We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

6,900
Open access books available

185,000
International authors and editors

200M
Downloads

Our authors are among the

154
Countries delivered to

TOP 1%
most cited scientists

12.2%
Contributors from top 500 universities



WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?
Contact book.department@intechopen.com

Numbers displayed above are based on latest data collected.
For more information visit www.intechopen.com



9

Structural and Vibrational Properties and NMR Characterization of (2'-furyl)-Imidazole Compounds

Ana E. Ledesma[1], Juan Zinczuk[2],
Juan J. López González[3] and Silvia A. Brandán[4*]
[1]*INQUINOA-UNSE, Facultad de Agronomía y Agroindustrias, Universidad Nacional de Santiago del Estero, Santiago del Estero*
[2]*Instituto de Química Rosario (CONICET-UNR), Facultad de Ciencias Bioquímicas y Farmacéuticas, Rosario, Santa Fé*
[3]*Departamento de Química Física y Analítica, Facultad de Ciencias Experimentales, Universidad de Jaén, Jaén*
[4]*Cátedra de Química general, Instituto de Química Inorgánica, Facultad de Bioquímica, Química y Farmacia, Universidad Nacional de Tucumán, San Miguel de Tucumán, Tucumán, República*
[1,2,4]*Argentina*
[3]*Spain*

1. Introduction

The furylimidazoles compounds have a great importance in biochemistry and pharmacology because many of them present interesting properties[1,2]. They are also found in artificial compounds[3], such as agrochemicals,[4] pharmaceuticals[5], dyes[6], plastics, solvents, photographic chemicals, electronics, corrosion inhibitors,[7] preservatives, and polymers[8]. They can be used in synthetic organic chemistry as building blocks, due to their presence as key structural units in many natural products and in important pharmaceuticals. For example, the nature of the N- atoms in the imidazole molecule makes possible an extraordinary variety of reactions and this is the main reason for the great biological importance of the amino acid, histidine.

* Corresponding Author
1 Salerno & Perillo, 2005
2 Szabo, 2002.
3 Gould et. al., 2006.
4 Higashio & Shoji, 2004.
5 Monterrey et al., 2004.
6 Ooyama et al., 2007.
7 Rohwerder & Michalik, 2007.
8 Stroganova, et al., 2000.

Polymers of these compounds, which have potential as semi-conducting material are of great importance, because of their good thermal and chemical stability and relative ease of functionalization, which potentially permit the fine tuning of their physical and electronic properties[9]

In fact, these compounds provide one of the best studied examples of annular tautomerism, such as the 4(5)-substituted imidazoles[10,11,12]. Recently, the theoretical and experimental studies on structure, electronic and vibrational properties for the (2'-furyl)-imidazole series were reported by us[13,14,15,16,17].

Examination of the spectroscopic data for the each furanics molecules indicated that Nuclear Magnetic resonance spectroscopy, coupled with IR spectroscopy, was potentially the best analytical technique to provide confirmatory structural evidence for their formation. On the other hand, in general, the chemical shifts for the substituted imidazole ring, relative to the unsubstituted rings, suggest that the mesomeric effect of the five-membered rings contributes less to the interaction between two rings than does their inductive effects. It would indicate which rings is more electron-withdrawing in its overall electronic effect than the furan ring, as well as observed in the pyridine-thiophenes and furans[18]. The downfield shifts of the ^{13}C NMR signals for the carbon atom at the point of substitution on the imidazole ring would be explicate of the significant inductive electron-withdrawing effects of the 2-heteroaryl rings.

For this, reason for predicting the reactivity of this molecules due to the different position of the substituent, in this chapter, a comparison of the structural and vibrational properties of the four molecules belong to the (2'-furyl)-imidazole series was performed in order to evaluate the experimental and theoretical results based on B3LYP calculations by using 6-31G* and 6-311++G** basis sets. The optimized geometries and frequencies for the normal modes of vibration were calculated using both theory levels. For a complete assignment of the compounds, the DFT (Density functional Theory) calculations were combined with the scaled quantum mechanical force field (SQMFF) methodology[19,20,21] in order to fit the theoretical wavenumbers to the experimental ones. In all molecules of this series, the changes in the chemical shifts of the hydrogen and carbon atoms were also studied. In addition, the electronic properties of those molecules were evaluated by means of natural bond orbital (NBO) and atoms in molecules (AIM) studies in order to analyze the nature and magnitude of the intramolecular interactions. In this chapter, the experimental and theoretical studies of

[9] Nevin et al., 2008.
[10] Bellina et al., 2007.
[11] Popov et al., 2004.
[12] Sztanke et al., 2005.
[13] Ledesma et al., 2008.
[14] Ledesma et al., 2010.
[15] Ledesma et al., 2009a.
[16] Ledesma et al., 2009b.
[17] Zinczuk et al., 2009.
[18] Jones & Civcir, 1997.
[19] Rauhut & Pulay,1995a.
[20] Rauhut & Pulay, 1995b.
[21] Kalincsak & Pongor, 2002.

structures and vibrational properties of 2-(2′-furyl)-imidazole, 4-(2′-furyl)-imidazole, 5-(2′-furyl)-imidazole and N-(2′-furyl)-imidazole are compared and analyzed.

2. Structure and properties of the (2'-furyl)-imidazole series

2.1 Structural analysis

All compounds of this series are present in two different stable conformations according to the syn and anti position of the oxygen atom with respect to the N—H bond, named syn and anti conformers, respectively, as show in Figure 1.

