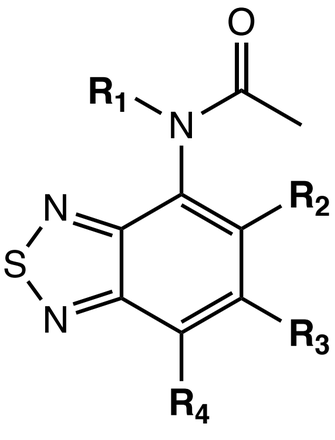
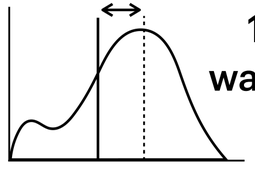
A) Design space



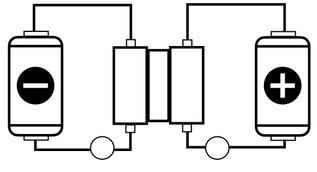
R_1 = -CCOC, -CF_2CF_3
R_2, **R_3** = -CH_3, -CF_3, -CN, -OCH_3, -OCF_3, -SCH_3, -SCF_3, -$N(CH_3)_2$
R_4 = -CH_3, -CF_3, -CN, -OCH_3, -OCF_3, -SCH_3, -SCF_3, -$N(CH_3)_2$, NO_2, -$SO_2N(CH_3)_2$

