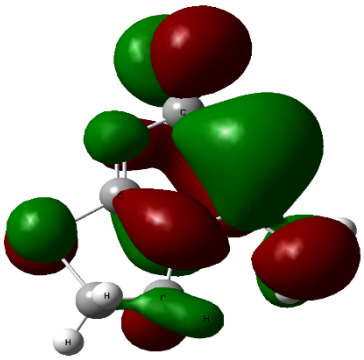
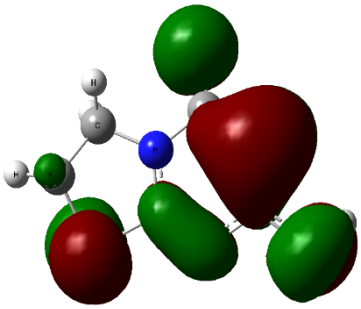
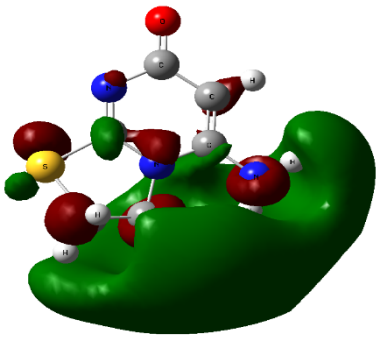
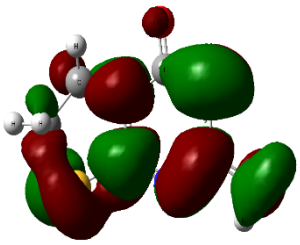
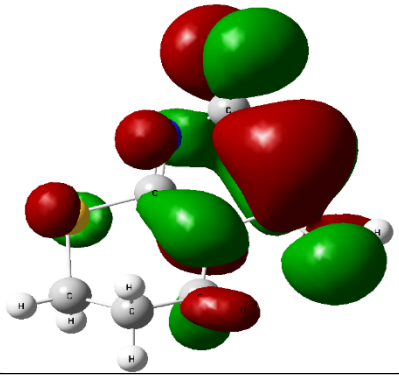
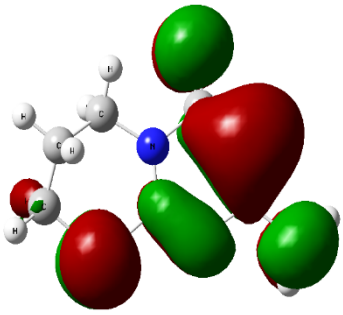
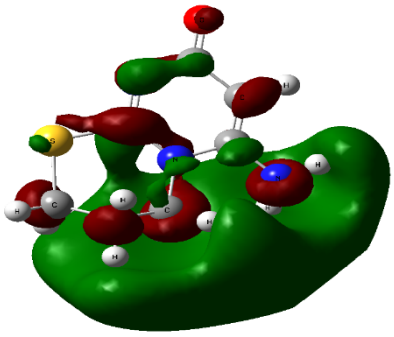
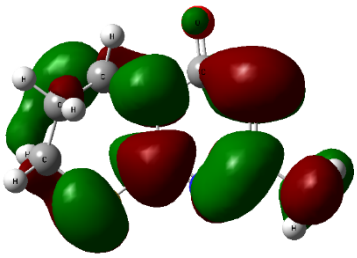
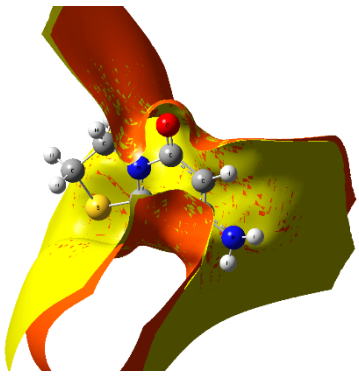
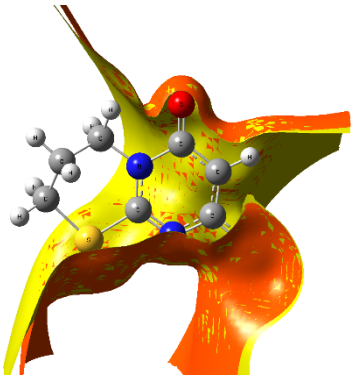
HOMO		
	11a	**12a**
LUMO		
	11a	**12a**
HOMO		
	11b	**12b**
LUMO		
	11b	**12b**

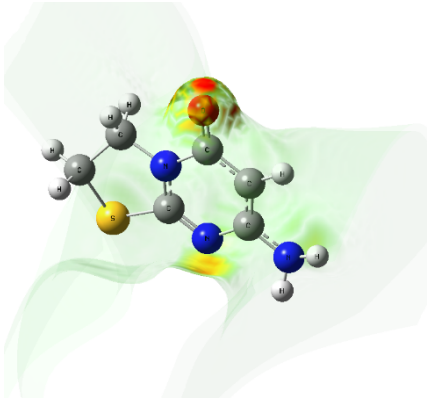
Fig. S1. HOMO, and LUMO maps, of different Regio isomer **11a & 12a** and **11b & 12b** compounds at the B3LYP/6-311++G(d,p).



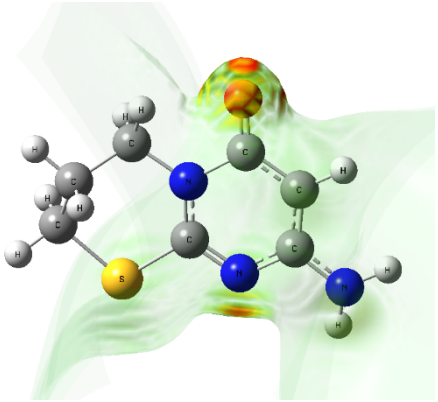
ESP



12a **12b**



3D-MEP



12a **12b**

Fig.S2. ESP, and MEP maps, for the studied compounds **12a** and **12b** at the B3LYP/6-311++G(d,p).

