**SUPPLEMENTARY TABLES**

*Table 1S.Chemical names, SMILES notations, and experimental and predicted log(RS) for 233 sweeteners compounds. ^ test set*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **ID** | **Chemical Name** | **SMILES** | **log(RS)** | **Eq. 1** | **Reference** |
| 1 | Sucrose | OCC1OC(C(C1O)O)(CO)OC1OC(CO)C(C(C1O)O)O | 0.000 | -0.106 | (a) |
| 2 | Sucralose | ClCC1OC(C(C1O)O)(CCl)OC1OC(CO)C(C(C1O)O)Cl | 2.778 | 2.198 |
| 3 | Alitame | CC(COCNC1C(C)(C)SC1(C)C)NCOCC(CC(=O)O)N | 3.301 | 3.201 |
| 4^ | Aspartame | COC(=O)C(NC(=O)C(CC(=O)O)N)Cc1ccccc1 | 2.255 | 3.001 |
| 5 | Tagatose | OCC1(O)OCC(C(C1O)O)O | -0.046 | -0.166 |
| 6^ | Maltitol | OCC(C(C(C(CO)O)O)OC1OC(CO)C(C(C1O)O)O)O | -0.046 | -0.230 |
| 7 | Isomaltulose | OCC1OC(OCC2OC(C(C2O)O)(O)CO)C(C(C1O)O)O | -0.319 | -0.277 |
| 8^ | Trehalose | OCC1OC(OC2OC(CO)C(C(C2O)O)O)C(C(C1O)O)O | -0.347 | -0.185 |
| 9 | Neohesperidine dihydrochalcone | OCC1OC(Oc2cc(O)c(c(c2)O)C(=O)CCc2ccc(c(c2)O)OC)C(C(C1O)O)OC1OC(C)C(C(C1O)O)O | 3.255 | 2.372 |
| 10 | Neotame | COC(=O)C(Cc1ccccc1)NC(=O)C(CC(=O)O)NCCC(C)(C)C | 3.903 | 4.021 |
| 11 | Lactitol | OCC(C(C(C(CO)O)O)OC1OC(CO)C(C(C1O)O)O)O | -0.398 | -0.230 |
| 12 | Isomalt | OCC(C(C(C(COC1OC(CO)C(C(C1O)O)O)O)O)O)O | -0.260 | -0.446 |
| 13 | Sorbitol | OCC(C(C(C(CO)O)O)O)O | -0.222 | -0.329 |
| 14^ | Mannitol | OCC(C(C(C(CO)O)O)O)O | -0.155 | -0.329 |
| 15 | Erythritol | OCC(C(CO)O)O | -0.155 | -0.098 |
| 16 | Xylitol | OCC(C(C(CO)O)O)O | 0.000 | -0.226 |
| 17 | Stevioside | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)OC2OC(CO)C(C(C2O)O)O)C(C(C1O)O)OC1OC(CO)C(C(C1O)O)O | 2.477 | 2.359 |
| 18 | Steviolbioside | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)O)C(C(C1O)O)OC1OC(CO)C(C(C1O)O)O | 2.051 | 2.350 |
| 19 | Rebaudioside A | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)OC2OC(CO)C(C(C2O)O)O)C(C(C1O)OC1OC(CO)C(C(C1O)O)O)OC1OC(CO)C(C(C1O)O)O | 2.544 | 2.468 |
| 20 | Rebaudioside B | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)O)C(C(C1O)OC1OC(CO)C(C(C1O)O)O)OC1OC(CO)C(C(C1O)O)O | 2.512 | 2.473 |
| 21^ | Rebaudioside C | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)OC2OC(CO)C(C(C2O)O)O)C(C(C1O)OC1OC(CO)C(C(C1O)O)O)OC1OC(C)C(C(C1O)O)O | 1.929 | 2.797 |
| 22 | Rebaudioside D | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)OC2OC(CO)C(C(C2OC2OC(CO)C(C(C2O)O)O)O)O)C(C(C1O)OC1OC(CO)C(C(C1O)O)O)OC1OC(CO)C(C(C1O)O)O | 2.512 | 2.485 |
| 23 | Rebaudioside E | OCC1OC(OC(=O)C2(C)CCCC3(C2CCC24C3CCC(C4)(C(=C)C2)OC2OC(CO)C(C(C2OC2OC(CO)C(C(C2O)O)O)O)O)C)C(C(C1O)O)OC1OC(CO)C(C(C1O)O)O | 2.352 | 2.384 |
| 24^ | Dulcoside A | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)OC2OC(CO)C(C(C2O)O)O)C(C(C1O)O)OC1OC(C)C(C(C1O)O)O | 1.929 | 2.682 |
| 25 | Glycyrrhizin | OC1C(OC2OC(C(=O)O)C(C(C2O)O)O)C(OC(C1O)C(=O)O)OC1CCC2(C(C1(C)C)CCC1(C2C(=O)C=C2C1(C)CCC1(C2CC(C)(CC1)C(=O)O)C)C)C | 1.875 | 2.183 |
| 26 | Hernandulcin | CC(=CCCC(C1CCC(=CC1=O)C)(O)C)C | 3.000 | 1.637 |
| 27 | Fructose | OCC1OC(C(C1O)O)(O)CO | 0.057 | -0.147 | (b) |
| 28 | Glucose | OCC1OC(O)C(C(C1O)O)O | -0.161 | -0.137 |
| 29 | Galactose | OCC1OC(O)C(C(C1O)O)O | -0.201 | -0.137 |
| 30^ | Mannose | OCC1OC(O)C(C(C1O)O)O | -0.229 | -0.137 |
| 31^ | Xylose | OC1COC(C(C1O)O)O | -0.174 | 0.002 |
| 32 | Maltose | OCC1OC(O)C(C(C1OC1OC(CO)C(C(C1O)O)O)O)O | -0.337 | -0.099 |
| 33^ | Lactose | OCC1OC(O)C(C(C1OC1OC(CO)C(C(C1O)O)O)O)O | -0.398 | -0.099 |
| 34^ | Lactulose | OCC1OC(C(C1OC1OC(CO)C(C(C1O)O)O)O)(O)CO | -0.222 | -0.120 |
| 35^ | Lactosucrose | OCC1OC(OC2(CO)OC(C(C2O)O)CO)C(C(C1OC1OC(CO)C(C(C1O)O)O)O)O | -0.347 | -0.074 |
| 36^ | Galactitol | OCC(C(C(C(CO)O)O)O)O | -0.387 | -0.329 |
| 37 | Raffinose | OCC1OC(C(C1O)O)(CO)OC1OC(COC2OC(CO)C(C(C2O)O)O)C(C(C1O)O)O | -0.658 | -0.238 |
| 38^ | Rhamnose | OC1C(C)OC(C(C1O)O)O | -0.481 | 0.155 |
| 39 | Glycerol | OCC(CO)O | -0.097 | 0.047 | (c) |
| 40 | 2-amino-4-nitro-propoxybenzene | CCCOc1ccc(cc1N)N(=O)=O | 3.602 | 3.060 |
| 41 | Dulcin | CCOc1ccc(cc1)NC(=O)N | 2.301 | 2.692 |
| 42^ | Dihydroquercetin 3-acetate 4'-(methylether) | COc1ccc(cc1O)C1Oc2cc(O)cc(c2C(=O)C1OC(=O)C)O | 2.602 | 2.052 | (d) |
| 43^ | 1,3-benzodioxane | COc1ccc(cc1O)C1OCc2c(O1)cccc2 | 3.477 | 1.751 |
