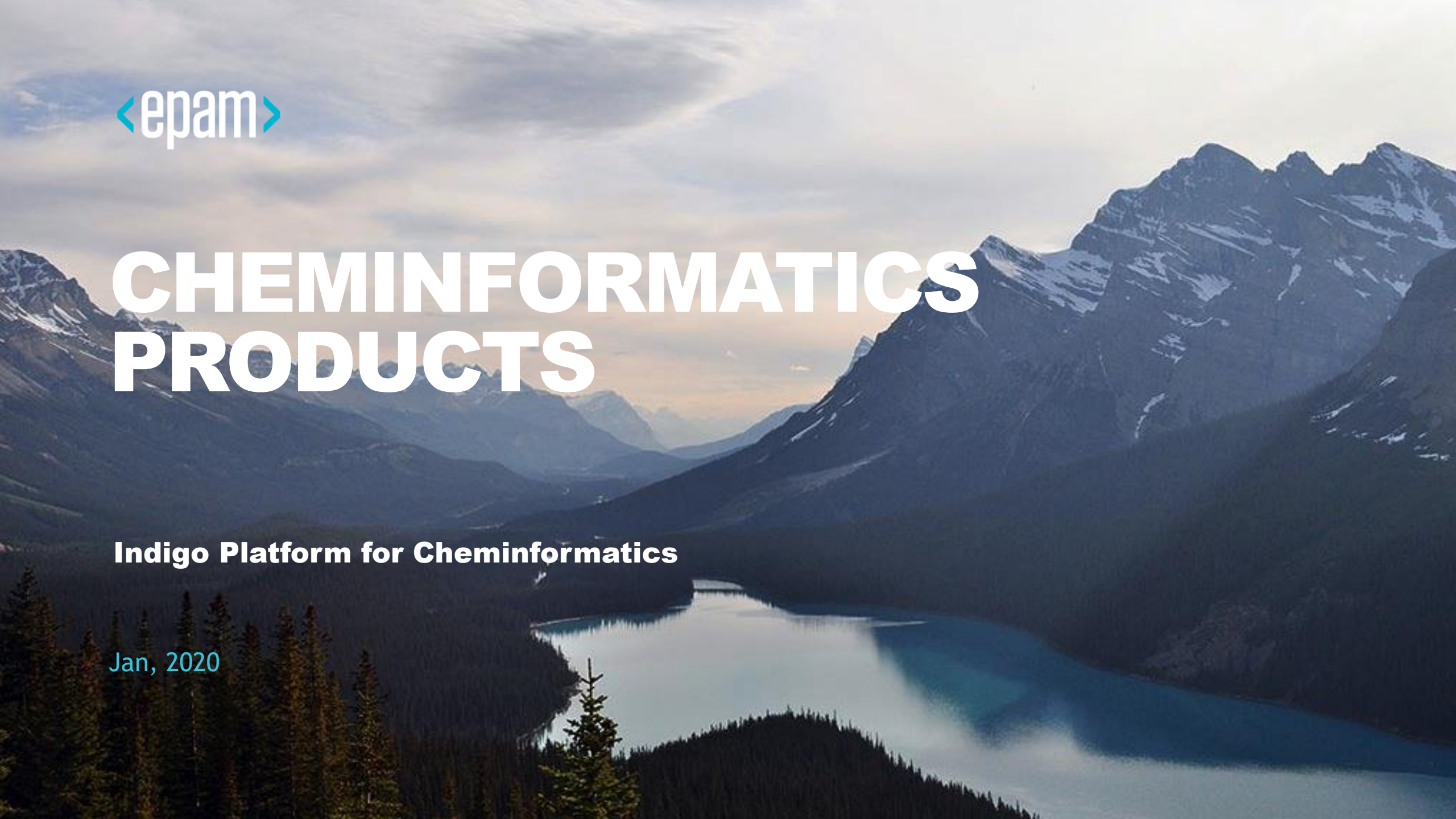


CHEMINFORMATICS PRODUCTS

Indigo Platform for Cheminformatics

Jan, 2020

INDIGO PLATFORM

Indigo Platform

Web (view)

KETCHER

Import chemistry	Export chemistry	Editing of chemical structures	Lightweight portable JavaScript

