**Table XXX: List of chemicals from the primary screen** (Total 164 Chemicals)

Green – Positive Hits (p<0.01)

Yellow – False Hits (p<0.01, but not significant (p<0.05) when re-bought and re-tested)

|  |  |  |
| --- | --- | --- |
| **Chemical Name** | **SMILES** | **Vendor and Catalogue Number** |
| D-(-)-Lactic acid | O[C@H](C)C(=O)O |  |
| Sedoheptulose anhydride monohydrate | O1[C@]2(OC[C@@H]1[C@H]([C@H]([C@@H]2O)O)O)CO.O |  |
| D-Galacturonic acid sodium salt | [Na+].[O-]C(=O)[C@H]1OC([C@@H]([C@H]([C@H]1O)O)O)O |  |
| DL-Glyceraldehyde | OC(CO)C=O |  |
| Lactobionic acid | O1[C@H]([C@@H]([C@H]([C@H]([C@H]1CO)O)O)O)O[C@@H]([C@H](O)[C@@H](O)C(=O)O)[C@H](O)CO |  |
| alpha-D-Glucose 1-phosphate disodium salt hydrate | [Na+].[Na+].[P](=O)([O-])([O-])O[C@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO.O |  |
| N-Acetylneuraminic acid | N([C@H]1[C@@H](O[C@](C[C@@H]1O)(O)C(=O)O)[C@H](O)[C@H](O)CO)C(=O)C |  |
| 2,3-dihydroxypropyl dihydrogen phosphate | [P](=O)(OCC(O)CO)(O)O |  |
| N-Acetylmuramic acid | N([C@H]([C@@H](O[C@H](C)C(=O)O)[C@H](O)[C@H](O)CO)C=O)C(=O)C |  |
| L-(+)-Erythrulose | O[C@@H](CO)C(=O)CO |  |
| D-(+)-Talose | O1[C@@H]([C@@H]([C@@H]([C@@H](C1O)O)O)O)CO |  |
| D-(+)-Arabitol | O[C@@H](C(O)[C@H](O)CO)CO |  |
| D-(+)-Cellobiose | O[C@@H]1[C@@H](O)C(O)O[C@H](CO)[C@H]1O[C@H](O2)[C@H](O)[C@@H](O)[C@H](O)[C@H]2CO |  |
| Sucralose | Cl[C@H]1[C@H](O[C@@H]([C@@H]([C@H]1O)O)O[C@@]2(O[C@@H]([C@H]([C@@H]2O)O)CCl)CCl)CO |  |
| D-Psicose | C1[C@H]([C@H]([C@H](C(O1)(CO)O)O)O)O |  |
| Gluconolactone | O1[C@@H]([C@H]([C@@H]([C@H](C1=O)O)O)O)CO |  |
| 6-Phosphogluconic acid trisodium salt | [Na+].[Na+].[Na+].[P](=O)([O-])([O-])OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C(=O)[O-] |  |
| D-Glucose 6-phosphate sodium salt | [Na+].[P](=O)([O-])(OC[C@H]1O[C@H]([C@@H]([C@H]([C@@H]1O)O)O)O)O |  |
| cis-Inositol | O[C@@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H]1O)O)O)O)O |  |
| D-Lactitol monohydrate | O1[C@H]([C@@H]([C@H]([C@H]([C@H]1CO)O)O)O)O[C@@H]([C@H](O)[C@@H](O)CO)[C@H](O)CO.O |  |
| DL-Lactic acid | OC(C)C(=O)O |  |
| Meglumine | N(C[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO)C |  |
| Glycerol | OC(CO)CO |  |
| D-(+)-Mannose | O1[C@@H]([C@H]([C@@H]([C@@H](C1O)O)O)O)CO |  |
| N-Acetyl-D-glucosamine | N([C@@H]1[C@H]([C@@H]([C@H](OC1O)CO)O)O)C(=O)C |  |
| alpha-D-Galactosamine 1-phosphate | C([C@@H]1[C@@H]([C@@H]([C@H]([C@H](O1)OP(=O)(O)O)N)O)O)O |  |
| L-Galactono-1,4-lactone | O1[C@@H]([C@H]([C@@H](C1=O)O)O)[C@@H](O)CO |  |
| alpha-D-Glucose 1,6-bisphosphate potassium salt hydrate | [K+].[K+].[K+].[K+].[P](=O)([O-])([O-])O[C@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO[P](=O)([O-])[O-] |  |
| D-Arabino-1,4-lactone | O1[C@@H]([C@H]([C@@H](C1=O)O)O)CO |  |
| 5-Thio-D-glucose | OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)C(O)S1 |  |
| Thioglycolic acid solution | SCC(=O)O |  |
| alpha-Lactose monohydrate | O1[C@H]([C@@H]([C@H]([C@H]([C@H]1CO)O)O)O)O[C@@H]2[C@H](O[C@@H]([C@@H]([C@H]2O)O)O)CO.O |  |
| myo-Inositol | O[C@@H]1[C@H]([C@H]([C@H]([C@@H]([C@H]1O)O)O)O)O |  |
| Amygdalin | N#CC(O[C@@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CO[C@@H]3O[C@@H]([C@H]([C@@H]([C@H]3O)O)O)CO)c1ccccc1 |  |
| D-Glucose 6-phosphate disodium salt hydrate | [Na+].[Na+].[P](=O)([O-])([O-])OC[C@H]1OC([C@@H]([C@H]([C@@H]1O)O)O)O.O |  |
| Isomaltose | O1[C@@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)OC[C@H]2OC([C@@H]([C@H]([C@@H]2O)O)O)O |  |
| D-(-)-3-Phosphoglyceric acid disodium salt | [Na+].[Na+].[P](=O)([O-])(OC[C@@H](O)C(=O)[O-])O |  |
| L-(+)-Threose | O1C([C@H]([C@@H](C1)O)O)O |  |
| (-)-Sinigrin hydrate | [K+].[S](=O)(=O)([O-])ONC(=CC=C)S[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO.O |  |
