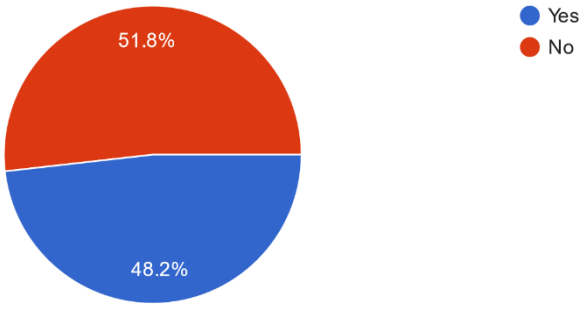
<u>Summary of WG1 Survey</u> (COST Action - CA21111 "OneHealthDrugs")

This survey is organized by WG1 (Compound libraries coordination and integration of compound design) of COST Action CA21111 "OneHealthDrugs" and collects information from COST Action members about the handling of chemical compound information and the usage of compound databases/repositories. The results will help to coordinate and integrate compound data from different resources for searching and screening purposes by the COST Action participants.

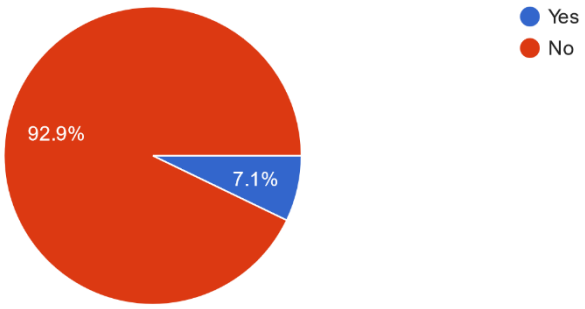
Do you use chemical compound databases or repositories for your daily work?

56 responses



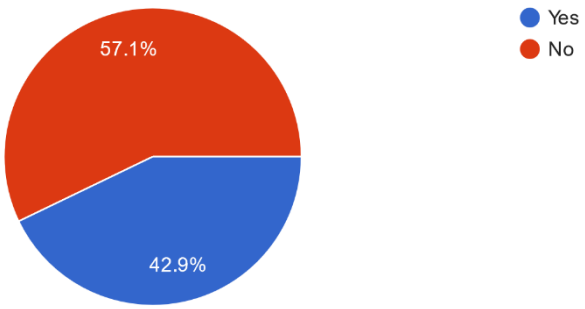
Have you already used the FAIRDOM-SEEK data management platform?

56 responses



Do you create your own compound information?

