Electronic Supplementary Materials For

Indium(III)-terpyridine complexes: synthesis, structures and remarkable antifungal and anticancer activities

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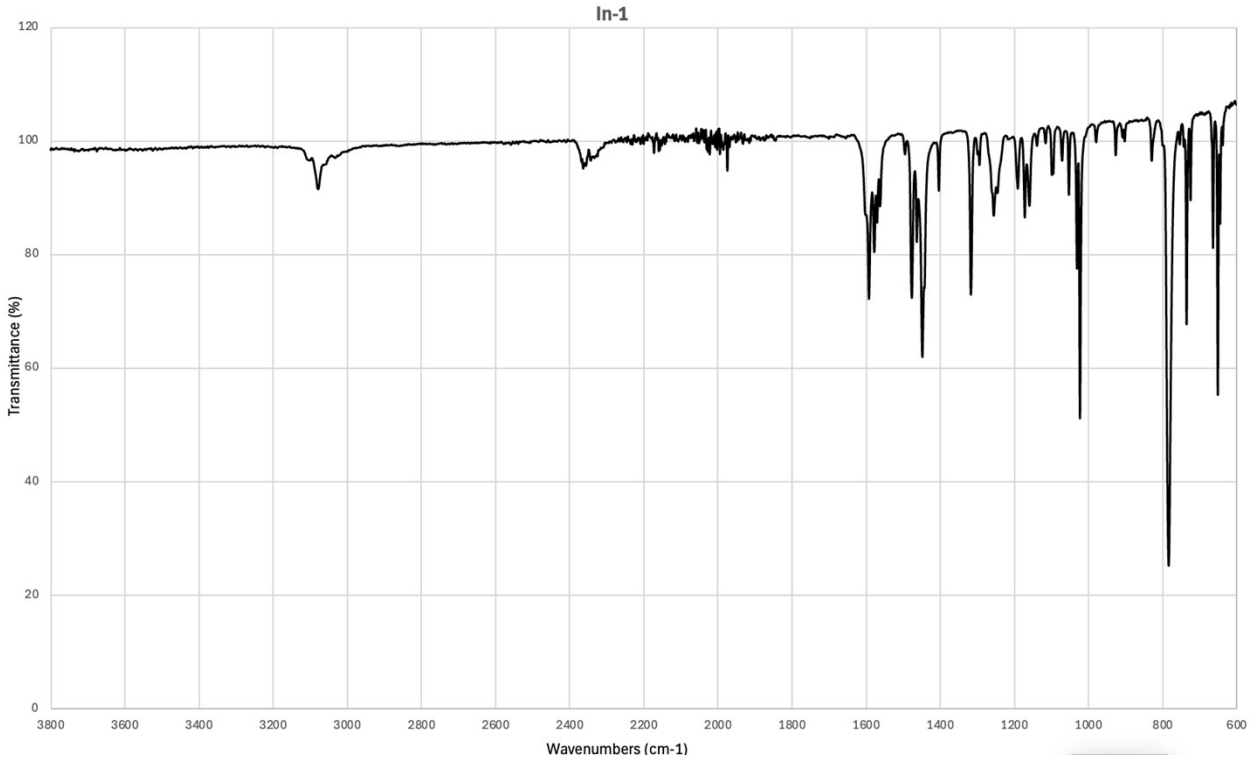

Fig. S1. The FT-IR spectrum of complex **In-1**.

