Supporting information for

An accurate density functional theory based estimation of pK_a value of polar residues combined with experimental data: from amino acids to minimal proteins

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This supporting information (SI) contains
SI 1: Full version of reference 14.
SI 2: The validities of SKE and HKT schemes
SI 3: Cartesian coordinate of optimized geometries.

Supporting information 1: Full version of reference 14

Gaussian 09, Revision A. 02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Supporting Information 2: The validities of SKE and HKT schemes

Table S1: Benchmark molecules, computed ΔE_{SCF} and each concerned term in Eq. (7) (in kJ).

	ΔE_{SCF}	ΔE_{ZPE}	$\Delta G_{0->298K}$	$\Delta E_{ZPE}+G_{0->298K}$	ΔG_0
COOH					
CH_3COOH	1222.27	-34.52	3.72	-30.79	1191.48
$CH_2ClCOOH$	1192.27	-33.64	0.96	-32.68	1159.55
$(COOH)_2$	1169.43	-34.77	-0.75	-35.48	1133.95
PhCOOH	1215.45	-34.27	-0.50	-34.81	1180.68
NH_3^+					
$CH_3NH_3^+$	1197.34	-41.76	-2.18	-43.93	1153.40
$NH_2CH_2CH_2NH_3^+$	1190.89	-41.42	0.59	-40.88	1150.06
$CNCH_2CH_2NH_3^+$	1168.72	-41.34	0.38	-40.96	1127.76
$NH_3(CH_3^+)_3NH_3^+$	1177.46	-45.73	3.39	-42.34	1135.12
SH					
$C_2H_5OCOCH_2SH$	1214.87	-23.56	4.18	-19.37	1195.49
C_2H_5SH	1242.56	-24.73	1.80	-22.93	1219.64
t-C_4H_9SH	1248.80	-24.98	1.42	-23.56	1225.24
$C_2H_5OC_2H_4SH$	1231.27	-24.06	3.89	-20.21	1211.06
Phenol					
Phenol	1261.48	-35.19	0.46	-34.77	1226.71
m-Cl-Phenol	1240.39	-35.82	0.08	-35.73	1204.66
p-NO_2-Phenol	1205.79	-34.69	0.54	-34.14	1171.65
o-CH_3-Phenol	1265.66	-35.35	0.75	-34.60	1231.06
Imidazole					
2-Methyl	1195.62	-37.53	-0.96	-38.45	1157.17
4-Hydroxymethyl	1181.98	-36.48	1.84	-34.69	1147.34
4-Brimidazole	1166.92	-36.23	0.04	-36.19	1130.77
Imidazole	1184.87	-36.69	0.21	-36.48	1148.38
Alcohol					
CF_3CH_2OH	1287.79	-36.99	5.40	-31.59	1256.20
$HOCH_2CH_2OH$	1327.54	-36.53	1.88	-34.64	1292.90
$HCCCH_2OH$	1311.18	-36.57	1.17	-35.40	1275.79
C_2H_5OH	1339.67	-37.36	1.30	-36.07	1303.61

Table S2: Benchmark molecules, computed $\Delta E'_{SCF}$ and each concerned term in Eq. (9) (in kJ).

	ΔE_{SCF}	ΔE_1-ΔE_2	$\Delta E'_{SCF}$
COOH			
CH_3COOH	1222.27	23.88	1246.15
$CH_2ClCOOH$	1192.27	23.04	1215.31
$(COOH)_2$	1169.43	30.58	1200.01
PhCOOH	1215.45	25.86	1241.31
NH_3^+			
$CH_3NH_3^+$	1197.34	1.11	1198.45
$NH_2CH_2CH_2NH_3^+$	1190.89	4.50	1195.39
$CNCH_2CH_2NH_3^+$	1168.72	4.93	1173.65
$NH_3(CH_3^+)_3NH_3^+$	1177.46	4.70	1182.16
SH			
$C_2H_5OCOCH_2SH$	1214.87	2.50	1217.36
C_2H_5SH	1242.56	2.07	1244.63
t-C_4H_9SH	1248.80	17.84	1266.64
$C_2H_5OC_2H_4SH$	1231.27	2.02	1233.29
Phenol			
Phenol	1261.48	17.57	1279.05
m-Cl-Phenol	1240.39	18.98	1259.36
p-NO_2-Phenol	1205.79	26.03	1231.81
o-CH_3-Phenol	1265.66	17.62	1283.28
Imidazole			
2-Methyl	1195.62	14.07	1209.69
4-Hydroxymethyl	1181.98	19.11	1201.09
4-Brimidazole	1166.92	0.05	1166.97
Imidazole	1184.87	14.03	1198.89
Alcohol			
CF_3CH_2OH	1287.79	11.14	1298.93
$HOCH_2CH_2OH$	1327.54	8.48	1336.03
$HCCCH_2OH$	1311.18	7.41	1318.59
C_2H_5OH	1339.67	8.06	1347.74

Table S3: Deprotonation Energy (in kJ/mol) and predicted pK_a value of each side chain of amino acid in each scheme.

	ΔE_{SCF}	pK_a (SKE)	ΔE_1-ΔE_2	$\Delta E'_{SCF}$	pK_a (HKT)
Asp	1210.04	3.92	-26.70	1236.74	4.04
Cys	1228.54	9.18	-20.42	1248.96	10.26
Glu	1215.70	4.29	-26.16	1241.86	4.41
His	1182.91	6.29	-16.29	1199.20	6.68
Lys	1200.18	10.91	-4.76	1204.94	11.18
Ser	1338.57	15.63	-11.45	1350.02	15.91
Tyr	1268.74	10.41	-17.08	1285.82	10.44

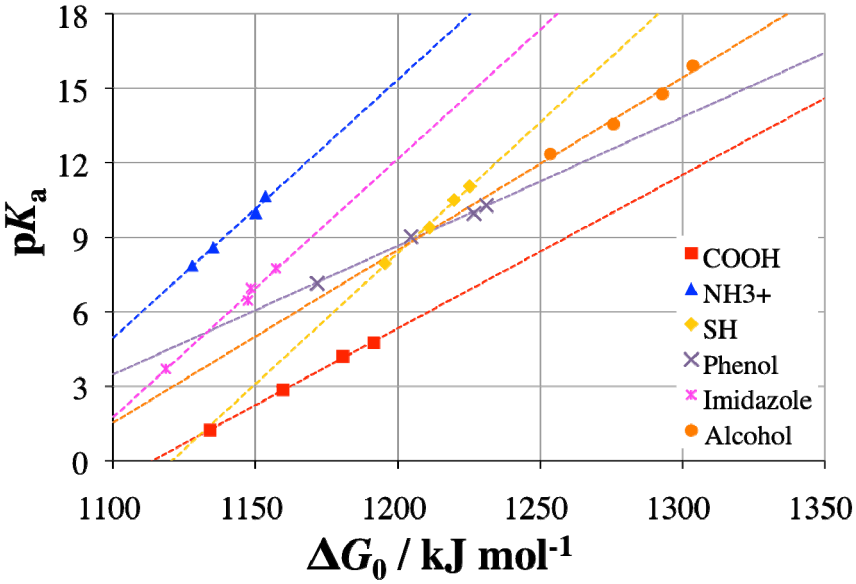

Figure S1: Scatter plot of ΔG_0 and observed pK_a for each chemical group.

