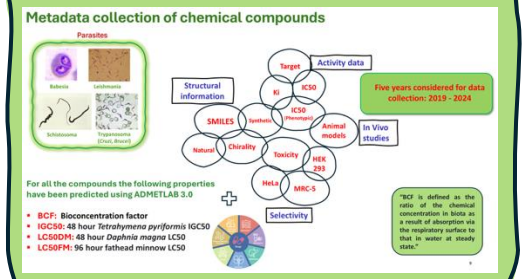
Virtual Chemotheca Project: Data Collection and Management:

https://www.cclab.unicz.it/ohd/index.php

Literature Compounds Collection:

- OHD2 *T. Brucei* 2019-2024
- OHD2 *T. Cruzi* 2019-2024
- OHD2 *Schistosoma* 2019-2024
- OHD2 *Babesia* 2019-2024
- OHD2 Leishmania 2019-2024

1498 compounds



Total Compounds Collected

12398

Virtual Chemotheca Data Collection and Management

GSK Kinetobox (KB)

Collection:

- KB- Chagas collection (GSK)
- KB- Leishmania collection (GSK)
- KB- HAT collection (GSK)

521 compounds

COST Member Contribution:

- Tydock Lib. – Prof. M.P. Costi group.
- ULFKKTLIB - Prof. C. Podlipnik group
- OSA_Lib - Prof. Outi Salo-Ahen, Dr. Seebacher group
- TC_lib – Dr. T. Calogeropoulou group
- UniSi_lib – Prof. S. Gemma group
- MAC-Lib – Prof. M. A. Carvalho group
- DCM –Lib – Prof. D. C. Magri group

One Health Drugs
Virtual Chemotheca

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Welcome to the OHD Virtual Chemotheca

This computational facility contains virtual compounds kindly provided by One Health Drugs COST Action CA21111 participants. The compounds are antimicrobials or they are considered good candidates for an antimicrobials activity. The Chemotheca contains different sections:

a. compounds from metadata;
b. compounds from proprietary collections obtained by synthetic chemistry
c. compounds from proprietary collections of natural origin (natural products)
d. IP protected compounds, only accessible through contact with the owner by email

Currently, **12398** compounds are stored and available for registered users.

For each entry, physico-chemical and ADME properties have been theoretically computed. Experimental activity data have been stored, if available.

To access the OHD Virtual Chemotheca all users must be registered by filling this **form**.

You will receive username and a randomly generated password from our administrative staff.

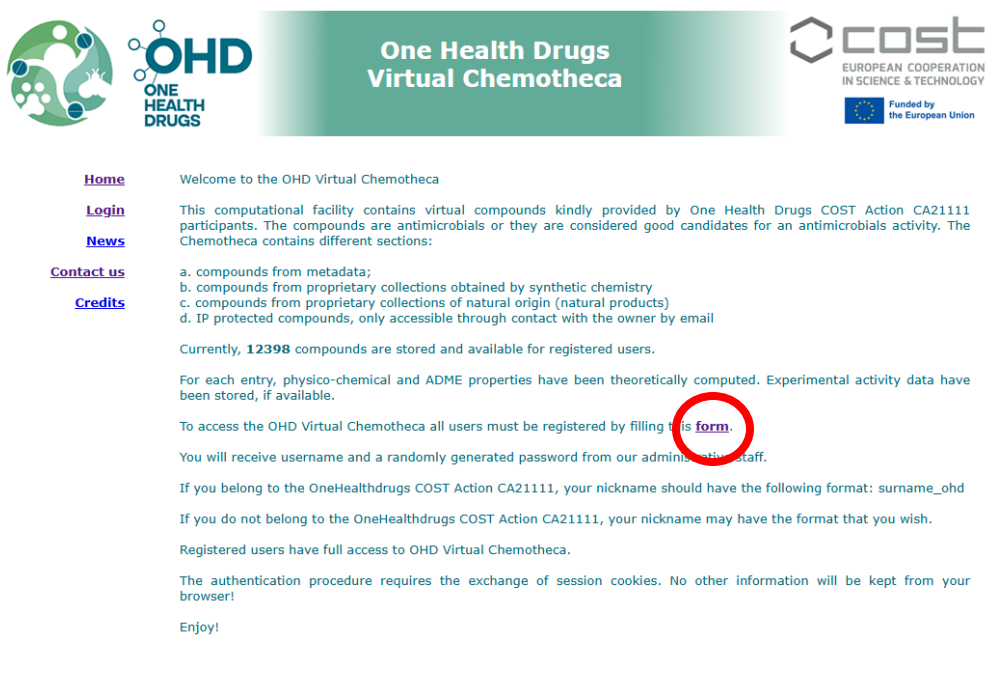
If you belong to the OneHealthdrugs COST Action CA21111, your nickname should have the following format: surname_ohd

If you do not belong to the OneHealthdrugs COST Action CA21111, your nickname may have the format that you wish.

