**Supporting Information**

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

Viet-Khoa Tran-Nguyen1, Pedro J. Ballester1,2\*

1 Centre de Recherche en Cancérologie de Marseille (CRCM), INSERM, U1068, Marseille, F-13009, France. CNRS, UMR7258, Marseille, F-13009, France. Institut Paoli-Calmettes, Marseille, F-13009, France. Aix-Marseille University, UM 105, F-13284, Marseille, France.

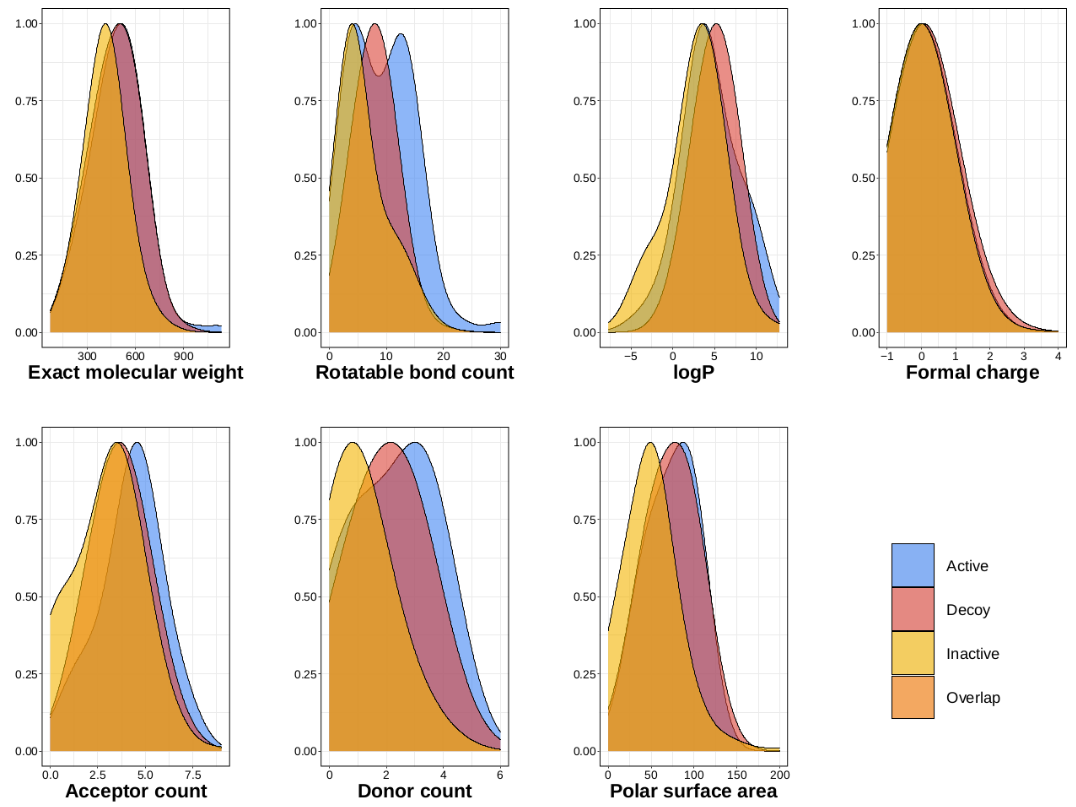
2 Department of Bioengineering, Imperial College London, London SW7 2AZ, UK.

\* Correspondence to: [pedro.ballester@inserm.fr](mailto:pedro.ballester@inserm.fr)

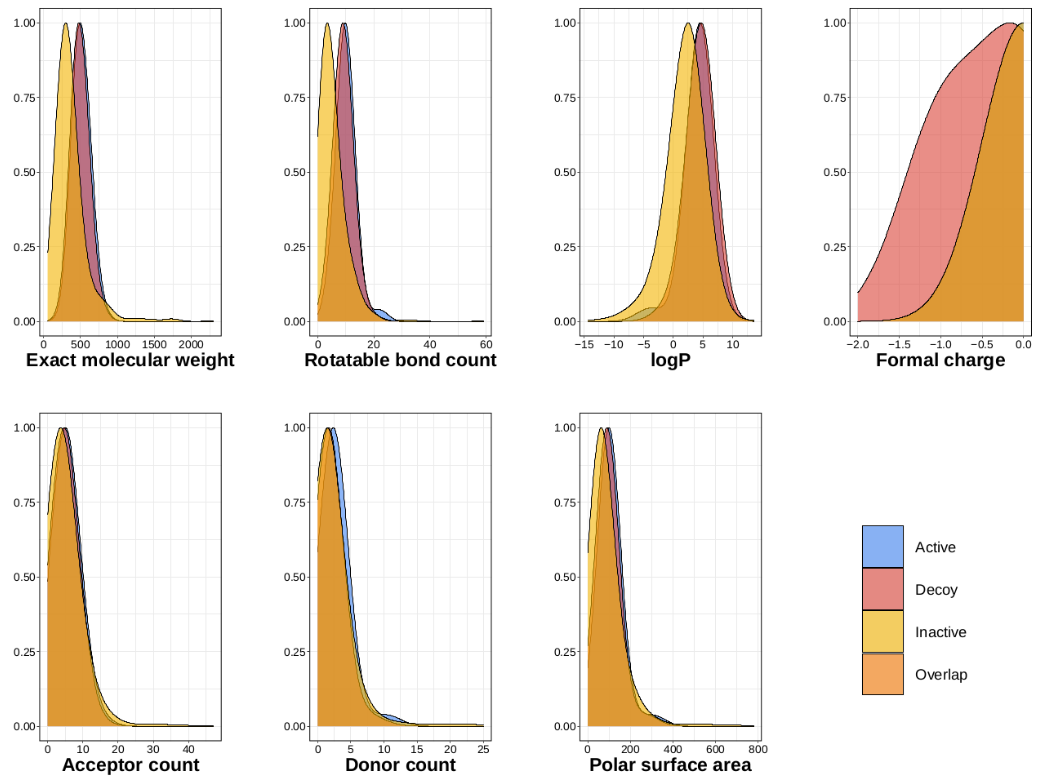
**Table S1.** SBVS performance of four generic SFs (Smina, IFP, CNN-Score, RF-Score-VS) on three DEKOIS 2.0 benchamarks (ACHE, HMGR, PPARA).

|  |  |  |  |
| --- | --- | --- | --- |
|  | **ACHE** | **HMGR** | **PPARA** |
| - Number of actives  - Number of decoys  - Total number of molecules  - PR-AUC of a random classifier  - Maximal EF1% | 40  1200  1240  0.032  30.00 | 40  1200  1240  0.032  30.00 | 40  1200  1240  0.032  30.00 |
| **Smina:**  - ROC-AUC  - PR-AUC  - EF1% | 0.649  0.195  15.00 | 0.780  0.080  2.50 | 0.679  0.063  0.00 |
| **IFP:**  - ROC-AUC  - PR-AUC  - EF1% | 0.735  0.167  15.00 | 0.714  0.125  10.00 | 0.631  0.052  0.00 |
| **CNN-Score:**  - ROC-AUC  - PR-AUC  - EF1% | 0.659  0.055  0.00 | 0.870  0.171  7.50 | 0.670  0.121  10.00 |
| **RF-Score-VS:**  - ROC-AUC  - PR-AUC  - EF1% | 0.690  0.083  2.50 | 0.945  0.763  30.00 | 0.652  0.167  12.50 |

**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 “own” PPARA benchamark (*n* = 1115) and their partition into the test set and the training set according to their clusters (Option 2.1).

