

# JET and iJET performance on a pool of proteins discussed in the text

| Proteins discussed in the text - with clustering |                     |       |      |       |      |       |      |       |                                       |             |             |            |             |            |             |             |
|--------------------------------------------------|---------------------|-------|------|-------|------|-------|------|-------|---------------------------------------|-------------|-------------|------------|-------------|------------|-------------|-------------|
| PDBCode                                          | JET on conservation |       |      |       |      |       |      |       | JET on conservation and pc properties |             |             |            |             |            |             |             |
|                                                  | Sen                 | ScSen | PPV  | ScPPV | Spe  | ScSpe | Acc  | ScAcc | Sen                                   | ScSen       | PPV         | ScPPV      | Spe         | ScSpe      | Acc         | ScAcc       |
| 1all :A                                          | 46.7                | 18.4  | 56.8 | 1.7   | 81.4 | 9.6   | 69.5 | 12.7  | 44.4                                  | 20.0        | 62.5        | 1.8        | 86.0        | 10.5       | 71.8        | 13.8        |
| 1all :B                                          | 51.1                | 23.0  | 60.5 | 1.8   | 83.3 | 11.5  | 72.6 | 15.3  | 66.7                                  | 36.3        | 73.2        | 2.2        | 87.8        | 18.1       | 80.7        | 24.2        |
| 1apm :E                                          | 52.2                | 41.2  | 85.7 | 4.8   | 98.1 | 9.0   | 89.8 | 14.8  | 43.5                                  | 33.7        | 80.0        | 4.5        | 97.6        | 7.4        | 87.9        | 12.1        |
| 1grn :A                                          | 81.8                | 54.2  | 45.0 | 3.0   | 82.1 | 9.7   | 82.1 | 16.5  | 68.2                                  | 48.2        | 51.7        | 3.4        | 88.6        | 8.6        | 85.5        | 14.6        |
| 1grn :B                                          | 65.5                | 47.2  | 70.4 | 3.6   | 93.2 | 11.6  | 87.8 | 18.6  | 62.1                                  | 43.7        | 66.7        | 3.4        | 92.4        | 10.7       | 86.4        | 17.2        |
| 1leh :A                                          | 3.8                 | -10.4 | 2.6  | 0.3   | 84.6 | -1.1  | 76.7 | -2.0  | 37.0                                  | 14.9        | 16.7        | 1.7        | 79.5        | 1.6        | 75.3        | 3.0         |
| 1shc :A                                          | 65.0                | 39.1  | 29.5 | 2.5   | 79.3 | 5.2   | 77.6 | 9.2   | 70.0                                  | 47.1        | 35.9        | 3.1        | 83.3        | 6.3        | 81.8        | 11.1        |
| 1ycr :A                                          | 58.8                | 19.7  | 37.0 | 1.5   | 67.3 | 6.4   | 65.2 | 9.7   | 76.5                                  | 30.1        | 40.6        | 1.6        | 63.5        | 9.8        | 66.7        | 14.8        |
| 2cjk :A                                          | 40.0                | 27.6  | 82.4 | 3.2   | 97.1 | 9.5   | 82.5 | 14.1  | 37.1                                  | 24.0        | 72.2        | 2.8        | 95.1        | 8.2        | 80.3        | 12.3        |
| 2ktq :A                                          | 43.5                | 32.3  | 45.5 | 3.9   | 93.1 | 4.3   | 87.3 | 7.6   | 39.1                                  | 27.4        | 39.1        | 3.3        | 91.9        | 3.6        | 85.8        | 6.4         |
| 2pol :A                                          | 25.4                | 10.5  | 39.0 | 1.7   | 88.2 | 3.1   | 73.8 | 4.8   | 30.2                                  | 13.8        | 42.2        | 1.8        | 87.7        | 4.1        | 74.5        | 6.3         |
| 2ptc :E                                          | 61.9                | 44.4  | 46.4 | 3.5   | 89.2 | 6.7   | 85.6 | 11.7  | 71.4                                  | 56.4        | 62.5        | 4.8        | 93.5        | 8.5        | 90.6        | 14.8        |
| average                                          | 49.6                | 28.9  | 50.1 | 2.6   | 86.4 | 7.1   | 79.2 | 11.1  | <b>53.4</b>                           | <b>32.5</b> | <b>53.3</b> | <b>2.9</b> | <b>87.1</b> | <b>8.0</b> | <b>80.4</b> | <b>12.3</b> |

TAB. 1 – JET performance on a set of proteins discussed individually in the text. Predictions based on conservation and on both conservation and physical-chemical signals are evaluated. Bold characters indicate best performance. The evaluations that we present correspond to the best performance over the 10 runs used to evaluate iJET in Table 2, where the "best performance" corresponds to the highest *PPV* and *Acc* values.

