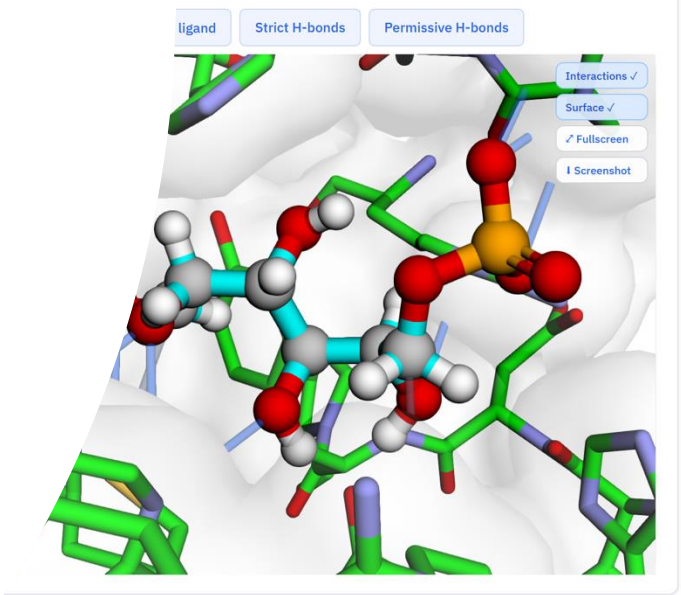
OHD Workshop

"Virtual Screening of OHD Compound Library to Antiparasitic Targets"

13 May 2026 hrs 14-16

- Background of Antiparasitics Target Selection from the aspects of structural biology (Why targets of our database are interesting for Antiparasitics drug design)
- Background of designing OHD-Chemoteque
- The strategy for virtual screening.
- The overview of the analysis of the results.
- System to present the data.



The OHD:LUB Project: Implementation Workflow

The OHD:LUB project represents the Action's proactive "success story," demonstrating how interdisciplinary collaboration can accelerate drug discovery under budget constraints.

Phase I: High-Standard Virtual Screening

Črtomir Podlipnik and Marko Jukić reported on the computational campaign executed on the **Vega HPC system**(10 petaflops):

Library Size: 36,000+ compounds (In-house + Commercial diversity sets like GSK Kineto Box).

Computational Status: 21 of 22 targets are fully docked.

Post-Docking Analysis: The team is utilizing a "3D Post Viewer" and interaction fingerprints to harmonize scores and define target-specific cutoffs.

Phase II: The "Eco-Aware" Triage (New Methodology)

A critical innovation discussed was the **Option B Triage**. Rather than filtering for toxicity at the start, machine-learning (ML) ecotoxicity models will be applied *post-docking*. This allows researchers to select hits that are both high-affinity and environmentally benign, creating a "Green Drug Score." This is developed in collaboration with Daniele Aiello.

Experimental Validation Strategy

The virtual shortlists must be validated experimentally before the end of the COST Action (October 2026).

Protein Production: A "call to action" was issued. Labs that proposed targets must verify their capacity to purify proteins immediately. Collaboration with the network's structural biologists (Cecilia, Andrea, Marco Mazzorana) is vital.

Testing Infrastructure: Sheraz Gul (Fraunhofer) confirmed availability for High-Throughput Screening (HTS) and ADMET/Ecotox testing in Hamburg.

Funding for Mobility: Remaining funds are allocated for **Short-Term Scientific Missions (STSMs)**. Young researchers are encouraged to visit host labs (Hamburg, Porto, etc.) to perform the physical assays on the shortlisted compounds.

Report of UL-OHD

OHD1:OHD2 project

Podlipnik, Črtomir, Marko Jukic and Daniele Aiello

Some preliminary overview ....

1.) Targets preparation:

- **Cleaning raw pdb with Schrodinger's PPW**
- **Cavity detection and grid - generation (CMDOCK's CMCAVITY)**
- **22 targets - done**

2.) Ligand preparation:

- **Schrodinger's Ligprep**
- **644 chunks with 50 ligands each**

3.) Docking:

- **CMDOCK – standard protocol**
- **"keep only best scored pose**
- **21 targets – done; 1 on queue**

4.) Analysing the results:

