Brandeis

Zizhang Chen <zizhang2@brandeis.edu>

Replacement of files in full directory

34 messages

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 20, 2022 at 8:30 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

No need to redownload every time I sent, just keeping a log in this email chain as I check things.

I just replaced DB8939.csv, it had a formatting issue.

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Dr. Ryan Badman
Postdoctoral Researcher
Pengyu Hong Lab
Computer Science Department
Brandeis University

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 20, 2022 at 8:38 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB9155.pdb was missing and added, DB9155.csv already there
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 21, 2022 at 1:10 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

Added DB9507 to directory online
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 21, 2022 at 3:48 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

repeat-4)-b-D-Galp-(1-4)-a-D-GlcpNAc-(1-4)-b-D-Galp-(1-3)-a-D-GlcpNAc-(1-2)-b-D-Ribf-(1-.pdb added to the drive, had csv but was missing pdb
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 21, 2022 at 3:54 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

added DB9917 both pdb and csv
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 3:42 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

b-D-Manp has two different C6 shifts actually, C6 should possibly be
omitted for this glycan:

http://www.glycosciences.de/database/start.php?action=explore_linucsid&linucsid=22593&show=17#nmr
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 24, 2022 at 3:47 PM

To: Zizhang Chen <zizhang2@brandeis.edu>

b-D-Glcp-(1-4)-b-D-Glcp had an error in the PDB, I corrected it in the drive.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 1:18 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26510 was missing, added it
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 1:56 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

(meaning the PDB of 26510 was missing in last)

Also the shift file for 26511 was corrupted, I fixed it
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 2:07 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-D-GalpA-(1-3)-a-D-GalpA-(1-3)-b-D-GlcpNAc-(1-4)-a-D-GlcpNAc had a
txt extension instead of csv, fixed
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Oct 26, 2022 at 2:30 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

Added new molecule DB26517
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Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 1:21 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-L-Rhap-(1-4)-a-D-GalpA-(1-3)-b-D-GlcpNAc-(1-2)-a-L-Rhap-(3-1)-a-L-Rhap
has an issue, the PDB and csv is offset by 1 in order.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 4:18 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-D-GlcpA-(1-2)-a-D-GalpA-(1-2)-b-D-Manp(1-4)-b-D-Galp-(1-2)-b-D-Rhap.pdb
had an issue, replaced it
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 4:24 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

For a-D-Galp-(1-2)-a-L-Rhap-(1-3)-b-D-Manp-(1-4)-b-D-Manp-(1-4)-a-D-Galp-(1-3)-b-D-Galp-(2-1)-a-D-Glcp
, the pdb only has an error in it that needs to be corrected. Residue
1 and 2 are flipped and need to be swapped back. GLC should be 1.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 4:33 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-L-Rhap-(1-4)-a-D-Glcp-(1-3)-b-L-Rhap-(1-4)-b-D-Glcp-(1-4)-a-D-Glcp-(3-1)-a-L-Rhap,

the pdb only has an error in it that needs to be corrected. Residue
1 and 2 are flipped and need to be swapped back. GLC should be 1.

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Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 5:30 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

b-D-Xylp-(1-4)-b-D-Xylp-(1-4)-a-L-Galp-(2-1)-b-D-Xylp the pdb only has
an error in it that needs to be corrected. Residue 1 and 2 are flipped
and need to be swapped back. GAL should be 1 not 2..
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 10:09 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

b-D-Fruf-(2-1)-b-D-Fruf-(2-1)-b-D-Fruf-(2-1)-b-D-Fruf-(2-1)-a-D-Glcp
PDB is missing too much and 1st and 2nd residue is swapped.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Oct 27, 2022 at 10:36 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

b-D-Galp-(1-3)-b-D-Glcp-(1-3)-b-D-Xylp-(1-4)-b-D-Xylp-(1-4)-a-L-Galp-(2-1)-b-D-Xylp
1st and 2nd residue is swapped.

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Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 2:41 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

Corrected a-D-Manp-(1-2)-b-D-manp-(1-3)-a-D-GlcpNAc-(1-6)-a-D-Manp.pdb,
H1o should be H62. Redownload the online data
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 4:48 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-D-Galp-(1-2)-a-L-Rhap-(1-3)-b-D-Manp-(1-4)-b-D-Manp(1-4)-a-D-Galp-(1-3)-b-D-Galp-(2-1)-a-D-Glcp
a-D-Galp-(1-2)-a-L-Rhap-(1-3)-b-D-Manp-(1-4)-b-D-Manp(1-4)-a-D-Galp-(1-3)-b-D-Galp-(2-1)-b-D-Glcp

were duplicates of :

a-D-Galp-(1-2)-a-L-Rhap-(1-3)-b-D-Manp-(1-4)-b-D-Manp-(1-4)-a-D-Galp-(1-3)-b-D-Galp-(2-1)-a-D-Glcp
a-D-Galp-(1-2)-a-L-Rhap-(1-3)-b-D-Manp-(1-4)-b-D-Manp-(1-4)-a-D-Galp-(1-3)-b-D-Galp-(2-1)-b-D-Glcp