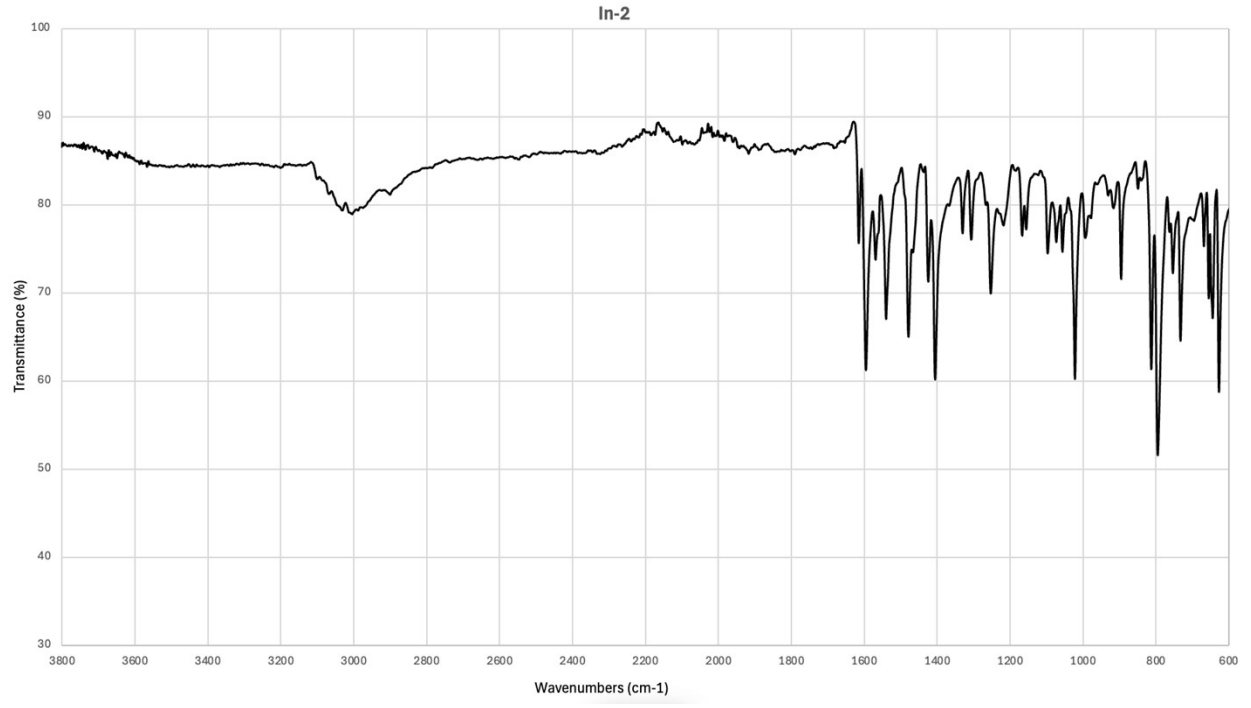

Fig. S2. The FT-IR spectrum of complex **In-2**.

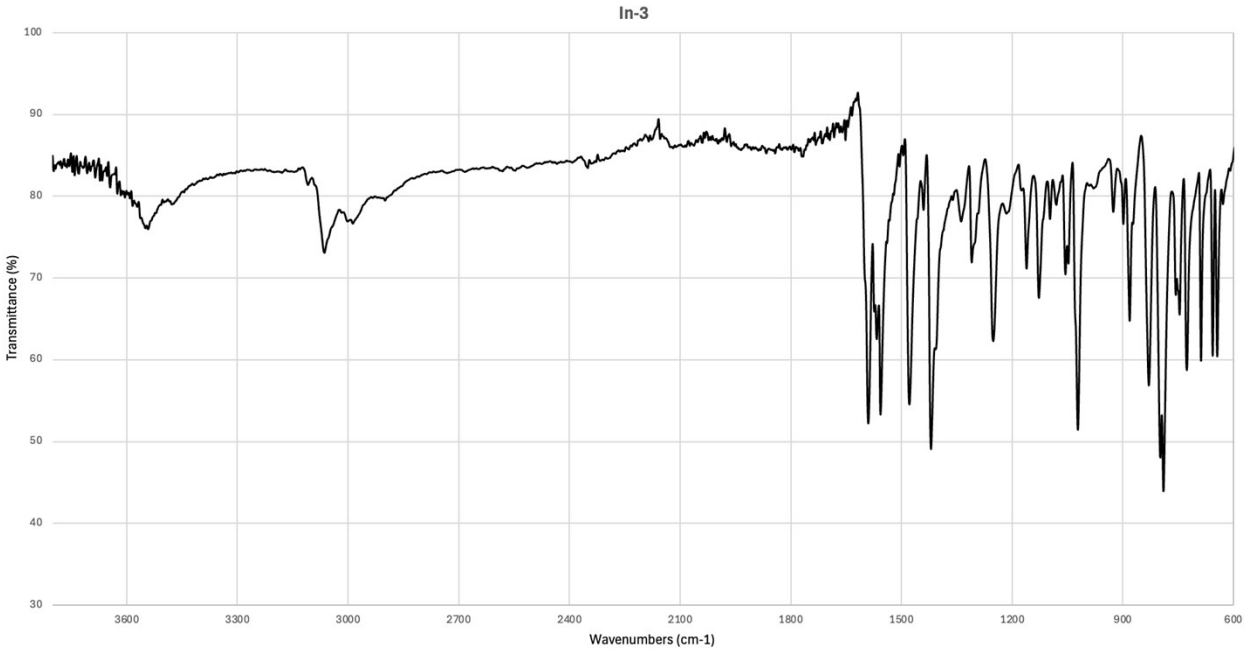

Fig. S3. The FT-IR spectrum of complex **In-3**.

