Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Privileged hydration sites in aromatic side chains: Effect on conformational equilibrium

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Table S1. Cartesian coordinates of the geometry optimized Phe and Phe+1W

Phenylalanine/continuum[a]				**Phenylalanine+1W/continuum[b]**			
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
N	-0.0929636039	0.1346016254	0.0768080332	N	-0.0437588894	0.1952227038	0.1233063478
C	0.0036696434	-0.0232124278	1.5775962443	C	-0.0351816292	-0.1015014741	1.6071729761
C	1.5316097659	-0.0768762960	1.9099455992	C	1.4739316151	-0.1559093659	2.0244508572
O	2.2893217293	-0.1835437541	0.9073190399	O	2.2920295069	-0.0484591778	1.0695726201
C	-0.7216737795	-1.2943972270	2.0508309094	C	-0.7732653852	-1.4083490073	1.9318033464
C	-2.1936070739	-1.3332016818	1.6944954642	C	-2.2468197665	-1.3957797960	1.5789303156
C	-2.6692778617	-2.2294898819	0.7305708137	C	-2.7439578585	-2.2095457291	0.5530879871
C	-3.1067030170	-0.4644717140	2.3091595056	C	-3.1433472090	-0.5671097248	2.2681246427
C	-4.0220240209	-2.2569537049	0.3830888154	C	-4.1010662528	-2.1913756926	0.2176044113
C	-4.4559001864	-0.4905405677	1.9654702209	C	-4.4956827220	-0.5470383157	1.9354968951
C	-4.9180798098	-1.3862483149	0.9982769083	C	-4.9793087418	-1.3579639297	0.9065902582
H	0.8819103256	-0.0760810736	-0.2386539630	H	0.9790973448	0.1598313616	-0.1107582808
H	-0.4385277208	0.8605057696	2.0336968043	H	-0.5097279366	0.7390618642	2.1112988046
H	-0.2169200874	-2.1721795245	1.6359278197	H	-0.2755712293	-2.2404262998	1.4240125538
H	-0.5874458168	-1.3342763027	3.1337119107	H	-0.6402088011	-1.5683007663	3.0037764879
H	-1.9812754951	-2.9222698604	0.2561992050	H	-2.0695747338	-2.8681002449	0.0146487342
H	-2.7618289045	0.2327480960	3.0661014366	H	-2.7829205225	0.0624106361	3.0753416854
H	-4.3710869705	-2.9607136555	-0.3641371930	H	-4.4659198597	-2.8291184419	-0.5795490650
H	-5.1487315581	0.1853852230	2.4541114527	H	-5.1742582117	0.0979784232	2.4822709709
H	-5.9686991947	-1.4058990622	0.7319129700	H	-6.0320938361	-1.3425491665	0.6492715924
H	-0.3257515419	1.0877366515	-0.2013850544	H	-3.4353056450	-4.0133240567	2.2495109163
H	-0.7714421318	-0.4928569915	-0.3586418038	O	-3.5583852061	-4.7430458076	2.8706251586
O	1.8283287710	-0.0278811354	3.1159540613	H	-3.1193057953	-4.4496856049	3.6768778796
				H	-0.4103013934	1.1207768641	-0.0960751299
				H	-0.5625198816	-0.4863549881	-0.4316529685
				O	1.6993125440	-0.3014016238	3.2370992680

Unit: angstroms

[a]Corresponding to the lowest energy conformer of Phe ($g^{-}g^{\pm}$, $\Delta E=0$), see for the graphical representation (Fig. 1A, main text).

[b]Corresponding to the lowest energy conformer of Phe+1W ($g^{-}g^{\pm}$, $\Delta E=0$), see for the graphical representation (Fig. 1D, main text).

