Supporting Information

Gas-Phase Geometry Optimization of Biological Molecules as a Reasonable Alternative to a Continuum Environment Description: Fact, myth or fiction?

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1. Gas-phase equilibrium structures

Alanine

N	19.640261	102.632326	56.700004
C	18.648045	102.802775	55.619607
C	19.253081	102.294212	54.289026
O	18.730764	102.481647	53.213286
C	18.095021	104.223162	55.470434
H	20.139715	103.498715	56.886463
H	17.817198	102.116485	55.826830
O	20.389255	101.594886	54.437139
H	17.414228	104.278189	54.618301
H	18.907731	104.938008	55.295537
H	17.559010	104.521796	56.376786
H	20.583475	101.618658	55.404846
H	19.213816	102.329541	57.569439

Arginine

N	20.379303	100.121699	58.950037
C	21.012211	101.205701	58.191039
C	20.097773	101.618466	57.005040
O	18.840364	101.179820	57.101225
C	22.435829	100.941768	57.669802
C	23.506176	100.906151	58.768227
C	24.899073	100.706188	58.164517
N	25.932238	100.705532	59.220570
C	27.246060	100.811023	59.016661
N	27.746665	100.773658	57.774207
N	28.082471	100.965896	60.057727
H	20.650600	99.195354	58.632075
H	18.797846	100.626848	57.913987
H	21.030816	102.089961	58.842247
O	20.495191	102.308544	56.093954
H	22.437031	99.994875	57.111674
H	22.665463	101.730515	56.946330
H	23.492041	101.850552	59.327995
H	23.297881	100.095769	59.480451
H	24.937204	99.756479	57.615397
H	25.120383	101.523184	57.469086
H	25.618875	100.555915	60.171335
H	28.707106	101.023071	57.587910
H	27.178115	100.503323	56.985757

Asparagine

N	37.916337	89.961586	61.971624
C	38.173998	88.639722	61.372649
C	38.497660	88.850661	59.874697
O	38.465576	87.959597	59.048026
C	37.058430	87.586951	61.603657
C	37.550321	86.139838	61.753629
O	37.435851	85.546889	62.824294
N	38.098691	85.582685	60.645295
H	38.199736	89.994042	62.945944
H	36.928781	90.204549	61.930635
H	39.108079	88.271799	61.817071
O	38.847732	90.099616	59.564405
H	36.559289	87.815178	62.547304
H	36.317948	87.645051	60.797235
H	38.460447	84.642703	60.713903
H	38.248971	86.136702	59.807495
H	38.735052	90.617631	60.399536

Aspartic acid

N	25.454552	91.031020	63.161693
C	25.701952	92.014125	62.078686
C	27.082542	91.731410	61.470447
O	27.687650	92.473067	60.722418
C	25.453225	93.464700	62.492863
C	23.980019	93.718130	62.977354
O	23.189877	92.726299	62.921031
O	23.746711	94.883261	63.373220
H	25.829033	91.414443	64.031120
H	26.866447	90.152592	62.419752
H	24.979257	91.772002	61.287818
O	27.565498	90.513975	61.809609
H	26.139061	93.752968	63.302543
H	25.668497	94.139075	61.657652
H	24.437580	91.053332	63.289093

Cysteine

N	89.901761	58.439133	53.085399
C	91.159833	59.149929	53.334733
C	92.318854	58.126010	53.420028
O	92.020451	56.923344	52.910435
C	91.186138	60.117154	54.530686
S	90.653084	59.356998	56.127424
H	89.240536	58.992028	52.549779
H	89.463687	58.165884	53.963953

H	91.385803	59.742290	52.437035
O	93.411345	58.405980	53.858716
H	92.212426	60.454073	54.686198
H	90.561646	60.991158	54.332959
H	89.358183	59.728450	56.064530
H	91.069053	56.969569	52.657226

