



Quantum-Aided Drug Design from POLARIS^{qb}

Launching a new job on QuADD
07/08/2025



Quantum Execution Controls

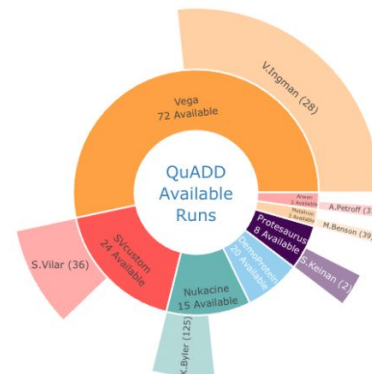
[Start New Job](#)[View Job Output](#)[View Dashboard](#)

Recent Runs

User & Project

A.Petroff - Arwen_37	Arwen_37	Fragment Library Generation	Quantum Annealing	Calculating Properties	Filtering	Ligand Geometry in Pocket
A.Petroff - Arwen_36	Arwen_36	Fragment Library Generation	Quantum Annealing	Calculating Properties	Filtering	Ligand Geometry in Pocket
A.Petroff - Arwen_35	Arwen_35	Fragment Library Generation	Quantum Annealing	Calculating Properties	Filtering	Ligand Geometry in Pocket
A.Petroff - Arwen_34	Arwen_34	Fragment Library Generation	Quantum Annealing	Calculating Properties	Filtering	Ligand Geometry in Pocket
A.Petroff - Arwen_33	Arwen_33	Fragment Library Generation	Quantum Annealing	Calculating Properties	Filtering	Ligand Geometry in Pocket

Available Runs



Run Details

[Next](#)

Arwen_37

1x7O_FIC T20240429220058 (Sub#22)

Fragment Library: Finished (1)

Quantum: Finished (18)

Arwen_36

1x7O_FIC T20240429220058 (Sub#22)

Fragment Library: Finished (1)

Quantum: Finished (18)

Arwen_35

1x7O_FIC T20240429220058 (Sub#22)

Fragment Library: Finished (1)

Quantum: Finished (22)

Finished Runs

Download	Project	Runs	Generated Molecules	Submission	User
	Vega	Vega_8	1237	7	V.Ingman
	Metatron	Metatron_32	40681	5	M.Benson

