

This README defines the Prolog data files used in the following paper:

Michael Sternberg, et. al. Gene function hypotheses for the *Campylobacter jejuni* glycome generated by a logic-based approach.

DATA

The data used for learning are arranged in the following files.

(Note genes have the suffix "c" after their number which was, for brevity, omitted in the paper).

background_pl

The background knowledge for the machine learning which includes the general rules, working assumptions and the abductive learning settings for Progol 5.0.

codes_pl

Known gene functions represented by instances of the 'codes' predicate

common_pl

Common predicate declarations for genes and strains

CPS_pathway_pl

The *C. jejuni* CPS pathway information compiled from KEGG and BioCyc augmented by some specific information about the *C. jejuni* capsul glycan structure that were extracted from publications.

glycan_structure_pl

The *C. jejuni* CPS glycan structures. This includes the definition of `struct_next` which states that one glycan structure is related to another by the addition of a single chemical group

mutants_pl

The gene knock-out experiments for *C. jejuni* CPS. The data is mainly compiled from previously published data. The data is represented by instances of the 'knockout_observable' predicate which states when a specific gene is knocked out this result causes a particular glycan structure to be the largest synthesised

strains_pl

The cross-strain genomic data for the CPS loci originate from an in-progress study in which 270 *C. jejuni* isolates were analysed by comparative phylogenomics (whole genome comparisons of bacteria using DNA microarrays, combined with Bayesian-based algorithms, to model the phylogeny), using a previously published method.

The data includes predicates 'absent' and 'occurs' which state that a particular gene is absent or present from a particular strain.

MACHINE LEARNING USING PROGOL

These files were prepared to be used with the Inductive Logic Programming (ILP) system Progol 5.0. The version of Progol used in this study can be downloaded from

<http://www.doc.ic.ac.uk/Campy>

The latest version of Progol is available from:

<http://www.doc.ic.ac.uk/~shm/Software/progol5.0/>

It is necessary to abduce the function of each gene in turn to obtain the independent compression values reported in the paper. As an example below we give the input to abduce the function of `cyj1416c` and the output obtained.

`learn_cj1416c_pl`

Example learning file for the reaction `cyj1416c` in the paper. This is an input file for Progol 5.0 which loads other files in this directory into Progol and does the learning.

`learn_cj1416c_out`

The output of running Progol 5.0 on the example file `learn_cj1416c.pl`

After compiling the source file, Progol 5.0 can be used to run the example learning file described above. Under UNIX, to run Progol, rename each file as `.pl` so for example, `codes_pl.txt` should be renamed as `codes.pl`

To initiate the learning, type the following at the command line:

```
$ progol learn_cj1416c.pl
```

Then you should obtain the same output as the one in `learn_cj1416c_out`.

VISUALISATION

We developed a portal-based workbench, WIBL (Workbench for Integrative Biological Learning) to browse the glycan structure, metabolic and protein-protein interaction networks as well as the underlying Prolog. WIBL is hosted at

<http://www.sbg.bio.ic.ac.uk/wibl> (username `guest`, project `campy`).

Lesk V, Taubert J, Rawlings C, Dunbar S, Muggleton S (2011)

WIBL: Workbench for Integrative Biological Learning.

Journal of integrative bioinformatics 8: 156

```

% FILE BACKGROUND_PL
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% A logic program for modelling genotype-phenotype
% relation in Campylobacter jejuni. This model
% integrates data from different sources, i.e. mutants
% data from gene knock-out experiments, cross-strain
% genomic data, glycan structures and pathways
% information compiled from KEGG and BioCyc
%
% N.B. This model was prepared to be used with Progol 5.0

% Abductive learning settings for Progol 5.0

:- modeh(1, codes(#any, #any))?

:- observable(knockout_observable/2)?

% The following rule models the effect of knocking-out a gene in terms
% of the absence of a glycan structure and the implications for assigning
% a gene to a specific reaction

knockout_observable(Gene, Observable):-
    unassigned_gene(Gene),
    struct_observable(Prs_Struct, Observable),
    struct_next(Prs_Struct, Abs_Struct),
    path3(R, Prs_Struct, Abs_Struct),
    unassigned_reaction(R),
    codes(Gene, R).

% The working assumption that if a pair of genes are present in two strains
% which share the same serotype, they both perform neighbour reactions in a
% path which synthesises a particular glycan

occurs(Strain1, Gene):-
    codes(Gene, R1),
    neighbour_reaction(R1, R2),
    codes(G2, R2),
    occurs0(Strain2, G2),
    have_same_serotype(Strain1, Strain2), !.

have_same_serotype(Strain1, Strain2):-
    Strain1 \= Strain2,
    strain_has_penner_serotype(Strain1, Serotype),
    strain_has_penner_serotype(Strain2, Serotype), !.

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% The definition of pathways in terms of steps of sequential reactions

path3(R, X, Y):-

```

reaction3(R,X,Y).

path3(R,X,Y):-

reaction3(R0,X,Y),
reaction3(R0,Z,Y),
not(X=Z),
leading_to(R,Z).

leading_to(R,X):-

reaction3(R,Z,X).

leading_to(R,X):-

reaction3(_,Z,X),
leading_to(R,Z).

reaction3(R,X,Y):-

reaction2(R,X,Y).

reaction2(R,X,Y):-

reaction(D,O,R,X,Y,Dir).

%%
%%

% Integrity constraints

:- codes(Gene, Reaction1),
codes(Gene, Reaction2),
not(Reaction1 = Reaction2).

:- codes(Gene1, Reaction),
codes(Gene2, Reaction),
not(chain(Reaction)),
not(Gene1 = Gene2).

```
% FILE CODES_PL
```

```
% Known gene functions represented by instances of the 'codes' predicate
```

```
codes(cj1421c,capsule_ngro36a).
```

```
codes(cj1422c,capsule_ngro21a).
```

```
codes(cj1426c,capsule_ngro21c).
```

```
codes(cj1430c,capsule_hep5).
```

```
codes(cj1431c,capsule_ngro1c).
```

```
codes(cj1439c,capsule_pre_pre_galfnac).
```

```
codes(cj1441c,capsule_pre_pre_glca).
```

% FILE COMMON_PL

% Common predicate declarations for genes and strains

gene(cj1413c).
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strain(strainTurkey8).
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penner_serogroup(serogroupE).
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penner_serotype(hs55).
penner_serotype(hs6).
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penner_serotype(hs67).

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clade(cladeB2).
clade(cladeB3).
clade(cladeB4).

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superclade(supercladeB).

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strain_has_penner_serogroup(strainClinical30280,serogroupD).

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strain_has_penner_serogroup(strainClinical38762,serogroupN).
strain_has_penner_serogroup(strainClinical38857,serogroupR).
strain_has_penner_serogroup(strainClinical40671,serogroupD).
strain_has_penner_serogroup(strainClinical40917,serogroupP).
strain_has_penner_serogroup(strainClinical41651,serogroupD).
strain_has_penner_serogroup(strainClinical43205,serogroupB).
strain_has_penner_serogroup(strainClinical43983,serogroupD).
strain_has_penner_serogroup(strainClinical44119,serogroupN).
strain_has_penner_serogroup(strainClinical44811,serogroupB).
strain_has_penner_serogroup(strainClinical44933,serogroupD).
strain_has_penner_serogroup(strainClinical44958,serogroupD).
strain_has_penner_serogroup(strainClinical45631,serogroupD).
strain_has_penner_serogroup(strainClinical48612,serogroupB).
strain_has_penner_serogroup(strainClinical52331,serogroupD).
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strain_has_penner_serogroup(strainClinical56832,serogroupD).
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strain_has_penner_serogroup(strainClinical59424,serogroupU).
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strain_has_penner_serogroup(strainClinicall38556,serogroupD).
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strain_has_penner_serogroup(strainOvine12481,serogroupD).
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strain_has_clade(strainGoose222,cladeB4).
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strain_has_clade(strainWaterSA5,cladeB4).

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strain_has_superclade(strainTurkey4,supercladeA).
strain_has_superclade(strainTurkey8,supercladeB).
strain_has_superclade(strainWaterS5,supercladeB).
strain_has_superclade(strainWaterSA5,supercladeB).

```
% CPS_PATHWAY_PL
% Campylobacter jejuni capsule pathway compiled from KEGG and BioCyc
% augmented by some specific information about the C. jejuni capsul
% glycan structure that were extracted from publications.
```

```
species_t(cje).
db_t(brendan).
```

```
pathway_t(capsule).
pathway_name(brendan,cje,capsule,'Capsule synthesis pathway').
```

```
subpathway_t(cap_hep).
subpathway(brendan,cje,cap_hep,capsule).
subpathway_name(brendan,cje,cap_hep,'Heptose biosynthesis').
```

```
%% Hep biosynthesis component (alternative to that given for LOS pathway above)
```

```
compound_t('gdp-dd-hep').
compound(brendan,cje,'gdp-dd-hep').
compound_name(brendan,'gdp-dd-hep','GDP-D,D-heptose').
```

```
compound_t('gdp-d-al-gluco-hep').
compound(brendan,cje,'gdp-d-al-gluco-hep').
compound_name(brendan,'gdp-d-al-gluco-hep','GDP-D-glycero-alpha-L-glucoheptose').
```

```
reaction_t(capsule_hep1).
reaction(brendan,cje,capsule_hep1,'d-sedohep-7-p','dd-hep-7-p',1).
reaction_gene(brendan,cje,capsule_hep1,cj1424c).
reaction_subpathway(brendan,cje,capsule_hep1,cap_hep).
reaction_pathway(brendan,cje,capsule_hep1,capsule).
```

```
gene_t(cj1424c).
gene(brendan,cje,cj1424c).
gene_name(brendan,cj1424c,'GmhA2').
```

```
reaction_t(capsule_hep2).
reaction_gene(brendan,cje,capsule_hep2,cj1425c).
reaction(brendan,cje,capsule_hep2,'dd-hep-7-p','dd-hep-17-pp',1).
reaction_subpathway(brendan,cje,capsule_hep2,cap_hep).
reaction_pathway(brendan,cje,capsule_hep2,capsule).
```

```
gene_t(cj1425c).
gene(brendan,cje,cj1425c).
gene_name(brendan,cj1425c,'HddA').
```

```
reaction_t(capsule_hep3).
reaction_gene(brendan,cje,capsule_hep3,cj1152c).
reaction(brendan,cje,capsule_hep3,'dd-hep-17-pp','dd-hep-1-p',1).
reaction_subpathway(brendan,cje,capsule_hep3,cap_hep).
reaction_pathway(brendan,cje,capsule_hep3,capsule).
```

```
reaction_t(capsule_hep4).
```

```
reaction_gene(brendan,cje,capsule_hep4,cj1423c).
reaction(brendan,cje,capsule_hep4,'dd-hep-1-p','gdp-dd-hep',1).
reaction_subpathway(brendan,cje,capsule_hep4,cap_hep).
reaction_pathway(brendan,cje,capsule_hep4,capsule).
```

```
gene_t(cj1423c).
gene(brendan,cje,cj1423c).
gene_name(brendan,cj1423c,'HddC').
```

```
reaction_t(capsule_hep5).
reaction_gene(brendan,cje,capsule_hep5,cj1427c).
reaction_gene(brendan,cje,capsule_hep5,cj1428c).
reaction_gene(brendan,cje,capsule_hep5,cj1430c).
reaction(brendan,cje,capsule_hep5,'gdp-dd-hep','gdp-d-al-gluco-hep',1).
reaction_subpathway(brendan,cje,capsule_hep5,cap_hep).
reaction_pathway(brendan,cje,capsule_hep5,capsule).
```

```
gene_t(cj1427c).
gene(brendan,cje,cj1427c).
gene_name(brendan,cj1427c,'Putative UDP-glucose 4-epimerase').
gene_t(cj1428c).
gene(brendan,cje,cj1428c).
gene_name(brendan,cj1428c,'Fcl').
gene_t(cj1430c).
gene(brendan,cje,cj1430c).
gene_name(brendan,cj1430c,'Putative dTDP-4-dehydrorhamnose 3,5-epimerase').
```

%% adding next unit to chain

```
compound_t('capsule_chain').
compound(brendan,cje,'capsule_chain').
compound_name(brendan,'capsule_chain','Capsule chain (X)').
```

```
compound_t('glca').
compound(brendan,cje,'glca').
compound_name(brendan,'glca','GlcA-X').
```

```
compound_t('glca6ngro').
compound(brendan,cje,'glca6ngro').
compound_name(brendan,'glca6ngro','GlcA6(NGro)-X').
```

```
compound_t('glca6etn').
compound(brendan,cje,'glca6etn').
compound_name(brendan,'glca6etn','GlcA6(EtN)-X').
```

%% for glca6ngro

%% side Hep group + phase variable modifications

```
compound_t('glca6ngro+hep').
compound(brendan,cje,'glca6ngro+hep').
compound_name(brendan,'glca6ngro+hep','GlcA6(NGro)+Hep-X').
```

```
compound_t('glca6ngro+hep+omepn').
compound(brendan,cje,'glca6ngro+hep+omepn').
compound_name(brendan,'glca6ngro+hep+omepn','GlcA6\(\NGro\)+\(\Hep+OMePN\)-X').
```

```
compound_t('glca6ngro+hep+3ome').
compound(brendan,cje,'glca6ngro+hep+3ome').
compound_name(brendan,'glca6ngro+hep+3ome','GlcA6\(\NGro\)+\(\Hep+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+6ome').
compound(brendan,cje,'glca6ngro+hep+6ome').
compound_name(brendan,'glca6ngro+hep+6ome','GlcA6\(\NGro\)+\(\Hep+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome').
compound_name(brendan,'glca6ngro+hep+omepn+3ome','GlcA6\(\NGro\)+\(\Hep+OMePN+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+6ome').
compound(brendan,cje,'glca6ngro+hep+omepn+6ome').
compound_name(brendan,'glca6ngro+hep+omepn+6ome','GlcA6\(\NGro\)+\(\Hep+OMePN+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+3ome+6ome').
compound(brendan,cje,'glca6ngro+hep+3ome+6ome').
compound_name(brendan,'glca6ngro+hep+3ome+6ome','GlcA6\(\NGro\)+\(\Hep+3OMe+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome+6ome').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome+6ome').
compound_name(brendan,'glca6ngro+hep+omepn+3ome+6ome','GlcA6\(\NGro\)+\(\Hep+OMePN+3OMe+6OMe\)-X').
```

%% GalfNAc group + phase variable group

```
compound_t('glca6ngro-galfnac').
compound(brendan,cje,'glca6ngro-galfnac').
compound_name(brendan,'glca6ngro-galfnac','GalfNAc-GlcA6\(\NGro\)-X').
```

```
compound_t('glca6ngro+hep-galfnac').
compound(brendan,cje,'glca6ngro+hep-galfnac').
compound_name(brendan,'glca6ngro+hep-galfnac','GalfNAc-GlcA6\(\NGro\)+Hep-X').
```

```
compound_t('glca6ngro+hep+omepn-galfnac').
compound(brendan,cje,'glca6ngro+hep+omepn-galfnac').
compound_name(brendan,'glca6ngro+hep+omepn-galfnac','GalfNAc-GlcA6\(\NGro\)+\(\Hep+OMePN\)-X').
```

```
compound_t('glca6ngro+hep+3ome-galfnac').
compound(brendan,cje,'glca6ngro+hep+3ome-galfnac').
compound_name(brendan,'glca6ngro+hep+3ome-galfnac','GalfNAc-GlcA6\(\NGro\)+\(\Hep+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+6ome-galfnac').
compound(brendan,cje,'glca6ngro+hep+6ome-galfnac').
compound_name(brendan,'glca6ngro+hep+6ome-galfnac','GalfNAc-GlcA6\(\NGro\)+\(\Hep+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome-galfnac').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome-galfnac').
compound_name(brendan,'glca6ngro+hep+omepn+3ome-galfnac','GalfNAc-GlcA6\(\NGro\)+\(\Hep+OMePN+3OMe\)-X').
```