| D-(+)-Glucosamine hydrochloride | Cl.N[C@@H]1[C@H]([C@@H]([C@H](OC1O)CO)O)O |  |
| DL-Xylose | O[C@@H]([C@H](O)CO)[C@@H](O)C=O |  |
| Maltitol | O1[C@@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@@H]([C@H](O)[C@@H](O)CO)[C@H](O)CO |  |
| Mannide monooleate | O1[C@@H]([C@@H]([C@H](C1)O)O)[C@H](O)COC(=O)CCCCCCC\C=C/CCCCCCCC |  |
| D-Sorbitol 6-phosphate barium salt | [Ba+2].[P](=O)([O-])([O-])OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)CO |  |
| D-Mannose 6-phosphate sodium salt | OC(O1)[C@@H](O)[C@@H](O)[C@H](O)[C@H]1COP(O)([O-])=O.[Na+] |  |
| D-Arabinose 5-phosphate disodium salt | C([C@@H]1[C@H]([C@@H](C(O1)O)O)O)OP(=O)([O-])[O-].[Na+].[Na+] |  |
| D-Xylono-1,4-lactone | O1[C@@H]([C@@H]([C@H](C1=O)O)O)CO |  |
| 3-O-Methyl-D-glucopyranose | O[C@@H]1[C@H](OC([C@@H]([C@H]1OC)O)O)CO |  |
| Xylitol | O[C@H]([C@@H](O)CO)[C@H](O)CO |  |
| sn-Glycerol 3-phosphate bis(cyclohexylammonium) salt | [P](=O)(OC[C@H](O)CO)(O)O.NC2CCCCC2.NC1CCCCC1 |  |
| DL-Glyceric acid hemicalcium salt hydrate | [Ca+2].[O-]C(=O)C(O)CO.[O-]C(=O)C(O)CO.O.O |  |
| beta-Lactose | O1[C@H]([C@@H]([C@H]([C@H]([C@H]1CO)O)O)O)O[C@@H]2[C@H](O[C@H]([C@@H]([C@H]2O)O)O)CO |  |
| D-Glucosamine 6-phosphate | C([C@@H]1[C@H]([C@@H]([C@H](C(O1)O)N)O)O)OP(=O)(O)O |  |
| Sodium L-lactate | [Na+].[O-]C(=O)[C@@H](O)C |  |
| D-Arabinonic acid sodium salt | [Na+].[O-]C(=O)[C@@H](O)[C@H](O)[C@H](O)CO |  |
| 3,5-dideoxy-5-(glycoloylamino)-D-glycero-beta-D-galacto-non-2-ulopyranosonic acid | N([C@H]1[C@@H](O[C@](C[C@@H]1O)(O)C(=O)O)[C@H](O)[C@H](O)CO)C(=O)CO |  |
| D-Glucosamine 3-sulfate | [S](=O)(=O)(O[C@H]1[C@@H]([C@H](OC([C@@H]1N)O)CO)O)O |  |
| Ethyl-beta-D-thiogalactopyranoside | S([C@@H]1O[C@@H]([C@@H]([C@@H]([C@H]1O)O)O)CO)CC |  |
| D-Erythronic acid gamma-lactone | O1C[C@H]([C@H](C1=O)O)O |  |
| Methyl-beta-D-glucopyranoside hemihydrate | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)OC |  |
| beta-Estradiol | O[C@@H]1[C@@]2([C@H]([C@H]3[C@H](CC2)c4c(cc(cc4)O)CC3)CC1)C |  |
| 2-hydroxymethyl-tetrahydro-pyran-3,4,5-triol | O1C(C(C(C(C1)O)O)O)CO |  |
| Adonitol | O[C@H]([C@H](O)CO)[C@@H](O)CO |  |
| meso-Erythritol | O[C@H]([C@H](O)CO)CO |  |
| N-Acetyl-alpha-D-glucosamine 1-phosphate disodium salt | CC(=O)N[C@@H]1[C@H]([C@@H]([C@H](O[C@@H]1OP(=O)(O)O)CO)O)O |  |
| Biotin | S1[C@H]([C@H]2NC(=O)N[C@H]2C1)CCCCC(=O)O |  |
| 2-Deoxy-D-ribonic acid lithium salt | O[C@@H]([C@@H](O)CC(=O)O)CO |  |
| Chloralose | ClC(Cl)(Cl)[C@H]1O[C@H]2O[C@@H]([C@@H]([C@H]2O1)O)[C@H](O)CO |  |
| p-Acetamidophenyl beta-D-glucuronide sodium salt | [Na+].N(c1ccc(cc1)O[C@@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)C(=O)[O-])C(=O)C |  |
| Arbutin | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)Oc2ccc(cc2)O |  |
| D-Sorbitol | O[C@@H]([C@H](O)[C@H](O)CO)[C@@H](O)CO |  |
| 2'-Hydroxy-4'-methoxyacetophenone | O(C)c1cc(c(cc1)C(=O)C)O |  |
| D-Mannitol | O[C@@H]([C@H](O)[C@H](O)CO)[C@H](O)CO |  |
| D-Mannose 6-phosphate disodium salt hydrate | [Na+].[Na+].[P](=O)([O-])([O-])OC[C@H]1OC([C@H]([C@H]([C@@H]1O)O)O)O.O |  |
| D-Fructose 1,6-bisphosphate trisodium salt hydrate | C([C@@H]1[C@H]([C@@H](C(O1)(COP(=O)(O)O)O)O)O)OP(=O)(O)O |  |
| 6-deoxy-l-galactonic acid sodium salt | [Na+].[O-]C(=O)[C@@H](O)[C@H](O)[C@H](O)[C@@H](O)C |  |
| L-(+)-Gulose | O1[C@H]([C@H]([C@@H]([C@@H](C1O)O)O)O)CO |  |
| Nigerose | O1[C@@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@H]2[C@@H]([C@H](OC([C@@H]2O)O)CO)O |  |
| Methyl alpha-D-mannopyranoside | O1[C@@H]([C@H]([C@H]([C@@H]([C@H]1CO)O)O)O)OC |  |
| 4-Aminophenyl beta-D-galactopyranoside | C1=CC(=CC=C1N)O[C@H]2[C@@H]([C@H]([C@H]([C@H](O2)CO)O)O)O |  |
| 1-Deoxy-1-morpholino-D-fructose | N1(CCOCC1)CC(=O)[C@@H](O)[C@H](O)[C@H](O)CO |  |