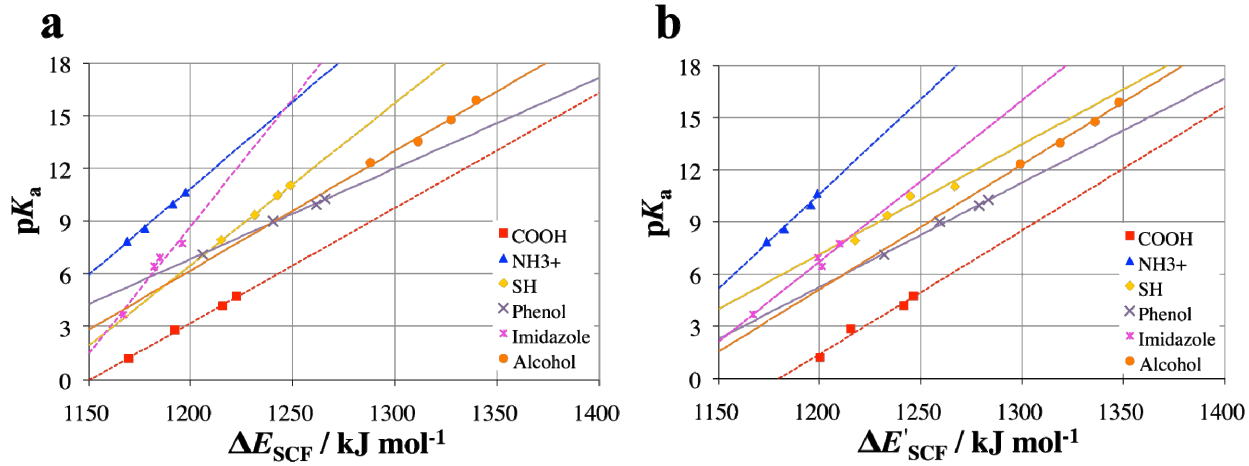

Figure S2: Scatter plots of (a) ΔE_{SCF} for SKE scheme, (b) $\Delta E'_{SCF}$ for HKT scheme and observed pK_a for each chemical group.

Supporting Information 3: Cartesian coordinate of optimized geometries.

Test in Chignolin:

Chignolin Tyr Protonated (Whole optimize)

Charge: -2

N	6.74254000	4.10573400	-1.27070200
C	5.44069900	4.52054700	-0.69021400
C	4.68835600	3.26404300	-0.23246400
O	5.27462000	2.17754000	-0.15586100
H	6.57929000	3.60099100	-2.23606700
H	7.17761100	3.40893100	-0.65700700
H	7.37792400	4.89978000	-1.37455500
H	5.61873500	5.17882800	0.16413800
H	4.88409100	5.07404700	-1.44886700
N	3.39837800	3.46333700	0.07709500
C	2.52668200	2.45380300	0.67809300
C	1.09620100	2.94323300	0.41537100
O	0.82849500	4.13917700	0.59457600
C	2.81296600	2.35008000	2.20506100
C	1.88630700	1.42856000	2.96521700
C	2.01350500	0.03275300	2.88210000
C	0.86357200	1.94738500	3.76972700
C	1.14221200	-0.81707300	3.55928000
C	-0.01299200	1.11128400	4.46380400
C	0.11916100	-0.27582400	4.34790200
O	-0.72327800	-1.15498900	4.97615300
H	3.00073200	4.39798900	0.05200500
H	2.70299500	1.49305100	0.18986400
H	3.85337700	2.02146500	2.30659100
H	2.74782400	3.36344900	2.61539200
H	2.80844400	-0.39913300	2.27859000
H	0.74714100	3.02463100	3.85976900
H	1.22600200	-1.89544500	3.46896300
H	-0.79648500	1.53539600	5.08784900
H	-1.40444500	-0.65851400	5.45953000
N	0.20919400	2.01991500	-0.00883500
C	-1.18075600	2.37686700	-0.27916100
C	-2.08533300	1.79739500	0.82229500
O	-2.00049400	0.59956300	1.13303900
C	-1.65088900	1.87956500	-1.66168800
C	-3.08797400	2.39482200	-1.91817000
O	-3.21246600	3.57542800	-2.30854900
O	-4.04194300	1.58910700	-1.64114300
H	0.50326800	1.05361600	-0.14456500
H	-1.21030300	3.46452400	-0.27217600
H	-0.97116900	2.29321400	-2.41404400
H	-1.61645700	0.78799700	-1.69777100
N	-2.97353800	2.63305000	1.41129000
C	-3.79589700	2.16187200	2.53424700
C	-5.01045100	1.29984300	2.14724600

O	-5.59009000	0.67294300	3.04127900
C	-4.22708200	3.47182600	3.22959700
C	-4.29321300	4.48285900	2.07486200
C	-3.09881100	4.09699500	1.19159300
H	-3.19064400	1.53143700	3.19006700
H	-5.17038400	3.35384100	3.76798300
H	-3.45780000	3.76724900	3.95163700
H	-5.22792000	4.35956300	1.51673800
H	-4.23305500	5.52175900	2.40961600
H	-3.26375300	4.31605000	0.13437600
H	-2.18053800	4.59955700	1.51857600
N	-5.41349000	1.31960200	0.85559700
C	-6.48924500	0.44394500	0.39212000
C	-5.95994700	-0.95379100	0.01650100
O	-6.58951800	-1.96619500	0.34180700
C	-7.30116400	1.12930800	-0.72775500
C	-8.57448800	0.37933500	-1.14245600
C	-8.40035100	-0.75622300	-2.19667200
O	-7.43979100	-0.63681500	-3.00762200
O	-9.27556800	-1.66292400	-2.18010600
H	-4.81540600	1.71838400	0.12765100
H	-7.14119500	0.26841500	1.25006800
H	-7.55982700	2.12454600	-0.34201700
H	-6.66438400	1.27161100	-1.60533400
H	-9.09828100	-0.02293500	-0.26627700
H	-9.26438600	1.10841400	-1.59438700
N	-4.77344800	-1.01197600	-0.64689800
C	-4.25418000	-2.30929700	-1.04126400
C	-3.46216100	-3.02280700	0.06695000
O	-3.32745700	-4.25112100	0.04310100
C	-3.36158000	-2.26710300	-2.30078100
O	-2.12488900	-1.61984800	-1.96696500
C	-4.02453900	-1.58065000	-3.49375500
H	-4.33670900	-0.14901500	-0.99683500
H	-5.10384200	-2.96195700	-1.26030200
H	-3.15896700	-3.31793100	-2.54397400
H	-1.39149700	-2.06662300	-2.44367400
H	-5.02819500	-1.97825500	-3.67766900
H	-3.41307200	-1.72815900	-4.39112900
H	-4.11708900	-0.50679400	-3.30832200
N	-2.87585000	-2.23581500	1.00247100
C	-1.93418000	-2.79204500	1.94970900
C	-0.55006300	-3.15039300	1.38694600
O	0.22354900	-3.83445500	2.06407200
H	-2.92688000	-1.22295000	0.92018100
H	-1.78863100	-2.08359000	2.77008700
H	-2.33696600	-3.71452000	2.37539600
N	-0.24738300	-2.66160100	0.15780400
C	0.98265500	-3.02457400	-0.51199400
C	1.86668200	-1.79008300	-0.80143900

