

Supplementary Files

Computer Aided Multi-Epitopes Vaccine Design against *Enterobacter Xiangfangensis*

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Table S1. T-cells epitopes for the B-cell epitopes.

| MHC-I | Percentile score | MHC-II | Percentile score |
|------------|------------------|---------------------|------------------|
| ETITVTAAPA | 0.15 | EETITVTAAPAAQES | 0.36 |
| TAAPAAQES | 3.4 | | |
| GPAPTIAAKR | 0.03 | AWGPAPTIAAKRTATA | 4.1 |
| ATKTDTPIEK | 0.02 | TATKTDTPIEKTPQ | 0.39 |
| VTREEMDMK | 0.46 | QSISSVVTREEMDMKQPGT | 8.01 |
| QSISSVVTRE | 4.3 | | |
| TEPLKEIQF | 0.31 | TTEPLKEIQFKMGT | 9.2 |
| QFKMGTDNLW | 1.2 | QFKMGTDNLWQTGFD | 20 |
| VVPYYDANGK | 0.89 | EGTVVPYYDANGKAH | 9.9 |
| EGDEDNKISR | 2.5 | TDFNEGDEDNKISRR | 36 |
| VVPYYDANGK | 0.89 | GTVVPYYDANGK | 6.2 |
| EGDEDNKISR | 2 | FNEGDEDNKISR | 20 |
| RNNGTTAEI | 2.9 | SAFNRNNGTTAEI | 0.94 |
| TTAEINDQA | 0.06 | NNGTTAEINDQAF | 9.1 |
| RNNGTTAEI | 2.9 | AFNRNNGTTAEI | 1.1 |
| RNNGTTAEI | 2.9 | NGTTAEINDQAF | 7.5 |
| ADPANPTSGF | 13 | ADPANPTSGFSV | 22 |
| ADPANPTSGF | 0.13 | VTYYSSASPKA | 0.29 |
| ASPKAYESF | 0.28 | ASPKAYESFNV | 11 |
| QARLQMQQL | 0.12 | EQARLQMQQLQQNNI | 0.06 |
| MQQLQQNNI | 2.3 | | |
| IVYFDLDKY | 0.15 | NNIVYFDLDKYDIRS | 0.71 |
| DLDKYDIRS | 6.5 | | |
| GMDANGNGNM | 6.7 | GTGMDANGNGNMSSE | 28 |
| ASNDQSGEGM | 1.5 | ASNDQSGEGMMGAGT | 14 |
| GTPEYNISL | 0.51 | ERGTPEYNISL | 50 |
| AVLGHDEAAY | 0.28 | KPAVLGHDEAAYSKN | 9.1 |
| YGKEKPAVL | 0.01 | SYGKEKPAVLGHDEA | 34 |

Table S2. Allele for major histocompatibility complex- I.

| Allele | Length |
|---------------|---------------|
| HLA-A*01:01 | 9 |
| HLA-A*01:01 | 10 |
| HLA-A*02:01 | 9 |
| HLA-A*02:01 | 10 |
| HLA-A*02:03 | 9 |
| HLA-A*02:03 | 10 |
| HLA-A*02:06 | 9 |
| HLA-A*02:06 | 10 |
| HLA-A*03:01 | 9 |
| HLA-A*03:01 | 10 |
| HLA-A*11:01 | 9 |
| HLA-A*11:01 | 10 |
| HLA-A*23:01 | 9 |
| HLA-A*23:01 | 10 |
| HLA-A*24:02 | 9 |
| HLA-A*24:02 | 10 |
| HLA-A*26:01 | 9 |
| HLA-A*26:01 | 10 |
| HLA-A*30:01 | 9 |
| HLA-A*30:01 | 10 |
| HLA-A*30:02 | 9 |
| HLA-A*30:02 | 10 |
| HLA-A*31:01 | 9 |
| HLA-A*31:01 | 10 |
| HLA-A*32:01 | 9 |
| HLA-A*32:01 | 10 |
| HLA-A*33:01 | 9 |

| | |
|-------------|----|
| HLA-A*33:01 | 10 |
| HLA-A*68:01 | 9 |
| HLA-A*68:01 | 10 |
| HLA-A*68:02 | 9 |
| HLA-A*68:02 | 10 |
| HLA-B*07:02 | 9 |
| HLA-B*07:02 | 10 |
| HLA-B*08:01 | 9 |
| HLA-B*08:01 | 10 |
| HLA-B*15:01 | 9 |
| HLA-B*15:01 | 10 |
| HLA-B*35:01 | 9 |
| HLA-B*35:01 | 10 |
| HLA-B*40:01 | 9 |
| HLA-B*40:01 | 10 |
| HLA-B*44:02 | 9 |
| HLA-B*44:02 | 10 |
| HLA-B*44:03 | 9 |
| HLA-B*44:03 | 10 |
| HLA-B*51:01 | 9 |
| HLA-B*51:01 | 10 |
| HLA-B*53:01 | 9 |
| HLA-B*53:01 | 10 |
| HLA-B*57:01 | 9 |
| HLA-B*57:01 | 10 |
| HLA-B*58:01 | 9 |
| HLA-B*58:01 | 10 |

Table S3. Allele for Major histocompatibility complex- II.

