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A DFT study for the structures and electronic spectra of 2,3-dihydropyridine-4-ones

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ABSTRACT

The molecular structure and electronic spectra of eleven dihydropyridones were theoretically studied utilizing density functional (DFT) method. The structures were optimized using B3LYP/6-31G(d,p) level of theory. The conformations of the molecules were analyzed with respect to substituents. The central six-membered dihydropyridone ring adopted a half-chair conformation. The geometries did not differ significantly except for conformations of the phenyl or styryl substituents. The only substituents that affected the structure of the central ring are those which have conjugation overlap with the -C=C-C=O system within the ring. Dipole moments and natural charges were calculated and it was found that in most cases substitution leads to higher dipoles, and both methyl and phenyl substituents have the same effect on the atomic charge distribution leading to decrease the atomic charge on the substitution site. Wiberg bond indices were also calculated and used to analyze the substitution effect on the electronic properties of the molecules. It is concluded that substitution on atoms that are not a part of the N-C=C-C=O system have practically no effect on both structural and electronic properties of the molecules. The electronic spectra were also calculated using the ZINDO method. The predicted spectra are in good agreement with experimental spectra concerning the long wavelength absorption band. The electronic transitions were either pure HOMO to LUMO transitions or comprises components of HOMO to LUMO and other transitions like H-1 to L, H to L+2, H-1 to L+1, H-2 to L+1.

1. Introduction

Dihydropyridones are important intermediates for the synthesis of natural products, particularly alkaloids, and have been investigated extensively as valuable building blocks for the construction of piperidines, perhydroquinolines, indolizidines, and other alkaloids ring systems possessing a wide range of biological and pharmacological properties [1]. Many synthetic ways were applied for their production, which includes different routes like hetero Diels-Alder reactions or stepwise, formal [4+2] transformation involving imines [2-4]. Comins has exploited the addition of Grignard reagents to 1-acyl-4-methoxy pyridimium salts [5-9]. They have been also synthesized via cyclization of α,β-unsaturated 1,3-diketones in acidic medium [10]. A facile route to functionalized dihydropyridones has been developed via formal [5C+1N] annulationsof α-alkynoyl ketene-(S,S)-acetals with aliphatic amines [11]. We previously reported the microwave-assisted formation of 2,3-dihydro-4-pyridinones from curcumins and simple primary amines [1,12].

Dihydropyridones are known as the most important class of calcium channels modulators [13]. They are also known for a variety of biological activities like antiproliferative and antitubiolin activities [14], and as potential selective inhibitors of receptor tyrosin kinase [15]. In addition they have the ability to induce leukaemic cell differentiation [16] and antimalarial activity [17] as well as their anticonvulsant activity against acutely elicited Seizures [18].

Theoretical studies using AM1 semi empirical method [13,19] depicted a twisted boat conformation for 3,4-dihydropyridones and that the 4-phenyl substituents in these compounds lies at a pseudo-axial position. This was confirmed by x-ray analyses [13,19] which showed also that the 4-phenyl ring is orthogonal to the main plane of the molecule concerned. The work presents a theoretical study for the investigation of the structural and electronic properties of 2,3-dihydropyridin-4-ones and the effect of the substitutes on these properties.

2. Experimental

UV-Visible spectra of compound **9** were taken from previously published work [20], while those of the compounds **10** and **11** were recorded from dilute solutions [5×10^{-5} M] in 1 cm quartz cuvettes, utilizing a T80+ UV/visible spectrophotometer.

The quantum chemical calculations were performed for 11 dihydropyridones (shown in Figure 1) with the Firefly QC package [21], which is partially based on the GAMESS (US) [22] source code. Geometrical optimizations were carried out using Density Functional Theory (DFT) method at B3LYP/6-31G(d,p) level of theory. B3LYP refers to the combination of functional hybrid exchange of Becke [23] with functional correlation gradient of Lee and Yang [24].

