Supplementary Material (ESI) for New Journal of Chemistry

Hydration Effect on Interaction Mode Between Glutamic Acid and Ca^{2+} and Its Biochemical Implication: A Theoretical Exploration

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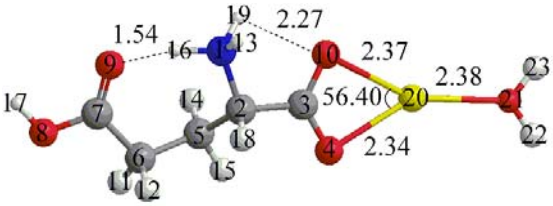
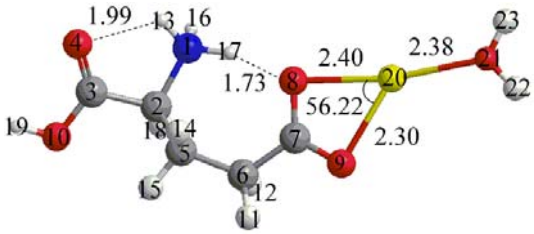
Supporting Information



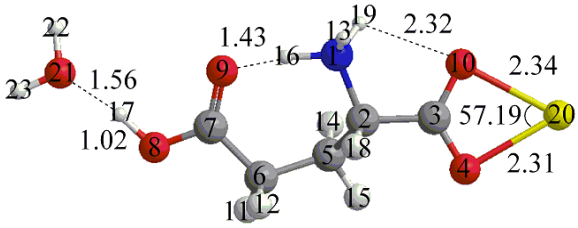
0.0

11-w



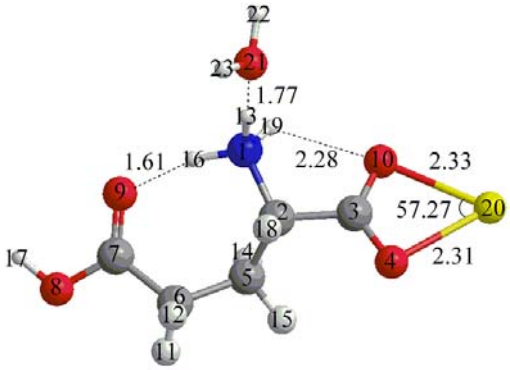
+4.1 kcal/mol

21-w



+19.2 kcal/mol

12-w



+19.8 kcal/mol

13-w

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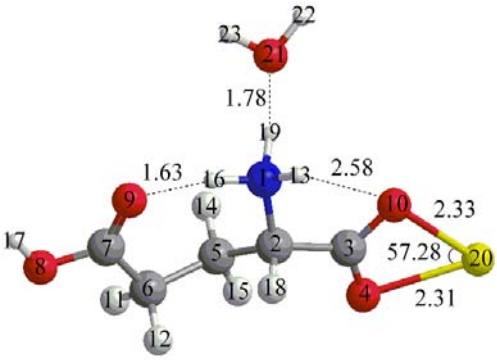
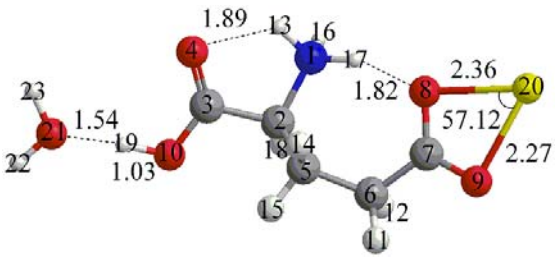