X').

```
compound_t('glca6ngro+hep+omepn+6ome-galfnac').  
compound(brendan,cje,'glca6ngro+hep+omepn+6ome-galfnac').  
compound_name(brendan,'glca6ngro+hep+omepn+6ome-galfnac','GalfNAc-GlcA6\(\NGro\)+\(\Hep+OMePN+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+3ome+6ome-galfnac').  
compound(brendan,cje,'glca6ngro+hep+3ome+6ome-galfnac').  
compound_name(brendan,'glca6ngro+hep+3ome+6ome-galfnac','GalfNAc-GlcA6\(\NGro\)+\(\Hep+3OMe+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome+6ome-galfnac').  
compound(brendan,cje,'glca6ngro+hep+omepn+3ome+6ome-galfnac').  
compound_name(brendan,'glca6ngro+hep+omepn+3ome+6ome-galfnac','GalfNAc-GlcA6\(\NGro\)+\(\Hep+OMePN+3OMe+6OMe\)-X').
```

```
compound_t('glca6ngro-galfnac+omepn').  
compound(brendan,cje,'glca6ngro-galfnac+omepn').  
compound_name(brendan,'glca6ngro-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)-X').
```

```
compound_t('glca6ngro+hep-galfnac+omepn').  
compound(brendan,cje,'glca6ngro+hep-galfnac+omepn').  
compound_name(brendan,'glca6ngro+hep-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)+Hep-X').
```

```
compound_t('glca6ngro+hep+omepn-galfnac+omepn').  
compound(brendan,cje,'glca6ngro+hep+omepn-galfnac+omepn').  
compound_name(brendan,'glca6ngro+hep+omepn-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)+\(\Hep+OMePN\)-X').
```

```
compound_t('glca6ngro+hep+3ome-galfnac+omepn').  
compound(brendan,cje,'glca6ngro+hep+3ome-galfnac+omepn').  
compound_name(brendan,'glca6ngro+hep+3ome-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)+\(\Hep+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+6ome-galfnac+omepn').  
compound(brendan,cje,'glca6ngro+hep+6ome-galfnac+omepn').  
compound_name(brendan,'glca6ngro+hep+6ome-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)+\(\Hep+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome-galfnac+omepn').  
compound(brendan,cje,'glca6ngro+hep+omepn+3ome-galfnac+omepn').  
compound_name(brendan,'glca6ngro+hep+omepn+3ome-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)+\(\Hep+OMePN+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+6ome-galfnac+omepn').  
compound(brendan,cje,'glca6ngro+hep+omepn+6ome-galfnac+omepn').  
compound_name(brendan,'glca6ngro+hep+omepn+6ome-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)+\(\Hep+OMePN+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+3ome+6ome-galfnac+omepn').  
compound(brendan,cje,'glca6ngro+hep+3ome+6ome-galfnac+omepn').  
compound_name(brendan,'glca6ngro+hep+3ome+6ome-galfnac+omepn','GalfNAc+OMePN-GlcA6\(\NGro\)+\(\Hep+3OMe+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome+6ome-galfnac+omepn').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome+6ome-galfnac+omepn').
compound_name(brendan,'glca6ngro+hep+omepn+3ome+6ome-galfnac+omepn','GalFNAC+OMePN-
GlcA6\(\NGro)\+\(Hep+OMePN+3OMe+6OMe\)-X').
```

%% Ribf group

```
compound_t('glca6ngro-galfnac-ribf').
compound(brendan,cje,'glca6ngro-galfnac-ribf').
compound_name(brendan,'glca6ngro-galfnac-ribf','Ribf-GalFNAC-GlcA6\(\NGro\)-X').
```

```
compound_t('glca6ngro+hep-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep-galfnac-ribf','Ribf-GalFNAC-GlcA6\(\NGro\)+Hep-X').
```

```
compound_t('glca6ngro+hep+omepn-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep+omepn-galfnac-ribf','Ribf-GalFNAC-GlcA6\(\NGro\)\+\(Hep+OMePN\)-X').
```

```
compound_t('glca6ngro+hep+3ome-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep+3ome-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep+3ome-galfnac-ribf','Ribf-GalFNAC-GlcA6\(\NGro\)\+\(Hep+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+6ome-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep+6ome-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep+6ome-galfnac-ribf','Ribf-GalFNAC-GlcA6\(\NGro\)\+\(Hep+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep+omepn+3ome-galfnac-ribf','Ribf-GalFNAC-
GlcA6\(\NGro)\+\(Hep+OMePN+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+6ome-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn+6ome-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep+omepn+6ome-galfnac-ribf','Ribf-GalFNAC-
GlcA6\(\NGro)\+\(Hep+OMePN+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+3ome+6ome-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep+3ome+6ome-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep+3ome+6ome-galfnac-ribf','Ribf-GalFNAC-
GlcA6\(\NGro)\+\(Hep+3OMe+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome+6ome-galfnac-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome+6ome-galfnac-ribf').
compound_name(brendan,'glca6ngro+hep+omepn+3ome+6ome-galfnac-ribf','Ribf-GalFNAC-
GlcA6\(\NGro)\+\(Hep+OMePN+3OMe+6OMe\)-X').
```

```
compound_t('glca6ngro-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro-galfnac+omepn-ribf','Ribf-GalFNAC+OMePN-GlcA6\(\NGro\)-X').
```

```
compound_t('glca6ngro+hep-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep-galfnac+omepn-ribf','Ribf-GalFNAC+OMePN-GlcA6\(\NGro\)+Hep-X').
```

```
compound_t('glca6ngro+hep+omepn-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep+omepn-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-
GlcA6\(\NGro\)+\(\Hep+OMePN\)-X').
```

```
compound_t('glca6ngro+hep+3ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep+3ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep+3ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-
GlcA6\(\NGro\)+\(\Hep+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+6ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep+6ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep+6ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-
GlcA6\(\NGro\)+\(\Hep+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep+omepn+3ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-
GlcA6\(\NGro\)+\(\Hep+OMePN+3OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-
GlcA6\(\NGro\)+\(\Hep+OMePN+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+3ome+6ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep+3ome+6ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep+3ome+6ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-
GlcA6\(\NGro\)+\(\Hep+3OMe+6OMe\)-X').
```

```
compound_t('glca6ngro+hep+omepn+3ome+6ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6ngro+hep+omepn+3ome+6ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6ngro+hep+omepn+3ome+6ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-
GlcA6\(\NGro\)+\(\Hep+OMePN+3OMe+6OMe\)-X').
```

%% now for EtN phase variable modification

%% side Hep group + phase variable modifications

```
compound_t('glca6etn+hep').
compound(brendan,cje,'glca6etn+hep').
compound_name(brendan,'glca6etn+hep','GlcA6\(\EtN\)+Hep-X').
```

```
compound_t('glca6etn+hep+omepn').
compound(brendan,cje,'glca6etn+hep+omepn').
compound_name(brendan,'glca6etn+hep+omepn','GlcA6\(\EtN\)+\(\Hep+OMePN\)-X').
```

```
compound_t('glca6etn+hep+3ome').
compound(brendan,cje,'glca6etn+hep+3ome').
compound_name(brendan,'glca6etn+hep+3ome','GlcA6\(\EtN\)+\(\Hep+3OMe\)-X').
```

```
compound_t('glca6etn+hep+6ome').
```

compound(brendan,cje,'glca6etn+hep+6ome').
compound_name(brendan,'glca6etn+hep+6ome','GlcA6(EtN)\(Hep+6OMe\)-X').

compound_t('glca6etn+hep+omepn+3ome').
compound(brendan,cje,'glca6etn+hep+omepn+3ome').
compound_name(brendan,'glca6etn+hep+omepn+3ome','GlcA6(EtN)\(Hep+OMePN+3OMe\)-X').

compound_t('glca6etn+hep+omepn+6ome').
compound(brendan,cje,'glca6etn+hep+omepn+6ome').
compound_name(brendan,'glca6etn+hep+omepn+6ome','GlcA6(EtN)\(Hep+OMePN+6OMe\)-X').

compound_t('glca6etn+hep+3ome+6ome').
compound(brendan,cje,'glca6etn+hep+3ome+6ome').
compound_name(brendan,'glca6etn+hep+3ome+6ome','GlcA6(EtN)\(Hep+3OMe+6OMe\)-X').

compound_t('glca6etn+hep+omepn+3ome+6ome').
compound(brendan,cje,'glca6etn+hep+omepn+3ome+6ome').
compound_name(brendan,'glca6etn+hep+omepn+3ome+6ome','GlcA6(EtN)\(Hep+OMePN+3OMe+6OMe\)-X').

%% GalfNAc group + phase variable group

compound_t('glca6etn-galfnac').
compound(brendan,cje,'glca6etn-galfnac').
compound_name(brendan,'glca6etn-galfnac','GalfNAc-GlcA6(EtN\)-X').

compound_t('glca6etn+hep-galfnac').
compound(brendan,cje,'glca6etn+hep-galfnac').
compound_name(brendan,'glca6etn+hep-galfnac','GalfNAc-GlcA6(EtN\)+Hep-X').

compound_t('glca6etn+hep+omepn-galfnac').
compound(brendan,cje,'glca6etn+hep+omepn-galfnac').
compound_name(brendan,'glca6etn+hep+omepn-galfnac','GalfNAc-GlcA6(EtN)\(Hep+OMePN\)-X').

compound_t('glca6etn+hep+3ome-galfnac').
compound(brendan,cje,'glca6etn+hep+3ome-galfnac').
compound_name(brendan,'glca6etn+hep+3ome-galfnac','GalfNAc-GlcA6(EtN)\(Hep+3OMe\)-X').

compound_t('glca6etn+hep+6ome-galfnac').
compound(brendan,cje,'glca6etn+hep+6ome-galfnac').
compound_name(brendan,'glca6etn+hep+6ome-galfnac','GalfNAc-GlcA6(EtN)\(Hep+6OMe\)-X').

compound_t('glca6etn+hep+omepn+3ome-galfnac').
compound(brendan,cje,'glca6etn+hep+omepn+3ome-galfnac').
compound_name(brendan,'glca6etn+hep+omepn+3ome-galfnac','GalfNAc-GlcA6(EtN)\(Hep+OMePN+3OMe\)-X').

compound_t('glca6etn+hep+omepn+6ome-galfnac').
compound(brendan,cje,'glca6etn+hep+omepn+6ome-galfnac').
compound_name(brendan,'glca6etn+hep+omepn+6ome-galfnac','GalfNAc-GlcA6(EtN)\(Hep+OMePN+6OMe\)-X').

compound_t('glca6etn+hep+3ome+6ome-galfnac').
compound(brendan,cje,'glca6etn+hep+3ome+6ome-galfnac').
compound_name(brendan,'glca6etn+hep+3ome+6ome-galfnac','GalfNAc-GlcA6(EtN)\(Hep+3OMe+6OMe\)-X').

compound_t('glca6etn+hep+omepn+3ome+6ome-galfnac').

compound(brendan,cje,'glca6etn+hep+omepn+3ome+6ome-galfnac').
compound_name(brendan,'glca6etn+hep+omepn+3ome+6ome-galfnac','GalfnAc-GlcA6(EtN)\+(Hep+OMePN+3OMe+6OMe)-X').

compound_t('glca6etn-galfnac+omepn').
compound(brendan,cje,'glca6etn-galfnac+omepn').
compound_name(brendan,'glca6etn-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)-X').

compound_t('glca6etn+hep-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep-galfnac+omepn').
compound_name(brendan,'glca6etn+hep-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)+Hep-X').

compound_t('glca6etn+hep+omepn-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep+omepn-galfnac+omepn').
compound_name(brendan,'glca6etn+hep+omepn-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)\+(Hep+OMePN)-X').

compound_t('glca6etn+hep+3ome-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep+3ome-galfnac+omepn').
compound_name(brendan,'glca6etn+hep+3ome-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)\+(Hep+3OMe)-X').

compound_t('glca6etn+hep+6ome-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep+6ome-galfnac+omepn').
compound_name(brendan,'glca6etn+hep+6ome-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)\+(Hep+6OMe)-X').

compound_t('glca6etn+hep+omepn+3ome-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep+omepn+3ome-galfnac+omepn').
compound_name(brendan,'glca6etn+hep+omepn+3ome-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)\+(Hep+OMePN+3OMe)-X').

compound_t('glca6etn+hep+omepn+6ome-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep+omepn+6ome-galfnac+omepn').
compound_name(brendan,'glca6etn+hep+omepn+6ome-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)\+(Hep+OMePN+6OMe)-X').

compound_t('glca6etn+hep+3ome+6ome-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep+3ome+6ome-galfnac+omepn').
compound_name(brendan,'glca6etn+hep+3ome+6ome-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)\+(Hep+3OMe+6OMe)-X').

compound_t('glca6etn+hep+omepn+3ome+6ome-galfnac+omepn').
compound(brendan,cje,'glca6etn+hep+omepn+3ome+6ome-galfnac+omepn').
compound_name(brendan,'glca6etn+hep+omepn+3ome+6ome-galfnac+omepn','GalfnAc+OMePN-GlcA6(EtN)\+(Hep+OMePN+3OMe+6OMe)-X').

%% Ribf group

compound_t('glca6etn-galfnac-ribf').
compound(brendan,cje,'glca6etn-galfnac-ribf').
compound_name(brendan,'glca6etn-galfnac-ribf','Ribf-GalfnAc-GlcA6(EtN)-X').

compound_t('glca6etn+hep-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep-galfnac-ribf').
compound_name(brendan,'glca6etn+hep-galfnac-ribf','Ribf-GalfnAc-GlcA6(EtN)+Hep-X').

compound_t('glca6etn+hep+omepn-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep+omepn-galfnac-ribf').
compound_name(brendan,'glca6etn+hep+omepn-galfnac-ribf','Ribf-GalfNAc-GlcA6(EtN)+(Hep+OMePN)-X').

compound_t('glca6etn+hep+3ome-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep+3ome-galfnac-ribf').
compound_name(brendan,'glca6etn+hep+3ome-galfnac-ribf','Ribf-GalfNAc-GlcA6(EtN)+(Hep+3OMe)-X').

compound_t('glca6etn+hep+6ome-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep+6ome-galfnac-ribf').
compound_name(brendan,'glca6etn+hep+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA6(EtN)+(Hep+6OMe)-X').

compound_t('glca6etn+hep+omepn+3ome-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep+omepn+3ome-galfnac-ribf').
compound_name(brendan,'glca6etn+hep+omepn+3ome-galfnac-ribf','Ribf-GalfNAc-GlcA6(EtN)+(Hep+OMePN+3OMe)-X').

compound_t('glca6etn+hep+omepn+6ome-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep+omepn+6ome-galfnac-ribf').
compound_name(brendan,'glca6etn+hep+omepn+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA6(EtN)+(Hep+OMePN+6OMe)-X').

compound_t('glca6etn+hep+3ome+6ome-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep+3ome+6ome-galfnac-ribf').
compound_name(brendan,'glca6etn+hep+3ome+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA6(EtN)+(Hep+3OMe+6OMe)-X').

compound_t('glca6etn+hep+omepn+3ome+6ome-galfnac-ribf').
compound(brendan,cje,'glca6etn+hep+omepn+3ome+6ome-galfnac-ribf').
compound_name(brendan,'glca6etn+hep+omepn+3ome+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA6(EtN)+(Hep+OMePN+3OMe+6OMe)-X').

compound_t('glca6etn-galfnac+omepn-ribf').
compound(brendan,cje,'glca6etn-galfnac+omepn-ribf').
compound_name(brendan,'glca6etn-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA6(EtN)-X').

compound_t('glca6etn+hep-galfnac+omepn-ribf').
compound(brendan,cje,'glca6etn+hep-galfnac+omepn-ribf').
compound_name(brendan,'glca6etn+hep-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA6(EtN)+Hep-X').

compound_t('glca6etn+hep+omepn-galfnac+omepn-ribf').
compound(brendan,cje,'glca6etn+hep+omepn-galfnac+omepn-ribf').
compound_name(brendan,'glca6etn+hep+omepn-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA6(EtN)+(Hep+OMePN)-X').

compound_t('glca6etn+hep+3ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6etn+hep+3ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6etn+hep+3ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA6(EtN)+(Hep+3OMe)-X').

compound_t('glca6etn+hep+6ome-galfnac+omepn-ribf').
compound(brendan,cje,'glca6etn+hep+6ome-galfnac+omepn-ribf').
compound_name(brendan,'glca6etn+hep+6ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-

GlcA6(EtN)\(Hep+6OMe)-X').

compound_t('glca6etn+hep+omepn+3ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca6etn+hep+omepn+3ome-galfnac+omepn-ribf').

compound_name(brendan,'glca6etn+hep+omepn+3ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-GlcA6(EtN)\(Hep+OMePN+3OMe)-X').

compound_t('glca6etn+hep+omepn+6ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca6etn+hep+omepn+6ome-galfnac+omepn-ribf').

compound_name(brendan,'glca6etn+hep+omepn+6ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-GlcA6(EtN)\(Hep+OMePN+6OMe)-X').

compound_t('glca6etn+hep+3ome+6ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca6etn+hep+3ome+6ome-galfnac+omepn-ribf').

compound_name(brendan,'glca6etn+hep+3ome+6ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-GlcA6(EtN)\(Hep+3OMe+6OMe)-X').

compound_t('glca6etn+hep+omepn+3ome+6ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca6etn+hep+omepn+3ome+6ome-galfnac+omepn-ribf').

compound_name(brendan,'glca6etn+hep+omepn+3ome+6ome-galfnac+omepn-ribf','Ribf-GalfNac+OMePN-GlcA6(EtN)\(Hep+OMePN+3OMe+6OMe)-X').