O	1.43891700	-0.63123200	-0.79329500
C	0.75025900	-3.85161700	-1.80049400
O	0.12647800	-2.98364700	-2.76772700
C	-0.07428700	-5.11247800	-1.56096300
H	-0.95532600	-2.14240500	-0.35969600
H	1.51947800	-3.67172700	0.18890300
H	1.73832600	-4.13129100	-2.18742900
H	0.05076500	-3.47123400	-3.60449600
H	0.43596500	-5.77380300	-0.85177300
H	-0.19660500	-5.66201000	-2.50149900
H	-1.06444200	-4.86977600	-1.16401200
N	3.15374800	-2.09745900	-1.07274000
C	4.16298000	-1.12174700	-1.44315700
C	3.86045000	-0.50699900	-2.82968600
O	3.25441500	-1.12673600	-3.70690900
C	5.55453800	-1.81236900	-1.49343700
C	5.92161000	-2.56003800	-0.24418000
C	6.04277300	-3.92682800	-0.12909300
C	6.20761600	-2.01679200	1.06431500
N	6.38578800	-4.26669100	1.16223100
C	6.49510000	-3.11976200	1.91981600
C	6.25883700	-0.71305000	1.59618500
C	6.82303700	-2.95447800	3.27127600
C	6.58445900	-0.54714000	2.93893900
C	6.86231400	-1.65562700	3.76804700
H	3.45860900	-3.05820100	-0.97795300
H	4.18346500	-0.32329400	-0.69419800
H	5.56181000	-2.50132900	-2.34720700
H	6.29387000	-1.03283100	-1.71298900
H	5.92416300	-4.69303100	-0.88362600
H	6.54156300	-5.20759500	1.49278200
H	6.05145800	0.15292400	0.97355800
H	7.03911100	-3.80944400	3.90594200
H	6.62864600	0.45412700	3.35950000
H	7.11327500	-1.49205100	4.81261000
N	4.36786900	0.72994700	-2.99857800
C	4.36795400	1.43788500	-4.26795300
C	5.32165200	2.65446100	-4.20239500
O	5.19510400	3.54287600	-5.05614600
O	6.17883000	2.59432400	-3.24860200
H	4.95217500	1.15470900	-2.28288700
H	4.68851200	0.76785700	-5.07701000
H	3.36209900	1.78796200	-4.52672400

Chignolin Tyr Deprotonated

N	-6.75469800	-4.03387300	-1.38215800
C	-5.46769200	-4.48286600	-0.79371400
C	-4.70542900	-3.24896700	-0.29074700
O	-5.27621300	-2.15278300	-0.21537900
H	-6.57289300	-3.51110000	-2.33262200

H	-7.18516900	-3.34245600	-0.75912100
H	-7.40184000	-4.81433900	-1.51176700
H	-5.66812900	-5.16284200	0.03816700
H	-4.90693800	-5.02215200	-1.55966100
N	-3.43056000	-3.47783300	0.05114900
C	-2.54450700	-2.49230200	0.67509600
C	-1.12193200	-2.97678700	0.37024700
O	-0.85068300	-4.17725600	0.51358900
C	-2.80055900	-2.42280200	2.21235000
C	-1.83406700	-1.54510100	2.96902500
C	-1.89712900	-0.13996300	2.90265300
C	-0.78904600	-2.09697500	3.73198000
C	-0.94500300	0.66922200	3.51034300
C	0.16679600	-1.30379300	4.35854400
C	0.18145600	0.13053000	4.23061400
O	1.11970300	0.86583100	4.70852800
H	-3.04792400	-4.41805200	0.01053000
H	-2.72612400	-1.51737900	0.21797700
H	-3.83819200	-2.08421800	2.33166900
H	-2.75140900	-3.45132700	2.58988400
H	-2.71443000	0.32689600	2.35028200
H	-0.72412700	-3.18198700	3.82684500
H	-1.01342500	1.75167700	3.42159100
H	0.96534900	-1.76583600	4.93896500
N	-0.24231500	-2.04781300	-0.06182400
C	1.14796300	-2.39392600	-0.34614600
C	2.05618700	-1.80687500	0.74835300
O	1.99130900	-0.60137200	1.02696800
C	1.61038300	-1.89035000	-1.72873600
C	3.05831800	-2.38178000	-1.97511700
O	3.20384100	-3.55554400	-2.37945600
O	3.99772200	-1.56791400	-1.67315200
H	-0.53074700	-1.07493500	-0.14940200
H	1.18463800	-3.48126600	-0.34129100
H	0.94077700	-2.31564800	-2.48356700
H	1.55584500	-0.79940500	-1.76312500
N	2.92122700	-2.64403800	1.36946800
C	3.72772600	-2.16600400	2.50108900
C	4.95999900	-1.32598000	2.12452100
O	5.54353000	-0.70941700	3.02348300
C	4.12846600	-3.47170000	3.22159600
C	4.20958300	-4.49759300	2.08089700
C	3.03896600	-4.10998600	1.16655200
H	3.11858600	-1.52000400	3.13834600
H	5.06039300	-3.35733100	3.78017500
H	3.33890500	-3.74916900	3.92887500
H	5.15770200	-4.39015300	1.54234600
H	4.13157600	-5.53186300	2.42628100
H	3.22724200	-4.33953100	0.11513600
H	2.10929800	-4.60330000	1.47481700

N	5.37235800	-1.34752500	0.83538500
C	6.45451900	-0.47361600	0.38404000
C	5.93662900	0.93603700	0.03687800
O	6.58366800	1.93543600	0.36896700
C	7.25727700	-1.14627900	-0.74980900
C	8.53540200	-0.39998400	-1.15615900
C	8.36829000	0.75039600	-2.19513600
O	7.40026200	0.65349200	-3.00009000
O	9.25550500	1.64528400	-2.17442400
H	4.77046900	-1.72992200	0.10187700
H	7.11096200	-0.31926800	1.24269900
H	7.50906500	-2.14988800	-0.38149800
H	6.61648000	-1.26903400	-1.62728700
H	9.06292000	-0.01246400	-0.27556900
H	9.22020100	-1.12756900	-1.61821700
N	4.74138100	1.01825000	-0.60763000
C	4.22839400	2.32704800	-0.97172400
C	3.44383100	3.02596300	0.15198400
O	3.31682700	4.25619500	0.13926000
C	3.34137100	2.32418600	-2.23708300
O	2.09523900	1.68206000	-1.93423200
C	4.00560900	1.66029000	-3.44266200
H	4.29218000	0.16610100	-0.96541800
H	5.08427400	2.97710200	-1.17384600
H	3.15292500	3.38318400	-2.45466500
H	1.36573100	2.17837100	-2.36519000
H	5.01828400	2.04333700	-3.60785100
H	3.40464300	1.84157100	-4.34096900
H	4.07772700	0.58039600	-3.28486900
N	2.86314000	2.23607800	1.08779100
C	1.93229800	2.79781200	2.04773900
C	0.57155700	3.21115400	1.47409300
O	-0.17100500	3.95151300	2.12672900
H	2.90067200	1.22356700	0.99091600
H	1.75343100	2.08157100	2.86284300
H	2.36079600	3.70178500	2.48864100
N	0.24112900	2.69952600	0.25889500
C	-0.98619800	3.07766000	-0.40538800
C	-1.85323000	1.84430000	-0.74321300
O	-1.40356800	0.69567500	-0.80449200
C	-0.75983900	3.95322000	-1.66313200
O	-0.13407200	3.12639100	-2.66472400
C	0.06195000	5.20624900	-1.37816600
H	0.92531300	2.14560200	-0.25211700
H	-1.53014200	3.69722500	0.31472000
H	-1.75023200	4.24341000	-2.03718900
H	-0.04148000	3.65467000	-3.47465400
H	-0.44431600	5.83624300	-0.63846900
H	0.17621200	5.79407300	-2.29653700
H	1.05538900	4.94905100	-0.99875100

