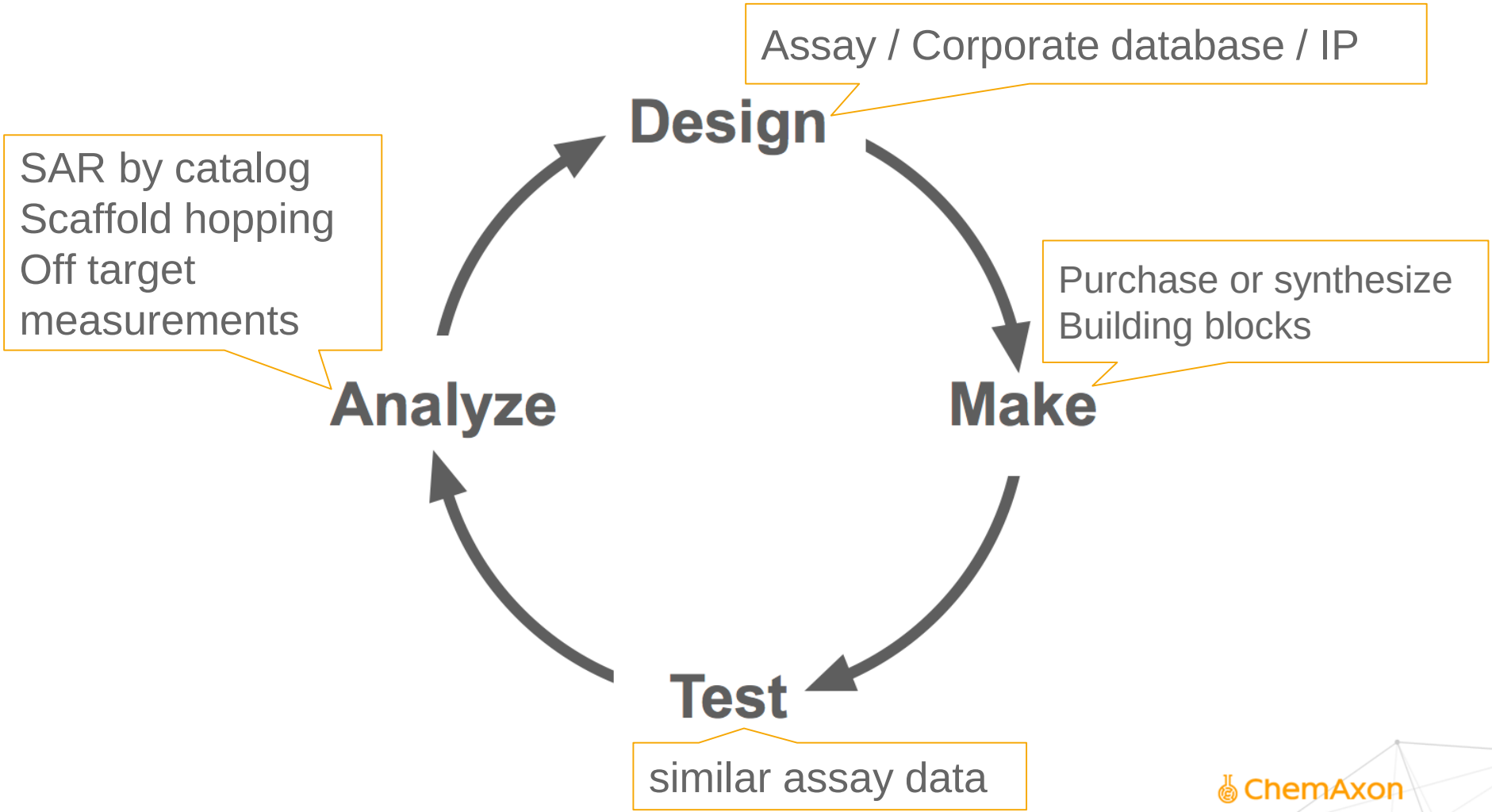
ChemAxon

András Volford
András Strácz
Iván Solt

Project Haystack


Assay / Corporate database / IP
Design
SAR by catalog
Scaffold hopping
Off target
measurements
Purchase or synthesize
Building blocks
Analyze
Make
Test
similar assay data

ChemAxon

Information you don’t know it exists

Universal, domain agnostic, simple access to the complete research history.