Glutamic acid

N	84.182548	58.275088	54.027763
C	83.871178	58.650572	52.621158
C	84.733113	59.913101	52.216484
O	84.515874	60.363439	51.068900
C	82.366680	58.891217	52.404577
C	81.720249	59.932501	53.352126
C	81.165438	59.388991	54.670216
O	80.040753	59.672872	55.063937
O	81.968014	58.596814	55.378269
H	82.884766	58.463657	54.899626
H	84.950299	58.921126	54.273093
H	84.180514	57.846379	51.940010
O	85.552355	60.306627	53.095561
H	82.263995	59.251398	51.376960
H	81.816970	57.941480	52.476500
H	82.456099	60.714186	53.586499
H	80.882455	60.427055	52.855238
H	84.541301	57.325499	54.084383

Glutamine

N	87.739117	58.292680	51.667099
C	88.548480	57.100414	51.374299
C	90.043778	57.441291	51.545359
O	90.940758	56.746633	51.119840
C	88.295769	56.414677	50.020066
C	86.819633	56.036806	49.757026
C	86.188554	55.247758	50.897253
O	85.826795	55.795479	51.939230
N	86.067649	53.902969	50.714763
H	86.831267	58.011069	52.030864
H	87.583832	58.857878	50.834767
H	88.329938	56.384065	52.175272
O	90.261698	58.563294	52.248363
H	88.625216	57.077646	49.209788
H	88.935060	55.528532	49.965678
H	86.216001	56.942441	49.641261
H	86.759700	55.485517	48.812077
H	85.685437	53.346117	51.466088

H	86.366597	53.441141	49.870639
H	89.363021	58.928196	52.436869

Glycine

N	23.320252	74.523594	62.744612
C	22.529243	73.317515	63.029416
C	22.047646	73.297274	64.489983
O	22.309679	74.426188	65.165933
H	24.312659	74.328447	62.664491
H	22.786763	75.008811	64.527926
H	21.632817	73.286533	62.402343
H	23.073604	72.385133	62.848335
O	21.472252	72.349381	64.973343
H	23.022484	74.999924	61.900817

Histidine

N	38.655311	86.964840	49.805393
C	38.503502	86.704045	48.362106
C	38.229686	88.057156	47.662382
O	37.780287	88.159951	46.537114
C	37.453194	85.617368	48.005487
C	37.648036	84.914275	46.697262
N	37.629107	85.543027	45.468449
C	37.842142	83.579691	46.405083
C	37.816771	84.584301	44.516104
N	37.944930	83.383003	45.046374
H	37.768696	86.876406	50.297774
H	38.841946	88.760962	49.270029
H	39.481819	86.376868	47.988104
O	38.557828	89.123186	48.394565
H	37.506080	84.850661	48.785637
H	36.449814	86.062220	48.066474
H	37.558565	86.550606	45.359288
H	37.903268	82.753053	47.100620
H	37.853891	84.815158	43.460591
H	39.314128	86.325521	50.238464

Isoleucine

N	36.433620	92.418481	57.654639
C	37.876472	92.173547	57.855039
C	38.251745	92.720286	59.247788
O	39.199982	92.323290	59.886762
C	38.695750	92.854167	56.716916

C	38.520215	92.065302	55.396552
C	40.183346	93.020345	57.065355
C	38.947985	92.829957	54.137165
H	36.192627	92.518808	56.674137
H	36.699925	93.733521	59.034575
H	38.130120	91.105379	57.871174
O	37.437706	93.696592	59.688330
H	38.261619	93.856865	56.579420
H	39.091719	91.129917	55.473816
H	37.471864	91.763828	55.270636
H	40.721805	93.464994	56.223862
H	40.644737	92.053744	57.294181
H	40.333549	93.666010	57.933121
H	38.761803	92.230562	53.239861
H	40.013261	93.079017	54.147561
H	38.387636	93.766776	54.033248
H	35.864015	91.667611	58.035361