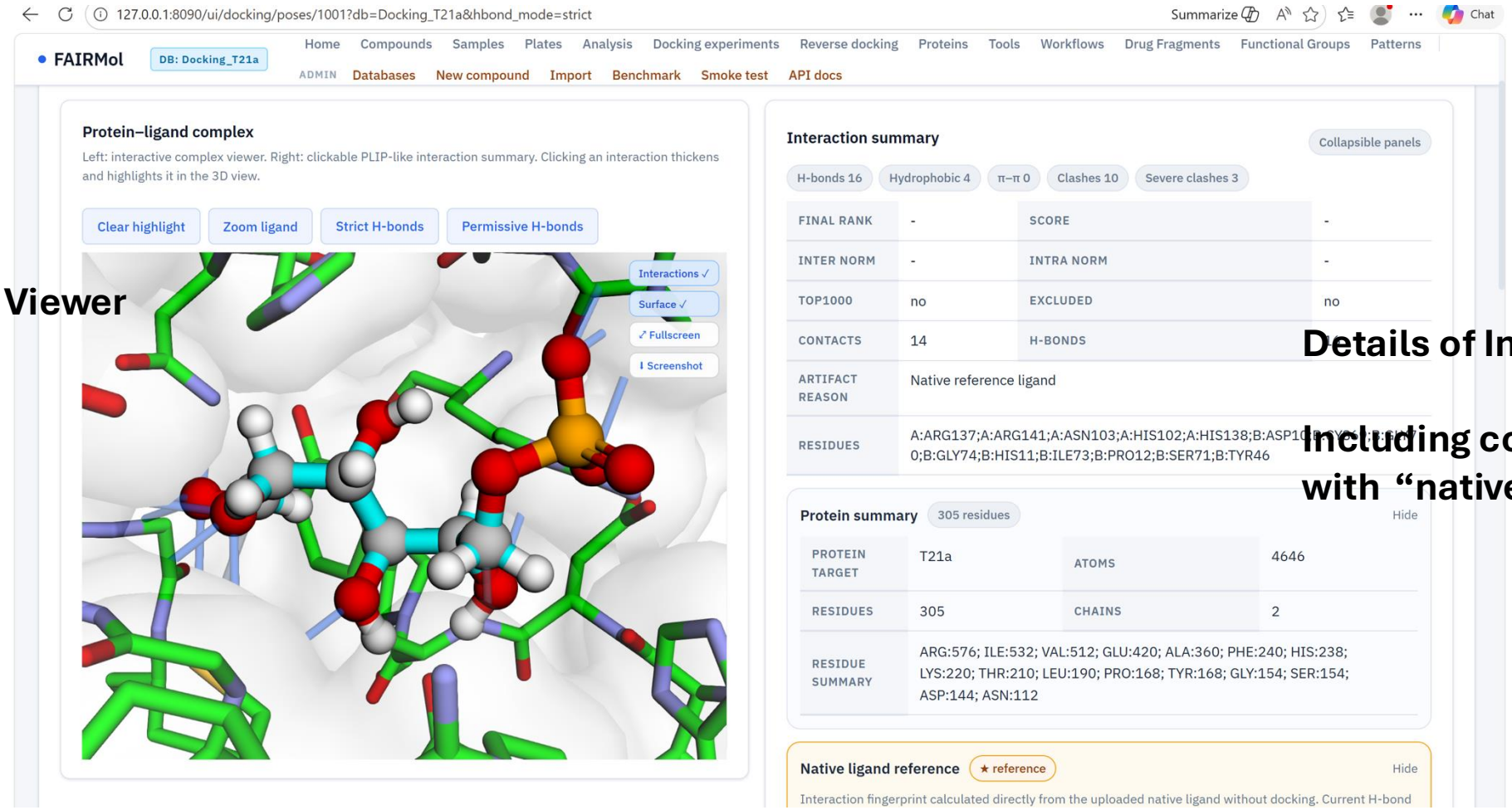
- **Jupyter notebook (to be constructed); Orange Workflow**

5.) Viewer of docked compounds – in progress

FairMol - Docking

Web tool for analysing and databasing – docking results (In development)

3D Pose Viewer



Details of Interaction

Including comparison with “native ligand”

FairMol - Docking

Web tool for analysing and databasing – docking results (In development)

FAIRMol DB: Docking_T21a

Home Compounds Samples Plates Analysis Docking experiments Docking results Reverse docking Proteins Tools Workflows Drug Fragments Functional Groups

Patterns ADMIN Databases New compound Import Benchmark Smoke test API docs

Docking results

Sortable table and score distributions for all docking poses. Select an experiment to filter and compare against the native ligand.

