Electronic Supplementary Material (ESI) for Analytical Methods.

Detection of Interaction between Protein Trytophan Residues and Small or Macromolecular Ligands by Synchrotron Radiation Magnetic Circular Dichroism

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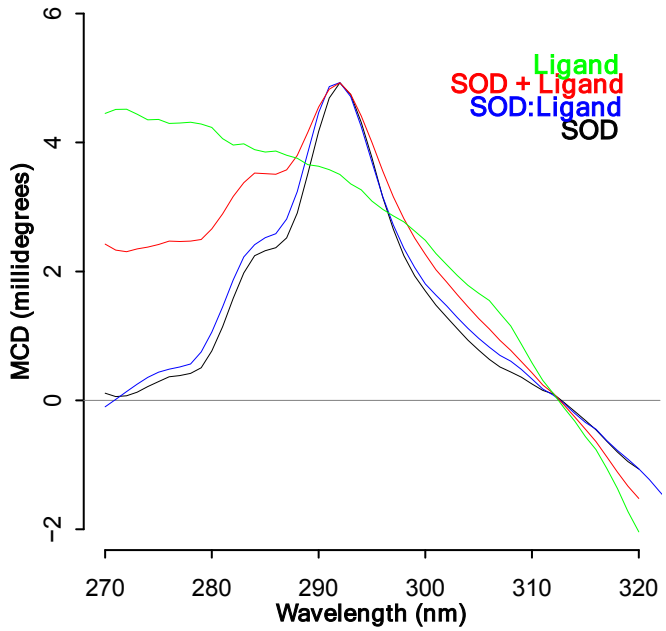
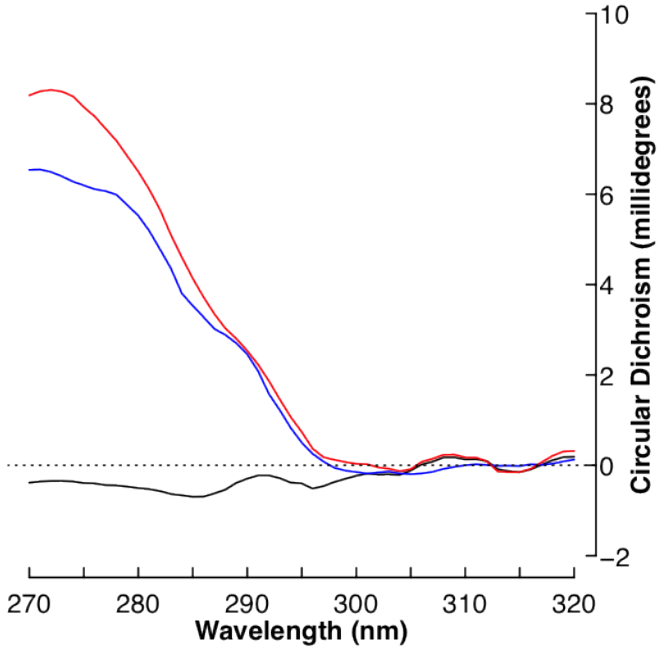
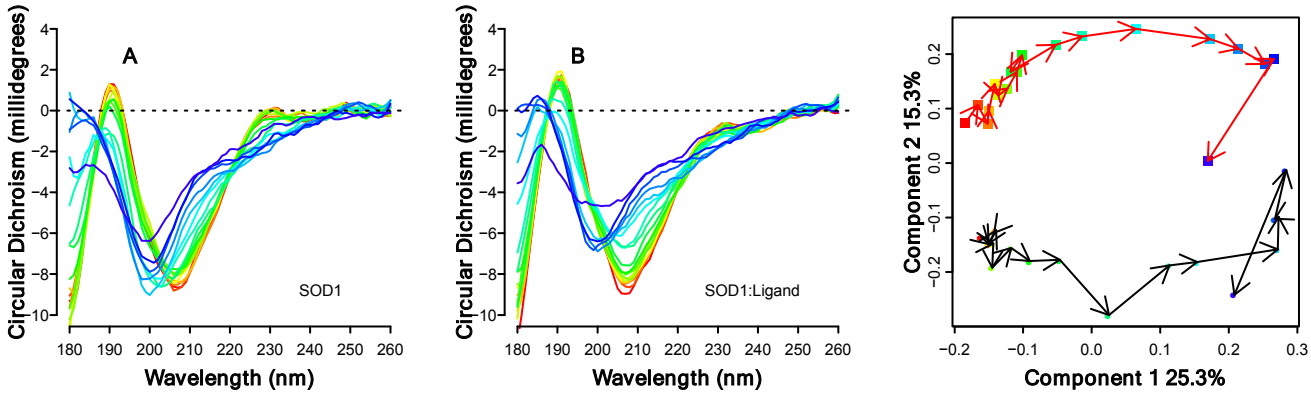


