Applying Machine Learning to Vibrational Spectroscopy

Supporting Information

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Table S1. The relative zero-point corrected energies ($ZPE_{rel.}$), enthalpy ($\Delta_{rel.}H$), entropy ($\Delta_{rel.}S$), and Gibbs free energies ($\Delta_{rel.}G$) of $(Phe/Ser + H)^+$. $ZPE_{rel.}$, $\Delta_{rel.}H$, and $\Delta_{rel.}G$ at 298 K are given in $kJ \cdot mol^{-1}$. $\Delta_{rel.}S$ at 298 K is given in $J \cdot K^{-1} \cdot mol^{-1}$. Calculations employed the B3LYP functional and 6-311++G(d,p) basis set.

Isomer List	$ZPE_{rel.}$ $kJ \cdot mol^{-1}$	$\Delta_{rel.}H$ $kJ \cdot mol^{-1}$	$\Delta_{rel.}S$ $J \cdot K^{-1} \cdot mol^{-1}$	$\Delta_{rel.}G$ $kJ \cdot mol^{-1}$
Isomer 1	0.00	0.00	0.00	0.00
Isomer 2	8.89	9.85	24.11	2.66
Isomer 3	9.19	10.68	32.81	0.89
Isomer 4	18.68	19.81	26.04	12.04
Isomer 5	22.38	23.88	29.85	14.98
Isomer 6	29.30	29.74	18.64	24.19
Isomer 7	32.81	33.26	7.74	30.95
Isomer 8	40.36	42.92	46.57	29.04
Isomer 9	40.62	40.71	10.04	37.71
Isomer 10	41.26	43.37	28.03	35.01
Isomer 11	42.09	44.65	50.60	29.56
Isomer 12	42.30	45.06	77.69	21.90
Isomer 13	43.45	45.84	44.34	32.62
Isomer 14	43.66	46.25	54.54	29.99
Isomer 15	48.88	49.93	23.52	42.92
Isomer 16	50.03	51.60	28.50	43.11
Isomer 17	50.73	51.13	10.29	48.07
Isomer 18	59.45	60.25	17.18	55.12
Isomer 19	59.72	62.30	49.92	47.41
Isomer 20	65.75	68.00	45.41	54.46
Isomer 21	111.08	113.09	40.68	100.96
Isomer 22	111.88	113.98	45.27	100.48
Isomer 23	113.09	115.25	45.94	101.55
Isomer 24	117.72	119.62	39.64	107.80
Isomer 25	118.62	120.42	29.15	111.73
Isomer 26	135.53	138.60	63.49	119.67
Isomer 27	135.73	138.80	64.98	119.43
Isomer 28	142.06	145.29	61.40	126.98
Isomer 29	145.05	147.06	58.31	129.68
Isomer 30	148.07	151.32	68.55	130.88
Isomer 31	149.78	152.80	52.78	137.06
Isomer 32	151.25	153.28	41.12	141.02
Isomer 33	155.24	157.04	47.51	142.88
Isomer 34	155.54	157.05	40.25	145.05
Isomer 35	163.88	167.02	51.46	151.68
Isomer 36	183.91	187.26	35.33	176.73
Isomer 37	194.48	197.87	54.98	181.48

Determining the appropriate scaling factor

To determine the appropriate scaling factor for the calculated spectra, we began by employing a scaling factor of 0.95. This scaling factor is commonly used for calculated harmonic spectra in the 2800 – 3800 cm^{-1} region. Using this initial guess to scale the calculated spectra, we used the cosine distances to judge which spectra best matched the various experimental spectra (as described in the article). Having identified several possible matches for each experimental spectrum, we then proceeded to calculate the cosine distances for the best matching calculated spectra as the scaling factor was varied from 0.92 to 1.0. Plots showing the cosine distances as a function of scaling factor are shown below for each experimental spectrum.

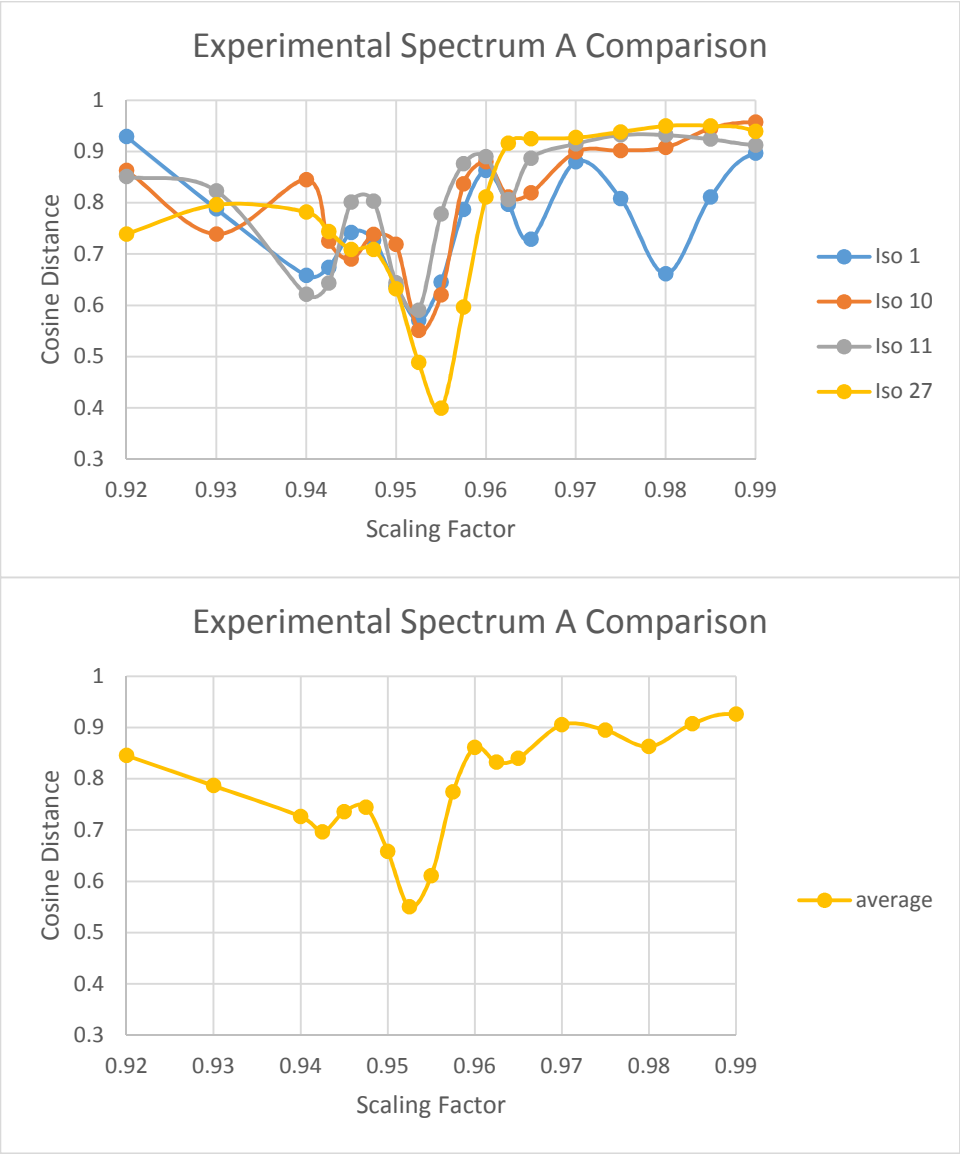


Figure S1. The cosine distances for experimental spectrum **A** and the harmonic spectra of several isomers of $(Phe/Ser + H)^+$ plotted as a function of scaling factor.

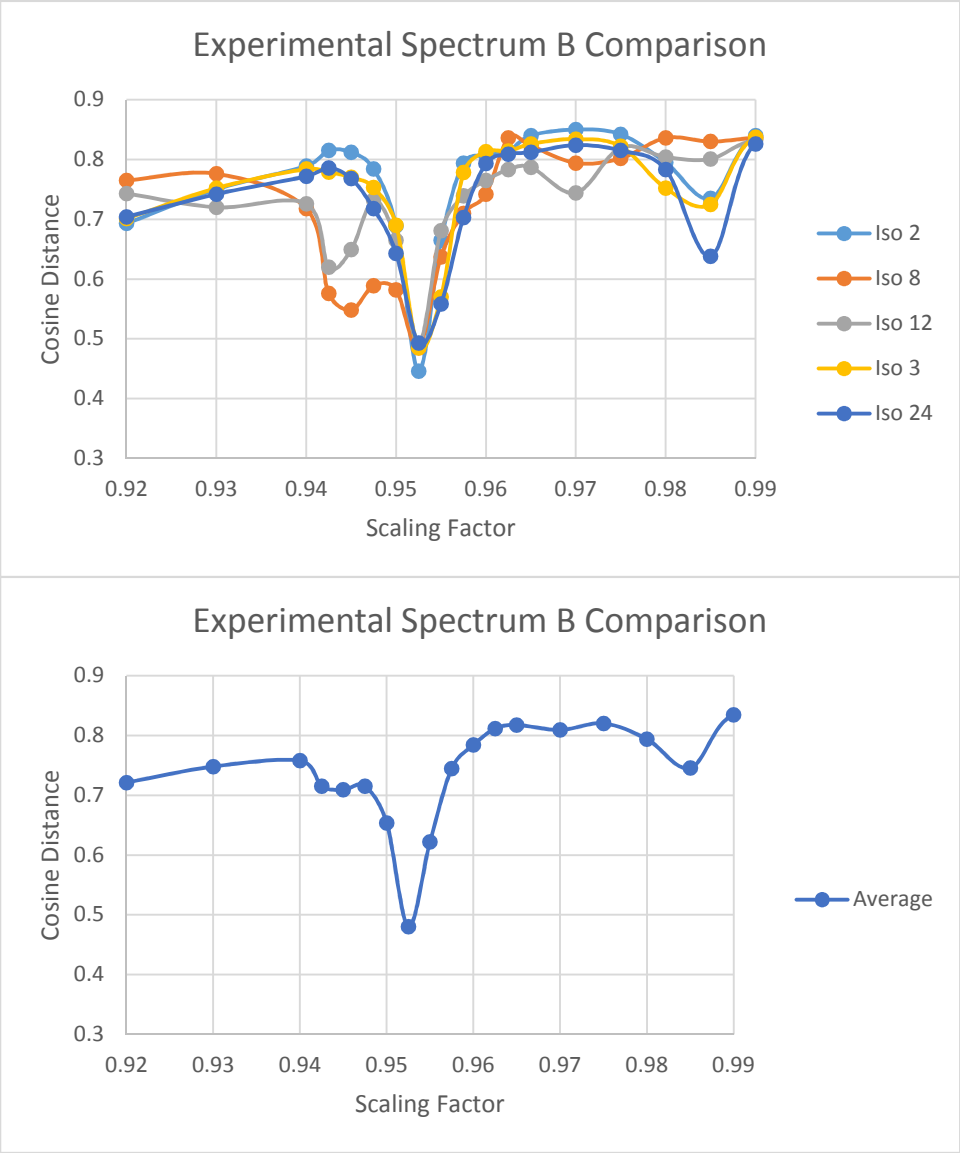


Figure S2. The cosine distances for experimental spectrum **B** and the harmonic spectra of several isomers of $(Phe/Ser + H)^+$ plotted as a function of scaling factor.

