

**Supplementary Data Set 1: Summary of Glycosyltransferase structures in PDB (January 2019)**

Glycosyltransferases structures in PDB as of January 1, 2019 have been previously catalogued in the CAZy database (1) and were used to populate the table below. Structure entries in the table are organized by CAZy family. Annotation information was assembled for each protein structure, including gene symbol, protein name, and UniProt accession number (all collected from the respective UniProt entry (2)), species and Kingdom for the coding region, and the species source of the expression system (derived from the respective PDB records (3)). The PDB ID codes for the respective CAZY family record and visual inspection of the protein structure. The glycosyltransferase mechanism (inverting or retaining catalytic mechanisms) were derived from the respective CAZY family record or the primary citation of the structure. The dependence for a metal cation in the catalytic mechanism (Metal dep) was determined by the requirement of a metal ion binding the donor analog in the respective protein structure for at least one member of the respective CAZY family. Donor and acceptor ligand structures were listed for analog complexes that bound to the respective substrates and do not include molecules bound to inhibitory or allosteric sites. Publications of the respective structures are listed by digital object identifiers (doi) based on citation information in the PDB record. If a publication is not available, then a PubMed ID is listed. In some instances no publication is listed if the 'Literature' field of the PDB record indicates that the structure is to be published.

| CAZy family | Gene symbol | Protein name                                       | UniProt   | Species             | Kingdom  | Expression system | PDB ID                     | Year first deposited | Year of subsequent deposits | Fold class | Mechanism | Metal dep | Donor ligand analog | Acceptor Ligand analog   | Pub doi or PubMed ID                                   |
|-------------|-------------|--|-----------|---------------------|----------|-------------------|----------------------------|----------------------|-----------------------------|------------|-----------|-----------|---------------------|--------------------------|--|
| 1           | ace2        | Ecto-N-acetylglucosaminidase                       | ADAM00999 | Actinomycetales     | Bacteria | E. coli           | S0042                      | 2003                 | 2009                        | GT-B       | Inverting | N.D.      | TDP, UDP-Glc, UDP   | Glc, vancomycin          | 10.1073/pnas.133377109; 10.1016/j.chembiol.2009.04.003 |
| gtfA        |             | UDP-galactose 4-epimerase                          | P09558    | Aspergillus oryzae  | Bacteria | E. coli           | S0783, S0791, S0461, S0471 | 2003                 | 2009                        | GT-B       | Inverting | no        |                     |                          | 10.1055/s-0029-102005-5                                |
| gtfB        |             | UDP-glucuronic acid 4-epimerase                    | P09559    | Aspergillus oryzae  | Bacteria | E. coli           | S0785                      | 2003                 | 2009                        | GT-B       | Inverting | no        |                     |                          | 10.1055/s-0029-102005-5                                |
| gtfC        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C7    | Armatobacter obesum | Bacteria | E. coli           | S0892                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | Glc, GlcNAc              | 10.1021/bj083130                                       |
| gtfD        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C8    | Armatobacter obesum | Bacteria | E. coli           | S0893                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfE        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0894                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfF        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0895                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfG        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0896                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfH        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0897                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfI        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0898                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfJ        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0899                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfK        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0900                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfL        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0901                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfM        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0902                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfN        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0903                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfO        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0904                