Middleware (controller)

INDIGO

• Import, export chemistry • Languages: Java, Python, C#	Transform chemistry: • API • Reactions	Calculate: • Properties • Layout • AAM • Scaffold	Render: • SVG • PNG • JPG • Grid

IMAGO

Convert images to chemistry:
- PNG
- JPG
- PDF

Storage (model)

BINGO

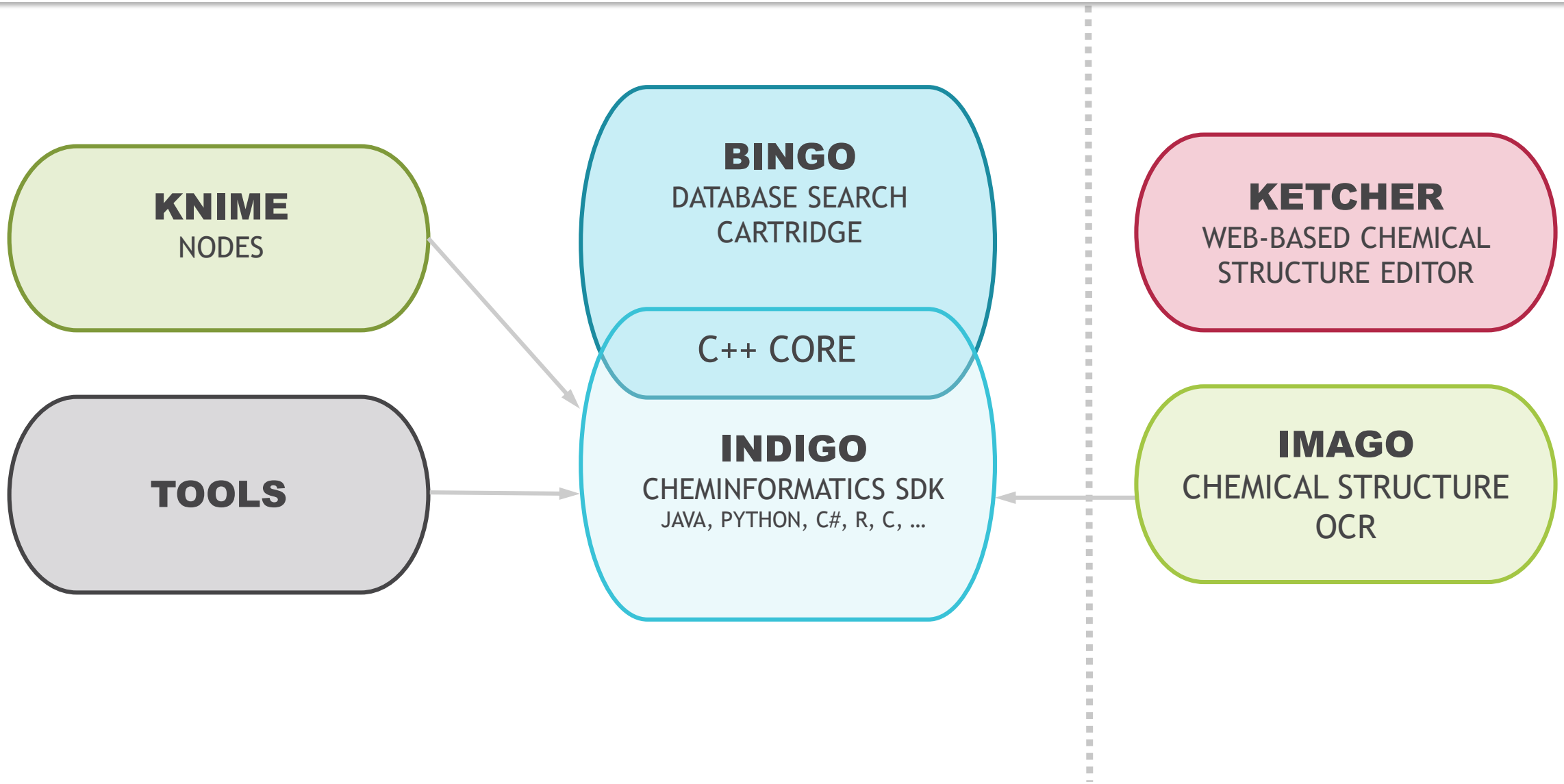
Import, export chemistry	RDBMS: • Oracle • PostgreSQL • Microsoft SQL Server	Search: • Sub • Exact • Similarity	Utility Properties: • SMILES • Aromatic • AAM