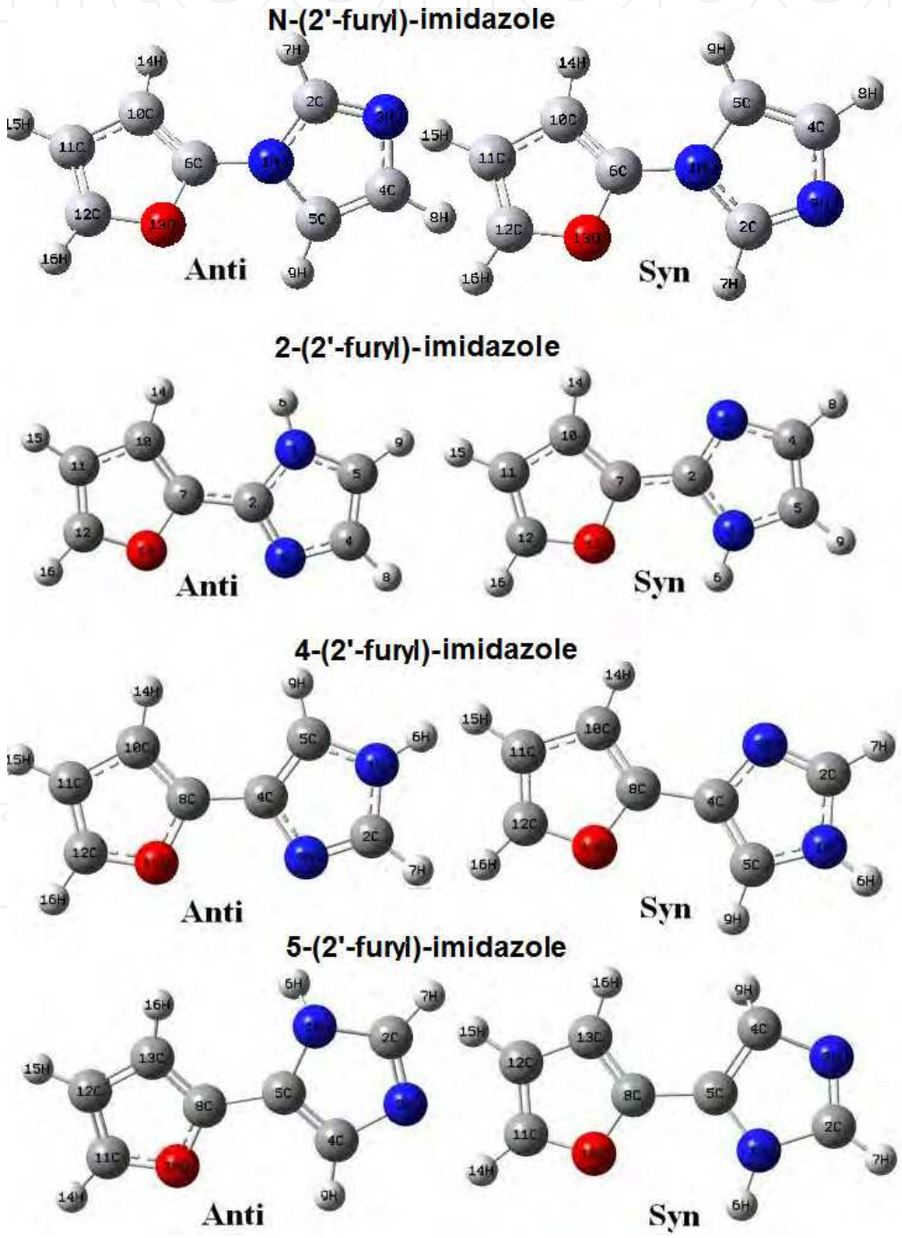


Fig. 1. Molecular structures of the (2′-furyl)-imidazole series

Experimentally, all molecules of this series have different characteristics or they are solid of different nature. Thus, the first series's member, N-(2′-furyl)-imidazole, is a liquid at room temperature and probably the two conformers are present in it. For the second series's member, 2-(2′-furyl)-imidazole, the crystallography analysis shows that both conformers are present in the crystalline lattice with equal occupancy and alternated arrangement in the N-H---N bonded polymeric chains along the crystal [101] direction. Only three units of the polymeric structure are shown in Figure 2. Finally, the 4-(2′-furyl)-imidazole and 5-(2′-furyl)-imidazole compounds are present in a tautomeric mixture in the solid state as a white power.

The calculation indicates that both conformers of N-(2′-furyl)-imidazole have C_1 symmetries, in the 2-(2′-furyl)-imidazole they have C_1 and C_s symmetries, while in the remaining molecules all conformers present C_s symmetries.

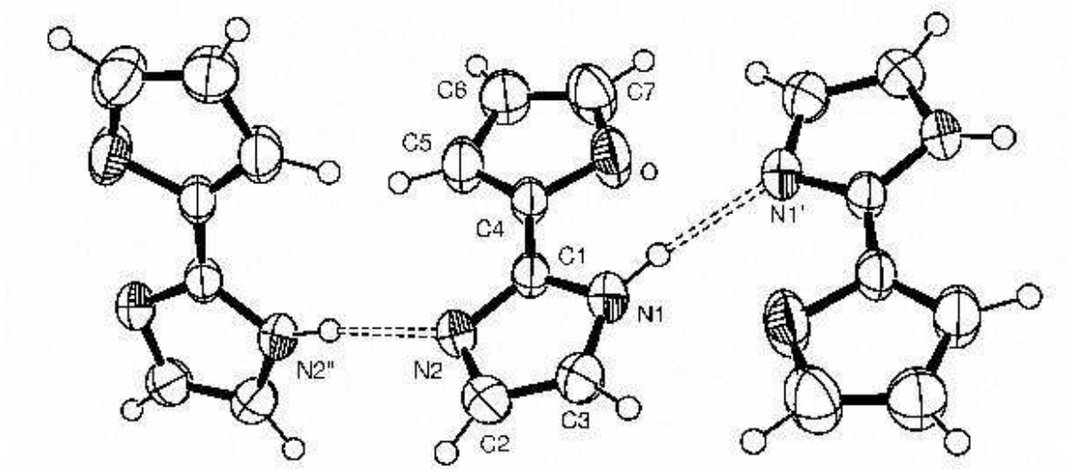


Fig. 2. View of a N—H---N bonded polymer chain in solid 2-(2′-furyl)-imidazole. The central monomer is related with the right and left side monomers through a crystallographic inversion center and a two fold axis rotation, respectively. The H-bonding is indicated by dashed lines

Table 1 shows a comparison of the total energy and dipole moment values for all molecules by using the 6-31 and 6-311++G** basis sets at B3LYP theory level. Note that all predicts values are similar between them and, only for the N-(2′-furyl)-imidazole, the calculation predicts that the anti conformation is the most stable, while that for the remaining compounds the syn conformation is the most stable.

