MOF-BAM DATABASE USER INTERFACE - http://mofdb-bam.de/

A quick introduction on how to get started with using the tool

The web version of the MOF-BAM database consists of three sections:

1. **Search parameters of MOFs**
2. **Search parameters of Organics**
3. **Results**
4. **Exporting**

1. The search parameters of MOFs are divided in:

Number of components: amount of metals (any, 0 – 3), amount of linkers (any, 0 – 3). It allows also including organic molecules that are not linkers, like structure directing agents, charge compensating ions, capping agents, etc., selecting the option "Allow MOFs with Non-Linker organics". Also the instruction "Keep order when searching for Used Organics" (see section XX)

Search parameters: The drop-down menu allows to select the search parameter and its value. Included parameters are MOF name, CSD reference code, porous properties like accessible surface area (ASA gravimetric and volumetric), pore volume, density, crystallographic properties, estimated hydrogen total uptake at 77 K and 100 bar, presence of open metal sites (OMS), specific metals, and price of linkers per gram. The total uptakes are estimated from the porous properties by following the procedure reported in https://doi.org/10.1016/j.ijhydene.2020.10.265.

It is possible to add (or delete, if needed) search parameters combining these parameters with the option "Add search parameter". Finally, the button "Reset search parameters" cleans all the search fields, and the button "Search" looks for matches within the database. The results from the search appear in section 3.a.