BINGO NO-SQL

Storages:
- File-based
- Lucene

Bingo and Indigo utilities

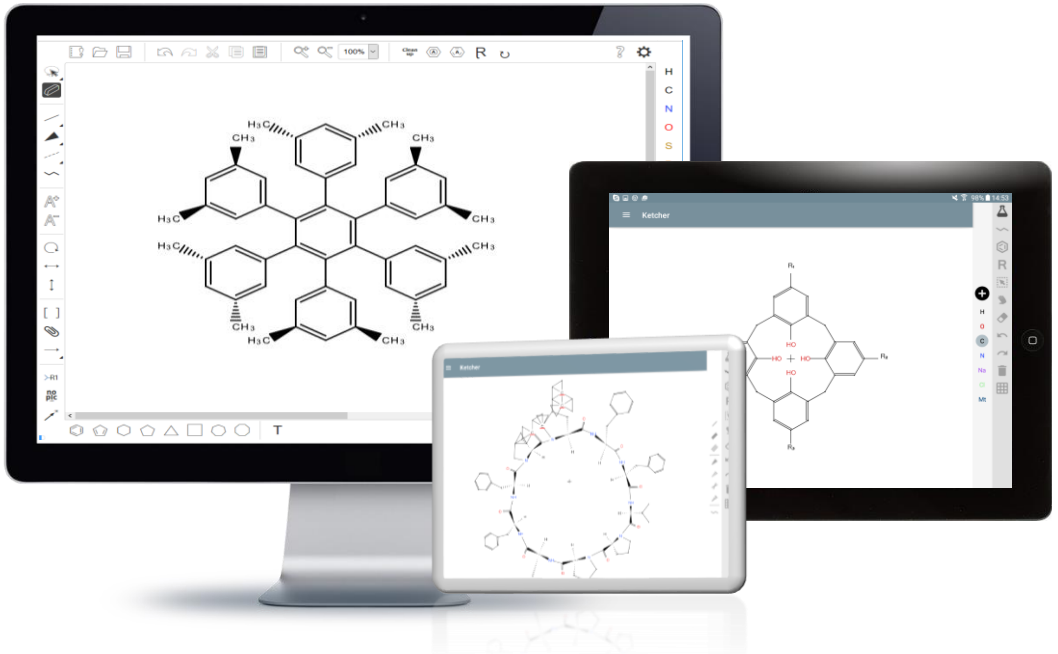
PRODUCTS OVERVIEW



KETCHER
WEB-BASED CHEMICAL STRUCTURE TOOL

SUMMARY

- EPAM developed an open-source web-based chemical structure editor incorporating high performance, good portability, light weight, and ability to easily integrate into a custom web-application.



KEY HIGHLIGHTS

- Use of SVG to achieve best quality in-browser chemical structure rendering
- Ability to load and save structures in MDL/Biovia molecular file format, InChI, ChemAxon Extended SMILES, ChemAxon Extended CML file formats
- Fast 2D structure representation that satisfies common chemical drawing standards
- 3D structure visualization
- OCR - ability to recognize structures at pictures (image files) and reproduce them
- Complete stereochemistry support during editing, loading, and saving chemical structures
- Storing full history of actions, with the ability to rollback to any previous state
- Direct input of atom label and charge
- Languages: JavaScript with third-party libraries

INDIGO CHEMINFORMATICS

SDK

- Indigo SDK is highly configurable and extensible and allows creating C/C++/C#/Java/Python plug-ins for it
- Excellent portability. Supported platforms: Windows/Linux/Mac - 32-bit and 64-bit
- Original Algorithms