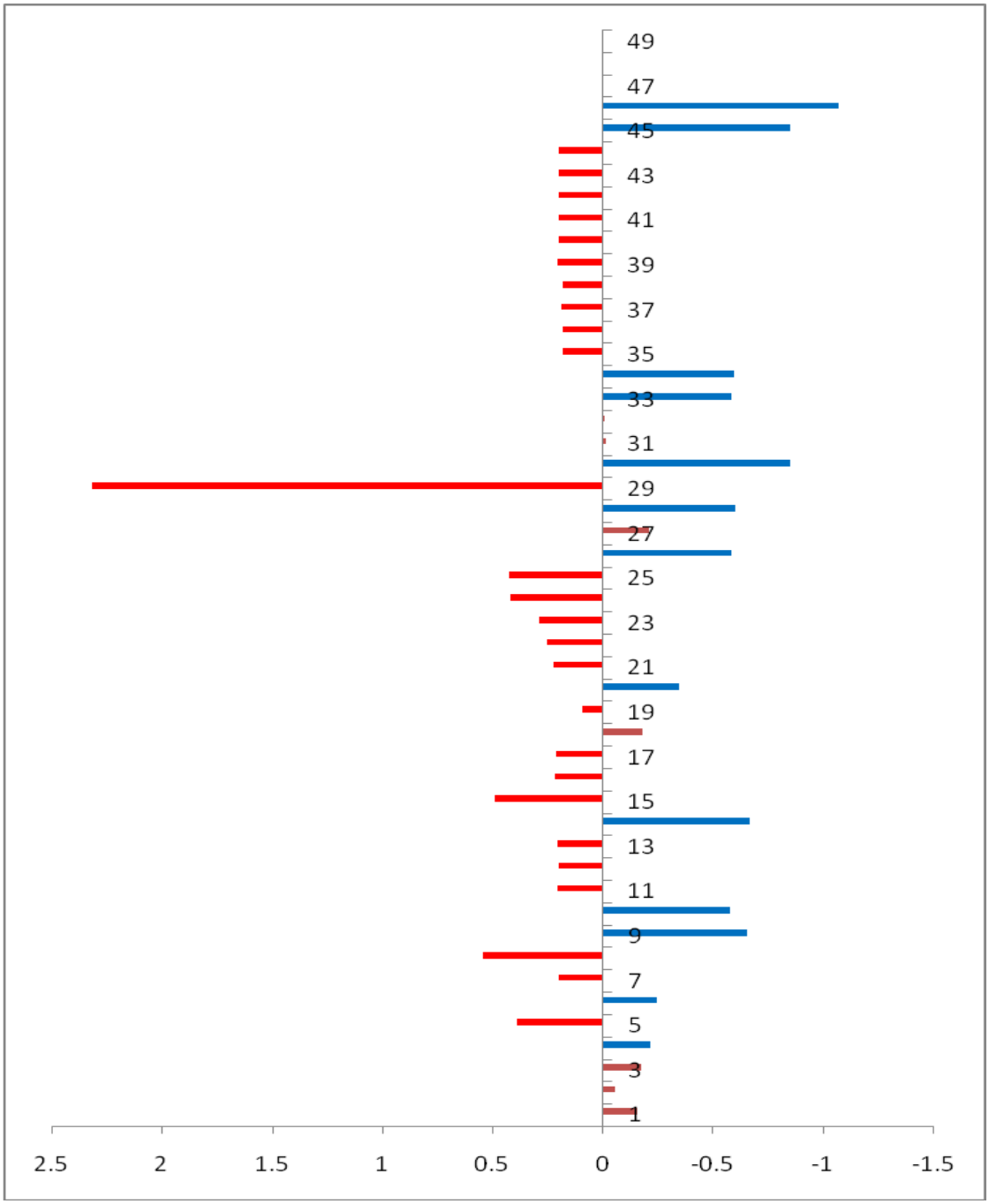
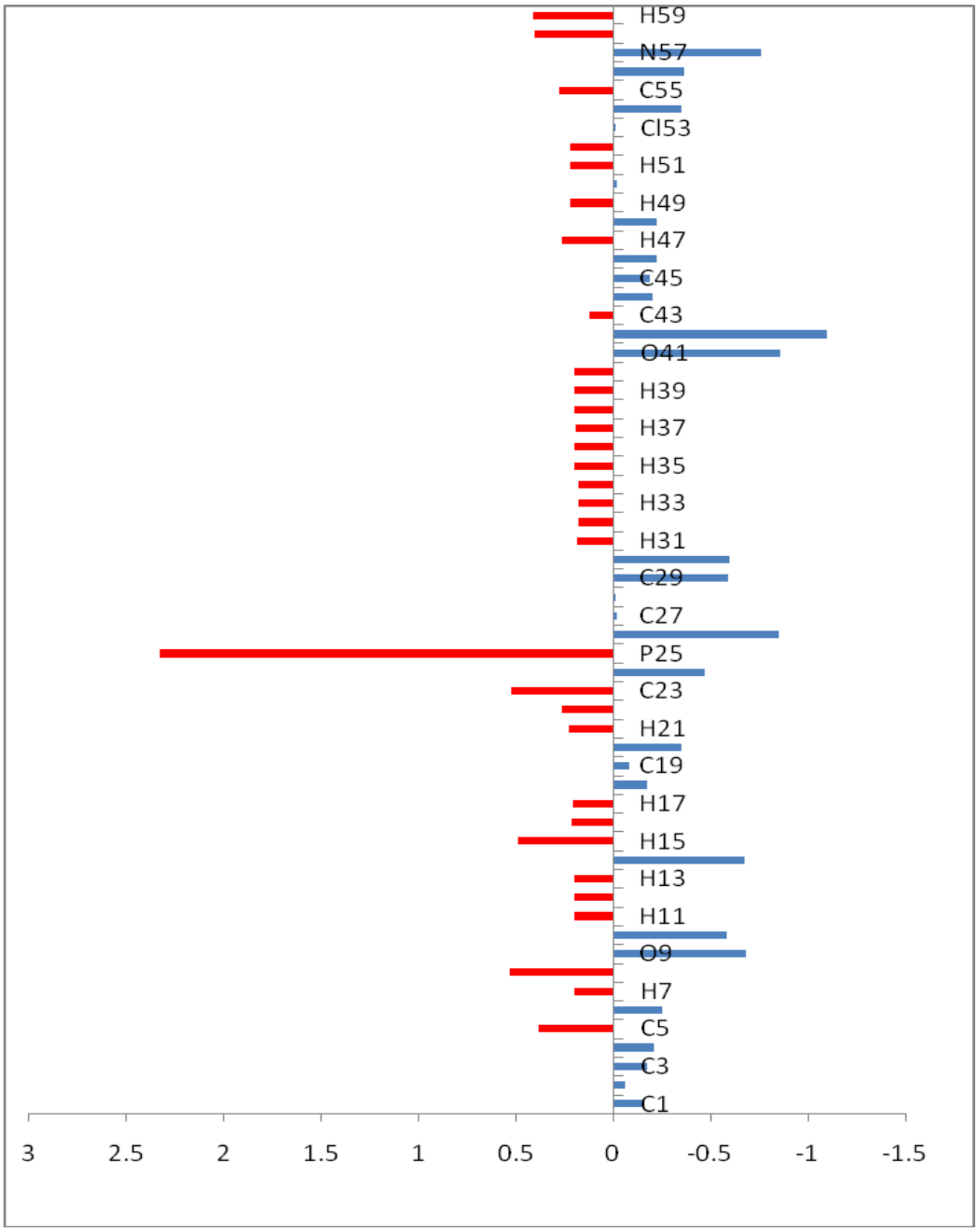


Fig.S3. Atomic charge distribution (e) for the studied compounds **12a** using B3LYP/6-311++G (d,p).

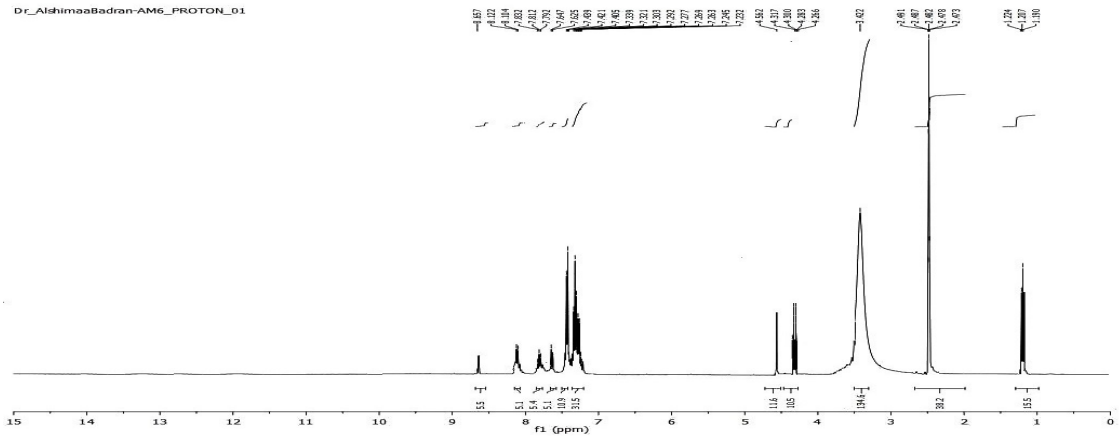


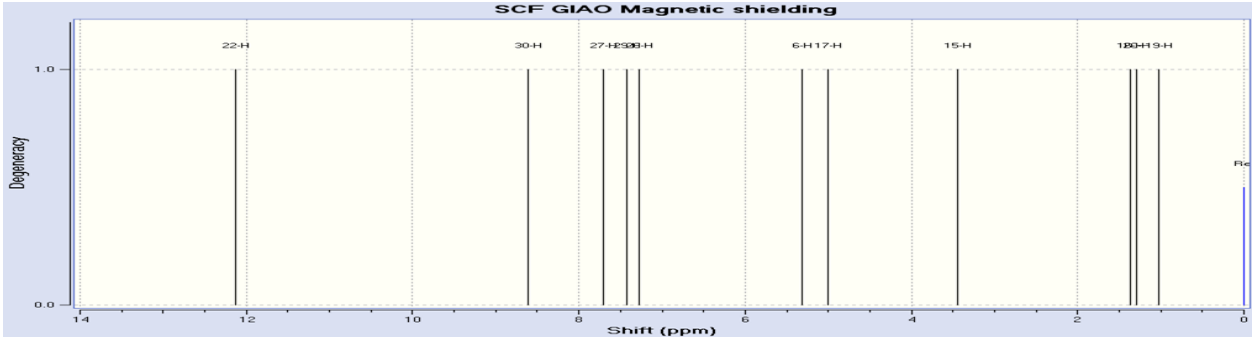
Atomic charge distribution

Negative Charge value

Positive Charge value

Fig.S4. Atomic charge distribution (e) for the studied compounds **12b** using B3LYP/6-311++G (d,p).