The comparison between the experimental geometrical parameters (obtained for 2-(2′-furyl)-imidazole) with the corresponding theoretical values are shown in Table 2. The analysis shows that the length of C=C bond of the furan ring, does not change for all molecules, while the length of C=C bond of the imidazole ring varies according the following order: (4)5-(2′-furyl)-imidazole > N-(2′-furyl)-imidazole > 2-(2′-furyl)-imidazole. This trend is explained taking into account the next of this bond respect to the furan ring, since in the first molecule that bond is in alpha position respect to C=C bond corresponding to the furan ring, favoring the electronic delocalization, while in the remaining structures those bonds

are in beta and gamma positions, respectively. This effect also explains the observed tendency for the C-N bond next to furan ring.

N-(2′-furyl)-imidazole						
Conf.	*E* (B3LYP/6-31G*) (Hartrees)	*ΔE* kJ/mol	*μ*	E (B3LYP/6-311++G**) (Hartrees)	*ΔE* kJ/mol	*μ*
anti	-455.03903057	0	3.63	-455.16243953	0	3.82
syn	-455.03834901	1.8	3.80	-455.16160715	2.2	3.99
2-(2′-furyl)-imidazole						
anti	-455.04955562	15.30	3.90	-455.17597057	15.42	4.08
syn	-455.05531501	0.0	2.97	-455.18185872	0.0	2.92
4-(2′-furyl)-imidazole						
anti	-455.0490477	12.25	3.94	-455.1754201	12.54	4.10
syn	-455.0537122	0.0	3.23	-455.1802136	0.0	3.24
5-(2′-furyl)-imidazole						
anti	-455.0512980	5.73	3.90	- 455.1772971	5.68	4.17
syn	-455.0534867	0.0	3.37	- 455.1794579	0.0	3.42

[a] In Debyes

Table 1. Total Energies (*E*) and relatives (*ΔE*) calculates (in Hartree), dipolar moments (*μ*) for all structures

Another very important difference between all series members is related to the dihedral angles. Thus, the angles values are 180° and 0° for the 2 and 4(5) isomers, while for the first isomer those values are between 30-40° and 160-170° respectively.

The stability of the different conformers were investigated using the Electrostatic Surface Potential, ESP maps[22,23] because these surfaces are important for describing overall molecular charge distributions as well as anticipating sites of electrophilic addition[23]. The molecular ESP values for the anti and syn conformers of each member's series by using 6-31G* basis set are given in Table 3 while Figure 3 shows the ESP maps for all conformers of this series. The red color represents negatively charged areas of the surface (i.e., those areas where accepting an electrophile is most favorable). The atomic charges derived from the ESPs (MK) and natural atomic charges were also analyzed and the corresponding values are given in Table 4. Note that the most important differences in all cases are observed on the imidazole ring. The important factor responsible for the lesser stability of same conformer is

[22] Sadlej-Sosnowska, 2007.
[23] Vektariene at al., 2007.

the electrostatic repulsion between the two lone pairs on N and O. Hence, a strong red color on both atoms is observed in the corresponding Figure 3.

Parameters	2-(2′-furyl)-Imidazole#	4-(2′-furyl)-Imidazole*		5-(2′-furyl)-Imidazole*		N-(2′-furyl)-Imidazole*	
Distances (Å)		*anti*	*syn*	*anti*	*syn*	*anti*	*syn*
$C=C_{furan}$	1.343 1.319	1.369 1.359	1.365 1.358	1.369 1.358	1.369 1.357	1.360 1.356	1.360 1.356
$C=C_{imidazole}$	1.345	1.379	1.377	1.380	1.380	1.367	1.367
C-N	1.374 1.369 1.342	1.382 1.377 1.366	1.383 1.378 1.366	1.385 1.373 1.367	1.385 1.372 1.366	1.380 1.379 1.390	1.380 1.379 1.392
C-C	1.413	1.429	1.432	1.431	1.431	1.435	1.435
C-O	1.362	1.361 1.364	1.365 1.370	1.365 1.367	1.364 1.367	1.370 1.359	1.372 1.360
C, N-$C_{inter-ring}$	1.438	1.450	1.445	1.439	1.439	1.392	1.389
Ángles (Degrees)							
N1-C2-N3	111.6 (2)	111.8	111.8	111.6	105.3	111.8	111.7
C2-N3-C4	105.6 (2)	105.5	105.3	105.6	111.8	105.6	105.7
N3-C4-C5	108.7 (2)	110.2	110.0	110.7	107.3	110.7	110.7
C4-C5-N1	108.4 (2)	105.1	110.8	104.6	104.4	105.3	105.4
C5-N1-C2	105.6 (2)	107.2	107.3	107.3	111.0	106.3	106.3
C6-C10-C11	107.1 (2)	106.6	106.4	106.4	106.5	105.6	105.5
C10-C11-C12	106.6(24)	106.0	106.0	106.2	106.2	106.5	106.6
C11-C12-O13	110.6(4)	110.5	110.6	110.3	110.4	110.0	111.1
C12-O13-C6	106.6(6)	107.3	106.9	107.3	107.2	106.5	106.6
O13-C6-C10	109.2 (2)	109.5	109.8	109.5	109.5	110.2	110.0

obtained by Ray X diffraction
* Theoretical parameters calculated at B3LYP/6-311++G** level of theory

