ELECTRONIC SUPPLEMENTARY INFORMATION

A "Hidden" Role of Amino and Imino Groups is Unveiled During the Micro-Solvation Study of Three Biomolecule Groups in Water

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Eqn (7) Analysis

Taking into consideration $A_1 = \left[\left(\frac{\mu_0}{4\pi}\right)^2 \frac{\hbar^2 \gamma_C^2 \gamma_H^2}{10 r_{CH}^2}\right]$ and $A_2 = \left(\frac{0.74\eta f_r}{kTN_A\rho}\right)$ constants while limiting the McLaurin series to the first two terms, eqn (6) becomes:

$$\begin{aligned}\frac{1}{NT_1} = {} & 36A_1A_2n\left[5 - 162A_2^2n^2\left(10\omega_C^2 + 10\omega_C\omega_H + 7\omega_H^2\right)\right] + \\ & + 2A_1A_2\left[5 - 486A_2^2n^2\left(10\omega_C^2 + 10\omega_C\omega_H + 7\omega_H^2\right)\right]Mw - \\ & - 54A_1A_2^3n\left(10\omega_C^2 + 10\omega_C\omega_H + 7\omega_H^2\right)Mw^2\end{aligned} \qquad (1S)$$

Defining $B = 10\omega_C^2 + 10\omega_C\omega_H + 7\omega_H^2$ and $K = A_1A_2$, eqn (1S) becomes:

$$\frac{1}{NT_1} = 36Kn\left(5 - 162A_2^2Bn^2\right) + 2K\left(5 - 486A_2^2Bn^2\right)Mw - 54A_2^2KBnMw^2 \qquad (2S)$$

Eqn (2S) is clearly represented by eqn (7):

$$\frac{1}{NT_1} = \alpha_0 + \alpha_1 Mw + \alpha_2 Mw^2 \ ,$$

where $a_0 = 36Kn\left(5 - 162A_2^2Bn^2\right)$, $a_1 = 2Kn\left(5 - 486A_2^2Bn^2\right)$ and $a_2 = -54A_2^2KBn$

Although the number of water molecules, *n*, can be obtained by the quotient of a_0 and a_1 values, we avoid such a procedure due to certain statistical reasons. However, the hydration number difference between biomolecules of interest is totally independent from the statistical treatment, resulting in its accurate measurement.

Calculation of correlation times (τ_c) through eqn (1)

1. From $^{13}C_\alpha$ T_1 measurements

Table S1. ^{13}C longitudinal (T_1) relaxation times and calculated correlation times (τ_c) in different ionization states (± indicates the StdDev with $N = 20$).

Compounds	Mw[a]	Acid[b] pH		pH = 6.0	
		T_1 (s)	τ_c (ps)	T_1 (s)	τ_c (ps)
Amino Acids					
Glycine	75.07	2.38 ± 0.06	10.3 ± 0.3	4.12 ± 0.04	5.9 ± 0.1
Alanine	89.10	3.16 ± 0.05	15.5 ± 0.3	4.54 ± 0.06	10.8 ± 0.1
Serine	105.09	2.46 ± 0.04	20.0 ± 0.6	3.34 ± 0.04	14.7 ± 0.03
Valine	117.15	2.19 ± 0.05	22.5 ± 0.5	2.65 ± 0.06	18.6 ± 0.4
Isoleucine	131.18	1.84 ± 0.08	26.8 ± 0.7	2.16 ± 0.06	22.8 ± 0.6
Aspartic Acid	133.11	1.74 ± 0.05	28.4 ± 1.1	2.53 ± 0.06	19.4 ± 0.5
Lysine	146.19	1.78 ± 0.17	27.7 ± 1.8	2.37 ± 0.22	20.8 ± 1.9
Histidine	154.11	1.52 ± 0.06	32.5 ± 1.2	1.76 ± 0.07	28.0 ± 0.9
Phenylalanine	165.19	1.51 ± 0.06	32.7 ± 1.2	1.71 ± 0.07	29.0 ± 0.8
Arginine	174.20	1.28 ± 0.04	38.7 ± 1.6	1.52 ± 0.05	32.5 ± 1.0
Tyrosine	181.19	1.12 ± 0.05	44.4 ± 1.7	1.22 ± 0.03	41.0 ± 1.8
Tryptophan	203.23	1.08 ± 0.05	46.2 ± 2.6	1.22 ± 0.05	41.0 ± 2.0
Ac-Amino Acids					
Ac-Glycine	117.10	1.32 ± 0.05	18.6 ± 1.1	1.48 ± 0.06	17.5 ± 3.3
Ac-Alanine	130.13	1.84 ± 0.04	26.8 ± 0.6	2.16 ± 0.06	22.8 ± 0.6
Ac-Valine	159.18	1.45 ± 0.05	34.0 ± 1.4	1.60 ± 0.06	30.8 ± 1.1
Ac-Leucine	173.21	1.26 ± 0.06	39.5 ± 1.9	1.34 ± 0.05	36.9 ± 1.5
Ac-Aspartic Acid	175.14	1.21 ± 0.06	41.2 ± 3.3	1.43 ± 0.06	34.6 ± 1.4
Ac-Glutamic Acid	189.17	1.28 ± 0.07	38.7 ± 1.7	1.47 ± 0.05	33.7 ± 1.6
Ac-Methionine	191.25	1.19 ± 0.05	41.7 ± 2.2	1.32 ± 0.05	37.5 ± 1.6

