

# Supplementary Materials for

## Polypyridyl Zinc(II)-Indomethacin Complexes with Potent Antibreast Cancer Stem Cell Activity

Tiffany K. Rundstadler, Arvin Eskandari, Sarah M. Norman, and Kogularamanan Suntharalingam\*

Department of Chemistry, King's College London, London, SE1 1DB, United Kingdom;  
tiffany.rundstadler@etu.unistra.fr (T.K.R.); arvin.eskandari@kcl.ac.uk (A.E.);  
sarah.norman@kcl.ac.uk (S.M.N.)

\* Correspondence: kogularamanan.suntharalingam@kcl.ac.uk; Tel.: +44-207-848-2595

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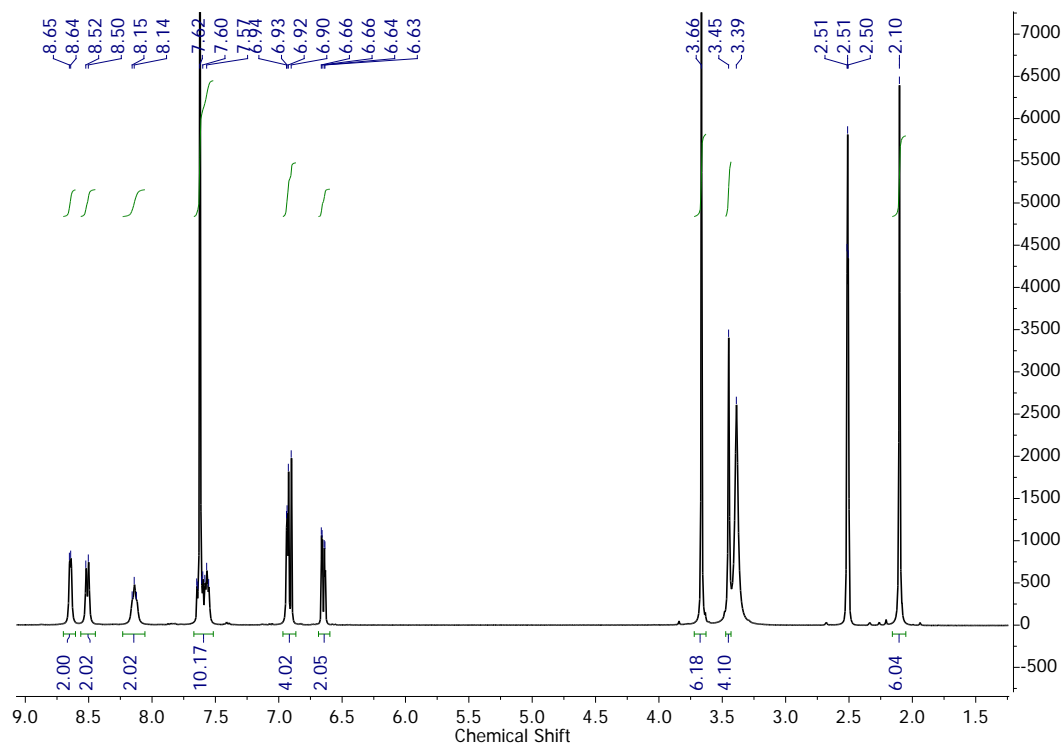


Figure S1.  $^1\text{H}$  NMR spectrum of **2** in  $\text{DMSO-d}_6$ .