| 44 | 1,4-benzodioxane | COc1ccc(cc1O)C1COc2c(O1)cccc2 | 2.653 | 2.009 |
| 45 | Isoflavan | COc1ccc(cc1O)C1COc2c(C1)cccc2 | 2.477 | 1.900 |
| 46 | 2-(3-hydroxy-4-methoxyphenyl)-1,3-benzodioxole | COc1ccc(cc1O)C1Oc2c(O1)cccc2 | 2.176 | 1.728 |
| 47^ | Bibenzyl derivative | COc1ccc(cc1O)CCc1ccccc1 | 2.477 | 1.643 |
| 48^ | Flavan | COc1ccc(cc1O)C1CCc2c(O1)cccc2 | 2.544 | 1.802 |
| 49^ | Compound 5 | COc1ccc(cc1O)C1OCc2c(C1)cccc2 | 2.544 | 1.613 |
| 50^ | 2-(3-Hydroxy-4-methoxyphenyl)-4H-1,3-benzoxathiine | COc1ccc(cc1O)C1SCc2c(O1)cccc2 | 2.699 | 2.245 | (e) |
| 51 | 2-(3-Hydroxy-4-methoxyphenyl)-4H-1,3-benzodithiole | COc1ccc(cc1O)C1Sc2c(S1)cccc2 | 2.301 | 2.599 |
| 52^ | 2-(3-Hydroxy-4-methoxyphenyl)-1,3-benzoxathiole | COc1ccc(cc1O)C1Oc2c(S1)cccc2 | 2.477 | 2.245 |
| 53^ | 2-(3-Hydroxy-4-methoxyphenyl)-2,3-dihydro-1,4-benzoxathiine | COc1ccc(cc1O)C1CSc2c(O1)cccc2 | 2.398 | 2.430 |
| 54 | 2-(3-Hydroxy-4-methoxyphenyl)-2,3-dihydro-1,4-benzodithiine | COc1ccc(cc1O)C1CSc2c(S1)cccc2 | 2.699 | 2.795 |
| 55^ | 2-(3-Hydroxy-4-methoxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol | COc1ccc(cc1O)C1CSc2c(O1)ccc(c2)O | 2.699 | 2.432 |
| 56 | 2-(3-Hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzothiopyran | COc1ccc(cc1O)C1CCc2c(S1)cccc2 | 2.301 | 2.285 |
| 57 | 2-(3-Mercapto-4-methoxyphenyl)-4H-3,1-benzoxathiine | COc1ccc(cc1S)C1OCc2c(S1)cccc2 | 1.699 | 2.642 |
| 58 | 2-(3-Hydroxy-4-methoxyphenyl)-2,3-dihydro-1,4-benzoxathiine S,S-Dioxide | COc1ccc(cc1O)C1Oc2ccccc2S(=O)(=O)C1 | 1.699 | 2.401 |
| 59^ | Haematoxylin | Oc1cc2CC3(C(c2cc1O)c1ccc(c(c1OC3)O)O)O | 2.079 | 1.858 | (f) |
| 60 | 9-Methoxy-7,11b-dihydrobenz[b]indeno[1,2-d]pyran-6a,10-diol | COc1cc2CC3(C(c2cc1O)c1ccccc1OC3)O | 1.699 | 1.593 |
| 61^ | Compound 8 | COc1ccc2c(c1O)CCC1C2CCC2(C1CCC2)C | 1.699 | 1.948 | (g) |
| 62 | Compound 18 | Oc1cccc(c1)C1OCc2c(S1)cccc2 | 2.079 | 1.917 |
| 63 | Compound 20 | COc1ccc(cc1OC(=O)Nc1ccccc1)C1OCc2c(S1)cccc2 | 2.778 | 3.365 |
| 64^ | Compound 21 | COc1ccc(cc1OC(=O)Nc1ccc(cc1)N(=O)=O)C1OCc2c(S1)cccc2 | 3.041 | 3.592 |
| 65 | 2-(4-methoxybenzoyl) benzoic acid | COc1ccc(cc1)C(=O)c1ccccc1C(=O)O | 2.176 | 1.314 | (h) |
| 66 | 2-(3,4-Dihydroxybenzoyl) benzoic acid | O=C(c1ccccc1C(=O)O)c1ccc(c(c1)O)O | 2.000 | 1.372 |
| 67 | 2-(3-Hydroxy-4-methoxybenzoyl) benzoic acid | COc1ccc(cc1O)C(=O)c1ccccc1C(=O)O | 2.398 | 1.590 |
| 68 | 2-(4-Methoxyphenylthio) benzoic acid S-Oxide | COc1ccc(cc1)S(=O)c1ccccc1C(=O)O | 1.699 | 1.645 |
| 69^ | Phthalic Acid Mono(4-methoxyphenyl) Ester | COc1ccc(cc1)OC(=O)c1ccccc1C(=O)O | 1.000 | 1.687 |
| 70 | Compound 9 | O=C(c1ccccc1C(=O)O)c1ccc(cc1)N(C)C | 2.301 | 2.769 |
| 71 | 3-Methoxy-1,3,5-estratrien-4-ol | COc1cc2CCC3C(c2cc1O)CCC1(C3CCC1)C | 1.699 | 2.047 | (i) |
| 72 | Spiro[(4-H-1,3-benzodithian)-2,1'-(5'-methoxy-6'hydroxy-[1*H*]-2',3'-dihydroindene)] | COc1cc2CCC3(c2cc1O)SCc1c(S3)cccc1 | 1.699 | 2.383 |
| 73^ | Compound 14 | COc1ccc(cc1O)C1OCc2c(S1)cccc2 | 4.255 | 2.260 |
| 74 | Compound 15 | COc1ccc(cc1O)C1SCc2c(S1)cccc2 | 4.301 | 2.610 |
| 75 | Phyllodulcin | COc1ccc(cc1O)C1OC(=O)c2c(C1)cccc2O | 2.903 | 1.838 | (j) |
| 76^ | Compound 4 | COc1ccc(cc1O)C1OCc2c(S1)cccc2 | 4.301 | 2.260 |
| 77 | Compound 6 | COc1ccc(cc1O)C1COc2c(S1)cccc2 | 3.176 | 2.524 |
| 78 | Compound 9 | COc1ccc(cc1O)C1SCC23C(O1)CC(C3(C)C)CC2 | 2.176 | 2.207 |
| 79 | Compound 10 | COc1ccc(cc1O)C1SCC23C(O1)CC(C3(C)C)CC2 | 2.000 | 2.207 |
| 80^ | 3',4'-dihydroxyphenyl-3,1-benzoxathiane | Oc1ccc(cc1O)C1OCc2c(S1)cccc2 | 2.301 | 2.062 | (k) |
| 81 | 2-[3-(4-nitrophenoxycarboxy)phenyl]-3,1-benzoxathiane | O=C(Oc1cc(ccc1O)C1OCc2c(S1)cccc2)Oc1ccc(cc1)N(=O)=O | 2.477 | 3.547 |
| 82 | 2-[3-(4-nitrophenylcarbonylmethoxy)-4-methoxyphenyl]-3,1-benzoxathiane | O=C(c1ccc(cc1)N(=O)=O)COc1cccc(c1)C1OCc2c(S1)cccc2 | 2.477 | 3.060 |
| 83 | 2-[3-(4-nitrophenylcarbamoyloxy-4-methoxy)phenyl]-3,1-benzodioxane | COc1ccc(cc1OC(=O)Nc1ccc(cc1)N(=O)=O)C1OCc2c(O1)cccc2 | 2.176 | 3.132 |
| 84 | 3-(3-Hydroxy-4-methoxyphenyl)-1-(3-carboxyphenyl)propan-1-one | COc1ccc(cc1O)CCC(=O)c1cccc(c1)C(=O)O | 1.903 | 1.857 |
| 85 | 2-(3-hydroxy-4-methoxyphenoxymethyl)benzoic acid | COc1ccc(cc1O)OCc1ccccc1C(=O)O | 1.000 | 1.849 |