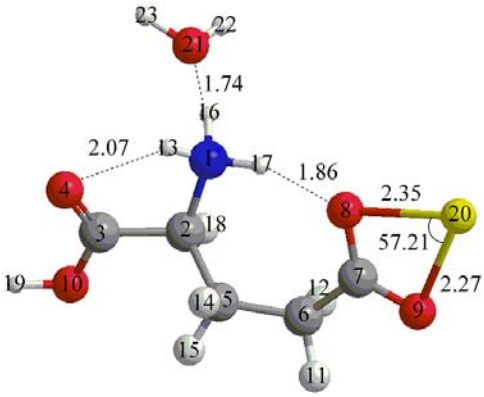
+21.1 kcal/mol

14-w



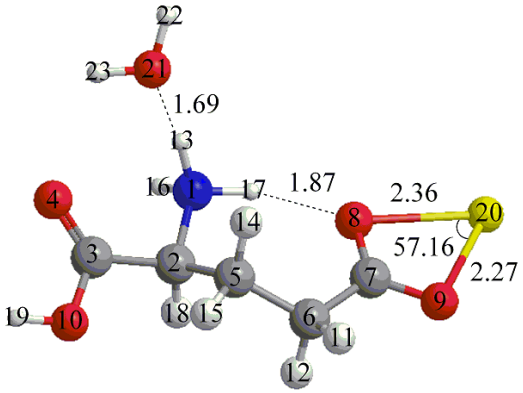
+22.1 kcal/mol

22-w



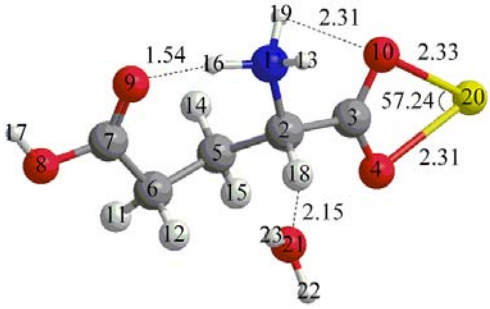
+22.6 kcal/mol

23-w



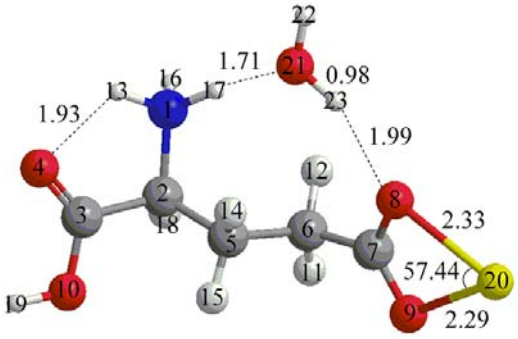
+24.1 kcal/mol

24-w



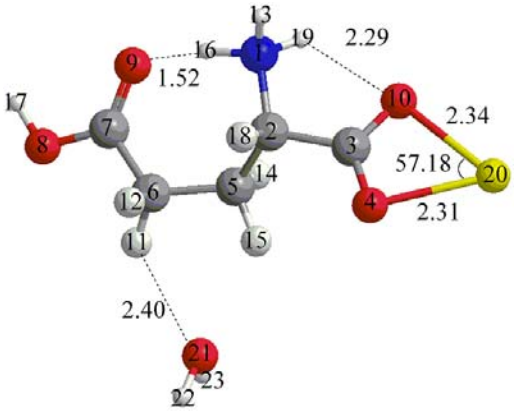
+24.8 kcal/mol

15-w



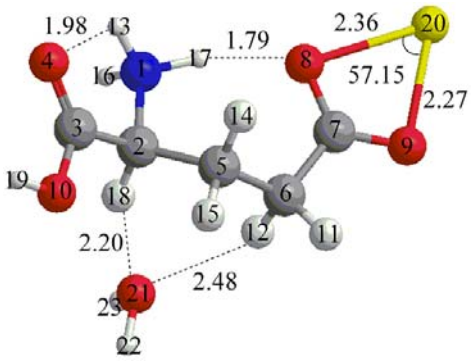
+25.1 kcal/mol

25-w



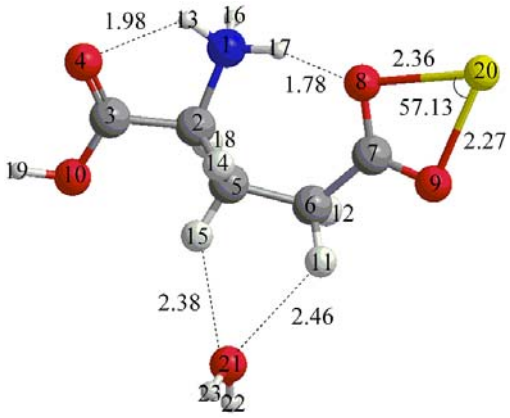
+27.6 kcal/mol

16-w



+28.8 kcal/mol

26-w



+30.8 kcal/mol

27-w

Figure S1. All of the B3LYP/6-31G (d, p)-optimized mono-hydrated complexes of the **1**- and **2**-series corresponding to the local minima points on the PES. Distances in the figure are given in angstroms, and the angles are given in degree. Here, the relative energies are listed below the different isomers with ZPVE corrections. The yellow ball is referred to Ca^{2+}, the red denotes O atom, the blue denotes N, the gray denotes C atom, and the white-gray denotes H atom, respectively.