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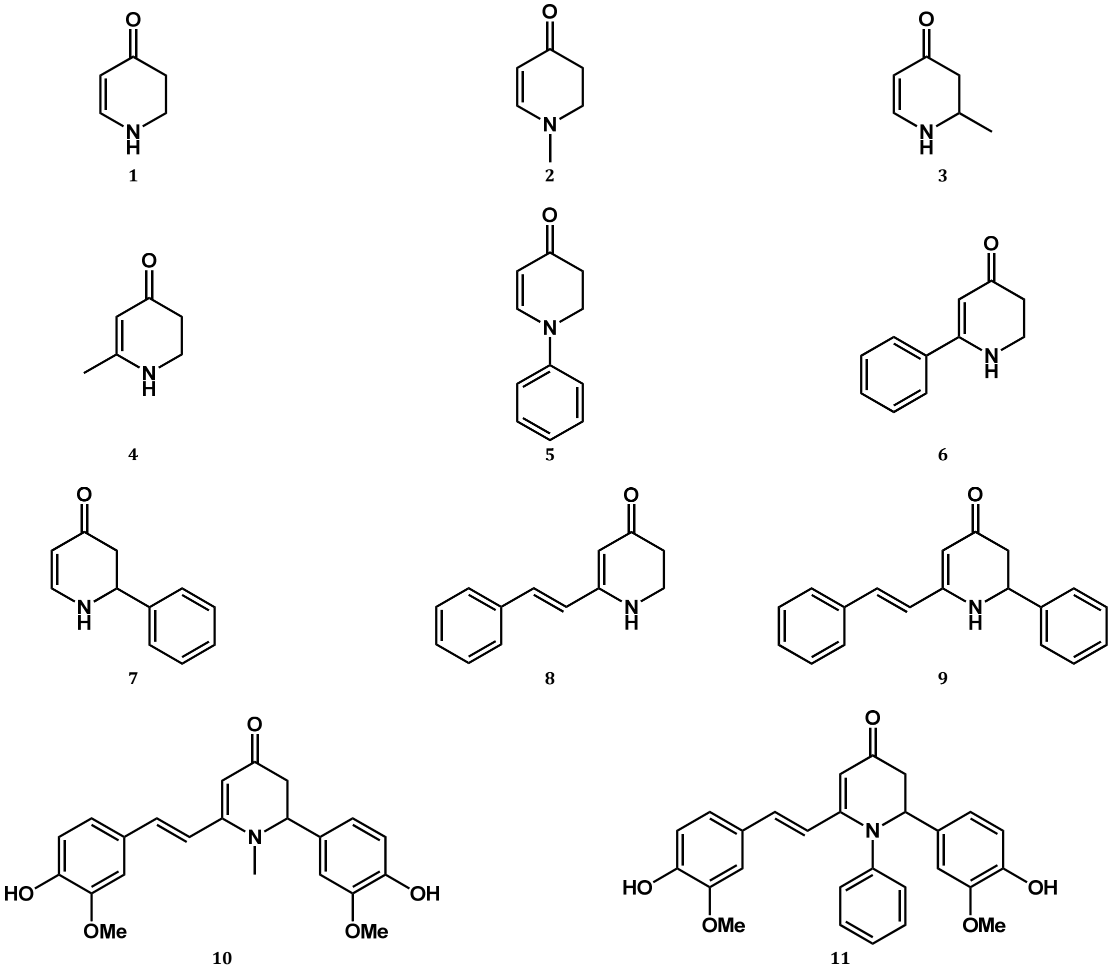


Figure 1. The chemical structures of dihydropyridones studied.

For the same level of theory, vibrational frequencies for all molecules were calculated to verify that the structure converged to a minimum using the zero imaginary frequencies criterion. Molecular orbitals, as well as the charges assigned to each atom, were made by natural population analysis phase of the natural bond analysis [25], using NBO software version 5 at B3LYP/6-31G(d,p) level of theory. Excited states were done with the semi empirical ZNDO method using the ORCA program package [26].

3. Results and discussion

3.1. Structures of dihydropyridones

The structures of dihydropyridones studied are shown in Figure 1. Selected structural properties calculated theoretically in this study are given in Table 1. Some of representative optimized geometries are given in Figure 2.