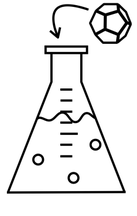
B) Objectives



1. Minimize absorption wavelength deviation from target

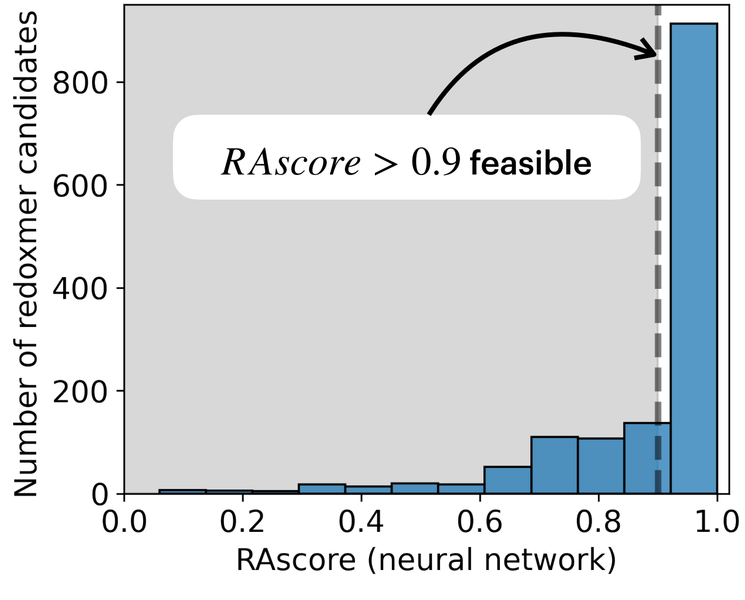
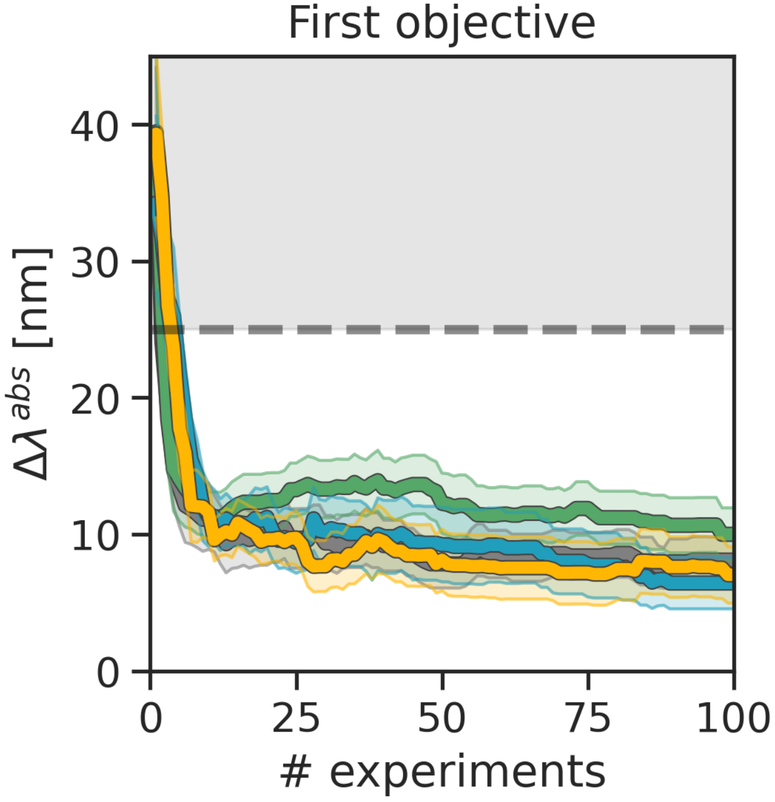
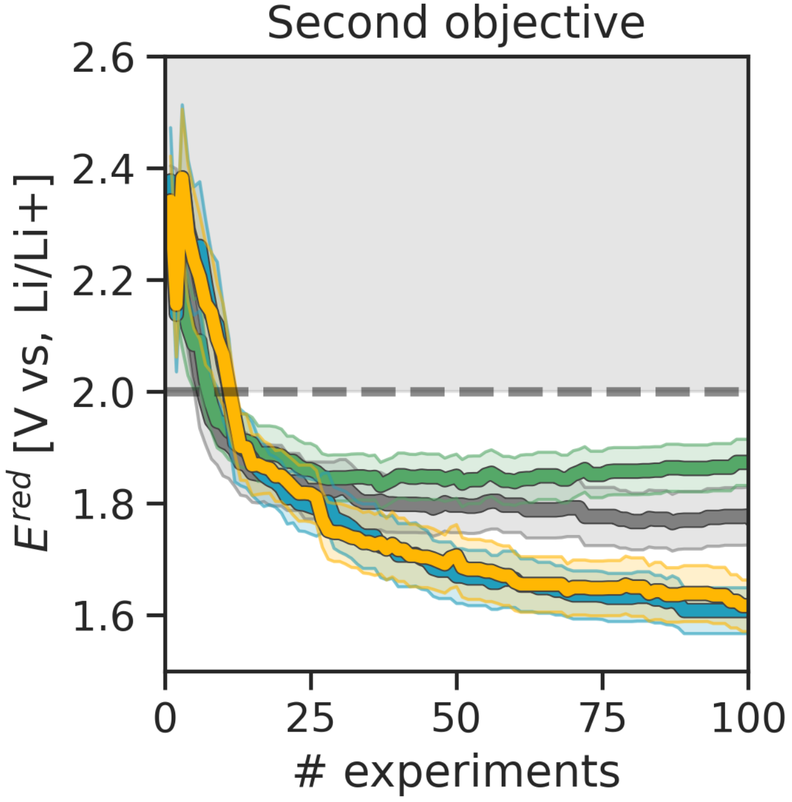
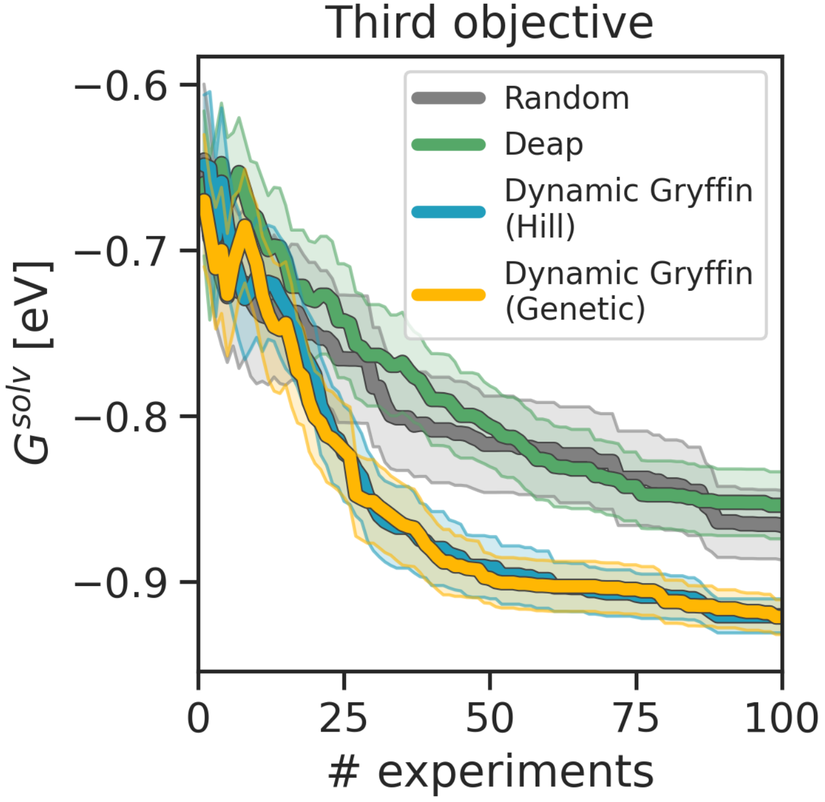
2. Minimize reduction potential





3. Minimize solvation free energy

C) Constraints



D) Optimization experiment results