**Supporting Information**

**A practical guide to machine-learning scoring for structure-based virtual screening**

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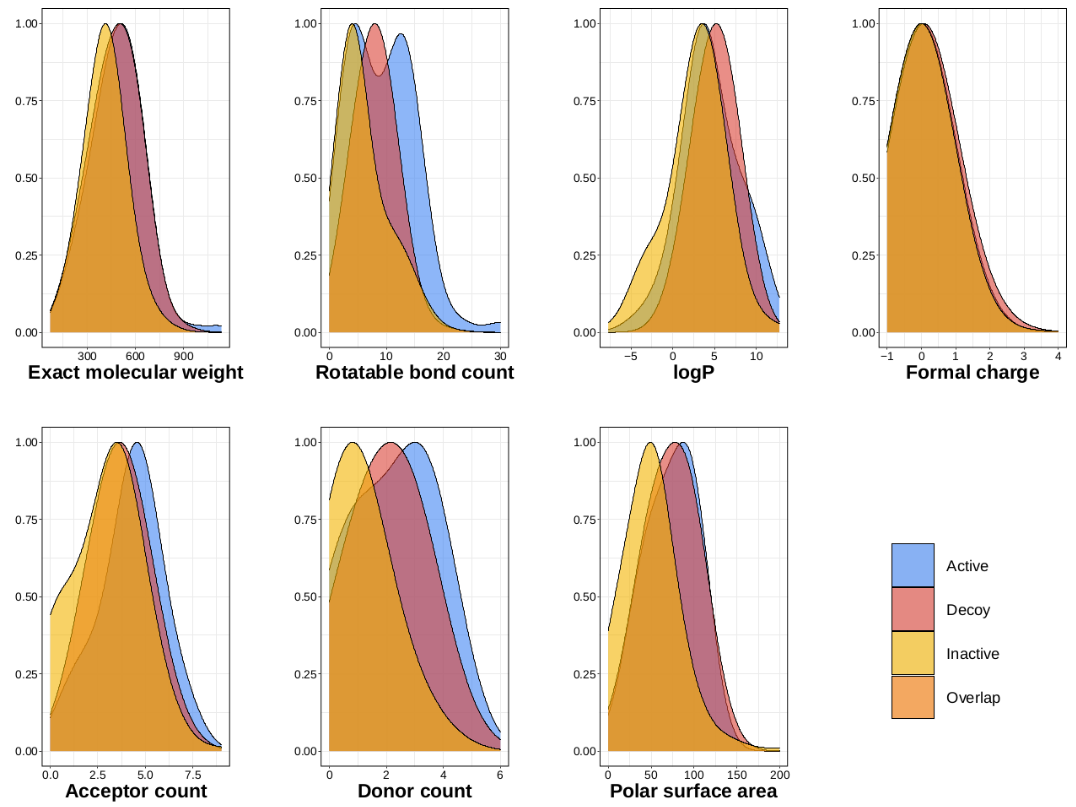
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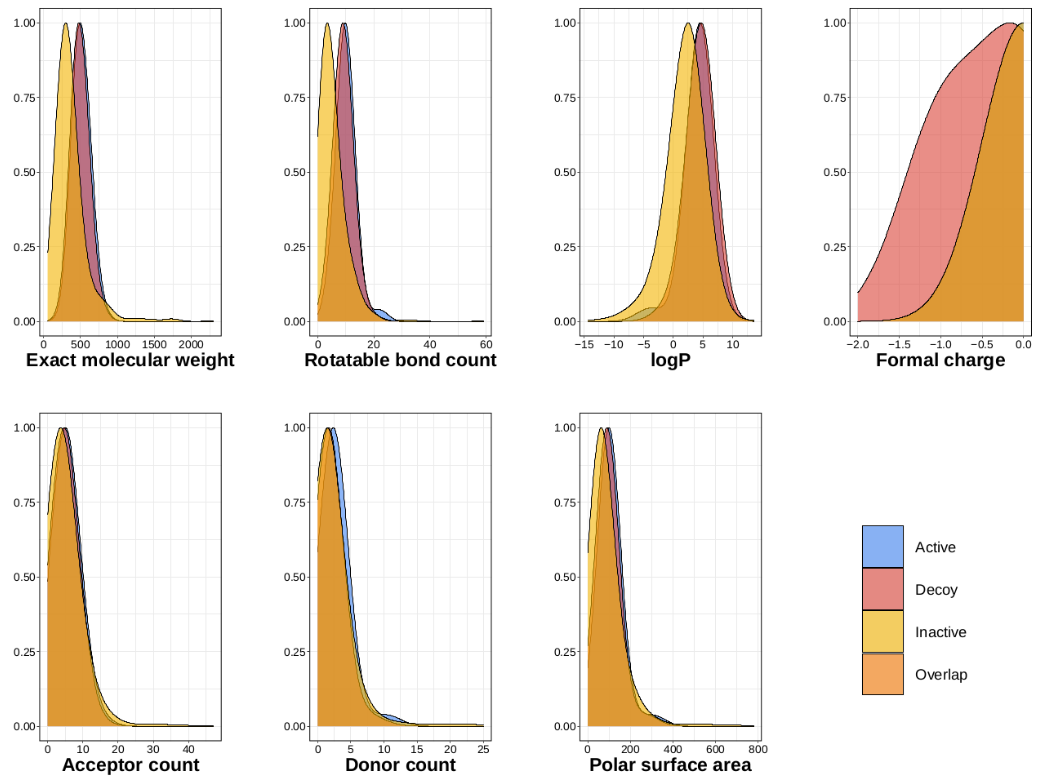
**Table S1.** SBVS performance of four generic SFs (Smina, IFP, CNN-Score, RF-Score-VS) on three DEKOIS 2.0 benchmarks (ACHE, HMGR, PPARA).