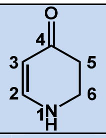
B3LYP has long been recognized as a good tool due to the fact that it is computationally less demanding for inclusion of electron correlation and could provide accurate geometries [27]; meanwhile, a previous study [28] also indicated, that for pyridinthiones, a related compound to pyridines, the predicted structural properties with B3LYP method were agreed well with the experimental X-ray data.

Accordingly B3LYP exchange-correlation functional is adopted for structural analysis. The geometries, with respect to molecule **1**, do not differ significantly, except for the conformation of the phenyl rings and the styryl residue at the atoms N1, C2 and C6. The values obtained for the lengths of bond of the same nature do not differ significantly within the molecules **1**-**4**. In these molecules the carbonyl bond length is 1.226 Å while the bonds C3-C4 and C2-C3 have lengths within the ranges 1.454-1.458 and 1.360-1.368 Å, respectively. Introducing the styryl group at the atom C2 leads to some changes in the geometry, for example in molecule **8** the bonds C=O, C4-C3 and C2-C3 become 1.228, 1.452 and 1.373 Å in length, respectively. This also is the case with molecules **9**-**11**. In general for molecules **8**-**11** the single bonds become shorter while double bonds become longer which presumably due to conjugation overlap. The six-membered dihydropyridone ring is bent at the atoms N1 and C5 adopting a half chair conformation (Figure 2) in which N1 is out of the main plane of the ring. The phenyl rings substituted at the atoms N1, C2 and C6 in all cases have their planes tilted to the plane of the dihydropyridone ring by dihedral angles within the range 36-77 °. The values calculated for the bonds C=O, N1-C2, C2-C3 and C3-C4, C4-C5 and C5-C6 in molecule **10** are in good agreement with reported experimental from X-ray data [29] which were 1.218, 1.390, 1.365, 1.456, 1.488 and 1.511 Å, respectively.

3.2. Polarity and charge distribution

The dipole moments obtained for the studied molecules are given in Table 2.

Table 1. Calculated bond lengths, valence angles and dihedral angles of dihydropyridones studied.

											
Molecule no	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
Bond lengths											
N1-C2	1.368	1.367	1.368	1.375	1.370	1.380	1.369	1.382	1.404	1.406	1.407
C2-C3	1.361	1.363	1.360	1.366	1.363	1.370	1.360	1.373	1.372	1.371	1.372
C3-C4	1.458	1.454	1.457	1.455	1.455	1.455	1.457	1.452	1.458	1.457	1.456
C4-C5	1.536	1.534	1.535	1.535	1.533	1.533	1.536	1.533	1.529	1.531	1.529
C5-C6	1.529	1.528	1.526	1.527	1.527	1.526	1.539	1.527	1.533	1.533	1.534
C6-N1	1.463	1.465	1.468	1.462	1.475	1.463	1.468	1.462	1.504	1.490	1.507
Valence angles											
N1-C2-C3	123.8	124.9	123.8	121.7	124.6	121.6	123.9	121.2	121.4	121.5	121.3
C5-C6-N1	109.7	111.2	108.4	109.6	111.3	110.0	108.3	109.8	110.0	110.9	109.8
Dihedral angles											
N1-C2-C3-C4	-4.4	-5.0	-4.2	-4.4	-7.1	-4.2	-4.2	-3.4	-10.7	-10.3	-10.4
C2-C3-C4-C5	-4.2	-4.8	-4.2	-3.3	-5.0	-3.9	-4.2	-3.8	4.3	4.1	4.5
C3-C4-C5-C6	32.4	32.3	32.8	31.7	33.9	32.2	32.7	31.6	29.7	29.0	29.3
C4-C5-C6-N1	-51.6	-50.7	-51.5	-51.8	-51.7	-52.2	-51.6	-52.0	-57.8	-56.9	-57.5
C5-C6-N1-C2	45.2	42.6	45.3	46.9	41.4	46.8	45.5	47.7	53.6	53.0	53.7
C6-N1-C2-C3	-17.7	-15.3	-18.4	-19.0	-12.3	-18.7	-18.5	-20.1	-19.3	-19.1	-19.8