N	-3.14998800	2.14211900	-0.98041400
C	-4.14846600	1.16715900	-1.38003200
C	-3.84207700	0.60008000	-2.78538600
O	-3.25381800	1.25757400	-3.64725900
C	-5.54725100	1.84494000	-1.40843100
C	-5.91970300	2.55298000	-0.13770600
C	-6.04472000	3.91540800	0.01887300
C	-6.20676100	1.96939200	1.15314700
N	-6.39127700	4.21476600	1.31932100
C	-6.49878100	3.04487400	2.04134000
C	-6.25513000	0.64983100	1.64447700
C	-6.82837900	2.83732300	3.38659200
C	-6.58256800	0.44195700	2.98087600
C	-6.86482500	1.52372000	3.84314700
H	-3.47299400	3.08841500	-0.82120200
H	-4.16113400	0.34458400	-0.65716200
H	-5.56242800	2.55818200	-2.24186000
H	-6.27913300	1.06459400	-1.64900200
H	-5.92711400	4.70454200	-0.71180600
H	-6.54942500	5.14474700	1.67838000
H	-6.04303000	-0.19555900	0.99573600
H	-7.04751100	3.67179700	4.04700200
H	-6.62414700	-0.57184000	3.37060700
H	-7.11672500	1.32747700	4.88185700
N	-4.32766200	-0.64069100	-2.98927700
C	-4.32636700	-1.30439600	-4.28237600
C	-5.29161100	-2.51359400	-4.26891500
O	-5.16503600	-3.36996400	-5.15536300
O	-6.15645900	-2.48184900	-3.32160800
H	-4.90355700	-1.09370200	-2.28392000
H	-4.63436200	-0.60180100	-5.06818400
H	-3.32224100	-1.65505400	-4.54768500

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Calc. for Trp-Cage:

Whole protonated

Charge: 1

N	-10.167107	-0.950178	0.598261
C	-9.501578	-1.919447	-0.305879
C	-8.158774	-1.429458	-0.841558
O	-7.167755	-2.105580	-0.603702
C	-10.451055	-2.416182	-1.411569
C	-11.561352	-3.268743	-0.800909
O	-11.556675	-3.521195	0.394093
N	-12.543391	-3.695590	-1.570377
H	-9.548471	-0.621786	1.358338
H	-10.559282	-0.117455	0.126803
H	-10.956995	-1.486344	1.028459
H	-9.268349	-2.777838	0.323083

H	-10.878265	-1.592485	-1.992877
H	-9.864842	-3.032434	-2.103714
H	-12.592172	-3.527221	-2.570275
H	-13.281156	-4.250883	-1.147101
N	-8.093750	-0.265161	-1.499492
C	-6.848351	0.342045	-2.000726
C	-5.672769	0.294843	-1.001888
O	-4.600524	-0.213413	-1.329449
C	-7.156650	1.762548	-2.524044
C	-7.899236	2.711087	-1.544417
C	-6.988361	3.797247	-0.980967
C	-9.083110	3.392051	-2.234049
H	-8.946933	0.204927	-1.795166
H	-6.482493	-0.256232	-2.842984
H	-6.211692	2.214212	-2.846585
H	-7.761981	1.631431	-3.430002
H	-8.303216	2.128489	-0.703998
H	-6.114861	3.376401	-0.477242
H	-6.633903	4.446107	-1.790085
H	-7.531445	4.417702	-0.257992
H	-8.730110	3.991753	-3.082229
H	-9.809127	2.661875	-2.612182
H	-9.600939	4.058627	-1.535508
N	-5.887921	0.747877	0.238945
C	-4.863876	0.736348	1.287109
C	-4.458705	-0.684408	1.725293
O	-3.302960	-0.920895	2.070084
C	-5.360877	1.562956	2.482342
C	-4.232972	2.242486	3.230340
C	-3.526867	1.549911	4.233250
C	-3.868089	3.560435	2.892969
C	-2.447666	2.170985	4.888837
C	-2.784323	4.182560	3.540616
C	-2.067120	3.482785	4.534093
O	-0.991963	4.053844	5.138925
H	-6.792087	1.139846	0.468509
H	-3.950372	1.182587	0.888229
H	-6.035552	2.338059	2.104142
H	-5.954098	0.933166	3.153814
H	-3.803763	0.535362	4.496316
H	-4.406225	4.103531	2.118542
H	-1.888897	1.649256	5.658383
H	-2.490461	5.189034	3.256628
H	-0.874556	4.961459	4.827301
N	-5.387072	-1.648488	1.661488
C	-5.139087	-3.070072	1.938037
C	-4.179113	-3.634219	0.880263
O	-3.193232	-4.288937	1.221895
C	-6.464968	-3.876759	1.986268
C	-7.599486	-3.194136	2.789988

C	-6.224963	-5.303125	2.507703
C	-7.255436	-2.830182	4.239663
H	-6.278199	-1.425378	1.220770
H	-4.618364	-3.153281	2.895739
H	-6.824484	-3.946419	0.952617
H	-7.912929	-2.279410	2.274486
H	-8.460752	-3.873357	2.770708
H	-5.470612	-5.826321	1.909252
H	-5.880366	-5.288504	3.547647
H	-7.156975	-5.874594	2.456560
H	-6.957776	-3.712802	4.815135
H	-6.436115	-2.103057	4.273664
H	-8.123715	-2.381052	4.734809
N	-4.434986	-3.325415	-0.399314
C	-3.566058	-3.711656	-1.511954
C	-2.177506	-3.044987	-1.442316
O	-1.201240	-3.641803	-1.881363
C	-4.250459	-3.396349	-2.854821
C	-3.880886	-4.423199	-3.940266
C	-4.699295	-5.709677	-3.834671
O	-4.244128	-6.735460	-3.342536
N	-5.928646	-5.704755	-4.318296
H	-5.286059	-2.800554	-0.622398
H	-3.367580	-4.783775	-1.445141
H	-5.337812	-3.403980	-2.710703
H	-3.982161	-2.385280	-3.175047
H	-4.050744	-3.976631	-4.925919
H	-2.823148	-4.682235	-3.864203
H	-6.350169	-4.890383	-4.753842
H	-6.496835	-6.544325	-4.241583
N	-2.066254	-1.835455	-0.877721
C	-0.769261	-1.201356	-0.602586
C	-0.034818	-1.853313	0.583317
O	1.167724	-2.112961	0.498328
C	-0.972488	0.304728	-0.386330
C	0.278962	1.065465	-0.061930
C	1.221381	1.456971	-0.949022
C	0.750084	1.522183	1.242118
N	2.251167	2.095056	-0.280175
C	2.002049	2.179258	1.067610
C	0.245274	1.451538	2.556520
C	2.715585	2.751305	2.129097
C	0.961095	2.003994	3.636499
C	2.183736	2.662969	3.425612
H	-2.911632	-1.301899	-0.664877
H	-0.104741	-1.358333	-1.455224
H	-1.429567	0.706454	-1.299313
H	-1.702818	0.439925	0.420018
H	1.247953	1.345291	-2.020317
H	3.064240	2.538548	-0.719463