| D-Fructose 6-phosphate dipotassium salt | [K+].[K+].[P](=O)([O-])([O-])OC[C@H]1OC([C@H]([C@@H]1O)O)(O)CO |  |
| D-Glucuronic acid | O=C(O)[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)C(O)O1 |  |
| 2-Keto-D-gluconic acid hemicalcium salt hydrate | [Ca+2].[O-]C(=O)C(=O)[C@@H](O)[C@H](O)[C@H](O)CO.[O-]C(=O)C(=O)[C@@H](O)[C@H](O)[C@H](O)CO.O |  |
| Melibiose | C([C@@H]1[C@@H]([C@@H]([C@H]([C@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@H](O2)O)O)O)O)O)O)O)O |  |
| Phthaldialdehyde | O=Cc1c(cccc1)C=O |  |
| D-Saccharic acid 1,4-lactone monohydrate | O1[C@@H]([C@@H]([C@H](C1=O)O)O)[C@H](O)C(=O)O.O |  |
| alpha-D-Glucoheptonic acid sodium salt | [Na+].[O-]C(=O)[C@H](O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO |  |
| D-(-)-Arabinose | O1C([C@H]([C@@H]([C@@H](C1)O)O)O)O |  |
| D-Xylonic acid lithium salt | O[C@@H]([C@H](O)CO)[C@@H](O)C(=O)O |  |
| Dulcitol | O[C@H]([C@H](O)[C@@H](O)CO)[C@H](O)CO |  |
| n-Dodecyl beta-D-glucopyranoside | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)OCCCCCCCCCCCC |  |
| D-(-)-Fructose | C1[C@H]([C@H]([C@@H](C(O1)(CO)O)O)O)O |  |
| L-(-)-Glucose | C([C@H]1[C@@H]([C@H]([C@@H](C(O1)O)O)O)O)O |  |
| Methyl-beta-D-galactopyranoside | O1[C@H]([C@@H]([C@H]([C@H]([C@H]1CO)O)O)O)OC |  |
| Methyl beta-D-xylopyranoside | O1[C@H]([C@@H]([C@H]([C@@H](C1)O)O)O)OC |  |
| Palatinose hydrate | O1[C@@H]([C@H]([C@@H](C1(O)CO)O)O)CO[C@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CO.O |  |
| Sucrose | O1[C@]([C@H]([C@@H]([C@H]1CO)O)O)(O[C@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CO)CO |  |
| 2-Azidoethyl beta-lactopyranoside | [N+](=[N-])=NCCO[C@@H]1OC([C@H](C(C1O)O)O[C@@H]2OC(C([C@@H](C2O)O)O)CO)CO |  |
| Calcium D-gluconate monohydrate | [Ca+2].[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO.[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO.O |  |
| epi-Inositol | O[C@@H]1[C@H]([C@H]([C@H]([C@H]([C@H]1O)O)O)O)O |  |
| Dithranol | Oc1c2c(cc3c1c(ccc3)O)cccc2O |  |
| 1,4-Dithioerythritol | SC[C@H](O)[C@H](O)CS |  |
| D-(+)-Fucose | C[C@@H]1[C@@H]([C@@H]([C@H]([C@@H](O1)O)O)O)O |  |
| L-(-)-Galactose | O1[C@H]([C@H]([C@H]([C@@H](C1O)O)O)O)CO |  |
| 2alpha-Mannobiose | O1[C@@H]([C@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@H]2[C@H]([C@@H]([C@H](OC2O)CO)O)O |  |
| 1-Thioglycerol | SCC(O)CO |  |
| 2-Phenylethyl beta-D-thiogalactoside | S([C@@H]2O[C@@H]([C@@H]([C@@H]([C@H]2O)O)O)CO)CCc1ccccc1 |  |
| Sodium salicylate | [Na+].[O-]C(=O)c1c(cccc1)O |  |
| Sodium thioglycolate | [Na+].SCC(=O)[O-] |  |
| Glycerol phosphate calcium salt | [CaH2].[P](=O)(OC(CO)CO)(O)O |  |
| DL-alpha-Glycerol phosphate magnesium salt hydrate | [Mg+2].[P](=O)([O-])([O-])OCC(O)CO.O |  |
| D-(+)-Xylose | O1C([C@@H]([C@H]([C@@H](C1)O)O)O)O |  |
| 2-Deoxyribose 5-phosphate sodium salt | C(C=O)[C@@H]([C@@H](COP(=O)([O-])[O-])O)O.[Na+].[Na+] |  |
| N-Acetyl-2,3-dehydro-2-deoxyneuraminic acid | N([C@H]1[C@@H](OC(=C[C@@H]1O)C(=O)O)[C@H](O)[C@H](O)CO)C(=O)C |  |
| D-Glucosaminic acid | N[C@H]([C@@H](O)[C@H](O)[C@H](O)CO)C(=O)O |  |
| beta-Glycerophosphate disodium salt hydrate | [Na+].[Na+].[P](=O)([O-])([O-])OC(CO)CO.O |  |
| L-(-)-Mannose | O1[C@H]([C@@H]([C@H]([C@H](C1O)O)O)O)CO |  |
| alpha-D-Mannose pentaacetate | CC(=O)OC[C@@H]1[C@H]([C@@H]([C@@H]([C@H](O1)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C |  |
| Ascorbyl Glucoside | C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)OC2=C([C@H](OC2=O)[C@H](CO)O)O)O)O)O)O |  |
| Sucrose 6'-monophosphate dipotassium salt | C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@]2([C@H]([C@@H]([C@H](O2)COP(=O)([O-])[O-])O)O)CO)O)O)O)O.[K+].[K+] |  |
| D-(-)-Tagatose | C1[C@H]([C@@H]([C@@H](C(O1)(CO)O)O)O)O |  |
| Magnesium D-gluconate hydrate | [Mg+2].[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO.[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO.O |  |