- Click the "Start New Job" button to begin your submission

Quantum

Execution Controls

Start New Job

View Job Output

View Dashboard

User Name

jchapman@polarisqb.com

Project Name

Quadd QA BETA - WJS

Belatrix

Run Description

Beta Protein Pose 2



Protein-Ligand PDB

Choose File

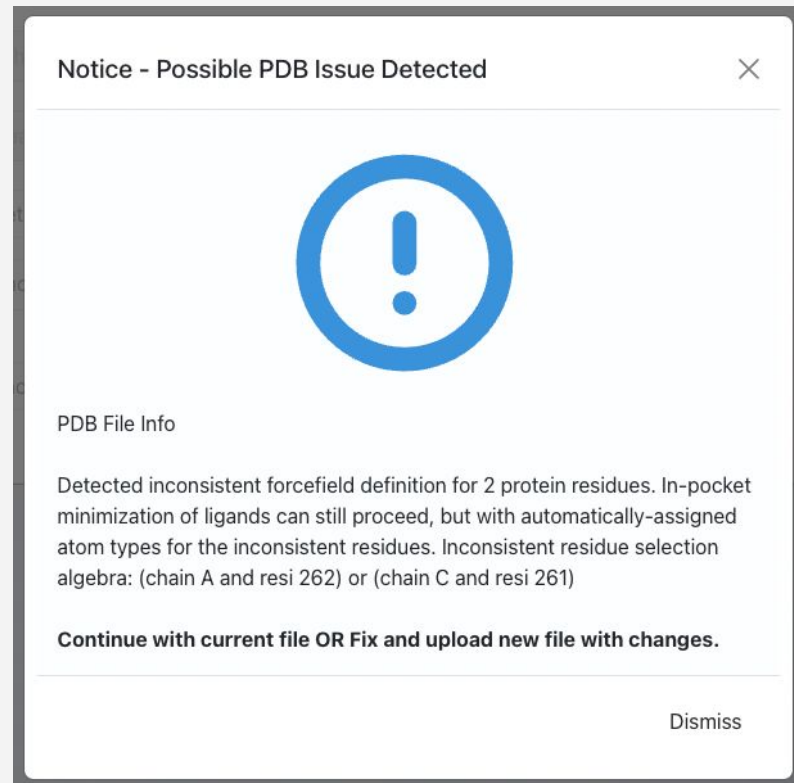
6chh.pdb

Upload



- Select your account under “Project Name”
- Enter a description for the run
- Use the "Choose File" dialog to select a Protein-Ligand complex PDB from your computer
- Click the "Upload" button
- QuADD will attempt to fix any detected issues with your input PDB, but using a PDB that has already been cleaned and protonated is preferred. It is also suggested to trim any unneeded chains prior to upload.

- In the input uploading process QuADD checks the input in a variety of ways
- One common occurrence is shown in this **Alert Box**
- This alert describes what was detected and provides references to the residues in PyMOL selection syntax
- Alternative you may see a message indicating the input was not able to be processed (**PDB Cleaning Failed**), please contact help@quadd.bio for more assistance



Quantum

Execution Controls

Start New Job

View Job Output

View Dashboard

User Name

S.Keinan

Project Name

NNMT - Quadd Analysis

Run Description

Example Run

Protein-Ligand PDB

Choose File 6chh.pdb

Upload

File Molecules

Choose Molecule to Fragment

Choose Molecule to Fragment

FOP_A_301

EDO_B_301

EDO_B_302

FOP_B_303

FOP_C_301

FOP_D_301

Submit

- Your PDB will be searched for small molecules
- Choose the ligand of interest from the dropdown menu
- The ligand names are built from the residue name, chain ID, and residue ID, as found in the PDB
- You will have the option to select another ligand on the next page

User Name

Project Name

Run Description

Protein-Ligand PDB

File Molecules

Objectives
☒ Standard ☐ Best In Class ☐ First In Class

Fragment Library
☒ Drug Space ☐ Drug-Like Space ☐ Combined Space

Fragmentation Options

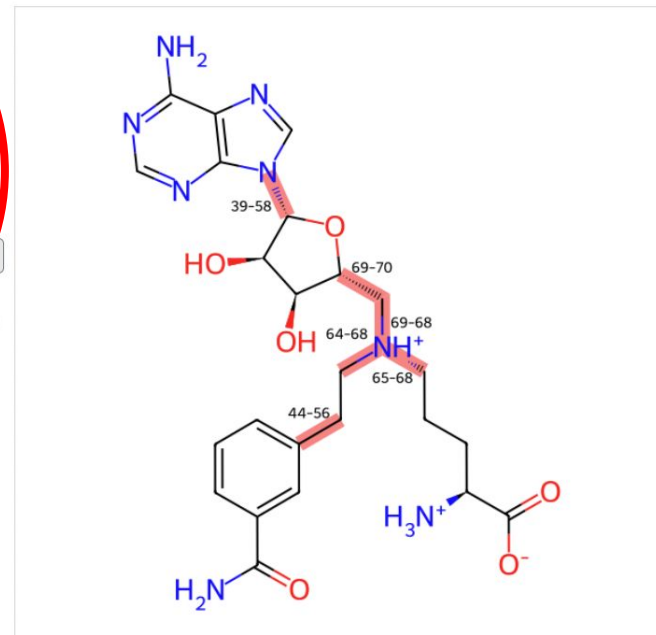
Select Scissile Bonds

- ☐ 39-58
- ☐ 44-56
- ☐ 64-68
- ☐ 65-68
- ☐ 69-68
- ☐ 69-70

Fragment Molecule

Minimum Heavy Atom Count

4



- Here you may choose your objectives, which fragment library to use, and various parameters for the fragmentation
- The highlighted bonds illustrate where the molecule may be split
- Some bonds may go unused depending on your fragmentation parameter selections (eg: the minimum heavy atom count can only be satisfied by excluding certain bonds)