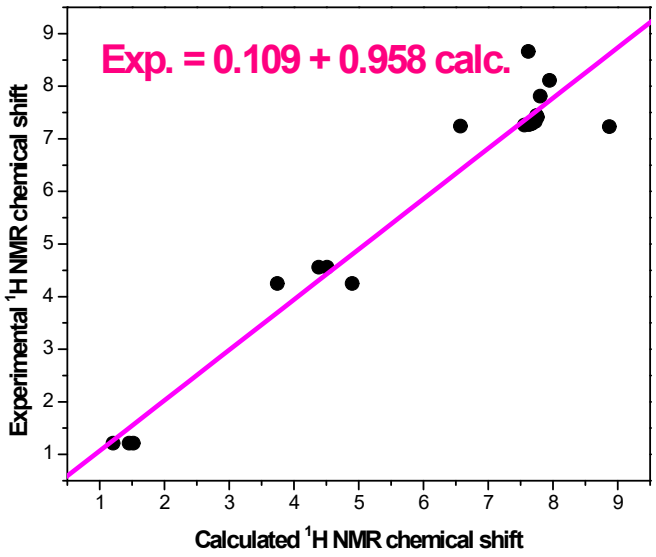


Fig. S5. (a) Experimental and (b) Calculated ^{1}H NMR spectrum, (c) Correlation graph between experimental and calculated ^{1}H-NMR chemical shifts of **12a** at B3LYP/6-311++G (d,p).

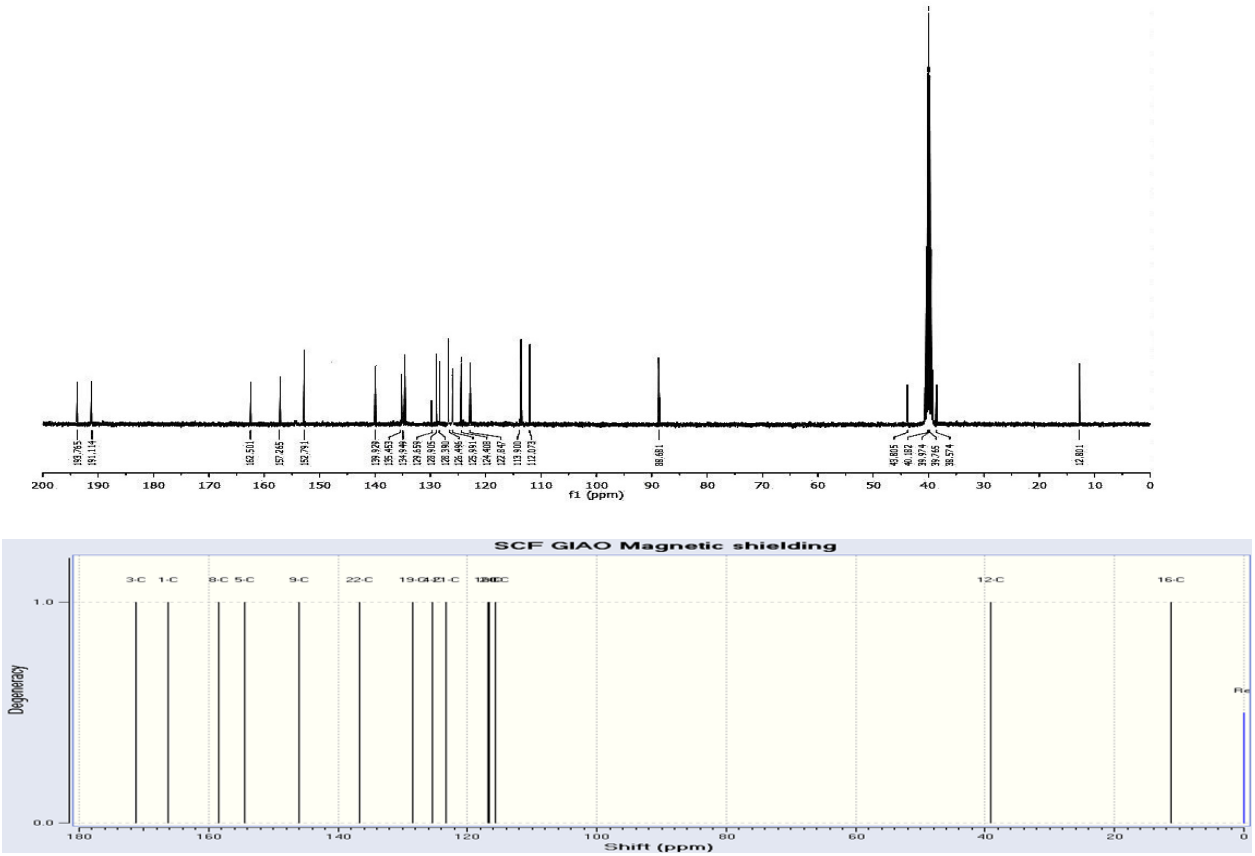
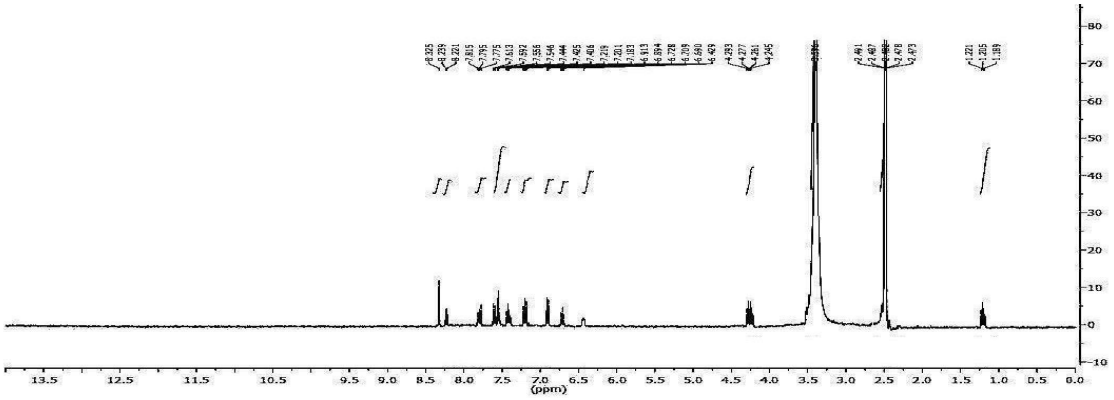
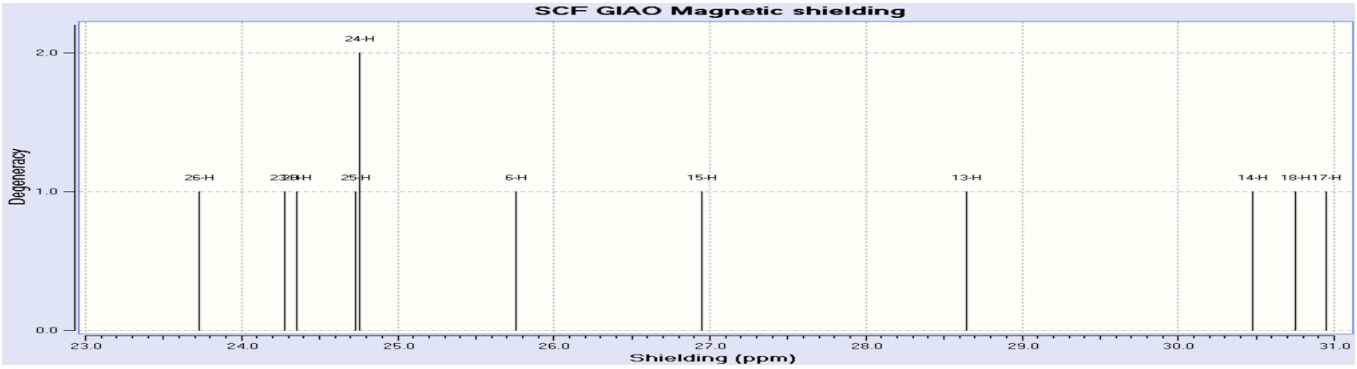


Fig. S6. (a) Experimental and (b) Calculated ^{13}C NMR spectrum, (c) Correlation graph between experimental and calculated ^{13}C NMR chemical shifts of **12a** at B3LYP/6-311++G (d,p).





