

Supporting Information

Oestradiol Post-Functionalized Gold(I) Bis(1,2,3-triazol-5-ylidene) Complex Exhibits high Activity for ER α -Positive Breast Cancer Cells (MCF-7)

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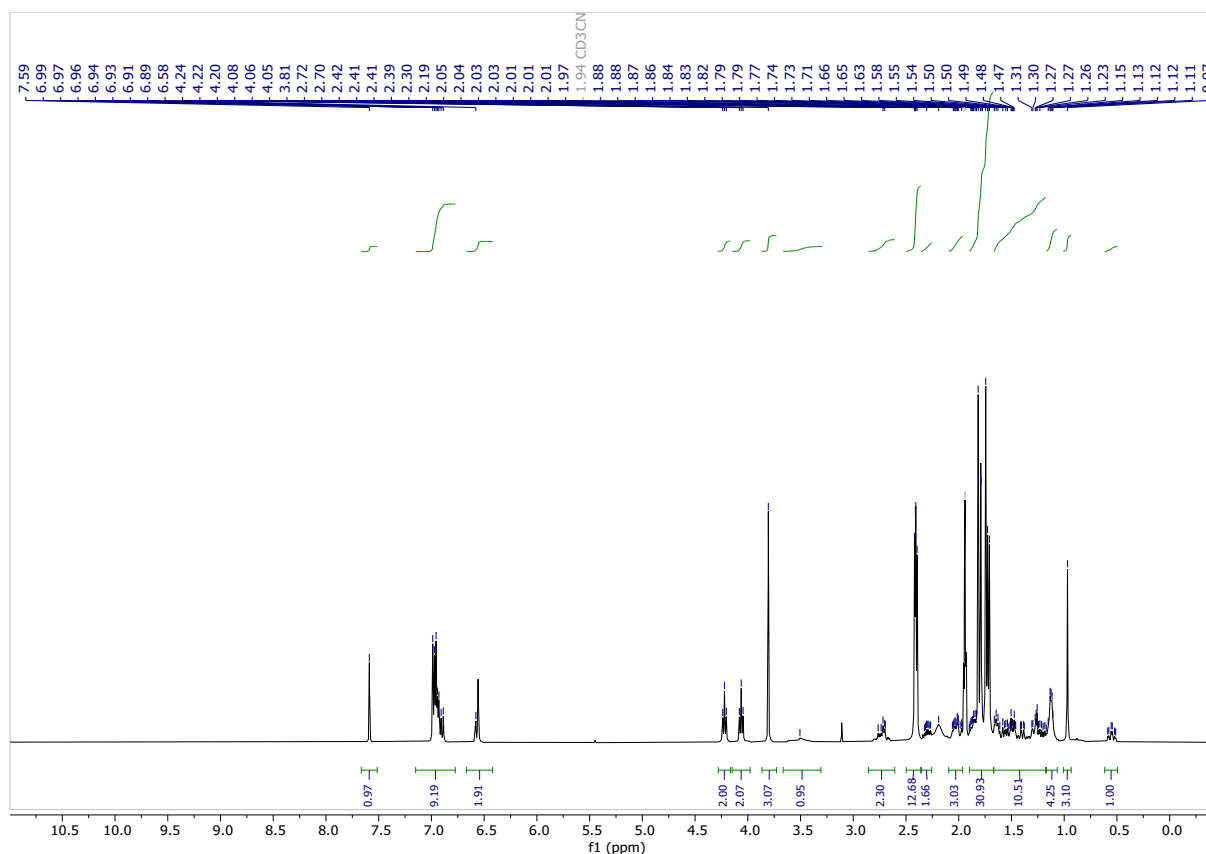


Figure S1: ¹H-NMR spectrum of 5 in acetonitrile-*d*₃.