| N-Acetyl-D-glucosamine 6-sulfate sodium salt | [Na+].[S](=O)(=O)([O-])OC[C@H]1OC([C@@H]([C@H]([C@@H]1O)O)NC(=O)C)O |  |
| L-(-)-Arabitol | O[C@H](C(O)[C@@H](O)CO)CO |  |
| L-(-)-Dithiothreitol | SC[C@H](O)[C@@H](O)CS |  |
| alpha-D-Galactose 1-phosphate dipotassium salt pentahydrate | [K+].[K+].[P](=O)([O-])([O-])O[C@H]1O[C@@H]([C@@H]([C@@H]([C@H]1O)O)O)CO.O.O.O.O.O |  |
| n-Heptyl beta-D-thioglucopyranoside | S([C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO)CCCCCCC |  |
| Methyl alpha-D-galactopyranoside | O1[C@@H]([C@@H]([C@H]([C@H]([C@H]1CO)O)O)O)OC |  |
| Methyl-beta-D-thiogalactoside | S([C@@H]1O[C@@H]([C@@H]([C@@H]([C@H]1O)O)O)CO)C |  |
| Lactulose | O1[C@@]([C@H]([C@@H]([C@H]1CO)O[C@@H]2O[C@@H]([C@@H]([C@@H]([C@H]2O)O)O)CO)O)(O)CO |  |
| D-Saccharic acid potassium salt | [K+].[O-]C(=O)[C@H](O)[C@H](O)[C@@H](O)[C@H](O)C(=O)O |  |
| D-(+)-Turanose | O1[C@@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@H]2[C@@H]([C@@H](COC2(O)CO)O)O |  |
| Catalpol | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@@H]2OC=C[C@@H]3[C@H]2[C@]4(O[C@H]4[C@H]3O)CO |  |
| L-Ascorbic acid | O1[C@@H](C(C(=O)C1=O)O)[C@@H](O)CO |  |
| Digalacturonic acid | [C@@H]1([C@H]([C@H](O[C@@H]([C@@H]1O)O[C@@H]2[C@@H]([C@H](C(O[C@@H]2C(=O)O)O)O)O)C(=O)O)O)O |  |
| DL-Dithiothreitol | SC[C@@H](O)[C@H](O)CS |  |
| D-(+)-Galactose | C([C@@H]1[C@@H]([C@@H]([C@H](C(O1)O)O)O)O)O |  |
| L-Iditol | O[C@@H]([C@H](O)[C@@H](O)CO)[C@@H](O)CO |  |
| N-Acetyl-D-galactosamine | N([C@@H]1[C@H]([C@H]([C@H](OC1O)CO)O)O)C(=O)C |  |
| Nonyl beta-D-glucopyranoside | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)OCCCCCCCCC |  |
| L-Rhamnose monohydrate | O[C@@H]1[C@H]([C@H](C(O[C@H]1C)O)O)O |  |
| D-(+)-Sorbose | C1[C@H]([C@@H]([C@H](C(O1)(CO)O)O)O)O |  |
| 2,3,5-Tri-O-benzyl-beta-D-arabinofuranose | O1[C@H]([C@H]([C@@H]([C@H]1COCc4ccccc4)OCc3ccccc3)OCc2ccccc2)O |  |
| Sodium gluconate | [Na+].[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO |  |
| Aucubin | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@@H]2OC=C[C@@H]3[C@H]2C(=C[C@H]3O)CO |  |
| N-Acetyl-D-lactosamine | N([C@@H]1[C@H]([C@@H]([C@H](OC1O)CO)O[C@@H]2O[C@@H]([C@@H]([C@@H]([C@H]2O)O)O)CO)O)C(=O)C |  |
| Decyl beta-D-glucopyranoside | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)OCCCCCCCCCC |  |
| L(+)-Erythrose | C1[C@@H]([C@@H]([C@@H](O1)O)O)O |  |
| D-(+)-Galactosamine hydrochloride | C([C@@H]1[C@@H]([C@@H]([C@H](C(O1)O)N)O)O)O |  |
| IPTG | S([C@@H]1O[C@@H]([C@@H]([C@@H]([C@H]1O)O)O)CO)C(C)C |  |
| Octyl alpha-D-glucopyranoside | O1[C@@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)OCCCCCCCC |  |
| L-(+)-Ribose | O1[C@H]([C@@H]([C@@H](C1O)O)O)CO |  |
| Gastrodin | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)Oc2ccc(cc2)CO |  |
| D-(+)-Trehalose dihydrate | O1[C@@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CO.O.O |  |
| L-(+)-Arabinose | C1[C@@H]([C@@H]([C@H](C(O1)O)O)O)O |  |
| 2-Deoxy-D-glucose | O[C@H]([C@H](O)CO)[C@H](O)CC=O |  |
| 5-Keto-D-gluconic acid potassium salt | [K+].[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)C(=O)CO |  |
| D-Mannosamine hydrochloride | Cl.N[C@H]1[C@H]([C@@H]([C@H](OC1O)CO)O)O |  |
| Paeoniflorin | O1[C@H]([C@@H]([C@H]([C@@H]([C@H]1CO)O)O)O)O[C@@]32[C@]4(O[C@@H]5O[C@@]([C@@H]([C@@]53COC(=O)c6ccccc6)C2)(C4)O)C |  |
| D-(-)-Ribose | C1[C@H]([C@H]([C@H](C(O1)O)O)O)O |  |
| 2-Azidoethyl beta-Galactopyranoside | [N+](=[N-])=NCCO[C@@H]1OC([C@@H](C(C1O)O)O)CO |  |
| Calcium D-gluconate | [Ca+2].[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO.[O-]C(=O)[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO |  |
| D-(+)-Glucose | C([C@@H]1[C@H]([C@@H]([C@H](C(O1)O)O)O)O)O |  |

