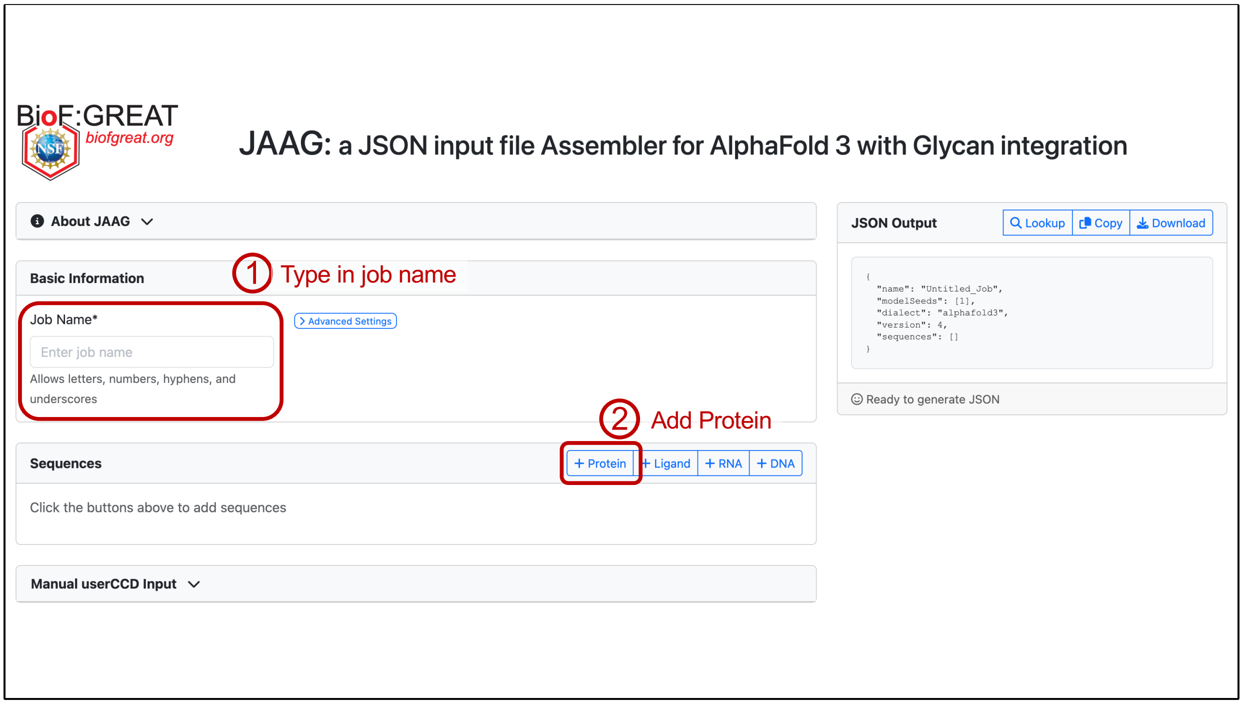
Modeling proteins only



JAAG: a JSON input file Assembler for AlphaFold 3 with Glycan integration

① Type in job name

Allows letters, numbers, hyphens, and underscores

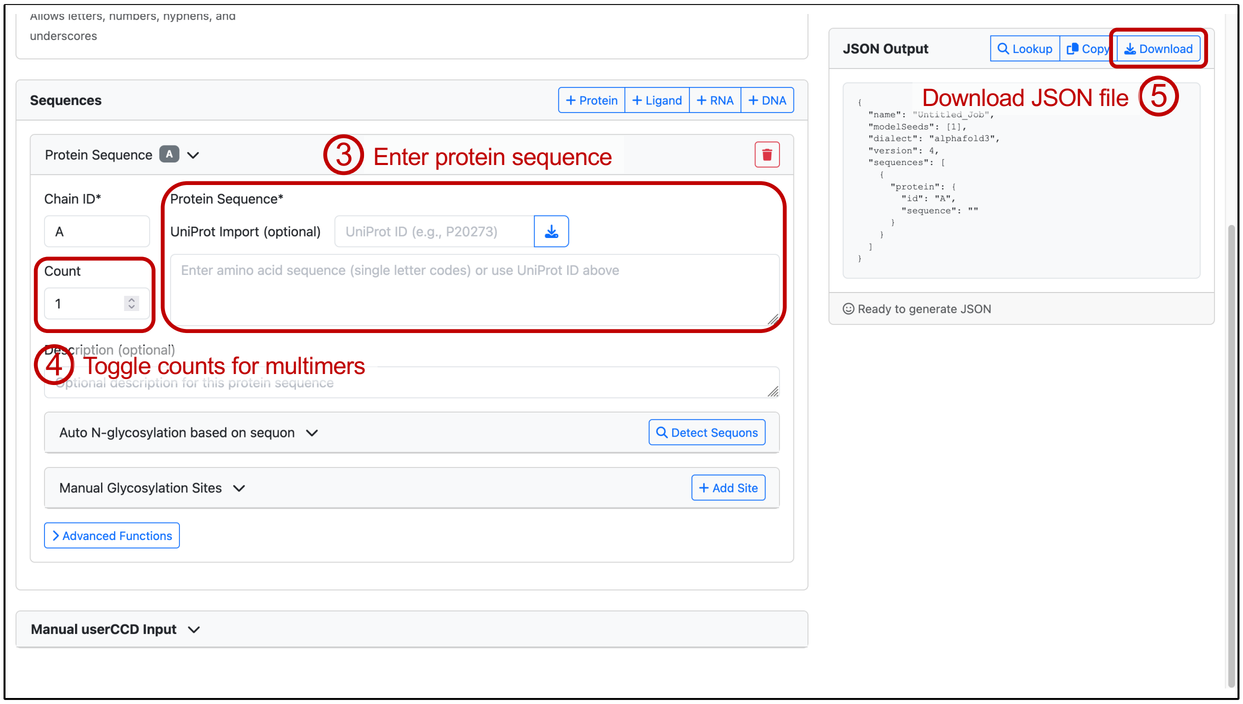
② Add Protein

Click the buttons above to add sequences

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": []
}
```

Ready to generate JSON

1. Enter job name. Space and other special symbols are not allowed.
2. Click the button to add a protein. If users are interested in a second protein, click the button again.



③ Enter protein sequence

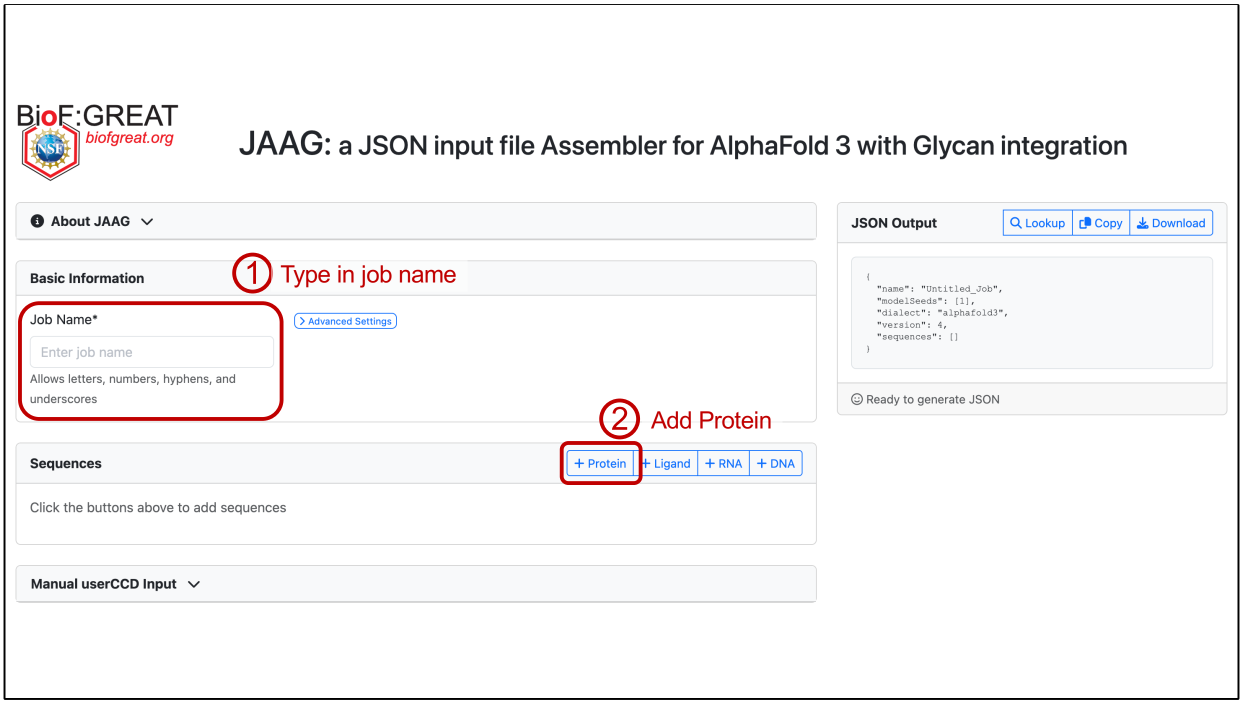
④ Toggle counts for multimers

Download JSON file ⑤

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence": ""
      }
    }
  ]
}
```

