ChemAxon

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CHEMICAL NAMING TOOLS

The naming family

- Convert structures to IUPAC and common names (Structure to Name)
- Convert names to structures (Name to Structure)
- Extract structures from documents (Document to Structure)
- Display documents in web browser (Document annotator)

Agenda

1. Recent improvements (focus on Name to Structure)
2. Architecture for custom document processing
3. Integration story by Questel

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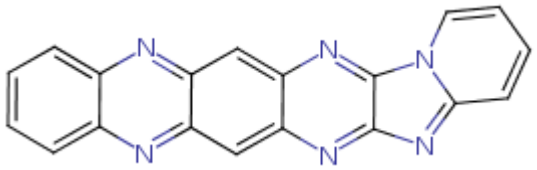
Name to Structure improvements

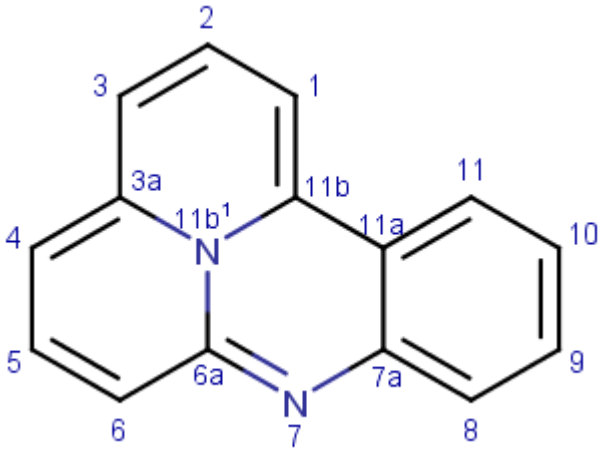
Multiple first-order and higher-order components

pyrido[1″,2″:1′,2′]imidazo[4′,5′:5,6]pyrazino[2,3-b]phenazine



Complex numbering

quinolizino[4,5,6-bc]quinazoline



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Document to Structure

API to detect and extract chemical structures from a document

Process a whole document or a single sentence or paragraph

Tens of options to control behaviour:

- include chemical elements?
- include fragments?
- …

Used by integrators and by ChemAxon products: ChemCurator and ChemLocator

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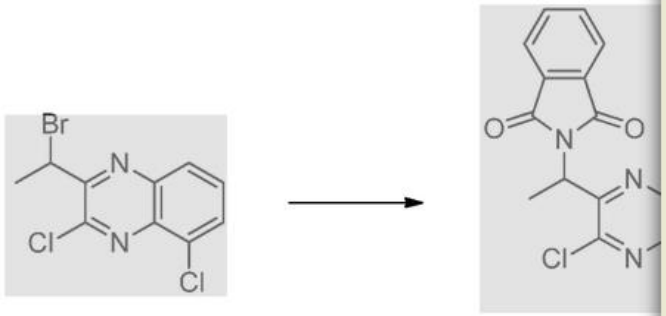
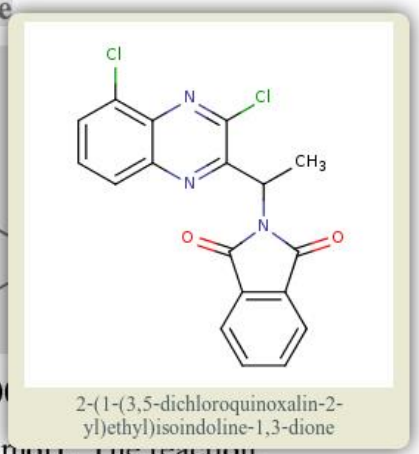
Document Annotator

2-(1-(3,5-dichloroquinoxalin-2-yl)ethyl)isoindoline-1,3-dione





2-(1-(3,5-dichloroquinoxalin-2-yl)ethyl)isoindoline-1,3-dione

To a solution of 2-(1-bromoethyl)-3,5-dichloroquinoxaline (1.0
DMF (8.2 L) was added potassium phthalimide (1.21 Kg, 6.54 mol). The reaction
mixture was stirred for 3 h. At this time LC-MS analysis showed that the reaction

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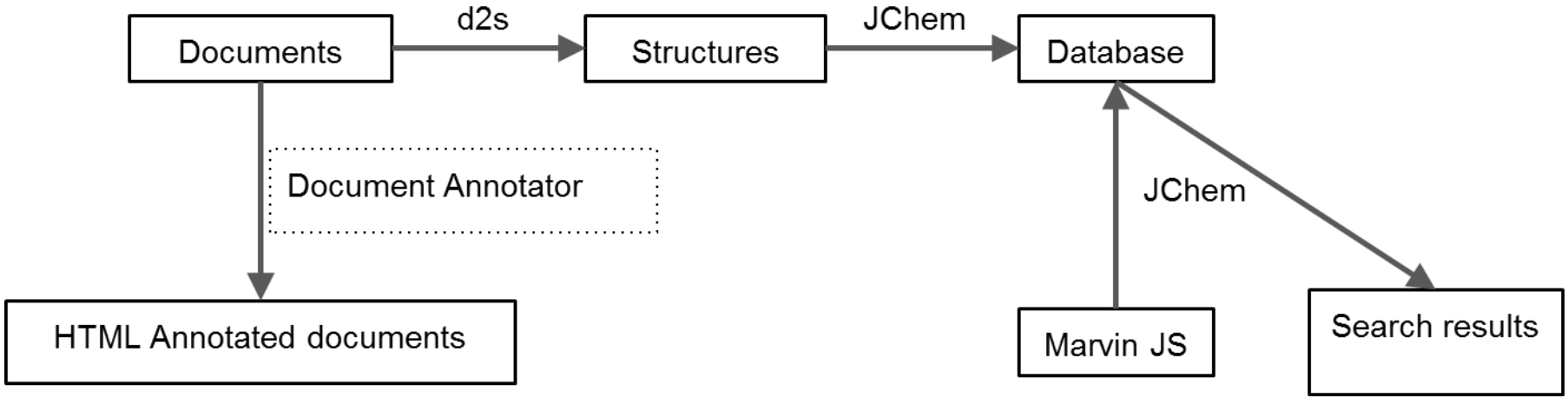
Document Annotator

Input: HTML, XML, Text or PDF document

Output: HTML, with chemical structures highlighted

Usage: Java and .NET API for integration in custom applications (also used in ChemCurator)

Chemical indexing and searching: architecture



THANK YOU

Continuing with Questel...

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