Electronic Supplementary Information (ESI)

Cytotoxic and antimicrobial effects of indium(III) complexes with 2-acetylpyridine-derived thiosemicarbazones

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Infrared spectra, ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of the complexes [In(2Ac4*o*ClPh)Cl_2(MeOH)] **(1)**, [In(2Ac4*p*FPh)Cl_2(MeOH)] **(2)**, [In(2Ac4*p*ClPh)Cl_2(MeOH)] **(3)** and [In(2Ac4*p*IPh)Cl_2(MeOH)] **(4)**

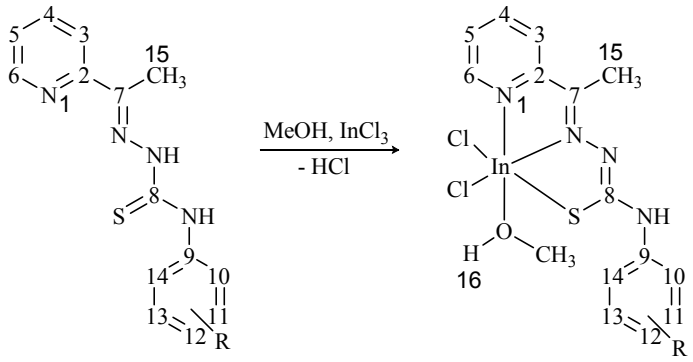

Figure S1. Syntheses of the indium(III) complexes with 2-acetylpyridine-derived thiosemicarbazones and carbon atom numbering.

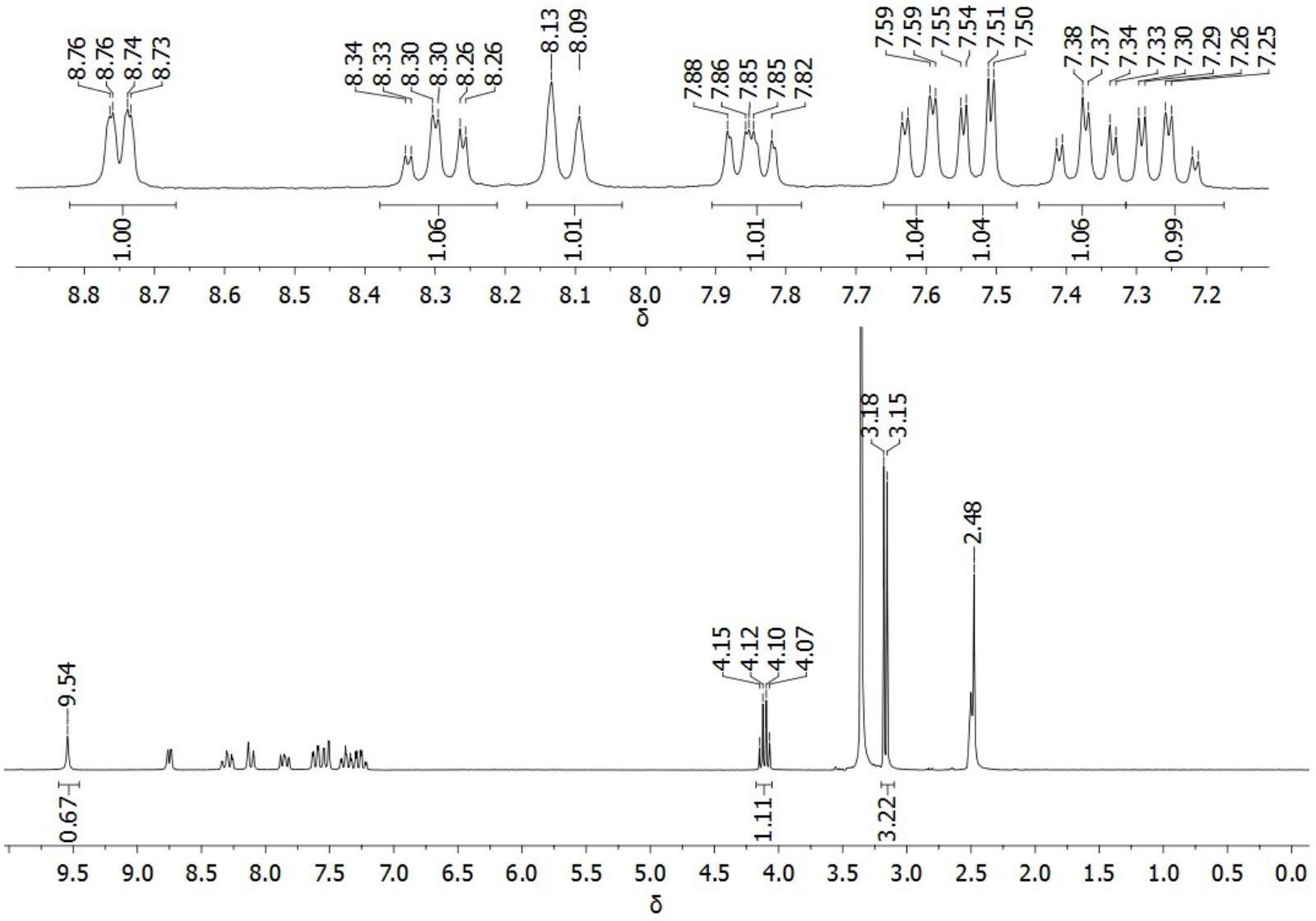

Figure S2. ^{1}H NMR spectrum of [In(2Ac4*o*ClPh)Cl_2(MeOH)] **(1)** in DMSO-d_6 (400 MHz) at room temperature

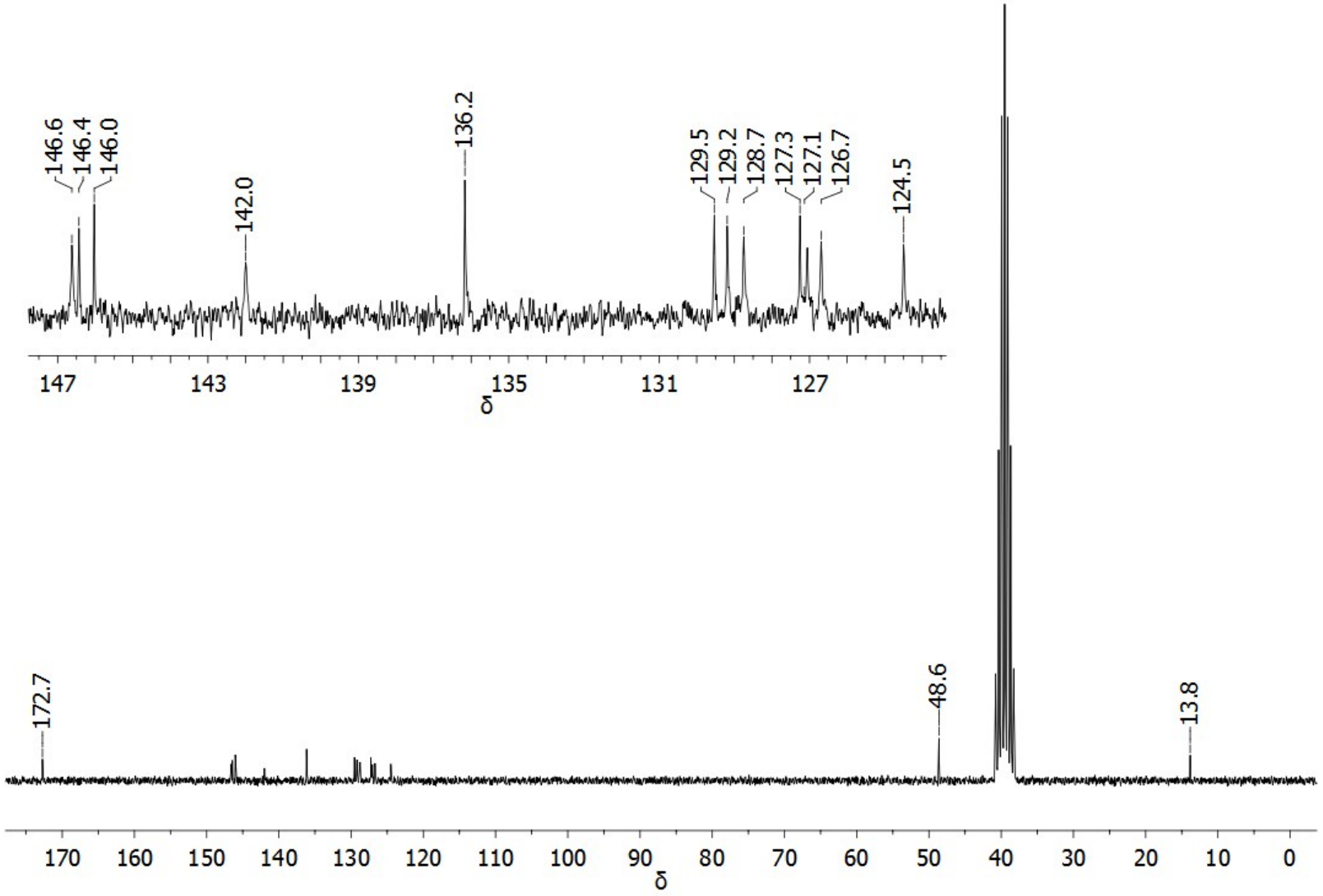

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of [In(2Ac4*o*ClPh)Cl_2(MeOH)] **(1)** in DMSO-d_6 (100 MHz) at room temperature

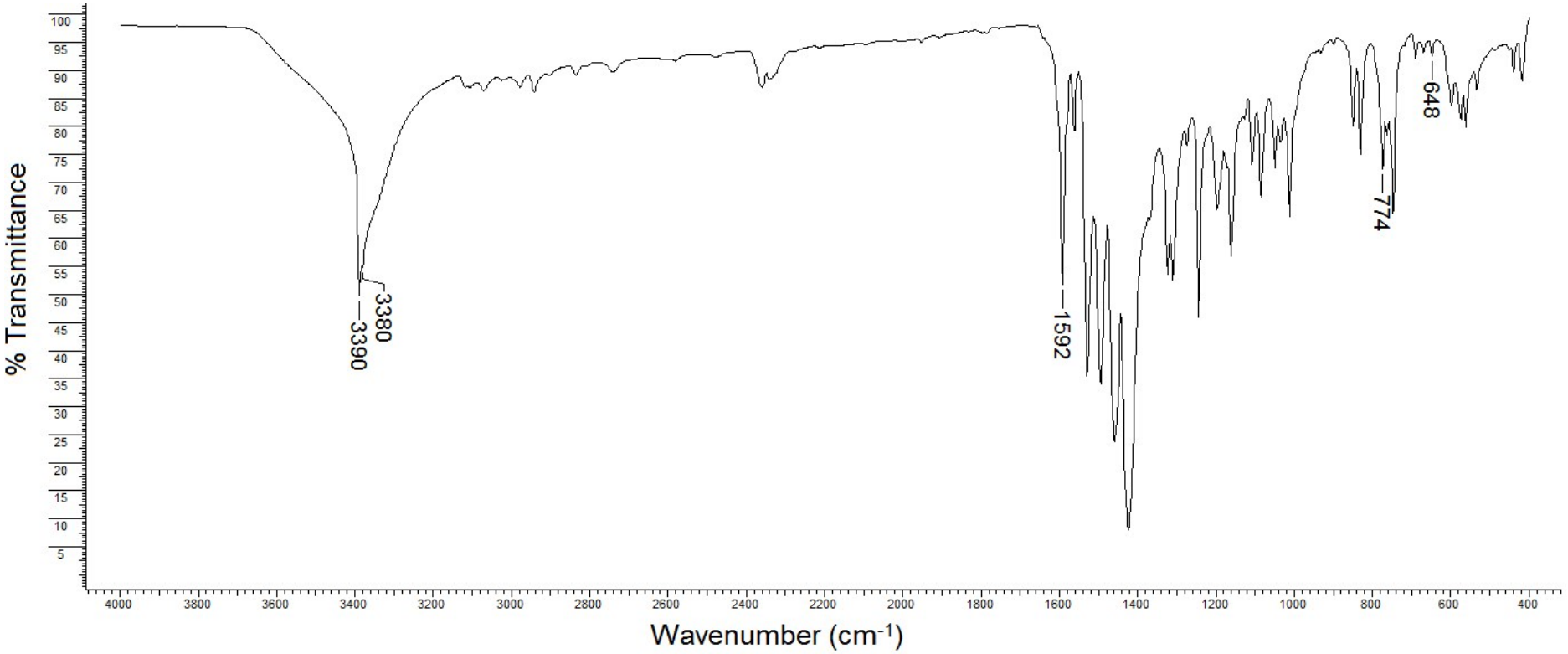

Figure S4. FT-IR spectrum of [In(2Ac4*o*ClPh)Cl_2(MeOH)] **(1)** (KBr pellet)

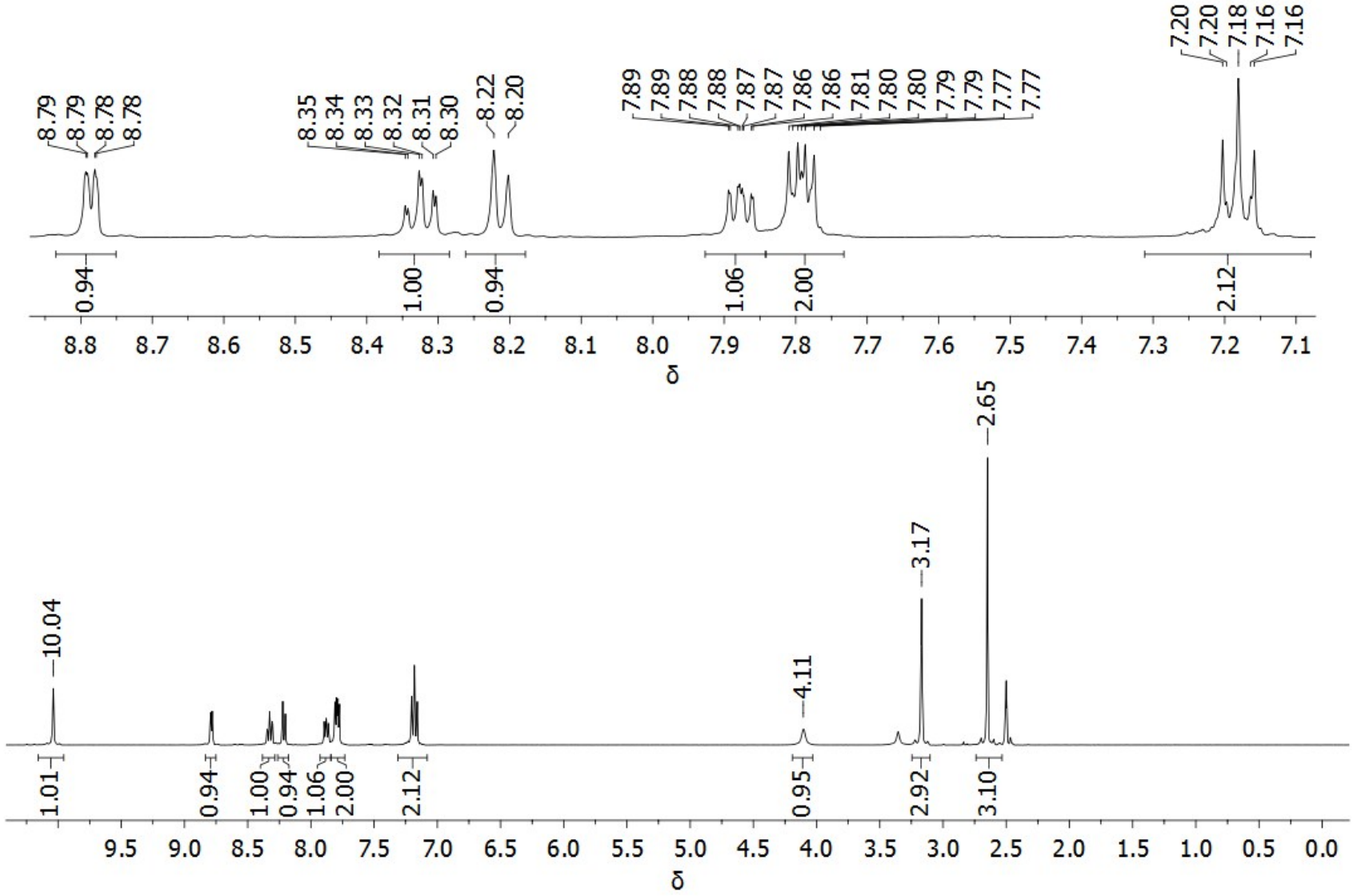

Figure S5. ^{1}H NMR spectrum of [In(2Ac4*p*FPh)Cl_2(MeOH)] **(2)** in DMSO-d_6 (400 MHz) at room temperature

