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Electrical Conductance And Theoretical Study Of Glutamic Acid In Different Solvents at 310.16k

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Abstract

The electrical conductivities of glutamic acid in the water, methanol, and ethanol are measured at 310.16 K and the conductivity parameters: Association constant (KA), equivalent conductance at infinite dilution (Λo) and the distance parameter (R). (Λo, KA, and R) are calculated. Values of Λo are found to be in the order: water > methanol > ethanol, but the order is reversed for the amount of KA and R. This indicates the increase of ion-solvent interaction and formation of solvent separated ion-pair in the above order. The main interest is to find an accurate yet efficient solvation model for semiempirical quantum-mechanical and Density Function Theory (DFT) methods applicable to amino acids (glutamic acid) in the context of computer-aided conductivity studying. It was reparametrization of the Conductor like Screening Model (COSMO) and Conductor-like Polarizable Continuum Model (CPCM) CPCM solvent model for Parameterization method three (PM3), Hartree- Fock (HF) & DFT calculation in Gaussian interface, version 16.0 which used to calculate many descriptors of the glutamic molecule and study the relationship between these descriptors and the association constant (KA). Molecular volume (MV), Connolly parameters, and the entropy were showed the same result corresponding with the experimental parameters.

Keywords: Electrical Conductivity, Lee-Wheaton equation, Theoretical Chemistry, Hartree- Fock , DFT;

1. INTRODUCTION

The amino acids and their compounds are used in biology, pharmacy, industry, and laboratory reagents [1]. They also control transamination, decarboxylation, and metabolism processes in the human body. On the other hand, non-essential amino acids are synthesized from intermediates of metabolism or, from essential amino acids. Glutamate can also be synthesized by reverse oxidative deamination, catalyzed by glutamate dehydrogenase. Synthesis from α-ketoacids. In a broad variety of biochemical processes, the connection of proteins with carbohydrates plays a crucial function. Much of these interactions are non-covalent in nature, such as hydrogen bonding and electrostatic interactions. The direct thermodynamic analysis is very complicated owing to the structural structure of proteins. So, molecules such as amino acids are analyzed in the low molecular weight model.

A comprehensive literature survey reveals that impressive experimental work has been published on the conductance of glycine, α, and, β-Alanine in aqueous and aqueous binary mixtures containing D-glucose (5,10,15,20 percent (w/w)) at distinct temperatures in the concentration range of $1 * 10^{-2}$ to $8* 10^{-2}$ mol dm^{-3} (298.15-313.15 K) [2]. Measurements of conductivity of electrolytes have been made nearly a century ago, and from the earliest times, interest has been restricted to aqueous solutions and very little on non-aqueous solutions or mixed electrolytes. However, only the conductance of single symmetrical electrolytes has been interpreted and far less attention, either functional or theoretical, has been paid to unsymmetrical electrolytes (especially associated ones) or to the electrolyte mixture. In the past few decades, some studies have been carried out on unsymmetrical electrolyte solutions [3].

In combination with refined experimental methods, computer simulations nowadays help to fill the above knowledge gaps. Monte Carlo models are often used in more context to analyze the functional and structural properties of polyelectrolyte solutions at specific stages [4-6]. Atomistic MD simulations are typically used for

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the study of molecular behaviour, provision a high level of detail and reliability for limited time and length scales [7-11]. Molecular methods simplify or even disregard molecular and chemical information for the sake of computational efficiency as compared to atomistic models, [12,13]. In particular, in recent years, the solvent- and ion-related effects on polyelectrolytes have drawn significant interest. Previous atomistic MD simulations, for example, showed that the behavior of molecular solving greatly influences the sum of dissociated counterions and hence the resulting conformational behaviour of repulsive electrostatic interactions or charge screening effects along the polyelectrolyte backbone [9,14,15]. The presence of the polyelectrolyte as expressed by local dielectric constant changes, asymmetry effects of charge hydration, or modified charge transfer mechanisms [16-18], affects the molecular structure of the solvent molecules.

The chemical structure of glutamic acid (Fig. 1-1) was therefore optimized in this work using the Gaussian 16.0 programme and the Quantum Mechanical Calculation Ab Initio. At B3LYP/6-311+G**, seme empirical and Hartree-Fock optimization were performed. The measured energies in various solvents of the highest occupied molecular orbital (εHOMO) and the lowest unoccupied molecular orbital (εLUMO) of the glutamic acid are associated. In addition to estimating multiple descriptors across all of the above approaches.

