Electronic Supplementary Information (ESI)

Neutron activation of In(III) complexes with thiosemicarbazones leads to the production of potential radiopharmaceuticals for the treatment of breast cancer

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Spectroscopic characterization

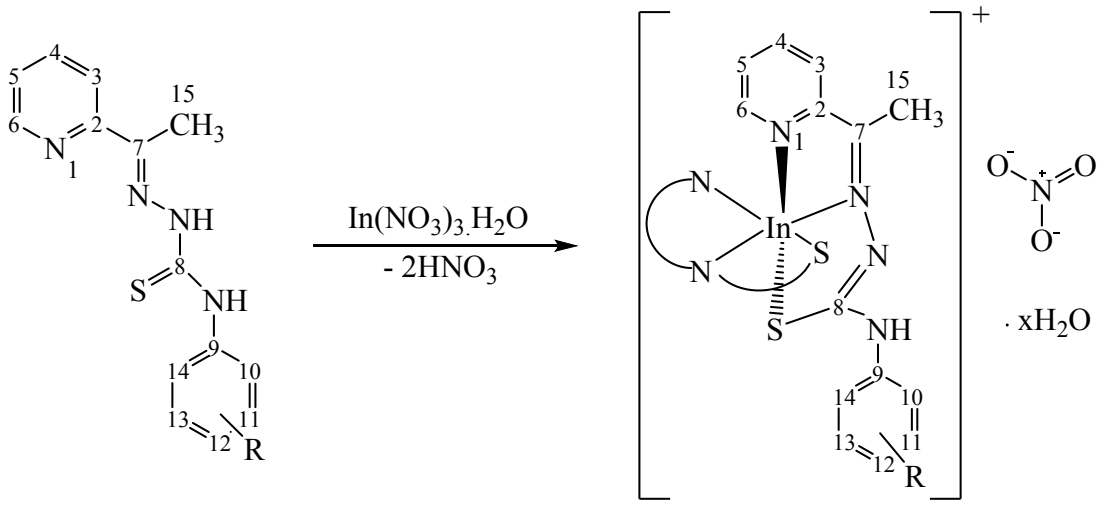

Figure S1. Syntheses of the In(III) complexes with 2-acetylpyridine-derived thiosemicarbazones and carbon atom numbering. R = *o*Cl (**1**) or *p*F (**2**).

