**Table 2.** Binding prediction accuracy of ISC-PLS algorithm for different MHC class II alleles when peptide length was incorporated

| DRB1*0101 | ISC-PLS | **Mod. 1**: Regression fit | **Alt. 1**: Length as variable |
|---|---|---|---|
| Combination rule | 0.291 ± 0.017[1] | 0.496 ± 0.014 | 0.411 ± 0.020 |
| Highest scoring register | 0.345 ± 0.009 | 0.501 ± 0.012 | 0.419 ± 0.017 |
| **Mod. 2**: Equilibrium formula | 0.440 ± 0.006 | 0.496 ± 0.017 | 0.463 ± 0.018 |

| DRB1*0401 | ISC-PLS | **Mod. 1**: Regression fit | **Alt. 1**: Length as variable |
|---|---|---|---|
| Combination rule | 0.459 ± 0.011[1] | 0.498 ± 0.018 | 0.486 ± 0.015 |
| Highest scoring register | 0.457 ± 0.011 | 0.502 ± 0.013 | 0.491 ± 0.004 |
| **Mod. 2**: Equilibrium formula | 0.501 ± 0.010 | 0.519 ± 0.003 | 0.513 ± 0.009 |

| DRB1*1501 | ISC-PLS | **Mod. 1**: Regression fit | **Alt. 1**: Length as variable |
|---|---|---|---|
| Combination rule | 0.147 ± 0.007[1] | 0.201 ± 0.023 | 0.136 ± 0.030 |
| Highest scoring register | 0.162 ± 0.008 | 0.219 ± 0.020 | 0.150 ± 0.014 |
| **Mod. 2**: Equilibrium formula | 0.157 ± 0.025 | 0.275 ± 0.025 | 0.147 ± 0.027 |

Five-fold cross-validation (5x-CV) was used and repeated five times. The mean Pearson correlation coefficient between predicted and experimentally determined $pIC_{50}$ values is shown along with standard errors of the mean. [1]The ISC-PLS algorithm with combination rule (Doytchinova 2003) was used as a baseline prediction.