Leucine

N	36.739370	92.834375	61.957196
C	36.118874	91.770358	62.772125
C	36.859999	90.435892	62.513411
O	36.471778	89.371787	62.941503
C	34.603634	91.598076	62.572605
C	33.732666	92.785712	63.027725
C	32.276699	92.565951	62.585808
C	33.805798	93.020842	64.545171
H	36.196859	93.030190	61.119416
H	38.047039	91.531411	61.589639
H	36.324088	91.997535	63.825047
O	37.989495	90.567896	61.801479
H	34.422967	91.405155	61.504598
H	34.297067	90.689118	63.101870
H	34.095701	93.695883	62.525686
H	31.645796	93.416212	62.867039
H	31.856917	91.668690	63.056943
H	32.202420	92.437144	61.500092
H	33.162553	93.857159	64.839762
H	34.819788	93.257355	64.886262
H	33.470020	92.132187	65.093509
H	36.845070	93.704371	62.467516

Lysine

N	69.914967	63.458551	55.498223
C	71.002465	63.767014	56.435321
C	70.924227	65.262390	56.826578

O	71.567284	65.722378	57.750475
C	72.374299	63.442296	55.796116
C	73.574047	63.947935	56.611297
C	74.935976	63.436305	56.115375
C	76.096866	64.274927	56.648665
N	76.013002	64.427484	58.170539
H	70.184342	62.804147	54.770225
H	69.714611	65.368218	55.414762
H	70.918158	63.205849	57.374921
O	70.131523	65.998922	56.052065
H	72.435623	62.352681	55.679154
H	72.410961	63.876349	54.788252
H	73.566385	65.043769	56.596640
H	73.418113	63.655120	57.658679
H	75.081067	62.378830	56.370663
H	75.000113	63.498429	55.022420
H	77.074358	63.835995	56.438964
H	76.070845	65.294933	56.257880
H	76.777675	65.004677	58.535185
H	76.055685	63.517658	58.642108
H	75.126276	64.872014	58.439518

Methionine

N	62.613002	80.345746	50.966048
C	62.136258	80.551497	52.345931
C	62.911240	79.619433	53.303108
O	63.981487	79.032416	52.746573
C	60.621340	80.405010	52.549588
C	59.774409	81.462877	51.831299
S	60.132436	83.212902	52.262080
C	59.619584	83.256060	54.017336
H	62.007157	79.720234	50.440638
H	63.980651	79.333536	51.806150
H	62.421849	81.569238	52.640643
O	62.601573	79.458495	54.463353
H	60.305218	79.412800	52.194151
H	60.423307	80.415778	53.624750
H	59.926594	81.418770	50.747159
H	58.711199	81.269323	52.009736
H	59.718932	84.294148	54.342355
H	60.256557	82.629900	54.646113
H	58.574199	82.952840	54.124332
H	62.690207	81.216596	50.451358

Phenylalanine

N	69.119201	74.147543	77.394520

C	68.219057	74.978335	78.216344
C	66.907232	75.187970	77.424226
O	66.130704	76.092537	77.634985
C	68.815860	76.315773	78.745501
C	68.464058	76.638576	80.186661
C	69.419281	76.466594	81.199587
C	67.186738	77.101793	80.540801
C	69.110909	76.742929	82.534897
C	66.877492	77.379020	81.874456
C	67.836258	77.200138	82.876444
H	69.675538	74.715565	76.758868
H	67.494685	73.689529	76.478080
H	67.930431	74.361064	79.076556
O	66.681602	74.246597	76.493843
H	69.905905	76.242397	78.663615
H	68.493514	77.132605	78.090915
H	70.418230	76.120891	80.941946
H	66.438816	77.233352	79.765200
H	69.866791	76.606039	83.303229
H	65.884575	77.738185	82.130373
H	67.593048	77.418681	83.912299
H	69.761274	73.608987	77.967653

Proline

N	60.332776	60.598003	64.349041
C	59.769173	59.279253	63.955652
C	59.739259	59.133637	62.426071
O	59.344828	58.132909	61.869460
C	58.346221	59.212709	64.577271
C	58.415557	60.212222	65.742963
C	59.327496	61.311227	65.178206
H	61.199999	60.478410	64.861664
H	60.389738	58.460650	64.336675
O	60.177728	60.219113	61.769471
H	57.598821	59.533133	63.843148
H	58.087813	58.196133	64.880024
H	57.430800	60.584926	66.041714
H	58.881684	59.748497	66.621489
H	58.752888	61.993816	64.539694
H	59.826439	61.914825	65.941391
H	60.447580	60.850136	62.483766

