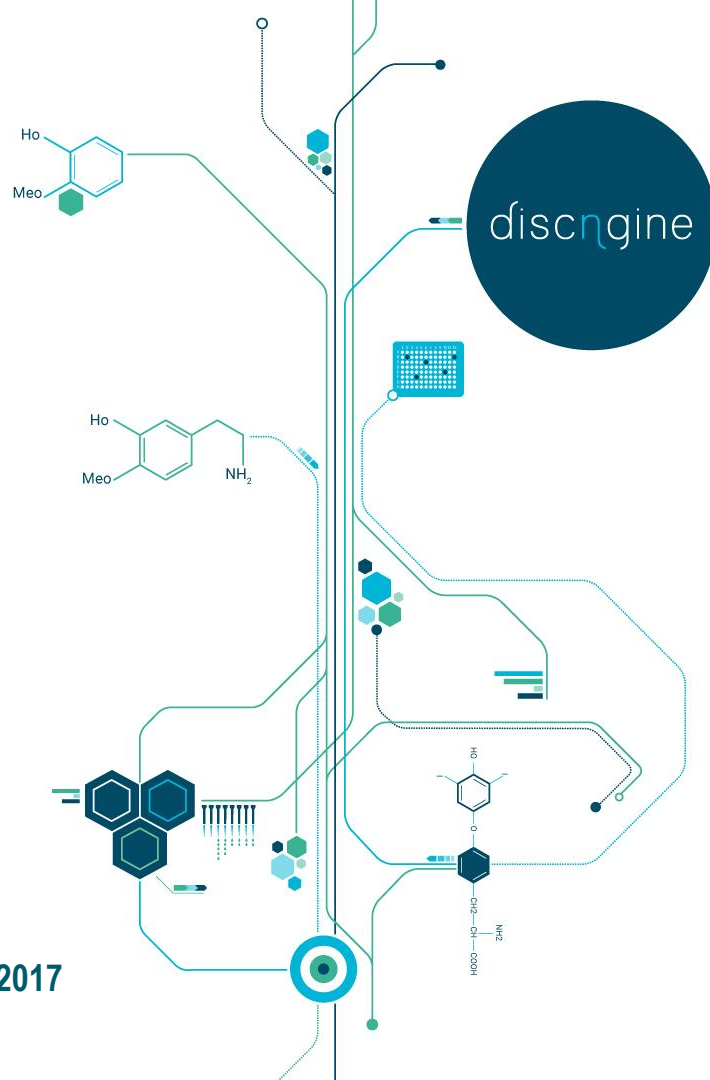


# ChemAxon MarvinJS sketcher integration in Discngine Decision

*Sandra Plumas* CHEMAXON'S 13<sup>TH</sup> EUROPEAN USER MEETING. 10 May 2017



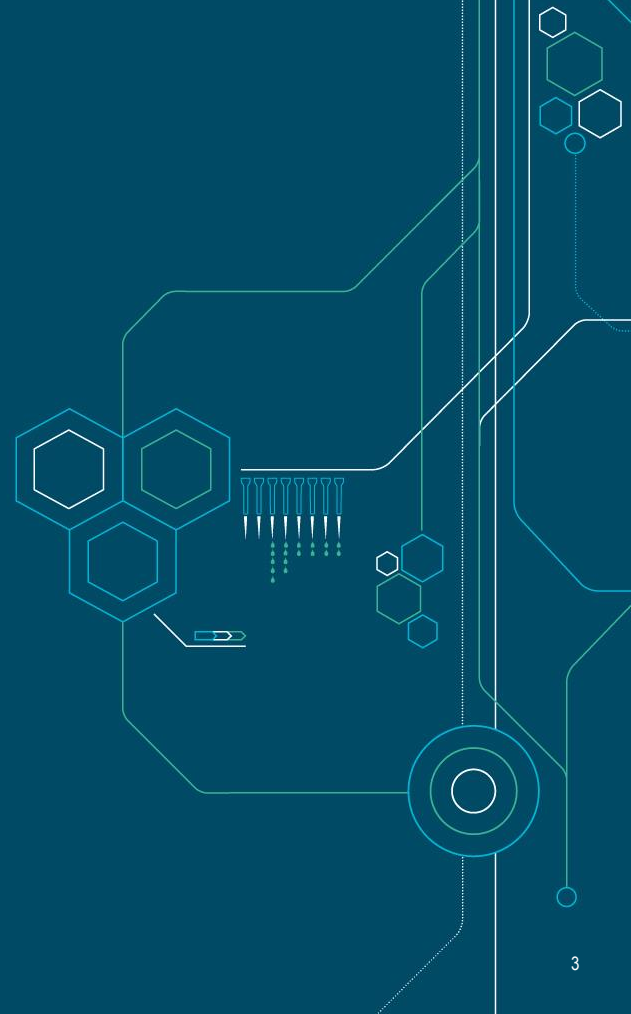


# Agenda

- Company overview
- Discngine Decision Platform
- ChemAxon MarvinJS sketcher in Discngine Decision

01

# COMPANY OVERVIEW





# Discngine



## Services and Solutions for Life Sciences Research Informatics

**Customers:** Sanofi, l'Oréal, IPSEN, Galderma, AbbVie, Merck & Co., GSK, Novartis, Roche, Pierre Fabre, CEREP, Servier, Chugai, DuPont, Galapagos...

*Founded in 2004 - Based in Paris, France - 37 employees*

*More Information: [www.discngine.com](http://www.discngine.com)*





# Discngine

## Business Expertise

- Pharmaceutical Discovery processes
- Screening data acquisition and analysis
- Sample Management
- Cheminformatics
- Decision Making & Reporting





# Integrated technologies



Oracle Application Express (APEX)



*Combine & integrate key research IT component to provide Scientific IT solutions*