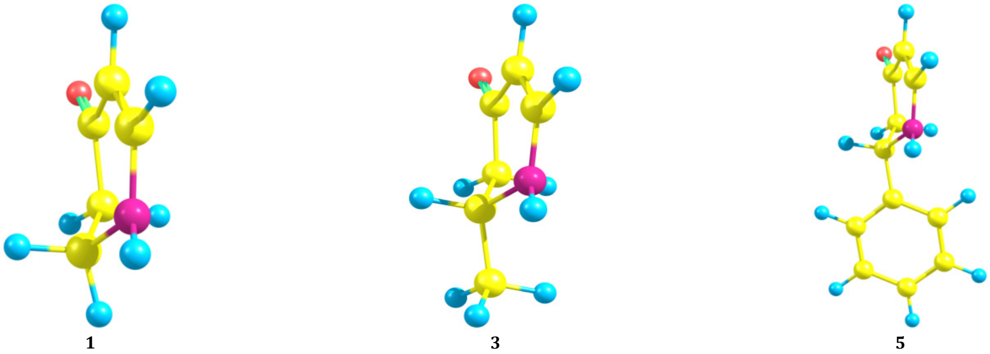


Figure 2. Representation of molecules **1**, **2** and **5** obtained from gas geometry optimization carry out B3LYP/6-31G(d,p) level of theory.

The substituted compounds in general are more polar than the parent molecule. In all cases (except for molecules **4** and **8**) the dipole moment is larger than that of molecule **1**. When the substituent is a phenyl group, substitution on C2 and C6 leads to higher dipole compared to substitution on N1. On the other hand when the substituent is methyl group the substitution at N1 and C2 leads to higher dipole compared to substitution at C6. The situation for the aromatic substituent is that substitution that leads to less symmetric molecule gives higher dipole, while in the case of methyl group mesomeric and inductive effects play the main role in determining the value of dipole moment.

The relative distribution of charges may indicate preferential binding sites on the hydrophilic or lipophilic regions of the receptor and can also determine sites of receptor regions at which polarity could be more easily induced. The atomic charges were calculated by natural population analysis using the same level of theory as for the geometrical optimizations. The values obtained for selected atoms in molecules studied are summarized in Table 2. The most negative atomic areas on the molecule become more sensitive to acidic coordination. Four sites have importance when taking charge distribution into account, namely N1, C2, C=O and C6. For N1, both phenyl and methyl groups have the same effect on the atomic charge distribution and lead to decrease the atomic charge. Practically they have identical effect since the atomic charge decreases from -0.630 in molecule **1** to -0.475 in molecules **2** and **3**. The atoms C2 and C6 are the most feasible for charge alteration upon substitution change and the charge difference is within 0.191-0.216 compared to 0.092 for N1. As is the case for N1 the phenyl and methyl groups have the same decreasing effect on the charge at C2 and C6 atoms. The charge on the carbonyl oxygen is substantially constant with changing substituent.

3.3. Wiberg bond index

Wiberg bond index affords a numerical picture about the kind of the bond and could be used to trace the electronic conjugation in molecules and interpreting changes in electronic structures and electronic spectra upon changing the substituent. The calculated Wiberg bond indices are gathered in Table 3.

As could be seen from Table 4 the most affected bonds by changing substitution are those directly connected to the atoms at which substitution takes place. These bonds are N1-C2, C2-C3 and C6-N1.

Substitution on N1 by phenyl or methyl group decreases Wiberg bond index of the bond N1-C2. This means that substitutions lead to transfer the electron density from the substituent to N1 by the inductive or mesomeric effect. This is more noticeable if the atoms N1 and C2 are both substituted.

Substitution on C2 affects both N1-C2 and C2-C3 bonds. According to Wiberg bond index, C2-C3 is not a pure double bond due to its conjugation with the carbonyl group and the unsaturated substituent on C2. It is clear from Table 4 that noticeable change in Wiberg bond index of this bond appears with substituent that conjugate with it leading to a decrease in its double bond character.

Table 2. Calculated dipole moments (deby) and atomic charges for dihydropyridones studied obtained at B3LYP/6-31G(d,p) level of theory.

