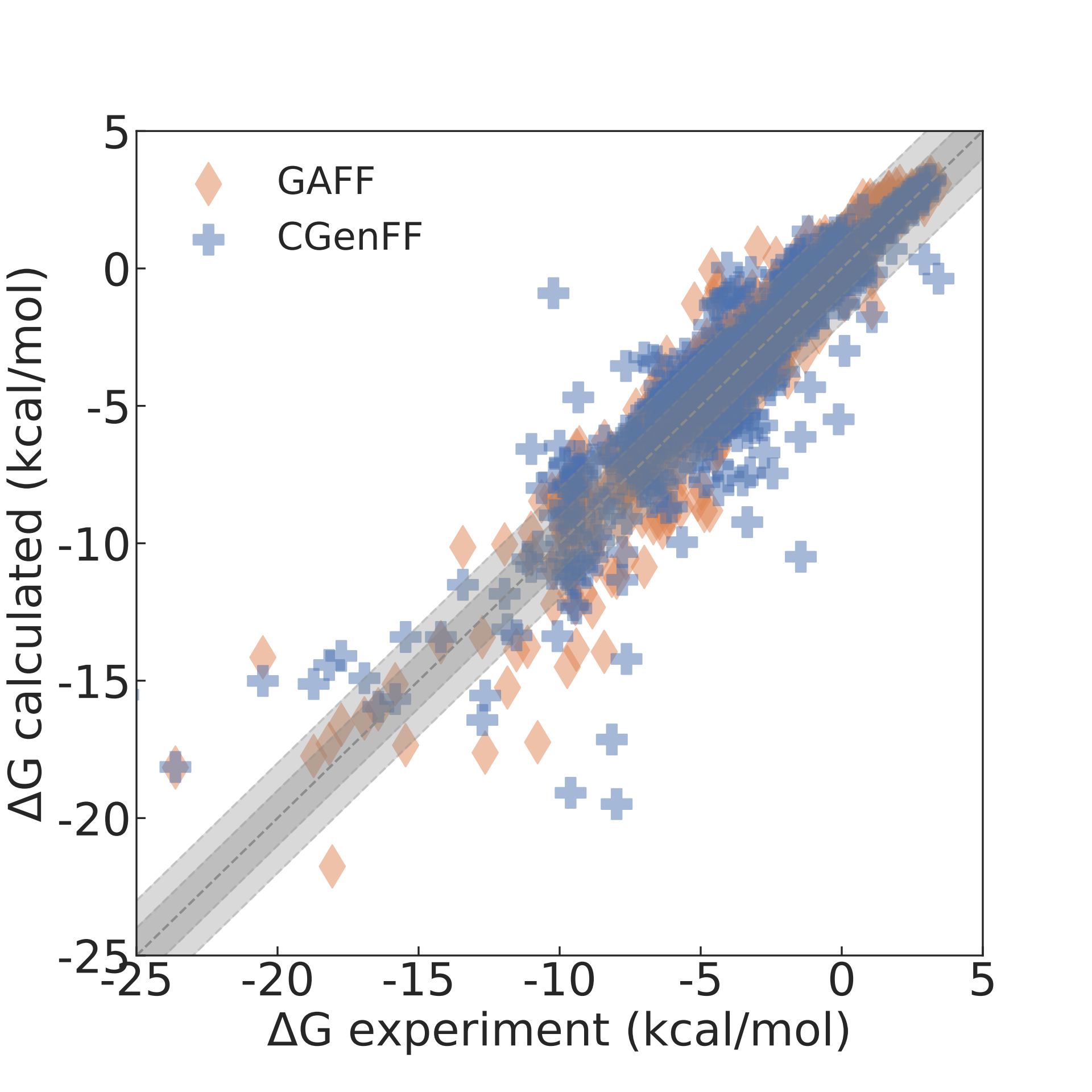
GAFF
CGenFF
ΔG calculated (kcal/mol)
ΔG experiment (kcal/mol)
5
0
-5
-10
-15
-20
-25
-25
-20
-15
-10
-5
0
5