SUPPORTING INFORMATION

Biological Evaluation, Chelation and Molecular Modeling Studies of Novel Metal-Chelating Inhibitors of NF-κB-DNA Binding: Structure Activity Relationship

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Contents

Figure 10. Energy minimized structures of the ATA analogs.

Figure 11. Molecular electrostatic potentials (MEP) of the energy minimized structures of the ATA analogs.

Figure 12. Antioxidant efficacies of the ATA analogs.
Figure 10. Energy minimized structures of the ATA analogs. a, CAS (Chrome Azurol S); b, ECR (Eriochrome Cyanine R); c, PV (Pyrocatechol Violet); d, AU (Aurin); e, PR (Pyrogallol Red); f, BPR (Bromopyrogallol Red); g, FL (Fluorescein).
Figure 11. Molecular electrostatic potentials (MEP) of the energy minimized structures of the ATA analogs. a, CAS (Chrome Azurol S); b, ECR (Eriochrome Cyanine R); c, PV (Pyrocatechol Violet); d, AU (Aurin); e, PR (Pyrogallol Red); f, BPR (Bromopyrogallol Red); g, FL (Fluorescein). Negative potentials are in red while positive potentials are depicted in blue. The maximum potential represented is $\phi_+ = 0.23$ au and the minimum is $\phi_- = -0.18$ au, over an electronic isodensity of $\rho = 0.02$ e Å$^{-3}$, for each surface represented.
Figure 12. Antioxidant efficacies of the ATA analogs. 1-5 represent BPR (Bromopyrogallol Red), PR (Pyrogallol Red), PV (Pyrocatechol Violet), ECR (Eriochrome Cyanine R) and CAS (Chrome Azurol S) respectively.