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfP        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0905                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfQ        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0906                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfR        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0907                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfS        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0908                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfT        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0909                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfU        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0910                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfV        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0911                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfW        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0912                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfX        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0913                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfY        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0914                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfZ        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0915                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfA        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0916                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfB        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0917                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfC        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0918                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfD        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0919                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfE        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0920                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfF        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0921                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfG        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0922                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfH        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0923                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfI        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0924                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfJ        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0925                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfK        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0926                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfL        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0927                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfM        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0928                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfN        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0929                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfO        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0930                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfP        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0931                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfQ        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0932                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfR        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0933                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfS        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0934                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfT        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0935                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfU        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0936                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfV        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0937                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfW        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0938                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfX        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0939                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfY        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0940                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfZ        |             | Vancomycin N-acetylglycosaminide acetyltransferase | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0941                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfA        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0942                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfB        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0943                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfC        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0944                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfD        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0945                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfE        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0946                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfF        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0947                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfG        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0948                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfH        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0949                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfI        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0950                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfJ        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0951                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfK        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0952                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfL        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0953                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfM        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0954                      | 2003                 | 2009                        | GT-B       | Inverting | no        | TDP                 | GlcNAc, GlcNAc-phosphate | 10.1021/bj084100                                       |
| gtfN        |             | Glucuronyl transferase                             | Q9H4C9    | Armatobacter obesum | Bacteria | E. coli           | S0955                      | 2003                 |                             |            |           |           |                     |                          |  |

|    |  |   |                              |                            |                  |  |   |             |             |           |                          |  |   |   |
|----|--|---|------------------------------|----------------------------|------------------|--|---|-------------|-------------|-----------|--------------------------|--|---|---|
| 16 | Probable mannose/transferrin XTR6                            | P05131  | Saccharomyces cerevisiae     | Eukaryota                  | <i>F. coli</i>   | 5407_5408  | 2015                                    | GT-A        | retaining   | yes       | GDP                      | 10_1371/journal.pone.0196239                                   |   |   |
| 16 | Mann-6-S-L-galactosaminidase 6-beta-N-acetylglucosaminidase  | Q16680  | Homo sapiens                 | Eukaryota                  | Homo sapiens     | TCMV_NUCA_SVCS   | 2018                                    | GT-A        | inverting   | yes       | UDP                      | 10_1073/journal.pone.0196811                                   |   |   |
| 18 | Alpha-L-5-mannosidase/protein 6-beta-N-acetylglucosaminidase | Q09328  | Homo sapiens                 | Eukaryota                  | Homo sapiens     | U26_52C  | 2018                                    | GT-B        | inverting   | no        | GDP-Mut, MuAc            | 10_1036/journal.pone.0193031.w                                 |   |   |
| 19 | Lipid-O-disaccharide synthase                                | P10641  | Escherichia coli             | Bacteria                   | <i>F. coli</i>   | EWBN_EWBS_WHXX   | 2017                                    | GT-B        | inverting   | no        | UDP                      | 10_1093/journal.pone.0172724.g                                 |   |   |
| 20 | utuA   | Trehalose-6-phosphate synthase  | A04093K3                     | Burkholderia multivorans   | Bacteria         | <i>F. coli</i>   | SIUF                                    | 2017        | GT-B        | retaining | N.D.                     | N.D.   | 10_1093/journal.pone.0194954  |   |
|    | IboxeUBP_2483  | Trehalose-6-phosphate synthase  | A04058                       | Burkholderia vietnamensis  | Bacteria         | <i>F. coli</i>   | STV5                                    | 2016        | GT-B        | retaining | no                       | UDP  | 10_1093/journal.pone.0194954  |   |
|    | utuA   | Trehalose-6-phosphate synthase  | P11377                       | Escherichia coli           | Bacteria         | <i>F. coli</i>   | 1025_1026_1107_20WTX                    | 2002        | 2004        | GT-B      | retaining                | no   | UDP, UDP-Glc, UDP-<br>Glc   | trehalose-6-PO4 mimetic<br>10_1036/journal.pone.0190596 |
|    | KEX_14123  | Alpha, alpha-trehalose-phosphate synthase   | G70572                       | Mycobacterium thermophilic | Bacteria         | <i>F. coli</i>   | SHJ_5HJ_5K4L_5K42_5K44_5K5C_5L3K        | 2016        | GT-B        | retaining | no                       | ADP, ADP-Glc, GDP-Glc  | Glc-6-PO4, trehalose-6-<br>PO4, Fru-6-P4  |   |
|    | Rse_A374   | Trehalose-6-phosphate synthase  | Q14248                       | Paraburkholderia venenosa  | Bacteria         | <i>F. coli</i>   | SHVA                                    | 2016        | GT-B        | retaining | no                       | GDP  | 10_1173/journal.pone.0194954  |   |