**Table XXX: List of chemicals from the secondary screen** (Total 8 Chemicals)

Green – Positive Hits (p<0.01)

|  |  |  |
| --- | --- | --- |
| **Chemical Name** | **SMILES** | **Vendor and Catalogue Number** |
| D-Glucamine | C([C@@H]([C@H]([C@@H]([C@@H](CO)O)O)O)O)N |  |
| L-Rhamnose | C[C@H]1[C@@H]([C@H]([C@H](C(O1)O)O)O)O |  |
| D-Lyxose | C1[C@H]([C@@H]([C@@H](C(O1)O)O)O)O |  |
| 3 Methyl-beta-D-xylopyranoside | CO[C@H]1[C@@H]([C@H]([C@@H](CO1)O)O)O |  |
| 1-Azido-1-deoxy-beta-D-glucopyranoside | C([C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)N=[N+]=[N-])O)O)O)O |  |
| 6-Deoxy-D-glucose | C[C@@H]1[C@H]([C@@H]([C@H](C(O1)O)O)O)O |  |
| 1-Amino-1-deoxy-D-fructose hydrochloride | C([C@H]([C@H]([C@@H](C(=O)CN)O)O)O)O.Cl |  |
| D-Mannoheptulose | C([C@H]([C@H]([C@@H]([C@@H](C(=O)CO)O)O)O)O)O |  |

**Table XXX: List of chemicals from the tertiary screen** (Total 13 Chemicals)

Green – Positive Hits (p<0.01)

|  |  |  |
| --- | --- | --- |
| **Chemical Name** | SMILES | **Vendor and Catalogue Number** |
| 1-Thio-beta-D-glucose sodium salt | C([C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)[S-])O)O)O)O |  |
| 2,5-Anhydro-D-mannitol | C([C@@H]1[C@H]([C@@H]([C@H](O1)CO)O)O)O |  |
| 1-Deoxynojirimycin | C1[C@@H]([C@H]([C@@H]([C@H](N1)CO)O)O)O |  |
| D-allose | C([C@@H]1[C@H]([C@H]([C@H](C(O1)O)O)O)O)O |  |
| 1-amino-1-deoxy-beta-D-mannopyranose | C([C@@H]1[C@H]([C@@H]([C@@H]([C@@H](O1)N)O)O)O)O |  |
| 2,5-Anhydro-D-glucitol | C([C@@H]1[C@H]([C@@H]([C@@H](O1)CO)O)O)O |  |
| 1,2-O-Isopropylidene-alpha-D-xylofuranose | CC1(O[C@@H]2[C@H]([C@H](O[C@@H]2O1)CO)O)C |  |
| 1-Amino-2,5-anhydro-1-deoxy-D-mannitol | C([C@@H]1[C@H]([C@@H]([C@H](O1)CO)O)O)N |  |
| 1-O-Methyl-2-deoxy-D-ribose | COC1C[C@@H]([C@H](O1)CO)O |  |
| 6-deoxy-D-glucose | C[C@@H]1[C@H]([C@@H]([C@H](C(O1)O)O)O)O |  |
| 1-Amino-1-deoxy-D-Fructose hydrochloride | C([C@@H]1[C@H]([C@@H](C(O1)(CN)O)O)O)O |  |
| Voglibiose | C1[C@@H]([C@@H]([C@H]([C@@H]([C@]1(CO)O)O)O)O)NC(CO)CO |  |
| 3-deoxy-1,2,5,6-di-O-isopropylidene alpha-D-glucofuranose | CC1(OCC(O1)[C@@H]2C[C@@H]3[C@H](O2)OC(O3)(C)C)C |  |