Goal

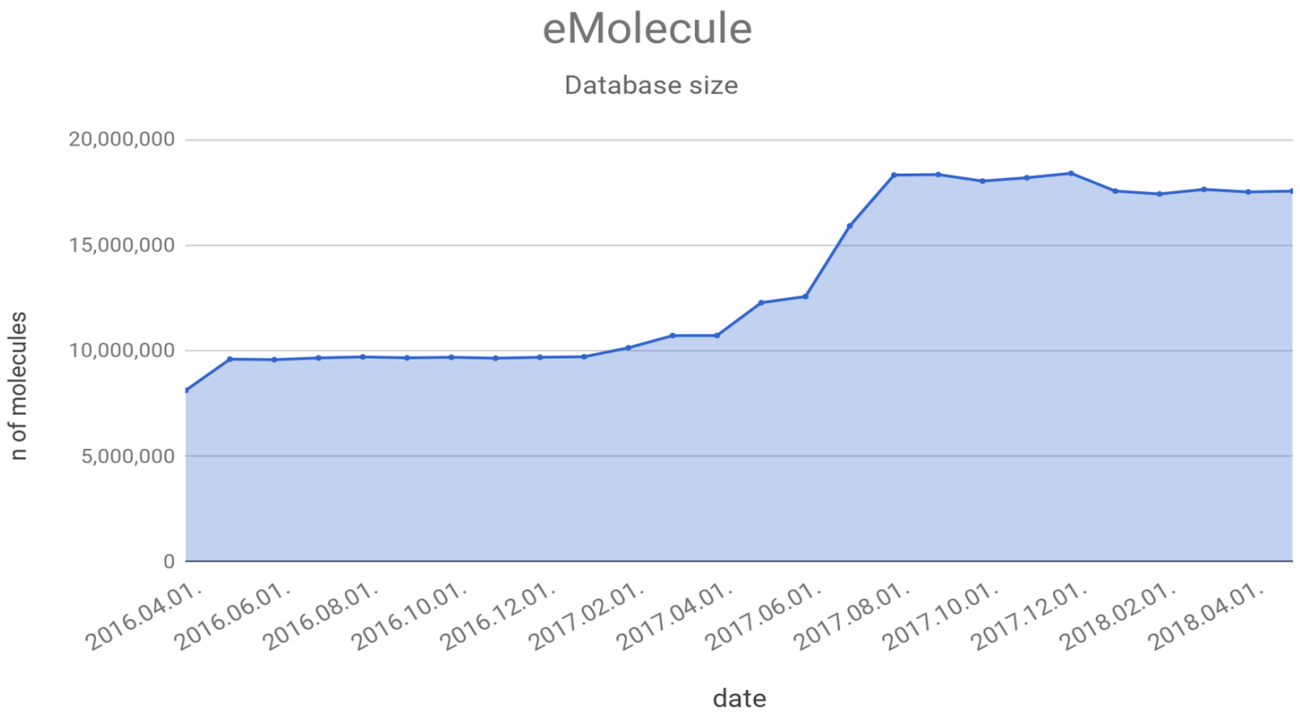
Indexing arbitrary amount of data and running substructure and similarity search.

Quickly explore your chemical space

Current, partial solutions

Some searchable implementations for specific databases.