# Scientific IT services

Provide consulting, design and development resources for research IT

- **Remote Services**

- > Managed by customer, assisted by discngine experts

- **On-site Services**

- > Managed by customer, assisted by discngine experts

- **Tokens**

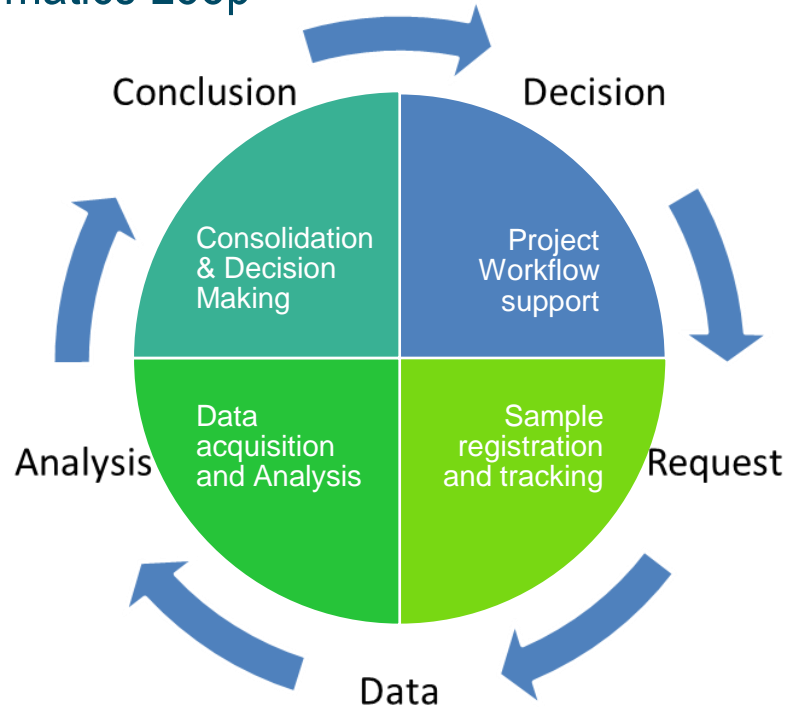
- > On-demand consulting days





# Products

## Research Informatics Loop

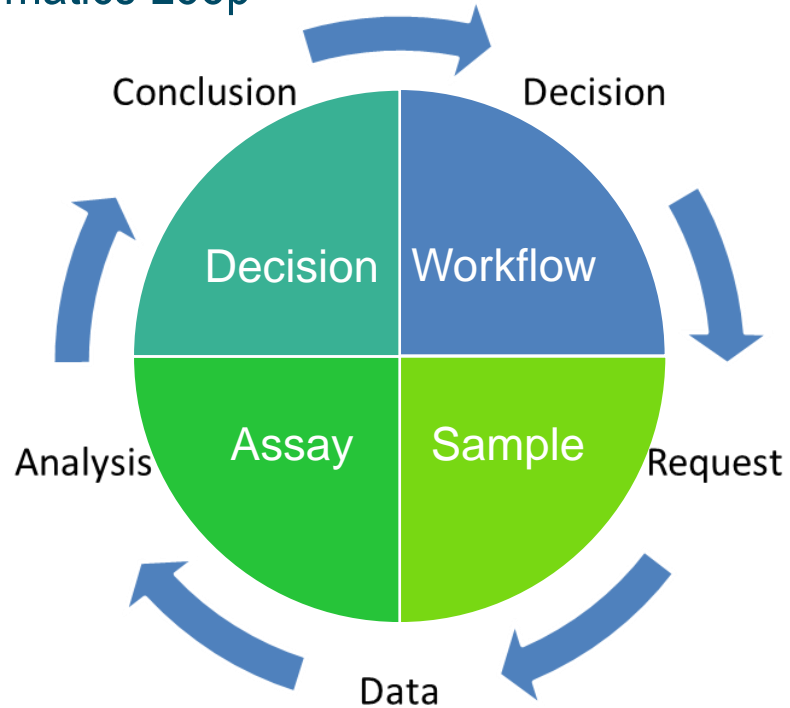






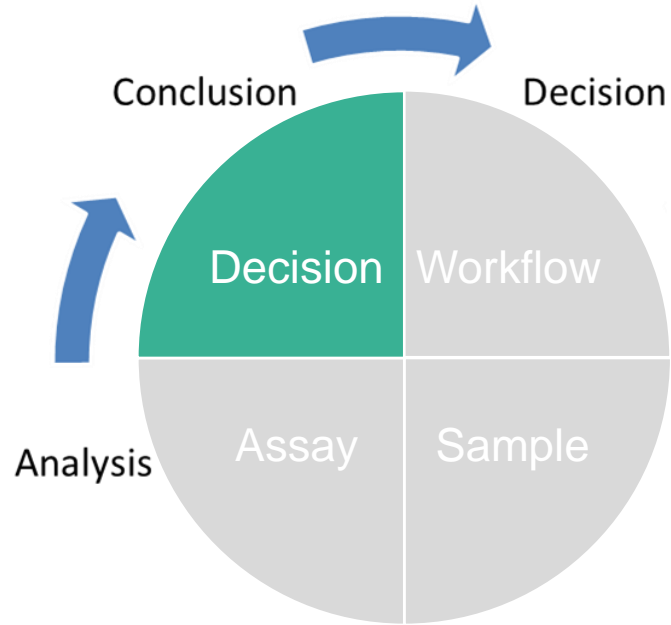
# Products

## Research Informatics Loop



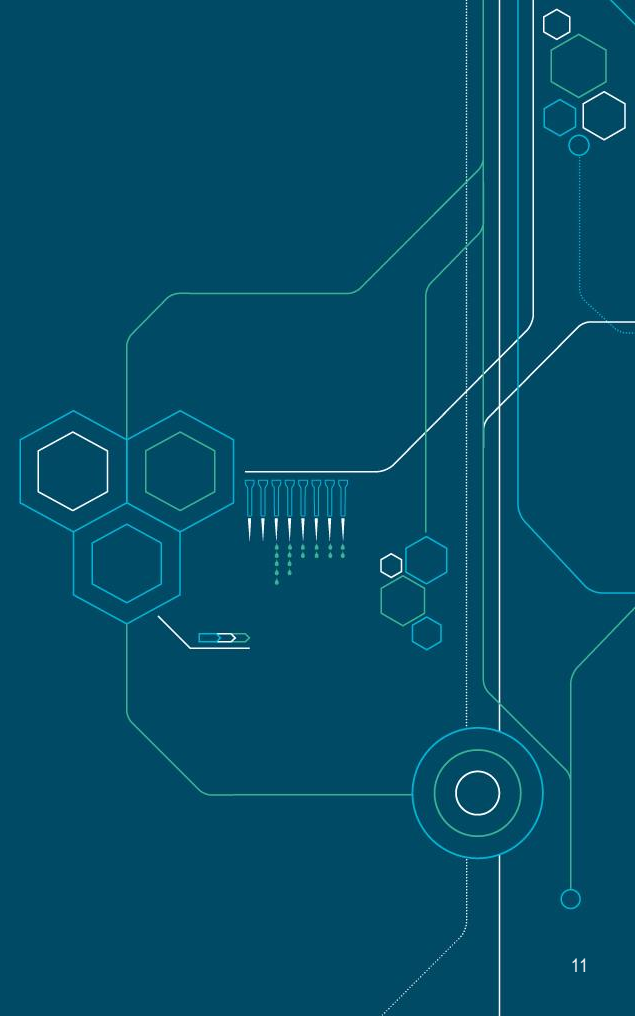