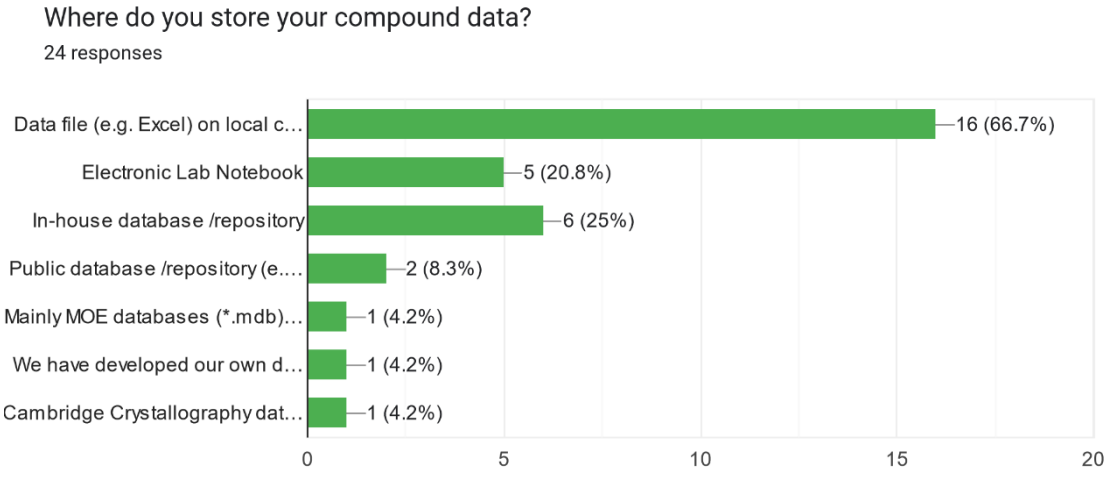
56 responses



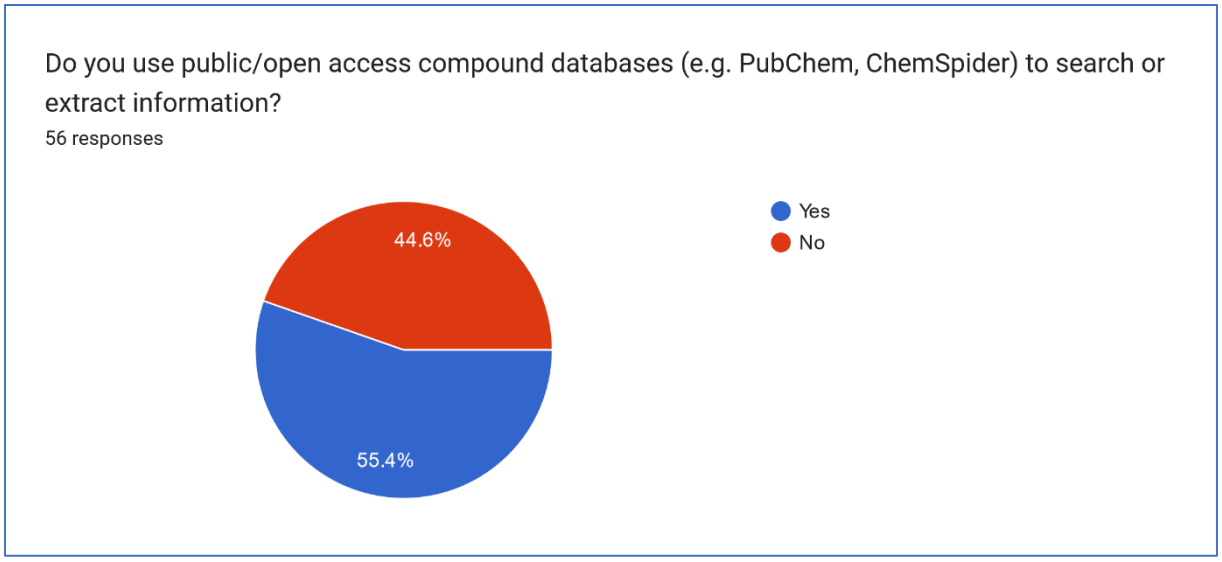
Your own compound information

Which kind of compound information are you creating/collecting? (18 responses)

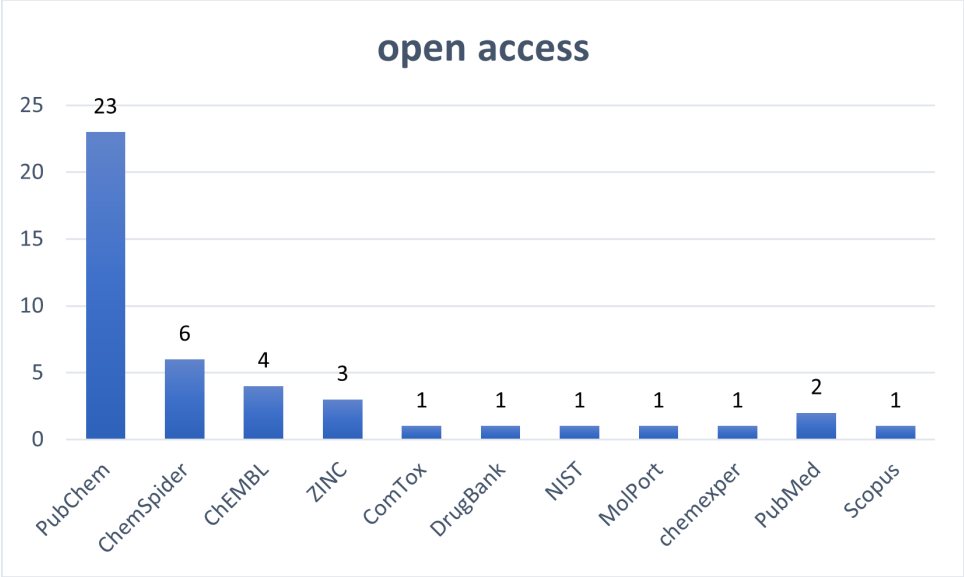
- MW, log P, logD, pKa, .sdf or .mol or any other file for 3 dimensional compound description
- Rational design series synthesized by med chem collaborator
- structures (2D and 3D) along with various molecular descriptors
- biological data (IC50 from phenotypic assays)
- .pdb for coordinates and .cif for the geometrical features
- endocrine disrupting compounds (aquatic animals and environment)
- parasite inhibitors
- name of the compound, CAS number, quantity, manufacturer, price
- various information properties of chemical compounds characterizing their drug-ability. Also models to predict these properties.
- Physicochemical data
- Name (Label), Structure, MW, Quantity, Physical property
- biguanide molecular structures, pyridoxine structures
- water solubilty, molecular weight, logP
- NMR data
- Code, structure, biological data
- Structure, code, quantity, aspect, MW (sometimes bio data)
- structure, name, date of preparation, reference to lab books for preparation procedures and analysis/characterization
- heterocyclic compounds
- chemistry, chemical analysis, physicochemical properties (if available), IC50 in antiparasitic tests

