Supplement Material to Improvement in protein functional site prediction using
all atom computational protein design

Table 1 Contributions from different sources of information on the accuracy of functional
site prediction

Model Name	Residual Deviance*
SCORECONS	10802
Natural/designed sequence profile difference	12753
Native-optimal residue energy difference	12539
SCORECONS + Profile Difference	10698
SCORECONS + Native/optimal residue energy difference	10706
SCORECONS + Natural/designed sequence profile difference + Native optimal residue energy difference	10606

*The residual deviance of different models were obtained using logistic regressions.
Residual deviance represents the how good the model is for the data.

Table 2 The statistics of the combined model.

	Coefficient	Z value*	Pr(>|z|)**
Scorecons score	6.0	38	<2e-16
Natural/designed sequence profile difference	1.0	9.5	<2e-16
Native/optimal residue energy difference	0.18	9.7	<2e-16

*Z value is from Ward test which represent the significance of the coefficient.

**Pr(Z) is the probability of the coefficient is random according to the Z value..