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Molecular Mechanics and Quantum Chemical Study on Sites of Action of Sanguinarine Using Vibrational Spectroscopy Based on Molecular Mechanics and Quantum Chemical Calculations

Ricardo Gobato[1] and Alireza Heidari[2*]

[1]Laboratory of Biophysics and Molecular Modeling Genesis, State Secretariat for Education of Parana, Bela Vista do Paraiso, Parana, 86130-000, Brazil

[2]Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA

*Corresponding author: (e-mail: Scholar.Researcher.Scientist@gmail.com; Alireza.Heidari@calsu.us)

Sanguinarine is an alkaloid studied in the treatment of cancer cell proliferation. Found in several plants with *Argemone mexicana* Linn, the plant is used in traditional medicine from several countries with Mexico and India in the natural treatment of wounds, conjunctivitis and as hallucinogen. Due to these studies of this alkaloid, a study was made on a molecular structure of the sanguinarine, through quantum chemistry, via computational methods such as molecular mechanics, PM3, Hartree-Fock, density functional theory and Møller-Plesset. The main site of molecular interaction was determined to be the hydrogen atoms. This has a strong antioxidant potential in its structure. It probably interacts with free radicals reducing their carcinogenic effect on cells. A study of the infrared spectrum complemented the paper.

Key words: Density functional theory; Hartree-Fock, Møller-Plesset; molecular geometry; quantum chemistry, PM3; sanguinarine

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Graphical Abstract

Figures (a) and (b) represent the structure of sanguinarine, obtained via molecular mechanics Mm+ optimized [16 – 20] obtained for computer programs HyperChem 7.5 Evaluation [51]. Below the Figures (c) and (d) representation of the molecular structure of sanguinarine via PM3 [43 – 47] obtained using computer programs HyperChem 7.5 and received using computer programs GAMESS [37]. Images obtained were from the softwares HyperChem 7.5 Evaluation [51] and Avogadro [109].

INTRODUCTION

Sanguinarine has been shown to inhibit proliferation of several types of human cancer cell including multidrug-resistant cells, whereas it has minimal cytotoxicity against normal cells such as neutrophils and keratinocytes [1].

Sanguinarine is an alkaloid studied in the treatment of cancer cell proliferation [1]. Found in several plants with *Argemone mexicana* Linn, the plant is used in traditional medicine from several countries including Mexico and India in the natural treatment of wounds, conjunctivitis and as hallucinogen [2].

Sanguinarine (13-methyl-[1,3]-benzodioxolo[5,6-c]-1,3-dioxolo-[4,5-i]-phenanthridinium chloride) (Figure 1), a benzophenan-thridine alkaloid derived from the plant *Sanguinaria canadensis*, found on *Argemone mexicana* Linn [2] has been shown to have antimicrobial, anti-inflammatory, antioxidant, and anticancer activities [3 – 13].

It was reported to inhibit proliferation of different types of cancer cell, including human prostate carcinoma cells (LNCaP, PC-3 and DU145),