| 86^ | Compound 32 | COc1ccc(cc1O)CCC(=O)c1c(O)cc(cc1O)O | 2.823 | 2.129 |
| 87 | Compound 42 | COc1ccc(cc1)C(=O)C=CC(=O)O | 1.699 | 1.567 |
| 88^ | Dihydroquercetin 4'-(methyl ether) | COc1ccc(cc1O)C1Oc2cc(O)cc(c2C(=O)C1O)O | 1.602 | 1.878 | (l) |
| 89 | Compound V | COc1ccc(cc1OC(=O)C)C1OC(=O)c2c(C1)cccc2OC(=O)C | 1.875 | 1.897 | (m) |
| 90 | Compound VII | COc1ccc(cc1O)C1OC(=O)c2c(C1)cccc2 | 2.000 | 1.706 |
| 91 | Compound XIV | COc1ccc(cc1O)CCCc1ccccc1 | 1.000 | 1.917 |
| 92^ | Compound XXI | COc1ccc(cc1O)CNc1ccccc1 | 2.477 | 2.878 |
| 93 | Compound XXII | COc1ccc(cc1O)COc1ccccc1 | 2.176 | 1.629 |
| 94 | Compound XXIII | COc1ccc(cc1O)CSc1ccccc1 | 2.176 | 2.110 |
| 95 | Compound XXIV | COc1ccc(cc1O)NCc1ccccc1 | 2.398 | 1.845 |
| 96^ | Compound XXVII | COc1ccc(cc1O)C(=O)Oc1ccccc1 | 1.000 | 1.646 |
| 97^ | Compound XXX | COc1ccc(cc1O)COC(=O)c1ccccc1O | 2.079 | 2.037 |
| 98 | Compound XXXI | COc1ccc(cc1O)CC(=O)c1ccccc1O | 1.477 | 1.646 |
| 99 | Compound XXXII | COc1ccc(cc1O)CCC1CCCCC1 | 1.477 | 1.938 |
| 100 | Compound XL | COc1ccc(cc1O)CCc1ccccc1C | 2.477 | 1.813 |
| 101^ | Compound XLI | COc1ccc(cc1O)CCc1ccccc1O | 2.176 | 1.950 |
| 102^ | Compound XLII | COc1ccc(cc1O)CCc1ccccc1OC | 2.097 | 2.207 |
| 103 | Compound XLIII | COc1ccc(cc1O)CCc1ccccc1CO | 1.000 | 1.677 |
| 104^ | Compound XLVII | COc1ccc(cc1O)CCc1cccc(c1)C | 1.000 | 1.815 |
| 105^ | Compound XLIX | COc1cccc(c1)CCc1ccc(c(c1)O)OC | 1.000 | 1.998 |
| 106^ | Compound LIV | COc1ccc(cc1O)CCc1ccc(cc1)O | 1.000 | 1.798 |
| 107 | Compound LIX | COc1ccc(cc1O)CCc1ccc(cc1)F | 1.477 | 2.178 |
| 108^ | Compound LXV | COc1ccc(cc1O)CCc1ccc2c(c1)OCO2 | 1.000 | 2.099 |
| 109^ | Compound LXVI | CCOc1ccc(cc1O)CCc1ccccc1 | 1.000 | 1.640 |
| 110 | Compound LXXVIII | COc1ccc(cc1O)C1OC(=O)c2c(O1)cccc2 | 2.000 | 1.808 |
| 111 | Compound LXXIX | COc1ccc(cc1O)C1OC(=O)c2c(S1)cccc2 | 2.398 | 2.341 |
| 112 | Compound LXXX | COc1ccc(cc1O)C1NC(=O)c2c(C1)cccc2O | 1.000 | 2.958 |
| 113 | Compound LXXXV | COc1ccc(cc1O)C1OCc2c(C1)cccc2O | 1.875 | 1.767 |
| 114^ | Compound LXXXIX | COc1ccc(cc1O)C1CC(=O)c2c(O1)cccc2O | 2.544 | 1.778 |
| 115 | Compound XC | CCOc1ccc(cc1O)C1CC(=O)c2c(O1)cccc2O | 2.176 | 1.776 |
| 116^ | Compound XCI | CCCOc1ccc(cc1O)C1CC(=O)c2c(O1)cccc2O | 1.778 | 1.908 |
| 117 | Compound XCV | COc1ccc(cc1O)CCC(=O)c1ccccc1O | 2.000 | 1.897 |
| 118^ | Compound XCVI | CCOc1ccc(cc1O)CCC(=O)c1ccccc1O | 1.000 | 1.889 |
| 119 | Glycol | OCCO | 0.114 | 0.165 | (n) |
| 120^ | Arabitol | OCC(C(C(CO)O)O)O | 0.000 | -0.226 |
| 121 | Stachyose | OCC1OC(C(C1O)O)(CO)OC1OC(COC2OC(COC3OC(CO)C(C(C3O)O)O)C(C(C2O)O)O)C(C(C1O)O)O | -1.000 | -0.371 |
| 122^ | 6-*O*-Methyl sucrose | COCC1OC(C(C1O)O)(CO)OC1OC(CO)C(C(C1O)O)O | 0.000 | 0.154 |
| 123 | 6,6'-di-*O*-Methyl sucrose | COCC1OC(C(C1O)O)(CO)OC1OC(COC)C(C(C1O)O)O | 0.000 | 0.423 |
| 124 | 6-Chloro-6-deoxy-D-fructofuranose | ClCC1OC(C(C1O)O)(O)CO | 0.000 | 0.808 |
| 125^ | 1,6-dichloro-1,6-deoxy-D-fructofuranose | ClCC1OC(C(C1O)O)(O)CCl | 0.000 | 1.586 |
| 126 | Methyl α-D-glucopyranoside | COC1OC(CO)C(C(C1O)O)O | -0.602 | 0.123 |
| 127 | 4-Chloro-galactosucrose | OCC1OC(C(C1O)O)(CO)OC1OC(CO)C(C(C1O)O)Cl | 0.699 | 0.704 |
| 128 | 6'-Chloro-sucrose | ClCC1OC(C(C1O)O)(CO)OC1OC(CO)C(C(C1O)O)O | 1.301 | 0.745 |
| 129 | 1'-Chloro-sucrose | OCC1OC(C(C1O)O)(CCl)OC1OC(CO)C(C(C1O)O)O | 1.301 | 0.773 |
| 130^ | 1',6'-Dichloro-sucrose | ClCC1OC(C(C1O)O)(CCl)OC1OC(CO)C(C(C1O)O)O | 1.845 | 1.551 |
| 131 | 1',4-Dichloro-galactosucrose | OCC1OC(C(C1O)O)(CCl)OC1OC(CO)C(C(C1O)O)Cl | 2.079 | 1.480 |
| 132 | 1,6-Di-S-1,6-dithio-D-fructofuranose | CSCC1OC(C(C1O)O)(O)CSC | 1.301 | 1.803 |
| 133 | Alanine | CC(C(=O)O)N | -0.005 | -0.031 |
| 134 | Arginine | NC(=N)NCCCC(C(=O)O)N | 0.624 | 1.077 |
| 135 | Asparagine | NC(=O)CC(C(=O)O)N | 0.301 | -0.225 |
| 136 | glutamine | OC(=O)CCC(C(=O)N)N | 0.322 | 0.727 |
| 137 | Glycine | NCC(=O)O | -0.182 | 0.000 |
| 138 | Histidine | NC(C(=O)O)Cc1c[nH]cn1 | 0.746 | 0.140 |
| 139 | Isoleucine | CCC(C(C(=O)O)N)C | -0.104 | 0.188 |
| 140 | Leucine | NC(C(=O)O)CC(C)C | 0.599 | 0.196 |
| 141 | Methionine | CSCCC(C(=O)O)N | 0.294 | 0.385 |
| 142 | Norvaline | CCCC(C(=O)O)N | 0.230 | 0.147 |