HLA-DRB1*01:01
HLA-DRB1*03:01
HLA-DRB1*04:01
HLA-DRB1*04:05
HLA-DRB1*07:01
HLA-DRB1*08:02
HLA-DRB1*09:01
HLA-DRB1*11:01
HLA-DRB1*12:01
HLA-DRB1*13:02
HLA-DRB1*15:01
HLA-DRB3*01:01
HLA-DRB3*02:02
HLA-DRB4*01:01
HLA-DRB5*01:01
HLA-DQA1*05:01/DQB1*02:01
HLA-DQA1*05:01/DQB1*03:01
HLA-DQA1*03:01/DQB1*03:02
HLA-DQA1*04:01/DQB1*04:02
HLA-DQA1*01:01/DQB1*05:01
HLA-DQA1*01:02/DQB1*06:02
HLA-DPA1*02:01/DPB1*01:01
HLA-DPA1*01:03/DPB1*02:01
HLA-DPA1*01:03/DPB1*04:01
HLA-DPA1*03:01/DPB1*04:02
HLA-DPA1*02:01/DPB1*05:01
HLA-DPA1*02:01/DPB1*14:01

Table S4. Pairs of amino acid residues opted for disulfide engineering with Chi3 energy in kal/mol and sum B-factors.

| Amino acid pair | Chi3 | Energy | Sum B-Factors |
|------------------------|-------------|---------------|----------------------|
| Ile2-Phe10 | -91.41 | 4.28 | 0 |
| Leu13-Ile26 | 113.98 | 4.19 | 0 |
| Ala17-26ile | 76.34 | 4.65 | 0 |
| Thr27-Thr40 | -65.95 | 5.22 | 0 |
| Cys30-Tyr39 | -59.73 | 4.07 | 0 |
| Ser47-Met58 | -62.7 | 4.74 | 0 |
| Thr49-Ile61 | -104.97 | 3.37 | 0 |
| Ala53-Val71 | 100.43 | 6.44 | 0 |
| Phe63-Ala67 | 106.67 | 5.37 | 0 |
| Met89-109 | -80.15 | 0.59 | 0 |
| Ile95-Thr99 | -75.18 | 4.45 | 0 |
| Glu100-Ile120 | 113.9 | 6.54 | 0 |
| Val103-Ala119 | 104.46 | 5.76 | 0 |
| Ala119-Ala132 | 74.01 | 2.77 | 0 |
| Ser121-Pro133 | 111.77 | 2.74 | 0 |
| Met122-Ala126 | 91.55 | 2.7 | 0 |
| Thr134-Ile168 | 95.21 | 1.38 | 0 |
| Ala136-Gly142 | -82.34 | 5.23 | 0 |

Table S5. Population coverage analysis of vaccine epitopes.

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| | | | | | | | | | |
|----------------------------|------------|------|----------|------------|------|----------|------------|-------|----------|
| Belarus Caucasoid | 0.0% | 0.0 | 0.0 | 43.81 % | 1.41 | 0.5 3 | 43.81 % | 1.41 | 0.5 3 |
| | | | | | | | | | |
| Belgium | 99.39 % | 6.66 | 4.6 7 | 79.39 % | 3.11 | 1.4 6 | 99.87 % | 9.77 | 6.9 5 |
| | | | | | | | | | |
| Belgium Caucasoid | 99.39 % | 6.66 | 4.6 7 | 79.39 % | 3.11 | 1.4 6 | 99.87 % | 9.77 | 6.9 5 |
| | | | | | | | | | |
| Bolivia | 0.0% | 0.0 | 0.0 | 77.82 % | 2.79 | 1.3 5 | 77.82 % | 2.79 | 1.3 5 |
| | | | | | | | | | |
| Bolivia Amerindian | 0.0% | 0.0 | 0.0 | 77.82 % | 2.79 | 1.3 5 | 77.82 % | 2.79 | 1.3 5 |
| | | | | | | | | | |
| Borneo | 0.0% | 0.0 | 0.0 | 49.02 % | 1.62 | 0.5 9 | 49.02 % | 1.62 | 0.5 9 |
| | | | | | | | | | |
| Borneo Austronesia n | 0.0% | 0.0 | 0.0 | 49.02 % | 1.62 | 0.5 9 | 49.02 % | 1.62 | 0.5 9 |
| | | | | | | | | | |
| Brazil | 96.1% | 5.85 | 3.6 9 | 63.8% | 2.3 | 0.8 3 | 98.59 % | 8.16 | 5.2 2 |
| | | | | | | | | | |
| Brazil Amerindian | 93.24 % | 4.12 | 3.1 9 | 48.6% | 1.55 | 0.5 8 | 96.52 % | 5.67 | 3.6 6 |
| | | | | | | | | | |
| Brazil Caucasoid | 99.32 % | 7.37 | 5.2 9 | 84.39 % | 3.49 | 1.9 2 | 99.89 % | 10.86 | 7.8 2 |
| | | | | | | | | | |
| Brazil Mixed | 97.02 % | 6.41 | 3.9 9 | 77.5% | 3.03 | 1.3 3 | 99.33 % | 9.44 | 6.4 1 |
| | | | | | | | | | |
| Brazil Mulatto | 0.0% | 0.0 | 0.0 | 74.09 % | 2.85 | 1.1 6 | 74.09 % | 2.85 | 1.1 6 |
| | | | | | | | | | |
| Bulgaria | 99.42 % | 7.1 | 5.1 | 57.23 % | 2.01 | 0.7 | 99.75 % | 9.11 | 6.4 6 |
| | | | | | | | | | |
| Bulgaria Caucasoid | 99.52 % | 7.2 | 5.2 6 | 57.23 % | 2.01 | 0.7 | 99.79 % | 9.21 | 6.5 3 |
| | | | | | | | | | |
| Bulgaria Other | 99.58 % | 6.19 | 4.3 1 | 0.0% | 0.0 | 0.0 | 99.58 % | 6.19 | 4.3 1 |