|  |  |  |
| --- | --- | --- |
| Cluster\_Group | ID | Data set |
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| 2 | CHEMBL112725 | Test |
| 3 | CHEMBL191275 | Test |
| 4 | CHEMBL247951 | Test |
| 6 | CHEMBL318351 | Test |
| 7 | CHEMBL482740 | Test |
| 9 | CHEMBL209546 | Test |
| 10 | CHEMBL81248 | Test |
| 11 | CHEMBL180019 | Test |
| 12 | CHEMBL76676 | Test |
| 13 | CHEMBL402840 | Test |
| 14 | CHEMBL173159 | Test |
| 15 | CHEMBL77502 | Test |
| 16 | CHEMBL230304 | Test |
| 17 | CHEMBL4463341 | Test |
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| 20 | CHEMBL454678 | Test |
| 21 | CHEMBL87307 | Test |
| 22 | CHEMBL373874 | Test |
| 24 | CHEMBL401616 | Test |
| 25 | CHEMBL217907 | Test |
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| 27 | CHEMBL219586 | Test |
| 28 | CHEMBL549723 | Test |
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| 34 | CHEMBL1087587 | Test |
| 35 | CHEMBL205665 | Test |
| 36 | CHEMBL255388 | Test |
| 37 | CHEMBL253416 | Test |
| 38 | CHEMBL3901479 | Test |
| 39 | CHEMBL589256 | Test |
| 40 | CHEMBL258766 | Test |
| 41 | CHEMBL1813003 | Test |
| 42 | CHEMBL469937 | Test |
| 43 | CHEMBL200840 | Test |
| 44 | CHEMBL187557 | Test |
| 45 | CHEMBL253109 | Test |
| 46 | CHEMBL21241 | Test |
| 47 | CHEMBL3103200 | Test |
| 48 | CHEMBL454651 | Test |
| 50 | CHEMBL201581 | Test |
| 51 | CHEMBL1080470 | Test |
| 53 | CHEMBL4062472 | Test |
| 54 | CHEMBL3318038 | Test |
| 55 | CHEMBL1630380 | Test |
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| 66 | CHEMBL3398446 | Test |
| 67 | CHEMBL2206302 | Test |
| 68 | CHEMBL1927473 | Test |
| 69 | CHEMBL1087471 | Test |
| 70 | CHEMBL20125 | Test |
| 72 | CHEMBL278590 | Test |
| 75 | CHEMBL220597 | Test |
| 77 | CHEMBL237519 | Test |
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| 79 | CHEMBL107367 | Test |
| 83 | CHEMBL200495 | Test |
| 85 | CHEMBL477095 | Test |
| 86 | CHEMBL118756 | Test |
| 87 | CHEMBL4449760 | Test |
| 88 | CHEMBL4073499 | Test |
| 89 | CHEMBL3906547 | Test |
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| 95 | CHEMBL446893 | Test |
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| 25 | CHEMBL220533 | Training |
| 25 | CHEMBL221123 | Training |
| 25 | CHEMBL221184 | Training |
| 25 | CHEMBL221474 | Training |
| 25 | CHEMBL221525 | Training |
| 25 | CHEMBL221641 | Training |
| 25 | CHEMBL221649 | Training |
| 25 | CHEMBL374448 | Training |
| 25 | CHEMBL386957 | Training |
| 25 | CHEMBL425639 | Training |
| 25 | CHEMBL426550 | Training |
| 25 | CHEMBL221388 | Training |
| 25 | CHEMBL218487 | Training |
| 25 | CHEMBL220655 | Training |
| 25 | CHEMBL221489 | Training |
| 26 | CHEMBL244573 | Training |
| 26 | CHEMBL244574 | Training |
| 26 | CHEMBL244575 | Training |
| 26 | CHEMBL395560 | Training |
| 26 | CHEMBL396496 | Training |
| 26 | CHEMBL428037 | Training |
| 26 | CHEMBL244786 | Training |
| 26 | CHEMBL258832 | Training |
| 26 | CHEMBL259055 | Training |
| 26 | CHEMBL259856 | Training |
| 26 | CHEMBL261555 | Training |
| 26 | CHEMBL408941 | Training |
| 26 | CHEMBL409355 | Training |
| 26 | CHEMBL409513 | Training |
| 26 | CHEMBL411045 | Training |
| 27 | CHEMBL221074 | Training |
| 27 | CHEMBL218094 | Training |
| 27 | CHEMBL218637 | Training |
| 27 | CHEMBL218687 | Training |
| 27 | CHEMBL218691 | Training |
| 27 | CHEMBL218784 | Training |
| 27 | CHEMBL219587 | Training |
| 27 | CHEMBL219626 | Training |
| 27 | CHEMBL220281 | Training |
| 27 | CHEMBL220926 | Training |
| 27 | CHEMBL221201 | Training |
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| 28 | CHEMBL551479 | Training |
| 28 | CHEMBL551884 | Training |
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| 28 | CHEMBL557342 | Training |
| 28 | CHEMBL558072 | Training |
| 28 | CHEMBL558141 | Training |
| 28 | CHEMBL560205 | Training |
| 28 | CHEMBL560484 | Training |
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| 29 | CHEMBL384746 | Training |
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| 29 | CHEMBL492535 | Training |
