Electron Impact Collision Estimations for Different Cross Sections On Atomic and Molecular Targets & Its Biological Relevance

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Abstract

In this article we have reported ionizing cross-sections of total electron impacts from the ionization threshold to 2000 eV for the bio-molecules, pyridine, n-propylamine, urea, formamide and N-methylformamide. The current calculations are based on the complex spherical optical formalism and complex ionization potential contribution method. For pyridine and pyrimidine, the results obtained are compared to available theoretical and experimental results and are in good agreement with existing data. For other molecules, the cross sections of ionization are first reported. There is also an interesting relationship between the inelastic peak and ionization sections with target parameters. It was found that the two cross-sections depend on those parameters as much as possible, which confirms the consistency of the values shown here.

Keywords: *Ionisation Cross Section; Spherical Complex Optical Potential; Complex Scattering Potential-Ionisation Contribution; Bio-Molecules*

1. INTRODUCTION

The most fundamental processes are electron-induced reactions, as they drive almost every physical and chemical phenomenon in the diverse sectors of applied science. It is well known to be important for areas such as plasma modeling of semiconductor etching and fusion devices, radiation chemistry and the atmosphere. The pioneering work by Sanche and colleagues[1-4], who have shown that low-energy electrons can induce strand breaks and therefore damage to dinetic diseases, has received much attention in the last decade in relation to the electron interaction with bio-molecules. Biomolecules are high-energy sensitive as they can lead to primary, secondary or greater processes of reaction. Electron ionization of biological molecules in radiation damage and therapy is one of the most common, important processes. Single and multiple ionization processes, which transport large parts of the impinged radiation power, are responsible for the secondary electrons produced in the irradiated cells. These energy-efficient electrons (0–20 eV) interact with the irradiated biomolecules directly or indirectly and produce single or double-strand breakages, thereby harming DNA and RNA. In the light of the fact that these cross sections are required as input in the Monte Carlo analysis for studying damage to living cellulars using ionizing radiation, the electron impact cross section for biomolecules at the low and intermediated energies is important[5,6]. In this paper we have notified the biological molecules / die total ionization cross section (Qion). The respective author. Author. Emails: pyritine (C5H5N), C-4H4N2 pyrimidine (C3H9N), n-propylamine (CH4N2O), CH3NO (formamine) and C-2H5NO from 2000 eV. Email: antony.bk.ap@ismdhanbad.ac. This work has been encouraged by the lack of adequate ionization cross-sectional data for the molecules in literature. The ionization section has been calculated with the improved binary-encounter-dipole (iBED) model in pyridine by Huo and coworkers [7,8]. In combination with the BORN Diploma cross section and the symmetrical Mot cross-section of the incident electron power is used the binary encounter model to obtain the iBED model.

Jiao et al. [9] used mass spectrometry transformation in Fourier to study dissociative electron impact ionization of pyridine. The total and partial ionization cross sections were measured as energy functions in the 10–200 eV range. The 2012 ionization cross section measurement for pyrimidine was carried out by Linert et al. [10]. Except for these two molécules, for the objectives studied here to the best of our knowledge no ionization cross-sections data are available. The cross section data for pyridine and pyrimidine is also fragmented. It is important to note here that It is difficult, either by direct measurement or by ab initio theoretical methods [11–13], to get cross-sectionally for these larger biomolecules. This difficulty or lack of data leads to empirical and semi-empirical models for the study of

ionization of these molecules by electron. In calculating the total inelastic cross section we employed a spherical complex optical (SCOP) formalism[14–18]. The whole cross section of ionization is then taken from the whole cross section of inelastic. using the complex CSP-ic method[16,19–22]. Method for scattered potential ionization contributions. The benefit of this approach is that the community of atomic and molecular physics produces cross-sectional information with the appropriate precision in a short period of time (see Figure 1).