3. Type in the UniProt accession ID to fetch the protein sequence, or paste the amino sequence directly. Only when fetching from UniProt will JAAG automatically import the ID into the "Description" field below.
4. If users are looking into protein homo-multimers, toggle the count to the desire number.
5. Click the button to download the whole JSON file.

Modeling glycoproteins



JAAG: a JSON input file Assembler for AlphaFold 3 with Glycan integration

① Type in job name

Allows letters, numbers, hyphens, and underscores

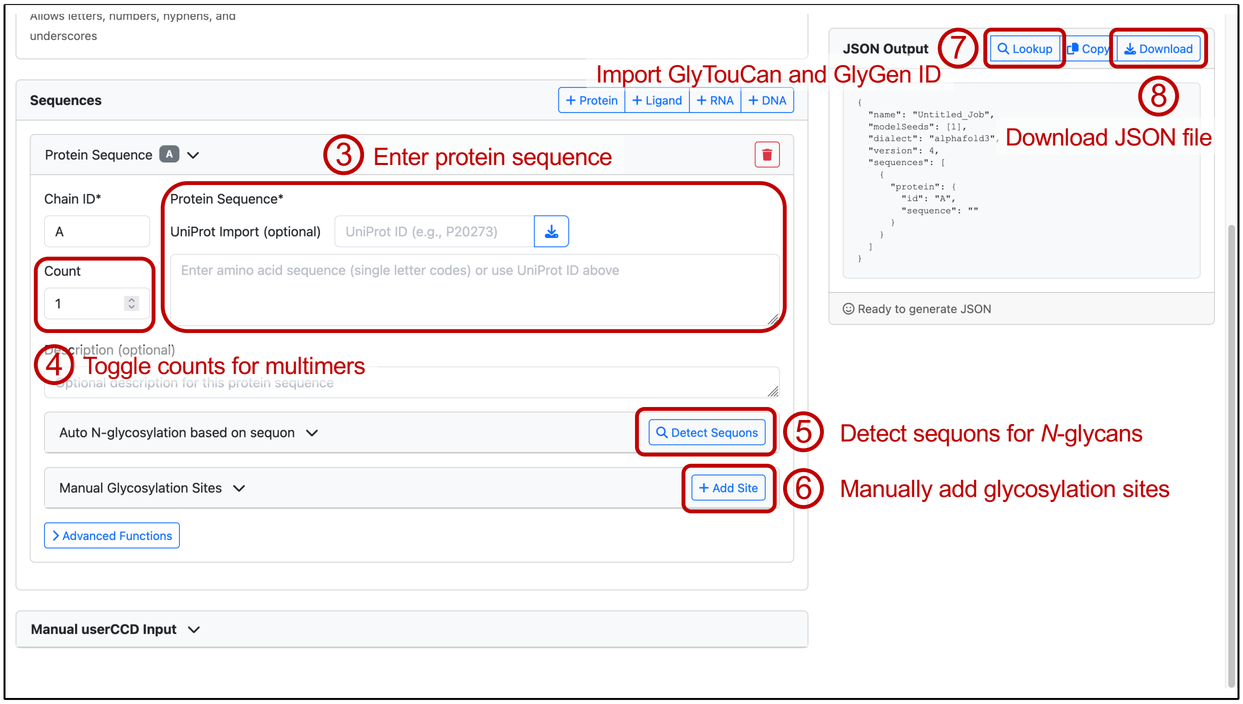
② Add Protein

Click the buttons above to add sequences

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": []
}
```

Ready to generate JSON

1. Enter job name. Space and other special symbols are not allowed.
2. Click the button to add a protein. If users are interested in a second protein, click the button again.



Chain ID*: A

Count: 1

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence": ""
      }
    }
  ]
}
```

Ready to generate JSON

③ Enter protein sequence

④ Toggle counts for multimers

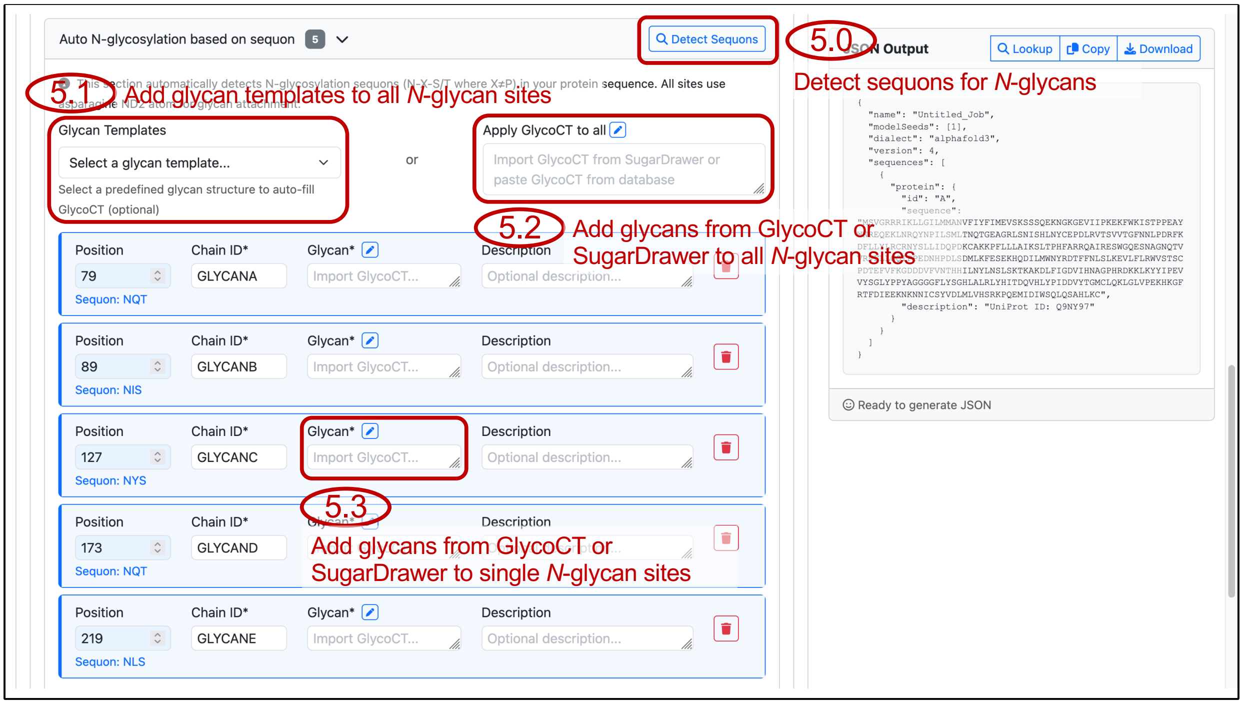
⑤ Detect sequons for *N*-glycans

⑥ Manually add glycosylation sites

⑦ Import GlyTouCan and GlyGen ID

⑧ Download JSON file

3. Type in the UniProt accession ID to fetch the protein sequence, or paste the amino sequence directly. Only when fetching by UniProt will JAAG automatically import the ID into the “description” field below.
4. If users are looking into protein homo-multimers, toggle the count to the desire number.
5. Click the button to automatically add N-glycosylation sites based on sequons. Please see the following pages for more details.
6. Click the button to manually add any glycosylation sites. Please see the following pages for more details.
7. Click the button to look up glycan structure in the GlyTouCan and GlyGen database and import the corresponding glycan into the JSON file. The IDs will be placed in the corresponding description field.
8. Click the button to download the whole JSON file.