# Discngine Decision

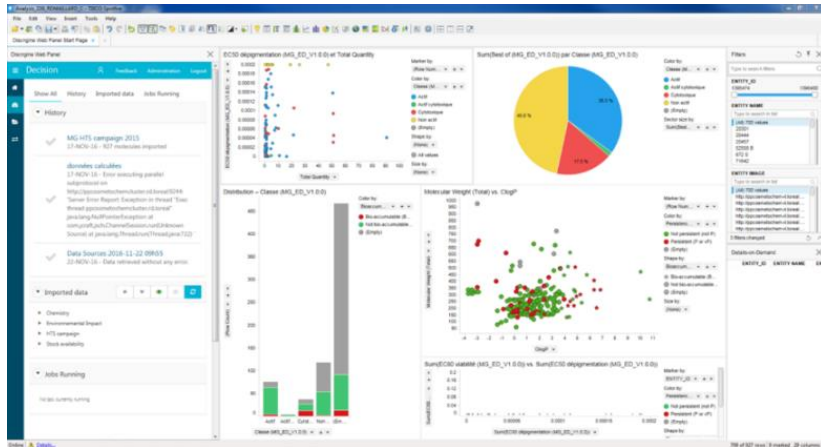


02

# DISCENGINE DECISION



# Discngine Decision



decision making platform...

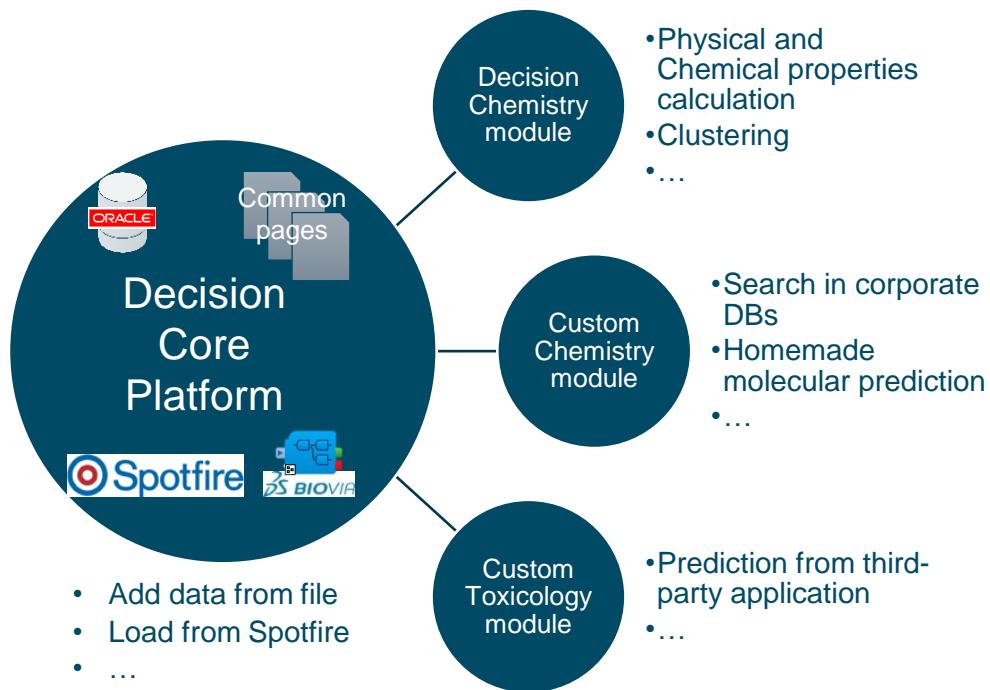
focused on entities of interest...

