**Identification of Highly Active Natural Thyroid Hormone Receptor Agonists by Pharmacophore-Based Virtual Screening**

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Table S1. The molecular docking results for screened compounds.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| UNPD\_ID | Chemical\_Name | Molecular\_Weight | Chemical\_Structure | binding energy  (kcal/mol) |
| 196655 | bisdehydrostemoninine B | 387.469 |  | -10.7 |
| 184785 | bisdehydrostemoninine A | 401.453 |  | -10.5 |
| 153863 | oxyphysodic acid | 500.538 |  | -10.4 |
| 188533 | ligulatrovine A | 460.518 |  | -10.4 |
| OEF |  |  |  | -10.4 |
| IH5 |  |  |  | -10.3 |
| T3 |  |  |  | -10.3 |
| 109028 | N/A | 809.98 |  | -9.9 |
| 105247 | tragopogonoside G | 1089.22 |  | -9.7 |
| 180643 | hederagenin 3-O-alpha-L-arabinofuranosyl-(1->3)-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranoside | 883.07 |  | -9.7 |
| 136867 | 3-O-[O-(beta-D-xylopyranosyl)-(1->2)-(beta-glucuronopyranosyl)]-3beta,22beta,24-trihydroxyolean-12-ene | 766.955 |  | -9.7 |
| 105249 | Cincholic acid 3beta-O-beta-6-deoxy-D-glucopyranoside-28-O-beta-D-glucopyranoside | 794.965 |  | -9.7 |
| 137310 | 3-O-2)>6)>-2-acetamido-2-deoxy-beta-D-glucopyranosyl echinocystic acid|3-O-[beta-D-xylopyranosyl (1->2)][beta-D-fucopyranosyl (1->6)]-2-acetamido-2-deoxy-beta-D-glucopyranosyl echinocysticacid | 954.148 |  | -9.7 |
| 100887 | Pseudoginsenoside RI2 | 1659.98 |  | -9.7 |
| 201011 | ivorenoside B | 1329.65 | CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C6C5(COC(O6)C(C)(C)CCC7(CCC8(C(=CCC9C8(CCC3C9(CC(C(C3(C)C(=O)O)O)O)C)C)C7)C)C(=O)OC3C(C(C(C(O3)CO)O)O)O)C)O)C)C)C2C1O)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)C | -9.7 |
| 139608 | oleanolic acid 3-O-(4-O-acetyl-beta-D-xylopyranosyl)-(1->3)-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranoside | 909.107 |  | -9.6 |
| 195668 | N/A | 795.01 |  | -9.6 |
| 109819 | saponin CP7 | 1029.21 |  | -9.5 |
| 158238 | 3-O-alpha-L-arabinopyranosyl(1-3)-alpha-L-rhamnopyranosyl(1-2)-alpha-L-arabinopyranosyl hederagenin | 883.07 |  | -9.5 |
| 119560 | Pseudo-ginsenoside-RI3 | 1089.22 |  | -9.5 |
| 174964 | 3-O-beta-D-xylopyranosyl-(1->3)-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranosyl-22alpha-hydroxyhederagenin | 899.07 |  | -9.4 |
| 173536 | hishoushi-saponin A | 867.071 |  | -9.4 |
| 187849 | (3beta)-28-hydroxy-28-oxoolean-12-en-3-yl-beta-D-xylopyranosyl-(1->3)-beta-D-galactopyranosyl-(1->3)-beta-D-glucopyranosiduronic acid | 927.08 |  | -9.4 |
| 175596 | momordin I | 763.931 |  | -9.4 |
| 18137 | azukisaponin I | 780.982 |  | -9.4 |
| 150683 | 3-O-[beta-D-xylopyranosyl-(1->2)-beta-D-galactopyranosyl-(1->2)-beta-D-glucuronopyranosyl]sophoradiol | 913.096 |  | -9.4 |
| 103902 | prosapogenin 1 | 929.096 |  | -9.2 |
| 140614 | scheffarboside B | 999.185 |  | -9.2 |
| 118386 | celosin C | 778.966 |  | -9.2 |
| 127988 | medicagenin 3-O-beta-D-glucopyranoside | 664.823 |  | -9.2 |
| 194922 | 3-O-alpha-L-rhamnopyranosyl-(1-2)-O-alpha-L-arabinopyranoside of echinocystic acid | 750.956 |  | -9.2 |
| 120381 | kalopanax-saponin A | 750.956 |  | -9.1 |
| 107217 | 3'alpha-[olean-12-ene-28-oyl-3beta-oxy]dihydronepetalactone | 622.917 |  | -9.1 |
| 1639 | triploside A | 1409.56 | CC1C(C(C(C(O1)OC2COC(C(C2OC3C(C(C(CO3)O)O)O)OC4C(C(C(C(O4)C)OC5C(C(C(CO5)O)O)O)OC6C(C(C(CO6)O)O)O)OC7C(C(C(CO7)O)O)O)OC8CCC9(C(C8(C)C)CCC1(C9CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C)O)O)O | -9.0 |
| 107455 | huzhangoside A | 867.071 |  | -9.0 |
| 100681 | N/A | 608.805 |  | -9.1 |
| 123323 | (3-O-trans-caffeoyl)oleanolic acid|3-O-(E)-caffeoyloleanolic acid | 618.842 |  | -9.1 |
| 200708 | blighoside A | 1087.25 |  | -9.1 |
| 111201 | 23-cis-p-coumaroyloxy-2alpha,3alpha-dihydroxyolean-12-en-28-oic acid | 634.842 |  | -9.1 |
| 102737 | 3-O-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranosyl gypsogenin | 748.94 |  | -9.1 |
| 129687 | stephanoic acid | 638.754 |  | -9.1 |
| 109815 | momordin I | 764.939 |  | -9.1 |
| 172044 | saponarioside D | 1267.36 |  | -9.1 |
| 153630 | oleanolic acid 3-O- 2)-O-beta-D-glucopyranosyl-(1 -> 3)-alpha-L-arabinopyranoside | 897.097 |  | -9.1 |
| 152222 | N/A | 941.106 |  | -9.1 |
| 112517 | <(alpha-L-arabinofuranosyl-(1 -> 4)-beta-D-galactopyranosyl-(1 -> 2))-beta-D-glucuronopyranosyl-(1 -> 3)>-3beta-hydroxyolean-12-en-28-oic acid | 927.08 |  | -9.1 |
| 127756 | impatienoside F | 1239.35 |  | -9.1 |
| 193563 | 23-hydroxy-3beta-[(O-alpha-L-rhamnopyranosyl-(1->2)-O-[O-beta-D-glucopyranosyl-(1->4)]-alpha-L-arabinopyranosyl)oxy]lup-20(29)-en-28-oic acid | 913.096 |  | -9.0 |
| 158649 | oleanolate 3beta-O-beta-D-glucopyranosyl-(1-> 4)-beta-d-xylopyranosyl-(1-> 3)-alpha-L-rhamnopyranosyl-(1 -> 2)-alpha-L-arabinopyranoside | 1029.21 |  | -9.0 |
| 111745 | 3beta-hydroxyolean-12-en-28-oic acid 3-O-{[alpha-L-rhamnopyranosyl(1->2)][beta-D-xylopyranosyl(1->2)-beta-D-glucopyranosyl(1->6)-beta-D-glucopyranosyl(1->3)]-beta-D-glucopyranoside} | 1221.38 |  | -9.0 |
| 174284 | foetidissimoside D | 1191.31 |  | -9.0 |
| 120456 | abrisaponin D1 | 943.122 |  | -9.0 |
| 160638 | caryocaroside V-1 | 810.964 |  | -9.0 |
| 174811 | deutzicoside B | 913.096 |  | -8.9 |
| 157154 | Esculentoic acid B | 454.684 |  | -8.9 |
| 1418 | N/A | 1235.36 |  | -8.9 |