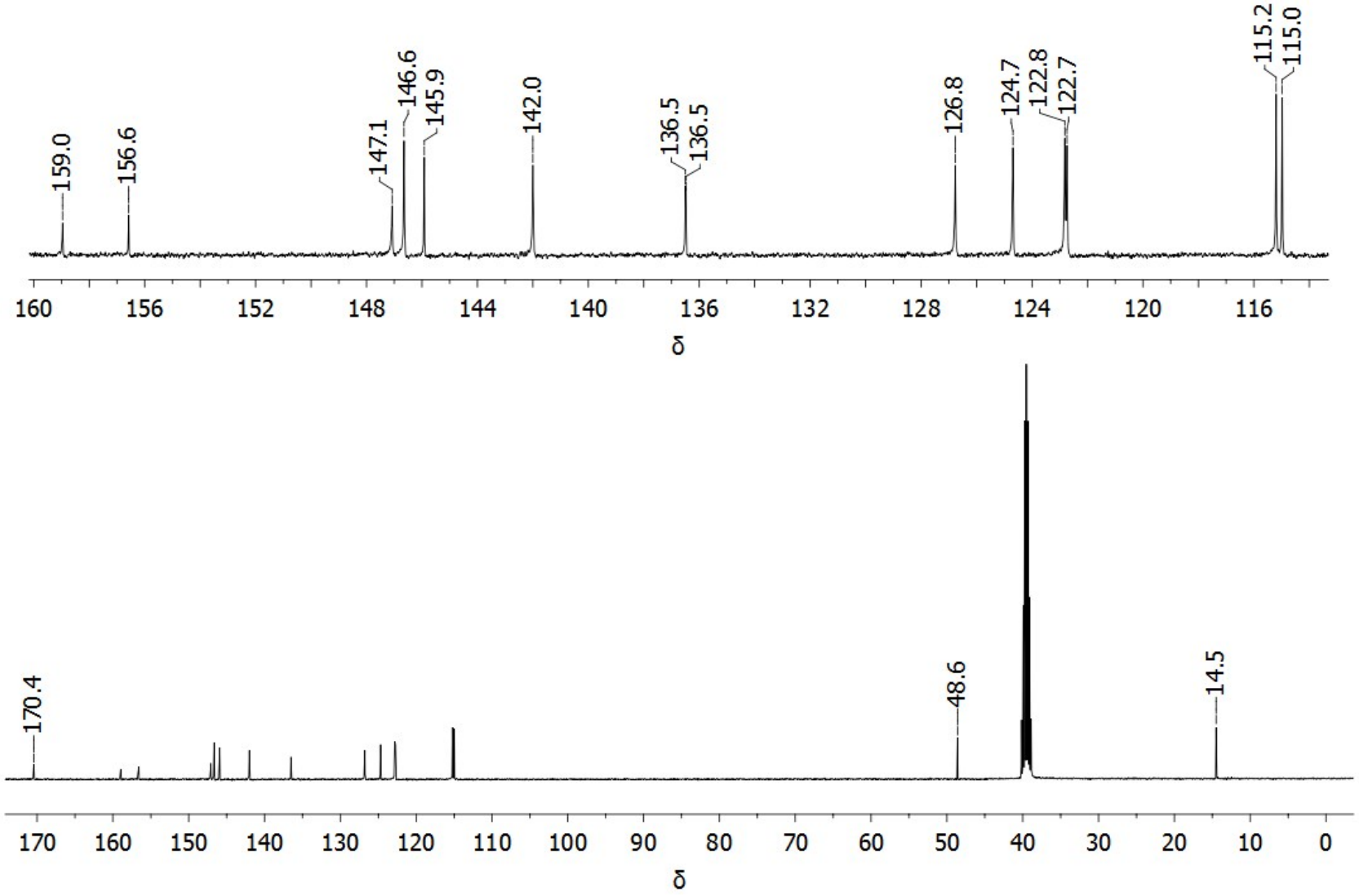

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of [In(2Ac4*p*FPh)Cl_2(MeOH)] **(2)** in DMSO-d_6 (100 MHz) at room temperature

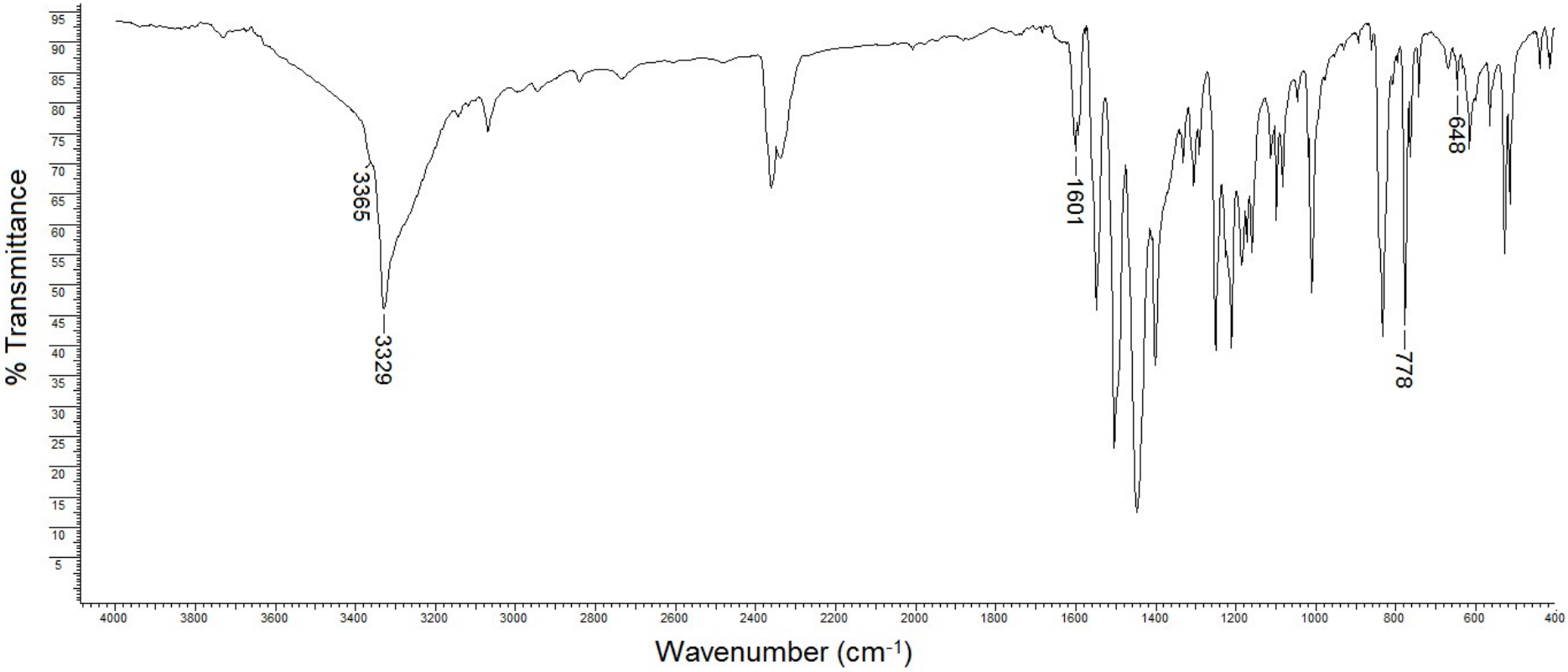

Figure S7. FT-IR spectrum of of [In(2Ac4*p*FPh)Cl_2(MeOH)] **(2)** (KBr pellet)

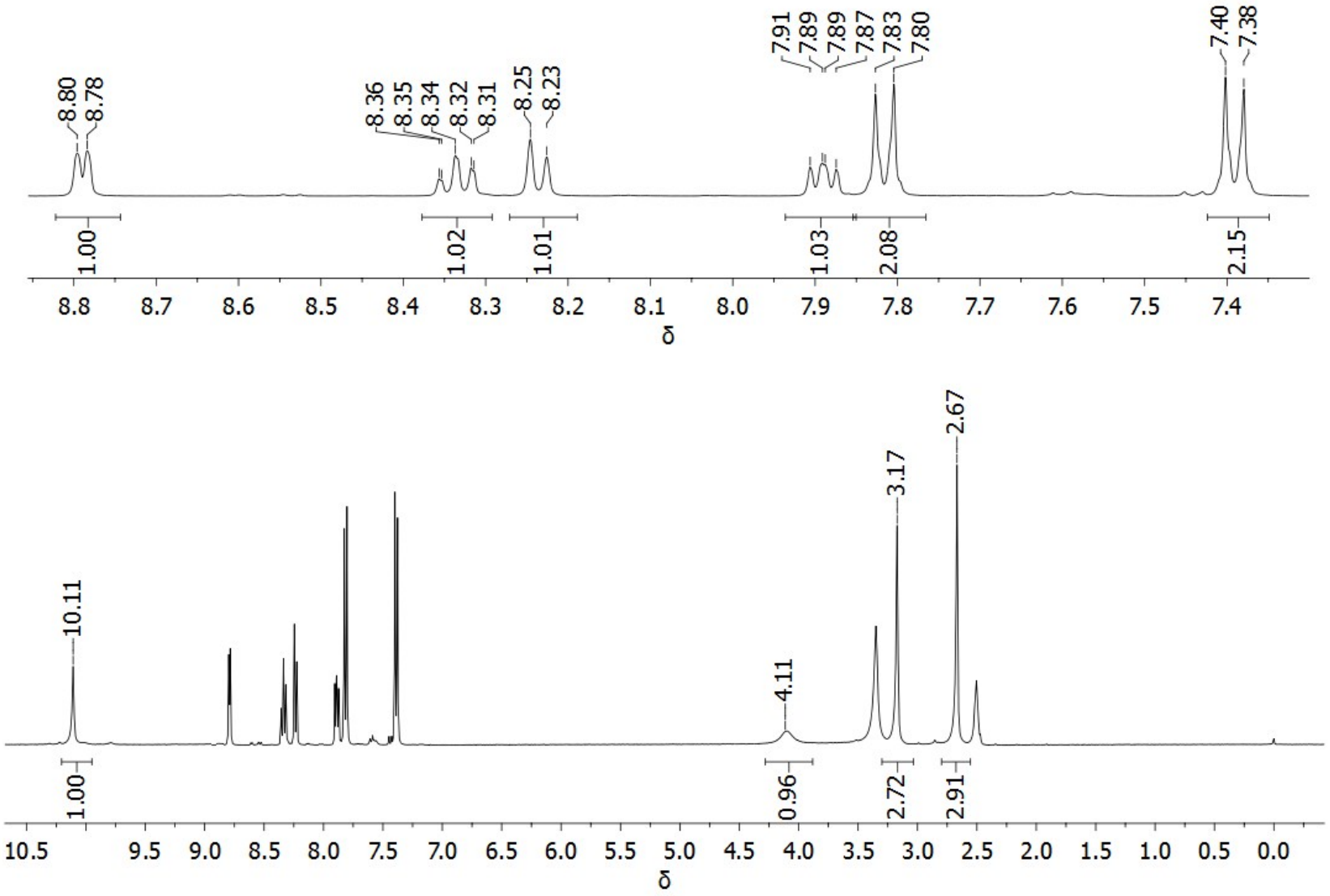

Figure S8. ^{1}H NMR spectrum of [In(2Ac4*p*ClPh)Cl_2(MeOH)] **(3)** in DMSO-d_6 (400 MHz) at room temperature

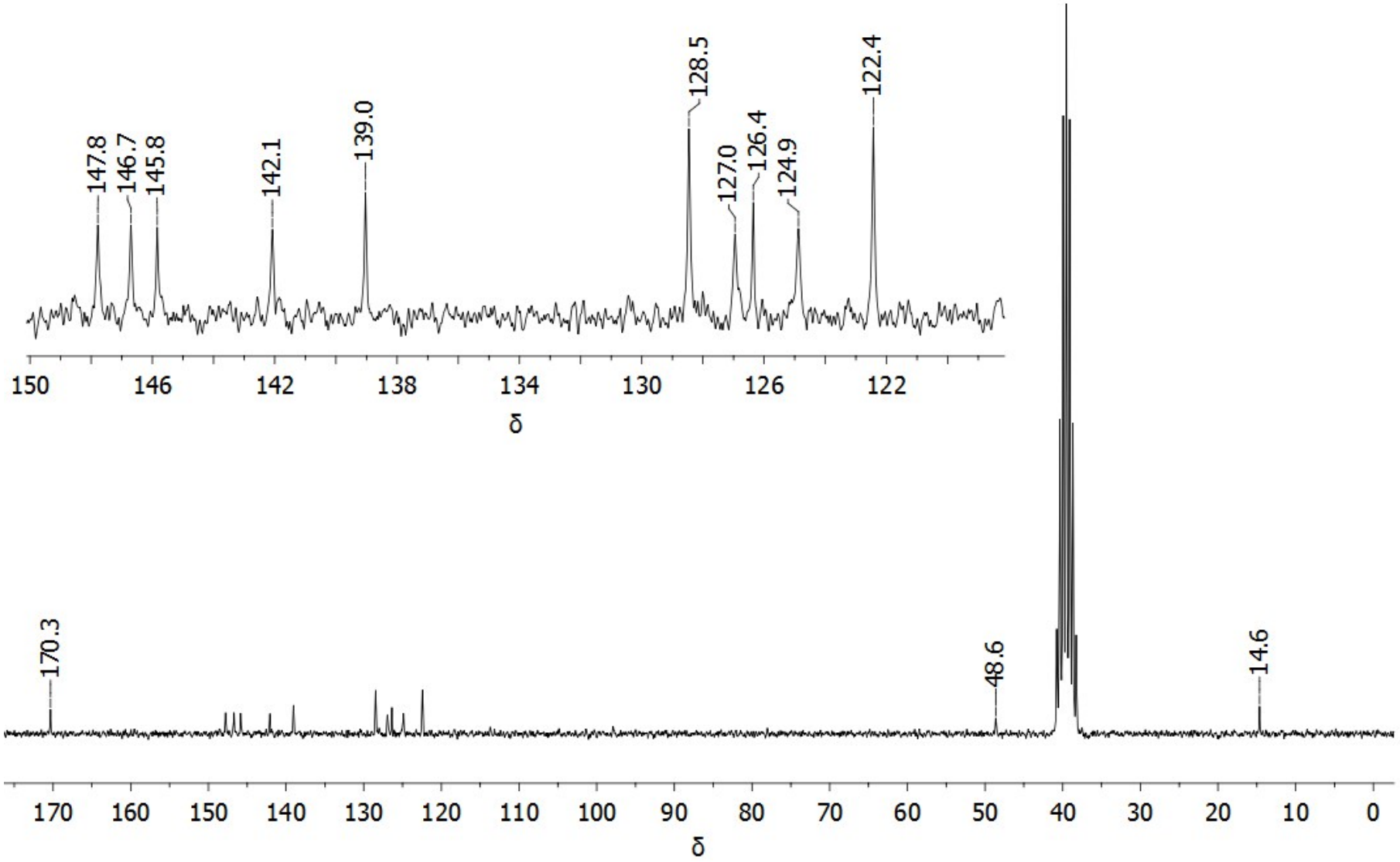

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of [In(2Ac4*p*ClPh)Cl_2(MeOH)] **(3)** in DMSO-d_6 (100 MHz) at room temperature