H	-0.700857	0.956824	2.747687
H	3.654386	3.259419	1.943724
H	0.546763	1.943112	4.633309
H	2.713778	3.116329	4.255077
N	-0.741779	-2.155311	1.682740
C	-0.150792	-2.824232	2.842982
C	0.323527	-4.249764	2.535208
O	1.430816	-4.598316	2.947121
C	-1.124374	-2.814752	4.035491
C	-1.227278	-1.457852	4.760175
C	-2.285329	-1.555089	5.862666
C	0.096547	-1.031406	5.409872
H	-1.733513	-1.913456	1.738615
H	0.771456	-2.308763	3.121972
H	-2.115941	-3.126217	3.686579
H	-0.779807	-3.563165	4.762528
H	-1.544032	-0.698979	4.037440
H	-3.265560	-1.830010	5.451897
H	-1.997873	-2.316391	6.599299
H	-2.390507	-0.599354	6.389461
H	0.432926	-1.801743	6.115788
H	0.888893	-0.860350	4.675195
H	-0.039938	-0.097075	5.966610
N	-0.453607	-5.065787	1.799292
C	-0.074746	-6.459191	1.482950
C	1.245601	-6.585049	0.708646
O	1.922626	-7.601882	0.823134
C	-1.232292	-7.193606	0.778021
C	-1.440678	-6.817891	-0.699889
C	-0.829360	-7.820320	-1.690213
C	-1.175368	-7.400555	-3.124297
N	-2.030716	-8.397074	-3.807672
H	-1.380280	-4.740098	1.508026
H	0.131926	-6.973829	2.427902
H	-1.039811	-8.268260	0.866966
H	-2.140696	-6.999262	1.357754
H	-2.518774	-6.784399	-0.896760
H	-1.078119	-5.809592	-0.911658
H	0.256428	-7.869595	-1.581972
H	-1.216758	-8.824713	-1.471503
H	-1.738643	-6.469877	-3.128728
H	-0.267857	-7.223006	-3.701107
H	-1.833020	-9.360143	-3.529811
H	-3.019770	-8.151609	-3.600926
H	-1.932869	-8.347054	-4.824542
N	1.625895	-5.542416	-0.034617
C	2.897681	-5.415514	-0.749232
C	4.085022	-5.039016	0.162210
O	5.224768	-5.055552	-0.307784
C	2.719583	-4.363996	-1.862862

C	2.319981	-4.970778	-3.210133
O	1.334337	-5.742353	-3.244237
O	3.026111	-4.648310	-4.194485
H	0.996890	-4.739184	-0.097629
H	3.153530	-6.386149	-1.186308
H	1.992783	-3.613487	-1.525973
H	3.670034	-3.854911	-2.014703
N	3.844741	-4.691259	1.436242
C	4.861891	-4.275635	2.410166
C	4.801491	-2.795950	2.812090
O	5.709749	-2.320390	3.495086
H	2.893826	-4.777083	1.822302
H	4.758522	-4.874037	3.321594
H	5.851936	-4.458329	1.986469
N	3.764656	-2.054910	2.395918
C	3.591677	-0.640851	2.729467
C	4.816040	0.204999	2.327697
O	5.212358	0.162186	1.159687
H	3.043493	-2.448449	1.787201
H	2.739741	-0.283764	2.147101
H	3.361049	-0.535888	3.790147
N	5.447159	0.961257	3.256115
C	6.642878	1.755518	2.954590
C	7.817621	0.926399	2.407358
O	8.613601	1.434618	1.618261
C	7.040840	2.447354	4.265957
C	5.781054	2.389348	5.125297
C	5.105945	1.099640	4.667056
H	6.411257	2.485188	2.172087
H	7.841780	1.877214	4.751107
H	7.397274	3.462550	4.085963
H	5.997400	2.375595	6.194863
H	5.132435	3.243626	4.903103
H	5.491319	0.243671	5.237284
H	4.024948	1.146906	4.804247
N	7.918455	-0.356699	2.780343
C	9.012949	-1.261360	2.405421
C	8.852262	-1.881397	1.006743
O	9.488460	-2.888972	0.712235
C	9.173805	-2.349904	3.477412
O	9.496090	-1.763472	4.724644
H	7.118063	-0.802515	3.232992
H	9.933762	-0.666823	2.360129
H	8.226640	-2.879285	3.611228
H	9.934182	-3.063681	3.151284
H	10.426351	-1.499786	4.721619
N	8.019856	-1.286415	0.141331
C	7.699016	-1.794872	-1.200408
C	7.979766	-0.787778	-2.330521
O	7.524889	-0.967077	-3.458291

C	6.249361	-2.285067	-1.204619
O	6.123897	-3.425092	-2.026227
H	7.369619	-0.596352	0.512155
H	8.346263	-2.658943	-1.373844
H	5.964045	-2.520739	-0.175137
H	5.581773	-1.489628	-1.549054
H	5.798589	-4.167750	-1.463392
N	8.718472	0.294032	-2.036522
C	9.140965	1.289609	-3.030499
C	7.998248	2.127616	-3.616869
O	8.117582	2.609391	-4.742205
H	9.047442	0.403430	-1.075418
H	9.865252	1.952596	-2.548598
H	9.625582	0.797159	-3.877337
N	6.886521	2.281796	-2.880572
C	5.648980	2.917884	-3.351225
C	4.957031	3.726907	-2.234134
O	4.767948	3.194795	-1.137175
C	4.724697	1.844302	-3.962529
C	4.333246	0.715752	-2.989967
C	3.502981	-0.415701	-3.614822
N	4.338641	-1.482943	-4.195215
C	4.814749	-1.581947	-5.428936
N	4.596443	-0.662491	-6.342124
N	5.519635	-2.631091	-5.767156
H	6.844077	1.877732	-1.947135
H	5.960644	3.580879	-4.161077
H	3.819818	2.329070	-4.353053
H	5.280271	1.426171	-4.809543
H	5.239201	0.274712	-2.571271
H	3.766799	1.134646	-2.158278
H	2.898408	-0.896482	-2.841730
H	2.808940	-0.037700	-4.374073
H	4.617374	-2.225028	-3.551838
H	4.084411	0.186733	-6.140183
H	4.885227	-0.794096	-7.305101
H	5.579935	-3.434346	-5.148541
H	5.960327	-2.716520	-6.675990
N	4.553570	4.989758	-2.483184
C	3.891601	5.823554	-1.479068
C	2.467496	5.321597	-1.170924
O	1.887522	4.602044	-1.987879
C	3.873442	7.232269	-2.085604
C	3.811830	6.969742	-3.588672
C	4.641797	5.697012	-3.753853
H	4.480042	5.794574	-0.555805
H	3.025366	7.817433	-1.722518
H	4.800692	7.753220	-1.826211
H	2.776341	6.768407	-3.881321
H	4.202640	7.793485	-4.187489

