Supporting Information for

Investigation of rotameric conformations of substituted imidazo- [1, 2-a] pyrazine: experimental and theoretical approaches

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Figure S23 Frontier Molecular orbital for conformer **2A** 18

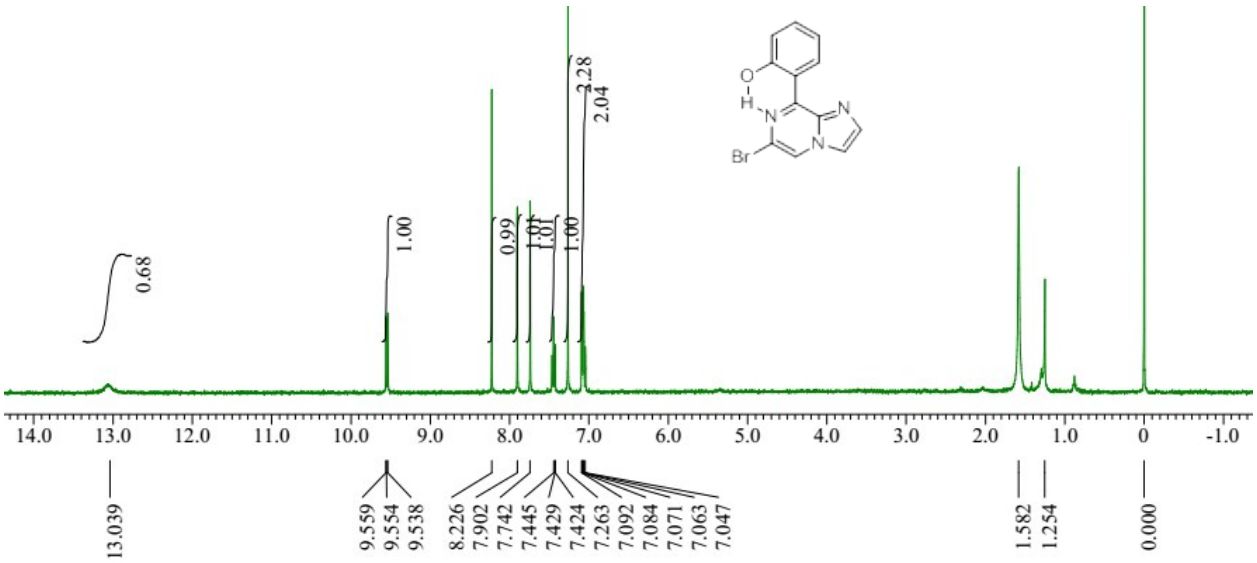


Figure S1: [1]H NMR spectra of Compound **1A**

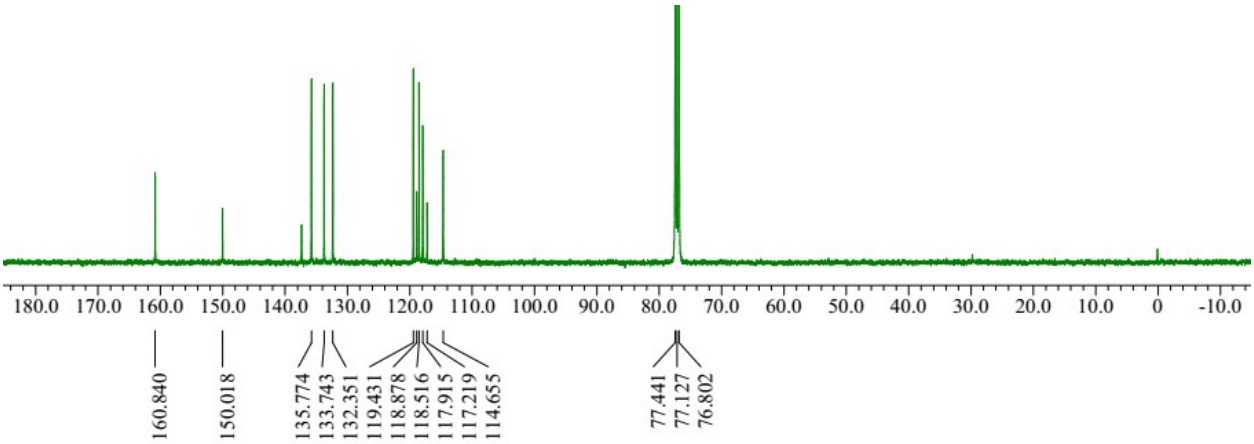


Figure S2: [13]C NMR spectra of Compound **1A**

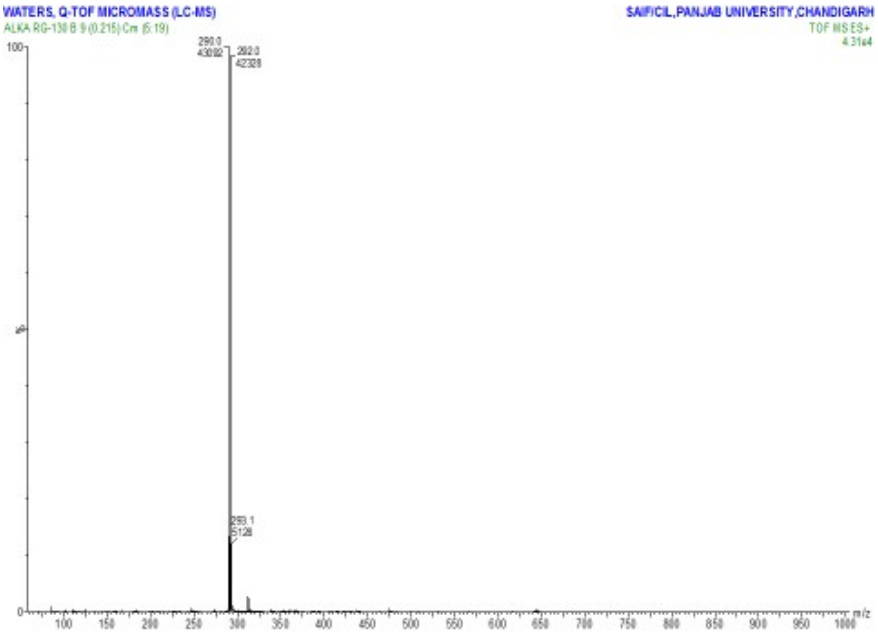


Figure S3: Mass spectra of compound **1A**

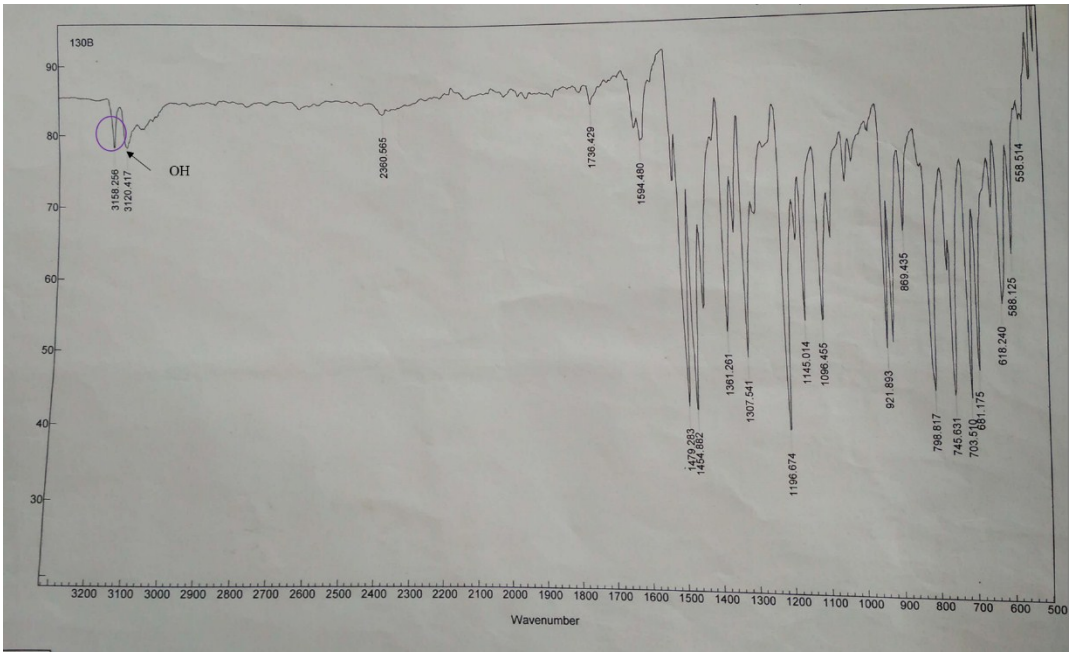
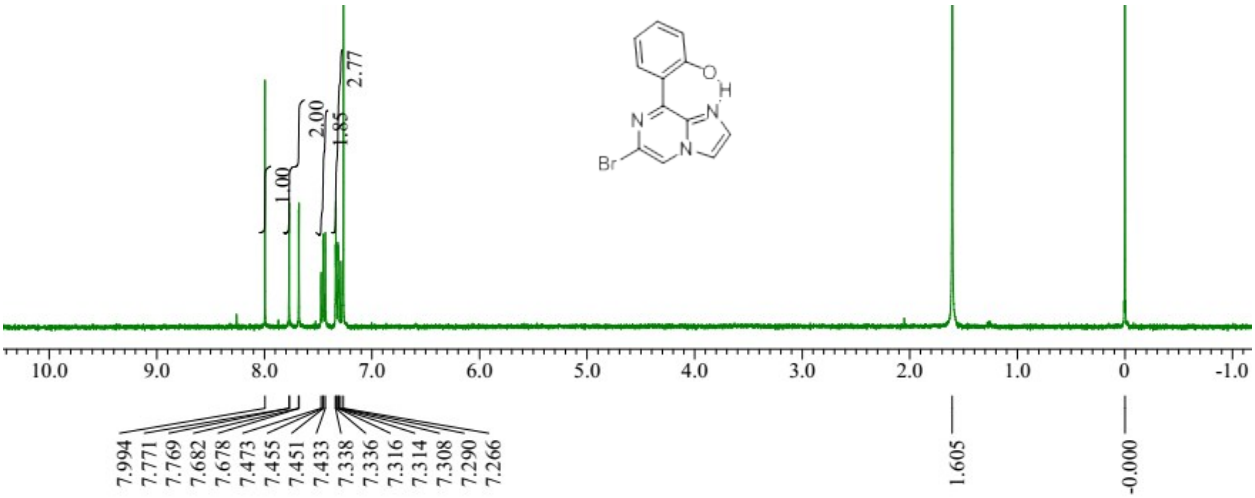


Figure S4: FTIR Spectra of compound **1A**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2.77
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H
N
N
N
Br
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
7.994
7.771
7.769
7.682
7.678
7.473
7.455
7.451
7.433
7.338
7.336
7.316
7.314
7.308
7.290
7.266
1.605
-0.000

