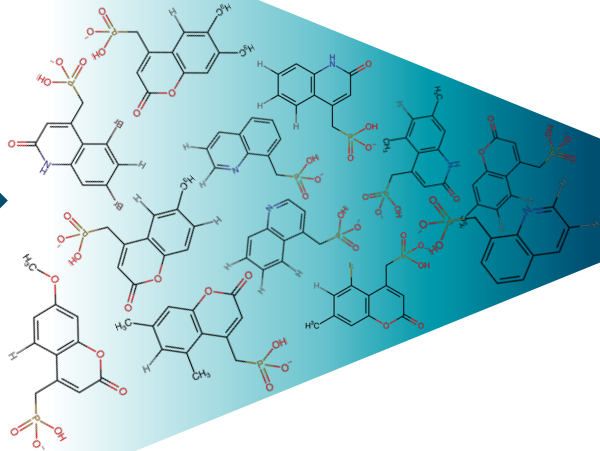
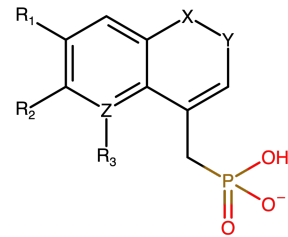


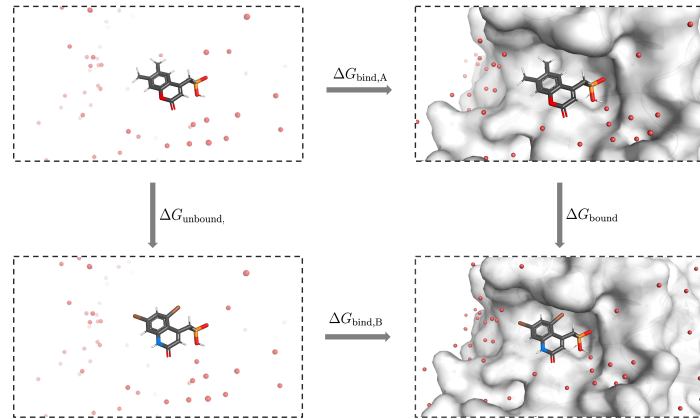
Target
crystal structure



Virtual screening with
molecular docking



Lead discovery



Lead optimisation with
alchemical free energy
calculations