Experiments Reverse docking

DB Docking_T21a

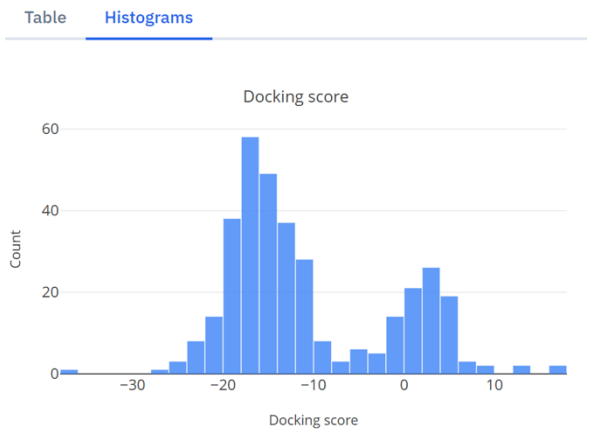
Experiment: T21a · T21a (1001 poses) | Target name: e.g. T21a | Include excluded | Apply | 349 poses | ★ Native available

Table Histograms

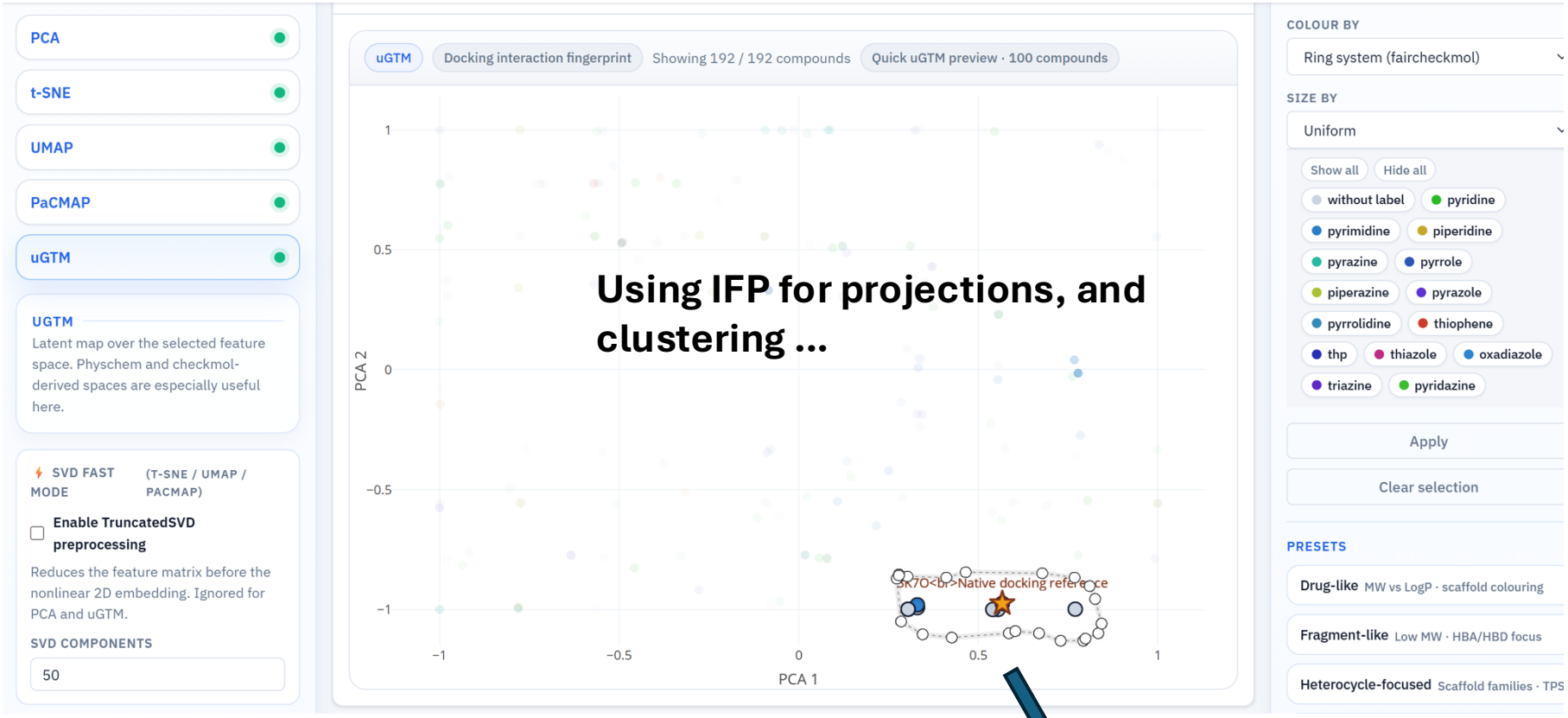
#	COMPOUND	SCORE ▲▲	FINAL RANK	INTER NORM	H-BONDS	CONTACTS	JACCARD	CONTACT RECALL	HB RECALL	HB ROLE RECALL	RMSD	
1	**OHD_Leishmania_216** T21a	-36.976	5.6405	-0.3969	10	15	0.53	0.71	0.33	0.33	-	Open
2	**OHD_Leishmania_19** T21a	-26.593	5.9341	-1.0965	11	19	0.74	1.00	0.50	0.67	-	Open
3	**OHD_Leishmania_193** T21a	-25.992	3.9769	-0.9210	8	16	0.76	0.93	0.42	0.56	-	Open
4	**OHD_Leishmania_346** T21a	-24.500	3.7081	-1.0710	5	18	0.78	[illegible]	[illegible]	[illegible]	-	Open
5	**OHD_Leishmania_110** T21a	-24.008	7.0370	-0.5981	8	16	0.67	0.86	0.33	0.44	-	Open
6	**OHD_Leishmania_97** T21a	-23.812	5.0397	-0.8070	8	19	0.74	1.00	0.58	0.67	-	Open
7	**OHD_Leishmania_363** T21a	-23.720	7.0466	-0.7972	7	14	0.75	0.86	0.25	0.22	-	Open