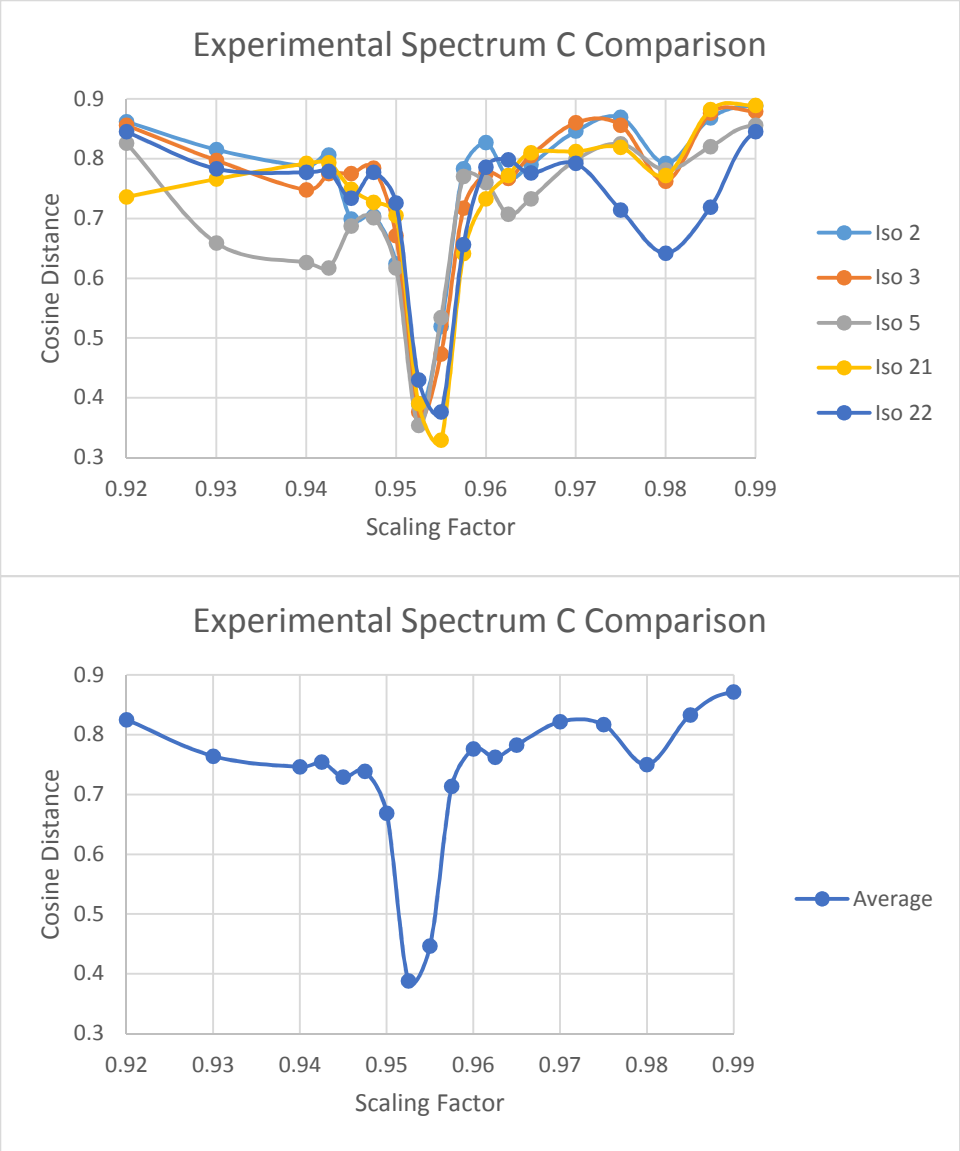


Figure S3. The cosine distances for experimental spectrum **C** and the harmonic spectra of several isomers of $(Phe/Ser + H)^+$ plotted as a function of scaling factor.

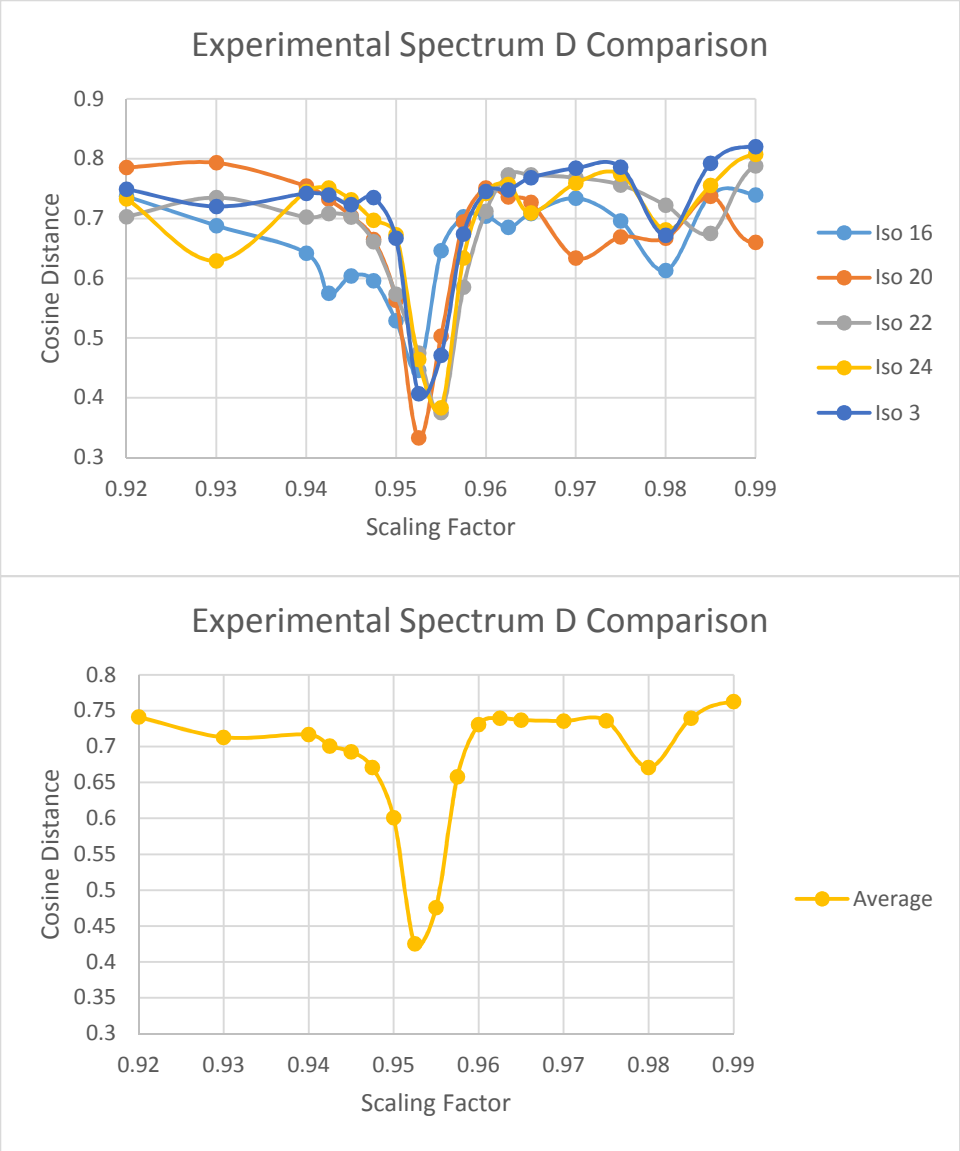


Figure S4. The cosine distances for experimental spectrum **D** and the harmonic spectra of several isomers of $(Phe/Ser + H)^+$ plotted as a function of scaling factor.

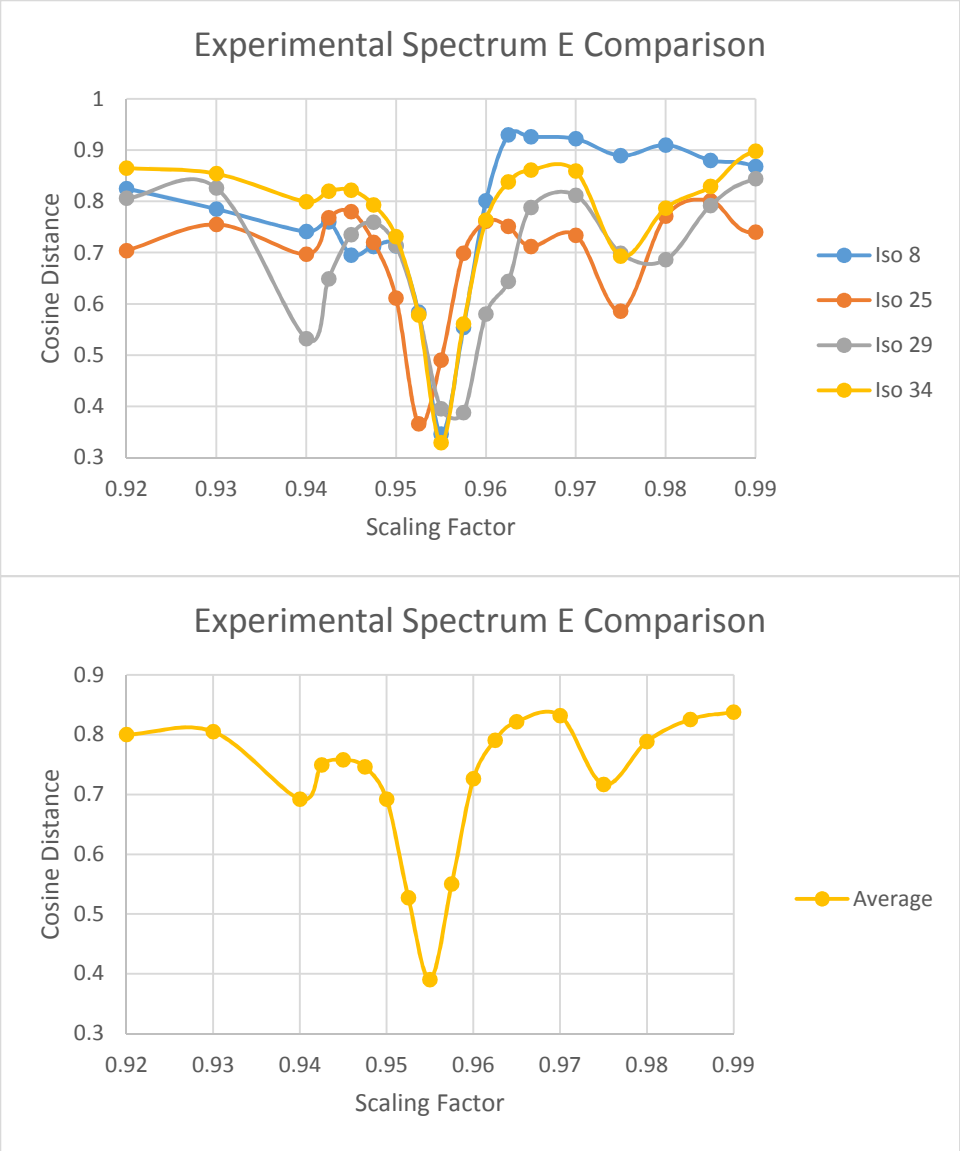
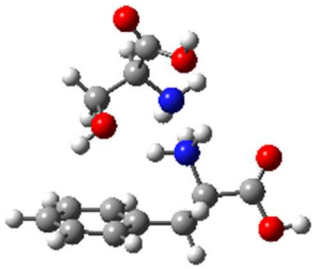


Figure S5. The cosine distances for experimental spectrum **E** and the harmonic spectra of several isomers of $(Phe/Ser + H)^+$ plotted as a function of scaling factor.

The atomic coordinates and structures of (Phe/Ser + H)$^+$

The *XYZ* atomic coordinates of all 37 isomers with relative zero-point corrected energies are provided. Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory.



Isomer 1, 0.0 kJ·mol^{-1}

N	-0.131652	1.102907	-0.587218
H	0.365403	1.794129	-1.150232
H	0.048453	0.161148	-0.966506
C	-1.582130	1.417015	-0.458589
H	-2.035687	1.314421	-1.447137
C	-2.275769	0.465452	0.538987
C	-1.694335	2.876735	-0.031597
H	-1.951586	0.714352	1.553487
H	-3.346018	0.680125	0.490860
C	-1.999365	-0.997471	0.257695
O	-0.739196	3.571182	0.204051
C	-1.474009	-1.817755	1.259344
C	-2.243413	-1.549071	-1.005731
H	-1.299177	-1.409999	2.249838
C	-1.187665	-3.158934	1.006427
C	-1.945046	-2.885005	-1.268120
H	-2.682176	-0.942805	-1.792176
H	-0.798666	-3.787573	1.799321
C	-1.409646	-3.693627	-0.262673
H	-2.144347	-3.299196	-2.249500
H	-1.191779	-4.736392	-0.461506
O	-2.972095	3.255366	0.043481
H	-3.017476	4.186785	0.315387
C	2.661190	-0.230980	0.906861
H	3.461694	-0.467735	1.617499
C	2.077020	-1.571902	0.453895
H	1.545236	-2.035627	1.292518
H	2.903499	-2.220760	0.151542
O	1.183229	-1.358136	-0.644184
H	0.713594	-2.180581	-0.833779
C	3.376282	0.420463	-0.277129
O	2.771938	1.558025	-0.716372

H	3.329177	1.925272	-1.422364
O	4.370096	-0.033121	-0.764833
H	0.401442	1.064439	0.338601
H	1.264636	0.194643	2.348653
H	2.043878	1.521815	1.808658
N	1.629272	0.641436	1.510743

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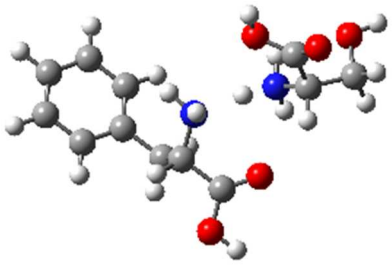

Isomer 2, 8.9 kJ·mol^{-1}

N	0.343825	0.128715	0.752637
H	-0.042177	0.175490	1.692843
H	0.993311	-0.657526	0.754049
C	1.095917	1.359603	0.443862
H	1.700000	1.692541	1.293508
C	2.048624	1.126001	-0.760693
C	0.127070	2.477369	0.089055
H	1.450467	0.886850	-1.645911
H	2.568438	2.064969	-0.962934
C	3.035947	0.015903	-0.481410
O	-1.008407	2.314188	-0.308276
C	2.876034	-1.248534	-1.057520
C	4.107923	0.229048	0.393824
H	2.064586	-1.422297	-1.758037
C	3.767093	-2.282241	-0.765336
C	4.997460	-0.800691	0.687112
H	4.256201	1.209206	0.836540
H	3.638312	-3.253573	-1.228557
C	4.827058	-2.060042	0.110028
H	5.829098	-0.619696	1.357996
H	5.523840	-2.858868	0.334515
O	0.699403	3.674636	0.222931
H	0.077954	4.364646	-0.060618
C	-3.124553	0.003683	-0.074333
H	-3.032048	1.014148	0.327085
C	-4.337402	-0.094511	-0.996735
H	-4.318927	0.726671	-1.724187
H	-5.241011	-0.012943	-0.387171

