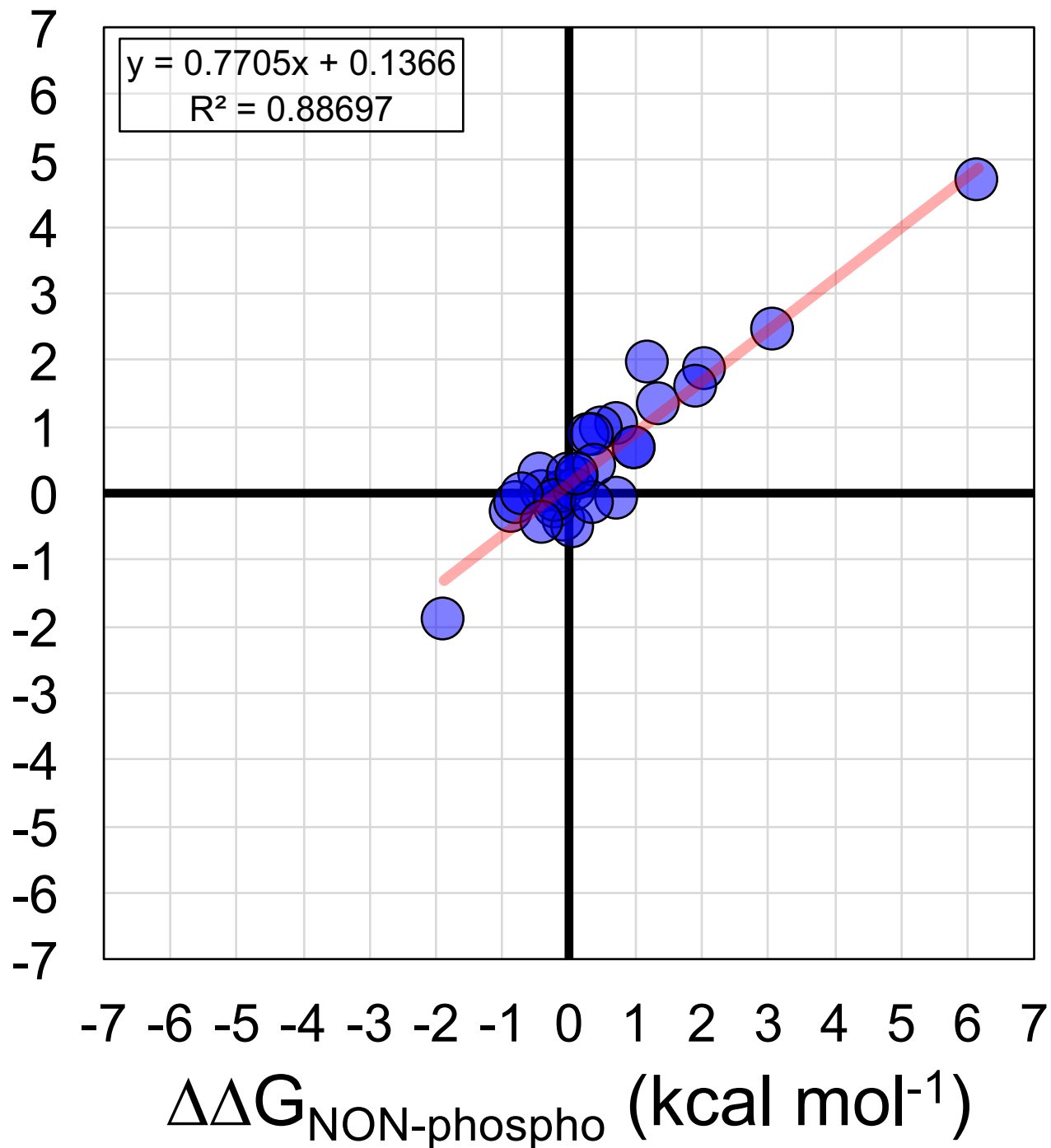


$\Delta\Delta G_{\text{phospho}}$  (kcal mol<sup>-1</sup>)



## Summary Statistics

Slope	0.77
Intercept (kcal mol <sup>-1</sup> )	0.14
Pearson's R	0.94
R <sup>2</sup>	0.89
RMSE (kcal mol <sup>-1</sup> )	0.50
MUE (kcal mol <sup>-1</sup> )	0.39
Accuracy (cut=1.36 kcal mol <sup>-1</sup> )	0.94
Specificity (cut=1.36 kcal mol <sup>-1</sup> )	0.96
Sensitivity (cut=1.36 kcal mol <sup>-1</sup> )	0.80

## Raw Data (adapted de Davis et al.)

TKI	ddG_NON-P (kcal mol <sup>-1</sup> )	ddG_phos (kcal mol <sup>-1</sup> )
axitinib	2.05	1.85
	1.37	1.32
	-0.86	-0.27
	0.74	1.02
	-1.88	-1.89
bosutinib	0.99	0.69
	-0.05	-0.40
	-0.39	0.00
	-0.20	-0.23
	3.08	2.47
dasatinib	0.74	-0.07
	0.06	-0.53
	-0.09	0.00
	0.15	0.20
	6.16	4.69
imatinib	1.20	1.98
	0.49	0.99
	1.00	0.67
	0.29	0.88
	ND	ND
nilotinib	0.35	0.87
	0.11	0.04
	-0.43	0.29
	0.00	0.29
	2.50	ND
gefitinib	1.92	1.59
	0.39	0.41
	-0.78	-0.16
	-0.22	-0.13
	0.38	-0.15
erlotinib	ND	1.36
	0.12	0.29
	-0.70	-0.03
	-0.41	-0.44
	ND	ND