- **Standard:** Balance between diversity and similarity
- **Best In Class:**
 - Fragments will be chosen based on the starting ligand
 - Great for exploring similar binding modes, while still having good diversity
- **First In Class:**
 - Fragments will be chosen based on the starting ligand and the protein pocket
 - Good for exploring new binding modes
- **Scaffold Hopping:** Option to hold certain template fragments constant

Quantum Execution Controls

User Name

Project Name

Run Description ?

Protein-Ligand PDB

File Molecules ?

Objectives

☒ Standard
 ☐ Best In Class
 ☐ First In Class

Fragment Library

☒ Drug Space
 ☐ Drug-Like Space
 ☐ Combined Space

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- ~~**Scaffold Hopping:** Option to hold certain template fragments constant~~

Quantum Execution Controls

User Name

Project Name

Quadd Project NNMT2

Run Description

?

Protein-Ligand PDB

File Molecules

▼
?

Objectives

☒ Standard
 ☐ Best In Class
 ☐ First In Class

Fragment Library

☒ Drug Space
 ☐ Drug-Like Space
 ☐ Combined Space

- **Minimum Heavy Atom Count**
 - Controls the size of fragments in accepted schemes
 - No smaller than 2 is advised
 - Between 2 and 4 is a good starting point
- **Minimum Number of Schemes**
 - If the number of schemes generated is less than this value, the Target Number of R Groups will be altered until enough schemes are produced
- **Target Number of R Groups**
 - The number of binding pocket sub-regions to consider in each scheme
 - Between 3 and 6 is a good starting point
 - It may be impossible to hit this number depending on the Minimum Heavy Atom Count chosen