O	-4.219294	-1.361091	-1.636632
H	-5.030112	-1.585794	-2.104352
C	-3.279000	-0.958821	1.104787
O	-2.200265	-1.755905	1.269304
H	-2.376177	-2.362048	2.007712
O	-4.252956	-0.969989	1.797910
H	-1.941805	-1.196111	-1.289730
H	-1.773194	0.435636	-1.581875
H	-0.986520	-0.186012	-0.235066
N	-1.875235	-0.273246	-0.854066

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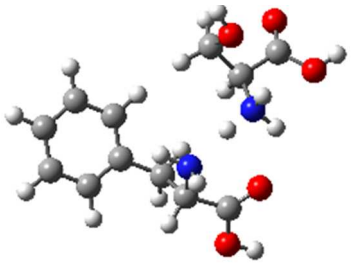

Isomer 3, 9.2 kJ·mol^{-1}

N	0.669382	-0.863910	-1.451309
H	0.683047	-1.308552	-2.367252
H	1.267440	-0.041522	-1.527192
C	1.263891	-1.771957	-0.449093
H	2.171590	-2.250633	-0.828565
C	1.630248	-0.996564	0.845980
C	0.270715	-2.866291	-0.084587
H	0.709761	-0.663366	1.335717
H	2.118498	-1.698462	1.526006
C	2.522275	0.190759	0.563603
O	-0.934170	-2.774522	-0.182904
C	2.038694	1.495795	0.699744
C	3.839885	0.002924	0.128485
H	1.030784	1.658264	1.069794
C	2.849353	2.592774	0.405894
C	4.650673	1.095405	-0.167766
H	4.239168	-1.002086	0.034130
H	2.465864	3.598798	0.531552
C	4.155870	2.393391	-0.033469
H	5.671416	0.935430	-0.494609
H	4.789944	3.242564	-0.258705
O	0.894351	-3.934405	0.416114
H	0.236039	-4.593412	0.690698

C	-2.192618	0.671099	0.156020
H	-1.506564	0.381571	0.955434
C	-1.839126	2.064610	-0.360453
H	-0.765858	2.121005	-0.577818
H	-2.091593	2.791651	0.415429
O	-2.615689	2.231420	-1.542128
H	-2.632954	3.153573	-1.817151
C	-3.604744	0.655266	0.752036
O	-4.334956	-0.377432	0.292934
H	-5.210962	-0.361657	0.712221
O	-3.968268	1.466523	1.552059
H	-2.539242	0.028671	-1.779588
H	-0.989311	-0.454460	-1.189034
H	-2.372539	-1.240418	-0.699741
N	-2.031156	-0.311529	-0.958825

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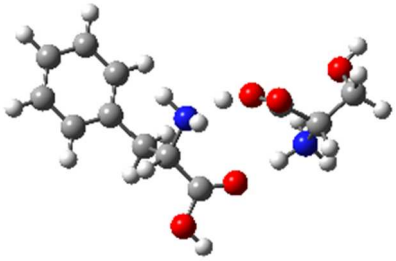

Isomer 4, 18.7 kJ·mol^{-1}

N	-0.527047	-0.106768	1.109275
H	-0.138459	-0.361612	2.015697
H	-1.293892	0.540994	1.286326
C	-1.059493	-1.280278	0.397204
H	-1.758456	-1.846439	1.019992
C	-1.812142	-0.826644	-0.886529
C	0.046467	-2.238016	-0.022147
H	-1.101081	-0.318636	-1.544366
H	-2.168913	-1.720012	-1.404552
C	-2.967751	0.088682	-0.552345
O	1.196223	-1.948035	-0.300962
C	-2.848772	1.474629	-0.700492
C	-4.162648	-0.439302	-0.049023
H	-1.933606	1.897112	-1.103715
C	-3.904203	2.318198	-0.352341
C	-5.216556	0.401348	0.298534
H	-4.274024	-1.513913	0.059040
H	-3.802551	3.389639	-0.479781
C	-5.088171	1.782886	0.149440

H	-6.139932	-0.020230	0.678174
H	-5.910237	2.436464	0.416169
O	-0.423324	-3.482232	-0.112186
H	0.273024	-4.072085	-0.442667
C	3.802241	0.073379	0.179147
H	4.178673	-0.778358	0.744879
C	4.875610	1.152687	0.055126
H	5.835742	0.700651	-0.226775
H	4.988994	1.628628	1.034321
O	4.412476	2.047985	-0.946467
H	4.955609	2.841972	-0.979409
C	2.515185	0.549594	0.872819
O	1.580621	0.909543	0.016248
H	0.651459	0.652196	0.432190
O	2.427410	0.512581	2.075088
H	3.163899	0.408949	-1.762827
H	4.182530	-0.907524	-1.666046
H	2.587919	-1.026431	-1.118983
N	3.417885	-0.413106	-1.202857

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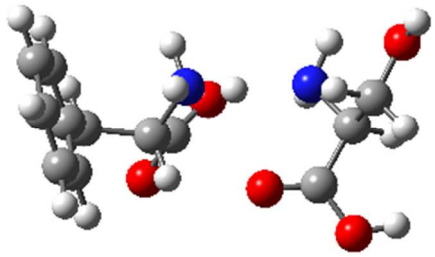

Isomer 5, 22.4 kJ·mol^{-1}

N	-0.244357	-0.318208	-0.947865
H	0.827368	-0.222274	-0.905365
H	-0.675816	0.590411	-0.760253
H	-0.485507	-0.587709	-1.904038
C	-0.791473	-1.315861	0.030084
H	-0.529875	-0.943473	1.020001
C	-2.323808	-1.434980	-0.111924
C	-0.056124	-2.626557	-0.193050
H	-2.567770	-1.922158	-1.061477
H	-2.670001	-2.096865	0.684158
C	-2.984844	-0.075571	-0.029824
O	0.788534	-2.785969	-1.041441
C	-3.536813	0.518761	-1.169669
C	-3.001960	0.630539	1.179660
H	-3.551878	-0.025695	-2.109271

C	-4.100431	1.793860	-1.103062
C	-3.563546	1.903179	1.246750
H	-2.588478	0.178999	2.076175
H	-4.537575	2.236767	-1.990286
C	-4.112408	2.488030	0.104563
H	-3.581776	2.434160	2.191218
H	-4.555439	3.475287	0.159619
O	-0.470028	-3.556755	0.666666
H	0.010010	-4.385067	0.503422
C	3.340295	0.489549	-0.063914
H	4.346271	0.065691	0.060528
C	3.507302	1.953575	-0.500897
H	4.095906	2.499846	0.245343
H	2.518471	2.425192	-0.577131
O	4.162641	1.909689	-1.758846
H	4.308545	2.801659	-2.091064
C	2.600865	0.449445	1.277767
O	3.321486	0.727791	2.371487
H	4.262506	0.833568	2.176312
O	1.420480	0.222408	1.366523
N	2.565828	-0.236305	-1.077140
H	2.926269	0.020766	-1.994744
H	2.691890	-1.242188	-0.985597

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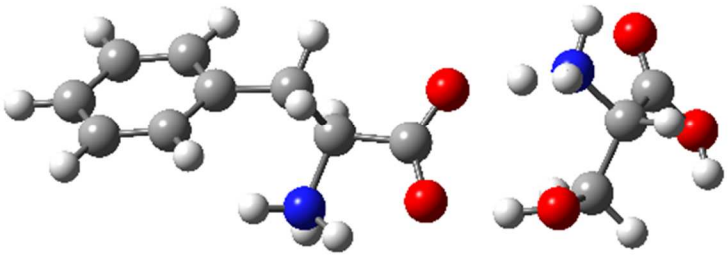

Isomer 6, 29.3 kJ·mol^{-1}

N	1.824398	1.171863	-1.293352
H	1.766134	0.992863	-2.295906
H	2.803015	1.379308	-1.055521
H	1.178187	1.958937	-1.067888
C	1.283990	0.016629	-0.469796
H	1.313474	-0.881647	-1.084514
C	2.137925	-0.169564	0.801604
C	-0.174264	0.388224	-0.114887
H	1.963444	0.674666	1.475924
H	1.756323	-1.062332	1.299827
C	3.609036	-0.289320	0.476895

O	-0.500026	1.580994	-0.337966
C	4.463891	0.806586	0.653800
C	4.125214	-1.467977	-0.076032
H	4.090630	1.713481	1.122223
C	5.808317	0.727725	0.281845
C	5.465744	-1.548065	-0.442619
H	3.479545	-2.331276	-0.204313
H	6.461462	1.578428	0.436892
C	6.308760	-0.448364	-0.269638
H	5.856634	-2.470197	-0.856556
H	7.352449	-0.515016	-0.552619
O	-0.853693	-0.531359	0.388889
H	-2.277994	-0.398596	0.989583
C	-4.295111	0.149279	0.508189
H	-5.120393	0.572270	1.088730
C	-3.681976	1.247177	-0.385483
H	-4.478651	1.729506	-0.964591
H	-2.977081	0.791767	-1.089384
O	-3.046302	2.187566	0.443293
H	-2.093557	2.178793	0.214601
C	-4.794770	-1.086617	-0.246971
O	-5.667224	-0.870026	-1.239723
H	-5.901571	0.061632	-1.344194
O	-4.424814	-2.191041	0.039708
N	-3.244963	-0.307746	1.472071
H	-3.136536	0.384677	2.213332
H	-3.492209	-1.223511	1.856598

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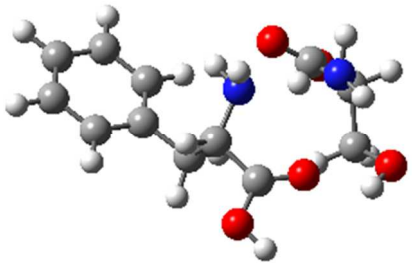

Isomer 7, 32.8 kJ·mol^{-1}

N	-0.122227	0.646989	-1.464489
H	-0.218862	1.037053	-2.399566
H	-0.742248	-0.162680	-1.430304
H	1.425060	0.033962	-1.338472
C	-0.568252	1.637079	-0.465287
H	-1.359896	2.281217	-0.858374
C	-1.122707	0.930797	0.803813

C	0.596540	2.525312	-0.061938
H	-0.349688	0.267600	1.204565
H	-1.321672	1.697337	1.556101
C	-2.381381	0.149952	0.498628
O	1.769418	2.215243	-0.151873
C	-2.345959	-1.237813	0.330217
C	-3.598927	0.823670	0.341485
H	-1.414246	-1.778204	0.456291
C	-3.508139	-1.940016	0.006280
C	-4.757772	0.123167	0.020533
H	-3.643498	1.899242	0.484187
H	-3.468615	-3.016151	-0.115745
C	-4.713675	-1.261541	-0.150667
H	-5.696146	0.654304	-0.088383
H	-5.617176	-1.806748	-0.396843
O	0.176175	3.677245	0.456899
H	0.937012	4.205919	0.747005
C	2.889650	-1.199872	-0.281022
H	3.837914	-1.671452	-0.555875
C	3.138854	-0.285699	0.939400
H	3.567564	-0.882235	1.750177
H	2.191419	0.133820	1.286779
O	4.053007	0.719616	0.559678
H	3.605106	1.574883	0.590819
C	1.817623	-2.259966	-0.022916
O	2.102042	-3.187103	0.897869
H	3.002934	-3.127481	1.243805
O	0.760249	-2.241997	-0.591994
N	2.450913	-0.354813	-1.431685
H	3.078245	0.453840	-1.485744
H	2.496582	-0.875713	-2.308054

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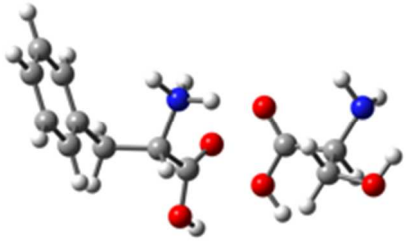

Isomer 8, 40.4 kJ·mol^{-1}

N	-0.801471	0.522174	1.167140
H	0.184687	0.149716	1.179060
H	-1.464185	-0.243577	1.336896

H	-0.876436	1.217513	1.917552
C	-1.104915	1.172533	-0.151941
H	-0.634895	0.565843	-0.925818
C	-2.631915	1.255357	-0.383668
C	-0.459487	2.550558	-0.120055
H	-3.067929	1.958654	0.332544
H	-2.781469	1.675431	-1.380118
C	-3.276905	-0.106294	-0.253958
O	-0.068859	3.069955	0.894956
C	-3.950273	-0.465154	0.920396
C	-3.156598	-1.048883	-1.282684
H	-4.085167	0.266204	1.712388
C	-4.491802	-1.744111	1.065286
C	-3.699292	-2.322920	-1.139372
H	-2.654351	-0.779222	-2.206726
H	-5.022684	-2.004816	1.973227
C	-4.363946	-2.674135	0.036871
H	-3.612990	-3.039345	-1.947817
H	-4.789808	-3.664548	0.144201
O	-0.437622	3.097119	-1.335254
H	-0.081485	3.998942	-1.276269
C	4.020886	-0.418599	0.215295
H	4.609159	0.438177	-0.131221
C	4.222123	-1.553442	-0.832877
H	3.820883	-1.268475	-1.809216
H	3.674323	-2.443066	-0.487306
O	5.587737	-1.806651	-1.011604
H	5.971139	-1.979911	-0.140533
C	2.552302	-0.021615	0.246397
O	2.073430	0.709656	-0.780712
H	2.768414	0.952164	-1.409087
O	1.775183	-0.369167	1.114176
N	4.556893	-0.866327	1.482095
H	4.773320	-0.102847	2.111535
H	3.922825	-1.502508	1.955126