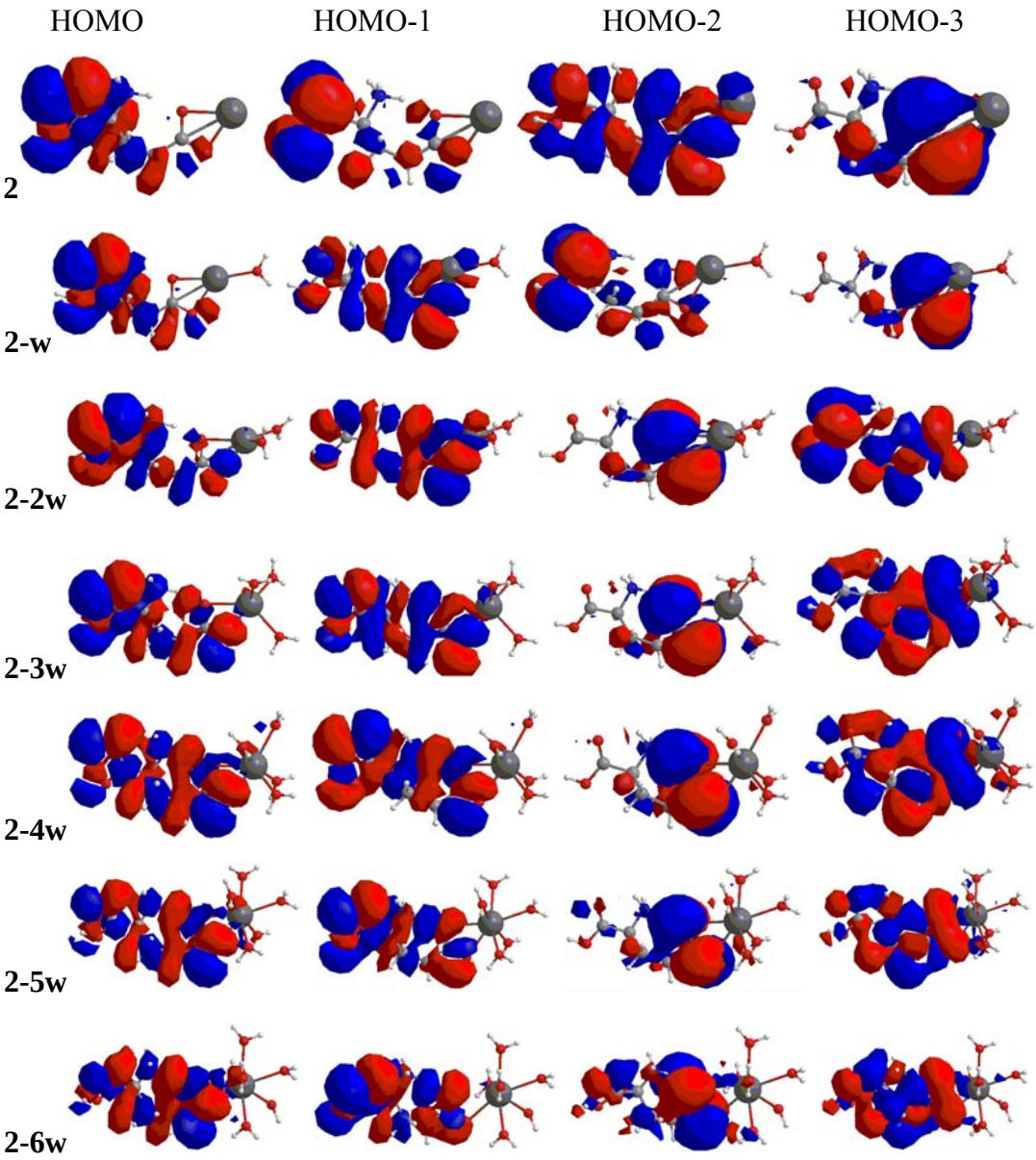


Figure S2. Diagrams of high energy level orbitals for the glutamic acid-Ca^{2+}-$(H_2O)_n$ (n=0-6) complex of the **2**-series. Isocontour value 0.01 is used. The order is HOMO, HOMO-1, HOMO-2 and HOMO-3 from left to right.