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| 31 | CHEMBL2037183 | Training |
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| 32 | CHEMBL2204600 | Training |
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| 33 | CHEMBL1934481 | Training |
| 33 | CHEMBL1934482 | Training |
| 33 | CHEMBL1934483 | Training |
| 33 | CHEMBL1934485 | Training |
| 33 | CHEMBL1934486 | Training |
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| 34 | CHEMBL1088099 | Training |
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| 34 | CHEMBL1088246 | Training |
| 34 | CHEMBL1088257 | Training |
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| 35 | CHEMBL424674 | Training |
| 35 | CHEMBL424685 | Training |
| 35 | CHEMBL202739 | Training |
| 35 | CHEMBL202973 | Training |
| 35 | CHEMBL203338 | Training |
| 35 | CHEMBL203408 | Training |
| 35 | CHEMBL203621 | Training |
| 35 | CHEMBL205803 | Training |
| 35 | CHEMBL206202 | Training |
| 35 | CHEMBL206759 | Training |
| 35 | CHEMBL382178 | Training |
| 36 | CHEMBL256468 | Training |
| 36 | CHEMBL257517 | Training |
| 36 | CHEMBL271240 | Training |
| 36 | CHEMBL271739 | Training |
| 36 | CHEMBL272336 | Training |
| 36 | CHEMBL272962 | Training |
| 36 | CHEMBL403847 | Training |
| 36 | CHEMBL404451 | Training |
| 36 | CHEMBL404646 | Training |
| 36 | CHEMBL411118 | Training |
| 36 | CHEMBL429734 | Training |
| 37 | CHEMBL253417 | Training |
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| 37 | CHEMBL398677 | Training |
| 37 | CHEMBL399629 | Training |
| 37 | CHEMBL252996 | Training |
| 37 | CHEMBL537921 | Training |
| 37 | CHEMBL554562 | Training |
| 37 | CHEMBL556643 | Training |
| 37 | CHEMBL562659 | Training |
| 37 | CHEMBL565198 | Training |
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| 38 | CHEMBL3981588 | Training |
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| 38 | CHEMBL4558447 | Training |
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| 39 | CHEMBL591534 | Training |
| 39 | CHEMBL592234 | Training |
| 39 | CHEMBL592235 | Training |
| 39 | CHEMBL592236 | Training |
| 39 | CHEMBL603612 | Training |
| 39 | CHEMBL606462 | Training |
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| 40 | CHEMBL260840 | Training |
| 40 | CHEMBL409215 | Training |
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| 41 | CHEMBL1813005 | Training |
| 41 | CHEMBL1813006 | Training |
| 41 | CHEMBL1813007 | Training |
| 41 | CHEMBL1813010 | Training |
| 41 | CHEMBL1813011 | Training |
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| 42 | CHEMBL1956364 | Training |
| 42 | CHEMBL2375947 | Training |
| 42 | CHEMBL2375948 | Training |
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| 43 | CHEMBL246204 | Training |
| 43 | CHEMBL246205 | Training |
| 43 | CHEMBL246206 | Training |
| 43 | CHEMBL246208 | Training |
| 43 | CHEMBL248261 | Training |
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| 44 | CHEMBL191276 | Training |
| 44 | CHEMBL364467 | Training |
| 44 | CHEMBL370021 | Training |
| 44 | CHEMBL371195 | Training |
| 44 | CHEMBL426451 | Training |
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| 45 | CHEMBL253520 | Training |
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| 45 | CHEMBL403637 | Training |
| 45 | CHEMBL404467 | Training |
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| 46 | CHEMBL21105 | Training |
| 46 | CHEMBL21706 | Training |
| 46 | CHEMBL281791 | Training |
| 46 | CHEMBL2088421 | Training |
| 46 | CHEMBL2088422 | Training |
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| 47 | CHEMBL3103197 | Training |
| 47 | CHEMBL3103198 | Training |
| 47 | CHEMBL3103194 | Training |
| 47 | CHEMBL3103195 | Training |
| 47 | CHEMBL3103196 | Training |
| 47 | CHEMBL3103199 | Training |
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| 48 | CHEMBL461145 | Training |
| 48 | CHEMBL461533 | Training |
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| 48 | CHEMBL516510 | Training |
| 49 | CHEMBL363006 | Training |
