Reaction Energetics and ^{13}C Fractionation of Alanine Transamination in the Aqueous and Gas Phases

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Table S1. Parameters for the QM/MM Potential and the Toukan-Rahman Water Potential.

QM/MM		SPC/E MM inter-atomic	
$A_{CO\text{^}}$	$4\sqrt{\varepsilon_C\varepsilon_O}\left(\frac{\sigma_C+\sigma_O}{2}\right)^{12}$	$q_{O\text{^}}$	-0.8476e
$B_{CO\text{^}}$	$4\sqrt{\varepsilon_C\varepsilon_O}\left(\frac{\sigma_C+\sigma_O}{2}\right)^{6}$	$q_{H\text{^}}$	0.4238e
$A_{NO\text{^}}$	$4\sqrt{\varepsilon_N\varepsilon_O}\left(\frac{\sigma_N+\sigma_O}{2}\right)^{12}$	r_{OH}	1Å
$N_{NO\text{^}}$	$4\sqrt{\varepsilon_N\varepsilon_O}\left(\frac{\sigma_N+\sigma_O}{2}\right)^{6}$	$\angle HOH$	109.47°
$A_{OO\text{^}}$	$4\varepsilon_O\sigma_O^{12}$	$A_{O\text{^}O\text{^}}$	$4\varepsilon_O\sigma_O^{12}$
$B_{OO\text{^}}$	$4\varepsilon_O\sigma_O^{6}$	$B_{O\text{^}O\text{^}}$	$4\varepsilon_O\sigma_O^{6}$
$A_{HO\text{^}}$	$4\sqrt{\varepsilon_H\varepsilon_O}\left(\frac{\sigma_H+\sigma_O}{2}\right)^{12}$	$A_{O\text{^}H\text{^}}, A_{H\text{^}H\text{^}}$	0.0
$B_{HO\text{^}}$	$4\sqrt{\varepsilon_H\varepsilon_O}\left(\frac{\sigma_H+\sigma_O}{2}\right)^{6}$	$B_{O\text{^}H\text{^}}, B_{H\text{^}H\text{^}}$	0.0
$A_{CH\text{^}}, A_{NH\text{^}}, A_{OH\text{^}}, A_{HH\text{^}}$	0.0		
$B_{CH\text{^}}, B_{NH\text{^}}, B_{OH\text{^}}, B_{HH\text{^}}$	0.0		
ε_C= 0.100 kcal/mol σ_C= 3.41Å ε_N= 0.069 kcal/mol σ_N= 3.26Å ε_O= 0.155 kcal/mol σ_O= 3.17Å ε_H= 0.044 kcal/mol σ_H= 0.70Å			

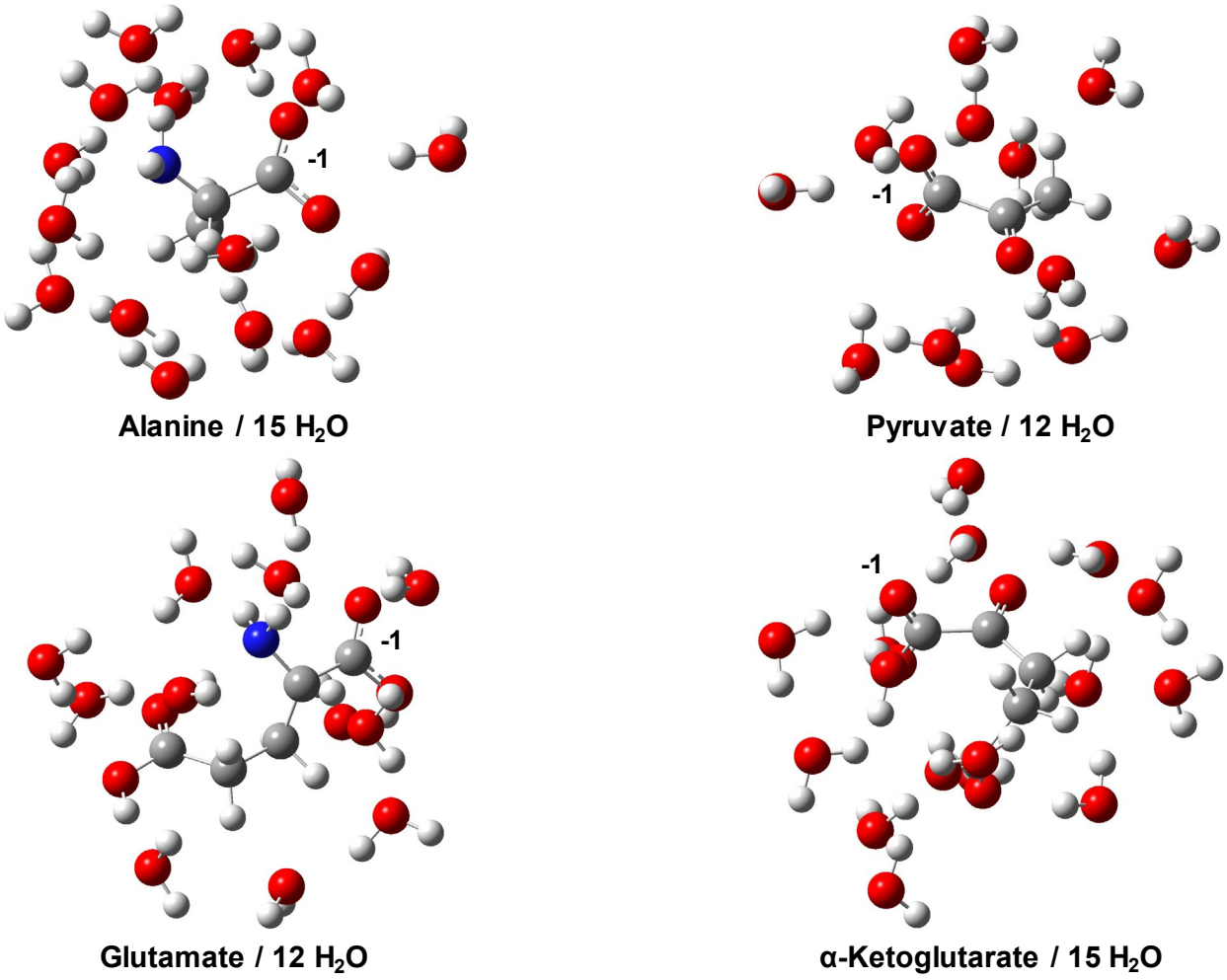


Figure S1. Starting explicitly solvated (single solvation shell) structures from MD simulations for deprotonated alanine, pyruvate, α-ketoglutarate, and glutamate.

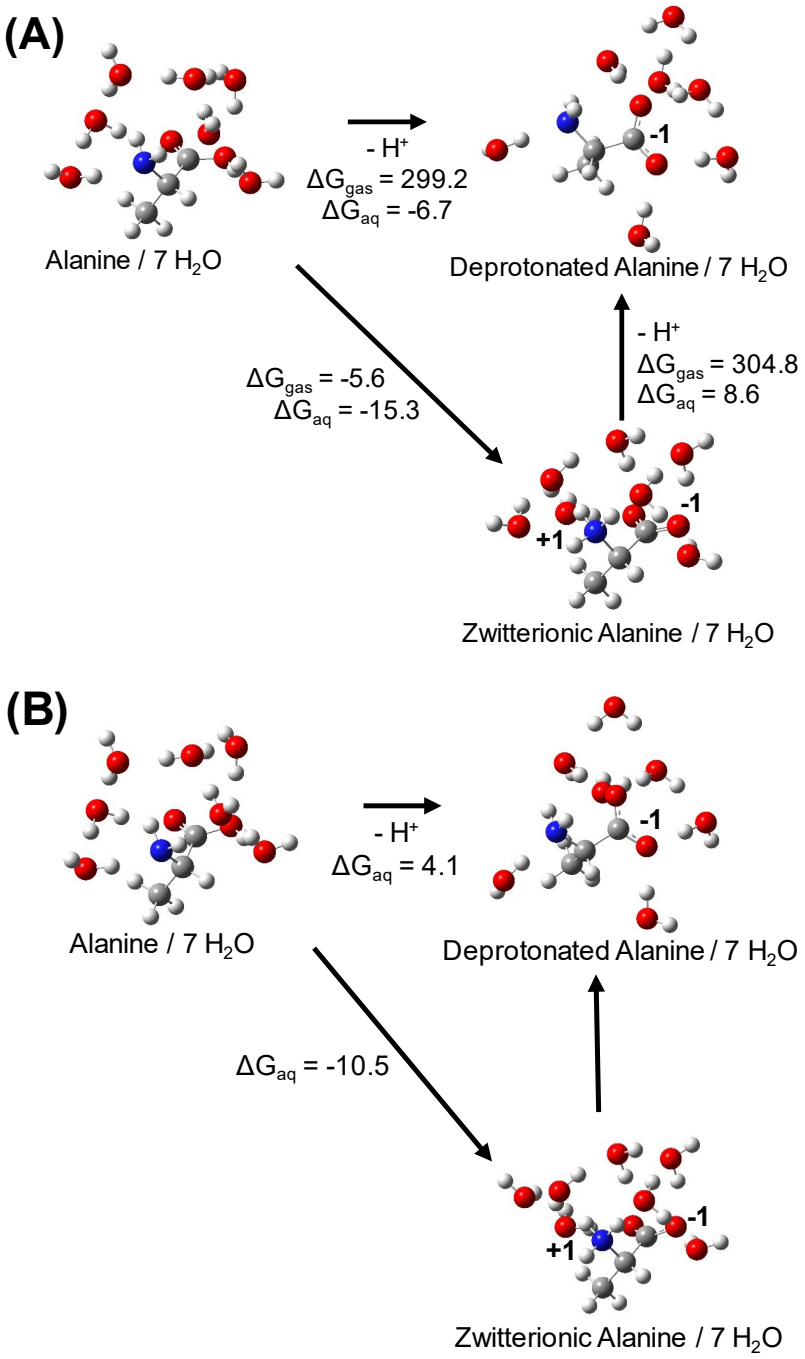
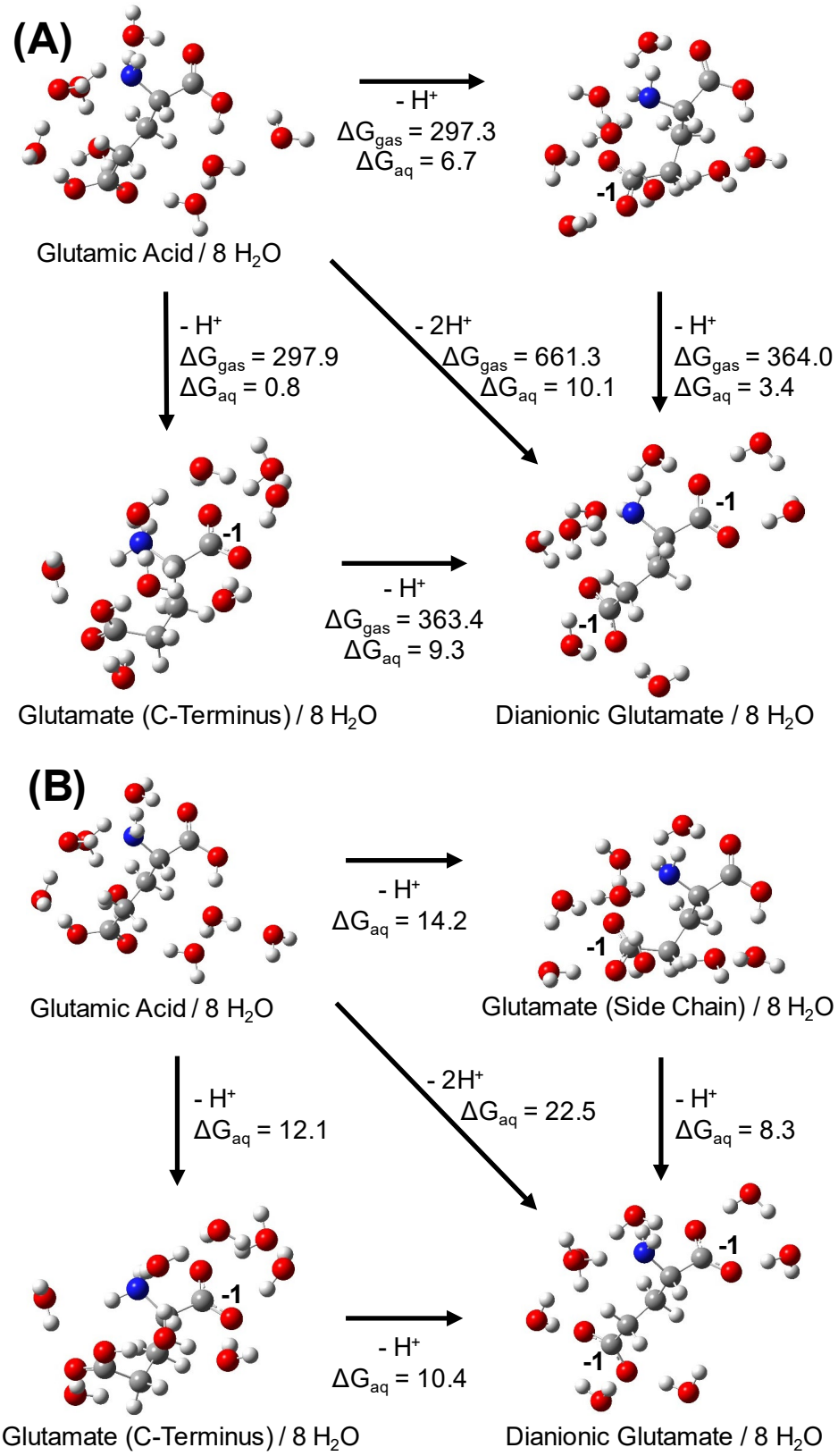
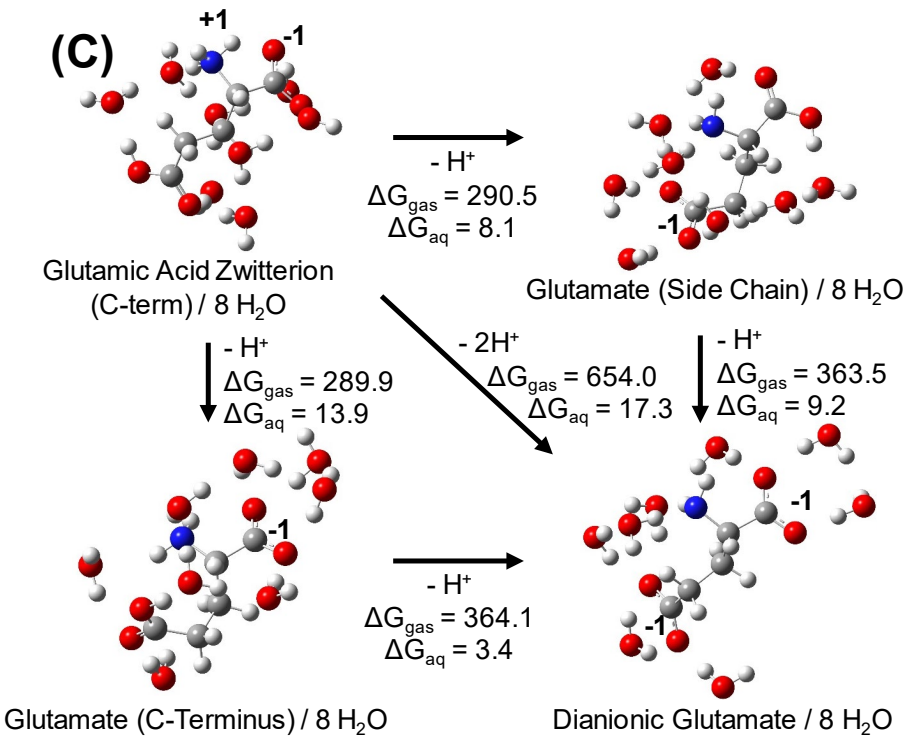
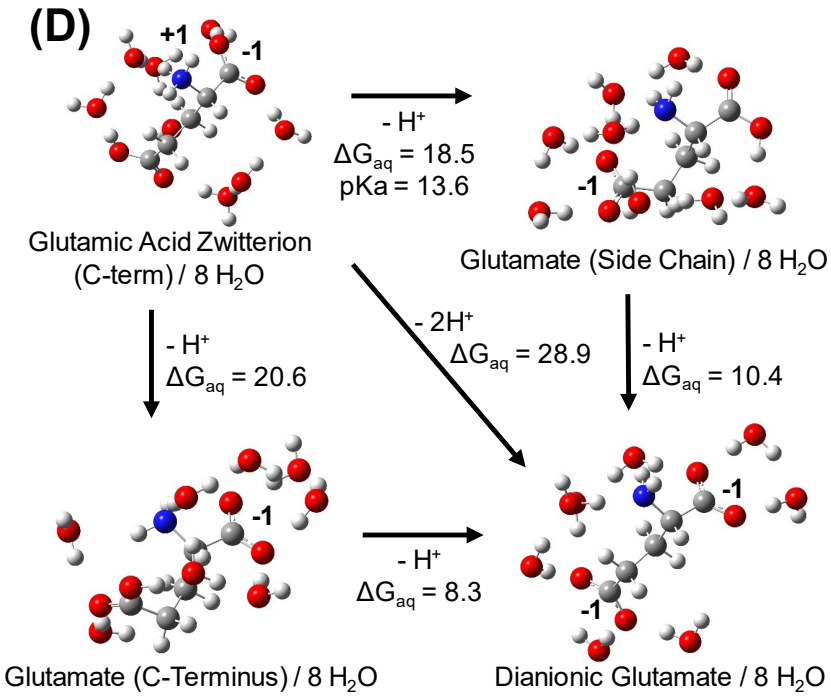
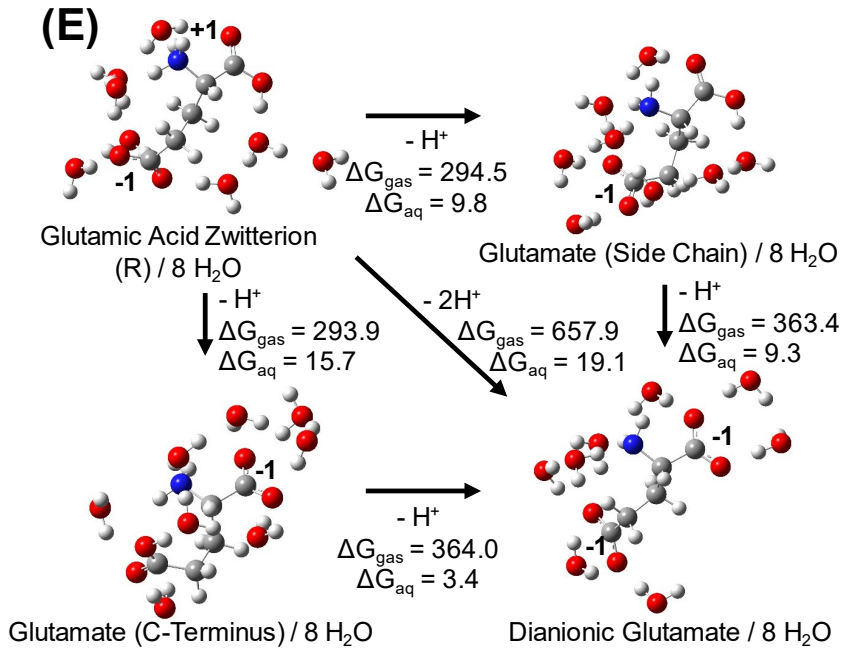