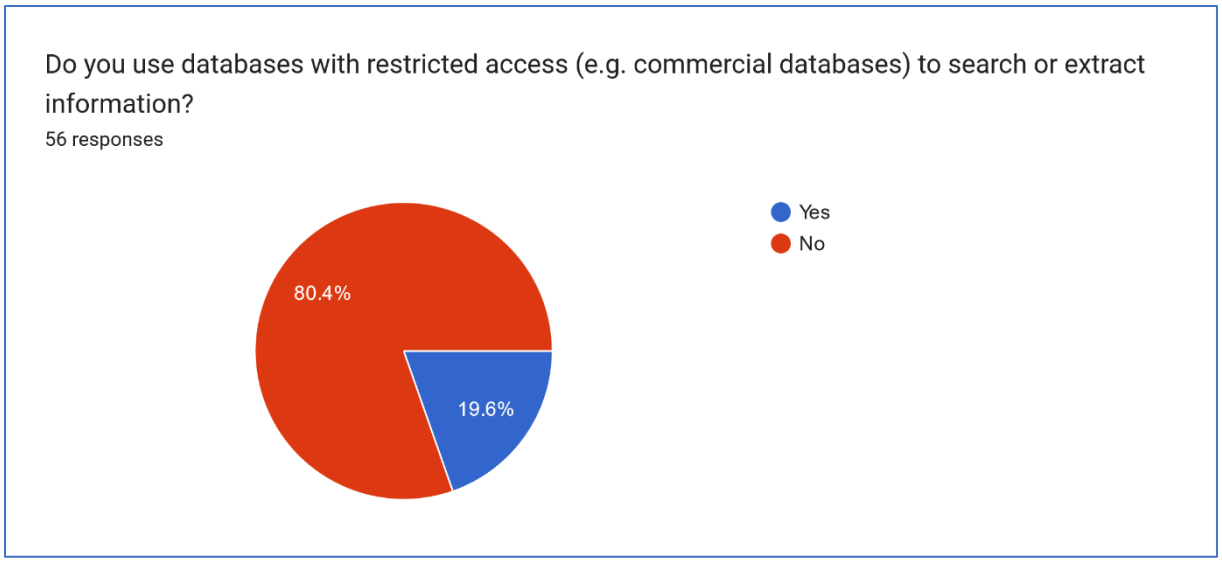


Compound data from external resource

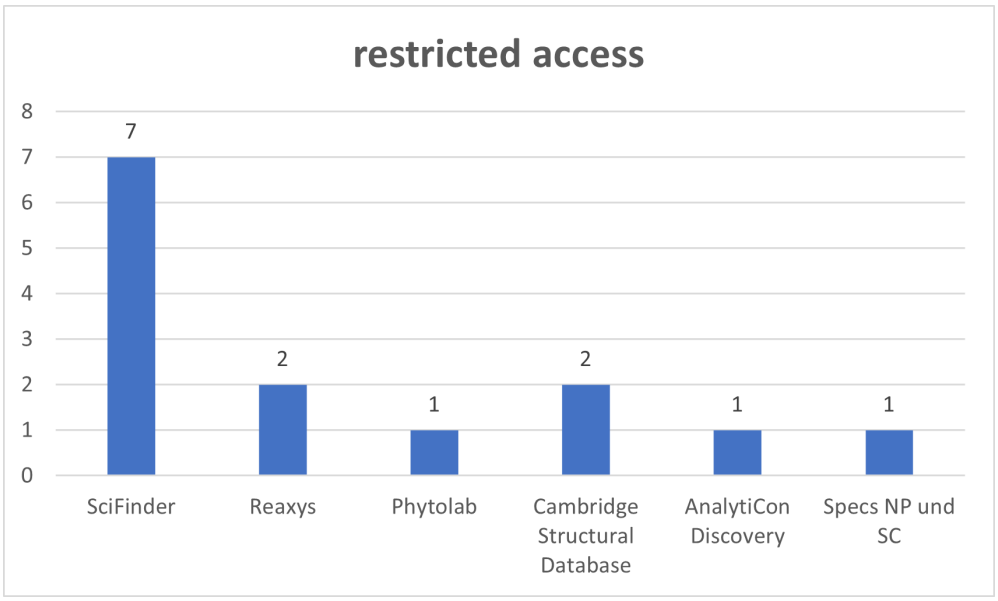


If yes, please specify the