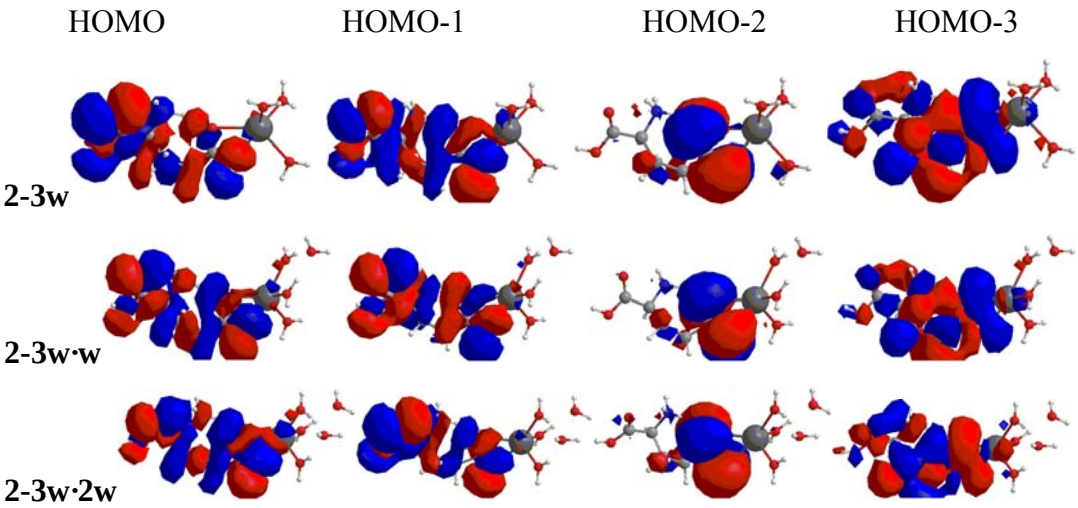


Figure S3. Diagrams of high energy level orbits for the (3, 0), (3, 1) and (3, 2) modes of the **2**-series. Isocontour value 0.01 is used. The order is HOMO, HOMO-1, HOMO-2 and HOMO-3 from left to right.

TABLE S1. The selected geometrical parameters of (n, 0), (n, 1), and (n, 2) Modes. The bond lengths (R), bond angles (A) are in angstroms and degrees, respectively. Atomic number used here is displayed in Figure 1.

1-series:

Complex	R (Ca-O)	R (N_1-H_{16})	R (O_9·····H_{16})	A (O-Ca-O)
1-2w	2.393	1.08	1.56	55.80
1-2w·2w	2.378	1.07	1.58	55.33
Complex	R (Ca-O)	R (N_1-H_{16})	R (O_9·····H_{16})	A (O-Ca-O)
1-3w	2.418	1.07	1.58	54.87
1-3w·w	2.412	1.07	1.59	54.76
1-3w·2w	2.410	1.07	1.60	54.57
Complex	R (Ca-O)	R (N_1-H_{16})	R (O_9·····H_{16})	A (O-Ca-O)
1-4w	2.447	1.07	1.59	54.30
1-4w·w	2.443	1.07	1.60	53.85

2-series:

Complex	R (Ca-O)	R (N_1-H_{17})	R (O_8·····H_{17})	A (O-Ca-O)
2-2w	2.390	1.06	1.68	55.56
2-2w·2w	2.373	1.06	1.63	55.05
Complex	R (Ca-O)	R (N_1-H_{17})	R (O_8·····H_{17})	A (O-Ca-O)
2-3w	2.416	1.06	1.64	54.38
2-3w·w	2.410	1.07	1.61	54.37
2-3w·2w	2.406	1.07	1.58	54.18
Complex	R (Ca-O)	R (N_1-H_{17})	R (O_8·····H_{17})	A (O-Ca-O)
2-4w	2.445	1.07	1.60	53.76
2-4w·w	2.445	1.08	1.57	53.11
2-4w·2w	2.445	1.09	1.53	53.22
Complex	R (Ca-O)	R (N_1-H_{17})	R (O_8·····H_{17})	A (O-Ca-O)
2-5w	2.486	1.08	1.57	51.82
2-5w·w	2.493	1.09	1.54	51.26

TABLE S2. Energy differences ΔE (kcal/mol) among (5,0) (4,1) and (3,2) modes of the **1**- and **2**-series at the different levels plus ZPVE corrections.

hydrates	ΔE (kcal/mol)			
	B3LYP/6-311++G(2d,p)	B3LYP/6-311+G(3df,2p)	MP2/6-311++G(2d,p)	MP2/6-311+G(3df,2p)
1-5w	0.0	0.0	0.0	0.0
1-4w·w	+0.2	+0.4	+3.0	+2.8
1-3w·2w	+3.4	+4.0	+9.5	+9.0
2-5w	+1.1	+0.9	0.0	0.0
2-4w·w	0.0	0.0	+1.7	+1.4
2-3w·2w	+3.8	+3.9	+8.5	+8.0