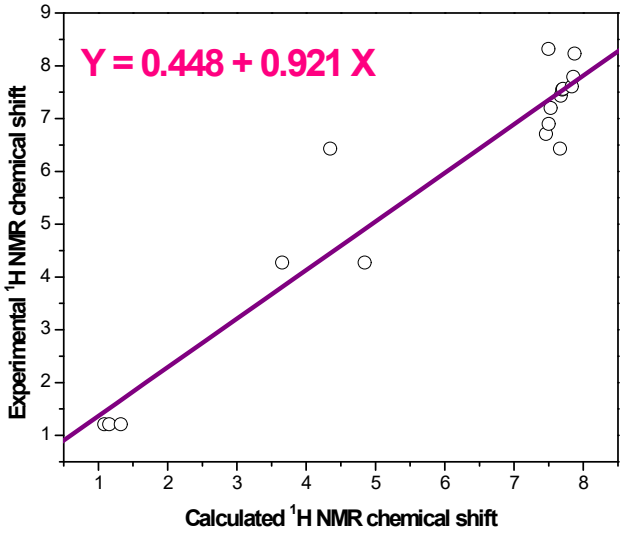


Fig. S7. (a) Experimental and (b) Calculated ^{1}H NMR spectrum, (c) Correlation graph between experimental and calculated ^{1}H-NMR chemical shifts of **12b** at B3LYP/6-311++G (d,p).

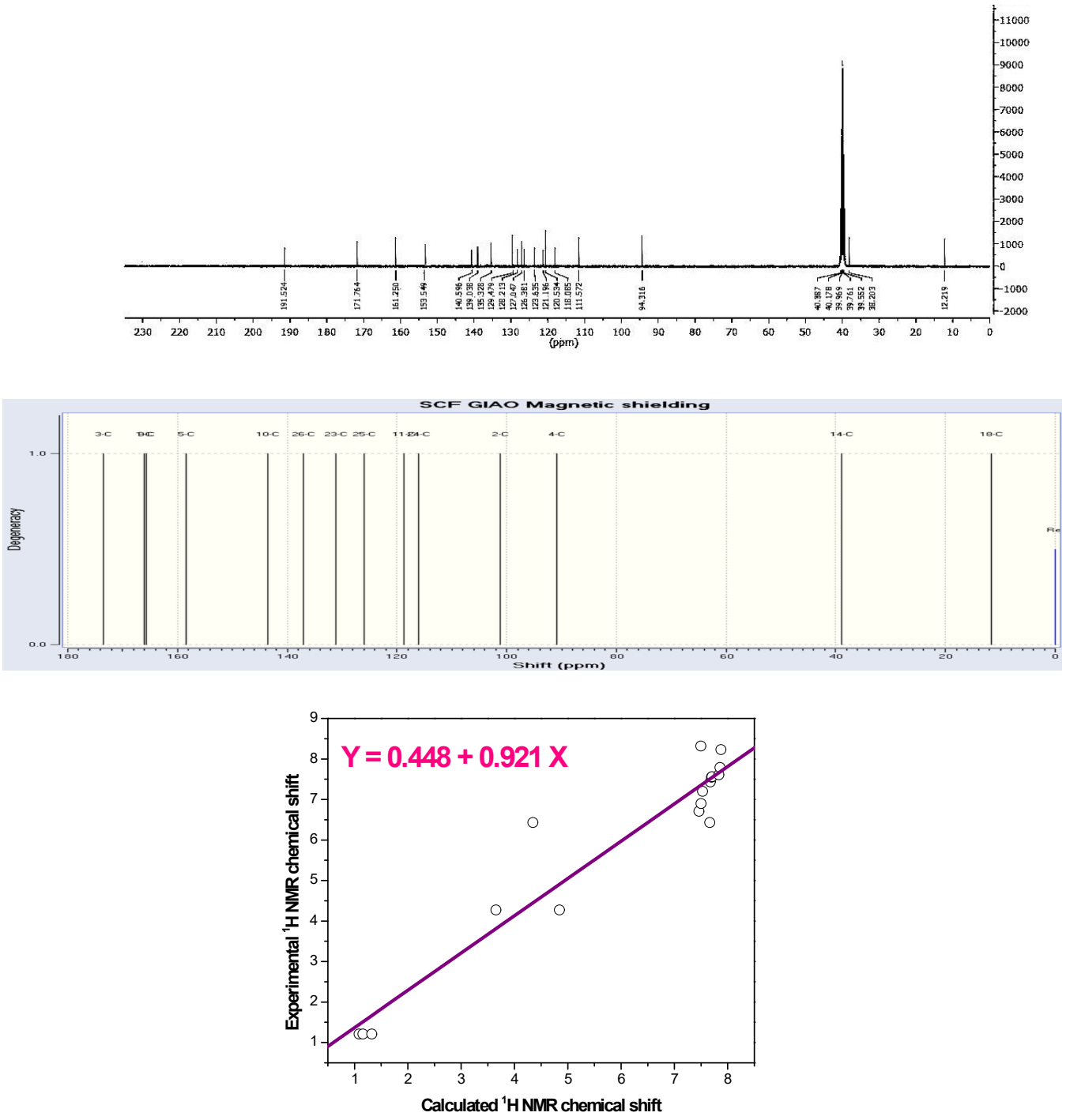


Fig. S8. (a) Experimental and (b) Calculated ^{13}C NMR spectrum, (c) Correlation graph between experimental and calculated ^{13}C NMR chemical shifts of **12b** at B3LYP/6-311++G (d,p).