Table 2. Geometrical parameters for all compounds of the series

Átom	N-(2′-furyl)-imidazole		2-(2′-furyl)-imidazole		4-(2′-furyl)-imidazole		5-(2′-furyl)-imidazole	
	anti	*syn*	*anti*	*syn*	*anti*	*syn*	*anti*	*syn*
N 1	-18.27	-18.26	-18.28	-18.28	-18.28	-18.28	-18.28	-18.28
C 2	-14.68	-14.68	-14.68	-14.67	-14.68	-14.68	-14.68	-14.68
N 3	-18.37	-18.37	-18.38	-18.38	-18.38	-18.37	-18.37	-18.37
C 4	-14.72	-14.72	-14.71	-14.72	-14.71	-14.71	-14.72	-14.72
C 5	-14.70	-14.70	-14.70	-14.71	-14.70	-14.70	-14.69	-14.69
H 6	-1.10	-1.10	-0.97	-0.98	-0.97	-0.97	-0.97	-0.98
C 7	-1.07	-1.08	-1.07	-1.10	-1.07	-1.07	-1.10	-1.10
H 8	-14.63	-14.63	-14.69	-14.68	-14.69	-14.69	-14.67	-14.67
H 9	-1.07	-1.07	-1.07	-1.07	-1.07	-1.07	-1.07	-1.07
C 10	-14.72	-14.72	-14.75	-14.74	-14.75	-14.75	-14.73	-14.73
C 11	-14.72	-14.72	-14.75	-14.73	-14.75	-14.75	-14.73	-14.73
C 12	-14.67	-14.67	-14.70	-14.68	-14.70	-14.70	-14.68	-14.68
O 13	-22.22	-22.22	-22.26	-22.24	-22.26	-22.25	-22.24	-22.23
H 14	-1.07	-1.07	-1.10	-1.09	-1.10	-1.11	-1.08	-1.08
H 15	-1.07	-1.07	-1.10	-1.09	-1.10	-1.10	-1.08	-1.08
H 16	-1.06	-1.06	-1.09	-1.07	-1.09	-1.08	-1.08	-1.07

Table 3. Molecular electrostatic potentials for all members of the series calculated at B3LYP/6-31G* level of theory

For the N-(2′-furyl)-imidazole a region can be observed where the delocalization of charge decrease (blue region between two rings) due to the breaking-off planarity of the both rings, while the remain molecules show π-electron delocalizated surfaces that evidence stables aromatic systems, being smaller for the N-(2′-furyl)-imidazole compound.

These results can be related with the energies of the HOMO and LUMO for all molecules. Table 4 shows the comparison of the HOMO and LUMO orbitals energies values as well as the GAP energies values of them.

The corresponding values for the N-(2′-furyl)-imidazole show that this compound is the most stable of the series, as expected, because it presents the longer GAP values. On the

other hand, the calculated energy HOMO orbital value for 4-(2'-furyl)-imidazole is higher than the other ones due to the fact that it is the most reactive compound of this series.

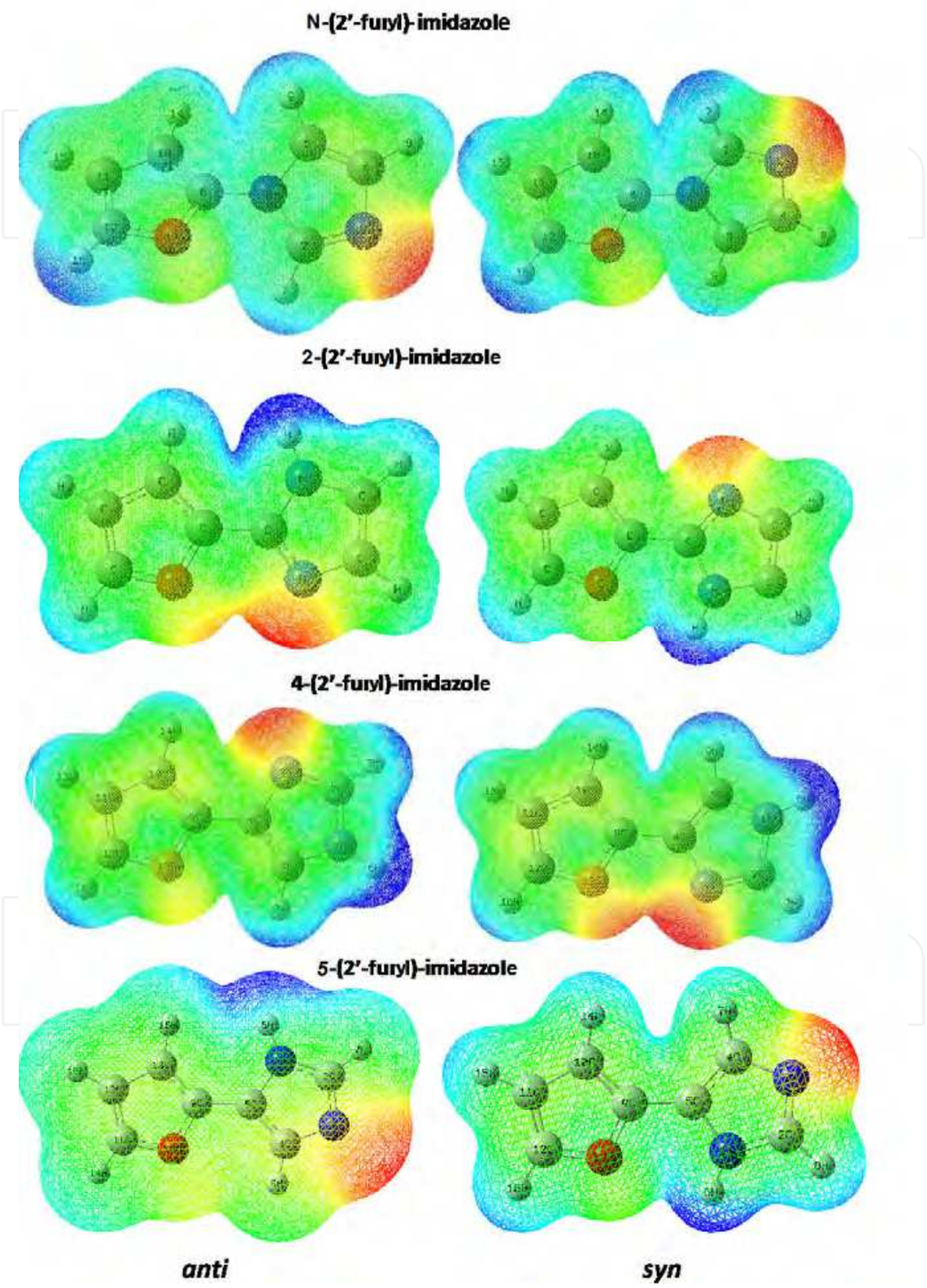


Fig. 3. Electrostatic Surface Potential calculated on the molecular surface of the conformers for all compounds of the series. Color, in u.a.: from red -0.103 to blue 0.103.