Table S2. Cartesian coordinates of the geometry optimized Tyr and Tyr+3W

Tyrosine/continuum[a]				**Tyrosine+3W/continuum[b]**			
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-0.0492369761	-0.0619134063	-0.1371358820	C	-0.1094636241	0.0219608538	0.0246420665
H	-0.0928217211	-0.2183473258	0.9449704935	H	-0.1051534306	0.0539678767	1.1182762321
C	1.3948043213	-0.055212128	-0.5939570190	C	1.3125665966	-0.0307778459	-0.4926257798
C	2.4422305868	0.0182265770	0.3321381285	C	1.5863564385	-0.3591232067	-1.8274165950
H	2.2189178979	0.0497546489	1.3939253843	H	0.7706366732	-0.6000270377	-2.5016133190
C	3.7748627928	0.0342317136	-0.0755548779	C	2.8882064497	-0.3965959773	-2.3150682606
C	3.0513853265	-0.0989476706	-2.3769188333	C	3.7103829796	0.2254023513	-0.1293210144
H	4.5775163279	0.0863829056	0.6505021194	H	3.0801990839	-0.6583425548	-3.3492056622
C	4.0812981922	-0.0236491927	-1.4342396183	C	3.9595206071	-0.0978620900	-1.4646431577
H	3.2860233804	-0.1493765437	-3.4352567205	H	4.5397897758	0.4598816416	0.5278772326
O	5.4036773897	-0.0075724660	-1.7884896674	O	5.2550633007	-0.1127105589	-1.8936124614
H	5.4913863561	-0.0673399081	-2.7474904324	H	5.3218954191	-0.3347513184	-2.8513093955
H	-0.5964781457	-0.8875303662	-0.5969592341	H	-0.6576452402	-0.8775638915	-0.2630752677
C	1.7260643516	-0.1141545233	-1.9539723864	O	5.5187411807	-0.7063166657	-4.5393691964
H	0.9409053429	-0.1799867153	-2.7001888956	H	5.8939373403	-0.0138125996	-5.0968516054
C	-0.8286600697	1.2165989164	-0.4920576748	H	6.0077519171	-1.5084423460	-4.7599310570
H	-0.8606338723	1.3570160652	1.5708276877	H	6.7927761354	-0.5196862104	-0.8680057728
N	-0.1718855289	2.4359029248	0.1138332201	O	7.5916542861	-0.7718993598	-0.3729023320
H	-0.133720193	3.2210644922	-0.5358397633	H	7.9493543457	0.0579455492	-0.0401274577
H	-0.8201334428	2.6846404261	0.8948356246	O	3.6497514522	-3.0805497454	1.0159451325
H	0.7767463661	2.2621511555	0.4512746403	H	3.5441283744	-2.1720590089	0.7035074352
C	-2.2831559375	1.1775633789	0.0799818456	H	4.5925536451	-3.2581744636	0.9237493868
O	-2.5009125594	1.9746383011	1.0329391692	C	2.3973517944	0.2567010056	0.3436428886
O	-3.0540474969	0.3569448868	-0.4473697222	H	2.2238769466	0.4992233116	1.3874799836
				C	-0.9307407807	1.2089646548	-0.5082055957
				H	-0.9837399005	1.1803294158	-1.5951019956
				N	-0.3022165980	2.5244349649	-0.1090614871
				H	-0.3014048708	3.2028632697	-0.8702977166
				H	-0.9455603700	2.8690570429	0.6395678383
				H	0.6568117590	2.4348731194	0.2313787941
				C	-2.3743750430	1.2188942975	0.0929333660
				O	-2.5981399923	2.1432919689	0.9215369668
				O	-3.1302162105	0.3096156505	-0.2907710735

Unit: angstroms

[a]Corresponding to the lowest energy conformer of Tyr (g^-g^-, $\Delta E=0$), see for graphical representation (Fig. 4A, main text).

[b]Corresponding to the lowest energy conformer of Tyr+3W (g^-g^-, $\Delta E=0$), see for graphical representation (Fig. 4G, main text).