Serine

N	56.743530	71.210065	69.891718
C	56.964886	69.868252	70.451506
C	56.368855	68.808476	69.501822

O	56.165941	67.660805	69.830748
C	56.461792	69.667962	71.879758
O	57.150578	70.615482	72.697867
H	55.858906	71.597792	70.215184
H	56.354795	70.229613	68.293988
H	58.048260	69.691565	70.453082
O	56.128585	69.268950	68.265708
H	55.373819	69.834875	71.917976
H	56.661833	68.637388	72.190315
H	56.922716	70.462508	73.623174
H	57.469404	71.851466	70.195654

Threonine

N	67.357270	68.099219	64.808634
C	68.032238	67.768527	66.071252
C	68.797649	69.020165	66.562141
O	69.682984	68.971801	67.390010
C	68.983392	66.553459	66.007467
O	69.964930	66.773326	64.983673
C	68.266917	65.250634	65.679733
H	67.963070	67.867138	64.022452
H	67.717368	69.889120	65.325055
H	67.266220	67.575580	66.833861
O	68.383142	70.162841	66.003289
H	69.476252	66.471869	66.982740
H	70.654156	67.352393	65.338489
H	68.983365	64.425234	65.675290
H	67.799580	65.293189	64.690216
H	67.492459	65.034826	66.423738
H	66.481110	67.601079	64.695062

Tryptophan

N	55.822270	69.934477	66.071419
C	56.110747	69.958037	64.628964
C	57.543110	69.450463	64.384668
O	57.948419	69.128666	63.289942
C	56.002126	71.402248	64.068377
C	54.631529	71.997572	64.205254
C	54.259028	73.005364	65.065586
C	53.441063	71.630182	63.471773
N	52.912556	73.284426	64.914450
C	52.383910	72.457466	63.941894
C	53.170958	70.695911	62.453307
C	51.081569	72.369938	63.435255
C	51.879525	70.605884	61.945723
C	50.844726	71.433368	62.433810

H	55.150141	70.659413	66.313529
H	57.722662	69.716308	66.222124
H	55.441820	69.308531	64.052356
O	58.315367	69.434659	65.484503
H	56.731286	72.034522	64.589836
H	56.308239	71.364772	63.017683
H	54.861694	73.567383	65.766396
H	52.407566	73.999442	65.412886
H	53.958866	70.058628	62.061830
H	50.285206	73.009750	63.805101
H	51.660603	69.890761	61.158502

Tyrosine

N	55.986568	73.370288	69.058071
C	56.996106	72.705391	68.216509
C	57.438828	71.389527	68.897942
O	58.404140	70.751450	68.542010
C	58.217200	73.569263	67.829688
C	57.858739	74.757142	66.963748
C	57.568594	74.588864	65.598560
C	57.788593	76.053958	67.486426
C	57.213757	75.664268	64.788269
C	57.436287	77.146608	66.687542
C	57.144803	76.951023	65.335177
O	56.793287	77.973941	64.493193
H	56.417179	74.045267	69.686502
H	55.948770	71.704098	69.972853
H	56.489079	72.388099	67.296293
O	56.632860	70.996497	69.896816
H	58.708764	73.909603	68.750400
H	58.932902	72.917154	67.320247
H	57.632734	73.597416	65.155861
H	58.026687	76.226298	68.533532
H	56.998576	75.527207	63.733557
H	57.396091	78.145076	67.117742
H	56.796783	78.813885	64.970671
H	55.305771	73.874977	68.499591

Valine

N	62.041885	79.100098	72.049775
C	61.354741	77.819667	72.318672
C	59.830534	78.063083	72.277540
O	59.477886	79.357114	72.352545
C	61.801566	77.224099	73.685329