Orbital	N-(2′-furyl)-Imidazole		2-(2′-furyl)-Imidazole		4-(2′-furyl)-Imidazole		5-(2′-furyl)-Imidazole	
	syn	*anti*	*syn*	*anti*	*syn*	*anti*	*syn*	*anti*
HOMO	-0.21	-0.22	-0.19	-0.19	-0.18	-0.18	-0.19	-0.19
LUMO	-0.01	-0.01	-0.01	-0.01	0.00	0.00	-0-01	-0-01
GAP	0.20	0.20	0.17	0.17	0.18	0.18	0.17	0.17
GAP (kJ/mol)	535.0	542.9	464.2	464.2	495.4	495.4	466.8	466.8

Table 4. HOMO and LUMO orbitals Energíes (u.a.) and gap of energy (u.a.) for all members of the series

2.2 Nuclear magnetic resonance characterization

All nuclear magnetic resonance spectra were recorded for diluted solutions in DMSD-d_6 and the calculated chemical shifts of the ^{1}H NMR and ^{13}C NMR for the two conformers of each compound were obtained by GIAO method[24] using the B3LYP/6-311++G** theory level, as it is usually used for chemical shift NMR calculations on reasonably large molecules[25,26]. The calculations have been performed using the geometries optimized for this theory level and by using TMS as reference. A comparison of the results is present in Table 5 and it shows that for 2-(2′-furyl)-imidazole the calculated ^{13}C chemical shifts from CSGT method are in accordance with the experimental values, while the closest values were obtained with the GIAO method and the 6-311++G** basis set. Furthermore, the calculated shifts with both methods for the C(2), C(7), and C(1) atoms are higher than the experimental values. One important observation is that the results obtained from the conformational average have better agreement with data experimental, as expected, due to the presence of the two conformers in the solution. On the other hand, a comparison is present in Table 6 and it shows the calculated shifts with the two methods used where, for the H atom show significant differences with the experimental results. The addition of the polarization and diffuses functions at the basis set improves the results; however, the CSGT method predicts shifts practically different than the GIAO method for this atom. This disparity would be attributed to the fact that the GIAO method uses basis functions which depend on the field while the CSGT method achieves gauge invariance by performing a continuous set of gauge transformations, for each point, obtaining an accurately description of the current density[17,18].

The peak belonging to H atom of the N–H bond appears at 11.37 ppm. A small shift of these peaks towards lower fields implies the existence of some intermolecular interaction between nonbonding electrons.

Table 7 shows the experimental and calculated chemical shifts for 4(5)-(2′-furyl)-imidazole. These chemical shift values indicate that in the H atom is weakly held by two imidazole rings. At an intermediate rate of exchange, the H atom is partially decoupled, and a broad

[24] Ditchfield, 1974.
[25] Cheeseman et al., 1996.
[26] Keith & Bader, 1993.

N–H peak results. The most intense peak of this spectrum belongs to the C atom of the reference, while the following four peaks belong to the C atoms of the furyl group. The calculated chemical shifts are in agreement with the experimental ones, with RMSD values of 2.53 and 0.32 ppm for the ^{13}C and ^{1}H atoms, respectively. The agreement with our experimental data in these solvents is good, except for the H atom of the H–N bond in chloroform. This is because the calculations are for the gas phase, while the experimental values are for the $CDCl_3$ solution, where the molecular interactions are important. It is important to mention that the registered NMR spectra at room temperature and low temperature were not sufficient to identify the tautomeric mixture of 1, because the speed of exchange of protons is higher than the response time of NMR.

Chem. Shift	C(10)	C(11)	C(5)	C(12)	C(2)	C(4)	C(7)
Exp.[a]	106.4	111.6	122.5	122.5	138.0	142.5	146.2
syn [b]	93.9	100.7	102.8	119.7	126.4	129.6	135.5
[c]	99.2	104.1	107.9	123.6	132.0	135.3	141.3
[d]	103.8	111.4	113.4	132.6	141.0	143.8	135.9
anti [b]	97.5	102.5	102.6	119.6	126.7	127.9	136.4
[c]	102.3	105.7	107.9	123.7	132.3	134.1	142.4
[d]	107.8	113.6	113.5	132.9	141.3	142.1	151.5
AVERAGE[b]	98.7	101.6	102.7	119.7	126.6	128.7	135.9
[c]	100.8	104.9	107.9	123.9	132.1	134.7	141.8
[d]	105.8	112.5	113.5	138.8	141.1	142.9	151.0

[#] In DMSO-d_6; [##]Related to TMS; [a] Experimental; [b] GIAO 6-31G**; [c] CSGT 6-31G**; [d] GIAO 6-311++G**

Table 5. Experimental[#] and calculated[##] ^{13}C chemical shifts in ppm

Chem. shifts	H C(10)	H C(11)	H C(12)	H C(4)	H C(5)
Exp.[a]	6.57	6.82	6.82	7.10	7.71
syn [b]	6.02	6.09	7.16	6.50	6.87
[c]	3.60	3.79	4.74	4.10	4.38
[d]	6.26	6.70	7.37	6.70	7.05
anti [b]	6.70	6.16	7.05	6.47	6.85
[c]	3.88	4.30	4.66	4.12	4.33
[d]	3.92	6.38	7.25	6.70	7.03
AVERAGE[B]	6.36	6.12	7.10	6.49	6.86
[c]	3.74	4.04	7.70	4.11	4.35
[d]	5.09	6.32	7.31	6.70	7.04

[#] In DMSO-d_6; [##]Related to TMS; [a] Experimental; [b] GIAO 6-31G**; [c] CSGT 6-31G**; [d] GIAO 6-311++G**

