Sigma-Aldrich®
Lab & Production Materials

MERCK

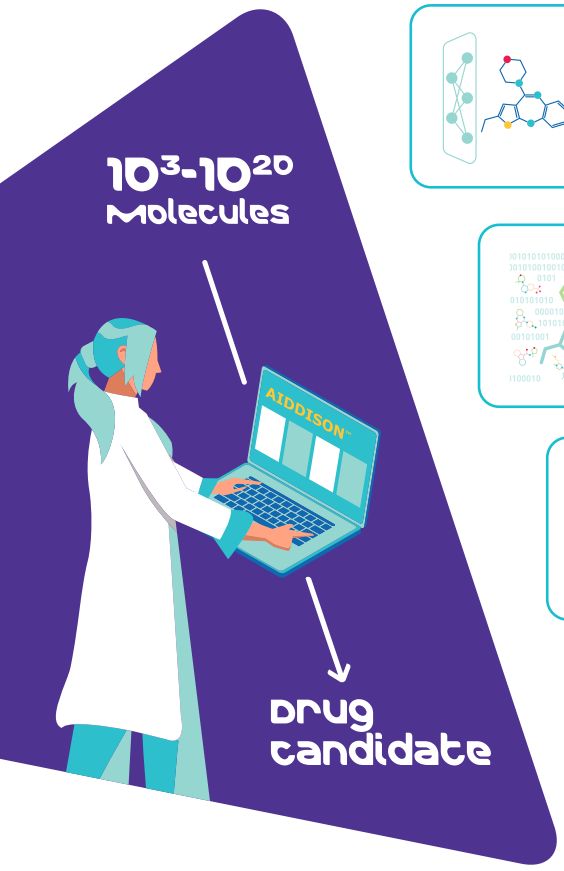
AIDDISON™

AI-powered Drug Discovery

Boldly go where no chemist has gone before

AIDDISON™ combines the power of artificial intelligence (AI) and computer-aided drug design (CADD) tools into a single integrated platform for virtual screening, scaffold hopping, hit identification, and lead optimization in medicinal chemistry. AIDDISON™ uses generative methods and ML models trained on experimentally validated ADMET data to guide search in ultra-large chemical spaces and *de novo* design of "drug-like" and synthetically viable compounds.

AIDDISON™ also encompasses SA-space™, a synthetically accessible chemical space of approximately 25 billion virtual compounds built on the Sigma-Aldrich® catalog of molecules, that are readily available for purchase, and well-known, robust chemical transformation rules.

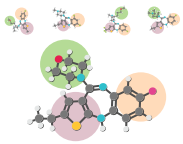


DE-NOVO MOLECULAR DESIGN

- Generate a set of virtual molecules with desired chemical properties from a target molecule of interest.
- Optimize synthesis accessibility score based on SYNTHIA™ retrosynthesis software.

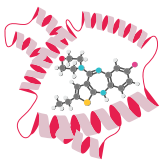
SIMILARITY & PHARMACOPHORE SEARCH

- Use 2D similarity search (Ftrees, BioSolveIT) for scaffold-hopping and ligand-based screening.
- Exploit ADME-Tox machine learning (ML) models to augment the pharmacokinetic profile search.



SHAPE-BASED SEARCH

- Evaluate the closest matching drug candidates based on electrostatic and shape properties (Flare™, Cresset).
- Quickly identify activity cliffs and 3D binding hypotheses to build 3D models of biological activity.



MOLECULAR DOCKING

- Visualize protein ligand complexes and propose innovative modifications.
- Confirm molecule interaction of desired drug candidates.
- Finalize 3D molecule alignment and 3D property evaluation with best protein ligand binding (Flare™, Cresset).

Unlock your ingenuity and learn more about AIDDISON™

See our webpage for further information, or contact us at aiddison@milliporesigma.com

The secure cloud infrastructure is ISO 27001-certified and scalable for cost-efficient, seamless access.

The Life Science business of Merck operates as MilliporeSigma in the U.S. and Canada.

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