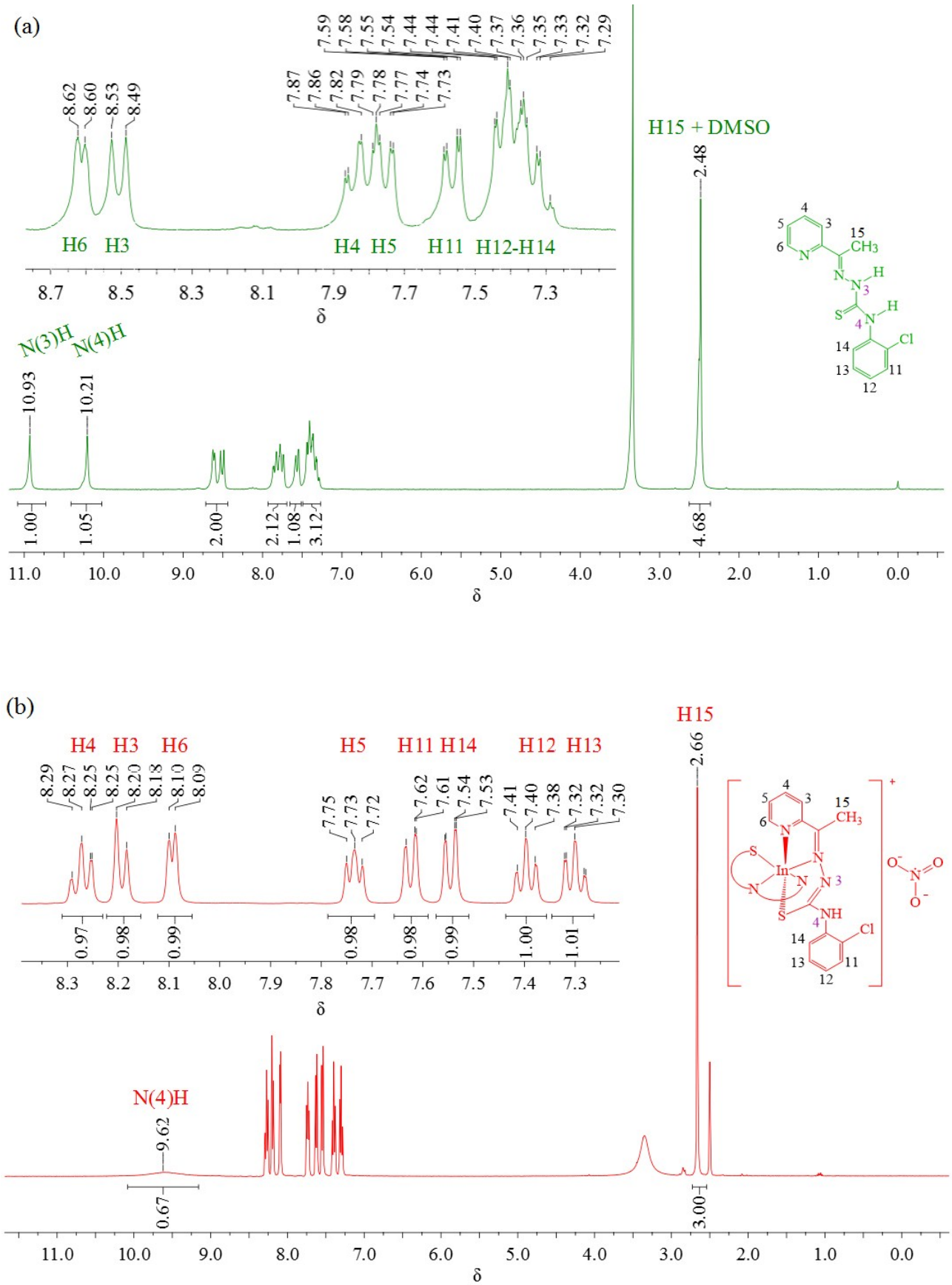

Figure S2. ^{1}H NMR spectra of (a) ligand H2Ac4*o*ClPh and (b) complex **1** (DMSO-d_6).

