ChemAxon

Dora Barna
Tim Parrott

How to reach the hidden world of chemistry in patents

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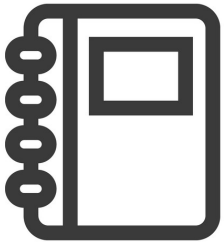
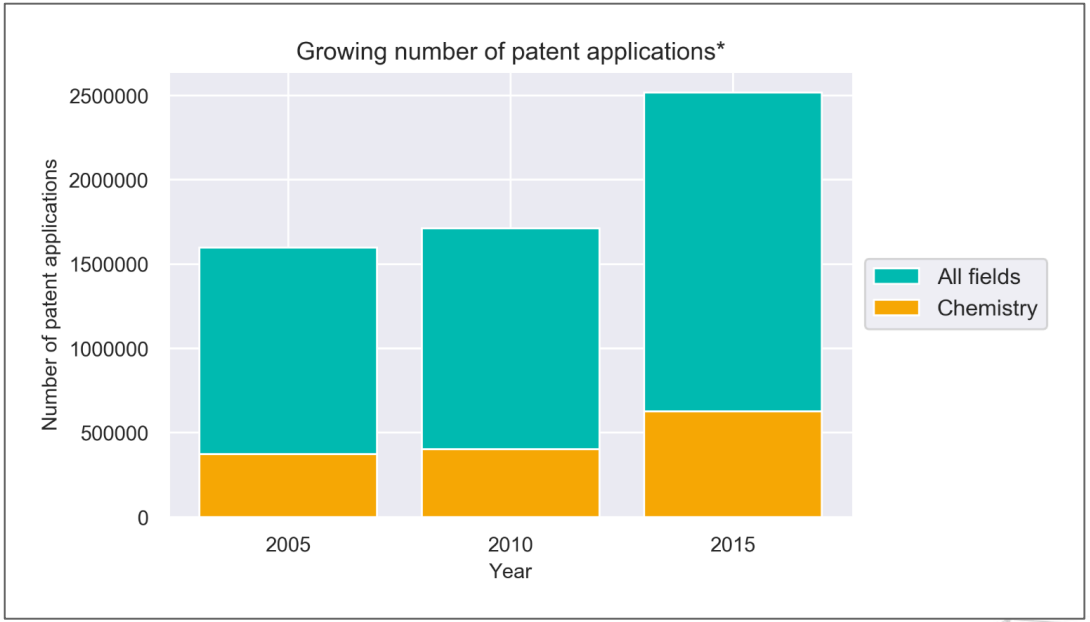
How to reach the hidden world of chemistry in documents

THE PROBLEM





*World Intellectual Property Indicators 2017 Patents,
https://www.wipo.int/edocs/pubdocs/en/wipo_pub_941_2017-chapter2.pdf

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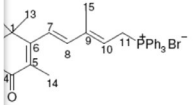
4–Oxo-β-ionylidene-ethyl-triphenylphosphonium bromide (38):

To a solution of PPh_3HBr (10.3 g, 28.6 mmol) in anhydrous methanol (100 mL) was added **36** (6.7 g, 28.6 mmol) in methanol (100 mL). After stirring for 75 h at room temp., the solvent was evaporated and **38** (10.57 g, 18.9 mmol, 66 %, lit.[30c] yield: 84 %) was obtained as a yellow solid. (m.p. 50 °C). The NMR spectra correspond to the



38

M⁺-Br].

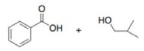
cm^{-1} (w), 1655 (s, C=O), 1588 (w),1480 (s), 1107 (s), 756

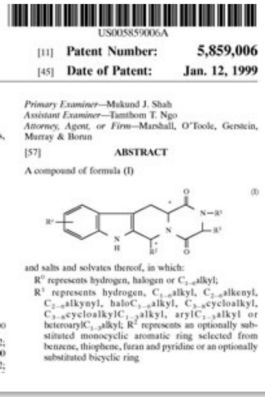
List of Schemes

1 Background

Our research project requires a target ester, whose starting material requires 15 synthetic steps. We decided to optimize the conditions of this Fischer esterification by preparing a closely related analogue **3**. The starting materials in this model reaction is the readily available benzoic acid (**1**) and *i*-PrOH (**2**).

f





US005859006A

United States Patent [19]