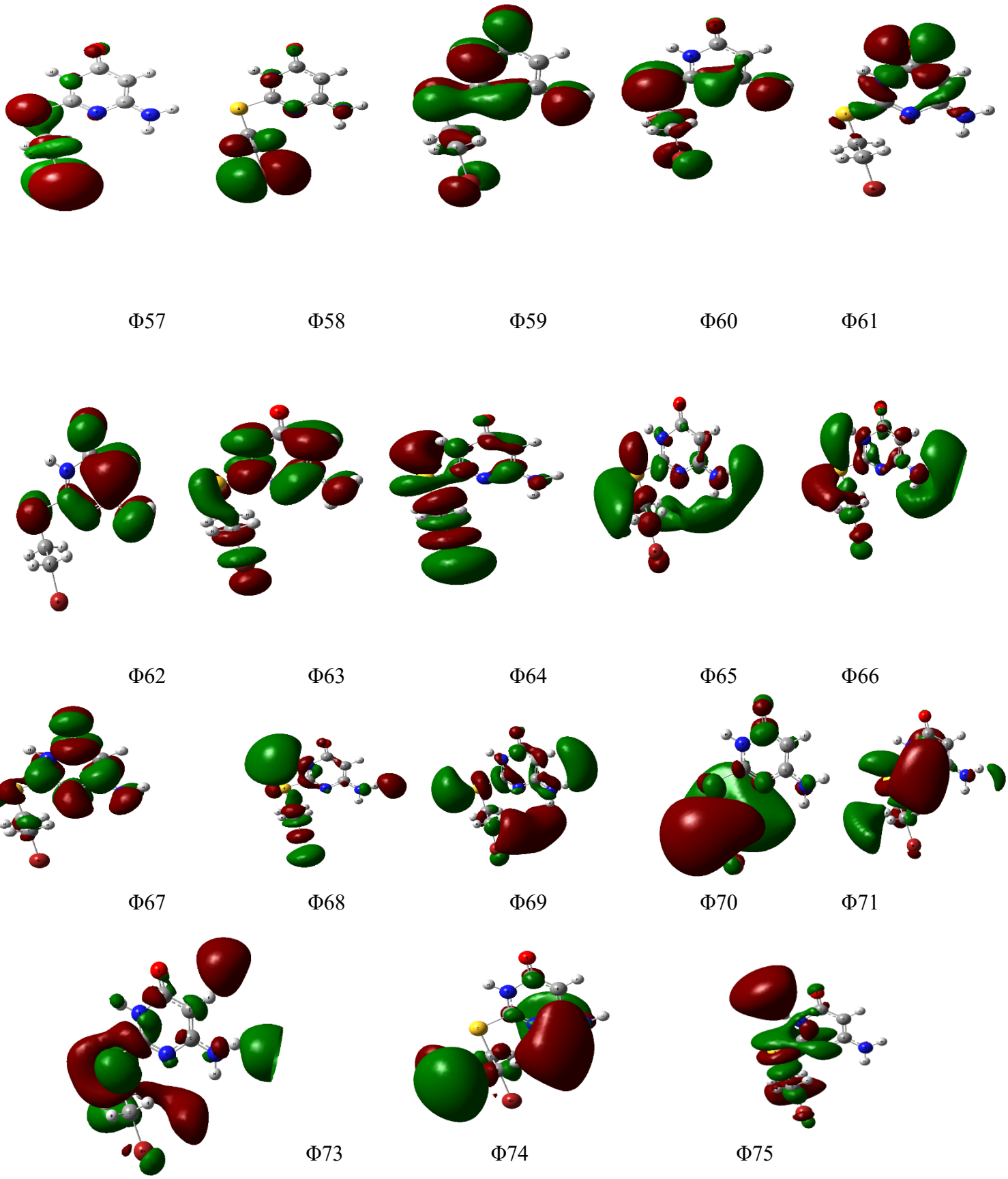


Fig. S9. Electron density contours of compound **12a**.

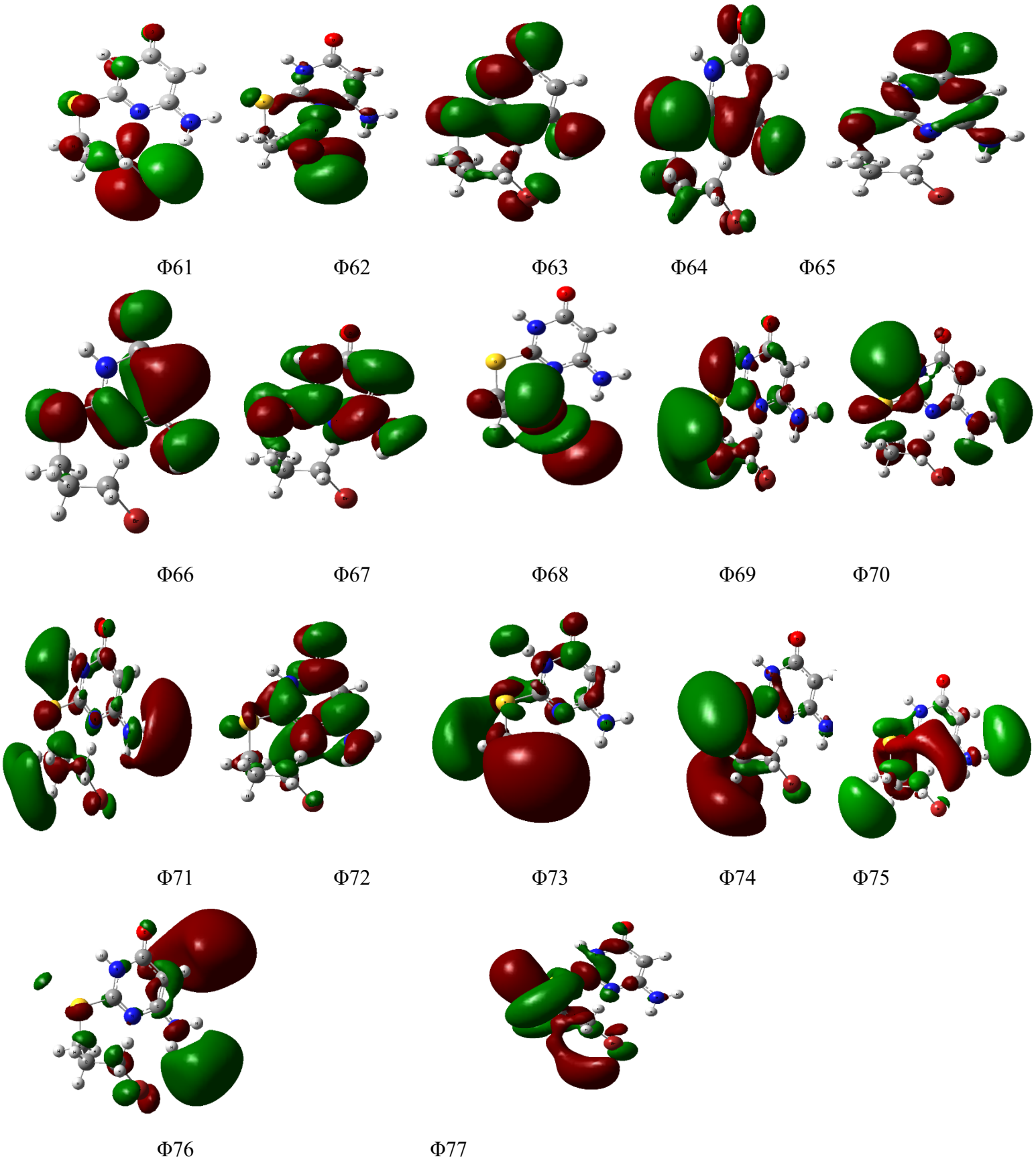


Fig. S10. Electron density contours of compound **12b**.

Table S1. Equilibrium bond lengths, (Å), bond angles, (°), Dihedral angles, (°), and Net charges, (°), for studied compounds **12a** and **12b** at the B3LYP/6-311++G(d,p).

Parameters	**12a**	**12b**	Exp. [92-94]
Bond lengths (Å)			
C1-N8	1.297	1.295	1.290
C2- N9	1.361	1.364	1.341
C1-S10	1.782	1.780	1.874
C4-O6	1.220	1.221	1.285
S10-C13	1.838	1.844	1.874
C13-C14	1.515	1.531	1.521
C14-C15	-------	1.520	1.440
Bond angles (°)			
<C2N9H12	119.05	116.85	117.61
<H12N9H11	119.45	117.74	118.44
<C2N9H11	121.47	119.55	117.61
<O6C4C3	128.98	128.90	125.21
<C1N8C2	116.98	117.34	115.52
<C1S10C13	101.16	102.86	105.35
<N7C4O6	118.56	118.53	117.56
<S10C13C14	111.54	114.68	110.21
Dihedral angles (°)			
<N8C1S10C13	0.33	0.29	
<C1S10C13C14	0.60	0.68	
<C13C14C15H22	179.89	179.99	
Mullikan net charges (°)			
O6	-0.364	-0.365	
N7	-0.157	-0.159	
N8	-0.091	-0.024	
N9	-0.332	-0.255	
S10	-0.005	-0.038	

Table S2. Second Order Perturbation Interaction Energy Values Computed in the NBO Basis for the studied compounds **12a** and **12b**, calculated at B3LYP/6-311++G (d, p).

Compound	Donor	Acceptor	$E^{(2)a}$ (kcal/mol)	NBO	Population
12a	πC1- N8	π*C2-C3	21.33	πC1- N8	1.86322
	πC2-C3	π*C4-O6	31.26	πC2-C3	1.76401
	LP (1) O6	RY*C4	16.84	LP (1) O6	1.97809
	LP (2) O6	σ*C3-C4	15.85	LP (2) O6	1.85119
	LP (2) O6	σ*C4-N7	31.56	LP (1) N7	1.61679
	LP (1) N7	π*C1-N8	67.41	LP (1) N8	1.89158
	LP (1) N7	π*C4-O6	40.65	LP (1) N9	1.76497
	LP (1) N8	σ*C1-N7	13.02	LP (2) S10	1.81885
	LP (1) N9	π*C2-C3	48.68	π*C1- N8	0.43454
	LP (2) S10	π*C1-N8	26.02	σ*C4-N7	0.10466
	π*C1- N8	π*C2-C3	57.47	π*C4-O6	0.37004
				σ*C3-C4	0.04818
				π*C2-C3	0.34154
				π*C1-N8	0.39644
				σ*C1-N7	0.04719
				RY*C4	0.01582
12b	πC1- N8	π*C2-C3	21.35	πC1- N8	1.86164
	πC2-C3	π*C4-O6	31.30	πC2-C3	1.76336
	LP (1) O6	RY*C4	16.83	LP (1) O6	1.97812
	LP (2) O6	π*C3-C4	15.81	LP (2) O6	1.85210
	LP (2) O6	π*C4-N7	31.37	LP (1) N7	1.61798
	LP (1) N7	π*C1-N8	66.54	LP (1) N8	1.88903
	LP (1) N7	σ*C4-O6	40.88	LP (1) N9	1.77240
	LP (1) N8	π*C1-N7	13.31	LP (2) S10	1.82710
	LP (1) N9	π*C2-C3	43.73	π*C1- N8	0.39664
	LP (2) S10	σ*C1-N8	25.56	σ*C4-N7	0.10404
	π*C1- N8	π*C2-C3	58.61	π*C4-O6	0.37093
				σ*C3-C4	0.04813
				π*C2-C3	0.33880
				π*C1-N8	0.39644
				σ*C1-N7	0.04793
				RY*C4	0.01580

[a]$E^{(2)}$ means energy of hyperconjugative interactions (stabilization energy).
$LP_{(n)}$ is a valence lone pair orbital (n) on atom.