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| | | | | | | | | | |
|-------------------------|---------|------|-------|---------|------|-------|---------|------|-------|
| Chile Mixed | 90.09 % | 4.82 | 3.0 1 | 52.65 % | 1.83 | 0.6 3 | 95.31 % | 6.64 | 3.7 3 |
| | | | | | | | | | |
| China | 94.57 % | 5.41 | 3.4 3 | 59.99 % | 2.15 | 0.7 5 | 97.83 % | 7.57 | 4.5 3 |
| | | | | | | | | | |
| China Oriental | 94.57 % | 5.41 | 3.4 3 | 59.99 % | 2.15 | 0.7 5 | 97.83 % | 7.57 | 4.5 3 |
| | | | | | | | | | |
| Colombia | 8.36% | 0.25 | 0.3 3 | 54.02 % | 1.88 | 0.6 5 | 57.86 % | 2.13 | 0.7 1 |
| | | | | | | | | | |
| Colombia Amerindian | 0.0% | 0.0 | 0.0 | 47.4% | 1.59 | 0.5 7 | 47.4% | 1.59 | 0.5 7 |
| | | | | | | | | | |
| Colombia Black | 3.65% | 0.11 | 0.3 1 | 65.25 % | 2.4 | 0.8 6 | 66.51 % | 2.51 | 0.9 |
| | | | | | | | | | |
| Colombia Mestizo | 14.07 % | 0.42 | 0.3 5 | 56.31 % | 1.97 | 0.6 9 | 62.45 % | 2.39 | 0.8 |
| | | | | | | | | | |
| Congo | 0.0% | 0.0 | 0.0 | 68.66 % | 2.54 | 0.9 6 | 68.66 % | 2.54 | 0.9 6 |
| | | | | | | | | | |
| Congo Black | 0.0% | 0.0 | 0.0 | 68.66 % | 2.54 | 0.9 6 | 68.66 % | 2.54 | 0.9 6 |
| | | | | | | | | | |
| Cook Islands | 0.0% | 0.0 | 0.0 | 78.59 % | 3.05 | 1.4 | 78.59 % | 3.05 | 1.4 |
| | | | | | | | | | |
| Cook Islands Polynesian | 0.0% | 0.0 | 0.0 | 78.59 % | 3.05 | 1.4 | 78.59 % | 3.05 | 1.4 |
| | | | | | | | | | |
| Costa Rica | 0.0% | 0.0 | 0.0 | 24.31 % | 0.76 | 0.4 | 24.31 % | 0.76 | 0.4 |
| | | | | | | | | | |
| Costa Rica Mestizo | 0.0% | 0.0 | 0.0 | 24.31 % | 0.76 | 0.4 | 24.31 % | 0.76 | 0.4 |
| | | | | | | | | | |
| Croatia | 99.79 % | 7.96 | 6.1 8 | 66.71 % | 2.45 | 0.9 | 99.93 % | 10.4 | 7.4 3 |
| | | | | | | | | | |
| Croatia Caucasoid | 99.79 % | 7.96 | 6.1 8 | 66.71 % | 2.45 | 0.9 | 99.93 % | 10.4 | 7.4 3 |