|    | Rse_A3142  | Trehalose-6-phosphate synthase  | Q19192B                      | Paraburkholderia venenosa  | Bacteria         | <i>F. coli</i>   | SIOT                                    | 2017        | GT-B        | retaining | no                       | UDP  | 10_1173/journal.pone.0194954  |   |
|    | utuE   | Trehalose-6-phosphate synthase  | Q15051                       | Streptomyces lividans      | Bacteria         | <i>F. coli</i>   | SI51_5T1D_5VBD_5VCD_5VDE_5VIF_4957      | 2011        | GT-B        | retaining | no                       | GDP  | 10_1093/journal.pone.0194954  |   |
|    | utuF   | Trehalose-6-phosphate synthase  | Q15052                       | Streptomyces lividans      | Bacteria         | <i>F. coli</i>   | SI51_5T1D_5VBD_5VCD_5VDE_5VIF_4957      | 2011        | GT-B        | retaining | no                       | UDP  | 10_1093/journal.pone.0194954  |   |
|    | TPS1A1A_651290B  | Trehalose-6-phosphate synthase  | Q24950                       | Neurospora crassa          | Eukaryota        | <i>F. coli</i>   | ShrA                                    | 2016        | GT-B        | retaining | no                       | UDP  | 10_1126/scientificreports.417   |   |
|    | AFU0204030   | Trehalose-6-phosphate synthase  | Q4999W0                      | Neurospora crassa          | Eukaryota        | <i>F. coli</i>   | ShrD                                    | 2017        | GT-B        | retaining | no                       | UDP  | 10_1126/scientificreports.417   |   |
|    | IT33   | Alpha,L-alpha-trehalose-phosphate synthase (UDP-<br>Glc)                          | P29348                       | Endomycetoma ulysseum      | Bacteria         | <i>F. coli</i>   | SHAU_SHUH_SHUV_SHUV                     | 2014        | GT-B        | retaining | no                       | UDP, UDP-Glc   | Glc-6-PO4, endomycetoma-<br>ulysseum  |   |
| 23 | modE   | Modulation protein Z  | P09417                       | Bacillus halodurans        | Bacteria         | <i>F. coli</i>   | ZHAC_2ZHC_3ZHL_3ZLW_3ZLX                | 2006        | GT-B        | inverting | no                       | GDP  | 10_1107/journal.pone.0190517_PMD_17762900   |   |
|    | FUT5   | Alpha-L-fucosidase  | Q9HVC5                       | Homo sapiens               | Eukaryota        | Spodoptera frugiperda                                  | 2000                                    | 2006        | GT-B        | inverting | N.D.                     | N.D.   | 10_1093/journal.pone.0190517  |   |
| 24 | CHTN_008890  | UDP glucose-glucuronide glucuronyltransferase-like                                | Q09538                       | Chromatium thermophilum    | Eukaryota        | Homo sapiens   | 2WZ_2WZ_3WZ_5WZ_5WZ_5WZ_5WZ             | 2017        | GT-A        | retaining | N.D.                     | N.D.   | 10_1075/journal.pone.0191114  |   |
|    | UDP-glucose-glucuronide glucuronyltransferase                | Q09539  | Thermomicrobium doncastrense | Eukaryota                  | <i>F. coli</i>   | 3YF7_3YF7_5H1R   | 2018                                    | GT-A        | retaining   | yes       | UDP, UDP-Glc             | 10_1093/journal.pone.0191228.w                                 |   |   |
| 27 | putative polyketide N-acetylglucosaminyltransferase 5        | Q8MRC5  | Drosophila melanogaster      | Kinorhabdida               | <i>posterior</i> | GE40_5E4R  | 2018                                    | GT-A        | retaining   | yes       | UDP                      | 10_1058/journal.pone.0195798                                   |   |   |
|    | GauH1  | Polyketide N-acetylglucosaminyltransferase 1                                      | Q09812                       | Mus musculus               | Eukaryota        | <i>posterior</i>                                       | 3X0B                                    | 2004        | GT-A        | retaining | yes                      | UDP, UDP-GlcNAc  | 10_1075/journal.pone.01905710   |   |
|    | GauH2  | Polyketide N-acetylglucosaminyltransferase 2                                      | Q10871                       | Homo sapiens               | Eukaryota        | <i>posterior</i>                                       | 2F7U_2F7V_4D0T_4D0Z_4D11_5A1N_5A1P_5A1O | 2005        | 2014, 2015, | GT-A      | retaining                | yes  | UDP, UDP-GlcNAc,<br>ethylene derivative of<br>UDP-GlcNAc  | 10_1047/journal.pone.01905071                           |
|    | GauH4  | Polyketide N-acetylglucosaminyltransferase 4                                      | Q10840                       | Homo sapiens               | Eukaryota        | <i>posterior</i>                                       | 5W0A_5H0R                               | 2017        | GT-A        | retaining | yes                      | UDP  | 10_1075/journal.pone.0190488  |   |
|    | GauH10   | Polyketide N-acetylglucosaminyltransferase 10                                     | Q10581                       | Homo sapiens               | Eukaryota        | <i>posterior</i>                                       | 2D57_2D57                               | 2005        | GT-B        | retaining | yes                      | UDP, UDP-Glc, UDP  | 10_1056/journal.pone.0191051  |   |
| 28 | putative polyketide N-acetylglucosaminyltransferase          | P12441  | Escherichia coli             | Bacteria                   | <i>F. coli</i>   | 3YK0_3YK1  | 2000                                    | GT-B        | inverting   | no        | UDP-GlcNAc               | 10_1110/journal.pone.0194045                                   |   |   |