| 164995 | caryocaroside IV-11 | 973.105 |  | -8.9 |
| 150567 | sapinmusaponin L | 925.107 |  | -8.9 |
| 184009 | lobatoside K | 1381.5 |  | -8.9 |
| 127446 | 3-O-(beta-glucuronopyranosyl)-3beta,22beta,24-trihydroxyolean-12-ene | 634.84 |  | -8.9 |
| 123874 | stipuleanoside R1 | 927.08 |  | -8.9 |
| 145944 | 3-O-[alpha-L-rhamnopyranosyl-(1->2)-beta-D-galactopyranosyl-(1->3)-beta-glucuronopyranosyl]oleanolic acid | 941.106 |  | -8.9 |
| 175962 | kalopanaxsaponin I | 883.07 |  | -8.8 |
| 129827 | hederagenin-3-O-beta-D-xylopyranosyl-(1-3)-alpha-L-rhamnopyranosyl-(1-2)-alpha-L-arabinopyranoside | 883.07 |  | -8.8 |
| 159007 | scheffarboside A | 911.08 |  | -8.7 |
| 105464 | 3-O-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranosyl-22alpha-hydroxyhederagenin | 766.955 |  | -8.7 |
| 104743 | saponin CP4 | 867.071 |  | -8.7 |
| 141360 | alpha-hederin | 750.956 |  | -8.7 |
| 153098 | 3-O-[alpha-L-rhamnopyranosyl-(1->4)-beta-D-glucuronopyranosyl]echinocystic acid | 794.965 |  | -8.7 |
| 141538 | O1-(17-carboxy-28-nor-olean-12-en-3beta-yl)-O4-(O4-alpha-L-rhamnopyranosyl-beta-D-glucopyranosyl)-beta-D-glucopyranuronic acid | 941.106 |  | -8.7 |
| 200707 | blighoside B | 1071.25 |  | -8.7 |
| 166611 | dianoside G | 973.105 |  | -8.7 |
| 155801 | repensoside A | 943.079 |  | -8.7 |
| 147368 | 3beta-(6-deoxy-beta-D-glucopyranosyloxy)-olean-12-ene-27,28-dioic acid | 632.824 |  | -8.7 |
| 149570 | 3-O-trans-p-coumaroyltormentic acid | 636.858 |  | -8.7 |
| 149113 | Z-senegin II | 1457.56 |  | -8.7 |
| 191187 | 23-trans-p-coumaroyloxy-2alpha,3beta-dihydroxyolean-12-en-28-oic acid | 634.842 |  | -8.7 |
| 197727 | N/A | 976.208 |  | -8.7 |
| 137497 | Thielocin A1alpha | 997.043 |  | -8.7 |
| 140717 | Thielocin B3 | 1131.18 |  | -8.7 |
| 145696 | N/A | 1029.21 |  | -8.7 |
| 116108 | N/A | 927.123 |  | -8.7 |
| 196920 | Mubenin B | 734.956 |  | -8.7 |
| 176326 | Mukurozisaponin E1 | 925.107 |  | -8.7 |
| 146115 | 3-O-[alpha-L-Rhamnopyranosyl(1->3)-beta-D-glucuronopyranosyl]-oleanolic acid | 778.966 |  | -8.7 |
| 186862 | N/A | 734.956 |  | -8.7 |
| 138806 | N/A | 672.888 |  | -8.7 |
| 180434 | oleanolic acid-3-O-neohesperidoside | 764.982 |  | -8.7 |
| 133249 | saponin A | 764.982 |  | -8.7 |
| 157534 | 3beta-O-trans-caffeoylmorolic acid | 586.844 |  | -8.7 |
| 174161 | (2alpha,3beta)-23-sulphonyl-2,3-dihydroxyurs-12-en-28-oic acid O-alpha-L-rhamnopyranosyl-(1->4)-O-beta-D-glucopyranosyl-(1->6)-O-beta-D-glucopyranosyl ester | 1039.18 |  | -8.7 |
| 144732 | (3beta,4alpha)-3-hydroxyolean-12-en-23,28-dioic acid 28-{[O-beta-D-glucopyranosyl-(1->2)-O-beta-D-glucopyranosyl]-(1->6)-beta-D-glucopyranosyl}-(1->3)-beta-D-galactopyranosyl ester | 1135.25 |  | -8.7 |
| 179503 | N/A | 666.796 |  | -8.7 |
| 11798 | momordin Ic 6'-methyl ester | 778.966 |  | -8.7 |
| 131765 | N/A | 634.842 |  | -8.7 |
| 111185 | AzII | 1099.22 |  | -8.7 |
| 183682 | Pastuchosid B | 943.122 |  | -8.7 |
| 121189 | abrisaponin A | 943.122 |  | -8.7 |
| 17013 | 3-O-[alpha-L-rhamnopyranosyl-(1->2)-beta-D-galactopyranosyl-(1->2)-beta-D-glucuronopyranosyl]-3beta,16beta,22alpha-trihydroxy-olean-12-ene | 943.122 |  | -8.7 |
| 138425 | (3-O-trans-caffeoyl)morolic acid | 618.842 |  | -8.7 |
| 175185 | Tragopogonsaponin A Methyl Ester | 662.85 |  | -8.7 |
| 137349 | beta-D-fucopyranosyl-(1->4)-(beta-D-glucopyranosyluronic acid)-(1->3)-oleanolic acid | 778.966 |  | -8.7 |
| 193382 | alternoside XI | 895.081 |  | -8.7 |
| 166845 | repensoside B | 1075.19 |  | -8.7 |
| 116573 | 3-O-{beta-D-apiofuranosyl-(1->4)-[alpha-L-arabinopyranosyl-(1->2)]-beta-D-glucuronopyranosyl}oleanolic acid | 897.054 |  | -8.7 |
| 135700 | assamsaponin D | 1233.35 |  | -8.7 |
| 16644 | hederagenin 3-O-beta-D-glucuronopyranoside 28-O-alpha-L-rhamnopyranosyl-(1->4)-O-beta-D-glucopyranosyl-(1->6)-beta-D-glucopyranosyl ester | 1119.25 |  | -8.7 |
| 185145 | N/A | 897.097 |  | -8.7 |
| 124846 | Pulchinenoside A | 750.956 |  | -8.7 |
| 191249 | 2'-O-methylnorobtusatic acid | 346.331 |  | -8.7 |
| 148086 | pesudoginsenoside RP1 methyl ester | 778.966 |  | -8.6 |
| 188368 | 3-O-[alpha-L-rhamnopyranosyl(1->4)-beta-D-xylopyranosyl]-hederagenin | 750.956 |  | -8.6 |
| 140574 | 3beta-[(O-beta-D-glucuronopyranosyl-(1->3)-O-[alpha-L-rhamnopyranosyl-(1->2)]-alpha-L-arabinopyranosyl)oxy]olean-12-en-28-oic acid | 911.08 |  | -8.6 |
| 12202 | Thermorubin A | 600.526 |  | -8.6 |
| 192428 | 3-O-beta-D-glucopyranosyl(1-3)-alpha-L-rhamnopyranosyl(1-2)-alpha-L-arabinopyranosyl hederagenin | 913.096 |  | -8.6 |
| 157599 | 3-O-[beta-glucopyranosyl-(1->3)-beta-glucopyranosyl]-28-O-[alpha-rhamnopyranosyl-(1->2)-alpha-arabinopyranoside] medicagenic acid | 1105.22 |  | -8.6 |
| 181221 | 3-O-(Z)-coumaroyl oleanolic acid|cis-3-O-p-hydroxycinnamoylursolic acid | 602.843 |  | -8.6 |
| 158977 | acanjaposide F | 973.105 |  | -8.6 |
| 200304 | 3-O-[alpha-L-arabinopyranosyl(1->2)-alpha-L-arabinopyranosyl(1->6)]-[beta-D-glucopyranosyl(1->2)]-beta-D-glucopyranoside echinocystic acid | 1059.24 |  | -8.6 |
| 109266 | licorice-saponin E2 | 820.916 |  | -8.6 |
| 128196 | hederagenin 3-O-beta-D-glucopyranosyl-(1-4)-beta-D-xylopyranosyl-(1-3)-alpha-L-rhamnopyranosyl-(1-2)-alpha-L-arabinopyranoside | 1045.21 |  | -8.6 |
| 1489 | narcissiflorinine | 911.08 |  | -8.6 |
| 12200 | eclalbasaponin V | 714.904 |  | -8.6 |
