The recommended directionality about the probability score for models using 129 optimum featuresf.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Score range | Directionality distribution‘Backward’/’Forward’/’Bidirectional’ | Recommendation\_1b,c | Confidence\_1a,d | Recommendation\_2 | Confidence\_2e |
| [0.00-0.02) | 0.00%/0.00%/0.00% | 'Forward' | N/A | 'Bidirectional' | High |
| [0.02-0.04) | 0.00%/0.00%/0.00% | 'Forward' | N/A | 'Bidirectional' | High |
| **[0.04-0.06)** | **0.00%/2.00%/2.09%** | **'Bidirectional'**  | **51%** | **'Forward'** | **100.00%** |
| [0.06-0.08) | 0.67%/2.67%/2.69% | 'Bidirectional'  | 45% | 'Forward' | 88.93% |
| **[0.08-0.10)** | **0.00%/5.33%/1.49%** | **'Forward'**  | **78%** | **'Bidirectional'** | **100.00%** |
| [0.10-0.12) | 0.67%/2.67%/3.28% | 'Bidirectional'  | 50% | 'Forward' | 89.92% |
| **[0.12-0.14)** | **0.00%/4.67%/2.69%** | **'Forward'**  | **63%** | **'Bidirectional'** | **100.00%** |
| **[0.14-0.16)** | **0.00%/4.00%/3.88%** | **'Forward'**  | **51%** | **'Bidirectional'** | **100.00%** |
| [0.16-0.18) | 0.67%/5.33%/2.09% | 'Forward'  | 66% | 'Bidirectional' | 91.76% |
| **[0.18-0.20)** | **0.00%/1.33%/2.69%** | **'Bidirectional'**  | **67%** | **'Forward'** | **100.00%** |
| [0.20-0.22) | 0.00%/3.33%/3.28% | 'Forward'  | 50% | 'Bidirectional' | 100.00% |
| [0.22-0.24) | 2.00%/4.00%/3.28% | 'Forward'  | 43% | 'Bidirectional' | 78.46% |
| [0.24-0.26) | 0.67%/2.00%/1.49% | 'Forward'  | 48% | 'Bidirectional' | 83.97% |
| [0.26-0.28) | 1.33%/5.33%/3.58% | 'Forward'  | 52% | 'Bidirectional' | 86.99% |
| **[0.28-0.30)** | **0.00%/3.33%/2.69%** | **'Forward'**  | **55%** | **'Bidirectional'** | **100.00%** |
| [0.30-0.32) | 0.67%/4.67%/1.49% | 'Forward'  | 68% | 'Bidirectional' | 90.23% |
| [0.32-0.34) | 1.33%/1.33%/3.28% | 'Bidirectional'  | 55% | 'Forward' | 77.59% |
| [0.34-0.36) | 0.67%/3.33%/4.48% | 'Bidirectional'  | 53% | 'Forward' | 92.14% |
| [0.36-0.38) | 0.67%/3.33%/2.69% | 'Forward'  | 50% | 'Bidirectional' | 90.03% |
| [0.38-0.40) | 2.67%/3.33%/2.09% | 'Forward'  | 41% | 'Backward' | 74.17% |
| [0.40-0.42) | 1.33%/2.67%/2.09% | 'Forward'  | 44% | 'Bidirectional' | 78.10% |
| [0.42-0.44) | 1.33%/3.33%/1.79% | 'Forward'  | 52% | 'Bidirectional' | 79.35% |
| [0.44-0.46) | 2.00%/1.33%/1.49% | 'Backward'  | 41% | 'Bidirectional' | 72.37% |
| [0.46-0.48) | 2.67%/2.00%/2.09% | 'Backward'  | 39% | 'Bidirectional' | 70.40% |
| [0.48-0.50) | 0.67%/1.33%/2.09% | 'Bidirectional'  | 51% | 'Forward' | 83.70% |
| [0.50-0.52) | 2.67%/2.00%/2.99% | 'Bidirectional'  | 39% | 'Backward' | 73.86% |
| [0.52-0.54) | 5.33%/1.33%/3.58% | 'Backward'  | 52% | 'Bidirectional' | 86.99% |
| [0.54-0.56) | 3.33%/2.00%/2.09% | 'Backward'  | 45% | 'Bidirectional' | 73.06% |
| [0.56-0.58) | 2.67%/2.00%/2.39% | 'Backward'  | 38% | 'Bidirectional' | 71.65% |
| **[0.58-0.60)** | **1.33%/0.00%/2.69%** | **'Bidirectional'**  | **67%** | **'Backward'** | **100.00%** |