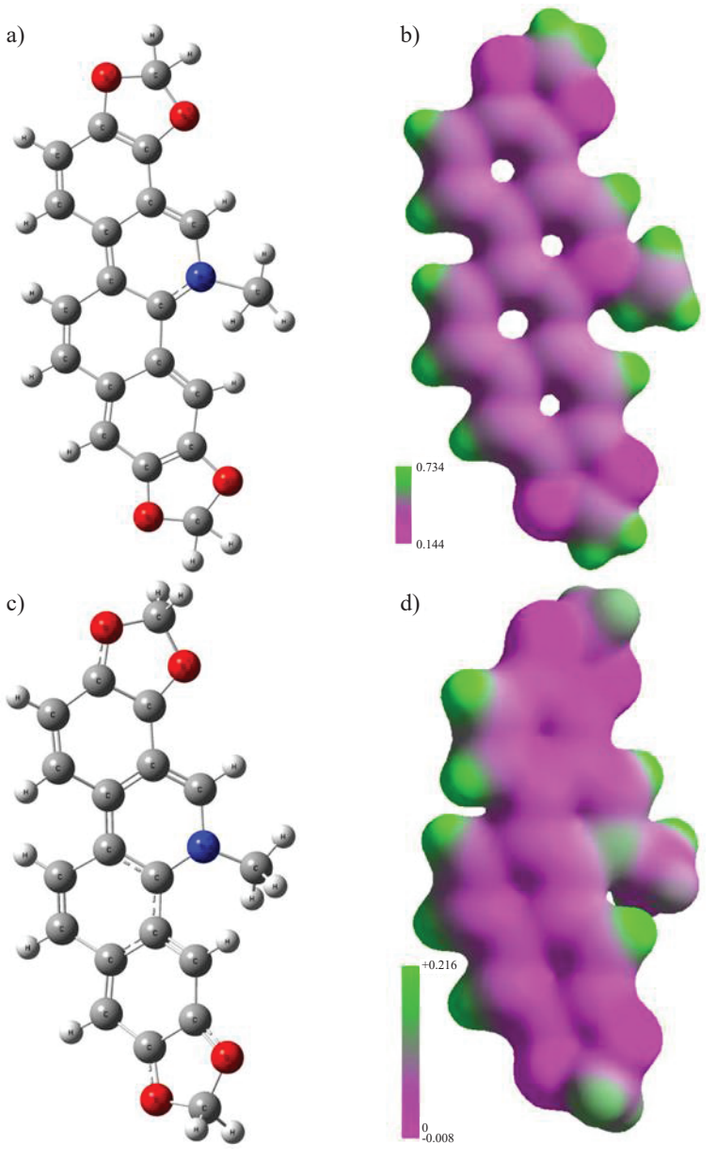

Figure 1. Above the Figures (a) and (b) representation of the structure of sanguinarine, obtained via molecular mechanics Mm+ optimized [16 – 20] obtained for computer programs HyperChem 7.5 Evaluation [51]. Below the Figures (c) and (d) represents of the molecular structure of sanguinarine via PM3 [43 – 47] obtained using computer programs HyperChem 7.5 and obtained using computer programs GAMESS [37]. Images were obtained in the softwares HyperChem 7 Evaluation [51] and Avogadro [109].

multidrug-resistant uterine cervical carcinoma cells, human epidermoid carcinoma A431 cells, human erythroleukemia K562 cells, and the premalignant cell-line HaCaT [8, 9]. However, sanguinarine was found to be less toxic towards normal cells such as normal human epidermal keratinocytes [5].

Alkaloids occupy an important position in chemistry and pharmacology. Among the various alkaloids, berberine and coralyne of the protoberberine group, sanguinarine of the benzophenanthridine group, and aristololactam-b -d-glucoside of the aristolochia group have potential to form molecular

complexes with nucleic acid structures and have attracted recent attention for their prospective clinical and pharmacological utility [14].

Dihydrosanguinarine (DHSA), a benzophenanthridines sanguinarine (SA) biosynthetic precursor and a less toxic benzophenanthridine, was also identified, based on chromatographic properties and further confirmed by gas chromatography coupled to mass spectrometry. The SA and DHSA display antimicrobiae and cytotoxic activities. These alkaloids are accumulated in roots and mature seeds, whereas berberine, a protoberberine alkaloid with antiviral properties, is accrued both in aerial and underground tissues [15].

The alkaloids allocryptopine, dihydrosanguinarine, protopine and sanguinarine have densities of similar negative and positive charges. Already the main local density of positive charges are the hydrogens atoms distributed by molecular contours, and the negative oxygens atoms in its longitudinal ends, and cross for allocryptopine and protopine [2].

Due to these studies of this alkaloid, a study was made on a molecular structure of the sanguinarine, through quantum chemistry, via computational methods such as molecular mechanics, and *ab initio* methods, as PM3 Hartree-Fock, density functional theory and Møller-Plesset [16 – 22]. A study of the infrared spectrum complemented the work.