Figure S2. Alanine and related structures with 7 explicit H_2O molecules optimized (A) in the gas phase. Energies are given in kcal/mol at the MP2/aD level with and without SCRF via COSMO and (B) in aqueous solution in kcal/mol at the MP2/aD/COSMO level.


(A)
- H+
ΔGgas = 297.3
ΔGaq = 6.7
-1
Glutamic Acid / 8 H2O
- H+
ΔGgas = 297.9
ΔGaq = 0.8
- 2H+
ΔGgas = 661.3
ΔGaq = 10.1
- H+
ΔGgas = 364.0
ΔGaq = 3.4
-1
-1
-1
- H+
ΔGgas = 363.4
ΔGaq = 9.3
Glutamate (C-Terminus) / 8 H2O
Dianionic Glutamate / 8 H2O
(B)
- H+
ΔGaq = 14.2
-1
Glutamic Acid / 8 H2O
Glutamate (Side Chain) / 8 H2O
- H+
ΔGaq = 12.1
- 2H+
ΔGaq = 22.5
- H+
ΔGaq = 8.3
-1
-1
-1
- H+
ΔGaq = 10.4
Glutamate (C-Terminus) / 8 H2O
Dianionic Glutamate / 8 H2O


(C)
+1
-1
Glutamic Acid Zwitterion
(C-term) / 8 H2O
- H+
ΔGgas = 290.5
ΔGaq = 8.1
-1
Glutamate (Side Chain) / 8 H2O
- H+
ΔGgas = 289.9
ΔGaq = 13.9
- 2H+
ΔGgas = 654.0
ΔGaq = 17.3
- H+
ΔGgas = 363.5
ΔGaq = 9.2
-1
- H+
ΔGgas = 364.1
ΔGaq = 3.4
-1
-1
Glutamate (C-Terminus) / 8 H2O
Dianionic Glutamate / 8 H2O


(D)
+1
-1
Glutamic Acid Zwitterion
(C-term) / 8 H2O
- H+
ΔGaq = 18.5
pKa = 13.6
-1
Glutamate (Side Chain) / 8 H2O
- H+
ΔGaq = 20.6
- 2H+
ΔGaq = 28.9
- H+
ΔGaq = 10.4
-1
- H+
ΔGaq = 8.3
-1
-1
Glutamate (C-Terminus) / 8 H2O
Dianionic Glutamate / 8 H2O



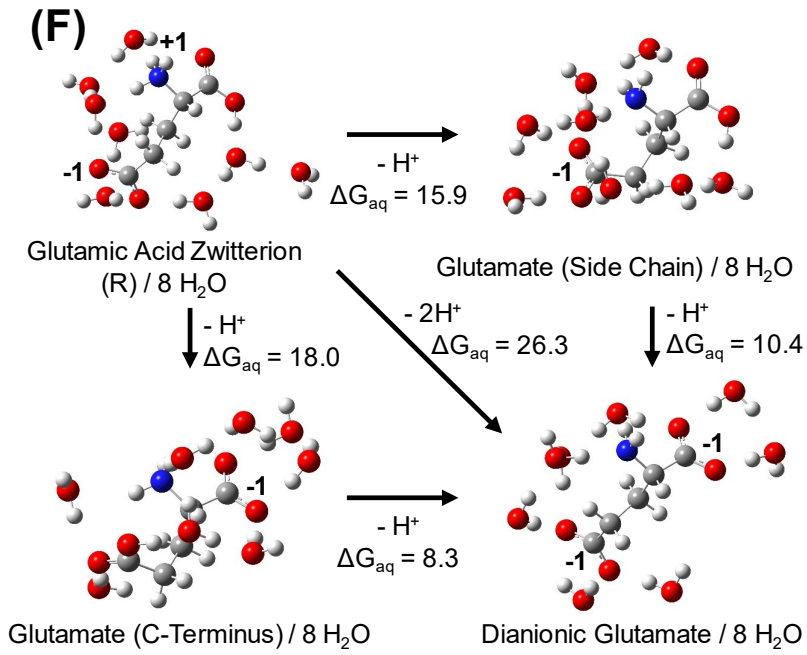


Figure S3. Glutamic acid and related structures with 8 explicit H_2O molecules optimized (A, C, E) in the gas phase and (B, D, F) in aqueous solution. Non-charge separated (NCS) glutamic acid deprotonation schemes are given in (A) and (B). Zwitterionic glutamic acid deprotonation reactions with the negative charge at the C-terminus are given in schemes (C) and (D). Zwitterionic glutamic acid deprotonation reactions with the negative charge at the side group are given in schemes (E) and (F). Energies are given in kcal/mol at the MP2/aD level with and without SCRF via COSMO and in aqueous solution in kcal/mol at the MP2/aD/COSMO level.

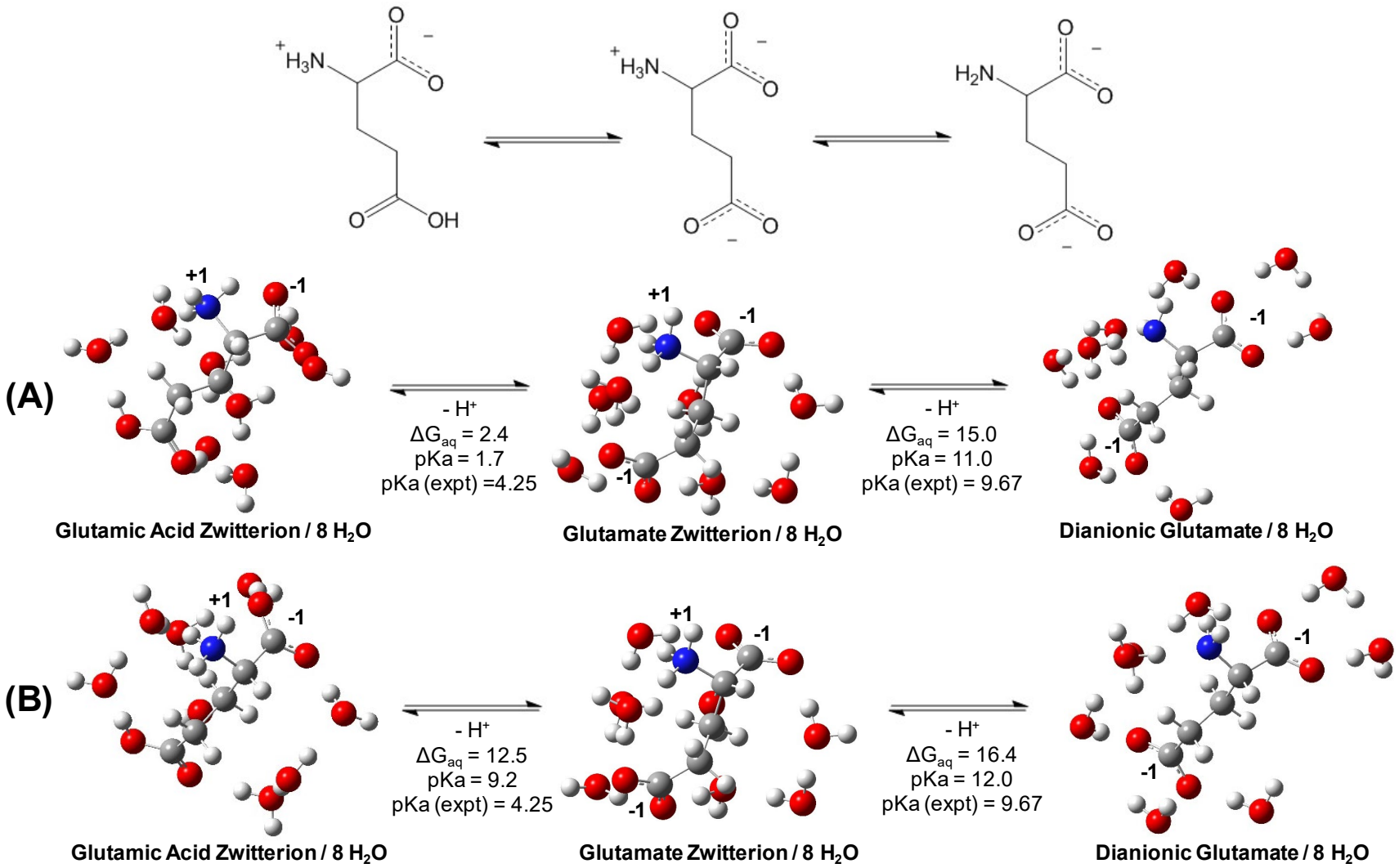


Figure S4. Zwitterionic glutamic acid deprotonation reactions and energetics compared to experimental pKa values for both (A) MP2/aD gas phase optimized and (B) MP2/aD/COSMO aqueous optimized clusters of glutamic acid or glutamate with 8 explicit H_2O molecules.

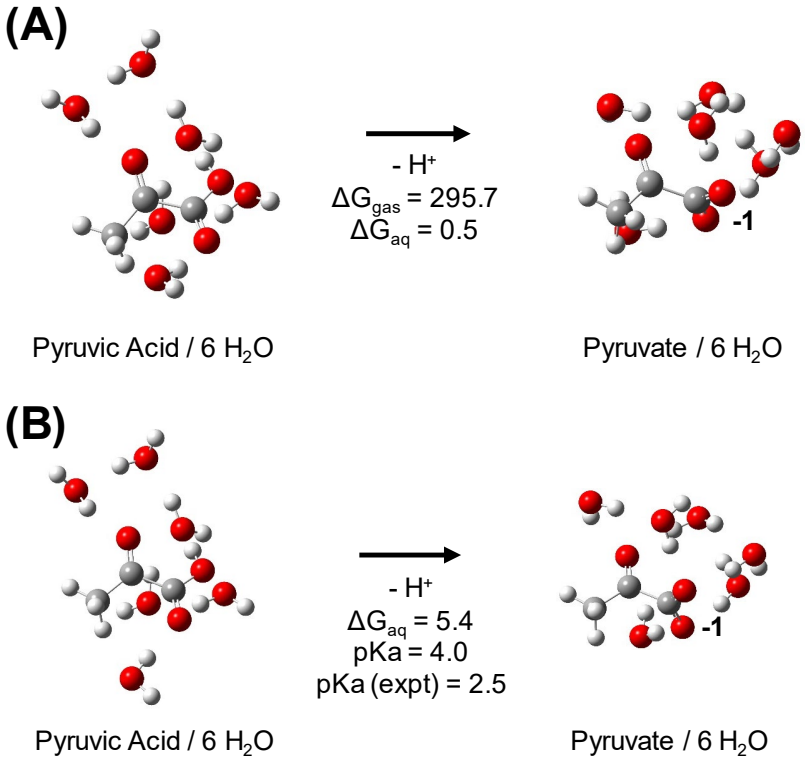


Figure S5. Pyruvic acid and pyruvate with 6 explicit H_2O molecules optimized (A) in the gas phase. Energies are given in kcal/mol at the MP2/aD level with and without SCRF via COSMO and (B) in aqueous solution in kcal/mol at the MP2/aD/COSMO level.