Information flood



ChemAxon

Databases

626 k

1.7 M

17.6 M

64 k

39.9 M

28.3 M

5.8 M

94.5 M

18 M

18.5 M

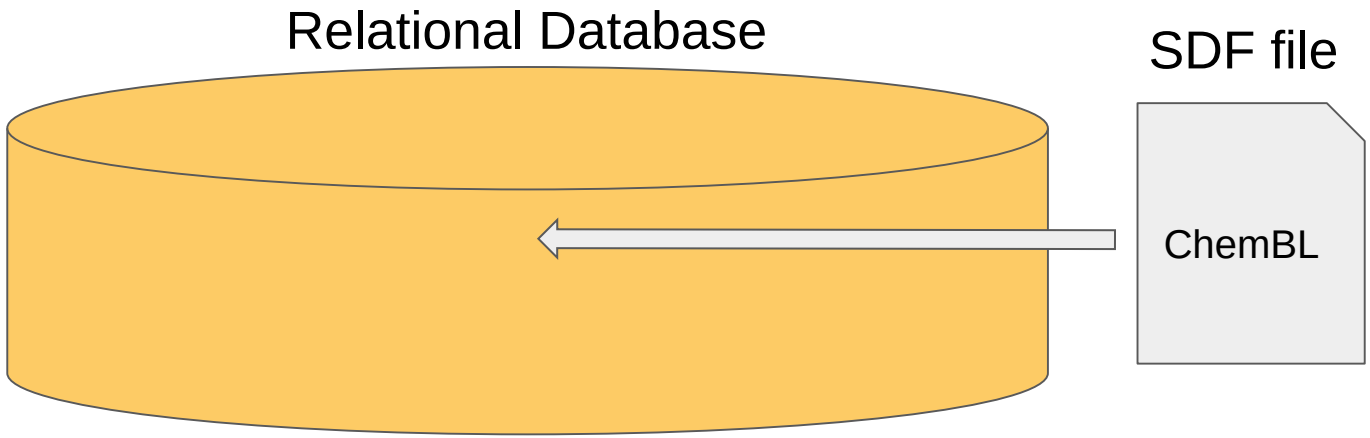