Ac-Phenylalanine	207.23	1.11 ± 0.06	45.0 ± 2.3	1.23 ± 0.05	40.5 ± 1.7
Betaines					
Glycine Betaine	117.15	2.13 ± 0.02	11.6 ± 1.5	2.38 ± 0.04	9.8 ± 1.3
Alanine Betaine	131.18	4.22 ± 0.07	13.7 ± 0.1	3.73 ± 0.04	13.0 ± 0.2
Valine Betaine	159.23	2.21 ± 0.05	22.3 ± 0.6	2.21 ± 0.05	22.3 ± 0.6
Threonine Betaine	161.21	1.99 ± 0.04	24.8 ± 0.5	2.07 ± 0.04	23.8 ± 0.5
Leucine Betaine	173.26	1.72 ± 0.05	28.7 ± 0.5	1.81 ± 0.05	27.2 ± 0.6
Phenylalanine Betaine	207.28	1.34 ± 0.05	37.0 ± 1.7	1.37 ± 0.04	36.2 ± 1.8

[a]Molecular weight (Mw) of the zwitterionic form. [b]Acid pH for AAs was adjusted to 0.5, for Ac-AAs to 1.8 and for betaines to 1.3.

2. From $^{13}C_\beta$ T_1 measurements

Table S2. ^{13}C longitudinal (T_1) relaxation times and calculated correlation times (τ_c) in different ionization states (± indicates the StdDev with $N = 20$).

Compounds	Mw[a]	Acid[b] pH		pH = 6.0	
		T_1 (s)	τ_c (ps)	T_1 (s)	τ_c (ps)
Amino Acids					
Glycine	75.07	-	-	-	-
Alanine	89.10	1.05 ± 0.01	15.6 ± 0.3	1.51 ± 0.01	10.8 ± 0.3
Serine	105.09	-	-	-	-
Valine	117.15	2.17 ± 0.05	22.7 ± 0.5	2.67 ± 0.06	18.4 ± 0.4
Isoleucine	131.18	1.85 ± 0.05	26.7 ± 0.6	2.17 ± 0.10	22.7 ± 0.8
Aspartic Acid	133.11	0.86 ± 0.04	29.0 ± 0.5	1.19 ± 0.03	20.7 ± 0.5
Lysine	146.19	0.90 ± 0.03	27.4 ± 0.4	1.20 ± 0.04	20.5 ± 0.4
Histidine	154.11	0.77 ± 0.03	32.1 ± 0.4	0.89 ± 0.02	27.7 ± 0.6
Phenylalanine	165.19	0.74 ± 0.02	33.4 ± 0.9	0.84 ± 0.02	29.4 ± 0.7
Arginine	174.20	0.65 ± 0.02	38.1 ± 1.3	0.77 ± 0.05	32.0 ± 1.0