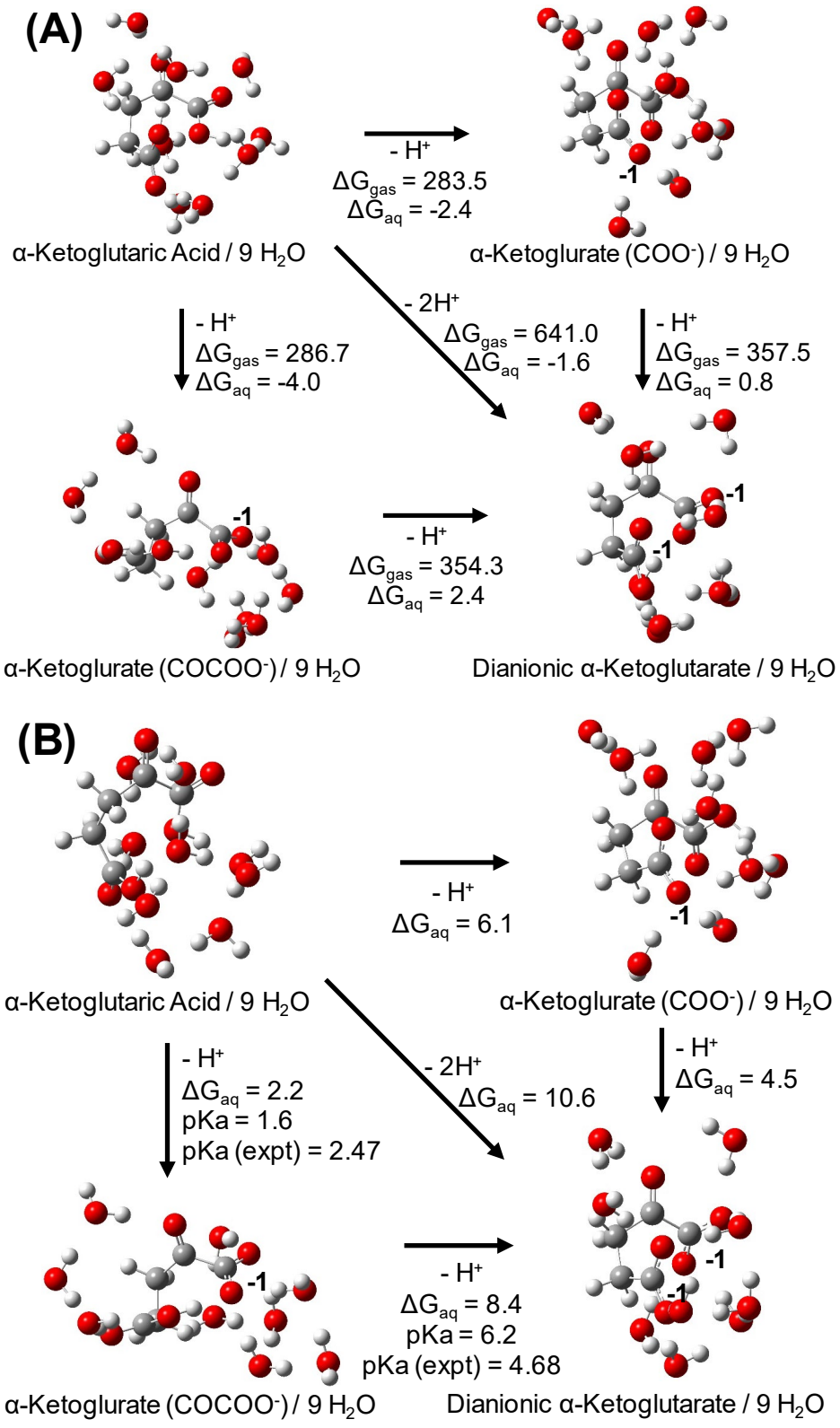


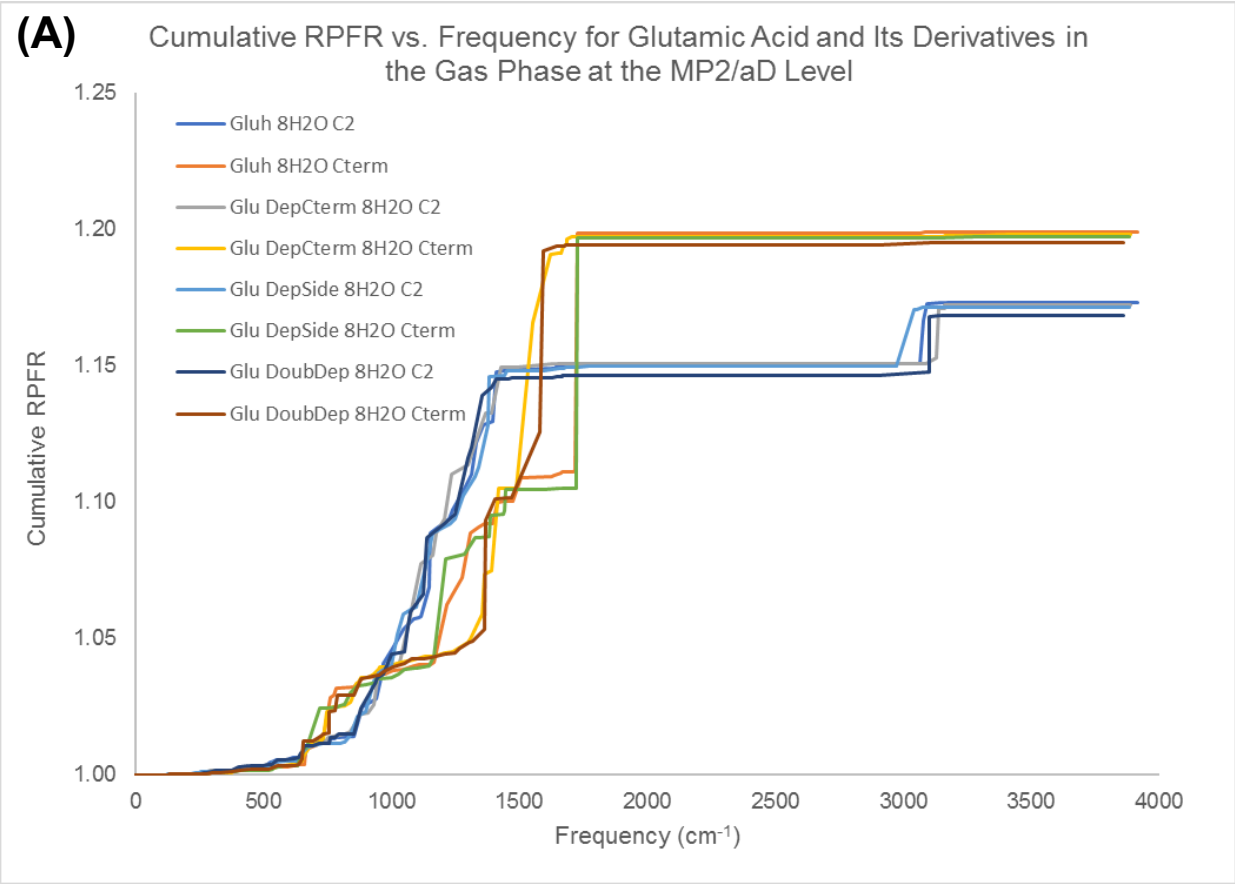
Figure S6. α-Ketoglutaric acid and related structures with 9 explicit H_2O molecules optimized (A) in the gas phase. Energies are given in kcal/mol at the MP2/aD level with and without SCRF via COSMO and (B) in aqueous solution in kcal/mol at the MP2/aD/COSMO level.

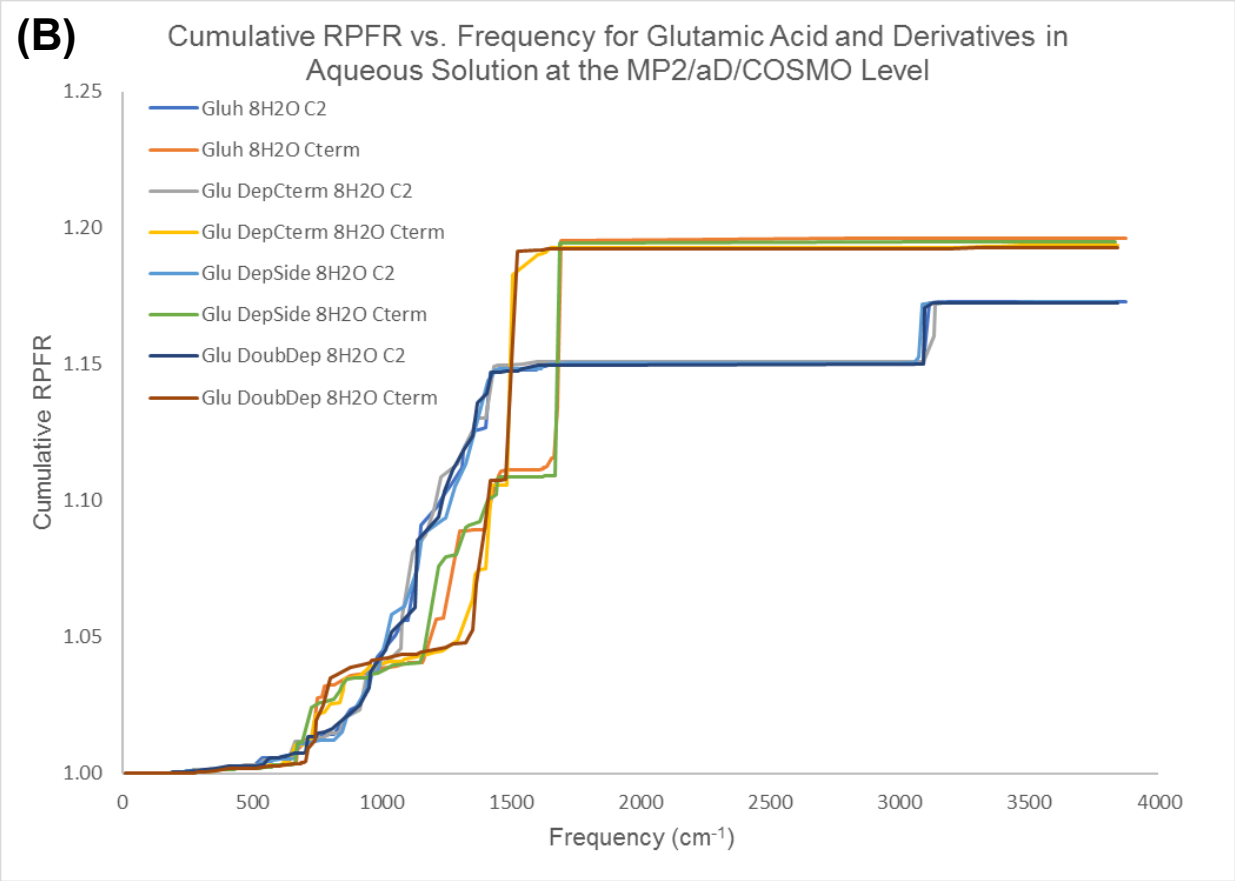
Table S2. Site Specific β Values for H_2CO, CH_3NH_2, $CH_3NH_3^+$, Alanine, Deprotonated Alanine, Pyruvic Acid, and Pyruvate in the Gas Phase at 298 K at the MP2/aD Level.

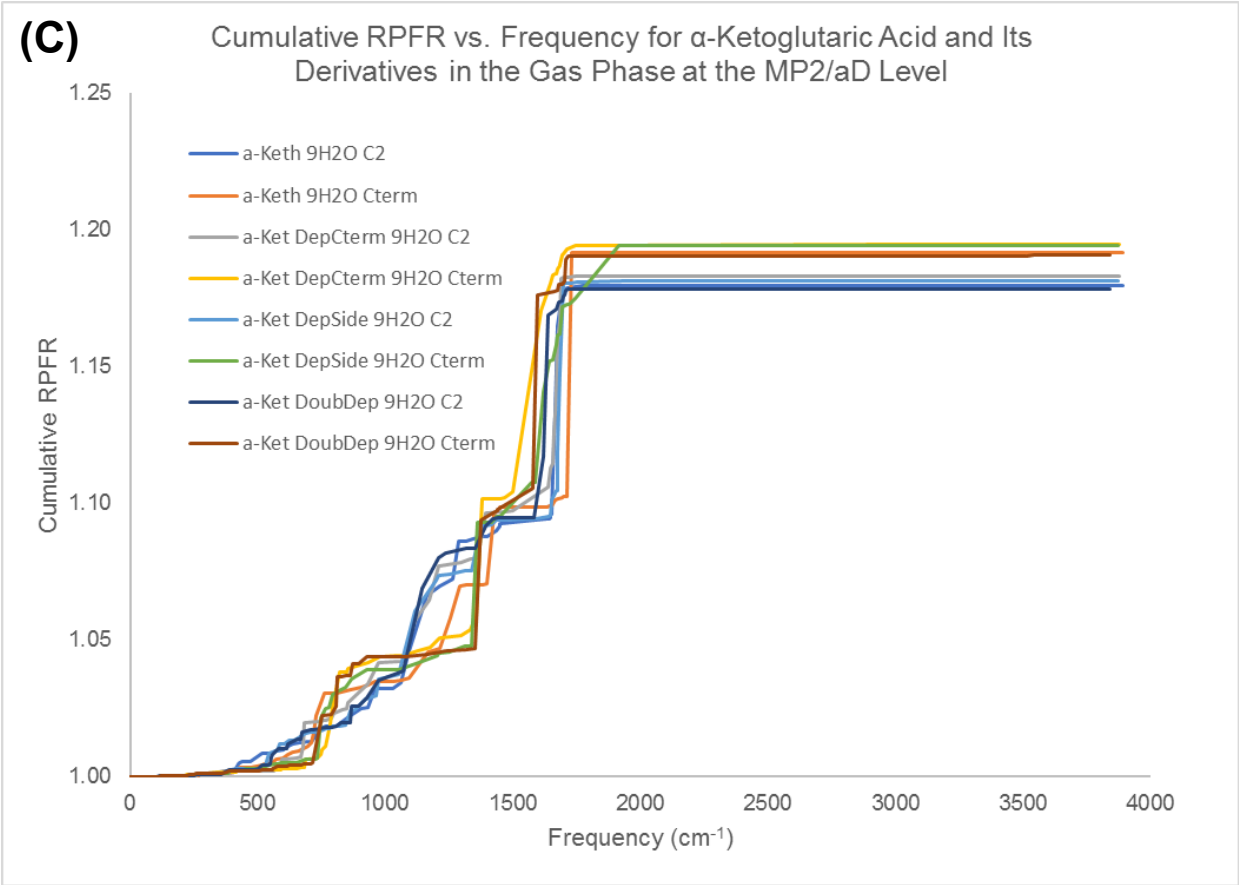
	$\beta = Q_h/Q_l$		
H_2CO	1.1504		
CH_3NH_2	1.1424		
$CH_3NH_3^+$	1.1415		
	^{13}C Methyl	^{13}C Central Carbon	^{13}C COOH/COO^-
Alanine	1.1405	1.1765	1.1983
Deprotonated Alanine	1.1414	1.1669	1.1990
Pyruvic Acid	1.1406	1.1810	1.1899
Pyruvate	1.1355	1.1788	1.1899

Table S3. $^{13}C/^{12}C$ Exchange Thermodynamics for Explicitly Solvated Pyruvate and Alanine in kcal/mol.

