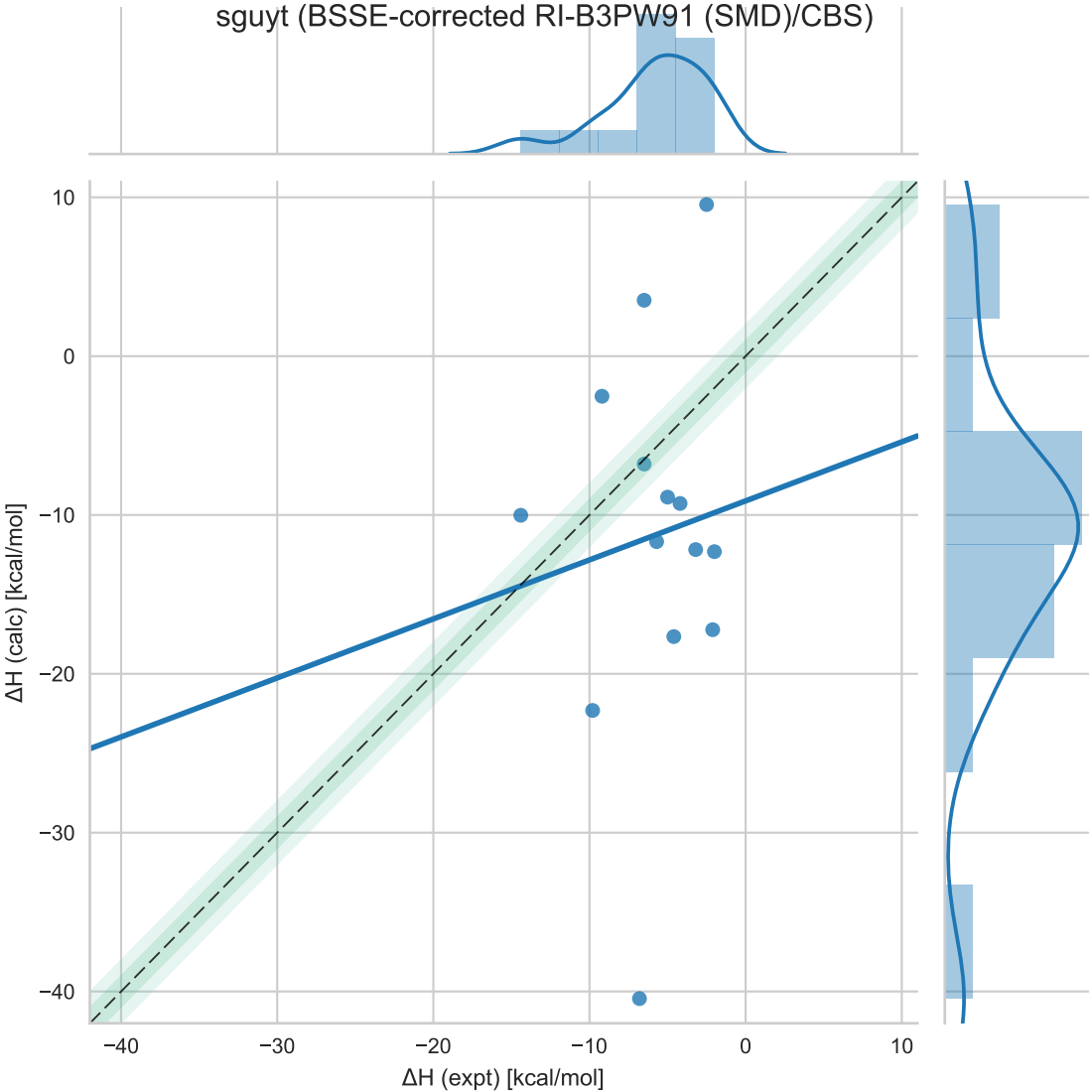
sguyt (BSSE-corrected RI-B3PW91 (SMD)/CBS)
ΔH (calc) [kcal/mol]
ΔH (expt) [kcal/mol]
10
0
−10
−20
−30
−40
−40
−30
−20
−10
0
10