|    | putative polyketide N-acetylglucosaminyltransferase          | P12442  | Parafomonas aerogenes        | Bacteria                   | <i>F. coli</i>   | 2WZU_2WZU_2WZU   | 2011                                    | GT-B        | inverting   | no        | UDP-GlcNAc               | 10_2174/journal.pone.0192006                                   |   |   |
|    | Mgd1   | Glucosidase, alpha-D-glucosidase  | Q18170                       | Anobolites thalassius      | Eukaryota        | <i>F. coli</i>   | 4WV9_4X1T                               | 2014        | GT-B        | inverting | no                       | UDP  | 10_1115/journal.pone.013129   |   |
| 29 | Isnt   | Beta-1,3-beta-D-glucuronidase   | Q18480                       | Habenaria speciosa         | Eukaryota        | <i>posterior</i>                                       | 4A95                                    | 2013        | GT-A        | inverting | no                       | GDP  | 10_1074/journal.pone.0190504  |   |
|    | Beta-D-glucuronidase   | P12007  | Habenaria speciosa           | Eukaryota                  | <i>posterior</i> | 4D1_4D2  | 2013                                    | GT-A        | inverting   | no        | CMP                      | Blumenthalia ciliolata   |   |   |
|    | ST364L1  | CMF-4-acetylureido-beta-D-glucuronidase   | Q02745                       | Cuscuta officinalis        | Eukaryota        | <i>F. coli</i>   | 2WZM_2WZM_2WZM                          | 2009        | GT-A        | inverting | no                       | Glc-GalNAc-pNP   | 10_1076/journal.pone.01985  |   |
|    | ST364ALN2  | Alpha-D-glucuronidase isozyme alpha-L-<br>beta-D-glucuronidase 2                  | Q19187                       | Habenaria speciosa         | Eukaryota        | <i>posterior</i>                                       | 4A91_4A91                               | 2018        | GT-A        | inverting | no                       | CMP  | 10_1056/journal.pone.01905006   |   |
|    | ST364AN2   | Alpha-D-glucuronidase isozyme alpha-L-<br>beta-D-glucuronidase 2                  | Q19173                       | Habenaria speciosa         | Eukaryota        | <i>posterior</i>                                       | 4WV9_4X1T                               | 2014        | GT-B        | inverting | no                       | CMP, CMP-3F-N-acetyl-CTD                                       | N-acAc/GlcNAc-5-OMe   |   |
| 30 | Wnk3   | 1-deoxy-D-xylulose-5-phosphate isomerase  | Q18480                       | Habenaria speciosa         | Eukaryota        | <i>posterior</i>                                       | 4A95                                    | 2013        | GT-B        | inverting | N.D.                     | N.D.   | 10_1074/journal.pone.0190504  |   |
|    | Wnk4   | 1-deoxy-D-xylulose-5-phosphate isomerase  | Q06663                       | Aquifex aeolicus           | Bacteria         | <i>F. coli</i>   | 2WZC_2WZC                               | 2010        | GT-B        | inverting | no                       | CMP  | 10_1078/journal.pone.011988409  |   |
| 31 | MtrA   | Delta-1,5-D-oxosuccinate mutase   | Q09008                       | Mus musculus               | Eukaryota        | Spodoptera frugiperda                                  | 2A1A_2B0B                               | 2006        | GT-A        | inverting | yes                      | UDP  | 10_1058/journal.pone.0191144  |   |
| 34 | XET1   | Galactosidase 6-sulfotransferase 1  | P06713                       | Anobolites thalassius      | Eukaryota        | Homo sapiens   | 4B51_B5B1_B5B5_W5B5                     | 2017        | GT-A        | retaining | yes                      | UDP  | 10_1073/journal.pone.01910515   |   |
| 35 | Maha_1-4 deoxy-chitosanase                                   | Q09506  | Cercozoa, Cercozoa           | Bacteria                   | <i>F. coli</i>   | 2C4M   | 2005                                    | GT-B        | retaining   | no        | Pentose-4-phosphate, P04 | 10_1078/journal.pone.01905006                                  |   |   |
|    | Maha_2-deoxy-alpha-L-glucosidase                             | P12007  | Habenaria speciosa           | Eukaryota                  | <i>posterior</i> | 1A4P_1E4D_1F5L_1G5V_1I5L_1J5W_1L5W_1M5V_2A5V_2A5V_2A5V | 1998, 1999,                             | 2002, 2005, | GT-B        | retaining | no                       | Malto-4,6-D-maltose, Pentosylate, PO4, PO4, NOL, VCA, VPC, VPC | 10_1038/journal.pone.01905002   |   |
|    | Maha_3-deoxy-alpha-L-glucosidase                             | P09890  | Escherichia coli             | Bacteria                   | <i>F. coli</i>   | 3YK1_3YK1  | 1997                                    | GT-B        | retaining   | no        | VCA, VPC, VPC            | 10_1038/journal.pone.01905003                                  |   |   |
|    | Maha_4-deoxy-alpha-L-glucosidase                             | P12007  | Habenaria speciosa           | Eukaryota                  | <i>posterior</i> | 4A91_4A91  | 2011                                    | GT-B        | retaining   | no        | VCA, VPC, VPC            | 10_1056/journal.pone.01905004                                  |   |   |