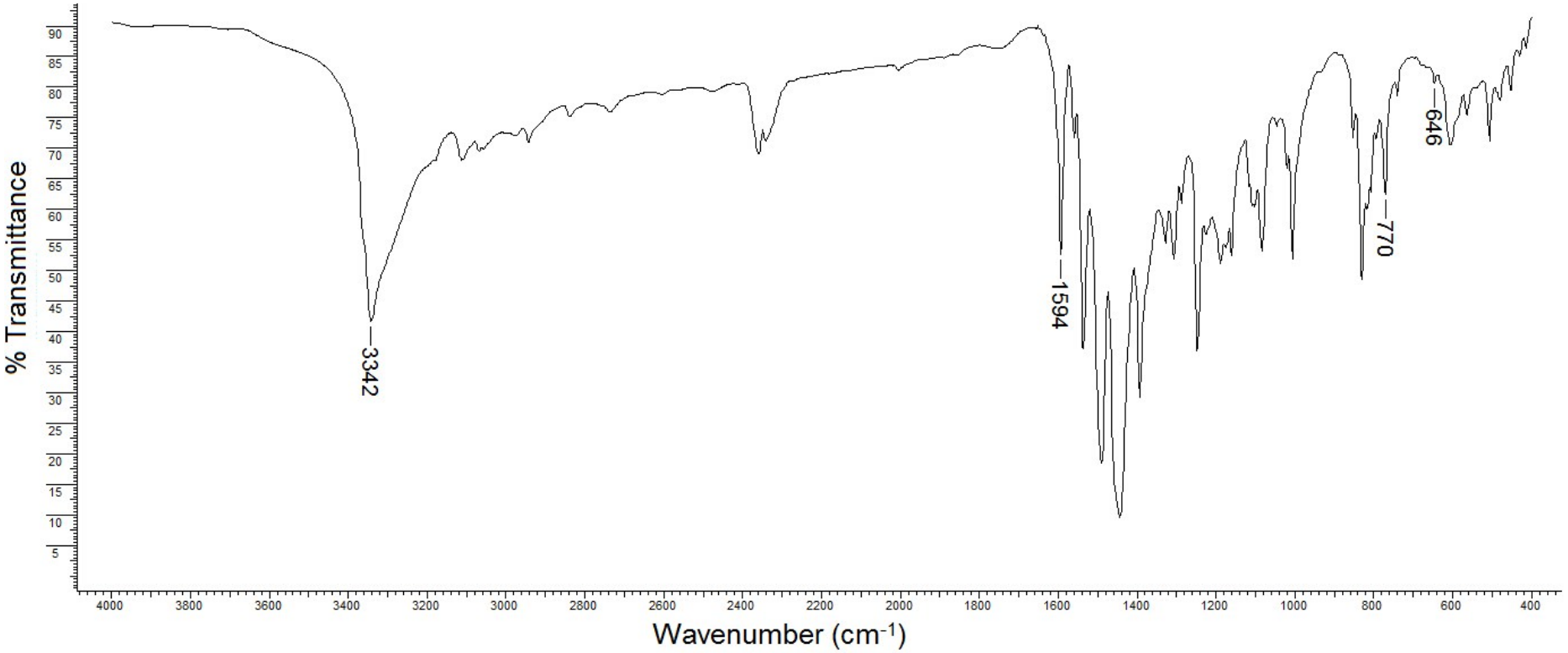

Figure S10. FT-IR spectrum of [In(2Ac4*p*ClPh)Cl_2(MeOH)] **(3)** (KBr pellet)

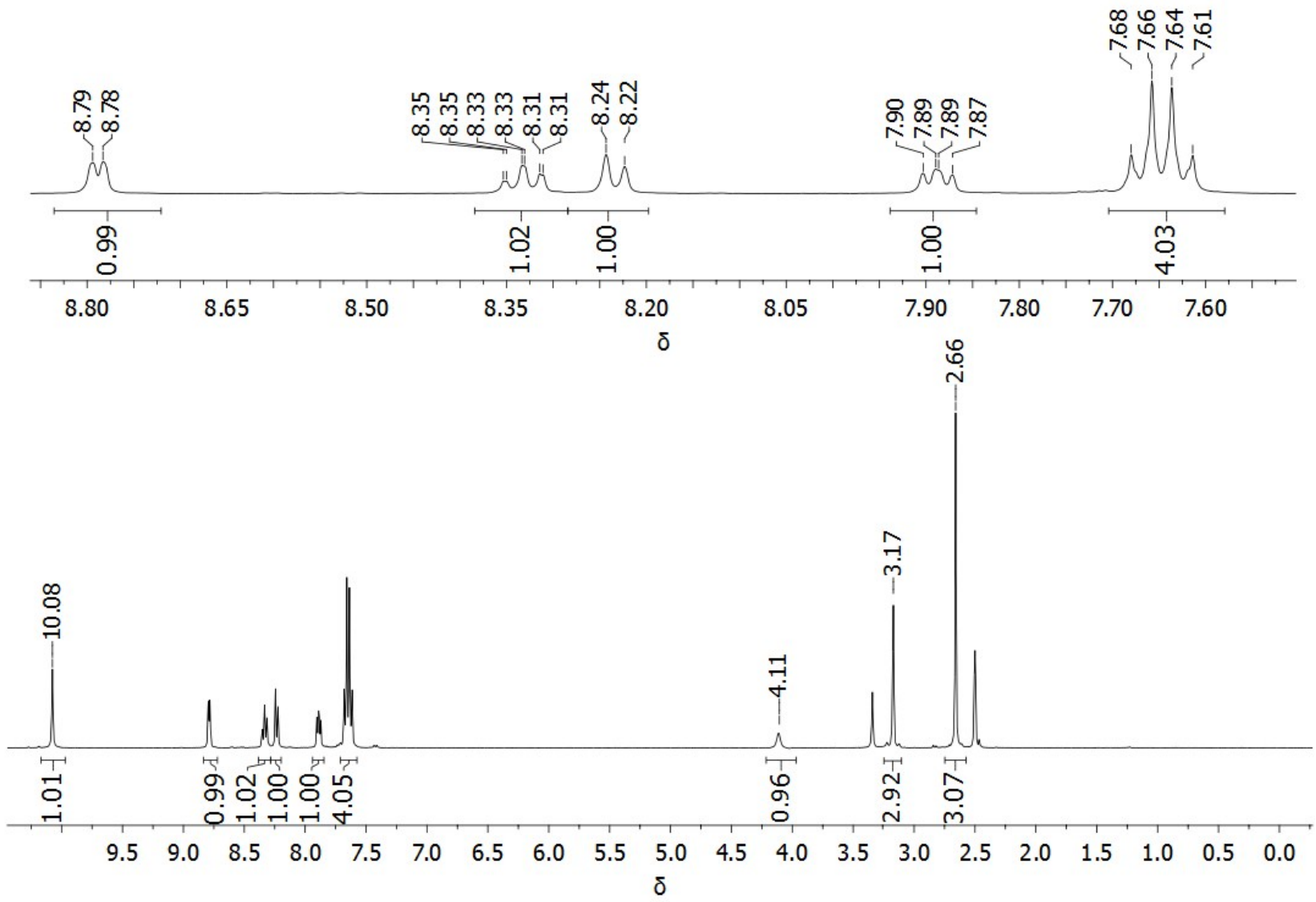

Figure S11. ^{1}H NMR spectrum of [In(2Ac4*p*IPh)Cl_2(MeOH)] **(4)** in DMSO-d_6 (400 MHz) at room temperature

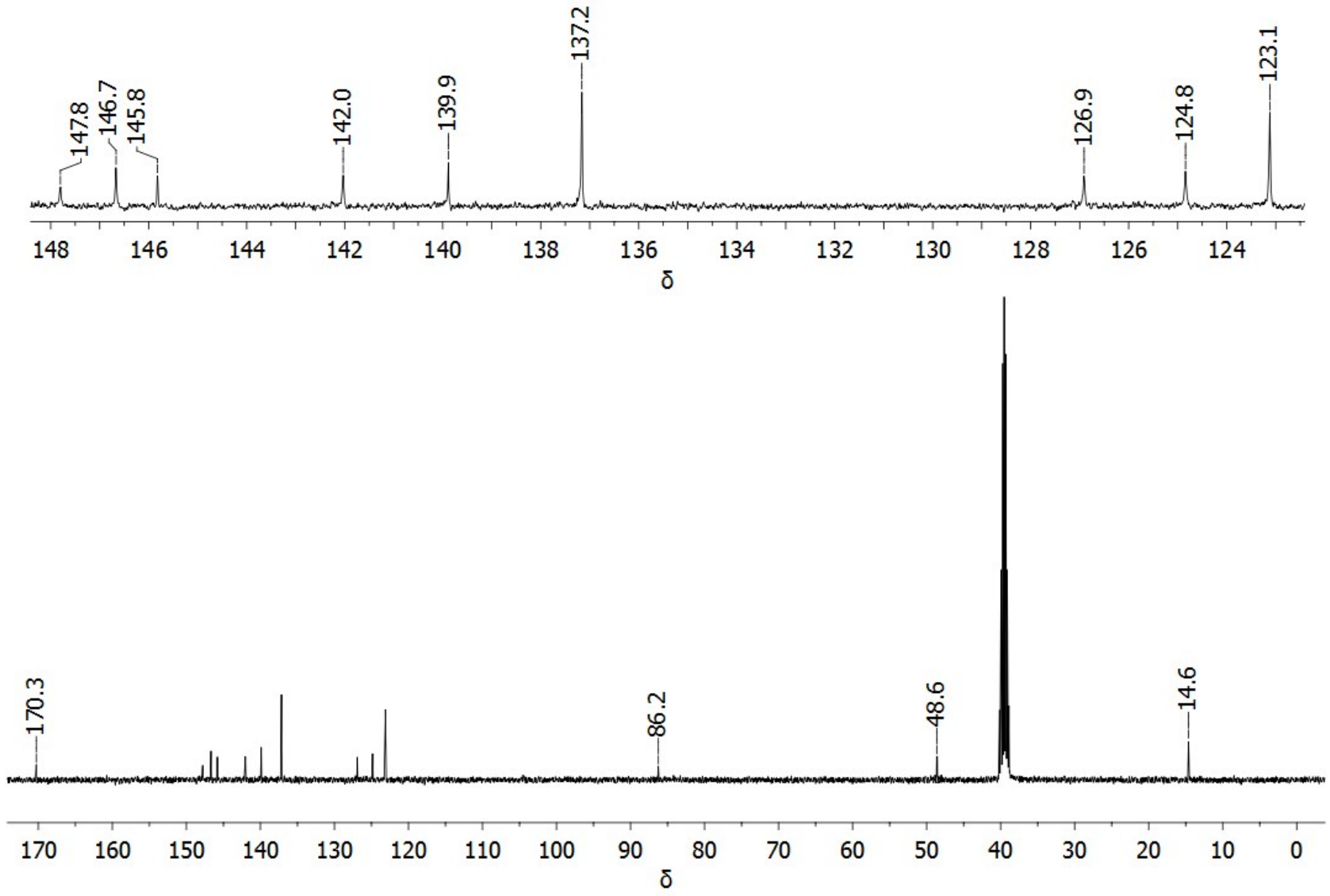

Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of [In(2Ac4*p*IPh)Cl_2(MeOH)] **(4)** in DMSO-d_6 (100 MHz) at room temperature

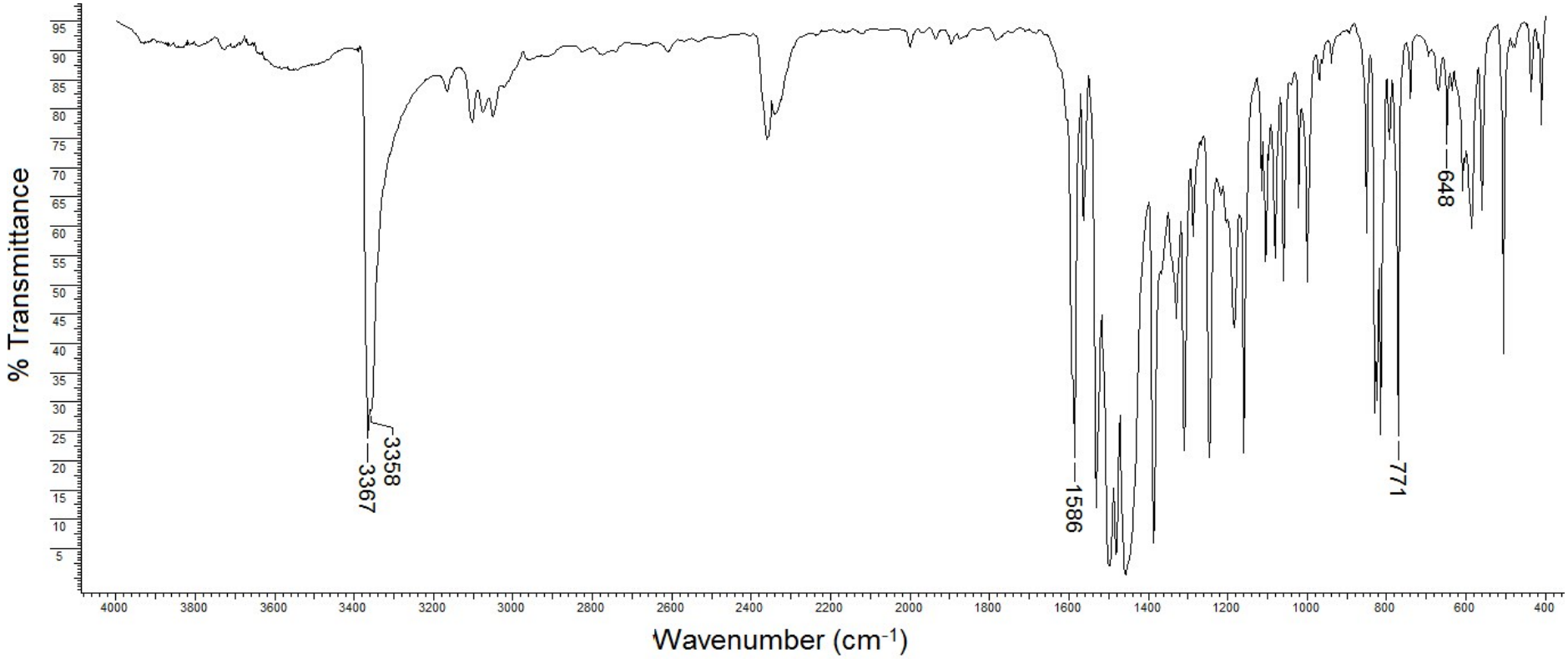

Figure S13. FT-IR spectrum of [In(2Ac4*p*IPh)Cl_2(MeOH)] **(4)** (KBr pellet)

Stability in solution

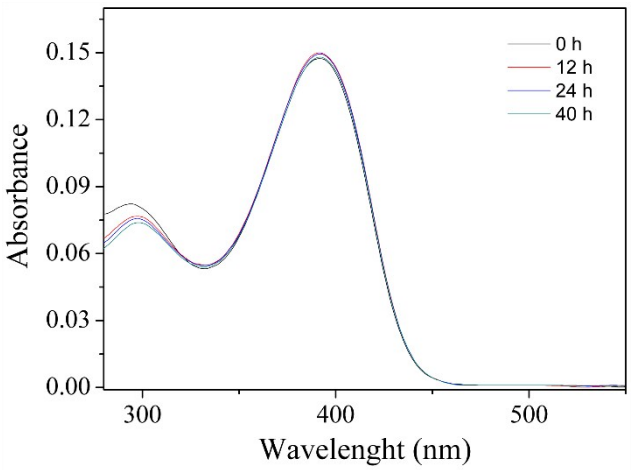

Figure S14. Electronic spectra of complex (**1**) as a function of time at 7.5 µM in DMSO

