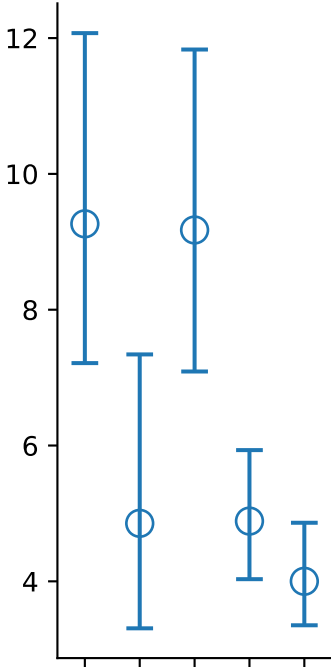


$G_{solv}$  (kJ/mol)

RMSE



FreeSolv ROH OpenFF 1.2.0

FreeSolv ROH after perturb\_32 BCC Fit

FreeSolv ROH after perturb\_5 BCC Fit

GSolv of perturb\_32 BCC Fit (Ether Sub-Set)

GSolv of perturb\_5 BCC Fit (Ether Sub-Set)