| 50 | CHEMBL201653 | Training |
| 50 | CHEMBL425766 | Training |
| 50 | CHEMBL202617 | Training |
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| 51 | CHEMBL1081355 | Training |
| 51 | CHEMBL1086861 | Training |
| 52 | CHEMBL4448919 | Training |
| 53 | CHEMBL4072395 | Training |
| 53 | CHEMBL4074391 | Training |
| 53 | CHEMBL4093146 | Training |
| 53 | CHEMBL4094877 | Training |
| 53 | CHEMBL4101596 | Training |
| 53 | CHEMBL4103575 | Training |
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| 54 | CHEMBL3318040 | Training |
| 54 | CHEMBL3318041 | Training |
| 54 | CHEMBL518038 | Training |
| 54 | CHEMBL3318037 | Training |
| 54 | CHEMBL456792 | Training |
| 55 | CHEMBL1630381 | Training |
| 55 | CHEMBL1630382 | Training |
| 55 | CHEMBL1630383 | Training |
| 55 | CHEMBL1630384 | Training |
| 55 | CHEMBL1630386 | Training |
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| 56 | CHEMBL1084321 | Training |
| 56 | CHEMBL1085062 | Training |
| 56 | CHEMBL1085795 | Training |
| 56 | CHEMBL1085796 | Training |
| 56 | CHEMBL1086515 | Training |
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| 57 | CHEMBL455853 | Training |
| 57 | CHEMBL476197 | Training |
| 57 | CHEMBL477644 | Training |
| 57 | CHEMBL514568 | Training |
| 57 | CHEMBL515666 | Training |
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| 58 | CHEMBL474157 | Training |
| 58 | CHEMBL491142 | Training |
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| 58 | CHEMBL474148 | Training |
| 58 | CHEMBL514007 | Training |
| 59 | CHEMBL467349 | Training |
| 59 | CHEMBL468160 | Training |
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| 59 | CHEMBL512789 | Training |
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| 60 | CHEMBL552240 | Training |
| 60 | CHEMBL560830 | Training |
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| 63 | CHEMBL119911 | Training |
| 64 | CHEMBL4466709 | Training |
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| 64 | CHEMBL4474407 | Training |
| 64 | CHEMBL4571498 | Training |
| 64 | CHEMBL4586557 | Training |
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| 65 | CHEMBL3948805 | Training |
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| 65 | CHEMBL3962832 | Training |
| 65 | CHEMBL4110590 | Training |
| 66 | CHEMBL3398449 | Training |
| 66 | CHEMBL3398451 | Training |
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| 67 | CHEMBL2206304 | Training |
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| 68 | CHEMBL2035068 | Training |
| 68 | CHEMBL2035069 | Training |
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| 68 | CHEMBL2035071 | Training |
| 69 | CHEMBL1087590 | Training |
| 69 | CHEMBL1087593 | Training |
| 69 | CHEMBL1087594 | Training |
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| 70 | CHEMBL281608 | Training |
| 71 | CHEMBL230519 | Training |
| 72 | CHEMBL248906 | Training |
| 72 | CHEMBL124842 | Training |
| 72 | CHEMBL125230 | Training |
| 72 | CHEMBL340011 | Training |
| 72 | CHEMBL435278 | Training |
| 73 | CHEMBL87928 | Training |
| 73 | CHEMBL89996 | Training |
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| 74 | CHEMBL111271 | Training |
| 75 | CHEMBL221850 | Training |
| 75 | CHEMBL222117 | Training |
| 75 | CHEMBL374296 | Training |
| 76 | CHEMBL220708 | Training |
| 77 | CHEMBL237307 | Training |
| 77 | CHEMBL236876 | Training |
| 77 | CHEMBL237085 | Training |
| 77 | CHEMBL237518 | Training |
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| 79 | CHEMBL147095 | Training |
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| 81 | CHEMBL482334 | Training |
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| 83 | CHEMBL118887 | Training |
| 83 | CHEMBL121206 | Training |
| 84 | CHEMBL381477 | Training |
| 85 | CHEMBL478725 | Training |
| 85 | CHEMBL593796 | Training |
| 85 | CHEMBL593801 | Training |
| 85 | CHEMBL594034 | Training |
| 86 | CHEMBL118251 | Training |
| 86 | CHEMBL122417 | Training |
| 86 | CHEMBL2037184 | Training |