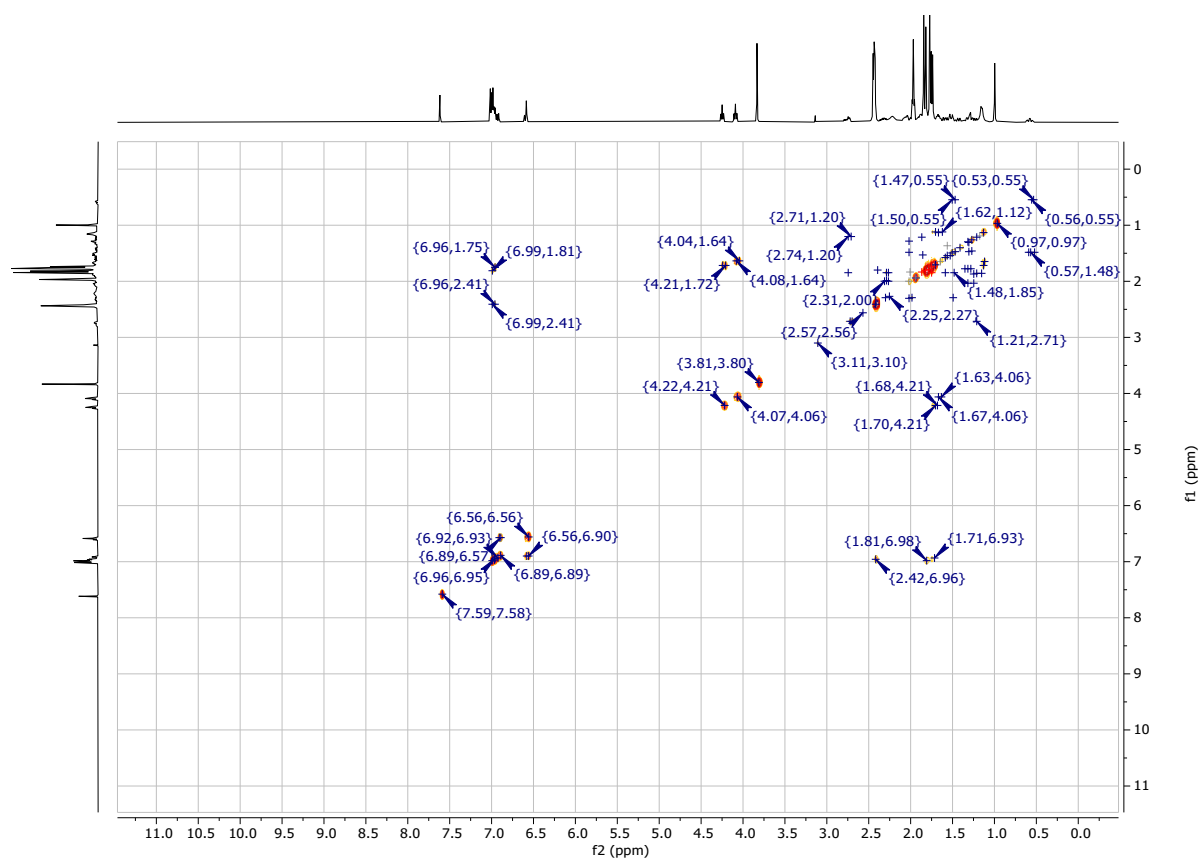


Figure S2: ^1H - ^1H -COSY NMR spectrum of complex **5** in acetonitrile- d_3 .

