Supplemental Information

Comparing Coordination Uranyl (VI)Complexes with 2-(1H-imidazo[4,5-b]phenazin-2-yl)phenol and Derivatives

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Single Crystal X-ray Diffraction

Datasets were collected on a Bruker SMART APEX CCD X-ray diffractometer unit using Mo Kα radiation, from crystals mounted in Paratone-N oil on glass fibers. SMART (v 5.624) was used for preliminary determination of cell constants and data collection control. All datasets were collected at 180K. Determination of integrated intensities and global cell refinement were performed with the Bruker SAINT software package using a narrow-frame integration algorithm.[1] The program suite SHELXL (v 5.1) was used for space group determination, structure solution, and refinement. Refinement was performed against F^2 by weighted full-matrix least squares, and empirical absorption correction (SADABS) was applied.[2] The olex2.refinement package using Gauss-Newton minimization was used for further refinement.3 Projections were generated using the Olex2.1-1 graphics program.[3]

L1 crystals were grown by dissolving 0.0200 grams of salimidizine in 1 ml of DMSO in a test tube, this test tube was placed in a 20-dram vial with hexanes as the diffusion solvent. After 3 weeks, quality single crystals were observed and used for X-ray diffraction.

L2 crystals were grown by dissolving 0.0200 grams of DTB-salimidizine in 8 ml of THF in a 20-dram slow evaporation of the solvent was allowed to occur. After a week, quality single crystals were observed and used for X-ray diffraction.

[L1]$UO_2(OAc)_2$(DMSO) crystals were grown by dissolving 0.0201 grams of salimidizine in 1 ml of DMSO in a test tube. This solution was then layered with an ethanol solution containing 0.0117 grams of $UO_2(OAc)_2{\cdot}2H_2O$. This solution was set up for slow diffusion in a 20-dram vial with hexanes as the diffusion solvent. After 4 days, quality single crystals were observed and used for X-ray diffraction.

NMR Spectra

^{1}H NMR were recorded on a Bruker AV 500 MHz spectrometer using DMF-d7 and DMSO-d6 (Cambridge Isotope Laboratories). Chemical shifts are reported in parts per million (δ) and are referenced residual internal solvent signals or with respect to tetramethyl silane (TMS) as the internal standard.

*

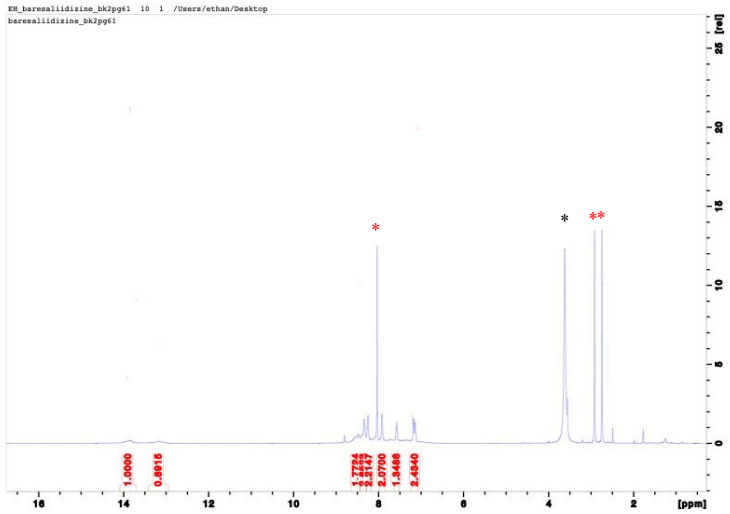

*Figure S1. H[1] NMR spectra of Salimidizine (**L1**) in DMF-d7, 600 MHz (*=H_2O, *=solvent)*