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| 87 | CHEMBL4461949 | Training |
| 87 | CHEMBL4471853 | Training |
| 88 | CHEMBL4092600 | Training |
| 88 | CHEMBL4064900 | Training |
| 88 | CHEMBL4100336 | Training |
| 89 | CHEMBL3916538 | Training |
| 89 | CHEMBL3919950 | Training |
| 89 | CHEMBL3982893 | Training |
| 90 | CHEMBL1934471 | Training |
| 90 | CHEMBL1934473 | Training |
| 91 | CHEMBL1934314 | Training |
| 92 | CHEMBL485155 | Training |
| 92 | CHEMBL485179 | Training |
| 92 | CHEMBL520508 | Training |
| 93 | CHEMBL468159 | Training |
| 94 | CHEMBL234819 | Training |
| 94 | CHEMBL393381 | Training |
| 94 | CHEMBL394031 | Training |
| 95 | CHEMBL147721 | Training |
| 95 | CHEMBL345009 | Training |
| 96 | CHEMBL355695 | Training |
| 96 | CHEMBL166637 | Training |
| 96 | CHEMBL166628 | Training |
| 97 | CHEMBL118577 | Training |
| 97 | CHEMBL118816 | Training |
| 97 | CHEMBL324027 | Training |
| 98 | CHEMBL491750 | Training |
| 98 | CHEMBL491751 | Training |
| 99 | CHEMBL23874 | Training |
| 99 | CHEMBL1783033 | Training |
| 100 | CHEMBL4519542 | Training |
| 100 | CHEMBL4535730 | Training |
| 100 | CHEMBL4593987 | Training |
| 101 | CHEMBL4464538 | Training |
| 101 | CHEMBL4519376 | Training |
| 102 | CHEMBL4436335 | Training |
| 102 | CHEMBL4470753 | Training |
| 102 | CHEMBL4516239 | Training |
| 103 | CHEMBL4454999 | Training |
| 103 | CHEMBL4457812 | Training |
| 103 | CHEMBL4543257 | Training |
| 104 | CHEMBL4160945 | Training |
| 104 | CHEMBL4167789 | Training |
| 104 | CHEMBL4174996 | Training |
| 105 | CHEMBL4060007 | Training |
| 106 | CHEMBL1828826 | Training |
| 106 | CHEMBL3752643 | Training |
| 106 | CHEMBL3753965 | Training |
| 107 | CHEMBL3601087 | Training |
| 107 | CHEMBL3601089 | Training |
| 107 | CHEMBL3601093 | Training |
| 108 | CHEMBL2022403 | Training |
| 108 | CHEMBL2022404 | Training |
| 108 | CHEMBL2022405 | Training |
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| 109 | CHEMBL1935495 | Training |
| 109 | CHEMBL1935608 | Training |
| 110 | CHEMBL1927474 | Training |
| 110 | CHEMBL1927475 | Training |
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| 111 | CHEMBL1080365 | Training |
| 111 | CHEMBL1080699 | Training |
| 112 | CHEMBL562786 | Training |
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| 113 | CHEMBL514544 | Training |
| 113 | CHEMBL522754 | Training |
| 114 | CHEMBL481549 | Training |
| 114 | CHEMBL481550 | Training |
| 114 | CHEMBL520272 | Training |
| 115 | CHEMBL101123 | Training |
| 115 | CHEMBL322690 | Training |
| 115 | CHEMBL443218 | Training |
| 116 | CHEMBL197684 | Training |
| 116 | CHEMBL198163 | Training |
| 116 | CHEMBL383607 | Training |
| 117 | CHEMBL117402 | Training |
| 117 | CHEMBL325844 | Training |
| 117 | CHEMBL331388 | Training |
| 118 | CHEMBL260627 | Training |
| 119 | CHEMBL252675 | Training |
| 119 | CHEMBL253486 | Training |
| 119 | CHEMBL253923 | Training |
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| 120 | CHEMBL120243 | Training |
| 121 | CHEMBL1090212 | Training |
| 121 | CHEMBL1091664 | Training |
| 122 | CHEMBL401534 | Training |
| 122 | CHEMBL256142 | Training |
| 122 | CHEMBL256358 | Training |
| 123 | CHEMBL364378 | Training |
| 123 | CHEMBL192521 | Training |
| 123 | CHEMBL193082 | Training |
| 124 | CHEMBL427530 | Training |
| 124 | CHEMBL191149 | Training |
| 124 | CHEMBL191556 | Training |
| 125 | CHEMBL400625 | Training |
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| 126 | CHEMBL391479 | Training |
| 126 | CHEMBL232396 | Training |
| 127 | CHEMBL2237300 | Training |
| 128 | CHEMBL4083589 | Training |
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| 129 | CHEMBL3890301 | Training |
| 130 | CHEMBL3601098 | Training |
| 130 | CHEMBL3601099 | Training |
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| 131 | CHEMBL3335661 | Training |
| 132 | CHEMBL1934468 | Training |
| 133 | CHEMBL1778839 | Training |
| 133 | CHEMBL1778840 | Training |
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| 134 | CHEMBL1732818 | Training |