C	61.393582	78.099134	74.882742
C	61.325698	75.775417	73.865067
H	62.918740	79.174657	72.557134
H	60.329495	79.856900	72.363192
H	61.565655	77.070850	71.545398
O	59.018274	77.167558	72.201593
H	62.901661	77.205693	73.635949
H	61.826306	77.697740	75.804915
H	60.305220	78.115224	75.008071
H	61.734873	79.134638	74.779734
H	61.722782	75.365764	74.799976
H	61.669817	75.137483	73.043758
H	60.234582	75.716104	73.895687
H	62.247504	79.216377	71.061523

2. CSD-Based reference structures

Alanine

N	19.573	102.566	56.621
C	18.571	102.787	55.582
C	19.051	102.136	54.287
O	18.336	101.323	53.697
C	18.372	104.28	55.374
H	19.268	102.9889	57.4742
H	17.6989	102.3817	55.8562
O	20.3987	102.4871	53.7299
H	17.6856	104.4293	54.6623
H	19.2372	104.6963	55.0946
H	18.0621	104.6976	56.2282
H	20.4415	102.9738	56.3393
H	19.6966	101.5837	56.762

Arginine

N	20.616	100.387	59.119
C	21.03	101.342	58.093
C	19.982	101.359	56.998
O	19.5	100.303	56.568
C	22.404	100.99	57.528
C	23.49	101.048	58.572
C	24.869	100.733	58.013

N	25.818	100.483	59.094
C	27.127	100.7	59.024
N	27.665	101.176	57.913
N	27.898	100.45	60.077
H	21.2987	100.3648	59.8493
H	20.5326	99.4767	58.7135
H	21.1079	102.252	58.5001
O	19.5241	102.6694	56.4294
H	22.3687	100.0635	57.1533
H	22.6259	101.6369	56.7984
H	23.5073	101.9683	58.9629
H	23.2779	100.3845	59.2895
H	24.8104	99.9205	57.433
H	25.1879	101.5091	57.469
H	25.4551	100.1208	59.9526
H	28.6506	101.338	57.8642
H	27.0861	101.3738	57.122
H	19.733	100.6652	59.4972
H	28.8832	100.613	60.0253
H	27.493	100.0989	60.9212

Asparagine

N	37.485	90.068	61.663
C	38.256	88.82	61.502
C	39.069	88.9	60.197
O	38.61	88.455	59.126
C	37.342	87.581	61.492
C	38.11	86.269	61.234
O	39.335	86.202	61.381
N	37.387	85.227	60.854
H	36.9533	90.0251	62.5088
H	36.8657	90.1804	60.8859
H	38.8726	88.7226	62.2832
O	40.4336	89.5225	60.2138
H	36.886	87.5142	62.3795
H	36.657	87.6961	60.7726
H	37.8312	84.3497	60.6724
H	36.3967	85.3173	60.7486
H	38.1128	90.8453	61.7036

Aspartic acid

N	26.231	90.877	63.268
C	25.415	91.75	62.427
C	26.138	91.967	61.101
O	25.543	91.777	60.043
C	25.143	93.075	63.137

C	24.633	94.151	62.203
O	23.446	94.129	61.837
O	25.429	95.035	61.856
H	25.7678	90.7266	64.1413
H	27.1192	91.3064	63.4319
H	24.5287	91.3224	62.2493
O	27.5708	92.4109	61.0892
H	24.4583	92.9203	63.8492
H	25.9938	93.393	63.5553
H	26.3653	89.9998	62.8071

Cysteine

N	90.028	58.388	52.839
C	91.247	59.095	53.227
C	92.318	58.098	53.675
O	92.071	56.884	53.756
C	90.948	60.029	54.404
S	90.537	59.151	55.949
H	89.3366	59.0494	52.5486
H	89.6824	57.8659	53.6187
H	91.5734	59.616	52.4383
O	93.6897	58.596	54.0222
H	91.754	60.5975	54.5687
H	90.1738	60.6114	54.1562
H	90.354	59.8165	56.6726
H	90.2299	57.7643	52.0838