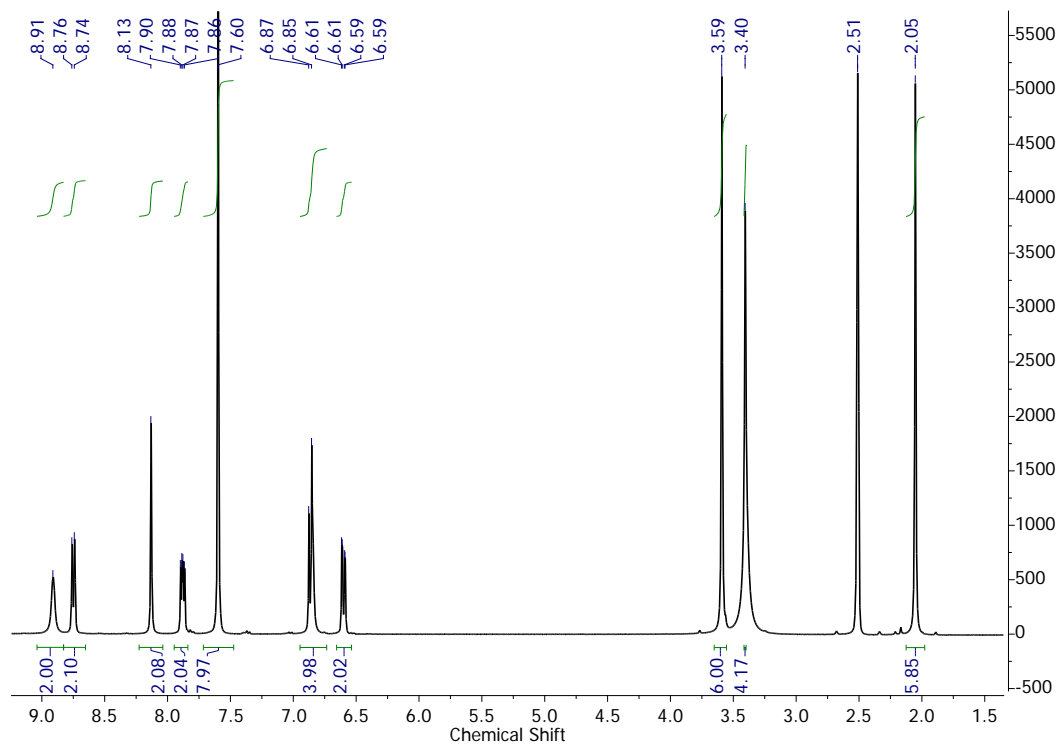


Figure S2.  $^1\text{H}$  NMR spectrum of **3** in  $\text{DMSO-d}_6$ .

