SpaceMACS – Substructure Matching

BioSolveIT
expect actives!

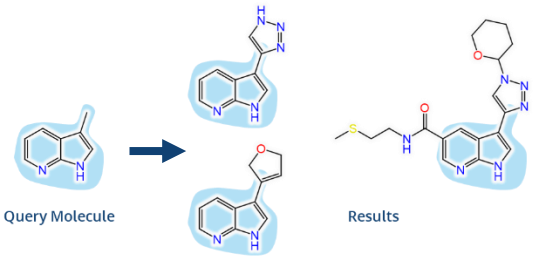
Retrieve compounds with a particular substructure from trillion-sized make-on-demand Chemical Spaces. SpaceMACS mines for results within seconds to present you the most relevant chemistry.

How does SpaceMACS work?

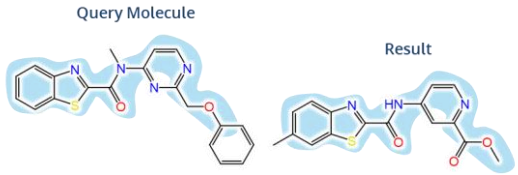
With a molecular structure as input, SpaceMACS extracts a specified number of compounds from a combinatorial Chemical Space. The matching process relies on maximum common substructure (MCS) similarity that surpasses straight-forward exact substructure search.
SpaceMACS not only retrieves compounds within the Chemical Space that contain the exact molecular substructure specified but also identifies closely-related candidates, providing relevant options in cases where exact matches are absent.

Advancing motif-driven campaigns

Securing access to all available molecules is crucial for progressing drug discovery campaigns. SpaceMACS serves a powerful tool, offering chemically accessible compounds and, in the case of BioSolveIT's partner Chemical Spaces, commercially available ones.
Especially fragment-based projects profit from this approach, as SpaceMACS enable the mining of both smaller and larger decorated compounds that contain the known fragment binder as a substructure.



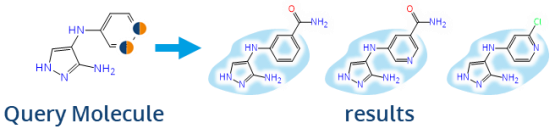
Users of SpaceMACS do not leave empty-handed even if an identical molecular motif is not found in the Chemical Space. The algorithm extends its capabilities beyond common exact substructure searches, uncovering similar molecules with minimal deviations.



Chemical Spaces serve as an appealing resource for molecules with novel IP and diverse substitution patterns. These molecules can then be employed to explore a range of potential alternatives to enhance affinity and show better ADME properties.

Versatile claw machine with SMARTS

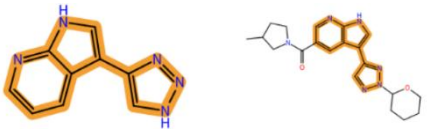
SpaceMACS holds a significant edge over alternative methods due to its capability to conduct searches using SMARTS definitions. This feature empowers users to utilize the method for retrieving diverse compound classes characterized by specific molecular and functional arrangements.



Users can tailor their approach based on the project's requirements, utilizing the pharmacophore-containing segment of the molecule as a query. This allows them to retrieve accessible compounds, expanding their discovery toolbox for exploring structure-activity relationships.

Molecule mining powerhouse

When provided with a set of query molecules (SD or SMILES), SpaceMACS delivers up to one million compounds for each entry in a single run. SpaceMACS yields results at unparalleled BioSolveIT speed, with a search taking only seconds, enabling the screening of trillion-sized Chemical Spaces.



Visual highlighting helps you to understand the motif matching with a single glance.

Literature

Schmidt, R.; Klein, R.; Rarey, M. Maximum Common Substructure Searching in Combinatorial Make-on-Demand Compound Spaces. *J. Chem. Inf. Model.* **2022**, 62 (9), 2133–2150. https://doi.org/10.1021/acs.jcim.1c00640.

Schmidt, R.; Krull, F.; Heinzke, A. L.; Rarey, M. Disconnected Maximum Common Substructures under Constraints. *J. Chem. Inf. Model.* **2021**, 61 (1), 167–178. https://doi.org/10.1021/acs.jcim.0c00741.