Glutamic acid

N	84.481	59.104	54.092
C	83.697	58.737	52.916
C	84.641	58.765	51.726
O	84.716	57.803	50.964
C	82.533	59.699	52.675
C	81.563	59.868	53.838
C	80.805	58.6	54.224
O	80.145	57.996	53.342
O	80.838	58.236	55.428
H	83.8929	59.0972	54.9007
H	84.8632	60.0195	53.966
H	83.2967	57.8309	53.0527
O	85.4892	59.9772	51.4785
H	82.9165	60.5977	52.462
H	82.0143	59.3625	51.889
H	82.0827	60.1752	54.6352
H	80.8935	60.5669	53.5864
H	85.2246	58.4469	54.2158

Glutamine

N	87.5	57.997	51.332
C	88.595	57.045	51.407
C	89.923	57.748	51.679
O	90.816	57.76	50.828
C	88.676	56.265	50.096
C	87.358	55.644	49.696
C	86.775	54.781	50.808
O	87.488	53.991	51.438
N	85.477	54.941	51.068
H	86.6454	57.5094	51.1535
H	87.673	58.6472	50.5921
H	88.4197	56.4176	52.1657
O	90.1441	58.4316	52.9957
H	88.9668	56.8896	49.3712
H	89.3529	55.5363	50.2002
H	86.7094	56.3738	49.4798
H	87.5016	55.0745	48.8867
H	85.0409	54.4008	51.7877
H	84.9396	55.6012	50.5433
H	87.4269	58.4906	52.1987

Glycine

N	23.339	74.524	62.901
C	22.635	73.282	63.172
C	21.847	73.388	64.461
O	22.039	74.337	65.207
H	23.8533	74.4369	62.0479
H	23.97	74.7206	63.6515
H	22.0074	73.0886	62.4179
H	23.299	72.5386	63.2527
O	20.8389	72.3367	64.8193
H	22.6788	75.2704	62.8169

Histidine

N	38.734	87.279	49.622
C	38.546	86.901	48.233
C	37.454	87.741	47.613
O	37.667	88.357	46.577
C	38.194	85.425	48.109
C	37.798	85.02	46.725
N	38.718	84.696	45.75

C	36.577	84.866	46.153
C	38.083	84.357	44.641
N	36.783	84.451	44.859
H	39.4578	86.7191	50.0253
H	37.8821	87.1348	50.1254
H	39.4059	87.0607	47.7481
O	36.1069	87.8202	48.268
H	38.9912	84.8858	48.3805
H	37.4322	85.2285	48.7263
H	39.7113	84.7146	45.8641
H	35.6923	85.0248	46.5913
H	38.5134	84.077	43.7829
H	38.9919	88.2438	49.6734

Isoleucine

N	36.482	92.478	57.752
C	37.906	92.208	57.869
C	38.404	92.687	59.214
O	39.28	92.061	59.811
C	38.689	92.884	56.724
C	38.501	92.078	55.431
C	40.162	93.041	57.077
C	38.927	92.83	54.18
H	36.1541	92.1608	56.8622
H	36.3208	93.4615	57.8348
H	38.0555	91.2217	57.7987
O	37.828	93.9306	59.8237
H	38.3274	93.8056	56.583
H	39.0447	91.2414	55.4978
H	37.5334	91.8412	55.3437
H	40.6421	93.4808	56.318
H	40.5623	92.1405	57.247
H	40.2502	93.6049	57.8981
H	38.7797	92.2525	53.377
H	39.8964	93.0666	54.2466
H	38.3855	93.6662	54.0925
H	35.9904	91.9977	58.4784

Leucine

N	36.651	92.765	61.905
C	36.153	91.773	62.83
C	36.907	90.437	62.81
O	36.909	89.727	63.814
C	34.662	91.561	62.576
C	33.782	92.756	62.977
C	32.374	92.6	62.478