%% for glca without ngro or etn phase variable modification

%% side Hep group + phase variable modifications

compound_t('glca+hep').

compound(brendan,cje,'glca+hep').

compound_name(brendan,'glca+hep','GlcA+Hep-X').

compound_t('glca+hep+omepn').

compound(brendan,cje,'glca+hep+omepn').

compound_name(brendan,'glca+hep+omepn','GlcA+\(Hep+OMePN)-X').

compound_t('glca+hep+3ome').

compound(brendan,cje,'glca+hep+3ome').

compound_name(brendan,'glca+hep+3ome','GlcA+\(Hep+3OMe)-X').

compound_t('glca+hep+6ome').

compound(brendan,cje,'glca+hep+6ome').

compound_name(brendan,'glca+hep+6ome','GlcA+\(Hep+6OMe)-X').

compound_t('glca+hep+omepn+3ome').

compound(brendan,cje,'glca+hep+omepn+3ome').

compound_name(brendan,'glca+hep+omepn+3ome','GlcA+\(Hep+OMePN+3OMe)-X').

compound_t('glca+hep+omepn+6ome').

compound(brendan,cje,'glca+hep+omepn+6ome').

compound_name(brendan,'glca+hep+omepn+6ome','GlcA+\(Hep+OMePN+6OMe)-X').

compound_t('glca+hep+3ome+6ome').

compound(brendan,cje,'glca+hep+3ome+6ome').

compound_name(brendan,'glca+hep+3ome+6ome','GlcA+\(Hep+3OMe+6OMe)-X').

```
compound_t('glca+hep+omepn+3ome+6ome').
compound(brendan,cje,'glca+hep+omepn+3ome+6ome').
compound_name(brendan,'glca+hep+omepn+3ome+6ome','GlcA+\(Hep+OMePN+3OMe+6OMe\)-X').
```

%% GalfNAc group + phase variable group

```
compound_t('glca-galfnac').
compound(brendan,cje,'glca-galfnac').
compound_name(brendan,'glca-galfnac','GalfNAc-GlcA-X').
```

```
compound_t('glca+hep-galfnac').
compound(brendan,cje,'glca+hep-galfnac').
compound_name(brendan,'glca+hep-galfnac','GalfNAc-GlcA+Hep-X').
```

```
compound_t('glca+hep+omepn-galfnac').
compound(brendan,cje,'glca+hep+omepn-galfnac').
compound_name(brendan,'glca+hep+omepn-galfnac','GalfNAc-GlcA+\(Hep+OMePN\)-X').
```

```
compound_t('glca+hep+3ome-galfnac').
compound(brendan,cje,'glca+hep+3ome-galfnac').
compound_name(brendan,'glca+hep+3ome-galfnac','GalfNAc-GlcA+\(Hep+3OMe\)-X').
```

```
compound_t('glca+hep+6ome-galfnac').
compound(brendan,cje,'glca+hep+6ome-galfnac').
compound_name(brendan,'glca+hep+6ome-galfnac','GalfNAc-GlcA+\(Hep+6OMe\)-X').
```

```
compound_t('glca+hep+omepn+3ome-galfnac').
compound(brendan,cje,'glca+hep+omepn+3ome-galfnac').
compound_name(brendan,'glca+hep+omepn+3ome-galfnac','GalfNAc-GlcA+\(Hep+OMePN+3OMe\)-X').
```

```
compound_t('glca+hep+omepn+6ome-galfnac').
compound(brendan,cje,'glca+hep+omepn+6ome-galfnac').
compound_name(brendan,'glca+hep+omepn+6ome-galfnac','GalfNAc-GlcA+\(Hep+OMePN+6OMe\)-X').
```

```
compound_t('glca+hep+3ome+6ome-galfnac').
compound(brendan,cje,'glca+hep+3ome+6ome-galfnac').
compound_name(brendan,'glca+hep+3ome+6ome-galfnac','GalfNAc-GlcA+\(Hep+3OMe+6OMe\)-X').
```

```
compound_t('glca+hep+omepn+3ome+6ome-galfnac').
compound(brendan,cje,'glca+hep+omepn+3ome+6ome-galfnac').
compound_name(brendan,'glca+hep+omepn+3ome+6ome-galfnac','GalfNAc-GlcA+\(Hep+OMePN+3OMe+6OMe\)-X').
```

```
compound_t('glca-galfnac+omepn').
compound(brendan,cje,'glca-galfnac+omepn').
compound_name(brendan,'glca-galfnac+omepn','GalfNAc+OMePN-GlcA-X').
```

```
compound_t('glca+hep-galfnac+omepn').
compound(brendan,cje,'glca+hep-galfnac+omepn').
compound_name(brendan,'glca+hep-galfnac+omepn','GalfNAc+OMePN-GlcA+Hep-X').
```

```
compound_t('glca+hep+omepn-galfnac+omepn').
compound(brendan,cje,'glca+hep+omepn-galfnac+omepn').
```


compound_name(brendan,'glca+hep+omepn-galfnac+omepn','GalfNAc+OMePN-GlcA+\(Hep+OMePN\) -X').

compound_t('glca+hep+3ome-galfnac+omepn').

compound(brendan,cje,'glca+hep+3ome-galfnac+omepn').

compound_name(brendan,'glca+hep+3ome-galfnac+omepn','GalfNAc+OMePN-GlcA+\(Hep+3OMe\) -X').

compound_t('glca+hep+6ome-galfnac+omepn').

compound(brendan,cje,'glca+hep+6ome-galfnac+omepn').

compound_name(brendan,'glca+hep+6ome-galfnac+omepn','GalfNAc+OMePN-GlcA+\(Hep+6OMe\) -X').

compound_t('glca+hep+omepn+3ome-galfnac+omepn').

compound(brendan,cje,'glca+hep+omepn+3ome-galfnac+omepn').

compound_name(brendan,'glca+hep+omepn+3ome-galfnac+omepn','GalfNAc+OMePN-GlcA+\(Hep+OMePN+3OMe\) -X').

compound_t('glca+hep+omepn+6ome-galfnac+omepn').

compound(brendan,cje,'glca+hep+omepn+6ome-galfnac+omepn').

compound_name(brendan,'glca+hep+omepn+6ome-galfnac+omepn','GalfNAc+OMePN-GlcA+\(Hep+OMePN+6OMe\) -X').

compound_t('glca+hep+3ome+6ome-galfnac+omepn').

compound(brendan,cje,'glca+hep+3ome+6ome-galfnac+omepn').

compound_name(brendan,'glca+hep+3ome+6ome-galfnac+omepn','GalfNAc+OMePN-GlcA+\(Hep+3OMe+6OMe\) -X').

compound_t('glca+hep+omepn+3ome+6ome-galfnac+omepn').

compound(brendan,cje,'glca+hep+omepn+3ome+6ome-galfnac+omepn').

compound_name(brendan,'glca+hep+omepn+3ome+6ome-galfnac+omepn','GalfNAc+OMePN-GlcA+\(Hep+OMePN+3OMe+6OMe\) -X').

%% Ribf group

compound_t('glca-galfnac-ribf').

compound(brendan,cje,'glca-galfnac-ribf').

compound_name(brendan,'glca-galfnac-ribf','Ribf-GalfNAc-GlcA-X').

compound_t('glca+hep-galfnac-ribf').

compound(brendan,cje,'glca+hep-galfnac-ribf').

compound_name(brendan,'glca+hep-galfnac-ribf','Ribf-GalfNAc-GlcA+Hep-X').

compound_t('glca+hep+omepn-galfnac-ribf').

compound(brendan,cje,'glca+hep+omepn-galfnac-ribf').

compound_name(brendan,'glca+hep+omepn-galfnac-ribf','Ribf-GalfNAc-GlcA+\(Hep+OMePN\) -X').

compound_t('glca+hep+3ome-galfnac-ribf').

compound(brendan,cje,'glca+hep+3ome-galfnac-ribf').

compound_name(brendan,'glca+hep+3ome-galfnac-ribf','Ribf-GalfNAc-GlcA+\(Hep+3OMe\) -X').

compound_t('glca+hep+6ome-galfnac-ribf').

compound(brendan,cje,'glca+hep+6ome-galfnac-ribf').

compound_name(brendan,'glca+hep+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA+\(Hep+6OMe\) -X').

compound_t('glca+hep+omepn+3ome-galfnac-ribf').

compound(brendan,cje,'glca+hep+omepn+3ome-galfnac-ribf').

compound_name(brendan,'glca+hep+omepn+3ome-galfnac-ribf','Ribf-GalfNAc-GlcA+\(Hep+OMePN+3OMe\) -X').

compound_t('glca+hep+omepn+6ome-galfnac-ribf').

compound(brendan,cje,'glca+hep+omepn+6ome-galfnac-ribf').

compound_name(brendan,'glca+hep+omepn+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA+\(Hep+OMePN+6OMe\) -X').

compound_t('glca+hep+3ome+6ome-galfnac-ribf').

compound(brendan,cje,'glca+hep+3ome+6ome-galfnac-ribf').

compound_name(brendan,'glca+hep+3ome+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA+\(Hep+3OMe+6OMe\) -X').

compound_t('glca+hep+omepn+3ome+6ome-galfnac-ribf').

compound(brendan,cje,'glca+hep+omepn+3ome+6ome-galfnac-ribf').

compound_name(brendan,'glca+hep+omepn+3ome+6ome-galfnac-ribf','Ribf-GalfNAc-GlcA+\(Hep+OMePN+3OMe+6OMe\) -X').

compound_t('glca-galfnac+omepn-ribf').

compound(brendan,cje,'glca-galfnac+omepn-ribf').

compound_name(brendan,'glca-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA-X').

compound_t('glca+hep-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA+Hep-X').

compound_t('glca+hep+omepn-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep+omepn-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep+omepn-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA+\(Hep+OMePN\) -X').

compound_t('glca+hep+3ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep+3ome-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep+3ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA+\(Hep+3OMe\) -X').

compound_t('glca+hep+6ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep+6ome-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep+6ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA+\(Hep+6OMe\) -X').

compound_t('glca+hep+omepn+3ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep+omepn+3ome-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep+omepn+3ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA+\(Hep+OMePN+3OMe\) -X').

compound_t('glca+hep+omepn+6ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep+omepn+6ome-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep+omepn+6ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA+\(Hep+OMePN+6OMe\) -X').

compound_t('glca+hep+3ome+6ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep+3ome+6ome-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep+3ome+6ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-GlcA+\(Hep+3OMe+6OMe\) -X').

compound_t('glca+hep+omepn+3ome+6ome-galfnac+omepn-ribf').

compound(brendan,cje,'glca+hep+omepn+3ome+6ome-galfnac+omepn-ribf').

compound_name(brendan,'glca+hep+omepn+3ome+6ome-galfnac+omepn-ribf','Ribf-GalfNAc+OMePN-

GlcA+\(Hep+OMePN+3OMe+6OMe\)-X').

%% what form of sugars and side groups are involved in reactions??

```
compound_t('pre-omepn').
compound(brendan,cje,'pre-omepn').
compound_name(brendan,'pre-omepn','Pre-OMePN').
```

```
compound_t('pre-ome').
compound(brendan,cje,'pre-ome').
compound_name(brendan,'pre-ome','Pre-OMe').
```

```
compound_t('pre-galfnac').
compound(brendan,cje,'pre-galfnac').
compound_name(brendan,'pre-galfnac','Pre-GalfNac').
```

```
compound_t('pre-ribf').
compound(brendan,cje,'pre-ribf').
compound_name(brendan,'pre-ribf','Pre-Ribf').
```

```
compound_t('pre-glca').
compound(brendan,cje,'pre-glca').
compound_name(brendan,'pre-glca','Pre-GlcA').
```

```
compound_t('pre-ngro').
compound(brendan,cje,'pre-ngro').
compound_name(brendan,'pre-ngro','Pre-NGro').
```

```
compound_t('pre-etn').
compound(brendan,cje,'pre-etn').
compound_name(brendan,'pre-etn','Pre-Etn').
```