Gas Phase Optimized, ^{13}C Substituted		
Pyruvate $\Delta ZPE_{gas,Me}$	0.1182	
Alanine Zwitterion $\Delta ZPE_{gas,Me}$	0.1220	
Deprotonated Alanine $\Delta ZPE_{gas,Me}$		0.1188
$\Delta\Delta ZPE_{gas,Me}$	0.0039	0.0007
$1000*\ln K_{ZPE,gas,Me}$ (‰)	-6.5	-1.1
Pyruvate $\Delta ZPE_{gas,C2}$	0.15451	
Alanine Zwitterion $\Delta ZPE_{gas,C2}$	0.1498	
Deprotonated Alanine $\Delta ZPE_{gas,C2}$		0.1491
$\Delta\Delta ZPE_{gas,C2}$	-0.0047	-0.0054
$1000*\ln K_{ZPE,gas,C2}$ (‰)	7.8	9.2
Pyruvate $\Delta ZPE_{gas,Cterm}$	0.1621	
Alanine Zwitterion $\Delta ZPE_{gas,Cterm}$	0.1648	
Deprotonated Alanine $\Delta ZPE_{gas,Cterm}$		0.1646
$\Delta\Delta ZPE_{gas,Cterm}$	0.0027	0.0025
$1000*\ln K_{ZPE,gas,Cterm}$ (‰)	-4.6	-4.3
Aqueous Optimized, ^{13}C Substituted		
Pyruvate $\Delta ZPE_{aq,Me}$	0.1181	
Alanine Zwitterion $\Delta ZPE_{gas,Me}$	0.1215	
Deprotonated Alanine $\Delta ZPE_{aq,Me}$		0.1188
$\Delta\Delta ZPE_{aq,Me}$	0.0035	0.0007
$1000*\ln K_{ZPE,aq,Me}$ (‰)	-5.8	-1.2
Pyruvate $\Delta ZPE_{aq,C2}$	0.1553	
Alanine Zwitterion $\Delta ZPE_{gas,C2}$	0.1496	
Deprotonated Alanine $\Delta ZPE_{aq,C2}$		0.1496
$\Delta\Delta ZPE_{aq,C2}$	-0.0057	-0.0057
$1000*\ln K_{ZPE,aq,C2}$ (‰)	9.6	9.5
Pyruvate $\Delta ZPE_{aq,Cterm}$	0.1612	
Alanine Zwitterion $\Delta ZPE_{gas,Cterm}$	0.1625	
Deprotonated Alanine $\Delta ZPE_{aq,Cterm}$		0.1624
$\Delta\Delta ZPE_{aq,Cterm}$	0.0013	0.0013
$1000*\ln K_{ZPE,aq,Cterm}$ (‰)	-2.2	-2.1


(A)
Cumulative RPFR vs. Frequency for Glutamic Acid and Its Derivatives in the Gas Phase at the MP2/aD Level
Gluh 8H2O C2
Gluh 8H2O Cterm
Glu DepCterm 8H2O C2
Glu DepCterm 8H2O Cterm
Glu DepSide 8H2O C2
Glu DepSide 8H2O Cterm
Glu DoubDep 8H2O C2
Glu DoubDep 8H2O Cterm
Cumulative RPFR
1.25
1.20
1.15
1.10
1.05
1.00
0
500
1000
1500
2000
2500
3000
3500
4000
Frequency (cm-1)


(B)
Cumulative RPFR vs. Frequency for Glutamic Acid and Derivatives in Aqueous Solution at the MP2/aD/COSMO Level
Gluh 8H2O C2
Gluh 8H2O Cterm
Glu DepCterm 8H2O C2
Glu DepCterm 8H2O Cterm
Glu DepSide 8H2O C2
Glu DepSide 8H2O Cterm
Glu DoubDep 8H2O C2
Glu DoubDep 8H2O Cterm
Cumulative RPFR
1.25
1.20
1.15
1.10
1.05
1.00
0
500
1000
1500
2000
2500
3000
3500
4000
Frequency (cm-1)


(C)
Cumulative RPFR vs. Frequency for α-Ketoglutaric Acid and Its Derivatives in the Gas Phase at the MP2/aD Level
Cumulative RPFR
1.25
1.20
1.15
1.10
1.05
1.00
0
500
1000
1500
2000
2500
3000
3500
4000
Frequency (cm-1)
a-Keth 9H2O C2
a-Keth 9H2O Cterm
a-Ket DepCterm 9H2O C2
a-Ket DepCterm 9H2O Cterm
a-Ket DepSide 9H2O C2
a-Ket DepSide 9H2O Cterm
a-Ket DoubDep 9H2O C2
a-Ket DoubDep 9H2O Cterm

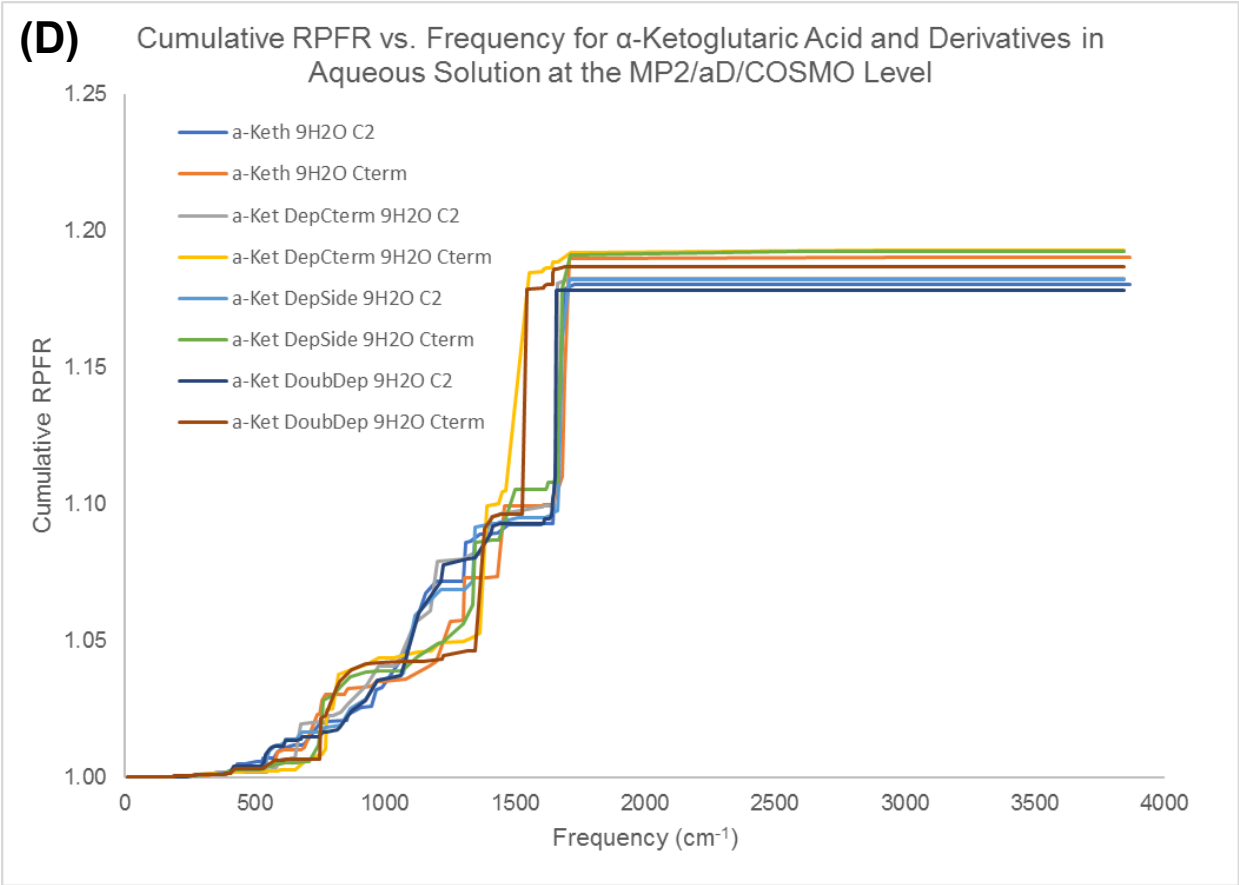


Figure S7. Cumulative reduced partition function ratio (RPFR) vs. vibrational frequency (cm^{-1}) at 298 K for ^{13}C at either the C2 site or the C-terminus. (A) and (B) are glutamic acid (Gluh) and its various deprotonated forms (Glu) with 8 explicit H_2O molecules in the gas phase and in aqueous solution, respectively. (C) and (D) are α-ketoglutaric (a-Keth) acid and its various deprotonated forms (a-Ket) with 9 explicit H_2O molecules in the gas phase and in aqueous solution, respectively. All results are optimized at the MP2/aD level for the gas phase and MP2/aD/COSMO for the aqueous solution.

Table S3. Q Values for All Species Optimized in the Gas Phase or in Aqueous Solution at the MP2/aD or MP2/aD/COSMO Level at 298 K.

Species	# of H_2O Molecules	$Q_{l,gas\ opt}$	$Q_{l,aq\ opt}$	^{13}C Site	$Q_{h,gas\ opt}$ [a]	$Q_{h,aq\ opt}$ [a]
Alanine	7	2.42680×10^{-71}	3.67591×10^{-70}	Methyl	2.77475×10^{-71}	4.20473×10^{-70}
				C2	2.84597×10^{-71}	4.31398×10^{-70}
				C-terminus	2.90870×10^{-71}	4.39408×10^{-70}
Alanine, Zwitterion	7	1.33845×10^{-71}	1.64825×10^{-70}	Methyl	1.53195×10^{-71}	1.88699×10^{-70}
				C2	1.57008×10^{-71}	1.93402×10^{-70}
				C-terminus	1.60421×10^{-71}	1.96818×10^{-70}
Alanine, Deprotonated	7	6.01801×10^{-68}	1.69660×10^{-66}	Methyl	6.87162×10^{-68}	1.93640×10^{-66}
				C2	7.05616×10^{-68}	1.99065×10^{-66}
				C-terminus	7.21309×10^{-68}	2.02582×10^{-66}
Glutamic Acid	8	5.67114×10^{-87}	2.50526×10^{-85}	Side Chain	6.81020×10^{-87}	2.99488×10^{-85}
				C2	6.65295×10^{-87}	2.93860×10^{-85}
				C-terminus	6.79896×10^{-87}	2.99665×10^{-85}
Glutamic Acid, Zwitterion (C-terminus)	8	7.25137×10^{-87}	6.52629×10^{-86}	Side Chain	8.70155×10^{-87}	7.80597×10^{-86}
				C2	8.46005×10^{-87}	7.64664×10^{-86}
				C-terminus	8.67348×10^{-87}	7.78964×10^{-86}
Glutamic Acid, Zwitterion (Side Chain)	8	1.16950×10^{-86}	1.64453×10^{-85}	Side Chain	1.40115×10^{-86}	1.96048×10^{-85}
				C2	1.37083×10^{-86}	1.93101×10^{-85}
				C-terminus	1.40321×10^{-86}	1.96801×10^{-85}
Glutamate, Zwitterionic Anion		2.13975×10^{-83}	1.71107×10^{-82}	Side Chain	2.50363×10^{-83}	2.00674×10^{-82}
				C2	2.56265×10^{-83}	2.03921×10^{-82}
				C-terminus	2.55844×10^{-83}	2.04140×10^{-82}
Glutamate, C-terminus Deprotonation	8	1.92245×10^{-83}	5.48760×10^{-82}	Side Chain	2.30675×10^{-83}	6.56171×10^{-82}
				C2	2.25362×10^{-83}	6.43344×10^{-82}
				C-terminus	2.30331×10^{-83}	6.54926×10^{-82}
Glutamate, Side Chain Deprotonation	8	2.30255×10^{-83}	6.00869×10^{-82}	Side Chain	2.75483×10^{-83}	7.15671×10^{-82}
				C2	2.69723×10^{-83}	7.04667×10^{-82}
				C-terminus	2.75644×10^{-83}	7.17956×10^{-82}
Glutamate,	8	5.15756×10^{-80}	1.01366×10^{-78}	Side Chain	6.16202×10^{-80}	1.20839×10^{-78}

Doubly Deprotonated				C2	6.02672×10^{-80}	1.18856×10^{-78}
				C-terminus	6.16349×10^{-80}	1.20920×10^{-78}
Pyruvic Acid	6	1.36071×10^{-55}	2.10712×10^{-54}	Methyl	1.55333×10^{-55}	2.40473×10^{-54}
				C2	1.61052×10^{-55}	2.49164×10^{-54}
				Carboxylic Acid	1.62413×10^{-55}	2.50838×10^{-54}
Pyruvate	6	2.47092×10^{-52}	3.25271×10^{-51}	Methyl	2.81494×10^{-52}	3.70508×10^{-51}
				C2	2.92504×10^{-52}	3.85147×10^{-51}
				Carboxylate	2.95373×10^{-52}	3.88193×10^{-51}
Pyruvate	8	1.93272×10^{-65}	7.01755×10^{-64}	Methyl	2.20140×10^{-65}	7.99402×10^{-64}
				C2	2.28601×10^{-65}	8.30790×10^{-64}
				Carboxylate	2.30922×10^{-65}	8.37321×10^{-64}
α-Ketoglutaric Acid	9	7.74812×10^{-84}	2.60672×10^{-82}	$-C(O)^{13}COOH$	9.23382×10^{-84}	3.10272×10^{-82}
				$-^{13}C(O)COOH$	9.14008×10^{-84}	3.07668×10^{-82}
				$-CH_2{}^{13}COOH$	9.28701×10^{-84}	3.11433×10^{-82}
α-Ketoglutarate, α-Keto Moiety Dep. ($-C(O)C(O)O^-$)	9	5.08207×10^{-81}	2.76222×10^{-79}	$-C(O)^{13}COO^-$	6.07198×10^{-81}	3.29494×10^{-79}
				$-^{13}C(O)COO^-$	6.01137×10^{-81}	3.26658×10^{-79}
				$-CH_2{}^{13}COOH$	6.08189×10^{-81}	3.30082×10^{-79}
α-Ketoglutarate, Glutarate Moiety Dep. ($-CH_2C(O)O^-$)	9	3.91551×10^{-80}	6.71130×10^{-79}	$-C(O)^{13}COOH$	4.67645×10^{-80}	8.00102×10^{-79}
				$-^{13}C(O)COOH$	4.62461×10^{-80}	7.93247×10^{-79}
				$-CH_2{}^{13}COO^-$	4.68027×10^{-80}	8.00338×10^{-79}
α-Ketoglutarate, Doubly Deprotonated	9	1.07394×10^{-77}	7.12808×10^{-76}	$-C(O)^{13}COO^-$	1.27869×10^{-77}	8.45961×10^{-76}
				$-^{13}C(O)COO^-$	1.26541×10^{-77}	8.39895×10^{-76}
				$-CH_2{}^{13}COO^-$	1.28365×10^{-77}	8.50191×10^{-76}

[a] "l" represents values for which all atoms are isotopically light and "h" denotes the presence of ^{13}C at the given carbon.

Discussion of β Values for Glutamic Acid and α-Ketoglutaric Acid.

Glutamic acid and its related species are modeled with 8 explicit H_2O molecules. Neutral glutamic acid is modeled as non-charge separated (NCS) and as a zwitterion with the positive charge at the N-terminus and the negative charge at either the C-terminus or the carboxylate of the side chain. All forms and derivatives of glutamic acid are modeled with all isotopically normal atoms and with ^{13}C at either the C-terminus, the C2 position, or the carboxylic acid/carboxylate of the side chain. All glutamic acid-related compounds have C-terminus and side chain β_{aq} values that are very similar to those for the C-terminus of alanine with the largest β_{aq} value 1.1967 for NCS zwitterionic glutamic acid with the negative charge on the side chain and the smallest β_{aq} value 1.1929 for doubly deprotonated glutamate. Additionally, the C2 position of all glutamic acid-related compounds have β_{aq} values that are very similar to those of the C2 position of alanine and its derivatives with the largest β_{aq} value 1.1742 for zwitterionic glutamic acid with the negative charge on the side chain and the smallest β_{aq} value 1.1717 for zwitterionic glutamic acid with the negative charge at the C-terminus. ^{13}C substitution at the C-terminus is the most favorable site for non-charge separated glutamic acid, the zwitterionic glutamic acid with the negative charge at the side chain, glutamate deprotonated at the C-terminus, and doubly deprotonated glutamate by 0.7, 4.6, 0.7, and 0.8 ‰, respectively. ^{13}C substitution at the side chain is the most favorable site for the zwitterionic glutamic acid with the negative charge at the C-terminus and glutamate deprotonated at the side chain by 2.5 and 1.8 ‰, respectively. The zwitterionic form of the glutamate anion has similar β values to the glutamate anions with NCS backbones. The differences between β_{aq} values for the zwitterionic glutamate anion vs the anions with NCS backbones are less than 0.5 ‰. The only exception is for ^{13}C substitution of the side chain carboxylic acid for the NCS glutamate anion deprotonated at the C-terminus, which is ~ 4 ‰ larger than the value for ^{13}C substitution in the zwitterionic glutamate anion. Thus, the zwitterionic backbone of glutamate makes only very minor differences in β. For gas phase optimized structures, the values for zwitterionic glutamate anion and glutamate anion deprotonated at the side chain with a NCS backbone are also very similar, with the largest difference less than 2 ‰ for ^{13}C substitution at the C2 position.