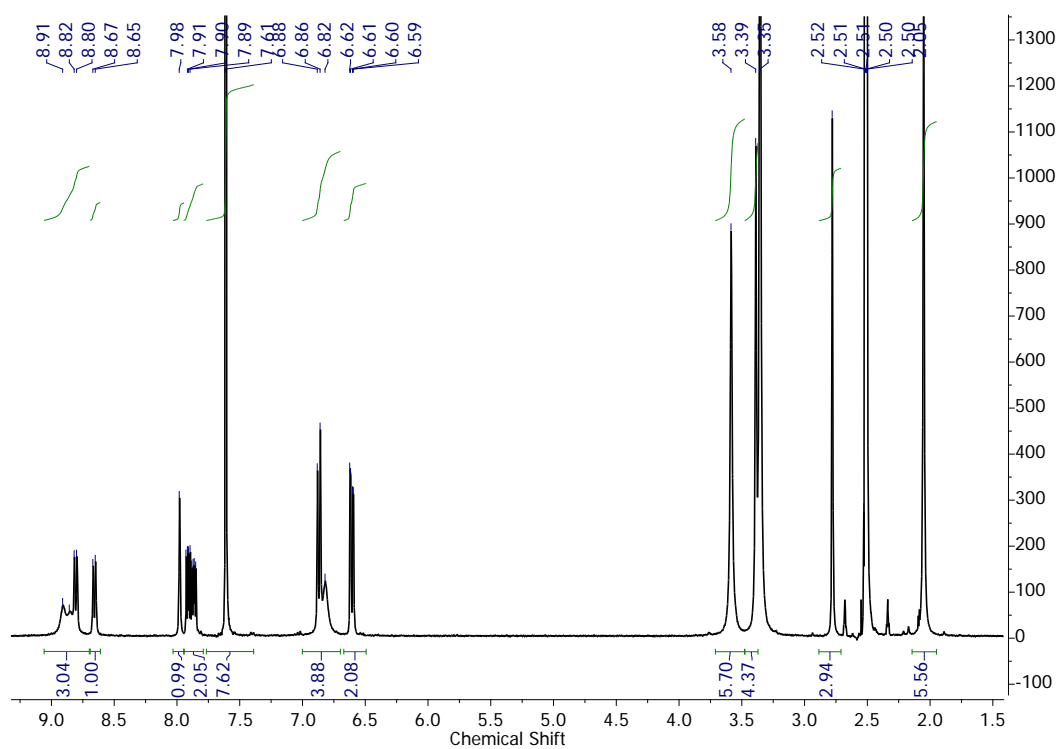


Figure S3.  $^1\text{H}$  NMR spectrum of **4** in  $\text{DMSO-d}_6$ .