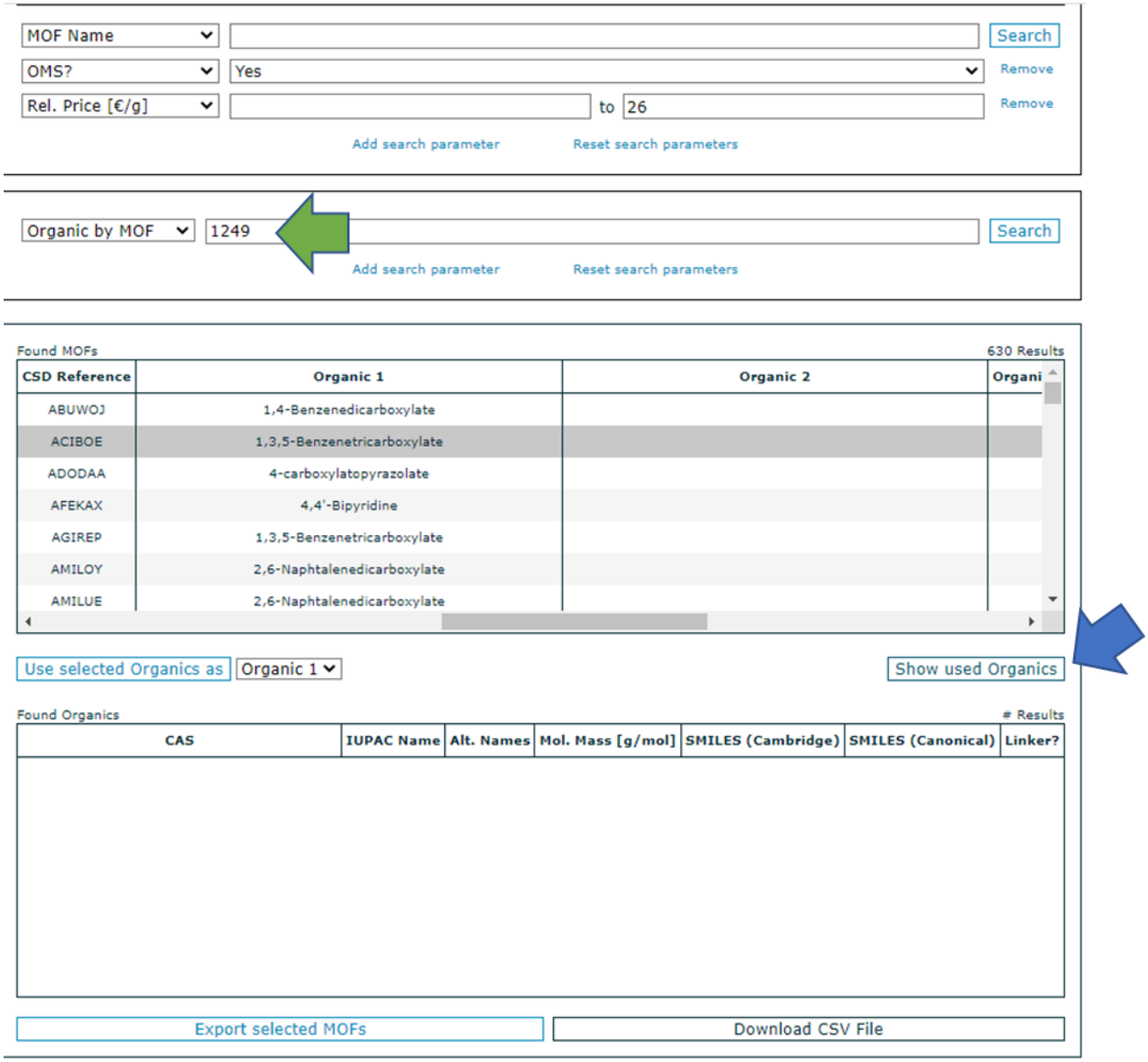
2. The search parameters of Organics

This field allows to look among organic components within MOF structures, even if they are linkers or not. It is possible to look for organics from their name (total name or fragments), CAS number, molar mass, their price (€/g), and the presence of specific chemical moieties (including carbonyl, amine, azolates, fluor,…).

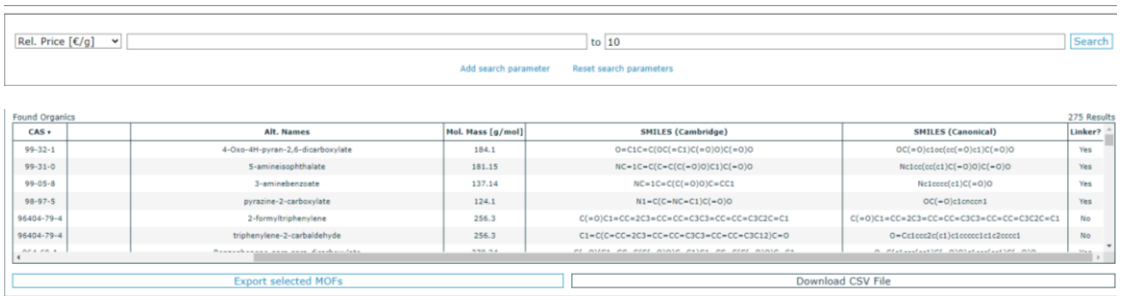
3. Results

Results are divided for MOFs structures (3.a) and organics (3.b). Both tables can be sorted by any attribute by clicking on the appropriate column header.

3.a: Found MOFs, the interface provides the CSD reference, MOF name (if available), porous and crystalline properties, density, gravimetric hydrogen excess in saturation, gravimetric and volumetric total uptakes at 77 K and 100 bar, metallic and organic composition, and the potential presence or not of OMS. It is also possible to select one or many structures from the results field to export or to select their organic components as a search criteria in 2.



3.b: Found Organics: The organic compounds matching the search parameters in section "2." appear here. For example, cheaper linkers than 10 €/g.



4. Exporting

Exportation buttons allow to export the MOF structures results into a csv file. After the selection is made (Selecting no MOFs will automatically result in all results in the MOF table to be exported), it is necessary to click on “Export selected MOFs”. This will generate a file containing the information on both the selected MOFs and the organics associated with them. Once the file is ready the “Download CSV File” button will turn clickable and upon its use the generated file will be downloaded. The file contains the following fields:

Identifiers of the structure: csd_ref, name, as identifiers of the structure.

Porous properties: asa_grav [m^2/g], asa_vol [m^2/cm^3], av_vf, pore_volume [cm^3/g],

density [g/cm^3]