Table S3. Natural Charge, Natural Population and Natural electronic Configuration of active sites in studied compounds **12a** and **12b** using B3LYP/6-311++G (d,p) .

Compound	Atom No.	Natural Charge	Natural Population				Natural electronic Configuration
			Core	Valence	Rydberg	total	
12a	O6	-0.62901	1.999	6.616	0.0137	8.629	[core]2S (1.70)2p (4.92)3p(0.01)3d
	N7	-0.61427	1.999	5.598	0.0171	7.614	[core]2S (1.27)2p (4.32)4p(0.01)
	N8	-0.61138	1.999	5.585	0.0272	7.611	[core]2S (1.36)2p (4.22)3p(0.01)3d
	N9	-0.76672	1.999	5.753	0.0146	7.767	[core]2S (1.29)2p (4.46)3p (0.01)
	S10	0.26751	9.999	5.697	0.0367	15.73	[core]3S (1.67)3p(4.02)3d(0.02)5S
12b	O6	-0.63173	1.999	6.618	0.0137	8.632	[core]2S(1.70)2p(4.92)3p(0.01)3d
	N7	-0.61512	1.999	5.599	0.0171	7.615	[core]2S(1.27)2p(4.32)4p(0.01)
	N8	-0.61097	1.999	5.585	0.0272	7.611	[core]2S(1.36)2p(4.23)3p(0.01)3d
	N9	-0.76830	1.999	5.753	0.0159	7.768	[core]2S(1.31)2p(4.44)3p(0.01)
	S10	0.24573	9.999	5.718	0.0367	15.75	[core]3S(1.67)3p(4.05)3d(0.02)5S

For numbering system, see Fig. 5

Table S4. Natural population of the total electrons in studied compounds **12a** and **12b** using B3LYP/6-311++G (d,p) .

Parameters	**12a**	**12b**
Core	57.99081 (99.984% of 58)	59.99007 (99.983% of 60)
Valence Lewis	64.13715 (97.178% of 66)	70.08560 (97.341% of 72)
Total Lewis	122.12796 (98.490% of 124)	130.07566 (98.542% of 132)
Valence non-Lewis	1.66999 (1.347% of 124)	1.70843 (1.294% of 132)
Rydberg non-Lewis	0.20205 (0.163% of 124)	0.21591 (0.164% of 132)
Total non-Lewis	1.87204 (1.510% of 124)	1.92434 (1.458% of 132)

Table S5: Total static dipole moment (μ), the mean polarizability (<α>), the anisotropy of the polarizability (Δα), and the mean first-order hyperpolarizability (<β>), for studied compounds **12a** and **12b** by B3LYP/6-311++G (d,p).

Property	PNA	**12a**	**12b**
μx		2.8426 Debye	-4.6592 Debye
μy		1.3018 Debye	1.1481 Debye
μz		-0.8187 Debye	0.1138 Debye
μ	2.44 Debye [a]	3.2319 Debye	4.7999 Debye
αXX		-124.2609 a.u.	-127.4420 a.u.
αXY		-9.6431 a.u.	-3.4665 a.u.
αYY		-75.6116 a.u.	-82.7208 a.u.
αZZ		-92.5943 a.u.	-98.1690 a.u.
αYZ		-1.1935 a.u.	0.0986 a.u.
αXZ		3.0791 a.u.	-4.0274 a.u.
<α>	22×10^{-24} esu[b]	35.25×10^{-24} esu	45.21×10^{-24} esu
Δα		46.31×10^{-24} esu	56.02×10^{-24} esu
βxxx		247.2045 a.u.	-237.0187 a.u.
βxxy		31.7250 a.u.	22.0527 a.u.
βxyy		5.0827 a.u.	-16.7915 a.u.
βyyy		54.4033 a.u.	-65.4942 a.u.
βxxz		-23.0361 a.u.	-16.5512 a.u
βxyz		-1.5676 a.u.	-0.4051 a.u.
βyyz		-3.6459 a.u.	-2.5183 a.u.
βxzz		41.5856 a.u.	-38.3195 a.u.
βyzz		1.5336 a.u.	--2.6481 a.u.
βzzz		5.7093 a.u.	4.8290 a.u.
<β>	15.5×10^{-30} esu[c]	25.16×10^{-30} esu	36.28×10^{-30} esu
DR		0.35	0.46
βHRS		45.25	56.12

[a, b, c] PNA results are taken from references [97–99].

Table S6: Calculated thermodynamically parameters for studied compounds **12a** and **12b** at the B3LYP/6-311++G(d,p).

Parameters	**12a**	**12b**
Zero Point Vibrational Energy (kcal.mol^{-1})	91.12637	109.44726
Rotational constant (GHz)		
A	1.23056	0.83593
B	0.24365	0.30103
C	0.20828	0.23050
Entropy Total (S) (cal mol^{-1} K^{-1})	114.061	120.565
Translational	42.437	42.600
Rotational	32.909	32.983
Vibrational	38.715	44.982
Thermal Energy Total (E) (kcal mol^{-1})	98.712	117.975
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	96.934	116.197
Specific heat (CV) (cal mol^{-1} K^{-1})	43.408	49.627
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	37.446	43.665

Table S7: Thermodynamic properties at different temperatures of **12a** and **12b** at the B3LYP/6-311++G(d,p).

T (K)	H^0_m (kcalmol^{-1})		$C^0_{p,m}$ (calmol^{-1}K^{-1})		S^0_m (calmol^{-1}K^{-1})	
	12a	**12b**	**12a**	**12b**	**12a**	**12b**
200	116.14	118.41	50.80	52.08	120.10	123.01
250	118.93	121.39	60.74	62.47	132.96	134.69
300	122.20	125.02	69.93	71.39	145.23	147.32
350	125.91	127.19	78.31	80.13	156.95	158.59
400	130.01	133.10	85.87	87.78	168.18	170.08
450	134.48	137.84	92.64	94.46	178.92	180.29
500	139.27	141.72	98.66	100.11	189.21	191.12
550	144.33	146.44	104.00	107.01	199.06	200.60
600	149.66	151.22	108.75	111.57	208.49	211.94

Table S8: Experimental and Computed excitation energies (in eV), electronic transition configurations, and oscillator strengths a (f) for the optical transitions of the absorption bands in the UV-vis. regions (involving HOMOs) of the compound **12a** at the CAM-B3LYP/6-311++G (d,p).

