

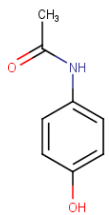
# Compound Registration

# Compound Registration

## *Scope*

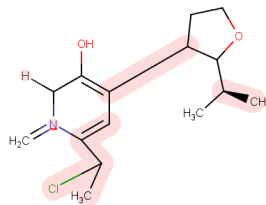
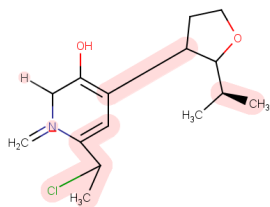
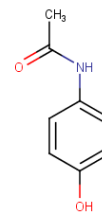
- Uniqueness of submitted entities
- Configurable business rules
- Automatic registration
- Upstream and downstream integration endpoints

INPUT

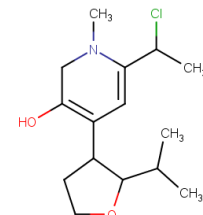


STAGING AREA

REGISTERED



FIX



LnbRef

U11-22-33



InvalidLnbRef - LnbRef U11-22-33 is not valid according to the regular expressions.

FIX

LnbRef  
U112233



# Registration UI

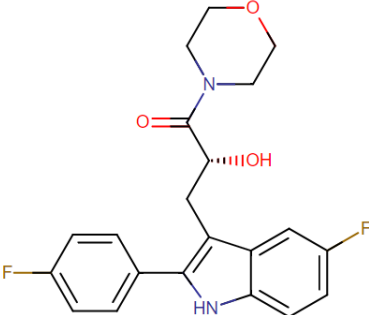
- Form-based input
- Basic/advanced registration
- Registration options
- Live Structure Checker/Stereo Analyzer

Registration Upload Staging Search

## Register new compound

Using source REGISTRAR · Created by rknispel@chemaxon.com · Advanced mode  ON · Virtual Compound  OFF

Single Structure View Find



No salts or solvates added.  
[+ Add new](#)

Chemically Significant Text

\*\*\* Actions

Submission Details

LnbRef

Additional Data ▼

Project

IUPAC name

Shipped  
 ON

Testing

Geometric isomerism

Structure Checker Stereo Analyzer

Stereo analyzer is  ON

STEREOCENTERS	
Single known enantiomer	
1 Total stereocenters	Fixers
0 Major	Major
1 Resolved known	Major as range

STEREO DOUBLE BONDS	
None	
0 Total stereo double bonds	Fixers
0 Cross/straight/squiggly	Cross
0 E configuration	E/Z

# New: Bulk upload improvements

- See own (user) or see all (admin) uploads
- Summary of error categories
- External bulk update of submissions
- Two-step registration
- Bulk submission deletion
- PDF report generation

Registration Upload Staging Search  rknispel@chemaxon.com

Upload > oxoazole-100k-ijc2-1-A-part4.sdf ⓘ [Update](#) [Delete All](#) [Download](#) [Register All](#)

⚠ Processing aborted at 1.4%

**221** / 15391

■ 25 Registered ■ 167 Ready ■ 27 Failed ■ 2 Deleted

**ERROR CATEGORIES**

- 26 Structural Error
- 1 Validation Error

Registered	25	REGISTERED	
Show All Error Categories ▾ <span style="float: right;"><a href="#">SELECT ALL</a> <a href="#">GO TO STAGING</a></span>			
<input type="checkbox"/> Unbalanced Charge	20	STRUCTURAL	<a href="#">OPEN IN STAGING</a> <a href="#">📄</a> <a href="#">🗑️</a> <a href="#">⌵</a>
<input type="checkbox"/> Positively Charged Structure	6	STRUCTURAL	<a href="#">OPEN IN STAGING</a> <a href="#">📄</a> <a href="#">🗑️</a> <a href="#">⌵</a>
<input type="checkbox"/> Duplicate LnbRef	1	VALIDATION	<a href="#">OPEN IN STAGING</a> <a href="#">📄</a> <a href="#">🗑️</a> <a href="#">⌵</a>

