SUPPORTING INFORMATION

**In Silico Design of Diacylglycerol acyl transferase-1 (DGAT1) inhibitors based on SMILES descriptors Using Monte Carlo Method**

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**Abstract**

The diabetes, obesity and other disease related to metabolic disorder are worldwide health problems. These syndromes can be well treated when a particular enzyme based therapy is developed. Diacylglycerol acyltransferase (DGAT; EC 2.3.1.20) is a microsomal enzyme which is responsible for the synthesis of triglycerides from 1,2-diacylglycerol by catalyzing the acyl-CoA-dependent acylation. The obesity and type-II diabetes can be checked by the inhibition of DGAT1 enzyme. QSAR modelling is an essential technique in drug design and development. To study the aspect of DGAT1 inhibitors, Monte Carlo method based QSAR is developed for 197 DGAT1 inhibitors. QSAR models were made by using the optimal descriptor based on SMILES notation. Different statistical parameters including novel Index of Ideality of Correlation (IIC) were applied to validate the generated QSAR models. Four random splits were prepared from the data set. The statistical criteria **R2 = 0.8129**, **CCC= 0.8979** and **Q2 = 0.7962** of the validation set of split 1 were best, therefore the developed QSAR model of split 1 was decided to be the leading model. The molecular fragments, which were promotor of endpoint increase and endpoint decrease, were also determined. Thirteen new DGAT1 inhibitors were designed from the lead compound DGAT011.

**Keywords:** Diacylglycerol acyltransferase, DGAT1 inhibitors, QSAR, IIC, SMILES

**Table S1**: Split distribution with SMILES notation, experimental pIC50, calculated pIC50, residual pIC50 and Applicability domain (AD) with IIC using equation 4