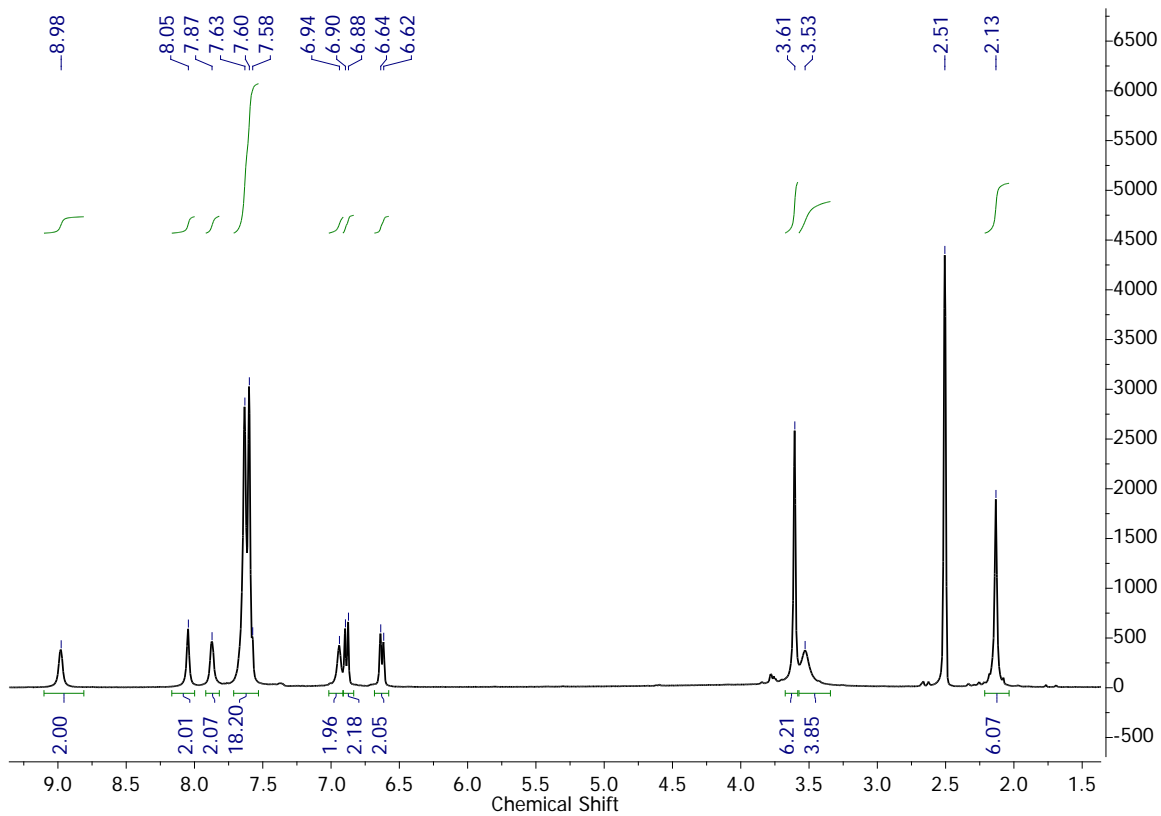
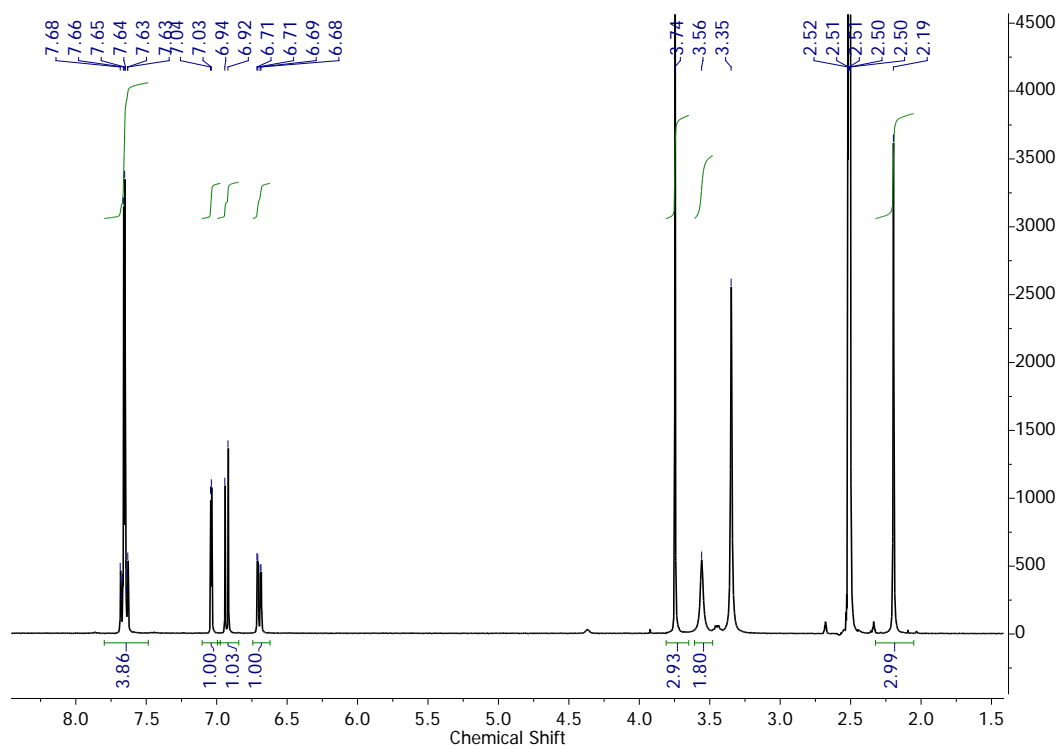
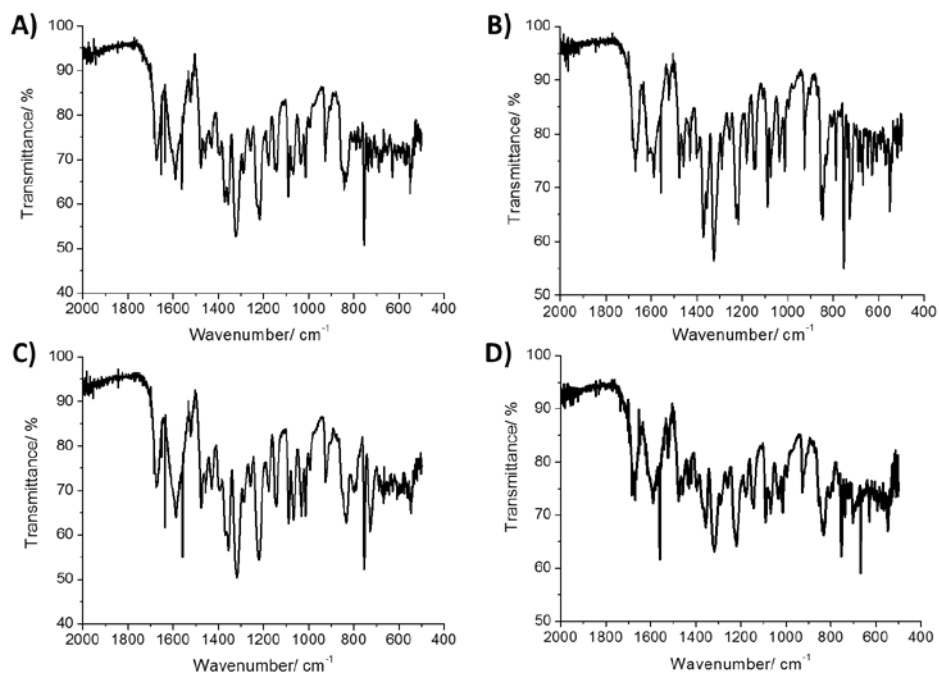