| 143 | Phenylalanine | NC(C(=O)O)Cc1ccccc1 | 0.689 | 0.612 |
| 144 | Proline | OC(=O)C1CCCN1 | -0.268 | 1.003 |
| 145 | Hydroxy proline | OC1CNC(C1)C(=O)O | 0.262 | 0.699 |
| 146 | Serine | OCC(C(=O)O)N | -0.210 | -0.277 |
| 147 | Threonine | CC(C(C(=O)O)N)O | -0.569 | -0.242 |
| 148 | Triptophane | OC(=O)C(Cc1c[nH]c2c1cccc2)N | 1.556 | 2.001 |
| 149^ | Tyrosine | OC(=O)C(Cc1ccc(cc1)O)N | 0.740 | 0.642 |
| 150 | Aspartyaminomalonic acid diester 1 | COC(=O)C(C(=O)OC1CCCC1)NC(=O)C(CC(=O)O)N | 2.778 | 2.844 |
| 151 | Aspartyaminomalonic acid diester 2 | COC(=O)C(C(=O)OC1CCCCC1)NC(=O)C(CC(=O)O)N | 2.944 | 3.025 |
| 152 | Aspartyaminomalonic acid diester 3 | COC(=O)C(C(=O)OC1C2(C)CCC(C1(C)C)C2)NC(=O)C(CC(=O)O)N | 4.521 | 3.543 |
| 153 | N-(L-aspartyl)-1,1-diaminoalkane 1 | CC(NC(=O)C(C)(C)C)NC(=O)C(CC(=O)O)N | 2.000 | 2.014 |
| 154 | N-(L-aspartyl)-1,1-diaminoalkane 2 | CC(NC(=O)C(C1CC1)C1CC1)NC(=O)C(CC(=O)O)N | 2.845 | 2.423 |
| 155 | N-(L-aspartyl)-1,1-diaminoalkane 3 | CC(NC(=O)C1CCCC1)NC(=O)C(CC(=O)O)N | 2.000 | 2.218 |
| 156 | N-(L-aspartyl)-1,1-diaminoalkane 4 | CC(NC(=O)C1C(C)(C)CCC1(C)C)NC(=O)C(CC(=O)O)N | 3.000 | 2.847 |
| 157 | N-(L-aspartyl)-1,1-diaminoalkane 5 | CC(NC(=O)c1ccccc1)NC(=O)C(CC(=O)O)N | 4.643 | 2.293 |
| 158 | N-(L-aspartyl)-1,1-diaminoalkane 6 | CC(NC(=O)C1CCCCC1)NC(=O)C(CC(=O)O)N | 1.875 | 2.382 |
| 159^ | N-(L-aspartyl)-1,1-diaminoalkane 7 | CC(NC(=O)C1C(C)CCCC1C)NC(=O)C(CC(=O)O)N | 2.301 | 2.733 |
| 160 | N-(L-aspartyl)-1,1-diaminoalkane 8 | CC(NC(=O)C1CC2CC1CC2)NC(=O)C(CC(=O)O)N | 2.000 | 2.297 |
| 161 | N-(L-aspartyl)-1,1-diaminoalkane 9 | CC(NC(=O)C12CC3CC(C2)CC(C1)C3)NC(=O)C(CC(=O)O)N | 1.176 | 2.596 |
| 162^ | Super aspartame | COC(=O)C(NC(=O)C(NC(=O)Nc1ccc(cc1)C#N)CC(=O)O)Cc1ccccc1 | 3.903 | 4.116 |
| 163 | Sucrononic acid | N#Cc1ccc(cc1)N=C(NC1CCCCCCCC1)NCC(=O)O | 5.301 | 4.865 |
| 164 | Cyanoarylurea aspartame | COC(=O)C(Cc1ccccc1)CC(=O)CNC(=O)Nc1ccc(cc1)C#N | 3.892 | 3.901 |
| 165^ | Aspartic acid fenchyl ester | COC(=O)C(C(=O)OC1C2(C)CCC(C1(C)C)C2)NC(=O)C(C(=O)O)N | 4.699 | 2.568 |
| 166 | Glycine analog of cyanosuosan | N#Cc1ccc(cc1)NC(=O)NCC(=O)O | 3.845 | 2.988 |
| 167 | Glycine analog of suosan | O=C(Nc1ccc(cc1)N(=O)=O)NCC(=O)O | 1.000 | 1.985 |
| 168 | Nitroaniline (2-amino-4-nitrobenzene) | Nc1cccc(c1)N(=O)=O | 1.602 | 1.866 |
| 169 | Methoxy-nitroaniline | COc1ccc(cc1N)N(=O)=O | 2.418 | 1.962 |
| 170 | Ethoxy-nitroaniline | CCOc1ccc(cc1N)N(=O)=O | 3.047 | 2.991 |
| 171^ | Butoxy-nitroaniline | CCCCOc1ccc(cc1N)N(=O)=O | 3.000 | 3.196 |
| 172 | Fluoro-nitroaniline | O=N(=O)c1ccc(c(c1)N)F | 1.602 | 2.439 |
| 173 | Chloro-nitroaniline | O=N(=O)c1ccc(c(c1)N)Cl | 2.602 | 2.667 |
| 174 | Bromo-nitroaniline | O=N(=O)c1ccc(c(c1)N)Br | 2.903 | 2.754 |
| 175^ | Iodo-nitroaniline | O=N(=O)c1ccc(c(c1)N)I | 3.097 | 2.868 |
| 176 | Allyl oxy-nitroaniline | C=COc1ccc(cc1N)N(=O)=O | 3.301 | 2.918 |
| 177^ | iso Propoxy-nitroaniline | CC(Oc1ccc(cc1N)N(=O)=O)C | 2.778 | 2.910 |
| 178 | Hydroxy-nitroaniline | O=N(=O)c1ccc(c(c1)N)O | 2.204 | 1.857 |
| 179 | Saccharine derivative 13 | Fc1ccc2c(c1)S(=O)(=O)NC2=O | 2.653 | 2.454 |
| 180 | Saccharine derivative 23 | O=C1NS(=O)(=O)c2c1c(Cl)ccc2 | 2.352 | 2.660 |
| 181 | Thiophenesaccharine | O=C1NS(=O)(=O)c2c1csc2 | 3.000 | 2.108 |
| 182^ | Suosan derivative 1 | O=C(Nc1ccc(cc1)N(=O)=O)NCCC(=O)O | 2.845 | 1.981 |
| 183 | Suosan derivative 11 | OC(=O)CCNC(=S)Nc1ccc(cc1)N(=O)=O | 3.380 | 2.748 |
| 184 | Suosan derivative 13 | OC(=O)CCNC(=O)Oc1ccc(cc1)N(=O)=O | 1.301 | 2.177 |
| 185 | Suosan derivative 16 | N#Cc1ccc(cc1)NC(=O)NCCC(=O)O | 2.653 | 2.976 |
| 186 | Oxathiazinon dioxide derivative 1 | O=C1C=C(C)OS(=O)(=O)N1 | 2.114 | 1.604 |
| 187 | Oxathiazinon dioxide derivative 2 | CCC1=CC(=O)NS(=O)(=O)O1 | 2.176 | 1.727 |
| 188 | Oxathiazinon dioxide derivative 3 | CC1=C(C)OS(=O)(=O)NC1=O | 2.114 | 1.669 |
| 189 | Oxathiazinon dioxide derivative 4 | CCC1=C(C)OS(=O)(=O)NC1=O | 2.398 | 1.912 |
| 190^ | Oxathiazinon dioxide derivative 5 | CCC1=C(C)C(=O)NS(=O)(=O)O1 | 2.114 | 1.869 |
| 191 | Oxathiazinon dioxide derivative 6 | O=C1NS(=O)(=O)OC=C1C | 1.301 | 1.591 |
| 192 | 2-aminobenzoic acid | OC(=O)c1ccccc1N | 2.079 | 1.468 |
