

## Supporting Information

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

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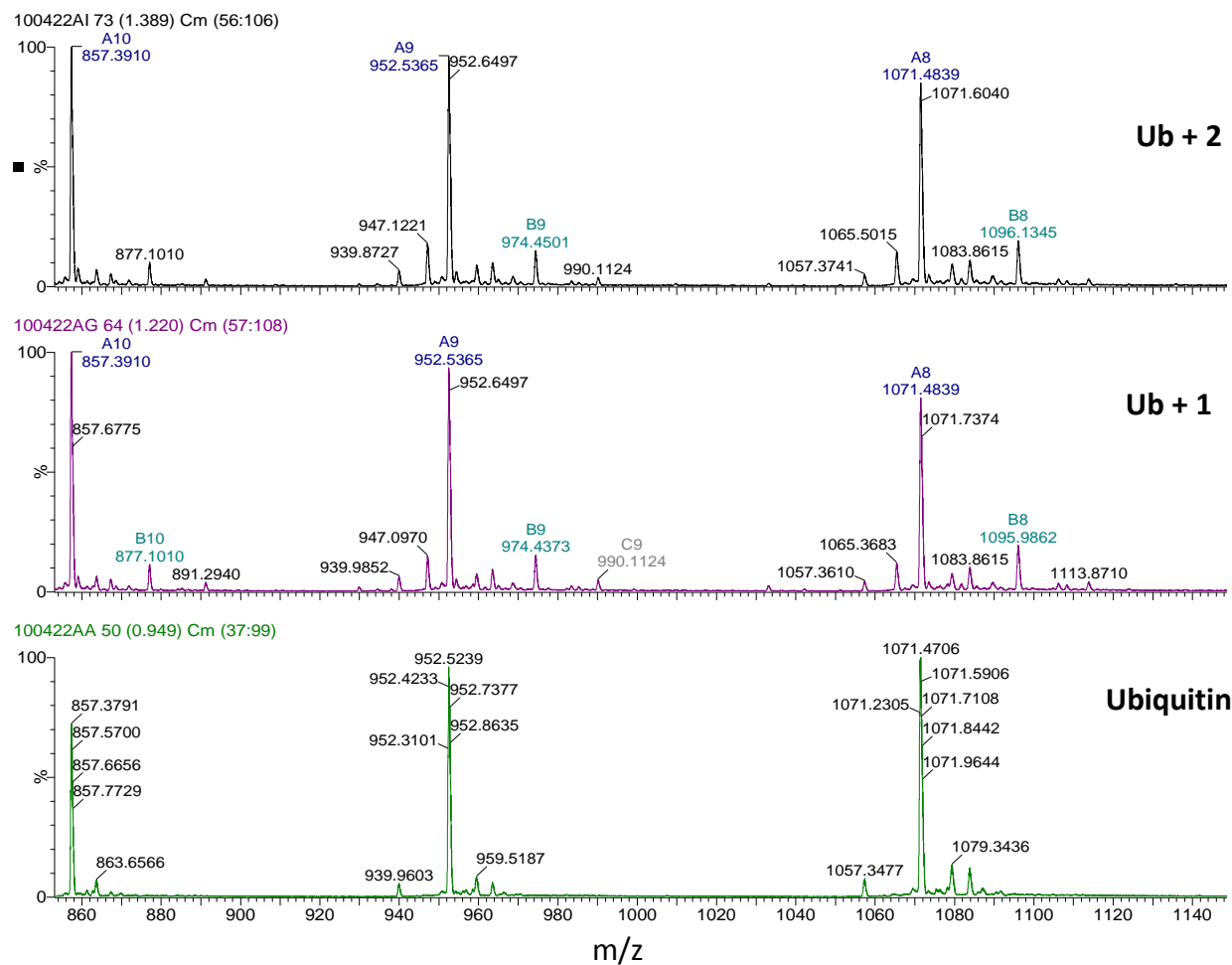
#### **Gold compounds analysis**

**Compound 1:** Anal. Calcd for C<sub>34</sub>H<sub>29</sub>AuBF<sub>7</sub>N<sub>3</sub>O<sub>2</sub>PS (915.42): C, 44.61; H, 3.19; N, 4.59. Found: C, 44.38; H, 3.19; N, 4.57. <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ 8.33 (br, 1H, H<sup>6</sup>), 7.74 (br, 2H, H<sup>3'</sup>, H<sup>6'</sup>), 7.53 (br, 15H, PPh<sub>3</sub>), 7.36 (m, J<sub>H-H</sub> = 9.1, 6.0, 3.0 Hz, 2H, H<sup>4'</sup>, H<sup>5'</sup>), 6.67 (d, J<sub>H-H</sub> = 5.6 Hz, 1H, H<sup>5</sup>), 4.76 (AB, J<sub>AB</sub> = 13.6 Hz, 2H, CH<sub>2</sub>SO), 4.36 (br, 2H, OCH<sub>2</sub>CF<sub>3</sub>), 2.18 (br, 3H, CH<sub>3</sub>). <sup>31</sup>P NMR (CDCl<sub>3</sub>): δ 31.2 ppm (s, PPh<sub>3</sub>). ESI-MS (CH<sub>3</sub>CN, pos. mode) for C<sub>34</sub>H<sub>29</sub>AuF<sub>3</sub>N<sub>3</sub>O<sub>2</sub>PS: exp. 305.1465 (calc. 305.1978).