Figure S5: [1]H NMR spectra of Compound **1B**

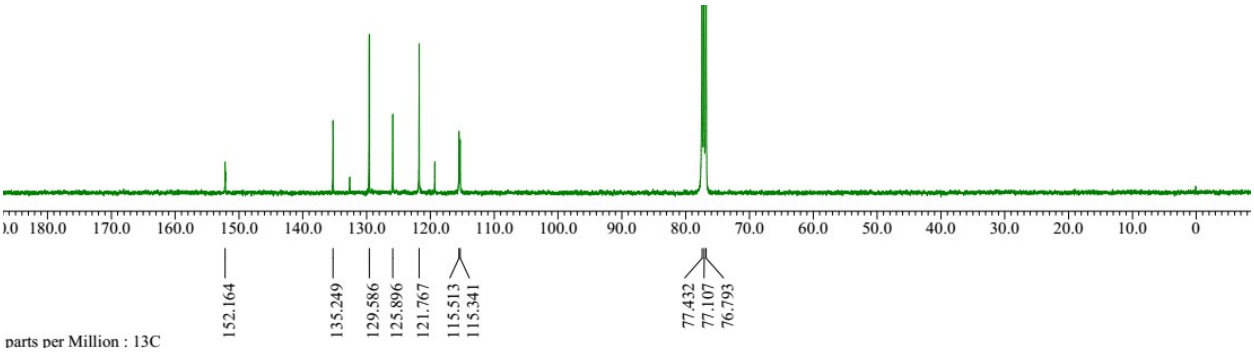


Figure S6: [13]C NMR spectra of Compound **1B**

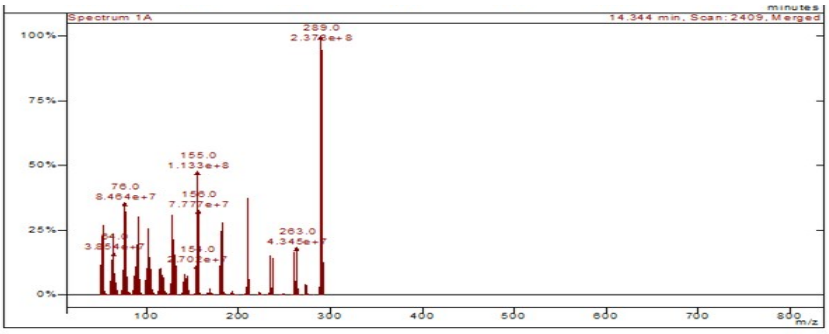


Figure S7: Mass spectra of compound **1B**

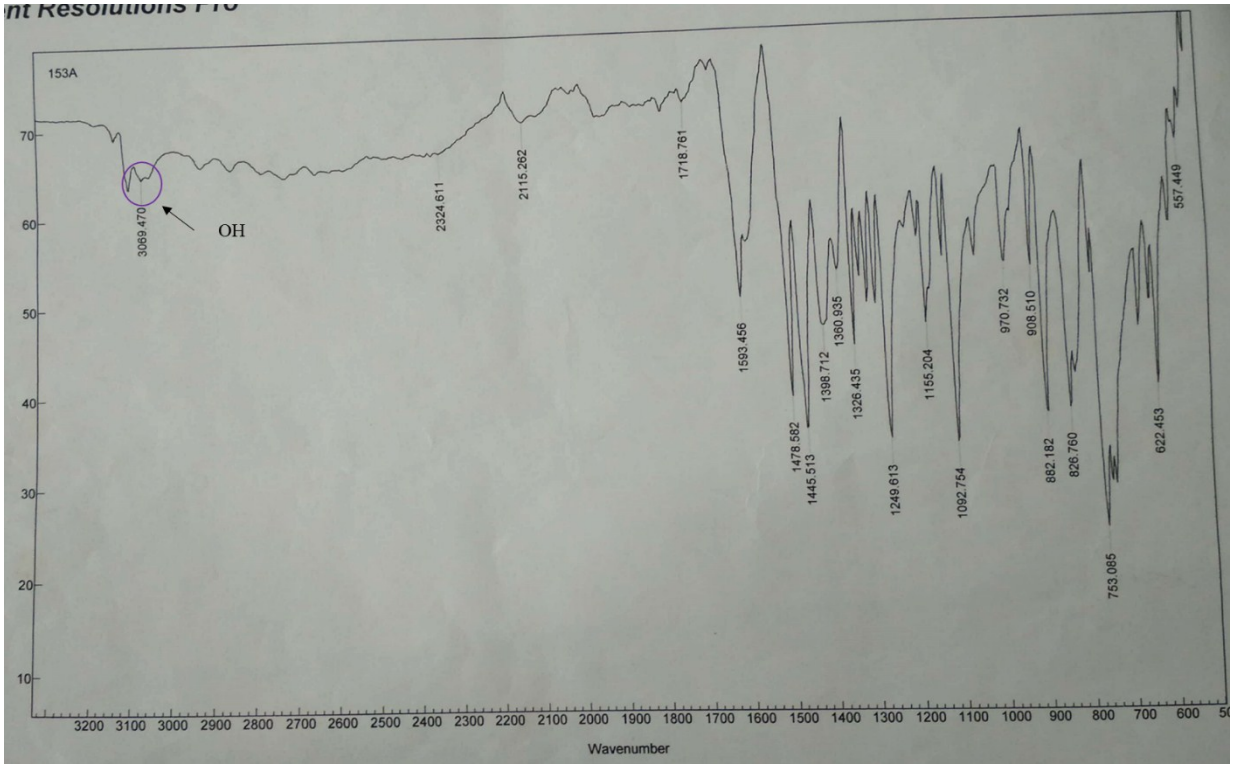


Figure S8: FTIR Spectra of compound **1B**

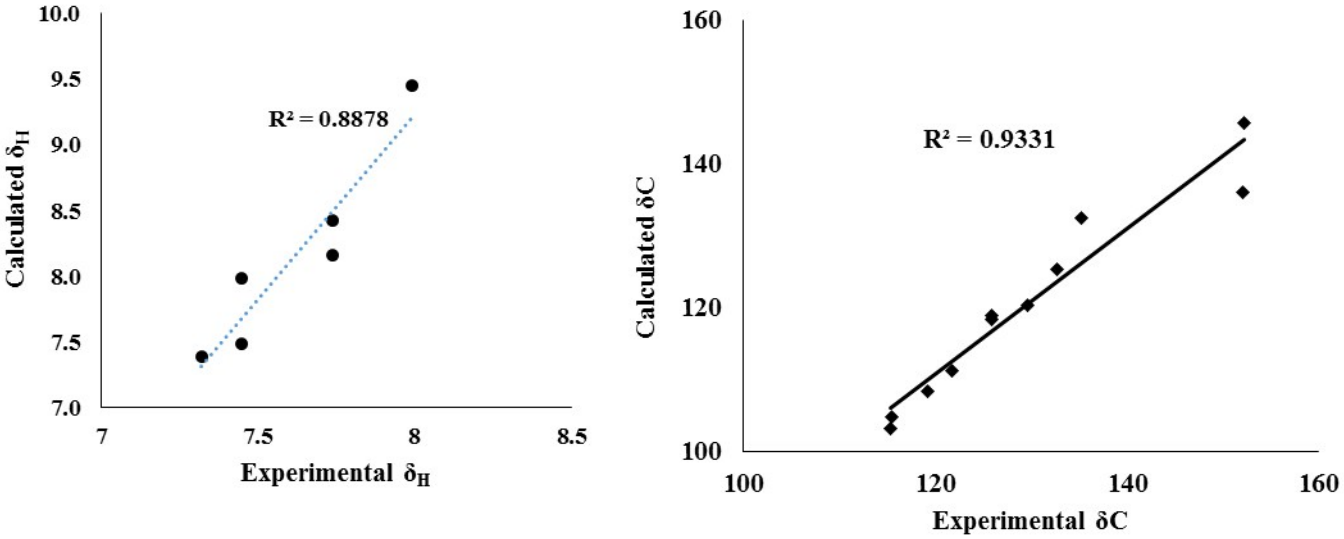
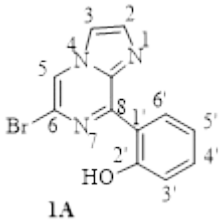
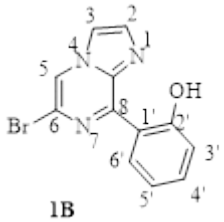


Figure S9: Experimental and theoretical ^{1}H NMR (left) and ^{13}C NMR (right) correlation for conformer **1B**

Table S1. Experimental ^{1}H NMR signals for conformer **1A** and **1B**		
H- position	 1A	 1B
	13.03	
6'	9.54	7.99
5	8.23	7.77
2	7.90	7.68
3	7.74	7.47
4'	7.45	7.43
3'	7.05	7.34
5'	7.09	7.29

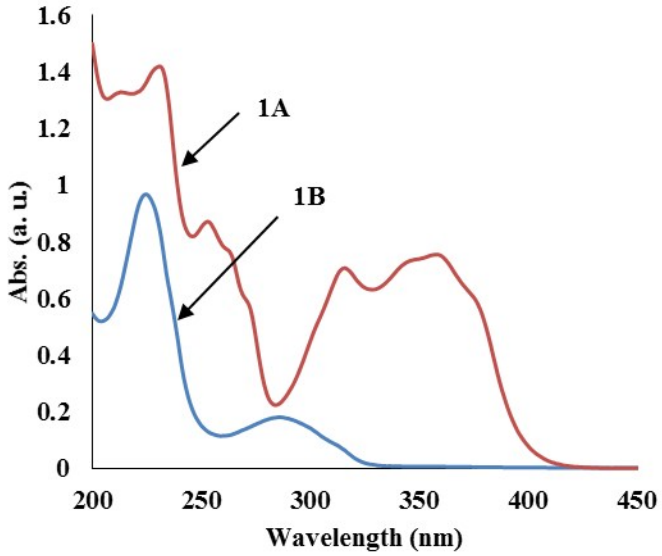


Figure S10: The absorption spectra of different compound **1A** and **1B** in CH_3CN**.**

