
C	1.92195800	-0.44056100	0.08246600
O	-2.18942600	-1.27316700	0.19863100
N	2.40829200	0.80190600	0.05365500
C	3.09484700	-1.28694500	-0.07587600
H	1.75194200	1.59574900	0.15663700
C	3.76001200	0.71930600	-0.10918500
N	4.17869300	-0.54757300	-0.18860300
H	3.10796900	-2.36643300	-0.10529500
H	4.39812000	1.58805600	-0.16462100
O	-2.74706500	0.84913000	-0.26659600
H	-3.67858300	0.50781900	-0.19096500
H	-0.67330700	2.35292100	-0.12905700
O	-5.11591500	-0.28413800	-0.12333300
H	-5.96397400	0.00827600	0.20897400
H	-4.99311100	-1.19089200	0.16155500

9c

N	1.00700500	1.17008900	1.01724600
H	1.91484000	1.62707200	0.97501600
C	1.16238600	-0.17513200	0.49387800
H	0.96434600	-0.92917000	1.25894100
C	0.22087000	-0.45315800	-0.72317200
C	2.61094900	-0.38975700	0.04362400
H	0.35239600	0.34970500	-1.44903700
H	0.50911900	-1.40076300	-1.17620700
C	-1.19031000	-0.53788900	-0.31821200
O	3.44698200	0.46078000	0.11734600
N	-2.03569400	0.49056500	-0.22461100
C	-1.98175200	-1.69174600	0.08484700
H	-1.75968700	1.48387600	-0.41227400
C	-3.23410200	0.00015100	0.19952600
N	-3.20758200	-1.32496500	0.38720600
H	-1.64214500	-2.71631800	0.12940200
H	-4.09729900	0.62874300	0.35765200
O	2.80743000	-1.61946500	-0.42035200
H	3.73243800	-1.71434900	-0.67860100
H	0.72463100	1.15909500	1.98662200
O	-0.72946800	2.72313900	-0.60529700

H	-0.01635100	2.45534200	0.00477100
H	-0.75619400	3.67649700	-0.67169400
9d			
N	-2.74065300	0.70237500	1.00253100
H	-3.11434300	-0.01438200	1.60415600
C	-1.49577900	0.39672200	0.39279500
H	-1.18639700	1.27101700	-0.18935500
C	-0.32963300	0.05061800	1.37803900
C	-1.58891600	-0.73590500	-0.63247600
H	-0.17220000	0.92739000	2.00869100
H	-0.63271000	-0.77537700	2.01997900
C	0.92623900	-0.30076000	0.69820800
O	-0.62512200	-1.39826700	-0.93913800
N	1.65955100	0.53698000	-0.05515400
C	1.68715100	-1.52851300	0.70062600
H	1.41703400	1.50783300	-0.29187800
C	2.75711400	-0.14890600	-0.47745800
N	2.78582100	-1.39765300	-0.01891000
H	1.41085900	-2.44470300	1.19927500
H	3.51156500	0.29633300	-1.10751100
O	-2.78146100	-0.88740600	-1.16268200
H	-2.74447900	-1.59534400	-1.81851400
H	-2.78130800	1.60480600	1.44493700
O	0.78325000	3.11322100	-0.65168400
H	0.58321700	3.41170000	-1.54015000
H	1.02532700	3.89889300	-0.15927100

9e			
N	0.46222000	-0.53981000	1.42501400
H	0.53785500	0.45802700	1.58315100
C	1.06996300	-0.94282100	0.16560000
H	1.23178900	-2.01688100	0.20025600
C	0.11889000	-0.60991400	-1.02245000
C	2.40753800	-0.23887300	-0.05453900
H	0.43213200	0.31051300	-1.51412000
H	0.14465500	-1.41140300	-1.75894300
C	-1.25999800	-0.42560700	-0.52471800
O	2.50021500	0.95854900	-0.18749100
N	-1.76784700	0.76192600	-0.18725300
C	-2.33655000	-1.36492700	-0.26593800
H	-1.19646700	1.62708700	-0.16592100
C	-3.03611000	0.55450100	0.26041800
N	-3.39089400	-0.73386600	0.20441300
H	-2.30896300	-2.43222700	-0.42697700
H	-3.66913400	1.35415100	0.61340600
O	3.43791000	-1.06023600	-0.04100800
H	4.25571500	-0.55632600	-0.14658800
H	0.88303200	-1.01450700	2.21098300
O	0.22864000	2.56894700	-0.01126900
H	1.11048700	2.17230000	-0.10962800
H	0.33802900	3.51929100	-0.01293300

10a			
N	-3.81238000	0.93635000	0.69072100
H	-4.30111100	0.23180400	1.22570000
C	-2.55706200	0.45404400	0.17179000
H	-2.15947600	1.22463200	-0.49603400

C	-1.56235000	0.25401400	1.33483900
C	-2.63843600	-0.81528200	-0.68113900
H	-1.59340900	1.17187500	1.92197600
H	-1.91430500	-0.56006700	1.96926000
C	-0.17542400	-0.00719600	0.88881000
O	-1.86851100	-1.73993200	-0.61634200
C	0.48081800	-1.27746700	0.87189300
C	0.75644600	0.90932700	0.35239400
H	0.08395800	-2.22639200	1.19264500
N	1.69115200	-1.15663800	0.37565300
C	1.92185900	0.18440500	0.02846700
C	0.71696600	2.28992500	0.11657900
H	2.36635000	-1.92122700	0.24930800
C	3.03217200	0.76666600	-0.51879000
C	1.83249600	2.89316100	-0.43751600
H	-0.16040100	2.87131300	0.36692000
H	3.91867100	0.19849900	-0.76277400
C	2.96653600	2.14666200	-0.75000500
H	1.82910100	3.95647400	-0.62915700
H	3.82397500	2.64452300	-1.18143600
O	-3.65872300	-0.77555600	-1.53096900
H	-3.65803300	-1.58522400	-2.05466400
H	-4.42731400	1.25326300	-0.04395800
O	3.59639300	-3.14418300	-0.02152600
H	3.61952100	-3.75572600	-0.75775600
H	4.22367300	-3.47390900	0.62212100