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Q

Start New Job

View Job Output

View Dashboard

Heavy Atom Count

6

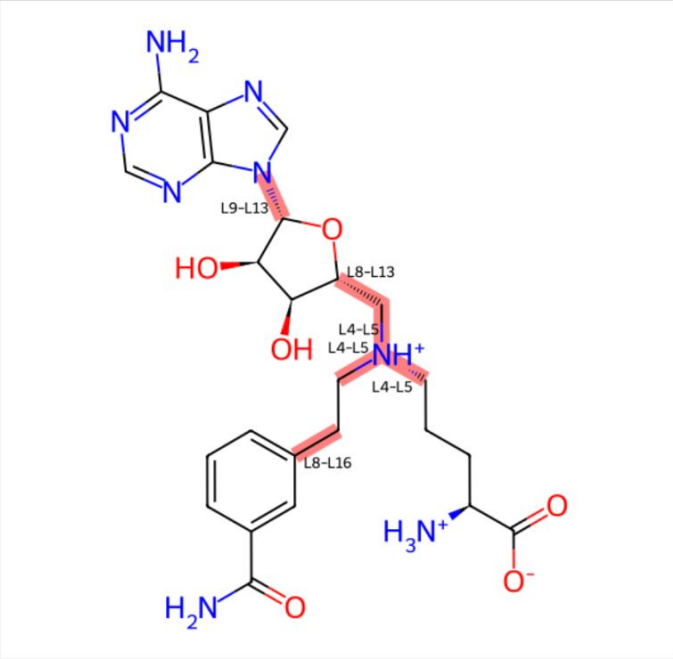
Minimum Number of Fragmentation Schemes

1

Target Number of R Groups

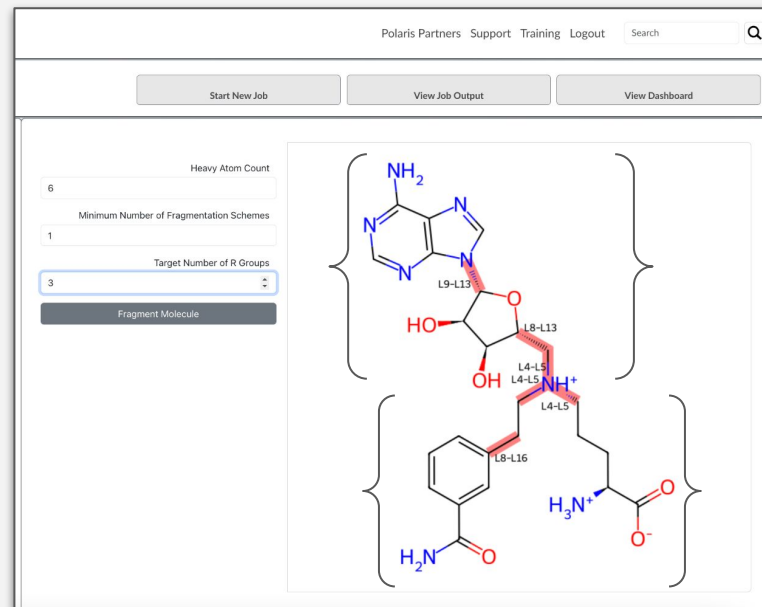
3

Fragment Molecule



Choosing Fragmentation Schemes

Using a variety of fragmentation schemes for a given template molecule gives QuADD the best opportunity to return novel chemistry. Where the template structure follows a simple A+B+C construction of fragments, QuADD will return structures according to this paradigm. Where combinations of fragments are sought, *e.g.* (A+B)+C or A+(B+C), the fragmentation scheme manager allows for this level of detail in constructing QuADD molecules. And where a more complete scan of chemical space is desired, using several combinations of fragment schemes is suggested (≤ 10).



Quantum Execution Controls

Start New Job

View Job Output

View Dashboard

User Name

Project Name

Run Description ?

Protein-Ligand PDB Upload

File Molecules ?

Objectives

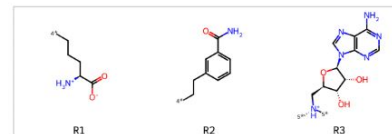
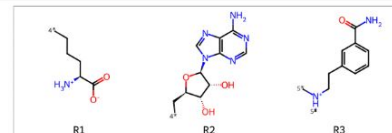
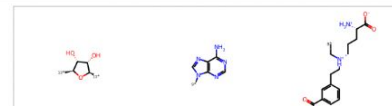
☒ Standard ☐ Best In Class ☐ First In Class ☐ Scaffold Hopping

Fragment Library

☒ Drug Space ☐ Drug-Like Space ☐ Combined Space

[Back to Fragment Options](#)

Select Desired Fragmentation Schemes

☐ 6_1_3_0☐ 6_1_3_1☐ 6_1_3_10☐ 6_1_3_11

- If you need to change your fragmentation parameters, click Back to Fragment Options in the top right corner
- Fragmentation schemes are presented in QuADD's estimated best priority order

Quantum
Execution Controls

Start New Job

View Job Output

View Dashboard

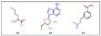
User Name Project Name Run Description ?Protein-Ligand PDB UploadFile Molecules ?

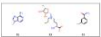
Objectives

☒ Standard ☐ Best In Class ☐ First In Class ☐ Scaffold Hopping

Fragment Library

☒ Drug Space ☐ Drug-Like Space ☐ Combined Space

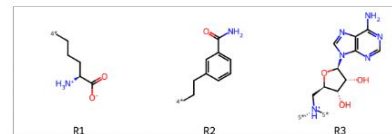
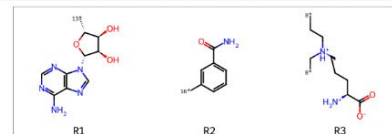
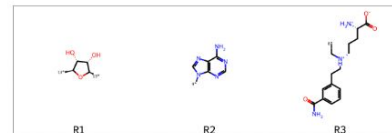
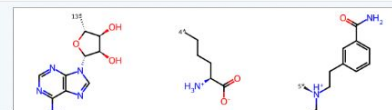
☐ 6_1_3_1 