Table S2: The calculated absorption value for conformer **1A** and **1B** in gas and CH_3CN solvent phase at B3LYP/6-31++G** level of theory, symmetry of frontier orbital and % contributions of Molecular orbitals

Excited State	λ_{ACN} (nm)	λ_{Gas} (nm)	λ_{Exp} (nm)	Osc. Strength	Symmetry	% Major Orbital Contribution	
				1A			
S_0–S_1	370.20	388.50	380,	0.2567	Singlet-A	H→L	94
S_0-S_2	329.15	326.29		0.1214	Singlet-A	H-1→L	89
S_0-S_3	311.03	309.84	361,	0.184	Singlet-A	H-2→L	86
S_0-S_4	274.96	281.59		0.0001	Singlet-A	H-4→L	96
S_0-S_5	270.69	281.16	318	0.155	Singlet-A	H-3→L	57
S_0-S_6	262.13	269.59		0.0688	Singlet-A	H→L+1	53
				1B			
S_0-S_1	381.54	402.60		0.2699	Singlet-A	H→L	94
S_0-S_2	333.23	336.02		0.1178	Singlet-A	H-1→L	94
S_0-S_3	300.16	300.28	290	0.1204	Singlet-A	H-2→L	81
S_0-S_4	280.89	288.76		0.0006	Singlet-A	H-4→L	95
S_0-S_5	278.85	288.73		0.1195	Singlet-A	H-3→L	44
S_0-S_6	265.55	274.51		0.0294	Singlet-A	H-3→L	43