gathered in reports...

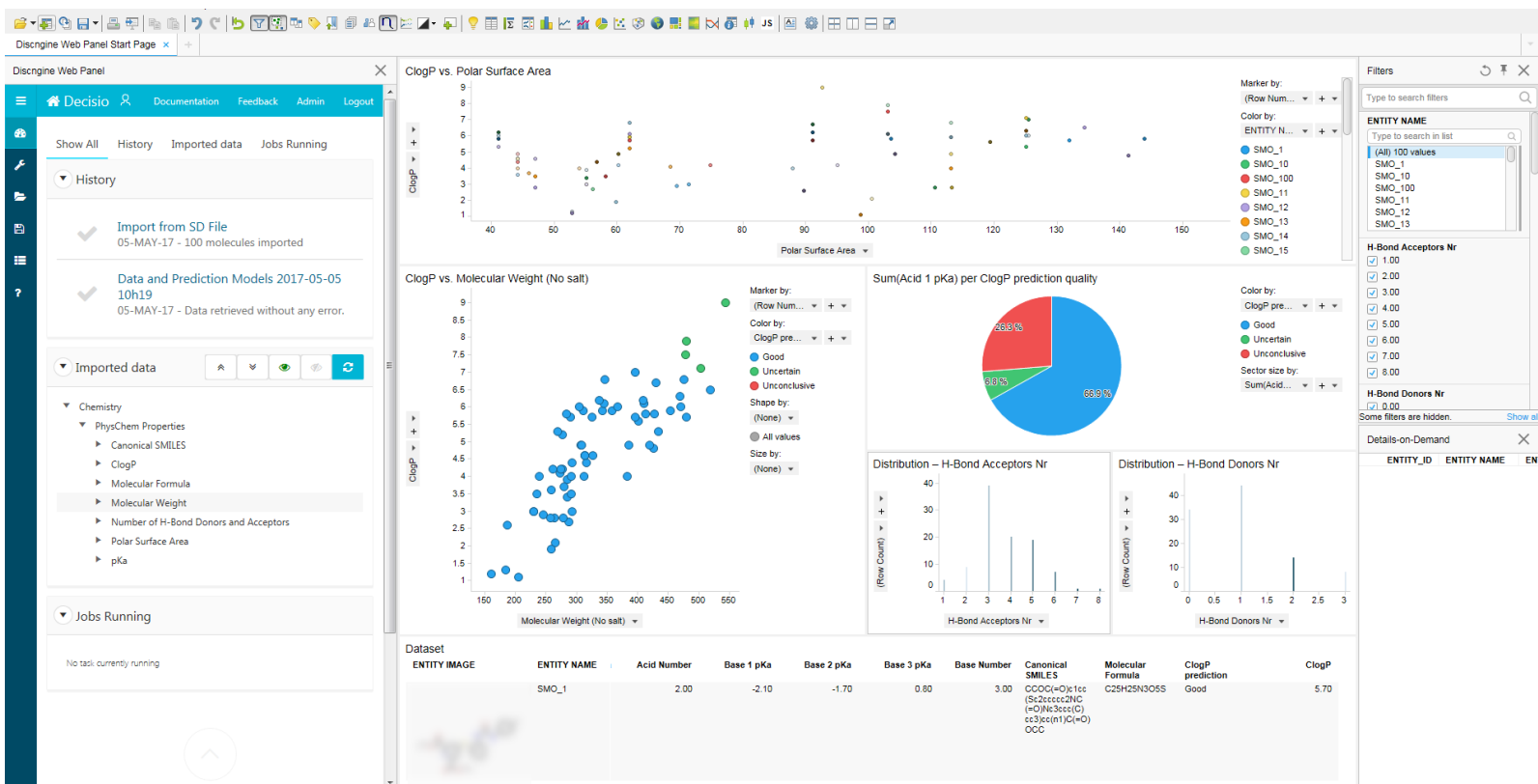
containing data from multiple sources...