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Split | | | | CHEMBL ID and other from reference 34\* | ID | SMILES | Expr pIC50 | Calc pIC50 | | | | Expr-Calc pIC50 | | | | **AD** | | | |
| **1** | **2** | **3** | **4** | **1** | **2** | **3** | **4** | **1** | **2** | **3** | **4** | **1** | **2** | **3** | **4** |
| - | + | + | - | CHEMBL3037924 | DGAT001 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc(cn1)-c1nc2ccc(Cl)cc2[nH]1 | 9.0000 | 8.0188 | 8.2273 | 7.7526 | 8.2503 | 0.9812 | 0.7727 | 1.2474 | 0.7497 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL2036730 | DGAT002 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(NC(=O)c2nnc(Nc3ccc(F)c(F)c3)o2)cc1 | 8.9590 | 8.8322 | 8.2183 | 7.7009 | 8.3362 | 0.1268 | 0.7407 | 1.2581 | 0.6228 | NO | YES | YES | YES |
| # | \* | + | - | CHEMBL3929522 | DGAT003 | CC(C)(NC(=O)c1cn2cc(ccc2n1)-c1ccc(cc1)C1CC[C@H](CC(O)=O)CC1)c1ccc(F)cc1 | 8.9210 | 8.0441 | 8.0889 | 8.1500 | 8.4721 | 0.8769 | 0.8321 | 0.7710 | 0.4489 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3233889 | DGAT004 | Cc1cc(C(=O)NCCCCCc2ccccc2)c2ccc(cc2n1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 8.8539 | 8.5691 | 8.7119 | 8.8106 | 8.8695 | 0.2848 | 0.1421 | 0.0434 | -0.0155 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL3613351 | DGAT005 | Cc1ccccc1-c1ccc(cc1)C(=O)NCCNC(=O)c1ccc(O[C@H]2C3CC4CC2C[C@](C4)(C3)C(O)=O)cc1 | 8.6990 | 8.5602 | 8.1047 | 8.1978 | 8.5232 | 0.1388 | 0.5943 | 0.5012 | 0.1758 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL2408630 | DGAT006 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C(F)(F)F | 8.6580 | 8.5657 | 8.7135 | 8.4888 | 8.5239 | 0.0923 | -0.0555 | 0.1692 | 0.1341 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3037925 | DGAT007 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C(F)(F)F | 8.5530 | 8.1327 | 8.1759 | 7.9983 | 8.2460 | 0.4203 | 0.3771 | 0.5547 | 0.3070 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL2408470 | DGAT008 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2cc(F)c(F)cc2[nH]1 | 8.4685 | 8.5569 | 9.1764 | 8.6650 | 8.5412 | -0.0884 | -0.7074 | -0.1960 | -0.0722 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL2408472 | DGAT009 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(F)cc2[nH]1 | 8.4690 | 8.3765 | 8.5638 | 8.2456 | 8.1723 | 0.0925 | -0.0948 | 0.2234 | 0.2967 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL2408632 | DGAT010 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(Cl)cc2[nH]1 | 8.4320 | 8.4518 | 8.7648 | 8.2431 | 8.5281 | -0.0198 | -0.3328 | 0.1889 | -0.0961 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL2408633 | DGAT011 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(Cl)cc2[nH]1 | 8.3770 | 8.3770 | 8.6161 | 8.3374 | 8.6409 | 0.0000 | -0.2391 | 0.0396 | -0.2639 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL2408620 | DGAT012 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2cc(F)c(F)cc2[nH]1 | 8.3665 | 8.4821 | 9.0278 | 8.7592 | 8.6540 | -0.1156 | -0.6608 | -0.3922 | -0.2870 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL2408631 | DGAT013 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C(F)(F)F | 8.3570 | 8.4909 | 8.5648 | 8.5831 | 8.6366 | -0.1339 | -0.2078 | -0.2261 | -0.2796 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL2408623 | DGAT014 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(OC(F)(F)F)cc2[nH]1 | 8.3370 | 8.4509 | 8.7586 | 8.4946 | 8.5502 | -0.1139 | -0.4216 | -0.1576 | -0.2132 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3613341 | DGAT015 | Cc1cccc(C)c1-c1ccc(cc1)C(=O)NCCNC(=O)c1ccc(O[C@H]2C3CC4CC2C[C@](C4)(C3)C(O)=O)cc1 | 8.3010 | 8.7117 | 8.2812 | 8.2263 | 8.7685 | -0.4107 | 0.0198 | 0.0747 | -0.4675 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3613349 | DGAT016 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)c1nc(oc1C(F)(F)F)-c1ccccc1)C(C3)C2 | 8.3010 | 8.3308 | 8.1736 | 7.9995 | 8.4182 | -0.0298 | 0.1274 | 0.3015 | -0.1172 | YES | YES | YES | No |
| # | + | # | \* | CHEMBL3613355 | DGAT017 | OC(=O)[C@@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1)C(C3)C2 | 8.3010 | 8.6095 | 8.3252 | 8.1444 | 8.5682 | -0.3085 | -0.0242 | 0.1566 | -0.2672 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3918850 | DGAT018 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)NCc1ccc(Oc2ccc(F)cc2)cc1 | 8.2760 | 8.4456 | 8.8795 | 8.8208 | 8.8206 | -0.1696 | -0.6035 | -0.5448 | -0.5446 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3924760 | DGAT019 | Cc1cccc(Cl)c1CNC(=O)c1cn2cc(ccc2n1)-c1ccc(cc1)C1CC[C@H](CC(O)=O)CC1 | 8.1190 | 8.1187 | 8.3625 | 8.3681 | 8.8958 | 0.0003 | -0.2435 | -0.2491 | -0.7768 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL2165819 | DGAT020 | OC(=O)[C@@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(ccc2[nH]1)C(F)(F)F | 8.0969 | 7.7409 | 7.7921 | 7.6884 | 7.5479 | 0.3560 | 0.3049 | 0.4086 | 0.5491 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL3233885 | DGAT021 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1)C(C3)C2 | 8.0970 | 7.8756 | 7.7778 | 7.5703 | 7.6796 | 0.2214 | 0.3192 | 0.5267 | 0.4174 | YES | YES | YES | YES |
| + | - | - | + | CHEMBL3342774 | DGAT022 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2c(cccc2c1)C(=O)Nc1ccccc1 | 8.0970 | 7.2786 | 7.1085 | 7.0231 | 7.0880 | 0.8184 | 0.9885 | 1.0739 | 1.0090 | YES | YES | YES | YES |
| + | + | - | + | CHEMBL3613340 | DGAT023 | Nc1c(cnc2ccnn12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 8.0970 | 7.2700 | 7.0501 | 6.5965 | 7.1677 | 0.8270 | 1.0469 | 1.5005 | 0.9293 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3613347 | DGAT024 | OC(=O)[C@@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc4ccccc4c1)C(C3)C2 | 8.0969 | 8.3628 | 7.8690 | 7.7224 | 7.7762 | -0.2659 | 0.2280 | 0.3746 | 0.3208 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL2408634 | DGAT025 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccccc2[nH]1 | 8.0910 | 7.8578 | 7.9207 | 7.8230 | 7.4622 | 0.2332 | 0.1703 | 0.2680 | 0.6288 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL2408471 | DGAT026 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(F)cc2[nH]1 | 8.0910 | 8.3017 | 8.4151 | 8.3398 | 8.2850 | -0.2107 | -0.3241 | -0.2488 | -0.1940 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3613350 | DGAT027 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)NCc1ccc2OCCCOc2c1 | 8.0040 | 7.2396 | 7.3950 | 7.7756 | 7.7548 | 0.7644 | 0.6090 | 0.2284 | 0.2492 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3233888 | DGAT028 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)Nc1ccc(Cl)c(Cl)c1 | 8.0044 | 7.9255 | 8.1223 | 8.3440 | 8.3665 | 0.0789 | -0.1183 | -0.3400 | -0.3625 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL3949646 | DGAT029 | OC(=O)[C@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1)C(C3)C2 | 8.0000 | 8.6875 | 8.3637 | 8.1421 | 8.6676 | -0.6875 | -0.3637 | -0.1421 | -0.6676 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3930018 | DGAT030 | Cc1cc(C(=O)Nc2ccccc2)c2ccc(cc2n1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 8.0000 | 7.9721 | 8.1051 | 8.0927 | 7.9338 | 0.0279 | -0.1051 | -0.0927 | 0.0662 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3342772 | DGAT031 | OC(=O)[C@@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(Cl)ccc2[nH]1 | 7.9590 | 7.6525 | 7.6927 | 7.4427 | 7.4792 | 0.3065 | 0.2663 | 0.5163 | 0.4798 | YES | YES | YES | No |
| \* | # | - | + | CHEMBL3975967 | DGAT032 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)Nc1cccc(Cl)c1 | 7.9318 | 7.5006 | 7.5094 | 7.8197 | 7.9199 | 0.4312 | 0.4226 | 0.1123 | 0.0121 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL2408635 | DGAT033 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccccc2[nH]1 | 7.9210 | 7.7830 | 7.7720 | 7.9172 | 7.5750 | 0.1380 | 0.1490 | 0.0038 | 0.3460 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL3946651 | DGAT034 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)NCc1ccc(F)c(Cl)c1 | 7.9140 | 7.7853 | 8.6641 | 8.6693 | 8.0493 | 0.1287 | -0.7501 | -0.7553 | -0.1353 | YES | YES | YES | No |
| # | \* | + | - | CHEMBL2408628 | DGAT035 | COc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@H](CC2)C(O)=O)nc1 | 7.8860 | 7.4339 | 7.4090 | 7.4206 | 7.5855 | 0.4521 | 0.4770 | 0.4654 | 0.3005 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL402721 | DGAT036 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccc(cc2)C(F)(F)F)cc1 | 7.8539 | 7.7813 | 7.6382 | 7.2831 | 7.5762 | 0.0726 | 0.2158 | 0.5709 | 0.2778 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL3287876 | DGAT037 | COc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@@H](CC2)C(O)=O)nc1 | 7.7960 | 7.5087 | 7.5577 | 7.3263 | 7.4728 | 0.2873 | 0.2383 | 0.4697 | 0.3232 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL254444 | DGAT038 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1C(F)(F)F | 7.7960 | 7.1908 | 7.0496 | 7.0169 | 7.1524 | 0.6052 | 0.7464 | 0.7791 | 0.6436 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL2408629 | DGAT039 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccccc2C(F)(F)F)cc1 | 7.7960 | 7.5772 | 6.9610 | 7.1214 | 7.0967 | 0.2188 | 0.8350 | 0.6746 | 0.6993 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL254445 | DGAT040 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cccc(c2)C(F)(F)F)cc1 | 7.7696 | 7.8655 | 7.7453 | 7.5120 | 7.6023 | -0.0959 | 0.0247 | 0.2580 | 0.1677 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL3287865 | DGAT041 | C[C@@H]1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.7450 | 7.4267 | 7.4048 | 7.3782 | 7.4847 | 0.3183 | 0.3402 | 0.3668 | 0.2603 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3905096 | DGAT042 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cccc(Cl)c2)cc1 | 7.7210 | 7.7679 | 7.6417 | 7.4045 | 7.6948 | -0.0469 | 0.0793 | 0.3165 | 0.0262 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3613348 | DGAT043 | OC(=O)[C@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc4ccccc4c1)C(C3)C2 | 7.7210 | 8.4408 | 7.9075 | 7.7202 | 7.8757 | -0.7198 | -0.1865 | 0.0008 | -0.1547 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL404419 | DGAT044 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)Nc1ccc(F)c(Cl)c1 | 7.7212 | 7.6238 | 8.2868 | 8.3665 | 7.7915 | 0.0974 | -0.5658 | -0.6455 | -0.0705 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL254865 | DGAT045 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cc(ccc2F)C(F)(F)F)cc1 | 7.6780 | 7.4978 | 7.2659 | 7.1337 | 7.4488 | 0.1802 | 0.4121 | 0.5443 | 0.2292 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3613339 | DGAT046 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc4ccccc4c1)C(C3)C2 | 7.6580 | 7.6288 | 7.3216 | 7.1483 | 6.8876 | 0.0292 | 0.3364 | 0.5097 | 0.7704 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3342775 | DGAT047 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2c(ccnc2c1)C(=O)Nc1ccccc1 | 7.6380 | 7.5911 | 7.1886 | 7.0544 | 7.3411 | 0.0469 | 0.4494 | 0.5836 | 0.2969 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3233887 | DGAT048 | OC(=O)[C@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(ccc2[nH]1)C(F)(F)F | 7.6383 | 7.6661 | 7.6434 | 7.7826 | 7.6607 | -0.0278 | -0.0054 | -0.1446 | -0.0227 | YES | YES | YES | No |
| - | + | - | + | CHEMBL3233886 | DGAT049 | Cc1cc(C(=O)Nc2ccccc2)c2ccc(cc2n1)-c1ccc(OCC(C)(C)C(O)=O)[n+]([O-])c1 | 7.6380 | 7.5268 | 7.6163 | 7.3830 | 7.3908 | 0.1112 | 0.0217 | 0.2550 | 0.2472 | YES | YES | YES | No |
| \* | - | \* | # | CHEMBL3233891 | DGAT050 | CC(C)c1cccc(NC(=O)c2ccnc3cc(ccc23)-c2ccc(cc2)[C@H]2CC[C@H](CC(O)=O)CC2)c1 | 7.6380 | 7.8522 | 7.7649 | 7.9535 | 7.6366 | -0.2142 | -0.1269 | -0.3155 | 0.0014 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL430405 | DGAT051 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccccc2)cc1 | 7.6200 | 6.9778 | 6.7751 | 6.8403 | 6.6495 | 0.6422 | 0.8449 | 0.7797 | 0.9705 | YES | YES | YES | YES |
| + | + | - | + | CHEMBL3342770 | DGAT052 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCN(CC1)C(=O)Nc1ccccc1Cl)N1CCCCC1 | 7.5850 | 6.3237 | 6.1723 | 6.3069 | 6.5591 | 1.2613 | 1.4127 | 1.2781 | 1.0259 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL2441208 | DGAT053 | OC(=O)[C@@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(F)ccc2[nH]1 | 7.5850 | 7.5517 | 7.6424 | 7.4451 | 7.1963 | 0.0333 | -0.0574 | 0.1399 | 0.3887 | YES | YES | YES | No |
| + | - | \* | # | CHEMBL3287884 | DGAT054 | CCCCCCCNC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.5690 | 7.0936 | 7.0210 | 6.8080 | 6.9368 | 0.4754 | 0.5480 | 0.7610 | 0.6322 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL254870 | DGAT055 | COc1ccc(NC(=O)Nc2ccc(cc2)-c2ccc(cc2)C(=O)[C@@H]2CCC[C@H]2C(O)=O)cc1 | 7.5530 | 7.4345 | 7.5256 | 7.4704 | 7.8805 | 0.1185 | 0.0274 | 0.0826 | -0.3275 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3342773 | DGAT056 | OC(=O)[C@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(Cl)ccc2[nH]1 | 7.5376 | 7.5777 | 7.5441 | 7.5369 | 7.5920 | -0.0401 | -0.0061 | 0.0011 | -0.0540 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL3915108 | DGAT057 | CC(NC(=O)c1cn2cc(ccc2n1)-c1ccc(cc1)C1CC[C@H](CC(O)=O)CC1)c1ccccc1 | 7.5210 | 7.2835 | 7.2672 | 7.7026 | 7.5617 | 0.2375 | 0.2538 | -0.1816 | -0.0407 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3287864 | DGAT058 | CC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.4810 | 6.9677 | 6.9577 | 7.0455 | 7.1487 | 0.5133 | 0.5233 | 0.4355 | 0.3323 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3287874 | DGAT059 | CCOc1ccc(NC(=O)N2CCOc3cc(ccc23)-c2ccc(cc2)[C@H]2CC[C@H](CC(O)=O)CC2)cc1 | 7.4680 | 7.2631 | 7.6623 | 7.7217 | 7.4974 | 0.2049 | -0.1943 | -0.2537 | -0.0294 | YES | YES | YES | YES |
| \* | # | # | + | CHEMBL3287878 | DGAT060 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccc(F)cc1C(F)(F)F | 7.4559 | 7.3418 | 7.5599 | 7.1282 | 7.5785 | 0.1141 | -0.1039 | 0.3278 | -0.1225 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL3287882 | DGAT061 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)NCCCCc1ccccc1 | 7.4440 | 7.0243 | 7.1389 | 7.1519 | 7.0220 | 0.4197 | 0.3051 | 0.2921 | 0.4220 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL2408621 | DGAT062 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C#N | 7.4440 | 7.2057 | 7.9013 | 7.7416 | 7.6843 | 0.2383 | -0.4573 | -0.2976 | -0.2403 | NO | YES | YES | YES |
| # | \* | + | - | CHEMBL1939631 | DGAT063 | CC(C)(COc1ccc(cn1)-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1)C(O)=O | 7.4320 | 6.3504 | 6.7608 | 6.7886 | 6.5875 | 1.0816 | 0.6712 | 0.6434 | 0.8445 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3287875 | DGAT064 | CCc1ccccc1NC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.4318 | 6.6806 | 6.8787 | 6.9836 | 6.9300 | 0.7512 | 0.5533 | 0.4484 | 0.5020 | NO | YES | YES | YES |
| - | + | # | \* | CHEMBL254658 | DGAT065 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cccc(F)c2)cc1 | 7.4090 | 7.6671 | 7.5913 | 7.4069 | 7.4118 | -0.2581 | -0.1823 | 0.0021 | -0.0028 | YES | YES | YES | YES |
| \* | # | - | + | 41 | DGAT066 | CCCc1c(-c2nc(CCO)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.7450 | 7.0012 | 6.8125 | 6.9537 | 6.8432 | -0.2562 | -0.0675 | -0.2087 | -0.0982 | YES | YES | YES | YES |
| - | + | - | + | CHEMBL3233884 | DGAT067 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 7.3980 | 6.4430 | 6.3723 | 6.4452 | 6.3698 | 0.9550 | 1.0257 | 0.9528 | 1.0282 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3287898 | DGAT068 | FC(F)(F)COc1ccc(cn1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 7.3565 | 6.5987 | 6.7182 | 6.8754 | 6.9424 | 0.7578 | 0.6378 | 0.4806 | 0.4136 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL1092385 | DGAT069 | CCc1ccccc1NC(=O)N1C[C@@H](C)Oc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.3560 | 7.1508 | 7.4960 | 7.2788 | 7.3491 | 0.2052 | -0.1400 | 0.0772 | 0.0069 | NO | YES | YES | YES |
| + | - | + | - | CHEMBL3287867 | DGAT070 | OC(=O)C[C@H]1CC[C@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 7.3470 | 6.3682 | 6.2237 | 6.5394 | 6.4825 | 0.9788 | 1.1233 | 0.8076 | 0.8645 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3287890 | DGAT071 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.3470 | 7.0863 | 7.0631 | 7.1416 | 7.2811 | 0.2607 | 0.2839 | 0.2054 | 0.0659 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3287896 | DGAT072 | CCc1ccccc1NC(=O)N1CC(C)Oc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.3010 | 6.6443 | 6.8179 | 7.1075 | 6.8542 | 0.6567 | 0.4831 | 0.1935 | 0.4468 | NO | YES | YES | YES |
| - | + | # | \* | CHEMBL3287897 | DGAT073 | CCc1ccccc1NC(=O)N1C[C@H](C)Oc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.2760 | 7.0760 | 7.3473 | 7.3730 | 7.4619 | 0.2000 | -0.0713 | -0.0970 | -0.1859 | NO | YES | YES | YES |
| + | - | \* | # | CHEMBL2408626 | DGAT074 | Cc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@H](CC2)C(O)=O)nc1 | 7.2080 | 7.3196 | 7.3429 | 7.4070 | 7.5281 | -0.1116 | -0.1349 | -0.1990 | -0.3201 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL402926 | DGAT075 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccc3OCOc3c2)cc1 | 7.2010 | 6.7220 | 6.7547 | 6.6584 | 6.7830 | 0.4790 | 0.4463 | 0.5426 | 0.4180 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3287877 | DGAT076 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCc2c1)C(=O)Nc1ccccc1 | 7.1612 | 6.4131 | 6.3681 | 6.4682 | 6.8045 | 0.7481 | 0.7929 | 0.6928 | 0.3565 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL3233883 | DGAT077 | Cc1cc(C(=O)Nc2ccccc2)c2ccc(cc2n1)-c1ccc(OCC(C)(C)C(O)=O)nc1 | 7.1610 | 7.0446 | 7.0587 | 7.0211 | 7.1360 | 0.1164 | 0.1023 | 0.1399 | 0.0250 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3613344 | DGAT078 | CC(C)c1ccccc1NC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.1610 | 6.6973 | 6.7441 | 6.9577 | 6.7400 | 0.4637 | 0.4169 | 0.2033 | 0.4210 | NO | YES | YES | YES |
| # | \* | + | - | CHEMBL3233890 | DGAT079 | OC(=O)CC1C2CC3CC1CC(C3)(C2)Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1 | 7.1610 | 7.1365 | 7.0731 | 7.1984 | 7.0621 | 0.0245 | 0.0879 | -0.0374 | 0.0989 | YES | YES | YES | YES |
| # | # | - | + | CHEMBL3287894 | DGAT080 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OCC(C)(C)C(O)=O)nc1 | 7.1370 | 6.1588 | 6.0166 | 6.0700 | 6.4833 | 0.9782 | 1.1204 | 1.0670 | 0.6537 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL1089874 | DGAT081 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 7.1140 | 6.2111 | 6.0852 | 6.1463 | 6.0180 | 0.9029 | 1.0288 | 0.9677 | 1.0960 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3233879 | DGAT082 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCCc2c1)C(=O)Nc1ccccc1 | 7.0760 | 6.5317 | 6.4734 | 6.5643 | 6.9368 | 0.5443 | 0.6026 | 0.5117 | 0.1392 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL1835919 | DGAT083 | CCOc1ccc(cn1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 7.0610 | 6.4301 | 6.4504 | 6.6971 | 6.4864 | 0.6309 | 0.6106 | 0.3639 | 0.5746 | YES | YES | YES | YES |
| # | # | - | + | CHEMBL1089498 | DGAT084 | Nc1ncnc2OCCN(c3ccc(cc3)[C@H]3CC[C@H](CC(O)=O)CC3)C(=O)c12 | 7.0560 | 6.9909 | 6.5808 | 6.9551 | 7.0303 | 0.0651 | 0.4752 | 0.1009 | 0.0257 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL3287892 | DGAT085 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OCC2(CC2)C(O)=O)nc1 | 7.0460 | 6.6248 | 6.5073 | 6.3987 | 6.6871 | 0.4212 | 0.5387 | 0.6473 | 0.3589 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL1089182 | DGAT086 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccn1 | 7.0410 | 6.3870 | 6.1626 | 6.2787 | 6.1480 | 0.6540 | 0.8784 | 0.7623 | 0.8930 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL2408622 | DGAT087 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C#N | 7.0180 | 7.1309 | 7.7526 | 7.8358 | 7.7970 | -0.1129 | -0.7346 | -0.8178 | -0.7790 | NO | YES | YES | YES |
| # | # | - | + | CHEMBL2178953 | DGAT088 | Cc1nc(C)c(nc1C(N)=O)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.0000 | 6.1531 | 6.3406 | 6.3956 | 6.3238 | 0.8469 | 0.6594 | 0.6044 | 0.6762 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL1939632 | DGAT089 | CC(C)(COc1ccc(cc1)-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1)C(O)=O | 6.9910 | 6.1314 | 6.3955 | 6.2378 | 6.1191 | 0.8596 | 0.5955 | 0.7532 | 0.8719 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3342771 | DGAT090 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Cc1ccccc1 | 6.9590 | 6.7252 | 6.6994 | 6.7329 | 6.5491 | 0.2338 | 0.2596 | 0.2261 | 0.4099 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3287893 | DGAT091 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)NCc1ccccc1 | 6.9590 | 6.6045 | 6.7497 | 6.7480 | 6.6276 | 0.3545 | 0.2093 | 0.2110 | 0.3314 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL3287881 | DGAT092 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OCC2(CCC2)C(O)=O)nc1 | 6.9586 | 6.7434 | 6.6126 | 6.4948 | 6.8195 | 0.2152 | 0.3464 | 0.4642 | 0.1395 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL3287869 | DGAT093 | OC(=O)[C@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(F)ccc2[nH]1 | 6.9590 | 7.4769 | 7.4937 | 7.5394 | 7.3091 | -0.5179 | -0.5347 | -0.5804 | -0.3501 | YES | YES | YES | No |
| + | - | + | - | CHEMBL2063280 | DGAT094 | COc1cc(C)c(-c2nc3ccc(cc3[nH]2)C(=O)Nc2ccc(C)c(C)c2)c(C)c1 | 6.9210 | 6.9713 | 6.8859 | 6.4547 | 6.0487 | -0.0503 | 0.0351 | 0.4663 | 0.8723 | NO | YES | YES | YES |
| - | + | # | \* | CHEMBL1939628 | DGAT095 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1ccc(OCC(C)(C)C(O)=O)nc1 | 6.9030 | 6.1296 | 6.1650 | 6.0375 | 5.7723 | 0.7734 | 0.7380 | 0.8655 | 1.1307 | YES | YES | YES | YES |
| # | # | - | + | CHEMBL2441209 | DGAT096 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCCN(CC1)C(=O)Nc1ccccc1Cl)N1CCCCC1 | 6.8730 | 6.4423 | 6.2777 | 6.4030 | 6.6915 | 0.4307 | 0.5953 | 0.4700 | 0.1815 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL3287868 | DGAT097 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)NC1CCCCC1 | 6.7960 | 6.3759 | 6.6381 | 6.2578 | 6.3778 | 0.4201 | 0.1579 | 0.5382 | 0.4182 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3287883 | DGAT098 | CCCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.7960 | 7.2049 | 7.1684 | 7.2377 | 7.4135 | -0.4089 | -0.3724 | -0.4417 | -0.6175 | YES | YES | YES | YES |