|  |  |  |  |
| --- | --- | --- | --- |
|  | **ACHE** | **HMGR** | **PPARA** |
| - Number of actives  - Number of decoys  - Total number of molecules  - Maximal EF1% | 40  1200  1240  30.00 | 40  1200  1240  30.00 | 40  1200  1240  30.00 |
| **Smina:**  - EF1%  - **NEF1%** | 15.00  **0.500** | 2.50  **0.083** | 0.00  **0.000** |
| **IFP:**  - EF1%  - **NEF1%** | 15.00  **0.500** | 10.00  **0.333** | 0.00  **0.000** |
| **CNN-Score:**  - EF1%  - **NEF1%** | 0.00  **0.000** | 7.50  **0.250** | 10.00  **0.333** |
| **RF-Score-VS:**  - EF1%  - **NEF1%** | 2.50  **0.083** | 30.00  **1.000** | 12.50  **0.417** |

**Fig. S1.** Distribution plots of seven physico-chemical properties calculated from all molecules of the ACHE ligand set.



**Fig. S2.** Distribution plots of seven physico-chemical properties calculated from all molecules of the HMGR ligand set.



**Table S2.** List of all active molecules of the users’ own PPARA benchmark (*n* = 1115) and their partition into the test set and the training set according to their clusters (OTS option).

|  |  |  |
| --- | --- | --- |
| **Cluster group** | **ID** | **Data set** |
| 118 | CHEMBL260627 | Test |
| 125 | CHEMBL400625 | Test |
| 127 | CHEMBL2237300 | Test |
| 128 | CHEMBL4083589 | Test |
| 132 | CHEMBL1934468 | Test |
| 144 | CHEMBL280897 | Test |
| 145 | CHEMBL252995 | Test |
| 150 | CHEMBL198579 | Test |
| 155 | CHEMBL205777 | Test |
| 156 | CHEMBL472451 | Test |
| 157 | CHEMBL192500 | Test |
| 158 | CHEMBL278994 | Test |
| 159 | CHEMBL410478 | Test |
| 160 | CHEMBL3780740 | Test |
| 161 | CHEMBL2037182 | Test |
| 162 | CHEMBL2037008 | Test |
| 163 | CHEMBL4571975 | Test |
| 164 | CHEMBL4104138 | Test |
| 165 | CHEMBL4101577 | Test |
| 166 | CHEMBL4100619 | Test |
| 167 | CHEMBL3982782 | Test |
| 168 | CHEMBL3735011 | Test |
| 169 | CHEMBL3601096 | Test |
| 170 | CHEMBL3397563 | Test |
| 171 | CHEMBL3354988 | Test |
| 172 | CHEMBL3354987 | Test |
| 173 | CHEMBL2069935 | Test |
| 174 | CHEMBL1934308 | Test |
| 175 | CHEMBL1927476 | Test |
| 176 | CHEMBL1760555 | Test |
| 177 | CHEMBL1720494 | Test |
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| 179 | CHEMBL1089633 | Test |
| 180 | CHEMBL1080361 | Test |
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| 182 | CHEMBL1075683 | Test |
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| 184 | CHEMBL572795 | Test |
| 185 | CHEMBL526740 | Test |
| 186 | CHEMBL438346 | Test |
| 187 | CHEMBL426883 | Test |
| 188 | CHEMBL401811 | Test |
| 189 | CHEMBL401562 | Test |
| 190 | CHEMBL374948 | Test |
| 191 | CHEMBL318696 | Test |
| 192 | CHEMBL306229 | Test |
| 193 | CHEMBL272017 | Test |
| 194 | CHEMBL250673 | Test |
| 195 | CHEMBL249865 | Test |
| 196 | CHEMBL219156 | Test |
| 197 | CHEMBL213355 | Test |
| 198 | CHEMBL207569 | Test |
| 199 | CHEMBL202631 | Test |
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| 201 | CHEMBL198786 | Test |
| 202 | CHEMBL194698 | Test |
| 203 | CHEMBL190739 | Test |
| 204 | CHEMBL190645 | Test |
| 205 | CHEMBL39687 | Test |
| 206 | CHEMBL496744 | Test |
| 207 | CHEMBL491039 | Test |
| 208 | CHEMBL391085 | Test |
| 209 | CHEMBL391084 | Test |
| 210 | CHEMBL593087 | Test |
| 211 | CHEMBL257345 | Test |
| 212 | CHEMBL221529 | Test |
| 213 | CHEMBL148797 | Test |
| 214 | CHEMBL2113219 | Test |
| 215 | CHEMBL383011 | Test |
| 216 | CHEMBL255872 | Test |
| 217 | CHEMBL3707395 | Test |
| 218 | CHEMBL592054 | Test |
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| 220 | CHEMBL242007 | Test |
| 221 | CHEMBL148319 | Test |
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| 223 | CHEMBL221044 | Test |
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| 154 | CHEMBL403432 | Training |