Table 6. The experimental and calculated ^{1}H chemical shifts in ppm

Position	δ C		δ H, multiplicidad in ppm	
	Exp.[b]	Theor[c]	Exp.[b]	Theor[c]
10	104.3	103.55	6.54 (d, J=3.3 Hz, 1H)	6.29
11	111.3	108.82	6.43 (dd, J=1.8, J=3.3 Hz, 1H)	6.17
5	114.7	111.03	7.33 (d, J=0.9 Hz, 1H)	6.98
4	131.6	132.40		
12	135.6	138.1	7.71 (d, J=0.9 Hz, 1H)	7.26
2	141.2	141.35	7.39 (dd, J=0.9, J=1.5 Hz, 1H)	7.16
8	149.0	153.20		
N-H			11.37 (bs,1H)	7.86

[a] B3LYP/6-311++G**, average values; [b] In $CDCl_3$; [c] Related to TMS

Table 7. Experimental and calculated Chemical shifts (in ppm) for 4(5)-(2'-furyl)-imidazole

A comparison between the experimental and calculated chemical shifts for the C and H atoms for N-(2'-furyl)-imidazole are given in Tables 8 and 9, respectively. The calculation results show that the GIAO method reproduces quite well the ^{13}C and ^{1}H experimental chemical shifts values as shown by the calculated root mean square deviations (RMSD) values for each conformer. Furthermore, the shifts of the H atoms for both structures are similar in both conformers and practically equal to the average values. As expected, the latter values have a better agreement with the experimental data, probably because both conformers are present in the solution.

Chem. Shifts	C10	C11	C5	C4	C12	C2	C6	RMSD
Exp.[a]	96.2	111.6	117.5	130.0	135.4	138.9	144.5	
anti [b]	96.5	112.7	117.7	133.2	135.4	140.4	149.5	*0.9*
syn [b]	93.6	112.7	116.1	132.9	134.7	139.1	149.7	*0.9*
AVERAGE[B]	95.0	112.7	116.9	133.1	135.0	139.7	149.6	*0.9*

[a] Related to $DCCl_3$; [b] GIAO, B3LYP/6-311++G*

Table 8. ^{13}C Experimental and calculated Chemical shifts (in ppm) for N-(2'-furyl)-imidazole

Chem. Shifts	H14	H15	H8	H9	H16	H7	RMSD
Exp.[a]	**6.14**	**6.44**	**7.13**	**7.22**	**7.26**	**7.81**	
anti [b]	5.87	6.29	7.05	7.05	7.16	7.30	*0.10*
syn [b]	5.73	6.28	6.81	7.01	7.08	7.62	*0.10*
AVERAGE[B]	5.80	6.29	6.93	7.03	7.12	7.46	*0.09*

[a] Related to $DCCl_3$; [b] GIAO, B3LYP/6-311++G*

Table 9. ^{1}H Experimental and calculated Chemical shifts (in ppm) for N-(2'-furyl)-imidazole

3. Vibrational analysis

For this analysis the vibrational frequencies were separated in two groups, the first group corresponds to the skeletal vibrations ring and the second ones to those vibrations related to the C-H groups, both are show in Tables 10 and 11, respectively. The analysis shows that the frequencies values for the C=C stretching of the imidazole ring is according to the respective length bonds. Furthermore, the frequencies values for the C=N stretching mode are longer for the N-(2'-furyl)-Imidazole, due to the highest p character of bound, which impedes the resonance effects between two rings. Changes in the frequencies values related to the C-O stretching modes are not observed, in accordance with the corresponding length bonds, where the variations were only observed for the imidazole ring. The vibrational ring modes are practically observed in the same region for all series molecules, while the corresponding torsions are in agreement with the imidazole ring in all series members and they are next to the reported values for the imidazole compound.

Description	N-(2'-furyl)-Imidazole	2-(2'-furyl)-Imidazole	4-(2'-furyl)-Imidazole	5-(2'-furyl)-Imidazole
	anti, syn	*anti, syn*		
ν $(C=C)_{furano}$	1625 1511	1625 1504	1638 1467	1638 1491
ν $(C=C)_{imidazol}$	1521	1547, 1538	1516	1518
ν (C=N)	1493	1462,1453	1484	1484
ν (C-N)	1305, 1285 1224 1104	1428, 1393 1365, 1358 1159, 1133	1304 1275 1120	1307 1342 1119
ν (C-C)	1374	1380	1378	1342
ν (C-O)	1162 1065	1181 1075	1162 1067	1162 1067
βR_f	904 892	897 894	885 868	885 868
βR_i	984 910	965,952 927,911	942 916	964 918
τR_i	656 650	665 650	685 655	655 634
τR_f	615 594	624,622 593,591	621 591	624 591
ν $(C, N-C)_{int}$	409	402	404	404

Table 10. Experimental Vibrational Frequencies for all modes of imidazole and furan rings of the series.

A notable difference between the frequencies of the C-H stretching modes is observed. The rotating of the imidazole ring with the furan ring increase or decrease the frequencies assigned to the alilic hydrogen.

Description	N-(2′-furyl)-imidazole	2-(2′-furyl)-imidazole	4-(2′-furyl)-imidazole	5-(2′-furyl)-imidazole
	anti, syn	*anti, syn*		
ν C-H	3155			
	3151	3149	3137	3137
	3126	3118	3122	3120
	3122	3109	3101	3101
	3120	3088	3081	3081
	3104	3011	3037	3037
B C-H	1410			
	1348	1300,1260	1225	1251
	1245	1229,1222	1204	1235
	1112	1106,1102	1081	1204
	1059	1084	1050	1081
	1014	1010	1006	1006
γ C-H	882			
	871	883,862	830	865
	816	843,835	813	813
	793	810,797	800	800
	737	748,733	750	776
	733	719	715	725