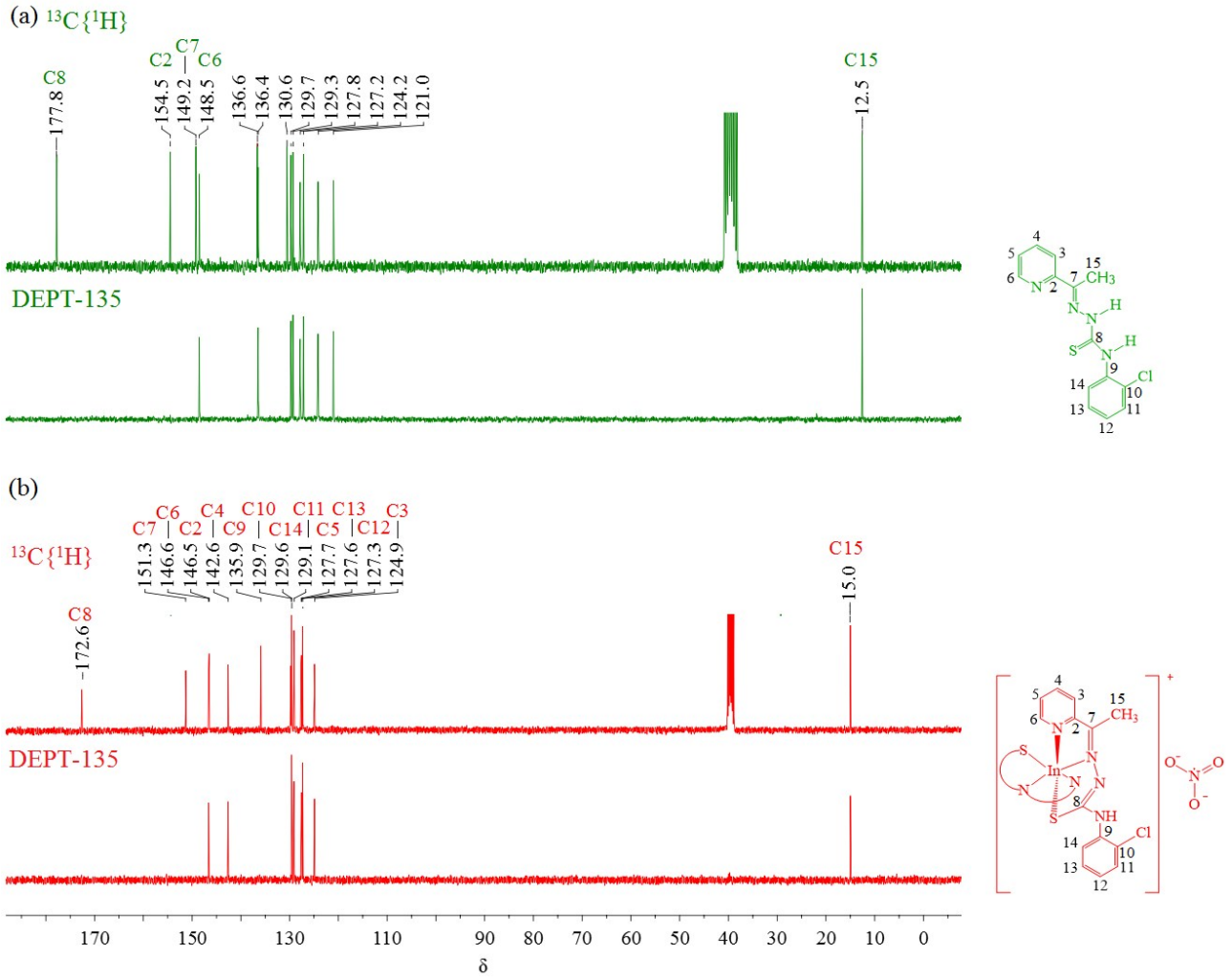

Figure S3. $^{13}C\{^{1}H\}$ NMR and DEPT-135 spectra of (a) ligand H2Ac4*o*ClPh and (b) complex **1** (DMSO-d_6).

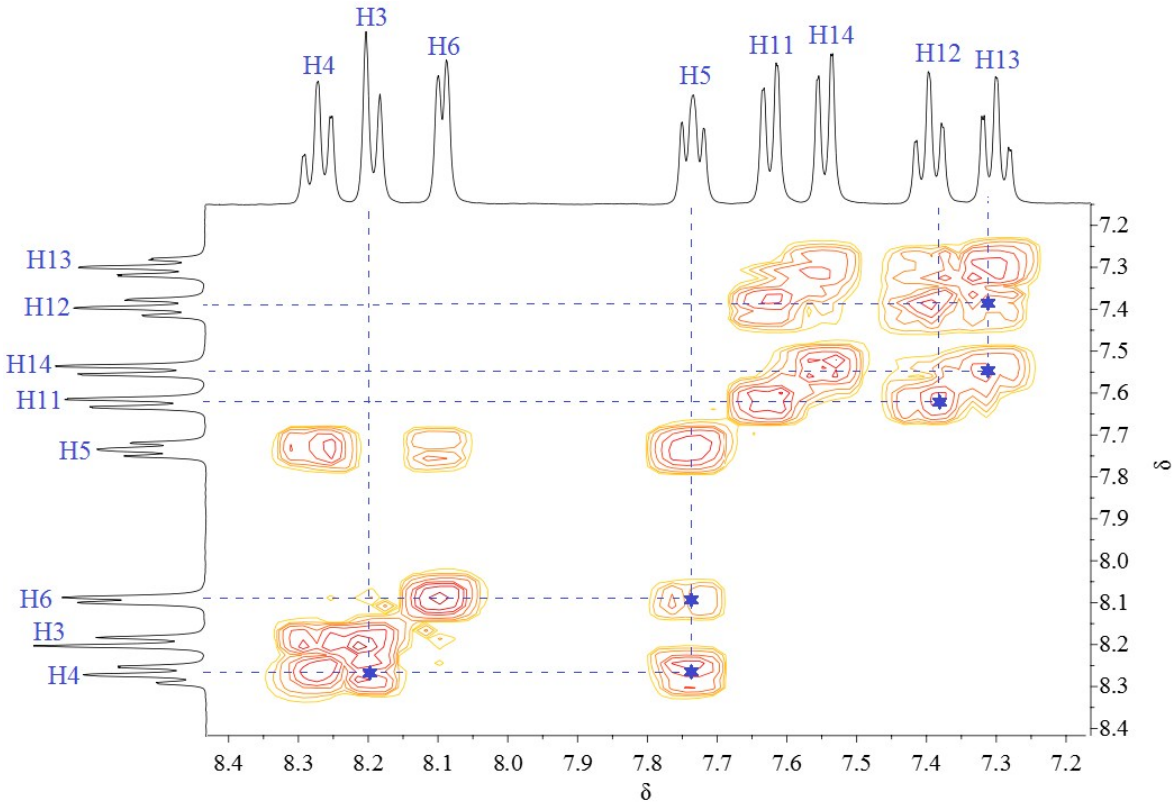

Figure S4. Contour map of 2D COSY experiment of the complex **1** (DMSO-d_6) exhibiting the homonuclear ^{1}H-^{1}H correlations.