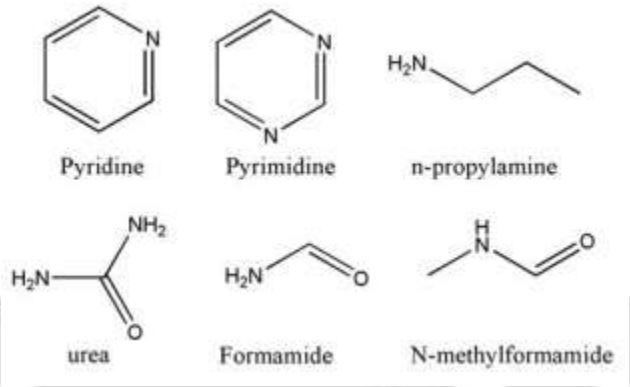

Figure 1. Structure of targets studied

1. Pyridine (C5H5N)

Pyridine is a basic organic heterocyclic, benzene-like compound, with a nitrogen substituted nitrogen group. It is also an important solvent and a reagent and is used as a precursor to agrochemicals and pharmaceuticals. In order to understand the processes of dissociative ionization in DNA damages by space radiation, the electron ionization cross section study of benzene and pyridine by Huo and collaborators was carried out[7,8]. Although pyridine is an important molecule, only few ionization cross-section studies have been conducted.

2. Pyrimidine (C4H4N2)

Pyrimidine is a pyridine-like organic aromatic compound with two atoms of nitrogen replacing benzene CH. It is the precursor to three DNA and RNA nuclei bases: cytosine, thymine and uracil. It has thus recently gained interest, particularly in gas photon and electron impact studies[10]. The experimental Qion reported by Linert et al.[10] is the only available data for this molecule.

3. n-propylamine (C3H9N)

n-propylamine means a C3H9N, a linear chain molecule. This can occur as a degrading biomass and as a volatile animal waste emission product. N-propylamine is used in the production of rubber chemicals, dyestuffs, pharmaceuticals, agricultural chemicals, resins for textiles and leather finishing. Literature contains a theoretical study on the mass spectrum of this molecule. However, for that molecule we were unable to find cross-sectional data. This calculation could certainly motivate other experimental and theoretical groups to calculate this molecule.

4. Urea (CH4N2O)

Urea is an organic compound with a biological atomic composition contained in the components carbon, hydrogen, nitrogen and oxygen and close to cellular density. There are 2 –NH2, together with a functional group of carbonyl (C=O). Urea is the main nitrogen-containing substance in the mammalian urine and is also an important chemical raw material. A recent study by Caleman et al. shows that urea produces 30% more electrons than water from a starter with the same energy. The first principles of this calculation are based on band structure, energy loss and an inelastic cross section. The highly accessible electrons play an important part in damaging bio-molecules by means of secondary single and multiple processes of ionisation. Electron ionisation impact cross-section data are therefore crucial for understanding the damage to bio-molecules caused by low-energy electron. Baldwin et al. also studied urea fragmentation under electron impact. However, the literature for this bio-molecule contains no electron impact ionization cross-section information at any stage.

5. Formamide (CH3NO) and N-methylformamide (C2H5NO)

Formamide and its derivative NMF have been very important in recent years as a prebiotic compound and the simplest of the peptide-bonding molécules. Species in star-forming areas, interstella media and the comet Hale-Bopp are detected. Formamide is considered to be a possible biological precursor because, in extreme high vacuum conditions, it can form nucleobases on TiO2 (001) single crystal surfaces. In the presence of largely available catalysts, formamide also provides a complete set of core fundamentals needed for the formation of nucleic acid through moderate heating. The dissociative electron attachment to formamide was studied in Seydou et al. and Goumans et al. The ab initio Schwinger multichannel and R matrix methods used by Bettege and Wang and Tian are to study formamide collision by low-energy electrons. Maljkovic et al. performed elastic differential cross section measurements/calculations for NMF. In addition, the electron impact on integral cross sections is calculated using the screen additivity rule procedure, but no ionization cross section measurement/calculation exists. In the present study, the Qion for both objectives is first calculated.

Table 1. Target properties

Target	IP (eV)	Polarisability (Å^3)	Bond length (Å)
Pyridine (C_5H_5N)	9.26	9.49	C–H = 1.075; C–C = 1.390; C–N = 1.340
Pyrimidine ($C_4H_4N_2$)	9.23	8.53	C–H = 1.087; C–C = 1.393; C–N = 1.350
n-propylamine (C_3H_9N)	8.78	7.70	C–H = 1.09; C–C = 1.524; C–N = 1.458; N–H = 1.01
Urea (CH_4N_2O)	9.70	5.52	C–O = 1.22; N–H = 1.02
Formamide (CH_3NO)	10.16	4.20	C–H = 1.09; N–H = 1.00; C–O = 1.21; N–C = 1.35
N-methylformamide (C_2H_5NO)	9.83	5.91	C–H = 1.09; N–H = 1.01; C–O = 1.29; C–N = 1.36; N–C = 1.459