C	33.766	92.882	64.487
H	36.1052	93.5991	61.9842
H	36.5869	92.4127	60.9713
H	36.3101	92.1352	63.7488
O	37.6366	89.9999	61.5744
H	34.5311	91.3881	61.5998
H	34.3647	90.7624	63.0992
H	34.1692	93.5788	62.5611
H	31.8316	93.3927	62.7561
H	31.9728	91.7698	62.865
H	32.3789	92.5336	61.4802
H	33.1942	93.6587	64.7511
H	34.6979	93.0264	64.8198
H	33.3953	92.0442	64.888
H	37.6061	92.9707	62.1184

Lysine

N	69.918	63.519	55.497
C	70.986	63.802	56.434
C	70.985	65.233	56.902
O	71.12	65.485	58.094
C	72.355	63.471	55.846
C	73.531	64.211	56.514
C	74.871	63.605	56.097
C	76.07	64.327	56.72
N	76.095	64.247	58.226
H	69.9636	62.5596	55.2187
H	70.0164	64.1041	54.692
H	70.8119	63.213	57.2232
O	70.8192	66.3476	55.912
H	72.508	62.4877	55.9444
H	72.3449	63.7118	54.8755
H	73.5087	65.1728	56.2412
H	73.4372	64.1435	57.5073
H	74.8911	62.6471	56.3835
H	74.949	63.6573	55.1014
H	76.9089	63.9136	56.3659
H	76.0343	65.2902	56.4536
H	76.8965	64.7341	58.5729
H	76.1397	63.2888	58.5087
H	75.2654	64.665	58.5963
H	69.0357	63.6977	55.9326

Methionine

N	62.596	80.138	50.933
C	62.277	80.579	52.281

C	63.055	79.849	53.372
O	63.431	78.676	53.229
C	60.79	80.402	52.535
C	59.938	81.459	51.922
S	60.429	83.035	52.584
C	59.343	83.125	54.062
H	62.0515	80.6572	50.2743
H	62.3881	79.164	50.8425
H	62.5445	81.5413	52.3293
O	63.3729	80.5682	54.6493
H	60.5108	79.5176	52.1609
H	60.6373	80.4097	53.5232
H	60.0606	81.4573	50.9295
H	58.9775	81.2863	52.14
H	59.512	83.982	54.5487
H	59.5392	82.3539	54.6678
H	58.3856	83.0881	53.7755
H	63.5682	80.289	50.7537

Phenylalanine

N	68.991	74.489	76.989
C	68.568	74.822	78.333
C	67.109	74.446	78.521
O	66.801	73.46	79.188
C	68.801	76.306	78.635
C	68.421	76.704	80.047
C	69.035	76.102	81.144
C	67.403	77.624	80.278
C	68.634	76.402	82.438
C	67.001	77.928	81.57
C	67.617	77.313	82.646
H	69.952	74.7384	76.8701
H	68.4326	74.9918	76.3291
H	69.1198	74.2978	78.9816
O	66.0364	75.2828	77.889
H	69.7711	76.5076	78.5
H	68.2553	76.8481	77.996
H	69.7744	75.4451	80.9965
H	66.956	78.0712	79.5033
H	69.0795	75.9604	83.2168
H	66.2676	78.5902	81.7238
H	67.3246	77.5291	83.5776
H	68.8809	73.5066	76.8382

Proline

N	60.281	60.558	64.256

C	59.755	59.221	63.947
C	59.702	59.029	62.414
O	59.843	57.904	61.911
C	58.348	59.261	64.525
C	58.467	60.244	65.665
C	59.378	61.308	65.148
H	61.1702	60.4607	64.703
H	60.3079	58.4741	64.3164
O	59.4776	60.2162	61.5251
H	57.6901	59.5813	63.8434
H	58.0719	58.3592	64.8574
H	57.5725	60.6265	65.8965
H	58.8605	59.8034	66.4718
H	58.8684	62.0041	64.6423
H	59.8854	61.7411	65.893
H	60.3903	61.068	63.4028