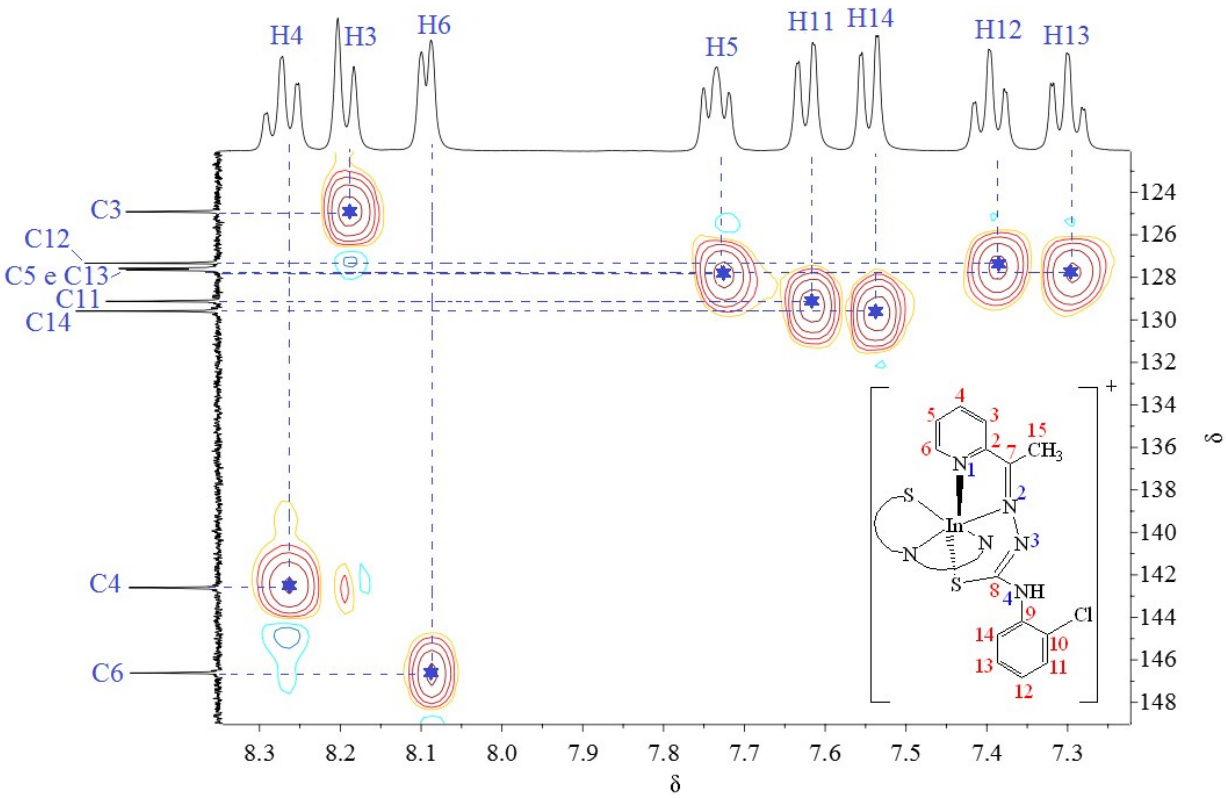

Figure S5. Contour map of 2D HMQC experiment of the complex **1** (DMSO-d_6) exhibiting the most important heteronuclear ^{1}H-^{13}C correlations.