%% Adding glca or glca6ngro or glca6etn to capsule chain

```
subpathway_t(cap_addngro).
subpathway(brendan,cje,cap_addngro,capsule).
subpathway_name(brendan,cje,cap_addngro,'Add NGro').
```

```
subpathway_t(cap_addetn).
subpathway(brendan,cje,cap_addetn,capsule).
subpathway_name(brendan,cje,cap_addetn,'Add EtN').
```

```
reaction_t(capsule_0).
reaction_gene(brendan,cje,capsule_0,cj1441c).
guess_rtn_gene(brendan,cje,capsule_0,cj1441c).
reaction(brendan,cje,capsule_0,'capsule_chain','glca',1).
reaction(brendan,cje,capsule_0,'pre-glca','glca',1).
reaction_pathway(brendan,cje,capsule_0,capsule).
```

```
reaction_t(capsule_ngro0).
reaction_gene(brendan,cje,capsule_ngro0,unknown).
reaction(brendan,cje,capsule_ngro0,'glca','glca6ngro',1).
reaction(brendan,cje,capsule_ngro0,'pre-ngro','glca6ngro',1).
```

```
reaction_subpathway(brendan,cje,capsule_ngro0,cap_addngro).
reaction_pathway(brendan,cje,capsule_ngro0,capsule).
```

```
gene_t(cj1441c).
gene(brendan,cje,cj1441c).
gene_name(brendan,cj1441c,'KfiD').
```

```
%% for glca6ngro
```

```
%% Adding Hep and associated phase-variable modifications
```

```
subpathway_t(cap_addhep).
subpathway(brendan,cje,cap_addhep,capsule).
subpathway_name(brendan,cje,cap_addhep,'Add Hep').
```

```
reaction_t(capsule_ngro1).
reaction_gene(brendan,cje,capsule_ngro1,cj1431c).
reaction(brendan,cje,capsule_ngro1,'glca6ngro','glca6ngro+hep',1).
reaction(brendan,cje,capsule_ngro1,'gdp-d-al-gluco-hep','glca6ngro+hep',1).
reaction_subpathway(brendan,cje,capsule_ngro1,cap_addhep).
reaction_pathway(brendan,cje,capsule_ngro1,capsule).
```

```
reaction_t(capsule_ngro1a).
reaction_gene(brendan,cje,capsule_ngro1a,cj1431c).
reaction(brendan,cje,capsule_ngro1a,'glca6ngro-galfnac','glca6ngro+hep-galfnac',1).
reaction(brendan,cje,capsule_ngro1a,'gdp-d-al-gluco-hep','glca6ngro+hep-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro1a,cap_addhep).
reaction_pathway(brendan,cje,capsule_ngro1a,capsule).
```

```
reaction_t(capsule_ngro1b).
reaction_gene(brendan,cje,capsule_ngro1b,cj1431c).
reaction(brendan,cje,capsule_ngro1b,'glca6ngro-galfnac-ribf','glca6ngro+hep-galfnac-ribf',1).
reaction(brendan,cje,capsule_ngro1b,'gdp-d-al-gluco-hep','glca6ngro+hep-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro1b,cap_addhep).
reaction_pathway(brendan,cje,capsule_ngro1b,capsule).
```

```
reaction_t(capsule_ngro1c).
reaction_gene(brendan,cje,capsule_ngro1c,cj1431c).
reaction(brendan,cje,capsule_ngro1c,'glca6ngro-galfnac+omepn-ribf','glca6ngro+hep-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro1c,'gdp-d-al-gluco-hep','glca6ngro+hep-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro1c,cap_addhep).
reaction_pathway(brendan,cje,capsule_ngro1c,capsule).
```

```
gene_t(cj1431c).
gene(brendan,cje,cj1431c).
gene_name(brendan,cj1431c,'HddC').
```

```
subpathway_t(cap_addhep3ome).
subpathway(brendan,cje,cap_addhep3ome,capsule).
subpathway_name(brendan,cje,cap_addhep3ome,'Add Hep 3-OMe').
```

```
subpathway_t(cap_addhep6ome).
```

```
subpathway(brendan,cje,cap_addhep6ome,capsule).
subpathway_name(brendan,cje,cap_addhep6ome,'Add Hep 6-OMe').
```

```
subpathway_t(cap_addhepomepn).
subpathway(brendan,cje,cap_addhepomepn,capsule).
subpathway_name(brendan,cje,cap_addhepomepn,'Add Hep OMePN').
```

```
%% 3-OMe
% ....
```

```
%% OMePN
```

```
reaction_t(capsule_ngro4).
reaction_gene(brendan,cje,capsule_ngro4,cj1422c).
reaction(brendan,cje,capsule_ngro4,'glca6ngro+hep','glca6ngro+hep+omepn',1).
reaction(brendan,cje,capsule_ngro4,'pre-omepn','glca6ngro+hep+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro4,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro4,capsule).
```

```
reaction_t(capsule_ngro5a).
reaction_gene(brendan,cje,capsule_ngro5a,cj1422c).
reaction(brendan,cje,capsule_ngro5a,'glca6ngro+hep+6ome','glca6ngro+hep+omepn+6ome',1).
reaction(brendan,cje,capsule_ngro5a,'pre-omepn','glca6ngro+hep+omepn+6ome',1).
reaction_subpathway(brendan,cje,capsule_ngro5a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro5a,capsule).
```

```
%% 6-OMe
```

```
reaction_t(capsule_ngro5c).
reaction_gene(brendan,cje,capsule_ngro5c,cj1426c).
reaction(brendan,cje,capsule_ngro5c,'glca6ngro+hep','glca6ngro+hep+6ome',1).
reaction(brendan,cje,capsule_ngro5c,'pre-ome','glca6ngro+hep+6ome',1).
reaction_subpathway(brendan,cje,capsule_ngro5c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_ngro5c,capsule).
```

```
reaction_t(capsule_ngro5e).
reaction_gene(brendan,cje,capsule_ngro5e,cj1426c).
reaction(brendan,cje,capsule_ngro5e,'glca6ngro+hep+omepn','glca6ngro+hep+omepn+6ome',1).
reaction(brendan,cje,capsule_ngro5e,'pre-ome','glca6ngro+hep+omepn+6ome',1).
reaction_subpathway(brendan,cje,capsule_ngro5e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_ngro5e,capsule).
```

```
%% 3-OMe
```

```
% ...
```

%% OMePN

```
reaction_t(capsule_ngro8).
reaction_gene(brendan,cje,capsule_ngro8,cj1422c).
reaction(brendan,cje,capsule_ngro8,'glca6ngro+hep-galfnac','glca6ngro+hep+omepn-galfnac',1).
reaction(brendan,cje,capsule_ngro8,'pre-omepn','glca6ngro+hep+omepn-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro8,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro8,capsule).
```

```
reaction_t(capsule_ngro9a).
reaction_gene(brendan,cje,capsule_ngro9a,cj1422c).
reaction(brendan,cje,capsule_ngro9a,'glca6ngro+hep+6ome-galfnac','glca6ngro+hep+omepn+6ome-galfnac',1).
reaction(brendan,cje,capsule_ngro9a,'pre-omepn','glca6ngro+hep+omepn+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro9a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro9a,capsule).
```

%% 6-OMe

```
reaction_t(capsule_ngro9c).
reaction_gene(brendan,cje,capsule_ngro9c,cj1426c).
reaction(brendan,cje,capsule_ngro9c,'glca6ngro+hep-galfnac','glca6ngro+hep+6ome-galfnac',1).
reaction(brendan,cje,capsule_ngro9c,'pre-ome','glca6ngro+hep+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro9c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_ngro9c,capsule).
```

```
reaction_t(capsule_ngro9e).
reaction_gene(brendan,cje,capsule_ngro9e,cj1426c).
reaction(brendan,cje,capsule_ngro9e,'glca6ngro+hep+omepn-galfnac','glca6ngro+hep+omepn+6ome-galfnac',1).
reaction(brendan,cje,capsule_ngro9e,'pre-ome','glca6ngro+hep+omepn+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro9e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_ngro9e,capsule).
```

%% 3-OMe

%% OMePN

```
reaction_t(capsule_ngro12).
reaction_gene(brendan,cje,capsule_ngro12,cj1422c).
reaction(brendan,cje,capsule_ngro12,'glca6ngro+hep-galfnac+omepn','glca6ngro+hep+omepn-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro12,'pre-omepn','glca6ngro+hep+omepn-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro12,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro12,capsule).
```

```
reaction_t(capsule_ngro13a).
reaction_gene(brendan,cje,capsule_ngro13a,cj1422c).
reaction(brendan,cje,capsule_ngro13a,'glca6ngro+hep+6ome-galfnac+omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro13a,'pre-omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro13a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro13a,capsule).
```

%% 6-OMe

```
reaction_t(capsule_ngro13c).
reaction_gene(brendan,cje,capsule_ngro13c,cj1426c).
reaction(brendan,cje,capsule_ngro13c,'glca6ngro+hep-galfnac+omepn','glca6ngro+hep+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro13c,'pre-ome','glca6ngro+hep+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro13c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_ngro13c,capsule).
```

```
reaction_t(capsule_ngro13e).
reaction_gene(brendan,cje,capsule_ngro13e,cj1426c).
reaction(brendan,cje,capsule_ngro13e,'glca6ngro+hep+omepn-galfnac+omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro13e,'pre-ome','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro13e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_ngro13e,capsule).
```

%% 3-OMe

%% OMePN

```
reaction_t(capsule_ngro16).
reaction_gene(brendan,cje,capsule_ngro16,cj1422c).
reaction(brendan,cje,capsule_ngro16,'glca6ngro+hep-galfnac-ribf','glca6ngro+hep+omepn-galfnac-ribf',1).
reaction(brendan,cje,capsule_ngro16,'pre-omepn','glca6ngro+hep+omepn-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro16,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro16,capsule).
```

```
reaction_t(capsule_ngro17a).
reaction_gene(brendan,cje,capsule_ngro17a,cj1422c).
reaction(brendan,cje,capsule_ngro17a,'glca6ngro+hep+6ome-galfnac-ribf','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_ngro17a,'pre-omepn','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro17a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_ngro17a,capsule).
```

%% 6-OMe

```
reaction_t(capsule_ngro17c).
reaction_gene(brendan,cje,capsule_ngro17c,cj1426c).
reaction(brendan,cje,capsule_ngro17c,'glca6ngro+hep-galfnac-ribf','glca6ngro+hep+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_ngro17c,'pre-ome','glca6ngro+hep+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro17c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_ngro17c,capsule).
```

```
reaction_t(capsule_ngro17e).
reaction_gene(brendan,cje,capsule_ngro17e,cj1426c).
reaction(brendan,cje,capsule_ngro17e,'glca6ngro+hep+omepn-galfnac-ribf','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_ngro17e,'pre-ome','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro17e,cap_addhep6ome).
```

reaction_pathway(brendan,cje,capsule_ngro17e,capsule).

%% 3-OMe

%% OMePN

reaction_t(capsule_ngro20).

reaction_gene(brendan,cje,capsule_ngro20,cj1422c).

reaction(brendan,cje,capsule_ngro20,'glca6ngro+hep-galfnac+omepn-ribf','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).

reaction(brendan,cje,capsule_ngro20,'pre-omepn','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro20,cap_addhepomepn).

reaction_pathway(brendan,cje,capsule_ngro20,capsule).

reaction_t(capsule_ngro21a).

reaction_gene(brendan,cje,capsule_ngro21a,cj1422c).

reaction(brendan,cje,capsule_ngro21a,'glca6ngro+hep+6ome-galfnac+omepn-ribf','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).

reaction(brendan,cje,capsule_ngro21a,'pre-omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro21a,cap_addhepomepn).

reaction_pathway(brendan,cje,capsule_ngro21a,capsule).

%% 6-OMe

reaction_t(capsule_ngro21c).

reaction_gene(brendan,cje,capsule_ngro21c,cj1426c).

reaction(brendan,cje,capsule_ngro21c,'glca6ngro+hep-galfnac+omepn-ribf','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).

reaction(brendan,cje,capsule_ngro21c,'pre-ome','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro21c,cap_addhep6ome).

reaction_pathway(brendan,cje,capsule_ngro21c,capsule).

reaction_t(capsule_ngro21e).

reaction_gene(brendan,cje,capsule_ngro21e,cj1426c).

reaction(brendan,cje,capsule_ngro21e,'glca6ngro+hep+omepn-galfnac+omepn-ribf','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).

reaction(brendan,cje,capsule_ngro21e,'pre-ome','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro21e,cap_addhep6ome).

reaction_pathway(brendan,cje,capsule_ngro21e,capsule).

gene_t(cj1422c).

gene(brendan,cje,cj1422c).

gene_name(brendan,cj1422c,'putative sugar transferase').

gene_t(cj1426c).

gene(brendan,cje,cj1426c).

gene_name(brendan,cj1426c,'putative methyltransferase family protein').

gene_t(unknown).


```
gene(brendan,cje,unknown).
gene_name(brendan,unknown,'Unknown gene or spontaneous reaction').
```

```
%% Adding galfnac and associated phase-variable modification
```

```
subpathway_t(cap_addgalf).
subpathway(brendan,cje,cap_addgalf,capsule).
subpathway_name(brendan,cje,cap_addgalf,'Add Galfnac').
```

```
reaction_t(capsule_ngro22).
reaction_gene(brendan,cje,capsule_ngro22,cj1439c).
guess_rtn_gene(brendan,cje,capsule_ngro22,cj1439c).
reaction(brendan,cje,capsule_ngro22,'glca6ngro','glca6ngro-galfnac',1).
reaction(brendan,cje,capsule_ngro22,'pre-galfnac','glca6ngro-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro22,cap_addgalf).
reaction_pathway(brendan,cje,capsule_ngro22,capsule).
```

```
reaction_t(capsule_ngro23).
reaction_gene(brendan,cje,capsule_ngro23,cj1439c).
guess_rtn_gene(brendan,cje,capsule_ngro23,cj1439c).
reaction(brendan,cje,capsule_ngro23,'glca6ngro+hep','glca6ngro+hep-galfnac',1).
reaction(brendan,cje,capsule_ngro23,'pre-galfnac','glca6ngro+hep-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro23,cap_addgalf).
reaction_pathway(brendan,cje,capsule_ngro23,capsule).
```

```
reaction_t(capsule_ngro24a).
reaction_gene(brendan,cje,capsule_ngro24a,cj1439c).
guess_rtn_gene(brendan,cje,capsule_ngro24a,cj1439c).
reaction(brendan,cje,capsule_ngro24a,'glca6ngro+hep+6ome','glca6ngro+hep+6ome-galfnac',1).
reaction(brendan,cje,capsule_ngro24a,'pre-galfnac','glca6ngro+hep+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro24a,cap_addgalf).
reaction_pathway(brendan,cje,capsule_ngro24a,capsule).
```

```
reaction_t(capsule_ngro25).
reaction_gene(brendan,cje,capsule_ngro25,cj1439c).
guess_rtn_gene(brendan,cje,capsule_ngro25,cj1439c).
reaction(brendan,cje,capsule_ngro25,'glca6ngro+hep+omepn','glca6ngro+hep+omepn-galfnac',1).
reaction(brendan,cje,capsule_ngro25,'pre-galfnac','glca6ngro+hep+omepn-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro25,cap_addgalf).
reaction_pathway(brendan,cje,capsule_ngro25,capsule).
```

```
reaction_t(capsule_ngro26a).
reaction_gene(brendan,cje,capsule_ngro26a,cj1439c).
guess_rtn_gene(brendan,cje,capsule_ngro26a,cj1439c).
reaction(brendan,cje,capsule_ngro26a,'glca6ngro+hep+omepn+6ome','glca6ngro+hep+omepn+6ome-galfnac',1).
reaction(brendan,cje,capsule_ngro26a,'pre-galfnac','glca6ngro+hep+omepn+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_ngro26a,cap_addgalf).
reaction_pathway(brendan,cje,capsule_ngro26a,capsule).
```

```
gene_t(cj1439c).
gene(brendan,cje,cj1439c).
gene_name(brendan,cj1439c,'Glf').
```

subpathway_t(cap_addgalfomepn).
subpathway(brendan,cje,cap_addgalfomepn,capsule).
subpathway_name(brendan,cje,cap_addgalfomepn,'Add Galfnac OMePN').

reaction_t(capsule_ngro27).
reaction_gene(brendan,cje,capsule_ngro27,cj1421c).
reaction(brendan,cje,capsule_ngro27,'glca6ngro-galfnac','glca6ngro-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro27,'pre-omepn','glca6ngro-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro27,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_ngro27,capsule).

reaction_t(capsule_ngro28).
reaction_gene(brendan,cje,capsule_ngro28,cj1421c).
reaction(brendan,cje,capsule_ngro28,'glca6ngro+hep-galfnac','glca6ngro+hep-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro28,'pre-omepn','glca6ngro+hep-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro28,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_ngro28,capsule).

reaction_t(capsule_ngro29a).
reaction_gene(brendan,cje,capsule_ngro29a,cj1421c).
reaction(brendan,cje,capsule_ngro29a,'glca6ngro+hep+6ome-galfnac','glca6ngro+hep+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro29a,'pre-omepn','glca6ngro+hep+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro29a,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_ngro29a,capsule).

reaction_t(capsule_ngro30).
reaction_gene(brendan,cje,capsule_ngro30,cj1421c).
reaction(brendan,cje,capsule_ngro30,'glca6ngro+hep+omepn-galfnac','glca6ngro+hep+omepn-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro30,'pre-omepn','glca6ngro+hep+omepn-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro30,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_ngro30,capsule).

reaction_t(capsule_ngro31a).
reaction_gene(brendan,cje,capsule_ngro31a,cj1421c).
reaction(brendan,cje,capsule_ngro31a,'glca6ngro+hep+omepn+6ome-galfnac','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_ngro31a,'pre-omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_ngro31a,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_ngro31a,capsule).

reaction_t(capsule_ngro32).
reaction_gene(brendan,cje,capsule_ngro32,cj1421c).
reaction(brendan,cje,capsule_ngro32,'glca6ngro-galfnac-ribf','glca6ngro-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro32,'pre-omepn','glca6ngro-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro32,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_ngro32,capsule).

reaction_t(capsule_ngro33).
reaction_gene(brendan,cje,capsule_ngro33,cj1421c).
reaction(brendan,cje,capsule_ngro33,'glca6ngro+hep-galfnac-ribf','glca6ngro+hep-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro33,'pre-omepn','glca6ngro+hep-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro33,cap_addgalfomepn).

reaction_pathway(brendan,cje,capsule_ngro33,capsule).

reaction_t(capsule_ngro34a).

reaction_gene(brendan,cje,capsule_ngro34a,cj1421c).

reaction(brendan,cje,capsule_ngro34a,'glca6ngro+hep+6ome-galfnac-ribf','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).

reaction(brendan,cje,capsule_ngro34a,'pre-omepn','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro34a,cap_addgalfomepn).

reaction_pathway(brendan,cje,capsule_ngro34a,capsule).

reaction_t(capsule_ngro35).

reaction_gene(brendan,cje,capsule_ngro35,cj1421c).

reaction(brendan,cje,capsule_ngro35,'glca6ngro+hep+omepn-galfnac-ribf','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).

reaction(brendan,cje,capsule_ngro35,'pre-omepn','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro35,cap_addgalfomepn).

reaction_pathway(brendan,cje,capsule_ngro35,capsule).

reaction_t(capsule_ngro36a).

reaction_gene(brendan,cje,capsule_ngro36a,cj1421c).

reaction(brendan,cje,capsule_ngro36a,'glca6ngro+hep+omepn+6ome-galfnac-ribf','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).

reaction(brendan,cje,capsule_ngro36a,'pre-omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro36a,cap_addgalfomepn).

reaction_pathway(brendan,cje,capsule_ngro36a,capsule).

gene_t(cj1421c).

gene(brendan,cje,cj1421c).

gene_name(brendan,cj1421c,'putative sugar transferase').