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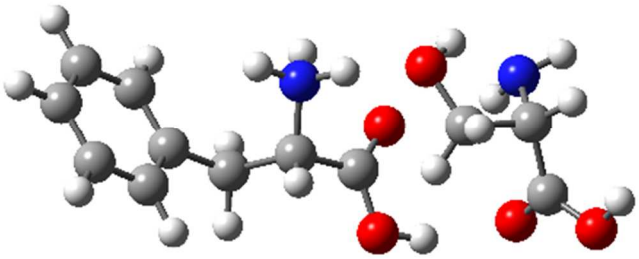

Isomer 9, 40.6 kJ·mol^{-1}

N	-0.896977	1.036149	-0.494268
H	-0.064433	1.548178	-0.084195
H	-1.787268	1.422189	-0.165067
H	-0.841615	1.151408	-1.510897
C	-0.807246	-0.428825	-0.155691
H	-0.758945	-0.498322	0.931275
C	-2.038720	-1.192091	-0.683983
C	0.501832	-0.916182	-0.768927
H	-2.015505	-1.194093	-1.778013
H	-1.938214	-2.229811	-0.357210
C	-3.321439	-0.573442	-0.172915
O	0.979567	-0.381167	-1.743622
C	-4.088964	0.256592	-0.998621
C	-3.725235	-0.774484	1.152808
H	-3.808204	0.394984	-2.038822
C	-5.239215	0.876626	-0.507584
C	-4.873742	-0.157444	1.642157
H	-3.151573	-1.432009	1.799061
H	-5.832847	1.505614	-1.160429
C	-5.630429	0.672394	0.813560
H	-5.184504	-0.331756	2.665509
H	-6.527100	1.146891	1.193851
O	1.014216	-1.928358	-0.094404
H	1.940062	-2.085982	-0.381359
C	3.707315	1.021050	0.266809
H	4.437099	1.747391	0.632498
C	2.369451	1.203204	1.075771
H	2.573462	1.645862	2.052281
H	1.891236	0.231860	1.231849
O	1.488205	2.058103	0.343705
H	1.977637	2.211287	-0.505572
C	4.204616	-0.417888	0.477149
O	5.193562	-0.626187	1.352214
H	5.553038	0.198010	1.705886
O	3.696755	-1.349665	-0.098860
N	3.443591	1.328548	-1.135325
H	4.269257	1.661342	-1.618383
H	3.064246	0.525355	-1.632787

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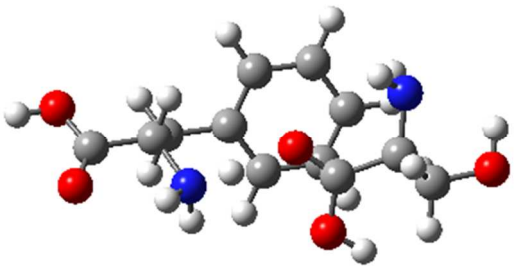

Isomer 10, 41.3 kJ·mol^{-1}

N	1.721401	1.351520	-0.476700
H	0.721383	1.272082	-0.127605
H	1.725565	1.107189	-1.469251
H	2.049274	2.322165	-0.410065
C	2.647124	0.460366	0.304899
H	2.278685	0.454226	1.333780
C	2.643498	-0.973095	-0.257536
C	4.022562	1.127772	0.296788
H	3.051111	-0.957765	-1.274141
H	3.339244	-1.554782	0.349688
C	1.264062	-1.595781	-0.244609
O	4.221987	2.204038	-0.207888
C	0.516850	-1.705559	-1.420175
C	0.712743	-2.059409	0.955388
H	0.940858	-1.381449	-2.365979
C	-0.760731	-2.265946	-1.399582
C	-0.558729	-2.624182	0.977982
H	1.287877	-1.998850	1.874005
H	-1.319291	-2.367326	-2.323176
C	-1.300970	-2.726107	-0.200564
H	-0.961095	-3.005931	1.909540
H	-2.281860	-3.188041	-0.187846
O	4.925639	0.378462	0.923027
H	5.783878	0.834368	0.924005
C	-3.090540	0.478611	0.162894
H	-3.444619	-0.289584	-0.533403
C	-4.070769	1.679149	0.042999
H	-4.032873	2.126549	-0.953623
H	-3.768880	2.449598	0.768382
O	-5.389512	1.247852	0.244281
H	-5.419493	0.773530	1.086431
C	-1.694271	0.894812	-0.274401
O	-1.482555	1.129313	-1.580502
H	-2.267200	0.944710	-2.115655
O	-0.766373	1.063454	0.495530
N	-3.170159	-0.048011	1.508065
H	-2.740262	-0.962738	1.579561

H	-2.703998	0.564710	2.170543

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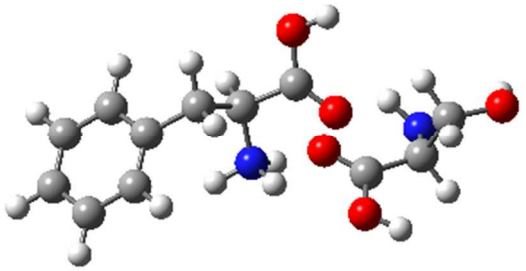

Isomer 11, 42.1 kJ·mol^{-1}

N	0.669319	-0.414936	-0.461224
H	-0.147113	-0.893089	0.007136
H	1.507512	-1.005943	-0.441560
H	0.383454	-0.267565	-1.434309
C	0.957119	0.898937	0.203821
H	0.991064	0.710885	1.278084
C	2.312384	1.471021	-0.273248
C	-0.207375	1.827274	-0.115199
H	2.232749	1.754622	-1.327400
H	2.491510	2.386190	0.294307
C	3.425539	0.466607	-0.071872
O	-1.033643	1.587754	-0.960486
C	3.911770	-0.282487	-1.150315
C	3.940128	0.227692	1.208453
H	3.545992	-0.086234	-2.154188
C	4.895040	-1.253777	-0.953062
C	4.922283	-0.739538	1.404738
H	3.586007	0.812672	2.051858
H	5.273538	-1.816916	-1.797929
C	5.398594	-1.484522	0.324756
H	5.322856	-0.906454	2.397641
H	6.166760	-2.232823	0.478916
O	-0.155863	2.924363	0.637454
H	-0.877820	3.525485	0.389877
C	-4.005969	-1.097847	0.107461
H	-4.593183	-1.709673	-0.585025
C	-4.386014	0.388348	-0.163210
H	-4.099428	0.695161	-1.171879
H	-3.831379	1.016533	0.550321
O	-5.772173	0.557563	-0.053418
H	-6.044623	0.187765	0.798250
C	-2.527219	-1.274604	-0.191407
O	-2.148665	-1.431325	-1.471525

H	-2.902793	-1.457946	-2.077101
O	-1.656960	-1.210864	0.658849
N	-4.396770	-1.427025	1.463187
H	-4.496428	-2.424050	1.612527
H	-3.732557	-1.066535	2.141156

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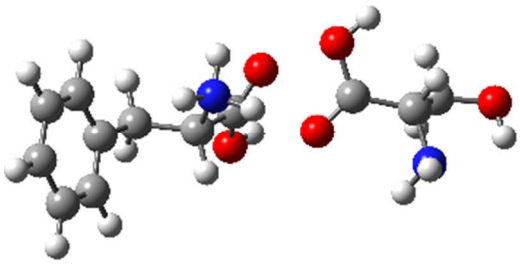

Isomer 12, 42.3 kJ·mol^{-1}

N	0.678237	-0.084985	-0.681475
H	-0.190894	-0.564382	-0.320309
H	1.454525	-0.751143	-0.760274
H	0.444252	0.280619	-1.610190
C	1.067464	1.041684	0.229842
H	0.983214	0.670195	1.252081
C	2.518785	1.497215	-0.048860
C	0.059200	2.160858	0.005096
H	2.567222	1.958703	-1.040025
H	2.756361	2.273623	0.680940
C	3.479926	0.332939	0.046665
O	-0.698522	2.186366	-0.932232
C	3.981658	-0.273691	-1.111352
C	3.832318	-0.192645	1.296072
H	3.745296	0.142450	-2.086529
C	4.820177	-1.386630	-1.022439
C	4.670116	-1.300945	1.384675
H	3.466123	0.277821	2.203507
H	5.213539	-1.838467	-1.925396
C	5.162441	-1.902136	0.225068
H	4.946978	-1.690510	2.357183
H	5.818661	-2.761277	0.296253
O	0.164570	3.091292	0.952158
H	-0.454521	3.816804	0.767219
C	-4.042541	-1.198233	0.033141
H	-4.587416	-1.826791	-0.679055
C	-4.704554	0.210968	-0.009358
H	-4.593706	0.672033	-0.994187
H	-4.193355	0.851966	0.725141

O	-6.077820	0.105037	0.244148
H	-6.185607	-0.393505	1.066326
C	-2.596583	-1.071957	-0.419741
O	-2.347712	-0.961903	-1.734265
H	-3.151598	-1.026119	-2.269107
O	-1.653738	-1.003847	0.349536
N	-4.218768	-1.744712	1.362574
H	-4.131533	-2.753574	1.388396
H	-3.555653	-1.348637	2.021248

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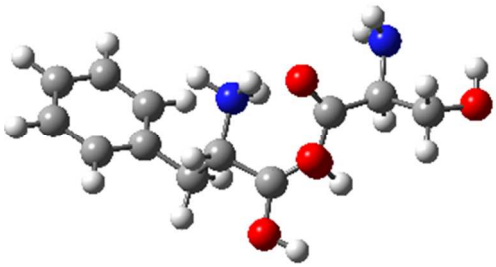

Isomer 13, 43.5 kJ·mol^{-1}

N	-0.825746	-0.548921	1.499471
H	-0.512768	-0.991122	2.365962
H	-1.592539	0.102689	1.693059
H	-0.009389	0.007910	1.124206
C	-1.273777	-1.571901	0.491735
H	-2.108155	-2.122556	0.933575
C	-1.742136	-0.869730	-0.800878
C	-0.108289	-2.534157	0.294337
H	-0.877484	-0.417538	-1.290946
H	-2.122448	-1.648665	-1.463750
C	-2.801908	0.168542	-0.503602
O	0.927193	-2.450510	0.904105
C	-2.457236	1.520967	-0.388599
C	-4.130278	-0.214544	-0.283001
H	-1.434860	1.835318	-0.577037
C	-3.423291	2.473154	-0.060167
C	-5.095043	0.735927	0.042777
H	-4.416380	-1.256932	-0.385922
H	-3.147177	3.518479	0.013653
C	-4.742435	2.081117	0.157447
H	-6.122681	0.429041	0.197641
H	-5.494988	2.820048	0.405341
O	-0.406633	-3.460870	-0.616139
H	0.335762	-4.081364	-0.700781
C	3.487829	1.200673	-0.366322

H	3.715046	1.459596	-1.406097
C	4.468834	0.059701	0.037834
H	4.291907	-0.843228	-0.552252
H	4.292679	-0.188053	1.095090
O	5.791053	0.454524	-0.203944
H	5.934345	1.296731	0.249613
C	2.063551	0.671841	-0.287168
O	1.634748	-0.128535	-1.279286
H	2.299730	-0.226292	-1.975647
O	1.316597	0.889483	0.648155
N	3.759555	2.352383	0.467141
H	3.415325	3.217858	0.069187
H	3.363404	2.245287	1.395560

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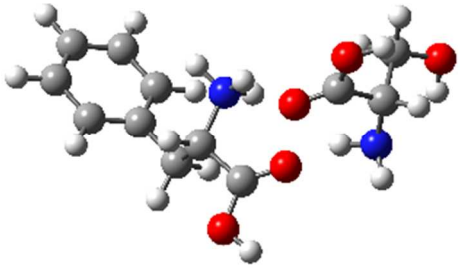