| [0.60-0.62) | 2.00%/4.00%/3.58% | 'Forward'  | 42% | 'Bidirectional' | 79.13% |
| [0.62-0.64) | 2.67%/0.67%/1.79% | 'Backward'  | 52% | 'Bidirectional' | 86.99% |
| [0.64-0.66) | 2.00%/2.00%/1.79% | 'Backward'  | 35% | 'Forward' | 69.07% |
| [0.66-0.68) | 6.67%/2.00%/2.99% | 'Backward'  | 57% | 'Bidirectional' | 82.84% |
| **[0.68-0.70)** | **6.00%/0.00%/1.19%** | **'Backward'**  | **83%** | **'Bidirectional'** | **100.00%** |
| **[0.70-0.72)** | **1.33%/0.00%/0.60%** | **'Backward'**  | **69%** | **'Bidirectional'** | **100.00%** |
| [0.72-0.74) | 2.00%/1.33%/1.49% | 'Backward'  | 41% | 'Bidirectional' | 72.37% |
| [0.74-0.76) | 2.00%/2.00%/0.60% | 'Backward'  | 44% | 'Forward' | 87.01% |
| [0.76-0.78) | 2.67%/0.67%/2.99% | 'Bidirectional'  | 47% | 'Backward' | 89.45% |
| **[0.78-0.80)** | **3.33%/0.00%/1.79%** | **'Backward'**  | **65%** | **'Bidirectional'** | **100.00%** |
| [0.80-0.82) | 2.00%/1.33%/0.90% | 'Backward'  | 47% | 'Forward' | 78.82% |
| [0.82-0.84) | 3.33%/0.67%/1.19% | 'Backward'  | 64% | 'Bidirectional' | 87.16% |
| [0.84-0.86) | 2.67%/0.67%/0.30% | 'Backward'  | 73% | 'Forward' | 91.78% |
| [0.86-0.88) | 2.67%/1.33%/0.90% | 'Backward'  | 54% | 'Forward' | 81.71% |
| [0.88-0.90) | 5.33%/0.67%/1.19% | 'Backward'  | 74% | 'Bidirectional' | 90.73% |
| [0.90-0.92) | 3.33%/1.33%/0.90% | 'Backward'  | 60% | 'Forward' | 83.90% |
| [0.92-0.94) | 4.67%/0.67%/0.90% | 'Backward'  | 75% | 'Bidirectional' | 89.30% |
| [0.94-0.96) | 1.33%/0.67%/0.30% | 'Backward'  | 58% | 'Forward' | 87.01% |
| **[0.96-0.98)** | **4.00%/0.00%/1.49%** | **'Backward'**  | **73%** | **'Bidirectional'** | **100.00%** |
| **[0.98-1.00]** | **4.67%/0.00%/0.60%** | **'Backward'**  | **89%** | **'Bidirectional'** | **100.00%** |

*a: N/A is placed for the lack of reference proteins with predicted probability scores located within corresponding ranges;*

*b: recommendation\_1 is determined according to the dominant class scored within the corresponding range;*

*c: in case the dominant class is not obvious, we recommend VIPs with probability score no less than 0.5 to be ‘Backward’ and those with probability score less than 0.5 to be ‘Forward’;*

*d: confidence\_1 is calculated as the occurrence frequency of dominant class divided by that of all classes;*

*e: confidence\_2 is calculated as the occurrence frequency of the major two classes divided by that of all classes; we can’t provide the exact confidence we have when getting a probability score lower than 0.04, but the tested HIV-1 interacting protein are very likely to have a ‘Forward’ or ‘Bidirectional’ tag;*

*f: rows are colored as red when we have confidence\_1 scored higher than 50%; texts in these rows are further bold when confidence\_2 reaches 100%.*

#Citation: Chai H, Gu Q, Hughes J, Robertson DL (2022) In silico prediction of HIV-1-host molecular interactions and their directionality. PLoS Comput Biol 18(2): e1009720. https://doi.org/10.1371/journal.pcbi.1009720.