Tyrosine	181.19	0.57 ± 0.02	43.6 ± 1.6	0.62 ± 0.03	40.0 ± 1.4
Tryptophan	203.23	0.54 ± 0.05	46.2 ± 2.2	0.61 ± 0.05	40.7 ± 2.0
Ac-Amino Acids					
Ac-Glycine	117.10	-	-	-	-
Ac-Alanine	130.13	0.62 ± 0.04	26.5 ± 0.6	0.72 ± 0.06	22.8 ± 1.0
Ac-Valine	159.18	0.72 ± 0.05	34.4 ± 1.3	0.80 ± 0.06	31.4 ± 1.1
Ac-Leucine	173.21	0.63 ± 0.04	39.4 ± 1.9	0.68 ± 0.05	36.4 ± 1.5
Ac-Aspartic Acid	175.14	0.59 ± 0.06	42.1 ± 2.3	0.71 ± 0.06	34.8 ± 1.4
Ac-Glutamic Acid	189.17	0.63 ± 0.07	39.4 ± 1.7	0.72 ± 0.05	34.4 ± 1.3
Ac-Methionine	191.25	0.57 ± 0.05	43.6 ± 1.2	0.65 ± 0.05	38.1 ± 1.4
Ac-Phenylalanine	207.23	0.54 ± 0.06	46.1 ± 1.8	0.61 ± 0.05	40.7 ± 1.6
Betaines					
Glycine Betaine	117.15	-	-	-	-
Alanine Betaine	131.18	1.23 ± 0.05	13.3 ± 0.2	1.25 ± 0.04	13.1 ± 0.2
Valine Betaine	159.23	2.37 ± 0.05	20.8 ± 0.3	2.42 ± 0.05	20.3 ± 0.3
Threonine Betaine	161.21	-	-	-	-
Leucine Betaine	173.26	0.91 ± 0.04	27.1 ± 0.5	0.92 ± 0.05	26.8 ± 0.4
Phenylalanine Betaine	207.28	0.73 ± 0.05	34.0 ± 1.2	0.74 ± 0.05	33.4 ± 1.1

[a]Molecular weight (Mw) of the zwitterionic form. [b]Acid pH for AAs was adjusted to 0.5, for Ac-AAs to 1.8 and for betaines to 1.3.

^{14}N $\Delta\nu_{1/2}$ titration of Glycine betaine

The titration of Glycine betaine reveals that ^{14}N $\Delta\nu_{1/2}$ values are independent of the pH, remaining constant at all pH values. Furthermore, that result certifies that the number of directly interacting water molecules with betaines is unaffected of their ionization state.

Table S3. Titration of Glycine betaine at 308 K.

pH	$\Delta\nu_{1/2}^{\alpha}$
1.35	41.17
1.54	41.15
1.70	41.15
2.08	40.35
2.17	40.98
2.40	40.50
2.60	40.64
3.00	40.10
3.46	40.32
3.88	40.12
4.36	40.20
4.70	40.01
5.30	40.17
6.10	41.32
6.80	40.61
7.65	40.88
9.20	40.45
10.00	40.53

$^{\alpha}$Linewidths at half-height, estimated errors < ±5%.

