Supplementary Information

Chemical Motifs that Redox Cycle and their Associated Toxicity

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Phenol red assay data

Phenol red redox cycling potency.xlsx

(see separate ESI file)

Calculation of HOMO-LUMO energies:

Initial 3D structures were obtained and the most likely protonation state at pH 7.0 was assigned for each compound using an internal tool. The minimum energy conformer for each molecule was obtained by generating up to 100 conformations using MacroModel v9.9,[1] with each conformer undergoing 500 iterations of energy minimization. Calculations of the HOMO, LUMO, and HOMO-LUMO gap energies were obtained from AM1 semiempirical calculations performed with MOPAC 7.0 as implemented in MOE v2011.10.[2]

References:

1) MacroModel, version 9.9, Schrodinger LLC, New York, NY (2012).
2) Molecular Operating Environment (MOE), 2011.10. Chemical Computing Group, Inc., 1010 Sherbooke St. West, Suite #910, Montreal, QC, Canada, H3A 2R7 (2011).

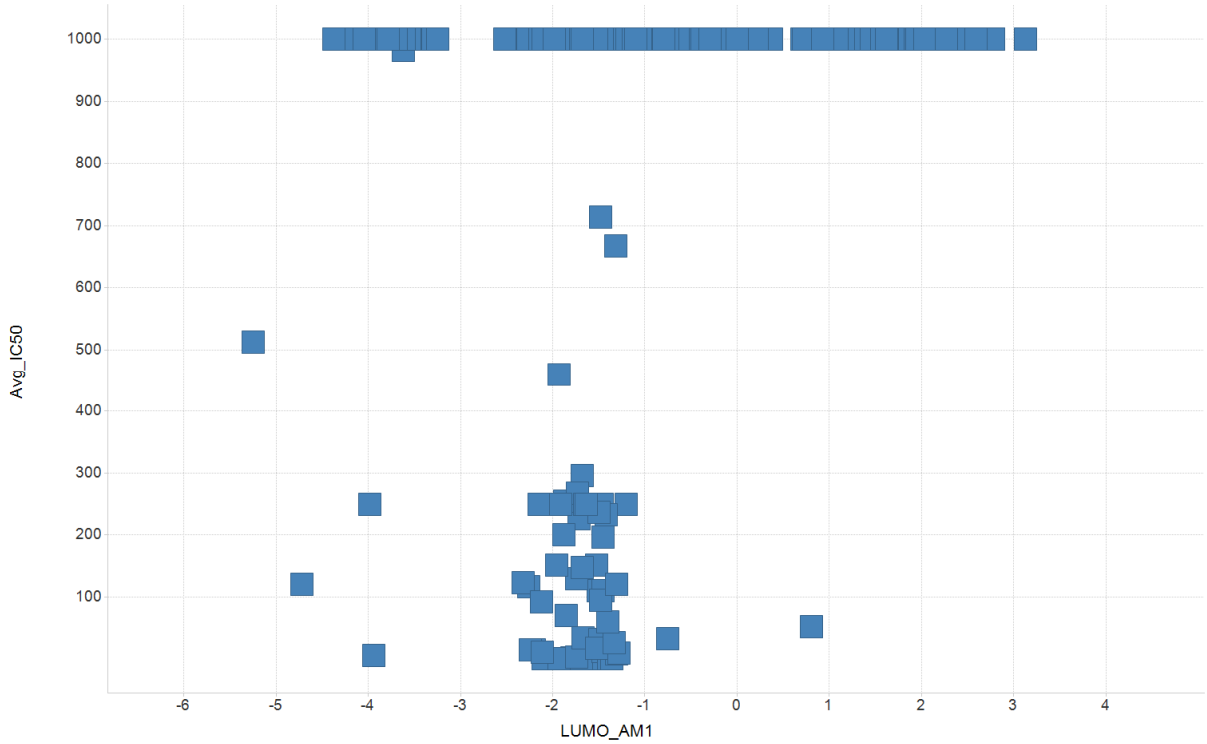

Figure S1 Phenol red redox cycling potency versus calculated LUMO energy level

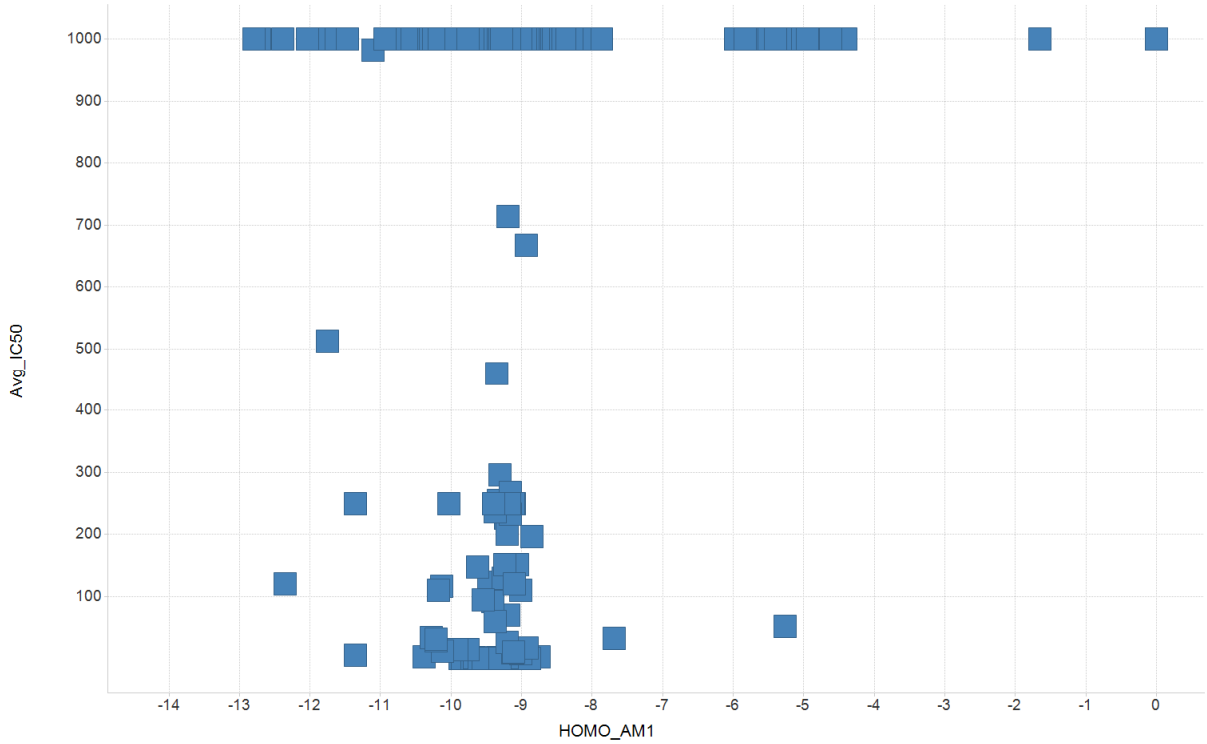

Figure S2 Phenol red redox cycling potency versus calculated HOMO energy level

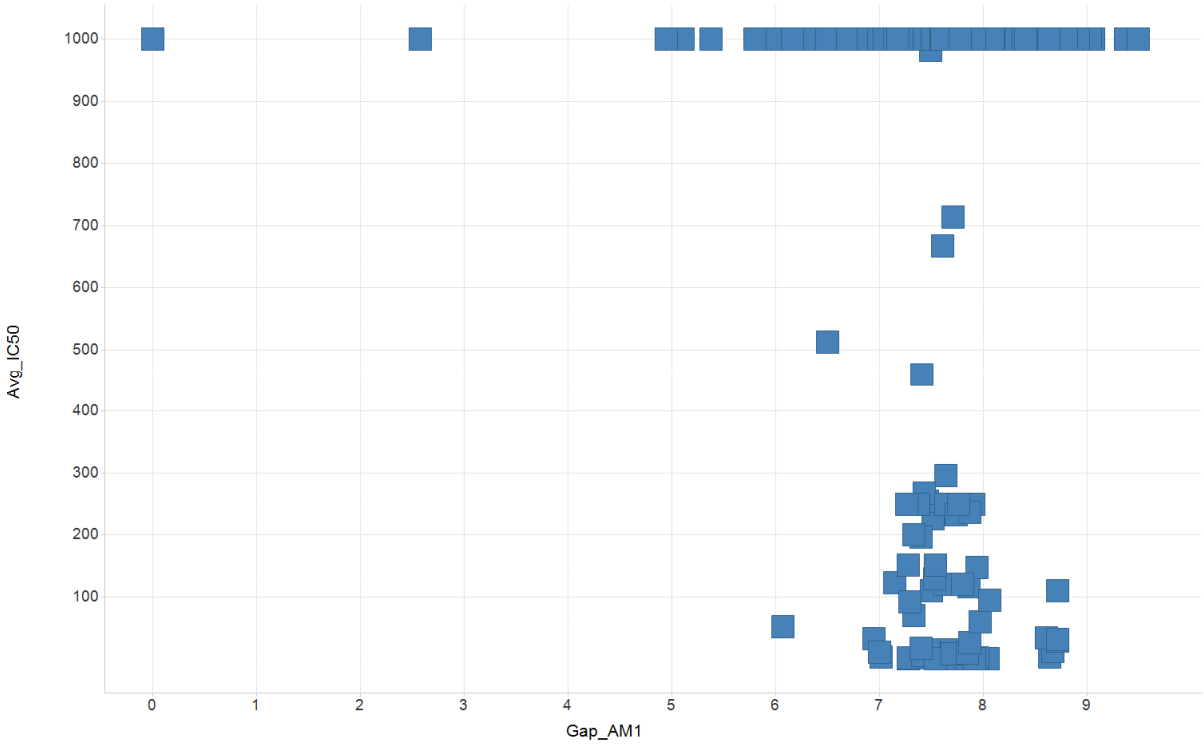

Figure S3 Phenol red redox cycling potency versus calculated HOMO-LUMO energy gap

Redox cycling versus ATP depletion plot

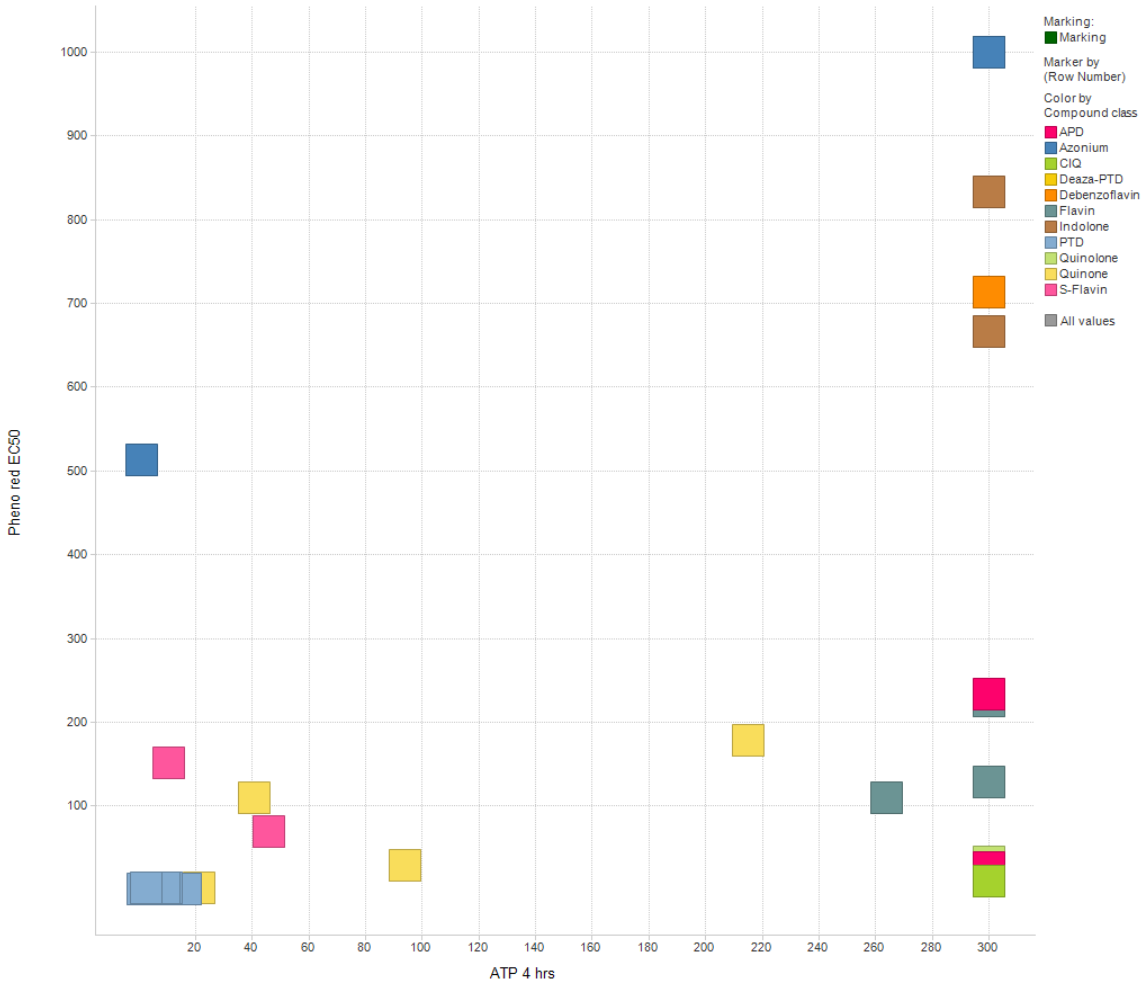

Figure S4 Phenol red redox cycling potency versus ATP depletion at 4 hours