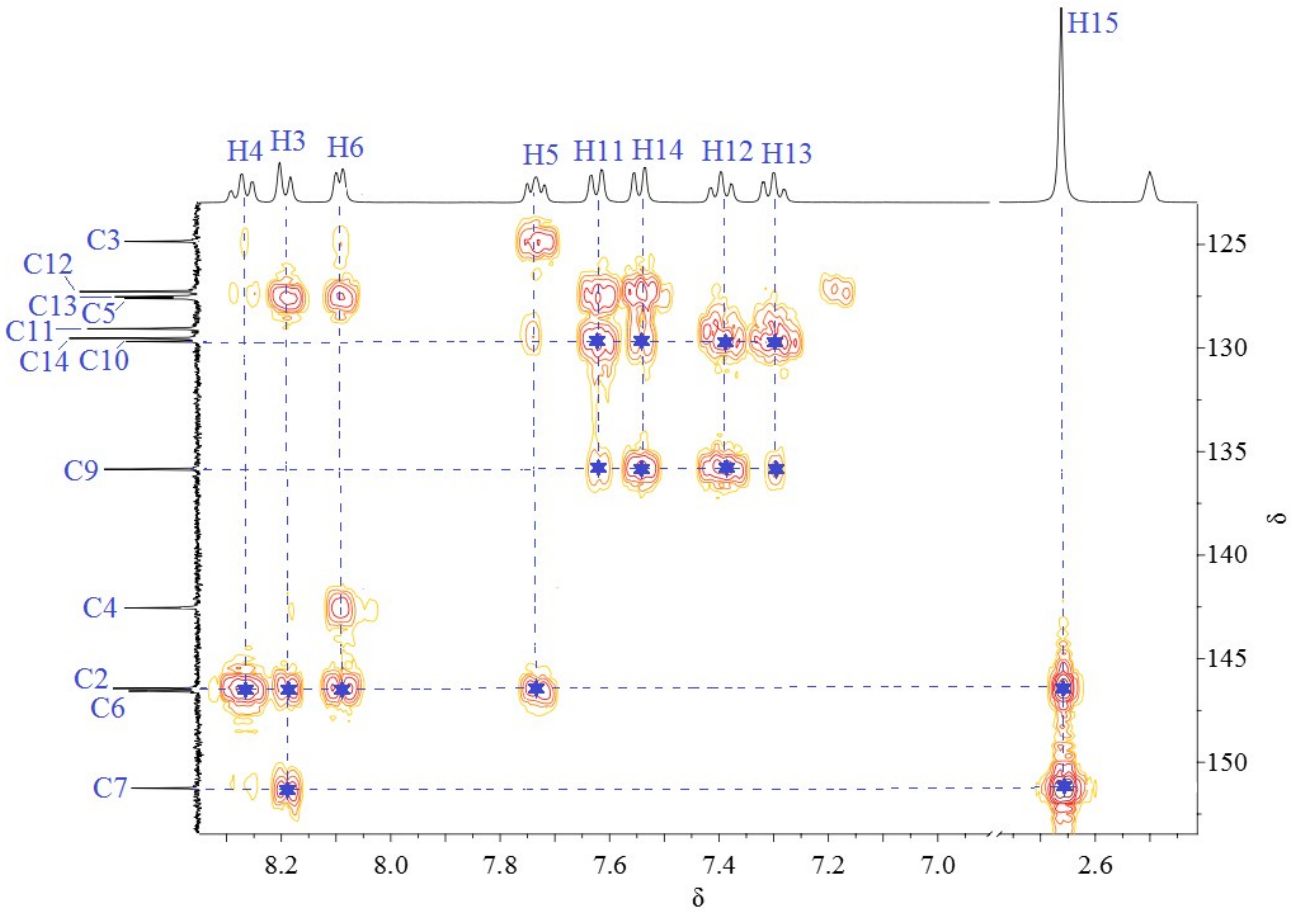

Figure S6. Contour map of 2D HMBC experiment of the complex **1** (DMSO-d_6) exhibiting the most important heteronuclear ^{1}H-^{13}C correlations.

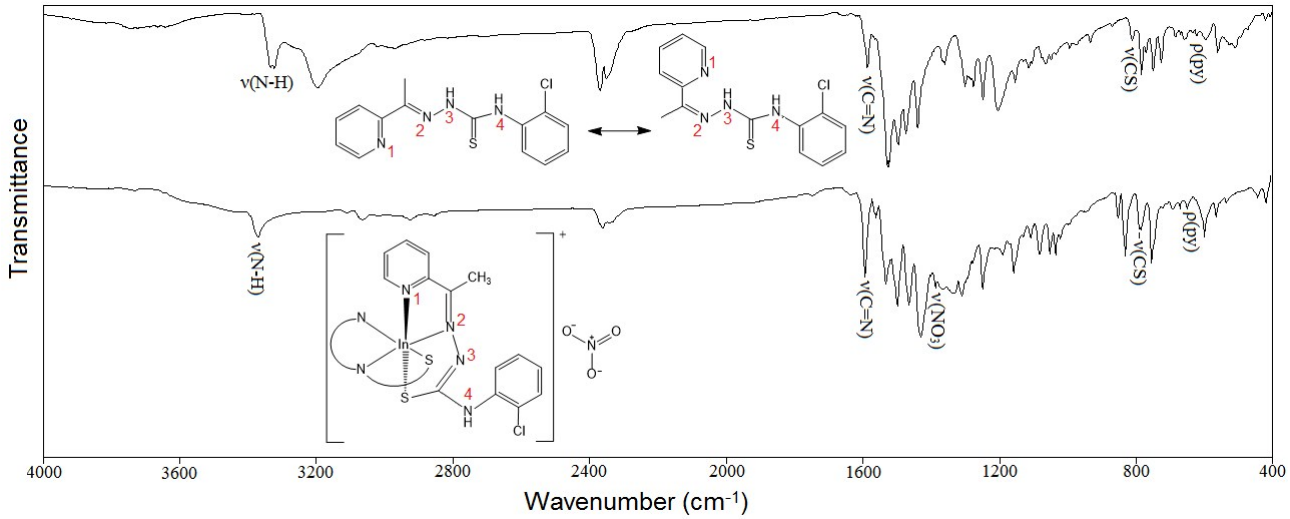

Figure S7. FT-IR spectrum of ligand H2Ac4*o*ClPh and complex **1** (KBr pellet).