Isomer 14, 43.7 kJ·mol^{-1}

N	-0.899353	-0.781826	1.311236
H	-0.610329	-1.347716	2.111814
H	-1.475085	0.006087	1.620736
H	-0.020173	-0.391513	0.868783
C	-1.653325	-1.596918	0.297204
H	-2.590044	-1.918232	0.758987
C	-1.952322	-0.731405	-0.946104
C	-0.804467	-2.826585	-0.001634
H	-1.011074	-0.504397	-1.453139
H	-2.552351	-1.341333	-1.623315
C	-2.672914	0.541887	-0.559000
O	0.261479	-3.036673	0.519642
C	-1.968023	1.745136	-0.433487
C	-4.041084	0.519784	-0.262840
H	-0.910311	1.776407	-0.676551
C	-2.621727	2.906997	-0.020466
C	-4.693099	1.679858	0.148723
H	-4.603639	-0.402385	-0.373614
H	-2.070090	3.836280	0.060876
C	-3.983443	2.874802	0.273141
H	-5.755149	1.654371	0.362329

H	-4.492923	3.777830	0.587564
O	-1.405630	-3.610212	-0.896349
H	-0.857704	-4.395116	-1.061332
C	3.697013	0.239903	-0.220926
H	4.421893	-0.515927	0.100424
C	4.263256	1.621068	0.222854
H	4.331203	1.689764	1.311586
H	3.572901	2.404872	-0.124142
O	5.559161	1.794790	-0.279448
H	5.526275	1.652224	-1.235496
C	2.379555	-0.013842	0.495518
O	2.418541	-0.351875	1.793046
H	3.322259	-0.481673	2.113960
O	1.286683	0.126043	-0.026164
N	3.619778	0.219791	-1.666296
H	3.583076	-0.718282	-2.046256
H	2.816859	0.738441	-2.007491

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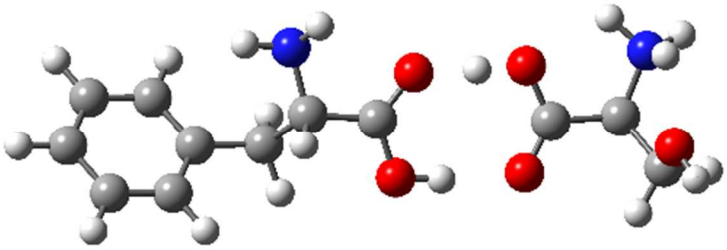

Isomer 15, 48.9 kJ·mol^{-1}

N	-1.960932	1.552328	0.919985
H	-1.416953	1.857939	1.718423
H	-2.945870	1.623693	1.150040
C	-1.638012	0.195620	0.520443
H	-1.833705	-0.567531	1.295405
C	-2.463392	-0.212057	-0.732277
C	-0.156993	0.074862	0.246726
H	-2.239605	0.499919	-1.531000
H	-2.139727	-1.202213	-1.057558
C	-3.945359	-0.219093	-0.435193
O	0.636708	0.995294	0.471270
C	-4.751426	0.874392	-0.767291
C	-4.528780	-1.313684	0.213777
H	-4.312766	1.726936	-1.274981
C	-6.111219	0.875544	-0.456018
C	-5.885996	-1.315042	0.525730
H	-3.918371	-2.175369	0.467395

H	-6.724320	1.728253	-0.724550
C	-6.680913	-0.218002	0.192534
H	-6.325088	-2.173150	1.021711
H	-7.738031	-0.219706	0.431434
O	0.208110	-1.103623	-0.214676
H	1.181035	-1.154678	-0.358163
C	5.051869	0.100242	-0.748134
H	5.137353	0.205533	-1.831384
C	5.849405	-1.101332	-0.245007
H	6.837267	-1.137534	-0.718607
H	5.290517	-2.004985	-0.499337
O	5.954885	-0.895290	1.161136
H	6.321440	-1.666452	1.606670
C	3.551870	-0.000556	-0.409383
O	3.055015	1.116939	0.038438
H	1.996813	1.043187	0.226859
O	2.962776	-1.042937	-0.611781
H	5.904403	1.092893	0.854326
H	6.413762	1.738565	-0.601542
H	4.861705	2.055803	-0.030238
N	5.610792	1.353995	-0.100364

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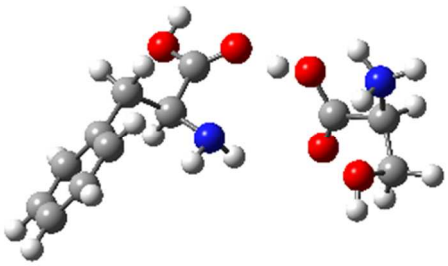

Isomer 16, 50.0 kJ·mol^{-1}

N	0.316837	0.174780	0.481374
H	-0.237435	0.250892	1.328687
H	0.835672	-0.696380	0.527966
C	1.246094	1.286887	0.350827
H	1.806238	1.514276	1.269181
C	2.288414	1.004812	-0.769048
C	0.486239	2.548682	-0.004103
H	1.751385	0.844573	-1.708112
H	2.914118	1.891950	-0.886962
C	3.141301	-0.199300	-0.441309
O	-0.677642	2.608305	-0.372371
C	2.919568	-1.430041	-1.066831
C	4.152326	-0.106129	0.522804

H	2.148706	-1.512575	-1.826436
C	3.689357	-2.545949	-0.735904
C	4.921368	-1.217834	0.855253
H	4.346036	0.845741	1.007733
H	3.512625	-3.491112	-1.236606
C	4.689992	-2.442482	0.227323
H	5.706744	-1.128212	1.596905
H	5.292864	-3.306335	0.481817
O	1.237317	3.641212	0.106503
H	0.715554	4.416791	-0.154815
C	-4.311704	-0.477556	0.104032
H	-5.154899	0.157824	0.381669
C	-4.368091	-1.818347	0.830198
H	-5.388592	-2.218620	0.833433
H	-4.037959	-1.653358	1.858423
O	-3.484422	-2.665097	0.097940
H	-3.319023	-3.490382	0.565120
C	-3.017445	0.310126	0.409683
O	-2.553585	0.897331	-0.675118
H	-1.718741	1.462389	-0.507282
O	-2.589432	0.364642	1.531012
H	-3.867252	-1.608980	-1.570107
H	-5.345758	-0.847176	-1.730240
H	-3.918169	0.034752	-1.881760
N	-4.388617	-0.736892	-1.390796

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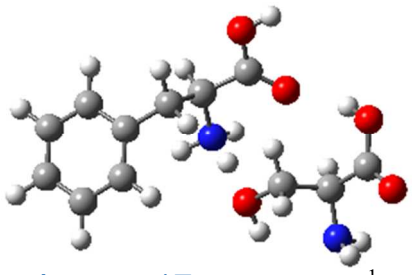

Isomer 17, 50.7 kJ·mol^{-1}

N	-0.769414	0.210162	-1.427924
H	-0.338107	0.481522	-2.313204
H	-1.661610	-0.262099	-1.610056
H	-0.131935	-0.505269	-0.950616
C	-1.027631	1.400605	-0.546136
H	-1.728558	2.054547	-1.070177
C	-1.659326	0.933180	0.787241
C	0.285715	2.144818	-0.353337
H	-0.918108	0.366475	1.357090

H	-1.895542	1.831351	1.360039
C	-2.891620	0.091685	0.535160
O	1.347673	1.745133	-0.777735
C	-2.810671	-1.306320	0.563507
C	-4.111221	0.700230	0.214973
H	-1.873101	-1.786912	0.826054
C	-3.934316	-2.082672	0.276534
C	-5.231871	-0.076436	-0.069947
H	-4.192247	1.783099	0.209473
H	-3.866137	-3.163518	0.314094
C	-5.143863	-1.468811	-0.042409
H	-6.175070	0.403603	-0.302348
H	-6.018178	-2.071254	-0.258005
O	0.099600	3.255536	0.344980
H	0.940789	3.727405	0.466589
C	3.047631	-0.957322	-0.368238
H	2.735121	-0.349396	-1.222103
C	1.856468	-1.052660	0.596035
H	1.555439	-0.080771	0.981740
H	2.104921	-1.702074	1.440521
O	0.730715	-1.601803	-0.117638
H	1.097593	-2.371578	-0.593603
C	4.215015	-0.259670	0.348319
O	4.112151	1.086507	0.437437
H	3.363554	1.417983	-0.080779
O	5.122019	-0.860218	0.846364
N	3.317236	-2.309981	-0.835791
H	3.837341	-2.307492	-1.706611
H	3.891208	-2.803557	-0.154585

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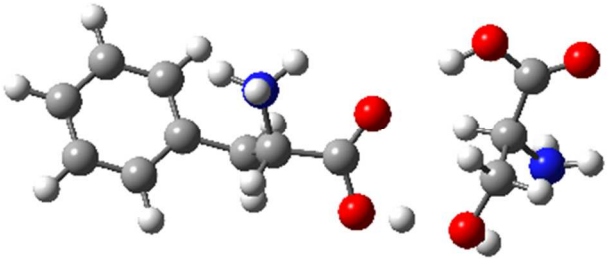

Isomer 18, 59.5 kJ·mol^{-1}

N	-1.640123	0.862791	1.347883
H	-1.625441	0.809260	2.368382
H	-2.560221	1.219629	1.043867
H	-0.884699	1.505072	1.063820
C	-1.370162	-0.479129	0.699150

H	-1.768612	-1.251072	1.356480
C	-2.068074	-0.537585	-0.681174
C	0.149980	-0.607460	0.572226
H	-1.555146	0.138241	-1.372426
H	-1.929492	-1.552534	-1.058018
C	-3.530782	-0.172961	-0.564683
O	0.855890	0.387151	0.685137
C	-3.966040	1.116652	-0.900343
C	-4.453938	-1.089886	-0.046837
H	-3.272510	1.824098	-1.347215
C	-5.302032	1.483201	-0.719377
C	-5.785811	-0.724528	0.128872
H	-4.135164	-2.097755	0.200518
H	-5.630634	2.477422	-0.997883
C	-6.210548	0.563891	-0.201868
H	-6.495324	-1.446359	0.515738
H	-7.248721	0.843187	-0.068355
O	0.510141	-1.821033	0.307871
H	1.534992	-1.960991	0.190454
C	3.852595	-0.024196	-0.569751
H	2.847816	0.139567	-0.971877
C	3.718315	-1.014364	0.595167
H	3.145443	-0.610196	1.427939
H	4.705012	-1.313754	0.958418
O	3.005167	-2.177209	0.130764
H	3.419768	-2.430179	-0.713160
C	4.380233	1.323132	-0.051396
O	3.481839	2.037455	0.669807
H	2.624954	1.586070	0.692110
O	5.496451	1.711615	-0.234801
N	4.655948	-0.669148	-1.595669
H	4.531994	-0.226947	-2.499927
H	5.644465	-0.589495	-1.366968

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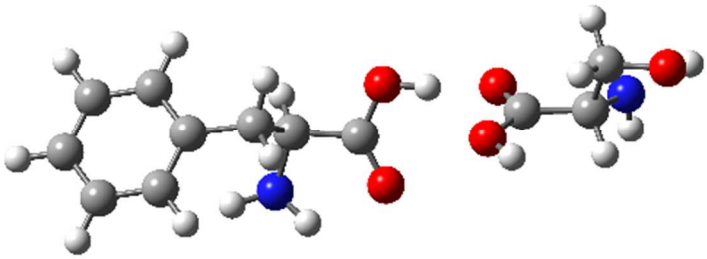

Isomer 19, 59.7 kJ·mol^{-1}

N	-2.465386	-1.825379	0.540526

H	-2.610292	-2.731514	0.092284
H	-3.373464	-1.472861	0.876663
H	-1.794818	-1.966941	1.318306
C	-1.817768	-0.822073	-0.391385
H	-2.069415	-1.099736	-1.414165
C	-2.332661	0.601189	-0.074850
C	-0.309715	-0.948066	-0.139704
H	-1.925236	0.923908	0.888068
H	-1.913493	1.259866	-0.837553
C	-3.843428	0.647080	-0.056374
O	0.095791	-1.541062	0.841457
C	-4.535527	0.630565	1.162196
C	-4.572542	0.628861	-1.251824
H	-3.985960	0.690311	2.097865
C	-5.932111	0.595477	1.184852
C	-5.964086	0.597499	-1.228376
H	-4.050621	0.658798	-2.203301
H	-6.456107	0.599387	2.133317
C	-6.646131	0.575515	-0.010096
H	-6.518338	0.598813	-2.159537
H	-7.729232	0.556102	0.004629
O	0.383659	-0.328802	-1.050356
H	1.381843	-0.370528	-0.869029
C	5.096489	-0.044244	0.309940
H	5.349380	-0.163245	1.369324
C	5.762515	1.277778	-0.166408
H	5.358733	2.141836	0.367682
H	5.544490	1.409919	-1.236801
O	7.140684	1.243863	0.092615
H	7.485224	0.423808	-0.288099
C	3.583098	0.076655	0.179853
O	2.937143	0.855578	1.058620
H	3.534595	1.211189	1.730944
O	2.949639	-0.457693	-0.710715
N	5.682917	-1.142644	-0.431014
H	5.560001	-2.034272	0.033862
H	5.281247	-1.215222	-1.360961