**Compound 2:** Anal. Calcd for C<sub>22</sub>H<sub>25</sub>AuF<sub>3</sub>N<sub>6</sub>O<sub>2</sub>PS (722.47): C, 36.57; H, 3.49; N, 11.63. Found C, 36.57; H, 3.43; N, 11.48. <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ 8.36 (d, J<sub>H-H</sub> = 5.6 Hz, 1H, H<sup>6</sup>), 7.74 (br, 2H, H<sup>3'</sup>, H<sup>6'</sup>), 7.23 (m, J<sub>H-H</sub> = 9.2, 6.0, 3.2 Hz, 2H, H<sup>4'</sup>, H<sup>5'</sup>), 6.68 (d, J<sub>H-H</sub> = 5.6 Hz, 1H, H<sup>5</sup>), 4.70 (q, AB, J<sub>AB</sub> = 13.5 Hz, 2H, CH<sub>2</sub>SO), 4.57 (q, AB, J<sub>AB</sub> = 13.5 Hz, 6H, NCH<sub>2</sub>N), 4.41 (q, J<sub>H-F</sub> = 8.0 Hz, 2H, OCH<sub>2</sub>CF<sub>3</sub>), 4.36 (s, 6H, N-CH<sub>2</sub>-P), 2.28 (s, 3H, CH<sub>3</sub>). <sup>1</sup>H NMR (acetone-*d*<sub>6</sub>): δ 8.34 (d, J<sub>H-H</sub> = 5.4 Hz, 1H, H<sup>6</sup>), 7.62 (m, AA' part of an AA'BB'), J<sub>H-H</sub> = 9.0, 6.0, 3.3 Hz, 2H, H<sup>3'</sup>, H<sup>6'</sup>), 7.12 (m, BB' part, J<sub>H-H</sub> = 9.0, 5.7, 2.7 Hz, 2H, H<sup>4'</sup>, H<sup>5'</sup>), 7.07 (d, J<sub>H-H</sub> = 5.4 Hz, 1H, H<sup>5</sup>), 4.83 (q, J<sub>H-F</sub> = 8.4 Hz, 2H, OCH<sub>2</sub>CF<sub>3</sub>), 4.71 (AB, J<sub>AB</sub> = 12.9 Hz, 6H, N-CH<sub>2</sub>-N), 4.57 (s, 2H, CH<sub>2</sub>SO), 4.52 (s, 6H, N-CH<sub>2</sub>-P), 2.27 (s, 3H, CH<sub>3</sub>). <sup>31</sup>P NMR (CDCl<sub>3</sub>): δ -58.6 ppm (s, PTA).

**Compound 3:** Anal. Calcd for C<sub>52</sub>H<sub>43</sub>Au<sub>2</sub>BF<sub>7</sub>N<sub>3</sub>O<sub>2</sub>P<sub>2</sub>S (1373.66): C, 45.47; H, 3.16; N, 3.06. Found: C, 45.43; H, 3.12; N, 3.05. <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ 7.95 (d, br, J<sub>H-H</sub> = 4.8 Hz, 1H, H<sup>6</sup>), 7.81 (m, AA' part of an AA'BB', J<sub>H-H</sub> = 8.8, 5.6, 2.8 Hz, 2H, H<sup>3'</sup>, H<sup>6'</sup>), 7.59 (m, br, 30H, PPh<sub>3</sub>), 7.39 (m, br, BB' part, J<sub>H-H</sub> = 9.2, 5.2, 3.2 Hz, 2H, H<sup>4'</sup>, H<sup>5'</sup>), 6.78 (d, J<sub>H-H</sub> = 5.6 Hz, 1H, H<sup>5</sup>), 4.78 (q, AB, J<sub>H-H</sub> = 13.2 Hz, 2H, CH<sub>2</sub>SO), 4.27 (qd, J<sub>H-F</sub> = 8.0, 3.2 Hz, 2H, CH<sub>2</sub>CF<sub>3</sub>), 1.93 (s, 3H, CH<sub>3</sub>). <sup>31</sup>P NMR (CDCl<sub>3</sub>): 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.