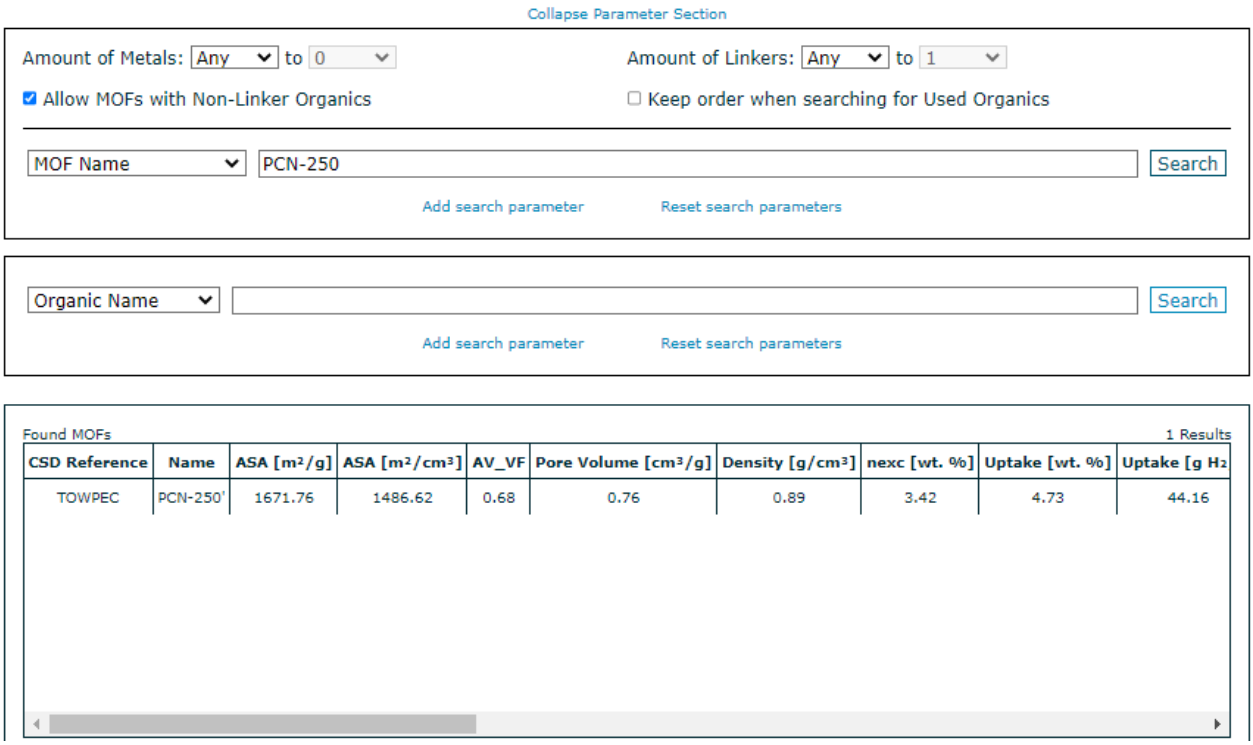
Hydrogen uptake: nexc [wt. %], uptake_grav [wt. %], uptake_vol [g H2/L],

Composition: metal1, metal2, metal3, cas1, norm_name1, name1, mol_mass1 [g/mol], smile_cam1, smile_can1, linker1, vendor_name1, max_amount1 [g], rel_price1 [€/g], min_purity1, cas2, norm_name2, name2, mol_mass2 [g/mol], smile_cam2, smile_can2, linker2, vendor_name2, max_amount2 [g], rel_price2 [€/g], min_purity2, cas3, norm_name3, name3, mol_mass3 [g/mol], smile_cam3, smile_can3, linker3, vendor_name3, max_amount3 [g], rel_price3 [€/g], min_purity3