In addition, important reactions in the fields of chemistry [19-21], chemical engineering [22,23] and biology are the dissociation and interaction of ions in a polar solvent, such as water.

Therefore, the conductance behaviour of glutamic acid in water, methanol and ethanol at 37oC was also studied and used Lee-Wheaton equation Conductance measurements were analyzed for NaClO4 and C6H5COONa solutions in 298.15 K acetonitrile + water. Using the Lee-Wheaton equation, Ka and R were obtained [24].

Fig (1-1) 3D structure of glutamic acid molecule

2. EXPERIMENTAL

2.1 Conductometric Measurements

Conductivity water was prepared by redistilling water three times with the addition of a little amount of potassium permanganate and small pellets of (KOH) [25]. Methanol and ethanol were put in the conductivity of solution were measured by WTW Inolab 740 computerized conductivity meter. A thermostat of type Hakke G3with a Thermo bath D3 was used for controlling the temperature of the conductance cell with ±0.1°C sensitivity. The cell constant of 0.5582 ms.cm-1. several additions of stock solution. A plastic syringe (1 ml) was used for injection of the stock solution into the conductivity cell. All stock solutions were generally prepared by weighing using freshly prepared solvents. For conductivity measurements, a known amount of the solvent was added to a dry, clean, and weighed conductivity cell, and the cell reweighed again then the cell was placed in a thermostated water bath at the required temperature. The resistance of the solvent was measured then a small amount of the stock solution was injected by a plastic syringe (which was weighed before and after each addition) into the cell. After the completion of all additions, the cell was dried, reweighed again to calculate the change in the weight which was found that the loss was not more than 0.02%.

2.2 Computational Details

In all of the chemical quantum computations carried out, Gaussian version 16.0, was used. The molecule in the gas phase is reminimized by the use of MM2 and MMFF94 in water, methanol, and ethanol after minimization of energy levels. The minimization is continued until a value smaller than 0.1 kcal/mol is reached by the root mean square (RMS) gradient value.

The optimizations have therefore been completed through the use of a semi-empirical approach based on the (AM1, and PM3). The wave function was adopted for optimization in addition to RHF (restricted Hartree-Fork: closed shell) until a value smaller than 0.01 kcal/mol is reached by the root mean square (RMS) gradient. Then all descriptors at 37˚C in three solvents are determined. First with the PM3 approach and then with the 6-311G(d) basis set by HF. Therefore, as the true sample representing the molecule for measurement, the optimum conformer with the least energy was considered and this sample was treated as a starting model for other calculations.

Afterward, the optimization structure and energy of the most stable conformer of the glutamic acid was further minimized using (DFT), employing (DFT/B3LYP), with a 6-311G(d,p) basis set. Before all calculations, as in order to classify the stationary points as local minima, frequency measurements were carried out at the same theory level as geometry optimizations (equilibrium structures). No protocols for scaling

were considered. Using the CPCM solvation model (conductor-like polarizable continuum model) and the COSMO continuum solvation model, the influence of the solvent was also taken into account [26,27].

2. RESULT AND DISCUSSION

3.1 Conductivity Measurements and Analysis

The glutamic acid solution promised symmetrical electrolytes of type (1:1) if the positive ion is denoted by(M+) and negative ion (X-) when using the equation for these solution can be explaining as follows.

$$M^{+}_{aq.} + X^{-}_{aq.} \xleftrightarrow{Ka} (M_{.aq}{}^{+n} X)$$

Ka: association constant

Kohlrausch has established the stability that the solution is weak electrolytes after electrical conductivity was measured at the above –mentioned temperature of the mother acid solution .The intent used is then to calculate the equivalent concentration for a glutamic acid solution using a special calculation program to extract the equivalent continuity after entering the conductivity information, physical parameter, temperature and weights of the additives, so it was shown that amino acid understudy the behavior of the weak electrolytes was demonstrated by the relationship between the square root of the different concentration of the glutamic acid solution versus the equivalent continuation calculated through the calculation program. Values indicating that solution behaves like weak electrolytes [28], figure (3-1) demonstrates this behavior. The lee-Wheaton equation was applied to the amino acid solution described above, where the equivalent continuity was calculation program after it announced the electrical conductivity of all studied fixed cell concentration (0.5cm), density (0.99707gm/cm3), the data including concentration and equivalent conductivity values, were analyzed using a special analysis software after giving information on both absolute temperature(T), the viscosity of solution (0.0089pois) and dielectric constant (78.3D). after completing the analysis of the data it was confirmed that these solutions were weak electrolytes .as a result of the analysis). The analysis shows that cation is associated with an anion to form a contact ion –pair (CIP) [29]. The values of stander deviation proved that the Lee-Wheaton equation suitable for this study.