Electron molecule collisions using quantemol

Collisions of electron molecules play an important part in many areas, from interstellar medium chemistry, ionizing radiation in the body to damage to the DNA. Where experiments are unable to offer cross-sections, simulation can be the answer for a number of potential reasons. This theory is based on the R-matrix method, where the space for calculation is divided into two areas. In a region with complicated physics – and in a region with large amounts of simplified equations [1]. [2]. The UKRmol Suite[2] collects the programs used for the calculation. The flexibility of the suite makes it possible to use many different models to better calculate special features or to adapt them to different molecules. Complexity comes with this flexibility too. Quantemol Ltd aims to offer users who are not familiar with the codes the means to calculate these cross sections and properties. First, by simplifying the calculation process - by using the Quantemol-N program, and secondly, by making home-made calculations for users and customers.

2. THEORY

The basics of R-matrix theory are division of space, the calculation of complex interactions between all electrons and the dispersing electron, and then the spread of the dispersing electric wave to a wider distance, whereas the target density is zero - the spread of asymptotic electron density Exchange and correlation effects are considered for all electrons in the internal region, the Eigen functions of the total Hamiltonian as like so:

$$\Psi_k^{N+1}(x_1 \cdots x_{N+1}) = A\sum_{ij} a_{ijk}\Phi_i(x_1 \cdots x_N)u_{ij}(x_{n+1}) + \sum_i b_{ik}\chi_i(x_1 \cdots x_{N+1})$$

where A is the antisymmetry operator, 1 Φi N ( ) x " x are the target orbitals, and 1 ( ) ij n + u x the continuum orbitals where xn are the spin coordinates of the nth electron. Continuum orbits are produced by a set of GTOs centered on the mass centre. GTOs are used to describe all the orbitals because they simplify and calculate to a higher precision the many integrations that have been made during the procedure. The terms () βi N'+x are known as the terms L2, representing the correlations between short-range and polarizing effects. The targets and virtual molecular orbits are used to construct them. We achieve various models that represent the target to a variety of degrees by limitation of the possible configurations. The simplest example of this is the ground status of the molecule with only one configuration. This is the model of static exchange. In this expansion we allow electronic excitedness, with more configurations included, - electrons can occupy every orbit, each different excitement is a

new configuration. In addition, they can be expanded to include more functions which are not true system autonomy - this is known as the Pseudo States R-Matrix (RMPS). The pseudo states are obtained through orthogonalization of an evenly tempered set of orbital centers. The R-Matrix is constructed with these wave functions and their own values, together with other target information. The R-Matrix is extended and matched to known asymptotic solutions in the outer region by a single center multipole expansion. The size of the base set used for the continuum determines the angular section of the partial wave expansion, which converges quickly in most cases. If the molecule has a permanent dipole, a correction is not applied by Born to account for the lack of higher partial waves [3]. Different matrices can be easily extracted and used as inputs to other codes by code modules in the external region during the calculation – K, T, etc.

Quantemol-N

Complexity comes with the flexibility of the codes. Sadly, this can lead to the time needed to execute codes competently. Without the steep learning curve Quantemol-N allows access to those codes. A graphical interface – the number of orbits in the model, symmetry, base set, etc – will be entered by the user and the calculation will be executed.

3. CALCULATED ELECTRON IMPACT TOTAL IONISATION CROSS SECTIONS FOR FURAN MOLECULES

Recent studies of radiation damage by DNA have shown that single-beach and double-beach breaks in DNA are the dominant elements in understanding the damage in living cells and tissues of low secondary electrons (less than 20 eV). This stimulated strong interest in the dispersion of electrons by molecules of biological importance. Theoretical and experimental groups have been working hard to provide a better insight into DNA damage mechanisms that include both the direct processes (ionisation, electronic, rotational and vibrational arousal) and compound processes such as resonances (disconnect and dissociation of electrons)[1]. In this document, we report the total ionization cross sections induced by the electron for Furan. For calculating total elastic cross-sections Qel, total inelastic cross-sectional Qinel and using the CSP-ic (Complex Scattering Potential) method [2], we used Spherical complex optical potential (SCOP) formalism to obtain Qion, the calculated Qinel, ionization cross-section. Compared with the available single measures of Szmytkowski[3], the calculated total cross-sections are considered as electron energy incident functions. We have also used the BEB method[4] to calculate Qion. Good agreement overall has been complied with.