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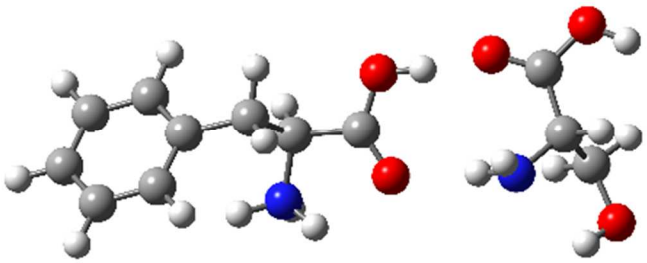

Isomer 20, 65.8 kJ·mol^{-1}

N	1.850367	-1.300823	1.019044
H	1.784484	-1.455324	2.026832
H	2.808618	-1.524783	0.709313
H	1.154149	-1.916974	0.567061
C	1.499440	0.121198	0.633329
H	1.751366	0.768245	1.472787
C	2.300438	0.535961	-0.624078
C	-0.008406	0.127868	0.370947
H	1.923608	-0.018184	-1.489241
H	2.083074	1.591417	-0.797561
C	3.778959	0.286547	-0.433827
O	-0.611418	-0.922511	0.231818
C	4.378947	-0.854052	-0.985189
C	4.551488	1.146948	0.356131
H	3.805784	-1.505482	-1.639662
C	5.728085	-1.130107	-0.749319
C	5.896817	0.872989	0.586906
H	4.105224	2.043703	0.774825
H	6.185071	-2.005818	-1.194734
C	6.485747	-0.268584	0.039264
H	6.489357	1.553586	1.186787
H	7.534110	-0.475980	0.217048
O	-0.476407	1.336524	0.283737
H	-1.466262	1.358609	0.091723
C	-4.533967	-0.258613	-0.561405
H	-5.410451	-0.264135	-1.218803
C	-4.955670	-0.943489	0.765872
H	-5.751066	-0.384472	1.264368
H	-4.082942	-0.961651	1.437157
O	-5.449363	-2.233820	0.512294
H	-4.821233	-2.665997	-0.083599
C	-4.146948	1.191754	-0.272570
O	-5.137137	2.073461	-0.119546
H	-6.002303	1.675882	-0.288807
O	-3.003712	1.576712	-0.128171
N	-3.499661	-1.066465	-1.175674
H	-3.354767	-0.839111	-2.151821

H	-2.613968	-0.994994	-0.682885

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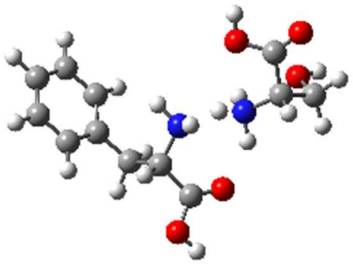

Isomer 21, 111.1 kJ·mol^{-1}

N	-0.378448	0.311559	-0.916625
H	-0.127240	0.395011	-1.899657
H	-0.930299	-0.543328	-0.846391
C	-1.241875	1.445723	-0.527241
H	-1.932667	1.718013	-1.331027
C	-2.088225	1.087686	0.726893
C	-0.402204	2.679333	-0.218175
H	-1.413722	0.878233	1.563035
H	-2.673678	1.969639	0.997049
C	-3.000045	-0.097225	0.487941
O	0.758107	2.679572	0.144728
C	-2.714978	-1.346194	1.050340
C	-4.144644	0.036390	-0.308743
H	-1.850019	-1.461732	1.696733
C	-3.549997	-2.440320	0.818738
C	-4.978061	-1.053883	-0.541585
H	-4.397469	1.002075	-0.735823
H	-3.322432	-3.398121	1.272181
C	-4.680785	-2.296391	0.019607
H	-5.865499	-0.932476	-1.151711
H	-5.334278	-3.142553	-0.156602
O	-1.117630	3.795921	-0.355651
H	-0.574321	4.558760	-0.098475
C	3.323103	-0.024476	-0.287377
H	3.354111	0.666969	-1.132524
C	4.537772	0.201567	0.613738
H	4.640513	1.268891	0.843307
H	5.430038	-0.140101	0.084065
O	4.275332	-0.558681	1.787659
H	5.057433	-0.607033	2.347201
C	3.336863	-1.446647	-0.858419
O	2.170174	-2.093307	-0.662332
H	2.247942	-2.987069	-1.035414

O	4.286582	-1.897082	-1.428228
H	2.098069	-0.286617	1.359488
H	1.995311	1.256849	0.714900
H	1.170002	0.080709	-0.047149
N	2.076361	0.255592	0.491543

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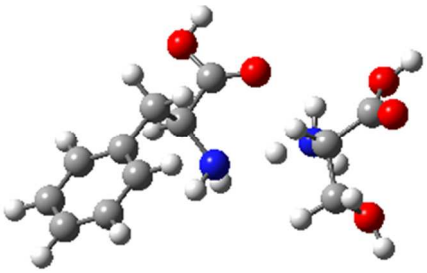

Isomer 22, 111.9 kJ·mol^{-1}

N	0.624527	0.523658	1.314522
H	0.590255	0.820147	2.288439
H	1.186350	-0.327791	1.307849
C	1.342912	1.542211	0.518029
H	2.184007	1.963596	1.077228
C	1.903987	0.923169	-0.791371
C	0.410020	2.694910	0.167317
H	1.069163	0.562986	-1.400945
H	2.391964	1.722253	-1.354190
C	2.877083	-0.206686	-0.527427
O	-0.801288	2.638233	0.134994
C	2.520891	-1.535077	-0.784080
C	4.153910	0.059043	-0.015570
H	1.548936	-1.757947	-1.214521
C	3.414650	-2.576730	-0.530716
C	5.046465	-0.978266	0.239282
H	4.460964	1.084008	0.168640
H	3.128213	-3.599259	-0.748039
C	4.677634	-2.299783	-0.014889
H	6.034153	-0.755578	0.625793
H	5.376061	-3.105575	0.177278
O	1.099851	3.794766	-0.143178
H	0.481533	4.496103	-0.405479
C	-2.594490	-0.821516	-0.197947
H	-1.862030	-0.887757	-1.006301
C	-2.653338	-2.144919	0.565346
H	-1.640458	-2.490629	0.802417
H	-3.148622	-2.884787	-0.066866
O	-3.388784	-1.860509	1.750574

H	-3.681685	-2.671226	2.179151
C	-3.947682	-0.504162	-0.849822
O	-4.307786	0.779203	-0.665485
H	-5.151591	0.941872	-1.118557
O	-4.565394	-1.316089	-1.473542
H	-2.678081	0.161858	1.613624
H	-1.103343	0.234757	0.944427
H	-2.306850	1.198181	0.356157
N	-2.153052	0.259093	0.738416

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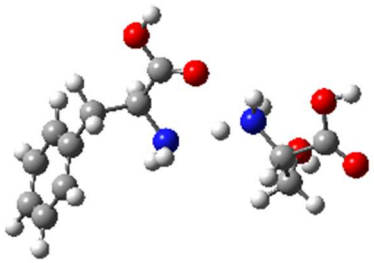

Isomer 23, 113.1 kJ·mol^{-1}

N	0.470545	-0.012909	-0.262553
H	1.015332	-0.849542	-0.058305
H	0.443081	0.043029	-1.280862
C	1.227181	1.149949	0.252006
H	1.388313	0.983729	1.322919
C	2.615179	1.342973	-0.416796
C	0.356026	2.397920	0.149755
H	2.467400	1.568638	-1.478406
H	3.090338	2.218295	0.030392
C	3.497972	0.122724	-0.263292
O	-0.797712	2.409375	-0.225223
C	3.726791	-0.740865	-1.339726
C	4.095339	-0.169108	0.969924
H	3.298660	-0.515460	-2.311870
C	4.528108	-1.873207	-1.188796
C	4.894321	-1.299388	1.123595
H	3.955139	0.502731	1.811706
H	4.705965	-2.524485	-2.036759
C	5.110270	-2.156355	0.044193
H	5.359661	-1.504117	2.080842
H	5.739343	-3.030826	0.161520
O	1.007097	3.493452	0.545817
H	0.412264	4.257679	0.475350
C	-3.143465	-0.865099	-0.399645
H	-2.738722	-0.931433	-1.412838

C	-3.117558	-2.240812	0.266479
H	-2.139338	-2.713837	0.121906
H	-3.889616	-2.860460	-0.194226
O	-3.368548	-1.992420	1.645670
H	-3.600967	-2.804784	2.106934
C	-4.582038	-0.344931	-0.531066
O	-4.680795	0.953660	-0.189954
H	-5.596723	1.249236	-0.321924
O	-5.478515	-1.027357	-0.930738
H	-2.475596	-0.070253	1.381764
H	-1.227761	-0.074738	0.201205
H	-2.448122	1.051741	0.147463
N	-2.276534	0.069920	0.385598

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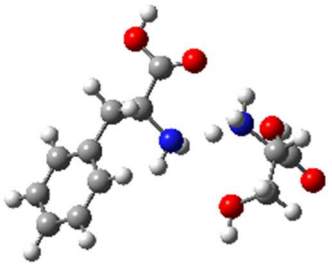

Isomer 24, 117.7 kJ·mol^{-1}

N	-0.022468	0.341103	-0.529753
H	0.399647	0.404345	-1.453662
H	-0.568686	-0.519440	-0.530267
C	-0.925938	1.487321	-0.305722
H	-1.439898	1.776799	-1.227380
C	-2.007086	1.141475	0.754958
C	-0.128800	2.696300	0.170221
H	-1.512366	0.906782	1.702774
H	-2.609892	2.037474	0.919469
C	-2.887477	-0.014970	0.330349
O	0.963920	2.657923	0.695461
C	-2.761354	-1.271458	0.932108
C	-3.844070	0.153802	-0.679176
H	-2.046813	-1.413579	1.737371
C	-3.567449	-2.338477	0.532407
C	-4.648021	-0.909311	-1.080184
H	-3.975395	1.126527	-1.143311
H	-3.467177	-3.302222	1.018298
C	-4.509560	-2.159848	-0.476742
H	-5.390583	-0.760247	-1.855401
H	-5.141365	-2.984657	-0.784404

O	-0.806124	3.830152	-0.028700
H	-0.294039	4.573812	0.328367
C	3.290926	-0.786832	0.747553
H	4.116022	-0.630975	1.449483
C	2.778503	-2.214961	0.902307
H	2.534270	-2.410694	1.954439
H	3.581292	-2.890565	0.597604
O	1.627516	-2.336424	0.076630
H	1.446672	-3.265884	-0.098320
C	3.872437	-0.559175	-0.652021
O	3.478654	0.616808	-1.182497
H	3.930775	0.739124	-2.033812
O	4.622555	-1.331460	-1.171116
H	1.310288	0.135898	0.446069
H	1.916393	0.102306	2.044522
H	2.501202	1.175102	0.943612
N	2.212515	0.200210	1.072190

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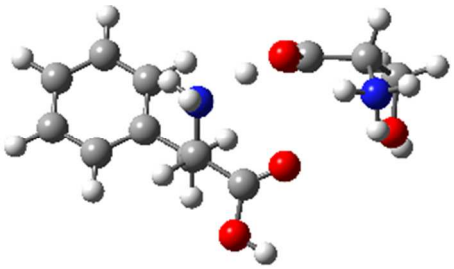

Isomer 25, 118.6 kJ·mol^{-1}

N	0.609520	0.687011	1.585455
H	0.585537	1.247122	2.435797
H	1.405556	0.053838	1.677050
C	0.847450	1.550684	0.406055
H	1.628559	2.285696	0.620447
C	1.308868	0.696322	-0.809057
C	-0.412563	2.325092	0.036754
H	0.511271	-0.001907	-1.074636
H	1.454069	1.375945	-1.651664
C	2.585258	-0.065035	-0.517938
O	-1.551218	2.024117	0.324340
C	2.545614	-1.434004	-0.227214
C	3.823047	0.590994	-0.521985
H	1.595336	-1.958436	-0.244172
C	3.720699	-2.131021	0.058919
C	4.994626	-0.104902	-0.236826
H	3.875173	1.647772	-0.766582

H	3.677567	-3.192667	0.273282
C	4.945208	-1.468029	0.057206
H	5.946685	0.412818	-0.253396
H	5.858220	-2.010061	0.273884
O	-0.100392	3.397321	-0.701061
H	-0.916267	3.852949	-0.962022
C	-3.472987	-1.265823	0.391691
H	-3.914986	-1.943659	1.124879
C	-3.922420	-1.613396	-1.023679
H	-4.976048	-1.914286	-1.036004
H	-3.302944	-2.441464	-1.374592
O	-3.725185	-0.430345	-1.794641
H	-3.744127	-0.625484	-2.736717
C	-1.933724	-1.279248	0.586465
O	-1.607397	-0.571961	1.642835
H	-0.615462	-0.117916	1.594705
O	-1.201660	-1.874314	-0.164464
H	-3.831709	0.713173	-0.123386
H	-4.892020	0.189838	1.059481
H	-3.276028	0.514166	1.436131
N	-3.927566	0.141658	0.728691