Table (3-1). Molar concentration (M) and Equivalent conductance of glutamic acid in water at 310.16K

Conc. Mole/L*10^{-7}	√Conc. Mole/L*10^{3}	Λ (Ohm^{-1} . equive^{-1}.cm^{2})
5.329623	0.730043	99.76132
10.43143	1.021344	96.41462
15.14089	1.230483	82.61713
19.87206	1.409683	74.25182
24.6716	1.57072	70.05385
29.59032	1.720184	66.6162
34.38385	1.854288	64.69787
38.84574	1.970932	63.04131
44.09012	2.099765	62.08043
48.23512	2.196250	61.35552

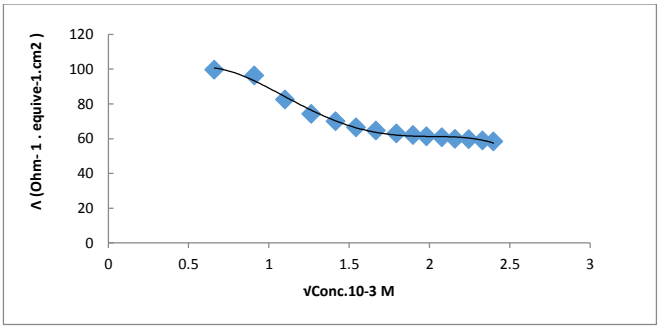


Fig (3-1): Equivalent conductance of glutamic acid in water at 310.16K

Table (3-2).
Molar concentration (M) and Equivalent conductance of glutamic acid in methanol at 310.16K

Conc.*10^{-7} M	√Conc. *10^{3} M	Λ (Ohm^{-1} . equive^{-1}.cm^{2})
5.329623	0.739051	137.3135
10.43143	1.03389	70.16389
15.14089	1.245534	61.76875
19.87206	1.426852	48.34492
24.6716	1.589768	39.56691
29.59032	1.740952	35.49579
34.38385	1.876578	32.99331
38.84574	1.994527	33.22483
44.09012	2.124783	31.42174
48.23512	2.222316	30.37248

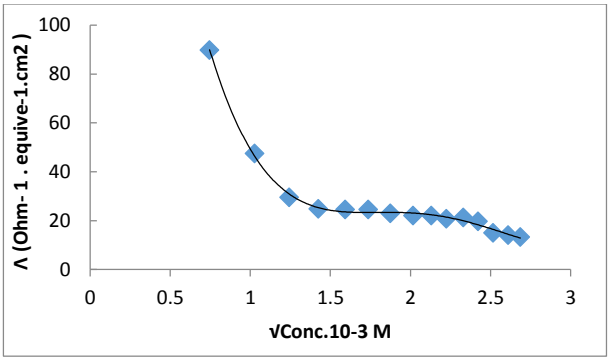


Fig (3-2): Equivalent conductance of glutamic acid in methanol at 310.16K

Table (3-3)
Molar concentration (M) and Equivalent conductance of glutamic acid in ethanol at 310.16K

Conc.*10^{-7} M	√Conc. *10^{3} M	Λ (Ohm^{-1} . equive^{-1}.cm^{2})
5.568882	0.746249422	89.78449
10.53321	1.026314279	47.46884
15.43805	1.242499497	29.53465

20.33422	1.425981066	24.85234
25.3939	1.59354636	24.58905
30.17824	1.737188533	24.58993
35.13575	1.874453254	23.01995
40.66705	2.016607299	22.00692
45.44023	2.13167141	22.02191
49.49994	2.224858198	20.79634