FIGURES

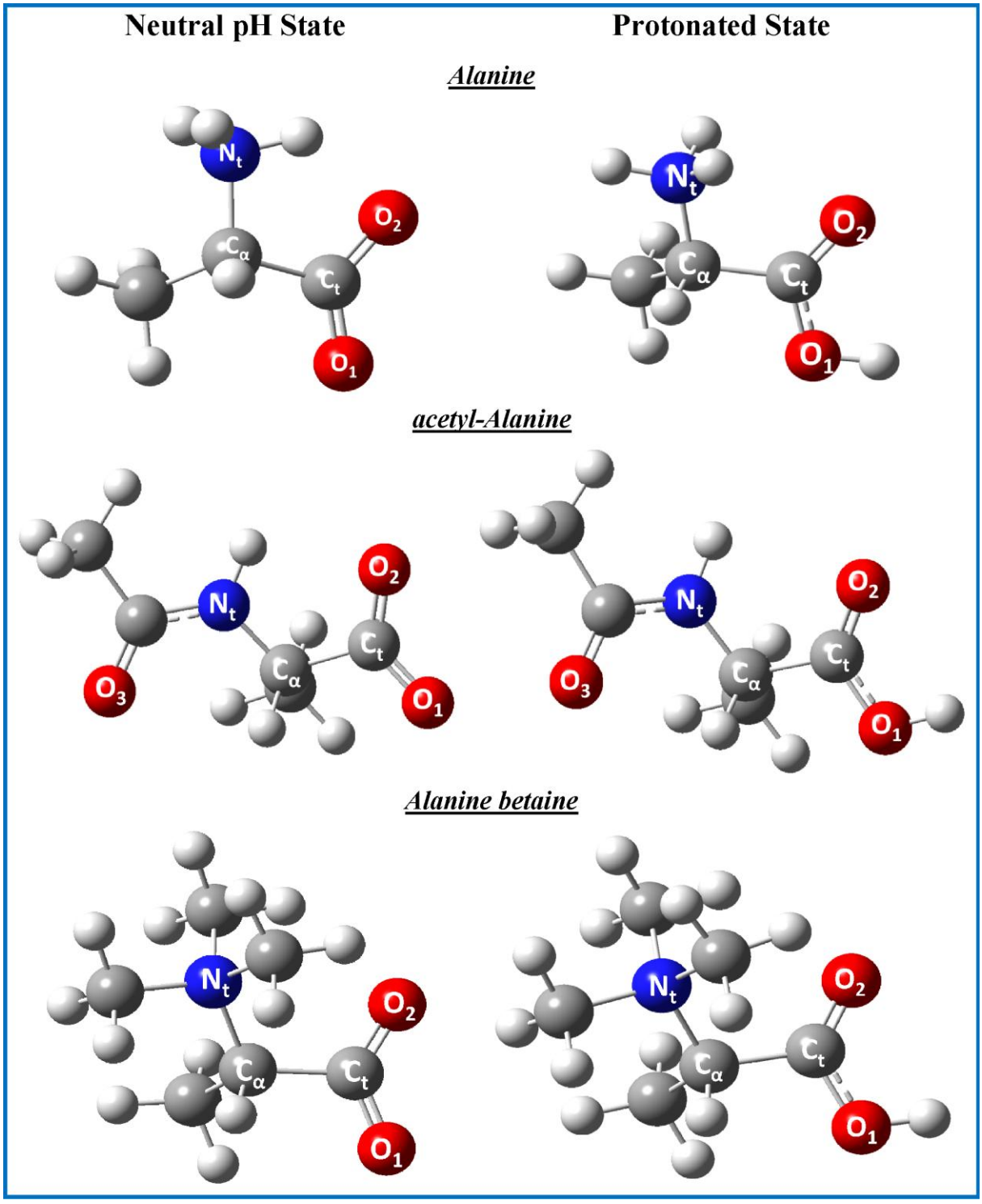

Fig. S1 Fully optimized structures of Ala, Ac-Ala and Ala betaine in aqueous solution (in their two studied ionization states, namely neutral pH and protonated) without their explicit first hydration shell, at the B3LYP/cc-pVTZ level of theory, applying the IEF-PCM model for bulk water.