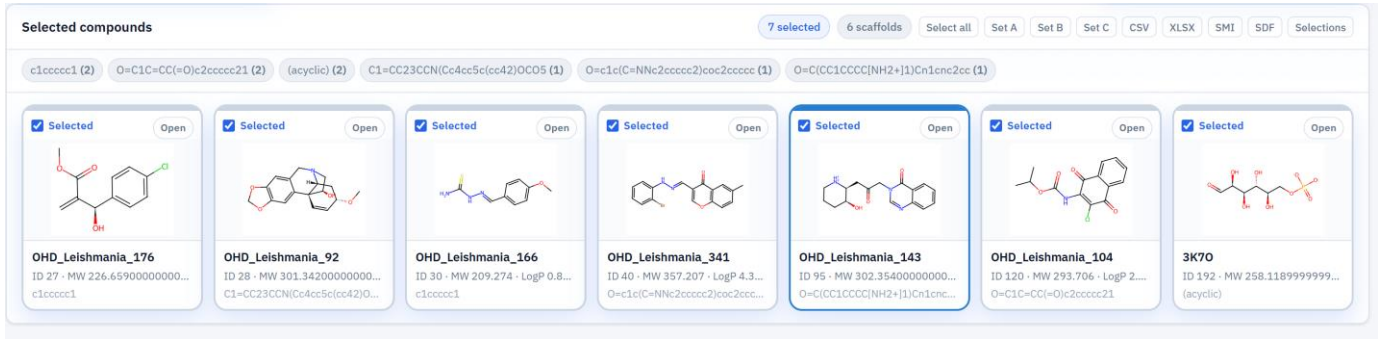
Table with results – sorting by ....