α-Ketoglutaric acid and its related species are modeled with 9 explicit H_2O molecules. The β_{aq} values of α-ketoglutaric acid and its derivatives for its ^{13}C substitution at the α-keto moiety carboxylic acid/carboxylate site and the glutarate moiety carboxylic acid/carboxylate site are in good agreement with similar ^{13}C sites in alanine, glutamic acid, and pyruvic acid. Substitution of ^{13}C at the carboxylic acid/carboxylate of the α-keto moiety yields a range of β_{aq} values from 1.1868 for doubly deprotonated α-ketoglutarate to 1.1929 for α-ketoglutarate deprotonated at the α-keto moiety. Substitution of ^{13}C at the carboxylic acid/carboxylate of the glutarate moiety yields a range of β_{aq} values from 1.1925 for α-ketoglutarate deprotonated at the glutarate moiety to 1.1950 for α-ketoglutarate deprotonated at the α-keto moiety. The β_{aq} values for C2 site ^{13}C substitution range from 1.1783 for doubly deprotonated α-ketoglutarate to 1.1826 for α-ketoglutarate deprotonated at the α-keto moiety. The average β_{aq} for the C2 site of α-ketoglutaric acid and its derivatives is 1.1808, which is 6.6 ‰ higher than the average β_{aq} of ^{13}C at the C2 position of alanine, indicating that this site is much more similar to the C2 position of pyruvic acid than that of alanine or glutamic acid.

Table S4. Reduced Partition Function Ratios at Various Carbon Atoms at 298 K for Glutamic Acid and α-Ketoglutaric Acid.

Species	# of H_2O Molecules	^{13}C Site	$\beta_{gas\ opt}$	$\beta_{aq\ opt}$	$\Delta\beta$ (‰) [a]
Glutamic Acid	8	Side Chain	1.2009	1.1954	5.416
		C2	1.1731	1.1730	0.151
		C-terminus	1.1989	1.1961	2.726
Glutamic Acid, Zwitterion (C-terminus)	8	Side Chain	1.2000	1.1961	3.906
		C2	1.1667	1.1717	-4.984
		C-terminus	1.1961	1.1936	2.538
Glutamic Acid, Zwitterion (Side Chain)	8	Side Chain	1.1981	1.1921	5.949
		C2	1.1721	1.1742	-2.060
		C-terminus	1.1998	1.1967	3.136
Glutamate, Zwitterion	8	Side Chain	1.1976	1.1918	5.862
		C2	1.1701	1.1727	-2.693
		C-terminus	1.1957	1.1931	2.619
Glutamate, C-terminus Deprotonation	8	Side Chain	1.1999	1.1957	4.166
		C2	1.1723	1.1724	-0.094
		C-terminus	1.1981	1.1935	4.643
Glutamate, Side Chain Deprotonation	8	Side Chain	1.1964	1.1911	5.367
		C2	1.1714	1.1727	-1.337
		C-terminus	1.1971	1.1949	2.265
Glutamate, Doubly Deprotonated	8	Side Chain	1.1948	1.1921	2.651
		C2	1.1685	1.1725	-4.022
		C-terminus	1.1950	1.1929	2.136
α-Ketoglutaric Acid	9	$-C(O)^{13}COOH$	1.1917	1.1903	1.473
		$-^{13}C(O)COOH$	1.1797	1.1803	-0.638
		$-CH_2{}^{13}COOH$	1.1986	1.1947	3.884
α-Ketoglutarate, α-Keto Moiety Dep. ($-C(O)C(O)O^-$)	9	$-C(O)^{13}COO^-$	1.1948	1.1929	1.924
		$-^{13}C(O)COO^-$	1.1829	1.1826	0.265
		$-CH_2{}^{13}COOH$	1.1967	1.1950	1.743
α-Ketoglutarate, Glutarate Moiety Dep. ($-CH_2C(O)O^-$)	9	$-C(O)^{13}COOH$	1.1943	1.1922	2.167
		$-^{13}C(O)COOH$	1.1811	1.1820	-0.857
		$-CH_2{}^{13}COO^-$	1.1953	1.1925	2.792
α-Ketoglutarate, Doubly Deprotonated	9	$-C(O)^{13}COO^-$	1.1907	1.1868	3.852
		$-^{13}C(O)COO^-$	1.1783	1.1783	-0.003
		$-CH_2{}^{13}COO^-$	1.1953	1.1927	2.532

[a] $\Delta\beta$ is calculated as $(\beta_{gas} - \beta_{aq})*1000$.

Table S5. Estimated Free Energy (A), ΔA, and ϵ_{ZPE} in kcal/mol for ^{12}C and ^{13}C Bonds with N, O, and H in kcal/mol at 310 K.

	A ^{12}C			A ^{13}C		
	ZPE	Thermal	Total	ZPE	Thermal	Total
C-N	1.57	-3.76×10^{-3}	1.57	1.54	-4.18×10^{-3}	1.54
C=O	2.50	-1.84×10^{-4}	2.50	2.45	-2.20×10^{-4}	2.45
C-H	4.29	-5.57×10^{-7}	4.29	4.28	-5.80×10^{-7}	4.28
	$^{12}C{=}O + {}^{13}CHNH_2 \leftrightarrows {}^{13}C{=}O + {}^{12}CHNH_2$					
	ΔA	K	ϵ_{ZPE} (‰)			
ZPE + Therm	-9.59×10^{-3}	-0.9845	15.6			
ZPE Only	-9.98×10^{-3}	-0.9839	16.2			

Gas Phase Optimized Geometries at the MP2/aD Level

Non-Charge Separated Neutral Alanine with 7 H_2O

C	-1.446039	-0.919471	-1.942966
C	-0.430739	-0.947200	-0.789574
C	0.423384	0.333167	-0.834761
O	-0.039277	1.467105	-0.656027
O	1.732050	0.198424	-1.060605
N	-1.105016	-1.124169	0.498990
H	-2.132069	-0.075443	-1.832076
H	-2.034784	-1.838987	-1.924478
H	-0.941062	-0.835210	-2.910504
H	0.239544	-1.800595	-0.931208
H	2.080000	-0.729976	-0.828430
H	-1.760092	-0.363643	0.688972
H	-0.422993	-1.163507	1.255080
O	-2.578420	2.655826	-0.566614
H	-2.814925	3.006876	-1.435185
H	-1.676362	2.279369	-0.650570
O	1.713019	-0.830068	2.194868
H	1.727448	-1.060831	3.133561
H	1.703259	0.156430	2.144228
O	-3.896942	-2.313669	0.344548
H	-4.153371	-1.382669	0.455960
H	-2.929565	-2.279910	0.456850
O	4.630627	0.380916	-0.702924
H	5.314448	0.593203	-1.352535
H	3.809091	0.790430	-1.022661
O	2.945601	-1.854498	-0.091482
H	2.658287	-1.676543	0.832127
H	3.811604	-1.412312	-0.184151
O	1.518907	1.904943	1.779485
H	1.000058	2.016432	0.958008
H	2.318014	2.437388	1.664004

O	-3.744562	0.640716	0.917744
H	-4.095405	0.990968	1.747293
H	-3.493676	1.421172	0.374658

Zwitterionic Neutral Alanine with 7 H_2O

C	-0.967262	-1.638534	-2.019039
C	0.152631	-1.156066	-1.102136
C	0.556821	0.338237	-1.293519
O	-0.373201	1.179219	-1.429634
O	1.798747	0.604351	-1.202377
N	-0.255934	-1.264945	0.348451
H	-1.936626	-1.636556	-1.517616
H	-0.758402	-2.651051	-2.381465
H	-1.033208	-0.978096	-2.887821
H	1.041562	-1.777463	-1.217698
H	-0.989969	-0.560909	0.592791
H	0.577201	-1.110695	0.978261
O	-3.096366	1.087865	-1.308406
H	-3.535932	1.872891	-1.660738
H	-2.134354	1.176226	-1.514025
O	3.470898	-1.389377	-0.475996
H	4.377996	-1.355844	-0.805665
H	2.974322	-0.632960	-0.883674
O	-2.348714	0.440321	1.274787
H	-2.854683	0.688815	0.466952
H	-1.812392	1.244398	1.474288
O	-2.381056	-2.298912	1.907622
H	-2.815270	-2.725085	2.657222
H	-2.603680	-1.346720	1.950292
O	2.043988	-0.812014	1.841684
H	2.735629	-1.133724	1.222506
H	2.183002	0.155757	1.869567
O	2.219673	1.986875	1.105125
H	2.935424	2.635481	1.147830
H	2.161550	1.680446	0.164304
O	-0.616537	2.604645	1.076226
H	-0.542748	2.420934	0.118802
H	0.311223	2.570881	1.376402
H	-0.681711	-2.167723	0.586230

Deprotonated Alanine with 7 H_2O

C	2.130144	-0.227282	0.045222
C	2.710811	-0.186818	-1.378437
N	2.039187	-1.628151	0.509335
H	3.692493	-0.668781	-1.395613
H	2.050011	-0.716157	-2.075140

H	2.812343	0.846862	-1.717337
C	0.776819	0.524507	0.067357
H	2.812518	0.307891	0.712128
H	1.735891	-1.628387	1.482831
H	1.264467	-2.065473	0.007161
O	0.830064	1.797461	0.072585
O	-0.284044	-0.168655	0.051623
O	-4.062790	-1.173682	1.522502
H	-3.724168	-0.286567	1.290968
H	-3.324235	-1.762588	1.268239
O	-2.759265	0.983739	0.021701
H	-2.574615	1.944805	0.009810
H	-1.847121	0.592301	0.044834
O	-1.328719	3.450615	-0.060450
H	-1.235314	3.844736	-0.937928
H	-0.544839	2.841205	0.024317
O	-4.122202	-1.033486	-1.443970
H	-4.546425	-1.253736	-0.594065
H	-3.678104	-0.187655	-1.221755
O	3.029988	3.437734	0.434652
H	2.282619	2.815727	0.263720
H	2.689841	4.034754	1.113769
O	4.398113	-3.255575	0.267224
H	4.131158	-3.934472	-0.366174
H	3.601187	-2.672985	0.361922
O	-1.924677	-2.463466	-0.052341
H	-2.536619	-2.161901	-0.752696
H	-1.253780	-1.752443	0.002589

Non-Charge Separated Neutral Glutamic Acid with 8 H_2O

C	0.041782	0.261655	-0.032567
C	-1.094412	1.125217	-0.602165
C	-1.860455	1.860957	0.486014
O	-1.302206	2.282333	1.510161
O	-3.160299	2.051831	0.317726
C	0.587111	-0.736794	-1.074834
C	1.964705	-1.274802	-0.631044
O	2.167454	-2.450673	-0.351226
O	2.963264	-0.386214	-0.593924
N	-0.395804	-1.805379	-1.302764
H	-0.321208	-0.316552	0.819270
H	0.841125	0.902186	0.335952
H	-1.783293	0.521991	-1.189881
H	-0.686513	1.890279	-1.275262
H	-3.522753	1.592973	-0.499157
H	0.765481	-0.206942	-2.020582

H	2.691403	0.571078	-0.783415
H	-0.698945	-2.169618	-0.388696
H	0.056506	-2.579321	-1.787185
O	-2.943636	-1.485224	-2.421701
H	-3.401974	-2.288284	-2.136205
H	-2.007859	-1.570592	-2.071138
O	2.722530	2.180036	-0.955124
H	3.683786	2.274392	-0.802565
H	2.264383	2.689089	-0.247778
O	-4.221861	0.779377	-1.744592
H	-4.581725	1.213911	-2.528747
H	-3.803237	-0.074149	-2.042179
O	0.972618	-4.128574	1.609040
H	1.447240	-3.648340	0.901618
H	1.628192	-4.311619	2.294748
O	-1.372548	-2.559661	1.455935
H	-0.646354	-3.141297	1.759875
H	-1.480129	-1.858070	2.124991
O	1.247200	3.362340	1.095115
H	1.263639	4.273460	1.415682
H	0.368100	2.994916	1.339265
O	-1.703543	-0.181199	3.190106
H	-1.527853	0.707936	2.832168
H	-2.533578	-0.102256	3.680165
O	5.352894	1.312085	-0.393642
H	4.981120	0.416645	-0.320631
H	6.167756	1.226775	-0.906380

Zwitterionic Neutral Glutamic Acid with 8 H_2O

C	0.223026	0.292850	-0.125073
C	-0.617556	1.303222	-0.931859
C	-1.697649	1.861006	-0.027132
O	-1.433471	2.442152	1.032488
O	-2.976922	1.665011	-0.356871
C	1.219421	-0.483077	-0.981653
C	1.987240	-1.520118	-0.105703
O	1.828571	-2.738977	-0.476846
O	2.618104	-1.082122	0.884470
N	0.526660	-1.334250	-2.018714
H	-0.430839	-0.425703	0.396183
H	0.805121	0.820923	0.642852
H	-1.075427	0.842438	-1.820532
H	0.039692	2.121704	-1.265297
H	-3.059841	1.109907	-1.177382
H	1.911377	0.205047	-1.487251
H	0.997432	-2.273810	-1.786901

H	0.673539	-1.020973	-2.978389
O	-2.096458	-2.099795	-1.130091
H	-2.033862	-2.064373	-0.115906
H	-2.331547	-3.018034	-1.321579
O	2.371817	2.585605	-1.209225
H	3.159439	2.086290	-0.918633
H	2.049781	2.983423	-0.379204
O	-3.272091	-0.027779	-2.419593
H	-4.183804	-0.136687	-2.719826
H	-3.030469	-0.872604	-1.972594
O	0.615237	-3.072874	2.091350
H	1.059018	-3.286741	1.246855
H	1.230457	-2.423237	2.465494
O	-1.863070	-2.053717	1.441411
H	-0.996315	-2.404249	1.759614
H	-2.035617	-1.236373	1.954245
O	1.198091	3.395380	1.280412
H	1.204961	4.284870	1.654387
H	0.258102	3.125912	1.285441
O	-2.283636	0.347194	2.822573
H	-2.089203	1.185672	2.365215
H	-3.136352	0.494967	3.250665
O	4.319239	0.753322	-0.284537
H	3.793470	0.149408	0.285283
H	5.127082	0.927405	0.212747
H	-0.482990	-1.465919	-1.820306

Zwitterionic Glutamate Anion with 8 H_2O

C	-0.619592	0.238645	0.319020
C	-1.248529	-1.018433	0.920490
C	-0.062290	1.260124	1.347433
N	-0.163870	-1.889187	1.485501
C	-2.003810	-1.763924	-0.213123
H	-1.940640	-0.763119	1.737185
H	-1.389703	0.712115	-0.302943
H	0.177694	-0.089122	-0.368622
C	1.396946	1.564492	1.007610
H	-0.649845	2.188604	1.285231
H	-0.142641	0.877242	2.376636
H	0.397989	-1.424387	2.238635
H	0.505289	-2.208785	0.721462
H	-0.569245	-2.744301	1.873996
O	-3.205805	-1.407855	-0.383270
O	-1.328255	-2.592865	-0.900164
O	1.609757	2.217914	-0.072004
O	2.318519	1.104662	1.760177

O	1.379999	-2.971645	-0.454162
H	0.508760	-3.022513	-0.900795
H	1.907525	-2.356307	-1.026138
O	2.574899	-1.182999	-2.110984
H	1.738136	-0.828632	-2.475464
H	3.036567	-0.419486	-1.700410
O	3.912839	0.941252	-0.804062
H	4.045862	0.638371	0.107254
H	3.161033	1.563391	-0.651492
O	1.477087	-0.702175	3.418588
H	2.259242	-1.207212	3.674185
H	1.841103	0.044941	2.831745
O	-0.076668	-0.510882	-2.942517
H	-0.295378	0.385128	-2.619780
H	-0.655577	-1.115142	-2.445721
O	-2.589350	3.217894	-0.327334
H	-2.999399	2.407474	0.030075
H	-1.888849	2.895673	-0.920528
O	-0.277164	2.238380	-1.952875
H	0.002806	2.892748	-2.605378
H	0.427058	2.279603	-1.241673
O	-3.871823	0.874818	0.844101
H	-4.818284	1.008493	0.711237
H	-3.681051	0.012098	0.380251

Glutamate Anion (C-terminus Deprotonation) with 8 H_2O

C	-0.796024	1.099225	-0.673373
C	-2.004942	0.478119	-1.423723
C	-3.088954	-0.010905	-0.479260
O	-3.901262	0.777735	0.030641
O	-3.148960	-1.296211	-0.159628
C	0.032969	0.075058	0.150601
C	1.543030	0.349640	-0.038621
O	2.166140	0.929629	0.895062
O	2.035669	-0.032692	-1.154588
N	-0.278757	-0.020473	1.590868
H	-1.134625	1.913386	-0.025043
H	-0.153164	1.541256	-1.439542
H	-1.652326	-0.331191	-2.067974
H	-2.460081	1.251285	-2.048255
H	-0.135306	-0.904870	-0.293340
H	-1.222200	0.290792	1.826528
H	0.390297	0.576894	2.080053
O	-0.209133	-2.775253	1.744409
H	0.683620	-3.071260	1.968417
H	-0.195394	-1.772239	1.840620

