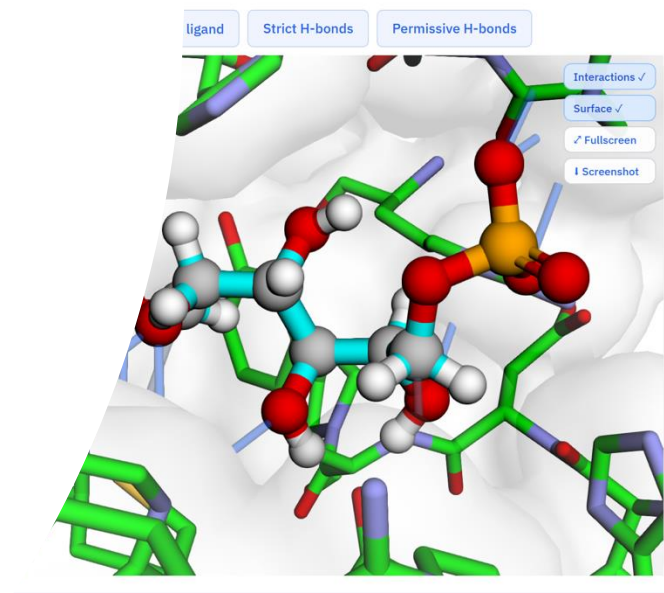


OHD Workshop

“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.



FINAL RANK	-	SCORE	-
INTER NORM	-	INTRA NORM	-
TOP1000	no	EXCLUDED	no
CONTACTS	14	H-BONDS	16
ARTIFACT REASON	Native reference ligand		
RESIDUES	A:ARG137;A:ARG141;A:ASN103;A:HIS102;A:HIS138;B:ASP10;B:CYS69;B:GLY70;B:GLY74;B:HIS11;B:ILE73;B:PRO12;B:SER71;B:TYR46		

Protein summary 305 residues Hide

PROTEIN TARGET	T21a	ATOMS	4646
RESIDUES	305	CHAINS	2
RESIDUE SUMMARY	ARG:576; ILE:532; VAL:512; GLU:420; ALA:360; PHE:240; HIS:238; LYS:220; THR:210; LEU:190; PRO:168; TYR:168; GLY:154; SER:154; ASP:144; ASN:112		

Native ligand reference ★ reference Hide

Interaction fingerprint calculated directly from the uploaded native ligand without docking. Current H-bond mode: strict.

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)

The screenshot displays the FairMol web interface. On the left is the 'Protein-ligand complex' 3D pose viewer, and on the right is the 'Interaction summary' table. The 3D viewer includes controls for 'Clear highlight', 'Zoom ligand', 'Strict H-bonds', and 'Permissive H-bonds'. The interaction summary table provides a detailed comparison of the docked ligand against a native reference ligand, including metrics like H-bonds, hydrophobic interactions, and protein residue counts.

3D Pose Viewer

Details of Interaction

Including comparison with “native ligand”

Interaction summary

H-bonds 16 Hydrophobic 4 $\pi-\pi$ 0 Clashes 10 Severe clashes 3

FINAL RANK	-	SCORE	-
INTER NORM	-	INTRA NORM	-
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Native ligand reference ★ reference Hide

Interaction fingerprint calculated directly from the uploaded native ligand without docking. Current H-bond

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](#)

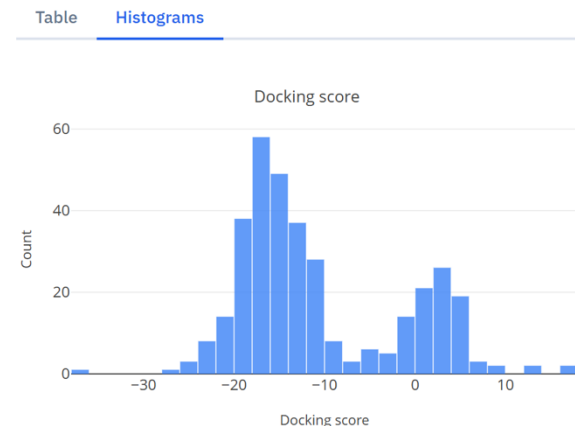
Experiment: Target name: Include excluded [Apply](#) 349 poses ★ Native available