METHODS

Classical molecular dynamics [16 - 20] using Equation 1:

$$E_{se} = E_{str} + E_{bend} + E_{str\text{-}bend} + E_{oop} + E_{tor} + E_{VdW} + E_{qq} \quad (1)$$

where, the steric energy E_{se} was defined as bond stretching, bending, stretch-bend, out of plane, and torsion interactions and Van der Waals and electrostatic [18 – 23].

The Hartree-Fock self-consistent method, [24] and one of the approaches to electron correlation is the Møller-Plesset (MP) perturbation [16, 24].

The density functional theory (DFT) [25 - 29]. A hybrid exchange-correlation functional is usually constructed as a linear combination of the Hartree–Fock exact exchange functional, given by Equation 2:

$$E_X^{HF} = -\frac{1}{2}\sum_{i,j}\iint \Psi_i^*(\boldsymbol{r}_1)\Psi_j^*(\boldsymbol{r}_1)\frac{1}{r_{12}}\psi_i(\boldsymbol{r}_2)\psi_j(\boldsymbol{r}_2)d\boldsymbol{r}_1 d\boldsymbol{r}_2 \quad (2)$$

and any number of exchange and correlation explicit density functionals. The parameters determining the weight of each individual functional are typically specified by fitting the functional's predictions to experimental or accurately calculated thermochemical data, although in the case of the 'adiabatic connection functionals' the weights can be set a priori [30].

The B3LYP (Becke, three-parameter, Lee-Yang-Parr) [31, 32] exchange-correlation functional is:

$$E_{XC}^{B3LYP} = E_X^{LDA} + a_0\,(E_X^{HF} - E_X^{LDA}) + a_x(E_X^{GGA} - E_X^{LDA}) + E_C^{LDA} + a_c(E_c^{GGA} - E_c^{LDA}) \quad (3)$$

are generalized gradient approximations: the Becke 88 exchange functional [33] and the correlation functional of Lee, Yang and Parr [34] for B3LYP, and E_c^{DA} is the VWN local-density approximation to the correlation functional [35].

The three parameters defining B3LYP have been taken without modification from Becke's original fitting of the analogous B3PW91 functional to a set of atomization energies, ionization potentials, proton affinities, and total atomic energies [36].

The first principles methods (i.e. HF and DFT) discussed above can be implemented with the aid of the GAMESS set of programs to study the electronic structure and to determine the various physical properties of many-electron systems [37]. A basis set is the mathematical description [38] 3-21G, 6-31G, 6-311G, 6-311G** are the basis sets used in the calculations. The functional Becke-style one parameter functional using modified Perdew-Wang exchange and Perdew-Wang 91 correlation is used for DFT Calculations [29, 39].

The vast literature associated with these methods suggests that the following is a plausible hierarchy:

HF << MP2 < CISD < CCSD < CCSD(T) < FCI

The extremes of 'best', FCI, and 'worst', HF, are irrefutable, but the intermediate methods are less clear and depend on the type of chemical problem being addressed [40, 41].

A cluster of six computers were used to perform the calculations from the Laboratory of Biophysics and Molecular Modeling Genesis [22, 42].

The dynamics was held in molecular mechanics force field (Mm+), Equation 1, after the quantum computation was optimized via PM3 [22, 43 – 47] and then by DFT, [16, 29] functional B3LYP [48] and base 6-311G** [22, 29, 37]. It was applied algorithm Polak-Ribiere [49], conjugate gradient, at the termination condition: RMS gradient of 0.1 kcal/A.mol or 405 maximum cycles in vacuum [22, 50].

The first principles calculations have been performed to study the equilibrium configuration of sanguinarine molecule using the Hyperchem 7.5 in trial version [51], Gaussview v.5 a general molecular and electronic structure processing program, an advanced semantic chemical editor, visualization, and analysis platform [52] and GAMESS is a computational chemistry software program [110–250].