O	0.690789	-1.921984	-2.480583
H	1.210251	-1.192081	-2.024784
H	1.343641	-2.448807	-2.959381
O	-1.296458	-2.976976	-0.826344
H	-0.581765	-2.715105	-1.454297
H	-0.862309	-3.075814	0.055377
O	4.821702	0.277960	-1.383691
H	3.843779	0.152403	-1.393445
H	4.921365	1.179184	-1.023458
O	4.586089	2.478530	0.610146
H	3.665120	2.143264	0.645113
H	5.054282	1.815674	1.147272
O	-4.250564	3.398757	-1.028735
H	-4.186683	2.497755	-0.648739
H	-3.792794	3.966401	-0.394876
O	-3.337917	0.197094	2.782119
H	-3.776257	0.413563	1.936071
H	-3.303588	-0.769928	2.790256
O	4.809089	-0.410726	1.437105
H	3.876902	-0.127118	1.472996
H	4.984720	-0.421404	0.472642
H	-2.404140	-1.882454	-0.539344

Glutamate Anion (Side Chain Deprotonation) with 8 H_2O

C	-1.229556	-0.126294	-1.293295
C	0.147460	0.291267	-1.835060
C	1.395289	-0.463232	-1.346102
O	1.308185	-1.697007	-1.057987
O	2.472762	0.217284	-1.311352
C	-1.525147	0.265109	0.180482
C	-3.053459	0.379001	0.334961
O	-3.761550	-0.543513	0.717063
O	-3.595806	1.563883	-0.001786
N	-0.935046	-0.664583	1.155312
H	-1.385237	-1.201813	-1.412712
H	-1.981082	0.364916	-1.921855
H	0.313827	1.359283	-1.669870
H	0.138377	0.149520	-2.924196
H	-1.107147	1.262987	0.358248
H	-2.906351	2.266142	-0.150002
H	-0.903893	-1.611074	0.772477
H	-1.538293	-0.717139	1.974029
O	1.638712	-0.001772	2.312382
H	2.212400	-0.751625	2.029689
H	0.756259	-0.226412	1.927599
O	-1.975126	3.714460	-0.238348

H	-2.347461	4.375503	0.360689
H	-0.986416	3.782440	-0.120888
O	2.364897	2.094893	0.697604
H	2.132113	1.425331	1.395443
H	2.432103	1.540081	-0.116194
O	-3.457959	-3.488163	0.004748
H	-3.614710	-2.573971	0.296874
H	-2.497218	-3.541223	-0.150444
O	-0.516424	-3.483243	-0.275993
H	0.003891	-4.079352	0.278960
H	0.141716	-2.854983	-0.677859
O	0.655636	4.017701	0.157363
H	1.286528	3.272966	0.423685
H	1.139305	4.536232	-0.498882
O	3.106839	-2.132142	1.098625
H	3.919702	-1.684344	0.787190
H	2.524410	-2.096607	0.305727
O	4.927918	-0.343410	-0.246747
H	4.083560	-0.220490	-0.752633
H	4.976733	0.448830	0.307245

Doubly Deprotonated Glutamate with 8 H_2O

C	-0.083781	-0.766764	0.128773
C	-1.457430	-0.716428	0.843053
C	-2.643292	-0.733216	-0.136051
O	-2.876793	0.354408	-0.771828
O	-3.319672	-1.802951	-0.260383
C	1.050346	-0.098090	0.927969
C	2.441350	-0.419503	0.301671
O	3.122094	0.554206	-0.154404
O	2.780036	-1.641819	0.331934
N	0.807972	1.360169	1.066746
H	-0.153820	-0.266867	-0.843293
H	0.203741	-1.803187	-0.063552
H	-1.530648	0.215735	1.409039
H	-1.545499	-1.552007	1.543487
H	1.076719	-0.543981	1.931557
H	0.368873	1.694810	0.204447
H	1.729324	1.801269	1.065566
O	-0.978556	2.415065	2.863225
H	-1.277334	1.692196	3.430946
H	-0.267004	2.005934	2.266608
O	-2.816714	-4.150170	1.055417
H	-1.912980	-4.331692	0.765348
H	-3.038853	-3.291173	0.605968
O	5.056977	-2.516220	-0.766011

H	4.213450	-2.199806	-0.318509
H	4.945188	-2.211510	-1.677043
O	1.992311	2.541980	-2.079480
H	2.382557	1.884173	-1.469301
H	1.027937	2.469383	-1.960960
O	-0.979828	2.358443	-1.482760
H	-1.444915	2.954575	-0.865248
H	-1.544356	1.554277	-1.427207
O	-5.235120	-0.791163	-2.126039
H	-4.777643	-1.424979	-1.534263
H	-4.640798	-0.031227	-1.985844
O	-2.861955	2.934057	0.677935
H	-3.010340	2.040020	0.303891
H	-2.291311	2.796884	1.462457
O	5.992859	0.210028	-0.085927
H	5.043090	0.460539	-0.117724
H	5.940545	-0.757442	-0.199503

Pyruvic Acid with 6 H_2O

C	-2.271427	-0.103087	1.651848
C	-1.453086	-0.288364	0.408465
O	-0.746571	-1.263812	0.181419
C	-1.570518	0.807000	-0.685781
O	-0.466730	1.155527	-1.317789
O	-2.671844	1.274464	-0.953897
H	-2.034422	-0.888971	2.369825
H	-3.338374	-0.122581	1.398295
H	-2.070862	0.884220	2.083028
O	-5.149934	0.278080	0.040561
H	-4.418176	0.726221	-0.424750
H	-5.937816	0.814970	-0.113691
O	0.920209	-3.516959	0.274140
H	0.221545	-2.836322	0.329991
H	0.478385	-4.355400	0.086556
O	2.871287	1.332851	2.044417
H	2.398704	0.766532	1.399970
H	3.373205	0.736181	2.616114
O	2.827564	-2.071997	-1.063195
H	2.942006	-2.353557	-1.980526
H	2.216971	-2.721733	-0.640736
O	3.746126	2.410256	-0.375604
H	3.658118	2.286790	0.593787
H	3.584407	3.346337	-0.554189
O	1.864654	0.388387	-0.455613
H	2.233442	-0.489140	-0.741139
H	2.519402	1.081608	-0.706233

H	0.385572	0.737165	-0.959012

Pyruvate with 6 H_2O

C	2.379581	0.851414	0.063224
C	1.116176	0.074887	-0.195784
O	1.091532	-0.996235	-0.817321
C	-0.199522	0.649642	0.353490
O	-0.826547	1.428991	-0.419180
O	-0.524584	0.250151	1.509084
H	3.241714	0.342900	-0.372460
H	2.505838	0.956545	1.147498
H	2.266628	1.856214	-0.360836
O	1.396762	0.179616	3.518992
H	0.711407	0.085633	2.817362
H	1.029662	0.841501	4.119365
O	3.510950	-2.407741	-1.429611
H	2.678480	-1.902370	-1.323111
H	3.445963	-3.113872	-0.773140
O	-1.673949	-2.227646	-1.113694
H	-0.756427	-1.900772	-1.066251
H	-2.025455	-2.139671	-0.202862
O	-2.985250	-1.226816	1.288393
H	-2.212467	-0.698996	1.575042
H	-3.385056	-0.672306	0.587388
O	0.578421	3.508912	-1.626832
H	0.186540	4.253269	-1.151699
H	0.058150	2.730478	-1.321488
O	-3.326557	0.201720	-1.222624
H	-2.844565	-0.599393	-1.511287
H	-2.604040	0.817561	-0.986759

Pyruvate with 8 H_2O

C	0.286660	-1.559695	1.552683
C	0.285989	-0.113680	1.136829
O	-0.420179	0.745776	1.686841
C	1.204221	0.281333	-0.029279
O	0.928641	-0.255556	-1.152278
O	2.134378	1.100762	0.229060
H	-0.326603	-1.694920	2.453506
H	1.329972	-1.872111	1.728379
H	-0.108844	-2.176315	0.730567
O	3.868505	-1.004780	1.408666
H	3.392309	-0.158335	1.416252
H	4.089655	-1.074451	0.462697
O	-3.203120	-0.175666	1.903655
H	-2.292599	0.121665	2.065759

H	-3.088994	-0.942367	1.304505
O	-3.061764	-1.932341	-0.337806
H	-3.285463	-1.072704	-0.754035
H	-2.222117	-2.182392	-0.769089
O	0.122398	3.258349	0.315407
H	-0.208376	2.581776	0.936110
H	1.038420	2.952194	0.200049
O	3.939811	-0.287689	-1.497080
H	3.486941	0.440611	-1.025415
H	3.173431	-0.711083	-1.913101
O	-3.577240	0.791889	-0.891588
H	-3.513490	0.812763	0.080450
H	-2.739505	1.196806	-1.203339
O	-0.554282	-2.476834	-1.637163
H	-0.697975	-2.477598	-2.591502
H	-0.019107	-1.661594	-1.471667
O	-1.111856	1.825604	-1.848481
H	-0.728176	2.453698	-1.202289
H	-0.463029	1.100498	-1.843101

α-Ketoglutaric Acid with 9 H_2O

C	0.673519	-1.301486	-1.351924
C	-0.646678	-0.584649	-1.649084
C	1.133457	-1.622238	0.067285
C	-0.814066	0.885364	-1.316494
H	-1.487015	-1.115005	-1.204042
H	-0.784338	-0.622002	-2.737742
H	0.630852	-2.279128	-1.839349
H	1.508266	-0.777839	-1.830480
C	0.572607	-0.931742	1.345615
O	2.087338	-2.369717	0.231793
O	0.228438	1.704179	-1.216149
O	-1.951377	1.381447	-1.234710
O	-0.473563	-0.135970	1.104655
O	1.123293	-1.046907	2.426499
H	1.118861	1.308412	-0.926499
H	-0.637120	0.480662	1.869697
O	2.517261	1.181555	-0.213246
H	3.256636	0.546535	-0.341134
H	2.501401	1.446994	0.737671
O	-0.739088	2.055598	2.640234
H	-1.230768	2.201935	3.460454
H	-1.159285	2.635476	1.941387
O	2.173221	1.721567	2.500459
H	2.124535	0.814168	2.848141
H	1.266839	2.063142	2.626744

O	4.364606	-0.883617	-0.576588
H	5.191185	-0.969865	-0.082587
H	3.809589	-1.644580	-0.319391
O	-1.821795	3.455251	0.627580
H	-1.255645	4.154489	0.271404
H	-1.928227	2.809632	-0.111231
O	1.207209	0.982726	-3.982384
H	1.116950	1.718940	-3.358771
H	1.980527	1.187397	-4.524914
O	-1.066704	-3.146225	0.401132
H	-0.902755	-4.024236	0.769500
H	-2.018812	-2.949963	0.562654
O	-3.742354	-2.448909	0.693481
H	-4.097191	-2.234953	1.566658
H	-3.943272	-1.666845	0.126939
O	-4.202491	-0.197204	-0.832588
H	-4.772543	-0.171722	-1.612321
H	-3.433655	0.386671	-1.026520

α-Ketoglutarate (α-Keto Moiety Deprotonation) with 9 H_2O

C	1.323152	-1.600478	-0.436471
C	1.212046	-0.466420	-1.490074
C	0.752322	-1.260959	0.925188
C	1.913151	0.822655	-1.074771
H	1.691249	-0.814579	-2.405398
H	0.160607	-0.258779	-1.705189
H	0.734059	-2.440608	-0.827108
H	2.365531	-1.904064	-0.320468
C	-0.715308	-0.792367	0.988468
O	1.402258	-1.348923	1.967703
O	1.270118	1.614811	-0.209400
O	3.022807	1.141506	-1.503846
O	-0.885531	0.459194	0.701371
O	-1.586617	-1.628249	1.278943
O	-3.823079	-1.735007	-2.037070
H	-4.208675	-1.856157	-1.143304
H	-3.634354	-0.779306	-2.040104
O	-3.352350	0.910907	-0.793949
H	-2.508329	0.746749	-0.326672
H	-3.508209	1.873145	-0.690707
O	-3.363567	3.681018	-0.063830
H	-2.732100	4.195328	-0.584764
H	-2.889675	3.447536	0.767442
O	-4.447773	-1.317366	0.738605
H	-4.365103	-0.407055	0.395486
H	-3.556354	-1.493583	1.099479

O	-1.963787	2.620300	2.091921
H	-1.242074	2.970188	2.630507
H	-1.634276	1.770565	1.721288
O	-1.476624	-3.225797	-1.305549
H	-2.232424	-2.765688	-1.730374
H	-1.611366	-3.049767	-0.360034
O	4.842603	-1.262255	-0.861482
H	4.471045	-0.415881	-1.159716
H	4.745677	-1.264133	0.110355
O	4.232542	-1.589005	1.987617
H	3.254912	-1.513983	2.037789
H	4.432539	-2.498728	2.245791
O	3.470090	3.942575	-0.750397
H	2.713322	3.916016	-0.148726
H	3.504608	3.025399	-1.083260
H	0.408485	1.193119	0.118549

α-Ketoglutarate (Glutarate Moiety Deprotonation) with 9 H_2O

C	-0.866835	-2.316812	0.028661
C	0.404410	-2.058627	0.860088
C	0.635919	-0.590474	1.258720
O	1.847464	-0.179174	1.275865
O	-0.374046	0.119849	1.551609
C	-1.088916	-1.411235	-1.172413
O	-2.190976	-1.207454	-1.665475
C	0.156944	-0.778303	-1.827664
O	1.121200	-1.485364	-2.120576
O	0.063144	0.525888	-1.999339
H	-1.776821	-2.255311	0.628374
H	-0.829346	-3.340842	-0.367027
H	1.292121	-2.428141	0.347271
H	0.319862	-2.627275	1.793601
O	-0.104473	2.981456	2.299041
H	-0.063618	2.005324	2.356993
H	-0.927937	3.115305	1.793136
O	3.575641	-0.555775	-0.929990
H	3.040463	-1.127454	-1.509021
H	3.011222	-0.464092	-0.127063
O	4.141184	-1.967268	1.887546
H	3.351028	-1.396535	1.927691
H	4.496307	-1.788243	1.003572
O	2.217839	1.724491	-1.866260
H	2.903059	1.032290	-1.710269
H	2.150353	2.179914	-0.971434
O	-2.124783	2.420770	-2.249316
H	-1.548082	1.633741	-2.300191

H	-1.544941	3.163869	-2.466754
O	-3.229090	-0.120036	2.162006
H	-2.260776	-0.250687	2.146394
H	-3.325844	0.737021	1.706867
O	2.147984	2.528687	0.667112
H	2.117732	1.610379	1.027553
H	1.405612	2.965897	1.139293
O	-4.385407	-2.077916	0.379062
H	-4.095329	-1.425757	1.050549
H	-3.909637	-1.817112	-0.425966
O	-2.250300	2.123270	0.589078
H	-1.560753	1.432603	0.631799
H	-2.370785	2.304686	-0.366405
H	1.033928	1.021729	-2.036217