☒ 6_1_3_12 

Submit

[Back to Fragment Options](#)

Select Desired Fragmentation Schemes

☐ 6_1_3_0☐ 6_1_3_10☐ 6_1_3_11☐ 6_1_3_2

- Review and select from the generated fragmentation schemes
- Your schemes chosen for submission will be visible on the left



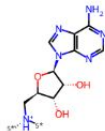
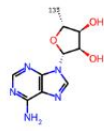

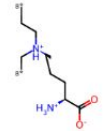


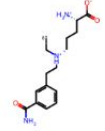
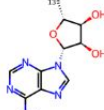

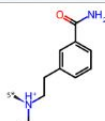
- You will be able to explore more chemical space by selecting different fragmentation schemes
- Tips for good scheme selection:
 - Varying the number of R Groups
 - Varying the number of connection points (noted with a "**") on analogous fragments
 - Functional moieties "moving" from one fragment to another or splitting alkyl chains at a different positions

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Training
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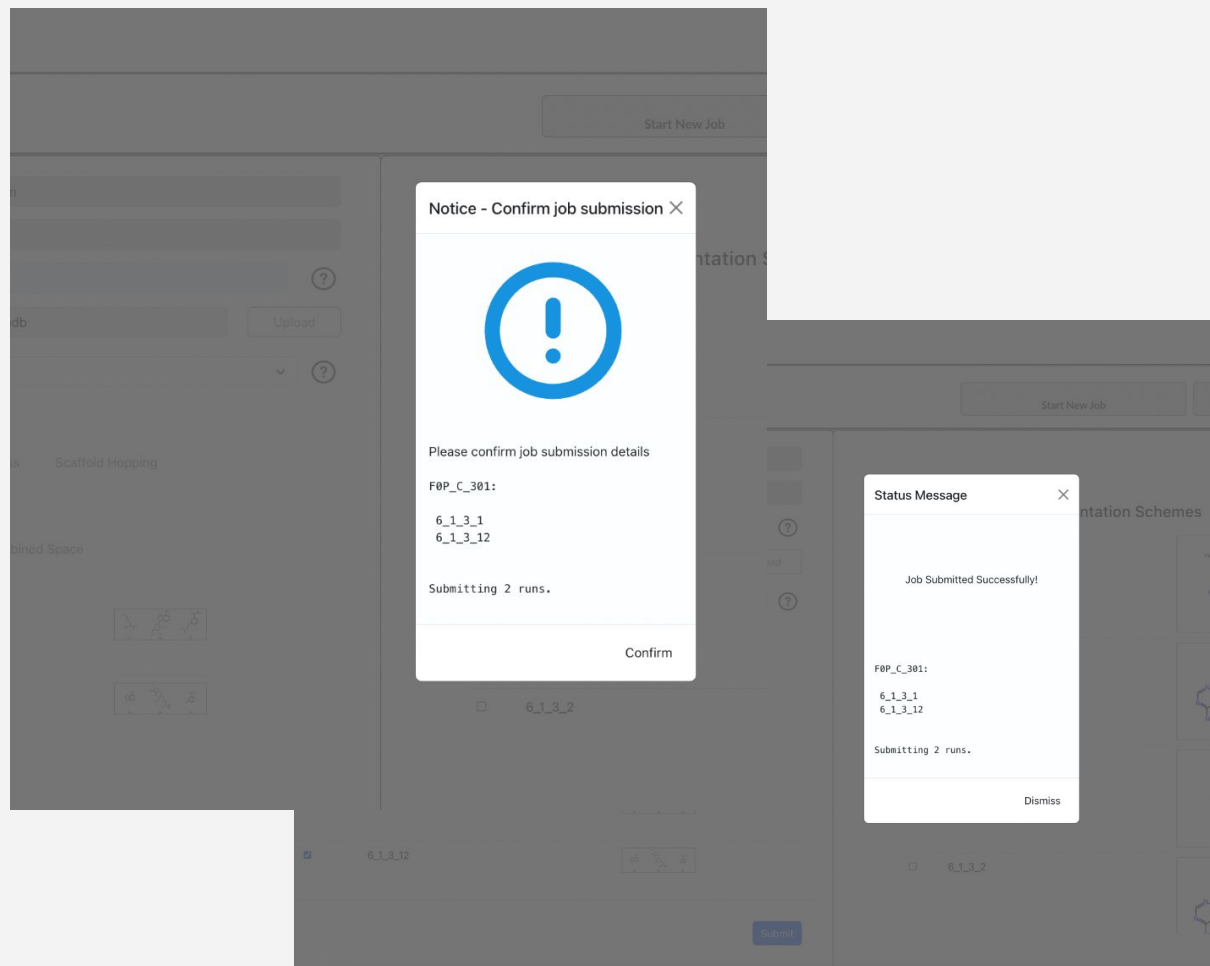
Start New Job
View Job Output
View Dashboard