FUNDAMENTALS

Geometry Optimization

The dynamics was held in molecular mechanics force field (Mm+), Equation 1 [22, 50]. Molecular properties: electrostatic potential 3D mapped isosurface, mapped function range, minimum 0.144 at maximum 0.734 and minimum –0.008 at maximum +0.216, Mm+ and PM3 methods, respectively. For display range legend, from positive colour lime green to negative colour pink, total charge density contour value of 0.05, gourand shaded surface.

Chemical Formula and Physico-chemical of Sanguinarine

Sanguinarine is a toxic quaternary ammonium salt from the group of benzylisoquinoline alkaloids. It is extracted from some plants, including bloodroot (*Sanguinaria canadensis*), Mexican prickly poppy *Argemone mexicana* [53], *Chelidonium majus* and *Macleaya cordata*. It is also found in the root, stem and leaves of the opium poppy but not in the capsule. Sanguinarine is a toxin that kills animal cells through its action on the Na+-K+-ATPase transmembrane protein [54]. Epidemic dropsy is a disease that results from ingesting sanguinarine [55]. If applied to the skin, sanguinarine kills cells and may destroy tissue. In turn, the bleeding wound may produce a massive scab, called an eschar. For this reason, sanguinarine is termed an escharotic [56].

CAS No. 2447-54-3

Chemical Name: Sanguinarine

Synonyms:13-Methyl-[1,3]benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridinium

Molecular Formula: $C_{20}H_{14}NO_4$

Molar Mass: 332.3295

Density: 0.0184 g/mol

Melting Point: 205–215ºC

Ecotoxicology: LD^{50}; 19.400 $mgDkg^{-1}$ (mouse, intravenous) [57]; 80 $mgDkg^{-1}$ (mouse, subcutaneous) [58]; 18 $mgDkg^{-1}$ (mouse, intraperitoneal) [59]

Solubility: soluble in alcohol, chloroform, acetone, ethyl acetate

UVmax: 234, 283, 325 nm in methyl alcohol [23, 60, 61]

DISCUSSIONS AND CONCLUSIONS

The Figures 1-b and 1-d show the distribution of charges in the sanguinarine molecule. The Figure 1-b represents the molecular dynamics by the Mm+ method, according to Equation 1. The charges range from 0.144, in pink, to 0.734, in lime green, to the distribution of charges in the molecule.

The Figure 1-d represents the molecular dynamics by the PM3 method. The load distribution in the molecule ranges from –0.008 negative, in pink, to +0.216 positive, in lime green, respectively.

By the Mm+ method, Figure 1-b, this indicates that the molecule has a positive potential, having a positive variation of charge distribution, $\Delta\delta = +0.59$, being strongly antioxidant. Likewise in Figure 1-d, by the PM3 method, a positive charge distribution variation, $\Delta\delta = + 0.224$, of lesser intensity, but more suitably distributed, occurs. This method represents the most appropriate displacement of charges in the molecule. As a result we have a better view of the action sites of the molecule. The Mm+ method is inappropriate for the representation of the displacements of charges in the molecule, but efficient in the deduction of an antioxidant molecule.

In Figure X-d it can be verified that the sites of antioxidant action are localized and distributed in the hydrogen atoms throughout the length of the molecule, presenting a strong electric potential of interaction in these sites. The nitrogen atom at the center of the molecule exerts the potential for moderate interaction compared to the hydrogens. Already the four oxygen atoms, located at both ends of the molecule, distributed two by two, have a negative potential, –0.008, represented in pink, also providing an antioxidant interaction, free radicals.

Although the Mm+ and PM3 methods are less sophisticated with others, with more accurate calculations, they give us an adequate vision for what the study proposed, and to determine the main sites of action of sanguinarine.

