Supplementary Figure Legends

**Figure S1.** Curve-fitting analysis of Au L₃ EXAFS data for KAuBr₄ (top) and KAuCl₄ (bottom). In all figures, thin black lines represent the observed data (Fourier transforms, FT, in full frames, EXAFS in insets) and bold red lines represent the best-fit simulation using feff v7 calculations based on crystal structure coordinates for five-atom (one Au, four halides) models. Simulations were generated using the parameters summarized in Fits 1 (KAuBr₄) and 2 (KAuCl₄) of Table 1 in the article. Fourier transforms were $k^3$ weighted over the $k = 2.0 – 14.0 \text{ Å}^{-1}$ range and were phase-corrected based on Br (KAuBr₄) or Cl (KAuCl₄). Both FTs exhibit peaks at approximately twice the first-shell distances (4.5-4.6 Å for KAuCl₄ and 4.8 Å for KAuBr₄) that arise predominantly from a multiple scattering path involving trans halide ligands (e.g., Au–Br₁–Au–Br₃–Au).

**Figure S2.** Curve-fitting analysis of Au L₃ EXAFS data for Na₃Au(S₂O₃)₂ (top) and auranofin in 50% DMSO (bottom). In all figures, thin black lines represent the observed data (Fourier transforms, FT, in full frames, EXAFS in insets) and bold red lines represent the best-fit simulation using feff v7 calculations based on crystal structure coordinates for Na₃Au(S₂O₃)₂ (one Au and four S's, but no O's, were included in the model) and based on a P-Au-P model for auranofin (P in place of S; see Figure 3B in article). Simulations were generated using the parameters summarized in Fits 3 (Na₃Au(S₂O₃)₂) and 4 (auranofin) of Table 1 in the article. Fourier transforms were $k^3$ weighted over the $k = 2.0 – 14.0 \text{ Å}^{-1}$ range (Na₃Au(S₂O₃)₂) or the $k = 2.0 – 13.0 \text{ Å}^{-1}$ range (auranofin) and were phase-corrected based on S. As in Figure S2, both FTs exhibit
peaks at approximately twice the first-shell Au-S(P) distance that arise predominantly from a multiple scattering path involving trans ligands (e.g., Au–S/P1–Au–S/P2–Au).

**Figure S3. Auranofin reduces growth yield of wild type *E. coli*, but not a *selD* mutant.** Both wild type (MC4100) and a *selD* mutant (WL400), which does not produce selenoproteins, were cultured in modified Luria broth under anaerobic conditions at 37ºC. Auranofin (dissolved in 95% ethanol) was added to the culture medium before inoculation (1, 5, 10, 25, 50 µM). Optical density of the cultures was measured after 24 hours of growth. Data shown is from at least three independent cultures. Error bars indicate standard deviation.

**Figure S4. Growth of *C. difficile* over a 24 hour time period in the presence of auranofin.** *C. difficile* (NAP1/O27) cultures were grown anaerobically at 37 ºC in BHI + cysteine in 96-well polystyrene plates. Auranofin in DMSO (0.25, 0.5, 0.75, 1.0, 1.5, and 2.0 µM) was added to the growth medium prior addition of a 1% inoculum from an overnight culture. Growth was measured as optical density at 600 nm at each time point. Data shown is from at least three independent cultures. Error bars indicate standard deviation.

**Figure S5. Inhibition of growth of *C. difficile*, *C. perfringens* and *C. tetani* by auranofin.** *C. perfringens* (ATCC 19406) and *C. tetani* (ATCC 10543) were grown anaerobically in BHI + cysteine. Auranofin in DMSO (1.0, 5.0 and 10.0 µM) was added to the growth medium prior to inoculation. Growth was measured as optical density at 600 nm after 24 hours at 37ºC. Percent growth (growth yield of inhibited cultures versus control) is plotted at the indicated concentrations of auranofin. Data shown is from at least three independent cultures. Error bars indicate standard deviation.
Figure S2

- Au L₃
- Na₃Au(S₂O₃)₂

FT Magnitude

R' (Å)

- Au L₃
- Auranofin

FT Magnitude

R' (Å)
Figure S3
Figure S4
Figure S5