SUPPLEMENTARY MATERIALS

The structural characterization, biological activity of sufamehtoxazolyl-azo-*p*-cresol; its copper(II) complex and their theoretical studies

Nilima Sahu, Dipankar Das, Sudipa Mondal, Suman Roy, Paramita Dutta, Nayim Sepay, Suvroma Gupta, Elena Lopez-Torres, and Chittaranjan Sinha*

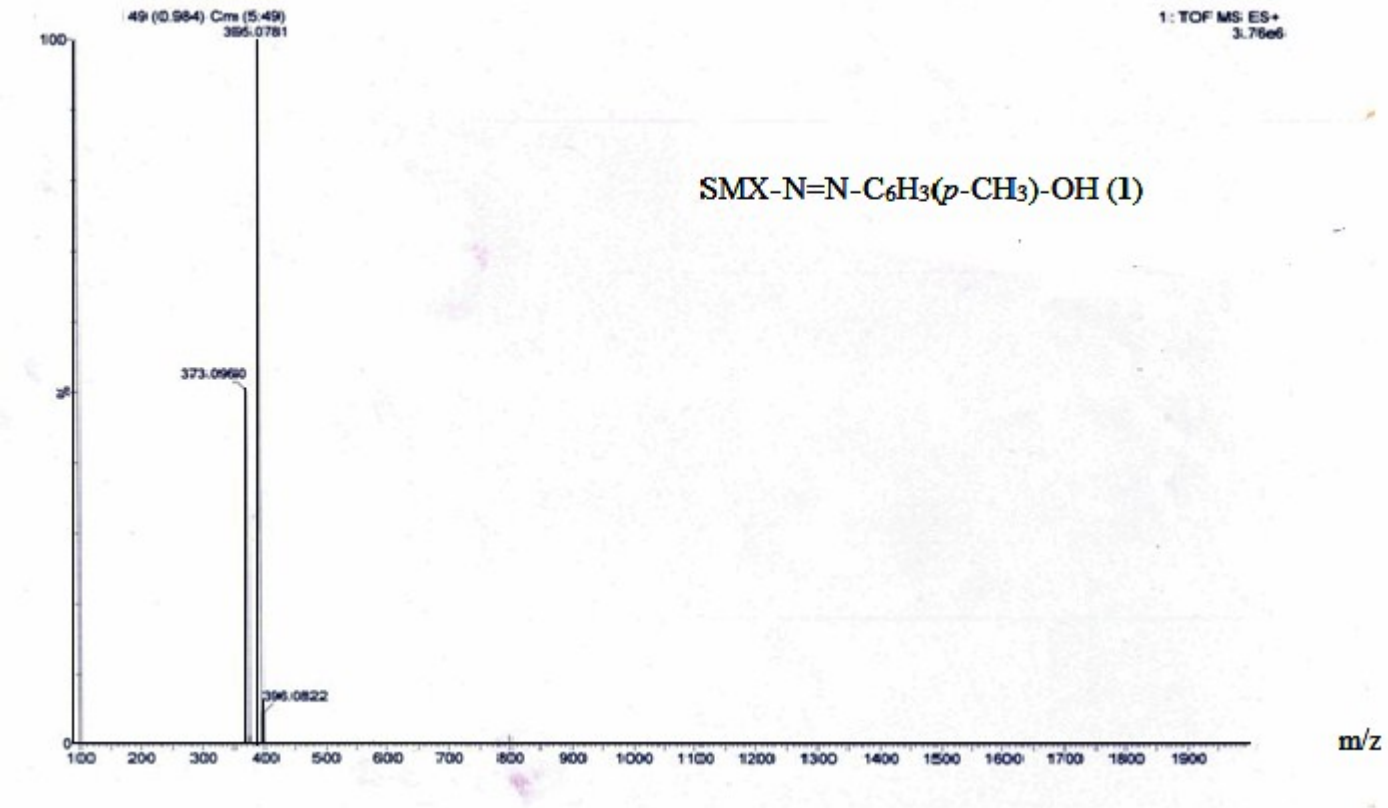


Fig. S1. Mass spectrum of SMX-N=N-C_6H_3(*p*-CH_3)-OH (**1**)

