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**Inquiro version 2.8 – December 2017**

# CHEMICAL ENTITIES DETECTION AND SEARCH

## 1.1 DETECTION OF CHEMICAL ENTITIES

Inquiro is now able to find chemical entities in your data thanks to a [ChemAxon](#) plugin. Those entities are displayed in a new metadata section once the document is indexed, see below.

File name : bcr1325.pdf



Custom Tag

Comment

Upload date 01/18/2018      Uploaded by Sébastien Rouanet      File Size 1.5 MB

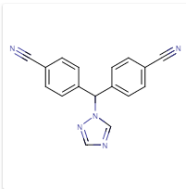
Number of download 0      Last download

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Chemical entities

<b>Molecule name</b>	letrozole, paclitaxel, estrogen, exemestane, goserelin, progesterone, epirubicin, methotrexate, fluorouracil, taxane, oncol, thalidomide, docetaxel, cyclophosphamide, doxorubicin, anastrozole, tamoxifen
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**LETROZOLE**



Hit count: 1  
Positions: p12  
Source name: letrozole  
Type: text

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[File metadata](#)

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[Technical Metadata](#)

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[Audit trail of the container](#)

You will be able to see the list of molecule names found in the document and also a picture of the molecular structure for each molecule along with some information (number of hits, page number, type text or OCR, source name).

## 1.2 STRUCTURAL AND SUBSTRUCTURAL SEARCH

This new version of Inquiro comes with a brand-new search capability which greatly improves the search feature by allowing to retrieve chemical information. New features detailed below will allow you to search for molecular entities by structure or substructure.

Here is the complete user guide of this feature: [Structural and sub structural search.](#)

### 1.2.1 MOLECULES' FACET

Once the user has entered a term in the search field, a new facet called "Molecule name" appears:

Project code (3) ↓Z A

Molecule name (252) ⊗ ↓Z A

- (.+.)-tartaric acid
- (+)-hematoxylin
- (2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl){(2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)(methyl)amino}ethyl)methylamine
- (3aS,3bR,9aS,9bS,11aS)-11a-methyl-tetradecahydro-1H-cyclopenta[a]phenanthrene-9,9-diol
- 1,2,3,4,5-pentaiodo-6-(triiodomethyl)benzene
- 2-phenyl-1H-indole-4,6-dicarboximidamide
- 200ne
- 3-deazaneplanocin A

Anatomy (4) ↓Z A

Molecule name (252) ⊗ ↓Z A

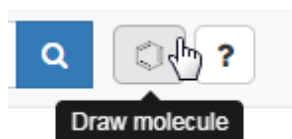
letro

letrozole

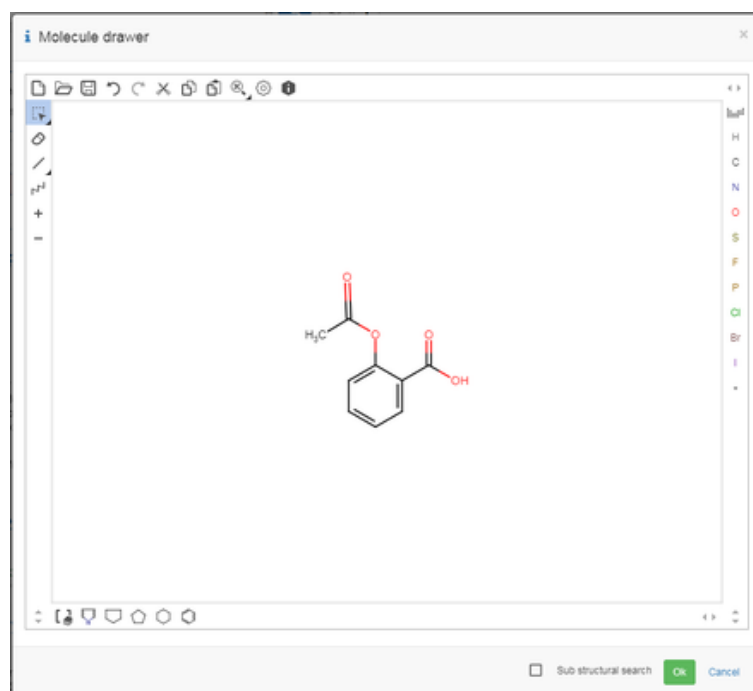
This facet displays all the molecule names pulled up in the search result's set.

### 1.2.2 STRUCTURAL AND SUBSTRUCTURAL DRAWING

You'll also be able to directly draw the structure or substructure of the molecules that you are searching for:



1.



2.

But also, to import an existing molecule from a file.