Compound	Medium	Transition	Excitation energies	Type of transition	$\lambda_{max/nm}$ $Th\ and$ Ex.	Oscillator strengths (f)	Configuration composition corresponding transition orbital
	Gas phase	3	4.85	n-π*	256	0.1691	0.65(62 ->63); -0.17(62 ->64); -0.14(62 ->65)
		22	6.17	n-π*	203	0.1665	0.17(57 ->63); 0.12(57 ->65); 0.47(60 ->63); -0.17(60 ->64); -0.21(61 ->63); -0.11(61 ->70); -0.12(62 ->65); -0.19(62 ->67); 0.10(62 ->70)
		29	6.45	π-π*	192	0.3208	0.51(59 ->63); -0.15(59 ->64); 0.10(62 ->65); -0.20(62 ->67); 0.22(62 ->68); 0.18(62 ->70)
		35	6.75	π-π*	184	0.0728	0.14(59 ->63); 0.12(60 ->63); -0.11(62 ->65); 0.26(62 ->67); -0.26(62 ->68); 0.11(62 ->69); 0.37(62 ->70); -0.11(62 ->71); 0.27(62 ->73); -0.12(62 ->75)
		4	4.94	n-π*	251 211	0.2534	0.66 (62 ->63); 0.18 (62 ->64)
		15	5.93	n-π*	209	0.2427	-0.20 (56 ->63); 0.10 (59 ->63); 0.57 (61 -

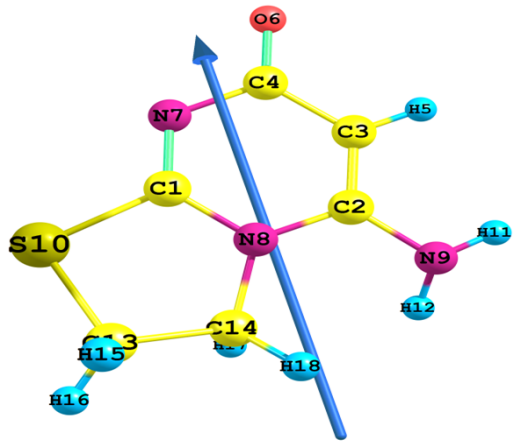
					208		>63); -0.12 (62 ->66)
		25	6.42	π-π*	193 170	0.3308	0.57 (60 ->63); 0.16 (60 ->64); 0.21 (62 ->67); -0.11 (62 ->68); 0.12 (62 ->70)
		38	6.97	π-π*	178 142	0.1441	-0.22(60 ->64); 0.17(60 ->67); -0.25(60 ->68); 0.23(60 ->70); -0.16(61 ->64); 0.13(61 ->65); 0.28(61 ->67); -0.22(61 ->68); 0.14(61 ->70); 0.14(62 ->67)
	Dioxane	3	4.84	n-π*	256 220	0.2467	0.65(62 ->63); -0.21(62 ->64)
		16	5.93	n-π*	209 211	0.1509	-0.15(56 ->63); -0.16(57 ->64); 0.12(58 ->63); 0.25(58 ->64); -0.10(58 ->65); -0.11(58 ->67); 0.49(61 ->63); 0.11(62 ->66)
		26	6.36	π-π*	195 180	0.3066	0.48(59 ->63); -0.15(59 ->64); 0.30(60 ->63); -0.14(60 ->70); -0.14(62 ->67); 0.14(62 ->68); -0.15(62 ->70)
		39	6.97	π-π*	178 150	0.0841	-0.19(59 ->68); 0.28(59 ->70); 0.26(60 ->64); -0.13(60 ->66); 0.26(60 ->67); 0.21(61 ->65); -0.15(61 ->68); 0.13(61 ->70); -0.11(62 ->66)
	DMSO	4	4.93	n-π*	252 212	0.2644	0.66 (62 ->63); -0.18 (62 ->64)
		15	5.92	n-π*	209 208	0.2715	-0.18 (56 ->63); 0.58 (61 ->63); -0.12 (62 ->66); -0.10 (62 ->67)
		24	6.41	π-π*	193 172	0.3481	-0.10 (57 ->63); 0.58 (60 ->63); -0.16 (60 ->64); -0.19 (62 ->67); 0.11 (62 ->68); -0.12 (62 ->70)
		38	6.97	π-π*	178 143	0.1553	-0.21(60 ->64); 0.18(60 ->67); -0.25(60 ->68); 0.23(60 ->70); -0.16(61 ->64); 0.13(61 ->65); 0.27(61 ->67); -0.22(61 ->68); 0.15(61 ->70); 0.12(62 ->67)
	1,2-dichloro-methan	3	4.91	n-π*	253 217	0.2582	0.66(62 ->63); 0.19(62 ->64)
		15	5.93	n-π*	209 212	0.2392	-0.19(56 ->63); 0.10(57 ->64); 0.13(59 ->63); 0.56(61 ->63); 0.11(62 ->66)
		24	6.40	π-π*	194 182	0.3576	-0.10(57 ->63); 0.57(60 ->63); 0.16(60 ->64); 0.18(62 ->67); 0.13(62 ->68); -0.13(62 ->70)
		38	6.99	π-π*	177 151	0.1228	-0.23(60 ->64); 0.13(60 ->67); 0.23(60 ->68); -0.23(60 ->70); -0.17(61 ->64); 0.17(61 ->65); 0.26(61 ->67); 0.19(61 ->68); -0.15(61 ->70); 0.15(62 ->67)

Table S9: Experimental and Computed excitation energies (in eV), electronic transition configurations, and oscillator strengths a (f) for the optical transitions of the absorption bands in the UV-vis. regions (involving HOMOs) of the compound **12b** at the CAM-B3LYP/6-311++G (d,p).

Compound	Medium	Transition	Excitation energies	Type of transition	$\lambda_{max/nm}$ $Th\ and$ Ex.	Oscillator strengths (f)	Configuration composition corresponding transition orbital
	Gas phase	3	4.84	n-π*	256	0.1645	0.65(66 ->67); -0.20(66 ->68)
		22	6.09	n-π*	204	0.1301	-0.11(64 ->75); 0.45(65 ->67); -0.18(65 ->68); -0.11(65 ->70); -0.14(65 ->75); -0.15(66 ->68); -0.15(66 ->71); -0.11(66 ->72); -0.17(66 ->74)
		30	6.48	π-π*	191	0.2592	0.43(63 ->67); -0.13(63 ->68); -0.13(63 ->70); -0.11(66 ->68); 0.14(66 ->71); 0.16(66 ->73); -0.18(66 ->74); -0.26(66 ->75); -0.14(66 ->76)
		34	6.65	π-π*	187	0.0375	-0.11(63 ->67); 0.13(65 ->68); 0.10(65 ->70); 0.11(65 ->73); 0.11(66->68); 0.10(66 ->71); -0.30(66 ->72); 0.17(66 ->73); -0.21(66 ->74); 0.12(66 ->75); 0.34(66 ->76); -0.13(66 ->77)

	Methanol	3	4.93	n-π*	252 212	0.2546	0.68 (66->67)
		15	5.90	n-π*	210 209	0.1291	0.36 (60 ->67); 0.11 (62 ->67); 0.22 (63 ->67); -0.39(65 ->70); 0.13(65 ->72); -0.11(65 ->72)
		24	6.41	π-π*	193 172	0.3157	0.17 (61 ->67); 0.57 (64 ->67); 0.11 (65 ->73); -0.15 (66 ->71); 0.19 (66 ->73)
		38	6.92	π-π*	179 145	0.0721	0.11(64 ->71); 0.25(64 ->73); 0.17(65 ->69); -0.18(65 ->71); 0.19(65 ->72); -0.21(65 ->73); 0.12(65 ->74); 0.10(66 ->70); 0.14(66 ->71); 0.27(66 ->76); -0.11(66 ->77); -0.13(66 ->78)
	Dioxane	3	4.84	n-π*	256 220	0.2466	0.68 (66->67)
		16	5.91	n-π*	210 215	0.1498	0.37(60 ->63); -0.18(62 ->64); 0.11(64 ->63); 0.42(65 ->64); -0.13(65 ->65); -0.11(66 ->67)
		25	6.34	π-π*	196 182	0.2618	-0.12(61 ->67); 0.52(63 ->67); -0.13(66 ->68); -0.19(66 ->69); 0.25(66 ->71); 0.13(66 ->74)
		40	6.96	π-π*	178 151	0.1169	0.13(63 ->73); 0.30(63 ->74); -0.18(63 ->75); -0.13(64 ->68); -0.21(64 ->70); -0.23(64 ->71); -0.17(65 ->68); -0.14(65 ->72); -0.14(65 ->73); -0.17(65 ->74); -0.10(66 ->68); 0.10(66 ->70)
	DMSO	4	4.92	n-π*	252 212	0.2658	0.68 (66->67)
		15	5.90	n-π*	210 209	0.1524	0.34 (60 ->67); 0.10 (62 ->67); -0.20 (63 ->67); 0.41(65 ->70); -0.13(65 ->72); -0.11(65 ->72)
		24	6.40	π-π*	194 173	0.3269	0.17 (61 ->67); 0.57 (64 ->67); 0.11 (65 ->73); -0.15 (66 ->71); 0.19 (66 ->73)
		38	6.92	π-π*	179 145	0.0698	0.12(64 ->71); 0.25(64 ->73); 0.14(65 ->69); 0.10(65 ->71); -0.17(65 ->72); 0.20(65 ->73); -0.19(65 ->74); 0.11(66 ->70); 0.14(66 ->71); 0.28(66 ->74); -0.11(66 ->76); -0.14(66 ->77)
	1,2-dichloro-methan	3	4.90	n-π*	253 217	0.2596	0.68 (66->67)
		15	5.90	n-π*	210 215	0.1348	0.36(60 ->67); 0.24(63 ->67); 0.40(65 ->67); -0.13(65 ->70); 0.14(66 ->72)
		24	6.39	π-π*	194 180	0.3241	0.16(61 ->67); 0.57(64 ->67); 0.11(65 ->73); -0.11(66 ->69); 0.15(66 ->71); 0.19(66 ->74)
		38	6.91	π-π*	179 152	0.0988	-0.10(64 ->68); 0.29(64 ->73); -0.13(64 ->74); 0.13(65 ->68); 0.25(65 ->69); -0.17(65 ->71); 0.12(65 ->72); -0.25(65 ->73); 0.15(65 ->74); 0.10(66 ->69); 0.11(66 ->71); 0.11(66 ->72)