| + | - | - | + | CHEMBL2408627 | DGAT099 | Cc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@@H](CC2)C(O)=O)nc1 | 6.7930 | 7.3944 | 7.4916 | 7.3128 | 7.4154 | -0.6014 | -0.6986 | -0.5198 | -0.6224 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3287887 | DGAT100 | O=C(Nc1ccccc1)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](Cc2nnn[nH]2)CC1 | 6.7700 | 6.8445 | 7.1621 | 7.1172 | 7.2404 | -0.0745 | -0.3921 | -0.3476 | -0.4704 | NO | YES | YES | YES |
| - | + | - | + | CHEMBL2409663 | DGAT101 | [H][C@@]1(CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1)C(C)C(O)=O | 6.6990 | 6.6099 | 6.6985 | 6.9181 | 6.5585 | 0.0891 | 0.0005 | -0.2191 | 0.1405 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3287885 | DGAT102 | OC(=O)CC1CCC(CC1)c1ccc(cc1)-c1nc2ccc(NC(=O)c3nc(oc3C(F)(F)F)-c3ccccc3C(F)(F)F)cc2[nH]1~ | 6.6970 | 6.5604 | 6.3165 | 6.5935 | 6.6096 | 0.1366 | 0.3805 | 0.1035 | 0.0874 | YES | NO | YES | YES |
| + | - | + | - | CHEMBL3287891 | DGAT103 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(Nc2nc3ccc(OC(F)(F)F)cc3s2)c(F)c1 | 6.6840 | 6.6549 | 8.1283 | 8.0209 | 8.0783 | 0.0291 | -1.4443 | -1.3369 | -1.3943 | NO | YES | YES | YES |
| + | - | \* | # | CHEMBL401117 | DGAT104 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OC[C@H]2C[C@@H]2C(O)=O)nc1 | 6.6780 | 6.8531 | 6.9985 | 7.3869 | 7.7351 | -0.1751 | -0.3205 | -0.7091 | -1.0571 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL1939623 | DGAT105 | Cn1c(OCC(C)(C)C(=O)Nc2ccccc2)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 6.6580 | 5.9894 | 6.4042 | 6.2944 | 6.2288 | 0.6686 | 0.2538 | 0.3636 | 0.4292 | NO | YES | YES | YES |
| + | - | - | + | CHEMBL1089875 | DGAT106 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C)-c1ccccc1 | 6.5850 | 6.0818 | 5.7440 | 5.7043 | 5.7667 | 0.5032 | 0.8410 | 0.8807 | 0.8183 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL2409568 | DGAT107 | OC(=O)CC1CCC(CC1)c1ccc(cc1)-c1nc2ccc(NC(=O)c3nc(oc3C(F)(F)F)-c3ccccc3Cl)cc2[nH]1 | 6.5580 | 6.2827 | 6.4528 | 6.5003 | 6.2779 | 0.2753 | 0.1052 | 0.0577 | 0.2801 | YES | YES | YES | No |
| \* | # | - | + | CHEMBL3233878 | DGAT108 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2c(c[nH]c2c1)C(=O)Nc1ccccc1 | 6.5467 | 6.6762 | 6.9300 | 6.6016 | 6.3603 | -0.1295 | -0.3830 | -0.0546 | 0.1867 | YES | YES | YES | No |
| - | + | - | + | CHEMBL3286412 | DGAT109 | CC(C)C1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.5230 | 7.1597 | 7.0567 | 7.3667 | 7.2782 | -0.6367 | -0.5337 | -0.8437 | -0.7552 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL3287895 | DGAT110 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1cnc(OCC(C)(C)C(O)=O)nc1 | 6.5090 | 6.4874 | 6.2219 | 6.1514 | 6.8400 | 0.0216 | 0.2871 | 0.3576 | -0.3310 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL2408624 | DGAT111 | CS(=O)(=O)c1ccc2nc([nH]c2c1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@H](CC2)C(O)=O)nc1 | 6.4460 | 6.6601 | 6.5829 | 6.4252 | 6.1767 | -0.2141 | -0.1369 | 0.0208 | 0.2693 | YES | YES | YES | No |
| - | + | + | - | CHEMBL3287866 | DGAT112 | C[C@H]1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.4440 | 7.3519 | 7.2561 | 7.4724 | 7.5974 | -0.9079 | -0.8121 | -1.0284 | -1.1534 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL1089169 | DGAT113 | FC(F)(F)c1nn(cc1C(=O)NCCNC(=O)c1ccc(Cl)nc1)-c1ccccc1 | 6.4320 | 6.1021 | 6.3404 | 5.9663 | 5.6585 | 0.3299 | 0.0916 | 0.4657 | 0.7735 | YES | YES | YES | No |
| + | - | \* | # | CHEMBL1092318 | DGAT114 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccc(OCC)cc1 | 6.4200 | 6.4030 | 6.2803 | 6.2827 | 6.4555 | 0.0170 | 0.1397 | 0.1373 | -0.0355 | YES | YES | YES | YES |
| + | - | - | + | CHEMBL2063284 | DGAT115 | Cc1cc(CCC(O)=O)cc(C)c1-c1nc2ccc(cc2[nH]1)C(=O)Nc1ccc(cc1)C(C)(C)C | 6.4090 | 6.5366 | 6.6563 | 6.7872 | 6.8533 | -0.1276 | -0.2473 | -0.3782 | -0.4443 | YES | YES | YES | YES |
| \* | # | # | + | CHEMBL1090842 | DGAT116 | FC(F)(F)c1nn(cc1C(=O)NCCNC(=O)c1ccc(cc1)-n1cccn1)-c1ccccc1 | 6.3979 | 6.7185 | 6.2793 | 6.8225 | 6.4148 | -0.3206 | 0.1187 | -0.4245 | -0.0168 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL1939621 | DGAT117 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1cnc(OCC(C)(C)C(O)=O)nc1 | 6.3640 | 6.4582 | 6.3703 | 6.1190 | 6.1290 | -0.0942 | -0.0063 | 0.2450 | 0.2350 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL1939625 | DGAT118 | CN(C)C(=O)C(C)(C)COc1nnc(-c2ccc(NC(=O)c3ccc4ccccc4c3)cc2)n1C | 6.3560 | 5.7320 | 5.7832 | 5.6248 | 5.7014 | 0.6240 | 0.5728 | 0.7312 | 0.6546 | NO | YES | YES | YES |
| + | - | - | + | CHEMBL3613336 | DGAT119 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)Nc1ccccc1)C(C3)C2 | 6.3090 | 6.9992 | 6.9906 | 6.9563 | 6.7972 | -0.6902 | -0.6816 | -0.6473 | -0.4882 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL3287861 | DGAT120 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2n1)C(=O)Nc1ccccc1 | 6.2600 | 6.7079 | 6.7882 | 7.1293 | 7.0442 | -0.4479 | -0.5282 | -0.8693 | -0.7842 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL2409564 | DGAT121 | OC(=O)CC1CCC(CC1)c1ccc(cc1)-c1nc2ccc(NC(=O)c3nc(oc3C(F)(F)F)-c3ccccc3)cc2[nH]1 | 6.2460 | 6.4881 | 6.1741 | 6.4800 | 6.4313 | -0.2421 | 0.0719 | -0.2340 | -0.1853 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL254871 | DGAT122 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1cccc(OCC)c1 | 6.2220 | 6.4328 | 6.3050 | 6.3983 | 6.4112 | -0.2108 | -0.0830 | -0.1763 | -0.1892 | YES | YES | YES | YES |
| + | - | - | + | CHEMBL1089832 | DGAT123 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccc(cc2)C#N)cc1 | 6.2200 | 6.2919 | 6.6249 | 6.4453 | 6.6401 | -0.0719 | -0.4049 | -0.2253 | -0.4201 | NO | YES | YES | YES |
| \* | # | # | + | CHEMBL1089208 | DGAT124 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1O | 6.2147 | 6.1861 | 6.0213 | 6.1718 | 6.1405 | 0.0286 | 0.1937 | 0.0432 | 0.0745 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL3287862 | DGAT125 | CC1COc2cc(ccc2N1C(=O)Nc1ccccc1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.2010 | 6.5644 | 6.4546 | 6.8103 | 6.2999 | -0.3634 | -0.2536 | -0.6093 | -0.0989 | YES | YES | YES | No |
| + | - | \* | # | CHEMBL1092303 | DGAT126 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)C1CCCCC1 | 6.1870 | 6.2746 | 6.3804 | 6.2218 | 6.0313 | -0.0876 | -0.1934 | -0.0348 | 0.1557 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL1939626 | DGAT127 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1ccc(OCC(C)(C)C(O)=O)nn1 | 6.1490 | 6.1456 | 6.2266 | 6.1163 | 5.6626 | 0.0034 | -0.0776 | 0.0327 | 0.4864 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL2408625 | DGAT128 | CS(=O)(=O)c1ccc2nc([nH]c2c1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@@H](CC2)C(O)=O)nc1 | 6.1385 | 6.7349 | 6.7316 | 6.3309 | 6.0640 | -0.5964 | -0.5936 | -0.1929 | 0.0740 | YES | YES | YES | No |
| - | + | # | \* | CHEMBL1092008 | DGAT129 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(Cc2ccccc2)nc1C(F)(F)F | 6.1140 | 6.5590 | 6.6674 | 6.4791 | 6.6108 | -0.4450 | -0.5534 | -0.3651 | -0.4968 | NO | YES | YES | YES |
| + | - | \* | # | CHEMBL3287889 | DGAT130 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 6.0810 | 6.5318 | 6.2861 | 6.7566 | 6.3551 | -0.4508 | -0.2051 | -0.6756 | -0.2741 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3287886 | DGAT131 | ONC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 6.0360 | 6.4433 | 6.1462 | 6.2817 | 6.1064 | -0.4073 | -0.1102 | -0.2457 | -0.0704 | YES | YES | YES | YES |
| # | # | - | + | CHEMBL3233877 | DGAT132 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2cc([nH]c2c1)C(=O)Nc1ccccc1 | 5.9630 | 6.8404 | 6.7246 | 6.2846 | 6.1979 | -0.8774 | -0.7616 | -0.3216 | -0.2349 | YES | YES | YES | No |
| - | + | + | - | CHEMBL2441200 | DGAT133 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1cc(ccc1F)C(F)(F)F | 5.9210 | 6.5296 | 7.0987 | 6.9644 | 7.2361 | -0.6086 | -1.1777 | -1.0434 | -1.3151 | NO | YES | YES | YES |
| + | - | \* | # | CHEMBL1089168 | DGAT134 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1nn(cc1C)-c1ccccc1 | 5.9210 | 6.0177 | 5.7240 | 5.8036 | 5.5528 | -0.0967 | 0.1970 | 0.1174 | 0.3682 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL3287873 | DGAT135 | FC(F)(F)c1nn(cc1C(=O)NCCNC(=O)c1ccc(Cl)cn1)-c1ccccc1 | 5.9210 | 6.3827 | 6.7473 | 6.7130 | 6.1686 | -0.4617 | -0.8263 | -0.7920 | -0.2476 | YES | YES | YES | No |
| \* | # | - | + | CHEMBL1089304 | DGAT136 | CC(C)OC(=O)N1CCN(CC1)c1ccc(NC(=O)c2oc(nc2C(F)(F)F)N2CCCCC2)cn1 | 5.9190 | 5.3487 | 5.9278 | 6.5864 | 5.6876 | 0.5703 | -0.0088 | -0.6674 | 0.2314 | YES | YES | YES | YES |
| - | + | # | \* | CHEMBL2441202 | DGAT137 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCN(CC1)C(=O)Oc1ccccc1Cl)N1CCCCC1 | 5.8580 | 6.5582 | 6.4879 | 6.4899 | 6.7051 | -0.7002 | -0.6299 | -0.6319 | -0.8471 | YES | YES | YES | No |
| + | - | + | - | CHEMBL1092009 | DGAT138 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccc(Cl)cc1 | 5.8240 | 6.3921 | 6.9612 | 6.3826 | 6.4277 | -0.5681 | -1.1372 | -0.5586 | -0.6037 | YES | YES | YES | No |
| + | - | \* | # | CHEMBL3233880 | DGAT139 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCC(=O)c2c1)C(=O)Nc1ccccc1 | 5.7780 | 6.4656 | 6.4419 | 6.6628 | 6.5387 | -0.6876 | -0.6639 | -0.8848 | -0.7607 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL1939618 | DGAT140 | Cn1c(OCC(C)(C)C(O)=O)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 5.7077 | 5.7209 | 5.9064 | 5.8361 | 5.7362 | -0.0132 | -0.1984 | -0.1281 | -0.0282 | NO | YES | YES | YES |
| - | + | # | \* | CHEMBL2063282 | DGAT141 | Cc1ccc(NC(=O)c2ccc3nc([nH]c3c2)-c2c(C)cc(NCC(O)=O)cc2C)cc1C | 5.6990 | 5.4383 | 5.9908 | 5.7420 | 5.6720 | 0.2607 | -0.2918 | -0.0430 | 0.0270 | YES | YES | YES | No |
| + | - | - | + | CHEMBL1939627 | DGAT142 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1cnc(OCC(C)(C)C(O)=O)cn1 | 5.6650 | 6.4788 | 6.5371 | 6.5854 | 6.3783 | -0.8138 | -0.8721 | -0.9204 | -0.7133 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL2441212 | DGAT143 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCN(CC1)c1ncccc1Cl)N1CCCCC1 | 5.6440 | 6.3875 | 6.2532 | 6.2450 | 6.3818 | -0.7435 | -0.6092 | -0.6010 | -0.7378 | YES | YES | YES | No |
| \* | # | - | + | CHEMBL1939622 | DGAT144 | CC(C)NC(=O)C(C)(C)COc1nnc(-c2ccc(NC(=O)c3ccc4ccccc4c3)cc2)n1C | 5.6308 | 5.7549 | 5.7624 | 5.5909 | 5.6122 | -0.1241 | -0.1314 | 0.0401 | 0.0188 | NO | YES | YES | YES |
| - | + | # | \* | CHEMBL3613334 | DGAT145 | CC(C)(C)OC(=O)NCCNC(=O)c1ccc(OC2C3CC4CC2CC(C4)(C3)C(O)=O)cc1 | 5.5770 | 6.1018 | 6.0724 | 6.2981 | 6.2885 | -0.5248 | -0.4954 | -0.7211 | -0.7115 | YES | YES | YES | YES |
| + | - | + | - | CHEMBL3233876 | DGAT146 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2n(ncc2c1)C(=O)Nc1ccccc1 | 5.5740 | 6.7763 | 6.5895 | 6.5844 | 6.6046 | -1.2023 | -1.0155 | -1.0104 | -1.0306 | YES | YES | YES | YES |
| # | \* | + | - | CHEMBL2441213 | DGAT147 | COCCN(C)c1ccc(NC(=O)c2oc(nc2C(F)(F)F)-c2ccccc2)cn1 | 5.5450 | 5.5844 | 5.9252 | 6.4576 | 5.1862 | -0.0394 | -0.3802 | -0.9126 | 0.3588 | YES | YES | YES | YES |
| \* | # | - | + | CHEMBL1089507 | DGAT148 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1cccnc1 | 5.4685 | 6.5742 | 6.1672 | 6.0274 | 6.2941 | -1.1057 | -0.6992 | -0.5594 | -0.8261 | YES | YES | YES | YES |
| - | + | + | - | CHEMBL3233873 | DGAT149 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2oc(Nc3ccccc3)nc2c1 | 5.4150 | 6.1530 | 6.4581 | 6.2345 | 6.1336 | -0.7380 | -1.0431 | -0.8195 | -0.7186 | YES | YES | YES | YES |
| + | - | \* | # | CHEMBL1939619 | DGAT150 | Cn1c(CCC(O)=O)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 5.3980 | 5.4901 | 5.6946 | 5.5576 | 5.2258 | -0.0921 | -0.2966 | -0.1596 | 0.1722 | NO | YES | YES | YES |
| - | + | - | + | CHEMBL3233881 | DGAT151 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCNc2c1)C(=O)Nc1ccccc1 | 5.3170 | 6.3932 | 6.2470 | 6.4767 | 6.3043 | -1.0762 | -0.9300 | -1.1597 | -0.9873 | YES | YES | YES | YES |
| - | # | - | + | CHEMBL1091721 | DGAT152 | CCOc1cccc(c1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 5.2920 | 6.2409 | 6.1098 | 6.2619 | 5.9737 | -0.9489 | -0.8178 | -0.9699 | -0.6817 | YES | YES | YES | YES |
| + | + | - | + | CHEMBL3287880 | DGAT153 | Nc1ccccc1NC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 5.2840 | 6.4074 | 6.4327 | 6.6614 | 6.5061 | -1.1234 | -1.1487 | -1.3774 | -1.2221 | NO | YES | YES | YES |
| + | - | + | - | CHEMBL1939624 | DGAT154 | CN(C)CCNC(=O)C(C)(C)COc1nnc(-c2ccc(NC(=O)c3ccc4ccccc4c3)cc2)n1C | 5.2300 | 5.9627 | 5.8609 | 5.7746 | 5.6847 | -0.7327 | -0.6309 | -0.5446 | -0.4547 | NO | YES | YES | YES |
| - | + | # | \* | CHEMBL1939620 | DGAT155 | Cn1c(OCC(C)(C)C(N)=O)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 5.2150 | 5.2741 | 5.4858 | 5.3643 | 5.3096 | -0.0591 | -0.2708 | -0.1493 | -0.0946 | NO | YES | YES | YES |
| \* | # | - | + | CHEMBL2063283 | DGAT156 | Cc1ccc(NC(=O)c2ccc3nc([nH]c3c2)-c2c(C)cc(CCC(O)=O)cc2C)cc1C | 5.1871 | 5.4676 | 6.0504 | 5.6285 | 5.7050 | -0.2805 | -0.8634 | -0.4415 | -0.5180 | YES | YES | YES | No |
| - | + | + | - | CHEMBL3287888 | DGAT157 | CS(=O)(=O)NC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 5.1370 | 5.7223 | 5.8842 | 6.1282 | 5.7406 | -0.5853 | -0.7472 | -0.9912 | -0.6036 | YES | YES | YES | YES |
| # | \* | + | - | 1 | DGAT158 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.9210 | 6.2156 | 6.4206 | 6.4645 | 6.2343 | 0.7054 | 0.5004 | 0.4565 | 0.6867 | YES | YES | YES | YES |
| \* | # | - | + | 2 | DGAT159 | CCOC(=O)c1c(C)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.2840 | 6.3620 | 6.4560 | 6.1637 | 6.2439 | -0.0780 | -0.1720 | 0.1203 | 0.0401 | YES | YES | YES | YES |
| - | + | # | \* | 3 | DGAT160 | CCOC(=O)c1c(CC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.6200 | 6.3300 | 6.3897 | 6.2258 | 6.1442 | 0.2900 | 0.2303 | 0.3942 | 0.4758 | YES | YES | YES | YES |
| + | - | \* | # | 4 | DGAT161 | CCOC(=O)c1c(CC=C)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 7.1250 | 7.0947 | 6.4218 | 6.2201 | 6.2094 | 0.0303 | 0.7032 | 0.9049 | 0.9156 | NO | YES | YES | YES |
| # | \* | + | - | 5 | DGAT162 | CCOC(=O)c1c(CCC(F)(F)F)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.9590 | 6.8200 | 6.7035 | 6.7639 | 6.4967 | 0.1390 | 0.2555 | 0.1951 | 0.4623 | YES | YES | YES | YES |
| \* | # | - | + | 6 | DGAT163 | CCCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.7960 | 6.3342 | 6.5259 | 6.5606 | 6.3666 | 0.4618 | 0.2701 | 0.2354 | 0.4294 | YES | YES | YES | YES |
| - | + | # | \* | 7 | DGAT164 | CCCCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.6580 | 6.4528 | 6.6313 | 6.6567 | 6.4990 | 0.2052 | 0.0267 | 0.0013 | 0.1590 | YES | YES | YES | YES |
| - | + | # | \* | 8 | DGAT165 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1C1CC1)N1CCOCC1)-c1ccccc1 | 6.2080 | 6.1351 | 5.9811 | 6.0542 | 5.8486 | 0.0729 | 0.2269 | 0.1538 | 0.3594 | YES | YES | YES | YES |
| \* | # | - | + | 9 | DGAT166 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1C1CCC1)N1CCOCC1)-c1ccccc1 | 5.6020 | 6.2537 | 6.0864 | 6.1503 | 5.9810 | -0.6517 | -0.4844 | -0.5483 | -0.3790 | YES | YES | YES | YES |
| - | + | # | \* | 10 | DGAT167 | CCOC(=O)c1c(COC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.6200 | 6.5216 | 6.8692 | 6.4375 | 6.6398 | 0.0984 | -0.2492 | 0.1825 | -0.0198 | YES | YES | YES | YES |
| + | - | \* | # | 11 | DGAT168 | CCOC(=O)c1c(CCCOC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.5690 | 6.7268 | 6.8765 | 6.6129 | 6.6518 | -0.1578 | -0.3075 | -0.0439 | -0.0828 | YES | YES | YES | YES |
| + | - | + | - | 12 | DGAT169 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccccc1)N1CCOCC1)-c1ccccc1 | 7.0920 | 6.5504 | 6.3146 | 6.5952 | 5.9431 | 0.5416 | 0.7774 | 0.4968 | 1.1489 | YES | YES | YES | YES |
| \* | # | - | + | 13 | DGAT170 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1cccc(OC)c1)N1CCOCC1)-c1ccccc1 | 6.3280 | 6.6854 | 6.6325 | 6.7679 | 6.4566 | -0.3574 | -0.3045 | -0.4399 | -0.1286 | YES | YES | YES | YES |
| - | + | # | \* | 14 | DGAT171 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1cccc(Cl)c1)N1CCOCC1)-c1ccccc1 | 6.5380 | 7.0488 | 7.1101 | 7.0628 | 6.8815 | -0.5108 | -0.5721 | -0.5248 | -0.3435 | YES | YES | YES | YES |
| # | \* | + | - | 15 | DGAT172 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(Cl)cc1)N1CCOCC1)-c1ccccc1 | 7.2010 | 7.0191 | 7.0855 | 6.9473 | 6.9258 | 0.1819 | 0.1155 | 0.2537 | 0.2752 | YES | YES | YES | YES |
| \* | # | - | + | 16 | DGAT173 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(O)cc1)N1CCOCC1)-c1ccccc1 | 6.2440 | 6.7513 | 6.5942 | 6.6781 | 6.4332 | -0.5073 | -0.3502 | -0.4341 | -0.1892 | YES | YES | YES | YES |
| - | + | # | \* | 17 | DGAT174 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(OC)cc1)N1CCOCC1)-c1ccccc1 | 7.2840 | 6.6557 | 6.6078 | 6.6523 | 6.5010 | 0.6283 | 0.6762 | 0.6317 | 0.7830 | YES | YES | YES | YES |
| \* | - | \* | # | 18 | DGAT175 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(N)cc1)N1CCOCC1)-c1ccccc1 | 6.2010 | 6.4853 | 6.2762 | 6.4748 | 6.1736 | -0.2843 | -0.0752 | -0.2738 | 0.0274 | YES | YES | YES | YES |
| + | - | \* | # | 19 | DGAT176 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(cc1)-c1ccccc1)N1CCOCC1)-c1ccccc1 | 6.6020 | 7.2881 | 6.8710 | 7.1133 | 6.7888 | -0.6861 | -0.2690 | -0.5113 | -0.1868 | YES | YES | YES | YES |
| \* | # | - | + | 20 | DGAT177 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(OCc2ccccc2)cc1)N1CCOCC1)-c1ccccc1 | 7.2220 | 7.5300 | 7.4577 | 7.6556 | 7.4675 | -0.3080 | -0.2357 | -0.4336 | -0.2455 | YES | YES | YES | YES |
| # | + | # | \* | 21 | DGAT178 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCC1)-c1ccccc1 | 5.8660 | 5.9693 | 6.2425 | 6.1903 | 6.1117 | -0.1033 | -0.3765 | -0.3243 | -0.2457 | YES | YES | YES | YES |
| - | + | - | + | 22 | DGAT179 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCCC1)-c1ccccc1 | 6.9210 | 6.0879 | 6.3478 | 6.2864 | 6.2440 | 0.8331 | 0.5732 | 0.6346 | 0.6770 | YES | YES | YES | YES |
| - | # | - | + | 23 | DGAT180 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCCCC1)-c1ccccc1 | 5.2150 | 6.2065 | 6.4532 | 6.3825 | 6.3764 | -0.9915 | -1.2382 | -1.1675 | -1.1614 | YES | YES | YES | YES |
| - | + | # | \* | 24 | DGAT181 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N(C)C)-c1ccccc1 | 6.0810 | 6.0778 | 6.1264 | 6.1845 | 6.1247 | 0.0032 | -0.0454 | -0.1035 | -0.0437 | YES | YES | YES | YES |
| + | - | \* | # | 25 | DGAT182 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1F | 6.2440 | 5.9900 | 6.4802 | 6.7162 | 6.4142 | 0.2540 | -0.2362 | -0.4722 | -0.1702 | NO | YES | YES | YES |
| # | \* | + | - | 26 | DGAT183 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1cccc(F)c1 | 6.5690 | 6.7527 | 7.0151 | 6.9345 | 6.7908 | -0.1837 | -0.4461 | -0.3655 | -0.2218 | YES | YES | YES | YES |
| \* | # | - | + | 27 | DGAT184 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccc(F)cc1 | 6.5380 | 6.7230 | 6.9904 | 6.8190 | 6.8351 | -0.1850 | -0.4524 | -0.2810 | -0.2971 | YES | YES | YES | YES |
| - | + | - | + | 28 | DGAT185 | CCCc1c(-c2nc(C)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.4200 | 6.8444 | 6.8356 | 6.7500 | 6.8540 | -0.4244 | -0.4156 | -0.3300 | -0.4340 | YES | YES | YES | YES |
| # | \* | + | - | 29 | DGAT186 | CCCc1c(-c2nc(CC)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.9590 | 6.8124 | 6.7692 | 6.8121 | 6.7543 | 0.1466 | 0.1898 | 0.1469 | 0.2047 | YES | YES | YES | YES |
| \* | # | - | + | 30 | DGAT187 | CCCc1noc(n1)-c1c(CCC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 7.1870 | 6.8366 | 6.6143 | 6.6305 | 6.7306 | 0.3504 | 0.5727 | 0.5565 | 0.4564 | NO | YES | YES | YES |
| - | + | # | \* | 31 | DGAT188 | CCCc1c(-c2nc(no2)C(C)C)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.2440 | 6.9381 | 6.6738 | 6.8000 | 6.8169 | 0.3059 | 0.5702 | 0.4440 | 0.4271 | YES | YES | YES | YES |
| + | - | \* | # | 32 | DGAT189 | CCCCc1noc(n1)-c1c(CCC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 7.1370 | 6.9552 | 6.7196 | 6.7266 | 6.8630 | 0.1818 | 0.4174 | 0.4104 | 0.2740 | NO | YES | YES | YES |
| # | \* | + | - | 33 | DGAT190 | CCCc1c(-c2nc(no2)C(C)(C)C)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.3190 | 7.0482 | 6.8757 | 6.8164 | 7.0875 | 0.2708 | 0.4433 | 0.5026 | 0.2315 | YES | YES | YES | YES |
| \* | # | - | + | 34 | DGAT191 | CCCCCc1noc(n1)-c1c(CCC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.9590 | 7.0738 | 6.8250 | 6.8227 | 6.9953 | -0.1148 | 0.1340 | 0.1363 | -0.0363 | NO | YES | YES | YES |
| - | + | # | \* | 35 | DGAT192 | CCCc1c(-c2nc(no2)-c2ccccc2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.7450 | 7.5134 | 7.2072 | 7.2610 | 7.3622 | -0.7684 | -0.4622 | -0.5160 | -0.6172 | YES | YES | YES | YES |
| # | \* | + | - | 36 | DGAT193 | CCCc1c(-c2nc(Cc3ccccc3)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.9210 | 7.2639 | 7.2077 | 7.3633 | 7.2355 | -0.3429 | -0.2867 | -0.4423 | -0.3145 | YES | YES | YES | YES |
| \* | # | - | + | 37 | DGAT194 | CCCc1c(-c2nc(no2)C2CCCC2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.3190 | 7.5016 | 7.4007 | 7.4058 | 7.3767 | -0.1826 | -0.0817 | -0.0868 | -0.0577 | YES | YES | YES | YES |
| - | + | # | \* | 38 | DGAT195 | CCCc1c(-c2nc(no2)C2CCCCC2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.2520 | 7.6202 | 7.5061 | 7.5019 | 7.5091 | -0.3682 | -0.2541 | -0.2499 | -0.2571 | YES | YES | YES | YES |
| + | - | \* | # | 39 | DGAT196 | CCCc1c(-c2nc(no2)N2CCCC2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.0000 | 7.1320 | 7.1260 | 7.2392 | 7.1268 | -0.1320 | -0.1260 | -0.2392 | -0.1268 | YES | YES | YES | YES |
| # | \* | + | - | 40 | DGAT197 | CCCc1c(-c2nc(no2)N(C)C)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.8540 | 6.5619 | 6.3901 | 6.5604 | 6.6301 | 0.2921 | 0.4639 | 0.2936 | 0.2239 | YES | YES | YES | YES |