| 173948 | 3beta-O-beta-D-glucopyranosyl-(1->3)-[beta-D-xylopyranosyl-(1->2)]-beta-D-glucuronopyranosyl-23-hydroxylup-20(29)-en-28-oic acid | 943.079 |  | -8.6 |
| 164481 | 3-O-alpha-L-rhamnopyranosyl-(1-2)-O-alpha-L-arabinopyranoside of ursolic acid | 750.956 |  | -8.6 |
| 132077 | 3-sulfate of 28-O-gentiobiosyl ester of oleanolic acid | 861.045 |  | -8.6 |
| 199883 | camellioside A | 1105.22 |  | -8.6 |
| 149059 | Kalopanaxsaponin A | 750.956 |  | -8.6 |
| 181985 | Licoricesaponin B2 | 808.949 |  | -8.6 |
| 199378 | N/A | 1205.34 |  | -8.6 |
| 145215 | alternoside VII | 812.98 |  | -8.6 |
| 148748 | momordin Id | 897.054 |  | -8.6 |
| 181726 | elatoside A | 927.08 |  | -8.6 |
| 130730 | momordin Ie | 897.054 |  | -8.5 |
| 119315 | giganteaside D | 734.956 |  | -8.5 |
| 170054 | hederagenin 3-O-beta-D-glucopyranosyl(1->3)-alpha-L-rhamnopyranosyl(1->2)-alpha-L-arabinopyranoside | 913.096 |  | -8.5 |
| 130898 | dictyodendrin A | 785.794 |  | -8.5 |
| 104712 | oleanolic acid 3-O-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranoside | 734.956 |  | -8.5 |
| 153606 | 3beta-[(O-beta-D-glucopyranosyl-(1->3)-O-[alpha-L-rhamnopyranosyl-(1->2)]-alpha-L-arabinopyranosyl)oxy]-23,29-dihydroxyolean-12-en-28-oic acid | 929.096 |  | -8.5 |
| 193433 | 3-O-{alpha-L-rhamnopyranosyl-(1->4)-[beta-D-galactopyranosyl-(1->2)]-beta-D-glucuronopyranosyl}oleanolic acid | 941.106 |  | -8.4 |
| 116193 | yunganoside G2 | 840.947 |  | -8.4 |
| 16117 | yunganoside K2 | 838.931 |  | -8.4 |
| 19258 | N/A | 634.885 |  | -8.4 |
| 176704 | N/A | 824.948 |  | -8.4 |
| 12251 | 3-O-cis-p-coumaroyltormentic acid | 634.842 |  | -8.4 |
| 178457 | 3-O-beta-D-glucuronopyranosyl-28-O-{beta-D-xylopyranosyl(1->4)-[alpha-L-arabinopyranoside(1->3)]-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranoside}zanhic acid | 1237.29 |  | -8.4 |
| 152032 | sulfapatrinoside II | 876.036 |  | -8.4 |
| 135102 | 3-O-(E)-feruloylursolic acid | 632.869 |  | -8.4 |
| 129187 | 3-O-(E)-p-coumaroyl tormentic acid | 634.842 |  | -8.4 |
| 180152 | yunganoside I1 | 955.09 |  | -8.4 |
| 136126 | albesoside-A | 1237.33 |  | -8.4 |
| 194587 | azukisaponin VI | 1135.25 |  | -8.4 |
| 117875 | silenorubicoside D | 1473.51 | CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C(=O)OC6C(C(C(C(O6)CO)O)O)OC7C(C(C(C(O7)C(=O)O)O)O)O)O)C)C)C2C1)C)C(=O)OC8C(C(C(C(O8)COC9C(C(C(C(O9)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)C | -8.4 |
| 140141 | abrisaponin Ca | 943.122 |  | -8.4 |
| 119513 | isocomplestatin | 1328.77 |  | -8.4 |
| 15707 | subproside IV | 1105.26 |  | -8.4 |
| 1308 | polyscioside B | 927.08 |  | -8.4 |
| 156793 | Hederagenin-3-O-β-glucuronopyranoside | 648.824 |  | -8.4 |
| 130776 | pulsatilla saponin A | 913.096 |  | -8.4 |
| 19450 | 3-beta-benzoyloxyoleana-11,13(18)-dien-28-oic acid | 558.79 |  | -8.4 |
| 126087 | N/A | 524.516 |  | -8.4 |
| 182504 | sapindoside C | 1045.21 |  | -8.4 |
| 195844 | 3-O-{alpha-L-Rhamnopyranosyl-(1->2)-O-[beta-D-galactopyranosyl-(1->3)]-beta-D-glucopyranosyl}oleanolic acid | 927.123 |  | -8.4 |
| 176744 | 23-trans-p-coumaroyloxy-2alpha,3alpha-dihydroxyolean-12-en-28-oic acid | 634.842 |  | -8.4 |
| 110456 | yunganoside E2 | 820.916 |  | -8.4 |
| 193221 | chionaeoside C | 780.938 |  | -8.4 |
| 122511 | Quinovic acid 3beta-O-beta-6-deoxy-D-glucopyranoside-28-O-beta-D-glucopyranoside | 794.965 |  | -8.4 |
| 116161 | 3-O-alpha-L-rhamnopyranosyl-(1->2)-beta-D-xylopyranosyl-(1->2)-beta-D-glucuronopyranosyl-22-O-beta-D-glucopyranosyl-21-epi-kudzusapogenol A | 1107.24 |  | -8.4 |
| 171265 | 2alpha,3beta-dihydroxyurs-12,20(30)-dien-28-oic acid 3-O-{O-beta-D-quinovopyranosyl-(1->2)-O-alpha-L-arabinopyranosyl-(1->2)-O-[beta-D-xylopyranosyl-(1->3)]beta-D-glucopyranoside} | 1043.19 |  | -8.4 |
| 19737 | 3-O-beta-D-glucopyranosyl-(1->2)-beta-D-glucuronopyranosyl-24-hydroxyoleanolic acid | 810.964 |  | -8.4 |
| 166587 | subproside V | 1137.26 |  | -8.4 |
| 166058 | subproside I | 959.122 |  | -8.4 |
| 179154 | Naucleosid; 3-(D-Xylose-L-rhamnose)-qunovaic acid | 764.939 |  | -8.4 |
| 148863 | N/A | 970.804 |  | -8.4 |
| 131721 | 3-O-beta-D-xylopyranosyl(1-3)-alpha-L-rhamnopyranosyl(1-2)-alpha-L-arabinopyranosyl hederagenin | 883.07 |  | -8.4 |
| 123141 | gypsogenic acid-28-O-beta-D-glucopyranosyl-(1->3)-[beta-D-glucopyranosyl-(1->2)-beta-D-galactopyranosyl-(1->6)]-beta-D-galactopyranoside | 1135.25 |  | -8.4 |
| 109284 | 3-O-alpha-L-rhamnopyranosyl(1-2)-alpha-L-arabinopyranosyl hederagenin | 750.956 |  | -8.4 |
| 164561 | saponarioside C | 1267.36 |  | -8.4 |
| 105930 | dianic acid 28-(6-O-(beta-D-galactopyranosy)-beta-D-glucopyranosyl) ester | 826.964 |  | -8.4 |
| 119581 | acacic acid 3-O-beta-D-xylopyranosyl-(1->2)-beta-D-fucopyranosyl-(1->6)-2-(acetylamino)-2-deoxy-beta-D-glucopyranoside | 970.147 |  | -8.4 |
| 193923 | N/A | 750.956 |  | -8.4 |
| 123118 | oleanolic acid 3-O-beta-D-glucuronopyranoside-6-O-butyl ester | 688.931 |  | -8.4 |
| 103503 | talinumoside I | 838.975 |  | -8.4 |
| 123065 | theasaponin E3 | 1189.29 |  | -8.4 |
| 152325 | saponin PG | 883.07 |  | -8.4 |
| 117463 | kaikasaponin I | 780.982 |  | -8.3 |
| 112005 | lupinoside PA4 | 1089.26 |  | -8.3 |
| 139252 | N/A | 973.105 |  | -8.3 |
| 142219 | sapinmusaponin K | 925.107 |  | -8.3 |