Analyzing the infrared spectrum, Figure 2, sanguinarine has absorption peaks at the frequencies 3009.4, 2984.3 (cm^{-1}) and 1501.1, 1471.0, 1275.5 and 1060.6 (cm^{-1}) for the method/base, MP2/6-31G [94, 95, 96, 97, 98, 99, 62, 63].

Analyzing the infrared spectrum, Figure 3, sanguinarine has absorption peaks at the frequencies 3115.3, 3109.7 (cm^{-1}) and 1484.6, 1295.4 (cm^{-1}) and 1027.5, 991.1 (cm^{-1}) for the method/base, B3LYP/6-311G** [17, 20, 28, 37, 49, 72, 91, 92] .

Therefore the found principal sites of interactions of the molecule. This has a strong antioxidant potential in its structure. It probably interacts with free radicals reducing their carcinogenic effect on cells.

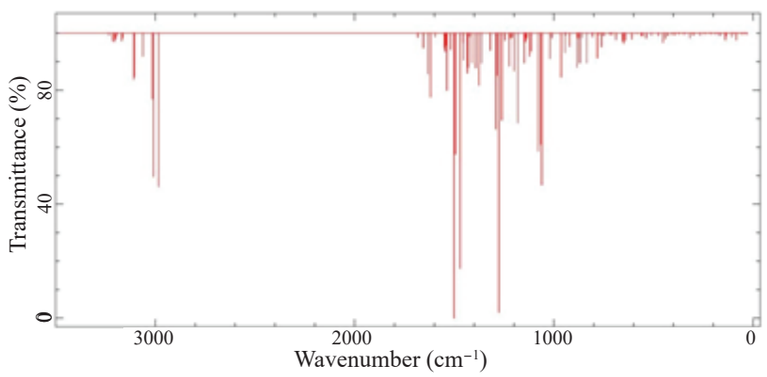

Figure 2. The figure represents the transmittance (%) in function with wavelength (cm^{-1}) for the infrared spectrum of the sanguinarine molecule, after optimization of the geometry with the method/base, B3LYP/6-311G** [17, 20, 28, 37, 49, 72, 91, 92] obtained using computer programs GAMESS [37]. The image was generated using the Avogadro program [109].

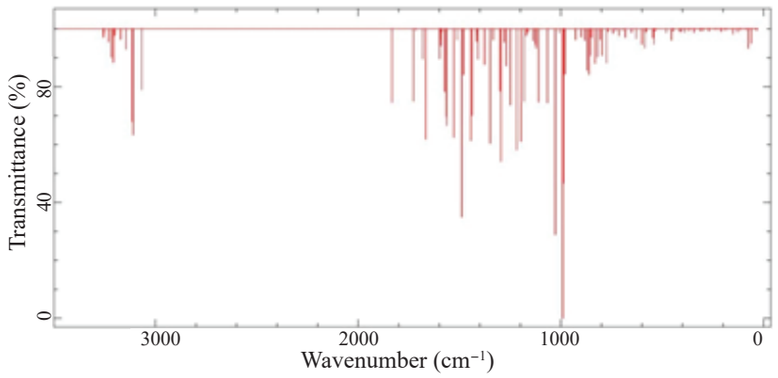

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Table 1. Thermochemical parameters of the sanguinarine obtained.

Methods and base	Thermochemistry parameters		
	$E_{Thermal}$ (Kcal/mol)	CV (cal/mol.K)	S (cal/mol.K)
B3LYP/6-311G	198.375	76.505	143.845
B3LYP/6-311G**	198.160	76.253	144.017
HF/6-21G	212.458	70.198	137.874
MP2/6-31G	200.357	76.830	144.219
B3LYP/STO-3G	207.813	74.557	142.422

Table 2. Table containing the dipole moments of the sanguinarine obtained.