ORIGINAL ALGORITHMS

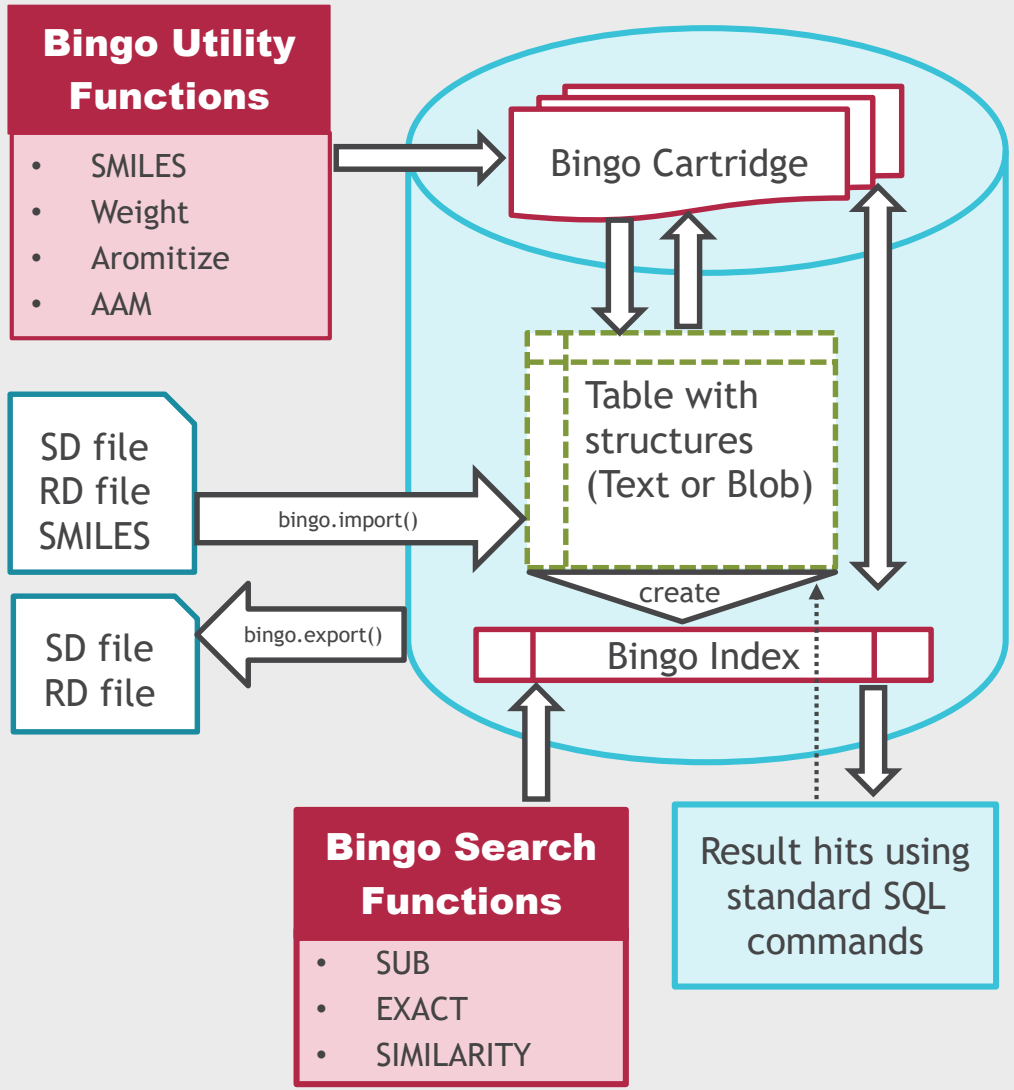
- Substructure matching (subgraph isomorphism)
- Aromaticity matching and de-aromatization
- Tautomer (sub)structure matching
- Chemical resonance (sub)structure matching
- Canonical SMILES (with stereochemistry)
- 2D molecule and reaction layout
- Reaction atom-to-atom mapping (AAM), based on maximum common substructure (MCS)
- Molecule and reaction fingerprints, based on sub-tree enumeration tree canonical codes

FEATURES

- Input formats support: Molfiles/Rxnfiles v2000 and v3000, SDF, RDF, SMILES, SMARTS
- Molecule and reaction rendering. Best picture quality among all available products. Easy SVG support
- Automatic layout for SMILES-represented molecules and reactions
- Canonical (isomeric) SMILES computation
- Exact matching, substructure matching, SMARTS matching. Highlighting support
- Matching of tautomers and resonance structures
- Molecule fingerprinting, molecule similarity computation
- Molecular weight, molecular formula computation
- R-Group deconvolution and scaffold detection