Registered users have full access to OHD Virtual Chemotheca.

The authentication procedure requires the exchange of session cookies. No other information will be kept from your browser!

Enjoy!



You can also send an e-mail with the same data to: onehealthdrugs.events@gmail.com

OHD
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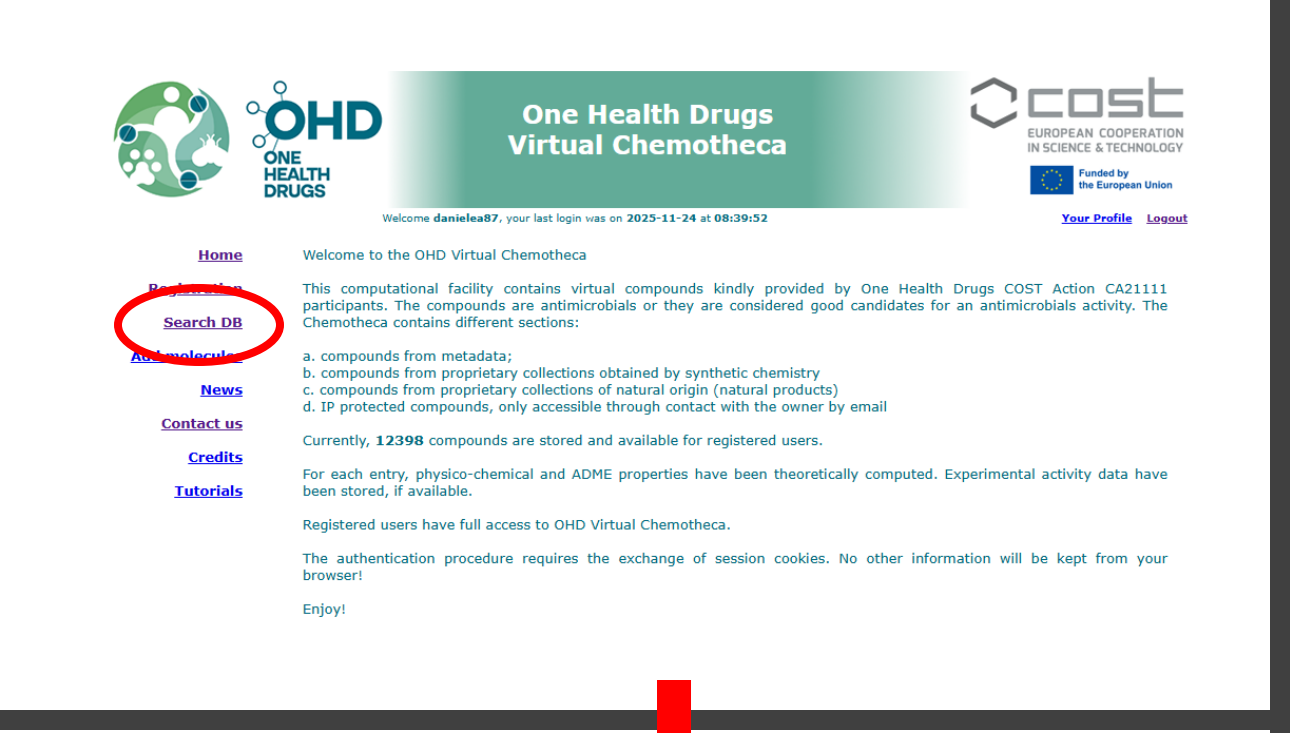
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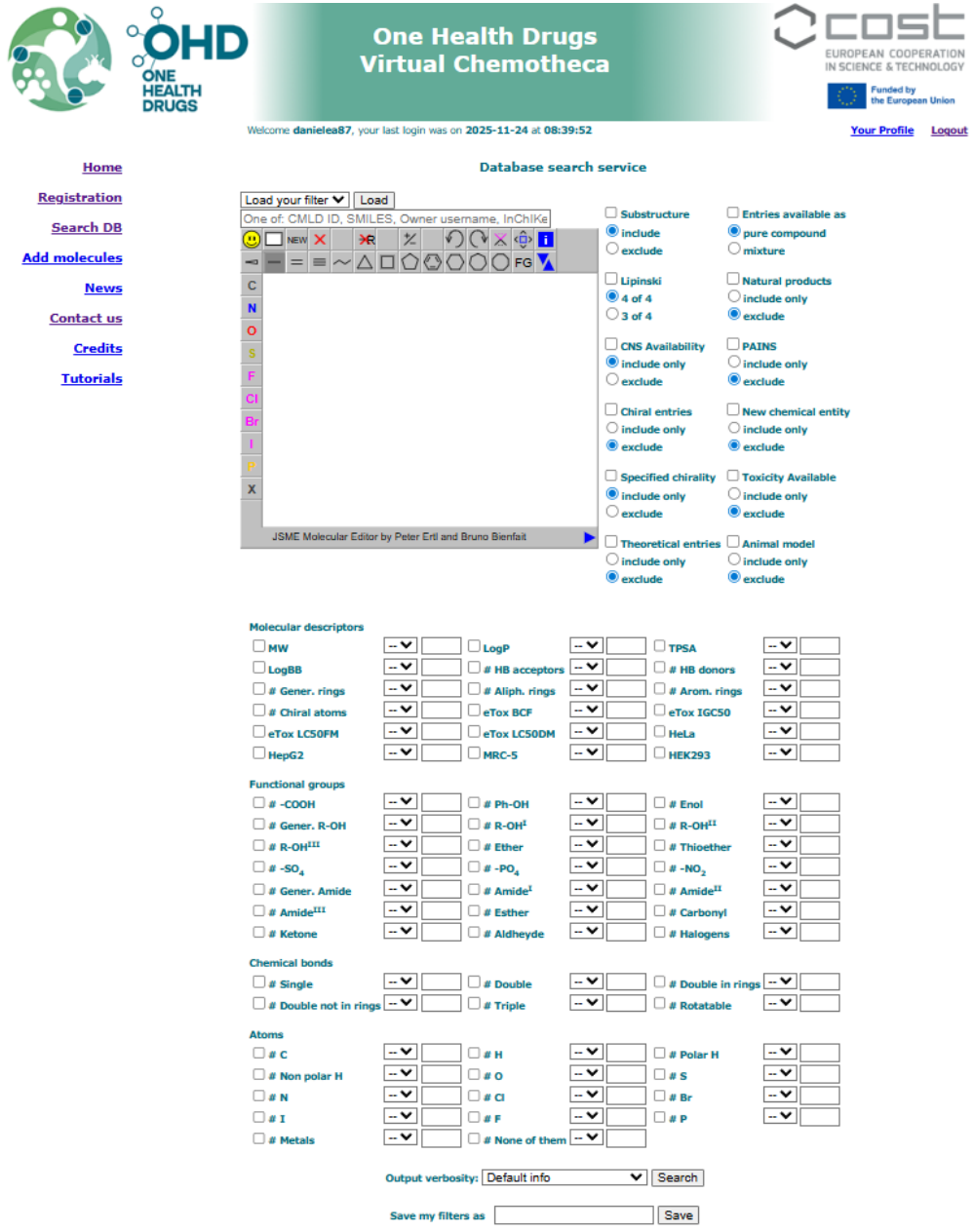
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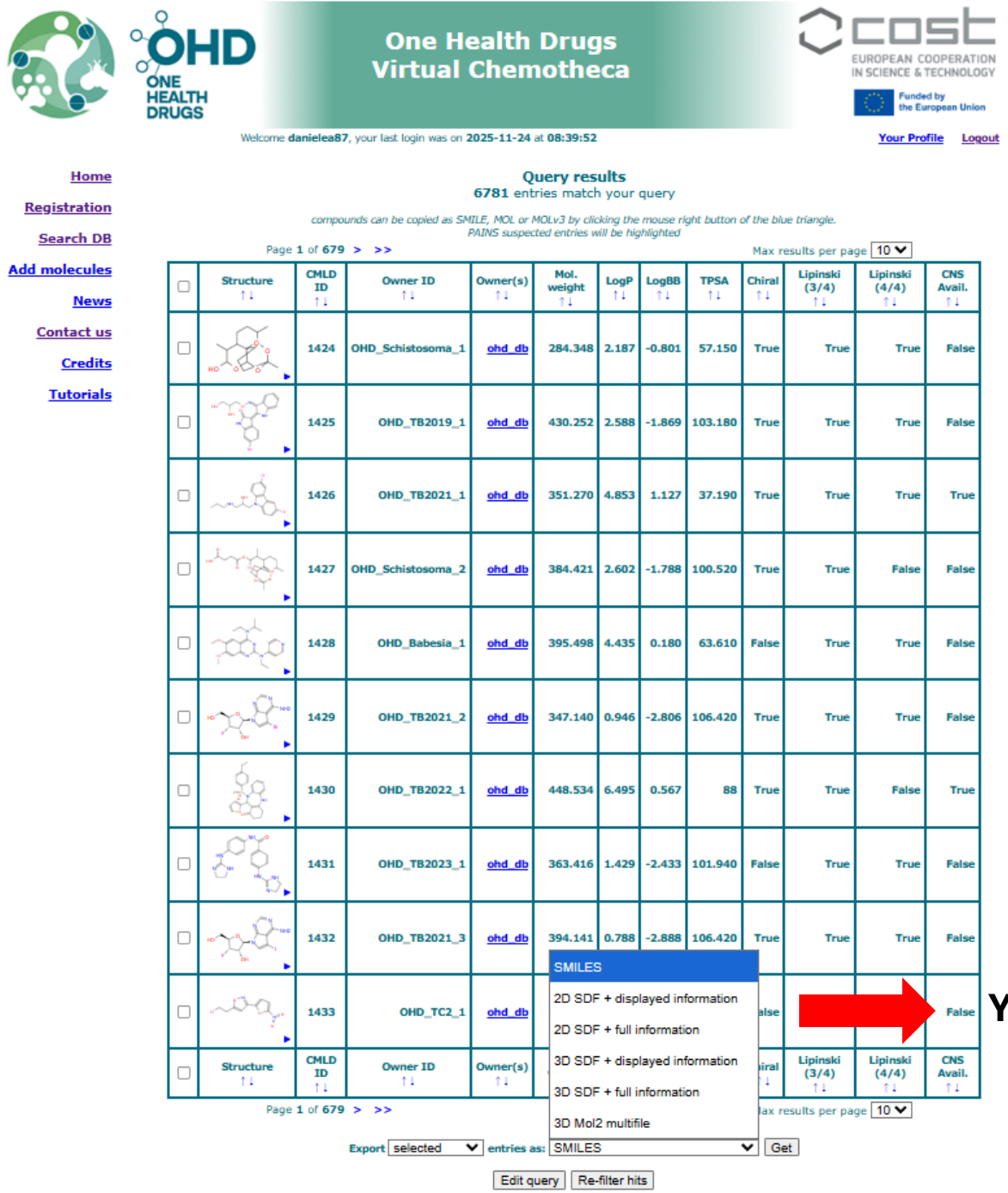
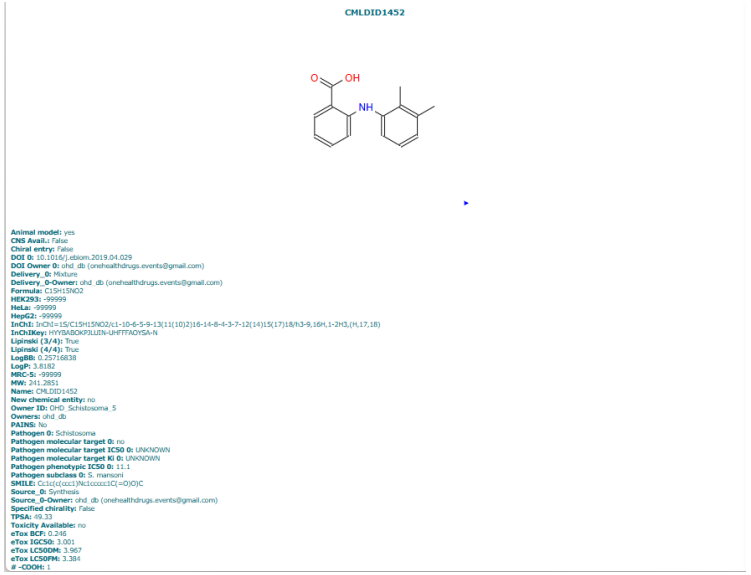
Load
One of: CMLD ID, SMILES, Owner username, InChIKey