\*R.B. Patil, E.G. Barbosa, J.N. Sangshetti, S.D. Sawant, and V.P. Zambre, *LQTA-R: A new 3D-QSAR methodology applied to a set of DGAT1 inhibitors*, Comput Biol Chem. 74 (2018), pp. 123-131.

**Table S2**: Split distribution with SMILES notation, experimental pIC50, calculated pIC50, residual pIC50 and Applicability domain (AD) without IIC using equation 3

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Split** | | | | **ID** | **SMILES** | **Expr pIC50** | **Calc pIC50** | | | | **Residual (Expr-Calc) pIC50** | | | | **AD** | | | |
| **1** | **2** | **3** | **4** | **1** | **2** | **3** | **4** | **1** | **2** | **3** | **4** | **1** | **2** | **3** | **4** |
| - | + | + | - | DGAT001 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc(cn1)-c1nc2ccc(Cl)cc2[nH]1 | 9.0000 | 8.5685 | 8.2167 | 8.2954 | 7.8736 | 0.4315 | 0.7833 | 0.7046 | 1.1264 | YES | YES | YES | YES |
| + | - | + | - | DGAT002 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(NC(=O)c2nnc(Nc3ccc(F)c(F)c3)o2)cc1 | 8.9590 | 9.0037 | 8.0511 | 8.1613 | 7.4456 | -0.0447 | 0.9079 | 0.7977 | 1.5134 | NO | YES | YES | YES |
| # | \* | + | - | DGAT003 | CC(C)(NC(=O)c1cn2cc(ccc2n1)-c1ccc(cc1)C1CC[C@H](CC(O)=O)CC1)c1ccc(F)cc1 | 8.9210 | 8.2065 | 8.1852 | 8.3796 | 8.3919 | 0.7145 | 0.7358 | 0.5414 | 0.5291 | YES | YES | YES | YES |
| \* | # | - | + | DGAT004 | Cc1cc(C(=O)NCCCCCc2ccccc2)c2ccc(cc2n1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 8.8539 | 9.3195 | 8.2713 | 9.2453 | 8.7979 | -0.4656 | 0.5827 | -0.3913 | 0.0561 | YES | YES | YES | YES |
| - | + | + | - | DGAT005 | Cc1ccccc1-c1ccc(cc1)C(=O)NCCNC(=O)c1ccc(O[C@H]2C3CC4CC2C[C@](C4)(C3)C(O)=O)cc1 | 8.6990 | 9.0042 | 8.1137 | 8.4895 | 8.2146 | -0.3052 | 0.5853 | 0.2095 | 0.4844 | YES | NO | NO | YES |
| + | - | \* | # | DGAT006 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C(F)(F)F | 8.6580 | 8.5868 | 8.6502 | 8.3861 | 8.4326 | 0.0712 | 0.0078 | 0.2719 | 0.2254 | YES | YES | NO | YES |
| # | \* | + | - | DGAT007 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C(F)(F)F | 8.5530 | 8.4999 | 8.0919 | 8.0245 | 8.0480 | 0.0531 | 0.4611 | 0.5285 | 0.5050 | YES | YES | NO | YES |
| \* | # | - | + | DGAT008 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2cc(F)c(F)cc2[nH]1 | 8.4685 | 8.9924 | 9.0466 | 8.6892 | 8.4860 | -0.5239 | -0.5776 | -0.2202 | -0.0170 | YES | YES | YES | YES |
| - | + | # | \* | DGAT009 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(F)cc2[nH]1 | 8.4690 | 8.6129 | 8.6859 | 8.2731 | 8.1159 | -0.1439 | -0.2169 | 0.1959 | 0.3531 | YES | YES | YES | YES |
| + | - | \* | # | DGAT010 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(Cl)cc2[nH]1 | 8.4320 | 8.6555 | 8.7749 | 8.6570 | 8.2582 | -0.2235 | -0.3429 | -0.2250 | 0.1738 | YES | YES | YES | YES |
| # | \* | + | - | DGAT011 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(Cl)cc2[nH]1 | 8.3770 | 8.6284 | 8.6717 | 8.7049 | 8.4432 | -0.2514 | -0.2947 | -0.3279 | -0.0662 | YES | YES | YES | YES |
| \* | # | - | + | DGAT012 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2cc(F)c(F)cc2[nH]1 | 8.3665 | 8.9653 | 8.9433 | 8.7371 | 8.6710 | -0.5988 | -0.5763 | -0.3701 | -0.3040 | YES | YES | YES | YES |
| - | + | + | - | DGAT013 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C(F)(F)F | 8.3570 | 8.5597 | 8.5469 | 8.4340 | 8.6176 | -0.2027 | -0.1899 | -0.0770 | -0.2606 | YES | YES | NO | YES |
| + | - | + | - | DGAT014 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(OC(F)(F)F)cc2[nH]1 | 8.3370 | 8.4612 | 8.7255 | 8.3521 | 8.3811 | -0.1242 | -0.3885 | -0.0151 | -0.0441 | YES | YES | YES | YES |
| # | \* | + | - | DGAT015 | Cc1cccc(C)c1-c1ccc(cc1)C(=O)NCCNC(=O)c1ccc(O[C@H]2C3CC4CC2C[C@](C4)(C3)C(O)=O)cc1 | 8.3010 | 9.1952 | 8.2426 | 8.3422 | 8.4426 | -0.8942 | 0.0584 | -0.0412 | -0.1416 | YES | NO | NO | YES |
| \* | # | - | + | DGAT016 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)c1nc(oc1C(F)(F)F)-c1ccccc1)C(C3)C2 | 8.3010 | 8.7255 | 7.8632 | 8.5891 | 8.0042 | -0.4245 | 0.4378 | -0.2881 | 0.2968 | YES | YES | YES | YES |
| # | + | # | \* | DGAT017 | OC(=O)[C@@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1)C(C3)C2 | 8.3010 | 8.1882 | 8.3572 | 8.3484 | 8.5069 | 0.1128 | -0.0562 | -0.0474 | -0.2059 | YES | YES | YES | YES |
| + | - | \* | # | DGAT018 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)NCc1ccc(Oc2ccc(F)cc2)cc1 | 8.2760 | 8.2536 | 8.9056 | 8.7683 | 8.5332 | 0.0224 | -0.6296 | -0.4923 | -0.2572 | YES | YES | YES | YES |
| # | \* | + | - | DGAT019 | Cc1cccc(Cl)c1CNC(=O)c1cn2cc(ccc2n1)-c1ccc(cc1)C1CC[C@H](CC(O)=O)CC1 | 8.1190 | 8.6731 | 8.5456 | 8.4071 | 8.6700 | -0.5541 | -0.4266 | -0.2881 | -0.5510 | YES | YES | YES | YES |
| \* | # | - | + | DGAT020 | OC(=O)[C@@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(ccc2[nH]1)C(F)(F)F | 8.0969 | 7.2976 | 7.4673 | 7.7106 | 7.7438 | 0.7993 | 0.6297 | 0.3864 | 0.3532 | YES | YES | NO | YES |
| - | + | # | \* | DGAT021 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1)C(C3)C2 | 8.0970 | 7.9020 | 7.7000 | 7.6260 | 7.6169 | 0.1950 | 0.3970 | 0.4710 | 0.4801 | YES | YES | YES | YES |
| + | - | - | + | DGAT022 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2c(cccc2c1)C(=O)Nc1ccccc1 | 8.0970 | 7.4311 | 6.9901 | 7.1187 | 6.9935 | 0.6659 | 1.1069 | 0.9783 | 1.1035 | YES | YES | YES | YES |
| + | + | - | + | DGAT023 | Nc1c(cnc2ccnn12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 8.0970 | 7.5452 | 6.7938 | 6.5574 | 6.6909 | 0.5518 | 1.3032 | 1.5396 | 1.4061 | YES | YES | YES | YES |
| \* | # | - | + | DGAT024 | OC(=O)[C@@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc4ccccc4c1)C(C3)C2 | 8.0969 | 7.9425 | 7.7057 | 7.7930 | 7.9033 | 0.1544 | 0.3913 | 0.3040 | 0.1937 | YES | YES | YES | YES |
| - | + | # | \* | DGAT025 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccccc2[nH]1 | 8.0910 | 7.9701 | 7.8504 | 7.7879 | 7.5238 | 0.1209 | 0.2406 | 0.3031 | 0.5672 | YES | NO | YES | YES |
| + | - | \* | # | DGAT026 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(F)cc2[nH]1 | 8.0910 | 8.5858 | 8.5827 | 8.3210 | 8.3009 | -0.4948 | -0.4917 | -0.2300 | -0.2099 | YES | YES | YES | YES |
| # | \* | + | - | DGAT027 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)NCc1ccc2OCCCOc2c1 | 8.0040 | 6.9736 | 7.4189 | 7.8757 | 7.5277 | 1.0304 | 0.5851 | 0.1283 | 0.4763 | YES | YES | YES | YES |
| \* | # | - | + | DGAT028 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)Nc1ccc(Cl)c(Cl)c1 | 8.0044 | 7.2220 | 8.5026 | 8.4069 | 8.0088 | 0.7824 | -0.4986 | -0.4029 | -0.0048 | YES | YES | YES | YES |
| - | + | + | - | DGAT029 | OC(=O)[C@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1)C(C3)C2 | 8.0000 | 8.4551 | 8.4073 | 8.2489 | 8.7346 | -0.4551 | -0.4073 | -0.2489 | -0.7346 | YES | NO | NO | YES |
| + | - | \* | # | DGAT030 | Cc1cc(C(=O)Nc2ccccc2)c2ccc(cc2n1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 8.0000 | 8.1340 | 7.7953 | 8.0910 | 7.9871 | -0.1340 | 0.2047 | -0.0910 | 0.0129 | YES | YES | YES | YES |
| # | \* | + | - | DGAT031 | OC(=O)[C@@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(Cl)ccc2[nH]1 | 7.9590 | 7.2189 | 7.6350 | 7.7454 | 7.5694 | 0.7401 | 0.3240 | 0.2136 | 0.3896 | YES | YES | YES | YES |
| \* | # | - | + | DGAT032 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)Nc1cccc(Cl)c1 | 7.9318 | 6.8575 | 7.9063 | 7.9318 | 7.6504 | 1.0743 | 0.0257 | 0.0002 | 0.2816 | YES | YES | YES | YES |
| - | + | # | \* | DGAT033 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccccc2[nH]1 | 7.9210 | 7.9430 | 7.7471 | 7.8358 | 7.7088 | -0.0220 | 0.1739 | 0.0852 | 0.2122 | YES | NO | YES | YES |
| + | - | + | - | DGAT034 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)NCc1ccc(F)c(Cl)c1 | 7.9140 | 7.6360 | 8.6025 | 8.2916 | 8.3929 | 0.2780 | -0.6885 | -0.3776 | -0.4789 | YES | YES | YES | YES |
| # | \* | + | - | DGAT035 | COc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@H](CC2)C(O)=O)nc1 | 7.8860 | 7.4994 | 7.4837 | 7.6280 | 7.2532 | 0.3866 | 0.4023 | 0.2580 | 0.6328 | YES | NO | YES | YES |
| \* | # | - | + | DGAT036 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccc(cc2)C(F)(F)F)cc1 | 7.8539 | 7.7246 | 7.5356 | 7.7631 | 7.5271 | 0.1293 | 0.3184 | 0.0909 | 0.3269 | YES | YES | YES | YES |
| - | + | # | \* | DGAT037 | COc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@@H](CC2)C(O)=O)nc1 | 7.7960 | 7.5266 | 7.5870 | 7.5801 | 7.0682 | 0.2694 | 0.2090 | 0.2159 | 0.7278 | YES | NO | YES | YES |
| + | - | + | - | DGAT038 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1C(F)(F)F | 7.7960 | 7.3775 | 6.9590 | 7.4921 | 6.9310 | 0.4185 | 0.8370 | 0.3039 | 0.8650 | YES | YES | YES | YES |
| + | - | + | - | DGAT039 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccccc2C(F)(F)F)cc1 | 7.7960 | 7.5376 | 7.1929 | 7.1916 | 7.1370 | 0.2584 | 0.6031 | 0.6044 | 0.6590 | YES | YES | YES | YES |
| \* | # | - | + | DGAT040 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cccc(c2)C(F)(F)F)cc1 | 7.7696 | 7.7279 | 7.5639 | 8.0067 | 7.5354 | 0.0417 | 0.2061 | -0.2367 | 0.2346 | YES | YES | YES | YES |
| - | + | # | \* | DGAT041 | C[C@@H]1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.7450 | 7.2801 | 7.2484 | 7.2978 | 7.4780 | 0.4649 | 0.4966 | 0.4472 | 0.2670 | YES | YES | YES | YES |
| + | - | \* | # | DGAT042 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cccc(Cl)c2)cc1 | 7.7210 | 7.7505 | 7.7778 | 7.9794 | 7.4810 | -0.0295 | -0.0568 | -0.2584 | 0.2400 | YES | YES | YES | YES |
| # | \* | + | - | DGAT043 | OC(=O)[C@]12CC3CC(C1)[C@H](Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc4ccccc4c1)C(C3)C2 | 7.7210 | 8.2095 | 7.7558 | 7.6935 | 8.1311 | -0.4885 | -0.0348 | 0.0275 | -0.4101 | YES | NO | NO | YES |
| \* | # | - | + | DGAT044 | OC(=O)C[C@H]1CCC(CC1)c1ccc(cc1)-c1ccc2nc(cn2c1)C(=O)Nc1ccc(F)c(Cl)c1 | 7.7212 | 7.3035 | 8.3704 | 8.0820 | 8.0885 | 0.4177 | -0.6494 | -0.3610 | -0.3675 | YES | YES | YES | YES |
| - | + | # | \* | DGAT045 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cc(ccc2F)C(F)(F)F)cc1 | 7.6780 | 7.3178 | 7.3822 | 7.2355 | 7.3256 | 0.3602 | 0.2958 | 0.4425 | 0.3524 | YES | YES | YES | YES |
| + | - | \* | # | DGAT046 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc4ccccc4c1)C(C3)C2 | 7.6580 | 7.6563 | 7.0485 | 7.0707 | 7.0133 | 0.0017 | 0.6095 | 0.5873 | 0.6447 | YES | YES | YES | YES |
| # | \* | + | - | DGAT047 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2c(ccnc2c1)C(=O)Nc1ccccc1 | 7.6380 | 7.6939 | 7.0764 | 7.1552 | 7.0514 | -0.0559 | 0.5616 | 0.4828 | 0.5866 | YES | YES | YES | YES |
| \* | # | - | + | DGAT048 | OC(=O)[C@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(ccc2[nH]1)C(F)(F)F | 7.6383 | 7.2705 | 7.3641 | 7.7585 | 7.9288 | 0.3678 | 0.2739 | -0.1205 | -0.2908 | YES | YES | NO | YES |
| - | + | - | + | DGAT049 | Cc1cc(C(=O)Nc2ccccc2)c2ccc(cc2n1)-c1ccc(OCC(C)(C)C(O)=O)[n+]([O-])c1 | 7.6380 | 7.7968 | 7.5278 | 7.0892 | 7.3093 | -0.1588 | 0.1102 | 0.5488 | 0.3287 | YES | YES | YES | YES |
| \* | - | \* | # | DGAT050 | CC(C)c1cccc(NC(=O)c2ccnc3cc(ccc23)-c2ccc(cc2)[C@H]2CC[C@H](CC(O)=O)CC2)c1 | 7.6380 | 7.9785 | 7.6704 | 7.1134 | 8.2457 | -0.3405 | -0.0324 | 0.5246 | -0.6077 | YES | YES | YES | YES |
| + | - | + | - | DGAT051 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccccc2)cc1 | 7.6200 | 7.0313 | 6.8678 | 7.0435 | 6.8520 | 0.5887 | 0.7522 | 0.5765 | 0.7680 | YES | YES | YES | YES |
| + | + | - | + | DGAT052 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCN(CC1)C(=O)Nc1ccccc1Cl)N1CCCCC1 | 7.5850 | 6.3045 | 6.2809 | 6.5463 | 6.4544 | 1.2805 | 1.3041 | 1.0387 | 1.1306 | YES | YES | YES | YES |
| - | + | # | \* | DGAT053 | OC(=O)[C@@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(F)ccc2[nH]1 | 7.5850 | 7.3237 | 7.5031 | 7.5977 | 7.4271 | 0.2613 | 0.0819 | -0.0127 | 0.1579 | YES | YES | YES | YES |
| + | - | \* | # | DGAT054 | CCCCCCCNC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.5690 | 7.3821 | 6.8225 | 7.1465 | 7.1722 | 0.1869 | 0.7465 | 0.4225 | 0.3968 | YES | YES | YES | YES |
| # | \* | + | - | DGAT055 | COc1ccc(NC(=O)Nc2ccc(cc2)-c2ccc(cc2)C(=O)[C@@H]2CCC[C@H]2C(O)=O)cc1 | 7.5530 | 7.4104 | 7.3707 | 7.7445 | 7.7252 | 0.1426 | 0.1823 | -0.1915 | -0.1722 | YES | YES | YES | YES |
| \* | # | - | + | DGAT056 | OC(=O)[C@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(Cl)ccc2[nH]1 | 7.5376 | 7.1917 | 7.5317 | 7.7933 | 7.7544 | 0.3459 | 0.0063 | -0.2553 | -0.2164 | YES | YES | YES | YES |
| - | + | # | \* | DGAT057 | CC(NC(=O)c1cn2cc(ccc2n1)-c1ccc(cc1)C1CC[C@H](CC(O)=O)CC1)c1ccccc1 | 7.5210 | 7.2418 | 7.4072 | 7.6141 | 7.7004 | 0.2792 | 0.1138 | -0.0931 | -0.1794 | YES | YES | YES | YES |
| + | - | \* | # | DGAT058 | CC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.4810 | 6.8697 | 6.8904 | 7.1430 | 7.1897 | 0.6113 | 0.5906 | 0.3380 | 0.2913 | YES | YES | YES | YES |
| # | \* | + | - | DGAT059 | CCOc1ccc(NC(=O)N2CCOc3cc(ccc23)-c2ccc(cc2)[C@H]2CC[C@H](CC(O)=O)CC2)cc1 | 7.4680 | 7.6493 | 7.5174 | 7.4443 | 8.0853 | -0.1813 | -0.0494 | 0.0237 | -0.6173 | YES | YES | YES | YES |
| \* | # | # | + | DGAT060 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccc(F)cc1C(F)(F)F | 7.4559 | 7.6059 | 7.3342 | 7.5868 | 7.3128 | -0.1500 | 0.1218 | -0.1308 | 0.1432 | YES | YES | YES | YES |
| - | + | # | \* | DGAT061 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)NCCCCc1ccccc1 | 7.4440 | 7.4980 | 6.9277 | 7.5418 | 7.2520 | -0.0540 | 0.5163 | -0.0978 | 0.1920 | YES | YES | YES | YES |
| + | - | + | - | DGAT062 | OC(=O)[C@@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C#N | 7.4440 | 7.1729 | 7.9826 | 7.3966 | 7.9374 | 0.2711 | -0.5386 | 0.0474 | -0.4934 | NO | YES | NO | YES |
| # | \* | + | - | DGAT063 | CC(C)(COc1ccc(cn1)-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1)C(O)=O | 7.4320 | 6.7056 | 6.6778 | 6.9491 | 6.4181 | 0.7264 | 0.7542 | 0.4829 | 1.0139 | YES | YES | YES | YES |
| \* | # | - | + | DGAT064 | CCc1ccccc1NC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.4318 | 6.8056 | 6.8253 | 6.9628 | 7.0673 | 0.6262 | 0.6067 | 0.4692 | 0.3647 | NO | YES | YES | YES |
| - | + | # | \* | DGAT065 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2cccc(F)c2)cc1 | 7.4090 | 7.8554 | 7.6459 | 7.8317 | 7.3387 | -0.4464 | -0.2369 | -0.4227 | 0.0703 | YES | YES | YES | YES |
| \* | # | - | + | DGAT066 | CCCc1c(-c2nc(CCO)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.7450 | 6.8910 | 6.9926 | 6.9885 | 6.8686 | -0.1460 | -0.2476 | -0.2435 | -0.1236 | YES | YES | YES | YES |
| - | + | - | + | DGAT067 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 7.3980 | 6.3826 | 6.4093 | 6.4318 | 6.3473 | 1.0154 | 0.9887 | 0.9662 | 1.0507 | YES | YES | YES | YES |
| \* | # | - | + | DGAT068 | FC(F)(F)COc1ccc(cn1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 7.3565 | 6.6730 | 6.5862 | 6.9068 | 6.6888 | 0.6835 | 0.7698 | 0.4492 | 0.6672 | YES | YES | YES | YES |
| - | + | # | \* | DGAT069 | CCc1ccccc1NC(=O)N1C[C@@H](C)Oc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.3560 | 7.2940 | 7.3869 | 6.8447 | 7.6038 | 0.0620 | -0.0309 | 0.5113 | -0.2478 | NO | NO | YES | YES |
| + | - | + | - | DGAT070 | OC(=O)C[C@H]1CC[C@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 7.3470 | 6.3555 | 6.3061 | 6.4797 | 6.5323 | 0.9915 | 1.0409 | 0.8673 | 0.8147 | YES | YES | YES | YES |
| # | \* | + | - | DGAT071 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.3470 | 7.0790 | 6.9907 | 7.3607 | 7.3292 | 0.2680 | 0.3563 | -0.0137 | 0.0178 | YES | YES | YES | YES |
| \* | # | - | + | DGAT072 | CCc1ccccc1NC(=O)N1CC(C)Oc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.3010 | 6.3911 | 6.9038 | 6.6487 | 7.1161 | 0.9099 | 0.3972 | 0.6523 | 0.1849 | NO | YES | YES | YES |
| - | + | # | \* | DGAT073 | CCc1ccccc1NC(=O)N1C[C@H](C)Oc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.2760 | 7.2669 | 7.2836 | 6.8926 | 7.7888 | 0.0091 | -0.0076 | 0.3834 | -0.5128 | NO | NO | YES | YES |
| + | - | \* | # | DGAT074 | Cc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@H](CC2)C(O)=O)nc1 | 7.2080 | 7.1124 | 7.4763 | 7.3807 | 7.2812 | 0.0956 | -0.2683 | -0.1727 | -0.0732 | YES | NO | YES | YES |
| # | \* | + | - | DGAT075 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccc3OCOc3c2)cc1 | 7.2010 | 6.6927 | 6.8153 | 6.8166 | 6.7642 | 0.5083 | 0.3857 | 0.3844 | 0.4368 | YES | YES | YES | YES |
| \* | # | - | + | DGAT076 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCc2c1)C(=O)Nc1ccccc1 | 7.1612 | 6.3939 | 6.4806 | 6.4394 | 6.5548 | 0.7673 | 0.6804 | 0.7216 | 0.6062 | YES | YES | YES | YES |
| - | + | # | \* | DGAT077 | Cc1cc(C(=O)Nc2ccccc2)c2ccc(cc2n1)-c1ccc(OCC(C)(C)C(O)=O)nc1 | 7.1610 | 7.0888 | 6.9924 | 7.0593 | 6.9836 | 0.0722 | 0.1686 | 0.1017 | 0.1774 | YES | YES | YES | YES |
| + | - | \* | # | DGAT078 | CC(C)c1ccccc1NC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.1610 | 6.5747 | 6.6398 | 6.5865 | 6.8544 | 0.5863 | 0.5212 | 0.5745 | 0.3066 | NO | YES | YES | YES |
| # | \* | + | - | DGAT079 | OC(=O)CC1C2CC3CC1CC(C3)(C2)Oc1ccc(cc1)C(=O)NCCNC(=O)c1ccc(cc1)-c1ccccc1 | 7.1610 | 6.9227 | 6.9823 | 7.1140 | 6.9706 | 0.2383 | 0.1787 | 0.0470 | 0.1904 | YES | YES | YES | YES |
| # | # | - | + | DGAT080 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OCC(C)(C)C(O)=O)nc1 | 7.1370 | 6.0338 | 6.1878 | 6.3291 | 6.3256 | 1.1032 | 0.9492 | 0.8079 | 0.8114 | YES | YES | YES | YES |
| - | + | + | - | DGAT081 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 7.1140 | 6.1747 | 6.1139 | 6.2747 | 6.0649 | 0.9393 | 1.0001 | 0.8393 | 1.0491 | YES | YES | YES | YES |
| + | - | \* | # | DGAT082 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCCc2c1)C(=O)Nc1ccccc1 | 7.0760 | 6.6033 | 6.5808 | 6.6572 | 6.6942 | 0.4727 | 0.4952 | 0.4188 | 0.3818 | YES | YES | YES | YES |
| # | \* | + | - | DGAT083 | CCOc1ccc(cn1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 7.0610 | 6.4881 | 6.3690 | 6.8834 | 6.5429 | 0.5729 | 0.6920 | 0.1776 | 0.5181 | YES | YES | YES | YES |
| # | # | - | + | DGAT084 | Nc1ncnc2OCCN(c3ccc(cc3)[C@H]3CC[C@H](CC(O)=O)CC3)C(=O)c12 | 7.0560 | 6.6579 | 6.5746 | 7.2759 | 7.0030 | 0.3981 | 0.4814 | -0.2199 | 0.0530 | YES | YES | YES | YES |
| - | + | # | \* | DGAT085 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OCC2(CC2)C(O)=O)nc1 | 7.0460 | 6.6826 | 6.6059 | 6.5974 | 6.5645 | 0.3634 | 0.4401 | 0.4486 | 0.4815 | YES | YES | YES | YES |
| + | - | \* | # | DGAT086 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccn1 | 7.0410 | 6.4107 | 6.1696 | 6.2935 | 6.2731 | 0.6303 | 0.8714 | 0.7475 | 0.7679 | YES | YES | YES | YES |
| + | - | + | - | DGAT087 | OC(=O)[C@H]1CC[C@@H](CC1)Oc1ccc(cn1)-c1ccc(cn1)-c1nc2ccc(cc2[nH]1)C#N | 7.0180 | 7.1458 | 7.8793 | 7.4445 | 8.1224 | -0.1278 | -0.8613 | -0.4265 | -1.1044 | NO | YES | NO | YES |
| # | # | - | + | DGAT088 | Cc1nc(C)c(nc1C(N)=O)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 7.0000 | 5.7326 | 6.2731 | 6.5011 | 6.5333 | 1.2674 | 0.7269 | 0.4989 | 0.4667 | YES | YES | YES | YES |
| - | + | # | \* | DGAT089 | CC(C)(COc1ccc(cc1)-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1)C(O)=O | 6.9910 | 6.3922 | 6.4227 | 6.3404 | 5.9400 | 0.5988 | 0.5683 | 0.6506 | 1.0510 | YES | YES | YES | YES |
| + | - | \* | # | DGAT090 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Cc1ccccc1 | 6.9590 | 6.6999 | 6.6663 | 6.4577 | 6.5493 | 0.2591 | 0.2927 | 0.5013 | 0.4097 | YES | YES | YES | YES |
| # | \* | + | - | DGAT091 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)NCc1ccccc1 | 6.9590 | 6.7152 | 6.6414 | 6.6414 | 6.6517 | 0.2438 | 0.3176 | 0.3176 | 0.3073 | YES | YES | YES | YES |
| \* | # | - | + | DGAT092 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OCC2(CCC2)C(O)=O)nc1 | 6.9586 | 6.8919 | 6.7061 | 6.8151 | 6.7039 | 0.0667 | 0.2529 | 0.1439 | 0.2551 | YES | YES | YES | YES |
| - | + | + | - | DGAT093 | OC(=O)[C@H]1CC[C@@H](CC1)OC1CCN(CC1)c1ccc(cn1)-c1nc2cc(F)ccc2[nH]1 | 6.9590 | 7.2966 | 7.3998 | 7.6456 | 7.6121 | -0.3376 | -0.4408 | -0.6866 | -0.6531 | YES | YES | YES | YES |
| + | - | + | - | DGAT094 | COc1cc(C)c(-c2nc3ccc(cc3[nH]2)C(=O)Nc2ccc(C)c(C)c2)c(C)c1 | 6.9210 | 6.9447 | 6.6807 | 6.2212 | 5.8231 | -0.0237 | 0.2403 | 0.6998 | 1.0979 | NO | YES | YES | YES |
| - | + | # | \* | DGAT095 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1ccc(OCC(C)(C)C(O)=O)nc1 | 6.9030 | 5.9123 | 6.1731 | 5.8021 | 5.8903 | 0.9907 | 0.7299 | 1.1009 | 1.0127 | YES | YES | YES | YES |
| # | # | - | + | DGAT096 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCCN(CC1)C(=O)Nc1ccccc1Cl)N1CCCCC1 | 6.8730 | 6.5139 | 6.3812 | 6.7640 | 6.5939 | 0.3591 | 0.4918 | 0.1090 | 0.2791 | YES | YES | YES | YES |
| - | + | # | \* | DGAT097 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)NC1CCCCC1 | 6.7960 | 6.4474 | 6.4424 | 6.4244 | 6.4443 | 0.3486 | 0.3536 | 0.3716 | 0.3517 | YES | YES | YES | YES |