Molecule	Dipole moment	Atomic charge						
		N1	C2	C3	C4	C5	C6	C=O
1	5.375	-0.630	0.043	-0.442	0.542	-0.562	-0.269	-0.567
2	6.080	-0.475	0.104	-0.407	0.515	-0.476	-0.167	-0.584
3	5.365	-0.635	0.047	-0.440	0.528	-0.559	-0.060	-0.567
4	5.598	-0.634	0.250	-0.436	0.527	-0.560	-0.265	-0.572
5	5.350	-0.430	0.045	-0.431	0.522	-0.561	-0.257	-0.565
6	5.507	-0.529	0.234	-0.417	0.525	-0.560	-0.265	-0.568
7	5.376	-0.534	0.047	-0.439	0.527	-0.548	-0.068	-0.564
8	5.822	-0.624	0.213	-0.414	0.521	-0.559	-0.265	-0.572
9	5.289	-0.477	0.204	-0.378	0.528	-0.559	-0.062	-0.557
10	5.373	-0.481	0.208	-0.382	0.531	-0.565	-0.070	-0.562
11	6.838	-0.474	0.204	-0.382	0.526	-0.557	-0.060	-0.562

Table 3. Wiberg bond indices for dihydropyridones studied obtained at B3LYP/31G(d,p) level of theory.

Molecule	Wiberg bond index						
	N1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-N1	C=O
1	1.2014	1.6451	1.1307	0.9688	1.0110	0.9639	1.7290
2	1.1874	1.6306	1.1365	0.9720	1.0176	0.9446	1.7165
3	1.1991	1.6466	1.1302	0.9695	0.9958	0.9475	1.7290
4	1.1774	1.6013	1.1367	0.9687	1.0109	0.9636	1.7230
5	1.1686	1.6392	1.1317	0.9682	1.0140	0.9293	1.7279
6	1.1948	1.6491	1.1291	0.9681	0.9834	0.9503	1.7302
7	1.1948	1.6491	1.1291	0.9681	0.9834	0.9503	1.7302
8	1.1586	1.5471	1.1475	0.9694	1.0108	0.9667	1.7120
9	1.0799	1.5806	1.1253	0.9707	0.9926	0.9082	1.7294
10	1.0827	1.5826	1.1292	0.9686	0.9950	0.9317	1.7259
11	1.0757	1.5747	1.1305	0.9703	0.9922	0.9036	1.7236

Table 4. Calculated and observed band maxima, intensities of the dihydropyridones studied.

Molecule	Excited state	Coefficient	Theoretical λ, nm	Oscillator strength	Experimental λ, nm
1	H → L	0.69152	272	0.4834	--- [a]
2	H → L	0.69251	283	0.4773	---
3	H → L	0.69065	275	0.5061	---
4	H → L	0.69065	275	0.5061	---
5	H → L	0.67326	301	0.6857	---
6	H → L	0.61457	274	0.4764	---
	H-1 → L	0.30324			
7	H → L	0.67685	299	0.6836	---
	H → L+2	-0.10338			
8	H → L	0.67819	337	0.8999	---
	H-1 → L+1	0.14204			
9	H → L	0.67263	335	1.1508	353
10	H → L	0.66998	347	1.1586	348
	H-2 → L+1	0.13266			
11	H → L	0.66843	349	1.1453	358

[a] Data not available.

Wiberg bond index decreases from 1.645 in molecule **1** to 1.183, 1.159, 1.083, 1.080 and 1.076 in molecules **7**-**11**, respectively. This suggests that an electron charge transfer occurs from the substituent to this bond. In this case the styryl group has more effect than the phenyl group.

Concerning C6, substitution effect is less pronounced and although it leads to some change on the bond C6-N1, it has practically no effect on the other sites of the molecule. This is of importance sequence when trying to discuss the electronic spectra of the molecules studied as it implies that substitution at C6 has practically no effect on these spectra.

3.4. Electronic spectra and electronic structure

The UV-Visible spectra of the molecules **9**, **10** and **11** have main bands at 353, 348 and 358 nm respectively in ethanol. The UV-Vis spectrum of compound 10 is presented in Figure 3.