| 135 | CHEMBL1644305 | Training |
| 135 | CHEMBL1644310 | Training |
| 136 | CHEMBL1644299 | Training |
| 136 | CHEMBL1644301 | Training |
| 137 | CHEMBL1079961 | Training |
| 137 | CHEMBL1079962 | Training |
| 138 | CHEMBL1075723 | Training |
| 138 | CHEMBL1075732 | Training |
| 139 | CHEMBL456912 | Training |
| 139 | CHEMBL514713 | Training |
| 140 | CHEMBL489768 | Training |
| 140 | CHEMBL489769 | Training |
| 141 | CHEMBL448996 | Training |
| 141 | CHEMBL450050 | Training |
| 142 | CHEMBL401560 | Training |
| 142 | CHEMBL403909 | Training |
| 143 | CHEMBL102004 | Training |
| 143 | CHEMBL317424 | Training |
| 144 | CHEMBL280897 | Training |
| 145 | CHEMBL252995 | Training |
| 146 | CHEMBL246209 | Training |
| 146 | CHEMBL248411 | Training |
| 147 | CHEMBL240868 | Training |
| 147 | CHEMBL241269 | Training |
| 148 | CHEMBL2113263 | Training |
| 148 | CHEMBL220223 | Training |
| 149 | CHEMBL214289 | Training |
| 149 | CHEMBL214295 | Training |
| 150 | CHEMBL198579 | Training |
| 151 | CHEMBL495904 | Training |
| 151 | CHEMBL498171 | Training |
| 152 | CHEMBL234659 | Training |
| 152 | CHEMBL391478 | Training |
| 153 | CHEMBL234588 | Training |
| 153 | CHEMBL234589 | Training |
| 154 | CHEMBL255309 | Training |
| 154 | CHEMBL403432 | Training |
| 155 | CHEMBL205777 | Training |
| 156 | CHEMBL472451 | Training |
| 157 | CHEMBL192500 | Training |
| 158 | CHEMBL278994 | Training |
| 159 | CHEMBL410478 | Training |
| 160 | CHEMBL3780740 | Training |
| 161 | CHEMBL2037182 | Training |
| 162 | CHEMBL2037008 | Training |
| 163 | CHEMBL4571975 | Training |
| 164 | CHEMBL4104138 | Training |
| 165 | CHEMBL4101577 | Training |
| 166 | CHEMBL4100619 | Training |
| 167 | CHEMBL3982782 | Training |
| 168 | CHEMBL3735011 | Training |
| 169 | CHEMBL3601096 | Training |
| 170 | CHEMBL3397563 | Training |
| 171 | CHEMBL3354988 | Training |
| 172 | CHEMBL3354987 | Training |
| 173 | CHEMBL2069935 | Training |
| 174 | CHEMBL1934308 | Training |
| 175 | CHEMBL1927476 | Training |
| 176 | CHEMBL1760555 | Training |
| 177 | CHEMBL1720494 | Training |
| 178 | CHEMBL1494365 | Training |
| 179 | CHEMBL1089633 | Training |
| 180 | CHEMBL1080361 | Training |
| 181 | CHEMBL1079489 | Training |
| 182 | CHEMBL1075683 | Training |
| 183 | CHEMBL584704 | Training |
| 184 | CHEMBL572795 | Training |
| 185 | CHEMBL526740 | Training |
| 186 | CHEMBL438346 | Training |
| 187 | CHEMBL426883 | Training |
| 188 | CHEMBL401811 | Training |
| 189 | CHEMBL401562 | Training |
| 190 | CHEMBL374948 | Training |
| 191 | CHEMBL318696 | Training |
| 192 | CHEMBL306229 | Training |
| 193 | CHEMBL272017 | Training |
| 194 | CHEMBL250673 | Training |
| 195 | CHEMBL249865 | Training |
| 196 | CHEMBL219156 | Training |
| 197 | CHEMBL213355 | Training |
| 198 | CHEMBL207569 | Training |
| 199 | CHEMBL202631 | Training |
| 200 | CHEMBL198929 | Training |
| 201 | CHEMBL198786 | Training |
| 202 | CHEMBL194698 | Training |
| 203 | CHEMBL190739 | Training |
| 204 | CHEMBL190645 | Training |
| 205 | CHEMBL39687 | Training |
| 206 | CHEMBL496744 | Training |
| 207 | CHEMBL491039 | Training |
| 208 | CHEMBL391085 | Training |
| 209 | CHEMBL391084 | Training |
| 210 | CHEMBL593087 | Training |
| 211 | CHEMBL257345 | Training |
| 212 | CHEMBL221529 | Training |
| 213 | CHEMBL148797 | Training |
| 214 | CHEMBL2113219 | Training |
| 215 | CHEMBL383011 | Training |
| 216 | CHEMBL255872 | Training |
| 217 | CHEMBL3707395 | Training |
| 218 | CHEMBL592054 | Training |
| 219 | CHEMBL426878 | Training |
| 220 | CHEMBL242007 | Training |
| 221 | CHEMBL148319 | Training |
| 222 | CHEMBL214921 | Training |
| 223 | CHEMBL221044 | Training |
| 224 | CHEMBL424133 | Training |
| 225 | CHEMBL280065 | Training |
| 226 | CHEMBL24458 | Training |

**Table S3.** SBVS performance of target-specific ML SFs trained on the “own” data sets ACHE and HMGR (Option 1) and tested on the corresponding DEKOIS 2.0 benchamarks (see Table S1 for the performance of four generic SFs).