[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	<div><div style="width: 53%;">0.53</div></div>	<div><div style="width: 71%;">0.71</div></div>	<div><div style="width: 33%;">0.33</div></div>	<div><div style="width: 33%;">0.33</div></div>	-	Open
2	OHD_Leishmania_19 T21a	-26.593	5.9341	-1.0965	11	19	<div><div style="width: 74%;">0.74</div></div>	<div><div style="width: 100%;">1.00</div></div>	<div><div style="width: 50%;">0.50</div></div>	<div><div style="width: 67%;">0.67</div></div>	-	Open
3	OHD_Leishmania_193 T21a	-25.992	3.9769	-0.9210	8	16	<div><div style="width: 76%;">0.76</div></div>	<div><div style="width: 93%;">0.93</div></div>	<div><div style="width: 42%;">0.42</div></div>	<div><div style="width: 56%;">0.56</div></div>	-	Open
4	OHD_Leishmania_346 T21a	-24.500	3.7081	-1.0710	5	18	<div><div style="width: 78%;">0.78</div></div>	<div><div style="width: 92%;">0.92</div></div>	<div><div style="width: 52%;">0.52</div></div>	<div><div style="width: 67%;">0.67</div></div>	-	Open
5	OHD_Leishmania_110 T21a	-24.008	7.0370	-0.5981	8	16	<div><div style="width: 67%;">0.67</div></div>	<div><div style="width: 86%;">0.86</div></div>	<div><div style="width: 33%;">0.33</div></div>	<div><div style="width: 44%;">0.44</div></div>	-	Open
6	OHD_Leishmania_97 T21a	-23.812	5.0397	-0.8070	8	19	<div><div style="width: 74%;">0.74</div></div>	<div><div style="width: 100%;">1.00</div></div>	<div><div style="width: 58%;">0.58</div></div>	<div><div style="width: 67%;">0.67</div></div>	-	Open
7	OHD_Leishmania_363 T21a	-23.720	7.0466	-0.7972	7	14	<div><div style="width: 75%;">0.75</div></div>	<div><div style="width: 86%;">0.86</div></div>	<div><div style="width: 25%;">0.25</div></div>	<div><div style="width: 22%;">0.22</div></div>	-	Open

Table with results – sorting by

Interactive histograms



FairMol - Docking



Selected compounds

7 selected 6 scaffolds Select all Set A Set B Set C CSV XLSX SMI SDF Selections

c1ccccc1 (2) O=C1C=CC(=O)c2ccccc21 (2) (acyclic) (2) C1=CC23CCN(Cc4cc5c(cc42)OC)O5 (1) O=c1c(C=Nnc2ccccc2)coc2ccccc1 (1) O=C(C1CCCC(NH2+1)Cn1cnc2cc (1)

Selected	Open
 OHD_Leishmania_176 ID 27 - MW 226.659000000000... <chem>c1ccccc1</chem>	 OHD_Leishmania_92 ID 28 - MW 301.342000000000... <chem>C1=CC23CCN(Cc4cc5c(cc42)O</chem>
 OHD_Leishmania_166 ID 30 - MW 209.274 · LogP 0.8... <chem>c1ccccc1</chem>	 OHD_Leishmania_341 ID 40 - MW 357.207 · LogP 4.3... <chem>O=c1c(C=Nnc2ccccc2)coc2ccccc</chem>
 OHD_Leishmania_143 ID 95 - MW 302.354000000000... <chem>O=C(C1CCCC(NH2+1)Cn1cnc2cc</chem>	 OHD_Leishmania_104 ID 120 - MW 293.706 · LogP 2... <chem>O=C1C=CC(=O)c2ccccc21</chem>
 3K70 ID 192 - MW 258.118999999999... (acyclic)	

FairMol - Docking

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

OHD_Leishmania_92

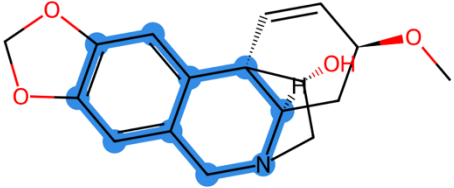
ID 28

DB Docking_T21a This detail page is pinned to the current database context.

2D 3D Properties Samples Containers Heterocycles & FG Structural Profile Drug Similarity PharmaFP-250 ADMET 3D Conformer Docking AI Analysis

Heterocycles & Functional Groups

Analysis powered by faircheckmol_nodb — click any item to highlight its atoms in the structure.