# New: Enhancements for No-structures

## Register new compound

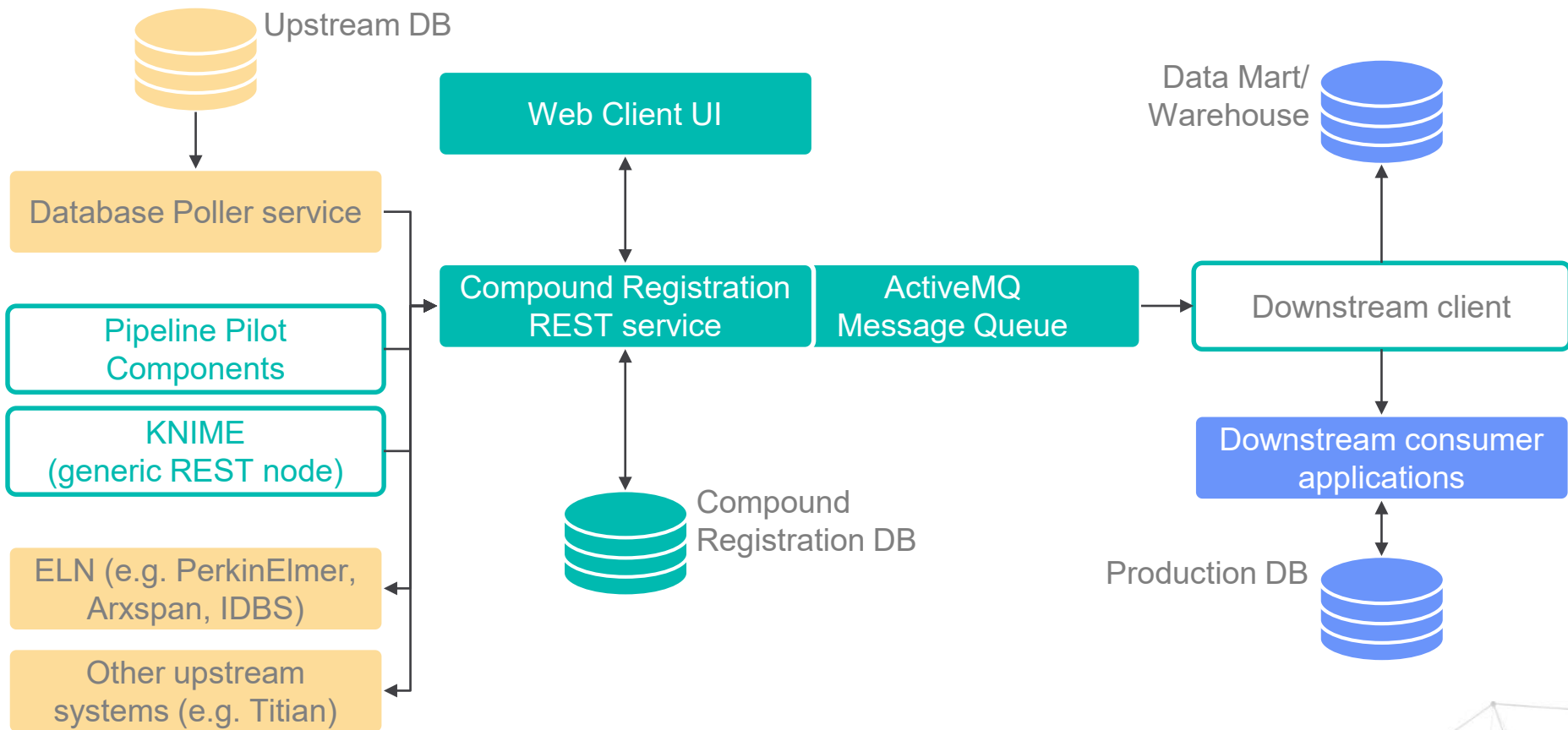
Using source REGISTRAR · Created by rknispel@chemaxon.com · Advanced mode  OFF

The screenshot shows a web interface for registering a new compound. On the left, a dropdown menu is open, listing structure types: 'No Structure' (selected), 'Single Structure', 'Mixture', 'Formulation', 'Alternate', 'Polymer', and 'No Structure'. The main area contains a 'View' dropdown, a search bar labeled 'Find', and a message: 'No salts or solvates added.' with a '+ Add new' link. Below this, there is a 'Chemically Significant' section with a 'Text' label and a text input field containing 'Enter any text val.'.