75 M
or
142 M

6.5 M
or
105 M

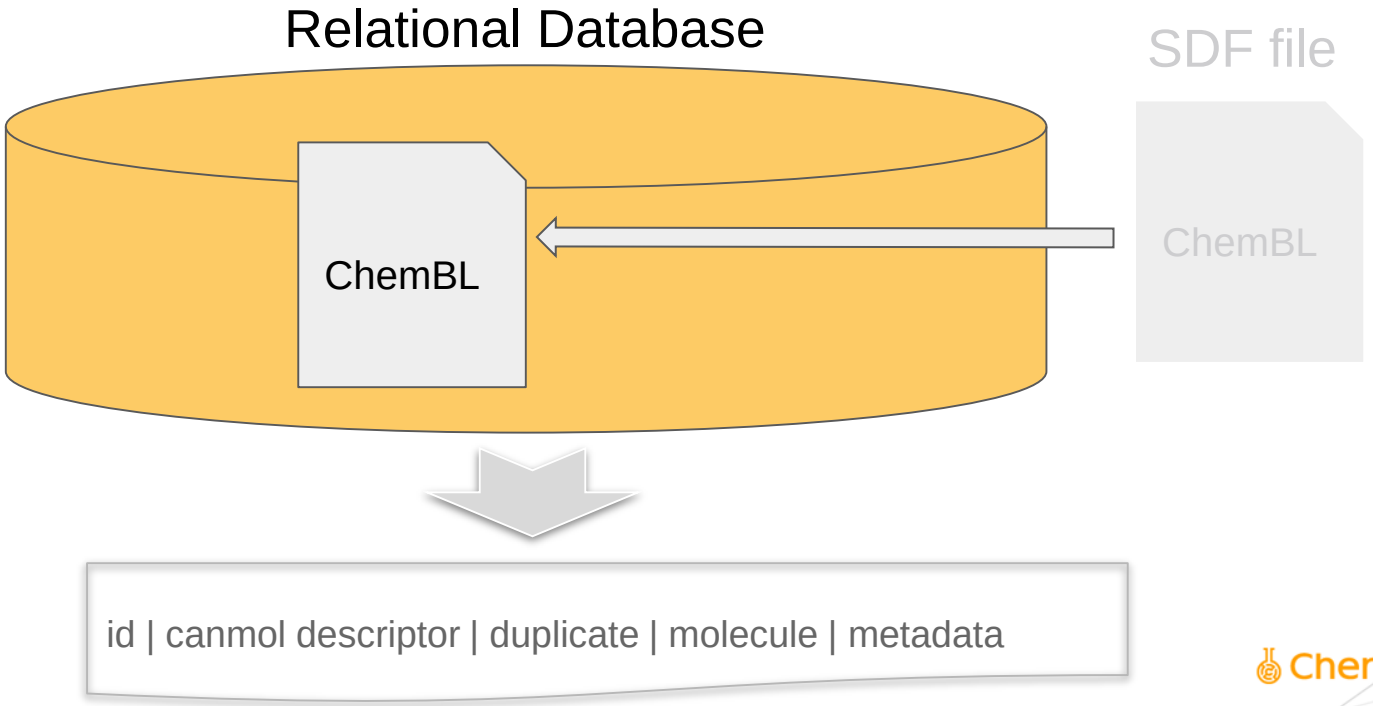
Your Corporate DB

ChemAxon

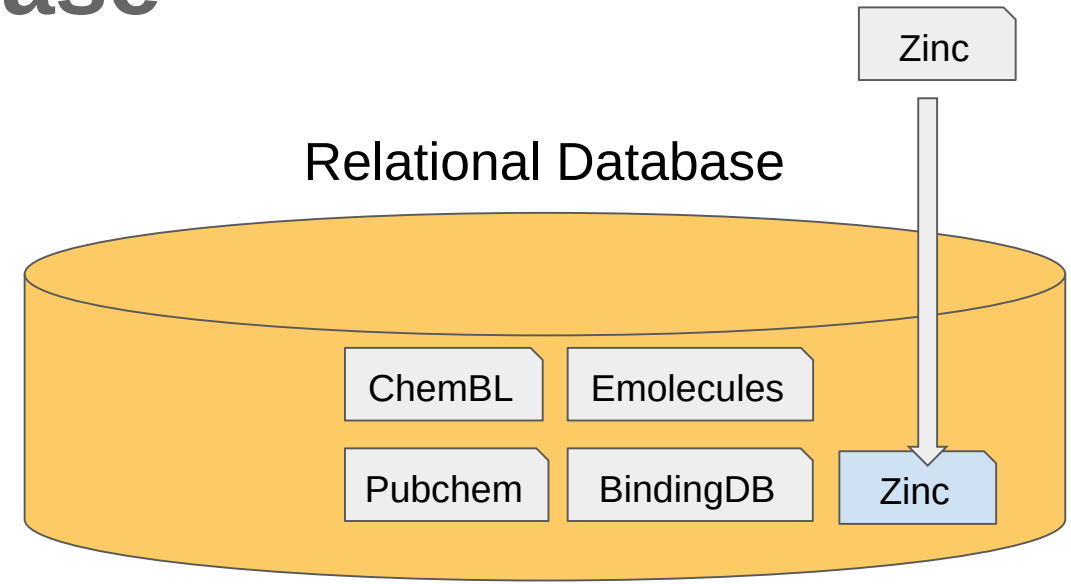