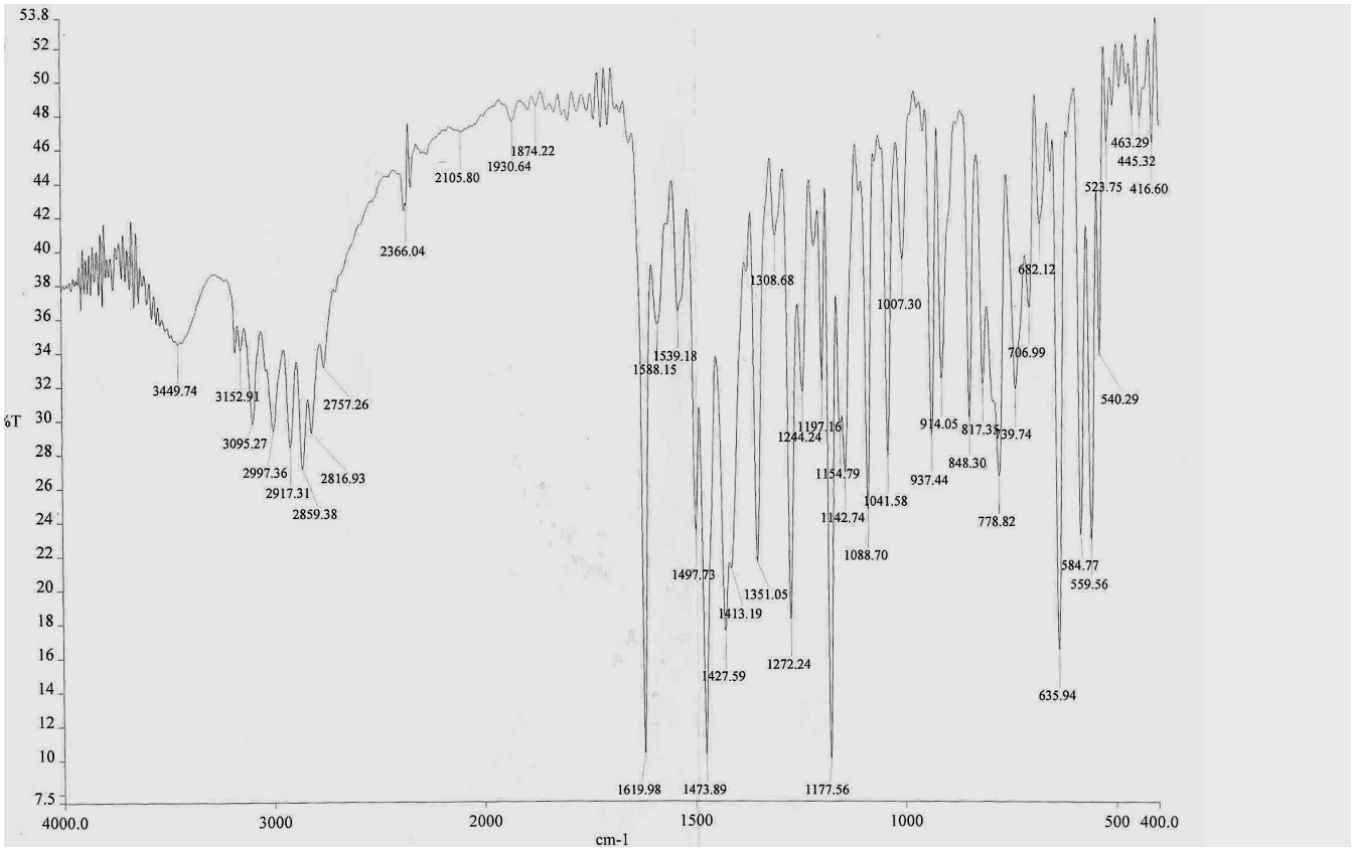
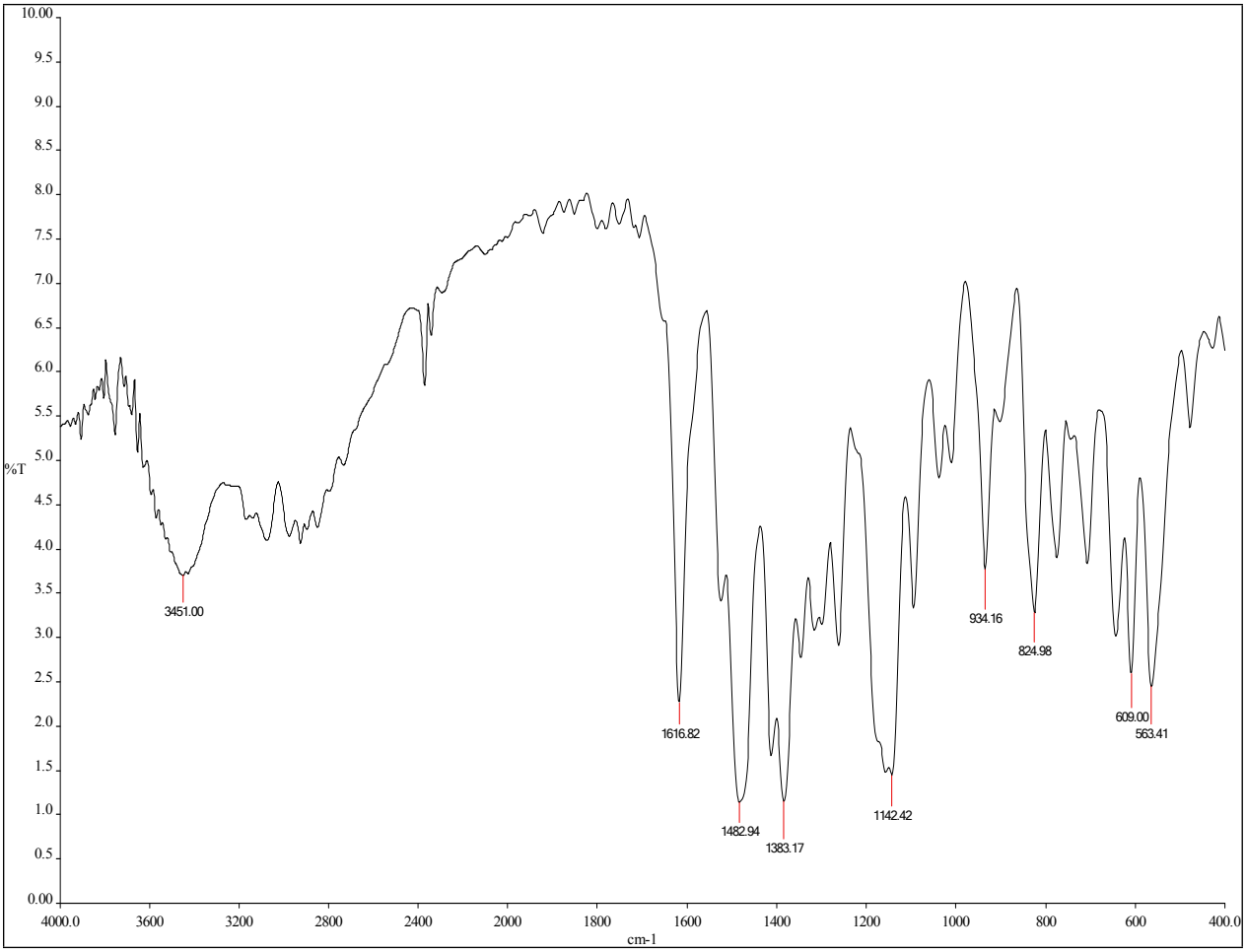


