

SUPPLEMENTARY MATERIAL

Kinetic Method Analysis of the Effect of *cis*- and *trans*-Hydroxylation on the Proton Affinity of Proline

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This Supplementary Material contains coordinates of X3LYP/6-311++G(d,p) optimized neutral and protonated proline, *cis*-4-hydroxyproline, and *trans*-4-hydroxyproline.

Page 2: neutral and protonated proline

Page 3: neutral and protonated *cis*-4-hydroxyproline

Page 4: neutral and protonated *trans*-4-hydroxyproline

proline

N	0.72100637	-1.03203921	0.57335306
C	1.99714556	-0.64096008	-0.07330159
C	-0.13202377	0.16839979	0.74936275
H	2.33951835	-1.42787343	-0.74851992
H	2.78445455	-0.46497527	0.67065780
C	1.65138260	0.66256340	-0.79722124
C	0.68644756	1.34776218	0.18087087
H	-0.39300380	0.33558363	1.79732687
C	-1.46916323	-0.01156857	0.00227489
H	1.14786768	0.44708249	-1.74436554
H	2.53532275	1.26258740	-1.01777117
H	0.04628588	2.10071537	-0.27743589
H	1.24708300	1.82730399	0.98786326
O	-1.58862351	-1.18996985	-0.61849738
O	-2.32236122	0.83612501	-0.01486144
H	0.86886919	-1.52881442	1.44227285
H	-0.73829665	-1.65375690	-0.42854306

protonated proline

N	0.79232729	-1.03473677	0.57106324
C	2.07891853	-0.55189910	-0.09305186
C	-0.13477417	0.16067517	0.75055197
H	2.45448398	-1.34112042	-0.74155015
H	2.79917444	-0.36001867	0.70217006
C	1.64965635	0.73024645	-0.79717796
C	0.65728280	1.36221050	0.19029966
H	-0.39016710	0.27318398	1.80400948
C	-1.39953490	-0.18432361	-0.03895551
H	1.16969621	0.50332940	-1.75264820
H	2.50379299	1.37563336	-0.99977040
H	-0.00660022	2.09361685	-0.26801961
H	1.18536343	1.85949740	1.00615478
O	-1.49256190	-1.20121077	-0.68220887
O	-2.32040385	0.75487906	0.08264291
H	0.97327641	-1.52039510	1.44991028
H	-3.11461222	0.51406594	-0.42395720
H	0.27373546	-1.68543806	-0.04721178

***cis*-4-hydroxyproline**

N	-0.44779969	1.42409608	0.18495136
C	-1.79379403	0.87245843	-0.11122222
C	0.36063891	0.39362545	0.87472179
H	-2.12139704	1.15210363	-1.11358628
H	-2.53973720	1.21932640	0.61249532
C	-1.62695265	-0.64154824	0.00072179
C	-0.59293995	-0.78895914	1.12267753
H	0.77550658	0.77190447	1.81257321
C	1.57804704	-0.01123557	0.01842566
H	-2.57516760	-1.13786642	0.23472917
H	-0.07141625	-1.74717653	1.11434547
H	-1.08756478	-0.68172162	2.09223390
O	1.75450973	0.73975440	-1.06849014
O	2.31618545	-0.90853219	0.33485443
H	-0.50293571	2.28240273	0.71667189
H	0.96618900	1.32912173	-1.09839230
O	-1.12408349	-1.09321138	-1.25655891
H	-0.83176853	-2.00689903	-1.17612022

Protonated *cis*-4-hydroxyproline

N	-0.52043487	1.36181816	0.21855059
C	-1.92370197	0.79366928	0.10025544
C	0.36559295	0.30286461	0.86411028
H	-2.41229915	1.21658159	-0.77459261
H	-2.47025011	1.04840533	1.00730488
C	-1.66260910	-0.70236303	-0.01080849
C	-0.54638450	-0.93259403	1.02225105
H	0.72973542	0.67417193	1.82244323
C	1.56429670	0.14202116	-0.07495795
H	-2.56430178	-1.27984218	0.20560009
H	0.00048530	-1.85826711	0.84901289
H	-0.95905289	-0.96877142	2.03260623
O	1.71316676	0.83798518	-1.04584419
O	2.38052605	-0.81212482	0.34430900
H	-0.50279950	2.24580773	0.72779320
H	3.14712396	-0.87688292	-0.24980277
H	-0.09790826	1.53725680	-0.71184243
O	-1.19233027	-0.90739127	-1.33259697
H	-1.22175363	-1.84052749	-1.57042151

***trans*-4-hydroxyproline**

N	-0.19931789	1.15878358	0.48853266
C	-1.18124589	1.10717440	-0.61176714
C	0.38649151	-0.20053588	0.58697222
H	-0.66947340	1.26582023	-1.56758326
H	-1.93109951	1.89223748	-0.49702069
C	-1.76204140	-0.31215437	-0.56094645
C	-0.53572384	-1.16060230	-0.21780175
H	0.44711680	-0.49984712	1.63541540
C	1.83218217	-0.19957173	0.06424428
H	-0.03331692	-1.50399901	-1.12343907
H	-0.82385030	-2.03969445	0.35627723
O	2.33185100	1.02574427	-0.14258787
O	2.45903326	-1.20738747	-0.12679556
H	-0.67935196	1.38412709	1.35165195
H	1.59415104	1.64168683	0.06948557
H	-2.22632730	-0.61427736	-1.50572092
O	-2.69252656	-0.44996237	0.51973335
H	-3.50746008	0.00944515	0.29419878

Protonated *trans*-4-hydroxyproline

N	-0.32124660	1.13083881	0.50022135
C	-1.39824010	1.12248084	-0.56924585
C	0.35455936	-0.23630555	0.48373024
H	-0.93657573	1.41710787	-1.51192023
H	-2.18289410	1.82557059	-0.29760093
C	-1.82458571	-0.34676391	-0.55459110
C	-0.47931022	-1.07949786	-0.50850484
H	0.31548150	-0.64979808	1.49088530
C	1.80398069	0.00546145	0.07779756
H	-0.01785792	-1.09074711	-1.49793675
H	-0.59019960	-2.10510182	-0.16365336
O	2.21890269	1.10704823	-0.18543088
O	2.49251169	-1.12281346	0.04997224
H	-0.74538680	1.29999008	1.41318677
H	3.41215561	-0.94762764	-0.21243781
H	0.40966965	1.83857449	0.32531273
H	-2.41915826	-0.61391012	-1.42968830
O	-2.49672485	-0.61761836	0.66759894
H	-3.45244850	-0.61511107	0.55006473