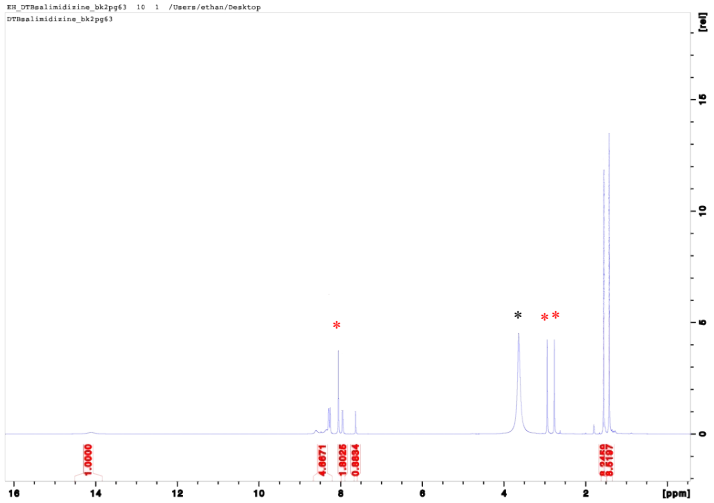

*Figure S2. H[1] NMR of DTB Salimidizine (**L2**) in DMF-d7, 600 MHz (*=H_2O, *=solvent)*

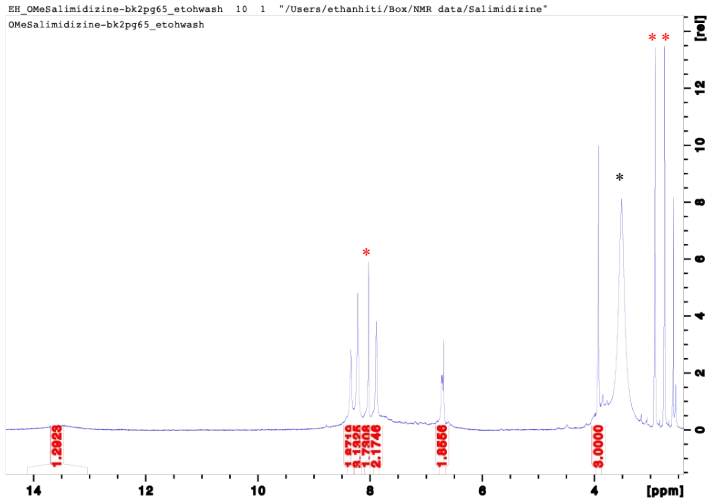

*Figure S3. H^1 NMR of OMe Salimidizine (**L3**) in DMF-d_7, 600 MHz (*=H_2O, *=solvent)*

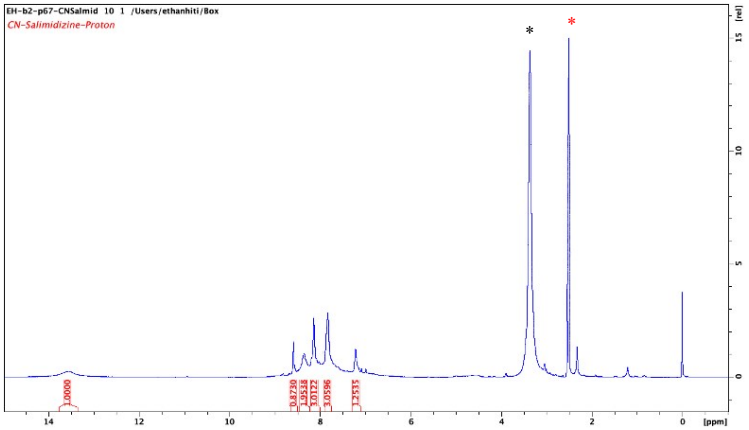

Figure S4. H^1 NMR of L4 in DMSO-d6, 500 MHz (=H_2O, *=solvent)*

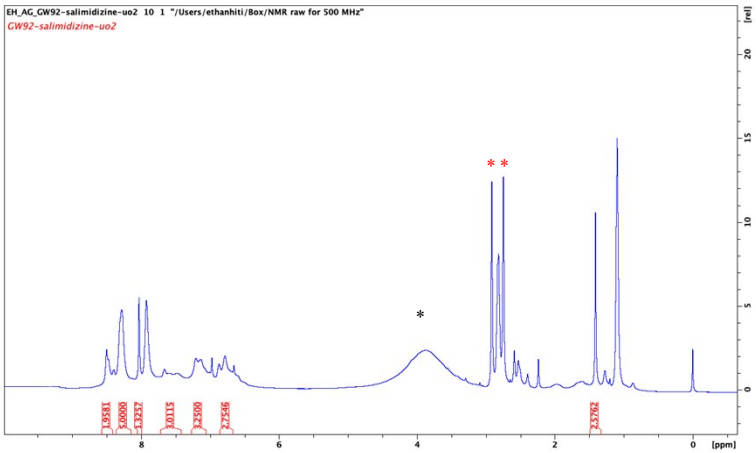

Figure S5. 1H NMR of Salimidizine (L1) UO2 complex in DMF-d7, 500 MHz (=H_2O, *=solvent)*