| + | - | \* | # | DGAT098 | CCCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.7960 | 7.2884 | 7.0909 | 7.5785 | 7.4686 | -0.4924 | -0.2949 | -0.7825 | -0.6726 | YES | YES | YES | YES |
| + | - | - | + | DGAT099 | Cc1ccc2[nH]c(nc2n1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@@H](CC2)C(O)=O)nc1 | 6.7930 | 7.1395 | 7.5795 | 7.3328 | 7.0962 | -0.3465 | -0.7865 | -0.5398 | -0.3032 | YES | NO | YES | YES |
| + | - | \* | # | DGAT100 | O=C(Nc1ccccc1)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](Cc2nnn[nH]2)CC1 | 6.7700 | 6.7278 | 7.0547 | 7.4733 | 6.7758 | 0.0422 | -0.2847 | -0.7037 | -0.0058 | NO | YES | YES | YES |
| - | + | - | + | DGAT101 | [H][C@@]1(CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1)C(C)C(O)=O | 6.6990 | 6.5651 | 6.6053 | 6.5408 | 6.5189 | 0.1339 | 0.0937 | 0.1582 | 0.1801 | YES | YES | NO | YES |
| + | - | \* | # | DGAT102 | OC(=O)CC1CCC(CC1)c1ccc(cc1)-c1nc2ccc(NC(=O)c3nc(oc3C(F)(F)F)-c3ccccc3C(F)(F)F)cc2[nH]1~ | 6.6970 | 6.4823 | 6.6619 | 6.5142 | 6.4663 | 0.2147 | 0.0351 | 0.1828 | 0.2307 | YES | YES | YES | YES |
| + | - | + | - | DGAT103 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(Nc2nc3ccc(OC(F)(F)F)cc3s2)c(F)c1 | 6.6840 | 6.6067 | 8.1816 | 7.6485 | 7.9876 | 0.0773 | -1.4976 | -0.9645 | -1.3036 | NO | YES | YES | YES |
| + | - | \* | # | DGAT104 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(OC[C@H]2C[C@@H]2C(O)=O)nc1 | 6.6780 | 6.7020 | 6.9544 | 6.9816 | 7.2445 | -0.0240 | -0.2764 | -0.3038 | -0.5665 | YES | YES | YES | YES |
| - | + | # | \* | DGAT105 | Cn1c(OCC(C)(C)C(=O)Nc2ccccc2)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 6.6580 | 6.0760 | 6.2224 | 6.2356 | 6.1365 | 0.5820 | 0.4356 | 0.4224 | 0.5215 | NO | YES | YES | YES |
| + | - | - | + | DGAT106 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C)-c1ccccc1 | 6.5850 | 6.3418 | 5.8317 | 5.8356 | 5.7860 | 0.2432 | 0.7533 | 0.7494 | 0.7990 | YES | YES | YES | YES |
| # | \* | + | - | DGAT107 | OC(=O)CC1CCC(CC1)c1ccc(cc1)-c1nc2ccc(NC(=O)c3nc(oc3C(F)(F)F)-c3ccccc3Cl)cc2[nH]1 | 6.5580 | 6.1655 | 6.7918 | 6.1992 | 6.5654 | 0.3925 | -0.2338 | 0.3588 | -0.0074 | YES | YES | YES | YES |
| \* | # | - | + | DGAT108 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2c(c[nH]c2c1)C(=O)Nc1ccccc1 | 6.5467 | 6.6863 | 6.7652 | 6.7608 | 6.5884 | -0.1396 | -0.2182 | -0.2138 | -0.0414 | YES | YES | YES | YES |
| - | + | - | + | DGAT109 | CC(C)C1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.5230 | 7.0136 | 6.9974 | 7.2611 | 7.4629 | -0.4906 | -0.4744 | -0.7381 | -0.9399 | YES | YES | YES | YES |
| + | - | \* | # | DGAT110 | CCC1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1cnc(OCC(C)(C)C(O)=O)nc1 | 6.5090 | 6.4864 | 6.4452 | 6.5280 | 6.5507 | 0.0226 | 0.0638 | -0.0190 | -0.0417 | YES | YES | YES | YES |
| # | \* | + | - | DGAT111 | CS(=O)(=O)c1ccc2nc([nH]c2c1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@H](CC2)C(O)=O)nc1 | 6.4460 | 5.9875 | 7.1205 | 6.0558 | 6.6818 | 0.4585 | -0.6745 | 0.3902 | -0.2358 | YES | YES | YES | YES |
| - | + | + | - | DGAT112 | C[C@H]1CN(C(=O)Nc2ccccc2)c2ccc(cc2O1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.4440 | 7.2530 | 7.1451 | 7.3457 | 7.6630 | -0.8090 | -0.7011 | -0.9017 | -1.2190 | YES | YES | YES | YES |
| - | + | + | - | DGAT113 | FC(F)(F)c1nn(cc1C(=O)NCCNC(=O)c1ccc(Cl)nc1)-c1ccccc1 | 6.4320 | 5.9819 | 6.3538 | 5.8916 | 5.9112 | 0.4501 | 0.0782 | 0.5404 | 0.5208 | YES | YES | YES | YES |
| + | - | \* | # | DGAT114 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccc(OCC)cc1 | 6.4200 | 6.3302 | 6.3288 | 6.2003 | 6.3532 | 0.0898 | 0.0912 | 0.2197 | 0.0668 | YES | YES | YES | YES |
| + | - | - | + | DGAT115 | Cc1cc(CCC(O)=O)cc(C)c1-c1nc2ccc(cc2[nH]1)C(=O)Nc1ccc(cc1)C(C)(C)C | 6.4090 | 6.6192 | 6.6757 | 6.7008 | 7.1812 | -0.2102 | -0.2667 | -0.2918 | -0.7722 | YES | YES | NO | YES |
| \* | # | # | + | DGAT116 | FC(F)(F)c1nn(cc1C(=O)NCCNC(=O)c1ccc(cc1)-n1cccn1)-c1ccccc1 | 6.3979 | 6.9303 | 6.4479 | 6.6418 | 6.3267 | -0.5324 | -0.0499 | -0.2438 | 0.0713 | YES | YES | YES | YES |
| - | + | # | \* | DGAT117 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1cnc(OCC(C)(C)C(O)=O)nc1 | 6.3640 | 6.3649 | 6.4305 | 6.0010 | 6.1154 | -0.0009 | -0.0665 | 0.3630 | 0.2486 | YES | YES | YES | YES |
| + | - | \* | # | DGAT118 | CN(C)C(=O)C(C)(C)COc1nnc(-c2ccc(NC(=O)c3ccc4ccccc4c3)cc2)n1C | 6.3560 | 5.6715 | 5.8059 | 5.6624 | 5.6542 | 0.6845 | 0.5501 | 0.6936 | 0.7018 | NO | YES | YES | YES |
| + | - | - | + | DGAT119 | OC(=O)C12CC3CC(C1)C(Oc1ccc(cc1)C(=O)NCCNC(=O)Nc1ccccc1)C(C3)C2 | 6.3090 | 6.6867 | 6.8745 | 7.1274 | 6.8813 | -0.3777 | -0.5655 | -0.8184 | -0.5723 | YES | YES | YES | YES |
| + | - | + | - | DGAT120 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2n1)C(=O)Nc1ccccc1 | 6.2600 | 6.6575 | 6.8534 | 7.1765 | 6.8912 | -0.3975 | -0.5934 | -0.9165 | -0.6312 | YES | YES | YES | YES |
| - | + | # | \* | DGAT121 | OC(=O)CC1CCC(CC1)c1ccc(cc1)-c1nc2ccc(NC(=O)c3nc(oc3C(F)(F)F)-c3ccccc3)cc2[nH]1 | 6.2460 | 6.3288 | 6.6565 | 6.4651 | 6.3320 | -0.0828 | -0.4105 | -0.2191 | -0.0860 | YES | YES | YES | YES |
| + | - | \* | # | DGAT122 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1cccc(OCC)c1 | 6.2220 | 6.4312 | 6.3358 | 6.2080 | 6.4750 | -0.2092 | -0.1138 | 0.0140 | -0.2530 | YES | YES | YES | YES |
| + | - | - | + | DGAT123 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc(NC(=O)Nc2ccc(cc2)C#N)cc1 | 6.2200 | 6.2923 | 6.7858 | 6.5857 | 6.8274 | -0.0723 | -0.5658 | -0.3657 | -0.6074 | NO | YES | YES | YES |
| \* | # | # | + | DGAT124 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1O | 6.2147 | 6.0430 | 6.1141 | 6.3040 | 6.1330 | 0.1717 | 0.1009 | -0.0890 | 0.0820 | YES | YES | YES | YES |
| - | + | + | - | DGAT125 | CC1COc2cc(ccc2N1C(=O)Nc1ccccc1)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 6.2010 | 6.5087 | 6.5563 | 6.4291 | 6.5472 | -0.3077 | -0.3553 | -0.2281 | -0.3462 | YES | YES | YES | YES |
| + | - | \* | # | DGAT126 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)C1CCCCC1 | 6.1870 | 6.2866 | 6.1074 | 6.3573 | 6.2839 | -0.0996 | 0.0796 | -0.1703 | -0.0969 | YES | YES | YES | YES |
| # | \* | + | - | DGAT127 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1ccc(OCC(C)(C)C(O)=O)nn1 | 6.1490 | 6.0284 | 6.1533 | 5.8581 | 5.8654 | 0.1206 | -0.0043 | 0.2909 | 0.2836 | YES | YES | YES | YES |
| \* | # | - | + | DGAT128 | CS(=O)(=O)c1ccc2nc([nH]c2c1)-c1ccc(nc1)-c1ccc(O[C@H]2CC[C@@H](CC2)C(O)=O)nc1 | 6.1385 | 6.0146 | 7.2238 | 6.0079 | 6.4968 | 0.1239 | -1.0858 | 0.1301 | -0.3588 | YES | YES | YES | YES |
| - | + | # | \* | DGAT129 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(Cc2ccccc2)nc1C(F)(F)F | 6.1140 | 6.6137 | 6.4121 | 6.3941 | 6.3369 | -0.4997 | -0.2981 | -0.2801 | -0.2229 | NO | YES | YES | YES |
| + | - | \* | # | DGAT130 | OC(=O)[C@@H]1CCC[C@H]1C(=O)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 6.0810 | 6.3935 | 6.5168 | 6.7299 | 6.4456 | -0.3125 | -0.4358 | -0.6489 | -0.3646 | YES | YES | YES | YES |
| # | \* | + | - | DGAT131 | ONC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 6.0360 | 6.0963 | 6.2525 | 6.0551 | 6.1252 | -0.0603 | -0.2165 | -0.0191 | -0.0892 | YES | YES | YES | YES |
| # | # | - | + | DGAT132 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2cc([nH]c2c1)C(=O)Nc1ccccc1 | 5.9630 | 6.8300 | 6.7191 | 6.4656 | 6.5060 | -0.8670 | -0.7561 | -0.5026 | -0.5430 | YES | YES | YES | YES |
| - | + | + | - | DGAT133 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1cc(ccc1F)C(F)(F)F | 5.9210 | 6.6932 | 7.0269 | 6.9160 | 6.9377 | -0.7722 | -1.1059 | -0.9950 | -1.0167 | NO | YES | YES | YES |
| + | - | \* | # | DGAT134 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1nn(cc1C)-c1ccccc1 | 5.9210 | 6.4316 | 5.7121 | 6.0028 | 5.6161 | -0.5106 | 0.2089 | -0.0818 | 0.3049 | YES | YES | YES | YES |
| # | \* | + | - | DGAT135 | FC(F)(F)c1nn(cc1C(=O)NCCNC(=O)c1ccc(Cl)cn1)-c1ccccc1 | 5.9210 | 6.5933 | 6.6982 | 6.5964 | 6.3351 | -0.6723 | -0.7772 | -0.6754 | -0.4141 | YES | YES | YES | YES |
| \* | # | - | + | DGAT136 | CC(C)OC(=O)N1CCN(CC1)c1ccc(NC(=O)c2oc(nc2C(F)(F)F)N2CCCCC2)cn1 | 5.9190 | 4.5313 | 5.9113 | 5.7905 | 6.0662 | 1.3877 | 0.0077 | 0.1285 | -0.1472 | YES | YES | YES | YES |
| - | + | # | \* | DGAT137 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCN(CC1)C(=O)Oc1ccccc1Cl)N1CCCCC1 | 5.8580 | 6.4235 | 6.5238 | 6.6568 | 6.6819 | -0.5655 | -0.6658 | -0.7988 | -0.8239 | YES | YES | YES | YES |
| + | - | + | - | DGAT138 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccc(Cl)cc1 | 5.8240 | 6.2875 | 6.7530 | 6.3399 | 6.6797 | -0.4635 | -0.9290 | -0.5159 | -0.8557 | YES | YES | YES | YES |
| + | - | \* | # | DGAT139 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCC(=O)c2c1)C(=O)Nc1ccccc1 | 5.7780 | 6.1585 | 6.5731 | 6.5161 | 6.5745 | -0.3805 | -0.7951 | -0.7381 | -0.7965 | YES | YES | YES | YES |
| \* | # | - | + | DGAT140 | Cn1c(OCC(C)(C)C(O)=O)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 5.7077 | 5.7506 | 5.8791 | 5.5697 | 5.7441 | -0.0429 | -0.1711 | 0.1383 | -0.0361 | NO | YES | YES | YES |
| - | + | # | \* | DGAT141 | Cc1ccc(NC(=O)c2ccc3nc([nH]c3c2)-c2c(C)cc(NCC(O)=O)cc2C)cc1C | 5.6990 | 5.5085 | 6.1300 | 5.2392 | 5.6379 | 0.1905 | -0.4310 | 0.4598 | 0.0611 | YES | YES | YES | YES |
| + | - | - | + | DGAT142 | Cc1cc(NC(=O)c2ccc3ccccc3c2)ccc1-c1cnc(OCC(C)(C)C(O)=O)cn1 | 5.6650 | 6.4924 | 6.6000 | 6.4189 | 6.3088 | -0.8274 | -0.9350 | -0.7539 | -0.6438 | YES | YES | YES | YES |
| + | - | + | - | DGAT143 | FC(F)(F)c1nc(oc1C(=O)Nc1ccc(nc1)N1CCN(CC1)c1ncccc1Cl)N1CCCCC1 | 5.6440 | 6.4094 | 6.1724 | 6.3707 | 6.3436 | -0.7654 | -0.5284 | -0.7267 | -0.6996 | YES | YES | YES | YES |
| \* | # | - | + | DGAT144 | CC(C)NC(=O)C(C)(C)COc1nnc(-c2ccc(NC(=O)c3ccc4ccccc4c3)cc2)n1C | 5.6308 | 5.5551 | 5.7702 | 5.6218 | 5.6174 | 0.0757 | -0.1392 | 0.0092 | 0.0136 | NO | YES | YES | YES |
| - | + | # | \* | DGAT145 | CC(C)(C)OC(=O)NCCNC(=O)c1ccc(OC2C3CC4CC2CC(C4)(C3)C(O)=O)cc1 | 5.5770 | 5.4686 | 6.1509 | 6.1984 | 6.2307 | 0.1084 | -0.5739 | -0.6214 | -0.6537 | YES | NO | YES | YES |
| + | - | + | - | DGAT146 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2n(ncc2c1)C(=O)Nc1ccccc1 | 5.5740 | 6.2929 | 6.7622 | 6.4350 | 6.5878 | -0.7189 | -1.1882 | -0.8610 | -1.0138 | YES | YES | YES | YES |
| # | \* | + | - | DGAT147 | COCCN(C)c1ccc(NC(=O)c2oc(nc2C(F)(F)F)-c2ccccc2)cn1 | 5.5450 | 5.5550 | 5.7310 | 5.9924 | 5.4875 | -0.0100 | -0.1860 | -0.4474 | 0.0575 | YES | YES | YES | YES |
| \* | # | - | + | DGAT148 | CCOc1ccc(cc1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1cccnc1 | 5.4685 | 6.6894 | 6.2716 | 6.1194 | 6.2250 | -1.2209 | -0.8036 | -0.6514 | -0.7570 | YES | YES | YES | YES |
| - | + | + | - | DGAT149 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2oc(Nc3ccccc3)nc2c1 | 5.4150 | 6.1205 | 6.3643 | 6.2728 | 6.1746 | -0.7055 | -0.9493 | -0.8578 | -0.7596 | YES | YES | YES | YES |
| + | - | \* | # | DGAT150 | Cn1c(CCC(O)=O)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 5.3980 | 5.5822 | 5.7615 | 5.2168 | 5.1840 | -0.1842 | -0.3635 | 0.1812 | 0.2140 | NO | YES | YES | YES |
| - | + | - | + | DGAT151 | OC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCNc2c1)C(=O)Nc1ccccc1 | 5.3170 | 6.1774 | 6.2950 | 6.2657 | 6.3844 | -0.8604 | -0.9780 | -0.9487 | -1.0674 | YES | YES | YES | YES |
| - | # | - | + | DGAT152 | CCOc1cccc(c1)C(=O)NCCNC(=O)c1cn(nc1C(F)(F)F)-c1ccccc1 | 5.2920 | 6.2757 | 6.1209 | 6.2825 | 6.1867 | -0.9837 | -0.8289 | -0.9905 | -0.8947 | YES | YES | YES | YES |
| + | + | - | + | DGAT153 | Nc1ccccc1NC(=O)N1CCOc2cc(ccc12)-c1ccc(cc1)[C@H]1CC[C@H](CC(O)=O)CC1 | 5.2840 | 6.2248 | 6.4861 | 6.4128 | 6.4927 | -0.9408 | -1.2021 | -1.1288 | -1.2087 | NO | YES | YES | YES |
| + | - | + | - | DGAT154 | CN(C)CCNC(=O)C(C)(C)COc1nnc(-c2ccc(NC(=O)c3ccc4ccccc4c3)cc2)n1C | 5.2300 | 5.8807 | 5.8097 | 5.7391 | 5.8366 | -0.6507 | -0.5797 | -0.5091 | -0.6066 | NO | YES | YES | YES |
| - | + | # | \* | DGAT155 | Cn1c(OCC(C)(C)C(N)=O)nnc1-c1ccc(NC(=O)c2ccc3ccccc3c2)cc1 | 5.2150 | 5.0243 | 5.5596 | 5.0910 | 5.3294 | 0.1907 | -0.3446 | 0.1240 | -0.1144 | NO | YES | YES | YES |
| \* | # | - | + | DGAT156 | Cc1ccc(NC(=O)c2ccc3nc([nH]c3c2)-c2c(C)cc(CCC(O)=O)cc2C)cc1C | 5.1871 | 5.5089 | 6.2549 | 5.0596 | 5.5496 | -0.3218 | -1.0679 | 0.1274 | -0.3626 | YES | YES | YES | YES |
| - | + | + | - | DGAT157 | CS(=O)(=O)NC(=O)C[C@H]1CC[C@@H](CC1)c1ccc(cc1)-c1ccc2N(CCOc2c1)C(=O)Nc1ccccc1 | 5.1370 | 5.0994 | 6.0484 | 5.6552 | 5.9110 | 0.0376 | -0.9114 | -0.5182 | -0.7740 | YES | YES | YES | YES |
| # | \* | + | - | DGAT158 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.9210 | 6.1687 | 6.2614 | 6.3282 | 6.3457 | 0.7523 | 0.6596 | 0.5928 | 0.5753 | YES | YES | YES | YES |
| \* | # | - | + | DGAT159 | CCOC(=O)c1c(C)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.2840 | 6.1477 | 6.4754 | 5.9941 | 6.1590 | 0.1363 | -0.1914 | 0.2899 | 0.1250 | YES | YES | YES | YES |
| - | + | # | \* | DGAT160 | CCOC(=O)c1c(CC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.6200 | 6.0312 | 6.4395 | 5.9904 | 6.1224 | 0.5888 | 0.1805 | 0.6296 | 0.4976 | YES | YES | YES | YES |
| + | - | \* | # | DGAT161 | CCOC(=O)c1c(CC=C)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 7.1250 | 7.1701 | 6.4646 | 5.9834 | 6.1366 | -0.0451 | 0.6604 | 1.1416 | 0.9884 | NO | YES | YES | YES |
| # | \* | + | - | DGAT162 | CCOC(=O)c1c(CCC(F)(F)F)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.9590 | 6.3135 | 6.7150 | 6.7066 | 6.5406 | 0.6455 | 0.2440 | 0.2524 | 0.4184 | YES | YES | YES | YES |
| \* | # | - | + | DGAT163 | CCCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.7960 | 6.3781 | 6.3616 | 6.5460 | 6.4851 | 0.4179 | 0.4344 | 0.2500 | 0.3109 | YES | YES | YES | YES |
| - | + | # | \* | DGAT164 | CCCCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.6580 | 6.5874 | 6.4618 | 6.7638 | 6.6245 | 0.0706 | 0.1962 | -0.1058 | 0.0335 | YES | YES | YES | YES |
| - | + | # | \* | DGAT165 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1C1CC1)N1CCOCC1)-c1ccccc1 | 6.2080 | 5.8752 | 6.0244 | 5.7454 | 5.8965 | 0.3328 | 0.1836 | 0.4626 | 0.3115 | YES | YES | YES | YES |
| \* | # | - | + | DGAT166 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1C1CCC1)N1CCOCC1)-c1ccccc1 | 5.6020 | 6.0846 | 6.1246 | 5.9631 | 6.0360 | -0.4826 | -0.5226 | -0.3611 | -0.4340 | YES | YES | YES | YES |
| - | + | # | \* | DGAT167 | CCOC(=O)c1c(COC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.6200 | 6.6427 | 6.7575 | 6.5843 | 6.5836 | -0.0227 | -0.1375 | 0.0357 | 0.0364 | YES | YES | YES | YES |
| + | - | \* | # | DGAT168 | CCOC(=O)c1c(CCCOC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.5690 | 6.9106 | 6.7864 | 6.7948 | 6.6831 | -0.3416 | -0.2174 | -0.2258 | -0.1141 | YES | YES | YES | YES |
| + | - | + | - | DGAT169 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccccc1)N1CCOCC1)-c1ccccc1 | 7.0920 | 6.5420 | 6.3354 | 6.3730 | 6.1043 | 0.5500 | 0.7566 | 0.7190 | 0.9877 | YES | YES | YES | YES |
| \* | # | - | + | DGAT170 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1cccc(OC)c1)N1CCOCC1)-c1ccccc1 | 6.3280 | 6.7399 | 6.6286 | 6.3136 | 6.5542 | -0.4119 | -0.3006 | 0.0144 | -0.2262 | YES | YES | YES | YES |
| - | + | # | \* | DGAT171 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1cccc(Cl)c1)N1CCOCC1)-c1ccccc1 | 6.5380 | 7.0845 | 7.1814 | 7.1170 | 6.8695 | -0.5465 | -0.6434 | -0.5790 | -0.3315 | YES | YES | YES | YES |
| # | \* | + | - | DGAT172 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(Cl)cc1)N1CCOCC1)-c1ccccc1 | 7.2010 | 6.9836 | 7.1744 | 7.1092 | 6.7476 | 0.2174 | 0.0266 | 0.0918 | 0.4534 | YES | YES | YES | YES |
| \* | # | - | + | DGAT173 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(O)cc1)N1CCOCC1)-c1ccccc1 | 6.2440 | 6.5067 | 6.6160 | 6.2835 | 6.4628 | -0.2627 | -0.3720 | -0.0395 | -0.2188 | YES | YES | YES | YES |
| - | + | # | \* | DGAT174 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(OC)cc1)N1CCOCC1)-c1ccccc1 | 7.2840 | 6.6390 | 6.6216 | 6.3058 | 6.4324 | 0.6450 | 0.6624 | 0.9782 | 0.8516 | YES | YES | YES | YES |
| \* | - | \* | # | DGAT175 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(N)cc1)N1CCOCC1)-c1ccccc1 | 6.2010 | 6.5306 | 6.3536 | 6.3795 | 6.2933 | -0.3296 | -0.1526 | -0.1785 | -0.0923 | YES | YES | YES | YES |
| + | - | \* | # | DGAT176 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(cc1)-c1ccccc1)N1CCOCC1)-c1ccccc1 | 6.6020 | 7.4357 | 7.0290 | 6.9892 | 6.7463 | -0.8337 | -0.4270 | -0.3872 | -0.1443 | YES | YES | YES | YES |
| \* | # | - | + | DGAT177 | CCOC(=O)c1c(C(=O)OCC)c2c(cc(nn2c1-c1ccc(OCc2ccccc2)cc1)N1CCOCC1)-c1ccccc1 | 7.2220 | 7.9237 | 7.2526 | 7.2588 | 7.1317 | -0.7017 | -0.0306 | -0.0368 | 0.0903 | YES | YES | YES | YES |
| # | + | # | \* | DGAT178 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCC1)-c1ccccc1 | 5.8660 | 5.6496 | 6.1863 | 5.9666 | 6.1037 | 0.2164 | -0.3203 | -0.1006 | -0.2377 | YES | YES | YES | YES |
| - | + | - | + | DGAT179 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCCC1)-c1ccccc1 | 6.9210 | 5.8589 | 6.2865 | 6.1844 | 6.2431 | 1.0621 | 0.6345 | 0.7366 | 0.6779 | YES | YES | YES | YES |
| - | # | - | + | DGAT180 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCCCC1)-c1ccccc1 | 5.2150 | 6.0683 | 6.3867 | 6.4022 | 6.3825 | -0.8533 | -1.1717 | -1.1872 | -1.1675 | YES | YES | YES | YES |
| - | + | # | \* | DGAT181 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N(C)C)-c1ccccc1 | 6.0810 | 5.9138 | 6.0467 | 6.0763 | 6.0438 | 0.1672 | 0.0343 | 0.0047 | 0.0372 | YES | YES | YES | YES |
| + | - | \* | # | DGAT182 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1F | 6.2440 | 6.3551 | 6.5648 | 6.7368 | 6.4309 | -0.1111 | -0.3208 | -0.4928 | -0.1869 | NO | YES | YES | YES |
| # | \* | + | - | DGAT183 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1cccc(F)c1 | 6.5690 | 6.9087 | 6.9328 | 6.8357 | 6.9458 | -0.3397 | -0.3638 | -0.2667 | -0.3768 | YES | YES | YES | YES |
| \* | # | - | + | DGAT184 | CCCc1c(C(=O)OCC)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccc(F)cc1 | 6.5380 | 6.8077 | 6.9258 | 6.8279 | 6.8240 | -0.2697 | -0.3878 | -0.2899 | -0.2860 | YES | YES | YES | YES |
| - | + | - | + | DGAT185 | CCCc1c(-c2nc(C)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.4200 | 6.7442 | 7.0315 | 6.8859 | 6.6834 | -0.3242 | -0.6115 | -0.4659 | -0.2634 | YES | YES | YES | YES |
| # | \* | + | - | DGAT186 | CCCc1c(-c2nc(CC)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.9590 | 6.6278 | 6.9955 | 6.8822 | 6.6468 | 0.3312 | -0.0365 | 0.0768 | 0.3122 | YES | YES | YES | YES |
| \* | # | - | + | DGAT187 | CCCc1noc(n1)-c1c(CCC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 7.1870 | 6.7896 | 6.8056 | 6.6588 | 6.6974 | 0.3974 | 0.3814 | 0.5282 | 0.4896 | NO | YES | YES | YES |
| - | + | # | \* | DGAT188 | CCCc1c(-c2nc(no2)C(C)C)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.2440 | 6.3890 | 6.8603 | 6.9449 | 6.7859 | 0.8550 | 0.3837 | 0.2991 | 0.4581 | YES | YES | YES | YES |
| + | - | \* | # | DGAT189 | CCCCc1noc(n1)-c1c(CCC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 7.1370 | 6.9990 | 6.9058 | 6.8766 | 6.8368 | 0.1380 | 0.2312 | 0.2604 | 0.3002 | NO | YES | YES | YES |
| # | \* | + | - | DGAT190 | CCCc1c(-c2nc(no2)C(C)(C)C)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.3190 | 6.5993 | 6.9134 | 7.4603 | 7.0902 | 0.7197 | 0.4056 | -0.1413 | 0.2288 | YES | YES | YES | YES |
| \* | # | - | + | DGAT191 | CCCCCc1noc(n1)-c1c(CCC)n2nc(cc(-c3ccccc3)c2c1C(=O)OCC)N1CCOCC1 | 6.9590 | 7.2084 | 7.0061 | 7.0943 | 6.9762 | -0.2494 | -0.0471 | -0.1353 | -0.0172 | NO | YES | YES | YES |
| - | + | # | \* | DGAT192 | CCCc1c(-c2nc(no2)-c2ccccc2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.7450 | 7.3234 | 7.3840 | 7.5430 | 7.1442 | -0.5784 | -0.6390 | -0.7980 | -0.3992 | YES | YES | YES | YES |
| # | \* | + | - | DGAT193 | CCCc1c(-c2nc(Cc3ccccc3)no2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.9210 | 6.8269 | 7.4409 | 7.4495 | 7.2037 | 0.0941 | -0.5199 | -0.5285 | -0.2827 | YES | YES | YES | YES |
| \* | # | - | + | DGAT194 | CCCc1c(-c2nc(no2)C2CCCC2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.3190 | 7.3598 | 7.4888 | 7.5782 | 7.5598 | -0.0408 | -0.1698 | -0.2592 | -0.2408 | YES | YES | YES | YES |
| - | + | # | \* | DGAT195 | CCCc1c(-c2nc(no2)C2CCCCC2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.2520 | 7.5692 | 7.5890 | 7.7960 | 7.6992 | -0.3172 | -0.3370 | -0.5440 | -0.4472 | YES | YES | YES | YES |
| + | - | \* | # | DGAT196 | CCCc1c(-c2nc(no2)N2CCCC2)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 7.0000 | 6.7868 | 7.3248 | 7.2873 | 7.2327 | 0.2132 | -0.3248 | -0.2873 | -0.2327 | YES | YES | YES | YES |
| # | \* | + | - | DGAT197 | CCCc1c(-c2nc(no2)N(C)C)c(C(=O)OCC)c2c(cc(nn12)N1CCOCC1)-c1ccccc1 | 6.8540 | 5.8588 | 6.7141 | 6.6641 | 6.5961 | 0.9952 | 0.1399 | 0.1899 | 0.2579 | YES | YES | YES | YES |

