| Training set | Surface measure | parameter | AUC on evaluation set |
|---|---|---|---|
| **2,3,4,5** | FS | $k$ = 18 | 0.6699 |
| | UHS | $k$ = 14 | 0.6092 |
| | Ta | $T$ = 18 | 0.6783 |
| | RSA | | 0.6437 |
| | HSE | $k$ = 18 | 0.6576 |
| **1,3,4,5** | FS | $k$ = 18 | 0.6875 |
| | UHS | $k$ = 14 | 0.6459 |
| | Ta | $T$ = 16 | 0.6935 |
| | RSA | | 0.664 |
| | HSE | $k$ = 16 | 0.6719 |
| **1,2,4,5** | FS | $k$ = 18 | 0.7047 |
| | UHS | $k$ = 14 | 0.6992 |
| | Ta | $T$ = 16 | 0.7071 |
| | RSA | | 0.6827 |
| | HSE | $k$ = 18 | 0.7035 |
| **1,2,3,5** | FS | $k$ = 22 | 0.6230 |
| | UHS | $k$ = 14 | 0.6343 |
| | Ta | $T$ = 16 | 0.6292 |
| | RSA | | 0.6347 |
| | HSE | $k$ = 18 | 0.6481 |
| **1,2,3,4** | FS | $k$ = 22 | 0.7051 |
| | UHS | $k$ = 12 | 0.7041 |
| | Ta | $T$ = 18 | 0.7234 |
| | RSA | | 0.6962 |
| | HSE | $k$ = 18 | 0.7402 |

**Table S3. Results of cross-validation of surface exposure measures.** The data were split in 5 datasets, where 4 were used for training of parameters and the remaining dataset for evaluation of surface measure performance. The surface exposure measures were tested for their ability to predict epitopes, and parameters were estimated by a one-dimensional grid search as described in methods.