Graphical user interface, application

Description automatically generated

**Figure XXX: Localization of selected SweetTrac1 mutants in yeast**

**Graphical user interface, application

Description automatically generated**

**Figure XXX: Localization of selected AtSWEET1 mutants tagged with EGFP in yeast**

**Graphical user interface, chart, application

Description automatically generated**

**Figure XXX: Steady State Kinetics of V69 SweetTrac1 Mutants**

**Graphical user interface, chart

Description automatically generated**

**Figure XXX: Steady State Kinetics of I72 SweetTrac1 Mutants**

**Graphical user interface, application

Description automatically generated**

**Figure XXX: Steady State Kinetics of V188 SweetTrac1 Mutants**

OsSWEET2b -----MDSLYDISCFAAGLAGNIFALALFLSPVTTFKRILKAKSTERFDGLPYLFSLLNC 55

AtSWEET1 ---------MNIAHTIFGVFGNATALFLFLAPSITFKRIIKNKSTEQFSGIPYPMTLLNC 51

AtSWEET2 MDVFAFNASLSMCKDVAGIAGNIFAFGLFVSPMPTFRRIMRNKSTEQFSGLPYIYALLNC 60

AtSWEET3 --------MGDKLRLSIGILGNGASLLLYTAPIVTFSRVFKKKSTEEFSCFPYVMTLFNC 52

AtSWEET4 ------MVNATVARNIAGICGNVISLFLFLSPIPTFITIYKKKKVEEYKADPYLATVLNC 54

AtSWEET5 ------MTDPHTARTIVGIVGNVISFGLFCAPIPTMVKIWKMKSVSEFKPDPYVATVLNC 54

AtSWEET6 ----MVHEQLNLIRKIVGILGNFISLCLFLSPTPTFIHIVKKKSVEKYSPLPYLATLLNC 56

AtSWEET7 ----MVFAHLNLLRKIVGIIGNFIALCLFLSPTPTFVRIVKKKSVEEYSPIPYLATLINC 56

AtSWEET8 ------MVDAKQVRFIIGVIGNVISFGLFAAPAKTFWRIFKKKSVEEFSYVPYVATVMNC 54

AtSWEET9 -----MFLKVHEIAFLFGLLGNIVSFGVFLSPVPTFYGIYKKKSSKGFQSIPYICALASA 55

AtSWEET10 -----MAISQAVLATVFGILGNIISFFVCLAPIPTFVRIYKRKSSEGYQSIPYVISLFSA 55

AtSWEET11 ---MSLFNTENTWAFVFGLLGNLISFAVFLSPVPTFYRIWKKKTTEGFQSIPYVVALFSA 57

AtSWEET12 ---MALFDTHNTWAFVFGLLGNLISFAVFLSPVPTFYRICKKKTTEGFQSIPYVVALFSA 57

AtSWEET13 -----MALTNNLWAFVFGILGNIISFVVFLAPVPTFVRICKKKSTEGFQSLPYVSALFSA 55

AtSWEET14 -----MVLTHNVLAVTFGVLGNIISFIVFLAPVPTFVRICKKKSIEGFESLPYVSALFSA 55

AtSWEET15 ---MGVMINHHFLAFIFGILGNVISFLVFLAPVPTFYRIYKRKSTESFQSLPYQVSLFSC 57

AtSWEET16 ---------MADLSFYVGVIGNVISVLVFLSPVETFWRIVQRRSTEEYECFPYICTLMSS 51

AtSWEET17 ---------MAEASFYIGVIGNVISVLVFLSPVETFWKIVKRRSTEEYKSLPYICTLLGS 51

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OsSWEET2b LICLWYGLPWVAD--G-RLL**V**AT**V**NGIGAVFQLAYICLFIFYADSRKTRMK-IIGLLVLV 111