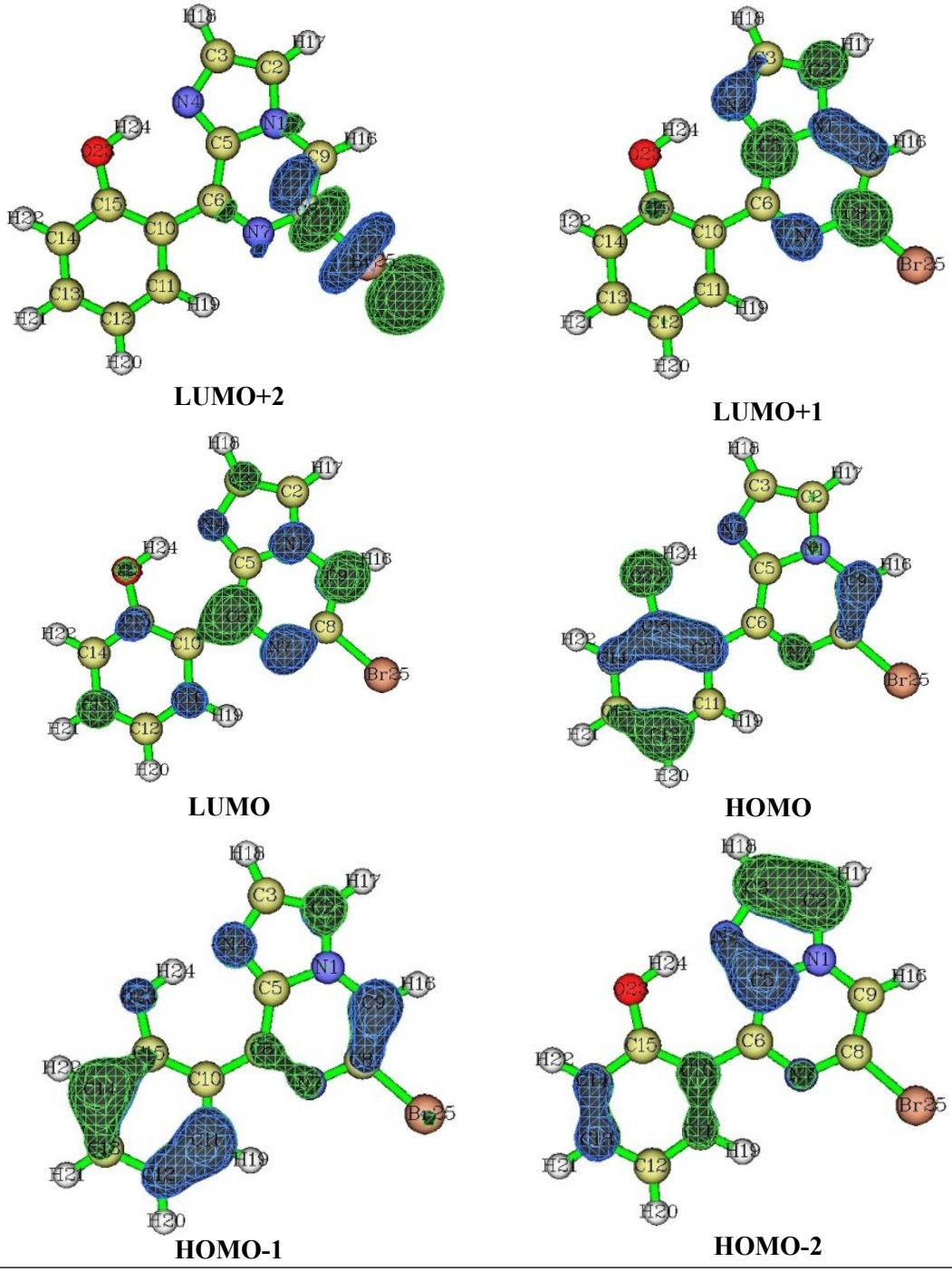


Figure S11: Frontier Molecular orbital for conformer **1B**

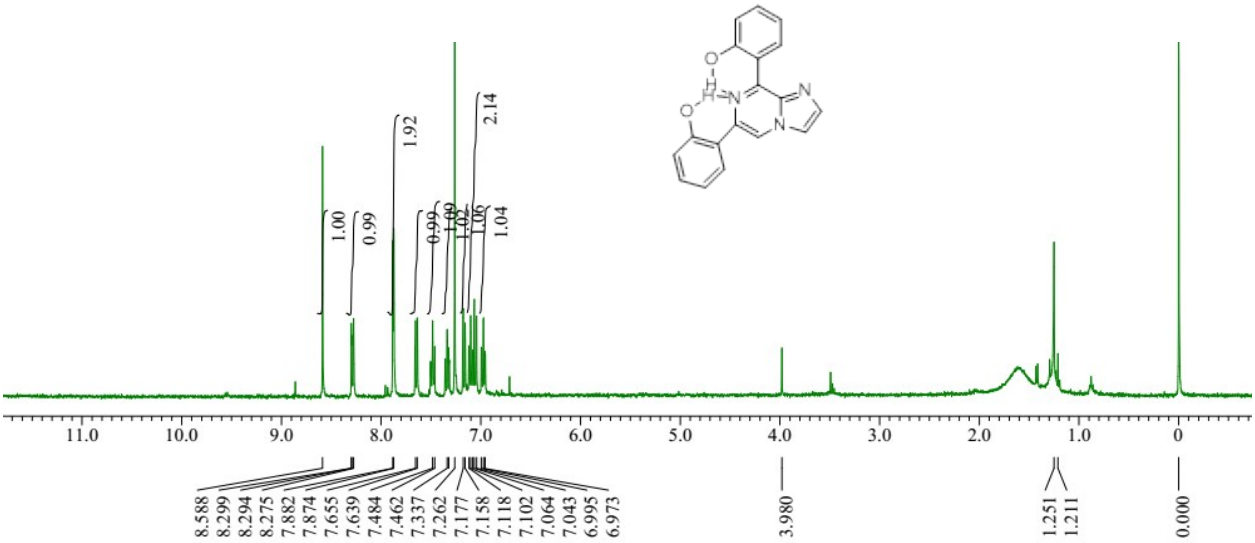

1.00
0.99
1.92
0.99
1.00
1.02
1.06
1.04
2.14
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.588
8.299
8.294
8.275
7.882
7.874
7.655
7.639
7.484
7.462
7.337
7.262
7.177
7.158
7.118
7.102
7.064
7.043
6.995
6.973
3.980
1.251
1.211
0.000