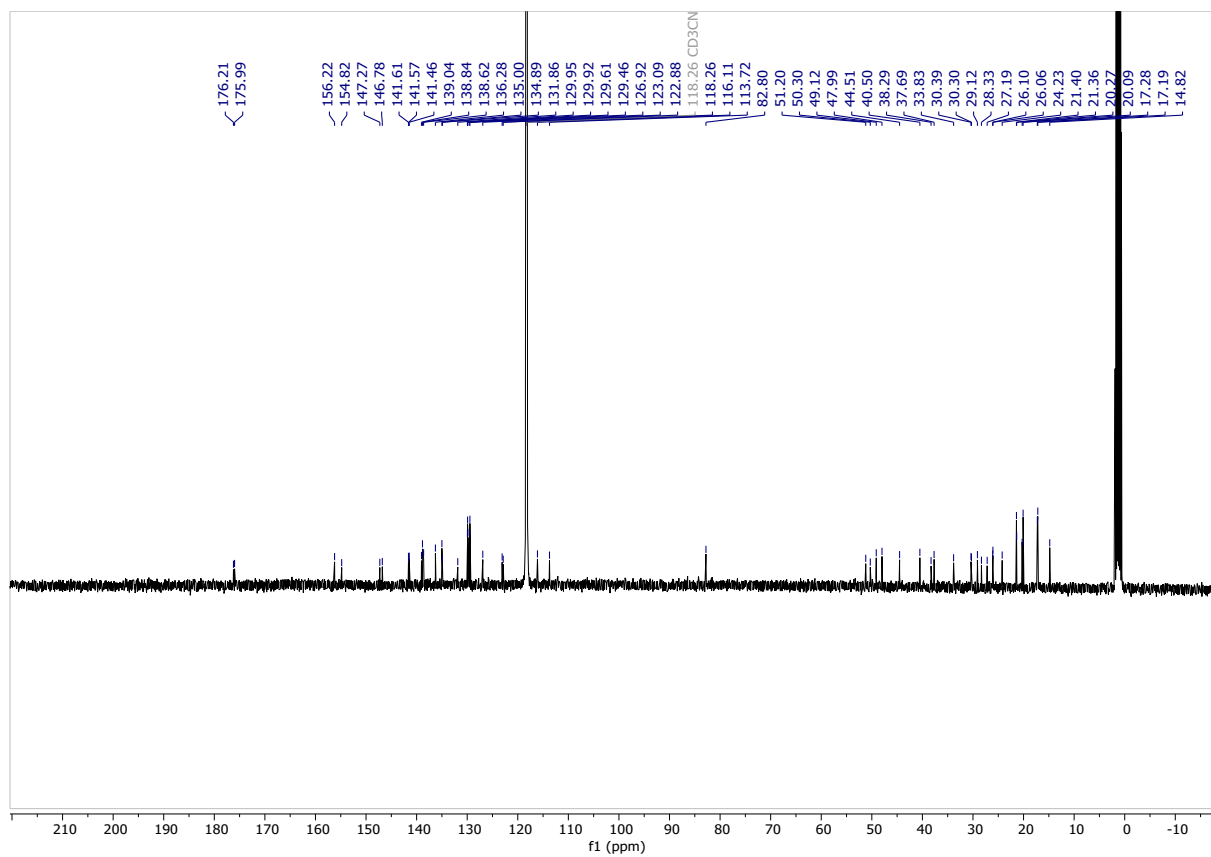


Figure S3: ^{13}C -NMR spectrum of complex **5** in acetonitrile- d_3 .

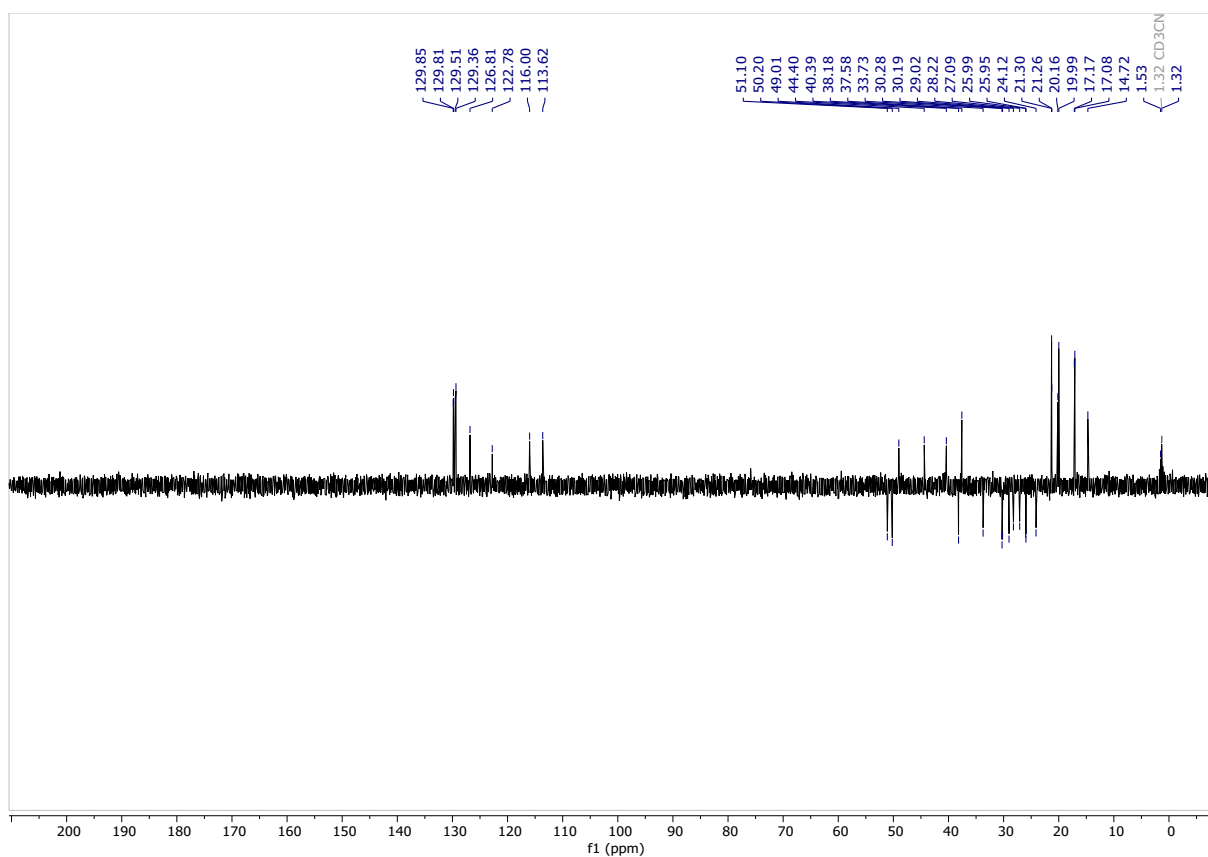


Figure S4: DEPT-135 NMR spectrum of complex **5** in acetonitrile-*d*₃.