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| | | | | | | | | | |
|-------------------------------|------------|------|----------|------------|------|----------|------------|-------|-----------|
| England Caucasoid | 99.93 % | 9.02 | 6.9 5 | 93.48 % | 4.21 | 3.2 2 | 100.0 % | 13.24 | 10. 42 |
| | | | | | | | | | |
| Equatorial Guinea | 0.0% | 0.0 | 0.0 | 47.58 % | 1.61 | 0.5 7 | 47.58 % | 1.61 | 0.5 7 |
| | | | | | | | | | |
| Equatorial Guinea Black | 0.0% | 0.0 | 0.0 | 47.58 % | 1.61 | 0.5 7 | 47.58 % | 1.61 | 0.5 7 |
| | | | | | | | | | |
| Ethiopia | 0.0% | 0.0 | 0.0 | 83.0% | 3.27 | 1.7 6 | 83.0% | 3.27 | 1.7 6 |
| | | | | | | | | | |
| Ethiopia Black | 0.0% | 0.0 | 0.0 | 83.0% | 3.27 | 1.7 6 | 83.0% | 3.27 | 1.7 6 |
| | | | | | | | | | |
| Europe | 99.68 % | 8.05 | 6.1 7 | 85.83 % | 3.57 | 2.1 2 | 99.96 % | 11.62 | 8.9 7 |
| | | | | | | | | | |
| Fiji | 0.0% | 0.0 | 0.0 | 79.87 % | 2.95 | 1.4 9 | 79.87 % | 2.95 | 1.4 9 |
| | | | | | | | | | |
| Fiji Melanesian | 0.0% | 0.0 | 0.0 | 79.87 % | 2.95 | 1.4 9 | 79.87 % | 2.95 | 1.4 9 |
| | | | | | | | | | |
| Finland | 99.99 % | 9.19 | 7.1 6 | 51.14 % | 1.75 | 0.6 1 | 100.0 % | 10.94 | 8.4 9 |
| | | | | | | | | | |
| Finland Caucasoid | 99.99 % | 9.19 | 7.1 6 | 51.14 % | 1.75 | 0.6 1 | 100.0 % | 10.94 | 8.4 9 |
| | | | | | | | | | |
| France | 99.8% | 8.26 | 6.3 4 | 88.54 % | 3.78 | 2.6 2 | 99.98 % | 12.04 | 9.3 1 |
| | | | | | | | | | |
| France Caucasoid | 99.8% | 8.26 | 6.3 4 | 88.54 % | 3.78 | 2.6 2 | 99.98 % | 12.04 | 9.3 1 |
| | | | | | | | | | |
| Gabon | 0.0% | 0.0 | 0.0 | 41.78 % | 1.35 | 0.5 2 | 41.78 % | 1.35 | 0.5 2 |
| | | | | | | | | | |
| Gabon Black | 0.0% | 0.0 | 0.0 | 41.78 % | 1.35 | 0.5 2 | 41.78 % | 1.35 | 0.5 2 |
| | | | | | | | | | |
| Georgia | 98.32 % | 6.77 | 4.4 1 | 75.05 % | 2.85 | 1.2 | 99.58 % | 9.62 | 6.6 3 |

| | | | | | | | | | |
|----------------------------|------------|------|----------|------------|------|----------|------------|-------|----------|
| Georgia Caucasoid | 98.94 % | 7.1 | 4.8 3 | 75.05 % | 2.85 | 1.2 | 99.74 % | 9.95 | 6.9 1 |
| | | | | | | | | | |
| Georgia Kurd | 98.19 % | 6.69 | 4.3 7 | 0.0% | 0.0 | 0.0 | 98.19 % | 6.69 | 4.3 7 |
| | | | | | | | | | |
| Germany | 99.93 % | 8.86 | 6.8 | 91.14 % | 4.0 | 3.0 7 | 99.99 % | 12.86 | 10. 0 |
| | | | | | | | | | |
| Germany Caucasoid | 99.93 % | 8.86 | 6.8 | 91.14 % | 4.0 | 3.0 7 | 99.99 % | 12.86 | 10. 0 |
| | | | | | | | | | |
| Greece | 0.0% | 0.0 | 0.0 | 66.92 % | 2.47 | 0.9 1 | 66.92 % | 2.47 | 0.9 1 |
| | | | | | | | | | |
| Greece Caucasoid | 0.0% | 0.0 | 0.0 | 66.92 % | 2.47 | 0.9 1 | 66.92 % | 2.47 | 0.9 1 |
| | | | | | | | | | |
| Guatemala | 7.76% | 0.24 | 0.3 3 | 49.16 % | 1.61 | 0.5 9 | 53.11 % | 1.85 | 0.6 4 |
| | | | | | | | | | |
| Guatemala Amerindian | 7.76% | 0.24 | 0.3 3 | 49.16 % | 1.61 | 0.5 9 | 53.11 % | 1.85 | 0.6 4 |
| | | | | | | | | | |
| Guinea- Bissau | 96.39 % | 6.37 | 3.8 9 | 71.16 % | 2.67 | 1.0 4 | 98.96 % | 9.04 | 6.1 1 |
| | | | | | | | | | |
| Guinea- Bissau Black | 96.39 % | 6.37 | 3.8 9 | 71.16 % | 2.67 | 1.0 4 | 98.96 % | 9.04 | 6.1 1 |
| | | | | | | | | | |
| Hong Kong | 96.05 % | 5.73 | 3.6 4 | 0.0% | 0.0 | 0.0 | 96.05 % | 5.73 | 3.6 4 |
| | | | | | | | | | |
| Hong Kong Oriental | 96.05 % | 5.73 | 3.6 4 | 0.0% | 0.0 | 0.0 | 96.05 % | 5.73 | 3.6 4 |
| | | | | | | | | | |
| India | 89.41 % | 4.74 | 2.8 3 | 74.99 % | 2.87 | 1.2 | 97.35 % | 7.6 | 4.4 6 |
| | | | | | | | | | |
| India Asian | 89.41 % | 4.74 | 2.8 3 | 74.99 % | 2.87 | 1.2 | 97.35 % | 7.6 | 4.4 6 |
| | | | | | | | | | |
| Indonesia | 86.79 % | 4.38 | 2.2 7 | 47.84 % | 1.62 | 0.5 8 | 93.11 % | 6.0 | 3.3 5 |