%% Adding ribf

subpathway_t(cap_addribf).

subpathway(brendan,cje,cap_addribf,capsule).

subpathway_name(brendan,cje,cap_addribf,'Add Ribf').

reaction_t(capsule_ngro37).

reaction_gene(brendan,cje,capsule_ngro37,unknown).

reaction(brendan,cje,capsule_ngro37,'glca6ngro-galfnac','glca6ngro-galfnac-ribf',1).

reaction(brendan,cje,capsule_ngro37,'pre-ribf','glca6ngro-galfnac-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro37,cap_addribf).

reaction_pathway(brendan,cje,capsule_ngro37,capsule).

reaction_t(capsule_ngro38).

reaction_gene(brendan,cje,capsule_ngro38,unknown).

reaction(brendan,cje,capsule_ngro38,'glca6ngro+hep-galfnac','glca6ngro+hep-galfnac-ribf',1).

reaction(brendan,cje,capsule_ngro38,'pre-ribf','glca6ngro+hep-galfnac-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro38,cap_addribf).

reaction_pathway(brendan,cje,capsule_ngro38,capsule).

reaction_t(capsule_ngro39a).

reaction_gene(brendan,cje,capsule_ngro39a,unknown).

reaction(brendan,cje,capsule_ngro39a,'glca6ngro+hep+6ome-galfnac','glca6ngro+hep+6ome-galfnac-ribf',1).

reaction(brendan,cje,capsule_ngro39a,'pre-ribf','glca6ngro+hep+6ome-galfnac-ribf',1).

reaction_subpathway(brendan,cje,capsule_ngro39a,cap_addribf).
reaction_pathway(brendan,cje,capsule_ngro39a,capsule).

reaction_t(capsule_ngro40).
reaction_gene(brendan,cje,capsule_ngro40,unknown).
reaction(brendan,cje,capsule_ngro40,'glca6ngro+hep+omepn-galfnac','glca6ngro+hep+omepn-galfnac-ribf',1).
reaction(brendan,cje,capsule_ngro40,'pre-ribf','glca6ngro+hep+omepn-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro40,cap_addribf).
reaction_pathway(brendan,cje,capsule_ngro40,capsule).

reaction_t(capsule_ngro41a).
reaction_gene(brendan,cje,capsule_ngro41a,unknown).
reaction(brendan,cje,capsule_ngro41a,'glca6ngro+hep+omepn+6ome-galfnac','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_ngro41a,'pre-ribf','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro41a,cap_addribf).
reaction_pathway(brendan,cje,capsule_ngro41a,capsule).

reaction_t(capsule_ngro42).
reaction_gene(brendan,cje,capsule_ngro42,unknown).
reaction(brendan,cje,capsule_ngro42,'glca6ngro-galfnac+omepn','glca6ngro-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro42,'pre-ribf','glca6ngro-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro42,cap_addribf).
reaction_pathway(brendan,cje,capsule_ngro42,capsule).

reaction_t(capsule_ngro43).
reaction_gene(brendan,cje,capsule_ngro43,unknown).
reaction(brendan,cje,capsule_ngro43,'glca6ngro+hep-galfnac+omepn','glca6ngro+hep-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro43,'pre-ribf','glca6ngro+hep-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro43,cap_addribf).
reaction_pathway(brendan,cje,capsule_ngro43,capsule).

reaction_t(capsule_ngro44a).
reaction_gene(brendan,cje,capsule_ngro44a,unknown).
reaction(brendan,cje,capsule_ngro44a,'glca6ngro+hep+6ome-galfnac+omepn','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro44a,'pre-ribf','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro44a,cap_addribf).
reaction_pathway(brendan,cje,capsule_ngro44a,capsule).

reaction_t(capsule_ngro45).
reaction_gene(brendan,cje,capsule_ngro45,unknown).
reaction(brendan,cje,capsule_ngro45,'glca6ngro+hep+omepn-galfnac+omepn','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro45,'pre-ribf','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro45,cap_addribf).
reaction_pathway(brendan,cje,capsule_ngro45,capsule).

reaction_t(capsule_ngro46a).
reaction_gene(brendan,cje,capsule_ngro46a,unknown).
reaction(brendan,cje,capsule_ngro46a,'glca6ngro+hep+omepn+6ome-galfnac+omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_ngro46a,'pre-ribf','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_ngro46a,cap_addribf).

reaction_pathway(brendan,cje,capsule_ngro46a,capsule).

%% now for glca6etn

%

%% now for glca

%% Adding Hep and associated phase-variable modifications

reaction_t(capsule_1).
reaction_gene(brendan,cje,capsule_1,cj1431c).
reaction(brendan,cje,capsule_1,'glca','glca+hep',1).
reaction(brendan,cje,capsule_1,'gdp-d-al-gluco-hep','glca+hep',1).
reaction_subpathway(brendan,cje,capsule_1,cap_addhep).
reaction_pathway(brendan,cje,capsule_1,capsule).

reaction_t(capsule_1a).
reaction_gene(brendan,cje,capsule_1a,cj1431c).
reaction(brendan,cje,capsule_1a,'glca-galfnac','glca+hep-galfnac',1).
reaction(brendan,cje,capsule_1a,'gdp-d-al-gluco-hep','glca+hep-galfnac',1).
reaction_subpathway(brendan,cje,capsule_1a,cap_addhep).
reaction_pathway(brendan,cje,capsule_1a,capsule).

reaction_t(capsule_1b).
reaction_gene(brendan,cje,capsule_1b,cj1431c).
reaction(brendan,cje,capsule_1b,'glca-galfnac-ribf','glca+hep-galfnac-ribf',1).
reaction(brendan,cje,capsule_1b,'gdp-d-al-gluco-hep','glca+hep-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_1b,cap_addhep).
reaction_pathway(brendan,cje,capsule_1b,capsule).

reaction_t(capsule_1c).
reaction_gene(brendan,cje,capsule_1c,cj1431c).
reaction(brendan,cje,capsule_1c,'glca-galfnac+omepn-ribf','glca+hep-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_1c,'gdp-d-al-gluco-hep','glca+hep-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_1c,cap_addhep).
reaction_pathway(brendan,cje,capsule_1c,capsule).

%% 3-OMe

%% OMePN

reaction_t(capsule_4).
reaction_gene(brendan,cje,capsule_4,cj1422c).
reaction(brendan,cje,capsule_4,'glca+hep','glca+hep+omepn',1).
reaction(brendan,cje,capsule_4,'pre-omepn','glca+hep+omepn',1).
reaction_subpathway(brendan,cje,capsule_4,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_4,capsule).

reaction_t(capsule_5a).
reaction_gene(brendan,cje,capsule_5a,cj1422c).
reaction(brendan,cje,capsule_5a,'glca+hep+6ome','glca+hep+omepn+6ome',1).
reaction(brendan,cje,capsule_5a,'pre-omepn','glca+hep+omepn+6ome',1).

reaction_subpathway(brendan,cje,capsule_5a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_5a,capsule).

%% 6-OMe

reaction_t(capsule_5c).
reaction_gene(brendan,cje,capsule_5c,cj1426c).
reaction(brendan,cje,capsule_5c,'glca+hep','glca+hep+6ome',1).
reaction(brendan,cje,capsule_5c,'pre-ome','glca+hep+6ome',1).
reaction_subpathway(brendan,cje,capsule_5c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_5c,capsule).

reaction_t(capsule_5e).
reaction_gene(brendan,cje,capsule_5e,cj1426c).
reaction(brendan,cje,capsule_5e,'glca+hep+omepn','glca+hep+omepn+6ome',1).
reaction(brendan,cje,capsule_5e,'pre-ome','glca+hep+omepn+6ome',1).
reaction_subpathway(brendan,cje,capsule_5e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_5e,capsule).

%% 3-OMe

%% OMePN

reaction_t(capsule_8).
reaction_gene(brendan,cje,capsule_8,cj1422c).
reaction(brendan,cje,capsule_8,'glca+hep-galfnac','glca+hep+omepn-galfnac',1).
reaction(brendan,cje,capsule_8,'pre-omepn','glca+hep+omepn-galfnac',1).
reaction_subpathway(brendan,cje,capsule_8,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_8,capsule).

reaction_t(capsule_9a).
reaction_gene(brendan,cje,capsule_9a,cj1422c).
reaction(brendan,cje,capsule_9a,'glca+hep+6ome-galfnac','glca+hep+omepn+6ome-galfnac',1).
reaction(brendan,cje,capsule_9a,'pre-omepn','glca+hep+omepn+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_9a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_9a,capsule).

%% 6-OMe

reaction_t(capsule_9c).
reaction_gene(brendan,cje,capsule_9c,cj1426c).
reaction(brendan,cje,capsule_9c,'glca+hep-galfnac','glca+hep+6ome-galfnac',1).
reaction(brendan,cje,capsule_9c,'pre-ome','glca+hep+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_9c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_9c,capsule).

reaction_t(capsule_9e).
reaction_gene(brendan,cje,capsule_9e,cj1426c).
reaction(brendan,cje,capsule_9e,'glca+hep+omepn-galfnac','glca+hep+omepn+6ome-galfnac',1).
reaction(brendan,cje,capsule_9e,'pre-ome','glca+hep+omepn+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_9e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_9e,capsule).

%% 3-OMe

%% OMePN

reaction_t(capsule_12).
reaction_gene(brendan,cje,capsule_12,cj1422c).
reaction(brendan,cje,capsule_12,'glca+hep-galfnac+omepn','glca+hep+omepn-galfnac+omepn',1).
reaction(brendan,cje,capsule_12,'pre-omepn','glca+hep+omepn-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_12,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_12,capsule).

reaction_t(capsule_13a).
reaction_gene(brendan,cje,capsule_13a,cj1422c).
reaction(brendan,cje,capsule_13a,'glca+hep+6ome-galfnac+omepn','glca+hep+omepn+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_13a,'pre-omepn','glca+hep+omepn+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_13a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_13a,capsule).

%% 6-OMe

reaction_t(capsule_13c).
reaction_gene(brendan,cje,capsule_13c,cj1426c).
reaction(brendan,cje,capsule_13c,'glca+hep-galfnac+omepn','glca+hep+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_13c,'pre-ome','glca+hep+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_13c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_13c,capsule).

reaction_t(capsule_13e).
reaction_gene(brendan,cje,capsule_13e,cj1426c).
reaction(brendan,cje,capsule_13e,'glca+hep+omepn-galfnac+omepn','glca+hep+omepn+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_13e,'pre-ome','glca+hep+omepn+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_13e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_13e,capsule).

%% 3-OMe

%% OMePN

reaction_t(capsule_16).
reaction_gene(brendan,cje,capsule_16,cj1422c).
reaction(brendan,cje,capsule_16,'glca+hep-galfnac-ribf','glca+hep+omepn-galfnac-ribf',1).
reaction(brendan,cje,capsule_16,'pre-omepn','glca+hep+omepn-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_16,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_16,capsule).

reaction_t(capsule_17a).
reaction_gene(brendan,cje,capsule_17a,cj1422c).
reaction(brendan,cje,capsule_17a,'glca+hep+6ome-galfnac-ribf','glca+hep+omepn+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_17a,'pre-omepn','glca+hep+omepn+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_17a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_17a,capsule).

%% 6-OMe

reaction_t(capsule_17c).

reaction_gene(brendan,cje,capsule_17c,cj1426c).
reaction(brendan,cje,capsule_17c,'glca+hep-galfnac-ribf','glca+hep+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_17c,'pre-ome','glca+hep+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_17c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_17c,capsule).

reaction_t(capsule_17e).
reaction_gene(brendan,cje,capsule_17e,cj1426c).
reaction(brendan,cje,capsule_17e,'glca+hep+omepn-galfnac-ribf','glca+hep+omepn+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_17e,'pre-ome','glca+hep+omepn+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_17e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_17e,capsule).

%% 3-OMe

%% OMePN

reaction_t(capsule_20).
reaction_gene(brendan,cje,capsule_20,cj1422c).
reaction(brendan,cje,capsule_20,'glca+hep-galfnac+omepn-ribf','glca+hep+omepn-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_20,'pre-omepn','glca+hep+omepn-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_20,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_20,capsule).

reaction_t(capsule_21a).
reaction_gene(brendan,cje,capsule_21a,cj1422c).
reaction(brendan,cje,capsule_21a,'glca+hep+6ome-galfnac+omepn-ribf','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_21a,'pre-omepn','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_21a,cap_addhepomepn).
reaction_pathway(brendan,cje,capsule_21a,capsule).

%% 6-OMe

reaction_t(capsule_21c).
reaction_gene(brendan,cje,capsule_21c,cj1426c).
reaction(brendan,cje,capsule_21c,'glca+hep-galfnac+omepn-ribf','glca+hep+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_21c,'pre-ome','glca+hep+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_21c,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_21c,capsule).

reaction_t(capsule_21e).
reaction_gene(brendan,cje,capsule_21e,cj1426c).
reaction(brendan,cje,capsule_21e,'glca+hep+omepn-galfnac+omepn-ribf','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_21e,'pre-ome','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_21e,cap_addhep6ome).
reaction_pathway(brendan,cje,capsule_21e,capsule).