**Table S3.** Percentage of identity of splits 1–4 DGAT1 inhibitors.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Split | SET | Split 1(%) | Split 2(%) | Split 3(%) | Split 4(%) |
| Split 1 | Total | 100 | 4.1 | 14.2 | 11.2 |
| Training | 100 | 4.9 | 27.6 | 16.0 |
| Invisible training | 100 | 0.0 | 15.4 | 20.3 |
| Calibration | 100 | 11.8 | 5.0 | 0.0 |
| Validation | 100 | 0.0 | 0.0 | 0.0 |
| Split 2 | Total |  | 100 | 11.2 | 13.7 |
| Training |  | 100 | 19.8 | 16.3 |
| Invisible training |  | 100 | 11.8 | 28.3 |
| Calibration |  | 100 | 6.9 | 0.0 |
| Validation |  | 100 | 0 | 0.0 |
| Split 3 | Total |  |  | 100 | 0.0 |
| Training |  |  | 100 | 0.0 |
| Invisible training |  |  | 100 | 0.0 |
| Calibration |  |  | 100 | 0.0 |
| Validation |  |  | 100 | 0.0 |
| Split 4 | Total |  |  |  | 100 |
| Training |  |  |  | 100 |
| Invisible training |  |  |  | 100 |
| Calibration |  |  |  | 100 |
| Validation |  |  |  | 100 |