Table 11. Experimental vibrational frequencies for C-H groups

4. Conclusions

All compounds studied in this chapter were synthesized and only, the 2-(2'-furyl)-1H-imidazole compound was isolated as a crystalline solid, which allowed the molecular structure's determination by means of the ray X diffraction. In all cases, the theoretical method that better reproduces the experimental data is the B3LYP/6-311++G** combination, for this, the calculated molecular geometries and vibrational spectra were performed at this theory level. Each molecule presents two stable conformations, anti and syn, according to the orientations of the furan and imidazole rings. The calculations predicted that the conformation syn is the most stable, with exception of the isomer one, for which the anti conformer was the most stable. The distances among both rings only present appreciable changes for the isomer one which because the union in this case is by means of the C-N instead C-C like in the remaining ones. In the 4(5)-(2'-Furyl) Imidazole isomers, the infrared spectra at low temperature allowed the complete assignment of the both member's series. The PEM analysis shows that when the π-electron delocalizated surface is longer, the hydrogen atoms are less retained by the carbon atoms and, for this reason, an increasing in

the respective length bonds is observed. Due to this, the H atom is very labile in consequence can be easily substituted. The later behavior is observed when the frequencies of the C-H groups in the N-(2'-Furyl)-imidazole are analyzed in reference to the other compounds of this series. Finally, the N-(2'-Furyl)-imidazole compound is the most stable member of the series.

5. References

[1] Salerno, A. ; Perillo, I. A., ^{1}H- and ^{13}C-NMR Analysis of a Series of 1,2-Diaryl-1H-4,5-dihydroimidazoles, 2005, *Molecules*, Vol 10, N° 2 (Febrary 2005), pp 435–443, ISSN: 1420-3049

[2] Szabo, B., Imidazoline antihypertensive drugs: a critical review on their mechanism of action, 2002, *Pharmacol. Therapeut*. Vol 93, N° 1 (January 2002) , pp. 1-35(35). ISSN: 0163 -7258

[3] Gould, S. L.; Kodis, G.; Liddell, P. A.; Palacios, R. E.; Brune, A.; Gust, D.; Moore, T. A; Moore, A. L., Artificial photosynthetic reaction centers with carotenoid antennas, *Tetrahedron* 2006, Vol 62, N° 9 (February 2006), pp 2074-2096. ISSN: 0040-4020

[4] Higashio, Y.; Shoji, T.; Erratum to "Heterocyclic compounds such as pyrrole, pyridines, piperidine, indole, imidazol and pyrazines" [Appl. Catal. A: Gen. 221 (2001) 197–207], *Applied Catalysis A: General* 2004, Vol 260, N° 2 (March 2004), pp 249-251. ISSN: 0926-860X

[5] Monterrey I. G.; Campiglia, P.; Lama, T.; La Colla, P.; Diurno, M. V.; Grieco, P.; Novellino, Synthesis of new pyrido [4,3- g and 3,4- g]quinoline-9,10-dione and dihydrothieno [2,3-g and 3,2-g]quinoline-4,9-dione derivatives and preliminary evaluation of cytotoxic activity, *E. Arkivoc* 2004 (v) 85 (February 2004), pp 85 – 96. ISSN: 1551-7004

[6] Ooyama, Y.; Mamura, T.; Yoshida, K., A facile synthesis of solid-emissive fluorescent dyes: dialkylbenzo[b]naphtho[2,1-d]furan-6-one-type fluorophores with strong blue and green fluorescence emission properties, *Tetrahedron Lett.* 2007, Vol 48 (June 2007), pp 5791–5793. ISSN: 0040-4039

[7] Rohwerder, M.; Michalik, A., Conducting polymers for corrosion protection: What makes the difference between failure and success?, *Electrochimica Acta*. 2007, Vol 53, N°20 (December 2007), pp 1300-1313. ISSN: 0013-4686

[8] Stroganova, T. A.; Butin, A. V.; Sorotskaya, J. N.; Kul'nevich, V. G., (Aryl)(2-furyl)alkanes and their derivatives, 20. Synthesis of symmetric bis- and tris(2-furyl)methanes, *E. Arkivoc 2000* (iv), 1, (September 2000), pp 641 – 659. ISSN 1551-7012.

[9] Nevin K.; Dilek E.; Pervin U. C., Synthesis and characterization of novel heterosubstituted pyrroles, thiophenes, and furans, *E. Arkivoc 2008* (xii) (March 2008), pp 17-29. ISSN 1551-7012.

[10] Bellina, F.; Cauteruccio, S.; Rossi, R., Efficient and Practical Synthesis of 4(5)-Aryl-1H-imidazoles and 2,4(5)-Diaryl-1H-imidazoles via Highly Selective Palladium-Catalyzed Arylation Reactions, 2007, *J. Org. Chem*., Vol 72, N° 22 (October 2007), pp 8543–8546. ISSN: 0022- 3263

[11] Popov, S. A.; Andreev, R. V.; Romanenko, G. V.; Ovcharenko, V. I.; Reznikov, V. A., Aminonitrone-N-hydroxyaminoimine Tautomeric Equilibrium in the Series of 1-

Hydroxy-2-imidazolines, 2004, *J.Mol. Struct.,* Vol 697, N° 1–3 (April 2004), pp 49-60. ISSN: 0022-2860

[12] Sztanke, K.; Fidecka, S.; dzierska, E. K; Karczmarzyk, Z.; Pihlaja, K.; Matosiuk, D., 2005, *Eur. J.Med. Chem., Vol* 40, N° 2, pp 127. ISSN: 0223- 5234

[13] Ledesma, A. E.; Brandán, S. A.; Zinczuk, J.; Piro, O. E.; López González, J. J.; Ben Altabef, A., 2008, Structural and vibrational study of 2-(2'-furyl)-1H- imidazole, *J. Phys. Org. Chem.*, Vol 21, N° 12 (December 2008), pp 1086–1097, ISSN: 1099-1395

[14] Ledesma, A. E.; Zinczuk, J.; López González, J. J.; Ben Altabef, A.; Brandán, S. A., Structural, vibrational spectra and normal coordinate analysis for two tautomers of 4(5)-(2'-furyl)-imidazole, *J. Raman Spectrosc.*, 2010, Vol 41, N°5 (Mayo 2010), pp 587–597, ISSN: 1097-4555