5.0 JSON Output

Detect sequons for *N*-glycans

This section automatically detects N-glycosylation sequons (N-X-S/T where X≠P) in your protein sequence. All sites use asparagine ND2 atom for glycan attachment.

5.1 Add glycan templates to all *N*-glycan sites

Glycan Templates: Select a glycan template...

Select a predefined glycan structure to auto-fill GlycoCT (optional)

Apply GlycoCT to all: Import GlycoCT from SugarDrawer or paste GlycoCT from database

5.2 Add glycans from GlycoCT or SugarDrawer to all *N*-glycan sites

Position: 79 | Chain ID*: GLYCANA | Glycan*: Import GlycoCT... | Description: Optional description... | Sequon: NQT

Position: 89 | Chain ID*: GLYCANB | Glycan*: Import GlycoCT... | Description: Optional description... | Sequon: NIS

Position: 127 | Chain ID*: GLYCANC | Glycan*: Import GlycoCT... | Description: Optional description... | Sequon: NYS

Position: 173 | Chain ID*: GLYCAND | Glycan*: | Description: | Sequon: NQT

5.3 Add glycans from GlycoCT or SugarDrawer to single *N*-glycan sites

Position: 219 | Chain ID*: GLYCANE | Glycan*: Import GlycoCT... | Description: Optional description... | Sequon: NLS

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPEAY
WNREQEKLNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLPDRFK
DFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESNAGNQTV
VRVFLLGQLIPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLFLRWVSTSC
PDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRDKKLKYYIPEV
VYSGLYPPYAGGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQKLGLVPEKHKGF
RTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC",
        "description": "UniProt ID: Q9NY97"
      }
    }
  ]
}
```

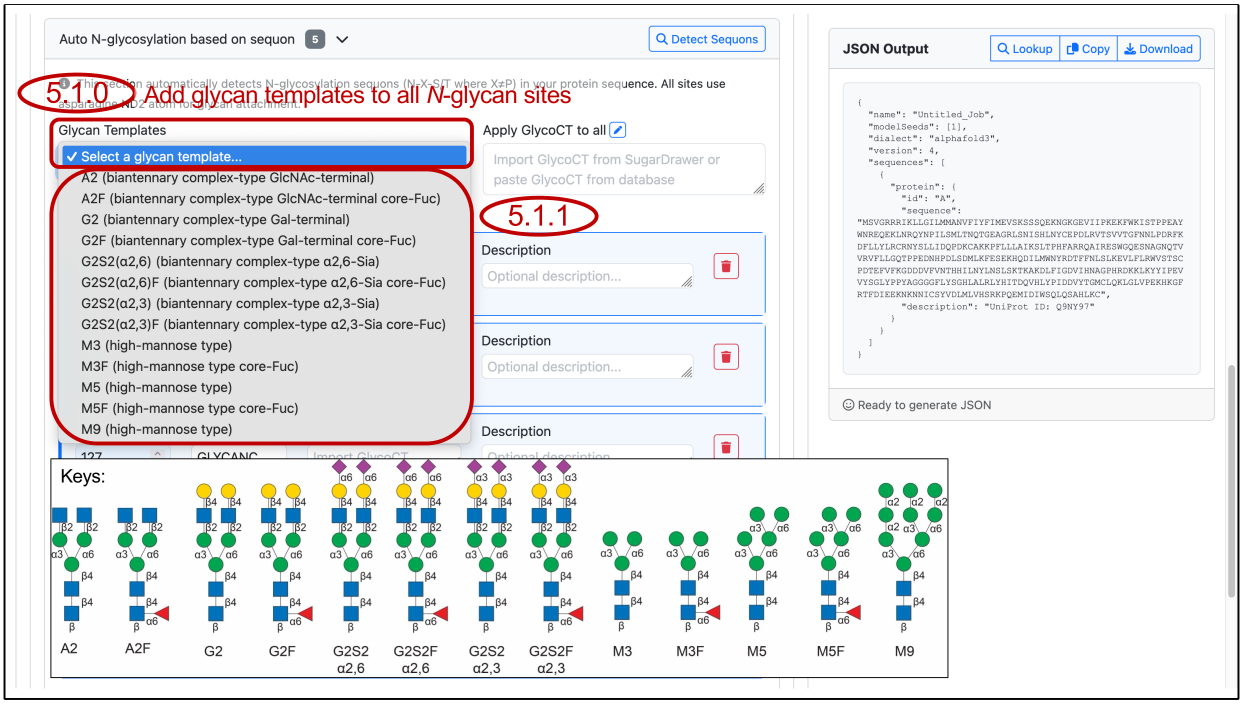
5.0. This tab will be added and expanded after clicking the “Detect Sequons” button.

Glycan structures can be introduced using the following three methods: 5.1, 5.2 and 5.3. Users can first use 5.1 or 5.2 to apply the same glycan to all N-glycan sites, then modify each site individually in 5.3.

5.1. Select glycan structures from a library of pre-built N-glycan templates. Please see the following pages for more details.

5.2. Paste in GlycoCT from your favorite glycoinformatics database or click the pencil icon to open the pop-up SugarDrawer tool to draw glycans. This will apply to all N-glycosylation sites. Please see the following pages for more details.

5.3. Paste in GlycoCT from your favorite glycoinformatics database or click the pencil icon to open the pop-up SugarDrawer tool to draw glycans. This will apply to individual N-glycosylation sites. Please see the following pages for more details.



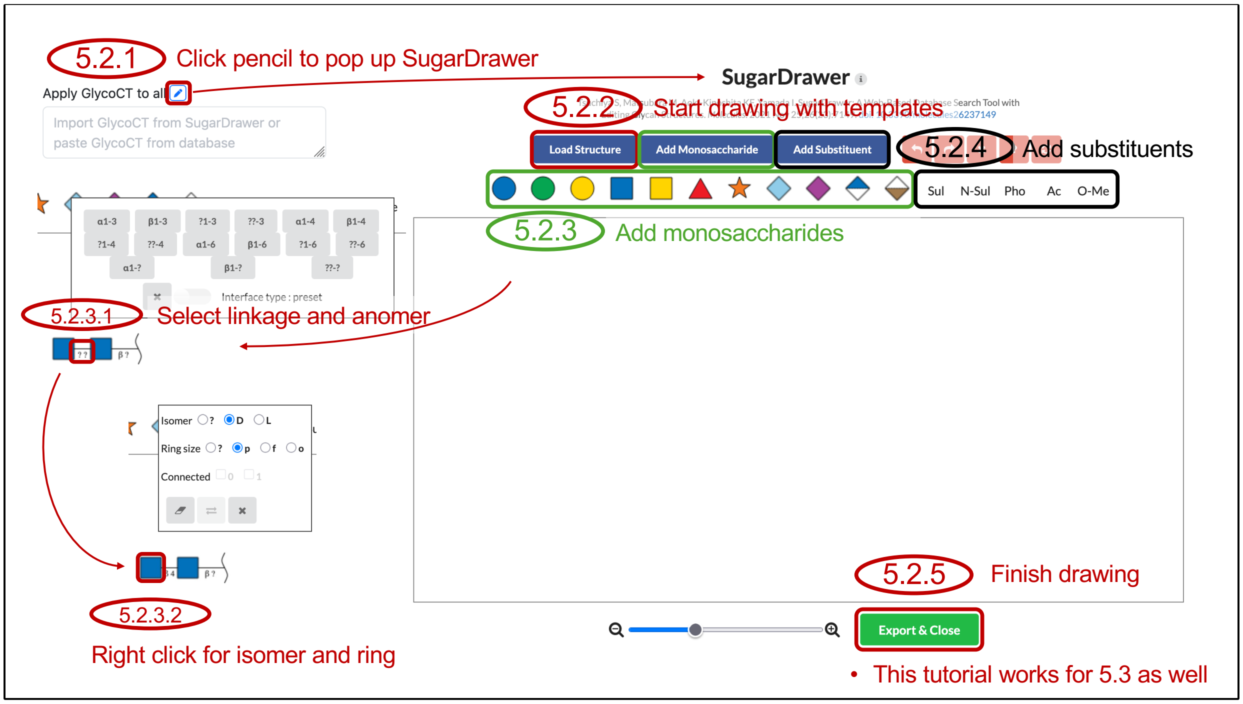
This section automatically detects N-glycosylation sequons (N-X-S/T where X≠P) in your protein sequence. All sites use asparagine ND2 atom for glycan attachment.

Glycan Templates

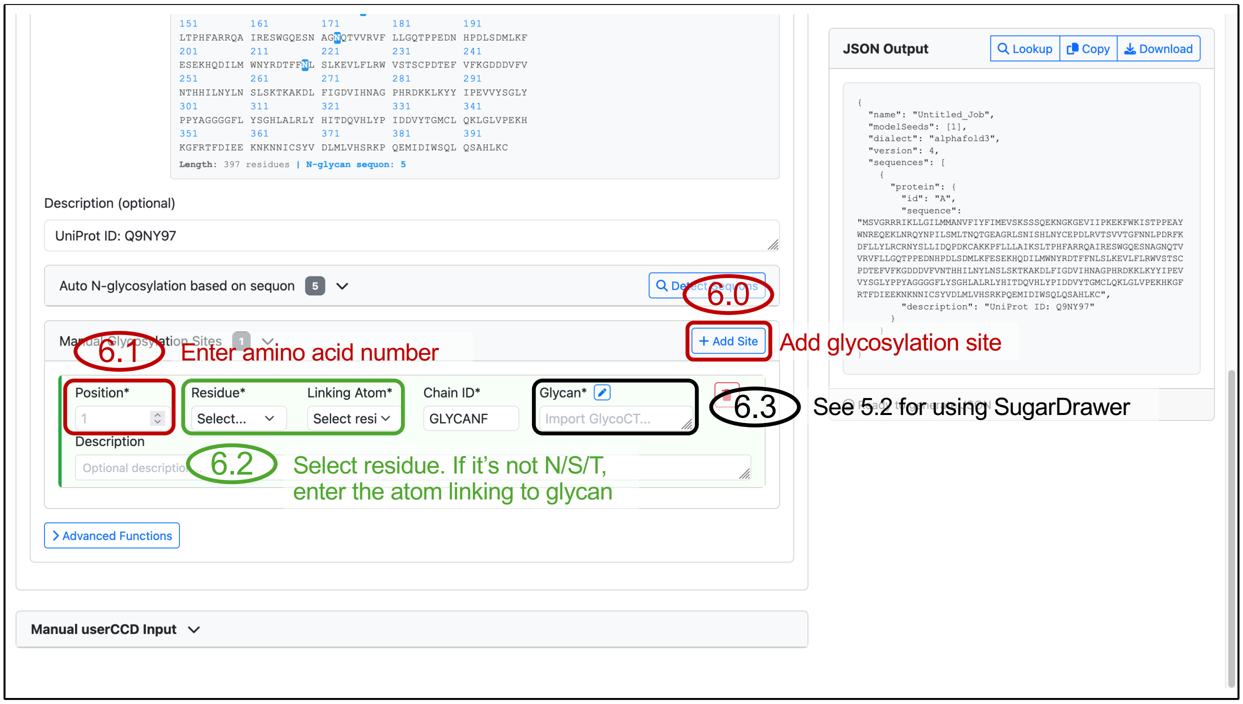
- ✓ Select a glycan template...
- A2 (biantennary complex-type GlcNAc-terminal)
- A2F (biantennary complex-type GlcNAc-terminal core-Fuc)
- G2 (biantennary complex-type Gal-terminal)
- G2F (biantennary complex-type Gal-terminal core-Fuc)
- G2S2(α2,6) (biantennary complex-type α2,6-Sia)
- G2S2(α2,6)F (biantennary complex-type α2,6-Sia core-Fuc)
- G2S2(α2,3) (biantennary complex-type α2,3-Sia)
- G2S2(α2,3)F (biantennary complex-type α2,3-Sia core-Fuc)
- M3 (high-mannose type)
- M3F (high-mannose type core-Fuc)
- M5 (high-mannose type)
- M5F (high-mannose type core-Fuc)
- M9 (high-mannose type)

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPEAY
WNREQEKLNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLPDRFK
DFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESNAGNQTV
VRVFLLGQTPPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLFLRWVSTSC
PDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRDKKLKYYIPEV
VYSGLYPPYAGGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQKLGLVPEKHKGF
RTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC",
        "description": "UniProt ID: Q9NY97"
      }
    }
  ]
}
```