Identity (%)= [Nij/0.5(Ni+Nj)]x100

Where:

Nij is the number of substances which are distributed into the same set for both i-th split and j-th split (set = training set, invisible training set, calibration set, validation set)

Ni is the number of substances which are distributed into the set for i-th split

Nj is the number of substances which are distributed into the set for j-th split

**Table S4:** Predicted statistical parameter for Split 1-4 using equation 3 and 4

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **SPLIT** | **EQUATION** | **SET** | **n** | **R2** | **CCC** | **IIC** | **Q2** | **s** | **MAE** | **F** | **CRp2** | **Y- test** | **RMSEP** | **Q2F1** | **Q2F2** | **Scaled**  **Avg.**  **Rm^2** | **Scaled**  **Delta**  **Rm^2** | **MODEL** |
| Split 1 | Equation 4  With IIC | Training | 60 | 0.6796 | 0.8092 | 0.7712 | 0.6625 | 0.501 | 0.374 | 123 | 0.6729 | 0.0133 |  |  |  |  |  | Endpoint = 1.9636813 (± 0.0487017) + 0.0365143 (± 0.0003197) \* DCW(1,23) |
| InvTrain | 57 | 0.6734 | 0.8095 | 0.5305 | 0.6506 | 0.530 | 0.432 | 113 | 0.6678 | 0.0112 |  |  |  |  |  |
| Calib | 39 | 0.7021 | 0.8202 | **0.8379** | **0.6669** | **0.478** | **0.37** | **87** | **0.6908** | **0.0225** | **0.4720** | **0.6710** | **0.6387** | **0.5984** | **0.1076** |
| validation | 41 | **0.8129** | **0.8979** | 0.6153 | 0.7962 | 0.398 | 0.301 | 169 | 0.7982 | 0.0291 | 0.3934 | 0.8149 | 0.8126 | 0.7377 | 0.1395 |
| Equation 3 | Training | 60 | 0.7333 | 0.8461 | 0.8011 | 0.7167 | 0.457 | 0.351 | 159 | 0.7250 | 0.0166 |  |  |  |  |  | Endpoint = 1.7901201 (± 0.0519123) + 0.0619099 (± 0.0005747) \* DCW(1,5) |
| InvTrain | 57 | 0.7166 | 0.8458 | 0.7984 | 0.6996 | 0.507 | 0.404 | 139 | 0.7101 | 0.0130 |  |  |  |  |  |
| Calib | 39 | 0.6796 | 0.7842 | 0.6647 | 0.6433 | 0.575 | 0.466 | 78 | 0.6526 | 0.0529 | 0.5677 | 0.5241 | 0.4773 | 0.5034 | 0.2490 |
| validation | 41 | 0.7059 | 0.8371 | 0.6837 | 0.6762 | 0.543 | 0.428 | 94 | 0.6921 | 0.0274 | 0.5361 | 0.6563 | 0.6521 | 0.6034 | 0.1136 |
|  |  |  |  | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** |  |
| Split 2 | Equation 4  With IIC | Training | 60 | 0.6378 | 0.7788 | 0.7986 | 0.6150 | 0.555 | 0.431 | 102 | 0.6258 | 0.0238 |  |  |  |  |  | Endpoint = 2.8334874 (± 0.0525059) + 0.0365509 (± 0.0004283) \* DCW(4,9) |
| InvTrain | 59 | 0.5742 | 0.7563 | 0.6207 | 0.5474 | 0.590 | 0.494 | 77 | 0.5572 | 0.0334 |  |  |  |  |  |
| Calib | 46 | 0.7183 | 0.8429 | **0.8467** | **0.6920** | **0.504** | **0.401** | **112** | **0.7128** | **0.0110** | **0.4989** | **0.7134** | **0.7134** | **0.6170** | **0.1479** |
| validation | 32 | **0.7717** | **0.8572** | 0.7048 | 0.7386 | 0.401 | 0.330 | 101 | 0.7542 | 0.0346 | 0.3946 | 0.7785 | 0.7415 | 0.6855 | 0.0578 |
| Equation 3 | Training | 60 | 0.6167 | 0.7629 | 0.7346 | 0.5931 | 0.571 | 0.458 | 93 | 0.6065 | 0.0202 |  |  |  |  |  | Endpoint = 3.3081390 (± 0.0482392) + 0.0285524 (± 0.0003437) \* DCW(2,3) |
| InvTrain | 59 | 0.5481 | 0.7375 | 0.7366 | 0.5202 | 0.607 | 0.508 | 69 | 0.5256 | 0.0442 |  |  |  |  |  |
| Calib | 46 | 0.6762 | 0.8112 | 0.7021 | 0.6461 | 0.538 | 0.438 | 92 | 0.6599 | 0.0322 | 0.5321 | 0.6740 | 0.6740 | 0.5603 | 0.2161 |
| validation | 32 | 0.7260 | 0.8359 | 0.6364 | 0.6863 | 0.430 | 0.353 | 79 | 0.7094 | 0.0329 | 0.4229 | 0.7457 | 0.7032 | 0.6272 | 0.0664 |
|  |  |  |  | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** |  |
| Split 3 | Equation 4 With IIC | Training | 61 | 0.5851 | 0.7382 | 0.5682 | 0.5574 | 0.621 | 0.514 | 83 | 0.5787 | 0.0128 |  |  |  |  |  | Endpoint = 2.8273046 (± 0.0611212) + 0.0452571 (± 0.0006322) \* DCW(10,13) |
| InvTrain | 60 | 0.5691 | 0.738 | 0.7527 | 0.5451 | 0.615 | 0.492 | 77 | 0.5616 | 0.0149 |  |  |  |  |  |
| Calib | 41 | 0.7586 | 0.8538 | **0.8706** | **0.7379** | **0.400** | **0.326** | **123** | **0.7455** | 0.0259 | **0.3955** | **0.7563** | **0.7410** | 0.6670 | 0.1092 |
| validation | 35 | **0.6940** | **0.8328** | 0.7321 | 0.6615 | 0.456 | 0.3776 | 75 | 0.6801 | 0.0275 | 0.4492 | 0.6761 | 0.6599 | 0.5902 | 0.0312 |
| Equation 3 | Training | 61 | 0.7215 | 0.8382 | 0.7207 | 0.7034 | 0.509 | 0.419 | 153 | 0.7076 | 0.0276 |  |  |  |  |  | Endpoint = 1.5918529 (± 0.0583141) + 0.0590010 (± 0.0005927) \* DCW(4,4) |
| InvTrain | 60 | 0.6446 | 0.7994 | 0.8010 | 0.6276 | 0.566 | 0.447 | 105 | 0.6428 | 0.0035 |  |  |  |  |  |
| Calib | 41 | 0.7186 | 0.8400 | 0.6525 | 0.6926 | 0.450 | 0.358 | 100 | 0.7101 | **0.0169** | 0.4449 | 0.6917 | 0.6724 | **0.6179** | **0.0995** |
| validation | 35 | 0.6933 | 0.8309 | 0.6426 | 0.6611 | 0.4690 | 0.3877 | 75 | 0.6811 | 0.0242 | 0.4623 | 0.6569 | 0.6398 | 0.5888 | 0.0873 |
|  |  |  |  | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | **Correct** | Wrong | **Correct** | **Correct** | **Correct** | Wrong | Wrong |  |
| Split 4 | Equation 4 With IIC | Training | 63 | 0.6931 | 0.8187 | 0.7568 | 0.6772 | 0.509 | 0.384 | 138 | 0.6821 | 0.0217 |  |  |  |  |  | Endpoint = 1.9535249 (± 0.0450836) + 0.0416621 (± 0.0003440) \* DCW(3,7) |
| InvTrain | 61 | 0.6345 | 0.7958 | 0.7731 | 0.6107 | 0.609 | 0.507 | 102 | 0.6253 | 0.0183 |  |  |  |  |  |
| Calib | 35 | 0.7249 | 0.8480 | **0.8513** | 0.6959 | 0.450 | 0.341 | 87 | 0.7124 | 0.0248 | 0.4434 | 0.6726 | 0.6686 | 0.6268 | 0.1283 |
| Validation | 38 | **0.7186** | **0.8335** | 0.6280 | 0.6882 | 0.445 | 0.352 | 92 | 0,7060 | 0.0250 | 0.4395 | 0.6931 | 0.6898 | 0.6187 | 0.0194 |
| Equation 3 | Training | 63 | 0.6336 | 0.7757 | 0.7711 | 0.615 | 0.556 | 0.426 | 105 | 0.6270 | 0.0132 |  |  |  |  |  | Endpoint = 2.0654314 (± 0.0493788) + 0.0455263 (± 0.0004202) \* DCW(6,3) |
| InvTrain | 61 | 0.5461 | 0.7338 | 0.6911 | 0.5173 | 0.667 | 0.565 | 71 | 0.5396 | 0.0130 |  |  |  |  |  |
| Calib | 35 | 0.7559 | 0.8666 | 0.6521 | **0.7291** | **0.412** | **0.325** | **102** | **0.7438** | **0.0240** | **0.4065** | **0.7249** | **0.7215** | **0.6665** | **0.1004** |
| validation | 38 | 0.7115 | 0.8298 | 0.7608 | 0.6802 | 0.4577 | 0.368 | 89 | 0.6988 | 0.0251 | 0.4517 | 0.6759 | 0.6724 | 0.6100 | 0.0316 |
|  |  |  |  | **Correct** | **Correct** | **Correct** | Wrong | Wrong | Wrong | Wrong | Wrong | Wrong | Wrong | Wrong | Wrong | Wrong | Wrong |  |