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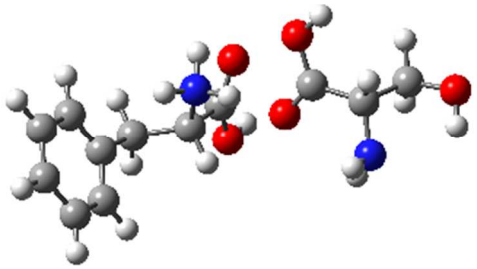

Isomer 26, 135.5 kJ·mol^{-1}

N	0.683671	0.486346	-0.828021
H	-0.249084	0.081404	-0.547980
H	1.326487	-0.278403	-1.066271
C	1.270888	1.323709	0.272847
H	0.953947	0.887726	1.220462
C	2.818226	1.347451	0.185566
C	0.676762	2.719351	0.110895
H	3.118728	1.906498	-0.705913
H	3.176698	1.908269	1.051187
C	3.406321	-0.047115	0.153256
O	0.132120	3.079463	-0.903134
C	3.853699	-0.599941	-1.053813
C	3.485319	-0.817487	1.320886

H	3.843337	-0.001777	-1.960780
C	4.365129	-1.898766	-1.094515
C	3.997407	-2.111232	1.280123
H	3.166966	-0.397963	2.270346
H	4.722219	-2.307806	-2.032305
C	4.434331	-2.655830	0.071557
H	4.067181	-2.691228	2.192852
H	4.839452	-3.660327	0.044071
O	0.876035	3.462793	1.195577
H	0.527173	4.357238	1.044451
C	-4.017191	-1.202592	0.036301
H	-4.460893	-1.984616	-0.589307
C	-4.996984	0.008619	0.003515
H	-5.093742	0.415472	-1.006054
H	-4.592425	0.799495	0.652209
O	-6.275531	-0.398080	0.404515
H	-6.183915	-0.846211	1.257075
C	-2.681558	-0.791456	-0.569899
O	-2.591368	-0.714077	-1.905646
H	-3.405231	-0.998256	-2.345859
O	-1.706631	-0.481900	0.093231
H	0.526655	1.084889	-1.648913
H	-3.641790	-2.657552	1.454446
H	-3.326035	-1.126652	1.970047
N	-3.944506	-1.692481	1.397717

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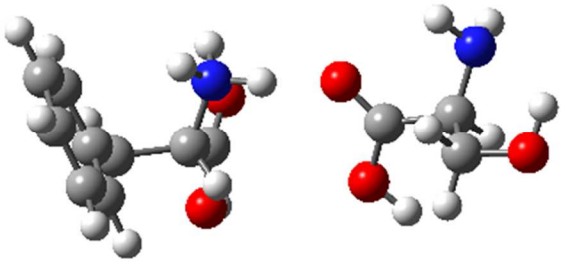

Isomer 27, 135.7 kJ·mol^{-1}

N	-0.810526	0.711493	1.103571
H	0.203931	0.442726	1.014246
H	-1.355585	-0.124265	1.347914
H	-0.881479	1.412502	1.852452
C	-1.337976	1.313367	-0.168472
H	-0.790708	0.862454	-0.996541
C	-2.857496	1.046642	-0.319154
C	-1.031933	2.805660	-0.093391
H	-3.399649	1.619982	0.439059

H	-3.154477	1.442066	-1.292627
C	-3.189184	-0.425499	-0.199756
O	-0.726362	3.355668	0.935531
C	-3.729744	-0.936048	0.987657
C	-2.932360	-1.305252	-1.259550
H	-3.979242	-0.262869	1.803209
C	-4.002764	-2.299582	1.115972
C	-3.207346	-2.663860	-1.132063
H	-2.537718	-0.924924	-2.196832
H	-4.434724	-2.678191	2.034823
C	-3.738718	-3.164284	0.057638
H	-3.018581	-3.331597	-1.964449
H	-3.958101	-4.221113	0.151653
O	-1.184881	3.395389	-1.276043
H	-1.030468	4.350373	-1.183208
C	4.104202	-0.261624	0.153260
H	4.742525	0.510047	-0.290882
C	4.294161	-1.549143	-0.703744
H	3.951218	-1.398566	-1.730502
H	3.692248	-2.354486	-0.257778
O	5.652178	-1.883413	-0.772623
H	5.986905	-1.928457	0.134052
C	2.653752	0.197147	0.067894
O	2.258192	0.831390	-1.050257
H	2.994471	0.982394	-1.660298
O	1.825060	-0.021662	0.931793
N	4.580118	-0.533209	1.493544
H	4.829159	0.306412	2.002732
H	3.898599	-1.050776	2.039547

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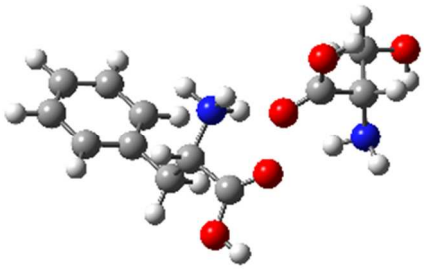

Isomer 28, 142.1 kJ·mol^{-1}

N	0.839461	0.792827	1.227261
H	0.583802	1.358954	2.039529
H	1.315871	-0.061281	1.532262
H	-0.066016	0.511004	0.756725
C	1.734717	1.557914	0.290163

H	2.647427	1.797802	0.842524
C	2.089142	0.689443	-0.934456
C	1.019700	2.867840	-0.029405
H	1.180062	0.488268	-1.508047
H	2.744571	1.288431	-1.569319
C	2.761605	-0.607326	-0.528134
O	-0.023847	3.188090	0.479984
C	2.045549	-1.810539	-0.518899
C	4.106072	-0.616762	-0.133832
H	1.012066	-1.826438	-0.851876
C	2.659546	-2.998552	-0.119016
C	4.718465	-1.802245	0.264774
H	4.686521	0.300713	-0.161178
H	2.097997	-3.925394	-0.129645
C	3.994977	-2.995092	0.275886
H	5.762704	-1.797805	0.554305
H	4.474752	-3.918030	0.579054
O	1.712714	3.592409	-0.907103
H	1.251178	4.432318	-1.066930
C	-3.888482	-0.200203	-0.174280
H	-4.649867	0.483321	0.217088
C	-4.353083	-1.643044	0.185588
H	-4.393532	-1.789888	1.267678
H	-3.624229	-2.355690	-0.227880
O	-5.645204	-1.867987	-0.305323
H	-5.641036	-1.648610	-1.247563
C	-2.565898	0.097610	0.520084
O	-2.593152	0.386639	1.830507
H	-3.495919	0.450259	2.173660
O	-1.481596	0.038132	-0.033067
N	-3.862777	-0.076525	-1.617220
H	-3.924499	0.884273	-1.932239
H	-3.029306	-0.494796	-2.017844

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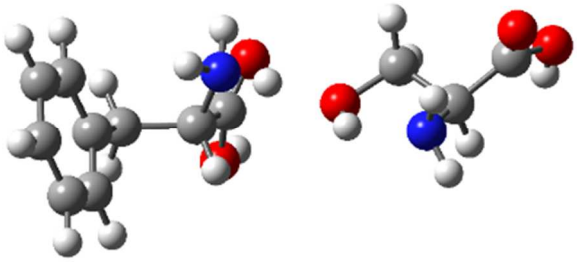

Isomer 29, 145.1 kJ·mol^{-1}

N	0.824202	0.520355	-0.789919

H	-0.127218	0.212610	-0.431999
H	1.382322	-0.307030	-1.032404
H	0.669033	1.094299	-1.627744
C	1.558275	1.347218	0.226788
H	1.288183	0.969562	1.213362
C	3.091133	1.247864	0.019622
C	1.053536	2.776669	0.060464
H	3.360439	1.747947	-0.915824
H	3.559110	1.810708	0.829822
C	3.566955	-0.189268	0.002999
O	0.432554	3.138671	-0.908406
C	3.868935	-0.822619	-1.209681
C	3.682579	-0.917919	1.194203
H	3.830162	-0.261146	-2.139063
C	4.272973	-2.159199	-1.232382
C	4.087797	-2.249539	1.171127
H	3.478587	-0.437430	2.146287
H	4.518259	-2.631696	-2.176214
C	4.379410	-2.873944	-0.042621
H	4.188209	-2.797599	2.100584
H	4.701510	-3.908300	-0.057041
O	1.416552	3.543914	1.084387
H	1.121155	4.456384	0.927326
C	-3.929761	-0.560184	0.600079
H	-4.045932	0.083907	1.476917
C	-2.867512	0.068852	-0.343376
H	-2.994974	1.147492	-0.441011
H	-2.934547	-0.391930	-1.334882
O	-1.575350	-0.186542	0.226510
H	-1.716816	-1.040238	0.705973
C	-5.259604	-0.698979	-0.161808
O	-6.034613	0.401525	-0.245468
H	-5.713565	1.117812	0.317021
O	-5.566861	-1.718520	-0.710031
N	-3.398562	-1.850394	1.038127
H	-3.726243	-2.095136	1.966063
H	-3.715408	-2.581612	0.402352

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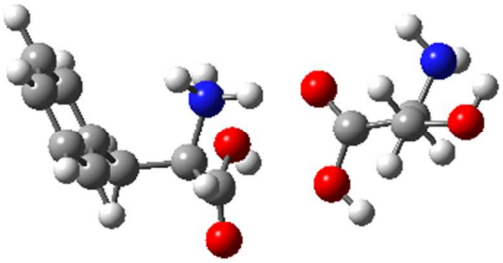

Isomer 30, 148.1 kJ·mol^{-1}

N	-0.781199	-0.682590	-1.085561
H	0.247718	-0.452217	-1.050902
H	-1.310429	0.178944	-1.273190
H	-0.937262	-1.338428	-1.855654
C	-1.257978	-1.274216	0.218069
H	-0.762871	-0.716022	1.012136
C	-2.794941	-1.132329	0.346223
C	-0.833482	-2.732476	0.345501
H	-3.282051	-1.770175	-0.397738
H	-3.064548	-1.523658	1.329562
C	-3.242476	0.304985	0.184579
O	-0.767094	-3.305075	1.392191
C	-3.812927	0.741955	-1.018178
C	-3.066283	1.227904	1.224249
H	-3.999499	0.031903	-1.819135
C	-4.195574	2.074983	-1.180894
C	-3.450009	2.556242	1.062314
H	-2.650445	0.902712	2.173025
H	-4.649936	2.395303	-2.111051
C	-4.011494	2.983151	-0.142022
H	-3.323038	3.256462	1.879570
H	-4.316103	4.015868	-0.262761
O	-0.603607	-3.292262	-0.865552
H	-0.392063	-4.233115	-0.749104
C	4.097743	0.314694	-0.091390
H	4.681277	-0.372017	0.531530
C	4.247677	1.731190	0.541793
H	3.820936	1.765090	1.547353
H	3.701320	2.450873	-0.085375
O	5.602819	2.061021	0.663072
H	6.009373	1.948718	-0.207634
C	2.635505	-0.109207	-0.045972
O	2.134911	-0.529215	1.128581
H	2.812526	-0.583914	1.817911
O	1.882155	-0.041517	-1.000643
N	4.683994	0.343539	-1.414933
H	4.958320	-0.573244	-1.747083

H	4.059288	0.760835	-2.097544

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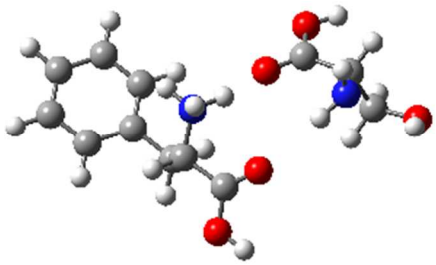

Isomer 31, 149.8 kJ·mol^{-1}

N	0.748012	0.612294	1.414056
H	0.519294	1.056369	2.305060
H	1.512062	-0.060066	1.553143
H	-0.094998	0.072126	1.100617
C	1.169571	1.620409	0.379105
H	1.974749	2.216312	0.815325
C	1.693216	0.891366	-0.880243
C	-0.027140	2.528887	0.119760
H	0.871386	0.336862	-1.341728
H	2.001724	1.663379	-1.587408
C	2.844236	-0.037724	-0.550172
O	-1.107281	2.366925	0.632464
C	2.625599	-1.411808	-0.384903
C	4.139013	0.469435	-0.379049
H	1.634775	-1.826763	-0.545325
C	3.682003	-2.260916	-0.049961
C	5.191775	-0.379127	-0.046847
H	4.332043	1.527484	-0.529017
H	3.502738	-3.323750	0.062085
C	4.964173	-1.745428	0.121504
H	6.191283	0.023121	0.069005
H	5.785962	-2.405151	0.373192
O	0.289846	3.502996	-0.728798
H	-0.482522	4.075019	-0.872907
C	-3.634271	-0.927809	0.349372
H	-4.357542	-1.651082	0.742034
C	-4.100902	-0.561487	-1.089459
H	-4.091688	-1.434063	-1.746790
H	-3.401777	0.181268	-1.503078
O	-5.417123	-0.081216	-1.063214
H	-5.461104	0.598583	-0.375756
C	-2.264740	-1.603754	0.285343
O	-2.221327	-2.871199	-0.132118