Enhanced name	Crinan,1,2-didehydro-
Heterocycle	Crinan,1,2-didehydro-
Family	fused heterocycle-like
Superclass	fused heterocycle
Scaffold	6-membered N-heterocycle
Substituents	hydroxy, trimethoxy

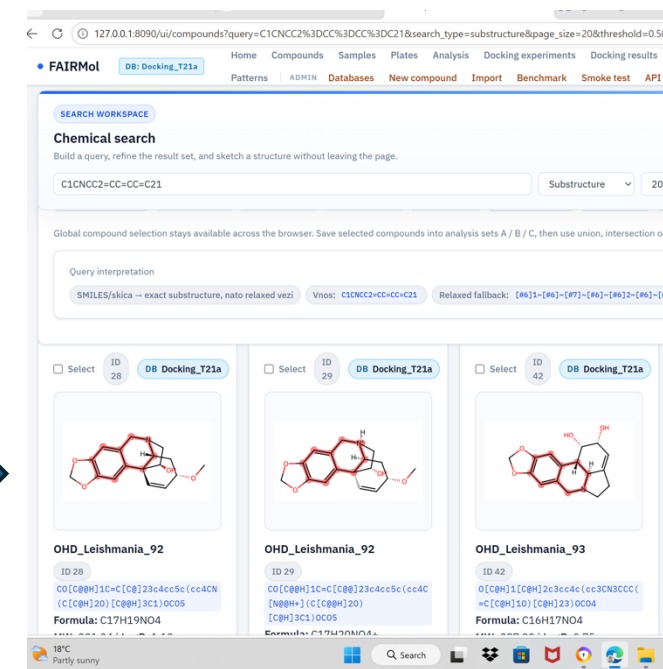
Heterocycles

6 heterocycles 6 functional groups 5 rings

- Crinan,1,2-didehydro-**
fused heterocycle-like · fused heterocycle · 1 match
Atoms: 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 17, 18, 19, 20, 21
[Search motif](#)
- 1,2,3,4-Tetrahydroisoquinoline**
isoquinoline-like · benzofused azine · 1 match
Atoms: 5, 6, 7, 8, 9, 10, 11, 12, 13, 17
[Search motif](#)
- 1,3-Benzodioxole**
fused heterocycle-like · fused heterocycle · 1 match
Atoms: 6, 7, 8, 9, 10, 11, 19, 20, 21
[Search motif](#)

Structural analysis

Substructure search



127.0.0.1:8090/ui/compounds?query=C1CNCC2%3DCC%3DCC%3DC21&search_type=substructure&page_size=20&threshold=0.50

FAIRMol DB: Docking_T21a

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Patterns ADMIN Databases New compound Import Benchmark Smoke test API docs

SEARCH WORKSPACE

Chemical search

Build a query, refine the result set, and sketch a structure without leaving the page.

C1CNCC2=CC=CC=C21 Substructure 20/

Global compound selection stays available across the browser. Save selected compounds into analysis sets A / B / C, then use union, intersection or

Query interpretation
SMILES/skica → exact substructure, nato relaxed vezi Vnos: C1CNCC2=CC=CC=C21 Relaxed fallback: [#6]1-[#6]-[#7]-[#6]-[#6]-[#6]-[#6]-[

<input type="checkbox"/> Select ID 28 DB Docking_T21a	<input type="checkbox"/> Select ID 29 DB Docking_T21a	<input type="checkbox"/> Select ID 42 DB Docking_T21a
OHD_Leishmania_92 ID 28 <chem>CO[C@@H]1C=C[C@]23c4cc5c(cc4CN(C[C@@H]2O)[C@@H]3C1)OCOS</chem> Formula: C17H19NO4	OHD_Leishmania_92 ID 29 <chem>CO[C@@H]1C=C[C@]23c4cc5c(cc4C[N@@H]1)[C@@H]23)OCOS</chem> Formula: C17H19NO4	OHD_Leishmania_93 ID 42 <chem>O[C@@H]1[C@@H]2c3cc4c(cc3CN3CCC(=C[C@@H]1O)[C@@H]23)OCOS</chem> Formula: C16H17NO4

18°C Partly sunny

See you virtually

May 13 2026