public/open access database name(s) (30 responses):

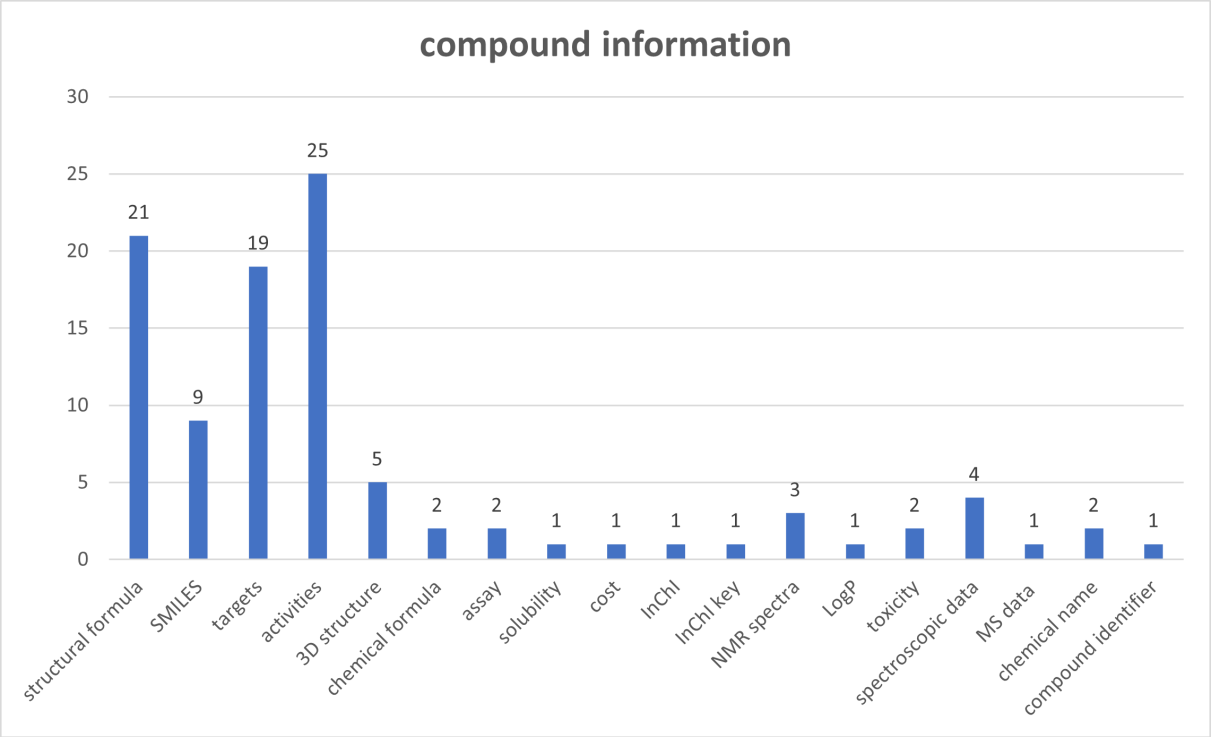




If yes, please specify the database name(s) (11 responses):