And needed to be removed. I edited the drive and fixed this.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Fri, Oct 28, 2022 at 5:36 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

In b-D-Galf-(1-3)-b-D-GalpNAc-(1-3)-b-D-Galp-(4-1)-a-D-Glcp-(6-1)-b-D-Glcp,
the shift order matches the name. The PDB top to bottom order matches
the shift, but the residue number is all jumbled. So just take the
residue order in the PDB relatively, rather than the number column.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 5:45 PM

To: Zizhang Chen <zizhang2@brandeis.edu>

DB26874 is too corrupted, unusable for atom-level prediction.
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Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 5:49 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

DB26878 is too corrupted, unusable for atom-level prediction.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 6:09 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-D-Kdop-(2-8)-a-D-Kdop-(2-4)-a-D-Kdop-(2-6)-b-D-GlcpN-(1-6)-a-D-GlcpN1PO4
the last residue in the PDB is PO3 and thus has no shifts, just note
that
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Mon, Oct 31, 2022 at 6:24 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

b-D-Galp-(3-1)-a-D-Manp has the order flipped between PDB and csv,
(e.g. Manp is 2 in PDB and 1 in shift).
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 3:56 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

I added DB26928, which is actually a linear molecule,
b-D-Kdop-(2-3)-a-D-Rhap-(1-3)-b-D-GlcpNAc-(1-3)-a-D-Rhap-(1-3)-b-D-GlcpNAc-(1-4)-a-D-Rhap-(1-3)-b-D-GlcpNAc-(1-4)-b-D-Glcp-(1-6)-a-D-Glcp-(1-4)-a-D-Manp
.

The PDB and csv order matches.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 4:14 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-L-Rhap-(1-2)-b-D-Glcp1OMe has a 3rd residue in the PDB which is
basically the Me group, that corresponds to the "B-D-GLCP1OME OMe
58.30 " row in the C list in the shifts.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 4:18 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

similar note for all these, not a real issue but just note it:

a-L-Fucp-(1-2)-b-D-Glcp1OMe
a-L-Rhap-(1-2)-b-D-Glcp1OMe
a-D-Manp-(1-2)-a-D-Glcp1OMe
b-D-Galp-(1-2)-a-D-Glcp1OMe
a-L-Fucp-(1-2)-a-D-Glcp1OMe
a-L-Rhap-(1-2)-a-D-Glcp1OMe
b-L-Fucp-(1-2)-a-D-Glcp1OMe
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 4:52 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

and for:

a-L-Fucp-(1-2)-b-D-Galp1OMe
b-L-Fucp-(1-2)-b-L-Galp1OMe
a-D-Manp-(1-3)-b-D-Glcp1OMe
b-D-Galp-(1-3)-b-D-Glcp1OMe
a-L-Fucp-(1-3)-b-D-Glcp1OMe
a-L-Rhap-(1-3)-b-D-Glcp1OMe
b-L-Fucp-(1-3)-b-D-Glcp1OMe
a-D-Manp-(1-3)-a-D-Glcp1OMe
b-D-Galp-(1-3)-a-D-Glcp1OMe
a-L-Rhap-(1-3)-a-D-Glcp1OMe
b-L-Fucp-(1-3)-a-D-Glcp1OMe
b-L-Fucp-(1-3)-b-D-Galp1OMe
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Tue, Nov 1, 2022 at 4:57 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

added b-D-Galp-(1-3)-b-D-Glcp1OMe , it was actually missing
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Wed, Nov 2, 2022 at 5:12 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-L-Rhap-(1-3)-b-D-Galp-(1-4)-b-D-GalpNAc-(3-1)-b-D-Galp residue 1 and 2 in the PDB are reversed, need to be flipped to match the csv.
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Nov 3, 2022 at 2:14 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-D-Glcp-(1-3)-a-L-Galp and a-D-Glcp-(1-3)-b-L-Galp might have the Glcp residues mislabeled, possibly should be GlcpA, just a note to check later. When the residues end with A that makes it an acid and those are more likely high C6 ppm
[Quoted text hidden]

Ryan Badman <ryanbadman@brandeis.edu> Thu, Nov 3, 2022 at 3:48 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

a-D-Apif is unusable, both the PDB and csv are super weird
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Ryan Badman <ryanbadman@brandeis.edu> Thu, Nov 3, 2022 at 3:48 PM
To: Zizhang Chen <zizhang2@brandeis.edu>

same with b-D-Apif
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