10b			
N	-2.74612400	-1.91869700	-1.13590900
H	-3.50657400	-1.28616700	-1.34451400
C	-1.68582300	-1.27545200	-0.38948200
H	-0.95731900	-2.04229000	-0.12104500
C	-1.01879000	-0.21687800	-1.28390500
C	-2.20085100	-0.66689700	0.91255200
H	-0.72235100	-0.73484400	-2.19733700
H	-1.74925000	0.54758400	-1.54950200
C	0.16683500	0.42219400	-0.66690800
O	-2.42464500	0.50460100	1.10013500
C	0.22995500	1.77550500	-0.20930400
C	1.43192400	-0.14054600	-0.39257600
H	-0.56280400	2.51482600	-0.25989900
N	1.42243500	2.01205100	0.30175100
C	2.22019900	0.85749800	0.21936400
C	1.98735500	-1.40839600	-0.62106400
H	1.71599600	2.89474800	0.68767200
C	3.51077500	0.64884400	0.61591800
C	3.29329000	-1.63652600	-0.22434300
H	1.41160800	-2.18619300	-1.10439300
H	4.10778600	1.41931100	1.08346600
C	4.03899300	-0.62985900	0.38315500
H	3.74472400	-2.60399200	-0.38982400
H	5.05793600	-0.83366400	0.68221400
O	-2.43177100	-1.60088300	1.82710500
H	-2.82642400	-1.18941100	2.60534800
H	-3.11543000	-2.72661800	-0.65650600
O	-2.53510700	2.79554300	-0.56675400
H	-2.81786000	2.14805300	0.08784800
H	-3.22519800	3.45416200	-0.62875200

10c

N	-2.31233800	2.61701100	0.28591000
H	-3.25208600	2.48958500	-0.06333900
C	-1.51203000	1.45340200	0.03816100
H	-0.86359300	1.54755600	-0.84434400
C	-0.58778500	1.19089400	1.27046300
C	-2.42083700	0.26714800	-0.26674900
H	-0.12743400	2.15200400	1.50294800
H	-1.21188500	0.91812700	2.12026000
C	0.47222300	0.19102800	1.03693200
O	-3.57932400	0.39376000	-0.56224000
C	0.49151200	-1.14158200	1.54231300
C	1.63756000	0.31579800	0.24667100
H	-0.23605000	-1.61768800	2.17950500
N	1.56450400	-1.77365600	1.10545800
C	2.31950200	-0.91690900	0.28654100
C	2.17541100	1.37238400	-0.49975400
H	1.80346400	-2.72695600	1.32468700
C	3.49291100	-1.14307300	-0.37777200
C	3.36181200	1.16045500	-1.18078700
H	1.67943200	2.33275000	-0.53798300
H	4.00917200	-2.09213500	-0.34113800
C	4.00670000	-0.07183200	-1.12145900
H	3.79754000	1.95888900	-1.76374200
H	4.93326900	-0.21048400	-1.66123600
O	-1.79771900	-0.90381100	-0.20476200
H	-2.43895400	-1.60883800	-0.48214600
H	-1.91821300	3.45985000	-0.09921800
O	-3.74334800	-2.44192200	-1.10080800
H	-4.21469100	-3.23070500	-0.83567000
H	-4.38387900	-1.72592700	-1.14303500

10d

N	-2.59073200	1.07543300	1.36428200
H	-3.26305000	0.53040300	1.88754600
C	-1.74160200	0.24315000	0.56565100
H	-1.20432200	0.88928700	-0.13301500
C	-0.69495300	-0.47782200	1.47101900
C	-2.48486700	-0.76536600	-0.31065200
H	-0.49763700	0.22036800	2.28433700
H	-1.12564700	-1.38018300	1.90538700
C	0.57343300	-0.77917900	0.77754000
O	-3.67313600	-0.84626700	-0.41284300
C	1.01805900	-2.05478000	0.32404300
C	1.57985000	0.13479100	0.39440800
H	0.51867800	-3.00503300	0.42310700
N	2.18722100	-1.93509700	-0.27829900
C	2.59073700	-0.58862700	-0.26909100
C	1.71656200	1.52004800	0.55817400
H	2.70988400	-2.69544100	-0.68198600
C	3.71751400	-0.00228800	-0.77262000
C	2.85194700	2.13073300	0.05151900
H	0.95406800	2.09428500	1.06788700
H	4.49013300	-0.56289300	-1.27993900
C	3.83060300	1.38608800	-0.59909500
H	2.98365400	3.19719700	0.16291800
H	4.70829900	1.88710500	-0.98359300

O	-1.64308700	-1.57185100	-0.98922900
H	-2.18097400	-2.14045000	-1.55288800
H	-3.10736600	1.70504700	0.76127000
O	-3.63298300	2.01258300	-1.29082400
H	-4.27007100	1.29619200	-1.31503300
H	-4.04111900	2.74556300	-1.75007700

11a

N	0.47669800	1.78586000	0.91675700
N	1.09349400	2.47805300	0.50775900
C	0.74796500	0.47268100	0.67231300
H	0.42659500	-0.19998000	1.46234400
C	-0.10544900	-0.11945800	-0.69983400
C	2.21386800	0.31418900	0.24829700
H	0.16639500	0.57366800	-1.49119000
H	0.37348000	-1.08807400	-0.82807700
C	-1.52966200	-0.20191000	-0.41958900
O	2.82062800	1.25354200	-0.19074800
C	-2.06127300	-1.34961700	0.19546700
C	-2.38933400	0.85964900	-0.74600600
H	-1.40307500	-2.17069000	0.45219700
C	-3.41244000	-1.44101800	0.45145300
C	-3.73861000	0.76536500	-0.48936600
H	-1.98703200	1.74638700	-1.22058400
H	-3.81984000	-2.33056200	0.91066900
C	-4.25174700	-0.38422800	0.11246800
H	-4.40154900	1.57635300	-0.75644100
H	-5.31155300	-0.45351500	0.31702800
O	2.63316800	-0.90828200	0.40470100
H	3.58183300	-0.99058100	0.09409500
H	-0.34916300	2.08210700	1.40950200
O	5.07319400	-1.02793500	-0.50354600
H	5.78759900	-1.58307100	-0.19088500
H	5.45009500	-0.17362100	-0.71819400

11b

N	-1.20993800	1.42891200	-0.05377500
H	-1.89573400	1.94666600	0.49651200
C	-1.51088200	0.09928100	-0.32400700
H	-1.21488400	-0.16523300	-1.34081500
C	-0.63744600	-0.87585800	0.62879300
C	-2.99092000	-0.13480500	-0.03553000
H	-0.92709600	-0.66408200	1.65645500
H	-0.99584900	-1.86716500	0.35210500
C	0.82848400	-0.72296500	0.40844400
O	-3.63153100	0.63676200	0.61693400
C	1.42814300	-1.25713100	-0.73091300
C	1.61011700	-0.02570700	1.32590000
H	0.83353500	-1.81521200	-1.44475400
C	2.78342000	-1.08805000	-0.95546600
C	2.96921500	0.13933700	1.10624800
H	1.15869200	0.38144200	2.22252700
H	3.24095300	-1.51095300	-1.83897300
C	3.55550000	-0.38538800	-0.03906200
H	3.57227900	0.66773100	1.83192600
H	4.61620700	-0.26037700	-0.20902100
O	-3.41375700	-1.26691700	-0.56276100
H	-4.34658500	-1.39853400	-0.34900200

H	-0.29979800	1.85219800	-0.35191200
O	1.17976400	2.30606100	-0.92500300
H	1.95904200	1.82017700	-0.64176800
H	1.47921400	3.11142500	-1.34664900

11c

N	2.48510700	-2.15266100	-0.09067700
H	3.10936200	-1.80635500	0.62564300
C	1.40046700	-1.39386200	-0.42220200
H	0.98985200	-1.62269300	-1.40084500
C	0.09003100	-1.76714400	0.66225600
C	1.69203100	0.08539700	-0.18630400
H	-0.08163600	-2.81469400	0.43238000
H	0.54075500	-1.63051400	1.64067600
C	-1.04162300	-0.90267200	0.39689800
O	2.39080800	0.43041900	0.73055400
C	-1.21981800	0.28154100	1.14038700
C	-1.96409300	-1.22280700	-0.61916400
H	-0.50239500	0.53848600	1.90953400
C	-2.30300000	1.09332800	0.90041000
C	-3.04311800	-0.40637500	-0.85728300
H	-1.82684900	-2.12687800	-1.19921200
H	-2.44991600	1.99152400	1.48314100
C	-3.21339400	0.75376600	-0.09977100
H	-3.76028600	-0.65998100	-1.62498800
H	-4.06161400	1.39693000	-0.29194200
O	1.09177700	0.84698300	-1.05702200
H	1.26182600	1.80638600	-0.83680700
H	2.58330600	-3.10557400	-0.39721300
O	1.57079400	3.30004900	-0.26868800
H	1.71336500	4.07280300	-0.81592000
H	2.27656400	3.28255100	0.38018400

11d

N	1.14392700	0.80533400	1.01559500
H	1.87317300	1.47372400	0.67959000
C	1.05282200	-0.47886100	0.53370100
H	0.57229300	-1.15838900	1.23413700
C	0.04738200	-0.51231100	-0.80626700
C	2.40041200	-0.98700100	0.03365100
H	0.48551900	0.19390000	-1.50736100
H	0.18202300	-1.53559100	-1.15495400
C	-1.34715200	-0.21182500	-0.44590700
O	3.27848400	-0.26627700	-0.33922600
C	-2.18965700	-1.23231500	0.00763100
C	-1.84215400	1.09209200	-0.54095400
H	-1.81559300	-2.24665200	0.07994300
C	-3.50150600	-0.95678100	0.34528000
C	-3.15264200	1.36595200	-0.20305000
H	-1.19911400	1.88670800	-0.90121600
H	-4.15142700	-1.75151100	0.68359100
C	-3.98270700	0.34144500	0.24307900
H	-3.53606100	2.37293000	-0.29136200
H	-5.00843400	0.55820700	0.50830600
O	2.42791800	-2.30851000	0.04169900
H	3.27609000	-2.61654600	-0.30242200
H	0.37903800	1.17207100	1.56537500
O	2.93006000	2.57423500	-0.02181100

H	3.27736500	3.42654800	0.24064300
H	3.65714300	2.06931300	-0.39169400

12a

N	4.10538600	-0.63638700	0.37734700
H	4.36666400	-0.13950300	1.21461100
C	2.75438400	-0.44334400	-0.03106400
H	2.59436900	-1.03236100	-0.93911100
C	1.67311600	-0.87541400	1.01651700
C	2.45701100	0.99321800	-0.46020100
H	1.87372900	-1.92602900	1.23869500
H	1.82619500	-0.30793600	1.93427000
C	0.27319000	-0.74080800	0.53938700
O	1.32997800	1.38708600	-0.63133700
C	-0.63423900	0.15641800	1.16434400
C	-0.19456500	-1.54541500	-0.53208500
H	-0.27804800	0.76953900	1.98047800
C	-1.92088900	0.26556300	0.74742200
C	-1.47414400	-1.45052500	-0.97145800
H	0.48244200	-2.24746700	-1.00039100
H	-2.61264600	0.95174100	1.21678100
C	-2.36656600	-0.53275800	-0.34325000
H	-1.85149300	-2.05238600	-1.78603900
O	-3.57372900	-0.47394400	-0.80819400
H	-4.15800300	0.18223500	-0.34048300
O	3.53088800	1.73951200	-0.63915100
H	3.24729400	2.61277900	-0.93615400
H	4.37772300	-1.60342700	0.44138000
O	-5.12606700	1.25925800	0.41608700
H	-5.41312900	2.04428200	-0.05304400
H	-5.88514100	0.94634400	0.91066100

12b

N	3.20882700	-1.68758600	-0.16275100
H	3.68092300	-1.29797200	0.63867800
C	1.92464400	-1.18578900	-0.40851600
H	1.57540400	-1.46357100	-1.40050700
C	0.81436000	-1.76090900	0.65487400
C	1.92883300	0.32693400	-0.24965800
H	0.79118200	-2.83278800	0.46827200
H	1.22529900	-1.55533900	1.64066600
C	-0.48864100	-1.13652700	0.45702400
O	2.53251900	0.86965500	0.64154100
C	-1.37607600	-1.61651900	-0.54254200
C	-0.86354000	0.00971200	1.20667200
H	-1.09164700	-2.48241600	-1.12584400
C	-2.57451000	-1.01432500	-0.76621900
C	-2.05645500	0.62522300	0.99785600
H	-0.18042400	0.39137300	1.95405100
H	-3.25551000	-1.38832200	-1.52025600
C	-2.93068700	0.12028000	0.00374000
H	-2.36342200	1.49308800	1.56390800
O	-4.06616900	0.75623400	-0.15793700
H	-4.61716000	0.36878200	-0.84589300
O	1.16527900	0.93065700	-1.13411400
H	1.16154800	1.90394700	-0.93570200
H	3.35614600	-2.67357200	-0.29212100
O	1.30165800	3.40321200	-0.20924000

H	1.49966800	4.22898800	-0.65141900
H	2.02234100	3.23437300	0.40403100

12c

N	-3.31183900	0.26902800	0.33634300
H	-3.68400400	-0.26410500	1.10634300
C	-1.96036800	-0.00319800	0.00916000
H	-1.68130100	0.65031200	-0.81915700
C	-0.92234000	0.27065100	1.16715300
C	-1.71816800	-1.41799900	-0.50831800
H	-1.13347300	1.29256300	1.48315000
H	-1.12029400	-0.40622700	1.99733000
C	0.47629800	0.17766000	0.70630500
O	-0.60586700	-1.83937600	-0.70902800
C	1.34261500	-0.86236400	1.14496400
C	0.98372300	1.16150400	-0.18528000
H	0.95402700	-1.61471100	1.81661300
C	2.63277800	-0.92522700	0.72606500
C	2.26786400	1.10919900	-0.62081200
H	0.32670000	1.96292700	-0.50142700
H	3.29065400	-1.71799000	1.05858000
C	3.11116200	0.05659000	-0.17397100
H	2.68010300	1.84575200	-1.29588400
O	4.33705800	0.05606400	-0.63698500
H	4.86130300	-0.67951600	-0.30304800
O	-2.81797400	-2.11620900	-0.72066100
H	-2.56838200	-2.98193100	-1.06666300
H	-3.49019900	1.25468300	0.44829400
O	-1.94136700	3.15229700	-0.30429800
H	-2.36542400	3.40097200	-1.12656400
H	-1.94300100	3.95097800	0.22421700

12d

N	3.04327200	1.28312200	0.14846900
H	3.53162300	0.58430000	-0.40630300
C	1.69834200	1.01486700	0.41577700
H	1.24620000	1.82327800	0.98442800
C	0.82554600	0.86120500	-0.97829000
C	1.55219700	-0.29101600	1.18618200
H	0.90385100	1.84458700	-1.43608900
H	1.36861900	0.12001200	-1.56162400
C	-0.55193400	0.48138200	-0.70497100
O	2.06673600	-1.32986500	0.87474800
C	-1.52379700	1.46201200	-0.37723500
C	-0.93950300	-0.88374700	-0.70456300
H	-1.23440300	2.50475000	-0.36310900
C	-2.81062600	1.11417900	-0.10011400
C	-2.22101600	-1.24958900	-0.43163300
H	-0.19917700	-1.63624900	-0.94222400
H	-3.55318800	1.86662000	0.13356200
C	-3.17624800	-0.25175300	-0.12423000
H	-2.53997700	-2.28210000	-0.44905100
O	-4.39712600	-0.66434400	0.13185700
H	-5.00067600	0.05893600	0.32877500
O	0.74938700	-0.14820300	2.23490500
H	0.69129600	-0.99461600	2.69593500
H	3.26645400	2.23208600	-0.10032400
O	3.53115300	-1.04961800	-1.52265800

H	4.22730900	-1.51566800	-1.98414700
H	3.27020200	-1.59679100	-0.77548000

13a

N	1.48508700	-1.67971500	-0.59710700
H	2.35276100	-1.62631900	-0.07765400
C	0.65971600	-0.62676200	-0.57085000
H	-0.08192900	-0.56767600	-1.35933100
C	-0.58161700	-0.86944200	0.92424600
C	1.33901400	0.64503400	-0.12212500
H	-1.07315600	-1.75532400	0.52621200
H	0.16316400	-1.02021700	1.69966700
O	-1.29803700	0.20569500	1.08276500
O	2.32880400	0.61741300	0.54833800
H	-2.10720100	0.21055600	0.50336300
O	0.69818100	1.71580600	-0.55320600
H	1.14521200	2.50857000	-0.22926400
H	1.25909800	-2.53188200	-1.08194600
O	-3.33404200	0.09346100	-0.55508200
H	-3.53927300	0.85887800	-1.09478500
H	-4.17621100	-0.27056100	-0.27666800

13b

N	-1.83687200	-1.45086100	0.04187200
H	-1.47673400	-1.74996100	0.94405100
C	-1.11652500	-0.53258300	-0.64246400
H	-1.22423500	-0.59407700	-1.72414400
C	-1.73435400	1.10447300	-0.40354000
C	0.31295600	-0.44101200	-0.08833500
H	-1.14229100	1.62001800	-1.15600500
H	-2.78894700	1.00356700	-0.65314000
O	-1.45347500	1.56760400	0.81735900
O	0.56423000	-0.92306600	0.98103000
H	-2.14946900	1.39058900	1.45547200
O	1.09550300	0.20381400	-0.89820900
H	2.03023300	0.24984800	-0.53167200
H	-2.66462000	-1.88654500	-0.33381500
O	3.49837700	0.22791400	0.06391800
H	3.64187600	-0.08549700	0.95721400
H	4.22274900	0.81269900	-0.15781200

13c

N	-1.04230200	-0.89392400	0.28006400
H	-0.76912400	-1.65228000	0.89864400
C	-0.05585800	-0.11490700	-0.23372000
H	-0.29835300	0.32685700	-1.19818100
C	0.09185200	1.35117700	0.70976900
C	1.29618000	-0.79909800	-0.12143700
H	-0.93984800	1.64253900	0.87774400
H	0.59942100	1.01841900	1.61643900
O	0.72126400	2.28579800	-0.01492500
O	1.45681300	-1.77986900	0.53970700
H	1.67492200	2.16236000	-0.02122700
O	2.23216000	-0.13917100	-0.79059100
H	3.07529500	-0.60403700	-0.70511100
H	-2.04017200	-0.70319900	0.08211900
O	-3.61461200	-0.14829800	-0.33097700
H	-4.05073000	-0.34010800	-1.16232400

H -4.31334700 0.03620200 0.29806300

13d

N 1.40615500 1.83381200 0.08555400
H 1.81054700 1.99644600 0.99655900
C 1.19804000 0.57139200 -0.37868400
H 1.01305600 0.54553200 -1.45246500
C 2.15283300 -0.50208800 0.10224400
C -0.37978700 0.10226100 0.18480100
H 3.14789400 -0.25030000 -0.28147000
H 2.18439900 -0.50611100 1.19735800
O 1.66547100 -1.69737700 -0.42964100
O -0.45451600 -0.29877400 1.29104800
H 2.20416100 -2.43572300 -0.14603000
O -1.21874400 0.33515800 -0.74902400
H -2.17536100 0.09506600 -0.46698200
H 1.03980200 2.63589600 -0.40364900
O -3.59398700 -0.19642700 -0.04702800
H -3.78884600 -0.78786100 0.68148500
H -4.29105400 -0.29965300 -0.69669700

13e

N -0.86589800 -0.99626600 0.94403100
H -1.73155700 -0.75325700 0.40930900
C 0.32096600 -0.37251000 0.72190000
H 1.03440800 -0.47193700 1.53658100
C 1.19299100 -1.21535400 -0.54957700
C 0.15353300 1.04153700 0.18858700
H 1.00480100 -2.26294900 -0.33991200
H 0.70080300 -0.86698200 -1.45895100
O 2.50054400 -0.95260400 -0.43730600
O -0.88944400 1.49412300 -0.17257000
H 2.72897400 -0.08573300 -0.78627700
O 1.32715800 1.66361600 0.14507600
H 1.19990900 2.56444000 -0.18085700
H -0.90140900 -1.78220200 1.57770300
O -3.05318300 -0.42928600 -0.55617400
H -3.93327400 -0.80222700 -0.60963500
H -3.12691000 0.50588900 -0.75384100

14a

N 1.10938500 2.25463100 -0.22200600
H 0.58781000 2.71985800 0.51126900
C 0.81424900 0.95452800 -0.49964300
H 1.09954700 0.64713600 -1.50049500
C 1.75645900 -0.06506700 0.54299900
C -0.63295900 0.63691000 -0.10170000
H 2.75902800 0.34506900 0.47288000
H 1.32238300 0.09696300 1.52550900
S 1.79646800 -1.71918500 0.02430100
O -1.18255600 1.29095900 0.74199000
H 0.60265300 -2.10115700 0.50245000
O -1.10053800 -0.39158600 -0.74953300
H -2.04425000 -0.58515700 -0.46203400
H 1.85921800 2.74618700 -0.67965300
O -3.49669000 -0.88153600 0.11453600
H -3.86203500 -0.20659800 0.68863000
H -4.22176200 -1.23867400 -0.39920700

14b

N 1.44014500 -0.81037900 -0.37091600
H 1.30784400 -1.45844500 -1.14044300
C 0.31550000 -0.31085100 0.23537300
H 0.49652300 0.00764500 1.25895300
C -0.10484800 1.10710100 -0.58366000
C -0.84350200 -1.29052500 0.06442200
H 0.74888400 1.76038400 -0.43709400
H -0.20841100 0.81878400 -1.62638500
S -1.61914000 1.80674500 -0.04854400
O -0.97153500 -1.92779700 -0.93830200
H -1.16520900 2.37964300 1.07614000
O -1.62160300 -1.31304400 1.12819700
H -2.35892600 -1.91970400 0.97926700
H 2.37644000 -0.43082900 -0.15982800
O 3.80405700 0.43247300 0.34430900
H 4.32210000 0.18289500 1.11082600
H 4.41573700 0.85695700 -0.25876200

14c

N -1.24663800 -0.57631300 1.31900400
H -2.01719100 -0.64092800 0.61809000
C -0.02492200 -0.04813100 0.97033100
H 0.59596700 0.17486400 1.83348600
C 0.79507700 -1.22379000 0.09217800
C -0.18998500 1.14854900 0.02816100
H 0.90551700 -2.06109800 0.77297200
H 0.13401300 -1.47399100 -0.73383400
S 2.32406700 -0.65792100 -0.55705600
O -0.93802300 1.14093200 -0.90424400
H 3.05335400 -0.78969800 0.56081300
O 0.60078700 2.13730400 0.39430900
H 0.51180300 2.87321300 -0.22591300
H -1.34115500 -1.08833400 2.18432500
O -3.03346600 -0.83470300 -0.70614300
H -3.94378400 -1.11214300 -0.80934400
H -2.87254200 -0.12898100 -1.33611400

14d

N 1.32612600 1.75289100 -0.73684600
H 2.24128400 1.47438300 -1.06630100
C 0.54754900 0.82515800 -0.10563600
H -0.21949100 1.25112300 0.53671500
C -0.39404400 0.00304100 -1.30200700
C 1.43084300 -0.23161800 0.54631900
H -1.03095200 0.80225600 -1.66615500
H 0.32088900 -0.33459400 -2.04672800
S -1.27842100 -1.34689700 -0.67373700
O 2.46480300 -0.57490100 0.05700500
H -2.20030200 -0.61551300 -0.00775700
O 0.89755700 -0.68428900 1.66832900
H 1.46899900 -1.36866300 2.04092500
H 0.96242500 2.64648600 -1.02266400
O -2.59406600 1.14857000 0.98474400
H -2.68987200 1.02934400 1.93122000
H -3.33356800 1.70075700 0.72578200

15a

N	0.54008300	2.67171200	-0.05294000
H	0.70810600	2.80019300	-1.03778800
C	0.00480100	1.41360300	0.32481600
H	-0.18564100	1.44001000	1.40363400
C	-1.31319000	1.03065000	-0.38274900
C	1.00383500	0.26433600	0.15735300
H	-2.12447400	1.67965400	-0.05969700
H	-1.21783000	1.09607000	-1.46621700
O	0.60589500	-0.90149800	0.11479300
O	2.23995500	0.59314400	0.10335600
H	2.84545700	-0.20479100	0.01775500
H	0.08241500	3.46915900	0.35443800
O	3.87653900	-1.39395400	-0.19064900
H	3.67601600	-2.30644100	0.01716700
H	4.82436100	-1.28448100	-0.10978100
Se	-1.83830500	-0.80424000	-0.02946000
H	-1.83839900	-0.68028500	1.43618600

15b

N	-2.35053900	-0.19255700	1.49277100
H	-2.68610400	-1.14235800	1.46965800
C	-1.16855700	0.06195400	0.74667900
H	-0.84722100	1.08950600	0.95026700
C	0.01436800	-0.87759800	1.06717300
C	-1.40042600	0.05750200	-0.76273500
H	0.37426200	-0.69097000	2.07736300
H	-0.27074600	-1.92541200	0.98241300
O	-0.48027200	-0.08823100	-1.55088600
O	-2.63112000	0.25979100	-1.13976100
H	-2.68110700	0.27718800	-2.10508900
H	-2.34193100	0.17074800	2.43051900
O	1.16098700	2.64270600	0.37363700
H	1.61151900	3.15273100	1.04897400
H	1.08564800	3.22680500	-0.38292200
Se	1.51623400	-0.63582600	-0.13949800
H	1.58843000	0.84247500	0.05174500

15c

N	-1.94869700	-1.11381800	1.16528800
H	-2.25077200	-1.56816900	0.31651700
C	-0.75101500	-0.36933800	1.02074800
H	-0.41646100	-0.05936400	2.01758700
C	0.39455900	-1.14767800	0.33932100
C	-0.94969800	0.95747100	0.28926000
H	0.77242900	-1.92489500	1.00041200
H	0.04664400	-1.59480300	-0.58968300
O	-0.02232400	1.53713400	-0.25504100
O	-2.14739400	1.46342400	0.35938000
H	-2.15960000	2.33100600	-0.06696800
H	-1.97230900	-1.72620800	1.96243300
O	-2.08601200	-0.79684400	-1.79606900
H	-1.98314900	-1.18049800	-2.66754600
H	-2.96502300	-0.41526500	-1.79394100
Se	1.89119500	-0.02513800	-0.17259400
H	2.15123500	0.51716100	1.17022400

15d

N	0.21317400	2.75710200	0.19781300
H	0.82214800	2.99694800	-0.57227200
C	0.01385700	1.42944400	0.48865600
H	-0.30809600	1.27028100	1.51324800
C	-1.22251700	0.84539400	-0.49048000
C	1.25162500	0.61080600	0.10193400
H	-2.05304500	1.53070600	-0.35257100
H	-0.84172100	0.88605000	-1.50656500
O	1.98034200	0.98147000	-0.77734100
O	1.34484500	-0.48789800	0.80124700
H	2.14527200	-1.01638600	0.50682200
H	-0.30177100	3.48750400	0.65796300
O	3.38544400	-1.81566300	-0.11468000
H	3.98416900	-2.36808400	0.38886800
H	3.92098200	-1.29321200	-0.71413500
Se	-1.82486700	-0.87971700	-0.01417200
H	-0.75751000	-1.62029200	-0.69865200

15e

N	-1.77723300	-0.51460400	1.38091900
H	-2.46324600	-0.80188100	0.65868600
C	-0.61130700	0.12468100	1.00619200
H	-0.05415700	0.49391200	1.86144500
C	0.33031500	-0.99537500	0.22687200
C	-0.89364600	1.22993400	-0.01739600
H	0.44176600	-1.82926000	0.91287800
H	-0.22636600	-1.29153900	-0.65731700
O	-1.60918900	1.07980400	-0.96357300
O	-0.22412400	2.32739200	0.28621100
H	-0.40824100	3.01220500	-0.37044500
H	-1.84523400	-0.92553000	2.29947500
O	-3.26251100	-1.30180700	-0.78397800
H	-4.06718700	-1.79208000	-0.95270200
H	-3.23118600	-0.57882100	-1.41398000
Se	2.07158000	-0.35457100	-0.18269900
H	1.67516300	0.37206800	-1.39598900

16a

N	1.27740100	1.85381800	0.09402300
H	0.96157200	2.05034900	1.03419200
C	0.63181800	0.94788700	-0.62068900
H	0.85787600	0.86578400	-1.67513700
C	1.45318200	-1.00843700	-0.00747500
C	-0.71173100	0.53961700	-0.10648600
H	0.60289000	-1.54080900	-0.42854600
C	2.75432500	-1.04764400	-0.70754700
O	1.51337800	-0.88201600	1.29309500
O	-0.96573300	0.62651700	1.07413600
H	3.43089600	-0.28492300	-0.32468000
H	3.21308800	-2.02176900	-0.51023500
H	2.63082200	-0.95022300	-1.78325300
H	0.64145000	-0.92043100	1.70888300
O	-1.47607800	0.05342000	-1.04312400
H	-2.35945200	-0.23267800	-0.66622900
H	2.11135800	2.30582600	-0.23976700
O	-3.73137500	-0.74468900	-0.00706300
H	-3.97816600	-0.37360800	0.84092400
H	-4.54123300	-0.88863200	-0.49748700

16b

N	-0.69638200	-1.08095100	0.55708400
H	-0.32376400	-1.23531600	1.48417200
C	0.12206700	-0.65895800	-0.38510100
H	-0.22664600	-0.66093500	-1.40879500
C	0.18809100	1.53874900	-0.16361200
C	1.57869500	-0.75055100	-0.09305300
H	1.10758300	1.63596400	-0.73685000
C	-1.09755200	1.92891900	-0.78100300
O	0.26205000	1.68862400	1.13617600
O	2.00510400	-0.74160400	1.03186300
H	-1.94079700	1.49630800	-0.24421600
H	-1.18558200	3.01802400	-0.71982300
H	-1.13323700	1.64599500	-1.82993900
H	1.14668000	1.51743900	1.48165300
O	2.30586500	-0.77793900	-1.19982100
H	3.24166700	-0.83690000	-0.96833700
H	-1.70566700	-1.16388900	0.39512300
O	-3.43429100	-1.11783600	-0.05815300
H	-4.12568900	-0.85013400	0.54848800
H	-3.83750300	-1.75881600	-0.64498300

16c

N	1.28008700	1.80949800	0.11012100
H	0.82574600	2.11887200	0.96154900
C	0.69026700	0.84036200	-0.58517600
H	0.93840500	0.76011900	-1.63750200
C	1.49372300	-0.96483200	-0.12997900
C	-0.72937000	0.55874700	-0.13663700
H	0.89631600	-1.46591000	-0.88590000
C	2.95264100	-0.78748600	-0.37036600
O	1.07300900	-1.27182600	1.08276300
O	-1.14564700	1.04889400	0.87865000
H	3.40648900	-0.12102800	0.36438300
H	3.42939000	-1.76730700	-0.28142900
H	3.15045600	-0.41328300	-1.37236400
H	1.70151200	-1.02201200	1.76819000
O	-1.34798100	-0.24641600	-0.95396600
H	-2.27779800	-0.42807300	-0.62643900
H	2.10466200	2.28626400	-0.21212200
O	-3.71807200	-0.71227800	0.01499800
H	-3.94236400	-0.17623700	0.77678700
H	-4.52745300	-0.86562000	-0.47260600

16d

N	-0.57293300	-1.02450500	1.70215200
H	-1.32493300	-1.65877600	1.47004200
C	-0.34241300	0.02338300	0.92568500
H	0.34946700	0.79124600	1.24812500
C	0.98387500	-0.70000200	-0.69836600
C	-1.42283300	0.35371400	-0.03942300
H	0.85569500	0.23199600	-1.24365300
C	2.23834500	-0.93371200	0.04382300
O	0.37660900	-1.77554600	-1.12630700
O	-2.20487500	-0.47087600	-0.43283300
H	2.14355300	-1.77935500	0.72329400
H	3.01216500	-1.18671900	-0.68819600

H	2.55265700	-0.03583200	0.56733500
H	-0.37972600	-1.58817800	-1.69477600
O	-1.37882200	1.62050000	-0.43805200
H	-2.10648700	1.77871700	-1.05321800
H	0.02083500	-1.24668800	2.48260300
O	1.56612800	2.32635800	0.09617800
H	2.37754200	2.82350200	0.20383800
H	0.89559300	2.97783000	-0.11266100

17a

N	1.19909100	2.70331700	-0.00219500
H	1.31592100	2.81575400	-0.99837800
C	0.32791300	1.61642100	0.35232900
H	0.23513100	1.62417800	1.44598800
C	-1.09137500	1.72033300	-0.23464400
C	0.99502500	0.27306800	0.07686200
H	-1.46408300	2.71020800	0.02850400
H	-1.04641400	1.69376700	-1.32621200
C	-2.10672600	0.70469500	0.28905600
O	0.35998300	-0.76358700	-0.13606200
H	-1.98056500	0.50662100	1.35300300
H	-3.12668600	1.05534600	0.12289100
S	-1.97638600	-0.84924400	-0.60079800
C	-2.18858700	-2.08531500	0.66173400
H	-3.16088700	-1.94447700	1.13396600
H	-2.14620500	-3.05788900	0.17822300
H	-1.38843000	-1.98886100	1.39281800
O	2.28119100	0.27782400	0.14059800
H	2.67033600	-0.63192000	0.01949400
H	0.90349800	3.57889600	0.39969300
O	3.48352800	-2.05555500	-0.05675300
H	4.39921200	-2.08690800	0.22255900
H	3.40258900	-2.65468400	-0.79869900

17b

N	0.14795500	1.99326000	-0.07483900
H	0.59168600	2.10543500	-0.98019900
C	0.55341300	0.75946200	0.54988700
H	0.53574400	0.87019800	1.63387300
C	-0.43431600	-0.35866800	0.14300100
C	1.95742800	0.32409900	0.11969600
H	-0.27001500	-0.60476900	-0.90919500
H	-0.27232500	-1.26040200	0.72964600
C	-1.84076900	0.20685100	0.33056000
O	2.48844900	0.77362800	-0.86314000
H	-2.15784800	0.28767400	1.37053100
H	-1.74373700	1.25559000	-0.07073700
S	-3.04287200	-0.62640600	-0.62009700
C	-4.54481000	-0.43515600	0.31803900
H	-4.72665500	0.62559800	0.49370700
H	-5.35438800	-0.86779700	-0.26408300
H	-4.44269900	-0.95582500	1.27076900
O	2.44804800	-0.59991300	0.91069600
H	3.33657000	-0.88607000	0.56759100
H	0.33634600	2.81048900	0.48568100
O	4.72314500	-1.22132000	-0.26984500
H	4.79358800	-0.55709900	-0.95842100
H	5.60118400	-1.35203600	0.08746600

17c

N	-2.88179500	-0.69355900	0.55834400
H	-3.14010800	-1.44268800	-0.06692400
C	-1.49035500	-0.34019800	0.48783700
H	-1.29685400	0.40674600	1.26726800
C	-0.51763800	-1.51305300	0.71686200
C	-1.18537900	0.42635000	-0.78824000
H	-0.84917800	-2.01098000	1.62792700
H	-0.61786300	-2.24865900	-0.08496900
C	0.94755200	-1.12970200	0.93201800
O	-0.07502300	0.50152000	-1.29614500
H	1.04430100	-0.21321500	1.51146400
H	1.48424600	-1.93469300	1.43789000
S	1.80673600	-0.89390300	-0.62630100
C	2.80070000	0.55248200	-0.34650800
H	3.61998600	0.27782900	0.32032300
H	3.19787500	0.86848000	-1.30784500
H	2.18488200	1.32549800	0.11161900
O	-2.20498500	1.06787000	-1.30044700
H	-1.91534000	1.54427700	-2.08922900
H	-3.17046900	-0.92765400	1.49483100
O	0.57756500	2.19161500	1.61916200
H	0.22761700	2.97212500	1.18790100
H	0.78595400	2.47698200	2.50978100

17d

N	0.80002900	2.63131100	-0.01616400
H	1.41588500	2.72838800	-0.81063800
C	0.53760100	1.34865700	0.45717000
H	0.34188700	1.33988000	1.52999300
C	-0.78607900	0.79557400	-0.26242600
C	1.70866800	0.43537200	0.09118600
H	-1.55595300	1.55268000	-0.12581700
H	-0.56889500	0.70558000	-1.32567800
C	-1.23326000	-0.55178800	0.34310600
O	2.42491900	0.68644500	-0.84113900
H	-0.48636100	-1.32251300	0.17138300
H	-1.42229600	-0.47007700	1.41213300
S	-2.69948500	-1.01615500	-0.53664100
C	-3.99628300	-0.20119800	0.38934500
H	-3.84908700	0.87808900	0.38933500
H	-4.93457100	-0.43153300	-0.10962100
H	-4.01550200	-0.57786700	1.41087800
O	1.78604300	-0.61367300	0.87294100
H	2.55011000	-1.18795600	0.58245400
H	0.28481800	3.43104800	0.30527600
O	3.76413700	-2.03809600	-0.08855800
H	4.20250400	-1.52357600	-0.76863800
H	4.44436000	-2.51994000	0.38210200

TS-Ala

N	0.96081700	-0.41648000	1.11577400
H	0.72891000	-1.06506400	1.86626800
C	0.26238700	0.67228600	0.94011500
H	-0.46550800	0.92537500	1.72037200
C	0.65405100	1.71187900	-0.04686700
C	-1.70580000	-0.14038000	-0.20493200

H	1.32056900	1.30497600	-0.81968600
H	-0.23164100	2.17751900	-0.50056300
H	1.19007100	2.50669300	0.50469000
O	-2.27504000	0.59711100	-0.92632700
O	-1.86631000	-1.37201700	0.18643900
H	-2.66825400	-1.77945400	-0.21168800
H	1.71905200	-0.67207900	0.44408400
O	2.86341000	-0.73697600	-0.83839100
H	2.84473200	-1.35490500	-1.58438300
H	3.79605100	-0.49535700	-0.73318700

