Chemical Space Docking™

BioSolveIT
expect actives!

Chemical Space Docking™ (C-S-D) is the next generation of structure-based virtual screening of ultra-vast, combinatorial Chemical Spaces for the most promising drug candidates.

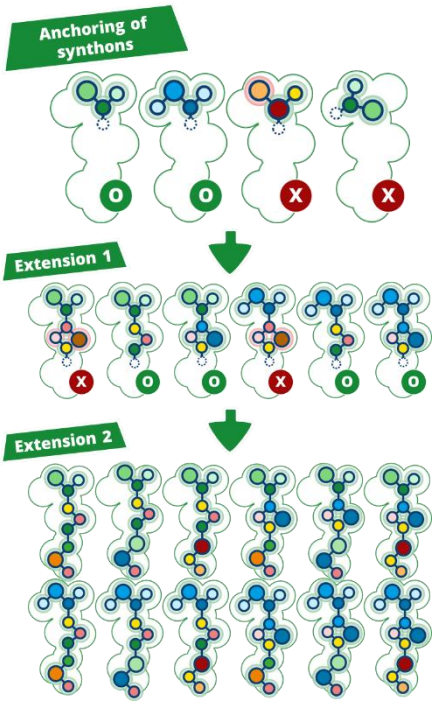
Docking billions or even trillions of molecules presents a significant computational challenge. As multiple poses are generated, the resulting file sizes can become enormous and difficult to handle. Furthermore, many compound poses tend to exhibit poor docking scores due to poor complementarity with the target's binding site, resulting in a substantial waste of computational resources.
We have developed C-S-D as an efficient method to retrieve relevant chemistry from vast compound clusters, applying a combinatorial built-up of molecules for tangible compounds that can also be ordered or synthesized.

How does C-S-D work?

C-S-D employs the synthon strategy: Starting with the docking of pre-processed building blocks of the selected Chemical Space, the smallest units containing an extension vector are assessed for their interaction potential within the target's binding site. After this anchoring step, users select the interesting candidates for extension. Here, they are supported by SeeSAR's enhanced assessment tools (e.g., for LLE, molecular torsions, clashes), as well as the position of the extension vector of the synthon, to make informed decisions.

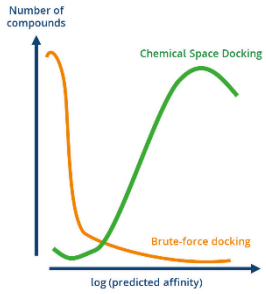
In the subsequent extension steps, the selected candidates are grown into complete drug candidates applying the encoded chemical reactions of the Chemical Space to ensure accessibility of the generated results. In each step, all the compounds that can emerge from the selected synthon are generated and re-docked into the binding site for the assessment of their interaction potential with the target structure.
After the final extensions, you can place an order for the compounds from our partners' Chemical Spaces to be synthesized and delivered to you.

By selecting initial starting fragments, you can focus on a small subset of the total compounds within the Chemical Space while still effectively covering the entire set of investigation. This approach significantly reduces computational times compared to commonly applied brute force methods.



More than Docking

The approach offers several advantages. First, and most important one, is the speed and efficiency that outperforms brute-force docking methods. As a result, C-S-D can operate without the need for server clusters or costly cloud computing, all while enriching high-scoring candidates.



Furthermore, two publications have demonstrated that C-S-D effectively retrieves diverse chemistries and various molecular scaffolds. Collaborations with multiple compound suppliers provide access to a wide array of Chemical Spaces, each featuring unique building blocks and reactions. This diversity ensures broader coverage of the chemical landscape, as the overlap among commercial Chemical Spaces is minimal.

Synergies of SeeSAR and HPSee

C-S-D was developed for cost-effective and secure in-house operations. For efficient handling of the whole workflow, users set up the docking and conduct the visual assessment of results within SeeSAR. Calculations for the anchoring and extensions steps are then handled by our HPSee product on external hardware. Both platforms efficiently communicate seamlessly, allowing for a streamlined and sophisticated user experience that enhances productivity and ease of use throughout the drug discovery process.

Literature

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