that can be manipulated in a visual analytics tool

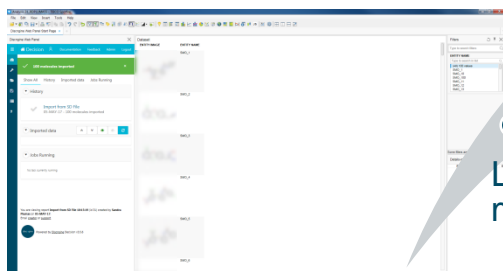
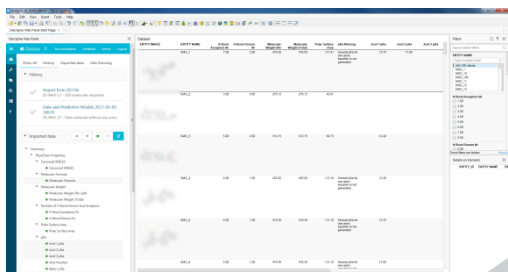
# Discngine Decision



# Example of Decision report



# Example of Decision workflow



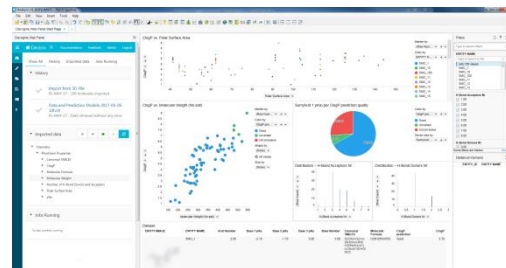
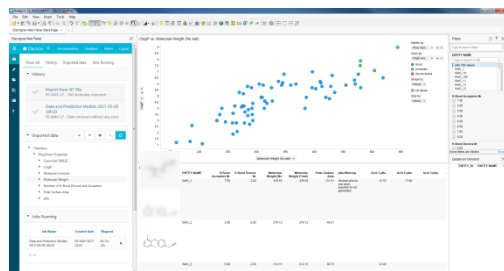
Load molecules