5.1.0. This pull-down menu will appear after clicking “Select a glycan template…”
5.1.1. Select one glycan from the template collection to apply it to all N-glycosylation sites. The nomenclature key for each glycan abbreviation is provided.



5.2.1. Click the pencil icon to pop up SugarDrawer.
5.2.2. In the SugarDrawer, there are pre-built glycan templates that users can load to start the drawing the glycan structure. In the case here, find the N-glycan structures to start with.
5.2.3. Click the monosaccharides in the shortcut to extend glycans. If the monosaccharides are not in the shortcut, click the “Add Monosaccharide” button to expand the monosaccharide table.
5.2.3.1. Click the linkage line at the reducing end or between monosaccharides to pop up the anomer/linkage selection panel. Anomer and linkages must be defined to properly export the glycan bondedAtomPairs.
5.2.3.2. Right click the monosaccharide to pop up the isomer panel if users are using rare monosaccharides.
*Note: not all monosaccharides have corresponding CCD IDs.
5.2.4. Sul (sulfation), N-Sul (N-sulfation), Pho (phosphorylation), Ac (acetylation) and O-Me (methylation) are supported for bondedAtomPairs generation.
5.2.5. Click the button to export GlycoCT. The glycan bondedAtomPairs will be converted automatically.
This tutorial works for 5.3 as well to customize individual N-glycosylation sites.



```
151        161        171        181        191
LTPHFARRQA IRESWGQESN AGNQTVVRVF LLGQTPPEDN HPDLSDMLKF
201        211        221        231        241
ESEKHQDILM WNYRDTFFNL SLKEVLFLRW VSTSCPDTEF VFKGDDDVFV
251        261        271        281        291
NTHHILNYLN SLSKTKAKDL FIGDVIHNAG PHRDKKLKYY IPEVVYSGLY
301        311        321        331        341
PPYAGGGGFL YSGHLALRLY HITDQVHLYP IDDVYTGMCL QKLGLVPEKH
351        361        371        381        391
KGFRTFDIEE KNKNNICSYV DLMLVHSRKP QEMIDIWSQL QSAHLKC
Length: 397 residues | N-glycan sequon: 5
```

Description (optional)

UniProt ID: Q9NY97

Position*: 1

Residue*: Select...

Linking Atom*: Select resi

Chain ID*: GLYCANF

Glycan*: Import GlycoCT...

Description: Optional description...