Fig. S2. FT-IR spectrum of SMX-N=N-C_6H_3(*p*-CH_3)-OH (**1**) in KBr disc

IR data of[(SMX-N=N-C_6H_3(*p*-CH_3)-O)$_2$Cu]$_n$ (2)



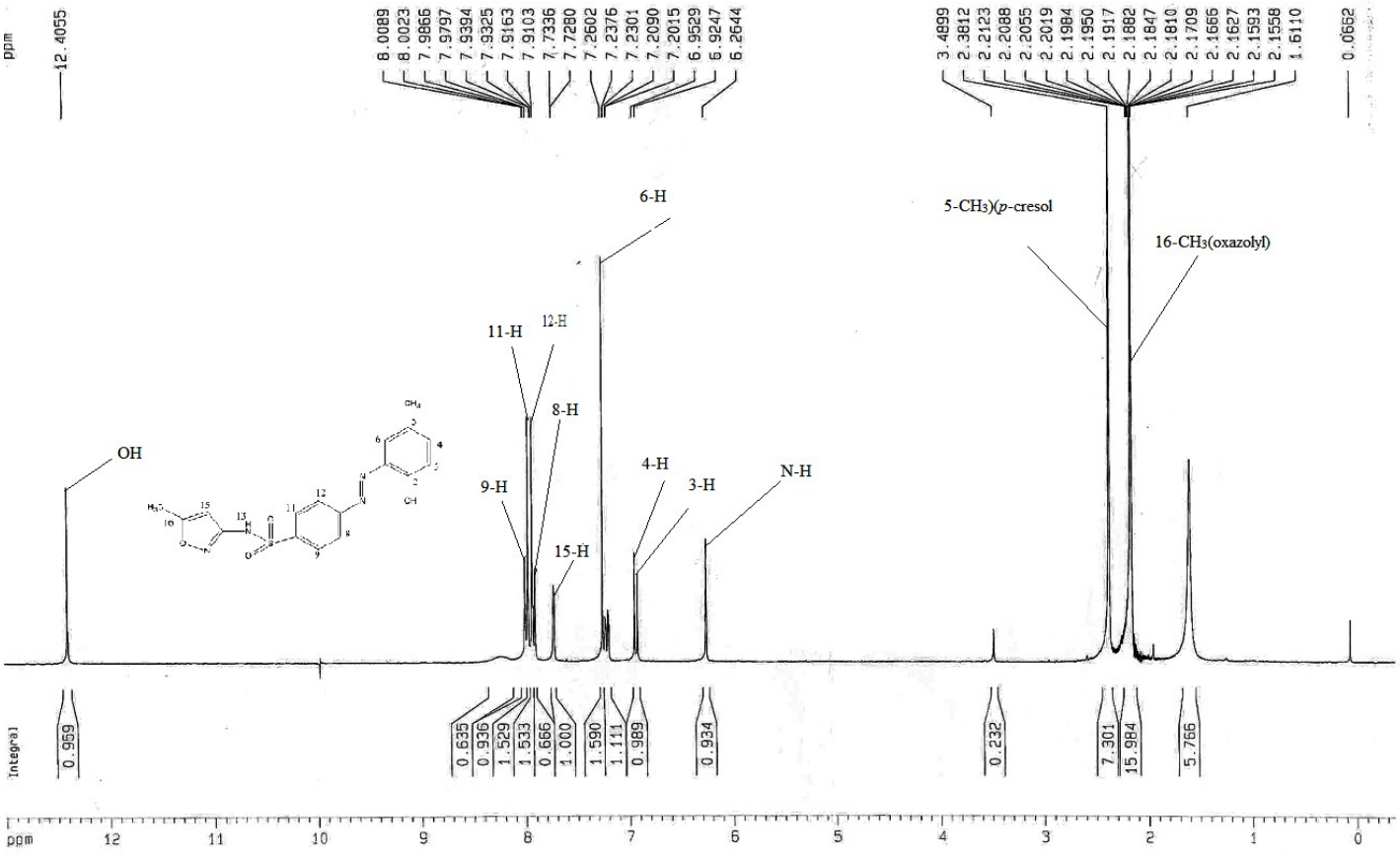
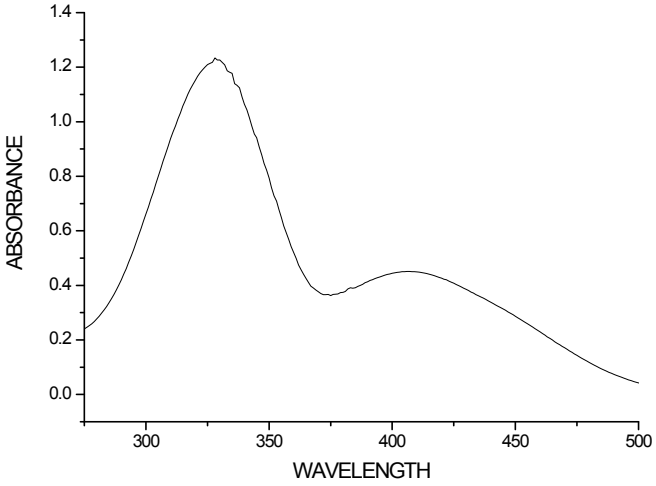
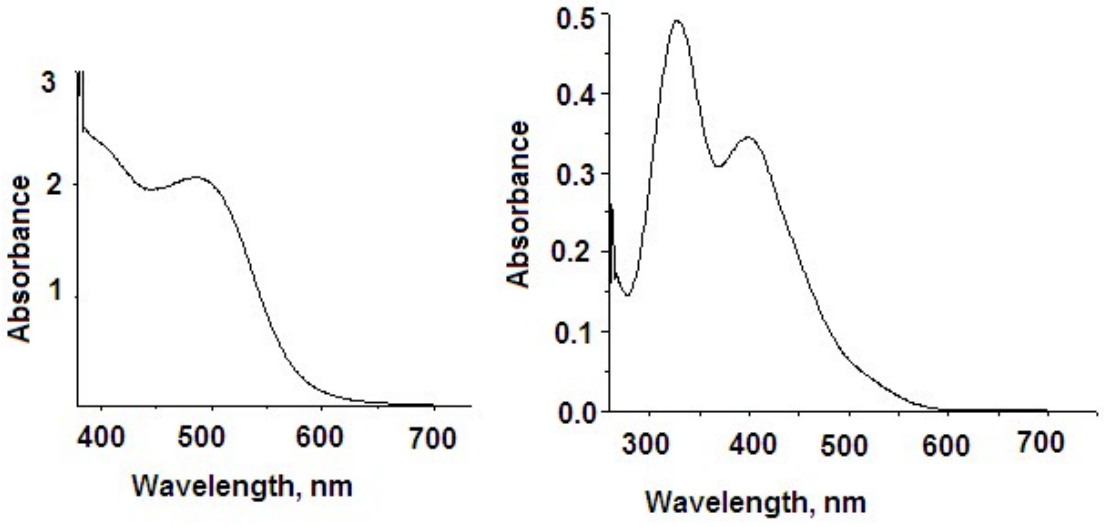


Fig. S3. ^{1}H NMR Spectra of SMX-N=N-C_6H_3(p-CH_3)-OH (**1**) in DMSO - d_6 solvent



(a)



(b/) (b)

Fig. S4. UV-Vis spectra of (a) SMX-N=N-C_6H_3(*p*-CH_3)-OH (**1**) in methanol **λmax at 329.2nm, ε = 1.524 X $10^4$$cm^2$$mol^{-1}$- (π-π*), λmax at 405.40nm, ε = 0.621X $10^4$$cm^2$$mol^{-1}$ - (n-π*)** and (b) and (b/) [Cu(SMX-N=N-C_6H_3(*p*-CH_3)-$O)_2]_n$ (**2**) in DMF solution. **λmax at 489.3 nm, ε = 1.023 X $10^4$$cm^2$$mol^{-1}$- (d-d),λmax at 327.5 nm, ε = 2.433 X $10^4$$cm^2$$mol^{-1}$- (π-π*),λmax at 400.5 nm, ε = 1.705 X $10^4$$cm^2$$mol^{-1}$ - (n-π*)**

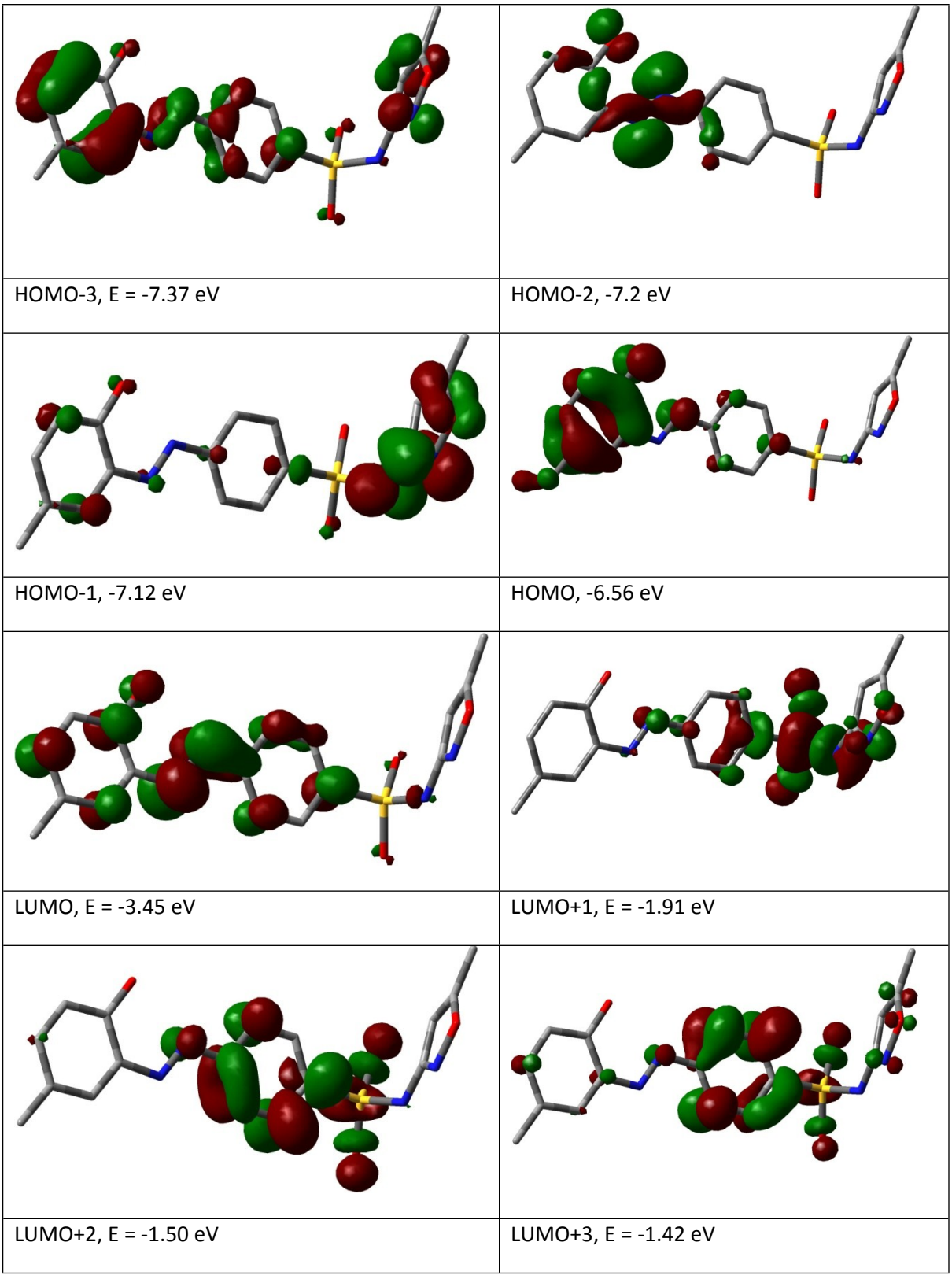


Fig. S5. Contour plots of some selected molecular orbitals of SMX-N=N-C_6H_3(*p*-CH_3)-OH (**1**)

Table S1. MO composition of SMX-N=N-C_6H_3(*p*-CH_3)-OH (**1**)

MO	Energy (eV)	Oxazole	Azo	4-methylphenol	Benzsulfonamide
LUMO+6	-0.23	04	04	58	34
LUMO+5	-0.6	02	04	90	04
LUMO+4	-0.89	79	00	05	16
LUMO+3	-1.42	06	02	07	85
LUMO+2	-1.5	00	05	03	92
LUMO+1	-1.91	11	03	03	83
LUMO	-3.45	00	43	28	29
HOMO	-6.56	01	07	82	10
HOMO-1	-7.12	54	01	11	34
HOMO-2	-7.2	00	68	24	08
HOMO-3	-7.37	20	08	52	20
HOMO-4	-7.53	78	01	05	16
HOMO-5	-8.17	00	00	00	100
HOMO-6	-8.34	02	00	00	98
HOMO-7	-8.35	04	02	11	83

Table S2. Assignment of transitions by TD-DFT data of SMX-N=N-C_6H_3(*p*-CH_3)-OH (**1**) in CH_3OH

Excitation energy (eV)	Wavelength (nm)	f	Key Transitions	Character
2.6813	462.41	0.2940	(97%) HOMO → LUMO	PACT, IPCT, PBCT
3.3788	366.94	0.7543	(96%) HOMO-2 → LUMO	APCT, ABCT
3.6343	341.15	0.1330	(97%) HOMO-3 → LUMO	PACT, IPCT, PBCT
4.0354	307.24	0.0210	(89%) HOMO-5 → LUMO	BACT, BPCT, IBCT
4.4007	281.74	0.0226	(81%) HOMO → LUMO+2	PBCT
4.6904	264.33	0.0136	(89%) HOMO → LUMO+3	PBCT
5.0141	247.27	0.0332	(45%) HOMO-2 → LUMO+2	ABCT
5.2312	237.01	0.0125	(55%) HOMO-7 → LUMO+1	IBCT
5.3335	232.46	0.0284	(63%) HOMO-2→ LUMO+3	ABCT

IPCT: Intra phenol charge transfer; PBCT: Phenol to benzene sulfonamide charge transfer; PACT: Phenol to azo charge transfer; APCT: Azo to phenol charge transfer; ABCT: Azo to benzene sulfonamide charge transfer; IBCT: Intra benzene sulfonamide charge transfer; BPCT: Benzene sulfonamide to phenol charge transfer; BACT: Benzene sulfonamide to azo charge transfer

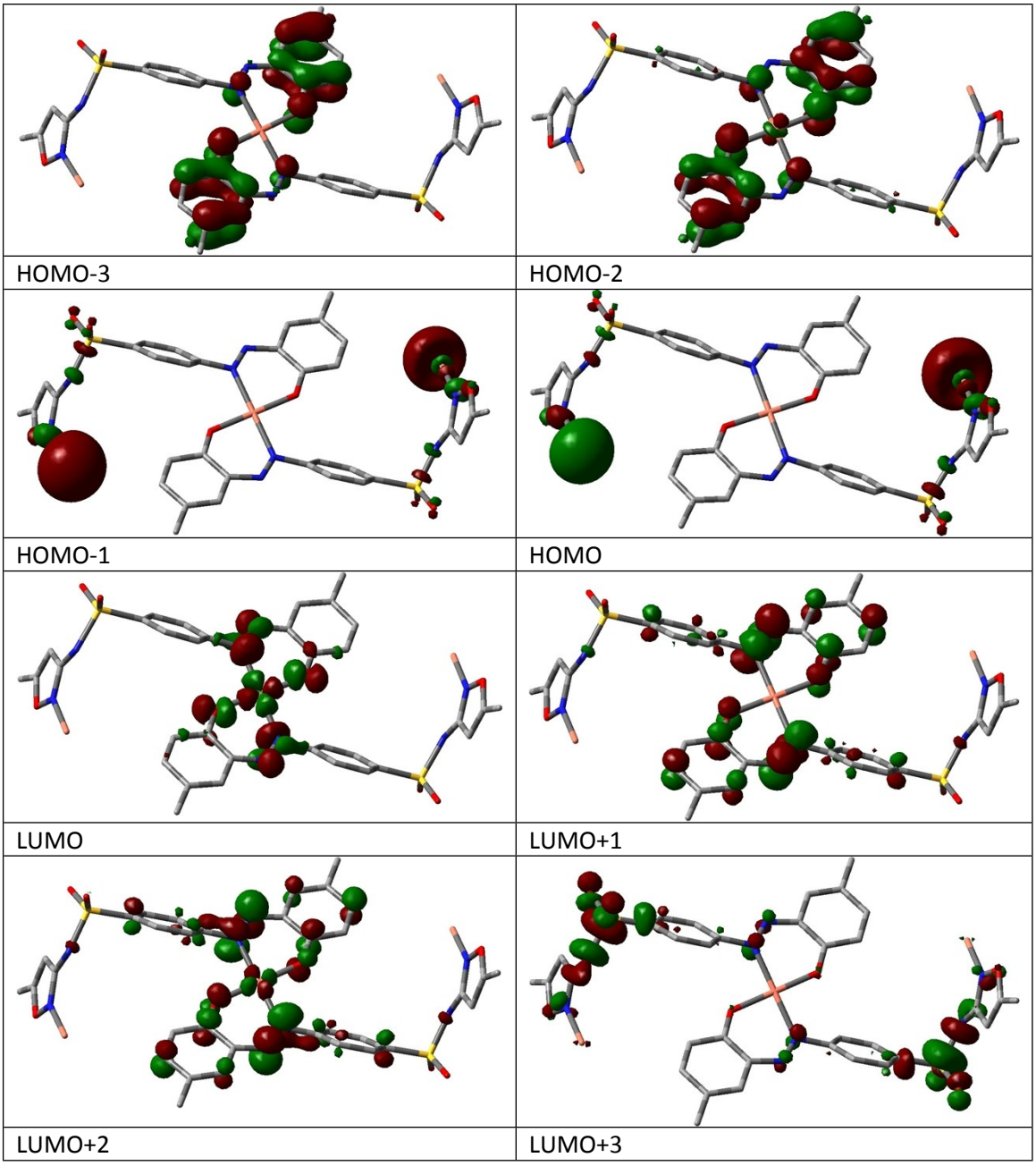


Fig. S6. Contour plots of some selected α-molecular orbitals of $[Cu(SMX\text{-}N{=}N\text{-}C_6H_3(p\text{-}CH_3)\text{-}O)_2]_n$ (**2**)

Table S3. MO composition of some selected α molecular orbitals of [Cu(SMX-N=N-C_6H_3(*p*-CH_3)-O)$_2$]$_n$ (**2**)

MO	Energy (eV)	4-methylphenol	Benzsulfonamide	Oxazle	Cu	Azo
LUMO+10	-1.24	01	86	13	00	00
LUMO+9	-1.25	00	86	13	01	00
LUMO+8	-1.5	02	44	51	01	02
LUMO+7	-1.51	03	43	51	01	02
LUMO+6	-1.66	04	63	28	01	04
LUMO+5	-1.67	02	66	29	00	03
LUMO+4	-2.56	04	72	17	01	06
LUMO+3	-2.56	04	72	18	00	06
LUMO+2	-3.2	31	23	05	07	34
LUMO+1	-3.26	35	21	04	00	40
LUMO	-3.47	25	03	00	46	26
HOMO	-3.98	01	11	88	00	00
HOMO-1	-3.99	01	12	86	00	01
HOMO-2	-6.13	79	08	00	03	10
HOMO-3	-6.41	85	04	00	02	09
HOMO-4	-6.68	00	04	96	00	00
HOMO-5	-6.69	00	04	96	00	00
HOMO-6	-6.74	01	04	95	0	0
HOMO-7	-6.74	00	04	96	00	00
HOMO-8	-6.99	15	02	67	01	15
HOMO-9	-6.99	00	00	100	00	00
HOMO-10	-7.0	09	01	81	00	09

Table S4. TD-DFT data of $[Cu(SMX\text{-}N{=}N\text{-}C_6H_3(p\text{-}CH_3)\text{-}O)_2]_n$ (**2**) considering α molecular orbitals in CH_3CN

Excitation energy(ev)	Wavelength(nm)	f	Key Transitions	Character
1.6203	765.19	0.0324	(30%) HOMO-2→LUMO	LMCT
1.8302	677.45	0.0452	(37%) HOMO-2→LUMO+1	ILCT
1.9503	635.72	0.0278	(32%) HOMO-2→LUMO+2	ILCT
2.2776	544.36	0.0279	(40%) HOMO-3→LUMO	LMCT
2.4816	499.62	0.0296	(56%) HOMO-1→LUMO+10	ILCT
2.5955	477.69	0.0279	(21%) HOMO-3→LUMO+1	ILCT
2.6990	459.37	0.0477	(30%) HOMO-5→LUMO	LMCT
2.7799	446.00	0.0984	(16%) HOMO-3→LUMO+2	ILCT
2.9029	427.10	0.0769	(28%) HOMO-5→LUMO+1	ILCT
2.9636	418.35	0.0241	(39%) HOMO-3→LUMO+3	ILCT
2.9964	413.77	0.0511	(25%) HOMO-3→LUMO+4	ILCT
3.2149	385.65	0.0624	(29%) HOMO-1→LUMO+3	ILCT

LMCT: Ligand to Metal charge transfer; ILCT: Inter Ligand charge transfer;

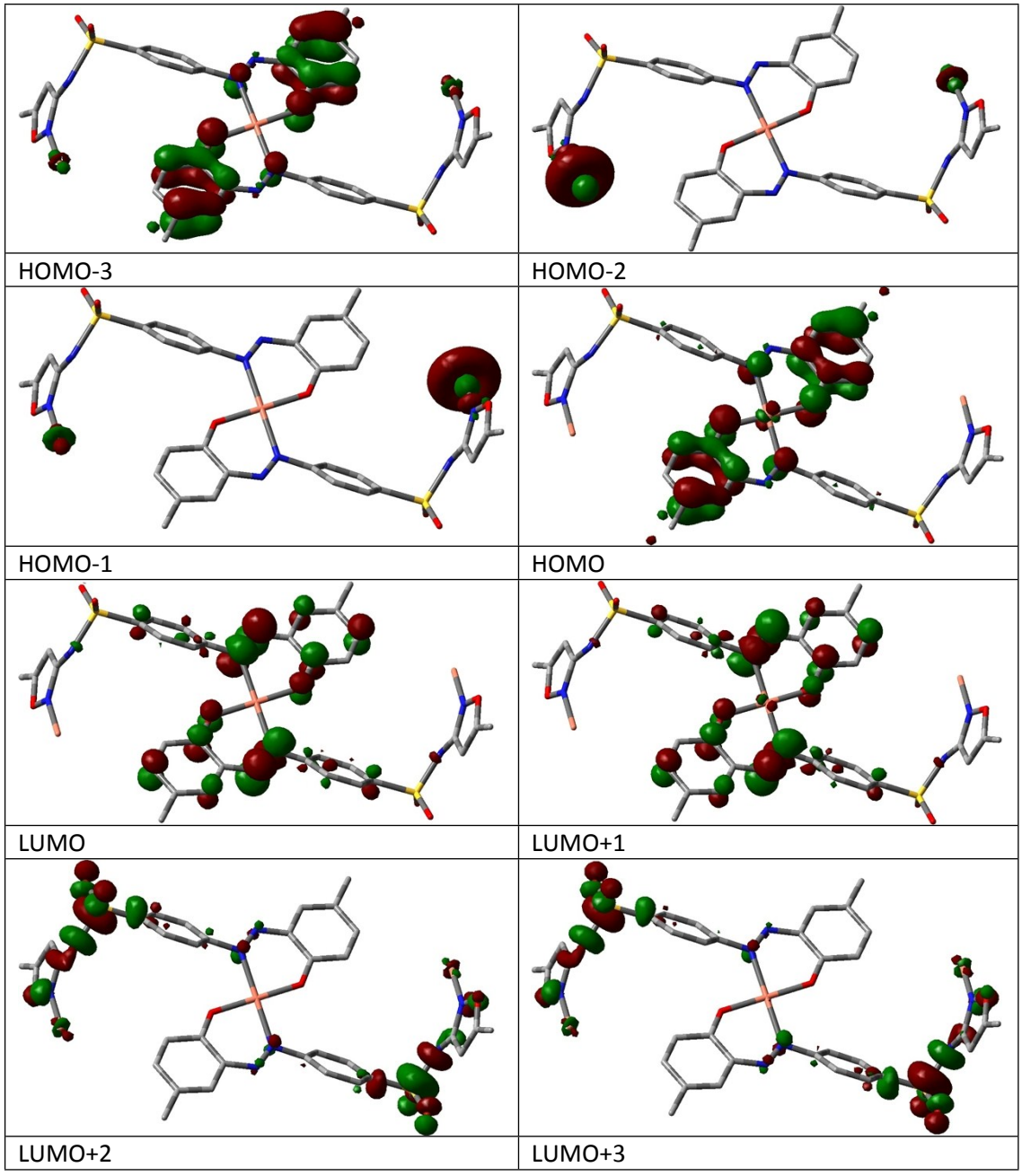


Fig. S7. Contour plots of some selected β-molecular orbitals of $[Cu(SMX\text{-}N{=}N\text{-}C_6H_3(p\text{-}CH_3)\text{-}O)_2]_n$ (**2**)

Table S5. MO composition of some selected β molecular orbitals of [Cu(SMX-N=N-C_6H_3(*p*-CH_3)-O)$_2$]$_n$ (**2**)

MO	Energy (eV)	4-methylphenol	Benzsulfonamide	Oxazle	Cu	Azo
LUMO+10	-1.24	00	81	18	01	00
LUMO+9	-1.47	01	41	55	01	02
LUMO+8	-1.48	01	38	59	01	01
LUMO+7	-1.64	02	73	22	00	03
LUMO+6	-1.64	04	73	19	01	03
LUMO+5	-1.95	02	15	82	00	01
LUMO+4	-1.96	02	16	81	00	01
LUMO+3	-2.54	03	70	23	00	04
LUMO+2	-2.55	03	70	23	00	04
LUMO+1	-3.25	35	20	01	01	43
LUMO	-3.28	37	20	01	00	42
HOMO	-6.18	80	07	00	02	11
HOMO-1	-6.41	02	01	97	00	00
HOMO-2	-6.41	01	01	98	00	00
HOMO-3	-6.43	82	04	04	02	08
HOMO-4	-6.54	38	08	03	13	38
HOMO-5	-6.65	01	07	92	00	00