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| | | | | | | | | | |
|-----------------------|---------|------|----------|---------|------|----------|---------|------|----------|
| Lebanon Arab | 0.0% | 0.0 | 0.0 | 70.46 % | 2.62 | 1.0 2 | 70.46 % | 2.62 | 1.0 2 |
| | | | | | | | | | |
| Macedonia | 26.72 % | 0.87 | 0.4 1 | 66.53 % | 2.45 | 0.9 | 75.47 % | 3.31 | 1.2 2 |
| | | | | | | | | | |
| Macedonia Caucasoid | 26.72 % | 0.87 | 0.4 1 | 66.53 % | 2.45 | 0.9 | 75.47 % | 3.31 | 1.2 2 |
| | | | | | | | | | |
| Malaysia | 81.38 % | 3.71 | 1.6 1 | 57.99 % | 2.05 | 0.7 1 | 92.18 % | 5.76 | 3.2 3 |
| | | | | | | | | | |
| Malaysia Austronesian | 63.18 % | 2.52 | 0.8 1 | 55.38 % | 1.94 | 0.6 7 | 83.57 % | 4.46 | 1.8 3 |
| | | | | | | | | | |
| Malaysia Oriental | 87.82 % | 4.26 | 2.4 6 | 70.35 % | 2.58 | 1.0 1 | 96.39 % | 6.84 | 3.9 7 |
| | | | | | | | | | |
| Mali | 96.02 % | 6.04 | 3.7 3 | 0.0% | 0.0 | 0.0 | 96.02 % | 6.04 | 3.7 3 |
| | | | | | | | | | |
| Mali Black | 96.02 % | 6.04 | 3.7 3 | 0.0% | 0.0 | 0.0 | 96.02 % | 6.04 | 3.7 3 |
| | | | | | | | | | |
| Martinique | 22.56 % | 0.68 | 0.3 9 | 74.51 % | 2.88 | 1.1 8 | 80.26 % | 3.56 | 1.5 2 |
| | | | | | | | | | |
| Martinique Black | 22.56 % | 0.68 | 0.3 9 | 74.51 % | 2.88 | 1.1 8 | 80.26 % | 3.56 | 1.5 2 |
| | | | | | | | | | |
| Mexico | 97.97 % | 5.98 | 3.9 5 | 55.04 % | 1.91 | 0.6 7 | 99.09 % | 7.89 | 5.2 3 |
| | | | | | | | | | |
| Mexico Amerindian | 99.87 % | 6.68 | 4.9 5 | 42.59 % | 1.38 | 0.5 2 | 99.93 % | 8.06 | 6.1 |
| | | | | | | | | | |
| Mexico Mestizo | 98.13 % | 6.24 | 4.0 9 | 68.51 % | 2.54 | 0.9 5 | 99.41 % | 8.77 | 6.1 6 |
| | | | | | | | | | |
| Mongolia | 95.31 % | 4.43 | 3.3 7 | 81.85 % | 3.34 | 1.6 5 | 99.15 % | 7.77 | 5.6 7 |
| | | | | | | | | | |
| Mongolia Oriental | 95.31 % | 4.43 | 3.3 7 | 81.85 % | 3.34 | 1.6 5 | 99.15 % | 7.77 | 5.6 7 |