|    | PHS2   | Alpha-L-glucan acetyltransferase 2  | Q19276                       | Anobolites thalassius      | Eukaryota        | <i>F. coli</i>   | 4B0F_4B0F_4B0I                          | 2013        | GT-B        | retaining | no                       | Pentose-4-P, PO4, PO4  | 10_1078/journal.pone.01905005   |   |
|    | PYGB   | Glycosen phosphohydrolase, brain form   | P11216                       | Homo sapiens               | Eukaryota        | <i>F. coli</i>   | 5K6D_5K6P                               | 2016        | GT-B        | retaining | no                       | Pentosid, PO4, PO4   | 10_1078/journal.pone.01905006   |   |
|    | PYGM   | Glycosen phosphohydrolase, muscle form  | P02489                       | Oryctolites curvatus       | Eukaryota        | <i>F. coli</i>   | 5A9B_5A9B_5A9C_5A9C                     | 2006        | 2005        | GT-B      | retaining                | no   | PO4   | 10_1000/journal.pone.01905007                           |
|    | PYGM   | Glycosen phosphohydrolase, muscle form  | P02489                       | Oryctolites curvatus       | Eukaryota        | <i>F. coli</i>   | 5A9B_5A9B_5A9C_5A9C                     | 2006        | 2005        | GT-B      | retaining                | no   | PYGM, PO4   | 10_1173/journal.pone.0174949                            |
|    | GHPI   | Glycosen phosphohydrolase   | P06738                       | Saccharomyces cerevisiae   | Eukaryota        | <i>F. coli</i>   | 5YGP                                    | 1996        | GT-B        | retaining | no                       | PYGM, PO4  | 10_1173/journal.pone.0174949  |   |
| 37 | FUT2   | Galactosidase 2-alpha-L-fucosidase  | Q195W5                       | Anobolites thalassius      | Eukaryota        | Homo sapiens   | SE01_5K0P_5K0V_5K0W_5K0X                | 2016        | GT-B        | inverting | no                       | GDP  | 10_1076/journal.pone.0191268  |   |
|    | utuE   | Galactosidase 2-alpha-L-fucosidase  | Q195W5                       | Anobolites thalassius      | Eukaryota        | <i>F. coli</i>   | SE02_5K0T_5K0U_5K0V_5K0W                | 2017        | GT-B        | inverting | no                       | GDP  | 10_1076/journal.pone.0191267  |   |
|    | Ttr_2822   | Tetracyclic peptide Ttr-2 repeat protein  | P12195                       | Thermobifidus terraneum    | Bacteria         | <i>F. coli</i>   | 5D05                                    | 2015        | GT-B        | inverting | no                       | UDP  | 10_1074/journal.pone.0190956  |   |
|    | NCC0865  | Uncharacterized protein   | Q8MC95                       | Bartramia longicauda       | Bacteria         | <i>F. coli</i>   | 2A8B_2A8C_2A8D_2A8E_2A8Z_2A8Z           | 2008        | 2010        | GT-B      | inverting                | no   | UDP-MurA, UDP-<br>allomuramidic acid, UDP-<br>alcanosaminidic acid, UDP-<br>threonosaminidic acid | 10_1038/journal.pone.01905010                           |
|    | utuE   | O-phosphotransferase  | P120048                      | Drosophila melanogaster    | Eukaryota        | <i>F. coli</i>   | 5A01                                    | 2015        | GT-B        | inverting | no                       | UDP-GlcNAc   | 10_1078/journal.pone.01905012   |   |
|    | OGT  | UDP-N-acetylgalactosamine-peptide N-acetylglucosaminyltransferase 120 kDa subunit | Q15294                       | Homo sapiens               | Eukaryota        | <i>F. coli</i>   | 5D45_5D46                               | 2010        | 2016, 2017  | GT-B      | inverting                | no   | Pyridoxal-PO4, PO4, PO4   | 10_1078/journal.pone.01905013                           |
| 42 | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2                                    | 2007        | GT-B        | inverting | no                       | GDP, NeAc, CMP   | 10_1074/journal.pone.01905014   |   |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905015                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905016                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905017                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905018                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905019                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905020                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905021                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905022                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905023                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905024                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905025                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905026                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905027                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905028                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, NeAc, CMP  | 10_1074/journal.pone.01905029                           |
|    | gtt1   | Glu-3-2-keto-3-phosphate  | Q19011                       | Candida parapsilosis       | Bacteria         | <i>F. coli</i>   | 3YK2_3YK2B_3YK2C_3YK2D_3YK2E_3YK2Z      | 2003        | 2011        | GT-A      | inverting                | no   | GDP, Ne   |   |

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