HOMO-6	-6.65	02	06	91	00	01
HOMO-7	-6.89	00	00	100	00	00
HOMO-8	-6.89	00	00	100	00	00
HOMO-9	-6.89	00	00	100	00	00
HOMO-10	-6.89	00	00	100	00	00

Table S6. TD-DFT data of of $[Cu(SMX\text{-}N{=}N\text{-}C_6H_3(p\text{-}CH_3)\text{-}O)_2]_n$ (**2**) considering β molecular orbitals in CH_3CN

Excitation energy (eV)	Wavelength (nm)	f	Key Transitions	Character
1.6203	765.19	0.0324	(26%) HOMO-1→LUMO	ILCT
1.8302	677.45	0.0452	(34%) HOMO-1→LUMO+1	ILCT
1.9503	635.72	0.0278	(33%) HOMO-1→LUMO+2	ILCT
2.2776	544.36	0.0279	(40%) HOMO-2→LUMO	ILCT
2.5804	480.49	0.0149	(39%) HOMO-8→LUMO+5	ILCT
2.6990	459.37	0.0477	(30%) HOMO-4→LUMO	ILCT
2.7799	446.00	0.0984	(32%) HOMO-2→LUMO+2	ILCT
2.9029	427.10	0.0769	(27%) HOMO-4→LUMO+1	ILCT
3.1341	395.60	0.0228	(21%) HOMO-1→LUMO+4	ILCT
3.1911	388.54	0.0245	(17%) HOMO-1→LUMO+4	ILCT

Table S7. Docking posed bonding parameters of SMX-N=N-C_6H_3(*p*-Me)-OH (**1**) with DNA

Compounds	Hydrogen bonds					π- Interactions			
	No. of hydrogen bonds	DNA End	Compound End	Bond Distances Å	D--H—A bond angle	No. of ionic interactions	DNA End	Compound End	Bond Distances Å
	1	Chain A, aromatic H of A6	N of azo	2.17	145.20	8	Chain B, H of sugar of G22	O of SO_2	2.32
							Chain A, H of sugar of A6	O of SO_2	2.64
							Chain A, H of sugar of A6	N of isooxazole ring	2.83
							Chain B, H of sugar of C21	N of azo	2.58
							Chain A, H of sugar of T8	O of carboxylic acid OH	2.83
							Chain B, H of sugar of T20	O of carboxylic acid C=O	3.07
							Chain B, H of sugar of T20	O of carboxylic acid C=O	2.96
							Chain A, H of sugar of T8	Aromatic OH	2.29

Table S8. Docking posed bonding parameters of $[Cu(SMX\text{-}N{=}N\text{-}C_6H_3(p\text{-}CH_3)\text{-}O)_2]_n$ (**2**) with DNA

Compounds	Hydrogen bonds					π- Interactions			
	No. of hydrogen bonds	DNA End	Compound End	Bond Distances Å	D--H—A bond angle	No. of ionic interactions	DNA End	Compound End	Bond Distances Å
	3	Chain A, NH_2 of G4	O of SO_2NH	2.72	129.6	7	Chain A, H of sugar of A6	O of SO_2NH	2.66
		Chain A, NH of A5	O of SO_2NH	1.55	147.18		Chain B, H of sugar of C21	O of SO_2NH	2.75
		Chain A, NH of A6	N of azo	3.08	160.01		Chain B, O of	isooxazole ring	4.51
							Chain B, O of phosphate of C21	CH3 containing Phenyl ring	4.59
							Chain A, O of phosphate of T8	CH_3 containing Phenyl ring	4.26
							Chain A, O of phosphate of T8	SO_2NH bearing phenyl ring	3.08

							Chain B, aromatic ring of T20	Aromatic CH_3	5.46

SMX AZO P-CRESOL 2-D

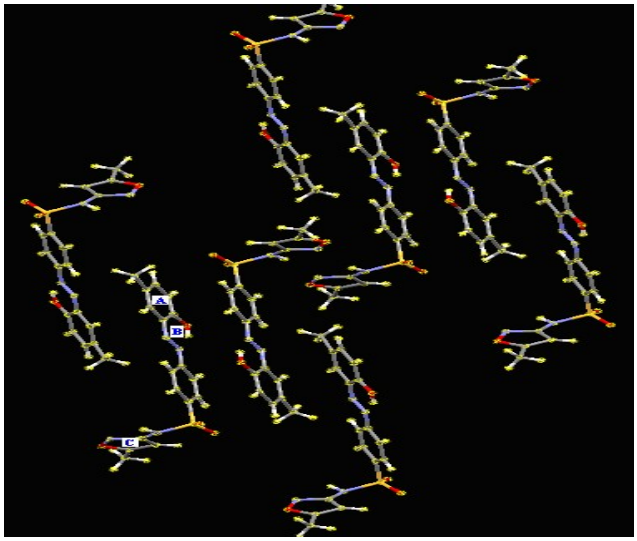


Table S9. ADMET data

Compds	Molecular Weight	ADMET Solubility (aqueous)	ADMET solubility level	ADMET absorption level≠	ADMET_ AlogP98	Molecular fractionalpolar surface area	No of H-bond acceptor	No. of H-bond donor	Lipniski's filter	Drug likeness inference	Ames Prediction
Ligand	372.4	-5.282	2	1 (moderate)	4.07	0.35	6	2	yes	Yes, low	non-mutagen