H	-3.105544	-3.233258	-0.285535
O	-1.212597	-1.047321	0.542558
N	-3.703343	0.267027	1.163966
H	-3.759275	0.071970	2.155798
H	-2.937093	0.909881	0.988883

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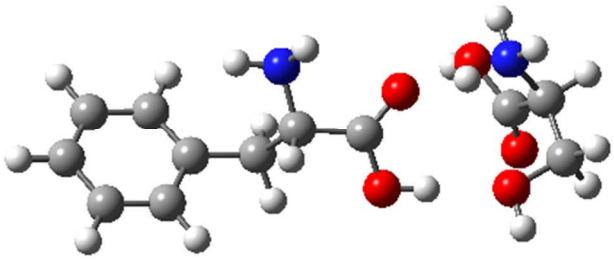

Isomer 32, 151.3 kJ·mol^{-1}

N	-1.544660	0.349648	1.867129
H	-1.152863	-0.028709	2.722045
H	2.594480	-0.020729	1.356044
H	-2.546603	0.448693	1.992085
C	-1.269956	-0.494406	0.718536
H	-1.626108	-1.535030	0.825751
C	-1.942247	0.085018	-0.557768
C	0.225772	-0.631693	0.533663
H	-1.564186	1.099791	-0.708999
H	-1.640281	-0.519251	-1.414950
C	-3.451750	0.108375	-0.447033
O	1.053365	-0.213779	1.342005
C	-4.131274	1.287493	-0.123470
C	-4.196090	-1.058994	-0.658325
H	-3.571283	2.204234	0.030100
C	-5.521432	1.299695	-0.007407
C	-5.583680	-1.049436	-0.542438
H	-3.689211	-1.980340	-0.929683
H	-6.033018	2.223253	0.238249
C	-6.250188	0.131069	-0.214166
H	-6.145664	-1.959815	-0.716879
H	-7.330505	0.140197	-0.128814
O	0.578942	-1.280288	-0.567000
H	1.551509	-1.390896	-0.584507
C	4.489037	0.197668	0.311728
H	5.478237	0.576801	0.588478
C	4.654741	-1.245767	-0.140406
H	5.197361	-1.813438	0.624124
H	5.245497	-1.233773	-1.059469

O	3.363819	-1.817917	-0.358668
H	3.467903	-2.701720	-0.732020
C	3.980971	1.117003	-0.811149
O	3.296375	2.156432	-0.299470
H	3.026357	2.756731	-1.014536
O	4.227911	0.938380	-1.965263
N	3.609578	0.308821	1.529540
H	3.989530	-0.230824	2.310046
H	3.533799	1.286677	1.822238

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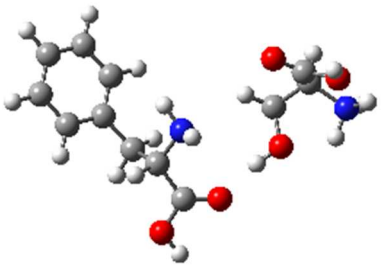

Isomer 33, 155.3 kJ·mol^{-1}

N	-0.416558	0.217700	-0.716124
H	0.041731	0.283164	-1.620643
H	-0.942818	-0.652288	-0.721459
C	-1.346910	1.328232	-0.526690
H	-1.974376	1.525620	-1.406591
C	-2.300559	1.045814	0.668690
C	-0.581530	2.614295	-0.262009
H	-1.694548	0.893879	1.566597
H	-2.915519	1.933642	0.830573
C	-3.182807	-0.160914	0.429680
O	0.598682	2.710723	0.019196
C	-2.931549	-1.375567	1.076106
C	-4.268511	-0.083127	-0.452116
H	-2.108440	-1.447851	1.780224
C	-3.740026	-2.489068	0.844260
C	-5.076233	-1.192535	-0.685834
H	-4.493835	0.855676	-0.948873
H	-3.536475	-3.420391	1.360370
C	-4.812216	-2.400449	-0.039472
H	-5.917422	-1.112896	-1.364783
H	-5.444686	-3.262253	-0.217408
O	-1.370271	3.687900	-0.362206
H	-0.847283	4.480772	-0.163199
C	3.732854	-0.943865	0.801657
H	3.832578	-1.752008	1.529082

C	2.459091	-0.119169	1.027605
H	2.301788	0.035535	2.103317
H	1.596910	-0.645769	0.613950
O	2.707146	1.099678	0.357623
H	1.876523	1.617101	0.218057
C	3.775479	-1.573117	-0.596354
O	4.990352	-1.425378	-1.170591
H	4.998513	-1.864551	-2.037186
O	2.850046	-2.154226	-1.074278
H	4.526712	0.927429	0.631838
H	5.166658	0.121214	1.958418
H	5.708087	-0.268525	0.423025
N	4.896604	0.016591	0.978621

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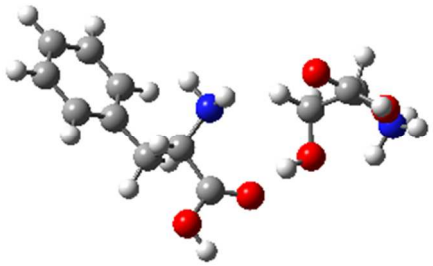

Isomer 34, 155.5 kJ·mol^{-1}

N	0.370655	-0.069491	0.625684
H	-0.142671	-0.005786	1.500731
H	1.061694	-0.805898	0.745781
C	1.068599	1.181159	0.336877
H	1.593328	1.596424	1.206984
C	2.122097	0.973550	-0.789349
C	0.083923	2.246953	-0.114296
H	1.605974	0.612862	-1.683512
H	2.560903	1.945098	-1.028468
C	3.207860	-0.002163	-0.388825
O	-1.029215	2.062199	-0.571793
C	3.232397	-1.301271	-0.906918
C	4.207933	0.378479	0.515213
H	2.478812	-1.605591	-1.626570
C	4.228286	-2.202351	-0.528016
C	5.201872	-0.518897	0.895571
H	4.219230	1.388419	0.913699
H	4.238483	-3.202259	-0.946637
C	5.213109	-1.813801	0.376270
H	5.973520	-0.205748	1.589408
H	5.990689	-2.510032	0.667879

O	0.590957	3.475013	0.025639
H	-0.045218	4.119330	-0.323683
C	-3.626164	-1.468722	-0.210295
H	-3.786374	-2.535070	-0.036465
C	-2.330821	-1.199693	-1.010292
H	-2.221580	-1.964418	-1.785737
H	-1.464711	-1.228320	-0.346337
O	-2.477681	0.065169	-1.624420
H	-1.871094	0.730109	-1.218146
C	-3.631179	-0.776321	1.156307
O	-4.804244	-0.150837	1.395825
H	-4.789709	0.247604	2.281901
O	-2.709972	-0.828323	1.914617
H	-4.315430	-0.122144	-1.562585
H	-5.065153	-1.615832	-1.768973
H	-5.551232	-0.623989	-0.511482
N	-4.753916	-0.936041	-1.072457

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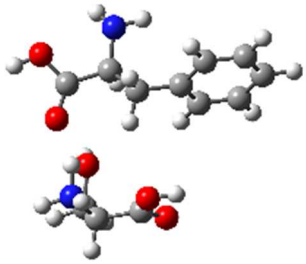

Isomer 35, 163.9 kJ·mol^{-1}

N	-1.914580	2.665711	0.790217
H	-1.692919	3.295657	1.552547
H	-2.692556	2.079551	1.072725
C	-0.786853	1.848810	0.385384
H	-0.365254	1.223058	1.192416
C	-1.210944	0.899167	-0.765448
C	0.396199	2.687505	-0.067294
H	-1.634048	1.510920	-1.566031
H	-0.316881	0.410080	-1.158299
C	-2.215946	-0.147456	-0.331504
O	1.438374	2.212968	-0.509569
C	-3.531767	-0.113239	-0.802991
C	-1.845981	-1.176633	0.545984
H	-3.836774	0.675811	-1.482220
C	-4.455147	-1.083662	-0.412169
C	-2.765731	-2.146724	0.937814
H	-0.834263	-1.217590	0.940354

H	-5.470554	-1.041432	-0.788846
C	-4.074741	-2.102557	0.457310
H	-2.462842	-2.934988	1.617635
H	-4.791420	-2.856555	0.760753
O	0.240853	3.994259	0.076886
H	1.048422	4.444947	-0.219452
C	3.284829	-1.132486	-0.364050
H	4.100994	-1.652121	-0.874592
C	3.696412	-0.822226	1.069109
H	4.670282	-0.315817	1.077813
H	3.790036	-1.774156	1.598508
O	2.675300	0.002325	1.605994
H	2.784881	0.089134	2.558892
C	2.064125	-2.062641	-0.419135
O	1.253807	-1.744317	-1.448077
H	0.497563	-2.355868	-1.468913
O	1.907473	-2.973292	0.336219
H	2.315905	0.787089	-0.660003
H	3.878568	0.689493	-1.232587
H	2.649627	-0.061697	-2.053649
N	3.020093	0.145036	-1.122494

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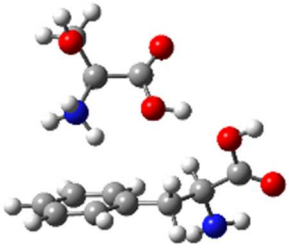

Isomer 36, 183.9 kJ·mol^{-1}

N	3.760729	0.516547	0.866056
H	4.393755	-0.103898	1.357880
H	3.501545	1.285365	1.471436
C	2.608968	-0.181488	0.322298
H	1.845660	-0.442553	1.076325
C	1.937143	0.660168	-0.789377
C	3.063879	-1.538253	-0.199252
H	2.744272	1.184095	-1.310334
H	1.467256	0.005709	-1.526498
C	0.899500	1.678272	-0.341404
O	4.169183	-1.985704	-0.156511
C	0.232768	2.425164	-1.329564
C	0.570635	1.929357	0.997179

H	0.483439	2.265371	-2.373659
C	-0.717707	3.388392	-0.993885
C	-0.383620	2.893665	1.339397
H	1.069965	1.392691	1.795752
H	-1.193844	3.968556	-1.776516
C	-1.033491	3.626511	0.347043
H	-0.594958	3.088426	2.385101
H	-1.747732	4.397369	0.613321
O	2.005646	-2.277089	-0.700676
H	2.361707	-3.135541	-0.982159
C	-2.560407	-0.717680	0.670770
H	-2.418262	-0.377746	1.698354
C	-3.976667	-1.257692	0.472123
H	-4.712868	-0.587685	0.931262
H	-4.035455	-2.238323	0.949866
O	-4.147578	-1.322967	-0.939795
H	-4.951557	-1.798687	-1.174397
C	-1.489564	-1.790634	0.400785
O	-0.551700	-1.339571	-0.435266
H	0.228165	-1.939284	-0.511507
O	-1.523101	-2.857914	0.939230
H	-2.835855	0.257947	-1.134606
H	-2.758844	1.333517	0.140933
H	-1.366320	0.645778	-0.427963
N	-2.366045	0.470361	-0.243600

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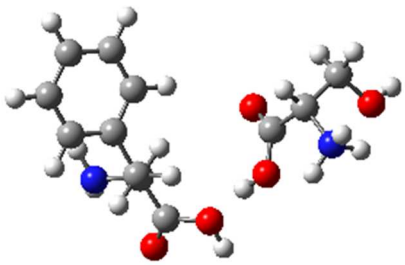

Isomer 37, 194.5 kJ·mol^{-1}

N	-3.073607	1.863891	0.859029
H	-3.115995	2.642048	1.506932
H	-3.512173	1.052725	1.278487
C	-1.716664	1.566079	0.440199
H	-1.089255	1.109704	1.226901
C	-1.741054	0.594172	-0.768945
C	-1.022064	2.871054	0.107409
H	-2.313648	1.067578	-1.569684
H	-0.722822	0.443929	-1.138064

C	-2.356149	-0.746468	-0.421872
O	-1.440531	3.976348	0.268173
C	-3.593861	-1.121601	-0.952154
C	-1.701845	-1.633511	0.443769
H	-4.118265	-0.442982	-1.616104
C	-4.163016	-2.354641	-0.632939
C	-2.269586	-2.863995	0.766681
H	-0.746668	-1.356433	0.880980
H	-5.123757	-2.627995	-1.053838
C	-3.502854	-3.229083	0.226585
H	-1.754178	-3.536495	1.443492
H	-3.946158	-4.185580	0.477839
O	0.270221	2.690674	-0.399579
H	0.620826	3.583933	-0.548893
C	3.314442	-1.185393	-0.335093
H	2.756788	-2.078048	-0.626083
C	4.331138	-1.503960	0.761730
H	4.844252	-2.449571	0.554222
H	3.792519	-1.583141	1.708315
O	5.240389	-0.407481	0.737773
H	5.835765	-0.422142	1.495045
C	2.284755	-0.126730	0.107536
O	2.058279	0.764762	-0.856927
H	1.353958	1.431277	-0.607435
O	1.753747	-0.186553	1.178218
H	4.886734	-0.155296	-1.198253
H	4.408038	-1.443321	-2.150270
H	3.472670	-0.050500	-2.092856
N	4.073083	-0.684827	-1.552270