Table S3. Cartesian coordinates of the geometry optimized Trp and Trp+3W

Tryptophan/continuum[a]				Tryptophan+3W/continuum[b]			
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
N	-0.2280204702	-0.1443876275	-0.9283624445	N	0.1902082803	-1.1803627889	-0.5655905069
H	0.7928905956	-0.1778071509	-0.8524959664	H	0.4676516865	-1.5504848304	0.3475925595
H	-0.4642863720	0.2381463055	-1.8437286539	H	0.6948922382	-1.7017833008	-1.2819542246
H	-0.6548219041	0.4684268455	-0.2030238074	H	0.4281122678	-0.1701941951	-0.6668470095
C	-0.8695494699	-1.4868153506	-0.6831210374	C	-1.3039054139	-1.2092197525	-0.7740519658
C	-2.1674784870	-1.2157176847	0.1395898518	C	-1.6828462707	0.1457687160	-1.4497879201
O	-2.2486956307	-0.0623953452	0.6424097044	O	-0.7739657068	1.0201949524	-1.4384168725
O	-2.9604941877	-2.1700981201	0.2342710204	O	-2.8405742480	0.2247485109	-1.8983810736
C	0.1004029375	-2.4036124797	0.0928797202	C	-2.0267127914	-1.3841761167	0.5782708084
H	0.2581303366	-1.9856507110	1.0921645553	H	-1.8328234508	-0.5036785009	1.1988358662
H	-0.4207769937	-3.3541369133	0.2295666806	H	-3.0965917068	-1.3817743325	0.3568256919
H	-1.1191970328	-1.9198249730	-1.6496495708	H	-1.5326195844	-2.0373003567	-1.4419012604
C	1.4243753420	-2.6058872122	-0.5829162936	C	-1.6318838021	-2.6251809827	1.3226945561
C	1.6974621591	-3.3808928143	-1.7706621092	C	-1.9777730753	-3.9886023789	1.0008970415
C	2.6279619354	-2.0684562877	-0.1873295472	C	-0.8472154960	-2.6849960578	2.4525091809
C	3.0906271183	-3.2653158008	-2.0320975313	C	-1.3616279034	-4.8147328897	1.9822502057
C	0.9096340069	-4.1711010474	-2.6265037603	C	-2.7630654465	-4.5879849289	0.0000960812
H	2.8546801973	-1.4465460127	0.6656933841	H	-0.4002114214	-1.8801495378	3.0175723509
N	3.6269674238	-2.4598745267	-1.051147444	N	-0.6924235483	-3.9918387156	2.8622682315
C	3.7027940765	-3.9045573911	-3.1147167833	C	-1.4980957866	-6.2070432030	1.9735873459
C	1.5145819072	-4.8088088209	-3.7012153924	C	-2.9061344284	-5.9688731076	-0.0075031634
H	-0.1542669888	-4.2886581404	-2.4520756913	H	-3.2578155034	-3.9854591066	-0.7537088138
H	4.5976215241	-2.2015239216	-0.9678347673	H	-0.0952962955	-4.2979143653	3.6320264280
C	2.8973427272	-4.6748007831	-3.9437437104	C	-2.2756350092	-6.7717407638	0.9678346881
H	4.7664852105	-3.8046303305	-3.2981611905	H	-1.0192760855	-6.8238815339	2.7252009341
H	0.9172214308	-5.4219213632	-4.3665487046	H	-3.5093107983	-6.4427418695	-0.7734450132
H	3.3404009526	-5.1848535330	-4.7916051583	H	-2.3950688668	-7.8486859589	0.9287864501
				H	0.7385242058	-4.7829680884	5.9565847750
				O	1.0088171793	-4.9061226413	5.0390555542
				H	1.9567058149	-4.7288380412	5.0279529772
				H	-2.6883289068	-3.8360680133	4.4888370340
				O	-3.5220864676	-4.0376764693	4.9294112417
				H	-3.9441957981	-4.7089567293	4.3605628119
				H	-4.0847408331	-6.2837827223	2.5825257006
				O	-4.7062506155	-6.0342889027	3.2824898958
				H	-5.5253778211	-5.8112113347	2.8250064060

Unit: angstroms

[a]Corresponding to the lowest energy conformer of Trp (g^-g^+, $\Delta E=0$), see for graphical representation (Fig. 6A, main text).

[b]Corresponding to the lowest energy conformer of Trp+3W (g^-g^+, $\Delta E=0$), see for graphical representation (Fig. 6G, main text).

Table S4. Cartesian coordinates of the geometry optimized His^0 and His^0+3W

Histidine/continuum[a]				**Histidine+3W/continuum[b]**			
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-0.0505974713	-0.0461649347	-0.0942542376	C	-0.1201859741	-0.0434645973	0.0232131535
H	-0.1049219134	-0.1182479666	0.9986110883	C	-0.1065838646	0.0637373867	1.3951893450
C	1.3837464582	-0.0083079087	-0.5277207311	H	0.7026549453	0.1855160627	2.0961856826
C	2.1095928582	-0.9139567732	-1.2572893848	N	-1.4228550391	0.0131121732	1.7963692378
H	1.8488125143	-1.8597558025	-1.7009699938	H	-1.7668408230	0.0587562332	2.7610161570
N	3.3779138088	-0.3818316663	-1.3517322073	C	-2.1808727073	-0.1252834273	0.6867715809
C	3.3829294488	0.8050198471	-0.6985219548	N	-1.4322259799	-0.1657571605	0.4031823872
N	2.1950485270	1.0628189391	-0.1837685336	C	1.0408587825	-0.0208154371	-0.9283399204
H	-0.5412291140	-0.9326266302	-0.4966558624	H	1.9467055679	-0.3193203990	-0.3996281918
H	4.2583403849	1.4309217108	-0.6275945571	H	0.8843733758	-0.7556127258	-1.7244867731
C	-0.8677648283	1.1780450391	-0.5487757209	H	-3.2564233860	-0.2014849451	0.7160329084
H	-0.8945251513	1.2309892072	-1.6360997390	H	-1.8043056958	-0.2082881376	-2.1327882912
N	-0.2208370872	2.4444876519	-0.0405973810	O	-1.7642879156	0.0098017349	-3.1032373736
H	-0.3615798981	3.2234712616	-0.6833246295	H	-1.6425341026	-0.8237851209	-3.5709666529
H	-0.7247281193	2.6698677594	0.8334686981	H	-2.6462316401	-0.6212588127	4.9703059757
H	0.8016183675	2.3061127454	0.1006328165	O	-2.3313964511	0.1694662721	4.5165925003
C	-2.3168003450	1.1267431540	0.0264352358	H	-2.9383112219	0.8720623672	4.7778604904
O	-2.5424055935	1.9117218425	0.9843811401	O	0.3446432718	-3.3667766968	1.3060180435
O	-3.0799540795	0.2949975313	-0.5024181136	H	0.4341714145	-3.7344854469	0.4195958864
H	4.1663296191	-0.8023609641	-1.8219807054	H	0.2687300986	-2.4127592411	1.1656110865
				C	1.3596350338	1.3473758055	-1.5515525652
				H	1.4363849470	2.0973053392	-0.7632086434
				N	0.3044320731	1.8273888183	-2.5187689218
				H	-0.2238425326	2.6230397747	-2.1646553869
				H	0.8706129157	2.1182976338	-3.3447276296
				H	-0.3796341950	1.0974121735	-2.8179670554
				C	2.7187098659	1.3536408959	-2.3362370218
				O	2.6572721453	1.8091409473	-3.5102970375