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPEAY
WNREQEKLNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLPDRFK
DFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESNAGNQTV
VRVFLLGQTPPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLFLRWVSTSC
PDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRDKKLKYYIPEV
VYSGLYPPYAGGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQKLGLVPEKHKGF
RTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC",
        "description": "UniProt ID: Q9NY97"
      }
    }
```

6.0

Add glycosylation site

6.1 Enter amino acid number

6.2 Select residue. If it's not N/S/T, enter the atom linking to glycan

6.3 See 5.2 for using SugarDrawer

6.0. This tab will be added and expanded after clicking “Add Site” button.

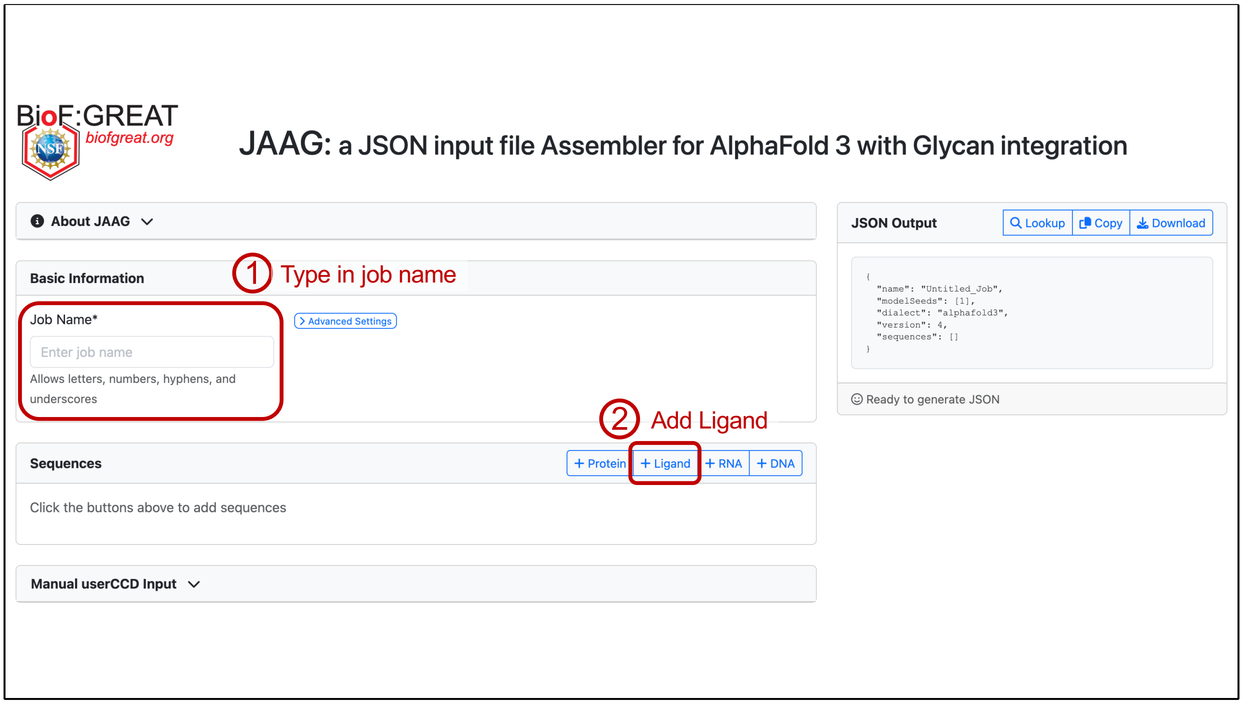
6.1. Users can type in amino acid numbers or toggle through the numbers.

6.2. When N/S/T are selected in 6.1, the amino acid atom linked to N- or O-glycan will appear automatically. If users are looking for other amino acid/atoms for glycosylation, look up PDBeChem for the atom: https://www.ebi.ac.uk/pdbe-srv/pdbechem/

6.3. Please refer to 5.2 for using SugarDrawer.

Modeling glycan as ligand

Referring to “modeling proteins only” or “modeling glycoproteins” sections to add protein



JAAG: a JSON input file Assembler for AlphaFold 3 with Glycan integration

① Type in job name

② Add Ligand

Basic Information

Job Name*

Enter job name

Allows letters, numbers, hyphens, and underscores

Sequences

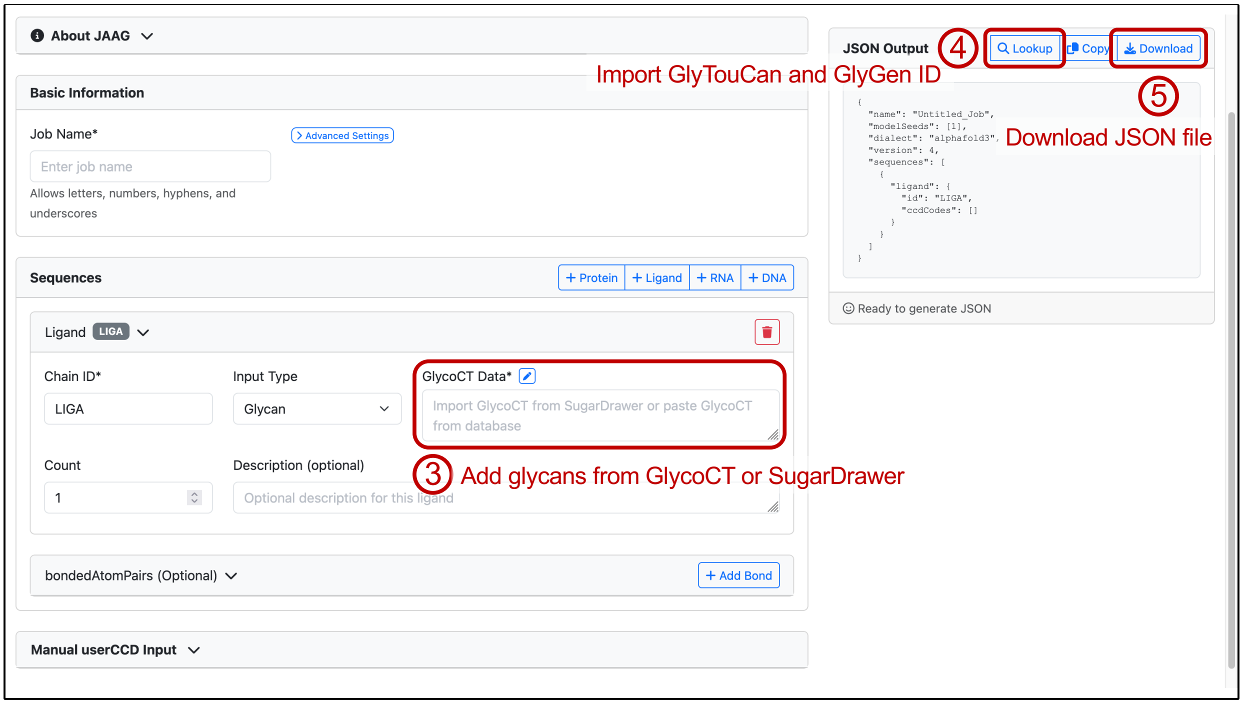
Click the buttons above to add sequences

JSON Output

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": []
}
```

Ready to generate JSON

1. Enter job name. Space and other special symbols are not allowed.
2. Click the button to add a ligand. If users are interested in a second ligand, click the button again.