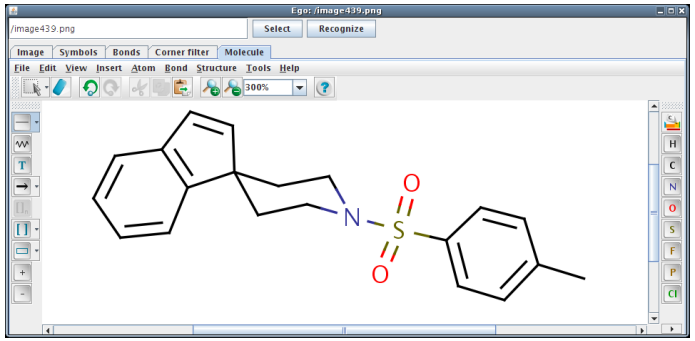
BINGO
DATABASE SEARCH CARTRIDGE

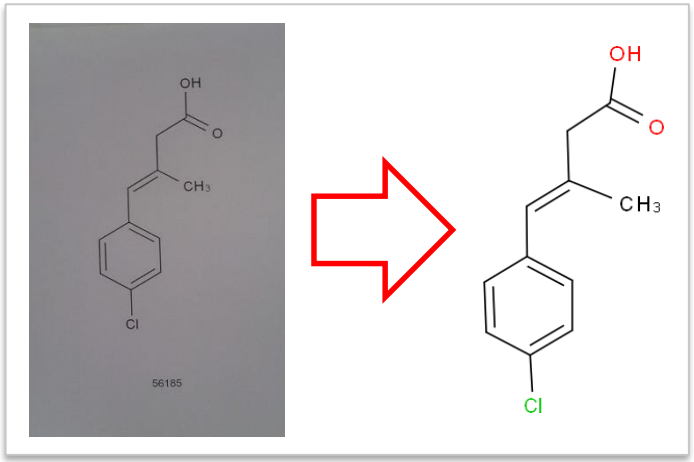
- Open-source chemistry cartridge for Oracle, SQL Server, PostgreSQL RDBMS.
- Store, index, and search molecules and reactions with ordinary SQL commands.
- Powerful cheminformatics functionality combined with all the comfort of relational database.
- Supports the most requested features for molecule and reaction databases: exact/substructure/similarity search, format conversion, canonical SMILES, reaction AAM.
- Performance, scalability, portability, and unique chemical features
- Supported platforms: Windows/Linux/Mac; 32-bit and 64-bit
- Supported database systems:
  - Oracle
  - Microsoft SQL Server
  - PostgreSQL
  - NoSql (Lucene SOLR, Sinequa)
- No problems with large databases like PubChem (> 40M entries)



IMAGO
CHEMICAL STRUCTURE OCR LIBRARY

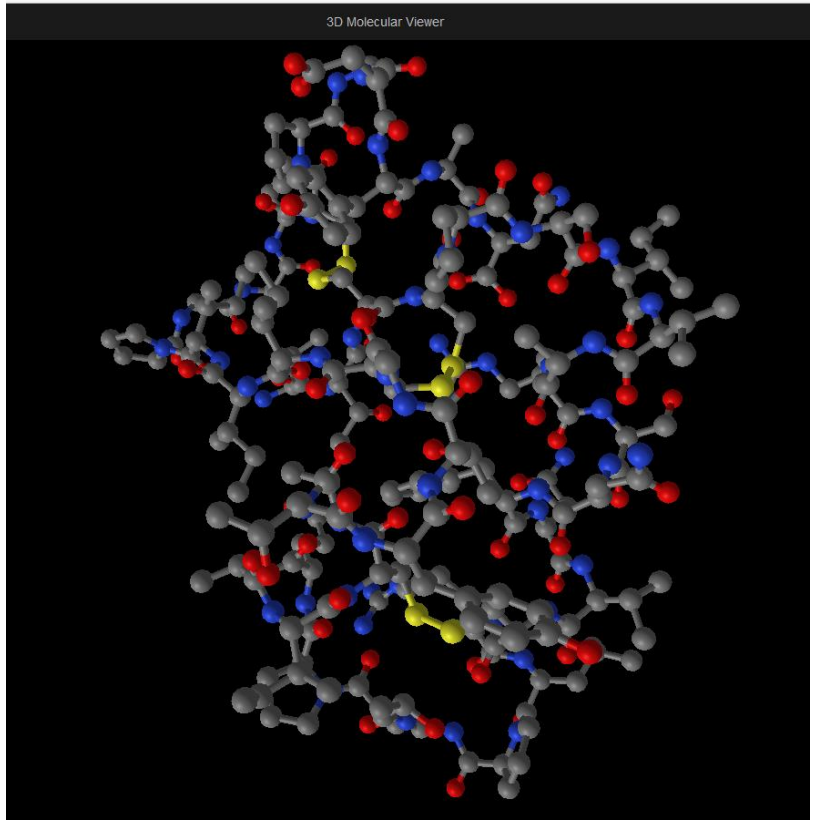
- Support for PNG files for input, each file containing one molecule
- Support for MDL/Symyx Molfile for output
- Recognized molecular elements: Single, double, triple bonds, Atom labels, subscripts, isotopes, charges, Superatoms, Aromatic rings, Touching characters
- Stereochemistry (up- and down-bonds)
- Java GUI and command-line utility
- OpenCV, C/C++
- Patent processing
- Mobile input via camera photos
- Papers indexing for molecule search
- Exposing C interface to applications
- Java wrapper available for all supported platforms