Retrieve data

Apply business analysis

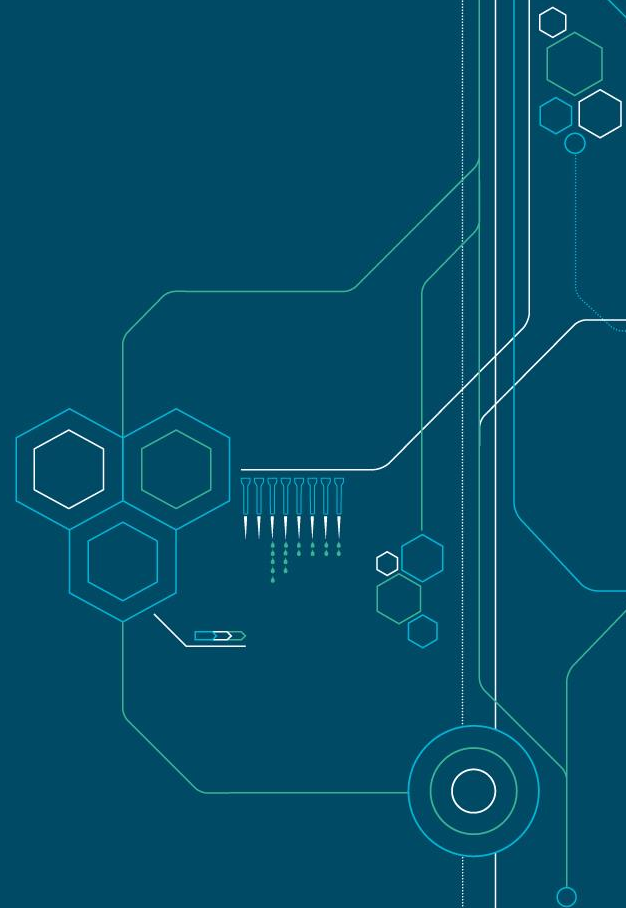
Analyse dataset

Share report



03

# CHEMAXON MARVINJS SKETCHER IN DISCENGINE DECISION







# A sketcher in Decision

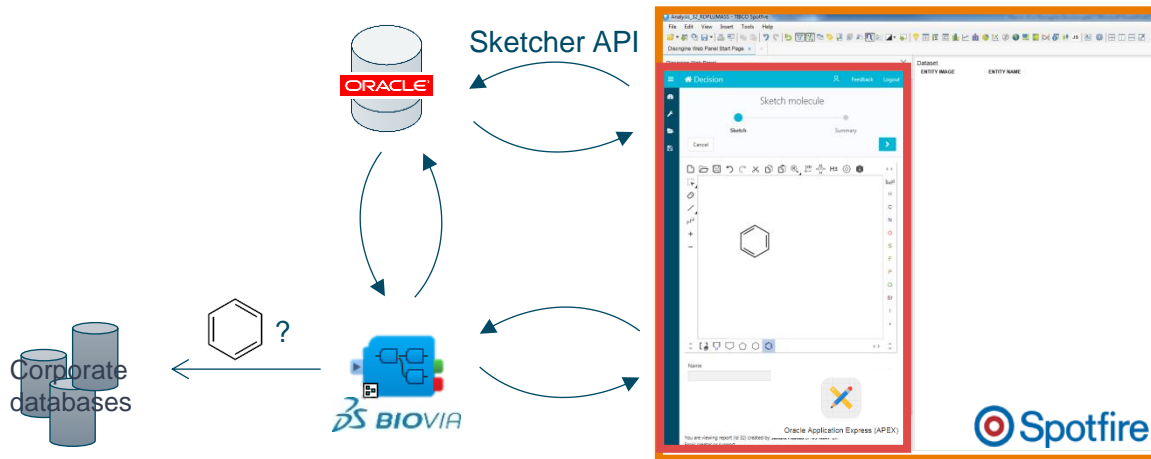
Several Decision features require a sketcher :

- Sketch a molecule to add it in a report
- Substructures searches in dataset
- Substructures searches in corporate databases



# Architecture of Decision

- Substructures searches in corporate databases



# Why MarvinJS ?

## On the developer side

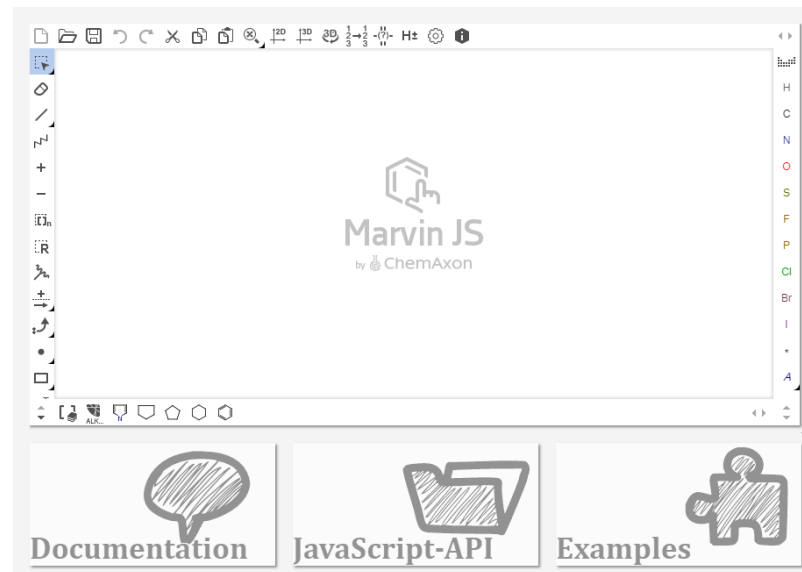
- Easy to integrate : complete and clean API, well documented
- No java !
- Many import/export formats in the API
- Listening to molecule changes in the sketcher