| Proteins discussed in the text - with clustering |      |       |      |       |      |       |      |       |                                       |             |             |            |             |            |             |             |
|--------------------------------------------------|------|-------|------|-------|------|-------|------|-------|---------------------------------------|-------------|-------------|------------|-------------|------------|-------------|-------------|
| PBDCode                                          | ET   |       |      |       |      |       |      |       | iJET : conservation and pc properties |             |             |            |             |            |             |             |
|                                                  | Sen  | ScSen | PPV  | ScPPV | Spe  | ScSpe | Acc  | ScAcc | Sen                                   | ScSen       | PPV         | ScPPV      | Spe         | ScSpe      | Acc         | ScAcc       |
| 1all :A                                          | 42.2 | 20.1  | 65.5 | 1.9   | 88.4 | 10.5  | 72.5 | 13.8  | 44.4                                  | 20.8        | 64.5        | 1.9        | 87.2        | 10.9       | 72.5        | 14.3        |
| 1all :B                                          | 40.0 | 15.6  | 54.5 | 1.6   | 83.3 | 7.8   | 68.9 | 10.4  | 62.2                                  | 32.6        | 70.0        | 2.1        | 86.7        | 16.3       | 78.5        | 21.7        |
| 1apm :E                                          | 58.7 | 39.9  | 56.3 | 3.1   | 90.0 | 8.8   | 84.4 | 14.4  | 43.5                                  | 33.3        | 76.9        | 4.3        | 97.1        | 7.3        | 87.5        | 12.0        |
| 1grn :A                                          | 40.9 | 23.7  | 36.0 | 2.4   | 87.0 | 4.2   | 80.0 | 7.2   | 77.3                                  | 51.1        | 44.7        | 2.9        | 82.9        | 9.1        | 82.1        | 15.5        |
| 1grn :B                                          | 34.5 | 18.8  | 43.5 | 2.2   | 89.0 | 4.6   | 78.2 | 7.4   | 62.1                                  | 43.0        | 64.3        | 3.3        | 91.5        | 10.6       | 85.7        | 17.0        |
| 1leh :A                                          | 3.7  | -15.1 | 2.0  | 0.2   | 79.5 | -1.7  | 72.0 | -3.0  | 3.7                                   | -12.2       | 2.3         | 0.2        | 82.8        | -1.3       | 74.9        | -2.4        |
| 1shc :A                                          | 70.0 | 50.0  | 41.2 | 3.5   | 86.7 | 6.7   | 84.7 | 11.8  | 60.0                                  | 34.7        | 27.9        | 2.4        | 79.3        | 4.6        | 77.1        | 8.2         |
| 1ycr :A                                          | 41.2 | 16.5  | 41.2 | 1.7   | 80.8 | 5.4   | 71.0 | 8.1   | 70.6                                  | 27.1        | 40.0        | 1.6        | 65.4        | 8.9        | 66.7        | 13.4        |
| 2cjk :A                                          | 54.3 | 32.4  | 63.3 | 2.5   | 89.2 | 11.1  | 80.3 | 16.5  | 34.3                                  | 21.9        | 70.6        | 2.8        | 95.1        | 7.5        | 79.6        | 11.2        |
| 2ktq :A                                          | 60.9 | 41.3  | 36.4 | 3.1   | 85.9 | 5.5   | 83.0 | 9.7   | 41.3                                  | 30.6        | 45.2        | 3.9        | 93.4        | 4.1        | 87.3        | 7.2         |
| 2pol :A                                          | 46.0 | 21.7  | 43.3 | 1.9   | 82.1 | 6.4   | 73.8 | 9.9   | 28.6                                  | 12.6        | 40.9        | 1.8        | 87.7        | 3.7        | 74.2        | 5.8         |
| 2ptc :E                                          | 38.1 | 28.1  | 50.0 | 3.8   | 94.2 | 4.2   | 86.9 | 7.4   | 71.4                                  | 57.1        | 65.2        | 5.0        | 94.2        | 8.6        | 91.3        | 15.0        |
| average                                          | 44.2 | 24.4  | 44.4 | 2.3   | 86.3 | 6.1   | 78.0 | 9.5   | <b>49.9</b>                           | <b>29.4</b> | <b>51.0</b> | <b>2.7</b> | <b>86.9</b> | <b>7.5</b> | <b>79.8</b> | <b>11.5</b> |

TAB. 2 – iJET is compared to ET on a set of proteins discussed individually in the text. Bold characters indicate best performance.

| pdb code | size | 20-39 | 40-59 | 60-79 | 80-98 |
|----------|------|-------|-------|-------|-------|
| 1all :A  | 160  | 219   | 14    | 10    | 12    |
| 1all :B  | 161  | 187   | 40    | 3     | 21    |
| 1apm :E  | 341  | 355   | 295   | 12    | 124   |
| 1grn :A  | 191  | 15    | 520   | 224   | 73    |
| 1grn :B  | 197  | 472   | 23    | 3     | 10    |
| 1leh :A  | 364  | 22    | 140   | 28    | 3     |
| 1shc :A  | 195  | 3     | 7     | 28    | 5     |
| 1ycr :A  | 85   | 0     | 14    | 6     | 11    |
| 2cjk :A  | 167  | 316   | 175   | 5     | 5     |
| 2ktq :A  | 528  | 475   | 139   | 0     | 13    |
| 2pol :A  | 366  | 459   | 153   | 46    | 17    |
| 2ptc :E  | 220  | 271   | 352   | 178   | 19    |

TAB. 3 – Size (amino-acids number) and number of sequences retrieved by PSI-BLAST for all proteins illustrated in the article. Number of sequences are considered after filtering and they are reported for each sequence identity class.