H	4.263708	5.083093	-4.576286
H	5.686616	5.953041	-3.969525
N	1.884584	5.701161	-0.016883
C	0.526489	5.307572	0.340914
C	-0.514678	6.001741	-0.555581
O	-0.328187	7.163325	-0.923274
C	0.354721	5.705733	1.808479
C	1.322655	6.874936	1.977471
C	2.469868	6.525188	1.030416
H	0.440654	4.225643	0.225610
H	-0.678776	5.975724	2.037234
H	0.654136	4.865993	2.441874
H	0.839944	7.793724	1.628927
H	1.664490	7.010947	3.005327
H	2.935099	7.427642	0.622656
H	3.243027	5.960018	1.568815
N	-1.631462	5.326867	-0.879093
C	-2.719916	5.910404	-1.654963
C	-3.578390	6.842594	-0.781405
O	-4.083446	6.426143	0.263421
C	-3.500472	4.702717	-2.176700
C	-3.330142	3.663336	-1.067692
C	-1.921061	3.935808	-0.551689
H	-2.288324	6.491894	-2.476019
H	-4.543617	4.945040	-2.386542
H	-3.028824	4.350892	-3.100572
H	-4.053716	3.856457	-0.275738
H	-3.445760	2.636338	-1.420949
H	-1.861088	3.754842	0.526728
H	-1.193672	3.277632	-1.041096
N	-3.725787	8.103033	-1.212874
C	-4.634605	9.108776	-0.636841
C	-6.083447	8.891051	-1.078792
O	-6.300261	8.806094	-2.307183
C	-4.202650	10.518687	-1.049035
O	-2.896786	10.775070	-0.579015
O	-6.944595	8.857853	-0.175374
H	-3.271776	8.368548	-2.083264
H	-4.594503	9.018460	0.451480
H	-4.189225	10.571866	-2.141719
H	-4.960646	11.226609	-0.679697
H	-2.911619	10.739616	0.413507

Tyr3 Deprotonated

N	-10.168094	-0.943148	0.602433
C	-9.503091	-1.911004	-0.303607
C	-8.160191	-1.420543	-0.838611
O	-7.169391	-2.097483	-0.602173
C	-10.452947	-2.405334	-1.410049
C	-11.563468	-3.258593	-0.800772

O	-11.558685	-3.513251	0.393762
N	-12.545803	-3.683644	-1.570858
H	-9.548713	-0.615120	1.362162
H	-10.561166	-0.109836	0.132480
H	-10.957582	-1.480020	1.032612
H	-9.270080	-2.770433	0.323979
H	-10.880187	-1.580148	-1.989460
H	-9.867158	-3.020022	-2.103824
H	-12.595602	-3.511766	-2.570117
H	-13.284041	-4.239113	-1.148645
N	-8.094831	-0.255060	-1.494409
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C	-5.673551	0.303096	-0.996187
O	-4.601557	-0.204967	-1.324869
C	-7.157127	1.774176	-2.515380
C	-7.899182	2.721191	-1.533877
C	-6.987793	3.805961	-0.968581
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H	-8.947891	0.217565	-1.786188
H	-6.484244	-0.244424	-2.838298
H	-6.211827	2.226036	-2.836837
H	-7.762619	1.645502	-3.421642
H	-8.303065	2.137231	-0.694319
H	-6.115838	3.383863	-0.463145
H	-6.631161	4.454632	-1.776905
H	-7.531431	4.426913	-0.246386
H	-8.729745	4.005516	-3.068830
H	-9.809010	2.674714	-2.602134
H	-9.600813	4.068923	-1.522083
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C	-4.864097	0.740068	1.293481
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O	-3.303685	-0.919216	2.073131
C	-5.360577	1.564661	2.490322
C	-4.232283	2.242376	3.239379
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H	-3.951167	1.189316	0.897582
H	-6.036367	2.338388	2.107915
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H	-3.809397	0.529130	4.490453
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C	-7.600961	-3.192130	2.789577
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H	-2.826344	-4.669809	-3.867989
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H	-2.912746	-1.296983	-0.657479

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H	2.711643	3.117870	4.263438
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C	-0.152117	-2.825185	2.841976
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H	0.770313	-2.310636	3.122427
H	-2.117190	-3.127695	3.684657
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H	-3.264246	-1.841621	5.453600
H	-1.995122	-2.317662	6.604674
H	-2.395636	-0.601504	6.382974
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H	0.888362	-0.865265	4.677141
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H	3.150246	-6.380845	-1.194620
H	1.990864	-3.606811	-1.528470
H	3.667806	-3.848864	-2.018419
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H	3.041586	-2.448457	1.786764
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H	5.580085	-1.485099	-1.549080
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N	1.886047	5.704687	-0.002508
C	0.527862	5.310959	0.354795
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C	0.356497	5.706479	1.823122
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C	2.471827	6.526556	1.046208
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Tyr3 and Ser13 Deprotonated

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H	-9.790965	2.685240	-2.619899
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C	-6.467257	-3.865062	1.977415
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H	-4.620804	-3.146361	2.891122
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H	-8.464655	-3.859104	2.757998
H	-5.477090	-5.816536	1.898829
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O	-1.195780	-3.634381	-1.879906
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H	-5.330375	-3.388274	-2.716592
H	-3.972190	-2.371236	-3.176947
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H	-2.815758	-4.669551	-3.866836
H	-6.341440	-4.870261	-4.763578
H	-6.492179	-6.524502	-4.253647
N	-2.059559	-1.827800	-0.875618
C	-0.761990	-1.196306	-0.597220
C	-0.030938	-1.851047	0.589252
O	1.171308	-2.112682	0.506217
C	-0.963010	0.309854	-0.379434
C	0.289147	1.067991	-0.051692
C	1.233928	1.458982	-0.936495
C	0.758578	1.522242	1.253826
N	2.263559	2.094429	-0.264886
C	2.012009	2.177361	1.082530