JSME Molecular Editor by Peter Ertl and Bruno Bienfait
Substructure
include
exclude
Entries available as
pure compound
mixture
Lipinski
4 of 4
3 of 4
Natural products
include only
exclude
CNS Availability
include only
exclude
PAINS
include only
exclude
Chiral entries
include only
exclude
New chemical entity
include only
exclude
Specified chirality
include only
exclude
Toxicity Available
include only
exclude
Theoretical entries
include only
exclude
Animal model
include only
exclude
Molecular descriptors
MW
LogP
TPSA
LogBB
HB acceptors
HB donors
Gener. rings
Aliph. rings
Arom. rings
Chiral atoms
eTox BCF
eTox IGC50
eTox LC50FM
eTox LC50DM
HeLa
HepG2
MRC-5
HEK293
Functional groups
-COOH
Ph-OH
Enol
Gener. R-OH
Ether
Thioether
Gener. Amide
Esther
Carbonyl
Ketone
Aldheyde
Halogens
Chemical bonds
Single
Double
Double in rings
Double not in rings
Triple
Rotatable
Atoms
C
H
Polar H
Non polar H
O
S
N
Cl
Br
I
F
P
Metals
None of them
Output verbosity:
Default info
Search
Save my filters as
Save



Compound Detailed Data Page



You can download the data in different formats

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Chemotheca's Video Tutorials

Part 1: Introduction and Registration

Part 2: Advanced Search Database

Part 3: Uploading-Editing Molecules