**Table S3.** SBVS performance of target-specific ML SFs trained on the users’ own data sets ACHE and HMGR and tested on the corresponding DEKOIS 2.0 benchmarks (PETS option, see Table S1 for the performance of four generic SFs). The values indicated here are median values obtained after 10 training-test runs of each ML algorithm on each training-test partition. Detailed results for each run can be downloaded from <https://github.com/vktrannguyen/MLSF-protocol> (Supporting Information folder).

|  |  |  |
| --- | --- | --- |
|  | **ACHE** | **HMGR** |
| **RF:**  - EF1%  - **NEF1%** | 30.00  **1.000** | 30.00  **1.000** |
| **XGB:**  - EF1%  - **NEF1%** | 10.00  **0.333** | 30.00  **1.000** |
| **SVM:**  - EF1%  - **NEF1%** | 30.00  **1.000** | 30.00  **1.000** |
| **ANN:**  - EF1%  - **NEF1%** | 5.00  **0.167** | 30.00  **1.000** |
| **DNN:**  - EF1%  - **NEF1%** | 7.50  **0.250** | 30.00  **1.000** |

**Table S4.** SBVS performance of target-specific ML SFs trained on the users’ own training sets ACHE, HMGR, PPARA and tested on the corresponding users’ own test sets (OTS option). The values related to target-specific ML SFs are the medians obtained after 10 training-test runs of each ML algorithm on each training-test partition. Detailed results for each run can be downloaded from <https://github.com/vktrannguyen/MLSF-protocol> (Supporting Information folder). The performance of four generic SFs (Smina, IFP, CNN-Score, RF-Score-VS) is also reported for comparison (only one run is performed on each test set for each of these SFs).

|  |  |  |  |
| --- | --- | --- | --- |
|  | **ACHE** | **HMGR** | **PPARA** |
| - Number of actives  - Number of inactives/decoys  - Total number of molecules  - Maximal EF1% | 37  2170  2207  59.46 | 31  2077  2108  67.74 | 80  2399  2479  30.00 |
| **RF:**  - EF1%  - **NEF1%** | 43.24  **0.727** | 54.84  **0.810** | 0.00  **0.000** |
| **XGB:**  - EF1%  - **NEF1%** | 45.95  **0.773** | 51.61  **0.762** | 1.25  **0.042** |
| **SVM:**  - EF1%  - **NEF1%** | 40.54  **0.682** | 54.84  **0.810** | 1.88  **0.063** |
| **ANN:**  - EF1%  - **NEF1%** | 37.84  **0.636** | 58.06  **0.857** | 2.50  **0.083** |
| **DNN:**  - EF1%  - **NEF1%** | 35.14  **0.591** | 54.84  **0.810** | 30.00  **1.000** |
| **Smina:**  - EF1%  - **NEF1%** | 8.11  **0.136** | 3.23  **0.048** | 1.25  **0.042** |
| **IFP:**  - EF1%  - **NEF1%** | 0.00  **0.000** | 16.13  **0.238** | 0.00  **0.000** |
| **CNN-Score:**  - EF1%  - **NEF1%** | 8.11  **0.136** | 0.00  **0.000** | 0.00  **0.000** |
| **RF-Score-VS:**  - EF1%  - **NEF1%** | 5.41  **0.091** | 9.68  **0.143** | 1.25  **0.042** |