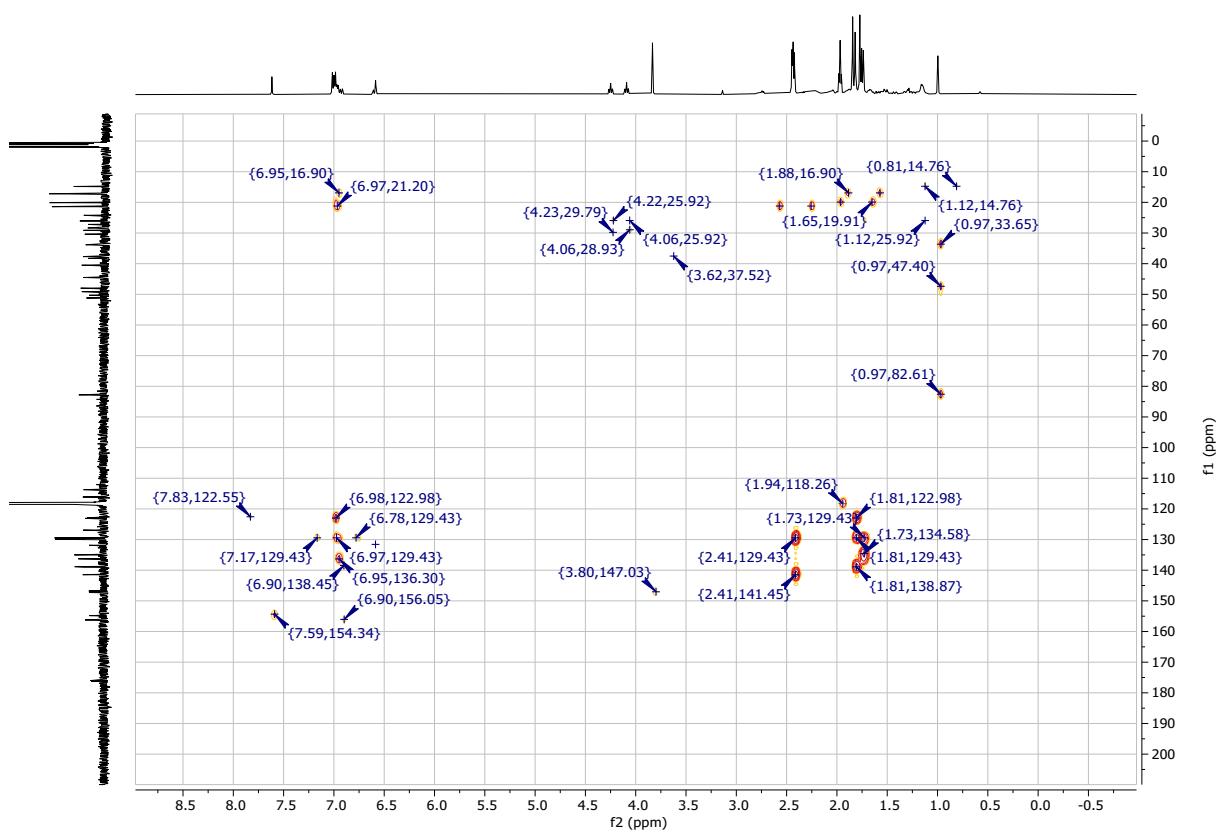


Figure S5: HMBC NMR spectrum of complex **5** in acetonitrile-*d*₃.