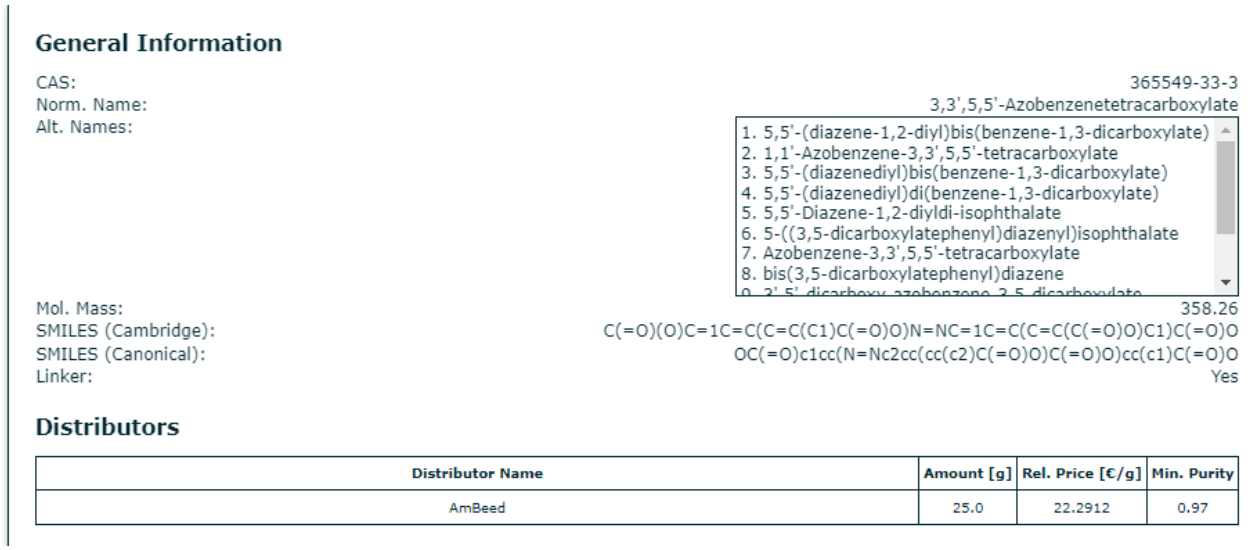
Structural/crystalline parameters: oms, lcd [Å…], pld [Å …], LFPD [Å …], symmetry_space_group, cell_length_a, cell_length_b, cell_length_c, cell_angle_alpha, cell_angle_beta, cell_angle_gamma, cell_volume [$Å^3$].

Example 1:

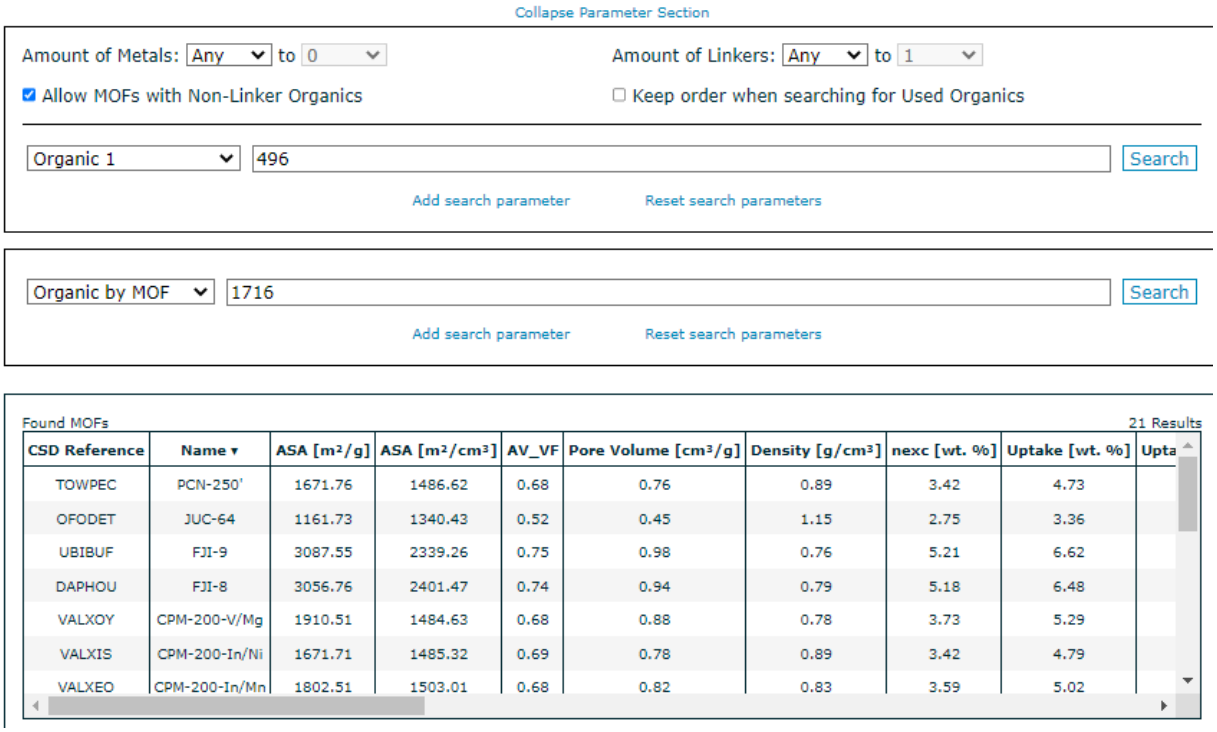
We want to search structures using the same linkers than material PCN-250. In the Structure search fields (1.), select “MOF Name”, and type “PCN-250”, then click on “Search”.



