Drug Discovery through Data Mining.

CCDC
advancing structural science

Effective mining of data can be used to generate new ideas in drug discovery.

What ligands show similar interaction patterns?

What modifications are tolerated?

Which structural motifs bind similar binding sites to your target?

By mining existing data you can answer these questions and generate new ideas for modifications or scaffold hops.

Discovery is getting harder.

Double the cost from 2010

$2.17 billion
Average cost of the R&D process per drug (USD)

10-12 years
The average time to take a molecule from discovery to market.

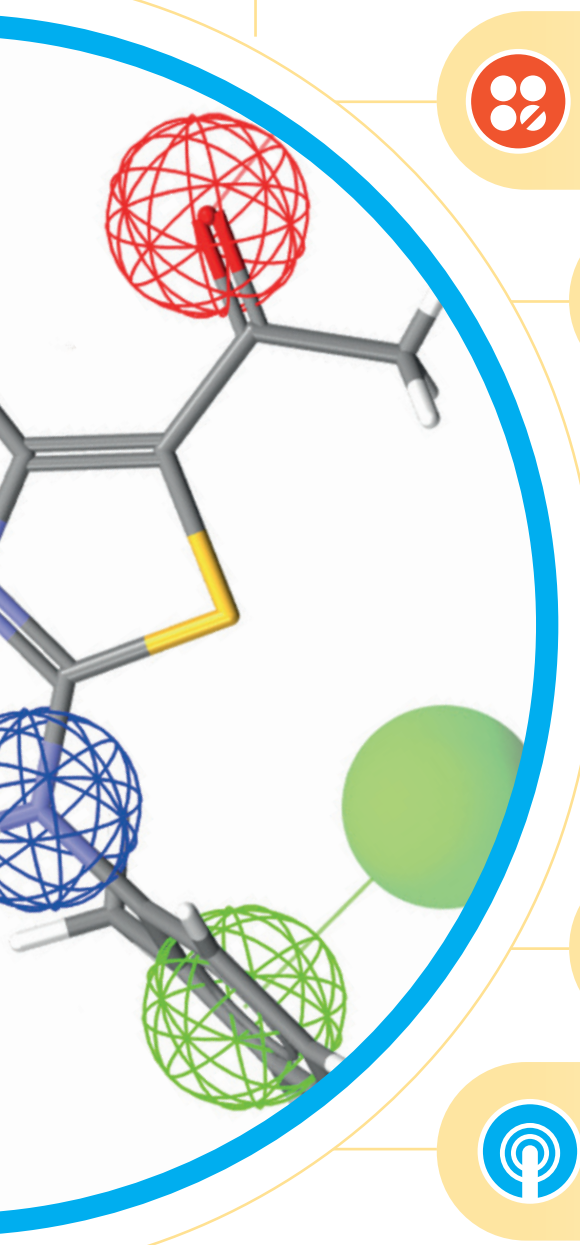
Innovative technologies could speed the process up
15 times

Source: 'Intelligent drug discovery - Powered by AI' (Deloitte Insights, 2019).

Innovation is required.

Here we describe the software CSD-CrossMiner, which allows you to mine public and proprietary databases by key pharmacophore features and generate new ideas in your drug discovery program.

1. Fast, flexible querying.
2. Timesaving, instantaneous results.
3. High-quality results produced from two highly trusted sources: The Cambridge Structural Database (CSD) and the Protein Data Bank (PDB).



User-editable feature definitions:
Tailor features per user and adjust as needed.

Excluded volume:
Define occupational volume - making it inaccessible to other molecules in the system.

(CSD) and (PDB) included:
Save time and money with a ready-to-use implementation of the most trusted databases for small and large molecules.

In-house database:
Search your own proprietary database by key pharmacophore features.

Customise feature definitions:
Improve the granularity of search and explore new chemistry.

Interactive user interface:
Receive instantaneous results - no need to wait for a completed search.

ORIGIN

Roche: A versatile pharmacophore query tool for successful modern drug discovery.

The CCDC developed CSD-CrossMiner in collaboration with Roche. It allows search of public and proprietary databases by pharmacophore. This closes an important gap in structural data mining, and allows scientists to learn from available crystal structures already solved.

Read more: Korb *et al*, J. Med. Chem.

CASE STUDY

University of Groningen.

In this paper, Dr Markella Konstantinidou *et al.* used CSD-CrossMiner to define a pharmacophore search against a reference PDB structure with a binding pattern very similar to their scaffold. The search returned 37 known structures that could serve as potential future scaffolds.

Read more: Case Study - Konstantinidou *et al*, Eur. JOC

CASE STUDY

Rediscovering through mining.

In this whitepaper the authors show how CSD-CrossMiner could be employed, and look to "re-discover" a known drug starting from a pharmacophore query against the target's natural ligand.

Read more: Whitepaper

The Cambridge Crystallographic Data Centre
www.ccdc.cam.ac.uk

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