Methods and base	Dipole moment (Debye)			
	X	Y	Z	Total
UHF/6-31G [49, 72, 17, 20, 28, 91, 92, 37]	0.5075	−0.1448	0.9548	1.0910
UBLYP/STO-3G [49, 72, 17, 20, 28, 91, 92, 37]	1.7949	−2.0135	0.7058	2.7882
UB3LYP/6-311** [49, 72, 17, 20, 28, 91, 92, 37]	1.9087	−1.5920	−0.0810	2.4868
UHF/3-21G [49, 72, 17, 20, 28, 91, 92, 37]	0.5075	−0.1448	0.9549	1.0910
UHF/6-311G** [49, 72, 17, 20, 28, 91, 92, 37]	−1.2776	−1.6030	−0.2325	2.0630
UMP2-FC/STO-3G [94, 95, 96, 97, 98, 99, 62, 63]	−1.8508	−1.4547	−0.1789	2.3609
UMP2-FC/6-31G [94, 95, 96, 97, 98, 99, 62, 63]	0.6840	−0.6053	0.8109	1.2214
B3LYP/STO-3G [49, 72, 17, 20, 28, 91, 92, 37, 62, 63]	1.7949	−2.0135	0.7058	2.7882

Table 3. pdb file sanguinarine (PM3 Methods).

HETATM	1	O	1	4.662	4.965	–0.264
HETATM	2	O	2	2.711	5.931	0.420
HETATM	3	O	3	5.744	–4.852	1.084
HETATM	4	O	4	3.970	–5.914	0.105
HETATM	5	N	5	5.145	0.433	–0.378
HETATM	6	C	6	3.986	–0.337	–0.105
HETATM	7	C	7	2.783	0.367	–0.026
HETATM	8	C	8	2.754	1.729	0.168
HETATM	9	C	9	3.941	–1.723	–0.046
HETATM	10	C	10	3.883	2.481	–0.093
HETATM	11	C	11	2.821	–2.401	–0.381
HETATM	13	C	13	3.792	3.963	–0.026
HETATM	14	C	14	1.549	–0.316	–0.553
HETATM	15	C	15	1.594	–1.621	–0.879
HETATM	16	C	16	4.946	–2.426	0.575
HETATM	17	C	17	1.502	2.410	0.694
HETATM	18	C	18	2.520	4.602	0.423
HETATM	19	C	20	4.935	–3.906	0.580
HETATM	22	C	22	6.470	–0.096	–0.716
HETATM	23	C	23	1.372	3.754	0.792
HETATM	24	C	24	4.030	6.203	–0.007
HETATM	25	C	25	5.178	–6.121	0.811
HETATM	26	H	26	5.920	2.453	–0.568
HETATM	27	H	27	0.670	0.230	–0.733
HETATM	28	H	28	0.739	–2.095	–1.267
HETATM	29	H	30	0.692	1.814	1.001
HETATM	31	H	31	1.822	–4.219	–0.950
HETATM	32	H	32	6.370	–0.862	–1.514
HETATM	33	H	33	6.951	–0.556	0.173
HETATM	34	H	34	7.154	0.695	–1.094
HETATM	35	H	35	0.485	4.186	1.151
HETATM	36	H	36	4.580	6.752	0.789
HETATM	37	H	37	4.010	6.820	–0.932
HETATM	38	H	38	5.880	–6.724	0.195
HETATM	39	H	39	4.972	–6.657	1.764
CONECT	1	13	24			
CONECT	2	18	24			
CONECT	3	20	25			
CONECT	4	21	25			
CONECT	5	6	12	22		
CONECT	6	5	7	9		
CONECT	7	6	8	14		
CONECT	8	7	10	17		
CONECT	9	6	11	16		
CONECT	10	8	12	13		
CONECT	11	9	15	19		
CONECT	12	5	10	26		
CONECT	13	1	10	18		
CONECT	14	7	15	27		
CONECT	15	11	14	28		
CONECT	16	9	20	29		
CONECT	17	8	23	30		
CONECT	18	2	13	23		
CONECT	19	11	21	31		
CONECT	21	4	19	20		
CONECT	22	5	32	33	34	
CONECT	23	17	18	35		
CONECT	24	1	2	36	37	
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CONECT	39	25				
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