[11] **Patent Number: 5,859,006**

[45] **Date of Patent: Jan. 12, 1999**

Primary Examiner—Mukund J. Shah
Assistant Examiner—Tamthom T. Ngo
Attorney, Agent, or Firm—Marshall, O'Toole, Gerstein, Murray & Borun

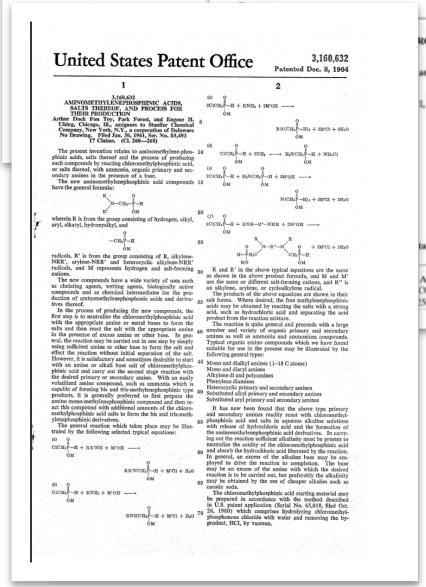
[57] **ABSTRACT**

A compound of formula (I)

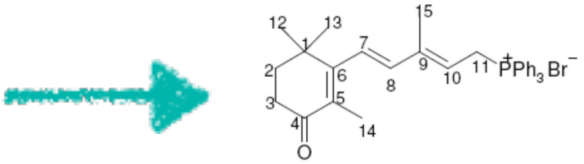
and salts and solvates thereof, in which:

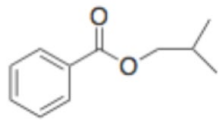
R^0 represents hydrogen, halogen or C_{1-4}alkyl;

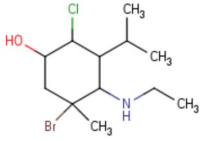
R^1 represents hydrogen, C_{1-6}alkyl, C_{2-6}alkenyl, C_{2-6}alkynyl, haloC_{1-6}alkyl, C_{1-6}cycloalkyl, C_{3-6}cycloalkylC_{1-3}alkyl, arylC_{1-3}alkyl or heteroarylC_{1-3}alkyl; R^2 represents an optionally substituted monocyclic aromatic ring selected from benzene, thiophene, furan and pyridine or an optionally substituted bicyclic ring

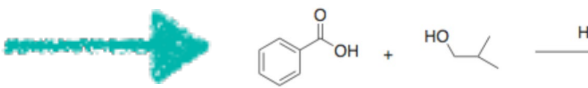


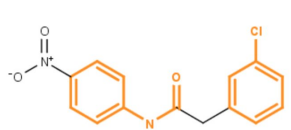
United States Patent Office 3,160,632 Patented Dec. 8, 1964

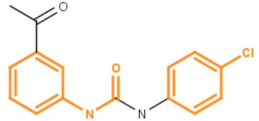


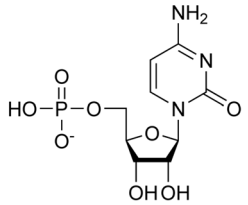












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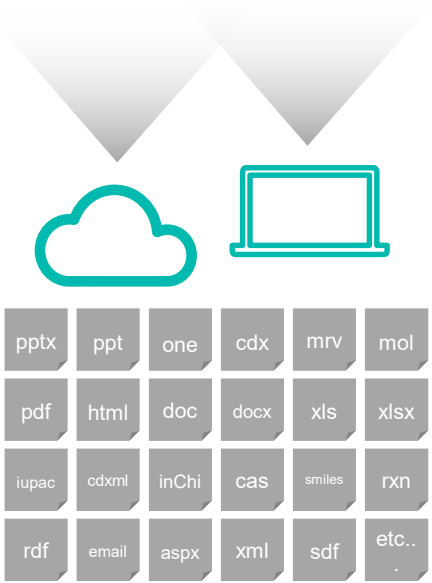
UNSTRUCTURED → STRUCTURED

ChemLocator

ChemLocator

Aspirin, also known as acetylsalicylic acid (ASA), is a medication used to treat pain, fever, or inflammation.[4] Specific inflammatory conditions in which aspirin is used include Kawasaki disease, pericarditis, and rheumatic fever.[4] Aspirin given …



Free text indexing

ChemAxon Naming +

Semantic indexing

Chemical NER*
OCR
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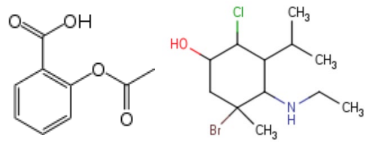
Metadata extraction
Tagging
Keywords
Biological NER
etc.