| 186766 | (2E)-2-(5-{(Z)-2-carboxy-2-[4-((E)-2-carboxyvinyl)-2-methoxyphenoxy]vinyl}-2-hydroxy-3-methoxyphenyl)-3-(4-hydroxy-3-methoxyphenyl)acrylic acid | 578.52 |  | -8.3 |
| 178940 | lancemaside D | 1089.22 |  | -8.3 |
| 174946 | fargoside D | 778.923 |  | -8.3 |
| 135219 | herniaria saponin C | 1321.41 |  | -8.3 |
| 162791 | gymnemic acid XVI | 847.04 |  | -8.3 |
| 131891 | [beta-D-galactopyranosyl-(1 -> 2)-beta-D-(6-O-methyl)-glucuronopyranosyl-(1 -> 3)]-3beta-hydroxyolean-12-en-28-oic acid | 808.992 |  | -8.2 |
| 194044 | phytolaccagenic acid 3-O-[alpha-L-arabinopyranosyl-(1''->3')-beta-D-glucuronopyranosyl]-28-O-beta-D-glucopyranoside | 987.089 |  | -8.2 |
| 165760 | Soyasaponin III | 796.981 |  | -8.2 |
| 192528 | 3-O-beta-D-galactopyranosyl-(1->3)2))-beta-D-glucopyranosylhederagenin | 943.122 |  | -8.2 |
| 16825 | N/A | 925.037 |  | -8.2 |
| 154445 | 23-hydroxy-3beta-[(O-beta-D-glucopyranosyl-(1->3)-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranosyl)oxy]lup-20(29)-enoic acid | 913.096 |  | -8.2 |
| 177094 | Glycyrrhizic acid | 822.932 |  | -8.2 |
| 162454 | 3alpha-O-trans-feruloyl-2alpha-hydroxy-12-ursen-28-oic acid | 648.868 |  | -8.2 |
| 146010 | N/A | 764.939 |  | -8.2 |
| 10928 | medinoside E | 1105.26 |  | -8.2 |
| 145832 | 3beta-trans-p-coumaroyloxy-2alpha,3beta,13beta-trihydroxy-urs-11-en-28-oic acid | 634.842 |  | -8.2 |
| 132093 | N/A | 824.948 |  | -8.2 |
| 191813 | fatsin | 618.841 |  | -8.2 |
| 118607 | oleanoic acid 3-O-28-O-beta-D-glucopyranoside | 927.08 |  | -8.2 |
| 143365 | 3-O-beta-D-glucopyranosyl 2-oxo-olean-12-en-23,28-dioic acid 28-O-{beta-D-xylopyranosyl(1->4)-beta-D-apiofuranosyl(1->3)-alpha-L-rhamnopyranosyl(1->2)-beta-D-glucopyranosyl} ester | 1235.32 |  | -8.2 |
| 118231 | copteroside D | 943.079 |  | -8.2 |
| 109687 | zygoeichwaloside H | 847.018 |  | -8.2 |
| 13664 | cynarasaponin H | 927.08 |  | -8.2 |
| 141551 | 3beta-cis-p-coumaroyloxy-2alpha,3beta,13beta-trihydroxy-urs-11-en-28-oic acid | 634.842 |  | -8.2 |
| 107995 | alternoside VIII | 812.98 |  | -8.2 |
| 191384 | herniaria saponin E | 1147.26 |  | -8.2 |
| 120910 | oleanolic acid 3-O-[alpha-L-arabinoranosyl-(1''->3')-beta-D-glucuronopyranosyl]-28-O-beta-D-glucopyranoside | 943.079 |  | -8.2 |
| 197766 | N/A | 1107.24 |  | -8.2 |
| 142429 | N/A | 1009.16 |  | -8.2 |
| 185624 | kaikasaponin III | 927.123 |  | -8.2 |
| 152663 | thielocin A1alpha | 997.043 |  | -8.2 |
| 149768 | Thielocin A1beta | 997.043 |  | -8.2 |
| 139513 | Digitoside B | 734.956 |  | -8.2 |
| 169477 | rarasaponin V | 925.107 |  | -8.2 |
| 166101 | momordin Ia | 778.966 |  | -8.2 |
| 139005 | eucalyptic acid | 648.868 |  | -8.2 |
| 188223 | 23-O-acetyl-hederagenin 3-O-(4-O-acetyl-beta-D-xylopyranosyl)-(1->3)-alpha-L-rhamnopyranosyl-(1->2)-alpha-L-arabinopyranoside | 967.143 |  | -8.2 |
| 162607 | hederoside C | 750.956 |  | -8.2 |
| 127869 | raddeanoside R23 | 1029.21 |  | -8.2 |
| 184370 | G2 | 1645.69 |  | -8.1 |
| 173904 | Scaberoside B4 | 911.08 |  | -8.1 |
| 139193 | N/A | 867.071 |  | -8.1 |
| 123401 | (3Z)-Coumaroylhederagenin | 618.842 |  | -8.1 |
| 153193 | N/A | 546.778 |  | -8.1 |
| 118015 | betavulgaroside IV | 794.922 |  | -8.1 |
| 129438 | N/A | 634.84 |  | -8.1 |
| 100938 | 28-deglucosyl-chikusetsusaponin IV | 764.939 |  | -8.1 |
| 193591 | myrioside C | 810.964 |  | -8.1 |
| 177090 | azukisaponin IV | 973.105 |  | -8.1 |
| 151404 | 3-O-{O-beta-D-glucopyranosyl-(1->2)-O-[alpha-L-rhamnopyranosyl-(1->3)]-(beta-D-glucopyranosyluronic acid)}oleanolic acid | 941.106 |  | -8.1 |
| 109321 | dianoside A | 810.964 |  | -8.1 |
| 149374 | oleanolic acid-(3)-beta-D-galactopyranosyl-(1->2)-beta-D-fucopyranoside | 764.982 |  | -8.1 |
| 112476 | 3-O-beta-D-glucopyranosylpresenegenin 28-O-beta-D-galactopyranosyl-(1->4)-[alpha-L-arabinopyranosyl-(1->3)]-beta-D-xylopyranosyl-(1->4)-[beta-D-apiofuranosyl-(1->3)]-alpha-L-rhamnopyranosyl-(1->2)-beta-D-fucopyranosyl ester | 1531.59 |  | -8.1 |
| 144030 | N/A | 792.949 |  | -8.1 |
| 18652 | complestatin | 1328.77 |  | -8.1 |
| 112842 | lablaboside F | 1395.53 | CC1C(C(C(C(O1)OC2C(OC(C(C2O)O)OC3C(C(C(OC3OC(=O)C45CCC(CC4C6=CCC7C8(CCC(C(C8CCC7(C6(CC5)C)C)(C)C)OC9C(C(C(C(O9)C(=O)O)O)O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)C)O)O)O)C)(C)C)CO)O)O)C)O)O)O | -8.1 |
| 157967 | quillaic acid 3-O-[beta-D-galactopyranosyl-(1->2)-beta-D-glucopyranosiduronic acid] | 824.948 |  | -8.1 |
| 147912 | Quinovic acid-3-O-beta-D-fucopyranosyl-(28->1)-beta-D-glucopyranosyl ester | 792.949 |  | -8.1 |
| 139026 | assamicin IV | 1235.36 |  | -8.1 |
| 161207 | theasaponin E2 | 1231.33 |  | -8.1 |
| 183004 | wistariasaponin A3 | 973.105 |  | -8.1 |
| 101784 | gymnemic acid VI | 927.08 |  | -8.1 |
| 187598 | soyasaponin III | 796.981 |  | -8.1 |
| 197729 | N/A | 976.208 |  | -8.1 |
| 175624 | 3-O-beta-D-xylopyranosyl-(1->3)2))-alpha-L-arabinopyranosylhederagenin | 883.07 |  | -8.1 |
| 193070 | 3beta,16alpha,23,28-tetrahydroxyoleana-11,13(18)-dien-30-oic acid 3-O-beta-D-glucopyranosyl-(1->2)-beta-D-glucopyranosyl-(1->3)-beta-D-fucopyranoside | 973.105 |  | -8.1 |
| 19501 | 3-O-alpha-L-rhamnopyranosyl-(1-2)-O-alpha-L-arabinopyranoside of oleanolic acid | 750.956 |  | -8.1 |
| 155236 | quillaic acid 3-O-{alpha-L-rhamnopyranosyl-(1->3)-[beta-D-galactopyranosyl-(1->2)]-beta-D-glucopyranosiduronic acid} | 971.089 |  | -8.1 |
| 132896 | rarasaponin IV | 1009.18 |  | -8.1 |
| 145173 | ligatoside A | 991.122 |  | -8.1 |
| 146483 | aceriphyllic acid K | 500.71 |  | -8.1 |
| 173177 | aceriphyllic acid C | 486.683 |  | -8.1 |
| 145097 | 3-O-sulfooleanolic acid 28-beta-glucopyranosyl ester | 698.904 |  | -8.1 |
| 174897 | vaccaroid A | 1135.25 |  | -8.1 |
| 173878 | thladioside H1 | 1351.43 |  | -8.1 |
| 166317 | N/A | 1544.95 |  | -8.1 |
| 115990 | N/A | 957.106 |  | -8.1 |
| 184154 | Gymnemic aicd XIII | 766.955 |  | -8.1 |
| 189918 | ageratoside A1 | 1265.34 |  | -8.1 |
| 106288 | 3-O-beta-D-glucuronopyranosyl-28-O-{beta-D-xylopyranosyl(1->4)-[beta-D-apiofuranosyl(1->3)]-alpha-L-rhamnopyranosyl(1->2)-alpha-L-arabinopyranoside}medicagenic acid | 1221.29 |  | -8.1 |
| 196396 | lancemaside-A | 1205.34 |  | -8.1 |
| 146670 | narcissiflorine methyl ester | 778.966 |  | -8.1 |
| 134908 | aceriphyllic acid D | 486.683 |  | -8.1 |
| 157560 | quillaic acid 3-O-glucuronide | 662.807 |  | -8.1 |
| 18863 | kudzusaponin SA1 | 812.98 |  | -8.1 |
| 187251 | N/A | 927.08 |  | -8.1 |
| 138643 | 3-O-[beta-D-Glucopyranosyl-(1?2)[alpha-L-rhamnopyranosyl-(1?3)]-beta-D-glucuronopyranoside],beta-D-glucopyranosyl ester -3beta-3-Hysroxy-12-oleanen-28-oic acid | 1103.25 |  | -8.1 |
| 180160 | 3alpha-hydroxylup-20(29)-ene-23,28-dioic acid 28-O-[beta-D-glucopyranosyl-(1->6)-beta-D-glucopyranosyl] ester | 810.964 |  | -8 |
| 16286 | quinovic acid 3-O-beta-D-rhamnopyranoside | 632.824 |  | -8 |
| 181330 | Polymastiamide B | 671.884 |  | -8 |
| 16235 | Gypsogenin | 486.683 |  | -8 |
| 129876 | Quinovic acid 3-O- β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranoside 27-O- β-D-glucopyranosyl ester | 957.106 |  | -8 |
| 152049 | 2beta,3beta,16alpha,28-tetrahydroxy olean-12-ene-23-oic acid | 504.699 |  | -8 |
| 170631 | Quinovic acid 3-O-β-D-quinovopyranoside 27-O- β-D-glucopyranosyl ester | 794.965 |  | -8 |
| 186856 | 3-O-beta-D-galactopyranosyl-(1->2)-[beta-D-xylopyranosyl-(1->3)]-beta-D-glucuronopyranosyl quilliac acid 28-O-(6-O-acetyl)-beta-D-glucopyranosyl-(1->3)-[beta-D-xylopyranosyl-(1->4)]-alpha-L-rhamnopyranosyl-(1->2)-beta-D-fucopyranoside | 1585.64 |  | -8 |
| 185714 | acanjaposide G | 957.106 |  | -8 |
| 155970 | N/A | 794.965 |  | -8 |
| 113892 | dianoside H | 648.824 |  | -8 |
| 18122 | N/A | 634.84 |  | -8 |
| 193641 | spinasaponin A methyl ester | 808.992 |  | -8 |
| 163771 | 3-O-[O-beta-D-galactopyranosyl-(1->2)-[O-beta-D-xylopyranosyl-(1->3)]-beta-D-glucopyranuronosyl]gypsogenin methyl ester | 955.09 |  | -8 |
| 128862 | Neobiliverdin IX delta | 582.646 |  | -8 |
| 159149 | clinopodic acid F | 552.483 |  | -8 |
| 197327 | N/A | 1006.18 |  | -8 |
| 155812 | spinacoside D | 764.896 |  | -8 |
| 17822 | bidentatoside II | 750.912 |  | -8 |
| 15551 | 3beta,23-dihydroxy-lup-20(29)-en-28-oic acid 3beta-caffeate | 634.842 |  | -8 |
| 117212 | sanguidioside C | 1343.63 | CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)C(=O)O)OC(=O)C6(C7CCC8(C(C7(CC(C6O)O)C)CC=C9C8(CCC3(C9C(C(CC3)(C)C)O)C(=O)OC3C(C(C(C(O3)CO)O)O)O)C)C)C)O)C)C)C2C1(C)O)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O | -8 |
| 169354 | Gymnemic aicd XIV | 764.939 |  | -8 |
| 115602 | saponarioside J | 1103.2 |  | -8 |
| 171537 | 3beta-hydroxyolean-12-en-23,28-dioic acid 28-O-beta-D-galactopyranoside | 1135.25 |  | -8 |
| 135766 | 3beta-[O-alpha-D-glucopyranosyl-(1->4)-beta-D-glucopyranosyl]-2beta-hydroxy-Delta12-oleanene-23,28-dioic acid | 826.964 |  | -8 |
| 105720 | acankoreoside E | 973.105 |  | -8 |
| 168062 | dianchinenoside D | 826.964 |  | -8 |
| 119945 | 3-O-[beta-D-glucopyranosyl-(1-2)-(beta-D-xylopyranosyl-(1-3))-beta-D-glucuronopyranosyl]-3beta-hydroxyolean-12-en-28-oic acid | 927.08 |  | -8 |
| 135259 | quinoa-saponin-9 | 810.964 |  | -8 |
| 120416 | 3-O-[beta-glucopyranosyl-(1->3)-beta-glucopyranosyl]-28-O-{beta-xylopyranosyl-(1->4)-[alpha-arabinopyranosyl-(1->3)]-alpha-rhamnopyranosyl-(1->2)-alpha-arabinopyranoside} zanhic acid | 1385.45 |  | -8 |
| 146283 | quinovic acid 3beta-O-beta-D-glucopyranosyl-(1->4)-beta-L-rhamnopyranoside | 794.965 |  | -7.9 |
| 112029 | goyasaponin III | 969.116 |  | -7.9 |
| 108028 | N/A | 780.982 |  | -7.9 |
| 157270 | lycoside P | 1381.46 |  | -7.9 |
| 197728 | N/A | 1020.22 |  | -7.9 |
| 101599 | N/A | 838.888 |  | -7.9 |
| 200185 | 12-O-[3'-(5'-methoxy-12'-hydroxy)-bibenzyl]-5-hydroxy-3-methoxybibenzyl-6-carboxylic acid | 514.566 |  | -7.9 |
| 130699 | N/A | 753.145 |  | -7.9 |
| 106327 | onjisaponin R | 1619.7 |  | -7.9 |
| 191042 | 3beta,23-dihydroxyolean-13(18)-en-28-oic acid 28-O-beta-D-glucopyranoside 3,23-disulfate ester | 794.967 |  | -7.9 |
| 182526 | 3beta-hydroxyurs-12-en-28-oic acid 3-O-beta-D-glucuranopyranoside 6'-O-methyl ester | 646.851 |  | -7.9 |
| 184124 | atomaric acid | 442.631 |  | -7.9 |
| 173110 | 3-O-[beta-glucopyranosyl-(1->3)-beta-glucopyranosyl]-28-O-[alpha-rhamnopyranosyl-(1->2)-alpha-arabinopyranoside] zanhic acid | 1121.22 |  | -7.9 |
| 185064 | polygalasaponin XXII | 1237.33 |  | -7.9 |
| 133921 | Porphyrin S 411 | 652.693 |  | -7.9 |
| 144488 | 3-O-[alpha-L-arabinopyranosyl(1->2)-beta-D-glucuronopyranosyl] oleanolic acid | 764.939 |  | -7.9 |
| 183200 | oleanolic acid sulfate | 536.763 |  | -7.9 |
| 179741 | kudzusaponin A1 | 1077.21 |  | -7.9 |
| 151037 | N/A | 634.842 |  | -7.9 |
| 152504 | acankoreoside A | 957.106 |  | -7.9 |
| 147883 | Licorice-saponin K2 | 822.932 |  | -7.9 |
| 17576 | acanjaposide A | 941.063 |  | -7.9 |
| 116268 | polygalasaponin H | 1075.19 |  | -7.9 |
| 119443 | Schizotenuin A | 712.652 |  | -7.9 |
| 111506 | saponarioside F | 1283.36 |  | -7.9 |
| 141855 | 3-epi-betulinic acid 3-O-sulfate | 536.763 |  | -7.9 |
| 18759 | Achyranthes saponin D | 1103.25 |  | -7.9 |
| 179273 | aesculioside IVb | 1143.31 |  | -7.9 |
| 133017 | abrisaponin D2 | 1105.26 |  | -7.9 |
| 184239 | N/A | 812.98 |  | -7.9 |
| 200844 | gypsogenin 3-O-sulfate 28-O-beta-D-glucopyranosyl ether | 712.888 |  | -7.9 |
| 145361 | theasaponin A4 | 1221.33 |  | -7.9 |
| 197767 | N/A | 798.954 |  | -7.9 |
| 106168 | |3-O-[beta-D-glucopyranosyl (1->2)-beta-D-galactopyranosyl (1->2)-beta-D-glucuronopyranosyl]-soyasapogenol E | 957.106 |  | -7.9 |
| 190965 | sasanquasaponin V | 1205.38 |  | -7.9 |
| 105007 | O4,O2II-Dimethyl-gyrophorsaeure | 496.463 |  | -7.9 |
| 64394 | Ovoic acid | 482.436 |  | -7.9 |
| 179360 | 3-O-trans-Feruloyleuscaphic acid | 664.868 |  | -7.9 |
| 175148 | 3-O-alpha-L-arabinofuranosyl-(1->3)2))-beta-D-xylopyranosylhederagenin | 883.07 |  | -7.9 |
| 124872 | 3beta-sulfate ester of gederagenin 28-O-beta-D-glucopyranosyl(1-2)-(beta-D-glucopyranosyl(1-6))-beta-D-glucopyranoside | 1039.18 |  | -7.9 |
| 170841 | N/A | 1990.13 |  | -7.9 |
| 169997 | Gypsogeninsaeure | 486.683 |  | -7.9 |
| 194940 | Atroxigenin | 553.127 |  | -7.9 |
| 109245 | azukisaponin II | 796.981 |  | -7.9 |
| 183057 | Arjunoside IV | 634.84 |  | -7.9 |
| 15191 | Pacidamycin 1 | 874.896 |  | -7.9 |
| 120980 | torvanol A | 451.424 |  | -7.9 |
| 144024 | N/A | 971.089 |  | -7.9 |
| 174223 | 3-O-[beta-D-glucopyranosyl(1->3)-beta-D-glucopyranosyl]-28-O-beta-D-glucopyranoside medicagenate | 989.104 |  | -7.9 |
| 158223 | buxifolioside I | 664.823 |  | -7.9 |
| 133866 | (3beta,4alpha,16alpha)-3-{{O-beta-D-galactopyranosyl-(1->4)-O-[beta-D-glucopyranosyl-(1->2)]-beta-D-glucopyranuronosyl}oxy}-16-hydroxy-23-oxoolean-12-en-28-oic acid | 987.089 |  | -7.9 |
| 102610 | silenoside C | 1543.6 |  | -7.9 |
| 156818 | Tenuifolsaeure | 537.128 |  | -7.9 |
| 138660 | soyasapogenol B 3-O-[beta-D-glucopyranosyl(1->2)][alpha-L-rhamnopyranosyl(1->2)-beta-D-glucopyranosyl(1->4)]-beta-D-glucuronopyranoside | 1105.26 |  | -7.9 |
| 191238 | N/A | 535.756 |  | -7.9 |
| 159201 | N/A | 957.106 |  | -7.9 |
| 108108 | 2alpha,3beta,19alpha,23-tetrahydroxyurs-12-en-28-oic acid 28-O-beta-D-glucopyranoside 23-sulfate ester|niga-ichigoside F1 23-sulfate ester | 746.902 |  | -7.9 |
| 114439 | impatienoside B | 945.095 |  | -7.9 |
| 163093 | N/A | 696.822 |  | -7.9 |
| 110393 | N/A | 810.964 |  | -7.9 |
| 154818 | Shaagrockol C | 710.938 |  | -7.8 |
| 122976 | alternoside II | 1001.16 |  | -7.8 |
| 194525 | N/A | 552.569 |  | -7.8 |
| 114153 | hederagenin 3-O-alpha-L-rhamnopyranosyl(1-->2)-alpha-L-arabinopyranoside | 750.956 |  | -7.8 |
| 17304 | lamellarin B 20-sulfate | 622.576 |  | -7.8 |
| 160348 | ilexhainanoside E | 664.823 |  | -7.8 |
| 1098 | Vaccarosid | 646.808 |  | -7.8 |
| 17303 | N/A | 426.459 |  | -7.8 |
| 157815 | ageratoside A4 | 1133.23 |  | -7.8 |
| 146705 | Symplocos glomerata saponin 3 | 969.116 |  | -7.8 |
| 1456 | arylomycin A2 | 824.959 |  | -7.8 |
| 144782 | polygalasaponin XXIII | 1103.2 |  | -7.8 |
| 200589 | 3-O-beta-D-glucopyranosyl gypsogenic acid 28-O-[beta-D-6-O-((3S)-3-hydroxyl-3-methylglutaryl)glucopyranosyl(1->6)]-beta-D-glucopyranoside | 1117.23 |  | -7.8 |
| 124371 | N/A | 969.03 |  | -7.8 |
| 110898 | gypsophilinoside | 728.887 |  | -7.8 |
| 147216 | arvensoside C | 939.09 |  | -7.8 |
| 174511 | shimadoside A | 1191.31 |  | -7.8 |
| 200843 | quillaic acid 3-O-sulfate | 566.746 |  | -7.8 |
| 137684 | 3-O-{[beta-D-glucopyranosyl-(1->2)]-[alpha-L-arabinofuranosyl-(1->4)]-(3-O-acetyl-beta-D-glucuronopyranosyl)}-28-O-[beta-D-glucopyranosyl]oleanolic acid | 1131.26 |  | -7.8 |
| 15751 | 3-O-(alpha-L-rhamnopyranosyl-(1->2)-beta-D-glucopyranosyl-(1->2)-beta-D-glucopyranosyl)serjanic acid | 971.132 |  | -7.8 |
| 200590 | 3-O-beta-D-glucopyranosyl gypsogenic acid 28-O-[7beta;-D-glucopyranosyl(1->3)][beta-D-6-O-((3S)-3-hydroxyl-3-methylglutaryl)glucopyranosyl(1->6)]-beta-D-glucopyranoside | 1279.37 |  | -7.8 |
| 189184 | 3-O-[beta-glucopyranosyl-(1->3)-beta-glucopyranosyl]-28-O-{beta-xylopyranosyl-(1->4)-[alpha-L-arabinopyranosyl-(1->3)]-alpha-rhamnopyranosyl-(1->2)-alpha-arabinopyranoside} medicagenic acid | 1369.45 |  | -7.8 |
| 178969 | caryocaroside IV-6 | 662.85 |  | -7.8 |
| 141387 | Mukurozisaponin G | 967.143 |  | -7.8 |
| 151609 | 5,4'-dihydroxy-3,3'-dimethoxy-6,7-methylenedioxyflavone 4'-O-beta-D-glucuronide | 534.423 |  | -7.8 |
| 163333 | 19-hydroxyaraplysillin-I N20-sulfamate | 812.095 |  | -7.8 |
| 116062 | Luciferin | 588.694 |  | -7.8 |
| 160801 | 2"-O-Methylgyrophoric acid | 482.436 |  | -7.8 |
| 117418 | 3beta-angeloyl-2beta,23-dihydroxyolean-12-en-28-oic acid | 570.8 |  | -7.8 |
| 149810 | madhucic acid | 596.88 |  | -7.8 |
| 172182 | MCLW | 1025.2 |  | -7.8 |
| 168231 | (23Z)-coumaroylhederagenin | 618.842 |  | -7.8 |
| 141624 | azukisaponin III | 810.964 |  | -7.8 |
| 166793 | Gymnemic acid IV | 764.939 |  | -7.8 |
| 155474 | lasalocid | 590.788 |  | -7.8 |
| 103382 | 3beta-hydroxyurs-12-en-28-oic acid 3-O-beta-D-glucuranopyranoside 6'-O-butyl ester | 688.931 |  | -7.8 |
| 149066 | onjisaponin Gg | 1601.68 |  | -7.8 |
| 126645 | N/A | 604.814 |  | -7.8 |
| 138391 | Acetyl-soyasaponin A2 | 1275.38 |  | -7.8 |
| 2008 | Vilaportine | 692.754 |  | -7.8 |
| 17671 | Parvodicin A | 1704.48 | CCCCCCCCCC(=O)NC1C(C(C(OC1OC2=C3C=C4C=C2OC5=C(C=C(C=C5)C(C6C(=O)NC(C7=CC(=CC(=C7C8=C(C=CC(=C8)C(C(=O)N6)NC(=O)C4NC(=O)C9C1=CC(=CC(=C1Cl)O)OC1=C(C=CC(=C1)C(C(=O)NC(CC1=CC=C(O3)C=C1)C(=O)N9)NC)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)C(=O)O)O)Cl)C(=O)O)O)O | -7.8 |
| 149734 | Egonsaeure | 340.327 |  | -7.8 |
| 107733 | Polymastiamide D | 657.857 |  | -7.8 |
| 113336 | amidepsine E | 581.567 |  | -7.8 |
| 194213 | Thielavin A | 538.542 |  | -7.7 |
| 113919 | N/A | 1513.62 |  | -7.7 |
| 182809 | Crossbyanol D | 1110.83 |  | -7.7 |
| 105848 | N/A | 524.516 |  | -7.7 |
| 20033 | Achyranthoside II | 794.922 |  | -7.7 |
| 120794 | N/A | 538.542 |  | -7.7 |
| 12822 | betavulgaroside III | 957.063 |  | -7.7 |
| 150756 | (-)-(R)-aristoquinoline A | 479.522 |  | -7.7 |
| 14134 | acantrifoic acid A | 544.719 |  | -7.7 |
| 181537 | Umbilicarsaeure | 482.436 |  | -7.7 |
| 130778 | 3beta-O-cis-p-coumaroyl-alphitolic acid | 618.842 |  | -7.7 |
| 173811 | kalidiumin | 516.709 |  | -7.7 |
| 166642 | O1-{4-[(1R,2S)-1-Aethyl-2-(4-hydroxy-phenyl)-butyl]-phenyl}-beta-D-glucopyranuronsaeure | 446.49 |  | -7.7 |
| 109476 | N/A | 1131.26 |  | -7.7 |
| 10200 | N/A | 927.08 |  | -7.7 |
| 12572 | 3-O-alpha-L-arabinofuranosyl-(1->3)-[alpha-L-arabinofuranosyl-(1->2)]-beta-D-glucuronopyranosyl-21beta,22alpha-di-O-angeloylprotoaescigenin | 1111.27 |  | -7.7 |
| 11296 | N/A | 620.814 |  | -7.7 |
| 102896 | Acetylsoyasaponin A5 | 1203.32 |  | -7.7 |
| 128794 | escin Ia | 1131.26 |  | -7.7 |
| 102597 | Acetyl-subproside II | 987.132 |  | -7.7 |
| 101664 | N/A | 828.68 |  | -7.7 |
| 131559 | 3-O-[beta-D-galactopyranosyl(1->2)-beta-D-glucuronopyranosyl]-28-O-beta-D-glucopyranoside bayogenin | 989.104 |  | -7.7 |
| 192735 | Dienestrol glucuronide | 442.458 |  | -7.7 |
| 19568 | Amidepsine D | 496.463 |  | -7.7 |
| 116182 | Polymastiamide A | 685.91 |  | -7.7 |
| 111072 | lamellarin C 20-sulfate | 624.592 |  | -7.7 |
| 142001 | lamellarin T 20-sulfate | 624.592 |  | -7.6 |
| 135616 | sandrosaponin VIII | 1052.16 |  | -7.6 |
| 132559 | (3beta,4alpha)-3,23,30-trihydroxyurs-20-en-28-al 3,23-di(sulfate) sodium salt | 631.818 |  | -7.6 |
| 167578 | N/A | 847.04 |  | -7.6 |
| 126682 | 3beta-O-cis-p-coumaroylmaslinic acid | 618.842 |  | -7.6 |
| 112036 | aceriphyllic acid J | 542.746 |  | -7.6 |
| 144242 | escin IVf | 1089.22 |  | -7.6 |
| 129390 | lamellarin alpha 20-sulfate|sodium 14-(3-hydroxy-4-methoxyphenyl)-2,11,12-trimethoxy-6-oxo-6H-[1]benzopyrano[4',3':4,5]pyrrolo[2,1-a]isoquinolin-3-yl sulfate | 592.55 |  | -7.6 |
| 184569 | (23E)-coumaroylhederagenin | 618.842 |  | -7.6 |
| 146468 | Z-senegasaponin b | 1427.53 |  | -7.6 |
| 192338 | arundifungin | 592.804 |  | -7.6 |
| 128420 | Sinocrassuloside VI | 1451.55 | CC1C(C(C(C(O1)OC2C(C(C(OC2OC(=O)C34CCC(CC3C5=CCC6C7(CCC(C(C7CCC6(C5(CC4O)C)C)(C)C=O)OC8C(C(C(C(O8)C(=O)O)O)OC9C(C(C(CO9)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)C)(C)C)C)OC(=O)C=CC1=CC=C(C=C1)OC)OC(=O)C)O)O)O | -7.6 |
| 179757 | acetyl-soyasaponin A3 | 1245.36 |  | -7.6 |
| 127718 | Orienticin A | 1557.99 |  | -7.6 |
| 12480 | zygophyloside P | 861.002 |  | -7.6 |
| 10147 | Polymastiamide A | 685.91 |  | -7.6 |
| 192478 | 2-(4-{2-carboxy-2-[4-(2-carboxyvinyl)-2-methoxyphenoxy]vinyl}-2-methoxyphenoxy)-3-(4-hydroxy-3-methoxyphenyl)acrylic acid | 578.52 |  | -7.6 |
| 192548 | 4,5-Di-O-methylhiascic acid | 512.462 |  | -7.6 |
| 114497 | Koproporphyrin III | 654.709 |  | -7.5 |
| 11982 | (2beta,3beta,4alpha)-3-(beta-D-glucopyranosyloxy)-2,27-dihydroxyolean-12-ene-23,28-dioic acid 28-{O-beta-D-galactopyranosyl-(1->4)-O-beta-D-xylopyranosyl-(1->4)-O-3-O-acetyl-6-deoxy-alpha-L-mannopyranosyl-(1->2)-O-[beta-D-glucopyranosyl-(1->3)]-6-deoxy-4-O-[(2E)-3-(3,4-dimethoxyphenyl)-1-oxoprop-2-en-1-yl]-beta-D-galactopyranosyl} ester | 1661.73 |  | -7.5 |
| 17928 | Porphyrin c | 804.974 |  | -7.5 |
| 121402 | N/A | 1101.23 |  | -7.5 |
| 185013 | 3beta,23-dihydroxyolean-12-en-28-oic acid 28-O-alpha-L-rhamnopyranosyl-(1->4)-beta-D-glucopyranosyl-(1->6)-beta-D-glucopyranoside 3-sulfate ester | 1023.19 |  | -7.5 |
| 157590 | glomelliferonic acid | 456.485 |  | -7.5 |
| 127327 | hederagenin 3-O-(6-O-caffeyl-beta-D-glucopyranosyl)-(1->4)-O-beta-D-xylopyranosyl-(1->3)-O-alpha-L-rhamnopyranosyl-(1->2)-O-alpha-L-arabinopyranoside | 1207.35 |  | -7.5 |
| 19896 | lamellarin G 8-sulfate | 580.539 |  | -7.5 |
| 110178 | 3-O-beta-D-glucopyranosyl presenegenin 28-O-beta-D-xylopyranosyl-(1-->4)-alpha-L-rhamnopyranosyl-(1-->2)-(4-O-acetyl)-beta-D-fucopyranosyl ester | 1147.26 |  | -7.5 |
| 57576 | Crossbyanol C | 1110.83 |  | -7.5 |
| 122848 | Aricicin B | 1803.39 | http://pubchem.ncbi.nlm.nih.gov/image/imagefly.cgi?cid=86278230&width=400&height=400 | -7.5 |
| 128014 | 3-O-alpha-L-arabinofuranosyl-(1->2)-beta-D-glucuronopyranosyl-21beta,22alpha-di-O-angeloylprotoaescigenin | 979.154 |  | -7.5 |
| 105895 | coproporphyrine I | 654.709 |  | -7.5 |
| 126674 | clinopodic acid G | 566.51 |  | -7.4 |
| 155747 | 4-Me ether, Me ester-Lecanoric acid | 390.341 |  | -7.4 |