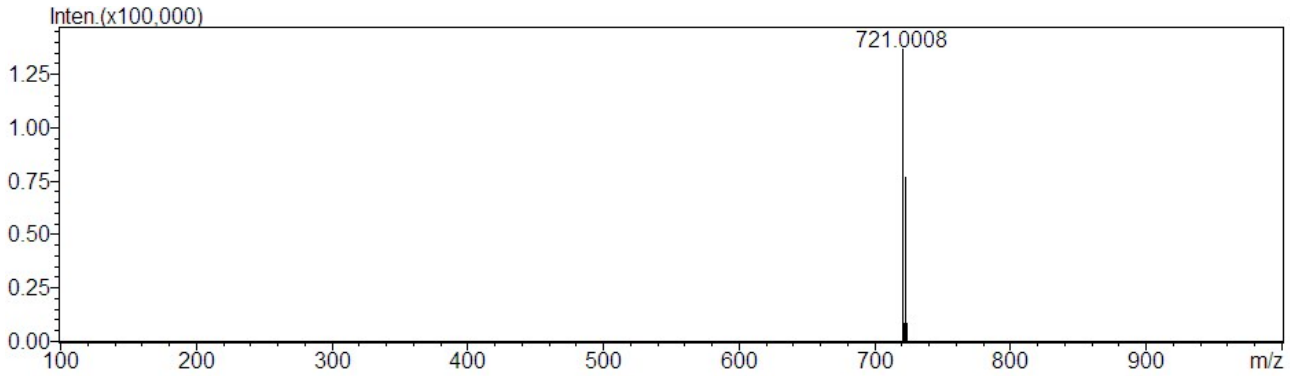

Figure S8. High Resolution Mass Spectra [ESI(+), IT-TOF] of **1**

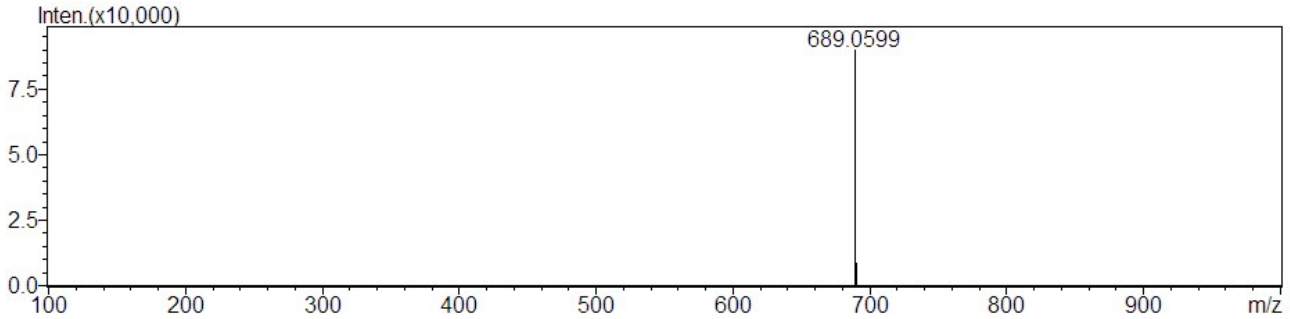

Figure S9. High Resolution Mass Spectra [ESI(+), IT-TOF] of **2**

X-ray crystallography

Table S10. Selected bond lengths (Å) and angles (°) for **1a** in comparison with the parent ligand[1]

Bond	**H2Ac4*o*ClPh**[a]	**1a**[b]
S1–C8	1.654(3)/1.654(3)	1.755(4)/1.756(4)
N2–C7	1.281(3)/1.278(3)	1.292(5)/1.292(4)
N2–N3	1.362(3)/1.361(3)	1.376(4)/1.381(4)
N3–C8	1.359(3)/1.351(3)	1.309(5)/1.315(5)
In1–N1	-	2.287(3)
In1–N2	-	2.264(3)
In1–S1	-	2.5028(10)
In1–N11	-	2.275(3)
In1–N12	-	2.264(3)
In1–S11	-	2.5018(10)
C7–N2–N3	119.1(2)/118.7(2)	117.6(3)/117.7(3)
N2–N3–C8	118.2(2)/118.9(2)	114.1(3)/114.7(3)
N3–C8–S1	121.0(2)/121.5(2)	128.9(3)/128.5(3)
N1–In1–N2	-	71.01(11)
N1–In1–S1	-	145.75(8)
N1–In1–N11	-	84.77(11)
N1–In1–N12	-	97.24(10)
N1–In1–S11	-	97.12(8)
N2–In1–S1	-	77.04(8)
N2–In1–N11	-	106.74(11)
N2–In1–N12	-	168.25(11)
N2–In1–S11	-	103.42(8)
S1–In1–N11	-	93.03(8)
S1–In1–N12	-	114.40(8)
S1–In1–S11	-	102.02(4)
N11–In1–N12	-	71.30(10)
N11–In1–S11	-	148.62(8)
N12–In1–S11	-	77.41(8)

[a] The two values of bond distances and angles in H2Ac4*o*ClPh refer to the two molecules in the asymmetric unit. [b] For **1a** the two values refer to the two ligands coordinated to the metal center.

