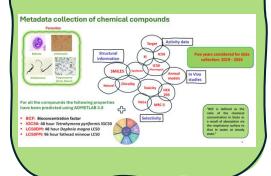
Virtual Chemotheca Project: Data Collection and Management:

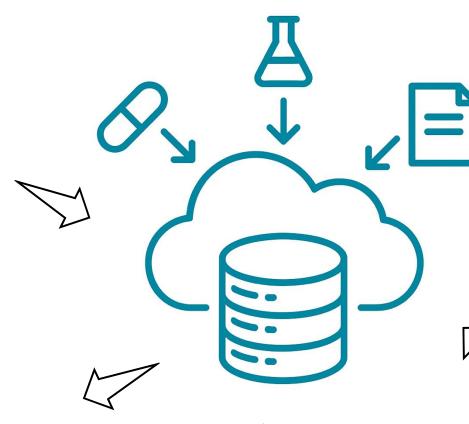
https://www.cclab.unicz.it/ohd/index.php

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







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







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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:

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a. compounds from metadata;

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- 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.

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Pre-registration form

Your data will be used by the web site management team for communication only. Submitted data will not be furnished to a third party. E-mail addresses will be readable by registered users only for allowing communication among them.

All fields are required!

Select ✓		
First Name		
Last Name		
Nickname for n	ext accesses	
Organization ty	pe	
Select ~		
Organization Na	ime	
Address		
Country		
Select		~
City		
ZIP code		
e-mail		
Retype e-mail		
Phone		
	Submit	

You can also send an e-mail with the same data

to: onehealthdrugs.events@gmail.com







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One of: CMLD ID, SMILES, Owner username, InChIKey Sea



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Load	your filter V Load	_	_
One	of: CMLD ID, SMILES, Owner username, InChIKe	Substructure	Entries available a
<u>Ф</u> Г	NEW X X % % () () X () ()	include	pure compound
		exclude	mixture
		Lipinski	☐ Natural products
C		4 of 4	_
N			include only
-		3 of 4	exclude
0		CNS Availability	PAINS
S			
F		include only	include only
		O exclude	exclude
CI		Chiral entries	☐ New chemical enti
Br			_
		include only	include only
•		exclude	exclude
P		☐ Specified chirality	☐ Toxicity Available
×			_
		include only	include only
		O exclude	exclude
	JSME Molecular Editor by Peter Ertl and Bruno Bienfait	☐ Theoretical entries	Animal model
		O include only	O include only
		exclude	exclude

Molecular descriptors					
□mw	🗸	LogP	V	☐ TPSA	🗸
LogBB	🗸	# HB acceptors	🗸	# HB donors	V
# Gener. rings	V	# Aliph. rings	V	# Arom. rings	V
# Chiral atoms	V	eTox BCF	V	eTox IGC50	V
eTox LC50FM	V	eTox LC50DM	V	HeLa	V
HepG2	V	☐ MRC-5	V	☐ HEK293	V
Functional groups					
□ # -соон	V	# Ph-OH	v	# Enol	V
# Gener. R-OH	🗸	# R-OHI	🗸	# R-OHII	🗸
# R-OHIII	🗸	# Ether	🗸	# Thioether	🗸
☐ # -SO ₄	🗸	☐ # -PO ₄	🗸	☐ # -NO ₂	🗸
# Gener. Amide	🗸	# Amide ^I		# Amide ^{II}	v
# AmideIII	🗸	# Esther	🗸	# Carbonyl	🗸
# Ketone	🗸	# Aldheyde	🗸	# Halogens	🗸
Chemical bonds					
# Single	V	# Double	V	# Double in rings	V
# Double not in rings	🗸	# Triple	🗸	# Rotatable	🗸
Atoms					
□#c	🗸	□#н	🗸	# Polar H	V
# Non polar H	🗸	□#0	🗸	□ # S	🗸
□ # N	🗸	□# a		□ # Br	🗸
□#I	🗸	□#E	~	□ # P	🗸
# Metals	🗸	# None of them	=	U#F	
— w Pictal5		- # Hone of them			

∨ Search Save

Output verbosity: Default info

Save my filters as









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Query results

6781 entries match your query

compounds can be copied as SMILE, MOL or MOLv3 by clicking the mouse right button of the blue triangle.

PAINS suspected entries will be highlighted

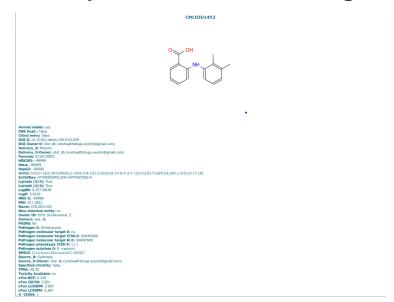
PAINS suspected entries will be highlighted Page 1 of 679 > >> Max results per page 10 ▼												
	Structure ↑↓	CMLD ID	Owner ID ↑↓	Owner(s) ↑↓	Mol. weight ↑↓	LogP ↑↓	LogBB ↑↓	TPSA ↑↓	Chiral ↑↓	Lipinski (3/4) ↑↓	Lipinski (4/4) ↑↓	CNS Avail. ↑↓
	HO TO THE	1424	OHD_Schistosoma_1	ohd_db	284.348	2.187	-0.801	57.150	True	True	True	False
	-100°	1425	OHD_TB2019_1	ohd_db	430.252	2.588	-1.869	103.180	True	True	True	False
0	- id	1426	OHD_TB2021_1	ohd_db	351.270	4.853	1.127	37.190	True	True	True	True
		1427	OHD_Schistosoma_2	ohd_db	384.421	2.602	-1.788	100.520	True	True	False	False
	aja	1428	OHD_Babesia_1	ohd_db	395.498	4.435	0.180	63.610	False	True	True	False
	10 X X X 10 10 10 10 10 10 10 10 10 10 10 10 10	1429	OHD_TB2021_2	ohd_db	347.140	0.946	-2.806	106.420	True	True	True	False
	- 025 - 025 - 025	1430	OHD_TB2022_1	ohd_db	448.534	6.495	0.567	88	True	True	False	True
	40.P	1431	OHD_TB2023_1	ohd_db	363.416	1.429	-2.433	101.940	False	True	True	False
	80 XX	1432	OHD_TB2021_3	ohd_db	394.141 SMILES	0.788	-2.888	106.420	True	True	True	False
	way.	1433	OHD_TC2_1	ohd_db			layed in	formation on	alse			False
	Structure ↑↓	CMLD ID ↑↓	Owner ID	Owner(s) ↑↓	1		layed in	formation on	iiral	Lipinski (3/4) ↑↓	Lipinski (4/4) ↑↓	CNS Avail. ↑↓
Page 1 of 679 > >>			3D Mol	2 multif	ile		lax n	lax results per page 10 ✔				

Export selected entries as: SMILES

Edit query Re-filter hits

∨ Get

Compound Detailed Data Page



You can download the data in different formats







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Part 2: Advanced Search Database





Part 3: Uploading-Editing Molecules