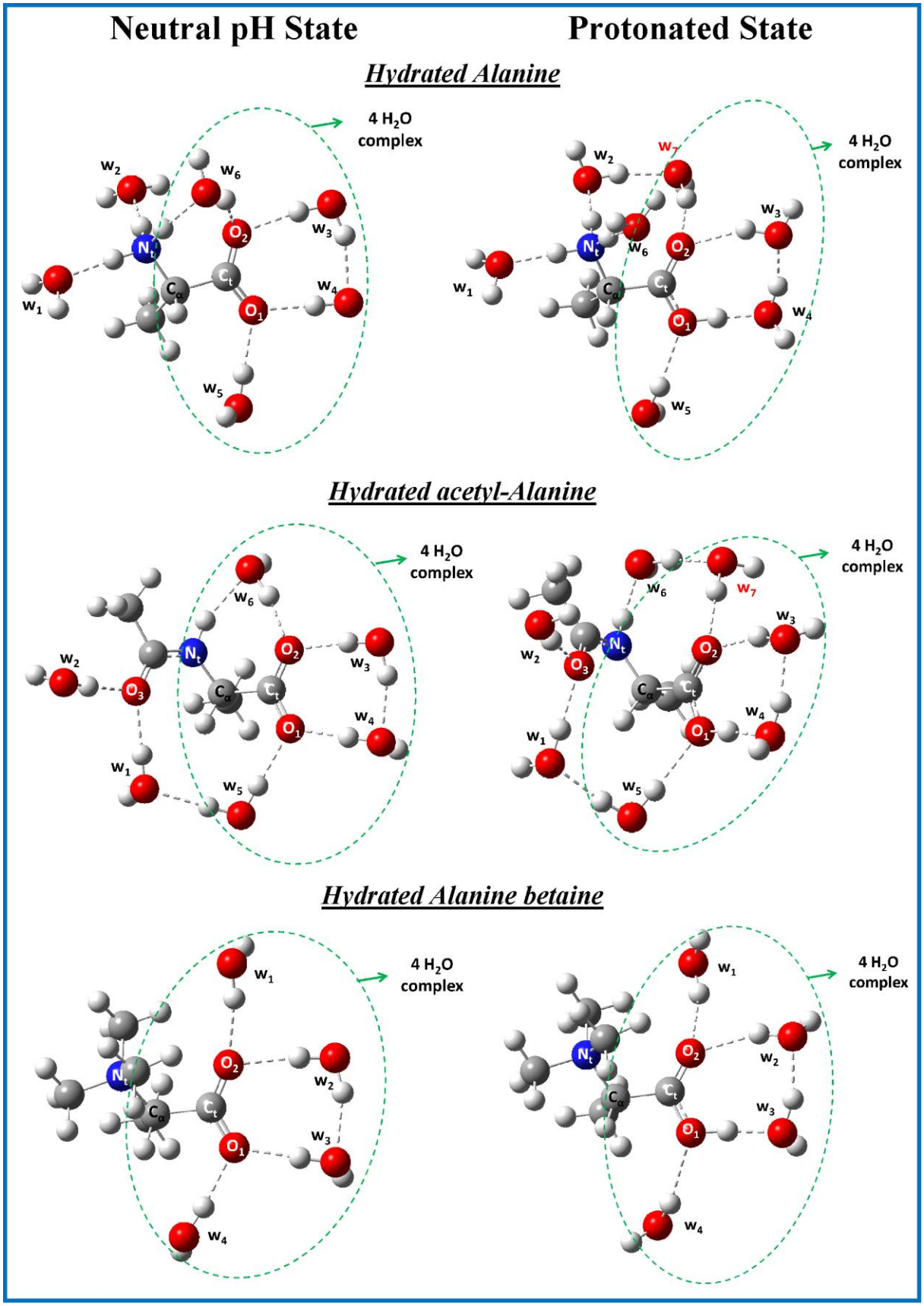

Fig. S2. The eight atom ring and two water molecules around the carboxyl group form similarly to the Ala, Ac-Ala and Ala betaine species, indicating the role of the amino group for the extra hydration of

protonated Ala and Ac-Ala. Amino group "controls" the water molecule 6 (**w6**) and "drives" an extra water molecule (**w7**) to interact with the protonated form of amino and acetyl-amino acids.

Geometrical details and energetics at the neutral pH and protonated states of Alanine, acetyl-Alanine and Alanine betaine fully optimized structures, depicted in **FIGURE S1** – Coordinates and absolute energies E (Hartree) calculated at the B3LYP/cc-pVTZ level of theory with the IEF-PCM model (bulk water).

Zwitterionic Alanine (Charge = 0)

13 Atoms

E = -323.895614

	X	Y	Z
N	1.224118	-1.179802	0.067500
H	1.806347	-1.150269	-0.776584
C	0.584352	0.147113	0.396565
H	0.649993	0.258533	1.481669
C	1.286512	1.299869	-0.298192
C	-0.925639	0.003998	0.035846
H	1.271088	1.172657	-1.382845
H	0.763525	2.222527	-0.059432
H	2.322722	1.392036	0.029152
O	-1.288925	-1.153614	-0.307151
O	-1.616738	1.029591	0.147148
H	0.399318	-1.792766	-0.122290
H	1.792137	-1.557802	0.832536

acetyl-Alanine neutral pH form (Charge = -1)

17 Atoms

E = -476.155007

	X	Y	Z
N	-0.587592	-0.321838	0.203352
C	0.597234	0.469227	-0.103374
H	0.451805	0.924698	-1.084483
C	0.812857	1.584844	0.927028
C	1.848265	-0.442096	-0.184697
H	0.954664	1.162430	1.923718
H	1.697047	2.165473	0.667334
H	-0.049779	2.250286	0.952889
O	1.752952	-1.605609	0.280904
O	2.865232	0.082642	-0.696728
H	-0.406239	-1.212793	0.651653
C	-1.832642	0.023276	-0.161787
C	-2.934450	-0.950522	0.201089
H	-3.439556	-1.266107	-0.712194
H	-2.574245	-1.830195	0.732234
H	-3.669253	-0.435773	0.820491
O	-2.093044	1.071275	-0.764759

Zwitterionic Alanine betaine (Charge = 0)

22 Atoms

E = -441.835160

	X	Y	Z
N	-1.032714	-0.140401	-0.081230
C	0.313930	0.585232	-0.337517
H	0.292823	0.781375	-1.410856
C	0.428323	1.902809	0.423205
C	1.587230	-0.278364	-0.056269
H	0.485764	1.750076	1.500386
H	1.358575	2.369194	0.105699
H	-0.379338	2.599471	0.205193
O	1.518548	-1.220414	0.764817
O	2.585545	0.121480	-0.688483
C	-2.159264	0.687105	-0.629510
H	-1.963797	0.898353	-1.677742
H	-3.080936	0.118923	-0.530372
H	-2.242058	1.611590	-0.068837
C	-1.292748	-0.403040	1.375387
H	-0.449675	-0.958329	1.768456
H	-1.410003	0.544361	1.891866
H	-2.214195	-0.975448	1.452801
C	-1.028774	-1.448830	-0.823653
H	-2.009614	-1.905615	-0.718959
H	-0.823245	-1.247951	-1.872471
H	-0.260233	-2.081194	-0.397082