Figure S4.  $^1\text{H}$  NMR spectrum of **5** in  $\text{DMSO-d}_6$ .



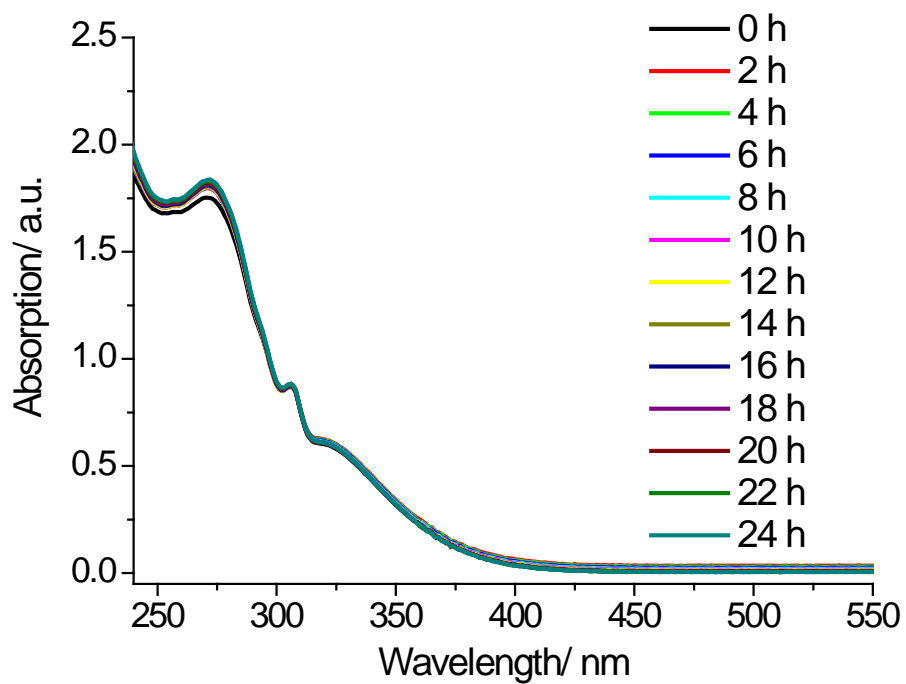
**Figure S5.**  $^1\text{H}$  NMR spectrum of **1** in  $\text{DMSO-d}_6$ .