AtSWEET1 LLSAWYGLPFVSK--D-NTL**V**ST**I**NGTGAVIETVYVLIFLFYAP-KKEKIK-IFGIFSCV 106

AtSWEET2 LICLWYGTPFISH--S-NAM**L**MT**V**NSVGATFQLCYIILFIMHTD-KKNKMK-MLGLLFVV 115

AtSWEET3 LIYTWYGLPIVSHLWE-NLP**L**VT**I**NGVGILLESIFIFIYFYYAS-PKEKIK-VGVTFVPV 109

AtSWEET4 ALWVFYGLPMVQP--D-SLL**V**IT**I**NGTGLAIELVYLAIFFFFSPTSRK-VK-VGLWLIGE 109

AtSWEET5 MMWTFYGLPFVQP--D-SLL**V**IT**I**NGTGLFMELVYVTIFFVFATSPVR-RK-ITIAMVIE 109

AtSWEET6 LVRALYGLPMVHP--D-STL**L**VT**I**SGIGITIEIVFLTIFFVFCGRQQH-RLVISAVLTVQ 112

AtSWEET7 LVWVLYGLPTVHP--D-STL**V**IT**I**NGTGILIEIVFLTIFFVYCGRQKQ-RLIISAVIAAE 112

AtSWEET8 MLWVFYGLPVVHK--D-SIL**V**ST**I**NGVGLVIELFYVGVYLMYCGHKKNHRRNILGFLALE 111

AtSWEET9 TLLLYYGI--MKT--H-AYL**I**IS**I**NTFGCFIEISYLFLYILYAPREAK-ISTLKLIVICN 109

AtSWEET10 MLWMYYAM--IKK--D-AMM**L**IT**I**NSFAFVVQIVYISLFFFYAPKKEK-TLTVKFVLFVD 109

AtSWEET11 TLWLYYAT--QKK--D-VFL**L**VT**I**NAFGCFIETIYISMFLAYAPKPAR-MLTVKMLLLMN 111

AtSWEET12 MLWLYYAT--QKK--D-VFL**L**VT**I**NSFGCFIETIYISIFVAFASKKAR-MLTVKLLLLMN 111

AtSWEET13 MLWIYYAM--QKD--GTAFL**L**IT**I**NAFGCVIETIYIVLFVSYANKKTR-ISTLKVLGLLN 110

AtSWEET14 MLWIYYAL--QKD--GAGFL**L**IT**I**NAVGCFIETIYIILFITYANKKAR-ISTLKVLGLLN 110

AtSWEET15 MLWLYYAL--IKK--D-AFL**L**IT**I**NSFGCVVETLYIAMFFAYATREKR-ISAMKLFIAMN 111

AtSWEET16 SLWTYYGI--VTP--G-EYL**V**ST**V**NGFGALAESIYVLIFLFFVPKSRF-LKTVVVVLALN 105

AtSWEET17 SLWTYYGI--VTP--G-EYL**V**ST**V**NGFGALVETIYVSLFLFYAPRHLK-LKTVDVDAMLN 105

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OsSWEET2b VCGFALVSHASVF-FFDQPLRQQFVGAVSMASLISMFASPLAVMGVVIRSESVEFMPFYL 170

AtSWEET1 LAVFATVALVSLF-ALQGNGRKLFCGLAATVFSIIMYASPLSIMRLVVKTKSVEFMPFFL 165

AtSWEET2 FAVVGVIVAGSLQ-IPDQLTRWYFVGFLSCGSLVSMFASPLFVINLVIRTKSVEFMPFYL 174

AtSWEET3 IVGFGLTTAISALVFDDHRHRKSFVGSVGLVASISMYGSPLVVMKKVIETRSVEYMPFYL 169

AtSWEET4 MVFVGIVATCTLLLFHTHNQRSSFVGIFCVIFVSLMYIAPLTIMSKVIKTKSVKYMPFSL 169

AtSWEET5 VIFMAVVIFCTMYFLHTTKQRSMLIGILCIVFNVIMYAAPLTVMKLVIKTKSVKYMPFFL 169

AtSWEET6 VVFVATLAVLVLTLEHTTDQRTISVGIVSCVFNAMMYASPLSVMKMVIKTKSLEFMPFLL 172

AtSWEET7 TAFIAILAVLVLTLQHTTEKRTMSVGIVCCVFNVMMYASPLSVMKMVIKTKSVEFMPFWL 172

AtSWEET8 VILVVAIILITLFALKGDFVKQTFVGVICDVFNIAMYGAPSLAIIKVVKTKSVEYMPFLL 171

AtSWEET9 IGGLGLLILLVNLLVPKQ-HRVSTVGWVCAAYSLAVFASPLSVMRKVIKTKSVEYMPFLL 168

AtSWEET10 VLGFGAIFVLTYFIIHAN-KRVQVLGYICMVFALSVFVAPLGIIRKVIKTKSAEFMPFGL 168

AtSWEET11 FGGFCAILLLCQFLVKGA-TRAKIIGGICVGFSVCVFAAPLSIIRTVIKTRSVEYMPFSL 170

AtSWEET12 FGGFCLILLLCQFLAKGT-TRAKIIGGICVGFSVCVFAAPLSIIRTVIKTKSVEYMPFSL 170

AtSWEET13 FLGFAAIVLVCELLTKGS-TREKVLGGICVGFSVSVFAAPLSIMRVVVRTRSVEFMPFSL 169

AtSWEET14 FLGFAAIILVCELLTKGS-NREKVLGGICVGFSVCVFAAPLSIMRVVIRTKSVEFMPFSL 169

AtSWEET15 VAFFSLILMVTHFVVKTPPLQVSVLGWICVAISVSVFAAPLMIVARVIKTKSVEYMPFTL 171

AtSWEET16 VCFPVIAIAGTRTLFGDANSRSSSMGFICATLNIIMYGSPLSAIKTVVTTRSVQFMPFWL 165

AtSWEET17 VFFPIAAIVATRSAFEDEKMRSQSIGFISAGLNIIMYGSPLSAMKTVVTTKSVKYMPFWL 165

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OsSWEET2b SLSTFLMSASFALYGLL-LRDFF**I**YFPNGLGLILGAMQLALYAYYSRKWRGQDSSAPLLL 229

