

Supplementary Table 1: Comparison of NetMHCIIpan-4.0 prediction to empirical data

| No | Pos | Seq | Computational (100-%Rank) | | Empirical (%competition) | | BA vs RIPPA | | EL vs RIPPA | | BA+EL vs RIPPA | | ELISA vs RIPPA | | IC50vHA306-318 | Comments |
|-----|-----|--------------------|---------------------------|-------------|--------------------------|--------------|-------------|----------|-------------|----------|----------------|------------------|----------------|-------------|----------------|------------------------|
| No | Pos | Seq | 100-%RankB | 100-%RankEL | RIPPA (Flow) | sDR4 (ELISA) | RIPPA false | BA false | RIPPA false | EL false | RIPPA false | Prediction false | RIPPA false | ELISA false | IC50 | Comments |
| 4 | 22 | TQLPPAYTNSFTRGVYY | 77.93 | 81.67 | 61.4352688 | 71.8123111 | | 1 | | 1 | | 1 | | | | binder |
| 5 | 29 | TNSFTRGVYYPDKVFRS | 96.34 | 93.44 | 68.2588881 | 80.2509847 | | | | | | | | | | binder |
| 6 | 36 | VYYPDKVFRSSVLHSTQ | 97.94 | 91.04 | 71.8359318 | 91.8338371 | | | | | | | | | | binder |
| 8 | 50 | STQDLFLPFFSNVTWFH | 96.65 | 75.36 | 0 | 26.4999542 | | 1 | | | | | | | | non-binder |
| 9 | 57 | PPFSNVTWFHAIHVSQT | 95.27 | 63.91 | 3.6033938 | 34.9821379 | | 1 | | | | | | | | non-binder |
| 10 | 64 | WFHAIHVSQTNGTKRFD | 94.55 | 93.9 | 74.4633008 | 70.3993771 | | | | | | | | | | binder |
| 13 | 85 | PFNDGVYFASTEKSNII | 95.54 | 98.94 | 75.3388373 | 67.2666483 | | | | | | | | | | strong binder |
| 15 | 99 | NIIRGWIFGTTLDLSTQ | 96.11 | 95.52 | 80.624436 | 76.1198131 | | | | | | | | | | strong binder |
| 17 | 113 | KTQSLILVNNATNVVVK | 99.16 | 91.99 | 0 | 0.6938719 | | 1 | | 1 | | | | | tested | non-binder |
| 21 | 141 | LGVYYHKNKNSWMESEF | 83.4 | 73.47 | 78.8901171 | 72.3619126 | | 1 | | 1 | | | | | tested | binder |
| 23 | 155 | SEFRVYSSANNCTFEYV | 97.08 | 74.95 | 7.93650794 | 26.7289548 | | 1 | | | | | | | | non-binder |
| 25 | 169 | EYVSQPFMLDLEKQGN | 77.5 | 92.03 | 63.8703408 | 79.5685628 | | 1 | | | | | | | | binder |
| 29 | 197 | IDGYFKIYSKHTPINLV | 90.51 | 85 | 0 | 15.6773839 | | 1 | | | | | | | | non-binder |
| 30 | 204 | YSKHTPINLVRDLPQGF | 86.29 | 94.72 | 51.2287105 | 75.4648713 | | 1 | | | | | | | | binder |
| 34 | 232 | GINITRFQTLALHRSY | 98.75 | 92.54 | 58.410649 | 67.4344186 | | | | | | | | | | binder |
| 35 | 239 | QTLALHRSYLTPGDSS | 84.13 | 53.11 | 63.6121879 | 56.5951259 | | 1 | | 1 | | | | | | binder |
| 40 | 274 | TFLLYNENGTITDAVD | 86.1 | 90.7 | 27.7886652 | 52.0289457 | | | | | | | | | | weak binder/non-binder |
| 41 | 281 | ENGTITDAVDCALDPLS | 37.79 | 58.56 | 57.8167308 | 25.5335715 | 1 | | 1 | | 1 | | 1 | | | non-binder |
| 44 | 302 | TLKSFTVEKGIYQTSNF | 95.98 | 97.15 | 87.7169907 | 89.1590247 | | | | | | | | | | strong binder |
| 45 | 309 | EKGIYQTSNFRVQPTES | 83.09 | 86.9 | 61.2305843 | 76.1312632 | | 1 | | 1 | | | | | | binder |
| 46 | 316 | SNFRVQPTESIVRFPNI | 99.03 | 95.98 | 61.452514 | 84.986718 | | | | | | | | | | strong binder |
| 50 | 344 | ATRFASVYAWNRKRISN | 91.5 | 74.24 | 0 | 17.149858 | | 1 | | | | | | | | non-binder |
| 52 | 358 | ISNCVADYSVLYNSASF | 97.12 | 91.96 | 61.169175 | 91.439956 | | | | | | | | | | strong binder |
| 53 | 365 | YSVLYNSASFSTFKCYG | 93.06 | 46.52 | 0 | 35.2294586 | | 1 | | | | | | | | non-binder |
| 57 | 393 | TNVYADSFVIRGDEVRO | 73.89 | 90.55 | 74.3406826 | 86.5828524 | | 1 | | | | | | | | strong binder |
| 62 | 428 | DFTGCVIAWNSNLDLSD | 93.58 | 92.87 | 0 | 35.6279198 | | 1 | | | | | | | | non-binder |
| 67 | 463 | PFERDISTEIQAGSTP | 72.19 | 65.58 | 74.8431367 | 62.041232 | | 1 | | 1 | | | | | tested | weak binder |
| 68 | 470 | TEIQAGSTPCNGVEGF | 68.56 | 81.88 | 85.4190191 | 79.270862 | | 1 | | 1 | | | | | | strong binder |
| 70 | 484 | EGFNCFPLQSYGFQPT | 72.79 | 58.57 | 58.2807658 | 72.9815759 | | 1 | | 1 | | | | | | binder |
| 71 | 491 | PLQSYGFQPTNGVGYQP | 91.79 | 98.8 | 90.203137 | 94.7787854 | | | | | | | | | | strong binder |
| 74 | 512 | VLSFELLHAPATVCGPK | 93.76 | 80.54 | 63.1536595 | 75.6358441 | | | | 1 | | | | | tested | strong binder |
| 83 | 575 | AVRDPQTLLEILITPCS | 56.5 | 48.44 | 54.9343159 | 60.4882294 | | 1 | | 1 | | | | | | weak binder |
| 84 | 582 | LEILDITPCSFQGVSVI | 54.62 | 9.87 | 60.6553144 | 46.8306311 | | 1 | | 1 | | | | | | weak binder |
| 88 | 610 | VLYQDVNCTEVPVAIHA | 63.52 | 77.88 | 63.6406444 | 53.2838692 | | 1 | | 1 | | | | | | weak binder |
| 90 | 624 | IHADQLTPTRVYSTGS | 59.82 | 37.46 | 59.2785919 | 29.7426033 | 1 | | 1 | | 1 | | | 1 | | non-binder/weak binder |
| 91 | 631 | PTWRVYSTGSNVFQTRA | 97.64 | 92.63 | 56.3157161 | 67.4758341 | | | | | | | | | | binder |
| 93 | 645 | TRAGCLIGAEHVNNSEYE | 65.31 | 86.93 | 87.0401274 | 59.4899093 | | 1 | | 1 | | | | | tested | binder |
| 94 | 652 | GAEHVNNSEYCDIPIGA | 54.09 | 72.2 | 70.6229467 | 0 | 1 | | 1 | | 1 | | | | tested | non-binder |
| 96 | 666 | IGAGICASYQTQTNNSPR | 58.48 | 49.66 | 56.9619623 | 5.4781777 | 1 | | 1 | | 1 | | | | | non-binder |
| 99 | 687 | VASQSIIAYTMLGAEN | 94.97 | 87.97 | 89.7061174 | 92.5010982 | | | | | | | | | tested | strong binder |
| 100 | 694 | AYTMLGAENSVAYSNN | 91.72 | 75.54 | 60.3482817 | 54.46877 | | | | 1 | | | | | | binder |

| | | | | | | | | | | | | | | |
|-----|------|---------------------|-------|-------|------------|------------|---|---|---|--|---|--|---|------------------------|
| 101 | 701 | AENSVAYSNNNSIAIPTN | 92.02 | 95.16 | 81.3993624 | 41.0062276 | | | | | | | 1 | binder |
| 103 | 715 | PTNFTISVTEILPVSM | 93.71 | 87.72 | 76.6549648 | 71.1284529 | | 1 | | | | | | binder |
| 106 | 736 | VDC'TMYICGDS'FECSNL | 55.33 | 56.64 | 71.3851967 | 31.8483682 | 1 | | 1 | | 1 | | 1 | non-binder/weak binder |
| 108 | 750 | SNLLQYGSFCTQLNRA | 85.97 | 51.66 | 67.1329343 | 2.7158325 | 1 | | 1 | | 1 | | 1 | non-binder |
| 109 | 757 | GSFCTQLNRALTGIAVE | 94.34 | 50.92 | 85.9082099 | 86.2037779 | | | 1 | | | | | strong binder |
| 110 | 764 | NRALTGIAVEQDKNTQE | 57.65 | 92.11 | 41.6959337 | 17.4085406 | | | 1 | | | | | non-binder |
| 115 | 799 | GFNFSQILPDPSPSKR | 95.51 | 99.08 | 78.9364026 | 79.2216853 | | | | | | | | strong binder |
| 122 | 848 | DLICAKFNGLTVLPPL | 94.32 | 73.22 | 3.0559766 | 0 | 1 | | | | | | | non-binder |
| 128 | 890 | AGAALQIPFAMQMAYRF | 92.34 | 31.21 | 44.0454506 | 1.2480943 | 1 | | | | | | | non-binder |
| 129 | 897 | PFAMQMAYRFNGIGVTQ | 93.09 | 60.87 | 0 | 0 | 1 | | | | | | | non-binder |
| 132 | 918 | ENQKLIANQFNSAIGKI | 96.2 | 87.79 | 79.1782757 | 41.4274271 | | | 1 | | 1 | | 1 | weak binder |
| 133 | 925 | NQFNSAIGKIQDLSLST | 79.18 | 86.87 | 80.2636166 | 20.5483346 | 1 | | 1 | | 1 | | 1 | weak binder |
| 134 | 932 | GKIQDLSLSTASALGKL | 90.72 | 90.4 | 91.6756734 | 94.340939 | | | | | | | | strong binder |
| 138 | 960 | NTLVKQLSSNFGAIVSV | 93.35 | 87.99 | 81.5863751 | 75.224166 | | | 1 | | | | | strong binder |
| 139 | 967 | SSNFGAIVSVLNDILSR | 97.63 | 88.04 | 71.9691514 | 28.2048632 | | | 1 | | 1 | | 1 | weak binder |
| 144 | 1002 | OSLQTYVVTQQLIRAAET | 97.2 | 91.7 | 81.3095383 | 93.1135171 | | | | | | | | strong binder |
| 145 | 1009 | TQQLIRAAEIRASANLA | 95.94 | 89.62 | 53.1983002 | 51.266312 | | | 1 | | | | | weak binder |
| 146 | 1016 | AEIRASANLAATKMSEC | 99.15 | 94.83 | 81.8672874 | 82.624874 | | | | | | | | strong binder |
| 150 | 1044 | GKGYHLMSFPQSAPHGV | 91.29 | 84.77 | 49.3835201 | 24.3055376 | 1 | | | | | | | non-binder |
| 152 | 1058 | HGVVFLHVTYVPAQEKV | 94.08 | 93.25 | 62.0561464 | 31.5201943 | | | | | | | 1 | weak binder |
| 154 | 1072 | EKNFTTAPAICHDKGAH | 92.68 | 90.41 | 41.3924826 | 10.4963953 | 1 | | 1 | | 1 | | 1 | non-binder |
| 157 | 1093 | GVFVSNQTHWFVTQRNF | 91.54 | 58.47 | 54.5194471 | 38.2568025 | | | | | | | | weak binder |
| 158 | 1100 | THWFVTQRNFYEPQIIT | 97.8 | 94.92 | 64.9437324 | 93.4778676 | | | | | | | | binder |
| 160 | 1114 | IITDNTFVSGNCDVVI | 65.75 | 56.61 | 57.2028519 | 10.9020905 | 1 | | 1 | | 1 | | 1 | non-binder |
| 165 | 1149 | KEELDKYFKNHTSPDVD | 80.45 | 95.49 | 31.951954 | 20.2640895 | | | 1 | | | | 1 | non-binder |
| 177 | 1233 | MLCCMTSCSCSLKCCS | 37.39 | 5 | 61.8346859 | 16.3854363 | 1 | | 1 | | 1 | | 1 | non-binder |
| 180 | 1254 | CKFDEDDSEPVLKGVKL | 35.84 | 75.5 | 69.1776149 | 60.7199152 | | 1 | 1 | | 1 | | 1 | weak binder |

False identification side-by-side (counts)

False identification side-by-side (%)

8 29 8 27 8 17 6 5
4.4198895 16.0221 4.4198895 14.917 4.41989 9.392265193 3.3149171 2.762431

| | | | | |
|------------------------------------|-----------|-------------|------------|------------|
| Potential false positives (counts) | 13 | 5 | 8 | 0 |
| Potential false negatives (count) | 17 | 23 | 1 | 7 |
| Potential false positives (%) | 7.1823204 | 2.762430939 | 4.4198895 | 0 |
| Potential false negatives (%) | 9.3922652 | 12.70718232 | 0.55248619 | 3.86740331 |
| False identification (counts) | 30 | 28 | 9 | 7 |
| False identification (FDR) | 16.574586 | 15.46961326 | 4.97237569 | 3.86740331 |

This number assumes ELISA identifies the rest 113 peptides as non-binder

18 agreements (red/pink fill), 50 disagreements between prediction and yeast display. The rest 113 non-binders were not evaluated by capture ELISA.

In the capture ELISA, 1 uM Bio-HA306-318 and 40 uM of a competitor peptide were used

Means of at least three independent experiments are shown