Supplementary Information

Heterocyclic ligated Co(II), Ni(II), Cu(II) and Zn(II) complexes for efficient photocatalyticand biological applications

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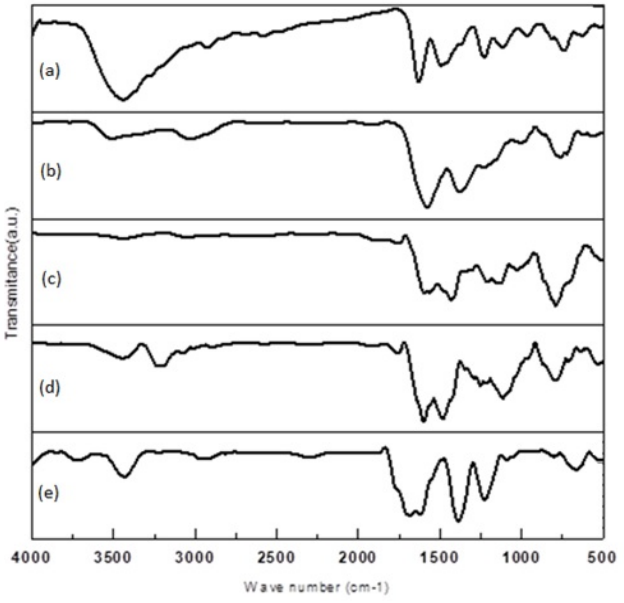

Fig. S1 — IR spectrum of (a) indal-2-abu, (b) [Co-(indal-2-abu)$_2$], (c) [Ni-(indal-2-abu)$_2$], (d) [Cu-(indal-2-abu)$_2$] and (e) [Zn-(indal-2-abu)$_2$] complexes

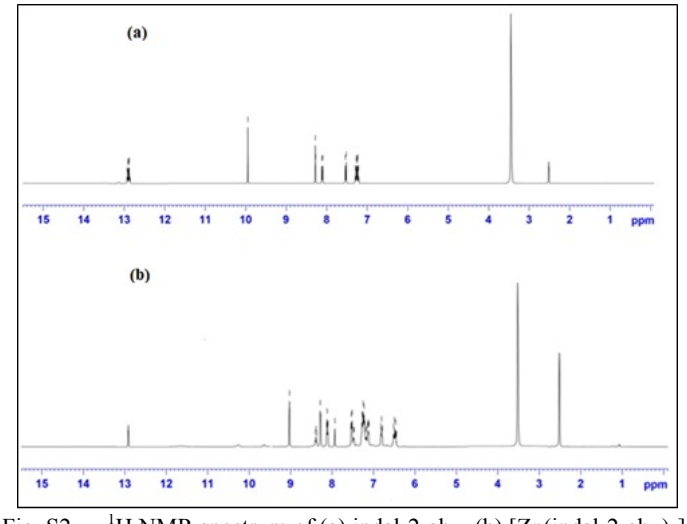

Fig. S2 — ^{1}H NMR spectrum of (a) indal-2-abu, (b) [Zn(indal-2-abu)$_2$]