Figure S12: ^{1}H NMR spectra of Compound **2A**

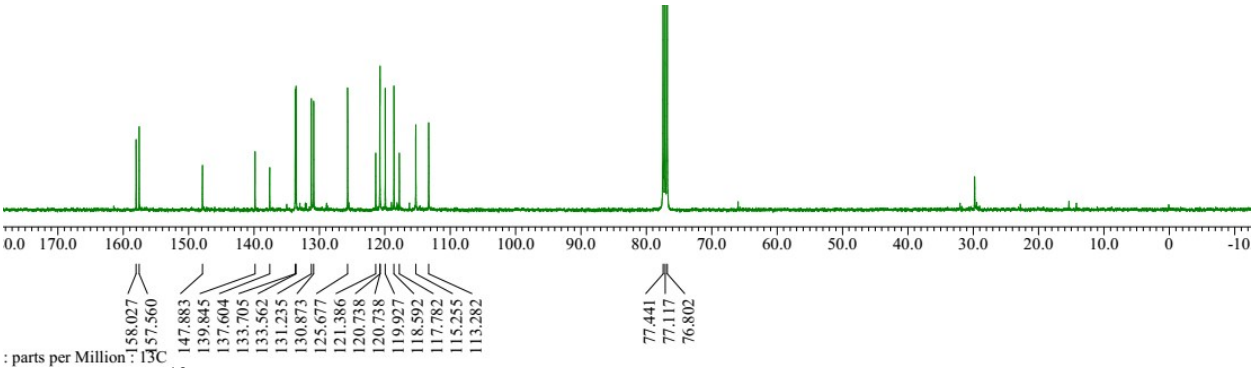


Figure S13: ^{13}C NMR spectra of Compound **2A**

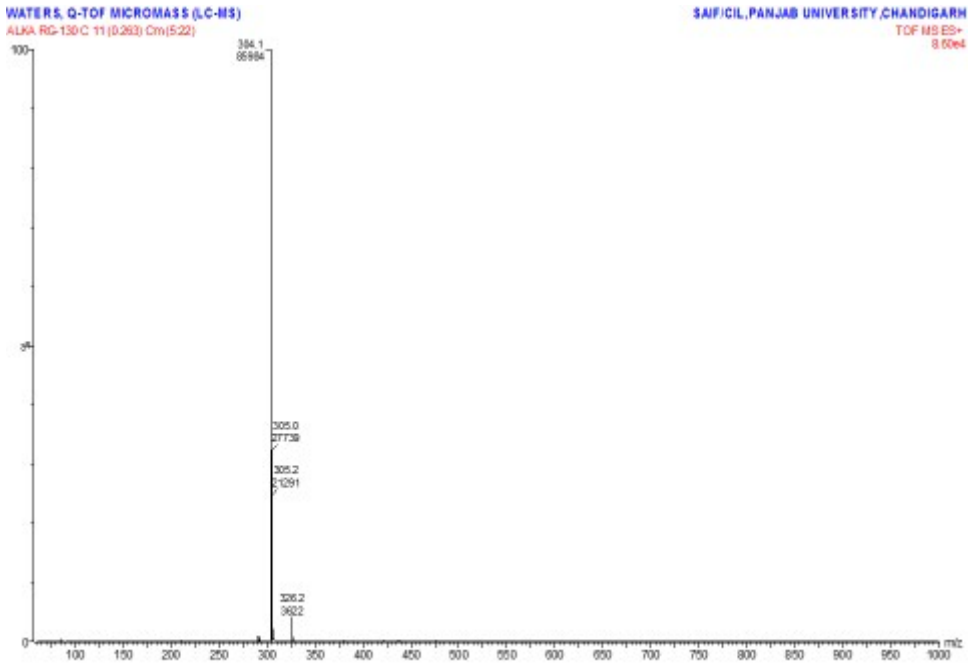


Figure S14: Mass spectra of compound **2A**

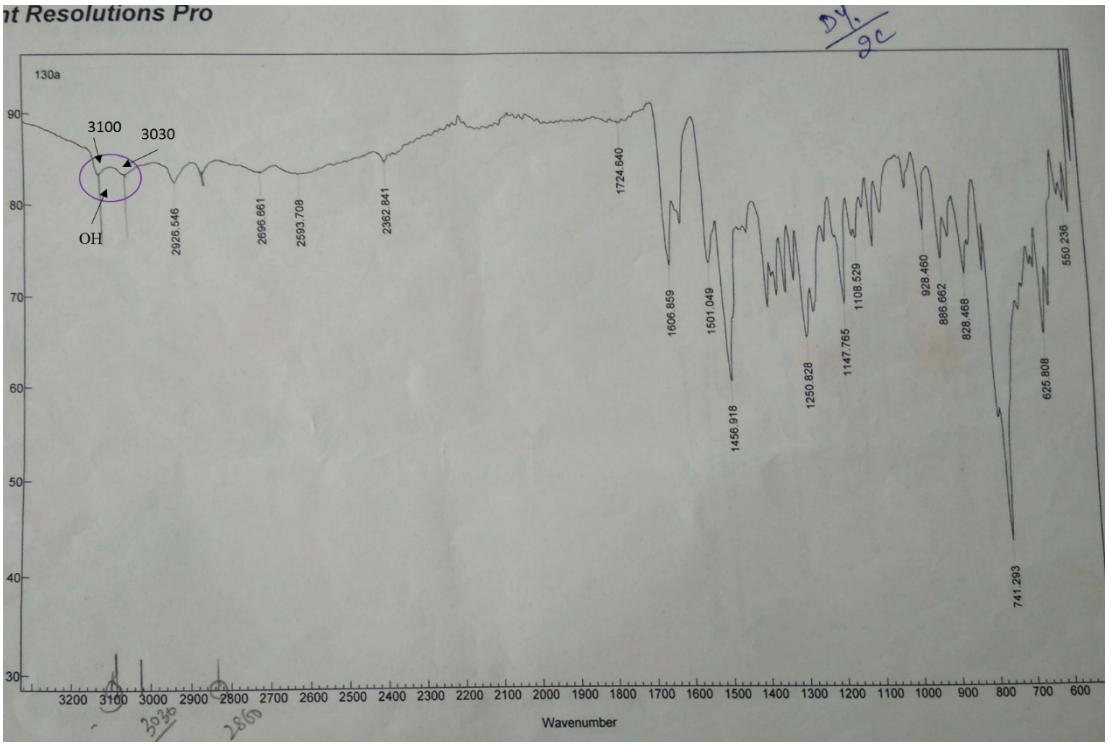


Figure S15: FTIR Spectra of compound **2A**

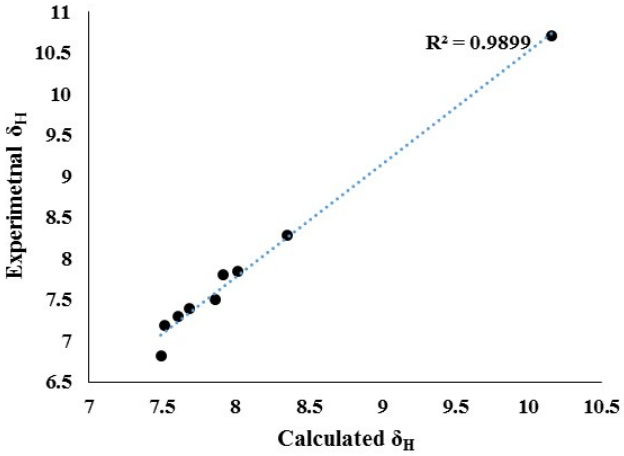
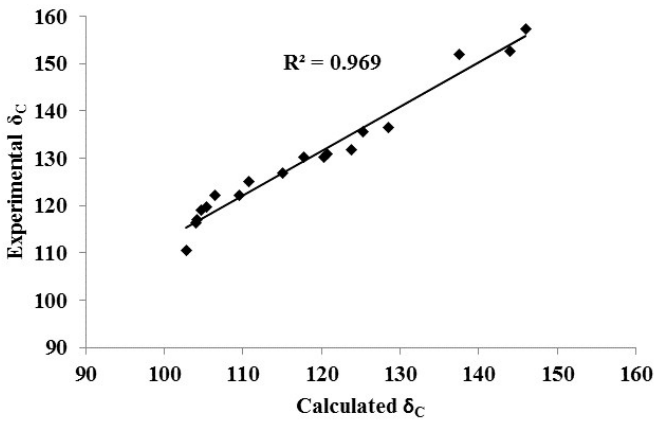