Back to Fragment Options

Select Desired Fragmentation Schemes

<input type="checkbox"/> 6_1_3_0	 R1	 R2	 R3
<input type="checkbox"/> 6_1_3_10	 R1	 R2	 R3
<input type="checkbox"/> 6_1_3_11	 R1	 R2	 R3
<input type="checkbox"/> 6_1_3_2	 R1	 R2	 R3

- Clicking the "Submit" button
- Confirm your selection
- You will be notified on successful submission
- Each fragmentation scheme is a separate run





Quantum Execution Controls

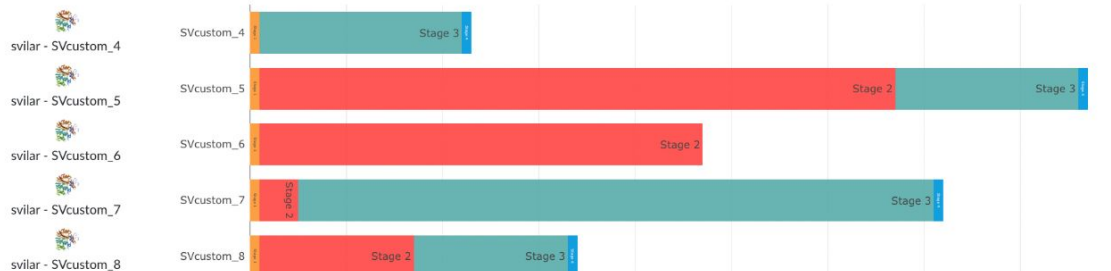
Start New Job

View Job Output

View Dashboard

Current Runs

User / Project



Available Runs



Run Details

Load More

Finished Runs

Protesaurus_1

(2) NNMT - SK test run...

Stage 1: enqueue 1

Stage 4: waiting 1

Protesaurus_2

(2) NNMT - SK test run...

Stage 1: enqueue 1

Stage 4: waiting 1

NNMT_205

(1) 7f58-melatonin-10f-st...

Stage 1: finish 1

Stage 2: finish 28

Stage 3: enqueue 28

User	Project	Submission	Runs	Generated Molecule Count	Download
svilar	SVcustom	2	SVcustom_1, SVcustom_2, SVcustom_3, SVcustom_4, SVcustom_5, SVcustom_6, SVcustom_7, SVcustom_8	7000747	Download
svilar	NNMT	1	NNMT_197, NNMT_198, NNMT_199, NNMT_200, NNMT_201, NNMT_202, NNMT_203, NNMT_204, NNMT_205, NNMT_206	2142502	Download
kbyler	Nukacine	1	Nukacine_3, Nukacine_4	485580	Download