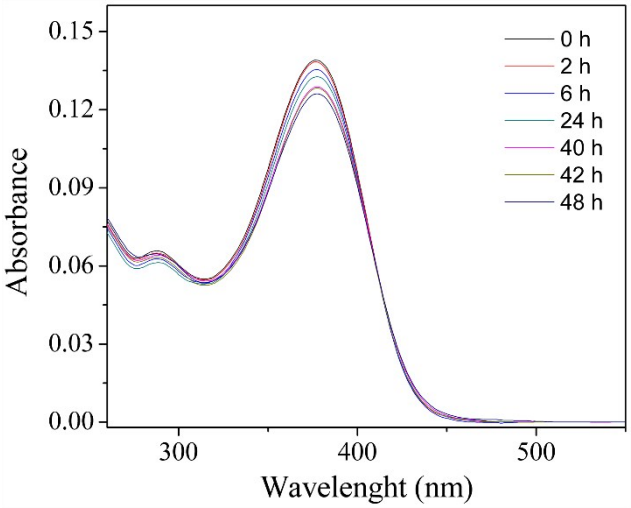

Figure S15. Electronic spectra of complex (**1**) as a function of time in DMSO 5%- Tris-HCl buffer pH 7.4 at 7.5 µM

X-ray crystallography

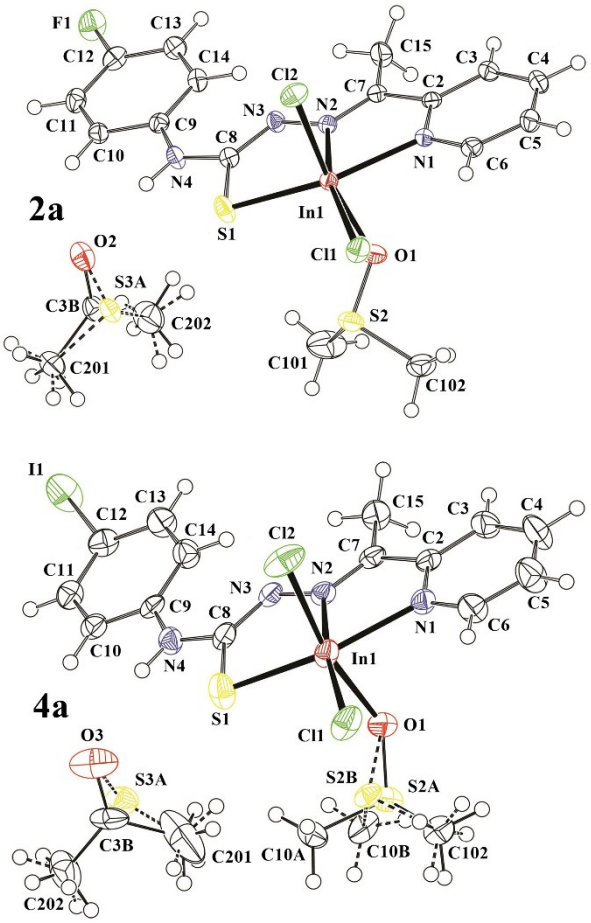

Figure S16. Molecular plots of complexes [In(2Ac4*p*FPh)Cl_2(DMSO)]·0.22DMSO·0.78C_3H_6O (**2a**) and [In(2Ac4*p*IPh)Cl_2(DMSO)]·0.41DMSO·0.59C_3H_6O (**4a**) showing the labeling scheme of the non–H atoms and their displacement ellipsoids at the 50 % probability level.

Table S1. Selected bond lengths (Å) and angles (°) for **1a**, **2a**, **3a** and **4a** in comparison with the parent free thiosemicarbazones

Bond	**H2Ac4*o*ClPh**[a] [1]	**1a**	**H2Ac4*p*FPh** [2]	**2a**	**H2Ac4*p*ClPh** [1]	**3a**	**H2Ac4*p*IPh** [2]	**4a**
S1–C8	1.654(3)/1.654(3)	1.7516(17)	1.672(2)	1.7640(17)	1.671(2)	1.7584(16)	1.670(3)	1.764(6)
N2–C7	1.281(3)/1.278(3)	1.287(2)	1.280(2)	1.294(2)	1.283(2)	1.290(2)	1.285(4)	1.287(7)
N2–N3	1.362(3)/1.361(3)	1.3784(19)	1.377(2)	1.3689(19)	1.374(2)	1.3700(18)	1.376(3)	1.369(6)
N3–C8	1.359(3)/1.351(3)	1.308(2)	1.349(2)	1.316(2)	1.352(2)	1.312(2)	1.352(4)	1.315(7)
In1–N1	-	2.2574(14)	-	2.2540(14)	-	2.2431(13)	-	2.252(5)
In1–N2	-	2.2410(14)	-	2.2581(13)	-	2.2540(13)	-	2.258(4)
In1–S1	-	2.5121(4)	-	2.5004(5)	-	2.5010(4)	-	2.4998(17)
In1–Cl1	-	2.4099(4)	-	2.4157(5)	-	2.4251(4)	-	2.4031(14)
In1–O1	-	2.2970(13)	-	2.2830(12)	-	2.2979(12)	-	2.297(4)
Angle	**H2Ac4*o*ClPh**[a]	**1a**	**H2Ac4*p*FPh**	**2a**	**H2Ac4*p*ClPh**	**3a**	**H2Ac4*p*IPh**	**4a**
C7–N2–N3	119.1(2)/118.7(2)	118.56(14)	118.91(13)	118.39(13)	118.86(15)	118.32(13)	118.1(2)	118.5(4)
N2–N3–C8	118.2(2)/118.9(2)	113.78(14)	119.18(14)	114.49(13)	118.66(15)	114.33(13)	118.7(2)	114.7 (4)
N3–C8–S1	121.0(2)/121.5(2)	130.53(13)	120.19(12)	128.97(13)	119.99(15)	129.26(12)	120.2(2)	128.7(4)
N1–In1–N2	-	72.04(5)	-	71.92(5)	-	72.41(5)	-	72.32(16)
N1–In1–Cl1	-	98.78(4)	-	96.25(4)	-	100.89(4)	-	101.55(12)
N1–In1–Cl2	-	92.23(4)	-	92.10(4)	-	89.70(3)	-	89.52(13)
N1–In1–S1	-	149.04(4)	-	148.83(4)	-	150.01(4)	-	148.93(13)
N2–In1–Cl1	-	163.69(7)	-	164.29(4)	-	164,05(4)	-	170.95(12)
N2–In1–Cl2	-	94.96(4)	-	95.84(4)	-	96.97(4)	-	91.44(12)
N2–In1–S1	-	78.15(4)	-	77.85(4)	-	77.76(3)	-	77.78(12)
Cl1–In1–S1	-	107.980(15)	-	111.867(16)	-	107.099(14)	-	107.05(6)
Cl2–In1–S1	-	98.568(16)	-	98.383(17)	-	97.039(14)	-	107.05(6)
O1–In1–S11	-	88.16(4)	-	88.40(4)	-	92.15(3)	-	88.89(12)

[a] The two bond distances and angles in H2Ac4*o*ClPh refer to the two molecules per asymmetric unit.

Albumin binding studies

Fluorescence quenching studies with HSA

The emission spectra of HSA at 298 K in the absence and in the presence of various concentrations of complex (**1**) are shown in Figure S17. HSA displays strong emission at 340 nm (excitation at 295 nm). By increasing the concentration of **1**, a decrease of the fluorescence maximum together with a hypsochromic shift (from 340 nm to 331 nm) were observed, indicating the presence of a more hydrophobic microenvironment around the Trp-214 residue upon formation of the HSA-**1** system.[3] Similar changes occurred for complexes (**2**-**4**).

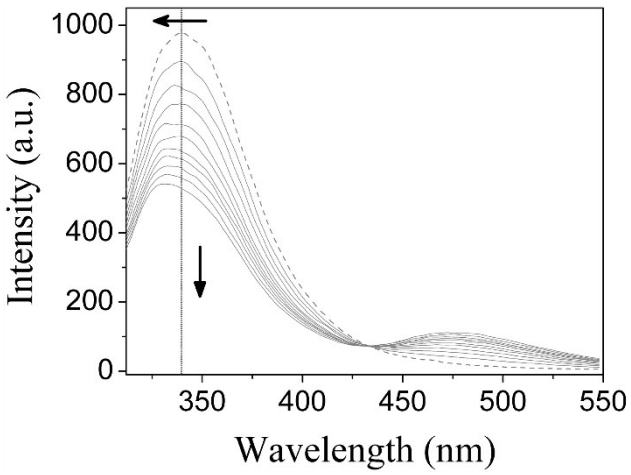

Figure S17. Emission spectra of HSA (1.92 μM) at 298 K in the absence (- - -) and in the presence (—) of increasing concentrations of **1** (0.24-2.34 μM), λ_{ex} = 295 nm. Arrows indicate the spectral changes.

In order to determine the fluorescence quenching mechanism, HSA titration experiments were performed at three different temperatures (293, 298 and 308 K). Based on the fluorescence intensity at λ_{em} = 340 nm for each different temperature, the Stern-Volmer quenching constant (K_{SV}) and the bimolecular quenching rate constant (K_q) were obtained using the classical Stern-Volmer Equation (S1):[4]

$$F_0/F = 1 + K_{SV}[Q] = 1 + Kq\tau_0[Q] \quad \text{(S1)}$$

in which F_0 and F are the fluorescence intensities in the absence and in the presence of the quencher, respectively, [Q] is the quencher concentration and τ_0 is the average lifetime of the fluorophore (Trp-214) in the absence of quencher ($\tau_0 = 10^{-8}$ s for most biomolecules).[5] K_{SV} is graphically obtained as the slope of the linear fit from the plot of F_0/F *vs* [Q] (Figure 3a, main article), and K_q is calculated as the K_{SV} / τ_0 ratio.

Binding constants

The fluorescence quenching was most probably preceded by complex formation between fluorophore (F) and quencher (Q). The binding constant (K_b) and the number of independent binding sites (n) on HSA were determined graphically using the Scatchard Equation (S2):[6]

$$F + nQ \rightleftharpoons FQ$$

$$log\left(\frac{F_0 - F}{F}\right) = logK_b + nlog[Q] \quad \text{(S2)}$$

The plot of $\log[(F_0-F)/F]$ *vs* log[complex] gives n and $\log K_b$ as the slope and intercept, respectively (Table S2, Figure 3b, main article).

Determination of thermodynamic parameters

Figure 3c (main article) shows the Van't Hoff diagram (lnK *vs* 1 / T) for the interaction between HSA and complexes (**1**-**4**). The standard enthalpy change (ΔH^o) and the standard entropy change (ΔS^o) were obtained from the Van't Hoff Equation (S3) by plotting $\ln K_b$ *vs* 1/T, where $-\Delta H^o$ / R is the angular coefficient and ΔS^o / R is the linear coefficient.

$$lnK_b = -\Delta H^o/RT + \Delta S^o/R \quad \text{(S3)}$$

Furthermore, the Gibbs free energy (ΔG) of the binding processes, at a given temperature, is calculated from Equation (S4):

$$\Delta G = -RTlnK_b \quad \text{(S4)}$$

As shown in Table S2, the variation in standard enthalpy (ΔHº) and standard entropy (ΔSº) are negative, suggesting that Van der Waals forces and / or hydrogen bonds play a major role in the interactions. The negative values for ΔG show that the binding processes are spontaneous.

Table S2. Fluorescence suppression constants (K_{SV}), binding constants logarithm ($logK_b$), number of binding sites (n) and thermodynamic parameters for the interaction between HSA and indium(III) complexes (**1-4**) at different temperatures

Compound		T (K)	K_{SV} (10^5 M^{-1})	$logK_b$	n	ΔG (kJ mol^{-1})	ΔHº (kJ mol^{-1})	ΔSº (J mol^{-1} K^{-1})
		293	(5.20 ± 0.09)	(5.86 ± 0.12)	(1.03 ± 0.02)	-32.87		
[In(2Ac4*o*ClPh)Cl_2(MeOH)]	**1**	298	(3.32 ± 0.07)	(5.32 ± 0.09)	(0.94 ± 0.02)	-30.35	-131.59	-338.05
		308	(2.40 ± 0.05)	(4.69 ± 0.16)	(0.86 ± 0.03)	-27.66		
		293	(4.88 ± 0.09)	(5.37 ± 0.09)	(0.95 ± 0.02)	-30.12		
[In(2Ac4*p*FPh)Cl_2(MeOH)]	**2**	298	(3.65 ± 0.07)	(5.30 ± 0.13)	(0.95 ± 0.02)	-30.24	-58.72	-96.82
		308	(2.61 ± 0.07)	(4.88 ± 0.10)	(0.90 ± 0.02)	-28.78		
		293	(4.69 ± 0.07)	(5.66 ± 0.14)	(0.98 ± 0.02)	-31.75		
[In(2Ac4*p*ClPh)Cl_2(MeOH)]	**3**	298	(3.13 ± 0.07)	(5.04 ± 0.12)	(0.91 ± 0.03)	-28.75	-139.60	-369.61
		308	(2.68 ± 0.05)	(4.41 ± 0.07)	(0.87 ± 0.01)	-26.00		
		293	(3.84 ± 0.08)	(5.38 ± 0.10)	(0.96 ± 0.02)	-30.18		
[In(2Ac4*p*IPh)Cl_2(MeOH)]	**4**	298	(3.42 ± 0.05)	(5.22 ± 0.10)	(0.95 ± 0.02)	-29.78	-40.63	-35.97
		308	(2.67 ± 0.04)	(5.02 ± 0.09)	(0.93 ± 0.01)	-29.60		

DNA binding studies

Electronic spectral studies

The absorption spectra of **1**-**4** in the absence and in the presence of increasing concentrations of CT-DNA are given in Figure S18. Upon addition of DNA, a significant hypochromism accompanied by a small bathochromic shift were observed at the wavelength of maximum absorption, in accordance with an intercalative binding mode, as in the case of classical intercalators such as ethidium bromide (EB).[7]

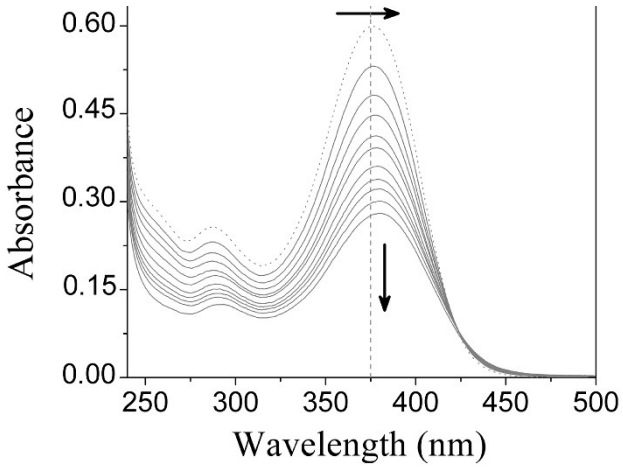

Figure S18. Electronic absorption spectra of **1** (initial concentration of 33 μM) in the absence (- - -) and in the presence (—) of increasing concentrations of CT-DNA (complex:DNA molar ratios ranging from 10:1 to 1:1). Arrows indicate the spectral changes.

In order to quantitatively compare the non-covalent binding strength, the intrinsic binding constants (K_b) of **1**-**4** with CT-DNA were obtained using Equation (S5):[6]

$$\frac{[DNA]}{(\varepsilon_a - \varepsilon_f)} = \frac{[DNA]}{(\varepsilon_b - \varepsilon_f)} + \frac{1}{K_b(\varepsilon_b - \varepsilon_f)} \quad \text{(S5)}$$

where [DNA] is the concentration of DNA base pairs, ε_a is the molar absorption coefficient of the complex at a given DNA concentration, ε_f and ε_b are the molar absorption coefficients of the complex unbound and fully bound to DNA, respectively. As shown in Figure 4a (main article), the plot of [DNA] / [ε_a - ε_f] *vs* [DNA] gives 1 / [ε_b - ε_f] as slope and 1 / (K_b[ε_b - ε_f]) as the intercept. The intrinsic binding constant K_b is calculated as the ratio between slope and intercept. The determined K_b values are shown in Table 6 (main article).