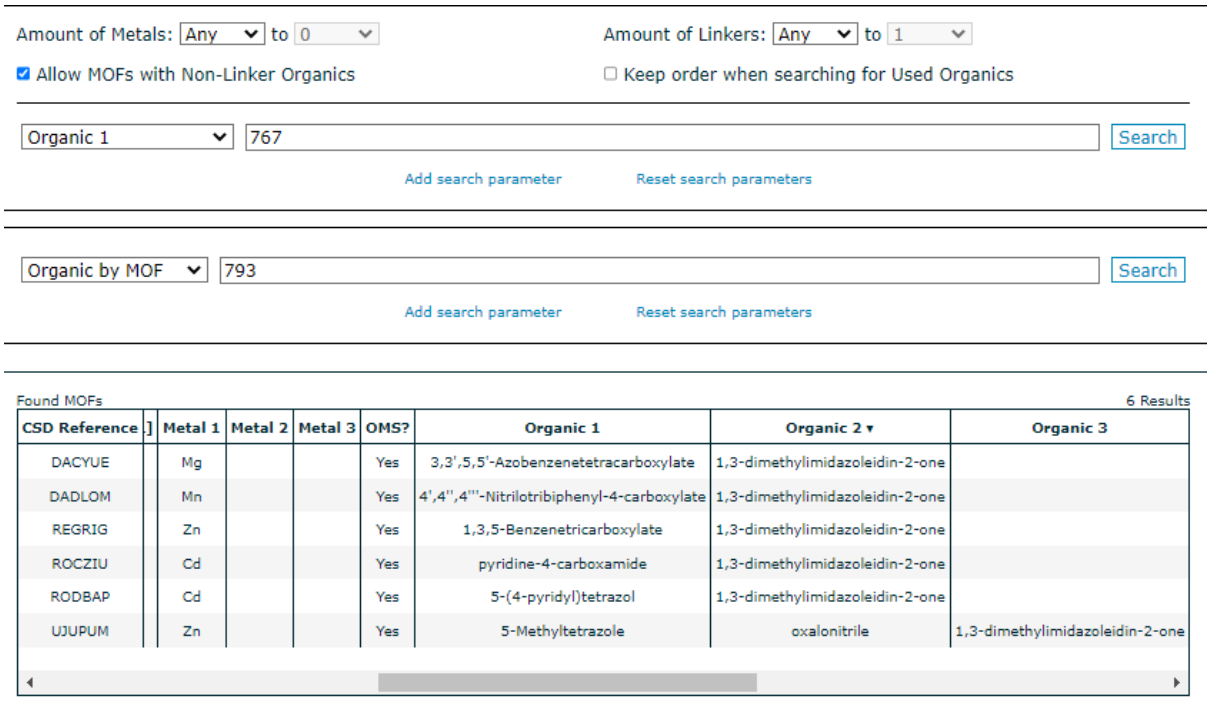
Now, select the structure with left click over it in the results field “3.a”and then, click on “Show Used organics”. An internal ID, assigned to this linker, will appear in the search field “2.” labeled as “Organic by MOF”. Click on “Search” button, and the information about this linker appears in the results box “3.b”. It is possible to check the information about a linker by double-clicking anywhere on its row in the results field. Clicking anywhere next to the opened information panel will close it again.



Now, reset search parameters in the structure search (1.), and click on “Use selected organic as” after selecting the position “Organic 1” in the drop-down menu rightwards. If the option “keep order when searching for Used Organics” is not selected in the field “1.”, then structures where the linker is in position 2 or 3 (if any) would also be displayed.