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| | | | | | | | | | |
|-----------------------------|---------|------|-------|---------|------|-------|---------|-------|-------|
| North America | 99.06 % | 7.34 | 5.1 | 87.89 % | 3.74 | 2.4 8 | 99.89 % | 11.09 | 8.0 4 |
| | | | | | | | | | |
| Northeast Asia | 94.7% | 5.45 | 3.4 5 | 59.99 % | 2.15 | 0.7 5 | 97.88 % | 7.6 | 4.5 6 |
| | | | | | | | | | |
| Norway | 0.0% | 0.0 | 0.0 | 94.71 % | 4.34 | 3.3 2 | 94.71 % | 4.34 | 3.3 2 |
| | | | | | | | | | |
| Norway Caucasoid | 0.0% | 0.0 | 0.0 | 94.71 % | 4.34 | 3.3 2 | 94.71 % | 4.34 | 3.3 2 |
| | | | | | | | | | |
| Oceania | 94.71 % | 4.99 | 3.3 7 | 59.87 % | 2.13 | 0.7 5 | 97.88 % | 7.12 | 4.3 1 |
| | | | | | | | | | |
| Oman | 99.69 % | 7.84 | 6.1 3 | 0.0% | 0.0 | 0.0 | 99.69 % | 7.84 | 6.1 3 |
| | | | | | | | | | |
| Oman Arab | 99.69 % | 7.84 | 6.1 3 | 0.0% | 0.0 | 0.0 | 99.69 % | 7.84 | 6.1 3 |
| | | | | | | | | | |
| Pakistan | 97.09 % | 4.77 | 3.6 1 | 1.18% | 0.04 | 0.3 | 97.13 % | 4.81 | 3.6 2 |
| | | | | | | | | | |
| Pakistan Asian | 96.75 % | 4.73 | 3.5 6 | 1.45% | 0.04 | 0.3 | 96.79 % | 4.77 | 3.5 8 |
| | | | | | | | | | |
| Pakistan Mixed | 97.73 % | 4.84 | 3.6 8 | 0.0% | 0.0 | 0.3 | 97.73 % | 4.84 | 3.6 8 |
| | | | | | | | | | |
| Papua New Guinea | 97.92 % | 4.45 | 3.4 5 | 69.15 % | 2.52 | 0.9 7 | 99.36 % | 6.97 | 4.6 2 |
| | | | | | | | | | |
| Papua New Guinea Melanesian | 97.92 % | 4.45 | 3.4 5 | 69.15 % | 2.52 | 0.9 7 | 99.36 % | 6.97 | 4.6 2 |
| | | | | | | | | | |
| Paraguay | 0.0% | 0.0 | 0.0 | 4.9% | 0.15 | 0.3 2 | 4.9% | 0.15 | 0.3 2 |
| | | | | | | | | | |
| Paraguay Amerindian | 0.0% | 0.0 | 0.0 | 4.9% | 0.15 | 0.3 2 | 4.9% | 0.15 | 0.3 2 |
| | | | | | | | | | |
| Peru | 99.99 % | 5.89 | 4.1 9 | 49.87 % | 1.64 | 0.6 | 100.0 % | 7.54 | 5.3 6 |

| | | | | | | | | | |
|---------------------------------|------------|------|----------|------------|------|----------|------------|-------|----------|
| Peru Amerindian | 99.99 % | 5.89 | 4.1 9 | 49.87 % | 1.64 | 0.6 | 100.0 % | 7.54 | 5.3 6 |
| | | | | | | | | | |
| Philippines | 94.98 % | 4.72 | 3.3 5 | 28.56 % | 0.91 | 0.4 2 | 96.41 % | 5.63 | 3.6 |
| | | | | | | | | | |
| Philippines Austronesia n | 94.98 % | 4.72 | 3.3 5 | 28.56 % | 0.91 | 0.4 2 | 96.41 % | 5.63 | 3.6 |
| | | | | | | | | | |
| Poland | 99.77 % | 8.06 | 6.2 1 | 84.46 % | 3.47 | 1.9 3 | 99.96 % | 11.53 | 8.8 7 |
| | | | | | | | | | |
| Poland Caucasoid | 99.77 % | 8.06 | 6.2 1 | 84.46 % | 3.47 | 1.9 3 | 99.96 % | 11.53 | 8.8 7 |
| | | | | | | | | | |
| Portugal | 98.72 % | 7.11 | 4.7 6 | 78.0% | 3.05 | 1.3 6 | 99.72 % | 10.15 | 7.0 2 |
| | | | | | | | | | |
| Portugal Caucasoid | 98.72 % | 7.11 | 4.7 6 | 78.0% | 3.05 | 1.3 6 | 99.72 % | 10.15 | 7.0 2 |
| | | | | | | | | | |
| Romania | 99.67 % | 7.7 | 6.0 2 | 0.0% | 0.0 | 0.0 | 99.67 % | 7.7 | 6.0 2 |
| | | | | | | | | | |
| Romania Caucasoid | 99.67 % | 7.7 | 6.0 2 | 0.0% | 0.0 | 0.0 | 99.67 % | 7.7 | 6.0 2 |
| | | | | | | | | | |
| Russia | 99.27 % | 7.18 | 5.0 7 | 77.62 % | 3.07 | 1.3 4 | 99.84 % | 10.25 | 7.1 8 |
| | | | | | | | | | |
| Russia Caucasoid | 3.96% | 0.12 | 0.3 1 | 88.52 % | 3.79 | 2.6 1 | 88.97 % | 3.91 | 2.7 2 |
| | | | | | | | | | |
| Russia Mixed | 5.05% | 0.15 | 0.3 2 | 0.0% | 0.0 | 0.0 | 5.05% | 0.15 | 0.3 2 |
| | | | | | | | | | |
| Russia Other | 99.98 % | 7.54 | 6.1 5 | 85.01 % | 3.48 | 2.0 | 100.0 % | 11.02 | 8.5 |
| | | | | | | | | | |
| Russia Siberian | 99.43 % | 7.64 | 5.7 | 78.83 % | 3.13 | 1.4 2 | 99.88 % | 10.77 | 7.6 6 |
| | | | | | | | | | |
| Rwanda | 24.87 % | 0.8 | 0.4 | 62.79 % | 2.24 | 0.8 1 | 72.05 % | 3.04 | 1.0 7 |