THEORY

The SCOP formalism provides Qel and Qinel such that,

$$Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i) \qquad (1)$$

We have deduced the Qion from Qinel using Complex Scattering Potential-ionization contribution (CSP-ic). We define the following energy dependent ratio of cross sections,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)} \qquad \text{such that } 0<R\leq 1 \qquad (2)$$

This dynamic ration is found to be,

$$R(E_i)\begin{cases} = 0 \; for \; E_i \leq I \\ = R_P \; at \; E_i = E_P \\ \cong 1 \; for \; E_i \gg E_P \end{cases} \qquad (3)$$

Here, Rp is the value of R at Ei = Ep where Ep stands for the incident energy at which, the Qinel attains its maximum value.

4. RESULTS AND DISCUSSION

For some important bio-molecules, we reported total ionization cross-section in this study, where very few works were previously reported. The current data are shown in Figures 2–6 with a Qion in A to 2 along y axis and the energy of incident in eV along the x axis (in logarithmic scale). Table 2 presents the values. Where available and a reasonable agreement is reached on all cases, our results are compared with existing experimental and theoretical data. A straight fit between the cross section and the target parameters such as polarization and IP is obtained in both cases.

The current Qion plot for the pyridine disperse system together with a comparison between Huo and his colleagues[7] and Jiao et al.[9] are shown in Figure 2. Figure 2. Our Qion has been very much in agreement with Jiao et al.[9experimental]'s results and also fits well with Huo and his coworkers' theoretical data[7]. At the peak of our information, Jiao et al.[9] and Huo and colleagues[7] are slightly overestimated but fall under experimental uncertainty across the entire power range.

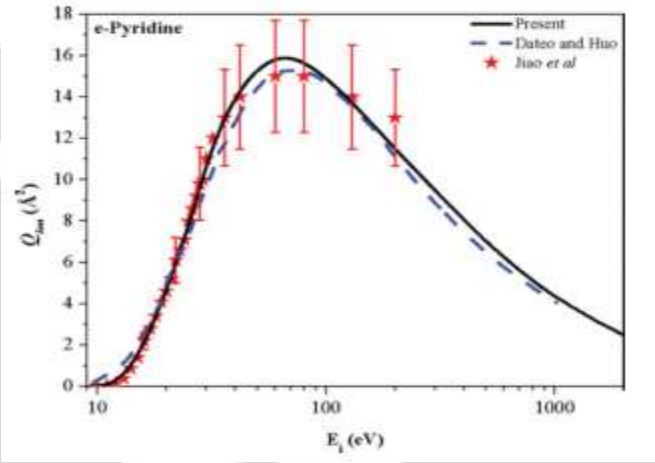

Figure 2. Total ionisation cross section for e-pyridine (C5H5N) scattering in A˚ 2. Solid line: present; dashed: Huo and co-workers [7]; stars: Jiao et al. [9].

In Figure 3, we have plotted the results of Qion for e-pyrimidine scattering from threshold up to 2 keV. The literature survey for this target clearly shows the scarcity of experimental and theoretical data. The lone comparison is due to a recent measurement by Linert et al. [10] from threshold to 150 eV. The present data for pyrimidine find excellent agreement with Linert et al. [10] throughout their energy and they are always within the experimental uncer tainty. The shape of the present curve, especially at the peak matches quite nicely with the measurement.

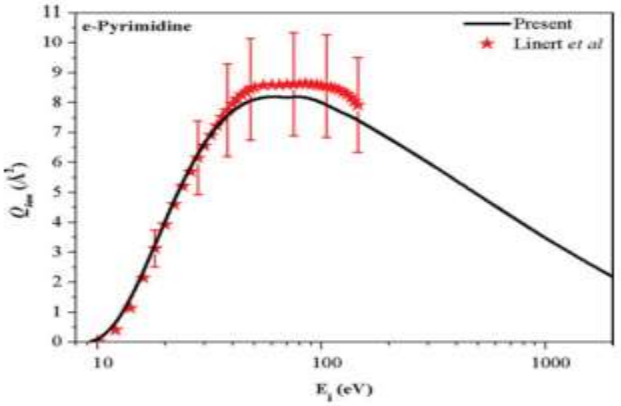

Figure 3. Total ionisation cross section for e-pyrimidine (C4H4N2) scattering in A˚ 2. Solid line: present; stars: Linert et al. [10].