Serine

N	56.818	71.032	69.851
C	57.096	69.763	70.477
C	56.577	68.794	69.448
O	57.126	67.714	69.302
C	56.356	69.624	71.81
O	56.755	70.69	72.661
H	57.1232	71.7731	70.4489
H	55.8345	71.117	69.691
H	58.0588	69.6256	70.7098
O	55.3896	69.1549	68.6055
H	55.3692	69.6684	71.654
H	56.5878	68.7488	72.2346
H	56.2796	70.6133	73.5374
H	57.3032	71.0871	68.9783

Threonine

N	67.327	68.085	64.938
C	67.977	67.806	66.199
C	68.558	69.076	66.773
O	68.479	69.311	67.984
C	69.065	66.726	66.049
O	70.09	67.182	65.16
C	68.473	65.448	65.521
H	66.9453	67.2394	64.5649
H	67.9939	68.4613	64.2948
H	67.2891	67.449	66.831
O	69.2363	70.0601	65.8667
H	69.4606	66.5507	66.9505

H	70.7914	66.4752	65.0687
H	69.1924	64.7594	65.4302
H	68.0587	65.6166	64.6266
H	67.7737	65.1172	66.1548
H	66.5917	68.7475	65.0809

Tryptophan

N	55.612	69.719	65.777
C	56.148	70.018	64.446
C	57.558	69.525	64.259
O	57.857	68.886	63.251
C	56.087	71.514	64.137
C	54.719	72.098	64.24
C	54.338	73.156	65.011
C	53.538	71.651	63.56
N	52.995	73.39	64.863
C	52.479	72.484	63.975
C	53.275	70.624	62.637
C	51.181	72.332	63.501
C	51.985	70.465	62.167
C	50.95	71.317	62.6
H	54.6771	70.067	65.8463
H	56.1823	70.1562	66.4725
H	55.5617	69.5244	63.8037
O	58.5979	69.8126	65.301
H	56.6828	71.9929	64.7817
H	56.4205	71.6566	63.2051
H	54.9496	73.6849	65.5994
H	52.4759	74.1068	65.3285
H	54.0081	70.0192	62.326
H	50.4437	72.9364	63.8028
H	51.784	69.7367	61.5119
H	50.0253	71.1813	62.2444
H	55.6104	68.7295	65.9216

Tyrosine

N	55.968	73.329	68.855
C	57.034	72.667	68.107
C	57.427	71.351	68.719
O	58.296	70.646	68.202
C	58.246	73.573	67.947
C	57.924	74.73	67.063
C	57.498	74.525	65.744
C	57.96	76.018	67.548
C	57.112	75.589	64.935
C	57.575	77.078	66.757

C	57.153	76.86	65.449
O	56.795	77.938	64.675
H	55.7398	74.1968	68.4137
H	56.2748	73.5021	69.7909
H	56.6671	72.4732	67.1971
O	56.752	70.8895	69.9765
H	58.5226	73.9133	68.8457
H	58.9962	73.0497	67.5428
H	57.4709	73.5953	65.3768
H	58.2688	76.1858	68.4842
H	56.8099	75.4299	63.9951
H	57.5989	78.0079	67.1242
H	56.8855	78.7779	65.2101
H	55.1586	72.7419	68.8731

Valine

N	61.917	79.141	72.104
C	61.32	77.82	72.31
C	59.789	77.99	72.287
O	59.273	79.082	72.537
C	61.802	77.233	73.682
C	61.371	78.147	74.852
C	61.311	75.816	73.881
H	62.9138	79.0621	72.114
H	61.6245	79.7572	72.8353
H	61.5984	77.1825	71.5916
O	58.9167	76.8151	71.9571
H	62.8014	77.2013	73.6672
H	61.6877	77.7552	75.7158
H	60.374	78.2228	74.8666
H	61.7722	79.0551	74.7315
H	61.6343	75.4714	74.7623
H	61.6626	75.2348	73.1471
H	60.3112	75.8039	73.8653
H	61.621	79.5072	71.2218