Despite their expanded structures, the electronic spectra of these molecules are not differing considerably from the spectrum of the less structurally expanded molecule named half curcumin. This molecule which has isoelctronic structure to the styryl part of the molecules **9**, **10** and **11** has an absorption band at 340 nm in ethanol. To discuss the origin of the spectra, singlet excited-state calculations were performed on B3LYP/6-31G(d,p) optimized geometries using the semi empirical ZINDO method for the molecules **9**, **10** and **11**. The spectra of molecules **1** to **8** were also calculated for comparison. The results are listed in Table 4.

The predicted spectra are in good agreement with the experimental spectra. The electronic transitions are either pure HOMO to LUMO transitions as is the case with molecules **1**, **2**, **3**, **4**, **5**, **9** and **11** or comprises components of HOMO to LUMO and other transitions like H-1 to L, H to L+2, H-1 to L+1, H-2 to L+1 as is the case of the molecules **6**, **7**, **8** and **10**, respectively.

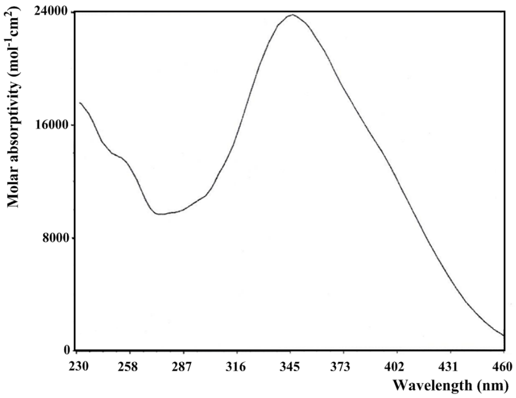
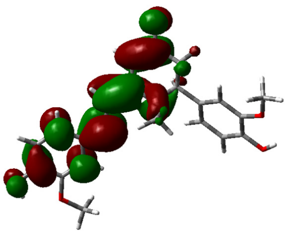
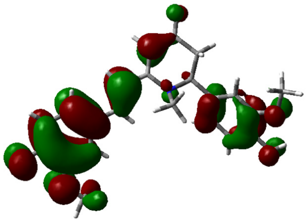


Figure 3. The UV-Vis spectrum of compound **10** in ethanol.



LUMO



HOMO

Figure 4. Representation of the HOMO and LUMO orbitals of molecule **10** determined by B3LYP/6-31G(d,p) level of theory.

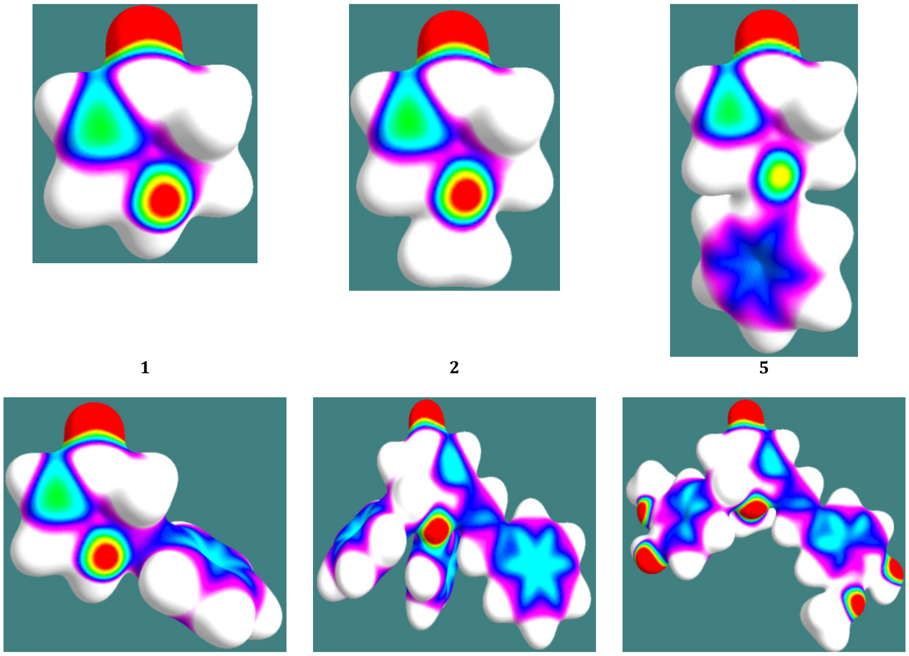


Figure 5. The electrostatic potential (ESP), mapped on an electron density surface that was given by (SCF) for the molecules **1**, **2**, **3**, **9** and **10**. The positively charged regions are blue and green while regions with higher electron density are mapped from red to blue.