The ionisation cross section data for n-propylamine is plotted in Figure 4. In a recent experiment done by the group of Krishnakumar [56], they have obtained the ionisation cross section for n-propylamine to peak at 73 eV with a value of 6.54 A˝ 2. They have mentioned only the position and magnitude of the cross section at the peak of ionisation. The overall uncertainty in their measurement was estimated to be 12%. Our cross section at the peak gives a value of 7.569 A˝ 2 at 70 eV

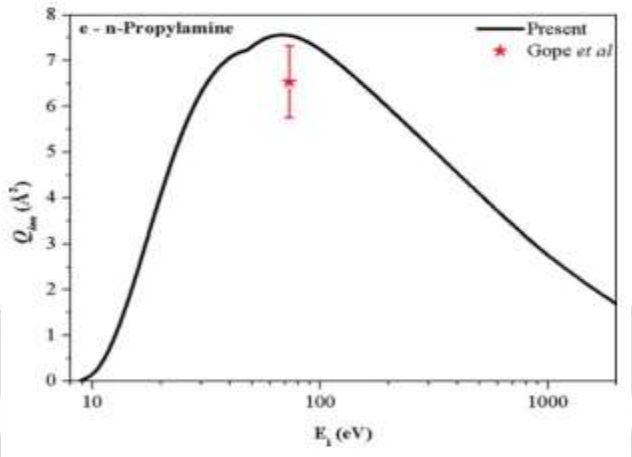

Figure 4. Total ionisation cross section for e-n-propylamine (C3H9N) scattering in A˝ 2. Solid line: present SCOP; star: Krishnakumar and co-workers

Figure 5 shows the results of Qion data for e-urea scattering. Caleman et al. [26] have obtained the inelastic cross section in crystalline state of urea, but there exists no measurement or calculation in gas phase to obtain either inelastic or ionisation cross section. In the present case, we have computed the ionisation cross section using SCOP formalism and also generated the Qion data using binaryencounter-Bethe (BEB) method [13]. The agreement between the SCOP and BEB calculations is good except that the BEB calculation overestimates the SCOP calculation at the peak. Also, the position of the peak from both calculations falls close to each other.

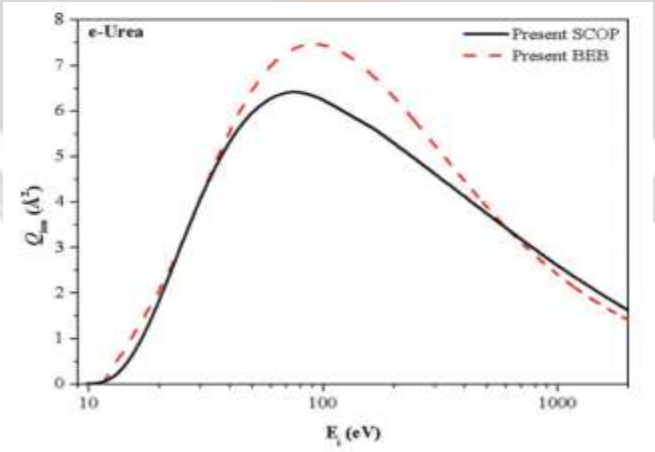

Figure 5. Total ionisation cross section for e-urea (CH4N2O) scattering in A˝ 2. Solid line: present SCOP; dashed line: present BEB.

In Figure 6, For formamide from threshold to 2 keV we presented the result of Qion. There is no other measurement or calculation in the ionization cross-section, although studies of the low-energies electron collision with formamide are mostly focused on dissociative electron fixture. Two formalisms were used to calculate Qion, namely SCOP and BEB[13]. In the entire range of energy, both theories agree quite correctly, except that the data used by the BEB are slightly changing to higher energy areas. Because data on this important biological target are not available for Qion,

the current calculations can very well fill up the void of bigger biomolecules in the database and motivate others to carry out the cross-section analysis.