- You can see the submitted runs and follow the runs progress on the Dashboard

Quantum Execution Controls

Start New Job

View Job Output

View Dashboard

Project Protein

NNMT

Job Run

NNMT - 98

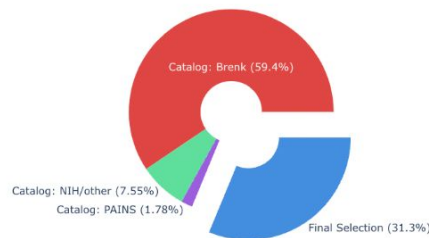
Result Space

Full Molecules

Figure Selection

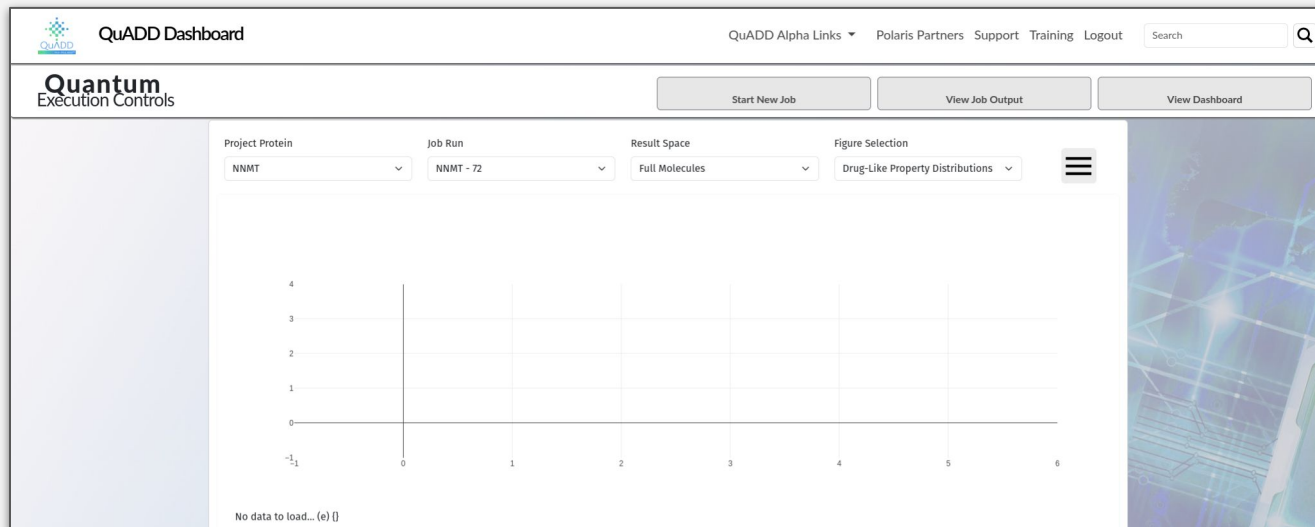
Drug-Like Filter Status

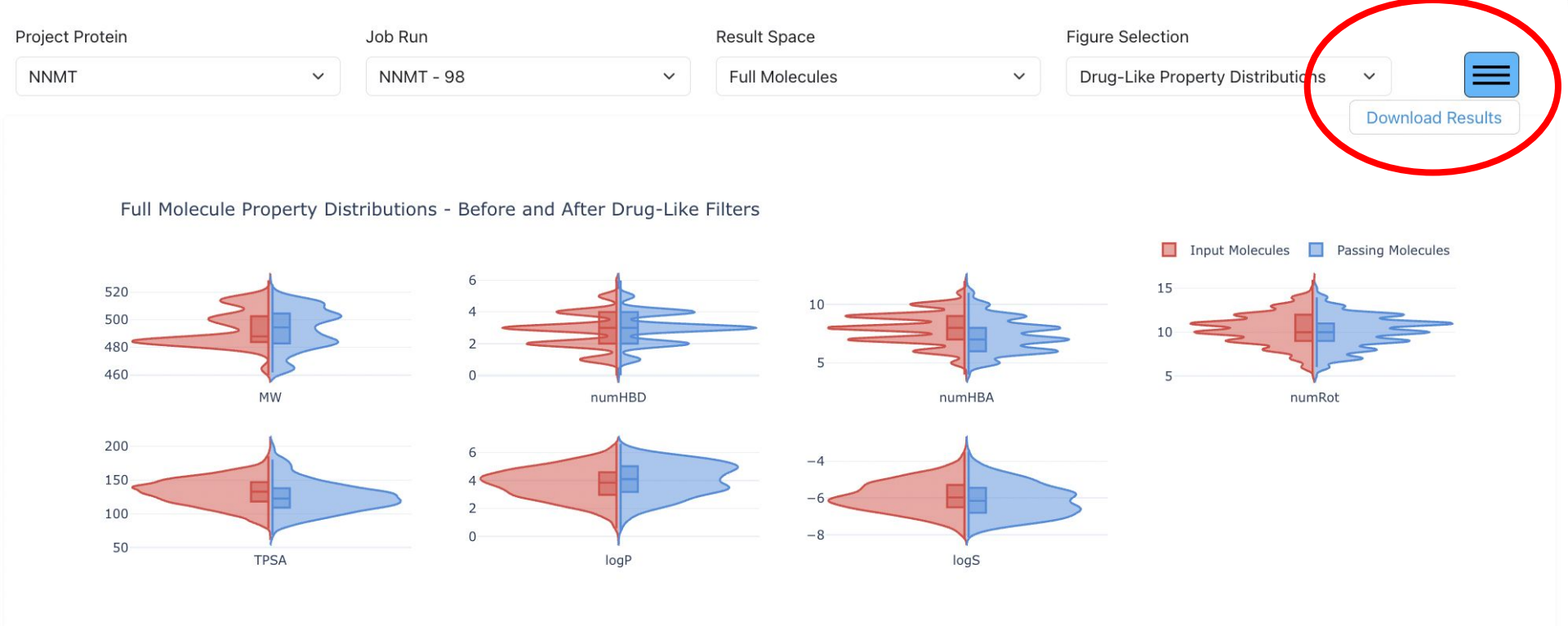
Full Molecule Drug-Like Filter Status Counts



- Use the "View Job Output" button to explore various visualizations for the results of a single fragmentation scheme
- "Full Molecules" Result Space will give you plots relevant to the fully built molecules
- "Fragments" Result Space will provide plots where you can compare the performance of various R-Groups