| | | | | | | | | | |
|--------------------------------------|------------|------|----------|------------|------|----------|------------|------|----------|
| Rwanda Black | 24.87 % | 0.8 | 0.4 | 62.79 % | 2.24 | 0.8 1 | 72.05 % | 3.04 | 1.0 7 |
| | | | | | | | | | |
| Samoa | 0.0% | 0.0 | 0.0 | 80.86 % | 3.18 | 1.5 7 | 80.86 % | 3.18 | 1.5 7 |
| | | | | | | | | | |
| Samoa Polynesian | 0.0% | 0.0 | 0.0 | 80.86 % | 3.18 | 1.5 7 | 80.86 % | 3.18 | 1.5 7 |
| | | | | | | | | | |
| Sao Tome and Principe | 97.02 % | 6.65 | 4.1 2 | 66.5% | 2.43 | 0.9 | 99.0% | 9.08 | 6.1 5 |
| | | | | | | | | | |
| Sao Tome and Principe Black | 97.02 % | 6.65 | 4.1 2 | 66.5% | 2.43 | 0.9 | 99.0% | 9.08 | 6.1 5 |
| | | | | | | | | | |
| Saudi Arabia | 98.26 % | 6.61 | 4.3 4 | 80.14 % | 3.15 | 1.5 1 | 99.65 % | 9.75 | 6.7 8 |
| | | | | | | | | | |
| Saudi Arabia Arab | 98.26 % | 6.61 | 4.3 4 | 80.14 % | 3.15 | 1.5 1 | 99.65 % | 9.75 | 6.7 8 |
| | | | | | | | | | |
| Scotland | 65.34 % | 2.62 | 0.8 7 | 90.82 % | 3.94 | 3.0 5 | 96.82 % | 6.56 | 3.9 5 |
| | | | | | | | | | |
| Scotland Caucasoid | 65.34 % | 2.62 | 0.8 7 | 90.82 % | 3.94 | 3.0 5 | 96.82 % | 6.56 | 3.9 5 |
| | | | | | | | | | |
| Senegal | 95.58 % | 5.94 | 3.6 5 | 30.28 % | 0.98 | 0.4 3 | 96.92 % | 6.91 | 4.0 8 |
| | | | | | | | | | |
| Senegal Black | 95.58 % | 5.94 | 3.6 5 | 30.28 % | 0.98 | 0.4 3 | 96.92 % | 6.91 | 4.0 8 |
| | | | | | | | | | |
| Serbia | 73.37 % | 2.8 | 1.1 3 | 0.0% | 0.0 | 0.0 | 73.37 % | 2.8 | 1.1 3 |
| | | | | | | | | | |
| Serbia Caucasoid | 73.37 % | 2.8 | 1.1 3 | 0.0% | 0.0 | 0.0 | 73.37 % | 2.8 | 1.1 3 |
| | | | | | | | | | |
| Singapore | 92.66 % | 5.13 | 3.2 3 | 65.78 % | 2.4 | 0.8 8 | 97.49 % | 7.53 | 4.4 4 |

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| | | | | | | | | | |
|-------------------------------|--------------|-------------|------------------|--------------|-------------|------------------|--------------|-------------|------------------|
| Venezuela Mestizo | 9.75% | 0.29 | 0.3 3 | 0.0% | 0.0 | 0.0 | 9.75% | 0.29 | 0.3 3 |
| | | | | | | | | | |
| Venezuela Mixed | 0.0% | 0.0 | 0.0 | 3.17% | 0.1 | 0.3 1 | 3.17% | 0.1 | 0.3 1 |
| | | | | | | | | | |
| Vietnam | 91.82 % | 5.0 | 3.1 5 | 54.44 % | 1.9 | 0.6 6 | 96.27 % | 6.89 | 3.9 4 |
| | | | | | | | | | |
| Vietnam Oriental | 91.82 % | 5.0 | 3.1 5 | 54.44 % | 1.9 | 0.6 6 | 96.27 % | 6.89 | 3.9 4 |
| | | | | | | | | | |
| Wales | 1.0% | 0.03 | 0.3 | 0.0% | 0.0 | 0.0 | 1.0% | 0.03 | 0.3 |
| | | | | | | | | | |
| Wales Caucasoid | 1.0% | 0.03 | 0.3 | 0.0% | 0.0 | 0.0 | 1.0% | 0.03 | 0.3 |
| | | | | | | | | | |
| West Africa | 95.49 % | 6.03 | 3.6 6 | 65.23 % | 2.4 | 0.8 6 | 98.43 % | 8.43 | 5.3 2 |
| | | | | | | | | | |
| West Indies | 98.98 % | 7.5 | 5.2 5 | 69.22 % | 2.59 | 0.9 7 | 99.69 % | 10.09 | 6.9 4 |
| | | | | | | | | | |
| World | 98.55 % | 6.9 | 4.5 4 | 81.81 % | 3.32 | 1.6 5 | 99.74 % | 10.22 | 7.0 7 |
| | | | | | | | | | |
| Zambia | 98.1% | 6.42 | 4.1 6 | 0.0% | 0.0 | 0.0 | 98.1% | 6.42 | 4.1 6 |
| | | | | | | | | | |
| Zambia Black | 98.1% | 6.42 | 4.1 6 | 0.0% | 0.0 | 0.0 | 98.1% | 6.42 | 4.1 6 |
| | | | | | | | | | |
| Zimbabwe | 93.79 % | 5.43 | 3.3 7 | 68.3% | 2.51 | 0.9 5 | 98.03 % | 7.95 | 4.8 4 |
| | | | | | | | | | |
| Zimbabwe Black | 93.79 % | 5.43 | 3.3 7 | 68.3% | 2.51 | 0.9 5 | 98.03 % | 7.95 | 4.8 4 |
| | | | | | | | | | |
| Average | 63.06 | 4.0 | 2.7 1 | 55.3 | 2.11 | 1.0 4 | 82.92 | 6.11 | 4.0 2 |
| Standard deviation | 43.68 | 3.13 | 2.2 7 | 30.26 | 1.26 | 0.8 3 | 25.25 | 3.59 | 2.8 5 |