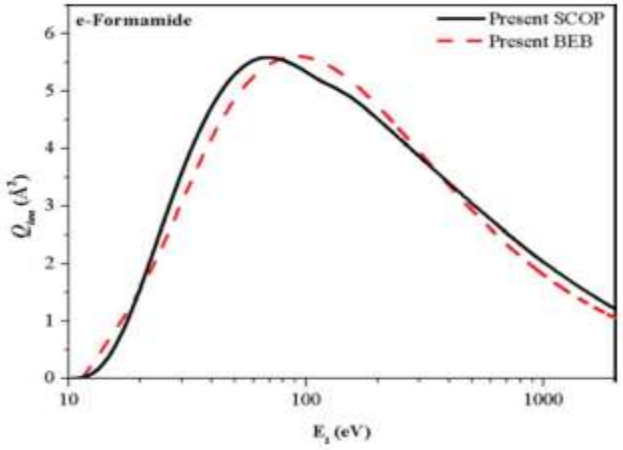

Figure 6. Total ionisation cross section for e-form amide (CH3NO) scattering in A´° 2. Solid line: present SCOP; dashed line: present BEB.

Table 2. Total ionisation cross section for all the targets studied in A˚ 2

E_i (eV)	Pyridine	Pyrimidine	n-propylamine	Urea	Formamide	N-methylformamide
10	0.008	0.091	0.123	–	–	–
11	0.088	0.315	0.391	0.016	0.004	0.02
12	0.289	0.637	0.751	0.076	0.039	0.111
15	1.557	1.912	2.07	0.558	0.428	0.901
20	4.678	4.041	4.095	1.847	1.575	3.079
25	7.792	5.609	5.47	3.094	2.706	5.211
30	10.679	6.645	6.31	4.08	3.599	6.912
40	13.897	7.715	7.068	5.335	4.731	9.045
50	15.275	8.108	7.309	5.977	5.3	9.909
60	15.819	8.205	7.529	6.286	5.545	10.139
70	15.864	8.164	7.569	6.403	5.595	10.063
80	15.633	8.199	7.506	6.403	5.543	9.84
90	15.278	8.129	7.387	6.338	5.446	9.571
100	14.88	8.003	7.245	6.238	5.336	9.302
150	12.983	7.36	6.535	5.726	4.93	8.296
200	11.495	6.805	5.964	5.294	4.514	7.388
250	10.374	6.365	5.512	4.923	4.155	6.678
300	9.466	5.997	5.138	4.616	3.86	6.111
400	8.052	5.396	4.542	4.125	3.397	5.255
500	7.019	4.92	4.083	3.743	3.043	4.629
600	6.238	4.54	3.715	3.435	2.761	4.145
700	5.62	4.215	3.411	3.177	2.529	3.758
800	5.121	3.937	3.157	2.958	2.336	3.44
900	4.706	3.695	2.94	2.767	2.169	3.172
1000	4.349	3.48	2.753	2.6	2.023	2.941
1500	3.173	2.695	2.093	1.998	1.518	2.165
2000	2.493	2.186	1.69	1.616	1.211	1.711

5. CONCLUSION

The electron effects cross-sectional ionization of some simple bio-molecules, from ionization threshold to 2keV, the SCOP and CSP-ic methods were successfully employed. SCOP formalism is an effective tool in the mid-to-high energy range of TCS calculations. This particular method for the calculation of TCS data is already employed by several groups. CSP-ic is a semi-empirical method designed to very quickly and fairly accurately find the whole ionization cross section. A large range of atomic and molecular systems have successfully employed this method.

The results achieved by this method for pyridine and pyrimidine are well compatible with Jiao et al [9] and Linert et al [10] experimental data. It is very obvious to correlate maximum Qion with polarization α and (α/IP)1/2 that this cross section confirms the consistency and reliability. The experimenting with large bio-molecules is very complicated and difficult. Calculations are also very complicated to perform using ab initio methods. Methods such as the one presented here are very important in this scenario. In addition, the cross section of ionization provided here can provide a guide to compare their values for others. Such a methodology is also very well integrated into database systems such as the virtual atomic and molecular data centre. We hope that this wok will certainly encourage other groups worldwide to carry out more studies into these bio-molecules that have many applications in the field of biology.

6. REFERENCES

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