## On the user side

- Responsive and compact design
- Intuitive and user-friendly
- Flexible and extensible interface
- Frequent releases

## On the customer side

- Flexible relationship
- Affordable



# MarvinJS APEX plugin

- APEX plugin : PL/SQL
- Easy to integrate : few parameters

```
HER
(with or without web services)
dge = 'marvinjs' THEN
etcher_type = 'mol' THEN
arvinjs_type := 'standard';
_sketcher_type = 'reaction' THEN
arvinjs_type := 'reaction';

hem_ws = 'Y' THEN
('<div class="sketcher-marvinjs-resizable" style="width: '||loc_width||
||loc_sketcher_name||'.initSketcher();" src="'||loc_jchem_source||'/e
('<div class="sketcher-marvinjs-resizable" style="width: '||loc_width||
||loc_sketcher_name||'.initSketcher();" src="'||loc_jchem_source||'/e
```

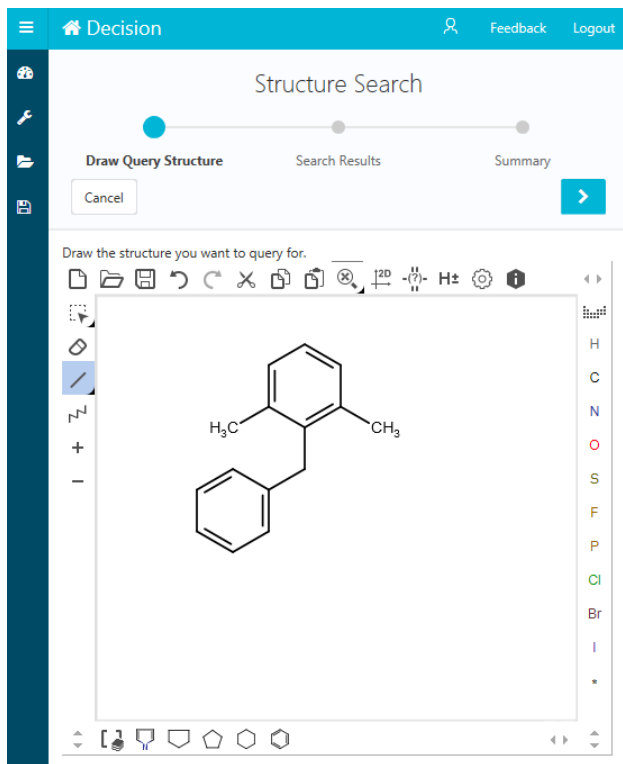
MarvinJS API



▼ Settings	
Cartridge	Marvin JS (chemaxon) ▾
Sketcher Width	500
Sketcher Height	450
Sketcher name	monsketcher
Marvin Path	&P1140_MARVINJS_URL.
JChem Web Services is available	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Sketcher Type	Molecule ▾

MarvinJS APEX plugin

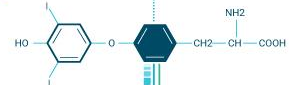
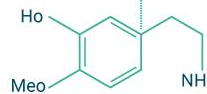
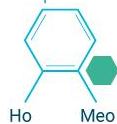
# Summary - A sketcher in Decision



- Sketcher used with the molecule mode
- Users can draw or import molecules
- MarvinJS API retrieves the structure in .mol format

Thanks

discngine



Contact : [sandra.plumas@discngine.com](mailto:sandra.plumas@discngine.com) or [support@discngine.com](mailto:support@discngine.com)