Table S10: The Optimized structures of studied compound **11a** at B3LYP/6-311++G (d,p).

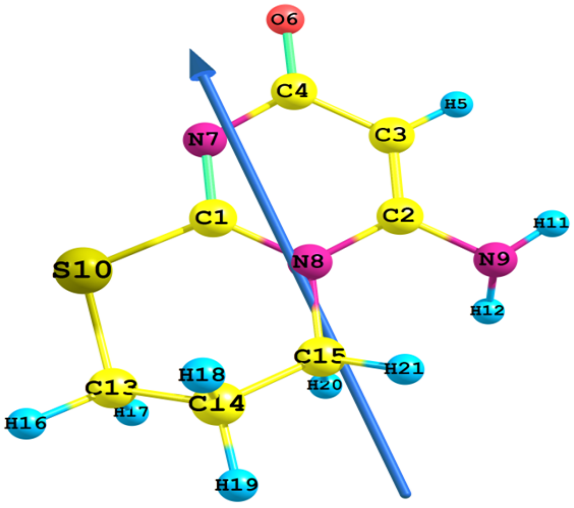


11a

C	0.293651000	-0.759893000	0.017650000
C	-1.012844000	1.220861000	-0.056294000
C	-2.116055000	0.429097000	-0.004455000

C	-2.014088000	-1.022316000	0.077566000
H	-3.105711000	0.865138000	-0.035272000
O	-2.982363000	-1.759257000	0.133926000
N	-0.696438000	-1.560394000	0.072590000
N	0.239764000	0.626776000	-0.006866000
N	-1.030966000	2.611095000	-0.069742000
S	1.985079000	-1.323157000	-0.050313000
H	-1.961365000	2.993031000	-0.168002000
H	-0.381810000	3.060309000	-0.701887000
C	2.593853000	0.369604000	0.326155000
C	1.516079000	1.318953000	-0.198669000
H	2.721655000	0.472410000	1.404356000
H	3.549024000	0.532465000	-0.169735000
H	1.672964000	1.530126000	-1.263873000
H	1.517000000	2.257547000	0.358083000

Table S11: The Optimized structures of studied compound **11b** at B3LYP/6-311++G (d,p).

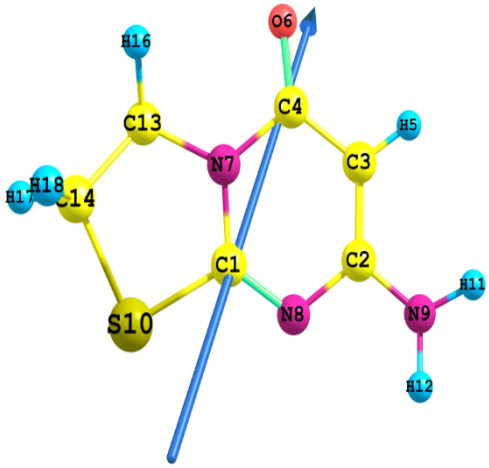


11b

C	0.096673000	0.701291000	0.134191000
C	-1.314374000	-1.196059000	0.012243000
C	-2.385239000	-0.365735000	0.063796000

C	-2.218635000	1.077083000	0.076658000
H	-3.389273000	-0.768851000	0.094171000
O	-3.148341000	1.866099000	0.042281000
N	-0.884738000	1.526744000	0.170397000
N	-0.014950000	-0.677202000	-0.006256000
N	-1.422375000	-2.583171000	-0.102883000
S	1.678802000	1.512641000	0.294595000
H	-2.385128000	-2.890476000	-0.078172000
H	-0.858958000	-3.123215000	0.542052000
C	2.902726000	0.154935000	0.133875000
C	2.366692000	-0.947236000	-0.763643000
C	1.128241000	-1.600743000	-0.169557000
H	3.794267000	0.619945000	-0.289661000
H	3.157550000	-0.233583000	1.122815000
H	2.144425000	-0.553381000	-1.759527000
H	3.124153000	-1.728978000	-0.882615000
H	1.381042000	-2.041383000	0.804003000
H	0.792092000	-2.403449000	-0.825075000

Table S12: The Optimized structures of studied compound **12a** at B3LYP/6-311++G (d,p).

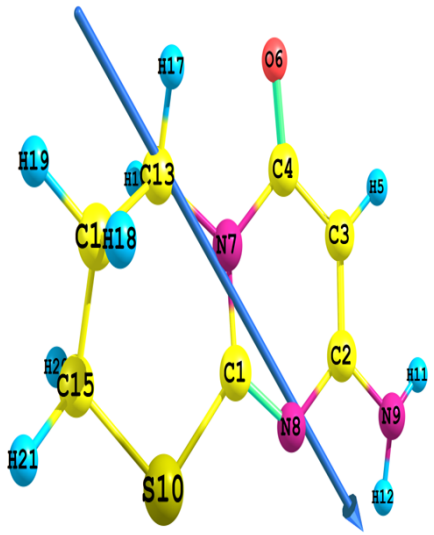


12a

C	-0.279668000	-0.698775000	0.050724000
C	1.983658000	-0.668033000	-0.009055000
C	2.021382000	0.712067000	-0.020995000
C	0.816217000	1.478089000	-0.020864000

H	2.954589000	1.257064000	-0.061913000
O	0.686590000	2.694115000	-0.070662000
N	-0.357751000	0.657200000	0.045708000
N	0.813945000	-1.391650000	0.037294000
N	3.107264000	-1.444068000	-0.069772000
S	-1.882301000	-1.457637000	0.070231000
H	4.005969000	-1.031324000	0.115171000
H	2.993705000	-2.423584000	0.136717000
C	-1.699740000	1.227709000	-0.084419000
C	-2.661680000	0.169952000	0.459177000
H	-1.896996000	1.446153000	-1.138797000
H	-1.745786000	2.163161000	0.471658000
H	-3.638772000	0.221435000	-0.017522000
H	-2.780101000	0.248318000	1.540384000

Table S13: The Optimized structures of studied compound **12b** at B3LYP/6-311++G (d,p).



12b

C	0.663145000	0.015429000	0.200055000
C	0.547248000	2.296702000	0.086901000

C	-0.770661000	2.270897000	-0.317946000
C	-1.444447000	1.032735000	-0.491360000
H	-1.331653000	3.172997000	-0.520246000
O	-2.599183000	0.859127000	-0.859046000
N	-0.628988000	-0.135553000	-0.188131000
N	1.263307000	1.164045000	0.345905000
N	1.240784000	3.457628000	0.295795000
S	1.733088000	-1.351462000	0.588109000
H	0.886132000	4.318550000	-0.085703000
H	2.239798000	3.373315000	0.396988000
C	-1.284559000	-1.441094000	-0.385243000
C	-0.806572000	-2.498782000	0.596777000
C	0.662605000	-2.833131000	0.386160000
H	-1.114180000	-1.769868000	-1.416872000
H	-2.351263000	-1.250307000	-0.285313000
H	-0.980401000	-2.165034000	1.624081000
H	-1.404358000	-3.402760000	0.442593000
H	0.826948000	-3.253088000	-0.608209000
H	1.026204000	-3.548314000	1.125704000