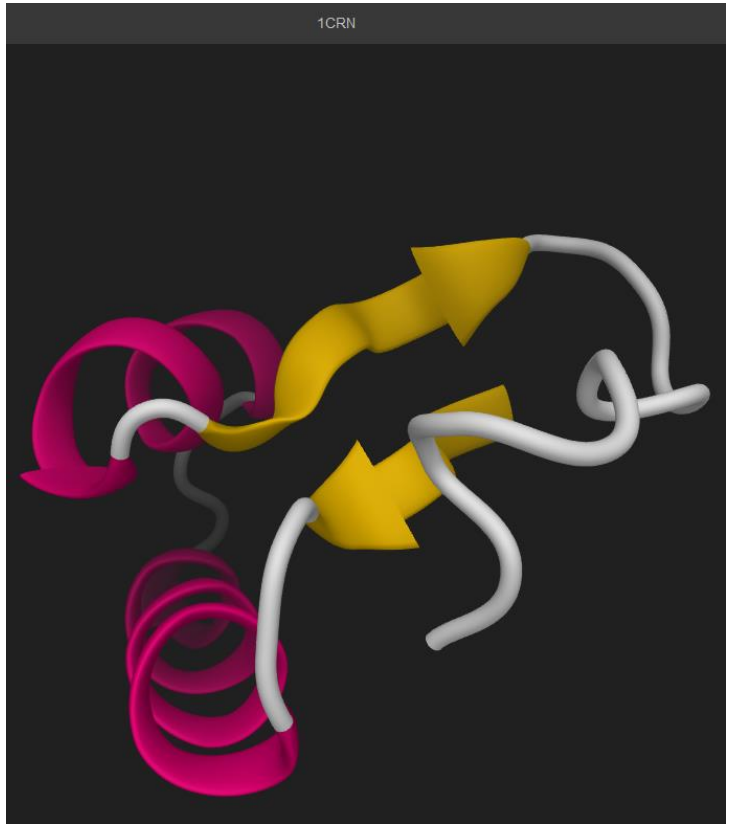




INDIGO PLATFORM PRESENT/FUTURE

- Ketcher 3D viewer integration
- Imago OCR algorithms and improvements
- Bingo and Indigo improvements
- Make it faster
- Make it more functional
- Indigo service