[15] Ledesma A. E.; Zinczuk, J.; López González, J. J.; Ben Altabef, A.; Brandán, S. A., Synthesis and vibrational analysis of N-(2'-Furyl)-Imidazole, *J. Raman Spectrosc.*, 2009, Vol 40, N°8 (August 2009), pp. 1004–1010, ISSN: 1097-4555

[16] Ledesma, A. E.; Zinczuk, J.; López González, J. J. ; Ben Altabef, A.; Brandán, S. A., Structural and vibrational study of 4-(2'-furyl)-1-methylimidazole *J. of Molecular Structure*, 2009, Vol 924–926 (April 2009), pp 322–331, ISSN: 0022-2860

[17] Zinczuk, J.; Ledesma, A. E.; Brandán, S. A.; Piro, O. E.; López-González, J. J.; Ben Altabef, A., Structural and vibrational study of 2-(2'- furyl)-4,5-1H-dihydroimidazole, *J. Phys. Org. Chem.*, 2009, Vol 21 (April 2010), pp 1–12, ISSN: 1099-1395.

[18] Jones, R. A.; Civcir, P. U. Extended Heterocyclic Systems 2. The Synthesis and Characterisation of (2-Furyl)pyridines, (2-Thienyl)pyridines, and Furan-Pyridine and Thiophene-Pyridine Oligomers, Tetrahedron 1997, Vol 53, N˚ 34 (August 1997), pp 11529- 11540. ISSN: 0040- 4020

[19] Rauhut, G.; Pulay, P., Transferable Scaling Factors for Density Functional Derived Vibrational Force Fields, *J. Phys. Chem*. 1995, Vol 99, N˚10 (March 1995), pp 3093-31100. ISSN: 1089-5639

[20] Rauhut, G.; Pulay, P., Transferable Scaling Factors for Density Functional Derived Vibrational Force Fields. [Erratum to document cited in CA122:199802], *J. Phys. Chem.* 1995, Vol 99, N˚ 39 (September 1995), pp 14572. ISSN: 1089-5639

[21] Kalincsak, F.; Pongor, G., Extension of the density functional derived scaled quantum mechanical force field procedure, *Spectrochim. Acta A* 2002, Vol 58, N˚ 5 (March 2002), pp 999- 1011(13), ISSN: 1386-1425

[22] Sadlej-Sosnowska, N., Molecular Similarity Based on Atomic Electrostatic Potential, *J. Phys. Chem. A*, 2007, Vol 111, N˚ 43 (October 2007), pp 11134–11140. ISSN: 1089-5639

[23] Vektariene, A. ; Vektaris, G.; Svoboda, J., 11th *International Electronic Conference on Synthetic Organic Chemistry* (ECSOC-11), 2007.

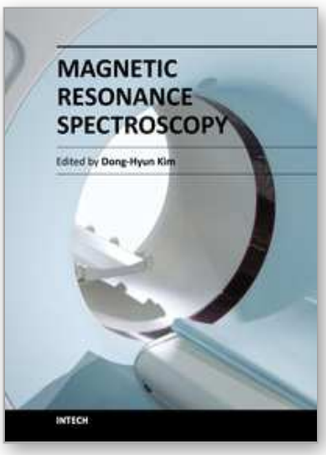
[24] Ditchfield, R., Self-consistent perturbation theory of diamagnetism, *Mol. Phys.*, 1974, Vol 27, N˚4 pp 789- 807. ISSN: 00268976

[25] Cheeseman, J.; Trucks, G. ; Keith, T.; Frisch, M., A comparison of models for calculating nuclear magnetic resonance shielding tensors, *J. Chem. Phys.,* 1996, Vol 104, N˚14 (April 1996), pp 5497–5509. ISSN: 1089-5639

[26] Keith, T. A.; Bader, R. F. W., Calculation of magnetic response properties using a continuous set of gauge transformations, *Chem. Phys.*, 1993, Vol 210, N˚1-3 (May 1993), pp 223–231. ISSN: 0301-0104

IntechOpen

IntechOpen



Magnetic Resonance Spectroscopy

Edited by Prof. Dong-Hyun Kim

ISBN 978-953-51-0065-2
Hard cover, 264 pages
Publisher InTech
Published online 02, March, 2012
Published in print edition March, 2012

Magnetic Resonance Spectroscopy (MRS) is a unique tool to probe the biochemistry in vivo providing metabolic information non-invasively. Applications using MRS has been found over a broad spectrum in investigating the underlying structures of compounds as well as in determining disease states. In this book, topics of MRS both relevant to the clinic and also those that are beyond the clinical arena are covered. The book consists of two sections. The first section is entitled 'MRS inside the clinic' and is focused on clinical applications of MRS while the second section is entitled 'MRS beyond the clinic' and discusses applications of MRS in other academic fields. Our hope is that through this book, readers can understand the broad applications that NMR and MRS can offer and also that there are enough references to guide the readers for further study in this important topic.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

Ana E. Ledesma, Juan Zinczuk, Juan J. López González and Silvia A. Brandán (2012). Structural and Vibrational Properties and NMR Characterization of (2'-furyl)-Imidazole Compounds, Magnetic Resonance Spectroscopy, Prof. Dong-Hyun Kim (Ed.), ISBN: 978-953-51-0065-2, InTech, Available from: http://www.intechopen.com/books/magnetic-resonance-spectroscopy/structural-and-vibrational-properties-of-2-furyl-imidazole-compounds

INTECH
open science | open minds

InTech Europe
University Campus STeP Ri
Slavka Krautzeka 83/A
51000 Rijeka, Croatia
Phone: +385 (51) 770 447
Fax: +385 (51) 686 166
www.intechopen.com

InTech China
Unit 405, Office Block, Hotel Equatorial Shanghai
No.65, Yan An Road (West), Shanghai, 200040, China
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元
Phone: +86-21-62489820
Fax: +86-21-62489821

© 2012 The Author(s). Licensee IntechOpen. This is an open access article distributed under the terms of the Creative Commons Attribution 3.0 License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

IntechOpen

IntechOpen