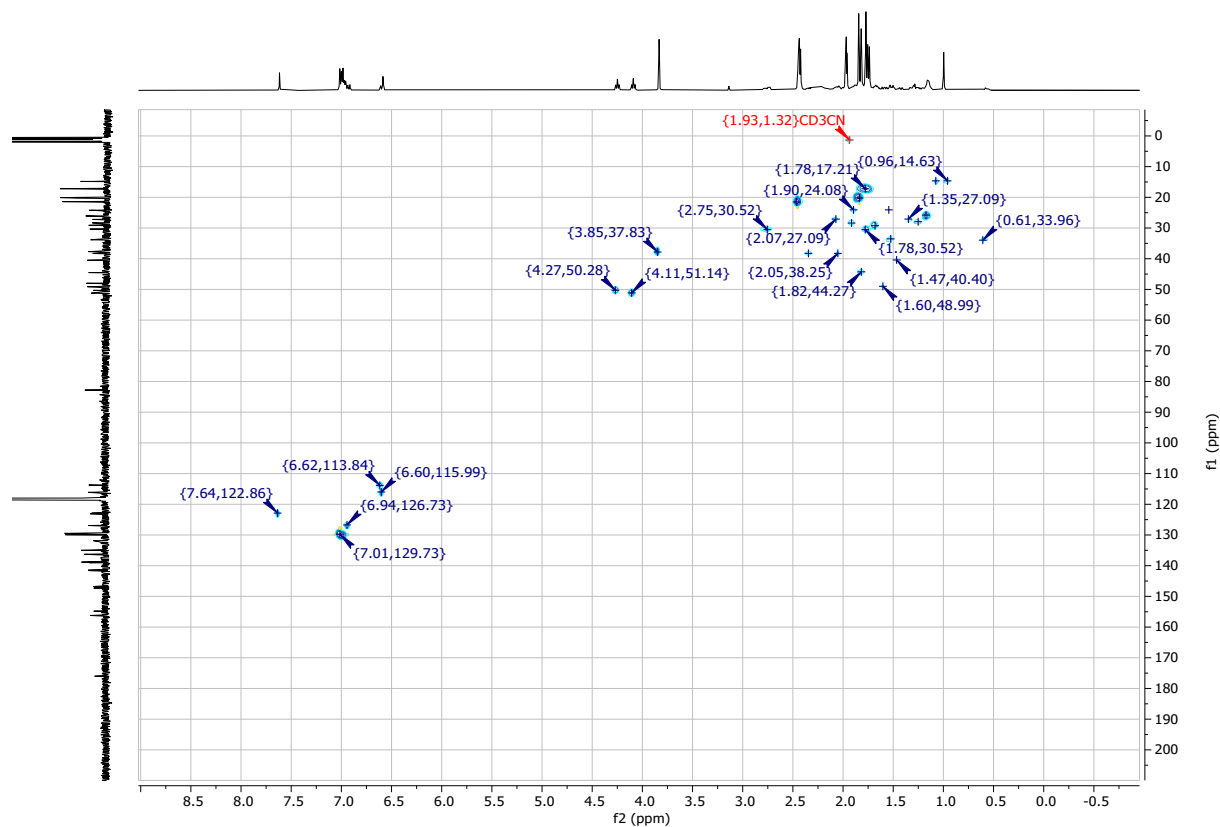


Figure S6: HSQC NMR spectrum of complex **5** in acetonitrile- d_3 .

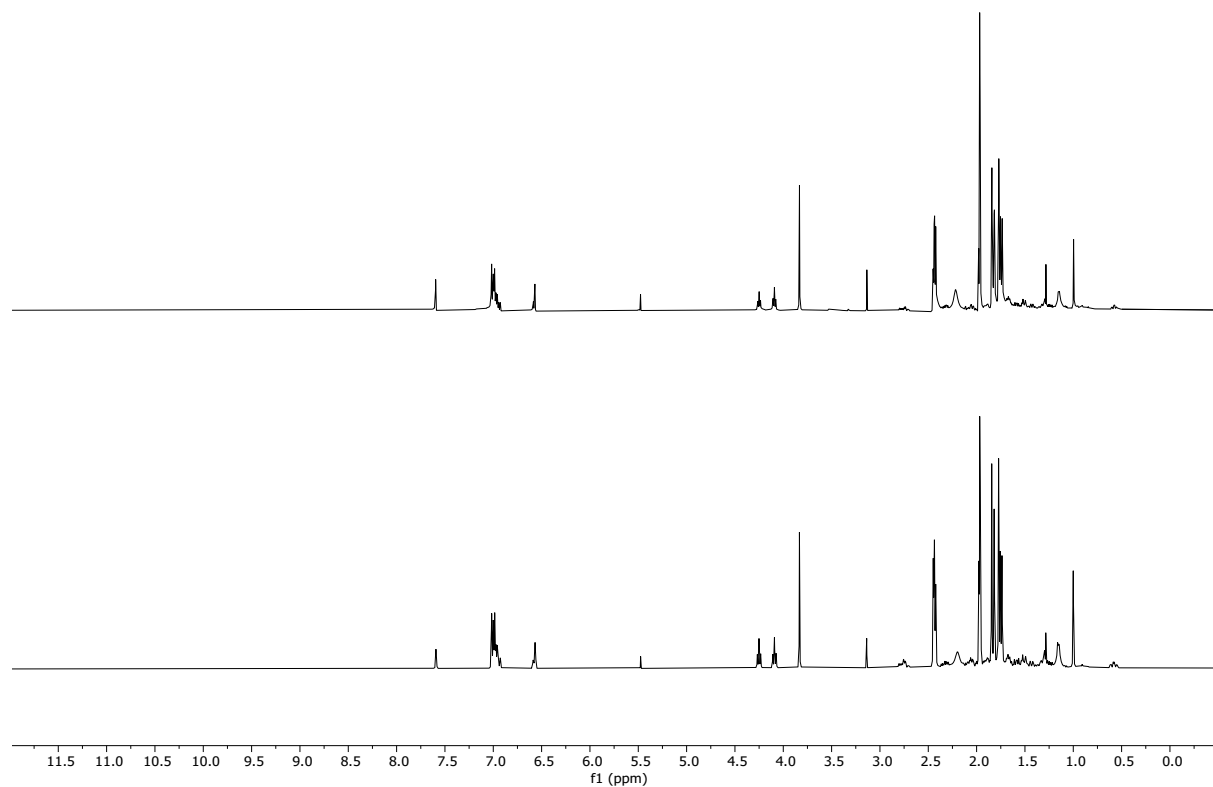


Figure S7: ^1H -NMR of complex **5** in acetonitrile- d_3 . Bottom: directly measured after solvation. Top: measured after four days.

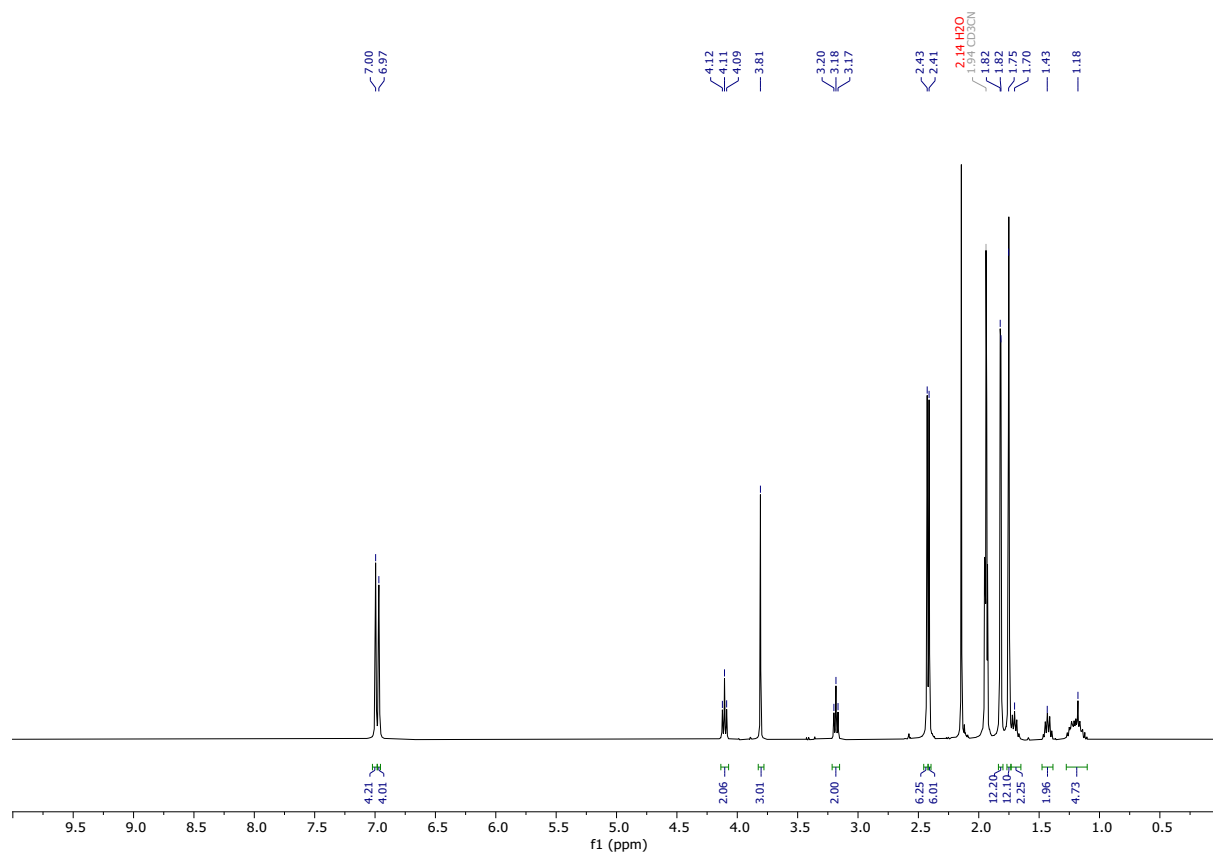


Figure S8: ¹H-NMR spectrum of complex **4** in acetonitrile-*d*₃.

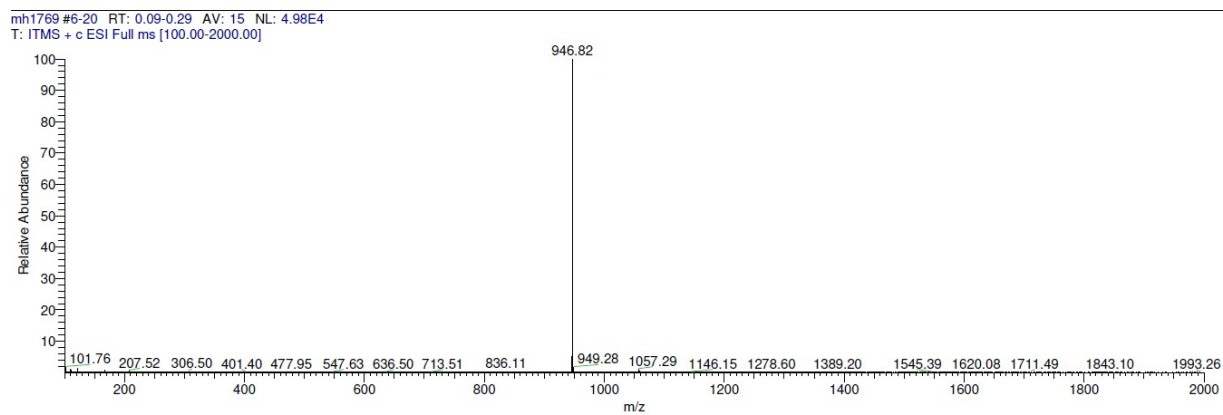


Figure S9: ESI-MS spectrum of complex **4**.

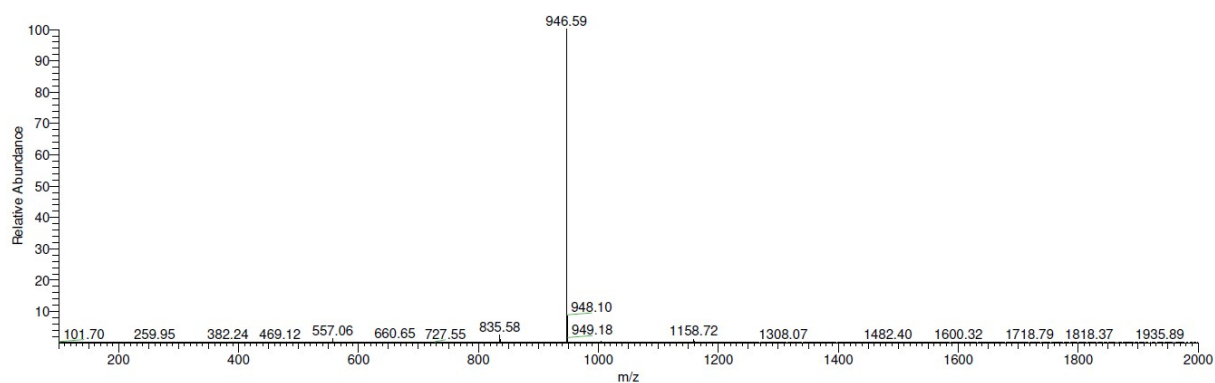


Figure S10: ESI-MS of crude **4** before column chromatography, showing mass signals for **1** (835.58 m/z) and **2** (1158 m/z).

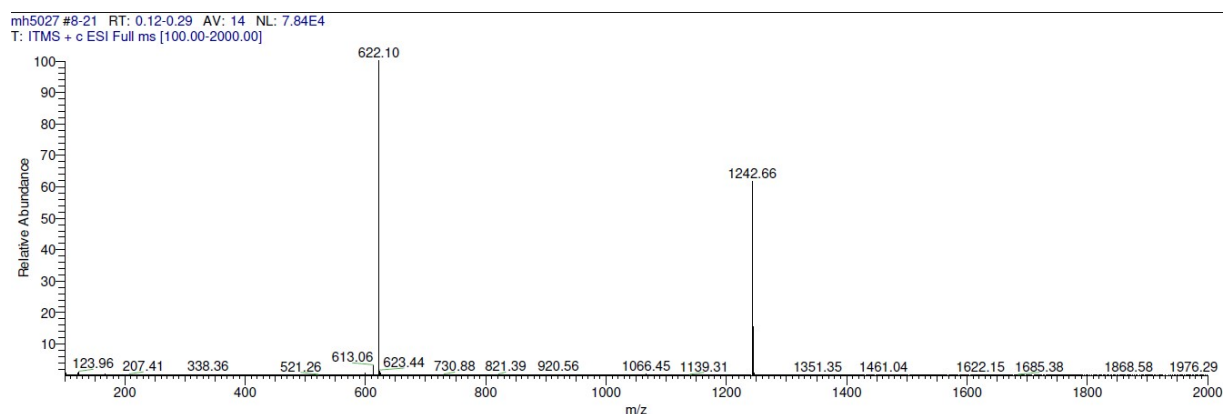


Figure S11: ESI-MS spectrum of complex **5**.