[1] J. A. Lessa, I. C. Mendes, P. R. O. Silva, M. A. Soares, R. G. Santos, N. L. Speziali, N. C. Romeiro, E. J. Barreiro, H. Beraldo, *Eur. J. Med. Chem.*, 2010, **45(12)**, 5671-5677.

Cytotoxic activity

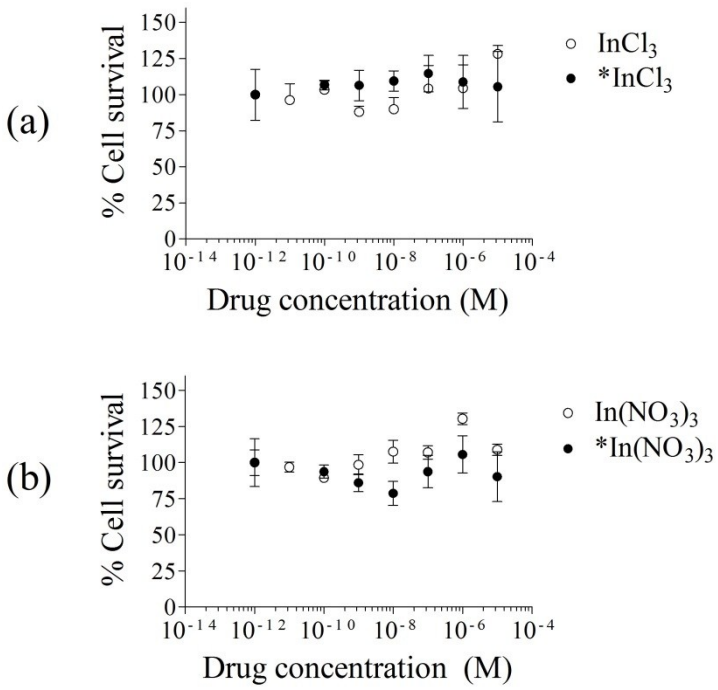

Figure S11. Percentage of cell survival of MCF-7 cells *vs* drug concentration for (a) $InCl_3$ and $*InCl_3$; (b) $In(NO_3)_3$ and $*In(NO_3)_3$