Figure S16:



NMR (right) correlation for conformer **2A**

Experimental and theoretical ^{1}H NMR (left) and ^{13}C

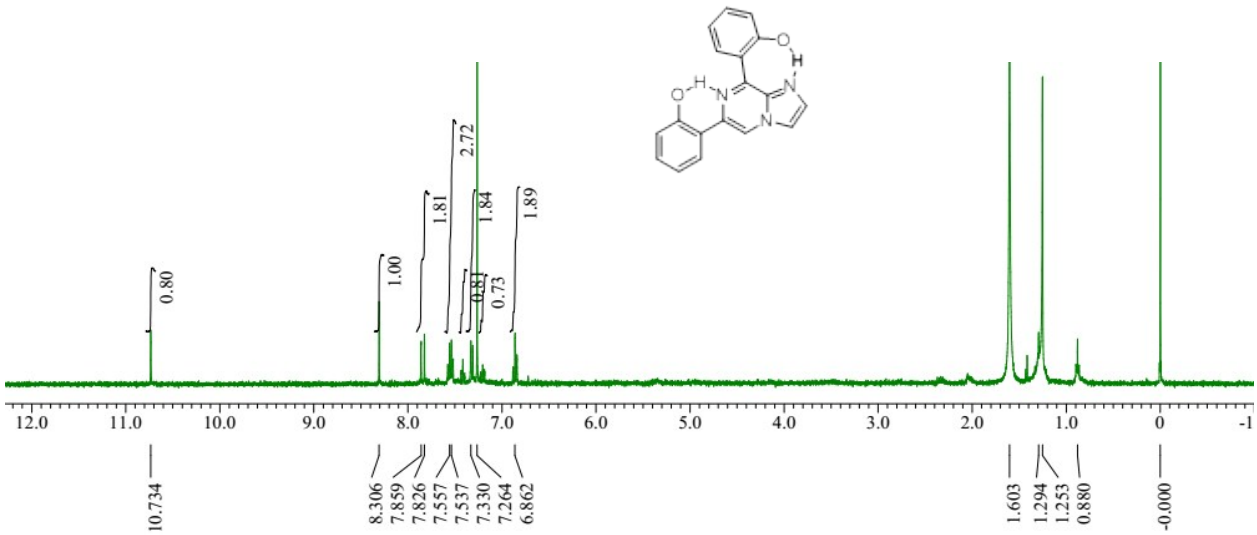


Figure S17: ^{1}H NMR spectra of Compound **2B**

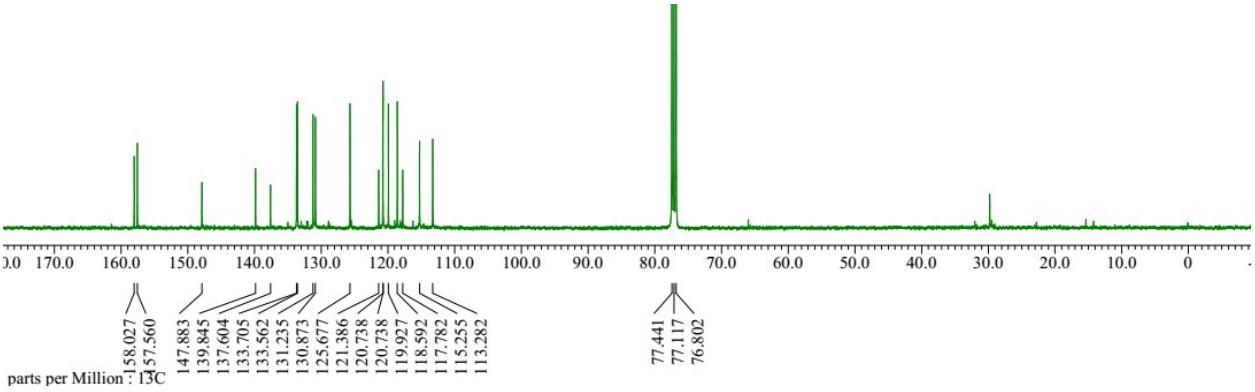


Figure S18: ^{13}C NMR spectra of Compound **2B**

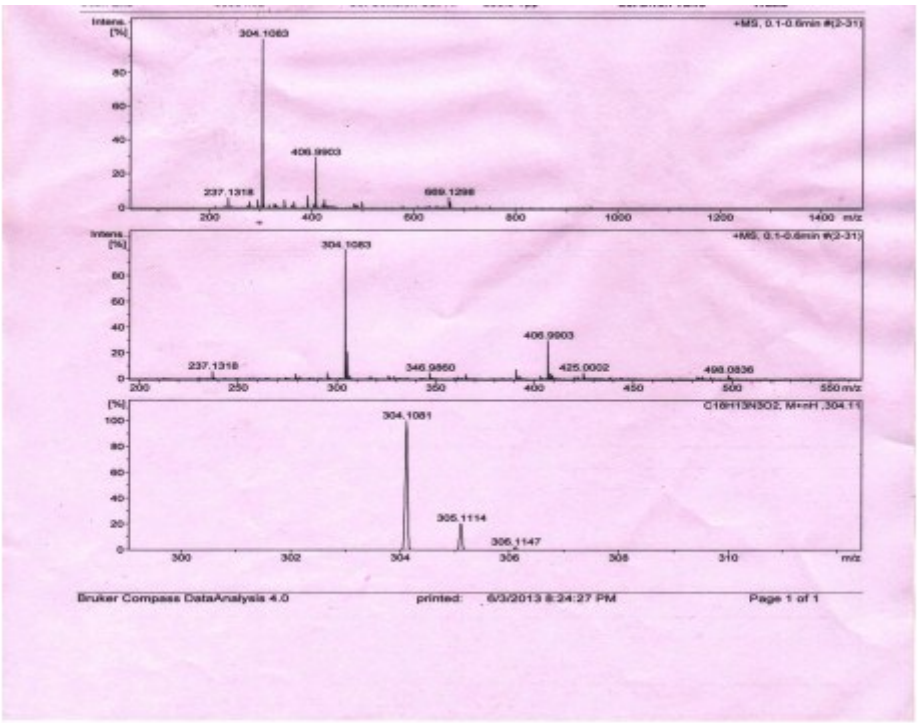


Figure S19: Mass spectra of compound **2B**

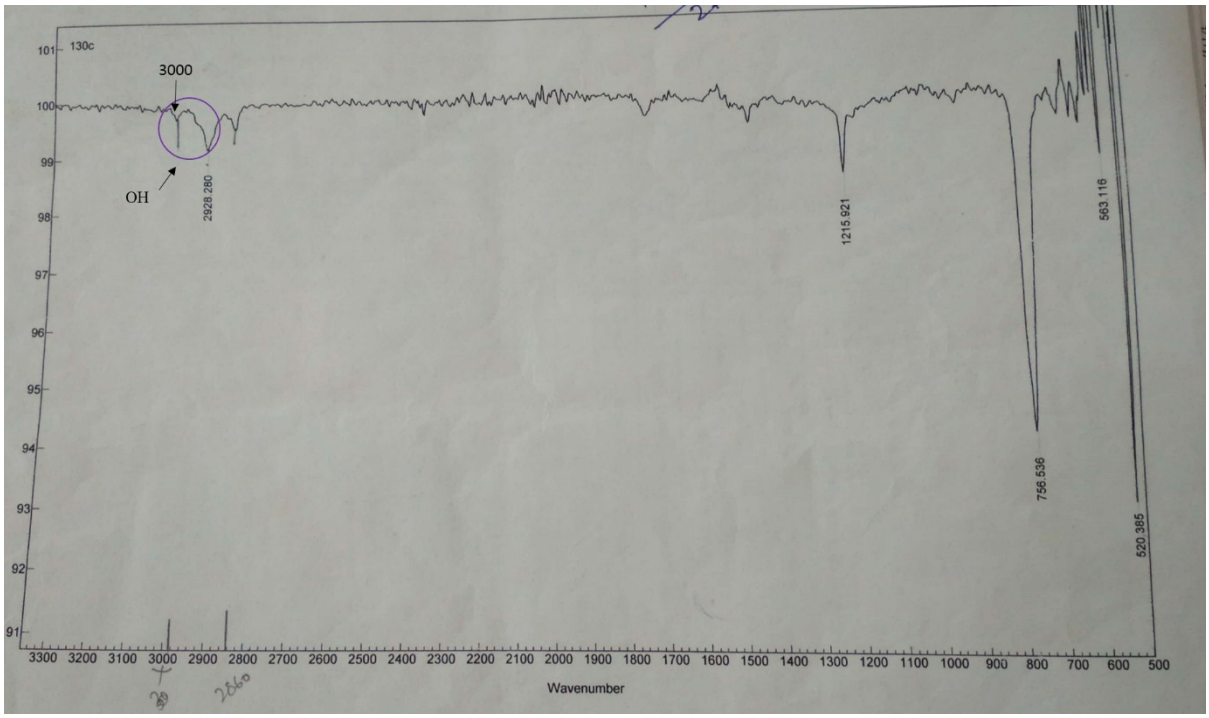
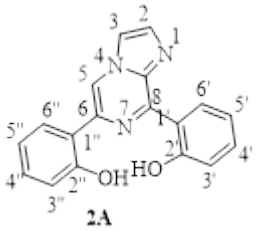
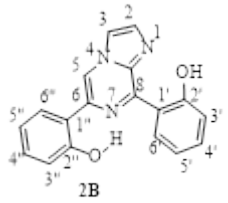


Figure S20: FTIR spectra of compound **2B**

Table S3. Experimental ^{1}H NMR signals for conformer **2A** and 2**B**		
	 2A	 2B
	2A	**2B**
6'	8.59	10.7
5	8.29	7.84
2	7.88	7.8
3	7.65	7.5
4'	7.48	7.39
4"	7.33	7.29
6"	7.26	
3'	7.18	
3"	7.12	
5'	7.06	7.18
5"	6.97	6.82

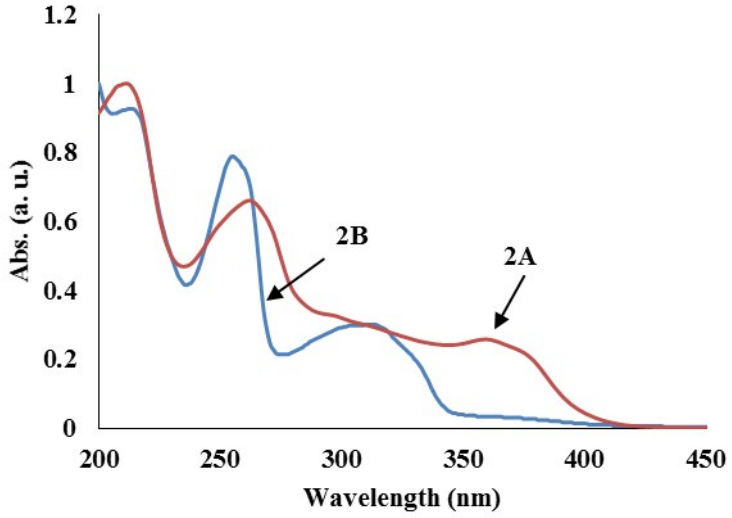
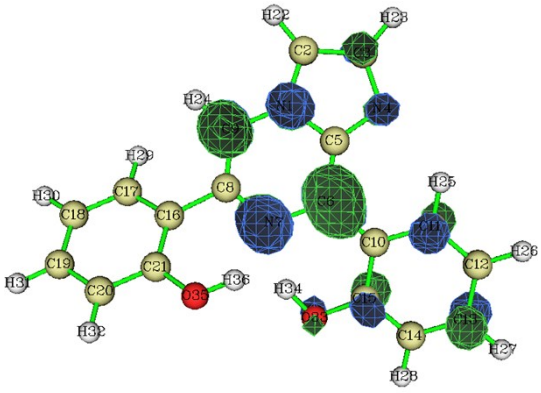


Figure S21: The absorption spectra of different conformers **2A** and **2B** in CH_3CN.