%% Adding galfnac and associated phase-variable modification

```
reaction_t(capsule_22).
reaction_gene(brendan,cje,capsule_22,cj1439c).
guess_rtn_gene(brendan,cje,capsule_22,cj1439c).
reaction(brendan,cje,capsule_22,'glca','glca-galfnac',1).
reaction(brendan,cje,capsule_22,'pre-galfnac','glca-galfnac',1).
reaction_subpathway(brendan,cje,capsule_22,cap_addgalf).
reaction_pathway(brendan,cje,capsule_22,capsule).
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reaction_t(capsule_23).
reaction_gene(brendan,cje,capsule_23,cj1439c).
guess_rtn_gene(brendan,cje,capsule_23,cj1439c).
reaction(brendan,cje,capsule_23,'glca+hep','glca+hep-galfnac',1).
reaction(brendan,cje,capsule_23,'pre-galfnac','glca+hep-galfnac',1).
reaction_subpathway(brendan,cje,capsule_23,cap_addgalf).
reaction_pathway(brendan,cje,capsule_23,capsule).
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reaction_t(capsule_24a).
reaction_gene(brendan,cje,capsule_24a,cj1439c).
guess_rtn_gene(brendan,cje,capsule_24a,cj1439c).
reaction(brendan,cje,capsule_24a,'glca+hep+6ome','glca+hep+6ome-galfnac',1).
reaction(brendan,cje,capsule_24a,'pre-galfnac','glca+hep+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_24a,cap_addgalf).
reaction_pathway(brendan,cje,capsule_24a,capsule).
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reaction_t(capsule_25).
reaction_gene(brendan,cje,capsule_25,cj1439c).
guess_rtn_gene(brendan,cje,capsule_25,cj1439c).
reaction(brendan,cje,capsule_25,'glca+hep+omepn','glca+hep+omepn-galfnac',1).
reaction(brendan,cje,capsule_25,'pre-galfnac','glca+hep+omepn-galfnac',1).
reaction_subpathway(brendan,cje,capsule_25,cap_addgalf).
reaction_pathway(brendan,cje,capsule_25,capsule).
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reaction_t(capsule_26a).
reaction_gene(brendan,cje,capsule_26a,cj1439c).
guess_rtn_gene(brendan,cje,capsule_26a,cj1439c).
reaction(brendan,cje,capsule_26a,'glca+hep+omepn+6ome','glca+hep+omepn+6ome-galfnac',1).
reaction(brendan,cje,capsule_26a,'pre-galfnac','glca+hep+omepn+6ome-galfnac',1).
reaction_subpathway(brendan,cje,capsule_26a,cap_addgalf).
reaction_pathway(brendan,cje,capsule_26a,capsule).
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reaction_t(capsule_27).
reaction_gene(brendan,cje,capsule_27,cj1421c).
reaction(brendan,cje,capsule_27,'glca-galfnac','glca-galfnac+omepn',1).
reaction(brendan,cje,capsule_27,'pre-omepn','glca-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_27,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_27,capsule).
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reaction_t(capsule_28).
reaction_gene(brendan,cje,capsule_28,cj1421c).
reaction(brendan,cje,capsule_28,'glca+hep-galfnac','glca+hep-galfnac+omepn',1).
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reaction(brendan,cje,capsule_28,'pre-omepn','glca+hep-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_28,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_28,capsule).

reaction_t(capsule_29a).
reaction_gene(brendan,cje,capsule_29a,cj1421c).
reaction(brendan,cje,capsule_29a,'glca+hep+6ome-galfnac','glca+hep+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_29a,'pre-omepn','glca+hep+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_29a,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_29a,capsule).

reaction_t(capsule_30).
reaction_gene(brendan,cje,capsule_30,cj1421c).
reaction(brendan,cje,capsule_30,'glca+hep+omepn-galfnac','glca+hep+omepn-galfnac+omepn',1).
reaction(brendan,cje,capsule_30,'pre-omepn','glca+hep+omepn-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_30,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_30,capsule).

reaction_t(capsule_31a).
reaction_gene(brendan,cje,capsule_31a,cj1421c).
reaction(brendan,cje,capsule_31a,'glca+hep+omepn+6ome-galfnac','glca+hep+omepn+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_31a,'pre-omepn','glca+hep+omepn+6ome-galfnac+omepn',1).
reaction_subpathway(brendan,cje,capsule_31a,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_31a,capsule).

reaction_t(capsule_32).
reaction_gene(brendan,cje,capsule_32,cj1421c).
reaction(brendan,cje,capsule_32,'glca-galfnac-ribf','glca-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_32,'pre-omepn','glca-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_32,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_32,capsule).

reaction_t(capsule_33).
reaction_gene(brendan,cje,capsule_33,cj1421c).
reaction(brendan,cje,capsule_33,'glca+hep-galfnac-ribf','glca+hep-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_33,'pre-omepn','glca+hep-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_33,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_33,capsule).

reaction_t(capsule_34a).
reaction_gene(brendan,cje,capsule_34a,cj1421c).
reaction(brendan,cje,capsule_34a,'glca+hep+6ome-galfnac-ribf','glca+hep+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_34a,'pre-omepn','glca+hep+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_34a,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_34a,capsule).

reaction_t(capsule_35).
reaction_gene(brendan,cje,capsule_35,cj1421c).
reaction(brendan,cje,capsule_35,'glca+hep+omepn-galfnac-ribf','glca+hep+omepn-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_35,'pre-omepn','glca+hep+omepn-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_35,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_35,capsule).

reaction_t(capsule_36a).

```
reaction_gene(brendan,cje,capsule_36a,cj1421c).
reaction(brendan,cje,capsule_36a,'glca+hep+omepn+6ome-galfnac-ribf','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_36a,'pre-omepn','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_36a,cap_addgalfomepn).
reaction_pathway(brendan,cje,capsule_36a,capsule).
```

%% Adding ribf

```
reaction_t(capsule_37).
reaction_gene(brendan,cje,capsule_37,unknown).
reaction(brendan,cje,capsule_37,'glca-galfnac','glca-galfnac-ribf',1).
reaction(brendan,cje,capsule_37,'pre-ribf','glca-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_37,cap_addrifb).
reaction_pathway(brendan,cje,capsule_37,capsule).
```

```
reaction_t(capsule_38).
reaction_gene(brendan,cje,capsule_38,unknown).
reaction(brendan,cje,capsule_38,'glca+hep-galfnac','glca+hep-galfnac-ribf',1).
reaction(brendan,cje,capsule_38,'pre-ribf','glca+hep-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_38,cap_addrifb).
reaction_pathway(brendan,cje,capsule_38,capsule).
```

```
reaction_t(capsule_39a).
reaction_gene(brendan,cje,capsule_39a,unknown).
reaction(brendan,cje,capsule_39a,'glca+hep+6ome-galfnac','glca+hep+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_39a,'pre-ribf','glca+hep+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_39a,cap_addrifb).
reaction_pathway(brendan,cje,capsule_39a,capsule).
```

```
reaction_t(capsule_40).
reaction_gene(brendan,cje,capsule_40,unknown).
reaction(brendan,cje,capsule_40,'glca+hep+omepn-galfnac','glca+hep+omepn-galfnac-ribf',1).
reaction(brendan,cje,capsule_40,'pre-ribf','glca+hep+omepn-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_40,cap_addrifb).
reaction_pathway(brendan,cje,capsule_40,capsule).
```

```
reaction_t(capsule_41a).
reaction_gene(brendan,cje,capsule_41a,unknown).
reaction(brendan,cje,capsule_41a,'glca+hep+omepn+6ome-galfnac','glca+hep+omepn+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_41a,'pre-ribf','glca+hep+omepn+6ome-galfnac-ribf',1).
reaction_subpathway(brendan,cje,capsule_41a,cap_addrifb).
reaction_pathway(brendan,cje,capsule_41a,capsule).
```

```
reaction_t(capsule_42).
reaction_gene(brendan,cje,capsule_42,unknown).
reaction(brendan,cje,capsule_42,'glca-galfnac+omepn','glca-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_42,'pre-ribf','glca-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_42,cap_addrifb).
reaction_pathway(brendan,cje,capsule_42,capsule).
```

```
reaction_t(capsule_43).
reaction_gene(brendan,cje,capsule_43,unknown).
reaction(brendan,cje,capsule_43,'glca+hep-galfnac+omepn','glca+hep-galfnac+omepn-ribf',1).
```

```
reaction(brendan,cje,capsule_43,'pre-ribf','glca+hep-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_43,cap_addribf).
reaction_pathway(brendan,cje,capsule_43,capsule).
```

```
reaction_t(capsule_44a).
reaction_gene(brendan,cje,capsule_44a,unknown).
reaction(brendan,cje,capsule_44a,'glca+hep+6ome-galfnac+omepn','glca+hep+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_44a,'pre-ribf','glca+hep+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_44a,cap_addribf).
reaction_pathway(brendan,cje,capsule_44a,capsule).
```

```
reaction_t(capsule_45).
reaction_gene(brendan,cje,capsule_45,unknown).
reaction(brendan,cje,capsule_45,'glca+hep+omepn-galfnac+omepn','glca+hep+omepn-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_45,'pre-ribf','glca+hep+omepn-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_45,cap_addribf).
reaction_pathway(brendan,cje,capsule_45,capsule).
```

```
reaction_t(capsule_46a).
reaction_gene(brendan,cje,capsule_46a,unknown).
reaction(brendan,cje,capsule_46a,'glca+hep+omepn+6ome-galfnac+omepn','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_46a,'pre-ribf','glca+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction_subpathway(brendan,cje,capsule_46a,cap_addribf).
reaction_pathway(brendan,cje,capsule_46a,capsule).
```

%% adding ngro

```
reaction_t(capsule_addngro1).
reaction_gene(brendan,cje,capsule_addngro1,unknown).
reaction_subpathway(brendan,cje,capsule_addngro1,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro1,capsule).
reaction(brendan,cje,capsule_addngro1,'glca+hep','glca6ngro+hep',1).
reaction(brendan,cje,capsule_addngro1,'pre-ngro','glca6ngro+hep',1).
```

```
reaction_t(capsule_addngro2).
reaction_gene(brendan,cje,capsule_addngro2,unknown).
reaction_subpathway(brendan,cje,capsule_addngro2,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro2,capsule).
reaction(brendan,cje,capsule_addngro2,'glca+hep+omepn','glca6ngro+hep+omepn',1).
reaction(brendan,cje,capsule_addngro2,'pre-ngro','glca6ngro+hep+omepn',1).
```

```
reaction_t(capsule_addngro4).
reaction_gene(brendan,cje,capsule_addngro4,unknown).
reaction_subpathway(brendan,cje,capsule_addngro4,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro4,capsule).
reaction(brendan,cje,capsule_addngro4,'glca+hep+6ome','glca6ngro+hep+6ome',1).
reaction(brendan,cje,capsule_addngro4,'pre-ngro','glca6ngro+hep+6ome',1).
```

```
reaction_t(capsule_addngro6).
reaction_gene(brendan,cje,capsule_addngro6,unknown).
reaction_subpathway(brendan,cje,capsule_addngro6,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro6,capsule).
```

reaction(brendan,cje,capsule_addngro6,'glca+hep+omepn+6ome','glca6ngro+hep+omepn+6ome',1).
reaction(brendan,cje,capsule_addngro6,'pre-ngro','glca6ngro+hep+omepn+6ome',1).

%% GalfNAc group + phase variable group

reaction_t(capsule_addngro9).
reaction_gene(brendan,cje,capsule_addngro9,unknown).
reaction_subpathway(brendan,cje,capsule_addngro9,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro9,capsule).
reaction(brendan,cje,capsule_addngro9,'glca-galfnac','glca6ngro-galfnac',1).
reaction(brendan,cje,capsule_addngro9,'pre-ngro','glca6ngro-galfnac',1).

reaction_t(capsule_addngro10).
reaction_gene(brendan,cje,capsule_addngro10,unknown).
reaction_subpathway(brendan,cje,capsule_addngro10,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro10,capsule).
reaction(brendan,cje,capsule_addngro10,'glca+hep-galfnac','glca6ngro+hep-galfnac',1).
reaction(brendan,cje,capsule_addngro10,'pre-ngro','glca6ngro+hep-galfnac',1).

reaction_t(capsule_addngro11).
reaction_gene(brendan,cje,capsule_addngro11,unknown).
reaction_subpathway(brendan,cje,capsule_addngro11,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro11,capsule).
reaction(brendan,cje,capsule_addngro11,'glca+hep+omepn-galfnac','glca6ngro+hep+omepn-galfnac',1).
reaction(brendan,cje,capsule_addngro11,'pre-ngro','glca6ngro+hep+omepn-galfnac',1).

reaction_t(capsule_addngro13).
reaction_gene(brendan,cje,capsule_addngro13,unknown).
reaction_subpathway(brendan,cje,capsule_addngro13,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro13,capsule).
reaction(brendan,cje,capsule_addngro13,'glca+hep+6ome-galfnac','glca6ngro+hep+6ome-galfnac',1).
reaction(brendan,cje,capsule_addngro13,'pre-ngro','glca6ngro+hep+6ome-galfnac',1).

reaction_t(capsule_addngro15).
reaction_gene(brendan,cje,capsule_addngro15,unknown).
reaction_subpathway(brendan,cje,capsule_addngro15,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro15,capsule).
reaction(brendan,cje,capsule_addngro15,'glca+hep+omepn+6ome-galfnac','glca6ngro+hep+omepn+6ome-galfnac',1).
reaction(brendan,cje,capsule_addngro15,'pre-ngro','glca6ngro+hep+omepn+6ome-galfnac',1).

reaction_t(capsule_addngro18).
reaction_gene(brendan,cje,capsule_addngro18,unknown).
reaction_subpathway(brendan,cje,capsule_addngro18,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro18,capsule).
reaction(brendan,cje,capsule_addngro18,'glca-galfnac+omepn','glca6ngro-galfnac+omepn',1).
reaction(brendan,cje,capsule_addngro18,'pre-ngro','glca6ngro-galfnac+omepn',1).

reaction_t(capsule_addngro19).
reaction_gene(brendan,cje,capsule_addngro19,unknown).
reaction_subpathway(brendan,cje,capsule_addngro19,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro19,capsule).
reaction(brendan,cje,capsule_addngro19,'glca+hep-galfnac+omepn','glca6ngro+hep-galfnac+omepn',1).
reaction(brendan,cje,capsule_addngro19,'pre-ngro','glca6ngro+hep-galfnac+omepn',1).

reaction_t(capsule_addngro20).
reaction_gene(brendan,cje,capsule_addngro20,unknown).
reaction_subpathway(brendan,cje,capsule_addngro20,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro20,capsule).
reaction(brendan,cje,capsule_addngro20,'glca+hep+omepn-galfnac+omepn','glca6ngro+hep+omepn-galfnac+omepn',1).
reaction(brendan,cje,capsule_addngro20,'pre-ngro','glca6ngro+hep+omepn-galfnac+omepn',1).

reaction_t(capsule_addngro22).
reaction_gene(brendan,cje,capsule_addngro22,unknown).
reaction_subpathway(brendan,cje,capsule_addngro22,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro22,capsule).
reaction(brendan,cje,capsule_addngro22,'glca+hep+6ome-galfnac+omepn','glca6ngro+hep+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_addngro22,'pre-ngro','glca6ngro+hep+6ome-galfnac+omepn',1).

reaction_t(capsule_addngro24).
reaction_gene(brendan,cje,capsule_addngro24,unknown).
reaction_subpathway(brendan,cje,capsule_addngro24,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro24,capsule).
reaction(brendan,cje,capsule_addngro24,'glca+hep+omepn+6ome-galfnac+omepn','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).
reaction(brendan,cje,capsule_addngro24,'pre-ngro','glca6ngro+hep+omepn+6ome-galfnac+omepn',1).

%% Ribf group

reaction_t(capsule_addngro27).
reaction_gene(brendan,cje,capsule_addngro27,unknown).
reaction_subpathway(brendan,cje,capsule_addngro27,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro27,capsule).
reaction(brendan,cje,capsule_addngro27,'glca-galfnac-ribf','glca6ngro-galfnac-ribf',1).
reaction(brendan,cje,capsule_addngro27,'pre-ngro','glca6ngro-galfnac-ribf',1).

reaction_t(capsule_addngro28).
reaction_gene(brendan,cje,capsule_addngro28,unknown).
reaction_subpathway(brendan,cje,capsule_addngro28,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro28,capsule).
reaction(brendan,cje,capsule_addngro28,'glca+hep-galfnac-ribf','glca6ngro+hep-galfnac-ribf',1).
reaction(brendan,cje,capsule_addngro28,'pre-ngro','glca6ngro+hep-galfnac-ribf',1).

reaction_t(capsule_addngro29).
reaction_gene(brendan,cje,capsule_addngro29,unknown).
reaction_subpathway(brendan,cje,capsule_addngro29,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro29,capsule).
reaction(brendan,cje,capsule_addngro29,'glca+hep+omepn-galfnac-ribf','glca6ngro+hep+omepn-galfnac-ribf',1).
reaction(brendan,cje,capsule_addngro29,'pre-ngro','glca6ngro+hep+omepn-galfnac-ribf',1).

reaction_t(capsule_addngro31).
reaction_gene(brendan,cje,capsule_addngro31,unknown).
reaction_subpathway(brendan,cje,capsule_addngro31,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro31,capsule).
reaction(brendan,cje,capsule_addngro31,'glca+hep+6ome-galfnac-ribf','glca6ngro+hep+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_addngro31,'pre-ngro','glca6ngro+hep+6ome-galfnac-ribf',1).