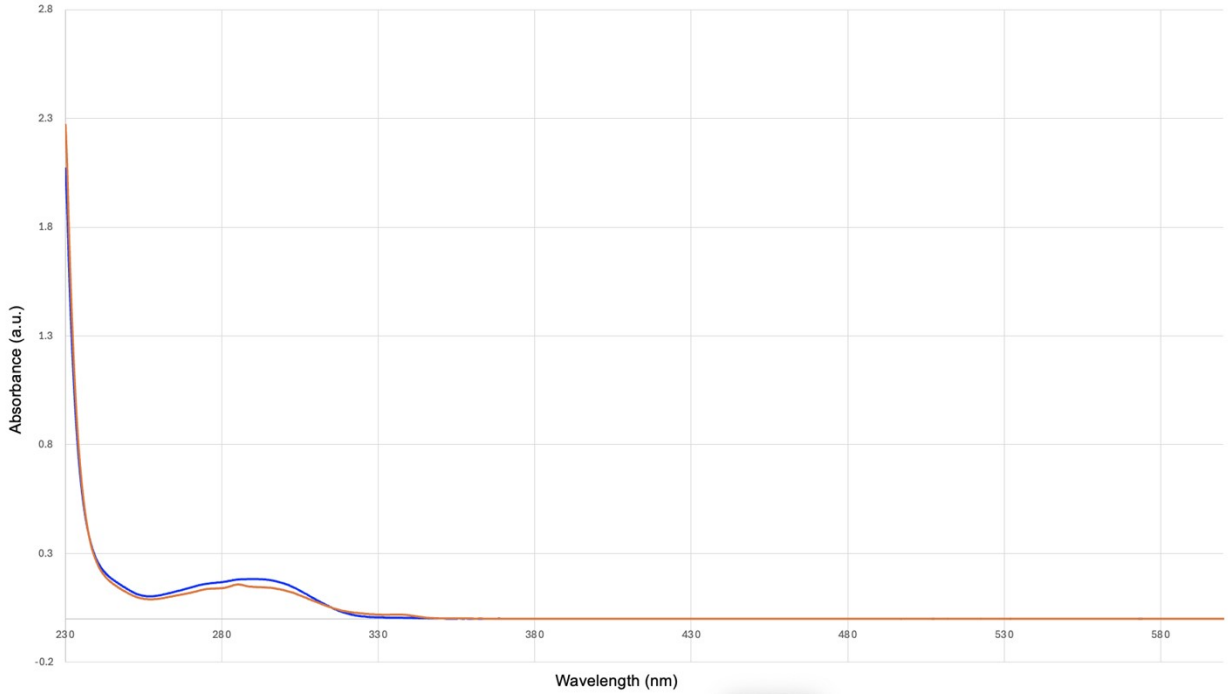

Figure S4. The UV-Vis spectra of compound **In-1** in aqueous solution (concentration: 1×10^{-5} M) as prepared (blue) and after 72 h (red).

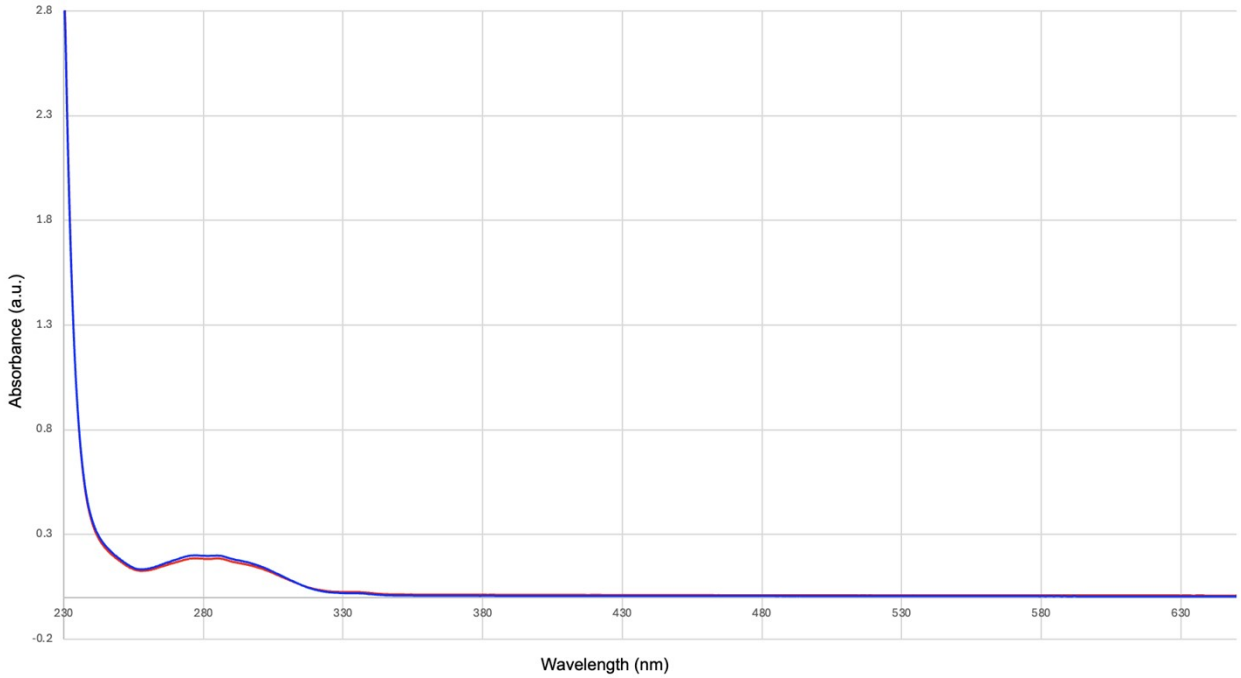

Figure S5. The UV-Vis spectra of compound **In-2** in aqueous solution (concentration: 1×10^{-5} M) as prepared (blue) and after 72 h (red).

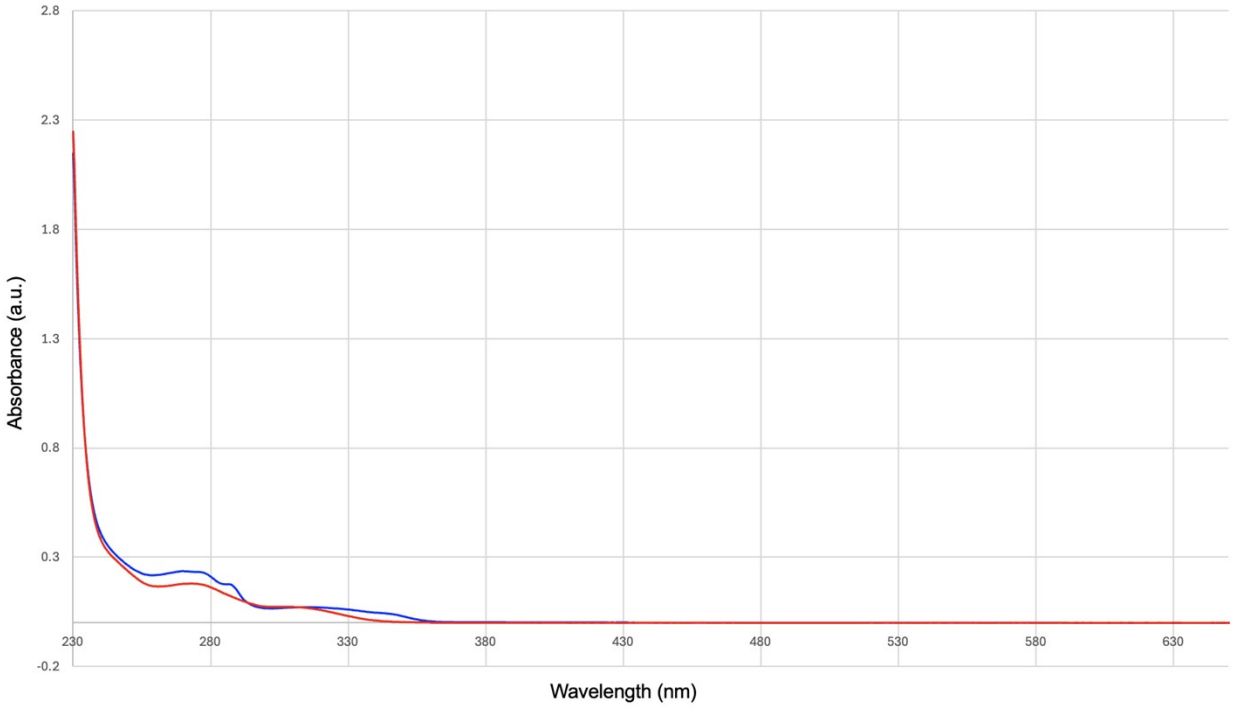

Figure S6. The UV-Vis spectra of compound **In-3** in aqueous solution (concentration: 1×10^{-5} M) as prepared (blue) and after 72 h (red).