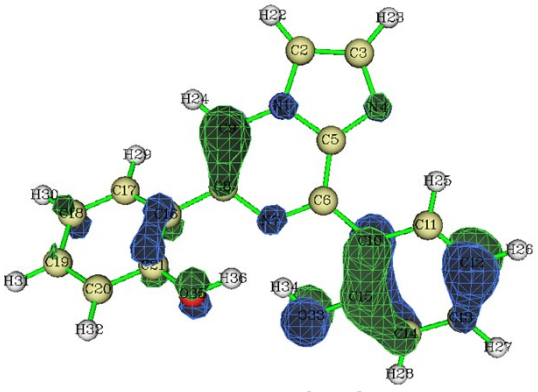
Table S4: The calculated absorption value for conformer **2A** and **2B** in gas and CH_3CN solvent phase at B3LYP/6-31++G** level of theory, symmetry of frontier orbital and % contributions of Molecular orbitals

Excitation S_0-S_n	λ_{Gas} (nm)	λ_{ACN} (nm)	λ_{Exp} (nm)	Osc. Strength	Symmetry	Major orbital contribs.	
2A							
1	387.15	377.15	380, 360, 265	0.1640	Singlet-A	H→L	96%
2	375.78	357.40		0.0624	Singlet-A	H-1→L	98%
3	326.38	325.97		0.0625	Singlet-A	H-2→L	89%
4	315.62	313.60		0.1080	Singlet-A	H-3→L	63%
5	297.45	290.59		0.4008	Singlet-A	H→L+1	55%
6	292.17	286.91		0.2020	Singlet-A	H-4→L	81%
2B							
1	406.33	391.19	375, 315, 260	0.1003	Singlet-A	H→L	91%
2	389.98	362.46		0.1141	Singlet-A	H-1→L	93%
3	335.74	329.86		0.073	Singlet-A	H-2→L	93%
4	321.73	317.88		0.1328	Singlet-A	H→L+1	80%
5	306.73	297.46		0.2859	Singlet-A	H-1→L+1	61%
6	301.69	292.03		0.2095	Singlet-A	H-3→L	59%