```
reaction_t(capsule_addngro33).
reaction_gene(brendan,cje,capsule_addngro33,unknown).
reaction_subpathway(brendan,cje,capsule_addngro33,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro33,capsule).
reaction(brendan,cje,capsule_addngro33,'glca+hep+omepn+6ome-galfnac-ribf','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
reaction(brendan,cje,capsule_addngro33,'pre-ngro','glca6ngro+hep+omepn+6ome-galfnac-ribf',1).
```

```
reaction_t(capsule_addngro36).
reaction_gene(brendan,cje,capsule_addngro36,unknown).
reaction_subpathway(brendan,cje,capsule_addngro36,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro36,capsule).
reaction(brendan,cje,capsule_addngro36,'glca-galfnac+omepn-ribf','glca6ngro-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_addngro36,'pre-ngro','glca6ngro-galfnac+omepn-ribf',1).
```

```
reaction_t(capsule_addngro37).
reaction_gene(brendan,cje,capsule_addngro37,unknown).
reaction_subpathway(brendan,cje,capsule_addngro37,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro37,capsule).
reaction(brendan,cje,capsule_addngro37,'glca+hep-galfnac+omepn-ribf','glca6ngro+hep-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_addngro37,'pre-ngro','glca6ngro+hep-galfnac+omepn-ribf',1).
```

```
reaction_t(capsule_addngro38).
reaction_gene(brendan,cje,capsule_addngro38,unknown).
reaction_subpathway(brendan,cje,capsule_addngro38,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro38,capsule).
reaction(brendan,cje,capsule_addngro38,'glca+hep+omepn-galfnac+omepn-ribf','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_addngro38,'pre-ngro','glca6ngro+hep+omepn-galfnac+omepn-ribf',1).
```

```
reaction_t(capsule_addngro40).
reaction_gene(brendan,cje,capsule_addngro40,unknown).
reaction_subpathway(brendan,cje,capsule_addngro40,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro40,capsule).
reaction(brendan,cje,capsule_addngro40,'glca+hep+6ome-galfnac+omepn-ribf','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_addngro40,'pre-ngro','glca6ngro+hep+6ome-galfnac+omepn-ribf',1).
```

```
reaction_t(capsule_addngro42).
reaction_gene(brendan,cje,capsule_addngro42,unknown).
reaction_subpathway(brendan,cje,capsule_addngro42,cap_addngro).
reaction_pathway(brendan,cje,capsule_addngro42,capsule).
reaction(brendan,cje,capsule_addngro42,'glca+hep+omepn+6ome-galfnac+omepn-ribf','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).
reaction(brendan,cje,capsule_addngro42,'pre-ngro','glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf',1).
```

```
%% adding etn
% .....
```

%% Lipooligosaccharide synthesis pathway

%%...

%% Capsule synthesis pathway

glycan_pathway(brendan,cje,capsule).
glycan_root(brendan,cje,capsule,'Chain').
glycan_part(brendan,cje,capsule,'Chain','Chain').
glycan_part(brendan,cje,capsule,'GlcA','GlcA').
glycan_part(brendan,cje,capsule,'NGro','NGro').
glycan_part(brendan,cje,capsule,'EtN','EtN').
glycan_part(brendan,cje,capsule,'Hep','Hep').
glycan_part(brendan,cje,capsule,'Hep OMePN','OMePN').
glycan_part(brendan,cje,capsule,'Hep 3-OMe','3-OMe').
glycan_part(brendan,cje,capsule,'Hep 6-OMe','6-OMe').
glycan_part(brendan,cje,capsule,'GalfNAc','GalfNAc').
glycan_part(brendan,cje,capsule,'GalfNAc OMePN','OMePN').
glycan_part(brendan,cje,capsule,'Ribf','Ribf').

part_precursor(brendan,cje,capsule,'GlcA','pre-glca').
part_precursor(brendan,cje,capsule,'NGro','pre-ngro').
part_precursor(brendan,cje,capsule,'EtN','pre-etn').
part_precursor(brendan,cje,capsule,'Hep','gdp-d-al-gluco-hep').
part_precursor(brendan,cje,capsule,'Hep OMePN','pre-omepn').
part_precursor(brendan,cje,capsule,'Hep 3-OMe','pre-ome').
part_precursor(brendan,cje,capsule,'Hep 6-OMe','pre-ome').
part_precursor(brendan,cje,capsule,'GalfNAc','pre-galfnac').
part_precursor(brendan,cje,capsule,'GalfNAc OMePN','pre-omepn').
part_precursor(brendan,cje,capsule,'Ribf','pre-ribf').

glycan_join(brendan,cje,capsule,'Chain','GlcA',cj1441c).
guess_glycan_join(brendan,cje,capsule,'Chain','GlcA',cj1441c).
glycan_join(brendan,cje,capsule,'GlcA','NGro',unknown).
glycan_join(brendan,cje,capsule,'GlcA','EtN',unknown).
glycan_join(brendan,cje,capsule,'GlcA','Hep',cj1431c).
glycan_join(brendan,cje,capsule,'Hep','Hep OMePN',cj1422c).
glycan_join(brendan,cje,capsule,'Hep','Hep 3-OMe',unknown).
glycan_join(brendan,cje,capsule,'Hep','Hep 6-OMe',cj1426c).
glycan_join(brendan,cje,capsule,'GlcA','GalfNAc',cj1439c).
guess_glycan_join(brendan,cje,capsule,'GlcA','GalfNAc',cj1439c).
glycan_join(brendan,cje,capsule,'GalfNAc','GalfNAc OMePN',cj1421c).
glycan_join(brendan,cje,capsule,'GalfNAc','Ribf',unknown).

%% Contains part

%% Chain

contains_part(brendan,cje,capsule,'capsule_chain','Chain').
contains_part(brendan,cje,capsule,'glca','Chain').
contains_part(brendan,cje,capsule,'glca6ngro','Chain').
contains_part(brendan,cje,capsule,'glca6etn','Chain').
contains_part(brendan,cje,capsule,'glca6ngro+hep','Chain').
contains_part(brendan,cje,capsule,'glca6ngro+hep+omepn','Chain').

contains_part(brendan,cje,capsule,'glca6etn+hep+omepn+3ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+omepn+6ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+3ome+6ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+omepn+3ome+6ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+omepn-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+3ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+6ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+omepn+3ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+omepn+6ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+3ome+6ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca6etn+hep+omepn+3ome+6ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+3ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+6ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn+3ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn+6ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+3ome+6ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn+3ome+6ome-galfnac-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+3ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+6ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn+3ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn+6ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+3ome+6ome-galfnac+omepn-ribf','Ribf').
contains_part(brendan,cje,capsule,'glca+hep+omepn+3ome+6ome-galfnac+omepn-ribf','Ribf').

%% Adds part

%% GlcA

adds_part(brendan,cje,capsule,capsule_0,'GlcA').

%% NGro

adds_part(brendan,cje,capsule,capsule_ngro0,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro1,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro2,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro3,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro4,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro5,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro6,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro7,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro8,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro9,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro10,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro11,'NGro').
adds_part(brendan,cje,capsule,capsule_addngro12,'NGro').

adds_part(brendan,cje,capsule,capsule_addetn19,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn20,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn21,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn22,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn23,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn24,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn25,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn26,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn27,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn28,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn29,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn30,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn31,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn32,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn33,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn34,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn35,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn36,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn37,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn38,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn39,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn40,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn41,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn42,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn43,'EtN').
adds_part(brendan,cje,capsule,capsule_addetn44,'EtN').

%% Hep

adds_part(brendan,cje,capsule,capsule_ngo1,'Hep').
adds_part(brendan,cje,capsule,capsule_ngo1a,'Hep').
adds_part(brendan,cje,capsule,capsule_ngo1b,'Hep').
adds_part(brendan,cje,capsule,capsule_ngo1c,'Hep').
adds_part(brendan,cje,capsule,capsule_etn1,'Hep').
adds_part(brendan,cje,capsule,capsule_etn1a,'Hep').
adds_part(brendan,cje,capsule,capsule_etn1b,'Hep').
adds_part(brendan,cje,capsule,capsule_etn1c,'Hep').
adds_part(brendan,cje,capsule,capsule_1,'Hep').
adds_part(brendan,cje,capsule,capsule_1a,'Hep').
adds_part(brendan,cje,capsule,capsule_1b,'Hep').
adds_part(brendan,cje,capsule,capsule_1c,'Hep').

%% Hep OMePN

adds_part(brendan,cje,capsule,capsule_ngo4,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo5,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo5a,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo5b,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo8,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo9,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo9a,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo9b,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo12,'Hep OMePN').
adds_part(brendan,cje,capsule,capsule_ngo13,'Hep OMePN').

adds_part(brendan,cje,capsule,capsule_9e,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_9f,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_13c,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_13d,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_13e,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_13f,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_17c,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_17d,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_17e,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_17f,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_21c,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_21d,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_21e,'Hep 6-OMe').
adds_part(brendan,cje,capsule,capsule_21f,'Hep 6-OMe').

%% GalfNAc

adds_part(brendan,cje,capsule,capsule_ngro22,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro23,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro24,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro24a,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro25,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro26,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro26a,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro26b,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_ngro26c,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn22,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn23,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn24,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn24a,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn25,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn26,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn26a,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn26b,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_etn26c,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_22,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_23,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_24,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_24a,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_25,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_26,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_26a,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_26b,'GalfNAc').
adds_part(brendan,cje,capsule,capsule_26c,'GalfNAc').

%% GalfNAc OMePN

adds_part(brendan,cje,capsule,capsule_ngro27,'GalfNAc OMePN').
adds_part(brendan,cje,capsule,capsule_ngro28,'GalfNAc OMePN').
adds_part(brendan,cje,capsule,capsule_ngro29,'GalfNAc OMePN').
adds_part(brendan,cje,capsule,capsule_ngro29a,'GalfNAc OMePN').
adds_part(brendan,cje,capsule,capsule_ngro30,'GalfNAc OMePN').
adds_part(brendan,cje,capsule,capsule_ngro31,'GalfNAc OMePN').
adds_part(brendan,cje,capsule,capsule_ngro31a,'GalfNAc OMePN').

neighbour_reaction(capsule_0,capsule_pre_pre_glca).
neighbour_reaction(capsule_pre_pre_glca,capsule_0).
neighbour_reaction(capsule_pre_pre_glca,capsule_pre_pre_glca).
neighbour_reaction(capsule_pre_pre_glca,capsule_pre_pre_glca).

neighbour_reaction(capsule_0,capsule_ngro1c).
neighbour_reaction(capsule_ngro1c,capsule_0).

neighbour_reaction(capsule_pre_pre_galfnac,capsule_22).
neighbour_reaction(capsule_22,capsule_pre_pre_galfnac).
neighbour_reaction(capsule_pre_pre_galfnac,capsule_pre_pre_galfnac).
neighbour_reaction(capsule_pre_pre_galfnac,capsule_pre_pre_galfnac).

neighbour_reaction(capsule_ngro36a,capsule_22).
neighbour_reaction(capsule_22,capsule_ngro36a).

neighbour_reaction(capsule_pre_pre_ribf,capsule_37).
neighbour_reaction(capsule_37,capsule_pre_pre_ribf).

neighbour_reaction(capsule_22,capsule_37).
neighbour_reaction(capsule_37,capsule_22).

neighbour_reaction(capsule_ngro36a,capsule_37).
neighbour_reaction(capsule_37,capsule_ngro36a).

neighbour_reaction(capsule_pre_glca,capsule_pre_hep).
neighbour_reaction(capsule_pre_hep,capsule_pre_glca).
neighbour_reaction(capsule_pre_glca,capsule_1).
neighbour_reaction(capsule_1,capsule_pre_glca).
neighbour_reaction(capsule_0,capsule_1).
neighbour_reaction(capsule_1,capsule_0).

neighbour_reaction(capsule_pre_glca,capsule_ngro21c).
neighbour_reaction(capsule_pre_glca,capsule_ngro21a).
neighbour_reaction(capsule_ngro21c,capsule_pre_glca).
neighbour_reaction(capsule_ngro21a,capsule_pre_glca).

neighbour_reaction(capsule_pre_pre_glca,capsule_pre_hep).
neighbour_reaction(capsule_pre_pre_glca,capsule_ngro21c).
neighbour_reaction(capsule_pre_pre_glca,capsule_ngro21a).
neighbour_reaction(capsule_pre_hep,capsule_pre_pre_glca).
neighbour_reaction(capsule_ngro21c,capsule_pre_pre_glca).
neighbour_reaction(capsule_ngro21a,capsule_pre_pre_glca).

neighbour_reaction(capsule_pre_hep,capsule_ngro21c).
neighbour_reaction(capsule_pre_hep,capsule_ngro21a).
neighbour_reaction(capsule_ngro21c,capsule_pre_hep).
neighbour_reaction(capsule_ngro21a,capsule_pre_hep).

neighbour_reaction(capsule_ngro21c,capsule_ngro21a).
neighbour_reaction(capsule_ngro21a,capsule_ngro21c).

neighbour_reaction(capsule_pre_pre_galfnac,capsule_ngro36a).
neighbour_reaction(capsule_pre_pre_galfnac,capsule_pre_pre_omepn).

neighbour_reaction(capsule_ngro36a,capsule_pre_pre_galfnac).
neighbour_reaction(capsule_pre_pre_omepn,capsule_pre_pre_galfnac).

neighbour_reaction(capsule_ngro21a,capsule_pre_pre_omepn).
neighbour_reaction(capsule_pre_pre_omepn,capsule_ngro21a).
neighbour_reaction(capsule_ngro36a,capsule_pre_pre_omepn).
neighbour_reaction(capsule_pre_pre_omepn,capsule_ngro36a).

neighbour_reaction(capsule_pre_pre_glca,capsule_pre_hep).
neighbour_reaction(capsule_pre_hep,capsule_pre_pre_glca).

neighbour_reaction(capsule_ngro1c,capsule_ngro1c).
neighbour_reaction(capsule_ngro1c,capsule_ngro21a).

%%%%%%%%
%%%%%%%%

% additional reaction information related to pre-cursors
%

reaction(brendan,cje,capsule_pre_pre_omepn,'pre-pre-omepn','pre-omepn',1).
chain(capsule_pre_pre_omepn).

reaction(brendan,cje,capsule_pre_pre_ribf,'pre-pre-ribf','pre-ribf',1).
chain(capsule_pre_pre_ribf).

reaction(brendan,cje,capsule_pre_pre_glca,'pre-pre-glca','pre-glca',1).

reaction(brendan,cje,capsule_pre_pre_galfnac,'pre-pre-galfnac','pre-galfnac',1).

%reaction(brendan,cje,capsule_pre_pre_omepn,'pre-pre-omepn','pre-omepn',1).

reaction(brendan,cje,capsule_pre_pre_hep,'pre-pre-hep','pre-hep',1).
chain(capsule_pre_pre_hep).

reaction(brendan,cje,capsule_pre_hep,'glca6ngro','glca6ngro+hep',1).
reaction(brendan,cje,capsule_pre_hep,'pre-hep','glca6ngro+hep',1).

