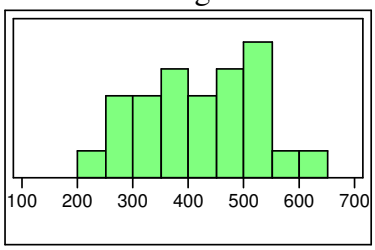
Figures and Tables

Figure 1: Histograms for molecular weight (a) and experimental free binding energy ΔG (b) of the training sets used for building the final COMBINE models of trypsin, thrombin, and urokinase. The molecular weight of the ligands were distributed between 100 and 650 Da and the experimental ΔG values (in kcal/mol) spanned in total a range of 11 log units with a maximum of 9 log units for a single training set. The training sets of thrombin and trypsin showed a larger distribution of the weight and the binding affinity than those of urokinase.

a) Weight distribution in Da.

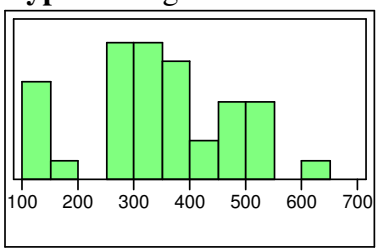
thrombin: weight



Moments

Mean	415,80422
Std Dev	108,00678
Std Err Mean	21,601357
upper 95% Mean	460,38723
lower 95% Mean	371,22121
N	25

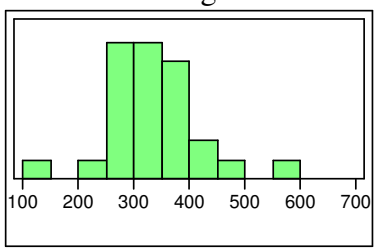
trypsin: weight



Moments

Mean	341,45241
Std Dev	129,48485
Std Err Mean	21,287179
upper 95% Mean	384,62481
lower 95% Mean	298,28001
N	37

urokinase: weight

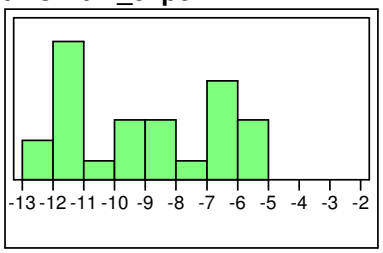


Moments

Mean	335,68962
Std Dev	87,581293
Std Err Mean	17,176105
upper 95% Mean	371,06447
lower 95% Mean	300,31477
N	26

b) Experimental ΔG values in kcal/mol.

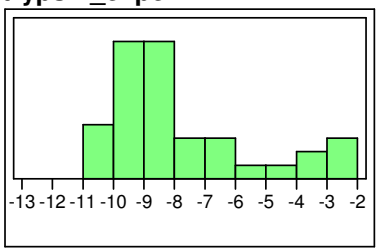
thrombin_exper



Moments

Mean	-9,122232
Std Dev	2,3496085
Std Err Mean	0,4699217
upper 95% Mean	-8,152362
lower 95% Mean	-10,0921
N	25

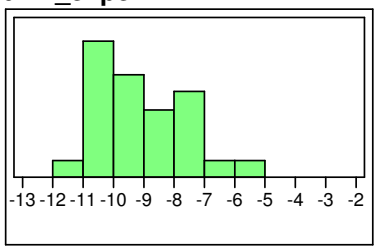
trypsin_exper



Moments

Mean	-7,807631
Std Dev	2,3617876
Std Err Mean	0,3882755
upper 95% Mean	-7,020172
lower 95% Mean	-8,595091
N	37

uPA_exper



Moments

Mean	-8,910829
Std Dev	1,5403823
Std Err Mean	0,3020938
upper 95% Mean	-8,288655
lower 95% Mean	-9,533003
N	26

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