|  |  |  |
| --- | --- | --- |
|  | **ACHE** | **HMGR** |
| **RF:**  - ROC-AUC  - PR-AUC  - EF1% | 0.737  0.525  30.00 | 0.997  0.964  30.00 |
| **XGB:**  - ROC-AUC  - PR-AUC  - EF1% | 0.729  0.165  10.00 | 0.979  0.886  30.00 |
| **SVM:**  - ROC-AUC  - PR-AUC  - EF1% | 0.786  0.566  30.00 | 0.977  0.961  30.00 |
| **ANN:**  - ROC-AUC  - PR-AUC  - EF1% | 0.666  0.094  5.00 | 0.994  0.940  30.00 |
| **DNN:**  - ROC-AUC  - PR-AUC  - EF1% | 0.627  0.086  7.50 | 0.936  0.840  30.00 |

**Table S4.** SBVS performance of target-specific ML SFs trained on the “own” training sets ACHE, HMGR, PPARA and tested on the corresponding test sets (Option 2). The performance of four generic SFs (Smina, IFP, CNN-Score, RF-Score-VS) is also reported for comparison.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **ACHE** | **HMGR** | **PPARA** |
| - Number of actives  - Number of inactives/decoys  - Total number of molecules  - PR-AUC of a random classifier  - Maximal EF1% | 37  2170  2207  0.017  59.46 | 31  2077  2108  0.015  67.74 | 80  2399  2479  0.032  30.00 |
| **RF:**  - ROC-AUC  - PR-AUC  - EF1% | 0.835  0.524  43.24 | 0.940  0.646  54.84 | 0.763  0.111  6.25 |
| **XGB:**  - ROC-AUC  - PR-AUC  - EF1% | 0.892  0.501  45.95 | 0.971  0.688  51.61 | 0.715  0.066  2.50 |
| **SVM:**  - ROC-AUC  - PR-AUC  - EF1% | 0.866  0.438  40.54 | 0.952  0.675  54.84 | 0.768  0.129  7.50 |
| **ANN:**  - ROC-AUC  - PR-AUC  - EF1% | 0.862  0.465  37.84 | 0.909  0.670  58.06 | 0.768  0.086  5.00 |
| **DNN:**  - ROC-AUC  - PR-AUC  - EF1% | 0.807  0.416  35.14 | 0.789  0.717  54.84 | 0.735  0.471  30.00 |
| **Smina:**  - ROC-AUC  - PR-AUC  - EF1% | 0.623  0.083  8.11 | 0.581  0.020  3.23 | 0.580  0.045  2.50 |
| **IFP:**  - ROC-AUC  - PR-AUC  - EF1% | 0.530  0.021  0.00 | 0.561  0.084  16.13 | 0.616  0.054  5.00 |
| **CNN-Score:**  - ROC-AUC  - PR-AUC  - EF1% | 0.524  0.030  8.11 | 0.671  0.026  0.00 | 0.581  0.056  2.50 |
| **RF-Score-VS:**  - ROC-AUC  - PR-AUC  - EF1% | 0.509  0.050  5.41 | 0.601  0.034  9.68 | 0.570  0.038  0.00 |

**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 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%.