Table S1. X-ray crystallographic refinement for **In-2a, In-2b** and **In-3**.

	In-2a	**In-2b**	**In-3**
lattice	Triclinic	Monoclinic	Monoclinic
formula	$C_{16}H_{14}Cl_4InN_3O$	$C_{16.5}H_{16}Cl_4InN_3O_{1.5}$	$C_{20}H_{14}Cl_3InN_4$
formula weight	520.92	536.94	531.52
space group	*P-1*	$P2_1/c$	$P2_1/c$
a/Å	8.6481(5)	13.1149(3)	10.6721(3)
b/Å	10.2867(6)	15.2796(3)	20.7727(6)
c/Å	10.9814(6)	19.7365(5)	8.6742(3)
α/°	104.902(2)	90	90
β/°	92.935(2)	90.9160(10)	90.7040(10)
γ/°	93.306(2)	90	90
V/Å^3	940.27(9)	3954.50(16)	1922.82(10)
Z	2	8	4
temperature (K)	130(2)	130(2)	130(2)
radiation (λ, Å)	0.71073	0.71073	0.71073
ρ (calcd.) g cm^{-3}	1.840	1.804	1.836
μ (Mo Kα), mm^{-1}	1.835	1.750	1.660
θ max, deg.	44.251	33.793	30.543
no. of data collected	72062	159273	58603
no. of data	14805	15835	5898
no. of parameters	231	481	253
R_1 [$I > 2\sigma(I)$]	0.0347	0.0295	0.0233
wR_2 [$I > 2\sigma(I)$]	0.0865	0.0770	0.0558
R_1 [all data]	0.0421	0.0383	0.0294
wR_2 [all data]	0.0919	0.0826	0.0585
GOF	1.037	1.015	1.033
R_{int}	0.0556	0.0625	0.0488

Table S2. The control experiments that determine the MIC (μg/mL) values of free ligands and $InCl_3$ salt against *C. albicans* SC5314.

Compound	MIC (μg/mL)
L1	8
L2	16
L3	>64
$InCl_3$	>64

Table S3. Yeast viability assay raw data. Data shown corresponds to the bar graphs shown in figure 2. The cell survival percentage values (# of CFUs for indium-treated experimental sample/# of CFUs for corresponding DMSO-treated control sample multiplied by 100) for each technical replicate (R1, R2, and R3) are shown. The mean and standard deviation values for replicates corresponding to each compound are shown.

Compound	R1	R2	R3	Mean/St Dev Percent of Cell Survival
DMSO	100	100	100	100 ± 0.0
In-1	0.78	0.39	0.95	0.71 ± 0.29
DMSO	100	100	100	100 ± 0.0
In-2	1.00	0.52	0.95	0.83 ± 0.26
DMSO	100	100	100	100 ± 0.0
In-3	2.05	1.75	0.90	1.57 ± 0.6

Table S4. SwissADME raw data. Numerical data points corresponding to bioavailability hexagonal visuals in Fig. 3 are presented in this table. The shaded region for each category corresponds to the range of the following categories: Lipo: -0.7 <XLOGP3< +5.0. Size: 150g/mol<MV<500g/mol. Polarity: 20Å^2 TPSA 130 Å^2. Insol: -6 <LogS< 0. Insatu: 0.25 <Fraction Csp3< 1. Flex: 0<Num. rotable bonds<9.

Compound	Size	Insatu	Flex	Polarity	Lipo	Insol
In-1	452.91	0	0	14.79	5.16	-6.51
In-2	488.89	0	0	14.79	5.79	-7.1
In-3	531.53	0	1	27.68	5.71	-7.3
Fluconazole	306.27	0.23	5	81.65	0.35	-2.17
Caspofungin	1093.31	0.75	24	412.03	0.34	-5.31