AtSWEET1 SLFVFLCGTSWFVYGLI-GRDPF**V**AIPNGFGCALGTLQLILYFIYCGNKGEKSADAQKDE 224

AtSWEET2 SLSTFLMSASFLLYGLF-NSDAF**V**YTPNGIGTILGIVQLALYCYYHRNSIEEETKEPLIV 233

AtSWEET3 SFFSFLASSLWLAYGLL-SHDLF**L**ASPNMVATPLGILQLILYFKYKNKKDLAPTTMVIT- 227

AtSWEET4 SLANFLNGVVWVIYALI-KFDLF**I**LIGNGLGTVSGAVQLILYACYYKTTPKDDEDEEDEE 228

AtSWEET5 SLANFMNGVVWVIYACL-KFDPY**I**LIPNGLGSLSGIIQLIIYITYYKTTNWNDDDEDKEK 228

AtSWEET6 SVVGFLNAGVWTIYGFV-PFDPF**L**AIPNGIGCVFGLVQLILYGTYYKSTKGIMEERKNRL 231

AtSWEET7 SVAGFLNAGVWTIYALM-PFDPF**M**AIPNGIGCLFGLAQLILYGAYYKSTKRIMAERENQP 231

AtSWEET8 SLVCFVNAGIWTTYSLIFKIDYY**V**LASNGIGTFLALSQLIVYFMYYKSTPKEKTVKPSEV 231

AtSWEET9 SLSLTLNAVMWFFYGLL-IKDKF**I**AMPNILGFLFGVAQMILYMMYQGSTKTDLPTENQLA 227

AtSWEET10 SFFLTLSAVMWFFYGLL-LKDMN**I**ALPNVLGFIFGVLQMILFLIYKKPGTKVLE--PPGI 225

AtSWEET11 SLTLTISAVIWLLYGLA-LKDIY**V**AFPNVLGFALGALQMILYVVYKYCKTSPHLGEK-EV 228

AtSWEET12 SLTLTISAVIWLLYGLA-LKDIY**V**AFPNVIGFVLGALQMILYVVYKYCKTPSDLVEK-EL 228

AtSWEET13 SLFLTISAVTWLFYGLA-IKDFY**V**ALPNVLGAFLGAVQMILYIIFKYYKTPVA-QKT-D- 225

AtSWEET14 SLFLTISAITWLFYGLA-IKDFY**V**ALPNILGAFLGAVQMILYVIFKYYKTPLVVDET-E- 226

AtSWEET15 SFFLTISAVMWFAYGLF-LNDIC**I**AIPNVVGFVLGLLQMVLYLVYRNSNEKPEKINSSEQ 230

AtSWEET16 SFFLFLNGAIWGVYALL-LHDMF**L**LVPNGMGFFLGIMQLLIYAYYRNAEPIVED------ 218

AtSWEET17 SFFLFLNGAIWAVYALL-QHDVF**L**LVPNGVGFVFGTMQLILYGIYRNAKPVGLSNGLSEI 224

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AtSWEET10 KLQDISEHVV---DVVRLSTMVCNSQ-------MRTLVPQDSA----DMEATIDIDEKI- 270

AtSWEET9 NKTDVNEVPIVAVELPDVGSDNVE----GSVRPMK------------------------- 258

AtSWEET15 QLKS----IV---VMSPLGVSEVHPVVTESVDPLSEAVHHE------DLSKVTKVEEPSI 277

AtSWEET11 EAAKLPEVSL---DMLKLGTVS-------SPEPIS--VVRQANKCTCGNDRRA---EI-- 271

AtSWEET12 EAAKLPEVSI---DMVKLGTLT-------SPEPVAITVVRSVNTCNCN-DRNA---EI-- 272

AtSWEET13 KSKDVSDHSI---DIAKLTTVI-------PGAVLDSAVHQPPA-LHNVPETKIQLTEVKS 274

AtSWEET14 KPKTVSDHSI---NMVKLSSTP-------ASGDLTVQPQTNPDVSHPIKT---------- 266

AtSWEET16 ----EEGLIP------N--QP------------------------------LL------- 229

AtSWEET17 AQDEEEGLTS------RV-EP------------------------------LL------- 240

AtSWEET8 EISATERV---------------------------------------------------- 239

AtSWEET6 GYVGEVGLS--------------------------NAIAQTEPENIPYLNKRV------- 258

AtSWEET7 GYVGLS-----------------------------SAIARTGSEKTANTNQEP------- 255

AtSWEET4 NLSKVN-----------------------------SQLQLSGNS---GQAKRV------- 249

AtSWEET5 RYSNAG-----------------------------IELGQA------------------- 240

AtSWEET3 KR-NDHDDKN------KA-TL-----------EFVVDVDRNSDTNEKNSNNAS------- 261

AtSWEET1 KSVEMKDDEK------KQ--------------------------NVVNGKQDL------- 245

AtSWEET2 SYV--------------------------------------------------------- 236

OsSWEET2b A----------------------------------------------------------- 230

AtSWEET10 -KGDIEKNKDEKEVFLISKN 289

AtSWEET9 -------------------- 258

AtSWEET15 ENGKCYVEATR---PETV-- 292

AtSWEET11 EDGQTPKHGKQSSSAAAT-- 289

AtSWEET12 ENGQGVRNSAATT------- 285

AtSWEET13 QNMTDPKDQINKDVQKQSQV 294

AtSWEET14 -HGGDLEDQMDKKMPN---- 281

AtSWEET16 --------------A----- 230

AtSWEET17 --------------S----- 241

AtSWEET8 -------------------- 239

AtSWEET6 --------------SGV--- 261

AtSWEET7 --------------NNV--- 258

AtSWEET4 --------------SA---- 251

AtSWEET5 -------------------- 240

AtSWEET3 --------------SI---- 263

AtSWEET1 --------------QV---- 247

AtSWEET2 -------------------- 236

OsSWEET2b -------------------- 230

**Figure XXX: Sequence alignment of AtSWEETs**