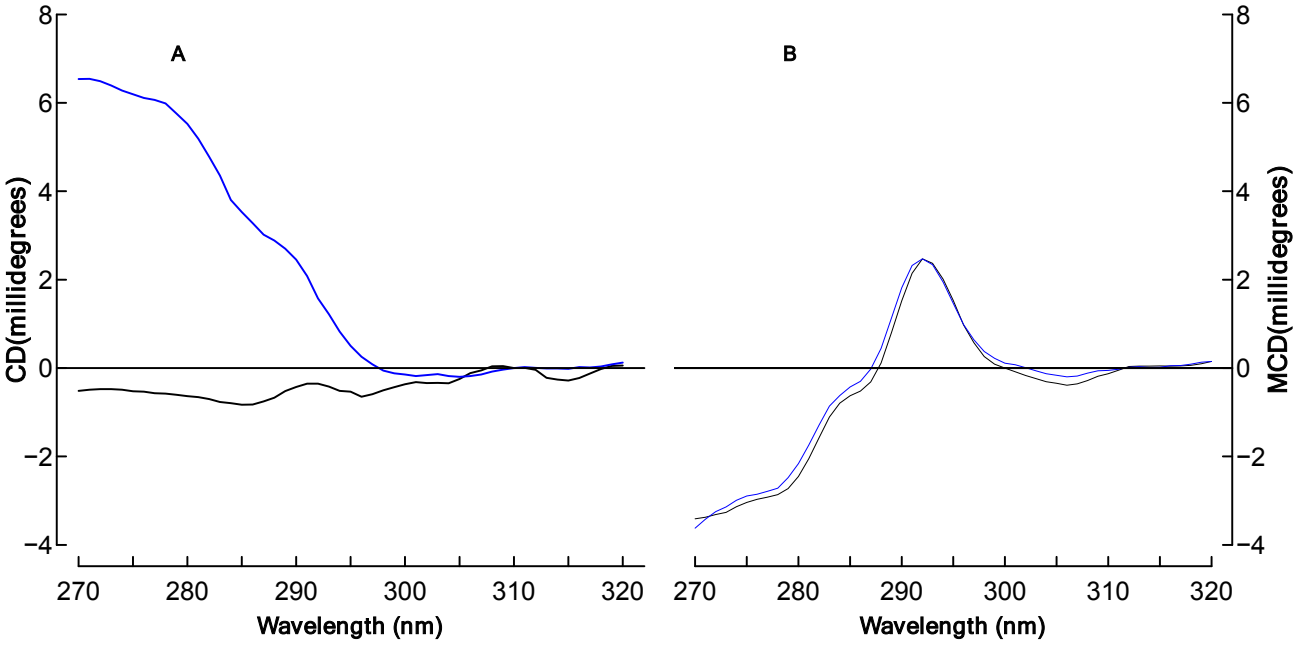
Supplementary Figure 1, MCD spectra (270-320 nm) of SOD1 alone (black), 5-fluorouridine ligand alone (green) SOD-1:ligand (blue) and the superposition of SOD-1 and ligand (red). The superposition has been normalised to the maximal value of the SOD spectrum. SOD-1 was at 0.16 μM and ligand at 1:1 molar ratio, with 3 s integration time and 1 mm path length.



Supplementary Figure 2. SRCD near UV spectra (270-320 nm) of SOD-1 alone (black), SOD-1:ligand (blue) and the ligand alone (red). SOD-1 was at 0.16 µM and ligand at 1:1 molar ratio, with 3 s integration time and 1 mm path length.



Supplementary Figure 3. A. Far UV SRCD spectra (180-260 nm) of the thermal degradation (10-90 ℃ in 5 steps, returning to 20 ℃) of; A. SOD-1 alone **B.** SOD-1 + ligand (1:1 molar ratio). SOD-1 was at 0.16 µM and ligand at 1:1 molar ratio with 0. 5 mm slit width, 1 s integration time and 0.1 mm path length. **C.** Principal component analysis (PCA) of the SRCD spectra in A and B, showing that the thermal degradation of SOD-1 (black arrows) alone differs from that of SOD-1 in the presence of ligand (5-fluorouridine at 1:1 molar ratio, red arrows). This demonstrates, independently of MCD, that SOD-1 and the ligand interact under these conditions.



Supplementary Figure 4. A. SRCD near UV spectra (270-320 nm) of SOD-1 alone (black), SOD-1:ligand (blue) and the ligand alone (red). SOD-1 was at 0.16 μM and ligand at 1:1 molar ratio, with 3 s integration time and 1 mm path length. The SOD-1 MCD and near UVCD spectra are of the same sample in the same cell in the presence and absence of the 1.4 T magnet. **B.** MCD spectra (270-320 nm) of SOD1 alone (black) and SOD-1:ligand (blue). SOD-1 was at 0.16 μM and ligand at 1:1 molar ratio, with 3 s integration time and 1 mm path length. Note the difference in signal intensity from the protein contributions, ~5.5 units for MCD and ~0.5 for standard far UVCD, demonstrating the extra sensitivity of MCD as a technique.