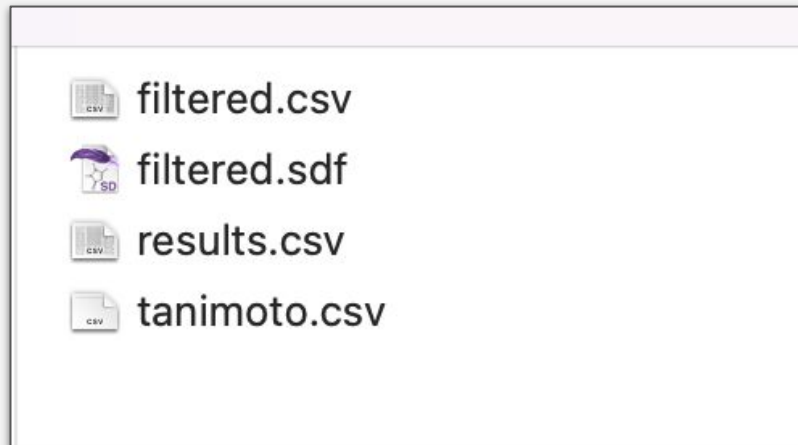
- Some plots may not be available until the run has progressed further
- If you see a blank plot, check back later





- You can download results for individual runs here too

- Downloaded results are in a zip file
- Results contents:
 - SDF with 3D structures of your passing molecules
 - CSVs with molecule smiles and properties, one with all fully-built molecules and one with just the passing molecules
- "Passing" molecules are those within the bounds of the drug-like filters (Rule of 5 properties, unwanted substructures, PAINS, etc.)



Thank You for using QuADD

Please don't hesitate to contact us if you have any questions

help@quadd.bio