Visualization-driven pipeline for drug design through generative AI

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Mots-clefs : *drug design, generative AI, visualization, interaction, fields, pharmacophore, pipeline, interpretable*

Designing and optimizing ligands for a known molecular target remains challenging, in part because generative methods often produce candidates that are hard to interpret. We present an interpretable pipeline **(figure 1)** which combine a synthesis-aware generative AI with two visualization tools to design new ligands. Starting from a receptor structure with a known ligand, the pipeline extracts ligand pharmacophore features and computes interaction fields once for the receptor binding pocket using smiffer. These fields show possible interaction inside a given pocket like hydrophobic or pi stacking. A Monte-Carlo tree-search generator then assembles molecular building blocks via known reactions encoded as SMARTS/SMILES, ensuring that molecules are synthetically feasible. Candidate molecules are evaluated by docking and by pairwise interaction analysis performed with strange, which computed ligand–receptor pharmacophore features, then possible interaction between these features. The pipeline produces docking scores, interaction fields, and direct interaction to facilitate interpretation. All components (smiffer, strange, and the pipeline) are open source and available online (GitLab, PyPI). The workflow is operational and currently being evaluated on ongoing benchmark, which aims to quantify the pipeline robustness.

Liens utiles :

- https://gitlab.galaxy.ibpc.fr/rouaud/smiffer / https://smiffer.mol3d.tech
- https://gitlab.galaxy.ibpc.fr/rouaud/strange / https://strange.mol3d.tech/
- https://gitlab.galaxy.ibpc.fr/prabakaran/synthemol

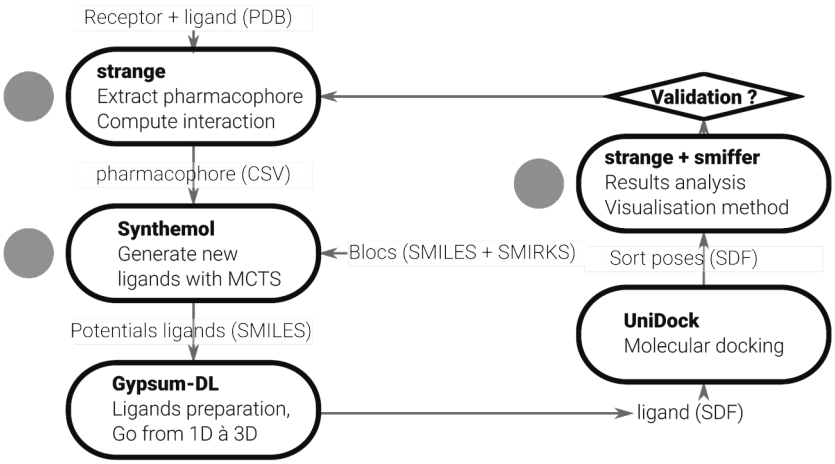

Figure 1 – Representation of the pipeline workflow.