| 193^ | 1',4',6'-3Cl-sucrose | ClCC1OC(C(C1Cl)O)(CCl)OC1OC(CO)C(C(C1O)O)O | 2.000 | 2.084 | (o) |
| 194^ | 1',4'-2Cl-sucrose | OCC1OC(C(C1Cl)O)(CCl)OC1OC(CO)C(C(C1O)O)O | 1.477 | 1.358 |
| 195 | 4'-F-4,1',6'-3Cl-sucrose | ClCC1OC(C(C1F)O)(CCl)OC1OC(CO)C(C(C1O)O)Cl | 3.000 | 2.790 |
| 196^ | 4,1',4',6'-4Cl-sucrose | ClCC1OC(C(C1Cl)O)(CCl)OC1OC(CO)C(C(C1O)O)Cl | 3.322 | 2.687 |
| 197 | 4,1',4'-3Cl-sucrose | OCC1OC(C(C1Cl)O)(CCl)OC1OC(CO)C(C(C1O)O)Cl | 2.342 | 2.011 |
| 198 | 4,1',6'-3Br-sucrose | BrCC1OC(C(C1O)O)(CBr)OC1OC(CO)C(C(C1O)O)Br | 2.903 | 2.778 |
| 199^ | 4,1',6'-3Cl-sucrose (trichlorosucrose) | ClCC1OC(C(C1O)O)(CCl)OC1OC(CO)C(C(C1O)O)Cl | 2.813 | 2.198 |
| 200 | 4,1',6'-3F-sucrose | FCC1OC(C(C1O)O)(CF)OC1OC(CO)C(C(C1O)O)F | 1.602 | 1.529 |
| 201^ | 4,4',6'-3Cl-sucrose | ClCC1OC(C(C1Cl)O)(CO)OC1OC(CO)C(C(C1O)O)Cl | 2.204 | 2.151 |
| 202 | 4,6,1',6'-4Cl-sucrose | ClCC1OC(C(C1O)O)(CCl)OC1OC(CCl)C(C(C1O)O)Cl | 2.301 | 2.826 |
| 203 | 4-F-1',4',6'-3Cl-sucrose | ClCC1OC(C(C1Cl)O)(CCl)OC1OC(CO)C(C(C1O)O)F | 2.778 | 2.687 |
| 204 | 4-Hydroxy glycosides DHC | OCC1OC(Oc2cc(O)c(c(c2)O)C(=O)CCc2ccc(c(c2)O)O)C(C(C1O)O)OC1OC(C)C(C(C1O)O)O | 2.000 | 2.188 |
| 205 | 6,1',6'-3Cl-sucrose | ClCC1OC(C(C1O)O)(CCl)OC1OC(CCl)C(C(C1O)O)O | 1.398 | 2.218 |
| 206^ | Psicose | OCC1OC(C(C1O)O)(O)CO | -0.155 | -0.147 |
| 207 | Ribose | OCC(C(C(C=O)O)O)O | -0.155 | -0.039 |
| 208 | DHQ-3-SIFA | CC(=O)OC1C(Oc2c(C1=O)c(O)cc(c2)O)c1ccc(c(c1)O)O | 1.903 | 1.850 |
| 209^ | Hesperidin-7-glucose DHC | OCC1OC(Oc2cc(O)c(c(c2)O)C(=O)CCc2ccc(c(c2)O)OC)C(C(C1O)O)O | 2.000 | 2.009 |
| 210 | Sorbose | OCC(C(C(C(=O)CO)O)O)O | 0.000 | -0.157 |
| 211 | Arabinose | OCC1OC(C(C1O)O)O | -0.161 | 0.015 |
| 212 | Fucose | OC1C(C)OC(C(C1O)O)O | -0.161 | 0.155 |
| 213 | Liquiritin | OCC1OC(Oc2ccc(cc2)C2CC(=O)c3c(O2)cc(cc3)O)C(C(C1O)O)O | 2.398 | 1.683 |
| 214^ | Naringin DHC | OCC1OC(Oc2cc(O)c(c(c2)O)C(=O)CCc2ccc(cc2)O)C(C(C1O)O)OC1OC(C)C(C(C1O)O)O | 2.000 | 2.255 |
| 215 | Periandrin I | O=CC12CCC(C(C1CCC1(C2CCC2C1(C)CCC1(C2=CC(C)(CC1)C(=O)O)C)C)(C)C)OC1OC(C(=O)O)C(C(C1OC1OC(C(=O)O)C(C(C1O)O)O)O)O | 1.929 | 2.020 |
| 216 | Periandrin II | O=CC12CCC(C(C1CCC1(C2CC=C2C1(C)CCC1(C2CC(C)(CC1)C(=O)O)C)C)(C)C)OC1OC(C(=O)O)C(C(C1OC1OC(C(=O)O)C(C(C1O)O)O)O)O | 2.000 | 1.901 |
| 217^ | Periandrin III | OCC12CCC(C(C1CCC1(C2CCC2C1(C)CCC1(C2=CC(C)(CC1)C(=O)O)C)C)(C)C)OC1OC(C(=O)O)C(C(C1OC1OC(C(=O)O)C(C(C1O)O)O)O)O | 2.000 | 2.100 |
| 218 | Periandrin IV | OCC12CCC(C(C1CCC1(C2CC=C2C1(C)CCC1(C2CC(C)(CC1)C(=O)O)C)C)(C)C)OC1OC(C(=O)O)C(C(C1OC1OC(C(=O)O)C(C(C1O)O)O)O)O | 2.000 | 1.978 |
| 219 | Perillartine | ON=CC1=CCC(CC1)C(=C)C | 3.301 | 2.810 |
| 220 | Polypodosides A | OCC1OC(OC2CCC3(C(C2)C(=O)CC2C3CCC3(C2CCC3C(C2CCC(C(O2)OC2OC(C)C(C(C2O)O)O)C)C)C)C)C(C(C1O)O)OC1OC(C)C(C(C1O)O)O | 2.778 | 2.905 |
| 221 | Rubusoside | OCC1OC(OC(=O)C2(C)CCCC3(C2CCC24C3CCC(C4)(C(=C)C2)OC2OC(CO)C(C(C2O)O)O)C)C(C(C1O)O)O | 2.057 | 2.300 |
| 222 | Siamenoside I | OCC1OC(OC2C(OC(C(C2O)O)COC2OC(CO)C(C(C2O)O)O)OC(C(O)(C)C)CCC(C2CCC3(C2(C)CC(O)C2(C3CC=C3C2CCC(C3(C)C)OC2OC(CO)C(C(C2O)O)O)C)C)C)C(C(C1O)O)O | 2.748 | 2.255 |
| 223 | Yang Li glycosides DHC | OCC1OC(Oc2cc(O)c(c(c2)O)C(=O)CCc2ccc(cc2)O)C(C(C1O)O)O | 1.602 | 1.882 |
| 224^ | Acesulfame potassium\_CH3CH2\_H | CCC1=COS(=O)(=O)NC1=O | 1.301 | 1.754 |
| 225 | Acesulfame potassium\_H\_H | O=C1C=COS(=O)(=O)N1 | 1.000 | 1.484 |
| 226 | Baiyunoside | OCC1OC(OC2CCC3(C(C2(C)C)CCC(=C3CCc2cocc2)C)C)C(C(C1O)O)OC1OCC(C(C1O)O)O | 2.699 | 2.793 |
| 227^ | Mogroside II | OCC1OC(OC2C(OC(C(C2O)O)COC2OC(CO)C(C(C2O)O)O)OC(C(O)(C)C)CCC(C2CCC3(C2(C)CC(=O)C2(C3CC=C3C2CCC(C3(C)C)OC2OC(COC3OC(CO)C(C(C3O)O)O)C(C(C2O)O)O)C)C)C)C(C(C1O)O)O | 1.924 | 1.943 |
| 228 | Mogroside IV | OCC1OC(OCC2OC(OC(C(O)(C)C)CCC(C3CCC4(C3(C)CC(O)C3(C4CC=C4C3CCC(C4(C)C)OC3OC(COC4OC(CO)C(C(C4O)O)O)C(C(C3O)O)O)C)C)C)C(C(C2O)O)O)C(C(C1O)O)O | 2.097 | 2.108 |
| 229 | Mogroside V | OCC1OC(OC2C(OC(C(C2O)O)COC2OC(CO)C(C(C2O)O)O)OC(C(O)(C)C)CCC(C2CCC3(C2(C)CC(O)C2(C3CC=C3C2CCC(C3(C)C)OC2OC(COC3OC(CO)C(C(C3O)O)O)C(C(C2O)O)O)C)C)C)C(C(C1O)O)O | 2.477 | 2.145 |
| 230^ | Osladin | OCC1OC(OC2CCC3(C(C2)C(=O)CC2C3CCC3(C2CCC3C(C2CCC(C(O2)OC2OC(C)C(C(C2O)O)O)C)C)C)C)C(C(C1O)O)OC1OC(C)C(C(C1O)O)O | 3.477 | 2.905 |
| 231 | Rebaudioside F | OCC1OC(OC23CCC4C(C2)(CC3=C)CCC2C4(C)CCCC2(C)C(=O)OC2OC(CO)C(C(C2O)O)O)C(C(C1O)OC1OC(CO)C(C(C1O)O)O)OC1OCC(C(C1O)O)O | 2.051 | 2.547 |
| 232^ | Saccharin | O=C1NS(=O)(=O)c2c1cccc2 | 2.653 | 1.943 |
| 233 | Xylobiose | OC1COC(C(C1O)O)OC1COC(C(C1O)O)O | -0.398 | 0.035 |
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*Table 2S. Brief of the mathematical equations used in present work.*

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|  |  |
| : standard deviation; : number of molecules;: experimental property for compound *i*; : predicted property for compound *i*; *d*: number of descriptors; *:* root mean square deviation; : leverage for compound *i*; *xi*: descriptor vector for *i*; :model matrix for the training set (train); : number of molecules in train; : number of molecules in test; : warning leverage; : regression coefficient for the *j*th descriptor;: standardized ; : standard deviation for the *j*th descriptor; : standard deviation for the experimental property; and : values of property in regressions through the origin ofagainst and against; and : the correlation coefficients for regression ofagainst and againstthrough the origin; : average value for  in test set; : average value for  in test set; : modified squared correlation coefficient; : squared correlation coefficient between observed and predicted values for the test set with b intercept. | |

*Table 3S. Correlation matrix for the descriptors of the linear QSPR model.*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | AAC | ATSC6p | CATS2D\_02\_PN | CATS2D\_05\_LL | B07[C-N] | ALOGP |
| AAC | 1 | 0.122 | 0.010 | 0.178 | 0.004 | 0.030 |
| ATSC6p |  | 1.000 | 0.036 | 0.788 | 0.013 | 0.020 |
| CATS2D\_02\_PN |  |  | 1.000 | 0.028 | 0.000 | 0.009 |
| CATS2D\_05\_LL |  |  |  | 1 | 0.021 | 0.026 |
| B07[C-N] |  |  |  |  | 1 | 0.003 |
| ALOGP |  |  |  |  |  | 1 |

*Table 4S. Numerical values for the molecular descriptors appearing in Eq. 1.*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| ID | AAC | ATSC6p | CATS2D\_02\_PN | CATS2D\_05\_LL | B07[C-N] | ALOGP |
| 1 | 1.510 | 6.484 | 0 | 0 | 0 | -4.311 |
| 2 | 1.762 | 9.096 | 0 | 0 | 0 | -0.700 |
| 3 | 1.566 | 8.911 | 0 | 0 | 1 | -0.003 |
| 4^ | 1.645 | 6.380 | 0 | 1 | 1 | 0.212 |
| 5 | 1.500 | 0.675 | 0 | 0 | 0 | -2.564 |
| 6^ | 1.488 | 7.045 | 0 | 0 | 0 | -4.687 |
| 7 | 1.510 | 5.156 | 0 | 0 | 0 | -4.311 |
| 8^ | 1.510 | 5.713 | 0 | 0 | 0 | -4.260 |
| 9 | 1.502 | 16.388 | 0 | 4 | 0 | -0.124 |
| 10 | 1.495 | 10.582 | 0 | 2 | 1 | 2.431 |
| 11 | 1.488 | 7.045 | 0 | 0 | 0 | -4.687 |
| 12 | 1.488 | 5.371 | 0 | 0 | 0 | -4.687 |
| 13 | 1.457 | 1.256 | 0 | 0 | 0 | -2.940 |
| 14^ | 1.457 | 1.256 | 0 | 0 | 0 | -2.940 |
| 15 | 1.436 | 0.167 | 0 | 0 | 0 | -1.919 |
| 16 | 1.449 | 0.581 | 0 | 0 | 0 | -2.430 |
| 17 | 1.436 | 34.430 | 0 | 17 | 0 | -1.729 |
| 18 | 1.409 | 28.789 | 0 | 17 | 0 | 0.175 |
| 19 | 1.453 | 40.513 | 0 | 17 | 0 | -3.476 |
| 20 | 1.436 | 34.823 | 0 | 17 | 0 | -1.571 |
| 21^ | 1.445 | 40.401 | 0 | 17 | 0 | -2.588 |
| 22 | 1.465 | 45.960 | 0 | 17 | 0 | -5.223 |
| 23 | 1.453 | 39.866 | 0 | 17 | 0 | -3.476 |
| 24^ | 1.425 | 34.317 | 0 | 17 | 0 | -0.841 |
| 25 | 1.410 | 43.614 | 0 | 42 | 0 | 2.415 |
| 26 | 1.196 | 6.983 | 0 | 7 | 0 | 3.446 |
| 27 | 1.500 | 0.817 | 0 | 0 | 0 | -2.564 |
| 28 | 1.500 | 0.740 | 0 | 0 | 0 | -2.513 |
| 29 | 1.500 | 0.740 | 0 | 0 | 0 | -2.513 |
| 30^ | 1.500 | 0.740 | 0 | 0 | 0 | -2.513 |
| 31^ | 1.500 | 0.215 | 0 | 0 | 0 | -2.003 |
| 32 | 1.510 | 6.376 | 0 | 0 | 0 | -4.260 |
| 33^ | 1.510 | 6.376 | 0 | 0 | 0 | -4.260 |
| 34^ | 1.510 | 6.376 | 0 | 0 | 0 | -4.311 |
| 35^ | 1.513 | 12.186 | 0 | 0 | 0 | -6.057 |
| 36^ | 1.457 | 1.256 | 0 | 0 | 0 | -2.940 |
| 37 | 1.513 | 10.913 | 0 | 0 | 0 | -6.057 |
| 38^ | 1.474 | 0.612 | 0 | 0 | 0 | -1.625 |
| 39 | 1.414 | 0.022 | 0 | 0 | 0 | -1.408 |
| 40 | 1.689 | 2.902 | 0 | 3 | 1 | 1.834 |
| 41 | 1.622 | 2.556 | 0 | 2 | 1 | 1.073 |
| 42^ | 1.510 | 8.588 | 0 | 6 | 0 | 2.115 |
| 43^ | 1.411 | 5.203 | 0 | 6 | 0 | 2.936 |
| 44 | 1.411 | 5.325 | 0 | 4 | 0 | 2.944 |
| 45 | 1.336 | 6.025 | 0 | 6 | 0 | 3.412 |
| 46 | 1.429 | 4.174 | 0 | 6 | 0 | 3.115 |
| 47^ | 1.269 | 5.148 | 0 | 8 | 0 | 3.977 |
| 48^ | 1.336 | 6.296 | 0 | 8 | 0 | 3.673 |
| 49^ | 1.336 | 5.905 | 0 | 7 | 0 | 3.037 |
| 50^ | 1.509 | 6.100 | 0 | 7 | 0 | 3.680 |
| 51 | 1.563 | 5.343 | 0 | 6 | 0 | 4.232 |
| 52^ | 1.538 | 4.741 | 0 | 6 | 0 | 3.673 |
| 53^ | 1.509 | 6.243 | 0 | 5 | 0 | 3.502 |
| 54 | 1.532 | 6.959 | 0 | 5 | 0 | 4.061 |
| 55^ | 1.561 | 6.287 | 0 | 5 | 0 | 3.235 |
| 56 | 1.415 | 7.064 | 0 | 8 | 0 | 4.231 |
| 57 | 1.532 | 6.509 | 0 | 6 | 0 | 4.121 |
| 58 | 1.600 | 6.866 | 0 | 4 | 0 | 2.487 |
| 59^ | 1.481 | 7.322 | 0 | 4 | 0 | 1.590 |
| 60 | 1.385 | 7.996 | 0 | 8 | 0 | 2.376 |
| 61^ | 1.195 | 11.337 | 0 | 14 | 0 | 4.898 |
| 62 | 1.468 | 4.726 | 0 | 7 | 0 | 3.510 |
| 63 | 1.580 | 8.297 | 0 | 6 | 0 | 5.101 |
| 64^ | 1.723 | 8.165 | 0 | 6 | 0 | 4.996 |
| 65 | 1.418 | 4.835 | 0 | 9 | 0 | 2.822 |
| 66 | 1.474 | 4.193 | 0 | 7 | 0 | 2.304 |
| 67 | 1.461 | 5.299 | 0 | 7 | 0 | 2.555 |
| 68 | 1.589 | 5.072 | 0 | 8 | 0 | 2.425 |
| 69^ | 1.461 | 4.192 | 0 | 6 | 0 | 2.850 |
| 70 | 1.490 | 5.629 | 0 | 9 | 1 | 3.001 |
| 71 | 1.195 | 11.172 | 0 | 13 | 0 | 4.898 |
| 72 | 1.494 | 8.569 | 0 | 11 | 0 | 4.489 |
| 73^ | 1.509 | 5.876 | 0 | 6 | 0 | 3.494 |
| 74 | 1.532 | 6.818 | 0 | 7 | 0 | 4.239 |
| 75 | 1.446 | 5.691 | 0 | 6 | 0 | 2.821 |
| 76^ | 1.509 | 5.876 | 0 | 6 | 0 | 3.494 |
| 77 | 1.509 | 6.042 | 0 | 4 | 0 | 3.502 |
| 78 | 1.396 | 7.294 | 0 | 7 | 0 | 3.764 |
| 79 | 1.396 | 7.294 | 0 | 7 | 0 | 3.764 |
| 80^ | 1.538 | 4.677 | 0 | 6 | 0 | 3.243 |
| 81 | 1.703 | 6.884 | 0 | 6 | 0 | 5.392 |
| 82 | 1.628 | 7.889 | 0 | 9 | 0 | 5.125 |
| 83 | 1.639 | 7.657 | 0 | 6 | 0 | 4.438 |
| 84 | 1.430 | 6.312 | 0 | 7 | 0 | 3.046 |
| 85 | 1.455 | 5.036 | 0 | 5 | 0 | 2.718 |
| 86^ | 1.471 | 6.280 | 0 | 4 | 0 | 2.639 |
| 87 | 1.473 | 2.762 | 0 | 2 | 0 | 1.772 |
| 88^ | 1.508 | 6.598 | 0 | 4 | 0 | 1.736 |
| 89 | 1.466 | 9.330 | 0 | 10 | 0 | 2.891 |
| 90 | 1.402 | 5.434 | 0 | 7 | 0 | 3.089 |
| 91 | 1.252 | 6.105 | 0 | 8 | 0 | 4.433 |
| 92^ | 1.440 | 4.667 | 0 | 6 | 1 | 2.938 |
| 93 | 1.362 | 4.453 | 0 | 6 | 0 | 3.113 |
| 94 | 1.451 | 5.051 | 0 | 6 | 0 | 3.672 |
| 95 | 1.440 | 4.549 | 0 | 5 | 0 | 2.938 |
| 96^ | 1.429 | 3.974 | 0 | 6 | 0 | 2.978 |
| 97^ | 1.455 | 4.644 | 0 | 3 | 0 | 2.718 |
| 98 | 1.411 | 5.071 | 0 | 6 | 0 | 2.718 |
| 99 | 1.216 | 6.143 | 0 | 8 | 0 | 4.650 |
| 100 | 1.252 | 6.129 | 0 | 9 | 0 | 4.463 |
| 101^ | 1.342 | 5.383 | 0 | 6 | 0 | 3.710 |
| 102^ | 1.323 | 6.881 | 0 | 6 | 0 | 3.961 |
| 103 | 1.323 | 6.472 | 0 | 8 | 0 | 3.373 |
| 104^ | 1.252 | 6.142 | 0 | 9 | 0 | 4.463 |
| 105^ | 1.323 | 6.191 | 0 | 7 | 0 | 3.961 |
| 106^ | 1.342 | 5.132 | 0 | 7 | 0 | 3.710 |
| 107 | 1.432 | 5.191 | 0 | 7 | 0 | 4.183 |
| 108^ | 1.392 | 5.651 | 0 | 6 | 0 | 3.745 |
| 109^ | 1.252 | 6.148 | 0 | 10 | 0 | 4.326 |
| 110 | 1.461 | 4.706 | 0 | 6 | 0 | 2.987 |
| 111 | 1.574 | 5.331 | 0 | 6 | 0 | 3.545 |
| 112 | 1.542 | 6.113 | 0 | 6 | 1 | 2.174 |
| 113 | 1.392 | 6.139 | 0 | 6 | 0 | 2.770 |
| 114^ | 1.446 | 6.086 | 0 | 6 | 0 | 2.549 |
| 115 | 1.430 | 7.072 | 0 | 8 | 0 | 2.898 |
| 116^ | 1.413 | 7.643 | 0 | 9 | 0 | 3.421 |
| 117 | 1.392 | 5.879 | 0 | 6 | 0 | 3.174 |
| 118^ | 1.374 | 6.856 | 0 | 8 | 0 | 3.523 |
| 119 | 1.371 | 0.000 | 0 | 0 | 0 | -0.897 |
| 120^ | 1.449 | 0.581 | 0 | 0 | 0 | -2.430 |
| 121 | 1.515 | 15.344 | 0 | 0 | 0 | -7.804 |
| 122^ | 1.497 | 7.422 | 0 | 0 | 0 | -3.902 |
| 123 | 1.485 | 8.408 | 0 | 0 | 0 | -3.494 |
| 124 | 1.690 | 1.498 | 0 | 0 | 0 | -1.360 |
| 125^ | 1.790 | 2.191 | 0 | 0 | 0 | -0.156 |
| 126 | 1.478 | 1.819 | 0 | 0 | 0 | -2.105 |
| 127 | 1.630 | 7.119 | 0 | 0 | 0 | -3.107 |
| 128 | 1.630 | 7.439 | 0 | 0 | 0 | -3.107 |
| 129 | 1.630 | 7.661 | 0 | 0 | 0 | -3.107 |
| 130^ | 1.706 | 8.728 | 0 | 0 | 0 | -1.903 |
| 131 | 1.706 | 8.176 | 0 | 0 | 0 | -1.903 |
| 132 | 1.640 | 6.527 | 0 | 0 | 0 | -0.257 |
| 133 | 1.669 | 0.000 | 1 | 0 | 0 | -0.601 |
| 134 | 1.669 | 1.370 | 1 | 0 | 1 | -1.107 |
| 135 | 1.808 | 0.258 | 1 | 0 | 0 | -1.847 |
| 136 | 1.743 | 0.565 | 0 | 0 | 0 | -1.526 |
| 137 | 1.761 | 0.000 | 1 | 0 | 0 | -0.978 |
| 138 | 1.782 | 0.873 | 1 | 0 | 0 | -1.015 |
| 139 | 1.477 | 0.591 | 1 | 0 | 0 | 0.699 |
| 140 | 1.477 | 0.868 | 1 | 0 | 0 | 0.631 |
| 141 | 1.739 | 1.111 | 1 | 0 | 0 | -0.273 |
| 142 | 1.529 | 0.471 | 1 | 0 | 0 | 0.379 |
| 143 | 1.542 | 2.074 | 1 | 0 | 0 | 0.955 |
| 144 | 1.609 | 0.168 | 0 | 0 | 0 | -0.057 |
| 145 | 1.676 | 0.191 | 0 | 0 | 0 | -1.147 |
| 146 | 1.724 | 0.028 | 1 | 0 | 0 | -1.489 |
| 147 | 1.659 | 0.120 | 1 | 0 | 0 | -1.111 |
| 148 | 1.604 | 3.070 | 1 | 1 | 1 | 1.249 |
| 149^ | 1.613 | 2.042 | 1 | 0 | 0 | 0.688 |
| 150 | 1.673 | 5.632 | 0 | 0 | 1 | -0.370 |
| 151 | 1.646 | 6.019 | 0 | 0 | 1 | 0.087 |
| 152 | 1.576 | 9.211 | 0 | 0 | 1 | 0.697 |
| 153 | 1.618 | 4.923 | 0 | 4 | 1 | -0.742 |
| 154 | 1.594 | 6.744 | 0 | 3 | 1 | -0.487 |
| 155 | 1.622 | 5.124 | 0 | 3 | 1 | -0.619 |
| 156 | 1.515 | 8.790 | 0 | 3 | 1 | 0.298 |
| 157 | 1.687 | 4.715 | 0 | 3 | 1 | -0.624 |
| 158 | 1.591 | 5.446 | 0 | 3 | 1 | -0.162 |
| 159^ | 1.538 | 7.414 | 0 | 3 | 1 | 0.341 |
| 160 | 1.594 | 5.765 | 0 | 3 | 1 | -0.487 |
| 161 | 1.543 | 7.429 | 0 | 4 | 1 | 0.267 |
| 162^ | 1.686 | 9.771 | 0 | 1 | 1 | 1.685 |
| 163 | 1.497 | 9.144 | 0 | 0 | 1 | 4.371 |
| 164 | 1.590 | 8.878 | 0 | 3 | 1 | 2.502 |
| 165^ | 1.598 | 8.494 | 1 | 0 | 1 | 0.662 |
| 166 | 1.794 | 2.144 | 0 | 0 | 1 | 0.495 |
| 167 | 1.876 | 1.863 | 0 | 0 | 0 | 0.510 |
| 168 | 1.811 | 0.471 | 0 | 0 | 0 | 0.978 |
| 169 | 1.802 | 1.415 | 0 | 0 | 0 | 0.961 |
| 170 | 1.742 | 2.262 | 0 | 2 | 1 | 1.310 |
| 171^ | 1.642 | 3.258 | 0 | 3 | 1 | 2.290 |
| 172 | 2.055 | 0.481 | 0 | 0 | 0 | 1.183 |
| 173 | 2.055 | 0.808 | 0 | 0 | 0 | 1.642 |
| 174 | 2.055 | 1.220 | 0 | 0 | 0 | 1.726 |
| 175^ | 2.055 | 2.641 | 0 | 0 | 0 | 1.556 |
| 176 | 1.785 | 1.864 | 0 | 2 | 1 | 1.046 |
| 177^ | 1.689 | 3.126 | 0 | 4 | 1 | 1.688 |
| 178 | 1.865 | 0.404 | 0 | 0 | 0 | 0.710 |
| 179 | 2.181 | 0.585 | 0 | 0 | 0 | 0.565 |
| 180 | 2.181 | 0.740 | 0 | 0 | 0 | 1.024 |
| 181 | 2.156 | 0.000 | 0 | 0 | 0 | 0.022 |
| 182^ | 1.836 | 2.337 | 0 | 0 | 0 | 0.545 |
| 183 | 1.960 | 3.540 | 0 | 0 | 0 | 1.444 |
| 184 | 1.809 | 2.247 | 0 | 0 | 0 | 1.192 |
| 185 | 1.750 | 2.629 | 0 | 0 | 1 | 0.530 |
| 186 | 2.066 | 0.245 | 0 | 0 | 0 | -0.857 |
| 187 | 1.989 | 0.753 | 0 | 0 | 0 | -0.334 |
| 188 | 1.989 | 0.547 | 0 | 0 | 0 | -0.411 |
| 189 | 1.914 | 2.163 | 0 | 0 | 0 | 0.045 |
| 190^ | 1.914 | 1.615 | 0 | 0 | 0 | 0.113 |
| 191 | 2.066 | 0.363 | 0 | 0 | 0 | -0.925 |
| 192 | 1.658 | 0.672 | 0 | 0 | 0 | 0.688 |
| 193^ | 1.762 | 9.143 | 0 | 1 | 0 | -0.700 |
| 194^ | 1.706 | 8.160 | 0 | 1 | 0 | -1.903 |
| 195 | 1.882 | 8.873 | 0 | 0 | 0 | 0.240 |
| 196^ | 1.803 | 9.399 | 0 | 1 | 0 | 0.504 |
| 197 | 1.762 | 8.571 | 0 | 1 | 0 | -0.700 |
| 198 | 1.762 | 12.228 | 0 | 0 | 0 | -0.263 |
| 199^ | 1.762 | 9.096 | 0 | 0 | 0 | -0.700 |
| 200 | 1.762 | 6.387 | 0 | 0 | 0 | -1.491 |
| 201^ | 1.762 | 8.730 | 0 | 0 | 0 | -0.700 |
| 202 | 1.803 | 9.552 | 0 | 0 | 0 | 0.504 |
| 203 | 1.882 | 8.997 | 0 | 1 | 0 | 0.240 |
| 204 | 1.512 | 15.597 | 0 | 4 | 0 | -0.375 |
| 205 | 1.762 | 9.250 | 0 | 0 | 0 | -0.700 |
| 206^ | 1.500 | 0.817 | 0 | 0 | 0 | -2.564 |
| 207 | 1.500 | 0.431 | 0 | 0 | 0 | -2.173 |
| 208 | 1.522 | 7.615 | 0 | 6 | 0 | 1.864 |
| 209^ | 1.503 | 10.848 | 0 | 4 | 0 | 0.735 |
| 210 | 1.500 | 1.152 | 0 | 0 | 0 | -2.693 |
| 211 | 1.500 | 0.309 | 0 | 0 | 0 | -2.003 |
| 212 | 1.474 | 0.612 | 0 | 0 | 0 | -1.625 |
| 213 | 1.491 | 9.666 | 0 | 5 | 0 | 0.661 |
| 214^ | 1.500 | 15.461 | 0 | 4 | 0 | -0.107 |
| 215 | 1.410 | 44.826 | 0 | 45 | 0 | 2.511 |
| 216 | 1.410 | 43.904 | 0 | 45 | 0 | 2.511 |
| 217^ | 1.402 | 46.381 | 0 | 45 | 0 | 2.255 |
| 218 | 1.402 | 45.431 | 0 | 45 | 0 | 2.255 |
| 219 | 1.354 | 2.347 | 0 | 2 | 1 | 2.755 |
| 220 | 1.381 | 40.907 | 0 | 27 | 0 | 0.780 |
| 221 | 1.409 | 28.890 | 0 | 17 | 0 | 0.018 |
| 222 | 1.404 | 54.263 | 0 | 37 | 0 | -2.232 |
| 223 | 1.500 | 9.859 | 0 | 4 | 0 | 0.751 |
| 224^ | 1.989 | 1.390 | 0 | 0 | 0 | -0.468 |
| 225 | 2.126 | 0.000 | 0 | 0 | 0 | -1.371 |
| 226 | 1.384 | 27.323 | 0 | 17 | 0 | 1.857 |
| 227^ | 1.426 | 57.119 | 0 | 37 | 0 | -4.019 |
| 228 | 1.404 | 53.117 | 0 | 37 | 0 | -2.232 |
| 229 | 1.421 | 58.646 | 0 | 37 | 0 | -3.979 |
| 230^ | 1.381 | 40.907 | 0 | 27 | 0 | 0.780 |
| 231 | 1.451 | 39.554 | 0 | 17 | 0 | -2.965 |
| 232^ | 1.969 | 0.558 | 0 | 0 | 0 | 0.360 |
| 233 | 1.512 | 4.172 | 0 | 0 | 0 | -3.239 |