Competitive binding between ethidium bromide (*EB) and complexes (**1-4**) for CT-DNA*

Figure S19 shows the emission spectra of EB bound to DNA in the absence and presence of complex (**1**). The EB-DNA system shows a strong emission at 595 nm when the excitation wavelength is 546 nm. In all cases a remarkable reduction in the emission intensity was observed in the presence of the indium(III) complex, presumably due to the reduction in the number of binding sites on DNA available for EB.

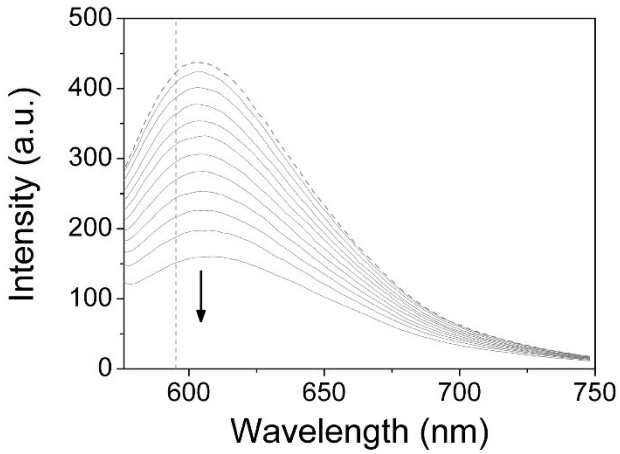

Figure S19. Emission spectra of EB-DNA system ([EB] = 1.26 μM; [DNA] = 2.00 μM) in the absence (- - -) and presence (—) of increasing concentrations of complex (**1**) (0 to 29 μM). Arrow indicates the spectral changes by increasing the concentration of **1** and the vertical line represents λ_{em} = 595 nm.

The apparent binding constants (K_{app}) for complexes (**1**-**4**) were calculated from Equation (S6):

$$K_{app} = \frac{K_{EB}\ x\ [EB]}{C_{50}} \qquad \text{(S6)}$$

where K_{EB} is the binding constant between ethidium bromide and DNA (9.5 x 10^6 M^{-1} per base pair), [EB] is the ethidium bromide concentration ([EB] = 1.26 μM) and C_{50} is the required concentration of the compound to reduce 50% of fluorescence of the EB-DNA system. As shown in Figure 4b (main article), the C_{50} values were obtained from the plot of fluorescence intensity *vs* [complex] when fluorescence is 50% of the initial fluorescence. The C_{50} values (μM) and K_{app} (10^5 M^{-1}) are shown in Table 6 (main article).

Cartesian coordinates of the B3LYP/TZVP optimized structures of the complexes

1-MeOH (MeOH Coordinated)

C	6.45598615756953	5.92998423310760	4.43951674444796
C	7.68140338205446	5.41986943586034	4.84714474438406
H	7.83497485973562	4.35452971527384	4.91987769579939
C	8.70905262949159	6.29664968376816	5.16943383866793
H	9.66544587028534	5.90954022799612	5.49523513403933
C	8.49215992306115	7.66184963391936	5.07550665015391
H	9.26198114755331	8.37962647408054	5.31959363890488
C	7.24715287947331	8.10143145777474	4.65685574642697
H	7.02832037894761	9.15729252648071	4.57298833168061
C	5.32471449711901	5.03608075992959	4.11389341124924
C	2.08868136788241	5.53608419044043	3.04792967674932
C	0.63069539521099	3.50013780601842	2.93559552844518
C	-0.35531368538090	2.92477579882450	2.11866982051264
C	-0.75703539181112	1.60752896898204	2.27220039016922
H	-1.51721652244517	1.20026455109689	1.61912775050555
C	-0.17185494721715	0.82378595736188	3.26011317668755
H	-0.48461069801714	-0.20514268077952	3.38444265137216
C	0.80554269791157	1.37350325432986	4.08346227137420
H	1.26210864846032	0.77310329086807	4.86011666425637
C	1.20122861765193	2.69537816210142	3.92907056204412
H	1.95134146742880	3.12009398082040	4.57599903297411
C	5.50041371858125	3.56082441175461	4.19732426284456
H	4.61538233242690	3.05016034426401	3.83150233770054
H	5.68585417696738	3.24776421558973	5.22819156360047
H	6.35687982399252	3.24010413188558	3.60134047371866
N	6.25949171682032	7.26323301805429	4.34853844464759
N	4.22139078096484	5.62037187335640	3.78112189275337
N	3.13072306402465	4.87168879184998	3.48754617342917
N	0.94341522839651	4.85815680205917	2.76486244102670
S	1.97509373959844	7.28348399077880	2.71689155874309

Cl	-1.12547896956469	3.89614997121924	0.85394582380056
Cl	4.63478866953780	10.21766006784791	3.15296535971875
Cl	3.54232280595082	8.26367050678616	6.11325203399446
In	4.24698090842631	7.82466973424912	3.69746116213207
H	0.23684966600528	5.40482455603278	2.29298797849831
C	5.76307640210391	8.23145129529371	0.59341929538341
H	6.29472529926434	7.68513309061527	-0.18620220825012
H	4.95037037633007	8.81341405154883	0.15678672771432
H	6.44848105912200	8.90349419663263	1.10164960357473
O	5.26373829864614	7.30262143856404	1.58199576266527
H	4.69506835743979	6.65929654836230	1.13805153645936

1-MeOH (MeOH intermolecular)

C	6.80489807337941	5.81100350775417	5.47980168602976
C	7.67317312271059	5.22538832451661	6.38974835322498
H	7.54030060920123	4.20122515320812	6.69893028867415
C	8.72981494184538	5.96933759152052	6.90117702805840
H	9.41223417991229	5.51876655816278	7.60899208410705
C	8.89335762085319	7.28440030971490	6.49754833775978
H	9.69434615155081	7.90397266124833	6.87340847833557
C	7.99308738496463	7.80255671194088	5.58133124569034
H	8.08457753078214	8.82221647793996	5.23315734782121
C	5.66275047368181	5.07490336163947	4.89905901753353
C	3.17242200942179	5.82285103039176	2.66144469650047
C	1.51707592024312	3.99929300060510	2.14475236302370
C	0.18863524266963	3.82323035317010	1.71823281604012
C	-0.44103862823559	2.59218183790909	1.76455007632402
H	-1.46470692369490	2.50233225893125	1.42638714193070
C	0.24876651463223	1.48450737206194	2.24450806255776
H	-0.24555713442787	0.52259322810367	2.28893313733152
C	1.56721446308348	1.63054347572581	2.65915305576038
H	2.11852138624952	0.77444527620916	3.02746430585981
C	2.19969378661457	2.86592056868286	2.60196671171042
H	3.22429866124850	2.97066854049501	2.91604095426115
C	5.36635985676128	3.66704709070972	5.27421006114734

H	4.29073777425544	3.49922890987883	5.27563930158849
H	5.76479176594876	3.40608944992832	6.24997074847444
H	5.80266080896394	2.98598724313496	4.53665208162442
N	6.98256535465867	7.09120355632729	5.08536710846126
N	4.95381943243589	5.72672964988585	4.03811416189301
N	3.90582532273670	5.09034394087337	3.46028630762824
N	2.08651472367633	5.27741485340850	2.04880700354990
S	3.41553247991914	7.54272151595246	2.27293954430106
Cl	-0.73115696493599	5.20824715744606	1.11078175229760
Cl	7.19425815096071	8.43838274874794	1.93084491175760
Cl	5.01954531158308	9.85305000148156	4.90421312514577
In	5.52147803378303	7.77990895726122	3.63230564377302
H	1.53910290524895	5.93651882405917	1.51295374925860
C	2.34082834225831	9.15215722375676	-1.00984779689732
H	1.50213541423458	8.49278821064223	-0.76591653684325
H	2.39061215279111	9.95602357883243	-0.26954943490769
H	2.16375412909048	9.59585242710805	-1.98946110258621
O	3.57486283504582	8.42226010103788	-1.08724821455058
H	3.73072191089793	8.01483781359588	-0.22071406765055

Compound 1a (in DMSO)

C	6.615325	5.978369	4.835647
C	7.785445	5.447532	5.364031
H	7.841436	4.410591	5.653311
C	8.899132	6.264744	5.512144
H	9.813411	5.858088	5.923490
C	8.824700	7.594440	5.130452
H	9.667108	8.264645	5.223214
C	7.625936	8.059765	4.616324
H	7.514282	9.090081	4.305948
C	5.404907	5.152174	4.622807
C	2.314457	5.713822	3.226455
C	0.925909	3.688544	2.666834
C	-0.098078	3.296014	1.785377
C	-0.445315	1.968181	1.608374

H	-1.232400	1.707875	0.913966
C	0.228805	0.981654	2.320410
H	-0.040571	-0.057135	2.178622
C	1.235209	1.346052	3.208251
H	1.759068	0.587382	3.776135
C	1.582953	2.680329	3.384086
H	2.363658	2.961198	4.070756
C	5.387374	3.702069	4.962520
H	4.397807	3.412639	5.311381
H	6.109635	3.450970	5.733442
H	5.616108	3.100379	4.077216
C	6.616939	8.597586	-0.243079
H	6.855015	9.454644	0.382749
H	6.450158	8.927281	-1.268259
H	7.402188	7.845540	-0.191832
C	4.911056	6.463875	-0.715952
H	5.828817	5.879174	-0.692360
H	4.702844	6.836757	-1.718500
H	4.065594	5.878269	-0.361638
N	6.555906	7.280944	4.479218
N	4.395324	5.758118	4.094087
N	3.289223	5.035958	3.786515
N	1.205574	5.055270	2.787119
O	5.466758	7.249003	1.769931
S	2.227076	7.469691	2.938341
S	5.065942	7.895054	0.384143
Cl	-0.972456	4.522924	0.852429
Cl	5.110705	10.293983	3.042968
Cl	3.973934	8.633093	6.123184
In	4.613924	7.918764	3.715789
H	0.518788	5.658674	2.356042

Compound 2a (in DMSO)

C	5.45637389927052	2.74304117216325	6.02129391528985
C	5.14278536876067	2.73382945654531	4.66766125449791
H	4.22049326690155	2.29250826305204	4.32332453853231

C	6.03039765979001	3.29221105594321	3.75670033715353
H	5.79290064233219	3.28812609377316	2.70135050074911
C	7.21141245272320	3.85401818344026	4.21560899278442
H	7.93146901368512	4.29934446356038	3.54470249655546
C	7.45905568041810	3.83240578446458	5.57794573934413
H	8.36718305069529	4.25366405736516	5.98775193703173
C	4.53994424720266	2.15796435298602	7.02828118986028
C	4.61616722737271	1.86727409918580	10.46346217970492
C	2.77374588241381	0.54434683187534	11.57952326373883
C	2.39137490955518	0.12882983812160	12.86411330353386
H	2.95204429250083	0.46954643850470	13.72663458487391
C	1.31422517123404	-0.72514002252940	13.04408621316800
H	1.02022572893811	-1.05782941039359	14.03104807678218
C	0.62339051250087	-1.15619581727521	11.92533907906141
C	0.95467001111339	-0.74843758567861	10.65039851920577
H	0.38355753817483	-1.09940801011946	9.80052395264063
C	2.03461579586873	0.11193287795816	10.47359141681681
H	2.31056847799859	0.44195363181333	9.48805108999808
C	3.24728318835954	1.56142135971623	6.58540115176452
H	2.72685739624227	1.11017282075286	7.42262662937892
H	3.40778413561518	0.79231344426060	5.82770522839774
H	2.60125783066109	2.32397138989222	6.14233434637021
C	4.27493599529176	6.74659469259946	9.99718394417938
H	3.72206278159484	7.01866157528059	9.10016231789933
H	4.33099007014994	7.58505996213608	10.69050139632757
H	3.82578736425931	5.89152047435870	10.49732064900541
C	6.41104836711265	7.73920260130466	8.56839812453634
H	7.42573900112887	7.59694341267848	8.20231117934110
H	6.37189518274001	8.60776885854764	9.22518199932356
H	5.70823307087075	7.83981635391001	7.74356481211091
N	6.61191616217161	3.29289723509963	6.45160096012855
N	4.93858469372923	2.21499395462937	8.25512632173368
N	4.16321531122156	1.69905535320386	9.24060775596173
N	3.91155784330881	1.37046530267024	11.51220165412686
O	5.81293020296504	5.12789563946214	8.49474268536425

F	-0.41949379167541	-2.02412905888146	12.09047107563570
S	6.10849188215584	2.70446634309986	10.97148764058858
S	5.97681456277587	6.28391856654994	9.55933642552590
Cl	9.04347070345405	4.47882252395828	8.92485154817918
Cl	8.22144164205096	0.95919203742146	8.26872566459033
In	6.90250188299782	3.17599677189019	8.60376735275801
H	4.32467369136794	1.57168763070288	12.41175355544898

Compound 3a (in DMSO)

C	2.94509290844456	3.42807662166706	9.34149338765200
C	3.19572887072722	2.18128501555510	9.90161222933038
H	2.69519884547955	1.30279019478616	9.52562614355492
C	4.10650639795974	2.07323546800755	10.94585618836340
H	4.31975848723892	1.10558552045575	11.38069302943089
C	4.73250877766414	3.21372688728654	11.42430547918663
H	5.44141452105030	3.17808919646442	12.23873765428081
C	4.43205548419558	4.42414291663584	10.82177418847926
H	4.89957301035597	5.34214470941823	11.15132169260664
C	2.00483384648004	3.59110711657352	8.20873279352374
C	1.02174308704201	6.27352974252747	6.28262551703226
C	-0.00011028324940	5.73406750129126	4.05256304758026
C	-0.53888940371564	4.46020114814787	4.24257039814997
H	-0.65757609170033	4.06249804379992	5.23754859127204
C	-0.92238938297874	3.69821789979205	3.14439536352970
H	-1.33973747782564	2.71191981619535	3.29535453363667
C	-0.78402257669702	4.21650101246779	1.86610307535699
C	-0.27174337499774	5.48984905271751	1.65707917072079
H	-0.16466047315864	5.89088861981188	0.65831763055742
C	0.11406138676149	6.24420434337501	2.75392043498179
H	0.53181446563185	7.23200729285879	2.59921021525256
C	1.32385261562694	2.39723824300157	7.63672304658784
H	2.05286511765205	1.71035386230826	7.19889657380204
H	0.78036289800846	1.85010493161140	8.40949963389204
H	0.62244658430856	2.69270368577412	6.86384666848589
C	-0.68838651115573	7.34987983911409	11.47785623517127

H	-1.23360970783993	7.09572153964949	10.57177574403228
H	-1.16660115755635	8.19239035812176	11.97591862877549
H	-0.61738450198820	6.49246890551031	12.14449481458076
C	1.71007641138079	8.06315415948153	12.63554385423216
H	1.61259758465493	7.12925010904912	13.18641086169121
H	1.17911644390209	8.87030481030273	13.13894003520305
H	2.75388446704727	8.33651688600253	12.50038982986450
N	3.57439245266901	4.52767015116994	9.80877819673520
N	1.86858980090702	4.79225420959837	7.75746714920201
N	1.09891367890798	5.01778704956589	6.66199733994968
N	0.41197383337365	6.57607803419358	5.10504906571519
O	1.61442504062192	6.54876749576946	10.40179421796574
S	1.63953447356917	7.71469019337843	7.12994182681297
S	0.97889294231397	7.87169538107944	10.98247109288054
Cl	4.52320374174267	8.06257735776661	9.87664915397698
Cl	4.98171504358277	5.83967611820039	7.02506617867702
Cl	-1.26732573345561	3.23815621872801	0.47103690804750
In	3.07386575536665	6.35927167634806	8.74096867013708
H	0.47652070165178	7.55229466443982	4.85386950910257

Compound 4a (in DMSO)

C	5.57460478175931	9.34743226510794	6.14591725173094
C	5.19132479591497	9.28636623240076	4.81134065053001
H	4.32678449587000	8.71622984481549	4.51150377064165
C	5.94368309552535	9.95320516406129	3.85320310669460
H	5.65104175024616	9.90667140094343	2.81264959060681
C	7.06106323579996	10.67389153976326	4.24389670820899
H	7.66977118333795	11.21463209733055	3.53379643780282
C	7.39587186644232	10.68015304075538	5.58827899604895
H	8.26780022786237	11.21174800098374	5.94540679450731
C	4.80393897972616	8.67422561028907	7.21426459909759
C	5.25692299658250	8.18686307976901	10.58710696736218
C	3.38860676399286	7.03022596070195	11.82749881313329
C	3.01157745346063	6.73965587272831	13.14635858420504
H	3.67920375302372	7.00524633364835	13.95727889288574

C	1.80284799449059	6.12963243939551	13.43039794343028
H	1.53608556212142	5.91627249989500	14.45679304918774
C	0.94498029521329	5.79885616403260	12.38464907734723
C	1.30142849245383	6.07560943702272	11.07070084829197
H	0.64113799072465	5.81600809810171	10.25353325794079
C	2.51672704656186	6.68976600065211	10.78916333754237
H	2.79255917628425	6.90626754071883	9.77206225970958
C	3.49017819344356	8.02552108355154	6.94180532663783
H	3.05468926632406	8.35376003791324	6.00317815176807
H	3.59106707582588	6.93661561359605	6.91333246847365
H	2.79256358888804	8.26686008363579	7.74411839818491
C	6.32662607361614	12.79951719768187	11.23750517942383
H	6.09165460413096	13.72539864662996	11.76162430776831
H	6.01904080308778	11.94934139575676	11.84138235909770
H	7.38519753667441	12.74350185026363	10.99233887466392
C	6.14503014931156	14.11052348268682	8.81018860514155
H	5.94772671934116	15.03546532676007	9.35191429825354
H	7.21239693411379	13.91518843438650	8.73159132709299
H	5.68070382060765	14.15897266640327	7.82745194524694
N	6.68388745908735	10.02993903330693	6.50625332788637
N	5.33378966564517	8.69934333305048	8.39076183999506
N	4.68055187199840	8.09037031159939	9.40895096355238
N	4.63639237533805	7.65142287419488	11.67059406097450
H	5.14541150495693	7.77365256623807	12.53451454002082
O	5.68310059949203	11.44543620510021	8.96046611033075
S	6.81511969798515	8.95262903034904	10.98130743525341
S	5.32420509457005	12.76898594023312	9.71959417016530
Cl	9.06391014295072	11.53163705286939	8.79322899234011
Cl	8.89304318841578	8.00183386501820	7.93203772448994
I	-0.85268656404728	4.90669255343560	12.76251262702351
In	7.19801526084847	9.85844679222219	8.62850202930876

Compound 1a (in H_2O)

C	6.63328328284009	6.01999993502274	4.87414620318335
C	7.80575082240221	5.49516313399374	5.40209851919095

H	7.87418763745319	4.45346189410578	5.67011845298946
C	8.90593408642485	6.32561958375071	5.57670785086473
H	9.82215967728798	5.92372030756953	5.98744347614414
C	8.81620731612425	7.66204448078710	5.22266013914621
H	9.64763272984088	8.34174846432848	5.33832024545894
C	7.61648471459439	8.12046785762064	4.70637978500999
H	7.49308562228952	9.15470445379255	4.41428628323019
C	5.43679045111560	5.18261126377214	4.63105517259572
C	2.35913954313931	5.73834098753703	3.20218386235308
C	0.97685526568654	3.71446004702366	2.60317213549778
C	-0.07523249157858	3.34055660836487	1.74755648045157
C	-0.42209198329830	2.01668495956674	1.54443902340337
H	-1.23189099701616	1.77284251449864	0.87097174350968
C	0.27934778353151	1.01375300681784	2.20542689846102
H	0.01063039390387	-0.02179193678993	2.04267962519185
C	1.31198515995716	1.35931605517788	3.06993107857097
H	1.85778875447074	0.58856204569177	3.59894098910284
C	1.65939238279612	2.69021604247394	3.27192935571270
H	2.45976447790106	2.95540918574560	3.94157061766134
C	5.44060983014694	3.72583533691797	4.93662305835985
H	4.44987453878552	3.40601312102080	5.25248988468981
H	6.15048002303876	3.47183809254239	5.71777918748803
H	5.70498095873989	3.15430769660187	4.04146315358764
C	6.65350683629350	8.33096855779404	-0.36037515613196
H	7.06721626046370	9.16506600856395	0.20206519744397
H	6.44312746718940	8.64429246081302	-1.38203238029517
H	7.32059456537325	7.47211861271134	-0.33377469567645
C	4.62731809277957	6.43423781421056	-0.53203342306925
H	5.44767147983286	5.72004674738059	-0.51667228940874
H	4.39168958838790	6.75374238595378	-1.54607844640498
H	3.73907205165563	6.01806738076816	-0.06061753092279
N	6.55974882146521	7.32851273331247	4.54344024275907
N	4.42439217852070	5.78630786122239	4.10469318017452
N	3.32931148151449	5.05836442829273	3.76691252674059
N	1.25470943671951	5.08050642916542	2.74577285772010

O	5.52055690657181	7.29419476960200	1.82579817194014
S	2.26135393268164	7.49579849736253	2.93973068826837
S	5.08109838114833	7.89952218450478	0.43040041937170
Cl	-0.99060270329961	4.58782051608659	0.88347776914535
Cl	5.13144511554327	10.33072933434583	3.10596156906766
Cl	3.94067624560544	8.66370834948443	6.15910714960794
In	4.62521903748283	7.95733813829398	3.76619242594678
H	0.56835084349321	5.68777565219691	2.31974450186793

Compound 2a (in H_2O)

C	5.44704424105952	2.74367141319491	6.02723496790954
C	5.13632099131140	2.73782640910081	4.67345998762532
H	4.21474720937091	2.29735926624947	4.32664776568341
C	6.02560363503691	3.29907095326542	3.76581114873704
H	5.79006126159587	3.29785750783478	2.71032613948973
C	7.20591330402064	3.85979167734055	4.22813542467687
H	7.92653800227686	4.30732170811749	3.55978986096911
C	7.45132805197221	3.83367683011547	5.59020470392231
H	8.35863919485026	4.25446997886476	6.00236859469661
C	4.52824658057501	2.16010309106783	7.03169107948225
C	4.59548214812706	1.87923261292287	10.46851392786827
C	2.76133559216500	0.54171228045116	11.58183417339085
C	2.38156084004603	0.12201644526425	12.86536010919589
H	2.93267003942228	0.47502680027555	13.72883541977792
C	1.31983951030752	-0.75179523188679	13.04287313894607
H	1.02803550736373	-1.08774603506754	14.02908391490161
C	0.64217646883713	-1.19819190448133	11.92206353585889
C	0.97097006919331	-0.78658589928099	10.64787556243095
H	0.40991013531605	-1.14947519057543	9.79668185810697
C	2.03498785554833	0.09410984946302	10.47404258657197
H	2.30728600780507	0.42786707750152	9.48892888161509
C	3.23573172688742	1.56814333727716	6.58554218020929
H	2.71253206808384	1.11472135669099	7.41965047574654
H	3.39722000546771	0.80272333395264	5.82467770484805
H	2.59503742572448	2.33562543092712	6.14409819242520

C	4.28948007681623	6.78830259615020	9.98443835998943
H	3.74718727919635	7.05802369842661	9.08058114766839
H	4.35604318398056	7.63199819191830	10.66960543173239
H	3.82641141486056	5.94228995448044	10.48660059484355
C	6.44874148782003	7.72819707189975	8.54879128897133
H	7.45389765775014	7.54805562645788	8.17364816967200
H	6.44106728615416	8.60303771543925	9.19745534444660
H	5.74045662372635	7.83748247046174	7.73012940359404
N	6.60270510988062	3.29091388772122	6.46071850475421
N	4.92464716301102	2.21558492676672	8.25958369220896
N	4.14469125806520	1.70479737735584	9.24551235846277
N	3.88506807297835	1.38932886483282	11.51815535690217
O	5.79562944323134	5.13128831813147	8.49874824218924
F	-0.38534991156001	-2.08527782978834	12.08376925604864
S	6.08555325460212	2.71350306898940	10.97629853554528
S	5.98379437315315	6.29493353101623	9.55599114725853
Cl	9.01886884176725	4.48951747903368	8.92943219246206
Cl	8.22466158093377	0.96694903413817	8.29391131002371
In	6.88783991673855	3.17331577033325	8.61149270662643
H	4.29596801452966	1.59192014764967	12.41816262151447

Compound 3a (in water)

C	2.97173280537958	3.41182854667416	9.31775771938839
C	3.22430830607667	2.16026816926972	9.86428852393442
H	2.73718044366055	1.28382367448186	9.46689188598923
C	4.11617292633311	2.04628176446654	10.92382665872096
H	4.33049230883048	1.07496360651167	11.34904246732869
C	4.72263212799275	3.18593644793837	11.42910662160829
H	5.41697506537212	3.14539732734210	12.25527841444441
C	4.42158325497211	4.40150095587884	10.83850618021768
H	4.87386587672686	5.31933294010340	11.18874269454947
C	2.04834407015463	3.58049806233003	8.17484025270296
C	1.04219548149702	6.28214197144925	6.28910657447544
C	-0.00444840401784	5.73878395864543	4.07347656840550
C	-0.57892162531715	4.48369276487223	4.28279808397729

H	-0.71206158109720	4.10505543700671	5.28318210453855
C	-0.98085492565309	3.71361972471158	3.19708132630464
H	-1.42579900966288	2.74214817793798	3.36315118438286
C	-0.82438859962709	4.20545552228087	1.91042054879364
C	-0.27901283164762	5.46127763971541	1.68171509080070
H	-0.16079313795663	5.84251794702531	0.67672467767057
C	0.12501897403216	6.22342511913637	2.76730379637154
H	0.56684069998445	7.19775698559211	2.59697200835340
C	1.39523996426874	2.38594908355360	7.57263224540168
H	2.14454376174986	1.67518046939132	7.21767905953273
H	0.77985831732682	1.86839320839775	8.31211343637927
H	0.76436859881892	2.67454258332371	6.73909313936060
C	-0.71050314369108	7.39036091783084	11.44760209849227
H	-1.23994639101063	7.12562627099404	10.53549106105887
H	-1.18980198310875	8.24222053706292	11.92726816506671
H	-0.65193658885425	6.54035550476832	12.12436042324419
C	1.68408583806117	8.08771562773461	12.62851649905331
H	1.56736744424243	7.15829015601851	13.18243221836732
H	1.15870227520593	8.90593066317604	13.11855952321405
H	2.73291866798650	8.34207979033934	12.49799534997112
N	3.58237104633102	4.51147027283645	9.81023424335114
N	1.89739867496702	4.78847322029454	7.74612374049871
N	1.13161120378744	5.02220819743379	6.65029803670687
N	0.41806065673635	6.58954285223341	5.11811986490386
O	1.59387538690851	6.55269811915591	10.41009807560616
S	1.64224356242858	7.71589647985794	7.15449162383989
S	0.96727478100571	7.89272148338158	10.97109140055520
Cl	4.52979978545684	7.99499012615123	10.00408489614298
Cl	4.98723005018263	5.93272617100802	7.03404024332802
Cl	-1.32881114891199	3.21522136585448	0.53176578085792
In	3.07940365933189	6.35525355237789	8.76465596295840
H	0.49866635474741	7.56152060345381	4.85626552915021

Compound 4a (in H_2O)

C	5.58073763472477	9.34483721421988	6.13708537576147

C	5.20204650607493	9.27932683136646	4.80186062316383
H	4.33745778339613	8.70967287875631	4.50190049379442
C	5.95950607154997	9.93999682667107	3.84338196075976
H	5.67046477484589	9.88921068380292	2.80236045109232
C	7.07736494591968	10.65989007169518	4.23467612608800
H	7.68996848192336	11.19529030878759	3.52435737976773
C	7.40668531505003	10.67236251810701	5.57988369928281
H	8.27766782780052	11.20515093944871	5.93733948803968
C	4.80721013686245	8.67491907318587	7.20421232756397
C	5.25914155213929	8.19624615768663	10.57908054076376
C	3.38577035789382	7.05015600150073	11.82549305019020
C	3.01275643849879	6.76065290769360	13.14524979315716
H	3.68264748780675	7.02799125953419	13.95345652950516
C	1.80589603346598	6.14906796330864	13.43379017871682
H	1.54283772853157	5.93653339443244	14.46099496093302
C	0.94563135594366	5.81521236042582	12.39099444070820
C	1.29814121866863	6.09173442549316	11.07588873327729
H	0.63632926235676	5.83054685582674	10.26086228140654
C	2.51185364920832	6.70748111941503	10.79019023550429
H	2.78307283381279	6.92420289957978	9.77201366648409
C	3.49249004573940	8.03114933608248	6.92854772053629
H	3.05711548292893	8.36870583590264	5.99345983553803
H	3.59330459015908	6.94278439012934	6.88921956168531
H	2.79712058523170	8.26548001471401	7.73423780367910
C	6.34949372965403	12.76443101498434	11.25158878393487
H	6.12583047011130	13.68658459870690	11.78633041788145
H	6.05774285706547	11.90909042036435	11.85537109353740
H	7.40104852620242	12.71228885974341	10.97771406833331
C	6.09448112564961	14.09795775415301	8.83910859901884
H	5.90891937901135	15.01710697121787	9.39369640208997
H	7.15908083311734	13.90528374152356	8.72565228752139
H	5.59929696175709	14.14625117219842	7.87205622845599
N	6.68948692776295	10.02809382224185	6.49855534228774
N	5.33842829694451	8.69597876610551	8.38043158137129
N	4.68337580610393	8.09112733837221	9.40095511458733

N	4.63538601007848	7.66977474519849	11.66615569432860
H	5.14160179649390	7.79939925222374	12.53036365432969
O	5.66011194126016	11.42971705146452	8.97565383989408
S	6.82238535353005	8.94683298450641	10.96855289765103
S	5.30920224010358	12.74543724058074	9.76071362269618
Cl	9.03819803946516	11.56701761429227	8.76589312793911
Cl	8.92267411716185	8.02837613767573	7.93603859150380
I	-0.84975837921922	4.91911044214957	12.77441046069295
In	7.19937286721279	9.86155180453085	8.62117693454573

Compound 1a-(H_2O) (in H_2O)

C	6.62049736200608	5.56428821028313	4.80638348303770
C	7.73922844550746	5.03583644320774	5.44303383223853
H	7.78297865149084	3.98581452432701	5.68921499233831
C	8.78990043268336	5.87861539973944	5.78120475854354
H	9.65983898709639	5.47934746225698	6.28695960239351
C	8.70847606635262	7.22968762817564	5.47465885156363
H	9.50150548544645	7.91945470310890	5.72642845967182
C	7.56400311976084	7.68929000894737	4.84328103679291
H	7.43607577270324	8.73668998843705	4.60429403132294
C	5.46184305479020	4.72976770563207	4.44026840610979
C	2.38068289024854	5.39191736675998	3.04683143260883
C	0.83884020753252	3.42570101523815	2.79969398471804
C	-0.13665431152861	2.94895874203953	1.91015585171528
C	-0.61373534876437	1.65113109912235	1.98777402264670
H	-1.36051883573655	1.31582884953374	1.28113981923356
C	-0.12310199058000	0.79932320603737	2.96995622480128
H	-0.49572741889862	-0.21455652621209	3.03332560497885
C	0.83364406559648	1.25903337848140	3.86854704377606
H	1.20837706141328	0.60360646946728	4.64390875153227
C	1.30929931624972	2.56050599338650	3.79131956380394
H	2.04225257635713	2.92053418481497	4.49367552126536
C	5.46615019132487	3.25603841059238	4.66943648028626
H	4.67366102986459	2.79215970529317	4.08941340394328
H	5.29268715558847	3.02707509599298	5.72591535342151

H	6.42041593787550	2.81151400953797	4.38524162366102
C	6.47755288540332	9.51668855720541	-0.11293097821030
H	6.45855153632866	10.33542993176439	0.60168782384591
H	6.22225448119696	9.88341387120460	-1.10758050476485
H	7.42808318094380	8.98640205521938	-0.11190642099169
C	5.37017204231694	7.04942899796605	-0.80321968682891
H	6.39874368044354	6.69337014969295	-0.80265407379312
H	5.08689980308707	7.45410237191217	-1.77557597775856
H	4.68325835690054	6.25418508683265	-0.52239531305648
N	6.55578177347918	6.88205456539207	4.51502336427328
N	4.45033660119176	5.36253733689695	3.93237338144071
N	3.34371165796969	4.68021669801149	3.60192815053173
N	1.23598798340142	4.77410268762686	2.68363642792239
O	5.78045109019359	7.74017739211998	1.74437100815122
S	2.37980395030903	7.13797137750218	2.70999705344586
S	5.16740134137540	8.37755420338911	0.42152395651807
Cl	-0.78717515775646	4.01938768088560	0.66765794898751
Cl	4.60413260895791	9.57366322006077	4.86475204497278
In	4.67032835531290	7.52284768344668	3.59290375998720
H	0.58548663229672	5.35667871547224	2.17215420205186
O	4.59654996846744	10.91087815050835	1.92668801179888
H	3.97372789257509	11.60306758059465	1.67859743142776
H	4.54960919422501	10.84847187509450	2.89399398364381

Compound 1a-$(H_2O)_2$ (in H_2O)

C	6.45286962086993	5.90003912467769	4.63821788029489
C	7.57613141558900	5.47480150717997	5.33126760150215
H	7.66830920650869	4.44741829185475	5.64614196625243
C	8.57827919481905	6.38922474156172	5.63256762154687
H	9.45198112534403	6.06704682065862	6.18161298050819
C	8.44306252496339	7.70741600134657	5.22748139482499
H	9.19616399909481	8.45118573437996	5.44106516409803
C	7.29987875688546	8.06467365889956	4.53299493088576
H	7.14964620281160	9.08012382205486	4.19342281378095
C	5.34666493528253	4.97218107015402	4.31232058474492

C	2.26273780115814	5.37750634571383	2.83703382115385
C	0.79031478962365	3.35578123996008	2.75690950341602
C	-0.13268226141256	2.72639247389937	1.90998556449902
C	-0.57022587243830	1.43125009864574	2.13711479365160
H	-1.27991990226886	0.97978145258427	1.45765057807877
C	-0.08754236674724	0.72893458425583	3.23523379598531
H	-0.42945330301769	-0.28112532349080	3.41850661271830
C	0.82433847698382	1.33615778408553	4.09246235365556
H	1.19876267717186	0.80150676381055	4.95562189167596
C	1.25641818934296	2.63520538809611	3.86209027798411
H	1.95362892457482	3.10550272299407	4.53564786869359
C	5.41032017168696	3.54658875277981	4.72608631852049
H	4.60783756260677	2.98183771893712	4.26328110145685
H	5.31480173364345	3.46146819017586	5.81225013719296
H	6.36422694244210	3.10153171915266	4.44181594185578
C	7.57441255459878	8.27219932986606	-0.28909522761664
H	8.20628587145854	8.54003046510825	0.55404658057336
H	7.78919396974146	8.92679188967557	-1.13203591418382
H	7.69249325459391	7.22544052635872	-0.56256406271920
C	5.00412551245930	7.99259249699018	-1.28228304276778
H	5.26569487844448	6.95100411255725	-1.45772811354714
H	5.32627153145368	8.62421721730390	-2.10870886941264
H	3.93721647841252	8.11566726214335	-1.11528568257170
N	6.33563535872335	7.18994678993078	4.24673564970664
N	4.34621692815817	5.49434015779882	3.68506286302893
N	3.26614945547773	4.73622073580592	3.38258588255020
N	1.13730361077101	4.69492803863451	2.50478996665739
O	5.57056521719149	7.47129978766382	1.30547937509478
S	2.15424724215945	7.12201288165095	2.45307272393440
S	5.85916025144600	8.58206434575790	0.19988831383317
Cl	-0.78130924609142	3.59940485245958	0.51510875032507
In	4.48223190145538	7.60209084348364	3.19733185840493
H	0.47398061206098	5.21264965879797	1.94536748737311
O	3.78685420464213	8.25767907319513	5.30424397597057
H	4.31896195002916	8.75926483163210	5.93776436799919

H	2.86572940817412	8.51304907136552	5.45642869372590
O	4.86158237641870	9.79205315251903	3.05754774204689
H	4.29505485938133	10.35468003278043	3.60584080055053
H	4.90929746632134	10.21735196815287	2.18795985606652

Compound 2a-(H_2O) (in H_2O)

C	5.39899316377540	2.80710470244864	6.14939065161383
C	5.13082379607917	2.79944661570896	4.78717326483033
H	4.24008004839230	2.32345843197461	4.40851756872756
C	6.02050389739138	3.40998431639209	3.91191245391368
H	5.81506784798736	3.41370785443725	2.85031876824732
C	7.16323784747428	4.01254618596322	4.41472910601076
H	7.88344848087757	4.49738278037061	3.77250510323591
C	7.36969009716088	3.98158817071870	5.78313582768795
H	8.24804142521890	4.43373972169669	6.22380857734088
C	4.47511938861306	2.17151753278182	7.11830324334875
C	4.47458382457022	1.83181004544427	10.55355307730277
C	2.71296638468496	0.36240797817212	11.61304739391906
C	2.33922337905688	-0.10051371306628	12.88304300686563
H	2.86051876983034	0.26349855183934	13.76043642895198
C	1.31746448205884	-1.02639518026364	13.02909675168272
H	1.02816146649473	-1.39220693421666	14.00537936487262
C	0.67688314662479	-1.48363020769470	11.89079641610485
C	1.00999556550774	-1.04079730056612	10.62811246851479
H	0.48219394033034	-1.41827249394411	9.76229730143873
C	2.03315179912740	-0.10771296624047	10.48582295758438
H	2.30496973577471	0.25399973265300	9.51036559102875
C	3.23860295168106	1.50742996104309	6.62381385502445
H	2.70212866777708	1.03590155794575	7.43923268007959
H	3.47820058700318	0.74578536295711	5.87985846267358
H	2.57963972214383	2.23534700018440	6.14438510534281
C	4.45778912919512	7.27658442372929	9.80430338715731
H	3.90349589959086	7.35971121320401	8.87204911130010
H	4.58640690218810	8.24813338694579	10.27891646236375
H	3.97065079966485	6.59065033192966	10.49280913436126

C	6.66573935369776	7.76099874655652	8.19176680662343
H	7.61216691883875	7.38225325295510	7.81240274603480
H	6.81857386738292	8.72766797336880	8.66922481934277
H	5.92248915284028	7.82082684893880	7.39956544346806
N	6.51479697823455	3.40098223792657	6.62331185149186
N	4.81714196803740	2.24801885676063	8.36157586016860
N	4.04328969547215	1.67848830597750	9.32061848512703
N	3.78589649942698	1.27605062618735	11.58149850547638
O	5.77643072545561	5.28283868695210	8.64364752806497
F	-0.32057185741007	-2.40943819845584	12.02146087444521
S	5.92843226919974	2.71061544974378	11.10377995109939
S	6.10284578879827	6.60149431493896	9.46458609708039
Cl	9.03420288738138	4.12095519224836	9.10647723434549
In	6.69583954970961	3.31474907981312	8.78250456174142
H	4.17943950310006	1.47497668157662	12.49021118871258
O	7.69748134232402	1.26096045658087	8.37700854045961
H	8.63117273123088	1.28434666403801	8.63629014460927
H	7.30729952000440	0.54368116034430	8.89749623918261

Compound 2a-$(H_2O)_2$ (in H_2O)

C	5.20734685493248	2.53202204310103	5.96312122943082
C	4.99994456882109	2.38612414893433	4.59987966475271
H	4.14005215850960	1.84818731994390	4.23335116288891
C	5.91448765679564	2.92882020135170	3.70535468341319
H	5.76023702362576	2.81368653568416	2.64129047628870
C	7.01807307419866	3.61007184239561	4.19409120804136
H	7.75627133033742	4.04620549124652	3.53768051976108
C	7.16460524945558	3.72470957883690	5.56615200165339
H	8.01015091723911	4.24646979222259	5.98995105667574
C	4.26849183959731	1.94871326630662	6.94860808132200
C	4.18463372270375	1.89161814141823	10.39702913533745
C	2.45613241836350	0.44372787336345	11.52887328601875
C	2.06355947977849	0.07176490831611	12.82252879168688
H	2.54849041524360	0.52336516780961	13.67971082772760
C	1.07142350795182	-0.87685918539600	13.01773456065799

H	0.76750478786276	-1.17390219549833	14.01262910336933
C	0.47666102306429	-1.44452392204397	11.90437442848412
C	0.82817159810500	-1.09086405197281	10.61845975097666
H	0.33546024187955	-1.55276111852402	9.77311915373768
C	1.82182652606729	-0.13542347723585	10.42601335061606
H	2.10829253071298	0.15547664816648	9.43133837676755
C	3.09500751916308	1.16783920824089	6.47565162376289
H	2.56128454217753	0.72779217823075	7.31020796431898
H	3.41037478489736	0.36845450679450	5.80298132189661
H	2.40732817057355	1.81087597173667	5.92089443750587
C	3.87936089068897	6.89267645904508	9.36969245119228
H	3.79064091645758	7.22750494685630	8.33772473036070
H	3.62861611027317	7.69204955829314	10.06472650692328
H	3.25129345609081	6.02697993015519	9.56552111393354
C	6.43658573975877	7.95131223472864	9.28181820176793
H	7.50223698084748	7.78787843468703	9.42302688081458
H	6.08451321740994	8.71509599079191	9.97273256548803
H	6.20606240693739	8.21491990979911	8.25131256175337
N	6.28865329971138	3.20254243345311	6.42752564648923
N	4.55658821943138	2.16325737217429	8.18906853050278
N	3.78166588980604	1.64261979123661	9.17234810031886
N	3.50322239717811	1.38612552432579	11.45154589181924
O	5.97751984825755	5.45339486683721	8.48157898203873
F	-0.49276638232111	-2.39052805764435	12.08463569432479
S	5.59885995700963	2.86874029116189	10.90893995748114
S	5.59248530512604	6.40849267133076	9.70743688241053
In	6.37547379618771	3.29690323476810	8.58988082477927
H	3.87229996991266	1.66170918036134	12.35057087380540
O	7.54500261653287	1.32871530790780	8.49320198216556
H	8.18334879320446	1.14511753191966	7.78957207606299
H	7.86626822103515	0.86981687958549	9.28222872800266
O	8.49261940298247	4.00478385340294	8.54123182571270
H	8.55321553054906	4.95188987400083	8.73369603001724
H	9.13053372987536	3.56087698639306	9.11893245974282

Compound 3a-(H_2O) (in H_2O)

C	3.51680023207552	3.54712127313912	9.41121857649564
C	3.80961690213702	2.34455006727815	10.03887187309057
H	3.52198853765675	1.40899546264673	9.58591352353413
C	4.47998631079183	2.35452724741672	11.25503914342074
H	4.72084865532626	1.42250575993149	11.74770384935536
C	4.83520374231235	3.56718550362934	11.82398126443979
H	5.35888176572074	3.62304389590875	12.76669205428210
C	4.50863804414692	4.73044253149196	11.14660469838798
H	4.77309599063378	5.69984895483710	11.54736533794330
C	2.81207290064013	3.57295902428140	8.11135096730527
C	1.97288182893703	6.07501194941972	5.90508150481974
C	0.11520524433858	5.68824010541302	4.24756169880811
C	-0.46142607183169	4.52456214472424	4.76297867521510
H	-0.01426835990484	4.02493508348744	5.60521712791281
C	-1.62331592009912	4.01265523555347	4.19503544479828
H	-2.07242379428416	3.11974626521970	4.60799146559031
C	-2.20340914759896	4.65787881250958	3.11596981163897
C	-1.63162867975619	5.79943238734109	2.57006928764121
H	-2.08532298113301	6.29578907669476	1.72344814174927
C	-0.47574072984957	6.30855579599781	3.13798837281064
H	-0.03024247953679	7.20511013862515	2.72368679156760
C	2.40758532737939	2.29395313645061	7.46836929758578
H	3.27907659612438	1.65658251884046	7.30642797932389
H	1.71524288478207	1.74131271730124	8.10718377777704
H	1.92719123835141	2.47781291408253	6.51321987394212
C	-0.77671779553063	8.11227089351181	9.88493452542905
H	-0.44786986276614	8.82304254300134	9.13108745040883
H	-1.37216229028374	8.62187334494888	10.64078884776543
H	-1.32670503274580	7.28811925931521	9.43515751895518
C	-0.05395538791543	6.23580397068892	11.78515121431556
H	-0.66768935372458	5.56453080042370	11.18760935243031
H	-0.65129192065540	6.77049112604784	12.52199421096747
H	0.74998118169442	5.69521158775027	12.27904491739776
N	3.86885284638503	4.72276881729457	9.97721318098690

N	2.60076633623849	4.74271425026588	7.60984699695898
N	1.92707510705401	4.87777995343918	6.43963208402719
N	1.23521678501984	6.34093863724859	4.79563948886272
O	1.38059550263948	6.57323905374726	9.57143833380082
S	2.95590855201759	7.46189008660730	6.44535984328537
S	0.70926451199199	7.46682944233481	10.69615303300111
Cl	4.33276296230801	8.31458422458531	10.08238076341057
Cl	-3.69732691214344	4.01586367764088	2.41767614585373
In	3.37530929984865	6.45716588610064	8.74031702623324
H	1.41653577054879	7.24817107551121	4.39071283084891
O	5.59594742785572	6.07794349124648	8.07503904426475
H	5.66008237920190	6.34599892965982	7.14559509473657
H	6.14548977460149	6.72007409140857	8.55010264662394

Compound 3a-$(H_2O)_2$ (in H_2O)

C	3.56187089086761	3.55177019046314	9.36926311762928
C	3.88661830718979	2.37621360158622	10.03007962330336
H	3.61111362879620	1.42119761714590	9.61143388269609
C	4.57414616348637	2.43867880765310	11.23569242971895
H	4.84003984603434	1.52802452367619	11.75411985444104
C	4.91690506376338	3.67467650583061	11.76110646068027
H	5.45308685769720	3.76942145480912	12.69347605024192
C	4.55714141981216	4.81014590951855	11.05600186908844
H	4.79922570913722	5.79458190988388	11.43108184744497
C	2.84247112652904	3.53306080070760	8.07568949136902
C	1.97380193781071	6.00144430541907	5.84441462802574
C	0.05413449595036	5.65555375293298	4.25444308857238
C	-0.52583109397554	4.50208897845865	4.78778390060041
H	-0.05729263070486	3.98942648476450	5.61047818546666
C	-1.71744168699827	4.01570702058650	4.26044353324972
H	-2.16775151657474	3.12934981660773	4.68575010120254
C	-2.32431673039507	4.67684230328068	3.20563426666447
C	-1.75163913610586	5.81128506194563	2.64541719579013
H	-2.22688512069897	6.32168585647863	1.81931398153795
C	-0.56612637935235	6.29509062084268	3.17256119787049

