

Supporting Information

***Ex vivo* toxicological evaluation of experimental anticancer gold(I) complexes with lansoprazole-type ligands**

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Gold compounds analysis

Compound 1: Anal. Calcd for C₃₄H₂₉AuBF₇N₃O₂PS (915.42): C, 44.61; H, 3.19; N, 4.59. Found: C, 44.38; H, 3.19; N, 4.57. ¹H NMR (CDCl₃): δ 8.33 (br, 1H, H⁶), 7.74 (br, 2H, H^{3'}, H^{6'}), 7.53 (br, 15H, PPh₃), 7.36 (m, *J*_{H-H} = 9.1, 6.0, 3.0 Hz, 2H, H^{4'}, H^{5'}), 6.67 (d, *J*_{H-H} 5.6 Hz, 1H, H⁵), 4.76 (AB, *J*_{AB} = 13.6 Hz, 2H, CH₂SO), 4.36 (br, 2H, OCH₂CF₃), 2.18 (br, 3H, CH₃). ³¹P NMR (CDCl₃): δ 31.2 ppm (s, PPh₃). ESI-MS (CH₃CN, pos. mode) for C₃₄H₂₉AuF₃N₃O₂PS: exp. 305.1465 (calc. 305.1978).

Compound 2: Anal. Calcd for C₂₂H₂₅AuF₃N₆O₂PS (722.47): C, 36.57; H, 3.49; N, 11.63. Found C, 36.57; H, 3.43; N, 11.48. ¹H NMR (CDCl₃): δ 8.36 (d, *J*_{H-H} = 5.6 Hz, 1H, H⁶), 7.74 (br, 2H, H^{3'}, H^{6'}), 7.23 (m, *J*_{H-H} = 9.2, 6.0, 3.2 Hz, 2H, H^{4'}, H^{5'}), 6.68 (d, *J*_{H-H} = 5.6 Hz, 1H, H⁵), 4.70 (q, AB, *J*_{AB} = 13.5 Hz, 2H, CH₂SO), 4.57 (q, AB, *J*_{AB} = 13.5 Hz, 6H, NCH₂N), 4.41 (q, *J*_{H-F} = 8.0 Hz, 2H, OCH₂CF₃), 4.36 (s, 6H, N-CH₂-P), 2.28 (s, 3H, CH₃). ¹H NMR (acetone-*d*₆): δ 8.34 (d, *J*_{H-H} = 5.4 Hz, 1H, H⁶), 7.62 (m, AA' part of an AA'BB', *J*_{H-H} = 9.0, 6.0, 3.3 Hz, 2H, H^{3'}, H^{6'}), 7.12 (m, BB' part, *J*_{H-H} = 9.0, 5.7, 2.7 Hz, 2H, H^{4'}, H^{5'}), 7.07 (d, *J*_{H-H} = 5.4 Hz, 1H, H⁵), 4.83 (q, *J*_{H-F} = 8.4 Hz, 2H, OCH₂CF₃), 4.71 (AB, *J*_{AB} = 12.9 Hz, 6H, N-CH₂-N), 4.57 (s, 2H, CH₂SO), 4.52 (s, 6H, N-CH₂-P), 2.27 (s, 3H, CH₃). ³¹P NMR (CDCl₃): δ -58.6 ppm (s, PTA).

Compound 3: Anal. Calcd for C₅₂H₄₃Au₂BF₇N₃O₂P₂S (1373.66): C, 45.47; H, 3.16; N, 3.06. Found: C, 45.43; H, 3.12; N, 3.05. ¹H NMR (CDCl₃): δ 7.95 (d, br, *J*_{H-H} = 4.8 Hz, 1H, H⁶), 7.81 (m, AA' part of an AA'BB', *J*_{H-H} = 8.8, 5.6, 2.8 Hz, 2H, H^{3'}, H^{6'}), 7.59 (m, br, 30H, PPh₃), 7.39 (m, br, BB' part, *J*_{H-H} = 9.2, 5.2, 3.2 Hz, 2H, H^{4'}, H^{5'}), 6.78 (d, *J*_{H-H} = 5.6 Hz, 1H, H⁵), 4.78 (q, AB, *J*_{H-H} = 13.2 Hz, 2H, CH₂SO), 4.27 (qd, *J*_{H-F} = 8.0, 3.2 Hz, 2H, CH₂CF₃), 1.93 (s, 3H, CH₃). ³¹P NMR (CDCl₃): δ 31.0 and 33.2 ppm.

Figures

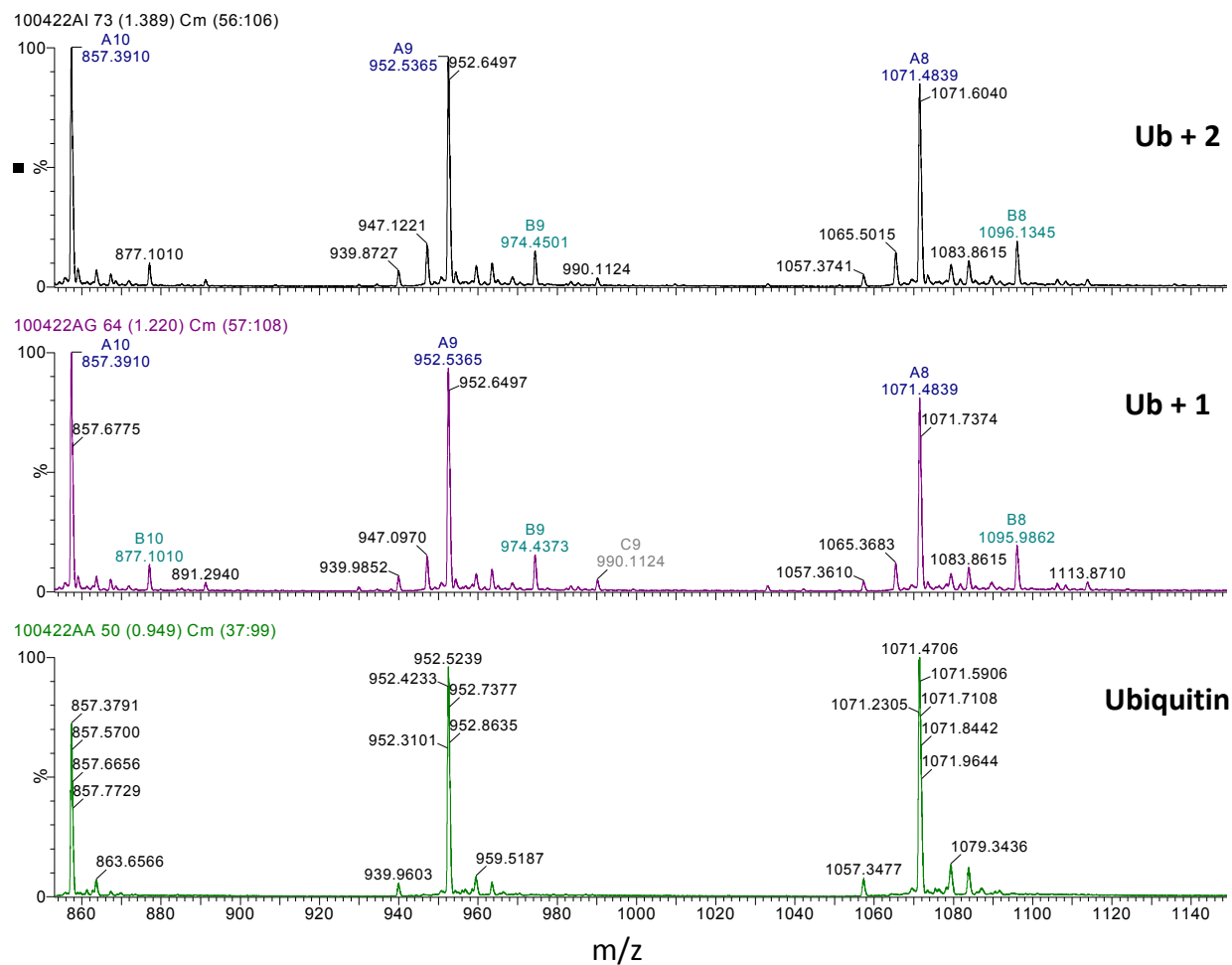


Figure S1 – Multicharged ESI mass spectra of Ub alone (bottom) or incubated with **1** and **2** (gold complex/Ub ratio = 3:1) for 24 h at 37 °C.