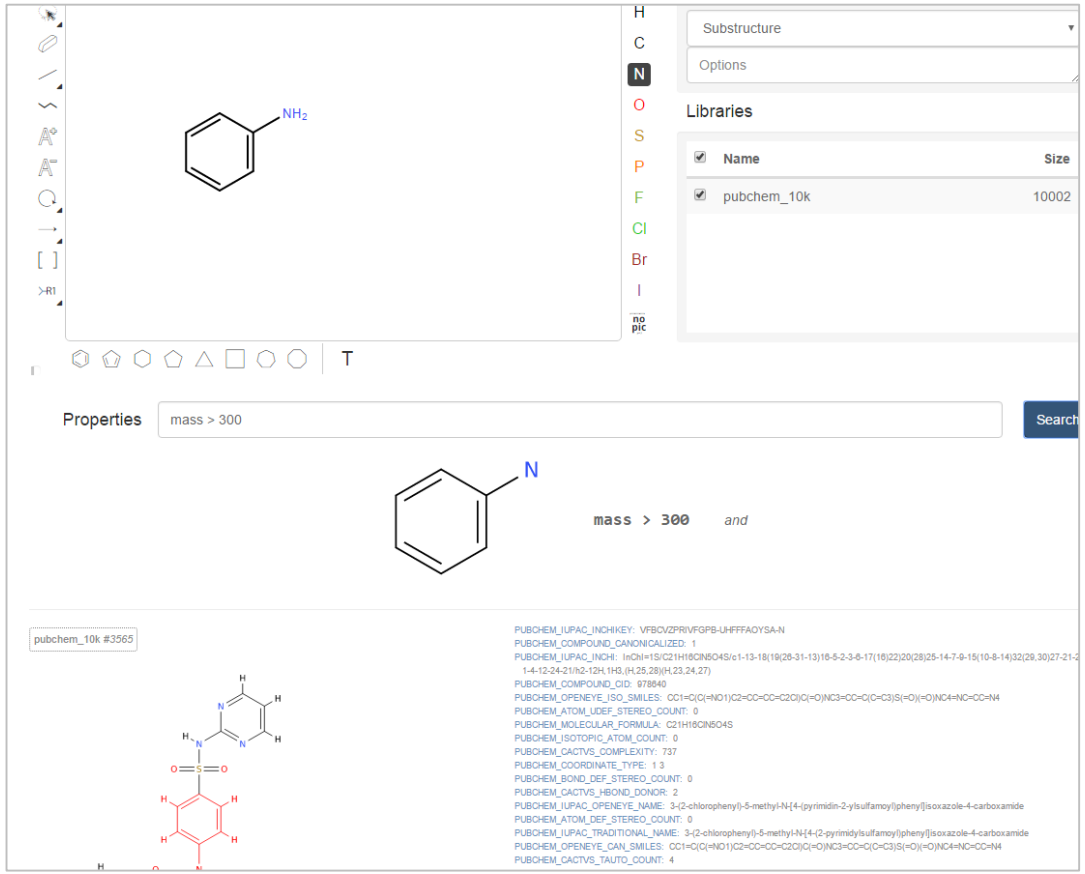
INDIGO PLATFORM PRESENT/FUTURE

INDIGO SERVICE

- Fast insert (about 10k per second)
- Google-like search
- Support users/projects
- Easy deploy REST (Docker)
- New technologies and features…

INNOVATIONS

- RESTful service (Python + Flask+Indigo)
- Easy deployment (Docker)
- Search chemistry (Bingo)
- Search properties (string and numbers)
- Fast upload* (>5000 structures/sec)
- Modern interface
- Etc.



OPEN SOURCE

- About 3 000 downloads in 2016
- 847 downloads by Industry
- Downloads from more than 40 countries
- Downloads from more than 250 companies
  Merck, Novartis, Lilly, BASF SE, Bayer, Royal Society of Chemistry, ChemBridge Corporation, IBM, Intel, other
- Downloads from more than 400 universities

Product \ Position		Business/Industry	C-Level	Manager	Other	Student/Academic	Totals
Bingo		166			1	204	**371**
ChemDiff	4	10				55	**69**
Imago		95				247	**342**
Indigo	7	209		1	1	753	**971**
Indigo ELN	7	177				482	**666**
Ketcher	5	78	1		1	211	**296**
Legio	3	7				28	**38**
Parso	4	105			1	95	**205**
Totals	**30**	**847**	**1**	**1**	**4**	**2,075**	**2,958**

BUSINESS DOWNLOADS

All around the world

Country	Totals
USA	199
India	154
China	128
France	53
UK	26
Germany	23
Japan	22
Switzerland	21
Spain	20
Denmark	17
Australia	16
Hungary	16
Italy	14
Korea, South	12
Anguilla	9
Canada	9

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