Job Name*: Enter job name

Allows letters, numbers, hyphens, and underscores

Chain ID*: LIGA

Input Type: Glycan

GlycoCT Data*: Import GlycoCT from SugarDrawer or paste GlycoCT from database

Count: 1

Description (optional): Optional description for this ligand

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "ligand": {
        "id": "LIGA",
        "ccdCodes": []
      }
    }
  ]
}
```

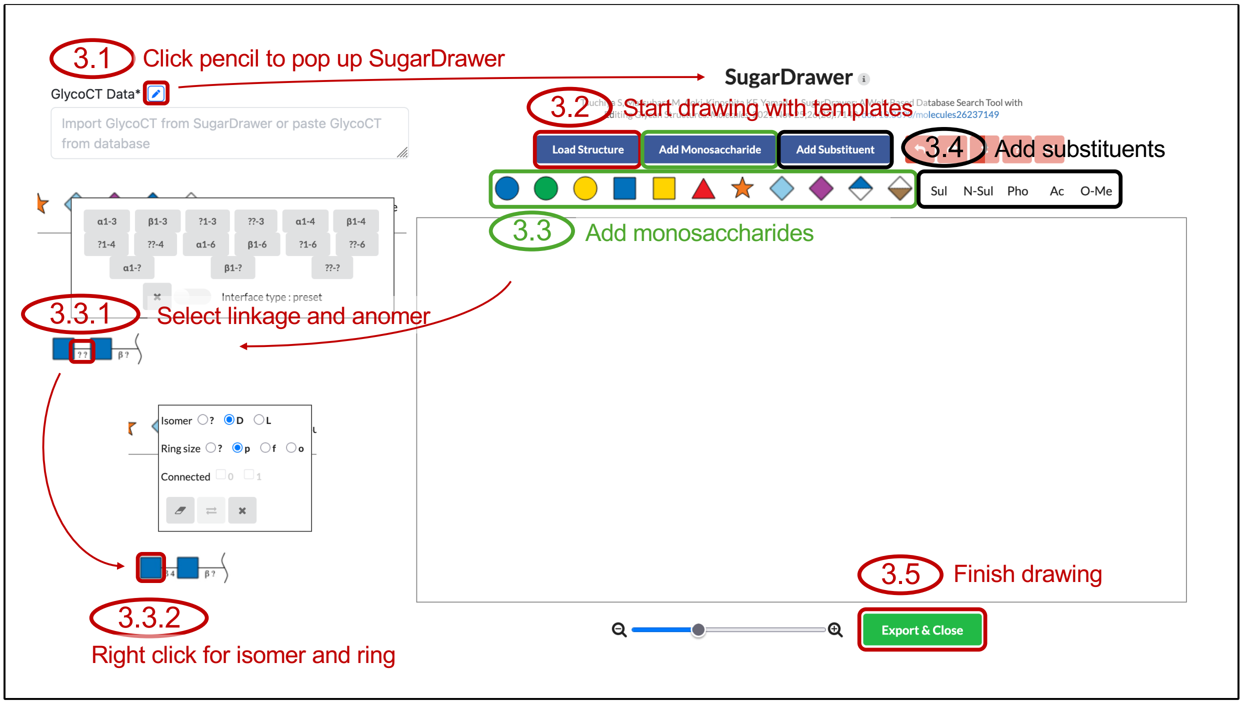
Ready to generate JSON

③ Add glycans from GlycoCT or SugarDrawer

④ Import GlyTouCan and GlyGen ID

⑤ Download JSON file

3. Paste in GlycoCT ID from your favorite glycoinformatics database or click the pencil icon to pop up SugarDrawer to draw glycans. Please see the following pages for more details.
4. Click the button to to look up glycan structures in GlyTouCan and GlyGen databases to import the corresponding glycan ID into the JSON file. The ID will be attached into the corresponding description field.
5. Click the button to download the whole JSON file.


3.1 Click pencil to pop up SugarDrawer

3.2 Start drawing with templates

3.3 Add monosaccharides

3.3.1 Select linkage and anomer

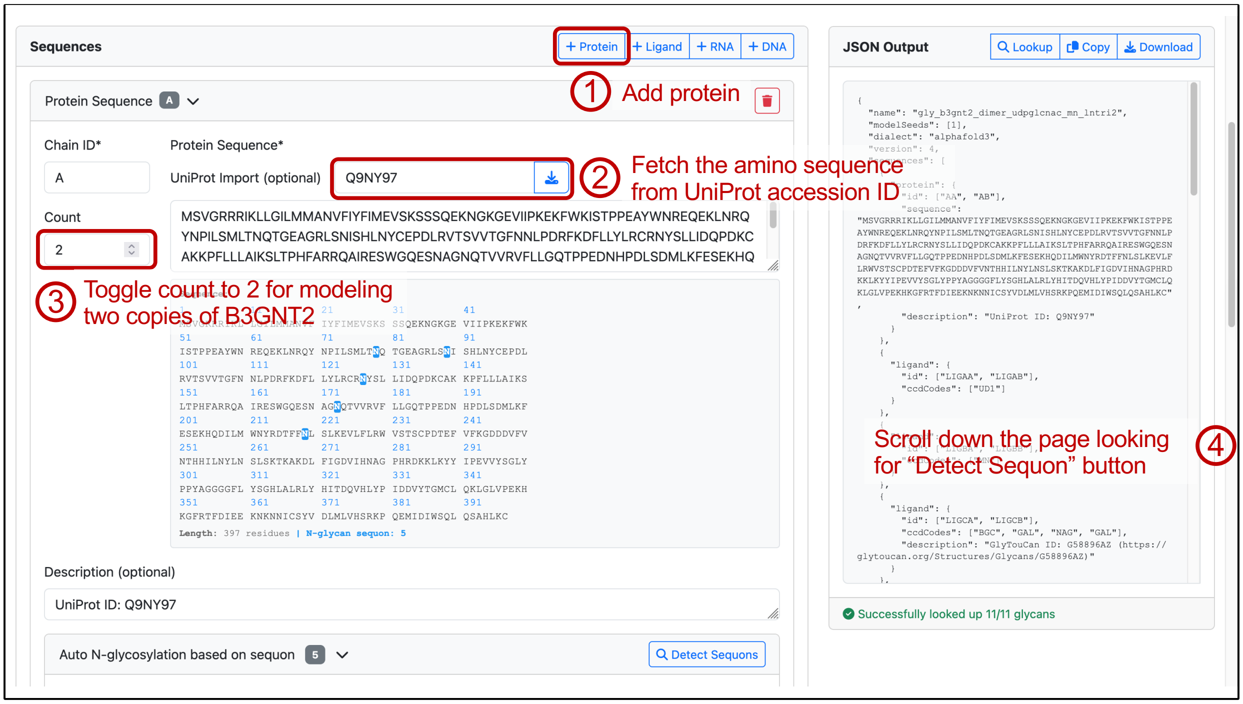
3.3.2 Right click for isomer and ring

3.4 Add substituents

3.5 Finish drawing

3.1. Click the pencil icon to pop up SugarDrawer.
3.2. In the SugarDrawer, there are pre-built glycan templates that users can load them to start the glycan drawing process.
3.3. Click the monosaccharides in the shortcut menu bar above to extend the glycan structure. If the monosaccharides are not in the shortcut, click the "Add Monosaccharide" button to expand the monosaccharide table.
3.3.1. Click the linkage line at the reducing end or between monosaccharides to pop up the anomer/linkage selection panel. Anomer and linkages must be defined to properly export the glycan bondedAtomPairs.
3.3.2. Right click the monosaccharide to pop up the isomer panel if users are using rare monosaccharides.
3.4. Sul (sulfation), N-Sul (N-sulfation), Pho (phosphorylation), Ac (acetylation) and O-Me (methylation) are the substituents that are supported for bondedAtomPairs generation.
3.5. Click the button to export GlycoCT. The glycan bondedAtomPairs will be converted automatically.

Example of building B3GNT2 homodimer-Mn^{2+}-UDP-GlcNAc-LNnT complex



① Add protein

② Fetch the amino sequence from UniProt accession ID

③ Toggle count to 2 for modeling two copies of B3GNT2

④ Scroll down the page looking for “Detect Sequon” button

Chain ID*: A

Count: 2

Protein Sequence*

UniProt Import (optional): Q9NY97

