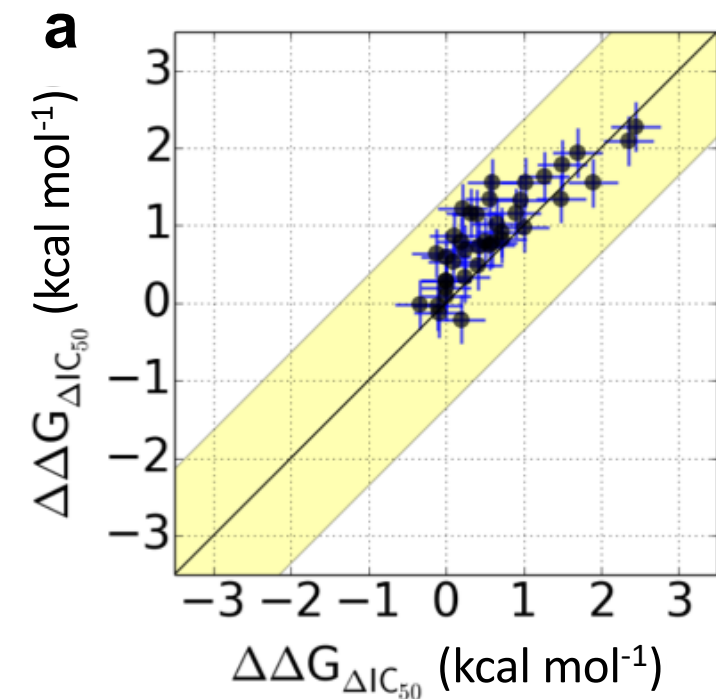
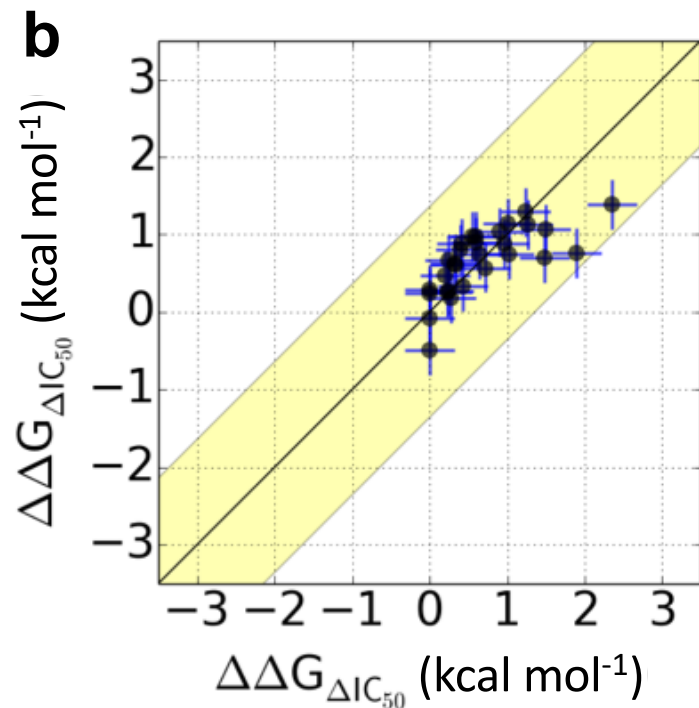


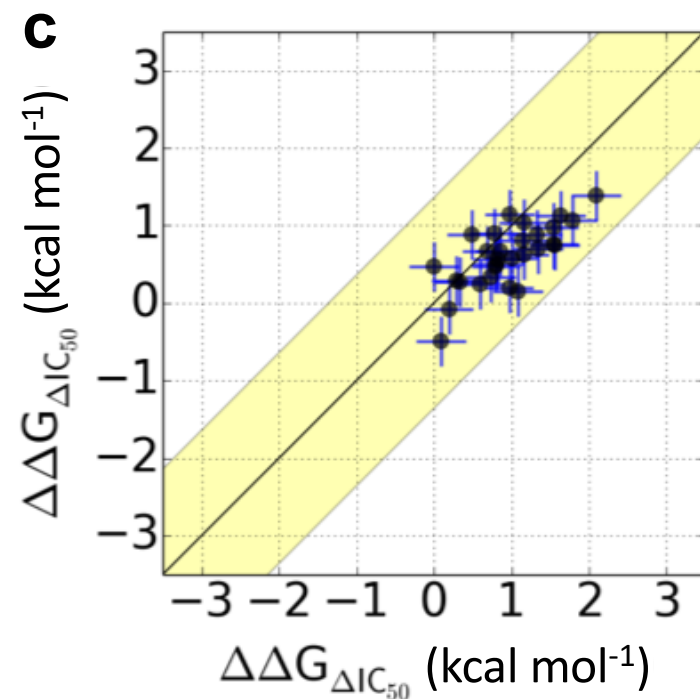
inter-lab ΔIC_{50}



N (samples)	39
RMSE (kcal mol ⁻¹)	0.45 ^{0.54} _{0.35}

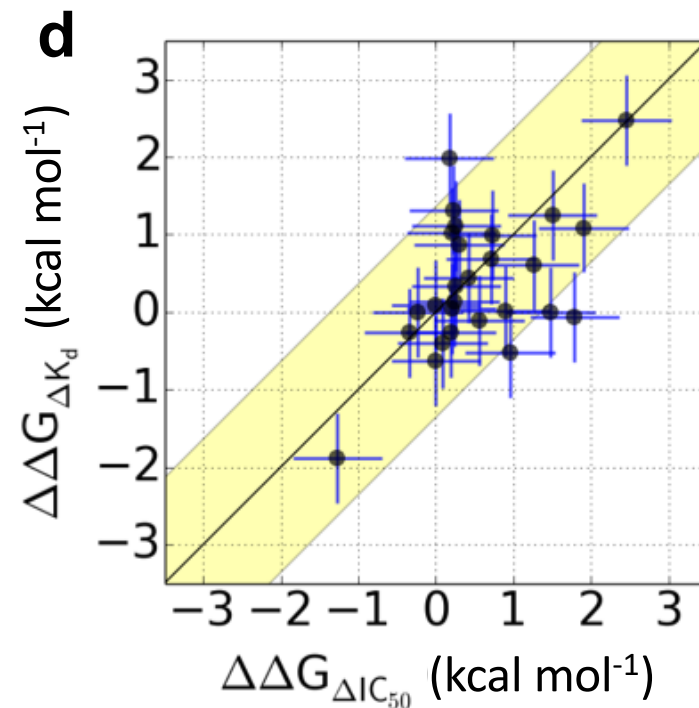


N (samples)	29
RMSE (kcal mol ⁻¹)	0.41 ^{0.54} _{0.28}



N (samples)	29
RMSE (kcal mol ⁻¹)	0.49 ^{0.57} _{0.40}

ΔK_d & ΔIC_{50}



N (samples)	27
RMSE (kcal mol ⁻¹)	0.81 ^{1.04} _{0.59}