Database



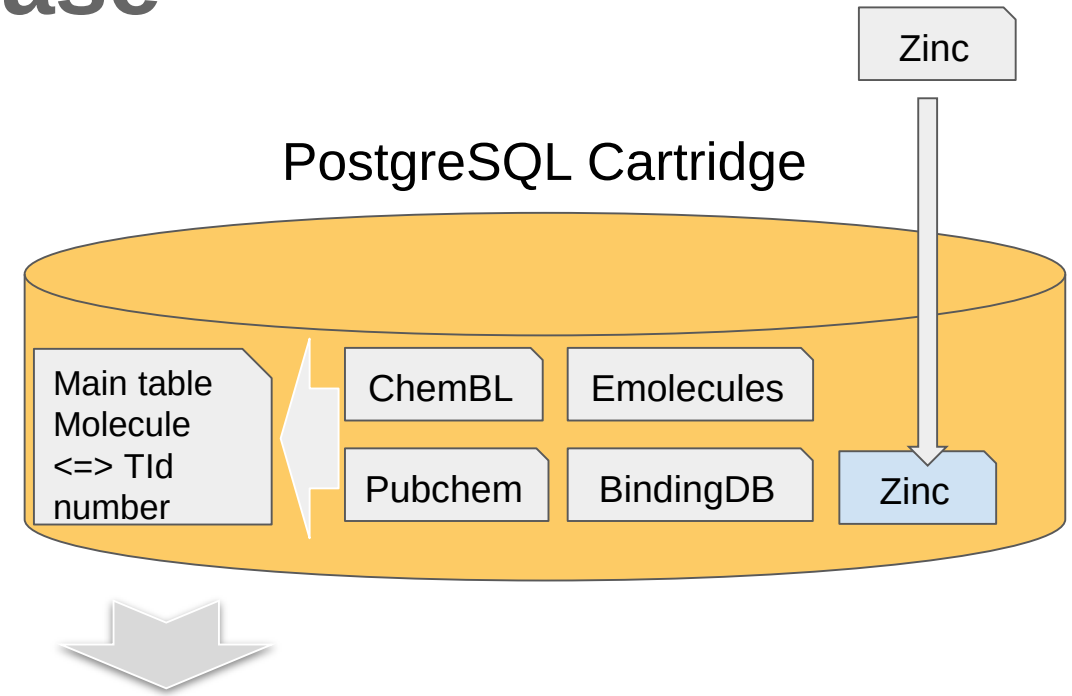
Database



Database

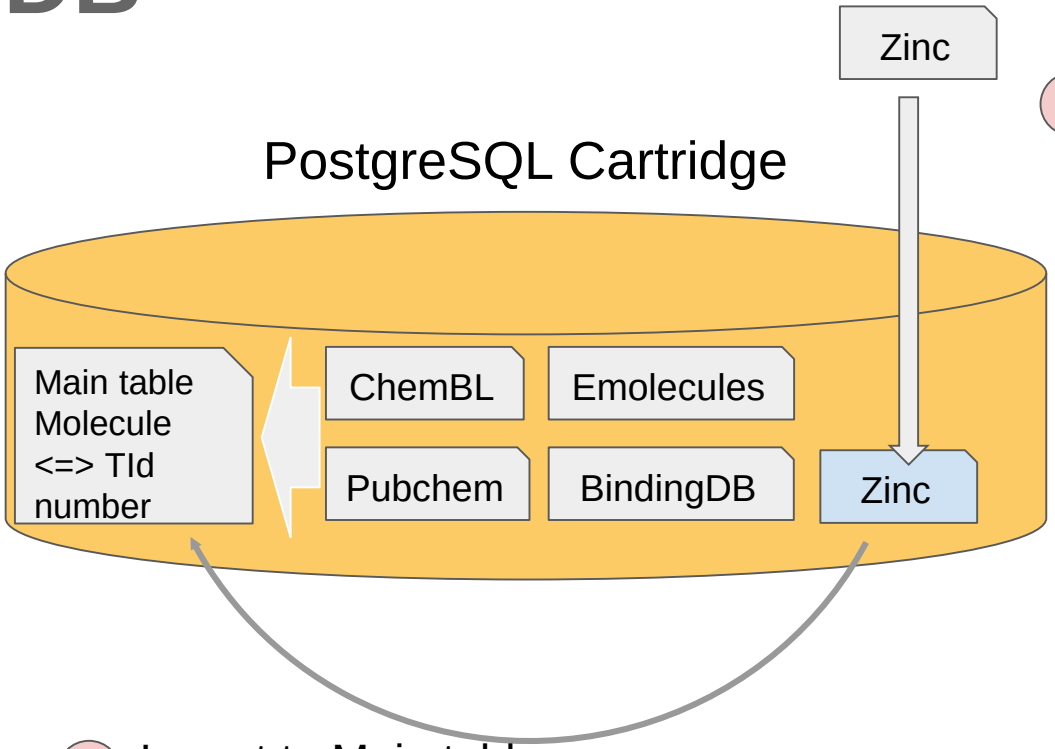


Database