- No-structures are new structure type
- Structure validations omitted for No-structures
- Bulk upload of No-structures
- Create new No-structure lots by mapping PCN during bulk upload



# USAGE SCENARIOS





# Extension points

- Custom ID generators
- Additional Data validators and generators
- Application UI links (e.g. Inventory system)
- Custom Downstream clients

## Registration Summary



Registration successful

### DETAILS

PCN	CXN817
CN	CXN817A
LN	CXN817-001
LnbRef	2648379629

Add to Inventory

View Details

Ok

# On-premise vs. cloud deployment

On-premise is deployed on local infrastructure

Cloud deployments are hosted on Amazon/Google/etc., otherwise identical to on-premise

Compound Registration on AWS Marketplace in 2018  
(zero installation, different pricing model)



aws marketplace

 ChemAxon



# ROADMAP

# Roadmap

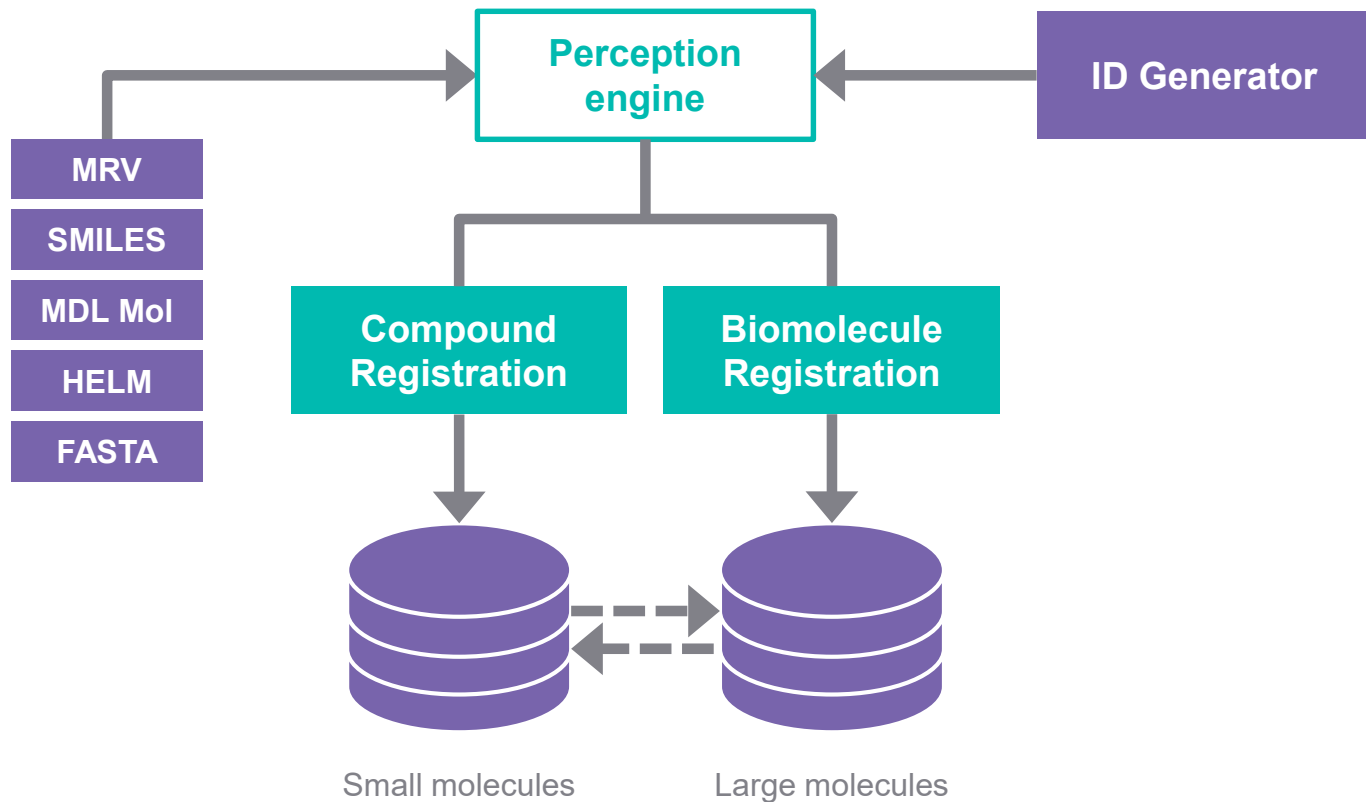
## H1 2019

- Enhancement for assigning/reviewing and commenting submissions
- User management change (enabling user management for internal and external users)
- History of all structure changes from drawing/import until registration
- Enhance suggestion list to multi-component structures