Doubly Deprotonated α-Ketoglutarate with 9 H_2O

C	1.224819	-0.605600	-1.781267
C	-0.248812	-0.231274	-1.973090
C	-0.755855	0.976637	-1.172379
O	-2.021269	1.056901	-1.012604
O	0.086978	1.817048	-0.728264
C	1.719503	-0.980479	-0.386242
O	2.937465	-1.072134	-0.185136
C	0.726094	-1.331301	0.752724
O	-0.103305	-2.240981	0.469177
O	0.855185	-0.698631	1.838959
H	1.891474	0.187480	-2.131501
H	1.443745	-1.486017	-2.401754
H	-0.894519	-1.082044	-1.761177
H	-0.406424	0.014003	-3.032115
O	-1.702334	-3.596238	-1.609524
H	-2.424352	-2.939898	-1.513455
H	-1.059250	-3.306352	-0.935380
O	-3.565057	-1.442611	-0.962779
H	-3.400424	-1.584861	-0.002141
H	-3.120153	-0.586187	-1.137298
O	-2.683622	-1.666224	1.741641
H	-1.764833	-1.912390	1.499397
H	-2.644437	-0.706675	1.939604
O	-3.667384	3.374974	-0.245970
H	-3.077431	2.755165	-0.721655
H	-3.611057	3.031816	0.661484
O	3.589358	-1.215920	2.739384
H	3.714659	-1.248559	1.774695
H	2.636933	-1.003139	2.775249
O	2.655075	2.744340	-0.562101

H	1.746076	2.405646	-0.756323
H	2.723863	2.647553	0.398958
O	-2.623671	1.260000	1.773341
H	-2.469064	1.170281	0.806640
H	-1.747641	1.567066	2.099599
O	4.598603	0.919089	-1.697370
H	4.007689	1.629902	-1.370973
H	4.224204	0.122411	-1.279628
O	0.109931	2.020095	2.090582
H	0.055996	2.179004	1.123205
H	0.452822	1.100247	2.131410

Aqueous Optimized Geometries at the MP2/aD/COSMO Level

Non-Charge Separated Neutral Alanine with 7 H_2O

C	-0.396232	-1.661078	-0.024725
C	-1.621261	-2.441210	-0.506846
C	0.227204	-0.897818	-1.192628
H	-2.387113	-1.761559	-0.906115
H	-1.334707	-3.154176	-1.296048
H	-2.045607	-2.999933	0.340406
N	-0.749482	-0.703047	1.058418
H	0.341418	-2.365665	0.383174
O	1.559412	-0.956644	-1.348758
O	-0.447052	-0.217959	-1.970072
H	-0.877294	0.232527	0.664311
H	0.044345	-0.611248	1.697372
H	2.010717	-1.415895	-0.567974
O	2.782001	-1.944122	0.739942
H	3.741223	-1.930299	0.600483
H	2.608866	-1.209737	1.382189
O	1.987352	0.083641	2.369386
H	2.580989	0.380126	3.074531
H	1.812860	0.892356	1.822896
O	1.433179	2.238335	0.807546
H	1.815809	2.111244	-0.086495
H	0.477483	2.400315	0.650696
O	-1.293046	2.796106	0.523217
H	-1.428381	3.721344	0.271854
H	-1.878718	2.285187	-0.083406
O	-2.873137	1.125318	-1.024527
H	-2.179837	0.577474	-1.439993
H	-3.217172	0.565637	-0.295009
O	2.645928	1.687439	-1.670129
H	2.281077	2.152668	-2.437754
H	2.296041	0.780571	-1.753110
O	-3.574281	-0.460902	1.261214
H	-3.822142	0.107199	2.006078
H	-2.614604	-0.645874	1.405633

Zwitterionic Neutral Alanine with 7 H_2O

C	0.315545	0.916141	-1.434731
N	-0.091824	-0.527782	-1.326320
C	-0.752766	1.693231	-2.191024
H	-0.936195	-0.644721	-0.724572
H	0.677521	-1.119641	-0.934218
H	-0.318755	-0.904246	-2.253779
C	0.566008	1.420038	0.007232
H	1.268410	0.924108	-1.980493

H	-0.471982	2.755528	-2.232359
H	-0.835903	1.310582	-3.220195
H	-1.728189	1.600960	-1.694729
O	1.755955	1.297865	0.451824
O	-0.419918	1.881215	0.659669
O	2.061405	-2.084189	-0.308296
H	2.021454	-1.854807	0.642225
H	2.755446	-1.472123	-0.637310
O	-2.327449	-0.947953	0.437960
H	-2.804401	-0.093345	0.353929
H	-1.822750	-0.830569	1.275000
O	-3.165750	1.727071	0.324759
H	-3.545960	1.997570	1.173860
H	-2.199884	1.888555	0.427435
O	-0.855818	-0.118629	2.665033
H	0.047226	-0.495271	2.689953
H	-0.716320	0.705929	2.155843
O	3.668597	0.086222	-1.106915
H	4.526238	0.184202	-0.667874
H	3.042553	0.605761	-0.546428
O	1.869093	-0.820725	2.253410
H	2.561667	-0.790921	2.930080
H	1.959052	0.024147	1.758918
O	-2.354767	-3.256715	-1.146262
H	-3.015988	-3.889764	-0.832670
H	-2.443967	-2.497229	-0.536690

Deprotonated Alanine with 7 H_2O

C	-1.791971	-0.088763	-0.251404
C	-1.748780	-0.239309	1.276976
N	-2.107310	-1.393376	-0.857320
H	-2.710784	-0.626672	1.645556
H	-0.951364	-0.946583	1.558770
H	-1.548576	0.729959	1.756574
C	-0.461980	0.536320	-0.706736
H	-2.596269	0.612209	-0.527471
H	-1.384188	-2.066424	-0.591134
H	-2.045325	-1.319600	-1.875555
O	-0.351654	1.802380	-0.575171
O	0.457633	-0.232206	-1.144049
O	1.177667	-2.550362	0.211308
H	1.439466	-2.088185	1.034486
H	0.814121	-1.809365	-0.322750
O	2.102324	-0.732003	2.217565
H	2.875412	-0.975841	2.747316
H	2.475048	-0.216555	1.465099

O	2.876959	0.545703	-0.134220
H	2.824898	1.523724	-0.132846
H	2.029793	0.296443	-0.581803
O	1.999792	3.208329	-0.416613
H	1.904879	3.753606	0.378121
H	1.136884	2.730148	-0.487995
O	3.819504	-2.104791	-0.831662
H	3.790822	-1.144705	-0.672414
H	2.936698	-2.384018	-0.512073
O	-2.341615	3.309813	0.583072
H	-2.282766	4.166198	0.136193
H	-1.647858	2.763460	0.143491
O	-4.715221	-2.069505	-0.108857
H	-4.725569	-2.056770	0.859065
H	-3.770881	-1.855754	-0.343387

Non-Charge Separated Neutral Glutamic Acid with 8 H_2O

C	-0.069377	0.059280	-0.029988
C	0.253216	-1.200508	-0.850911
C	-0.653670	1.161728	-0.939748
C	0.902278	-2.251394	0.023471
H	0.890805	-0.952843	-1.708607
H	-0.688282	-1.632515	-1.231113
H	-0.781932	-0.193996	0.768991
H	0.840253	0.456462	0.448303
C	-1.373812	2.165584	-0.039736
N	0.407677	1.789158	-1.746860
H	-1.396266	0.708366	-1.613976
O	2.073950	-2.764728	-0.331908
O	0.373290	-2.636937	1.080865
O	-2.590780	1.832502	0.384989
O	-0.849713	3.223020	0.327615
H	0.691013	2.656214	-1.280255
H	0.019592	2.084148	-2.644691
H	2.442629	-2.353661	-1.181636
O	3.267314	-1.730878	-2.392660
H	2.828359	-1.828596	-3.251223
H	3.215173	-0.757270	-2.182250
O	3.065230	0.807336	-1.581036
H	3.161273	0.780136	-0.600884
H	2.123884	1.091226	-1.708420
O	3.289658	0.908628	1.201408
H	2.830882	0.237896	1.748747
H	2.757403	1.724200	1.326009
O	1.860836	3.314209	1.319265
H	1.793546	3.738387	2.187483

H	0.939887	3.288349	0.995625
O	1.927018	-0.924898	2.892124
H	2.529209	-1.423354	3.464613
H	1.413857	-1.613844	2.433442
O	-3.339177	-0.493719	-0.466850
H	-4.319072	-0.563185	-0.502291
H	-3.049962	-1.169873	0.189286
O	-2.383253	-2.259719	1.436931
H	-2.776770	-3.144811	1.432660
H	-1.422778	-2.420154	1.314196
O	-6.112105	-0.517858	-0.655944
H	-6.479454	-1.293187	-1.107122
H	-6.545593	-0.531028	0.211045
H	-2.881345	0.925028	0.023171

Zwitterionic Neutral Glutamic Acid (C-terminus) with 8 H_2O

C	0.284704	0.158465	-0.215070
C	0.198524	1.506407	-0.963377
C	-0.456415	2.507456	-0.037148
O	0.119403	2.953605	0.968357
O	-1.714002	2.867637	-0.274023
C	0.737025	-1.015038	-1.092256
C	0.779018	-2.286290	-0.219695
O	-0.174772	-3.112811	-0.369978
O	1.735747	-2.363714	0.609293
N	-0.242044	-1.229675	-2.206982
H	-0.692784	-0.096074	0.225625
H	1.005529	0.247756	0.610876
H	-0.383460	1.424755	-1.891244
H	1.212251	1.858822	-1.204417
H	-2.102509	2.394563	-1.078198
H	1.719716	-0.821969	-1.545800
H	-0.097611	-2.147783	-2.640397
H	-0.145368	-0.520910	-2.941677
O	-2.857373	-0.882653	-1.161426
H	-2.863189	-0.845150	-0.167442
H	-3.552298	-1.514824	-1.399365
O	3.814019	1.263286	-0.986387
H	3.931715	0.319836	-0.747597
H	3.460875	1.659351	-0.163767
O	-2.839622	1.611001	-2.276965
H	-3.734210	1.960593	-2.408769
H	-2.973940	0.702801	-1.913244
O	-1.597653	-3.266824	1.975346
H	-1.003811	-3.309873	1.190121
H	-1.004206	-3.378949	2.732608

O	-2.778112	-0.784714	1.535208
H	-2.320691	-1.618698	1.787065
H	-2.257261	-0.074481	1.965726
O	2.794833	2.288939	1.450588
H	3.235785	3.092060	1.764360
H	1.867172	2.567110	1.295092
O	-1.268454	1.184307	2.905302
H	-0.822987	1.895312	2.411769
H	-1.809430	1.655673	3.556591
O	4.131742	-1.448406	-0.307146
H	3.279541	-1.760125	0.085653
H	4.785242	-1.582358	0.394618
H	-1.222958	-1.202949	-1.849386

Zwitterionic Neutral Glutamic Acid (Side Chain) with 8 H_2O

C	-0.155095	-0.110826	0.256172
C	-0.109276	0.853930	1.459871
C	0.838753	2.007849	1.146901
O	0.388877	2.950572	0.395569
O	2.026706	1.949555	1.589887
C	-0.726903	-1.477481	0.675504
C	-1.355668	-2.235027	-0.494188
O	-0.854949	-3.254512	-0.964798
O	-2.477815	-1.713478	-0.983159
N	0.376344	-2.304955	1.246965
H	0.854682	-0.277516	-0.155011
H	-0.759653	0.323581	-0.551704
H	0.241340	0.329435	2.360559
H	-1.123506	1.232942	1.654442
H	-1.492303	-1.346030	1.455298
H	0.022257	-3.034769	1.872916
H	1.064708	-1.713991	1.763661
O	3.660102	-1.012768	-0.579659
H	3.263573	-0.326709	-1.171653
H	4.601443	-1.027104	-0.806079
O	-3.318136	0.359205	0.287360
H	-4.288529	0.437579	0.146992
H	-2.928997	1.197059	-0.062735
O	2.620117	-0.711312	2.051050
H	2.427759	0.256614	1.995964
H	3.074035	-0.873459	1.198029
O	2.193246	-3.352981	-0.636403
H	1.717376	-3.424952	-1.477609
H	2.752834	-2.549460	-0.735980
O	2.472883	0.780072	-2.263275
H	1.555023	0.513402	-2.421336

H	2.405261	1.723087	-1.979813
O	-2.055965	2.593527	-0.698667
H	-2.548250	3.418609	-0.576881
H	-1.177038	2.758985	-0.263583
O	2.259773	3.426786	-1.500827
H	1.635303	3.350604	-0.734923
H	3.077363	3.772226	-1.113064
O	-6.069703	0.385710	-0.053826
H	-6.337785	0.517386	-0.975996
H	-6.527425	1.095570	0.421803
H	0.929447	-2.767663	0.485305
H	-2.785290	-0.884415	-0.468918

Zwitterionic Glutamate Anion with 8 H_2O

C	-0.452800	0.045086	0.492693
C	-1.292986	-1.211906	0.754098
C	0.130331	0.693856	1.774044
N	-0.379631	-2.368760	1.015693
C	-2.171361	-1.454994	-0.490073
H	-1.929935	-1.093396	1.641035
H	-1.087797	0.767878	-0.035271
H	0.353920	-0.234814	-0.205974
C	1.581334	1.097279	1.529009
H	-0.456431	1.590428	2.026919
H	0.075054	0.005402	2.629290
H	0.279882	-2.185637	1.806686
H	-0.909547	-3.215490	1.247209
O	-1.640081	-2.047792	-1.485991
O	-3.337168	-0.956407	-0.450484
O	1.789297	2.032836	0.671291
O	2.507610	0.470952	2.132849
O	1.584815	-1.912917	3.026133
H	2.293293	-2.568868	2.946373
H	1.999008	-1.055655	2.739747
O	0.036852	2.570993	-1.321603
H	0.438412	3.294055	-1.826779
H	0.678007	2.395265	-0.582398
O	-0.312775	0.261827	-2.948178
H	-0.814136	-0.419365	-2.463019
H	-0.287501	1.040243	-2.350854
O	-3.572838	1.155602	1.275160
H	-4.514442	1.329713	1.420178
H	-3.558820	0.366271	0.679586
O	0.988289	-2.910334	-1.448566
H	0.075832	-2.630617	-1.681084
H	1.540327	-2.149975	-1.740456

O	2.308453	-0.684913	-2.491400
H	1.438481	-0.270622	-2.680068
H	2.792063	-0.020005	-1.953845
O	3.740454	1.247599	-1.043362
H	4.496486	0.888003	-0.556618
H	3.119717	1.558464	-0.337370
O	-2.349411	3.404593	0.037931
H	-1.544431	3.100920	-0.426124
H	-2.738008	2.594432	0.427863
H	0.202908	-2.577550	0.176252

Glutamate Anion (C-terminus Deprotonation) with 8 H_2O

C	0.012509	-0.357072	-0.082766
C	0.995026	-0.975144	-1.105731
C	-1.399665	-0.924554	-0.285191
C	2.046281	0.048666	-1.598892
H	0.440122	-1.316929	-1.993279
H	1.490604	-1.851487	-0.655714
N	0.414804	-0.460169	1.333302
H	-0.084786	0.708961	-0.327863
O	-1.988482	-0.569312	-1.366626
O	-1.890437	-1.684592	0.606646
C	2.907014	0.538907	-0.457746
H	2.714350	-0.434037	-2.327863
H	1.532289	0.890291	-2.086330
H	0.023047	-1.329655	1.705416
H	1.428883	-0.531121	1.439618
O	2.607916	1.691296	0.136892
O	3.862931	-0.127540	-0.025901
O	3.504512	-0.523608	2.778344
H	3.440400	0.314927	3.258634
H	3.775136	-0.256294	1.879707
O	0.447560	3.025515	-0.443687
H	-0.121664	2.672406	-1.167015
H	-0.041024	2.784051	0.382657
O	-0.675898	2.058613	1.896008
H	-1.624147	1.823071	1.822199
H	-0.243502	1.162390	1.858942
O	-1.118708	1.814992	-2.411886
H	-1.928118	2.302247	-2.626600
H	-1.442838	0.945806	-2.063458
O	-3.240188	0.798476	1.775106
H	-2.798640	-0.069059	1.766100
H	-3.758735	0.763515	0.941563
O	-4.548258	0.262063	-0.690200
H	-4.862939	-0.595447	-0.340223

H	-3.667793	0.000290	-1.046238
O	-4.530876	-2.418022	0.319369
H	-4.837871	-2.622221	1.214756
H	-3.574236	-2.193081	0.435544
O	4.362868	-2.735732	-1.033645
H	3.604701	-2.982738	-1.582929
H	4.144463	-1.831720	-0.729985
H	1.778169	2.144998	-0.232168