**Table S5.**  External prediction criteria values for developed QSAR models of calibration and validation sets. Without IIC, using equation 3

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | Calibration set | | | | Validation set | | | |
| r2m(x,y): | Split 1 | Split 2 | Split 3 | Split 4 | Split 1 | Split 2 | Split 3 | Split 4 |
| r2 | 0.6796 | 0.6762 | 0.7186 | 0.7559 | 0.7059 | 0.7260 | 0.6933 | 0.7115 |
| r20 | 0.6794 | 0.5505 | 0.7036 | 0.7489 | 0.6975 | 0.6604 | 0.6823 | 0.6749 |
| rr20 | 0.5466 | 0.6756 | 0.6857 | 0.7242 | 0.6529 | 0.7236 | 0.6398 | 0.6968 |
| (r2-r20)/r2 | 0.0003 | 0.1860 | 0.0208 | 0.0093 | 0.0119 | 0.0903 | 0.0160 | 0.0514 |
| (r2-rr20)/r2 | 0.1957 | 0.0009 | 0.0457 | 0.0419 | 0.0750 | 0.0033 | 0.0772 | 0.0206 |
| k | 0.9661 | 0.9996 | 0.9833 | 0.9910 | 0.9907 | 0.9817 | 0.9962 | 0.9786 |
| kk | 1.0295 | 0.9947 | 1.0131 | 1.0057 | 1.0036 | 1.0155 | 0.9994 | 1.0179 |
| R2m(test) | 0.6698 | 0.4364 | 0.6307 | 0.6926 | 0.6413 | 0.5401 | 0.6204 | 0.5754 |
| r2m(y, x): |  | | | | | | | |
| r2 | 0.6796 | 0.6762 | 0.7186 | 0.7559 | 0.7059 | 0.7260 | 0.6933 | 0.7115 |
| r20 | 0.5466 | 0.6756 | 0.6857 | 0.7242 | 0.6529 | 0.7236 | 0.6398 | 0.6968 |
| rr20 | 0.6794 | 0.5505 | 0.7036 | 0.7489 | 0.6975 | 0.6604 | 0.6823 | 0.6749 |
| (r2-r20)/r2 | 0.1957 | 0.0009 | 0.0457 | 0.0419 | 0.0750 | 0.0033 | 0.0772 | 0.0206 |
| (r2-rr20)/r2 | 0.0003 | 0.1860 | 0.0208 | 0.0093 | 0.0119 | 0.0903 | 0.0160 | 0.0514 |
| k | 1.0295 | 0.9947 | 1.0131 | 1.0057 | 1.0036 | 1.0155 | 0.9994 | 1.0179 |
| kk | 0.9661 | 0.9996 | 0.9833 | 0.9910 | 0.9907 | 0.9817 | 0.9962 | 0.9786 |
| R\*2m(test) | 0.4317 | 0.6594 | 0.5884 | 0.6214 | 0.5434 | 0.6905 | 0.5329 | 0.6252 |
| R2m(av) | 0.5508 | 0.5479 | 0.6095 | 0.6570 | 0.5924 | 0.6153 | 0.5767 | 0.6003 |
| ∆R2m | 0.2381 | 0.2230 | 0.0424 | 0.0712 | 0.0978 | 0.1504 | 0.0875 | 0.0498 |

(r2-r20)/r2 should be <0.1; (r2-rr20)/r2 should be <0.1; Should be 0.85 < k < 1.15; Should be 0.85 < kk < 1.1565; R2m(test) and R\*2m(test) should be >0.566; R2m (av) is average value of R2m and should be >0.5; ∆R2m should be < 0.267

**Table S6.**  External prediction criteria values for developed QSAR models of calibration and validation sets. For SMILES with IIC using equation 4

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Parameters | Calibration set | | | | Validation set | | | |
| r2m(x,y): | Split 1 | Split 2 | Split 3 | Split 4 | Split 1 | Split 2 | Split 3 | Split 4 |
| r2 | 0.7021 | 0.7183 | 0.7586 | 0.7249 | 0.8129 | 0.7717 | 0.6940 | 0.7186 |
| r20 | 0.6781 | 0.6519 | 0.6902 | 0.7207 | 0.7757 | 0.7184 | 0.6723 | 0.6686 |
| rr20 | 0.6741 | 0.7153 | 0.7585 | 0.6687 | 0.8128 | 0.7712 | 0.6599 | 0.7115 |
| (r2-r20)/r2 | 0.0342 | 0.0925 | 0.0903 | 0.0059 | 0.0457 | 0.0691 | 0.0313 | 0.0695 |
| (r2-rr20)/r2 | 0.0399 | 0.0042 | 0.0001 | 0.0776 | 0.0001 | 0.0006 | 0.0492 | 0.0098 |
| k | 0.9757 | 1.0008 | 0.9823 | 0.9949 | 0.9985 | 0.9791 | 0.9962 | 0.9798 |
| kk | 1.0209 | 0.9942 | 1.0150 | 1.0011 | 0.9985 | 1.0187 | 0.9997 | 1.0169 |
| R2m(test) | 0.5933 | 0.5332 | 0.5601 | 0.6776 | 0.6562 | 0.5935 | 0.5917 | 0.5580 |
| r2m(y, x): |  | | | | | | | |
| r2 | 0.7021 | 0.7183 | 0.7586 | 0.7249 | 0.8129 | 0.7717 | 0.6940 | 0.7186 |
| r20 | 0.6741 | 0.7153 | 0.7585 | 0.6687 | 0.8128 | 0.7712 | 0.6599 | 0.7115 |
| rr20 | 0.6781 | 0.6519 | 0.6902 | 0.7207 | 0.7757 | 0.7184 | 0.6723 | 0.6686 |
| (r2-r20)/r2 | 0.0399 | 0.0042 | 0.0001 | 0.0776 | 0.0001 | 0.0006 | 0.0492 | 0.0098 |
| (r2-rr20)/r2 | 0.0342 | 0.0925 | 0.0903 | 0.0059 | 0.0457 | 0.0691 | 0.0313 | 0.0695 |
| k | 1.0209 | 0.9942 | 1.0150 | 1.0011 | 0.9985 | 1.0187 | 0.9997 | 1.0169 |
| kk | 0.9757 | 1.0008 | 0.9823 | 0.9949 | 0.9985 | 0.9791 | 0.9962 | 0.9798 |
| R\*2m(test) | 0.5846 | 0.6790 | 0.7506 | 0.5530 | 0.8042 | 0.7548 | 0.5658 | 0.6582 |
| R2m(av) | 0.5890 | 0.6061 | 0.6554 | 0.6153 | 0.7302 | 0.6742 | 0.5788 | 0.6081 |
| ∆R2m | 0.0087 | 0.1458 | 0.1905 | 0.1246 | 0.1480 | 0.1614 | 0.0259 | 0.1002 |

**Table S7.** Y-randomization results for four splits For Smiles Without IIC using equation 3

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Split 1** | | | **Split 2** | | | **Split 3** | | | **Split4** | | |
| Train | InvTrain | Calib | Train | InvTrain | Calib | Train | InvTrain | Calib | Train | InvTrain | Calib |
| n | 60 | 57 | 39 | 60 | 59 | 46 | 61 | 60 | 41 | 63 | 61 | 35 |
| R2 | 0.7333 | 0.7166 | 0.6796 | 0.6167 | 0.5481 | 0.6762 | 0.7215 | 0.6446 | 0.7186 | 0.6336 | 0.5461 | 0.7559 |
| 1 | 0.0075 | 0.0130 | 0.0390 | 0.0065 | 0.0111 | 0.0407 | 0.0028 | 0.0027 | 0.0400 | 0.0299 | 0.0002 | 0.0036 |
| 2 | 0.0003 | 0.0003 | 0.0002 | 0.0115 | 0.1929 | 0.0000 | 0.0294 | 0.0102 | 0.0108 | 0.0004 | 0.0039 | 0.1079 |
| 3 | 0.0002 | 0.0093 | 0.0015 | 0.0186 | 0.0049 | 0.0580 | 0.0736 | 0.0026 | 0.0059 | 0.0054 | 0.0040 | 0.0174 |
| 4 | 0.0020 | 0.0001 | 0.0806 | 0.0080 | 0.0059 | 0.0004 | 0.0523 | 0.0112 | 0.0888 | 0.0069 | 0.0002 | 0.0211 |
| 5 | 0.0837 | 0.0031 | 0.1604 | 0.0280 | 0.1073 | 0.0318 | 0.0183 | 0.0012 | 0.0017 | 0.0360 | 0.0002 | 0.0114 |
| 6 | 0.0051 | 0.0173 | 0.0957 | 0.0078 | 0.0608 | 0.0012 | 0.0241 | 0.0008 | 0.0033 | 0.0122 | 0.0408 | 0.0466 |
| 7 | 0.0157 | 0.0008 | 0.0050 | 0.0043 | 0.0008 | 0.0754 | 0.0097 | 0.0000 | 0.0009 | 0.0050 | 0.0003 | 0.0049 |
| 8 | 0.0511 | 0.0125 | 0.0000 | 0.1128 | 0.0201 | 0.0229 | 0.0398 | 0.0022 | 0.0122 | 0.0240 | 0.0006 | 0.0247 |
| 9 | 0.0010 | 0.0466 | 0.1273 | 0.0020 | 0.0044 | 0.0434 | 0.0000 | 0.0020 | 0.0037 | 0.0020 | 0.0655 | 0.0008 |
| 10 | 0.0000 | 0.0270 | 0.0195 | 0.0025 | 0.0336 | 0.0480 | 0.0256 | 0.0021 | 0.0014 | 0.0101 | 0.0138 | 0.0012 |
| Rr2\* | 0.0166 | 0.0130 | 0.0529 | 0.0202 | 0.0442 | 0.0322 | 0.0276 | 0.0035 | 0.0169 | 0.0132 | 0.0130 | 0.0240 |
| CR2p# | 0.7249 | 0.7100 | 0.6526 | 0.6065 | 0.5256 | 0.6599 | 0.7076 | 0.6428 | 0.7101 | 0.6270 | 0.5396 | 0.7438 |

\* Average randomized R2; # CR2p = R × (R2 − R2r)1/2 where CR2p should be greater than 0.5

**Table S8.** Y-randomization results for four splits For Smiles With IIC using equation 4

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Split 1** | | | **Split 2** | | | **Split 3** | | | **Split4** | | |
| Train | InvTrain | Calib | Train | InvTrain | Calib | Train | InvTrain | Calib | Train | InvTrain | Calib |
| n | 60 | 57 | 39 | 60 | 59 | 46 | 61 | 60 | 41 | 63 | 61 | 35 |
| R2 | 0.6796 | 0.6734 | 0.7021 | 0.6378 | 0.5742 | 0.7183 | 0.5851 | 0.5691 | 0.7586 | 0.6931 | 0.6345 | 0.7249 |
| 1 | 0.0635 | 0.0018 | 0.0199 | 0.0041 | 0.0527 | 0.0145 | 0.0151 | 0.0573 | 0.0197 | 0.0033 | 0.0515 | 0.0050 |
| 2 | 0.0017 | 0.0021 | 0.0115 | 0.0256 | 0.0386 | 0.0312 | 0.0060 | 0.0452 | 0.0914 | 0.0345 | 0.0247 | 0.0682 |
| 3 | 0.0004 | 0.0053 | 0.0290 | 0.0454 | 0.0115 | 0.0305 | 0.0001 | 0.0000 | 0.0084 | 0.0073 | 0.0126 | 0.0038 |
| 4 | 0.0216 | 0.0280 | 0.0261 | 0.0329 | 0.0033 | 0.0130 | 0.0150 | 0.0100 | 0.0183 | 0.0005 | 0.0304 | 0.0246 |
| 5 | 0.0011 | 0.0081 | 0.0585 | 0.0255 | 0.0461 | 0.0022 | 0.0110 | 0.0022 | 0.0758 | 0.0118 | 0.0002 | 0.0025 |
| 6 | 0.0011 | 0.0227 | 0.0522 | 0.0064 | 0.0017 | 0.0024 | 0.0618 | 0.0077 | 0.0061 | 0.0337 | 0.0267 | 0.0520 |
| 7 | 0.0034 | 0.0228 | 0.0009 | 0.0482 | 0.0328 | 0.0002 | 0.0041 | 0.0230 | 0.0050 | 0.0043 | 0.0027 | 0.0508 |
| 8 | 0.0029 | 0.0094 | 0.0033 | 0.0067 | 0.0039 | 0.0001 | 0.0000 | 0.0026 | 0.0024 | 0.0176 | 0.0020 | 0.0282 |
| 9 | 0.0345 | 0.0113 | 0.0012 | 0.0429 | 0.0967 | 0.0000 | 0.0031 | 0.0005 | 0.0005 | 0.0872 | 0.0268 | 0.0003 |
| 10 | 0.0031 | 0.0009 | 0.0227 | 0.0000 | 0.0467 | 0.0156 | 0.0121 | 0.0000 | 0.0315 | 0.0172 | 0.0054 | 0.0129 |
| Rr2\* | 0.0133 | 0.0112 | 0.0225 | 0.0238 | 0.0334 | 0.0110 | 0.0128 | 0.0149 | 0.0259 | 0.0217 | 0.0183 | 0.0248 |
| CR2p# | 0.6729 | 0.6678 | 0.6907 | 0.6258 | 0.5572 | 0.7128 | 0.5786 | 0.5616 | 0.7456 | 0.6821 | 0.6253 | 0.7124 |

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**Figure S1:** The homology model of the proteinDGAT1

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**Figure S2: Interaction of Designed molecules (DM01-DM13) with DGAT1**