id | canmol descriptor | molecule | reference IDs

Insert DB



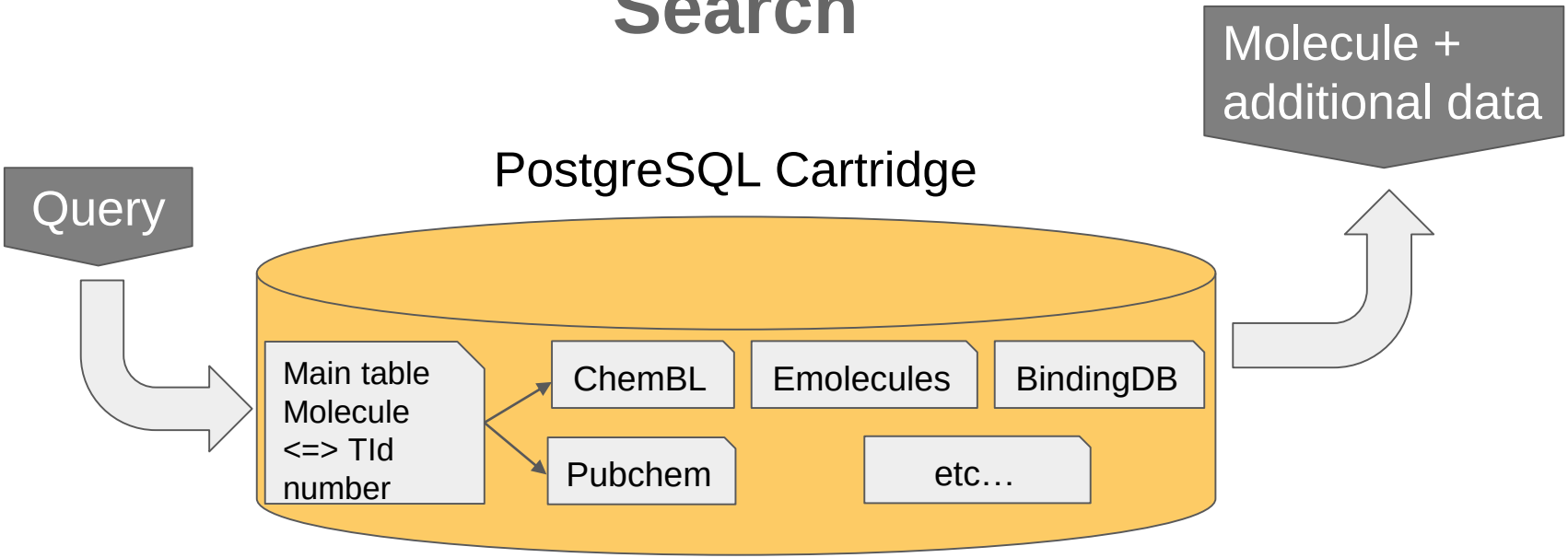
1 Load into new table
mark duplicates based on inchikey