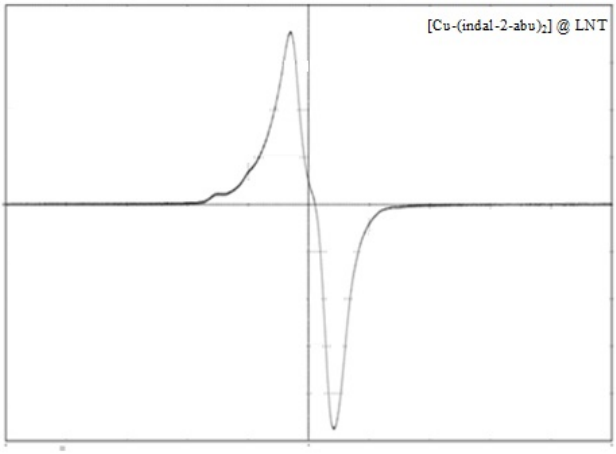

Fig. S3 — ESR spectrum of [Cu-(indal-2-abu)$_2$] at LNT

Table S1

Table S1—PASS prediction for the activity spectrum of indal-2-abu

Pa	Pi	Activity
0.842	0.003	Histidinol-phosphatase inhibitor
0.764	0.017	Mucositis treatment
0.699	0.005	Pyroglutamyl-peptidase II inhibitor
0.709	0.026	Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
0.692	0.060	Mucomembranous protector
0.632	0.036	Pseudolysin inhibitor
0.593	0.008	Antinociceptive
0.581	0.008	Cyclic AMP agonist
0.649	0.088	Gluconate 2-dehydrogenase (acceptor) inhibitor
0.595	0.043	Kidney function stimulant
0.545	0.002	L-Serine ammonia-lyase inhibitor
0.531	0.007	Serine-pyruvate transaminase inhibitor
0.530	0.009	Phenylalanine(histidine) transaminase inhibitor
0.508	0.003	Dimethylhistidine N-methyltransferase inhibitor
0.508	0.005	8-Amino-7-oxononanoate synthase inhibitor
0.511	0.031	Fibroblast growth factor agonist
0.478	0.004	Histidine decarboxylase inhibitor
0.527	0.058	Proteasome ATPase inhibitor
0.557	0.097	Nootropic
0.511	0.058	Glutamate-5-semialdehyde d

Pa represents the probability of being active and Pi isthe probability of being inactive

Table S2 ―The binding energy of indal-2-abu with target proteins

SI. No.	PDB	Binding energy (kcal/mol)
1	(3T88)	-6.9
2	(2RJG)	-7.7
3	(3TTZ)	-7.2
4	(3A8U)	-7.1
5	(3SRW)	-7.5
6	(2VEG)	-6.2
7	(1QI3)	-7.1
8	(5X2L)	-6.8
9	(3UGC)	-8.0
10	(1JS3)	-8.3

Table S3― Favourable non-covalent bond interaction between indal-2-abu and target proteins

PDBID	Residue name	Bond distance	Type of interaction	from	To
1JS3	Gly354	2.97	H-bond	A:GLY354:N	:UNK0:O
	Ala148	3.16	H-bond	B:ALA148:N	:UNK0:O
	Ser149	2.98	H-bond	B:SER149:N	:UNK0:O
	Phe103	3.83	Hydrophobic	:UNK0	A:PHE103
	Phe103	3.84	Hydrophobic	:UNK0	A:PHE103
	His192	4.73	Hydrophobic	:UNK0	B:HIS192
	His192	5.41	Hydrophobic	B:HIS192	:UNK0
	Ile101	4.18	Hydrophobic	:UNK0:C	A:ILE101
	Leu353	5.01	Hydrophobic	:UNK0	A:LEU353
	His302	4.51	Hydrophobic	B:HIS302	:UNK0:C
	Phe309	4.88	Hydrophobic	B:PHE309	:UNK0:C
1QI3	Ser64	2.16	H-bond	:UNK0:H	A:SER64:OG
	Gln305	2.49	H-bond	A:GLN305:NE2	:UNK0:O
	Glu76	2.68	H-bond	:UNK0:H6	A:GLU76:OE1
	Phe79	3.98	Hydrophobic	:UNK0	A:PHE79
	Phe79	5.05	Hydrophobic	:UNK0	A:PHE79