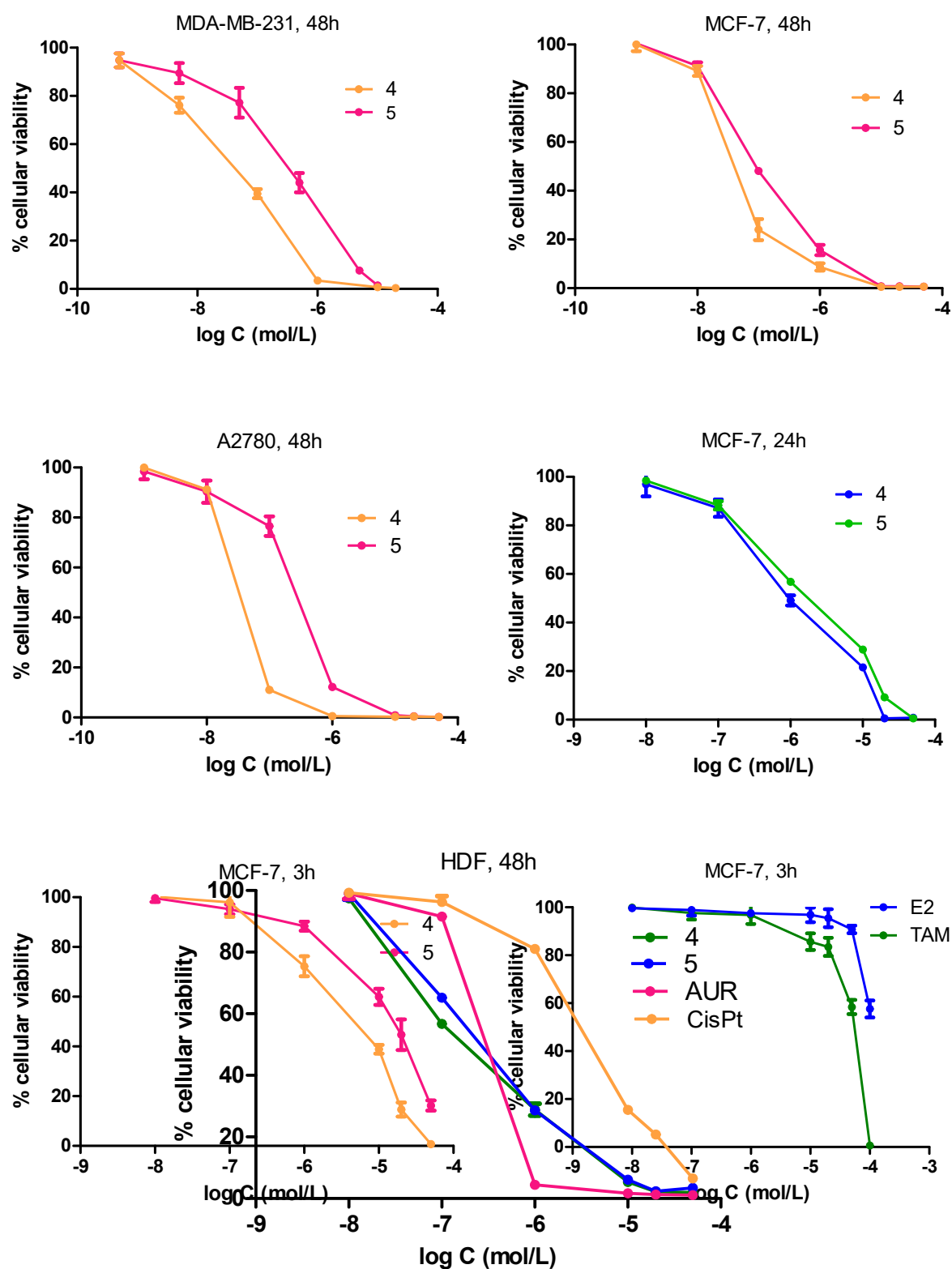


Figure S12: Dose-response curves for calculation of the IC_{50} values of 4 and 5, oestradiol (E2) and tamoxifen (TAM) in the cancer cells using the GraphPad Prism software (vs. 5.0). Results represent the mean $\pm$ SD of two independent experiments done with at least four replicates per condition.

Table S1: IC₅₀ values (± SD) of **4** and **5** in MCF-7 cells after 3, 24 and 48 h incubation determined by the MTT assay.

Compound	3 h	24 h	48 h
4	10.1 ± 0.9 µM	1.07 ± 0.3 µM	43.1 ± 9.0 nM
5	20.2 ± 1.8 µM	1.52 ± 0.4 µM	80.9 ± 8.2 nM

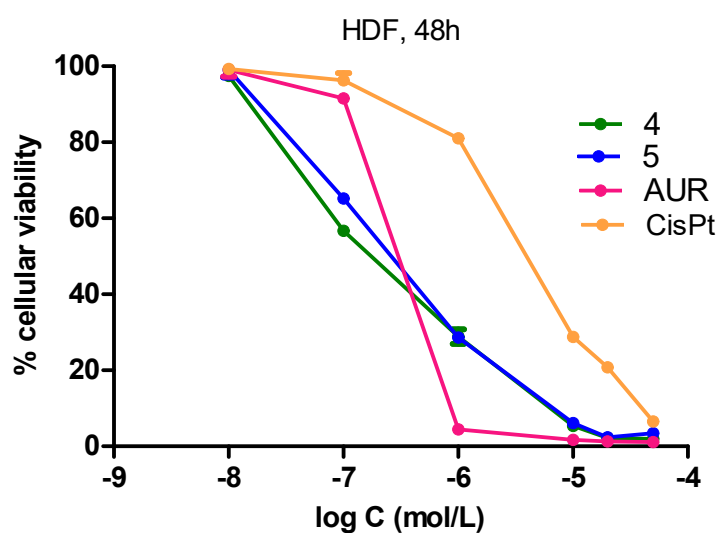


Figure S13: Dose-response curves for calculation of the IC₅₀ values of **4** and **5**, auranofin (AUR) and cisplatin (CisPt) in the human dermal fibroblasts using the GraphPad Prism software (vs. 5.0). Results represent the mean ± SD of two independent experiments done with at least four replicates per condition.