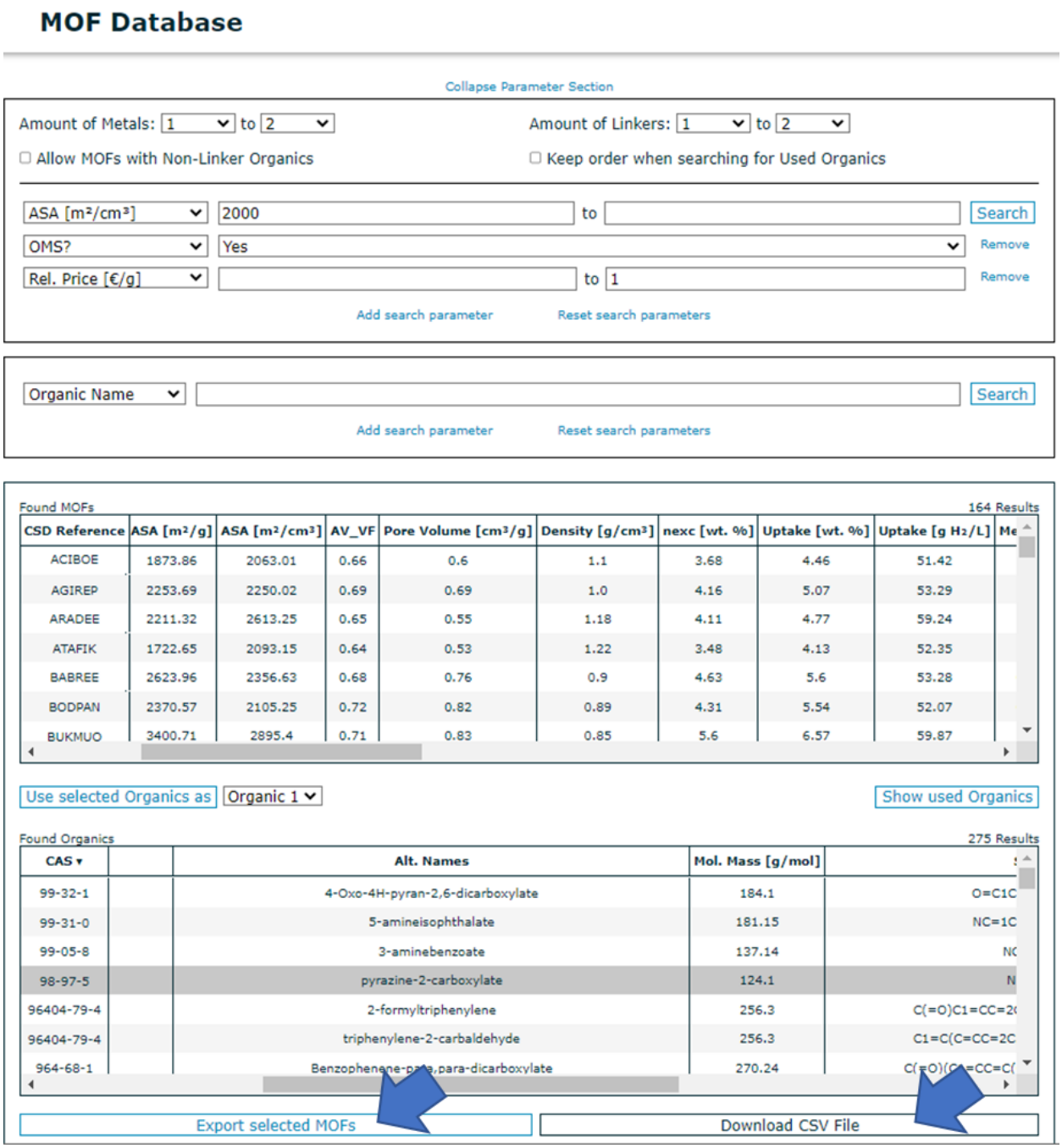


The structure DACYUE uses a mixture of linkers. By clicking on it and on “Show used Organics”, it would include this organic compound in the results field “3.b”. First, we need to Reset search parameters on fields “1.” and “2.”.



Example 2:

Now, let us search for MOF structures with higher volumetric area than 2,000 m^2/cm^3, with OMS, and using a cheaper linker than 1 €/g. The interface gives 164 MOF structures fulfilling this criteria.



To export this data, click first on “Export Selected MOFs”, and then on “Download CSD File”. It will generate a .csv file using comma as data delimiters. In some regions importing this file in other programs like EXCEL may require the user to set the appropriate delimiter for the columns to be displayed properly (for EXCEL

see https://support.microsoft.com/en-us/office/import-or-export-text-txt-or-csv-files-5250ac4c-663c-47ce-937b-339e391393ba).

After separating the fields, the selection looks like this: