SOMD/AM1BCC-GAFF-TIP3P/MBAR/C (f7duk + ibhca + wfs4v) ΑII -4 OA **TEMOA** CB8 -6 ΔG (calc) [kcal/mol] -8 -10 -12 -14 -16

-10

ΔG (expt) [kcal/mol]

-8

-6

-4

-12

-16

-14