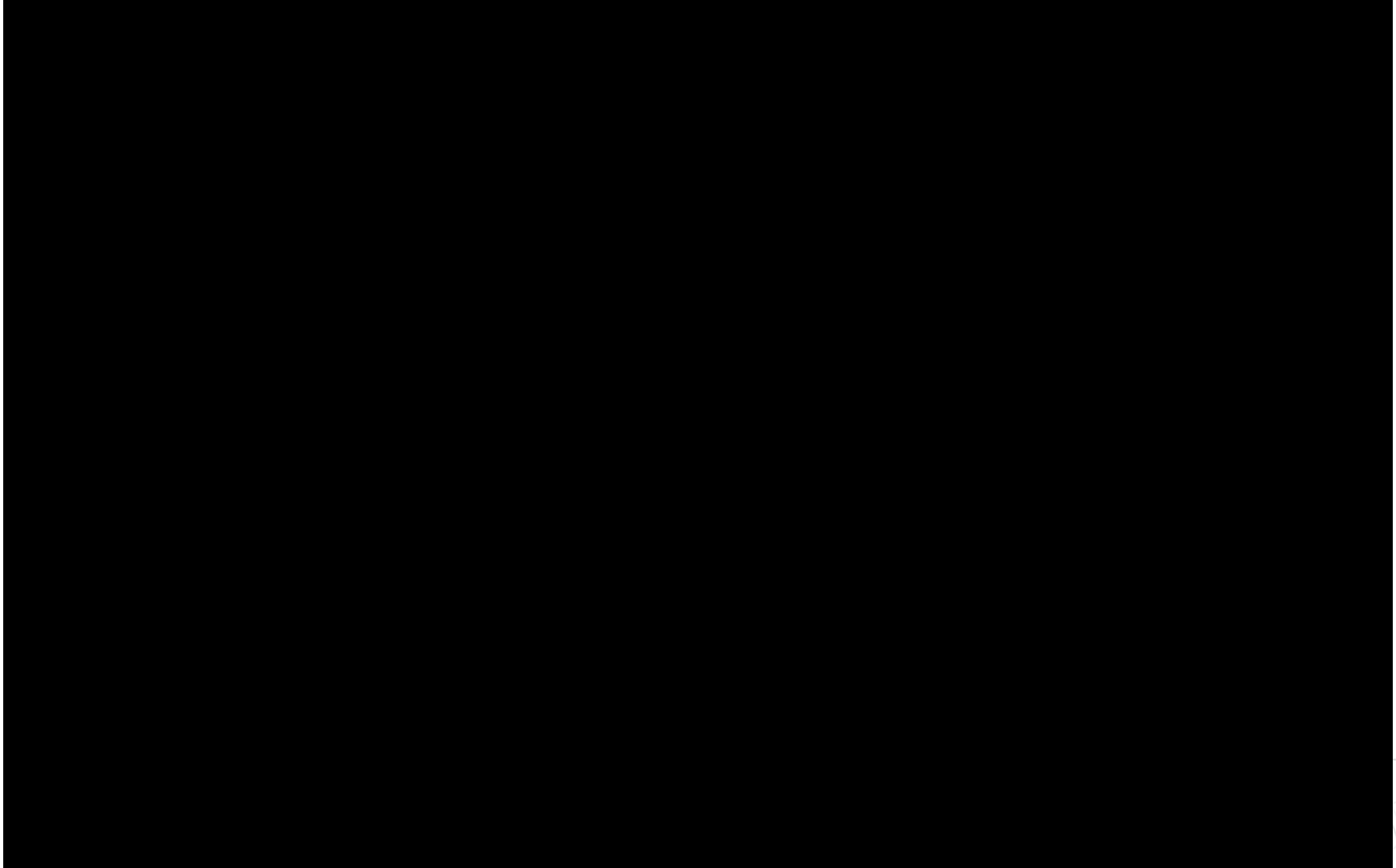
2 Import to Main table
For non duplicate structures
If new entry created insert molecule
else update TId numbers