3.5. Effect of substituent on the electronic spectra

For methyl as substituent, it has the largest effect when the substitution occurs at N1, so the calculated band is shifted from 272 in molecule **1** to 283 nm in molecule **2**. Substitution by methyl at the atoms C2 and C6 essentially has no important effect and the predicted bands in molecules **3** and **4** are 275 nm. As it is the case with the methyl group the phenyl group has its largest effect at the position N1 compared to C2 and C6 positions. Substitution with phenyl ring at N1 leads to much more red shift and the band occurs at 301 nm. Substitution at C2 has essentially the same effect and the band appears at 299.5 nm. This red shift is a result of the conjugation through the electronic systems N1-C2-C3-C4=O and C2-C3-C4=O, respectively, in which the electron density transferred from the phenyl groups to these electronic systems. Wiberg bond index values supported this conclusion. In accordance with the conclusion based on Wiberg bond index, substitution of phenyl group at position C6 has negligible effect on the spectra and the band in molecule **7** occurs at 274 nm. Substitution a styryl group at C2 has more pronounced effect on the spectra and molecule **8** has its main absorption band at 337 nm (Table 4) which is comparable in position to that predicted for molecule **9**. In molecule **10** the predicted band red shifted with respect to that of molecule **9** as result of the presence of the hydroxyl group in the styryl substituent which expands the electronic structure even more leading to more conjugation effect. The frontier orbitals, namely the HOMO and the LUMO of molecule **10** calculated for optimized B3LYP/6-31G(d,p) level of theory are shown in Figure 4.

The HOMO orbital is spread over the whole skeleton of the molecule and is antibonding at the bond C5-C6 while the LUMO orbital spreads over the styryl side only. This may accounts for the finding that the aromatic substituent at C6 has negligible effect on the main absorption band in the electronic spectra of the molecules studies.

3.6. Isoelectronic potential surfaces

The electronic potential surfaces obtained for some representative molecules are depicted in Figure 5. The large red region around the carbonyl, hydroxyl and alkoxyl groups and N1 is indicative of the existence of higher negative electrostatic potential indicating favorable interaction energy with electronic density acceptors. This suggest that dihydropyridones that are derived from curcumin (molecules **10** and **11**) are probably more active compare to the other studied dihydropyridones due to the presence of sites that are strong attractors of electron density.

4. Conclusion

The results obtained in this work lead to the conclusion that for substitution to be affective in compounds studied it must be occurring at the atoms N1 and C2. Substitution on C6 practically has no effects on the structural or the electronic properties. Accordingly the electronic spectra are solely affected by substituent on N1 and C2. According to isoelectronic potential surfaces dihydrpiridones seem to be more active compared to the other molecules due to the presence of sites that are strong attractors of electron density.