Glutamate Anion (Side Chain Deprotonation) with 8 H_2O

C	1.536068	-0.107344	0.286946
C	1.161209	0.149968	-1.191010
C	3.041492	0.127830	0.436507
C	-0.109368	-0.571559	-1.653814
H	1.991491	-0.206427	-1.821493
H	1.084266	1.237896	-1.353656
N	0.731673	0.705526	1.206539
H	1.349588	-1.168313	0.523514
O	3.843941	-0.848756	-0.004532
O	3.527566	1.155720	0.913731
C	-1.459705	0.037006	-1.278228
H	-0.092781	-1.620308	-1.318222
H	-0.112469	-0.600106	-2.759053
H	0.693286	1.670176	0.869020
H	1.204135	0.750219	2.113559
H	3.318080	-1.632508	-0.357563
O	-2.449861	-0.773716	-1.241596
O	-1.560736	1.294829	-1.094574
O	2.539344	-2.904837	-1.018005
H	3.135624	-3.663818	-1.106761
H	1.822900	-3.219006	-0.411020
O	0.621764	-3.623004	0.772292
H	0.470823	-4.577969	0.828631
H	-0.287893	-3.228897	0.747452
O	-1.869526	-2.530504	0.813443
H	-2.083212	-2.087964	-0.037698
H	-1.838477	-1.752297	1.420607
O	-1.705409	-0.172984	2.253100
H	-2.370013	0.445993	1.881445
H	-0.859877	0.132412	1.825099
O	-3.410292	1.704934	0.933050
H	-4.142070	1.128676	0.632971
H	-2.787718	1.641730	0.170350
O	-4.990038	-0.224482	-0.434757
H	-5.255240	-1.008339	0.068358
H	-4.075908	-0.437222	-0.753677

O	-0.195990	3.524234	-0.381586
H	-0.719194	3.835655	0.371673
H	-0.637585	2.686238	-0.657721
O	2.594690	3.703847	-0.132985
H	2.866913	2.858128	0.265996
H	1.621818	3.619716	-0.210646

Doubly Deprotonated Glutamate with 8 H_2O

C	0.004232	0.317734	-0.355050
C	1.057650	-0.384670	-1.229615
C	-1.403679	0.296036	-0.974652
N	0.787020	-1.837617	-1.318061
C	2.432854	-0.066308	-0.614650
H	1.023315	0.034372	-2.247474
H	-0.014321	-0.171135	0.632808
H	0.317412	1.364350	-0.199830
C	-2.394680	0.877751	0.027729
H	-1.689470	-0.735164	-1.216091
H	-1.407168	0.895054	-1.898960
H	1.151182	-2.262119	-0.458788
H	1.371174	-2.227122	-2.063222
O	2.813821	-0.808385	0.356465
O	3.064585	0.935708	-1.078569
O	-2.537016	2.148422	0.058521
O	-2.996285	0.072976	0.820715
O	-1.602166	-3.222113	-1.232925
H	-1.363564	-4.138990	-1.433773
H	-0.758044	-2.695651	-1.360563
O	1.159379	-2.103933	2.244391
H	0.233282	-2.095549	1.921833
H	1.676222	-1.630806	1.558465
O	-1.566668	-2.256029	1.477139
H	-1.586640	-2.727654	0.620221
H	-2.048113	-1.421899	1.272350
O	-4.159460	-1.962300	-0.807806
H	-3.807039	-1.256013	-0.227523
H	-3.357247	-2.470520	-1.032038
O	5.236925	2.125521	0.032957
H	4.905434	2.881445	0.538934
H	4.419884	1.700845	-0.337600
O	-1.004913	3.776100	-1.528630
H	-0.195165	3.295221	-1.752562
H	-1.518653	3.137371	-0.977106
O	5.320358	-0.381174	1.435687
H	5.499282	0.516367	1.096102
H	4.426800	-0.556071	1.055822

H	-3.557461	2.732320	1.357575
O	-4.107038	3.175355	2.050244
H	-4.380683	2.450226	2.629754

Pyruvic Acid with 6 H_2O

C	-0.744692	-0.960067	-0.142307
C	-1.627773	-1.648691	0.850741
C	-1.314567	0.286239	-0.849040
H	-2.085160	-0.912699	1.526449
H	-2.440218	-2.151155	0.299449
H	-1.044525	-2.392078	1.408617
O	0.367898	-1.358780	-0.491658
O	-0.436496	1.101296	-1.419320
O	-2.527885	0.472805	-0.932069
H	0.503874	0.908473	-1.120220
O	1.964883	1.060401	-0.360089
H	2.256989	1.984169	-0.296614
H	2.761780	0.501276	-0.529273
O	4.021050	-0.702270	-0.641244
H	4.192323	-0.984520	-1.551844
H	3.593148	-1.481351	-0.218866
O	2.581963	-2.643649	0.731574
H	2.710714	-3.583330	0.534634
H	1.700765	-2.437784	0.366429
O	1.103600	3.675759	0.751163
H	0.469571	4.201818	0.242432
H	0.564467	2.952194	1.123231
O	0.042786	1.113752	1.621783
H	0.133570	0.796816	2.532808
H	0.887171	0.876468	1.187881
O	-4.914686	-0.706304	0.195966
H	-5.609726	-0.118494	-0.133162
H	-4.097448	-0.328784	-0.177178

Pyruvate with 6 H_2O

C	-0.537209	1.265296	-0.176984
C	-1.146952	2.476770	-0.815202
C	0.359244	0.384468	-1.052539
H	-1.764400	2.149680	-1.668776
H	-0.339870	3.109592	-1.218953
H	-1.753920	3.034593	-0.090241
O	-0.731990	0.944328	1.005810
O	-0.211240	-0.600324	-1.618923
O	1.583548	0.711484	-1.117162
O	-2.558080	-1.638135	-0.584748
H	-2.257787	-2.389137	-0.051327

H	-1.724447	-1.257201	-0.945857
O	2.384993	2.736459	0.620973
H	2.352770	2.323593	1.496237
H	2.102287	2.016623	0.014711
O	1.039455	-2.951739	-0.655559
H	1.897822	-2.581611	-0.380019
H	0.641769	-2.206619	-1.151856
O	3.002459	-1.083179	0.684239
H	2.224919	-1.165419	1.272073
H	2.689127	-0.437904	0.022523
O	0.391808	-1.564354	1.874476
H	-0.038734	-0.731890	1.594613
H	0.345042	-2.128443	1.078703
O	-3.679503	0.325668	1.094455
H	-2.895524	0.835542	1.351021
H	-3.301150	-0.372282	0.517011

Pyruvate with 8 H_2O

C	0.315562	-0.197995	1.065593
C	0.329904	-1.653313	1.428409
C	1.241182	0.250151	-0.068857
H	0.002441	-2.241771	0.556477
H	1.368749	-1.947876	1.652032
H	-0.322788	-1.845920	2.289487
O	-0.400587	0.639606	1.638819
O	0.857974	-0.025322	-1.250892
O	2.299393	0.850697	0.282345
O	-0.650513	-2.257497	-1.885104
H	-0.837881	-2.204030	-2.833914
H	-0.135067	-1.441133	-1.692222
O	4.338603	-1.007969	1.309264
H	3.546309	-0.443046	1.326434
H	4.677606	-0.822810	0.415023
O	4.494009	0.281290	-1.347021
H	4.219002	-0.180054	-2.152824
H	3.647795	0.557999	-0.930022
O	-3.044967	-2.019339	-0.441406
H	-2.201621	-2.122989	-0.934426
H	-3.374439	-1.148649	-0.743098
O	-3.794034	0.746892	-0.645799
H	-3.611759	0.632412	0.305951
H	-2.946218	1.091364	-1.009049
O	-1.409885	1.714620	-1.732238
H	-0.714142	1.031030	-1.678600
H	-1.127936	2.350393	-1.039153
O	-0.618793	3.225992	0.508005

H	0.243808	3.663515	0.450988
H	-0.434423	2.395320	0.993256
O	-3.092331	-0.458254	1.953393
H	-2.199809	-0.090284	2.081531
H	-2.950465	-1.152253	1.276335

α-Ketoglutaric Acid with 9 H_2O

C	-1.712262	0.982134	-1.490472
C	-0.339934	0.940308	-2.174690
C	-1.845047	1.584983	-0.103174
C	0.645325	-0.155274	-1.830424
H	0.185644	1.897714	-2.073864
H	-0.521644	0.795944	-3.255384
H	-2.395646	1.568397	-2.123156
H	-2.154279	-0.027899	-1.430104
C	-0.818910	1.302544	1.017052
O	-2.845188	2.233676	0.203839
O	0.227943	-1.353352	-1.422748
O	1.855993	0.003987	-2.052388
O	0.268229	0.683560	0.571121
O	-1.040722	1.608218	2.184899
H	-0.657436	-1.353064	-0.960064
H	0.868855	0.433018	1.346833
O	-1.772276	-1.875817	0.192322
H	-2.610454	-1.433404	0.453821
H	-1.248978	-1.982704	1.022749
O	1.785410	-0.223949	2.486313
H	1.905041	0.342889	3.263278
H	2.701193	-0.424049	2.153217
O	4.181841	-0.779356	1.409066
H	4.722327	-1.401860	1.917416
H	3.988251	-1.250630	0.563327
O	3.570323	-1.931139	-1.010532
H	3.091315	-2.768242	-0.918179
H	2.913859	-1.322408	-1.416008
O	-0.145133	-2.290098	2.361325
H	-0.595181	-2.382453	3.214212
H	0.521920	-1.589196	2.513368
O	-4.139853	-0.624675	0.909690
H	-4.906131	-1.089013	0.539027
H	-4.243515	0.284900	0.589613
O	0.054398	3.639948	-0.316311
H	0.055275	4.131935	0.518279
H	0.961400	3.269086	-0.375978
O	2.592351	2.437834	-0.666017
H	3.200005	2.972291	-1.199006

H	2.432560	1.645247	-1.214073
O	-2.123716	-4.143909	-1.427686
H	-2.004229	-3.366543	-0.843439
H	-1.541995	-3.957567	-2.178765

α-Ketoglutarate (α-Keto Moiety Deprotonation) with 9 H_2O

C	-0.549501	0.934723	1.025354
C	-1.103285	1.330210	-0.323172
C	0.900566	0.437186	1.079515
C	-0.921480	0.244506	-1.412697
H	-2.163544	1.597608	-0.207862
H	-0.542696	2.226161	-0.642130
O	-1.205123	0.996255	2.073158
O	1.060425	-0.802130	0.772629
O	1.794482	1.254685	1.412884
C	-1.682923	-1.016099	-1.054214
H	-1.327338	0.628252	-2.357964
H	0.144985	0.013284	-1.554009
O	-1.144552	-1.829816	-0.143191
O	-2.786067	-1.290879	-1.544280
H	-0.259265	-1.467225	0.193684
O	3.255040	-2.003735	2.063096
H	2.884052	-2.659949	2.671420
H	2.468740	-1.591299	1.644148
O	4.671096	-2.920606	-0.135161
H	4.619156	-3.884362	-0.214862
H	4.203062	-2.718309	0.707311
O	2.747839	-1.433275	-1.534288
H	2.105559	-1.348041	-0.805612
H	3.440129	-2.013681	-1.147613
O	3.500141	1.202979	-0.951991
H	3.100807	1.238228	-0.061770
H	3.318614	0.277634	-1.232893
O	1.811095	3.009638	-2.185403
H	1.055669	2.532856	-2.559712
H	2.395533	2.296967	-1.833037
O	1.382584	3.954501	0.479547
H	1.492612	3.091062	0.921356
H	1.460148	3.714118	-0.466323
O	-4.804760	0.763294	-0.859549
H	-4.151079	0.129593	-1.200362
H	-4.541322	0.879743	0.076480
O	-4.080315	1.080418	1.876150
H	-4.419709	1.900891	2.263753
H	-3.110645	1.156555	1.972171
O	-4.283702	-3.357041	-0.276336

H	-3.676524	-3.889113	0.257919
H	-3.702655	-2.688430	-0.690912

α-Ketoglutarate (Glutarate Moiety Deprotonation) with 9 H_2O

C	-1.093581	-0.811915	-1.465565
C	-0.550813	-2.165183	-1.061323
C	-0.070596	0.276446	-1.815465
C	0.842433	-2.112754	-0.415840
H	-1.298061	-2.614779	-0.391253
H	-0.514343	-2.783110	-1.976674
O	-2.293165	-0.556772	-1.591486
O	-0.328904	1.440219	-1.227974
O	0.868475	0.034426	-2.574394
C	0.978893	-1.010835	0.635544
H	1.634025	-1.980509	-1.166599
H	1.040015	-3.070962	0.094180
O	2.160789	-0.605411	0.922711
O	-0.085410	-0.556375	1.166448
O	1.841586	2.752992	-0.885026
H	2.521804	2.098212	-1.161780
H	1.876478	2.657711	0.099792
O	2.148159	2.054006	1.757910
H	1.379515	2.050658	2.363436
H	2.207430	1.099912	1.515777
O	-0.083551	1.227852	3.316923
H	-0.915405	1.673348	3.087541
H	-0.028965	0.526922	2.626777
O	3.509314	0.494512	-1.345893
H	2.928857	0.192479	-2.064699
H	3.114833	0.053890	-0.563174
O	-2.281795	1.430630	1.318275
H	-1.491398	1.044326	0.901541
H	-2.699904	1.915628	0.577913
O	-3.072480	2.636379	-1.135483
H	-3.005312	3.602364	-1.174565
H	-2.199504	2.330132	-1.437333
O	-4.160265	-2.264601	-0.069901
H	-3.662267	-1.805666	-0.768168
H	-3.660287	-2.000791	0.732434
O	-2.635911	-1.314237	2.103821
H	-2.821164	-0.363233	1.974686
H	-1.714664	-1.358545	1.777516
O	4.203735	-2.500446	0.780941
H	4.350601	-2.690090	-0.156951
H	3.472384	-1.845280	0.774053
H	0.522696	2.027446	-1.223548

Doubly Deprotonated α-Ketoglutarate with 9 H_2O

C	1.254103	-1.269279	-0.666009
C	0.916555	-0.584802	-1.974917
C	0.117204	-1.782591	0.254767
C	-0.302914	0.347495	-1.938672
H	1.823952	-0.050487	-2.292421
H	0.733403	-1.389455	-2.710719
O	2.422782	-1.520152	-0.346826
O	-0.958358	-2.126297	-0.326817
O	0.365857	-1.856621	1.497815
C	-0.380839	1.207286	-0.683036
H	-1.240913	-0.210468	-2.032264
H	-0.256267	1.038557	-2.798247
O	-1.507196	1.751846	-0.405453
O	0.677003	1.350833	0.016242
O	-2.904602	-2.084673	-2.421823
H	-2.140611	-2.215545	-1.829733
H	-3.293673	-1.261526	-2.059606
O	-3.808573	0.236397	-1.009286
H	-3.735887	-0.323437	-0.204893
H	-3.024969	0.822247	-0.916836
O	-3.178168	-1.373381	1.238959
H	-2.401539	-1.744525	0.765349
H	-2.805246	-0.589829	1.702879
O	-2.194910	1.041746	2.265659
H	-1.276611	0.915767	2.589177
H	-2.037005	1.391924	1.363654
O	0.587869	0.721718	2.697671
H	0.663770	1.130919	1.806222
H	0.597247	-0.226821	2.458578
O	2.885085	2.419672	-1.241836
H	3.161907	3.147895	-0.666583
H	2.102344	2.035626	-0.784309
O	-0.940362	4.235410	0.748493
H	-0.158574	4.109627	1.305502
H	-1.111841	3.337231	0.387237
O	4.566329	0.147559	-1.333639
H	4.055641	0.983455	-1.305695
H	3.898239	-0.511319	-1.067761
O	2.885306	-2.169214	2.648803
H	3.577471	-2.065026	1.980359
H	2.060017	-2.032206	2.133630