Unit: angstroms

[a]Corresponding to the lowest energy conformer of His^0(NεH) (g^-g^+, ΔE=0), see for graphical representation (Fig. 8A, main text).

[b]Corresponding to the lowest energy conformer of His^0(NεH) (g^-g^+, ΔE=0), see for graphical representation (Fig. 9A, main text).

Table S5. Cartesian coordinates of the geometry optimized His^{1+} and His^{1+} +3W

Protonated histidine/continuum[a]				**Protonated histidine+2W/continuum[b]**			
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	0.0157644042	0.0174534010	0.0555004127	C	-0.1964057745	-0.0076339142	-0.0738968252
H	0.0191387566	0.0515984748	1.1467678585	C	-0.1268305498	0.0240734679	1.2925231477
C	1.4455281020	0.0024113912	-0.3850753758	H	0.7251925089	0.0576978412	1.9497014925
C	2.6015120194	-0.1655342820	0.3214942107	N	-1.4172911212	-0.0284999323	1.7725726716
H	2.7763738165	-0.3051752322	1.3735419426	H	-1.6944463322	-0.0299982504	2.7704582114
N	3.6313197135	-0.1358193619	-0.5982555022	C	-2.2580869961	-0.0960445591	0.7430506971
C	3.1331610362	0.0503795247	-1.8237155343	N	-1.5481370210	-0.0824098149	-0.3833051133
N	1.8129535369	0.1297957331	-1.7110822531	C	0.9045405701	0.0132142064	-1.0890295844
H	-0.4675793881	-0.9213779100	-0.2350210234	H	1.8133015962	-0.3546574882	-0.6088848952
H	3.7046240618	0.1265652685	-2.7323265452	H	0.6760949984	-0.6740706563	-1.9047629747
C	-0.8031499437	1.2074340275	-0.4841801922	H	-3.3309497576	-0.1561348770	0.8086287786
H	-0.2238369608	2.1289883714	-0.4072326205	H	-1.9713764877	-0.1595049667	-1.3349925794
N	-2.0387887911	1.4161340063	0.3548025489	H	-2.4405010022	-0.8292755072	4.8765202110
H	-1.9155631737	2.1125588085	1.0901881633	O	-2.0613119932	-0.0363622590	4.4786552168
H	-2.7559659684	1.7220964081	-0.3373108081	H	-2.5464868536	0.7044882941	4.8613583361
H	-2.3739778754	0.5531313117	0.7877950921	H	-1.9114075734	0.3276069713	-3.3425256635
C	-1.3149972018	1.0969811019	-1.9673145562	O	-2.6550616563	-0.1456399845	-2.9044355865
O	-2.5024496655	1.4396220268	-2.1427069168	H	-2.7533285457	-0.9872489010	-3.3639226563
O	-0.4885766465	0.7129631512	-2.8301665642	C	1.2010473462	1.3788425495	-1.7372033496
H	4.6155243322	-0.2333406434	-0.3861072472	H	2.0871641397	1.2653883500	-2.3617199962
H	1.0735488004	0.3315401537	-2.4267874082	N	1.5179917116	2.4495103929	-0.7239353994
				H	2.5168034001	2.6201018825	-0.6087415946
				H	1.0371000252	3.2926939014	-1.1055418155
				H	1.1183874033	2.2530507625	0.1970614822
				C	0.0729957962	1.9581991626	-2.6524656822
				O	-0.2140244109	3.1600937107	-2.4598741001
				O	-0.3916505774	1.1625662296	-3.5001595550

Unit: angstroms

[a]Corresponding to the lowest energy conformer of His^{1+}(NεH) (tg^-, ΔE=0), see for graphical representation (Fig. 11A, main text).

[b]Corresponding to the lowest energy conformer of His^{1+}(NεH) (g^+g^+, ΔE=0), see for graphical representation (Fig.11G, main text).