Protonated Alanine (Charge = 1)

14 Atoms

E = -324.353162

	X	Y	Z
N	-1.455502	-1.005060	-0.183237
H	-1.435535	-1.321782	0.797938
C	-0.597552	0.207204	-0.393166
H	-0.630959	0.429776	-1.464610
C	-1.123108	1.385973	0.418404
C	0.828242	-0.177380	-0.021084
H	-1.100908	1.169999	1.487679
H	-0.501721	2.257446	0.227065
H	-2.146017	1.621549	0.124950
O	1.116608	-1.238327	0.481147
H	-1.130749	-1.796197	-0.759211
H	-2.435208	-0.815113	-0.440326
O	1.674347	0.796506	-0.314480
H	2.596479	0.529532	-0.049087

Protonated acetyl-Alanine (Charge = 0)

18 Atoms

E = -476.625284

	X	Y	Z
N	-0.671959	-0.203114	0.384908
C	0.536989	0.492476	-0.006189
H	0.360476	0.919284	-0.995264
C	0.898351	1.627205	0.967424
C	1.687874	-0.495251	-0.133265
H	1.060082	1.236572	1.973071
H	1.800997	2.141581	0.642369
H	0.079695	2.344385	1.002060
O	1.672690	-1.634946	0.273009
H	-0.601517	-0.880926	1.140605
O	2.741339	0.066293	-0.730579
H	3.482018	-0.592322	-0.765449
C	-1.867355	0.020850	-0.204960
O	-2.018403	0.830471	-1.120386
C	-3.029175	-0.792397	0.318516
H	-3.842723	-0.114849	0.576164
H	-3.385286	-1.445090	-0.479528
H	-2.775137	-1.398671	1.186106

Protonated Alanine betaine (Charge = 1)

23 Atoms

E = -442.292392

	X	Y	Z
N	-1.066381	-0.152153	-0.087064
C	0.259959	0.587751	-0.325481
H	0.276590	0.781990	-1.401355
C	0.375446	1.909808	0.435101
C	1.483189	-0.273004	0.006635
H	0.412517	1.761776	1.513106
H	1.306119	2.384498	0.129614
H	-0.433202	2.594544	0.191269
O	1.522549	-1.157416	0.828369
O	2.515694	0.143021	-0.712992
H	3.332647	-0.360710	-0.444529
C	-2.189315	0.676312	-0.655540
H	-3.105568	0.098190	-0.572054
H	-2.287750	1.596756	-0.090893
H	-1.975476	0.889945	-1.699828
C	-1.052140	-1.463428	-0.831827
H	-0.817272	-1.265236	-1.875091
H	-0.311196	-2.117739	-0.388496
H	-2.040256	-1.908079	-0.751014
C	-1.358720	-0.412942	1.368032
H	-2.296336	-0.960726	1.419037

H	-0.549884	-0.996916	1.789034
H	-1.462730	0.534944	1.886107

Geometrical details and energetics at the neutral pH and protonated states of Alanine, acetyl-Alanine and Alanine betaine with their explicit first hydration shell fully optimized structures (with the presence of bulk water), depicted in **FIGURE 8** – Coordinates and absolute energies E (Hartree) calculated at the B3LYP/cc-pVTZ level of theory with the IEF-PCM model (bulk water).

Zwitterionic Alanine + **6(H_2O)** (Charge = 0)

31 Atoms

E = -782.777157

	X	Y	Z
N	-1.888117	-0.387634	-0.208629
H	-1.924313	-0.887471	0.700847
C	-0.851041	0.692549	-0.171888
H	-0.907940	1.209184	-1.134621
C	-1.170652	1.666891	0.957664
C	0.567392	0.088791	-0.063129
H	-1.104738	1.173202	1.928231
H	-0.468027	2.495463	0.935830
H	-2.178471	2.066485	0.840744
O	0.674235	-1.161312	-0.023797
O	1.506647	0.921505	-0.033098
H	-1.672243	-1.089872	-0.937150
H	-2.820302	0.024439	-0.402245
H	-0.127272	-2.196841	-1.366229
O	-0.846605	-2.373905	-2.000818
H	-1.161385	-3.269699	-1.791453
O	4.212775	0.332756	0.058175
H	3.255266	0.548443	0.021457

H	4.475406	0.541566	0.968869
H	3.784207	-1.538271	0.049692
O	3.262923	-2.359255	0.066959
H	2.351282	-2.016108	0.060329
H	-4.385901	1.539278	-1.398136
O	-4.398048	0.787822	-0.779331
H	-4.944202	1.088690	-0.031781
H	-1.161577	-1.952515	2.669072
O	-2.024171	-1.740267	2.271659
H	-2.541234	-1.341796	2.993524
O	1.486298	3.714119	-0.269605
H	1.000103	3.919288	-1.082636
H	1.481530	2.738878	-0.220982

acetyl-Alanine neutral pH form + **6(H_2O)** (Charge = -1)