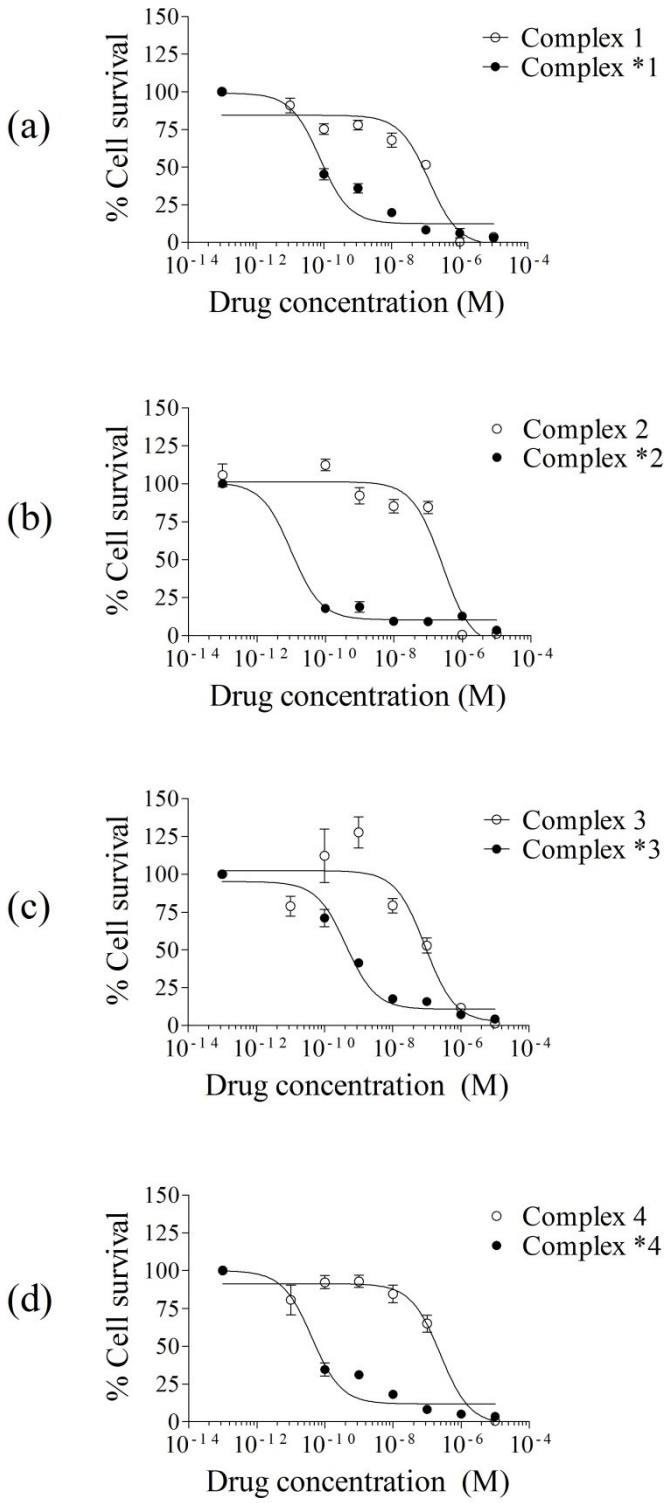

Figure S12. Percentage of cell survival of MCF-7 cells *vs* drug concentration for (a) **1** and ***1**; (b) **2** and ***2**; (c) **3** and ***3**; (d) **4** and ***4**.

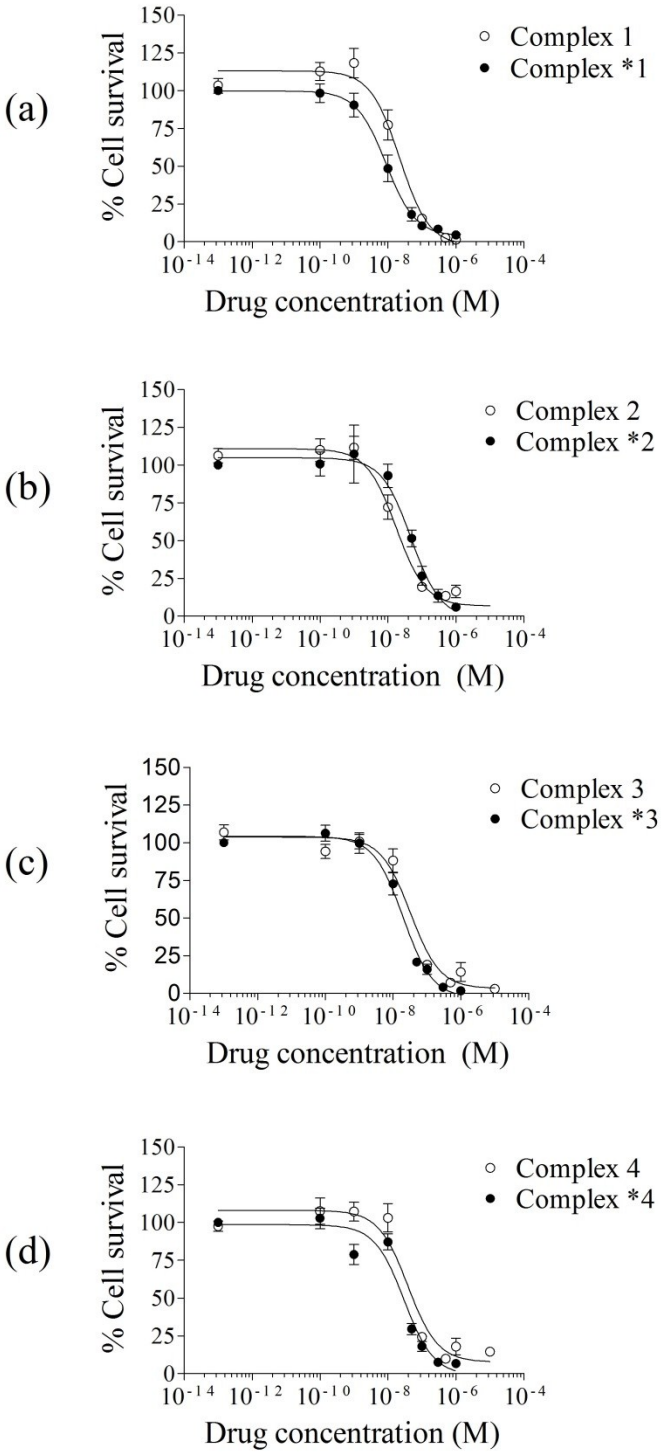

Figure S13. Percentage of cell survival of MRC-5 cells *vs* drug concentration for (a) **1** and ***1**; (b) **2** and ***2**; (c) **3** and ***3**; (d) **4** and ***4**.