**Table S5.** SBVS performance of target-specific ML SFs issued from the five “Dissimilar” (D) training-test partitions. A “Dissimilar” partition includes a full training set for a target, and a part of its corresponding test set composed only of molecules whose similarity (Morgan fingerprints, 2048 bits, radius 2) to any training molecule is lower than 0.7. The values related to target-specific ML SFs are the medians obtained after 10 training-test runs of each ML algorithm on each training-test partition. The performance of four generic SFs (Smina, IFP, CNN-Score, RF-Score-VS) is also reported for comparison (only one run is performed on each test set for each of these SFs).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **ACHE-PETS-D** | **ACHE-OTS-D** | **HMGR-PETS-D** | **HMGR-OTS-D** | **PPARA-OTS-D** |
| - Number of actives  - Number of inactives/decoys  - Total number of molecules  - Maximal EF1% | 39  1200  1239  30.77 | 12  2136  2148  100.00 | 8  1199  1207  100.00 | 7  2026  2033  100.00 | 65  1698  1763  26.15 |
| **RF:**  - EF1%  - **NEF1%** | 30.77  **1.000** | 41.67  **0.417** | 87.50  **0.875** | 71.43  **0.714** | 1.54  **0.059** |
| **XGB:**  - EF1%  - **NEF1%** | 7.69  **0.250** | 41.67  **0.417** | 62.50  **0.625** | 71.43  **0.714** | 0.00  **0.000** |
| **SVM:**  - EF1%  - **NEF1%** | 30.77  **1.000** | 41.67  **0.417** | 87.50  **0.875** | 71.43  **0.714** | 1.54  **0.059** |
| **ANN:**  - EF1%  - **NEF1%** | 5.13  **0.167** | 33.33  **0.333** | 100.00  **1.000** | 71.43  **0.714** | 3.08  **0.118** |
| **DNN:**  - EF1%  - **NEF1%** | 5.13  **0.167** | 33.33  **0.333** | 68.75  **0.688** | 71.43  **0.714** | 26.15  **1.000** |
| **Smina:**  - EF1%  - **NEF1%** | 15.38  **0.500** | 16.67  **0.167** | 0.00  **0.000** | 0.00  **0.000** | 1.54  **0.059** |
| **IFP:**  - EF1%  - **NEF1%** | 15.38  **0.500** | 0.00  **0.000** | 37.50  **0.375** | 14.29  **0.143** | 1.54  **0.059** |
| **CNN-Score:**  - EF1%  - **NEF1%** | 0.00  **0.000** | 16.67  **0.167** | 25.00  **0.250** | 0.00  **0.000** | 0.00  **0.000** |
| **RF-Score-VS:**  - EF1%  - **NEF1%** | 2.56  **0.083** | 0.00  **0.000** | 62.50  **0.625** | 28.57  **0.286** | 0.00  **0.000** |

**Additional Information.** Comparing the ligand binding sites of the ACHE human-extracted and *Tetronarce californica*-extracted variants.

The UniProt ID of the ACHE human-extracted variant is P22303 (representative PDB ID: 4M0E).

The UniProt ID of the ACHE *Tetronarce californica*-extracted variant is P04058 (representative PDB ID: 1E66).

The binding site of each PDB structure is composed of all amino acid residues that contain at least one heavy atom found within 5 Å from any heavy atom of the co-crystallized ligand.

The “Align” tool of UniProt is used to align the two amino acid sequences that correspond to the two binding sites of P22303 and P04058. The aligned sequences are as follows (the different amino acids are marked in bold red):

|  |  |
| --- | --- |
| **P22303 (4M0E)** | **P04058 (1E66)** |
| D74 | D72 |
| G82 | G80 |
| **T83** | **S81** |
| W86 | W84 |
| G120 | G117 |
| G121 | G118 |
| G122 | G119 |
| Y124 | Y121 |
| S125 | S122 |
| Y133 | Y130 |
| E202 | E199 |
| S203 | S200 |
| F297 | F290 |
| **Y337** | **F330** |
| F338 | F331 |
| Y341 | Y334 |
| W439 | W432 |
| M443 | M436 |
| **P446** | **I439** |
| H447 | H440 |
| G448 | G441 |
| Y449 | Y442 |

There are 19 (out of 22) similar positions after sequence alignment. The percentage sequence identity for the binding sites is therefore 86.36%.