

Table 4. Binding prediction accuracy of ISC-PLS algorithm for MHC class II alleles having small data sets

	ISC-PLS	ISC-PLS of 0401 ¹	Mod. 1: Regression fit	Mod. 1: Regression fit of 0401 ²	Alt. 1: Length as variable	Mod. 2: Equil. formula
DRB1*0404	0.462 ± 0.017	0.468	0.410 ± 0.033	0.458 ± 0.029	0.390 ± 0.020	0.439 ± 0.032
DRB1*0405	0.664 ± 0.014	0.542	0.682 ± 0.013	0.625 ± 0.008	0.680 ± 0.015	0.742 ± 0.010

Five-fold cross-validation (5x-CV) was used and repeated five times. Mean A_{ROC} scores between predicted and experimentally determined $pI_{C_{50}}$ values are shown with standard errors of the mean. Highest scores are shown in bold with multiple scores in bold if pair-wise differences were not statistically significant. A threshold of 500 nM (Sette 1994) was used to distinguish binding from non-binding peptides. ¹The ISC-PLS algorithm was derived for the DRB1*0401 data set first and then used to make predictions on the peptides in the *0404 or *0405 data sets. Note: no standard error is listed in this case due to the lack of different training and test sets which provide the basis for obtaining multiple AROC scores and subsequently standard error. ²The regression fit for DRB1*0401 was used as the basis of the modification rather than the regression fit for *0404 or *0405.