```
% FILE GLYCAN_STRUCTURE_PL
% The Campy CPS glycan structures. This includes the definition of struct_next
% which states that one glycan structure is related to another by the addition
% of a single chemical group
```

```
struct_next('pre-glca','glca').
struct_next('pre-galfnac','galfnac').
struct_next('pre-ribf','ribf').
```

```
struct_next('glca','glca-galfnac').
```

```
struct_next('glca-galfnac',
            'glca-galfnac-ribf').
```

```
struct_next('galfnac-ribf',
            'glca-galfnac-ribf').
```

```
struct_next('glca-ribf',
            'glca-galfnac-ribf').
```

```
struct_next('glca-galfnac-ribf',
            'glca6ngro-galfnac-ribf').
```

```
struct_next('glca6ngro-galfnac-ribf',
            'glca6ngro-galfnac+omepn-ribf').
```

```
struct_next('glca6ngro-galfnac+omepn-ribf',
            'glca6ngro+hep-galfnac+omepn-ribf').
```

```
struct_next('glca6ngro+hep-galfnac+omepn-ribf',
            'glca6ngro+hep+6ome-galfnac+omepn-ribf').
```

```
struct_next('glca6ngro+hep+6ome-galfnac-ribf',
            'glca6ngro+hep+6ome-galfnac+omepn-ribf').
```

```
struct_next('glca6ngro+hep+6ome-galfnac-ribf',
            'glca6ngro+hep+omepn+6ome-galfnac-ribf').
```

```
struct_next('glca6ngro+hep+omepn+6ome-galfnac-ribf',
            'glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf').
```

```
struct_next('glca6ngro+hep+6ome-galfnac+omepn-ribf',
            'glca6ngro+hep+omepn+6ome-galfnac+omepn-ribf').
```

```
struct_observable('glca6ngro+hep+6ome-galfnac-ribf',
                  'glca6ngro+hep+6ome-galfnac-ribf').
```

```
struct_observable('glca6ngro+hep+6ome-galfnac+omepn-ribf',
                  'glca6ngro+hep+6ome-galfnac+omepn-ribf').
```

```
struct_observable('glca6ngro+hep+omepn+6ome-galfnac-ribf',
```

```
'glca6ngro+hep+omepn+6ome-galfnac-ribf').  
struct_observable('glca6ngro-galfnac+omepn-ribf',  
  'glca6ngro-galfnac+omepn-ribf').  
struct_observable('glca6ngro+hep-galfnac+omepn-ribf',  
  'glca6ngro+hep-galfnac+omepn-ribf').  
struct_observable('glca6ngro-galfnac+omepn-ribf',  
  'glca6ngro-galfnac+omepn-ribf').
```

```
struct_observable('glca-galfnac','acapsular').  
struct_observable('galfnac-ribf','acapsular').  
struct_observable('glca-ribf','acapsular').  
struct_observable('glca','acapsular').  
struct_observable('pre-glca','acapsular').
```

```
struct_observable('pre_pre-glca','pre_pre-glca').  
struct_observable('pre_pre-galfnac','pre_pre-galfnac').  
struct_observable('pre_pre-hep','pre_pre-hep').
```

```
struct_observable('glca-galfnac','glca-galfnac').  
struct_observable('galfnac-ribf','galfnac-ribf').  
struct_observable('glca-ribf','glca-ribf').
```

% FILE MUTANTS_PL
% The gene knock-out experiments for Campy CPS. The data is mainly compiled from
% previously published data (McNally, 2007). The data is represented by instances
% of the 'knockout_observable' predicate which states when a specific gene is
% knocked out this result causes a particular glycan structure to be the largest
% synthesised

knockout_observable(cj1416c,'glca6ngro+hep+6ome-galfnac-ribf').
knockout_observable(cj1417c,'glca6ngro+hep+6ome-galfnac-ribf').
knockout_observable(cj1418c,'glca6ngro+hep+6ome-galfnac-ribf').
knockout_observable(cj1421c,'glca6ngro+hep+6ome-galfnac+omepn-ribf').
knockout_observable(cj1422c,'glca6ngro+hep+omepn+6ome-galfnac-ribf').
knockout_observable(cj1423c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1424c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1425c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1426c,'glca6ngro+hep-galfnac+omepn-ribf').
knockout_observable(cj1427c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1428c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1430c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1431c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1432c,'acapsular').
knockout_observable(cj1434c,'acapsular').
knockout_observable(cj1435c,'acapsular').
knockout_observable(cj1437c,'acapsular').
knockout_observable(cj1438c,'acapsular').
knockout_observable(cj1439c,'acapsular').
knockout_observable(cj1440c,'acapsular').
knockout_observable(cj1441c,'acapsular').
knockout_observable(cj1442c,'acapsular').
knockout_observable(cj1448c,'acapsular').

% FILE STRAINS_PL
% The cross-strain genomic data for the CPS loci originate from an in-progress study
% in which 270 *C. jejuni* isolates were analysed by comparative phylogenomics (whole
% genome comparisons of bacteria using DNA microarrays, combined with Bayesian-based
% algorithms, to model the phylogeny), using a previously published method (Champion,
% 2005).The data includes predicates 'absent' and 'occurs' which state that a particular
% gene is absent or present from a particular strain.

occurs(strainClinicalG1,cj1413c).
occurs(strainClinicalG3,cj1413c).
occurs(strainChickenicken11974,cj1413c).
occurs(strainChickenicken13249,cj1413c).
occurs(strainChickenicken13411,cj1413c).
occurs(strainClinical44811,cj1413c).
occurs(strainClinical48612,cj1413c).
occurs(strainClinical58473,cj1413c).
occurs(strainChicken11848,cj1413c).
occurs(strainChicken12567,cj1413c).
occurs(strainChicken11919,cj1413c).
occurs(strainChicken11973,cj1413c).
occurs(strainChicken13713,cj1413c).
occurs(strainBeach1791,cj1413c).
occurs(strainClinical43205,cj1413c).
occurs(strainClinical33106,cj1413c).
occurs(strainClinical38556,cj1413c).
occurs(strainClinical39182,cj1413c).
occurs(strainClinical44933,cj1413c).
occurs(strainClinical45631,cj1413c).
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```
% FILE LEARN_H_PL
% Example learning file for the reaction ?H in the paper. This is an input file
% for Progol 5.0 which loads other files in this directory into Progol and does the
% learning.
```

```
:-set(r,10)?
:-set(h,10000)?
```

```
:-['background.pl']?
:-['codes.pl']?
:-['common.pl']?
:-['CPS_pathway.pl']?
:-['glycan_structure.pl']?
:-['mutants.pl']?
:-['strains.pl']?
```

```
%%%%%%%%%%
%%%%%%%%%
```

```
unassigned_reaction(capsule_pre_pre_ribf). % reaction A
unassigned_reaction(capsule_37). % reaction B
unassigned_reaction(capsule_0). % reaction C
unassigned_reaction(capsule_22). % reaction D
unassigned_reaction(capsule_pre_pre_omepn). % reaction H
```

```
unassigned_gene(cj1416c).
%unassigned_gene(cj1417c).
%unassigned_gene(cj1418c).
```

```
%unassigned_gene(cj1432c).
%unassigned_gene(cj1434c).
%unassigned_gene(cj1438c).
%unassigned_gene(cj1440c).
%unassigned_gene(cj1442c).
```

FILE LEARN_H_OUT
CProgol Version 5.0

[:- set(r,10)? - Time taken 0.00s]
[:- set(h,10000)? - Time taken 0.00s]
[:- modeh(1,codes(#any,#any))? - Time taken 0.00s]
[:- observable(knockout_observable/2)? - Time taken 0.00s]
[Testing for contradictions]
[No contradictions found]
[:- [background.pl]? - Time taken 0.00s]
[Testing for contradictions]
[No contradictions found]
[:- [codes.pl]? - Time taken 0.00s]
[Testing for contradictions]
[No contradictions found]
[:- [common.pl]? - Time taken 0.01s]
[Testing for contradictions]
[No contradictions found]
[:- [CPS_pathway.pl]? - Time taken 0.02s]
[Testing for contradictions]
[No contradictions found]
[:- [glycan_structure.pl]? - Time taken 0.00s]
[Testing for contradictions]
[No contradictions found]
[:- [mutants.pl]? - Time taken 0.00s]
[Testing for contradictions]
[No contradictions found]
[:- [strains.pl]? - Time taken 0.04s]
[Testing for contradictions]
[No contradictions found]
[Generalising knockout_observable/2]
[Generalising knockout_observable(cj1416c,'glca6ngro+hep+6ome-galfnac-ribf').]
[Generalising <codes(cj1416c,capsule_pre_pre_omepn).>]
[Most specific clause is]

codes(cj1416c,capsule_pre_pre_omepn).

[C:1211,138,0,0 codes(cj1416c,capsule_pre_pre_omepn).]
[1 explored search nodes]
f=1211,p=138,n=0,h=0
[Result of search is]

codes(cj1416c,capsule_pre_pre_omepn).

[Result of search is]

codes(cj1416c,capsule_pre_pre_omepn).

[1 redundant clauses retracted from knockout_observable/2]
[130 redundant clauses retracted from occurs/2]
[Generalising knockout_observable(cj1417c,'glca6ngro+hep+6ome-galfnac-ribf').]
[Generalising knockout_observable(cj1418c,'glca6ngro+hep+6ome-galfnac-ribf').]
[Generalising knockout_observable(cj1421c,'glca6ngro+hep+6ome-galfnac+omepn-ribf').]

[Generalising knockout_observable(cj1422c,'glca6ngro+hep+omepn+6ome-galfnac-ribf').]
[Generalising knockout_observable(cj1423c,'glca6ngro-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1424c,'glca6ngro-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1425c,'glca6ngro-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1426c,'glca6ngro+hep-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1427c,'glca6ngro-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1428c,'glca6ngro-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1430c,'glca6ngro-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1431c,'glca6ngro-galfnac+omepn-ribf').]
[Generalising knockout_observable(cj1432c,acapsular).]
[Generalising knockout_observable(cj1434c,acapsular).]
[Generalising knockout_observable(cj1435c,acapsular).]
[Generalising knockout_observable(cj1437c,acapsular).]
[Generalising knockout_observable(cj1438c,acapsular).]
[Generalising knockout_observable(cj1439c,acapsular).]
[Generalising knockout_observable(cj1440c,acapsular).]
[Generalising knockout_observable(cj1441c,acapsular).]
[Generalising knockout_observable(cj1442c,acapsular).]
[Generalising knockout_observable(cj1448c,acapsular).]
knockout_observable(Gene,Observable) :- unassigned_gene(Gene),
 struct_observable(Prs_Struct,Observable), struct_next(Prs_Struct,
 Abs_Struct), path3(R,Prs_Struct,Abs_Struct), unassigned_reaction(R),
 codes(Gene,R).

knockout_observable(cj1417c,'glca6ngro+hep+6ome-galfnac-ribf').
knockout_observable(cj1418c,'glca6ngro+hep+6ome-galfnac-ribf').
knockout_observable(cj1421c,'glca6ngro+hep+6ome-galfnac+omepn-ribf').
knockout_observable(cj1422c,'glca6ngro+hep+omepn+6ome-galfnac-ribf').
knockout_observable(cj1423c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1424c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1425c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1426c,'glca6ngro+hep-galfnac+omepn-ribf').
knockout_observable(cj1427c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1428c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1430c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1431c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1432c,acapsular).
knockout_observable(cj1434c,acapsular).
knockout_observable(cj1435c,acapsular).
knockout_observable(cj1437c,acapsular).
knockout_observable(cj1438c,acapsular).
knockout_observable(cj1439c,acapsular).
knockout_observable(cj1440c,acapsular).
knockout_observable(cj1441c,acapsular).
knockout_observable(cj1442c,acapsular).
knockout_observable(cj1448c,acapsular).

[Total number of clauses = 23]

[Time taken 0.050s]

[The following definitions changed]

codes(cj1421c,capsule_ngo36a).

codes(cj1422c,capsule_ngro21a).
codes(cj1426c,capsule_ngro21c).
codes(cj1430c,capsule_hep5).
codes(cj1431c,capsule_ngro1c).
codes(cj1439c,capsule_pre_pre_galfnac).
codes(cj1441c,capsule_pre_pre_glca).
codes(cj1416c,capsule_pre_pre_omepn).

knockout_observable(Gene,Observable) :- unassigned_gene(Gene),
struct_observable(Prs_Struct,Observable), struct_next(Prs_Struct,
Abs_Struct), path3(R,Prs_Struct,Abs_Struct), unassigned_reaction(R),
codes(Gene,R).

knockout_observable(cj1417c,'glca6ngro+hep+6ome-galfnac-ribf').
knockout_observable(cj1418c,'glca6ngro+hep+6ome-galfnac-ribf').
knockout_observable(cj1421c,'glca6ngro+hep+6ome-galfnac+omepn-ribf').
knockout_observable(cj1422c,'glca6ngro+hep+omepn+6ome-galfnac-ribf').
knockout_observable(cj1423c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1424c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1425c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1426c,'glca6ngro+hep-galfnac+omepn-ribf').
knockout_observable(cj1427c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1428c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1430c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1431c,'glca6ngro-galfnac+omepn-ribf').
knockout_observable(cj1432c,acapsular).
knockout_observable(cj1434c,acapsular).
knockout_observable(cj1435c,acapsular).
knockout_observable(cj1437c,acapsular).
knockout_observable(cj1438c,acapsular).
knockout_observable(cj1439c,acapsular).
knockout_observable(cj1440c,acapsular).
knockout_observable(cj1441c,acapsular).
knockout_observable(cj1442c,acapsular).
knockout_observable(cj1448c,acapsular).

occurs(Strain1,Gene) :- codes(Gene,R1), neighbour_reaction(R1,
R2), codes(G2,R2), occurs0(Strain2,G2), have_same_serotype(Strain1,
Strain2), !.

occurs(strainClinicalG1,cj1413c).
occurs(strainClinicalG3,cj1413c).
occurs(strainChickenicken11974,cj1413c).
occurs(strainChickenicken13249,cj1413c).
occurs(strainChickenicken13411,cj1413c).
occurs(strainClinical44811,cj1413c).
occurs(strainClinical48612,cj1413c).
occurs(strainClinical58473,cj1413c).
occurs(strainChicken11848,cj1413c).
occurs(strainChicken12567,cj1413c).
occurs(strainChicken11919,cj1413c).
occurs(strainChicken11973,cj1413c).
occurs(strainChicken13713,cj1413c).
occurs(strainBeach1791,cj1413c).
occurs(strainClinical43205,cj1413c).
occurs(strainClinical33106,cj1413c).

occurs(strainClinical38556,cj1413c).
occurs(strainClinical39182,cj1413c).
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occurs(strainClinical30328,cj1413c).
occurs(strainClinical41651,cj1413c).
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occurs(strainClinical64555,cj1413c).
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occurs(strainClinicalM1,cj1445c).
occurs(strainClinical36860,cj1445c).
occurs(strainClinical40917,cj1445c).
occurs(strainClinical38857,cj1445c).
occurs(strainCjejuniRM1221,cj1445c).
occurs(strainChicken47693,cj1445c).
occurs(strainClinical63326,cj1445c).

occurs(strainClinical64555,cj1445c).
occurs(strainClinical59364,cj1445c).
occurs(strainClinical59424,cj1445c).
occurs(strainClinical33084,cj1445c).
occurs(strainClinical31481,cj1445c).
occurs(strainBeach1771,cj1445c).
occurs(strainClinical53250,cj1445c).
occurs(strainClinical45557,cj1445c).
occurs(strainClinical47939,cj1445c).
occurs(strainChickenicken13411,cj1447c).
occurs(strainClinical44811,cj1447c).
occurs(strainClinical48612,cj1447c).
occurs(strainClinical58473,cj1447c).
occurs(strainChicken11848,cj1447c).
occurs(strainChicken12567,cj1447c).
occurs(strainChicken11919,cj1447c).
occurs(strainChicken11973,cj1447c).
occurs(strainChicken13713,cj1447c).
occurs(strainBeach1791,cj1447c).
occurs(strainClinical43205,cj1447c).
occurs(strainClinical55703,cj1447c).
occurs(strainClinical30280,cj1447c).
occurs(strainClinical30328,cj1447c).
occurs(strainChickenicken12912,cj1447c).
occurs(strainChickenicken12450,cj1447c).
occurs(strainChickenicken12487,cj1447c).
occurs(strainChickenicken13082,cj1447c).
occurs(strainChicken40209,cj1447c).
occurs(strainClinical81116,cj1447c).
occurs(strainCjejuniRM1221,cj1447c).
occurs(strainChickenicken13411,cj1448c).
occurs(strainClinical44811,cj1448c).
occurs(strainClinical48612,cj1448c).
occurs(strainClinical58473,cj1448c).
occurs(strainChicken11848,cj1448c).
occurs(strainChicken12567,cj1448c).
occurs(strainChicken11919,cj1448c).
occurs(strainChicken11973,cj1448c).
occurs(strainChicken13713,cj1448c).
occurs(strainBeach1791,cj1448c).
occurs(strainClinical43205,cj1448c).
occurs(strainClinical55320,cj1448c).
occurs(strainClinical55703,cj1448c).
occurs(strainClinical30280,cj1448c).
occurs(strainClinical30328,cj1448c).
occurs(strainChickenicken12912,cj1448c).
occurs(strainChickenicken12450,cj1448c).
occurs(strainChickenicken12487,cj1448c).
occurs(strainChickenicken13082,cj1448c).
occurs(strainChicken40209,cj1448c).
occurs(strainBeach1793,cj1448c).
occurs(strainClinical81116,cj1448c).
occurs(strainClinical36860,cj1448c).
occurs(strainClinical53250,cj1448c).

[Total time taken 0.050s]