```
MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPEAYWNREQEKLNRQ
YNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLPDRFKDFLLYLRCRNYSLLIDQPDKC
AKKPFLLLAIKSLTPHFARRQAIRESWGQESNAGNQTVVRVFLLGQTPPEDNHPDLSDMLKFESEKHQ
```

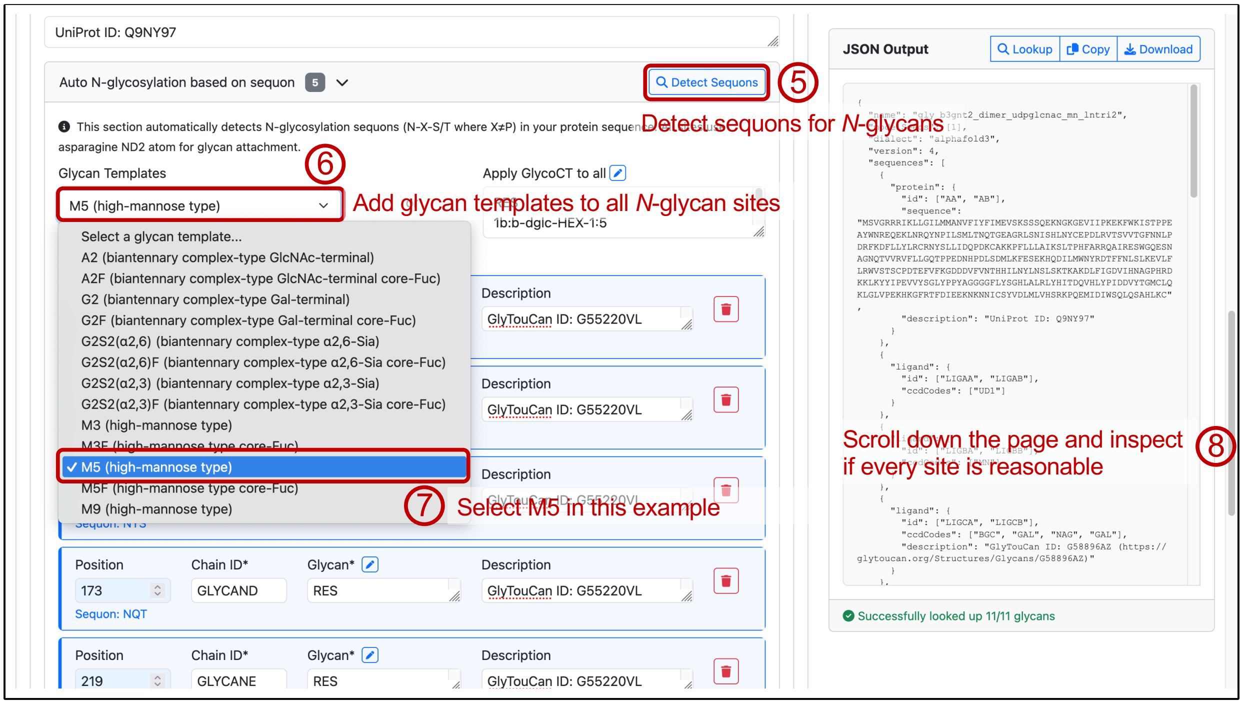
```
Sequence:
1          11         21         31         41
MSVGRRRIKL LGILMMANVF IYFIMEVSKS SSQEKNGKGE VIIPKEKFWK
51         61         71         81         91
ISTPPEAYWN REQEKLNRQY NPILSMLTNQ TGEAGRLSNI SHLNYCEPDL
101        111        121        131        141
RVTSVVTGFN NLPDRFKDFL LYLRCRNYSL LIDQPDKCAK KPFLLLAIKS
151        161        171        181        191
LTPHFARRQA IRESWGQESN AGNQTVVRVF LLGQTPPEDN HPDLSDMLKF
201        211        221        231        241
ESEKHQDILM WNYRDTFFNL SLKEVLFLRW VSTSCPDTEF VFKGDDDVFV
251        261        271        281        291
NTHHILNYLN SLSKTKAKDL FIGDVIHNAG PHRDKKLKYY IPEVVYSGLY
301        311        321        331        341
PPYAGGGGFL YSGHLALRLY HITDQVHLYP IDDVYTGMCL QKLGLVPEKH
351        361        371        381        391
KGFRTFDIEE KNKNNICSYV DLMLVHSRKP QEMIDIWSQL QSAHLKC
Length: 397 residues | N-glycan sequon: 5
```

Description (optional): UniProt ID: Q9NY97

Auto N-glycosylation based on sequon 5

```
{
  "name": "gly_b3gnt2_dimer_udpglcnac_mn_lntri2",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPE
AYWNREQEKLNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLP
DRFKDFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESN
AGNQTVVRVFLLGQTPPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLF
LRWVSTSCPDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRD
KKLKYYIPEVVYSGLYPPYAGGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQ
KLGLVPEKHKGFRTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC"
,
        "description": "UniProt ID: Q9NY97"
      }
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccdCodes": ["UD1"]
      }
    },
    {
      "ligand": {
        "id": ["LIGBA", "LIGBB"],
        "ccdCodes": ["MN"]
      }
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccdCodes": ["BGC", "GAL", "NAG", "GAL"],
        "description": "GlyTouCan ID: G58896AZ (https://
glytoucan.org/Structures/Glycans/G58896AZ)"
      }
    },
```

✓ Successfully looked up 11/11 glycans



UniProt ID: Q9NY97

This section automatically detects N-glycosylation sequons (N-X-S/T where X≠P) in your protein seque… asparagine ND2 atom for glycan attachment.

Glycan Templates: M5 (high-mannose type)

Apply GlycoCT to all: RES 1b:b-dglc-HEX-1:5

Description: GlyTouCan ID: G55220VL

Description: GlyTouCan ID: G55220VL

Description: GlyTouCan ID: G55220VL

Sequon: NYS

Position: 173 Chain ID*: GLYCAND Glycan*: RES Description: GlyTouCan ID: G55220VL

Sequon: NQT

Position: 219 Chain ID*: GLYCANE Glycan*: RES Description: GlyTouCan ID: G55220VL