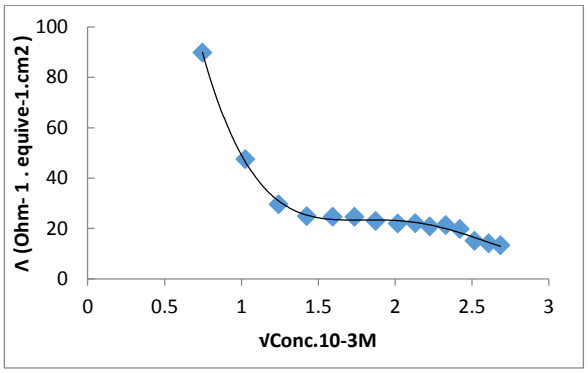


Fig (3-3): Equivalent conductance of glutamic acid in ethanol at 310.16K

The correlations between the concentration of the aqueous solution of the compound above and their equivalent conductance are shown in Figs. (3-1,2, and 3) which shows a non-linear relation, which means they are weak electrolytes. The conductance data obtained were first analyzed in accordance with the Lee-Wheaton equation.

Table (3-4).
Values of constant Ka, Λ,the distance between R(A°) and σΛ of glutamic acid in different solvents at 310.16K

Solvents	R	Λo	Ka	бΛ
water	$1*10^{-6}$	104.88	2372974	3.4999
methanol	$1*10^{-6}$	67.33	2857629	18.208
ethanol	$1.05*10^{-6}$	87.108	1414375	8.9057

3.2 Theoretical analysis

From first principles, Ab initio quantum chemistry makes the study of gas-phase molecular properties feasible. However, these properties can change significantly in liquid solutions, especially in polar solvents. While solving results can be modeled it by using explicit solvent molecules in the quantum chemical calculation, the glutamic amino acid molecule has been studied theoretically according to a series of theoretical calculations and in a series of sequences, starting with the minimization of the energy level through molecular mechanics MM2 and MMMFF94 to facilitate the start of quantum mechanical calculations that are more accurate.

When applying quantum mechanics and making the necessary calculations to bring the molecule to the lowest energy level so that it is more stable, Ab initio methods were started to simplify and reduce the calculation time. Firstly, two methods were used: AM1 and PM3 to minimization the energy of the molecule. In addition, the minimiza the frequencies of the molecule also were calculated, and then the various descriptors of the glutamic molecule were calculated. Descriptors were calculated with more than one model of solvents, the most important and most accurate of which was COSMO. Therefore, this method was adopted to compare the values calculated by quantum mechanical methods [30]. Tables (3-5), (3-6), and (3-7), show the values of the most important descriptors that were calculated by following two solvation models, namely (COSMO & CPCM) by applying PM3 methods, HF 6-311G (d, p) database, and finally by theoretical DFT with bases set 6-311G (d, p) in water, methanol, and ethanol.

Where the values of the most important descriptors related to the solvent have been included and may change according to the solvent molecules, as we notice that there is a slight difference when comparing the results of the two models of solvation used to calculate the descriptors using the PM3 method, as it is a quasi-experimental method that can only be used for comparison. From table (3-1) can notice a great convergence or the same Connolly three values for all solvents in the CPCM pattern. The difference in the molecular volume of the glutamic molecule according to the difference in the solvent indicates the effect of the solvent on the volume of the association molecule, which is considered as an indication of the extent to which the solvent molecules are gathered around the glutamic molecule. The results were more accurate in terms of the difference between the solvent and this method, which can be said to be simple as it is a semi-experimental method. And the COSMO model was adopted to measure the descriptors in the rest of the methods because the CPCM values were very close and maybe equal in different solvents.

Table (3-5): Values of descriptors in ethanol, methanol, and water were calculated by PM3 (CPCM, COSMO) models.