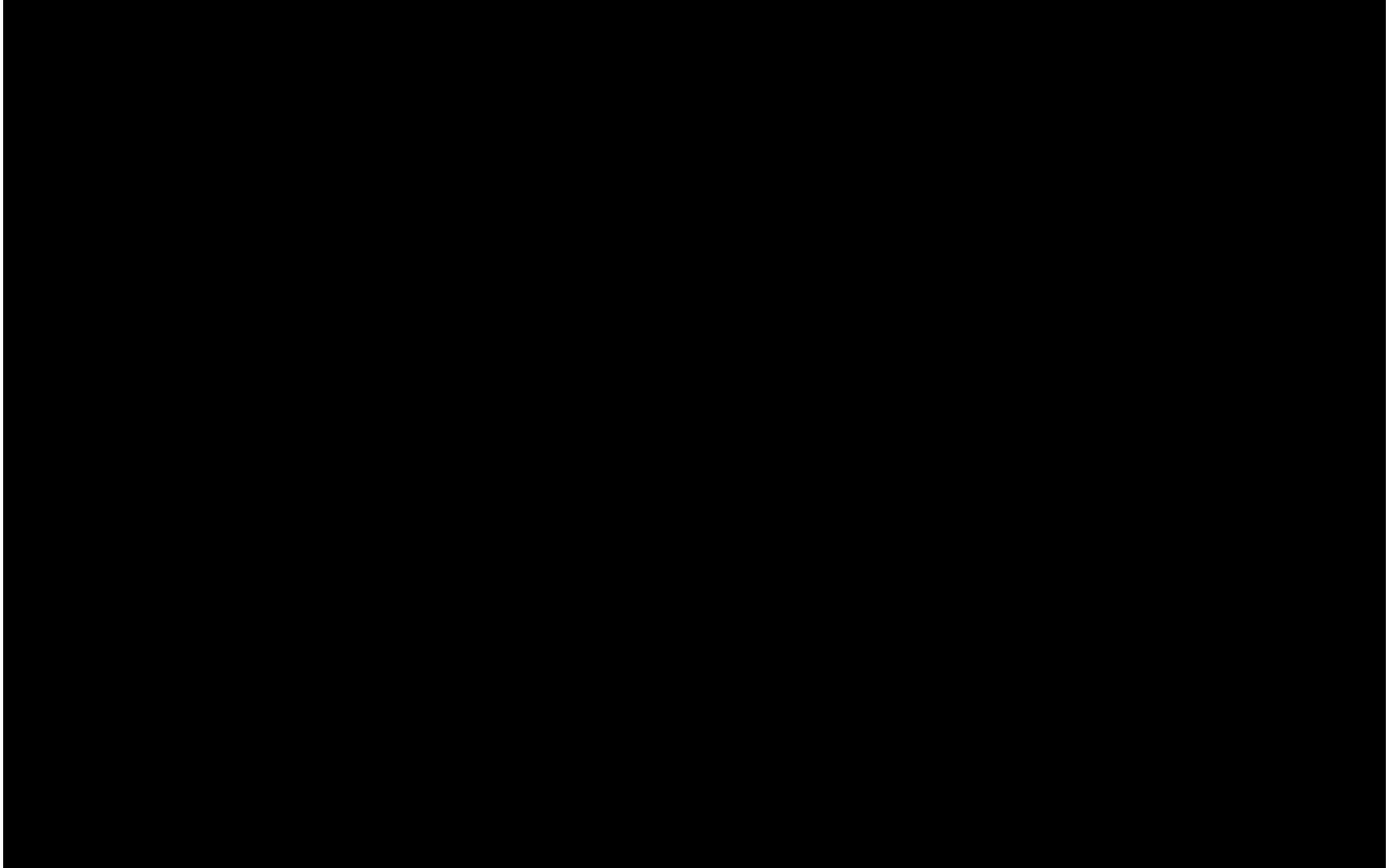
ChemAxon

Technical

Search







See it live at BOOTH # 543

ChemAxon