C	0.251148	1.450813	2.567176
C	2.724525	2.746812	2.146097
C	0.965872	2.000654	3.649214
C	2.190057	2.657764	3.441486
H	-2.904178	-1.294754	-0.658458
H	-0.096245	-1.353687	-1.448790
H	-1.418221	0.713216	-1.292805
H	-1.694817	0.444799	0.425688
H	1.262128	1.349686	-2.008083
H	3.077039	2.538327	-0.702339
H	-0.700926	0.968679	2.759263
H	3.664528	3.253683	1.962312
H	0.525904	1.974725	4.635795
H	2.716604	3.114453	4.271508
N	-0.740540	-2.153184	1.686952
C	-0.152900	-2.824621	2.847459
C	0.319524	-4.250585	2.538776
O	1.425446	-4.601588	2.952328
C	-1.128732	-2.814954	4.038127
C	-1.230651	-1.458794	4.764335
C	-2.290967	-1.555583	5.864689
C	0.092673	-1.035478	5.417088
H	-1.730744	-1.903623	1.744600
H	0.769790	-2.311248	3.129296
H	-2.120108	-3.124027	3.686280
H	-0.786940	-3.565517	4.764511
H	-1.546090	-0.696460	4.045194
H	-3.269078	-1.835425	5.452100
H	-2.002913	-2.312352	6.606068
H	-2.400758	-0.595828	6.382488
H	0.426291	-1.806052	6.124330
H	0.886534	-0.865377	4.683683
H	-0.045142	-0.099611	5.970585
N	-0.457642	-5.064318	1.800350
C	-0.080592	-6.457982	1.482966
C	1.241006	-6.585161	0.711011
O	1.916041	-7.603314	0.825492
C	-1.238069	-7.189486	0.774901
C	-1.442993	-6.811538	-0.702922
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C	-1.174085	-7.391599	-3.127557
N	-2.029862	-8.385755	-3.813824
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H	0.123603	-6.974308	2.427571
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H	-2.147237	-6.994454	1.353209
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H	-1.078429	-5.803600	-0.913045
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H	-1.843773	-9.348433	-3.526274
H	-3.019060	-8.132170	-3.616867
H	-1.920783	-8.344666	-4.829793
N	1.624527	-5.542250	-0.030206
C	2.897889	-5.416659	-0.742242
C	4.084144	-5.043383	0.171932
O	5.224772	-5.061285	-0.295949
C	2.723739	-4.363425	-1.854874
C	2.325643	-4.967804	-3.203669
O	1.338725	-5.737615	-3.240626
O	3.034206	-4.645321	-4.186269
H	0.997052	-4.737772	-0.093203
H	3.152850	-6.387136	-1.180222
H	1.998115	-3.611688	-1.518011
H	3.675674	-3.856248	-2.004306
N	3.842017	-4.696822	1.445973
C	4.858071	-4.284203	2.422319
C	4.799473	-2.804926	2.826013
O	5.707256	-2.331814	3.511337
H	2.889979	-4.780005	1.829863
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H	5.848523	-4.467282	1.999880
N	3.764723	-2.061554	2.408812
C	3.593570	-0.647618	2.743823
C	4.820166	0.196603	2.345457
O	5.218629	0.154579	1.178148
H	3.044443	-2.451902	1.797320
H	2.742987	-0.287661	2.161254
H	3.361599	-0.543218	3.804329
N	5.450832	0.950585	3.276031
C	6.648500	1.743145	2.977784
C	7.822841	0.912674	2.431735
O	8.621203	1.420504	1.644799
C	7.045170	2.432622	4.290784
C	5.783653	2.375728	5.147656
C	5.107176	1.087779	4.686494
H	6.417717	2.475110	2.196847
H	7.844163	1.859776	4.775931
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H	5.997041	2.360588	6.217978
H	5.136432	3.231046	4.925057
H	5.490502	0.230618	5.256595
H	4.025911	1.136956	4.821763
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C	9.014354	-1.277166	2.429290
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O	9.490265	-2.903450	0.734948
C	9.171283	-2.367335	3.500208

O	9.492217	-1.783050	4.748791
H	7.143045	-0.811301	3.293863
H	9.940832	-0.691444	2.404987
H	8.229286	-2.951986	3.520138
H	9.953423	-3.052450	3.128335
N	8.025537	-1.297615	0.163290
C	7.706357	-1.803828	-1.179693
C	7.991020	-0.795787	-2.307999
O	7.537971	-0.972864	-3.436856
C	6.255870	-2.291471	-1.187301
O	6.129963	-3.430278	-2.010536
H	7.378798	-0.606403	0.537122
H	8.353527	-2.668497	-1.351685
H	5.969681	-2.528332	-0.158479
H	5.589317	-1.494957	-1.531607
H	5.803182	-4.172751	-1.449006
N	8.731041	0.284362	-2.011224
C	9.157153	1.280461	-3.003131
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O	8.139327	2.604187	-4.715104
H	9.057845	0.389143	-1.048580
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H	9.643753	0.789442	-3.849694
N	6.904158	2.276380	-2.856231
C	5.668625	2.915221	-3.328425
C	4.975959	3.724032	-2.211625
O	4.783857	3.190859	-1.115703
C	4.743639	1.844023	-3.942847
C	4.348375	0.714928	-2.972460
C	3.517338	-0.414284	-3.600331
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C	4.830519	-1.580518	-5.413427
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N	5.534224	-2.630459	-5.751638
H	6.859194	1.870136	-1.923805
H	5.983186	3.578696	-4.136783
H	3.840158	2.331193	-4.333894
H	5.298912	1.425707	-4.789977
H	5.252520	0.271126	-2.552767
H	3.780987	1.133730	-2.141232
H	2.911662	-0.895645	-2.828491
H	2.823990	-0.033720	-4.359031
H	4.607546	-2.238571	-3.544122
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H	4.935605	-0.775135	-7.280939
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H	5.951309	-2.729107	-6.670186
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O	1.907515	4.604202	-1.970093
C	3.898191	7.231087	-2.060707
C	3.838978	6.970567	-3.564220
C	4.667046	5.696606	-3.729440
H	4.499320	5.790232	-0.531536
H	3.050317	7.817035	-1.698275
H	4.825686	7.750429	-1.798943
H	2.803745	6.771422	-3.859083
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N	1.902738	5.700829	0.002287
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O	-0.305756	7.167989	-0.906451
C	0.369416	5.705753	1.824745
C	1.339059	6.873054	1.997055
C	2.487464	6.522508	1.051741
H	0.455932	4.227503	0.240520
H	-0.663983	5.964827	2.062989
H	0.677019	4.867044	2.452706
H	0.860587	7.794766	1.649847
H	1.679337	7.005689	3.025829
H	2.955948	7.424277	0.645807
H	3.258308	5.954879	1.591021
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C	-2.698265	5.920164	-1.644272
C	-3.556777	6.852741	-0.771163
O	-4.064542	6.435850	0.272172
C	-3.479927	4.714499	-2.169025
C	-3.313515	3.673424	-1.061012
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H	-4.522223	4.959163	-2.380994
H	-3.007071	4.363165	-3.092531
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H	-3.429667	2.647033	-1.416253
H	-1.850038	3.761844	0.536754
H	-1.177179	3.283793	-1.029719
N	-3.701161	8.113980	-1.201314
C	-4.609322	9.120575	-0.625733
C	-6.057696	8.905935	-1.070710
O	-6.272320	8.822910	-2.299618
C	-4.174129	10.530251	-1.035315
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O	-6.920617	8.873093	-0.168974
H	-3.245086	8.379694	-2.070551
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H	-4.158361	10.584868	-2.127982
H	-4.931818	11.238952	-0.666816

H	-2.887393	10.755289	0.430206

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N	-10.165061	-0.925221	0.604185
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C	-10.453796	-2.385704	-1.408980
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H	-10.556608	-0.091049	0.134579
H	-10.955242	-1.460652	1.034721
H	-9.270992	-2.754318	0.324337
H	-10.879154	-1.559383	-1.988044
H	-9.869487	-3.001599	-2.102989
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O	-4.597635	-0.198029	-1.324727
C	-7.149351	1.787271	-2.513251
C	-7.889006	2.735359	-1.530972
C	-6.975072	3.817852	-0.965421
C	-9.071505	3.420974	-2.218350
H	-8.943306	0.233435	-1.785192
H	-6.480976	-0.232545	-2.837557
H	-6.203180	2.237241	-2.834713
H	-7.755427	1.660441	-3.419376
H	-8.293756	2.151766	-0.691613
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H	-6.617304	4.466195	-1.773505
H	-7.517109	4.439581	-0.242685
H	-8.717351	4.022262	-3.064961
H	-9.799323	2.693570	-2.598486
H	-9.587682	4.086804	-1.517849
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C	-4.857192	0.746161	1.294226
C	-4.455409	-0.676662	1.728809
O	-3.300088	-0.916909	2.072421
C	-5.351459	1.571180	2.491689
C	-4.221434	2.246053	3.240704
C	-3.516567	1.549296	4.241585
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O	-0.974822	4.044606	5.151873

H	-6.782324	1.161844	0.477926
H	-3.943496	1.193636	0.898120
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H	-5.950814	0.937500	3.155879
H	-3.801603	0.531142	4.490552
H	-4.397285	4.101159	2.128852
H	-1.867231	1.643353	5.660451
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C	-4.183771	-3.625152	0.876606
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C	-6.469653	-3.864511	1.983247
C	-7.602007	-3.180921	2.789194
C	-6.233005	-5.292722	2.501155
C	-7.256270	-2.821300	4.239549
H	-6.276523	-1.411054	1.223280
H	-4.620390	-3.148316	2.893252
H	-6.829878	-3.930638	0.949592
H	-7.913088	-2.264163	2.275971
H	-8.465215	-3.857740	2.768733
H	-5.480849	-5.816472	1.900393
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H	-6.960282	-3.706049	4.812690
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H	-8.123038	-2.371186	4.736476
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C	-3.572173	-3.698447	-1.516114
C	-2.181892	-3.035481	-1.445627
O	-1.207380	-3.633730	-1.886615
C	-4.256476	-3.378199	-2.857862
C	-3.890089	-4.403396	-3.945946
C	-4.711714	-5.688037	-3.842981
O	-4.258900	-6.716145	-3.353533
N	-5.941302	-5.678834	-4.325939
H	-5.287074	-2.781233	-0.622688
H	-3.376226	-4.771195	-1.451755
H	-5.343805	-3.383289	-2.713060
H	-3.985683	-2.366998	-3.175556
H	-4.059212	-3.954263	-4.930606
H	-2.832993	-4.665329	-3.870638
H	-6.361090	-4.862128	-4.758822
H	-6.511794	-6.516986	-4.250727
N	-2.067265	-1.827584	-0.878212
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C	-0.035113	-1.854093	0.581698
O	1.166720	-2.116596	0.495451
C	-0.967797	0.308632	-0.382306
C	0.285757	1.065407	-0.056762

C	1.228702	1.456627	-0.943419
C	0.758725	1.517816	1.248120
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C	2.012267	2.172118	1.074512
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H	-1.697489	0.443207	0.424792
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H	-0.697436	0.963518	2.756462
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H	0.534833	1.966438	4.631227
H	2.725139	3.105353	4.262831
N	-0.742261	-2.156910	1.680774
C	-0.152369	-2.830096	2.839105
C	0.318159	-4.256093	2.527684
O	1.424774	-4.608441	2.938177
C	-1.125296	-2.820982	4.032151
C	-1.224364	-1.465556	4.760120
C	-2.282079	-1.562728	5.862939
C	0.100883	-1.044028	5.410127
H	-1.732372	-1.908431	1.740178
H	0.771777	-2.317994	3.118560
H	-2.117873	-3.128648	3.682455
H	-0.782291	-3.572652	4.756822
H	-1.540893	-0.702236	4.042539
H	-3.261466	-1.840888	5.452220
H	-1.993108	-2.321010	6.602431
H	-2.389687	-0.603678	6.382578
H	0.435369	-1.815590	6.115916
H	0.893153	-0.874449	4.674886
H	-0.034589	-0.108432	5.964672
N	-0.461437	-5.068380	1.790240
C	-0.086291	-6.461985	1.470379
C	1.233324	-6.589356	0.695074
O	1.907819	-7.608178	0.806779
C	-1.246073	-7.191771	0.764318
C	-1.454279	-6.812005	-0.712582
C	-0.846036	-7.813623	-1.705616
C	-1.191729	-7.389563	-3.138512
N	-2.049970	-8.382271	-3.823804
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H	0.118095	-6.979508	2.414555
H	-1.055547	-8.267250	0.849947
H	-2.154547	-6.997956	1.344354

H	-2.532561	-6.775512	-0.908931
H	-1.089840	-5.803868	-0.920697
H	0.239575	-7.864675	-1.597264
H	-1.235249	-8.817978	-1.489177
H	-1.754200	-6.458308	-3.138070
H	-0.284054	-7.208351	-3.714377
H	-1.865272	-9.345101	-3.536121
H	-3.038404	-8.126339	-3.625001
H	-1.942375	-8.341845	-4.839946
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C	4.076384	-5.049254	0.150812
O	5.215837	-5.067569	-0.319827
C	2.711602	-4.365938	-1.871920
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O	1.322125	-5.737469	-3.255837
O	3.016178	-4.645472	-4.204377
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H	3.135713	-6.391003	-1.201640
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O	5.709778	-2.342722	3.489289
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H	5.840905	-4.469405	1.960533
N	3.764789	-2.069675	2.391792
C	3.595585	-0.655979	2.728800
C	4.821886	0.187708	2.328394
O	5.217479	0.146671	1.160075
H	3.047853	-2.466847	1.780733
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H	3.366148	-0.552114	3.790039
N	5.455416	0.940144	3.258275
C	6.652995	1.732076	2.958006
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O	8.622191	1.409350	1.619868
C	7.053405	2.419770	4.270806
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H	6.010594	2.346502	6.200256
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C	9.015090	-1.289504	2.400391
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C	9.173738	-2.381006	3.469701
O	9.498171	-1.798370	4.718154
H	7.118671	-0.829489	3.223463
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C	3.504125	-0.415485	-3.614886
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H	4.753084	-2.138998	-3.515070
H	4.121072	0.208489	-6.127044
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N	4.569065	4.984572	-2.470935
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C	4.658423	5.694626	-3.739962
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H	2.795647	6.771107	-3.863867
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H	5.703732	5.948516	-3.955990
N	1.903196	5.696883	-0.001526
C	0.544292	5.305898	0.356054
C	-0.495576	6.004849	-0.538231
O	-0.306322	7.166827	-0.903255
C	0.374310	5.700996	1.824655
C	1.345306	6.867326	1.995916
C	2.491127	6.516920	1.047420
H	0.455815	4.224442	0.238644
H	-0.658278	5.960686	2.065698
H	0.682879	4.861258	2.450757
H	0.866690	7.789844	1.650976
H	1.688177	6.998582	3.024004
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H	3.262826	5.948071	1.584196
N	-1.614245	5.333591	-0.862755
C	-2.701617	5.921743	-1.636653
C	-3.557256	6.854029	-0.760420
O	-4.062820	6.436376	0.283680
C	-3.485519	4.717292	-2.160849
C	-3.317252	3.674841	-1.054412
C	-1.907211	3.942497	-0.538511
H	-2.269003	6.504477	-2.456424
H	-4.528144	4.963030	-2.369859
H	-3.015173	4.366591	-3.085864
H	-4.038870	3.865615	-0.260160
H	-3.435019	2.648943	-1.410542
H	-1.849877	3.760411	0.539889
H	-1.181179	3.283451	-1.028712
N	-3.701672	8.115864	-1.188807
C	-4.607623	9.122540	-0.609897
C	-6.057247	8.909556	-1.051593
O	-6.274923	8.828079	-2.280068
C	-4.172298	10.532326	-1.018960
O	-2.865538	10.784265	-0.549026
O	-6.918001	8.876396	-0.147799

H	-3.248297	8.381968	-2.059330
H	-4.567137	9.029679	0.478174
H	-4.159179	10.588139	-2.111550
H	-4.928479	11.241291	-0.647616
H	-2.878767	10.738563	0.443119