PM3 (CPCM)			
DESCRIPTORS	In Ethanol	In Methanol	In water
Connolly Accessible Area (CAA) Å²	294.406	294.422	294.43
Connolly Molecular Area (CMA) Å²	131.753	131.763	131.764
Connolly Solvent Excluded Volume (CSEV) Å³	96.649	96.66	96.658
Molecular Volume (MV) bohr**3/mol	1257.855	1365.345	1411.615
Entropy Cal/Mol.Kelvin	90.788	90.802	93.633
Thermodynamic Energy (εth) Kcal/Mol	106.986	106.986	106.985
Finished Energy (εf) Kcal/Mol	-200.16 (-0.318976 Hartrees)	-200.24 (-0.319109 Hartrees)	- 200.4 (-0.31936 Hartrees)
RMS Force Kcal/Mol	0.0308	0.0194	0.0011
Dipole Debye	1.7854	1.7894	1.7957
HOMO (a.u)	- 0.37178	- 0.37177	-0.37096
LUMO (a.u)	0.02453	0.02450	0.02439
PM3 (COSMO)			
DESCRIPTORS	In Ethanol	In Methanol	In water
Connolly Accessible Area (CAA) Å²	289.512	293.199	294.458
Connolly Molecular Area (CMA) Å²	130.119	131.647	131.777
Connolly Solvent Excluded Volume(CSEV) Å³	96.498	95.928	96.662
Molecular Volume (MV) bohr**3/mol	1153.314	1229.312	1166.028
Entropy Cal/Mol.Kelvin	93.633	90.331	90.794
Thermodynamic Energy (εth) Kcal/Mol	108	108.176	106.986
Finished Energy (εf) Kcal/Mol	-193.39 (-0.308116 Hartress)	-200.29 (-0.319109 Hartrees)	-200.4 (-0.31936 Hartrees)
RMS Force Kcal/Mol	0.0308	0.0011	0.0045
Dipole Debye	1.7854	2.715	1.7935
HOMO (a.u)	-0.37113	-0.37498	-0.37107
LUMO (a.u)	0.02226	0.02065	0.02263

Table (3-6): Values of descriptors in ethanol, methanol, and water were calculated by HF (CPCM, COSMO) models.

HF 6-311G (CPCM)			
DESCRIPTORS	In Ethanol	In Methanol	In Water
Connolly Accessible Area (CAA) Å²	277.036	288.542	288.554
Connolly Molecular Area (CMA) Å	125.411	128.886	128.889
Connolly Solvent Excluded Volume (CSEV) Å³	96.639	95.196	95.203
Molecular Volume (MV) bohr**3/mol	1229.664	1227.593	1103.2
Entropy Cal/Mol.Kelvin	90.596	92.162	92.174
Thermodynamic Energy (εth) Kcal/Mol	108.466	108.292	108.295
Finished Energy (ε_f) Kcal/Mol	-344307.17 (-548.688857 Hartrees)	-344309.23 (-548.692138 Hartrees)	-344309.45 (-548.692494 Hartrees)
RMS Force Kcal/Mol	0.0086	0.0044	0.0040
Dipole Debye	2.3257	1.8072	1.812
HOMO (a.u)	-0.40174	- 0.39840	-0.40101
LUMO (a.u)	0.14459	0.15795	0.15269
HF 6-311G (COSMO)			
DESCRIPTORS	In Ethanol	In Methanol	In Water
Connolly Accessible Area (CAA) Å²	277.022	288.587	288.580
Connolly Molecular Area (CMA) Å²	125.388	128.862 d	128.854
Connolly Solvent Excluded Volume (CSEV) Å³	94.621	95.213	95.206
Molecular Volume (MV) bohr**3/mol	1118.51	1125.127	1120.186
Entropy Cal/Mol.Kelvin	92.06	93.65	93.632
Thermodynamic Energy (ε_{th}) Kcal/Mol	108.489	108.313	108.313
Finished Energy (ε_f) Kcal/Mol	-344291.13 (-548.663289 Hartrees)	-344293.37 (-548.666859 Hartrees)	-344293.6 (-548.667232 Hartrees)
RMS Force Kcal/Mol	0.0047	0.0086	0.0095
Dipole Debye	1.9179	1.833	1.8378
HOMO (a.u)	-0.40624	-0.40905	-0.39896
LUMO (a.u)	0.14032	0.1459	0.15242

Table (3-7): Values of descriptors in ethanol, methanol, and water were calculated by DFT (CPCM, COSMO) models.