| 168378 | escin IIa | 1101.23 |  | -7.4 |
| 192825 | escin IIb | 1101.23 |  | -7.4 |
| 135787 | ianthesine C | 1583.14 |  | -7.4 |
| 106026 | dichotomoside B | 608.631 |  | -7.4 |
| 14823 | 3,3',5-trimethoxy-4,4'-oxyneolign-9,9'-dioic acid|apteniol D | 404.41 |  | -7.4 |
| 126695 | ianthesine B | 761.05 |  | -7.4 |
| 192144 | Viscosid | 1689.74 |  | -7.4 |
| 106412 | ianthesine D | 840.105 |  | -7.3 |
| 120487 | Phycocyanobilin | 588.694 |  | -7.3 |
| 128574 | Z-senegin III | 1573.67 |  | -7.3 |
| 130194 | cryptoporic acid E | 849.012 |  | -7.3 |
| 109880 | beta-escin|escin Ib | 1131.26 |  | -7.3 |
| 12662 | assamsaponin G | 1261.36 |  | -7.3 |
| 120580 | 3-O-beta-D-xylopyranosyl-(1->2)-beta-D-glucuronopyranosyl-21beta,22alpha-di-O-angeloylprotoaescigenin | 979.154 |  | -7.3 |
| 134840 | psammaplin A2 | 822.498 |  | -7.3 |
| 168672 | apteniol E | 434.436 |  | -7.3 |
| 132681 | hederagenin-3-O-(3,4-di-O-acetyl-beta-D-xylopyranosyl)-(1-3)-alpha-L-rhamnopyranosyl-(1-2)-alpha-L-arabinopyranoside | 967.143 |  | -7.2 |
| 103541 | 3,5,3'-Triiodothyronine | 650.973 |  | -7.2 |
| 192275 | N/A | 858.963 |  | -7.2 |
| 109490 | diethylstilbestrol monoglucuronide | 444.474 |  | -7.2 |
| 146347 | N/A | 806.976 |  | -7.2 |
| 195901 | aesculioside IIb | 1059.19 |  | -7.2 |
| 152636 | bisaprasin 11'-sulfate | 1484.71 |  | -7.2 |
| 111861 | N/A | 1105.26 |  | -7.2 |
| 148050 | 4-Me ether,4'-Ac-(alphaZ)-3-(4-Hydroxygeranyl)-p-coumaric acid | 372.455 |  | -7.2 |
| 199397 | N/A | 386.352 |  | -7.2 |
| 185476 | tubulysin D | 828.069 |  | -7.2 |
| 180303 | denticin B | 531.621 |  | -7.2 |
| 45574 | 4'-O-Sulfate-Jaceidin | 440.378 |  | -7.2 |
| 175602 | 3,23-disulfate ester of stachlic acid A | 664.825 |  | -7.2 |
| 100468 | Lasalocid C | 604.814 |  | -7.2 |
| 161903 | Lasalocid E | 604.814 |  | -7.2 |
| 107266 | 2-Hydroxy-4-(2-hydroxy-4-methoxy-3,6-dimethyl-benzoyloxy)-3,6-dimethyl-benzoesaeure | 360.358 |  | -7.2 |
| 138305 | bunkankasaponin A | 1157.29 |  | -7.2 |
| 145035 | assamsaponin B | 1273.37 |  | -7.2 |
| 130281 | xanifolia-Y8 | 1141.29 |  | -7.2 |
| 143714 | 3-O-alpha-L-arabinofuranosyl-(1->3)-[beta-D-xylopyranosyl-(1->2)]-beta-D-glucuronopyranosyl-21beta,22alpha-di-O-angeloylprotoaescigenin | 1111.27 |  | -7.2 |
| 177534 | (2E)-3-(4-{1-carboxy-2-[5'-((E)-2-carboxyvinyl)-2',6-dihydroxy-3',5-dimethoxybiphenyl-3-yl]-2-hydroxyethoxy}-3-methoxyphenyl)acrylic acid | 596.536 |  | -7.2 |
| 111277 | Haematoporphyrin | 598.689 |  | -7.2 |
| 116211 | N/A | 330.418 |  | -7.1 |
| 175666 | araplysillin III | 761.05 |  | -7.1 |
| 158939 | glomellonic acid | 470.469 |  | -7.1 |
| 113802 | 2-O-Methylsekikaic acid | 432.464 |  | -7.1 |
| 200186 | 3-O-{12'-[12''-O-(3'',5''-dimethoxy-6''-carboxybibenzyl)]-5'-methoxy-6'-carboxybibenzyl}-12-hydroxy-5-methoxybibenzyl-6-carboxylic acid | 842.882 |  | -7.1 |
| 190437 | 4-Me ether, 4'-Ac-(alphaE)-3-(4-Hydroxygeranyl)-p-coumaric acid | 372.455 |  | -7.1 |
| 113755 | hexadellin C | 803.13 |  | -7.1 |
| 123499 | escin VIb | 1131.26 |  | -7.1 |
| 126078 | geomycin B | 678.593 |  | -7.1 |
| 157191 | N/A | 520.698 |  | -7.1 |
| 145872 | ianthesine A | 789.103 |  | -7.1 |
| 171115 | 3-O-Methylphysodic acid | 484.538 |  | -7.0 |
| 101688 | Thielavin C | 580.622 |  | -7.0 |
| 135511 | N/A | 372.455 |  | -7.0 |
| 106592 | 3-O-α-L-Arabinopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranosylgypsogenin-28-O-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosi| | 1497.57 |  | -7.0 |
| 188174 | dichotomoside C | 608.631 |  | -7.0 |
| 14724 | viridiofungin C | 614.726 |  | -6.9 |
| 128974 | 3beta-malonyloxy-15-(3-methylvaleryloxy)-ent-labda-7,13E-diene|3beta-malonyloxy-15-<3-methylvaleryloxy>-ent-labda-7,13E-diene | 490.672 |  | -6.9 |
| 155376 | cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-6-O-(trans-feruloyl)-beta-D-glucopyranoside]-5-O-[6-O-(maloyl)-beta-D-glucopyranoside] | 1006.86 |  | -6.9 |
| 148504 | alpha-alectoronic acid | 512.548 |  | -6.9 |
| 145254 | 22-O-acetyl-21-O-(3',4'-di-O-angeloyl)-beta-D-fucopyranosylprotoaescigenin 3-O-beta-D-glucuronopyranoside | 1035.22 |  | -6.9 |
| 109721 | micropeptin KT946 | 947.059 |  | -6.9 |
| 178886 | guaiacylglycerol-beta-ferulic acid ether | 390.384 |  | -6.9 |
| 105111 | Amonabactin T 789 | 789.831 |  | -6.8 |
| 163181 | 3-Chlorodivaricatic acid | 422.856 |  | -6.8 |
| 10765 | 3",3"'-bispolycerasoidol | 714.927 |  | -6.8 |
| 186081 | cryptoporic acid G | 834.986 |  | -6.8 |
| 151546 | alpha-Collatolsaeure | 526.575 |  | -6.7 |
| 193041 | 2-O-Methylperlatolic acid | 458.544 |  | -6.7 |
| 188758 | hyperplanaic acid | 500.624 |  | -6.7 |
| 140099 | CRM646-B | 704.801 |  | -6.7 |
| 123901 | cryptoporic acid C | 833.013 |  | -6.7 |
| 182223 | Epiphorellic acid 2 | 488.527 |  | -6.7 |
| 118666 | 18-dihydrocinnamoyloxy-labda-7,13E-dien-15-oic acid | 452.625 |  | -6.6 |
| 128418 | 2-O-Methylconfluentinsaeure | 514.607 |  | -6.6 |
| 1901 | Planaic acid | 472.571 |  | -6.5 |
| 11748 | Physodsaeure | 470.512 |  | -6.5 |
| 177219 | denticin A | 579.664 |  | -6.4 |
| 135708 | N/A | 614.726 |  | -6.4 |
| 157341 | 24-palmityloxyoleanonic acid | 709.093 |  | -6.3 |
| 167658 | 2-hydroxy-4-methoxy-6-(13-hydroxy-2-oxotridecyl)benzoic acid | 380.475 |  | -6.3 |
| 134728 | Antibiotic A 32724A | 694.937 |  | -6.2 |
| 120205 | N/A | 807.322 |  | -6.2 |