References

[1]. Saeed, B. A.; Radhi, W. A.; Elias, R. S. *Tetrahedron Lett.* **2010**, *51*, 2798-2880.
[2]. Waldman, H.; Braun, M. *J. Org. Chem.* **1992**, *57*, 4444-4451.
[3]. Huang, Y; Rawal, V. H. *Org. Lett.* **2000**, *2*, 3321-3323.
[4]. Alaimo, P. J.; O'Brien, R.; Johanson, A. W.; Slauson, S. R.; O'Brien, J. M. *Org. Lett.* **2008**, *10*, 5111-5114.
[5]. Comins, D. L.; Zhang, Y.; Joseph, S. P. *J. Org. Chem.* **1999**, *1*, 657-659.
[6]. Comins, D. L.; Kueth, J. T.; Hong, H.; Lakner, F. J. *J. Am. Chem. Soc.* **1999**, *121*, 2651-2651.
[7]. Comins, D. L.; Ollinger, G. C. *Tetrahedron Lett.* **2001**, *42*, 4115-4118.
[8]. Young, D. W.; Comins, D. L. *Org. Lett.* **2005**, *7*, 5661-5664.
[9]. McCall, W. S.; Grillo, T. A.; Comins, D. L. *J. Org. Chem.* **2008**, *73*, 9744-9751.
[10]. Mc Donald, F. K., Burnell, D. J. *J. Org. Chem.* **2009**, *74*, 6973-6979.
[11]. Dong, D.; Bi, X.; Liu, Q.; Cong, F. *Chem. Commun.* **2005**, 3580-3582.
[12]. Elias, R. S.; Saeed, B. A.; Saour, K. Y.; Al-Masoudi, N. A. *Tetrahedron Lett.* 2**008**, *49*, 3049-3051.
[13]. Ochoa, E, ; Suarez, M.; Verdicia, Y, ; Pita, B.; Martin, N.; Quinteiro, M.; Seoane, C.; Soto, J. L.; Duque, J.; Pomes, R. *Tetrahedron* **1998**, *54*, 12409-12420.
[14]. Magedov, I. V.; Manapadi, M.; Ogasawara, M. A.; Dhwan, A. S.; Rogdi, S. *J. Med. Chem.* **2008**, *51*, 2561-2570.
[15]. Hu, E.; Tasker, A.; White, R. D.; Kunz, R. K.; Hutman, J. *J. Med. Chem.* **2008**, *51*, 3065-3068.
[16]. Pierce, J. B.; Ariyan, Z. S.; Ovenden, G. S. *J. Med. Chem.* **1981**, *25*, 131-136.
[17]. Yeats, C. L.; Betchelor, J. F.; Capon, E. C.; Cheesman, N. J.; Fry, M. *J. Med. Chem.* **2008**, *51*, 2845-2852.
[18]. Revas, F. M.; Stables, J. P.; Murphree, L.; Edwanker, R. V.; Edwanker, C. R. *J. Med. Chem.* **2009**, *52*, 1795-1798.
[19]. Ochoa, E.; Suarez, M.; Verdicia, Y.; Gonzales, L.; Martin, N.; Quinteiro, M.; Seoane, C.; Soto, J. L. *J. Heterocycl. Chem.* **1996**, *33*, 103-107.
[20]. Sugiyama, N.; Yamamato, M.; Kashima, C. *Bull. Chem. Soc. Jpn.* **1970**, *43*, 3937-3938.
[21]. Alex A. Granovsky, Firefly version 7. 1. G, http://classic.chem.msu.su/gran/firefly/index.html
[22]. Scmidt, M. W.; Baldridge, K. K.; Boatz, J. A.; Elbert, S. T.; Gordon, M. S.; Jensen, J. H.; Koseki, S.; Matsunaga, N.; Nguyen, K. A.; Su, S.; Windus, T. L.; Dupuis, M.; Montgomery, J. A. *J. Comput. Chem.* **1993**, *14*, 1347-1363.
[23]. Becke, A. D. *J. Chem. Phys.* **1997**, *107*, 8554-8560.
[24]. Lee, C.; Yang, W.; Parr, G. R. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1998**, *37*, 785-789.
[25]. Carpenter, J. E.; Weinhold, F. *J. Mol. Struct. Theochem.* **1998**, *169*, 41-62.
[26]. ORCA - An ab initio, Density Functional and Semiempirical program package, Version 2.8; University of Bonn, 2011.
[27]. Wang, Y. H.; Zou, J. W.; Zhang, B.; Lu, Y. X.; Jin, H. X.; Yu, Q. S. *J. Mol. Struct. Theochem*. **2005**, *755*, 31-37.
[28]. Zhang, Y. A.; Monga, V.; Orvig, C.; Wang, Y. A. *J. Phys. Chem. A.* **2008**, *112*, 3231-3238.
[29]. Saeed, B. A.; Saour, K. Y.; Elias, R. S.; Xiaodi, D. *Am. J. Appl. Sci.* **2010**, *7*, 916- 919.