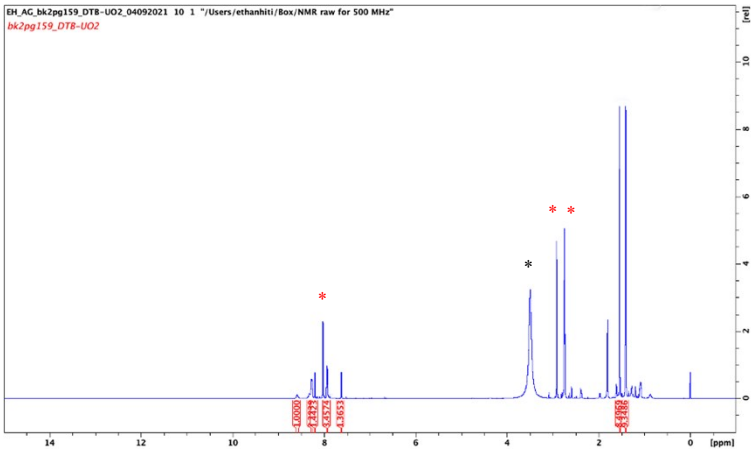

Figure S6. 1H NMR of DTB salimidizine (L2) UO2 complex in DMF-d7, 500 MHz (=H_2O, *=solvent)*

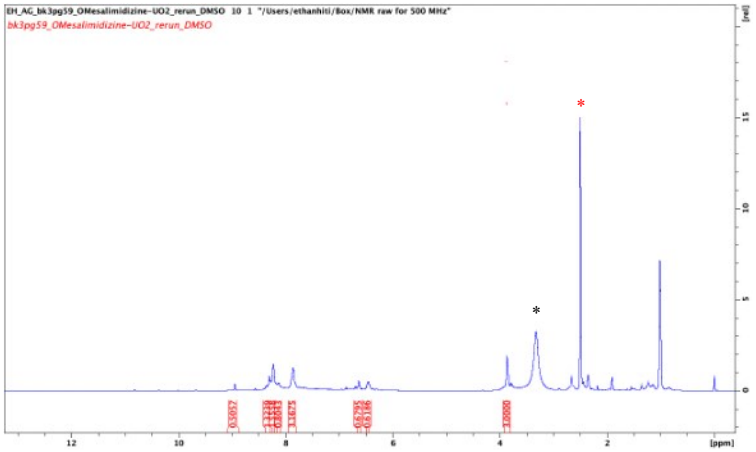

Figure S7. 1H NMR of OMe salimidizine (L3) UO2 complex in DMSO-d6, 500 MHz (=H_2O, *=solvent)*

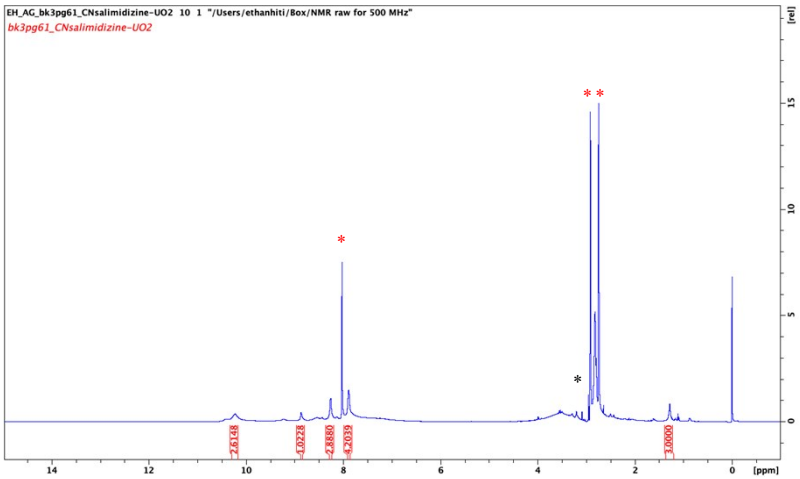

Figure S8. 1H NMR of CN salimidizine (L4) UO2 complex in DMF-d7, 500 MHz (=H_2O, *=solvent)*