2A

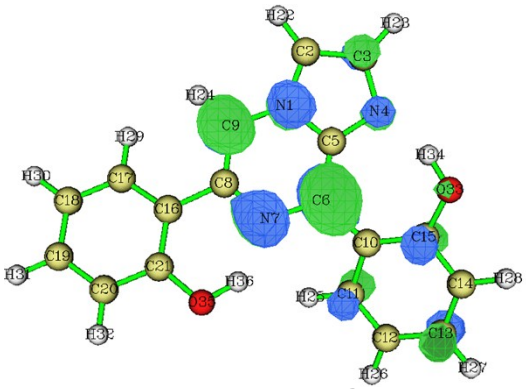


LUMO

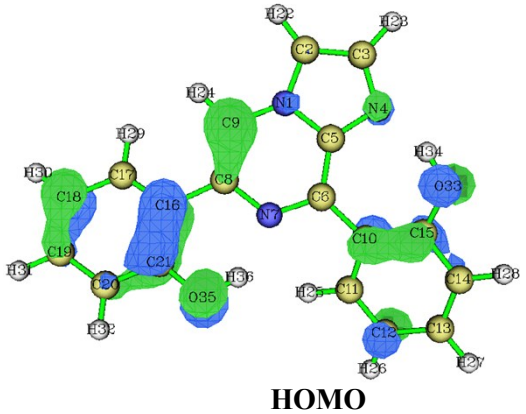


HOMO

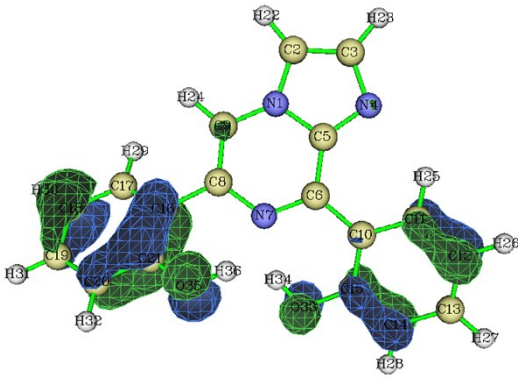
2B



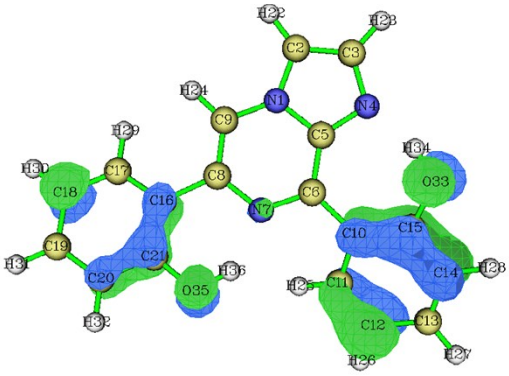
LUMO



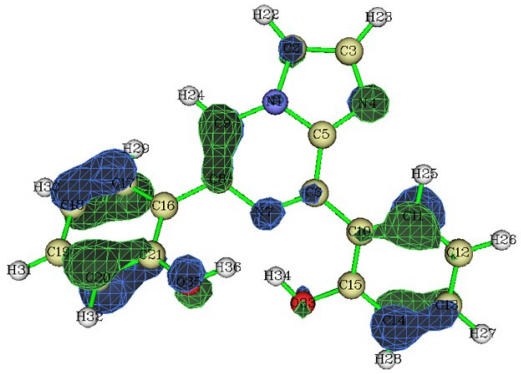
HOMO



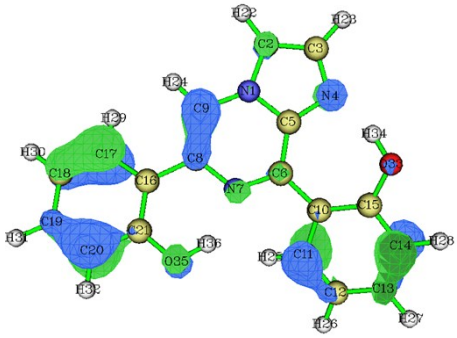
HOMO-1



HOMO-1

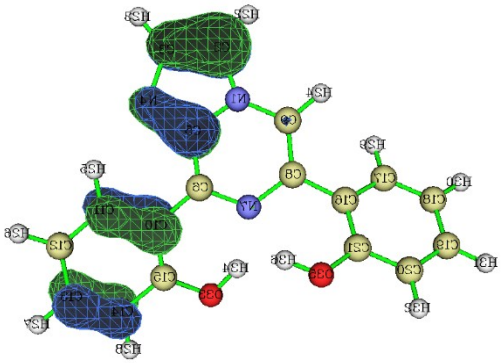


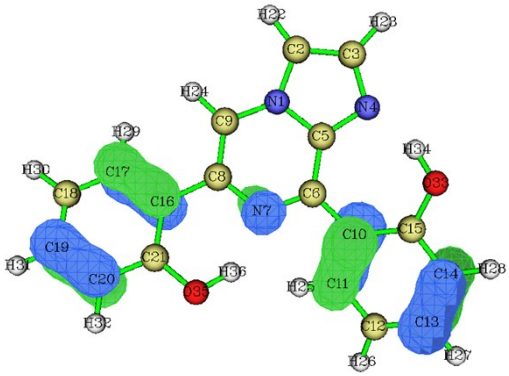
HOMO-2



HOMO-2

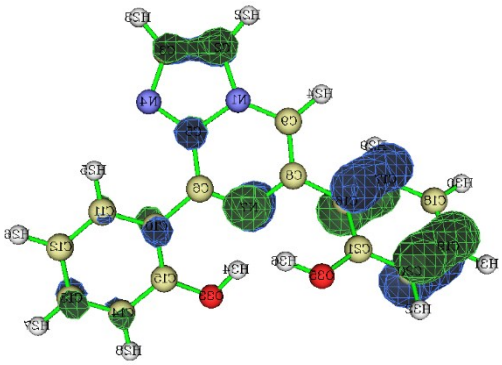
HOMO-3





HOMO-3

HOMO-4



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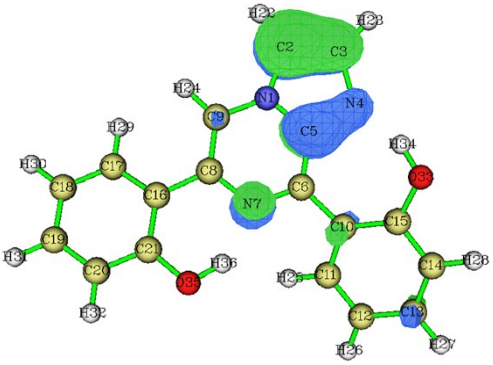
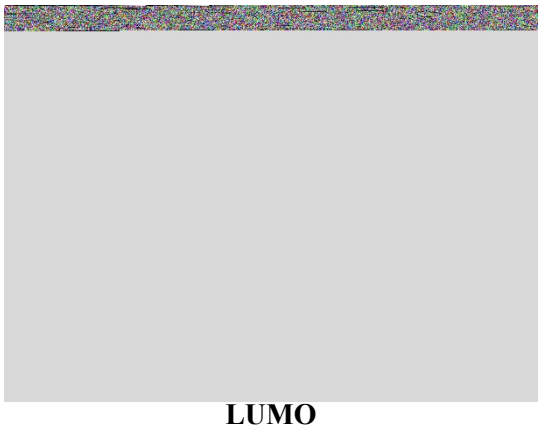


Figure S22: Frontier Molecular orbital for conformer **2B**



LUMO

HOMO

HOMO-1

HOMO-2

HOMO-3

HOMO-4

Figure S23: Frontier Molecular orbital for conformer **2A**