	Trp66	4.77	Hydrophobic	:UNK0	A:TRP66
	Trp66	5.06	Hydrophobic	A:TRP66	:UNK0
	Tyr78	4.97	Hydrophobic	A:TYR78:C,O	:UNK0
	Tyr78	5.04	Hydrophobic	A:TYR78	:UNK0:C
	Phe156	5.22	Hydrophobic	A:PHE156	:UNK0:C
2RTG	Ser45	3.00	H-bond	:UNK0:O	D:SER45:OG
	Asn23	2.30	H-bond	D:ASN23:HD21	:UNK0:O
	Ser27	2.82	H-bond	D:SER27:HG	:UNK0:O
	Tyr43	2.07	H-bond	D:TYR43:HH	:UNK0:O
	Ser45	2.92	H-bond	B:SER45:HB1	:UNK0:O
	Ala50	4.73	Hydrophobic	:UNK0	D:ALA50
	Leu110	5.37	Hydrophobic	:UNK0	D:LEU110
	Leu110	4.96	Hydrophobic	:UNK0	B:LEU110
	Trp92	5.01	Hydrophobic	B:TRP92	:UNK0:C
	Trp92	4.64	Hydrophobic	B:TRP92	:UNK0:C
	Trp108	3.76	Hydrophobic	B:TRP108	:UNK0:C
	Trp108	3.96	Hydrophobic	B:TRP108	:UNK0:C
2VEG	Asp91	2.36	H-bond	:UNK0:H	B:ASP91:OD1
	His248	3.13	H-bond	:UNK0:O	B:HIS284:NE2
	Arg282	3.29	H-bond	B:ARG282:NH1	:UNK0:N
	Arg282	3.24	H-bond	B:ARG282:NH1	:UNK0:O
	Arg282	3.08	H-bond	B:ARG282:NH2	:UNK0:N
	Arg282	3.23	H-bond	B:ARG282:NH2	:UNK0:O
	Arg282	4.17	Electrostatic	B:ARG282:NH2	:UNK0
	Asp91	3.74	Electrostatic	B:ASP91:OD2	:UNK0
	Phe206	5.11	Hydrophobic	:UNK0	B:PHE206
	Phe206	5.22	Hydrophobic	:UNK0	B:PHE206
	Ile112	5.35	Hydrophobic	:UNK0	B:ILE112
	Met135	-	Hydrophobic	:UNK0	B:MET135
	Ile112	-	Hydrophobic	:UNK0	B:ILE112
3A8U	Asp259	1.97	H-bond	:UNK0:H	X:GLY87:O
	Tyr152	2.84	H-bond	:UNK0:H	X:SER329:O
	Gly154	3.51	H-bond	X:GLY154:CA	:UNK0:O
	Val261	3.79	Hydrophobic	X:VAL261:CG1	:UNK0
	Val261	3.72	Hydrophobic	X:VAL261:CG1	:UNK0
	Tyr152	4.88	Hydrophobic	:UNK0	X:TYR152
	Tyr152	5.13	Hydrophobic	:UNK0	X:TYR152
	His153	4.10	Hydrophobic	X:HIS153:C,O	:UNK0
	Ile262	5.25	Hydrophobic	:UNK0	X:ILE262

	Tyr152	4.98	Hydrophobic	X:TYR152	:UNK0:C
3SRW	Asn19	2.99	H-bond	:UNK0:O	X:ASN19:OD1
	Ser50	2.71	H-bond	:UNK0:O	X:SER50:OG
	Thr47	3.20	H-bond	X:THR47:N	:UNK0:O
	Thr47	3.32	H-bond	X:THR47:OG1	:UNK0:N
	Thr47	2.87	H-bond	X:THR47:OG1	:UNK0:O
	Ile15	4.59	Hydrophobic	:UNK0	X:ILE15
	Ile15	5.00	Hydrophobic	:UNK0	X:ILE15
	Leu21	5.20	Hydrophobic	:UNK0:C	X:LEU21
3T88	Thr117	2.94	H-bond	A:THR117:OG1	:UNK0:N
	Arg113	2.95	H-bond	E:ARG113:NE	:UNK0:O
	Asp110	3.08	H-bond	:UNK0:H6	E:ASP110:OD1
	Glu248	4.91	Electrostatic	A:GLU248:OE1	:UNK0
	Asp110	4.93	Electrostatic	E:ASP110:OD2	:UNK0
	Arg113	4.60	Hydrophobic	:UNK0:C	E:ARG113
	Leu109	4.63	Hydrophobic	:UNK0	E:LEU109
3TTZ	Glu58	2.85	H-bond	:UNK0:O	A:GLU58:OE2
	Arg84	3.24	H-bond	A:ARG84:N	:UNK0:O
	Gly85	2.88	H-bond	A:GLY85:N	:UNK0:O
	Thr173	3.33	H-bond	A:THR173:OG1	:UNK0:N
	Thr173	3.09	H-bond	A:THR173:OG1	:UNK0:O
	Ser55	2.79	H-bond	:UNK0:H6	A:SER55:OG
	Asp81	2.22	H-bond	:UNK0:H6	A:ASP81:OD2
	Asn54	3.49	H-bond	A:ASN54:ND2	A:ASP81:OD2
	Ile86	3.94	Hydrophobic	A:ILE86:CD1	:UNK0
	Thr173	3.94	Hydrophobic	A:THR173:CG2	:UNK0
	Asn54	5.08	Hydrophobic	A:ASN54:C,O	:UNK0
	Ile51	5.10	Hydrophobic	:UNK0	B:ILE51
	Ile175	5.02	Hydrophobic	:UNK0	B:ILE175
	Ile51	5.45	Hydrophobic	:UNK0	B:ILE51
	Ile175	5.13	Hydrophobic	:UNK0	B:ILE175
3UGC	Leu932	2.38	H-bond	:UNK0:H	A:LEU932:O
	Leu855	3.73	Hydrophobic	A:LEU855:CD1	:UNK0
	Leu855	3.82	Hydrophobic	A:LEU855:CD1	:UNK0
	Leu855	3.91	Hydrophobic	A:LEU855:CD2	:UNK0
	Leu983	4.92	Hydrophobic	:UNK0:C	A:LEU983
	Ala880	4.83	Hydrophobic	:UNK0	A:ALA880
	Leu983	5.31	Hydrophobic	:UNK0	A:LEU983
	Phe995	3.89	Hydrophobic	A:PHE995	:UNK0:C