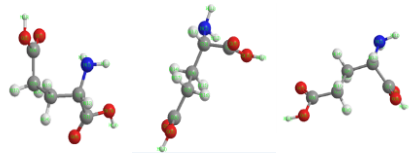
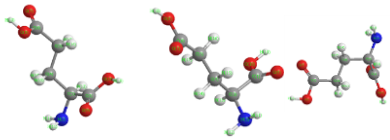
DFT / 6-311G(d,p) (CPCM)			
DESCRIPTORS	In Ethanol	In Methanol	In water
Connolly Accessible Area (CAA) Å²	290.192	289.987	289.989
Connolly Molecular Area (CMA) Å²	130.152	130.216	130.205
Connolly Solvent Excluded Volume (CSEV) Å³	95.34	96.164	96.150
Molecular Volume (MV) bohr**3/mol	1427.396	1223.22	1114.98
Entropy Cal/Mol.Kelvin	97.625	101.549	101.65
Thermodynamic Energy (ε_{th}) Kcal/Mol	108.59	108.785	108.784
Finished Energy (ε_f) Kcal/Mol	-346168.32 (-551.6547 Hartrees)	-346263.31 (-551.806168 Hartrees)	- 346263.51 (-551.806484 Hartrees)
RMS Force Kcal/Mol	0.0041	0.0041	0.0033
Dipole Debye	2.6628	2.6471	2.6592
HOMO (a.u)	-0.24682	-0.25605	0.25462-
LUMO (a.u)	-0.00092	-0.00853	-0.00968
DFT / 6-311G (d,p) (COSMO)			
DESCRIPTORS	In Ethanol	In Methanol	In water
Connolly Accessible Area (CAA) Å²	291.775	291.768	291.766
Connolly Molecular Area (CMA) Å²	130.907	130.906	130.904
Connolly Solvent Excluded Volume (CSEV) Å³	96.772	96.771	96.761
Molecular Volume (MV) bohr**3/mol	1057.188	1150.551	1141.652
Entropy Cal/Mol.Kelvin	97.021	96.999	96.877
Thermodynamic Energy (ε_{th}) Kcal/Mol	108.384	108.382	108.381
Finished Energy (ε_f) Kcal/Mol	-346174.2 (-551.664167 Hartrees	-346174.33 (-551.664367 Hartrees	-346174.57 (-551.664743 Hartrees
RMS Force Kcal/Mol	0.0062	0.0055	0.0047
Dipole Debye	2.6387	2.6456	2.6602
HOMO (a.u)	-0.26253	-0.26263	-0.26271
LUMO (a.u)	-0.02070	-0.02070	-0.02076

It is noted in the tables (3-1) and (3-2) the values of the descriptors computed using the PM3 method, as well as the HF of the COSMO model that showed values close to the practical results of conductivity measurements and the calculation of the ionic assembly constant, which showed that the largest value of KA was in methanol, then water and finally ethanol, which corresponds with the molecular volume MV of the glutamic molecule from theoretical calculations where it was greater in methanol, water and ethanol, which confirms the accuracy of the calculations. Entropy values that indicated increasing the association reduce their value can be seen in the same tables above.

Finally, the results of the DFT theory were the same as the base rule used by the HF method, which is 6-311G (d, p) for the COSMO solvation model. The molecular volume of the glutamic molecule in water was slightly larger than that of methanol and finally, it was lower in ethanol. What supports the concert of the theoretical and practical results is that these results coincide with the entropy values as they were maximum value in ethanol, methanol, and water, respectively. In

addition to the difference in (MV) values, the difference in the molecule geometry can also be observed in the solvents as shown in Table (3-4), which conforms with all results having from this study.

Table (3-8).
The final geometrical form of the glutamic acid molecule in the solvents, as a COSMO model

	Ethanol	Methanol	Water
HF			
DFT			

CONCLUSION

In this paper, the effect of solvents on the ionic behavior of glutamic acid was studied, through the practical results of conductivity measurements of dilute concentrations of glutamic acid in ethanol, methanol, and water at a temperature of 37 ° C, which was analyzed according to the Lee-Wheaton equation for dilute solutions to find the conductivity values: the association constant KA and the distance parameter R which were differentiated due to different dielectric constant and viscosity of each solvent. The main interest is to find an accurate and effective solution model for quasi-experimental quantum mechanics and DFT methods applied to amino acids (glutamic acid) in the context of a computer-aided conduction study. PM3, HF, and DFT methods were used together with CPCM and COSMO models to calculate various glutamic molecule descriptors and study the relationship between these descriptors and the (KA). The molecular size, Connolly parameters, and entropy showed the same corresponding result as the experimental parameters.

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