35 Atoms

E = -935.033088

	X	Y	Z
N	-0.926023	-1.040062	0.607020
C	-0.009157	0.039810	0.947403
H	-0.494974	0.968858	0.674785
C	0.289815	0.054626	2.451585
C	1.319759	-0.045213	0.158421
H	0.770968	-0.873899	2.762255
H	0.952778	0.885791	2.689134
H	-0.633059	0.172353	3.019484
O	1.757309	-1.179007	-0.164756
O	1.890440	1.054452	-0.063615
H	-0.599221	-1.990394	0.767942
H	1.162066	-2.751700	0.396982
O	0.619531	-3.508836	0.709184
H	1.013948	-3.781250	1.553063
O	4.427598	1.408774	-1.063929
H	3.516699	1.284513	-0.711446
H	4.982194	1.518583	-0.275366
H	4.480807	-0.456252	-1.509141
O	4.211434	-1.388116	-1.579885
H	3.357491	-1.383259	-1.108625
C	-2.113171	-0.875693	0.019765
C	-2.895570	-2.135897	-0.260650
H	-3.316563	-2.076859	-1.262761

H	-2.290676	-3.034826	-0.163569
H	-3.729421	-2.193445	0.441487
O	-2.591057	0.237824	-0.278692
H	-2.316488	2.010497	0.055151
O	-2.180599	2.960407	0.237414
H	-2.560350	3.098877	1.120541
O	-4.822087	0.264010	-2.011065
H	-4.065323	0.276494	-1.396306
H	-5.580713	0.037084	-1.452090
O	0.629909	3.558926	0.421524
H	-0.321709	3.374678	0.341680
H	1.063812	2.701334	0.259077

Zwitterionic Alanine betaine + **4(H_2O)** (Charge = 0)

34 Atoms

E = -747.747229

	X	Y	Z
N	2.116164	0.077011	-0.190628
C	0.950026	-0.787197	0.342470
H	1.049791	-1.719817	-0.207919
C	1.047179	-1.066854	1.839669
C	-0.467188	-0.222891	0.042317
H	0.861521	-0.173286	2.433319
H	0.274989	-1.795049	2.082460
H	2.002917	-1.499107	2.130559
O	-0.661345	1.010211	0.088643
O	-1.324494	-1.116810	-0.159877
C	3.377550	-0.741387	-0.154775
H	3.231934	-1.641599	-0.745975
H	4.181339	-0.144767	-0.578241
H	3.617894	-0.998540	0.870944
C	2.348978	1.336018	0.599625
H	1.449275	1.936159	0.583330
H	2.623258	1.072166	1.615846
H	3.170429	1.870896	0.129058
C	1.851888	0.437536	-1.626915
H	2.730358	0.943247	-2.019223
H	1.670180	-0.476897	-2.186719
H	0.989649	1.090814	-1.674148

H	-2.497036	1.625266	0.284647
O	-3.443708	1.836119	0.341403
H	-3.856983	0.984777	0.115316
H	-3.118776	-0.969958	-0.280878
O	-4.092478	-0.861905	-0.308388
H	-4.409553	-1.290036	0.503254
H	-0.375514	2.851854	-0.238874
O	-0.089538	3.769757	-0.358756
H	-0.326954	4.205625	0.475075
H	-0.593874	-4.241936	0.235561
O	-0.546018	-3.766146	-0.607873
H	-0.877947	-2.870051	-0.408546

Protonated Alanine + **7(H_2O)** (Charge = 1)

35 Atoms

E = -859.713324

	X	Y	Z
N	1.846971	-0.294279	0.373522
H	1.841830	-0.948960	-0.442032
C	0.922976	0.853637	0.162853
H	1.028887	1.518518	1.026470
C	1.284660	1.607898	-1.117918
C	-0.515189	0.354887	0.150564
H	1.154653	0.975285	-1.996065
H	0.659898	2.492065	-1.215965
H	2.325323	1.926786	-1.071038
O	-0.799273	-0.833780	0.116067
H	1.599091	-0.820561	1.236967
H	2.815656	0.067291	0.483981
O	-1.386357	1.332177	0.176687
H	-2.367912	1.000618	0.169730
O	-3.820782	0.588270	0.162570
H	-3.830804	-0.343191	0.489900
H	-4.349134	1.106217	0.796468
H	-0.964800	-2.020218	-1.459688
O	-0.705298	-2.563177	-2.218196
H	-1.141918	-2.153840	-2.985757
H	0.808919	-2.419898	2.730967
O	1.188844	-1.526670	2.804379