	Gly185	3.17	H-bond	A:GLY185:N	:UNK0:O
	Gly186	2.83	H-bond	A:GLY186:N	:UNK0:O
	Gly187	2.95	H-bond	A:GLY187:N	:UNK0:O
5X2L	Ser242	3.49	H-bond	A:SER242:OG	:UNK0
	Lys56	5.12	Hydrophobic	:UNK0:C	A:LYS56
	Pro153	4.90	Hydrophobic	:UNK0	A:PRO153
	Phe55	4.82	Hydrophobic	A:PHE55	:UNK0:C

Table S4—Magnetic susceptibility data of metal complexes

Complex	($ergG^{-2}mol^{-1}$)			(B.M.)
	χ_M $\times 10^{-3}$	χ_D $\times 10^{-3}$	$\chi_A = \chi_M + \chi_D$ $\times 10^{-3}$	μ_{eff}
[Co-(indal-2-abu)$_2$]	6.3745	2.8384	6.6584	3.95
[Ni-(indal-2-abu)$_2$]	4.9738	2.8384	5.2576	3.51
[Cu-(indal-2-abu)$_2$]	1.1297	2.8384	1.4136	1.82

χ_M =molar susceptibility, χ_D =diamagnetic correction, χ_A = molar susceptibility corrected for diamagnetic components.

Table S5 — Percentage degradation of MB with time for ligand and its complexes.

Ligand/Complex	**% degradation** Irradiation time (min.)			
	30	60	90	120
indal-2-abu	18.15	62.23	63.15	22.12
[Co-(indal-2-abu)$_2$]	17.25	60.15	85.28	24.12
[Ni-(indal-2-abu)$_2$]	16.12	65.01	80.1	22.13
[Cu-(indal-2-abu)$_2$]	17.75	76.2	84.23	30.21
[Zn-(indal-2-abu)$_2$]	20.12	63.21	78.12	25.22

Table S6— MIC data of the compounds against the growth of microbes

Ligand/Complex	*E. coli*	*S. aureus*	*B. subtilis*	*A. niger*	*C. albicans*
indal-2-abu	70	65	64	72	73
[Co-(indal-2-abu)$_2$]	24	32	34	18	27
[Ni-(indal-2-abu)$_2$]	17	18	20	32	28
[Cu-(indal-2-abu)$_2$]	18	32	35	30	33
[Zn-(indal-2-abu)$_2$]	16	18	16	19	20
Ciprofloxacin[#]	10	15	16	-	-
Fluconazole[#]	-	-	-	10	16

Standards