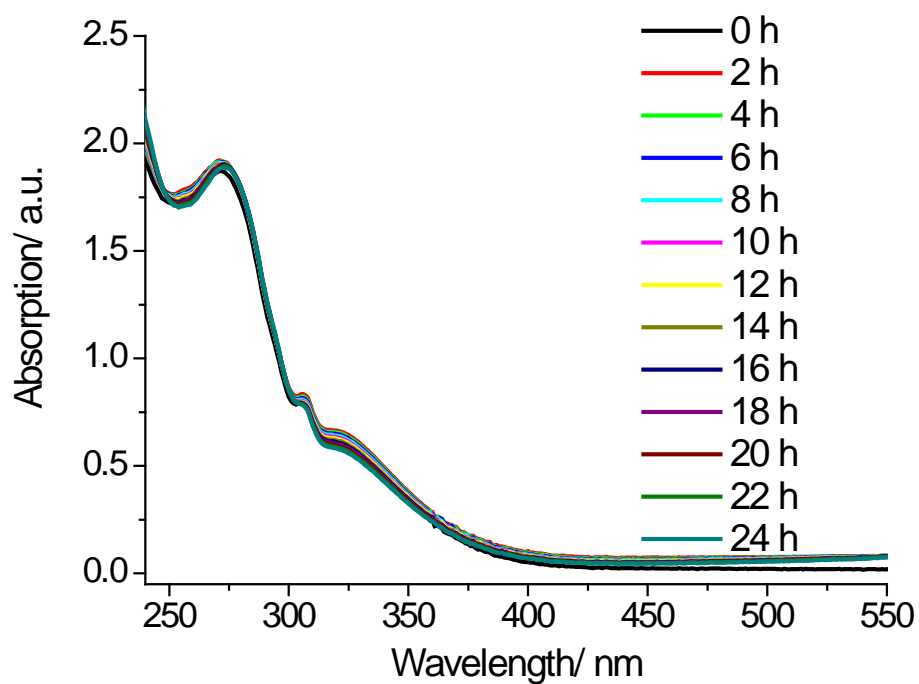
**Figure S6.** IR spectrum of (A) **2**, (B) **3**, (C) **4**, and (D) **5** in the solid form.

**Table S1.** Experimentally determined  $\text{Log}P$  values for 2–5.

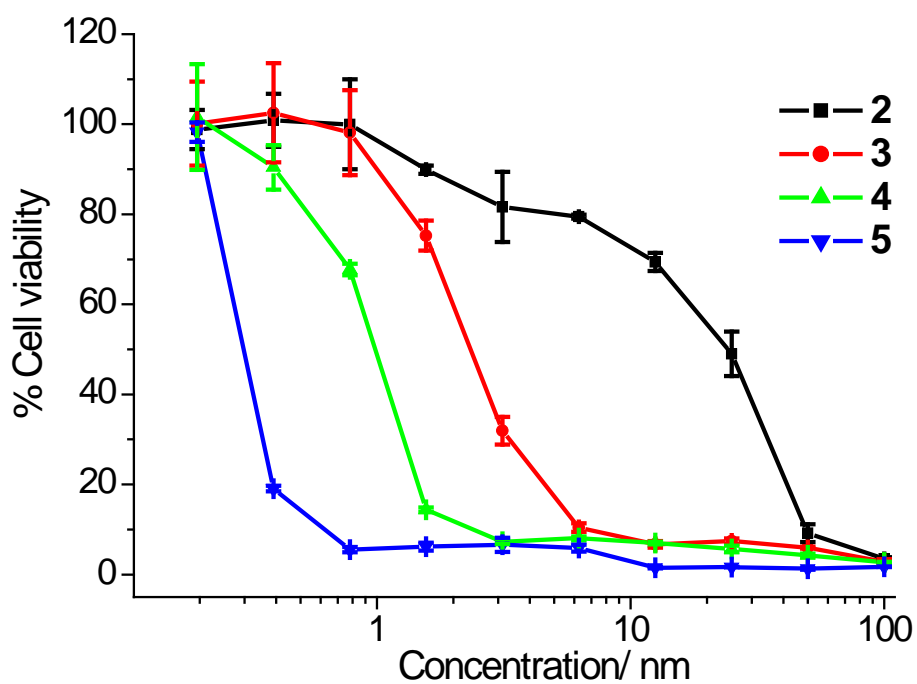
Zn(II) Complex	$\text{Log}P$
2	0.89
3	0.97
4	1.24
5	1.67



**Figure S7.** UV-Vis spectrum of 2 (50 μM) in PBS:DMSO (200:1) over the course of 24 h at 37 °C.



**Figure S8.** UV-Vis spectrum of **2** (50  $\mu$ M) in mammary epithelial cell growth medium (MEGM):DMSO (200:1) over the course of 72 h at 37  $^{\circ}$ C.



**Figure S9.** Representative dose response curves of **2–5** against HEK 293T cells after 72 h incubation.