Table S6. Docking score of vaccine with MHC-I.

| Cluster | Members | Representative | Weighted Score |
|---------|---------|----------------|----------------|
| 0 | 138 | Center | -733.6 |
| | | Lowest Energy | -799.3 |
| 1 | 95 | Center | -586.8 |
| | | Lowest Energy | -638.1 |
| 2 | 71 | Center | -608.9 |
| | | Lowest Energy | -608.9 |
| 3 | 59 | Center | -596.1 |
| | | Lowest Energy | -624.6 |
| 4 | 42 | Center | -556.0 |
| | | Lowest Energy | -642.2 |
| 5 | 39 | Center | -590.9 |
| | | Lowest Energy | -627.9 |
| 6 | 36 | Center | -650.3 |
| | | Lowest Energy | -658.9 |
| 7 | 35 | Center | -674.5 |
| | | Lowest Energy | -674.5 |
| 8 | 34 | Center | -665.4 |
| | | Lowest Energy | -665.4 |
| 9 | 31 | Center | -579.0 |
| | | Lowest Energy | -606.3 |
| 10 | 30 | Center | -699.5 |
| | | Lowest Energy | -699.5 |

Table S7. Docking score of vaccine with MHC-II.

| Cluster | Members | Representative | Weighted Score |
|---------|---------|----------------|----------------|
| 0 | 87 | Center | -696.0 |
| | | Lowest Energy | -821.4 |
| 1 | 76 | Center | -648.9 |

| Cluster | Members | Representative | Weighted Score |
|---------|---------|----------------|----------------|
| | | Lowest Energy | -789.4 |
| 2 | 68 | Center | -743.2 |
| | | Lowest Energy | -743.2 |
| 3 | 64 | Center | -796.4 |
| | | Lowest Energy | -796.4 |
| 4 | 53 | Center | -748.8 |
| | | Lowest Energy | -748.8 |
| 5 | 46 | Center | -755.9 |
| | | Lowest Energy | -794.5 |
| 6 | 40 | Center | -645.6 |
| | | Lowest Energy | -713.9 |
| 7 | 38 | Center | -786.6 |
| | | Lowest Energy | -786.6 |
| 8 | 37 | Center | -696.5 |
| | | Lowest Energy | -752.1 |
| 9 | 29 | Center | -650.5 |
| | | Lowest Energy | -789.0 |
| 10 | 29 | Center | -642.3 |
| | | Lowest Energy | -790.5 |

Table S8. Docking score of vaccine with TLR-4.

| Cluster | Members | Representative | Weighted Score |
|---------|---------|----------------|----------------|
| 0 | 82 | Center | -691.7 |
| | | Lowest Energy | -783.6 |
| 1 | 46 | Center | -758.5 |
| | | Lowest Energy | -758.5 |
| 2 | 44 | Center | -607.5 |

| Cluster | Members | Representative | Weighted Score |
|-----------|---------|----------------|----------------|
| | | Lowest Energy | -803.3 |
| 3 | 36 | Center | -646.0 |
| | | Lowest Energy | -699.0 |
| 4 | 35 | Center | -637.6 |
| | | Lowest Energy | -704.1 |
| 5 | 34 | Center | -695.4 |
| | | Lowest Energy | -703.4 |
| 6 | 32 | Center | -678.9 |
| | | Lowest Energy | -752.2 |
| 7 | 31 | Center | -667.6 |
| | | Lowest Energy | -832.6 |
| 8 | 31 | Center | -704.5 |
| | | Lowest Energy | -711.0 |
| 9 | 30 | Center | -709.4 |
| | | Lowest Energy | -709.4 |
| 10 | 30 | Center | -691.2 |
| | | Lowest Energy | -691.2 |