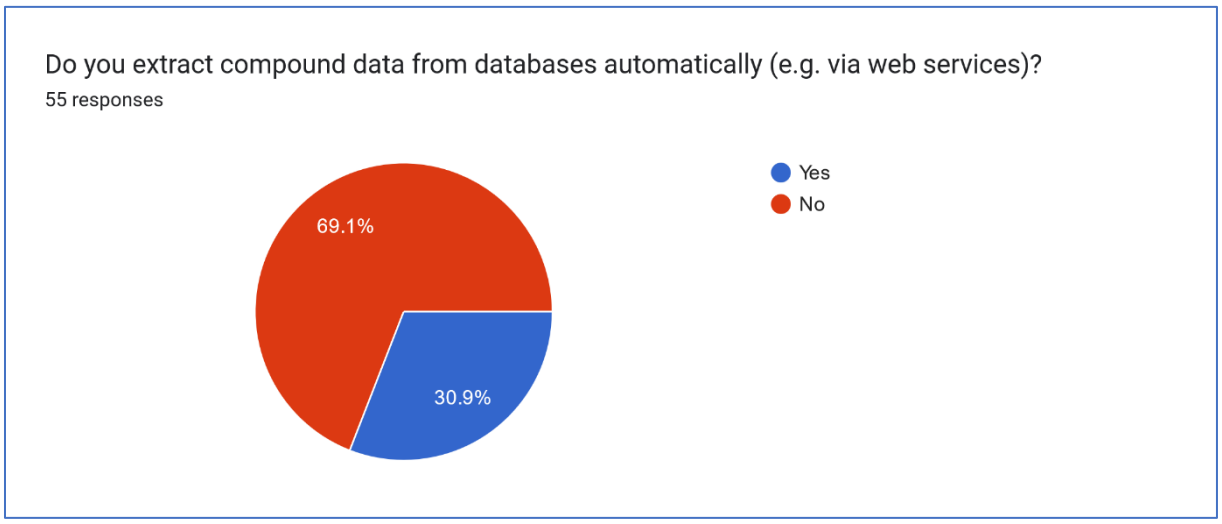


Which compound information are you interested in if you're searching in external resources (e.g. structural formula, SMILES, targets, activities)? (38 responses)



More general data:

- physiochemical properties
- constants
- synthetic procedures
- substructures
- spectral data
- spectrometric data
- everything available



Comments

- Decision on whether we will deposit is with the med chem partner

- We use the compounds mainly for virtual screening campaigns.

- There is a number of important issues to be considered/solved in WG1 and WG2 before data/compounds are collected. For example: Which quantity of a compound is available? How much should be available in order for the compound to be in the collection? How pure should it be, how pure IS it and how was the purity assessed? Is it available to anyone in the COST action? What are the criteria for making the compound available to another group? Must the compound have proven activity against a target or pathogen already? Or should we just add any compound we have in the fridges? After all, such compounds could be interesting, too. Lots of things to discuss and I hope we can have such a general discussion soon. It is really nice to have a platform for jointly collecting the data. But we must know what happens with the data and the compounds once they enter into this pool. I think it would be wise to know this before starting to collect data and compounds. Just my view on this. Best regards. Thomas

- I work with secondary plant metabolites in cell and animal disease models. I receive these compounds from other laboratories.

- As of now only looking at compounds -after- they have been crystallized with proteins, so structural databases for searching them are my primary source

- I am registered in FAIRdom seek, but I haven ´t used it before. I am rather new to this field of compounds libraries, so far we have tested only compounds from direct collaboration with all the necessary information obtained. For our new project we plan to include also in silico docking experiments, therefore we will need SMILEs and many more information about the compounds.