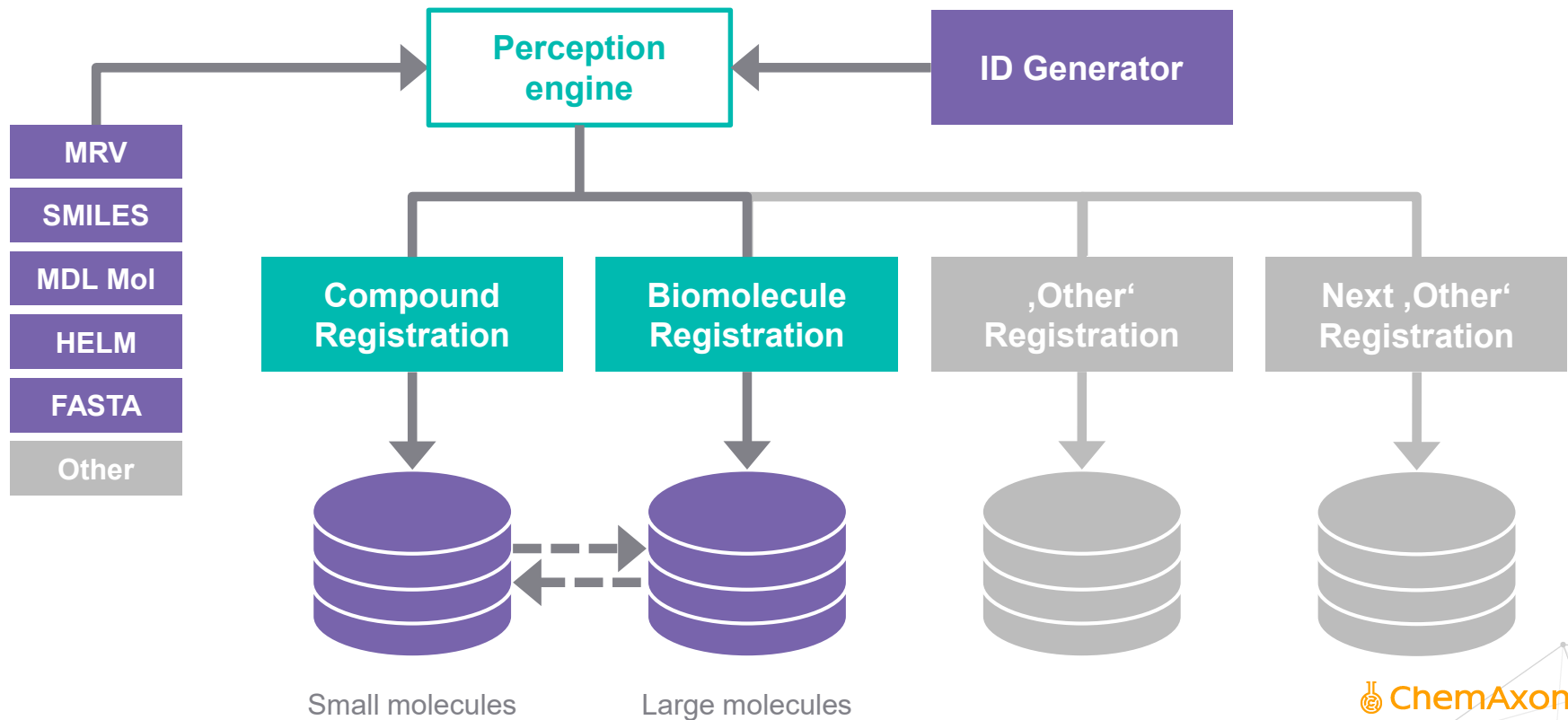
## H2 2019

- Bulk edits of additional data
- Bulk structure tree modifications (merging, splitting compounds)
- Bulk structure deletion
- Users can modify only their own registration records
- Agnostic registration and dependent requirements

# 2019 – Agnostic registration



# 2019 – Agnostic registration





# GET IN TOUCH

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