Imaginary Frequency: -78.42 cm⁻¹**TS-Gly**

N	1.48095500	1.17337000	0.47684800
H	1.59038400	1.70941100	1.33971300
C	0.67974100	1.55433600	-0.44900900
C	-1.40858700	-0.14682100	0.01059300
H	0.12737300	2.49696600	-0.37383900
H	0.62654800	0.95496800	-1.36213400
O	-0.83996500	-1.14748300	0.30051900
O	-2.64932200	0.19952200	-0.11076700
H	-3.26645800	-0.54386300	0.07804000
H	1.94129700	0.22417600	0.36623000
O	2.08441400	-1.27662100	-0.23457600
H	1.35844500	-1.87938900	-0.00877800
H	2.86777900	-1.82429400	-0.38807300

Imaginary Frequency: -43.57 cm⁻¹**TS-Cys**

N	-1.57150000	-0.01323800	1.43296100
H	-2.24509600	-0.02801400	0.63101600
C	-0.39348700	-0.54260300	1.27967800
H	0.33512100	-0.42167600	2.09049600
C	-0.12657800	-1.55011600	0.20749200
C	0.68688600	1.30929200	-0.02354000
H	-0.19494900	-2.55321600	0.66573100
H	-0.89441700	-1.48069100	-0.57711200
S	1.48874900	-1.35089600	-0.62874400
O	-0.11945900	1.67504200	-0.81584300
H	2.27005200	-1.58767800	0.45302400
O	1.78627900	1.82528600	0.44137100
H	1.99452200	2.68198300	0.00621400
H	-1.76957000	0.58890500	2.23103800
O	-2.63304900	0.05971200	-1.03266700
H	-3.45602100	-0.04264200	-1.53210400
H	-2.13022200	0.77028700	-1.46380400

Imaginary Frequency: -66.84 cm⁻¹**TS-Ser**

N	0.82837400	-1.37802500	0.92651900
H	0.53957200	-1.66912200	1.85986000
C	-0.02543000	-1.08524500	-0.00778200
H	0.40548400	-0.83641300	-0.98333700
C	-1.49209900	-1.36357900	0.05376300
C	-0.18195700	1.35168600	0.07727500

H	-1.59523800	-2.45931600	-0.11871500
H	-1.87757700	-1.15823200	1.07377900
O	-2.09041800	-0.59452400	-0.94582900
O	0.77781700	1.85310900	-0.40064000
H	-3.03363300	-0.79751600	-1.00493100
O	-1.23036800	1.78133800	0.70491600
H	-1.23894400	2.76220900	0.77719300
H	1.82643900	-1.16772500	0.70798700
O	2.89472800	-0.34736600	-0.38975400
H	2.80161300	0.60740800	-0.53192500
H	3.75651300	-0.59273800	-0.75462500

Imaginary Frequency: -63.82 cm⁻¹

PRC-Ala

N	1.37822600	0.01733800	1.07803500
H	1.10210300	-0.28007400	2.00315100
C	0.87195800	1.06975800	0.56054900
H	0.15868200	1.62469000	1.15889100
C	1.21966300	1.55990000	-0.77727900
C	-2.42771400	-0.55017300	0.10969900
H	1.93635100	0.92039300	-1.28603300
H	0.29769200	1.63980800	-1.35663400
H	1.61513700	2.57445800	-0.68554400
O	-1.77258100	0.41937200	-0.09650700
O	-3.66278300	-0.83320900	-0.17217200
H	-4.10361500	-0.09831800	-0.62987800
H	2.06237800	-0.56519800	0.56369400
O	3.20232400	-1.43226300	-0.41526000
H	3.01111700	-2.23774100	-0.89739300
H	4.15345400	-1.40749600	-0.30279800

PRC-Gly

N	-3.06273500	-0.14395500	0.50726900
H	-3.42474700	-0.24165500	1.44869800
C	-3.70272100	-0.61850600	-0.47517300
C	2.69577800	0.14323800	-0.21827800
H	-4.64451500	-1.13459000	-0.32856100
H	-3.29190100	-0.50004700	-1.47146700
O	1.64520800	-0.18902200	0.23462100
O	3.88087600	-0.35965900	-0.08536900
H	3.87940100	-1.14027500	0.49309500
H	-2.13680200	0.36221100	0.35665900
O	-0.81218800	1.03699500	-0.11370600
H	0.06253000	0.62469300	-0.00390800
H	-0.67432000	1.98245400	-0.16905200

PRC-Cys

N	-1.78736100	1.60291600	0.82090700
H	-0.89940200	1.79295300	0.29943200
C	-2.60309400	0.70227600	0.42377700
H	-3.50788500	0.54233900	1.00189100
C	-2.33888400	-0.16554400	-0.73813000
C	3.17154000	-0.51453400	0.01462200
H	-3.21523300	-0.27061800	-1.37184100
H	-1.49082600	0.18203300	-1.32369800
S	-1.88766300	-1.77069400	0.00838800
O	2.82906500	0.62472600	0.03978500

H	-3.13375300	-2.24661700	0.13033300
O	4.32384000	-1.06494800	0.23557600
H	5.00206000	-0.40289900	0.44963100
H	-1.97627000	2.12391800	1.66559300
O	0.42693900	1.84606300	-0.68294900
H	0.65631500	2.58879500	-1.24144800
H	1.26300900	1.42086500	-0.43136200

PRC-Ser

N	-1.65805100	-1.00085200	0.54299600
H	-1.99184400	-1.38913000	1.41669100
C	-2.37215000	-0.18255500	-0.11832600
H	-1.95335100	0.21798600	-1.03778600
C	-3.74463600	0.24229400	0.26019900
C	3.59684500	0.68339300	-0.14105100
H	-4.41742800	-0.53675700	-0.13217300
H	-3.85165800	0.24892900	1.35213700
O	-3.95662600	1.48720100	-0.32389800
O	3.09533000	-0.34184800	0.19640100
H	-4.87787500	1.73887800	-0.25558200
O	4.77070400	1.17804300	0.09745800
H	5.30809200	0.57882800	0.64169800
H	-0.70513000	-1.28311700	0.18694000
O	0.68732100	-1.52542100	-0.55118100
H	1.51917300	-1.09655300	-0.29136100
H	0.92220000	-2.31569800	-1.03670900

V. References

1. S. F. Boys and F. Bernardi, The calculation of small molecular interactions by the differences of separated total. *Mol. Phys.* 1970, **19**, 553–566.