H	1.937909	-1.625303	3.418621
H	1.041238	-2.213836	-2.130879
O	1.940737	-1.880669	-1.922301
H	2.507337	-2.667831	-1.855881
H	-3.699526	-2.676777	0.575180
O	-3.367760	-1.905993	1.068299
H	-2.427157	-1.837479	0.844733
H	4.537903	1.560544	1.184943
O	4.446591	0.719138	0.703276
H	5.008937	0.818540	-0.085402
O	-1.093304	4.285017	-0.407546
H	-1.546812	4.326615	-1.265458
H	-1.250196	3.382326	-0.103323

Protonated acetyl-Alanine + **7(H_2O)** (Charge = 0)

39 Atoms

E = -1011.974906

	X	Y	Z
N	-1.248263	0.814420	-0.742436
C	-0.146574	0.111280	-1.369810
H	-0.468608	-0.897972	-1.620132
C	0.287646	0.834398	-2.649685
C	1.055441	-0.016768	-0.429898
H	0.609618	1.852537	-2.431633
H	1.110222	0.301580	-3.123393
H	-0.547026	0.874834	-3.348312
O	1.328317	0.811851	0.428067
H	-1.398839	1.799803	-0.972856
O	1.777202	-1.084056	-0.683043
H	2.609095	-1.179630	-0.084740
O	3.884622	-1.424739	0.735025
H	3.929395	-0.668733	1.367534
H	3.807326	-2.228835	1.279424
H	0.990357	2.681955	0.444831
O	0.845808	3.643207	0.411654
H	1.635280	4.003694	-0.027022
H	-0.651467	3.819060	-0.569604
O	-1.502703	3.662266	-1.030909
H	-1.430012	4.115305	-1.886713
H	4.158898	1.526453	1.993198

O	3.557040	0.799287	2.229602
H	2.752888	0.949145	1.703208
C	-2.000386	0.255134	0.213428
O	-1.806077	-0.907914	0.612928
C	-3.113255	1.097825	0.779516
H	-3.038212	2.140859	0.482753
H	-4.064768	0.694560	0.427438
H	-3.105701	1.011164	1.864802
H	-2.503679	-1.342308	2.298193
O	-2.801844	-1.511323	3.209318
H	-2.045236	-1.250463	3.756784
O	-1.770368	-3.509957	-0.468492
H	-2.558404	-3.553398	-1.035165
H	-1.778301	-2.608101	-0.099688
O	0.662474	-3.603745	-1.881462
H	-0.204589	-3.653810	-1.435482
H	1.036608	-2.778860	-1.549180

Protonated Alanine betaine + **4(H_2O)** (Charge = 1)

35 Atoms

E = -748.198943

	X	Y	Z
N	-2.108408	-0.277173	-0.481766
C	-1.069782	0.765927	-0.028347
H	-1.196415	1.595198	-0.728821
C	-1.282974	1.259354	1.403614
C	0.378157	0.279073	-0.160816
H	-1.039442	0.494893	2.139443
H	-0.627469	2.114995	1.559517
H	-2.302857	1.601210	1.567446
O	0.734106	-0.873631	0.021221
O	1.172886	1.278656	-0.445620
H	2.161483	1.027892	-0.459503
C	-1.708906	-0.863530	-1.811847
H	-0.835271	-1.489876	-1.679976
H	-2.540854	-1.456626	-2.181544
H	-1.499786	-0.048750	-2.501575
C	-3.424305	0.430510	-0.683531
H	-4.149239	-0.303409	-1.024964
H	-3.756644	0.861818	0.254547
H	-3.294112	1.206755	-1.433285
C	-2.316634	-1.390727	0.510529
H	-2.747176	-0.980443	1.418201
H	-3.013419	-2.097328	0.066430

H	-1.372423	-1.875852	0.722954
H	4.139298	1.082099	0.237753
O	3.666319	0.780992	-0.559133
H	3.772608	-0.199107	-0.586402
H	2.492232	-1.794448	-0.398397
O	3.420254	-1.909220	-0.653364
H	3.832312	-2.399478	0.080260
H	0.381862	-3.991619	1.102589
O	0.345899	-3.288151	1.772227
H	0.663661	-2.503169	1.311026
O	0.793937	4.041305	0.855325
H	0.163803	4.617722	0.392038
H	1.006167	3.354491	0.211756