H	-0.12008043559153	7.18639621013746	2.74767557559336
C	2.45463769888857	2.23630388432855	7.46318701917137
H	3.33613262609062	1.61110419994823	7.30795930922277
H	1.77705963662288	1.68641020237530	8.11981044408487
H	1.96366137088542	2.39306187764509	6.50839795575842
C	-0.85716643955275	8.12821143093946	9.73851101105052
H	-0.54109335808910	8.83559483992140	8.97616259019679
H	-1.44207142140996	8.64004446048821	10.50108641769596
H	-1.41039364719925	7.29851637656718	9.30337934529747
C	-0.08864580614064	6.27716497882782	11.65779809306554
H	-0.71256010184389	5.59514017165178	11.08365240118311
H	-0.67102927889713	6.82154817163259	12.39950018780130
H	0.73038125296176	5.74951560239254	12.14060562235933
N	3.89993244505353	4.75346465068617	9.89425743872383
N	2.60721506780394	4.68998889301587	7.55719926761280
N	1.92050124588053	4.81196683334478	6.39509446179186
N	1.20958358421028	6.28169737690314	4.76044157097373
O	1.30119277364397	6.59048195210890	9.40476384919109
S	3.01165219690286	7.37482368565073	6.34002478268916
S	0.64081859832316	7.49405996874582	10.53224852820660
Cl	-3.85339593996433	4.06577808673629	2.55780629406999
In	3.31900164465249	6.43334229151121	8.63031271929573
H	1.39919091227522	7.18218905157751	4.34389793391503
O	5.63948180469975	6.65564483552483	8.49378730934536
H	5.92902948002047	6.98276735458430	7.62880262590238
H	6.10948757370389	5.81925209919271	8.62279697602430
O	3.85772079593147	7.93491847091143	10.14939390838875
H	4.75303474195072	8.28167322038941	10.01729906827360
H	3.28934826091832	8.69021552766990	10.35833006252107

Compound 4a-(H_2O) (in H_2O)

C	5.56594086245302	9.33464618190398	6.06615048305313
C	5.20333168948630	9.22618299933576	4.73054997391908
H	4.35874163171981	8.62134650132562	4.44173003389041
C	5.93885893277375	9.90214156961464	3.76517920721257

H	5.66097279103158	9.82195004437356	2.72311309446498
C	7.02257122174125	10.67449903930855	4.15243814146714
H	7.62216261849363	11.21765382697230	3.43697252587827
C	7.33263469250284	10.73701839303924	5.50077175178648
H	8.17174868498717	11.32016341780339	5.85510237835281
C	4.80371964163386	8.63098282741860	7.12338263655033
C	5.20630952384706	8.30716581973744	10.53345195696358
C	3.41459725300735	7.12238876798702	11.85969783450579
C	3.09737190732971	6.84914107967898	13.19654978452226
H	3.77895566491938	7.16792714185878	13.97589717754293
C	1.93151379901516	6.18704639638541	13.53585889118212
H	1.70994517566343	5.98681170684017	14.57512171174980
C	1.06002670260268	5.78553877769383	12.52653684537018
C	1.35862242451831	6.04730344688146	11.19521211945803
H	0.68648372291894	5.73513723141380	10.40719980044246
C	2.53050553866506	6.71513186846064	10.85853408214103
H	2.75893374615517	6.92382900417127	9.82839748730948
C	3.59948501847419	7.83862211708278	6.75219057782340
H	2.86398729949314	8.47273260189437	6.25268497988069
H	3.86159570850894	7.03521692003221	6.06065728903288
H	3.14389207726350	7.39838002426832	7.63220844221170
C	5.76889528556339	12.73060059121034	11.28310763407584
H	5.53085588875047	13.63626194175808	11.83944696678089
H	5.14043927600442	11.91471457454837	11.62848983391323
H	6.82346581423287	12.48007935487846	11.37527560597234
C	6.67122064624648	14.18566600848682	9.10756601493906
H	6.52841207036493	15.09072428264463	9.69645161287374
H	7.63605527937291	13.72761636814918	9.31497528303742
H	6.56276517735261	14.41206703298021	8.04960557336242
N	6.62786212822444	10.08759855317959	6.42758123349122
N	5.24643537505940	8.77033950129926	8.32741154774465
N	4.61739359532396	8.16276256442265	9.36698851700282
N	4.62821877217298	7.79510864717833	11.64816972710440
H	5.15834891909253	7.95557928381176	12.49283579620683
O	5.63076898681408	11.70269259477075	8.77238041426616

S	6.76444252214346	9.10172773701513	10.88742915644418
S	5.33184320943488	13.04442177169664	9.54927290236014
Cl	9.14656848913507	11.33767294782936	8.61029910064555
I	-0.67241740766583	4.80932988183764	12.98838481374324
In	7.02653473421875	10.04600451573980	8.56566755147208
O	8.32088966422207	8.16073476672528	8.00430120956656
H	9.24968791811667	8.40682052232996	7.87593071032470
H	8.32717654561423	7.56166635602572	8.76588099196107

Compound 4a-$(H_2O)_2$ (in H_2O)

C	5.52934641444087	9.29415379252906	6.05250530433074
C	5.17489411007992	9.14899080333577	4.71923451987746
H	4.36183148644764	8.49892229536793	4.43786287633098
C	5.87415290968446	9.85446131851334	3.74721790237069
H	5.60104554545849	9.74901742364970	2.70634528039684
C	6.91174458667598	10.69214556136368	4.12604784362477
H	7.47574432593838	11.26441717738406	3.40460156867673
C	7.22387574838933	10.78259212985894	5.47228016962011
H	8.02821455480879	11.41711151790155	5.81701423271617
C	4.79443345503339	8.58436964083031	7.12465254885655
C	5.14891058975504	8.46256054048393	10.55551485702178
C	3.41946019752178	7.22085354926606	11.90528016957905
C	3.06409334730209	7.02461485734234	13.24579559189858
H	3.67380305347144	7.46686399735557	14.02436464459241
C	1.94801690471898	6.28254224268355	13.58901759062031
H	1.69301719685341	6.14623231447439	14.63096897547084
C	1.17042426305912	5.71643556392837	12.58128148502973
C	1.51054477365487	5.89879894986767	11.24647603407161
H	0.91288779476810	5.45864927361264	10.45956194274475
C	2.62779031202166	6.65211463003805	10.90537544251304
H	2.88164283794951	6.80545158821835	9.87169313612432
C	3.66708540222037	7.68348049779412	6.76901777558846
H	2.87873631827058	8.23957089109529	6.25713337258474

H	4.00704793286722	6.89579321981298	6.09377718719318
H	3.24845173571766	7.22135046765269	7.65618208695287
C	5.01651724786012	12.86427084613640	10.97885084584406
H	4.80805681843217	13.78137472178234	11.52812664319241
H	4.09338529624838	12.31034260417510	10.82674728922102
H	5.75979618402402	12.25861646093591	11.49071240049880
C	7.26531055839403	13.95568386123335	9.79424608102374
H	7.13198577975740	14.87227030959082	10.36715024784510
H	7.78285119887271	13.21451172758679	10.40111582180858
H	7.79220371349395	14.18692947682933	8.87149541725335
N	6.55716948271104	10.10104675344367	6.40564228388704
N	5.19918983751321	8.81235341134569	8.32923414285858
N	4.58958657484991	8.22667993113943	9.39016872471653
N	4.57974872962946	7.98470659393448	11.68609873087448
H	5.07182674255475	8.23220514170464	12.53307422784680
O	5.86082765571894	12.00770579624860	8.54378225877687
S	6.66464268682428	9.36230509334217	10.89248605583861
S	5.61439879430679	13.35704755418791	9.33754543533614
I	-0.48557232511828	4.61966307298105	13.05131497850530
In	6.91588621290588	10.13860832641247	8.54186808879056
O	8.51177441568429	8.57915089001695	8.07934286827555
H	8.52436465459828	8.18504559238692	7.19519921305759
H	8.57453810434411	7.84342042876533	8.70566290666654
O	8.83164025954061	11.27953244217196	8.39417799437597
H	9.03203627804377	12.10461352185107	8.85792451257776
H	9.61032998470113	10.70994887743732	8.48572862414198

Structure Activity Relationships results

Table S3. Correlation Matrix between the IC_{50} data obtained for the HL-60 cell line and the Stereo-Electronic properties of the unsubstituted complexes **1a-4a**

	HL-60	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	V (Å^3)	LogP
HL-60	1							
EHOMO (eV)	0.85252	1						
ELUMO (eV)	0.71493	0.61920	1					
ΔE (eV)	-0.80818	-0.98911	-0.49692	1				
μ (D)	-0.95034	-0.97191	-0.66178	0.95009	1			
SA (Å^2)	0.78523	0.35626	0.44092	-0.31109	-0.56610	1		
V (Å^3)	0.80951	0.48057	0.27149	-0.48023	-0.65963	0.94293	1	
LogP	0.45428	0.01164	-0.05658	-0.02347	-0.22699	0.86962	0.88166	1

Table S4. Correlation Matrix between the IC_{50} data obtained for the HL-60 cell line and the Stereo-Electronic properties of the monoaqua derivatives of complexes **1a-4a**

	HL-60	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	V (Å^3)	LogP
HL-60	1							
EHOMO (eV)	0.94963	1						
ELUMO (eV)	0.54021	0.77187	1					
ΔE (eV)	-0.98249	-0.99035	-0.67628	1				
μ (D)	0.31716	0.10257	-0.23886	-0.17092	1			
SA (Å^2)	0.86984	0.67746	0.05636	-0.77264	0.48001	1		
V (Å^3)	0.81974	0.60815	0.02303	-0.69960	0.73207	0.94593	1	
LogP	0.52521	0.23446	-0.39469	-0.35771	0.78121	0.84115	0.90937	1

Table S5. Correlation Matrix between the IC_{50} data obtained for the HL-60 cell line and the Stereo-Electronic properties of the diaqua derivatives of complexes **1a-4a**

	HL60	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	V (Å^3)	LogP
HL-60	1							
EHOMO (eV)	0.94318	1						
ELUMO (eV)	-0.95173	-0.85460	1					
ΔE (eV)	-0.94782	-0.99986	0.86332	1				
μ (D)	0.94383	0.82184	-0.85300	-0.82665	1			
SA (Å^2)	0.67729	0.39721	-0.70766	-0.40922	0.81783	1		
V (Å^3)	0.78568	0.54021	-0.78938	-0.55087	0.90001	0.98640	1	
LogP	0.53038	0.21903	-0.62811	-0.23345	0.66204	0.96913	0.92177	1

Table S6. Correlation Matrix between the IC_{50} data obtained for the HL-60 cell line and the Stereo-Electronic properties of the free-ligands (*E*-configuration).

	HL-60	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	LogP
HL-60	1						
EHOMO (eV)	-0.00707	1					
ELUMO (eV)	0.49223	-0.78852	1				
ΔE (eV)	0.28732	-0.93496	0.95541	1			
μ (D)	-0.73107	0.67153	-0.93811	-0.86354	1		
SA (Å^2)	0.49199	0.57908	-0.45845	-0.54248	0.12335	1	
LogP	0.58714	0.17648	-0.14951	-0.17097	-0.19322	0.90460	1

Table S7. Correlation Matrix between the IC_{50} data obtained for *Candida* strains and the Stereo-Electronic properties of the free-ligands (*E*-configuration)

	C. Albicans	*C. Parapsilosis*	*C. Lusitaniae*	*C. Dubliniensis*	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	LogP
C. Albicans	1									
C. Parapsilosis	0.81784	1								
C. Lusitaniae	0.17015	0.68870	1							
C. Dubliniensis	0.59543	0.94744	0.88292	1						
EHOMO (eV)	0.72881	0.21430	-0.55072	-0.10905	1					
ELUMO (eV)	-0.32724	0.25114	0.73642	0.50623	-0.78852	1				
ΔE (eV)	-0.53868	0.04197	0.68920	0.34436	-0.93496	0.95541	1			
μ (D)	0.04032	-0.53901	-0.91765	-0.76408	0.67153	-0.93811	-0.86354	1		
SA (Å^2)	0.87252	0.69124	0.22973	0.52338	0.57908	-0.45845	-0.54248	0.12335	1	
LogP	0.66709	0.71341	0.55861	0.67974	0.17648	-0.14951	-0.17097	-0.19322	0.90460	1

Table S8. Correlation Matrix between the IC_{50} data obtained for *Candida* strains and the Stereo-Electronic properties of the complexes (**1a-4a**)

	C. Albicans	*C. Parapsilosis*	*C. Lusitaniae*	*C. Dubliniensis*	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	V (Å^3)	LogP
C. Albicans	1										
C. Parapsilosis	0.04703	1									
C. Lusitaniae	-0.58444	0.52147	1								
C. Dubliniensis	-0.03706	-0.80652	-0.06815	1							
EHOMO (eV)	-0.62131	0.23511	0.94885	0.24586	1						
ELUMO (eV)	0.22495	0.23782	0.55918	0.36851	0.61921	1					
ΔE (eV)	0.72880	-0.21527	-0.94384	-0.20265	-0.98911	-0.49692	1				
μ (D)	0.52105	-0.45228	-0.98927	-0.05309	-0.97191	-0.66178	0.95009	1			
SA (Å^2)	0.09064	0.97665	0.60745	-0.66343	0.35626	0.44092	-0.31109	-0.56610	1		
V (Å^3)	-0.23182	0.95461	0.73205	-0.70541	0.48057	0.27149	-0.48023	-0.65963	0.94293	1	
LogP	0.03495	0.95478	0.32658	-0.94573	0.01164	-0.05658	-0.02347	-0.22699	0.86962	0.88166	1

Table S9. Correlation Matrix between the IC_{50} data obtained for *Candida* strains and the Stereo-Electronic properties of the monoaqua derivatives of complexes (**1a-4a**)

	C. Albicans	*C. Parapsilosis*	*C. Lusitaniae*	*C. Dubliniensis*	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	V (Å^3)	LogP
C. Albicans	1										
C. Parapsilosis	0.04703	1									
C. Lusitaniae	-0.58444	0.52147	1								
C. Dubliniensis	-0.03706	-0.80652	-0.06815	1							
EHOMO (eV)	-0.36512	0.41329	0.94287	0.15422	1						
ELUMO (eV)	-0.52944	-0.24886	0.67466	0.68398	0.77187	1					
ΔE (eV)	0.30761	-0.53310	-0.94535	-0.02955	-0.99035	-0.67628	1				
μ (D)	-0.56966	0.64163	0.41579	-0.80013	0.10257	-0.23886	-0.17092	1			
SA (Å^2)	-0.00429	0.94437	0.71636	-0.56941	0.67746	0.05636	-0.77264	0.48001	1		
V (Å^3)	-0.26182	0.94411	0.75152	-0.69011	0.60815	0.02303	-0.69960	0.73207	0.94593	1	
LogP	-0.03217	0.96835	0.41082	-0.92127	0.23446	-0.39469	-0.35771	0.78121	0.84115	0.90937	1

Table S10. Correlation Matrix between the IC_{50} data obtained for *Candida* strains and the Stereo-Electronic properties of the diaaqua derivatives of complexes (**1a-4a**)

	C. Albicans	*C. Parapsilosis*	*C. Lusitaniae*	*C. Dubliniensis*	EHOMO (eV)	ELUMO (eV)	ΔE (eV)	μ (D)	SA (Å^2)	V (Å^3)	LogP
C. Albicans	1										
C. Parapsilosis	0.04703	1									
C. Lusitaniae	-0.58444	0.52147	1								
C. Dubliniensis	-0.03706	-0.80652	-0.06815	1							
EHOMO (eV)	-0.32023	0.40076	0.92396	0.17959	1						
ELUMO (eV)	0.00163	-0.78387	-0.80224	0.26586	-0.85460	1					
ΔE (eV)	0.31126	-0.41517	-0.92424	-0.16581	-0.99986	0.86332	1				
μ (D)	-0.49821	0.74362	0.95356	-0.36217	0.82184	-0.85300	-0.82665	1			
SA (Å^2)	-0.21562	0.96110	0.60663	-0.82859	0.39721	-0.70766	-0.40922	0.81783	1		
V (Å^3)	-0.28178	0.94327	0.72696	-0.72537	0.54021	-0.78938	-0.55087	0.90001	0.98640	1	
LogP	-0.00475	0.97386	0.40649	-0.91640	0.21903	-0.62811	-0.23345	0.66204	0.96913	0.92177	1

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