```
{
  "name": "gly_b3gnt2_dimer_udpglcnac_mn_lntri2",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPE
AYWNREQEKLNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLP
DRFKDFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESN
AGNQTVVRVFLLGQTPPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLF
LRWVSTSCPDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRD
KKLKYYIPEVVYSGLYPPYAGGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQ
KLGLVPEKHKGFRTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC"
,
        "description": "UniProt ID: Q9NY97"
      }
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccdCodes": ["UD1"]
      }
    },
    {
      "ligand": {
        "id": ["LIGBA", "LIGBB"],
        "ccdCodes": ["MN"]
      }
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccdCodes": ["BGC", "GAL", "NAG", "GAL"],
        "description": "GlyTouCan ID: G58896AZ (https://
glytoucan.org/Structures/Glycans/G58896AZ)"
      }
    },
```

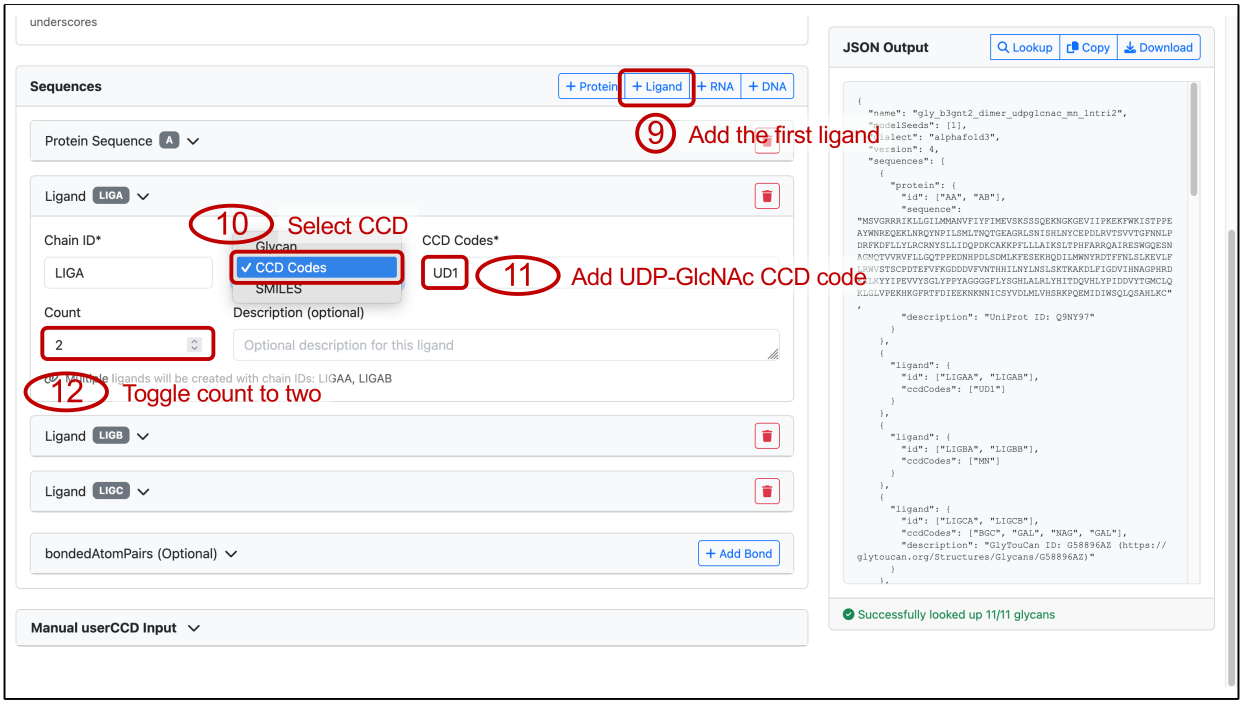
Successfully looked up 11/11 glycans

⑤ Detect sequons for *N*-glycans

⑥ Add glycan templates to all *N*-glycan sites

⑦ Select M5 in this example

⑧ Scroll down the page and inspect if every site is reasonable



9 Add the first ligand

10 Select CCD

11 Add UDP-GlcNAc CCD code

12 Toggle count to two

Chain ID*: LIGA

✓ CCD Codes

CCD Codes*: UD1

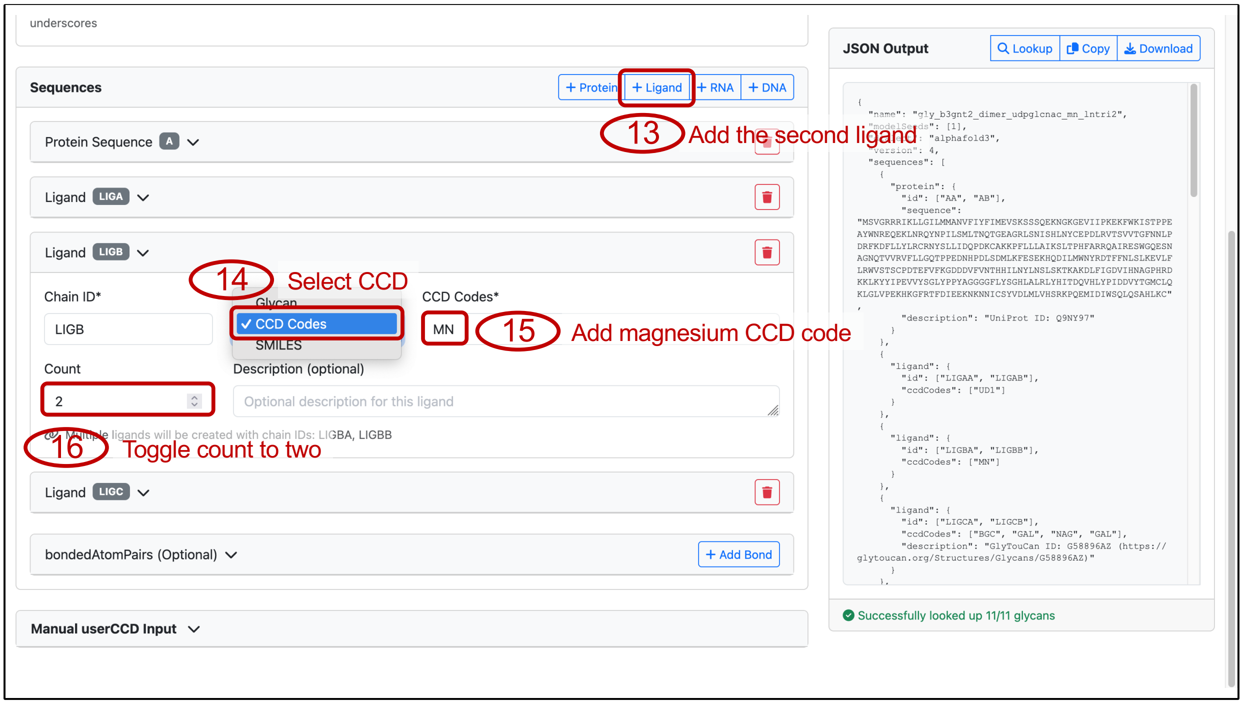
Count: 2

Description (optional)

Multiple ligands will be created with chain IDs: LIGAA, LIGAB

```
{
  "name": "gly_b3gnt2_dimer_udpglcnac_mn_lntri2",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPE
AYWNREQEKLNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLP
DRFKDFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESN
AGNQTVVRVFLLGQTPPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLF
LRWVSTSCPDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRD
KKLKYYIPEVVYSGLYPPYAGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQ
KLGLVPEKHKGFRTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC"
,
        "description": "UniProt ID: Q9NY97"
      }
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccdCodes": ["UD1"]
      }
    },
    {
      "ligand": {
        "id": ["LIGBA", "LIGBB"],
        "ccdCodes": ["MN"]
      }
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccdCodes": ["BGC", "GAL", "NAG", "GAL"],
        "description": "GlyTouCan ID: G58896AZ (https://
glytoucan.org/Structures/Glycans/G58896AZ)"
      }
    },
```

Successfully looked up 11/11 glycans



13 Add the second ligand

14 Select CCD

15 Add magnesium CCD code

16 Toggle count to two

Chain ID*: LIGB

CCD Codes*: MN

Count: 2

Description (optional): Optional description for this ligand

Multiple ligands will be created with chain IDs: LIGBA, LIGBB

```
{
  "name": "gly_b3gnt2_dimer_udpglcnac_mn_lntri2",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPE
AYWNREQEKLNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLP
DRFKDFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESN
AGNQTVVRVFLLGQTPPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLF
LRWVSTSCPDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRD
KKLKYYIPEVVYSGLYPPYAGGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQ
KLGLVPEKHKGFRTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC"
,
        "description": "UniProt ID: Q9NY97"
      }
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccdCodes": ["UD1"]
      }
    },
    {
      "ligand": {
        "id": ["LIGBA", "LIGBB"],
        "ccdCodes": ["MN"]
      }
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccdCodes": ["BGC", "GAL", "NAG", "GAL"],
        "description": "GlyTouCan ID: G58896AZ (https://
glytoucan.org/Structures/Glycans/G58896AZ)"
      }
    },
```

Successfully looked up 11/11 glycans

Chain ID*: LIGC

Input Type: Glycan

GlycoCT Data*:

```
RES
1b:b-dglc-HEX-1:5
```

Count: 2

Description (optional): GlyTouCan ID: G58896AZ (https://glytoucan.org/Structures/Glycans/G58896AZ)

Multiple ligands will be created with chain IDs: LIGCA, LIGCB

```
{
  "name": "gly_b3gnt2_dimer_udpglcnac_mn_lntri2",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence":
"MSVGRRRIKLLGILMMANVFIYFIMEVSKSSSQEKNGKGEVIIPKEKFWKISTPPE
AYWNREQEKLNRQYNPILSMLTNQTGNAGRLSNISHLNYCEPDLRVTSVVTGFNNLP
DRFKDFLLYLRCRNYSLLIDQPDKCAKKPFLLLAIKSLTPHFARRQAIRESWGQESN
AGNQTVVRVFLLGQTPPEDNHPDLSDMLKFESEKHQDILMWNYRDTFFNLSLKEVLF
LRWVSTSCPDTEFVFKGDDDVFVNTHHILNYLNSLSKTKAKDLFIGDVIHNAGPHRD
KKLKYYIPEVVYSGLYPPYAGGGGFLYSGHLALRLYHITDQVHLYPIDDVYTGMCLQ
KLGLVPEKHKGFRTFDIEEKNKNNICSYVDLMLVHSRKPQEMIDIWSQLQSAHLKC"
,
        "description": "UniProt ID: Q9NY97"
      }
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccdCodes": ["UD1"]
      }
    },
    {
      "ligand": {
        "id": ["LIGBA", "LIGBB"],
        "ccdCodes": ["MN"]
      }
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccdCodes": ["BGC", "GAL", "NAG", "GAL"],
        "description": "GlyTouCan ID: G58896AZ (https://
glytoucan.org/Structures/Glycans/G58896AZ)"
      }
    },
```

Successfully looked up 11/11 glycans

17 Add the third ligand

18 Paste the LNnT GlycoCT or draw from SugarDrawer by clicking the pencil icon

19 Toggle count to two

20 Look up GlyTouCan and GlyGen ID by clicking “Lookup” button

21 Download JSON file