Interactive histograms

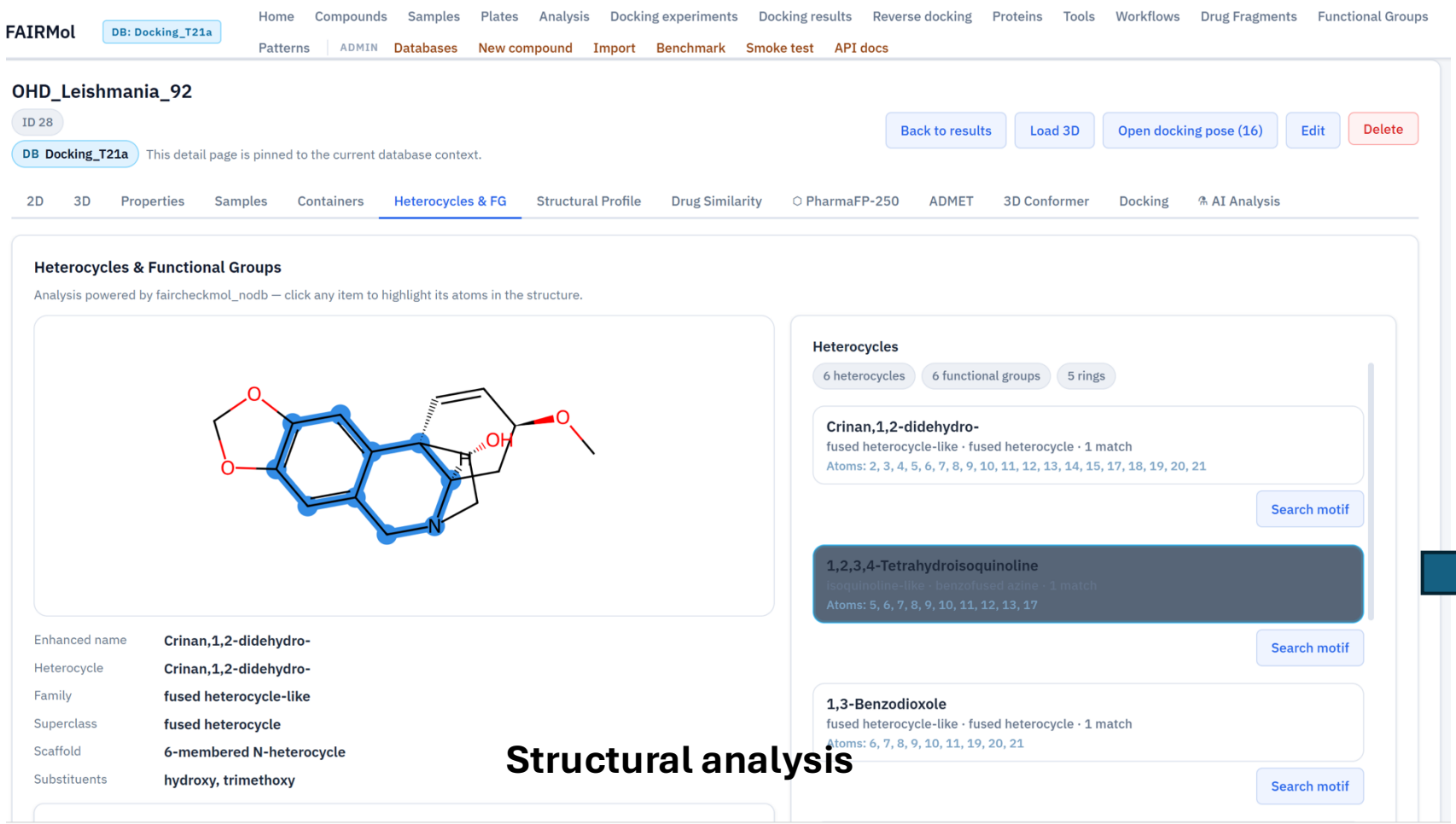


FairMol - Docking



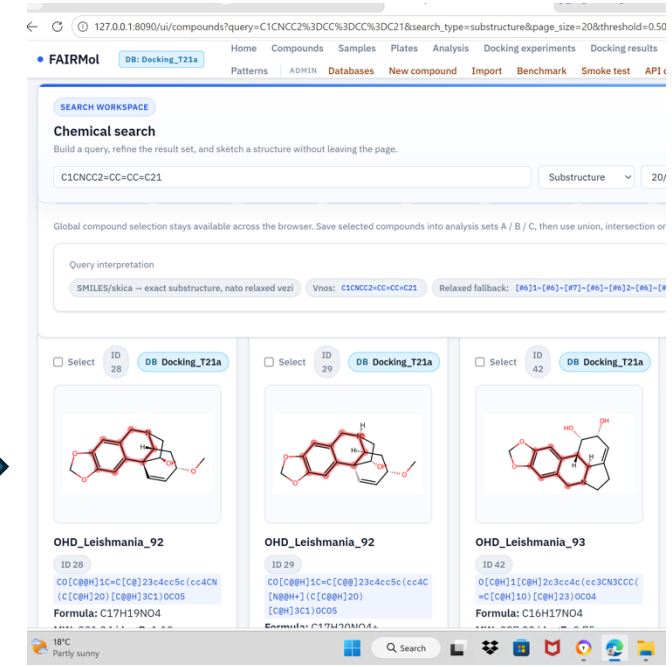


FairMol - Docking



Structural analysis

Substructure search ....



See you virtually

May 13 2026