***NER:** Named Entity Recognition

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An Experiment

24,000 patent documents

- From the **USPTO** patent database
- Medicinal chemistry patents from 2015

771,000 unique molecules

- exact molecules: 740,000
- fragments: 23,000
- generic structures: 8,800

3.1 million molecules in total

Processing

- Indexing time: 7.08 days
- Chemical database: 13.5 GB
- Elastic database: 25 GB

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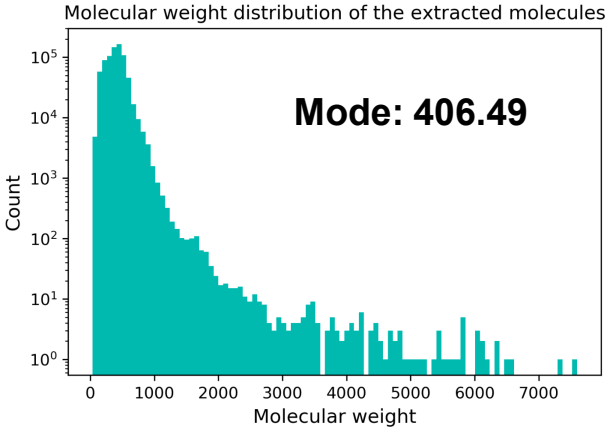
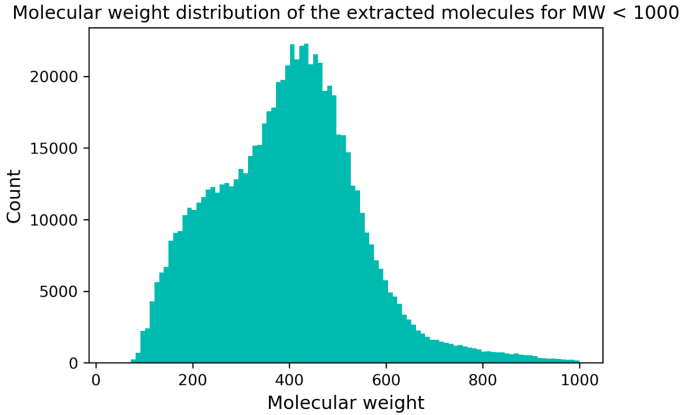
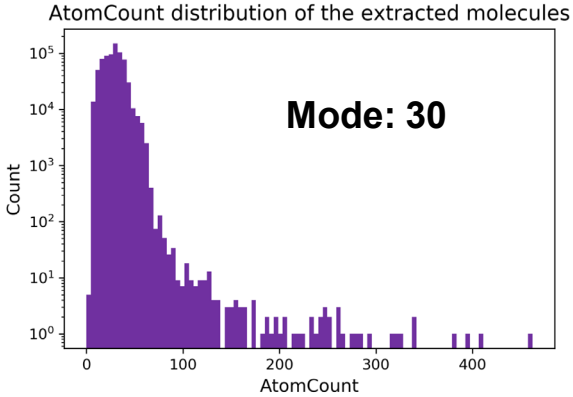
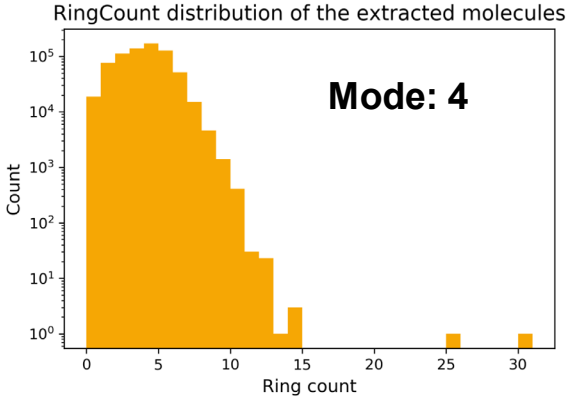
Chemical space - Basic properties



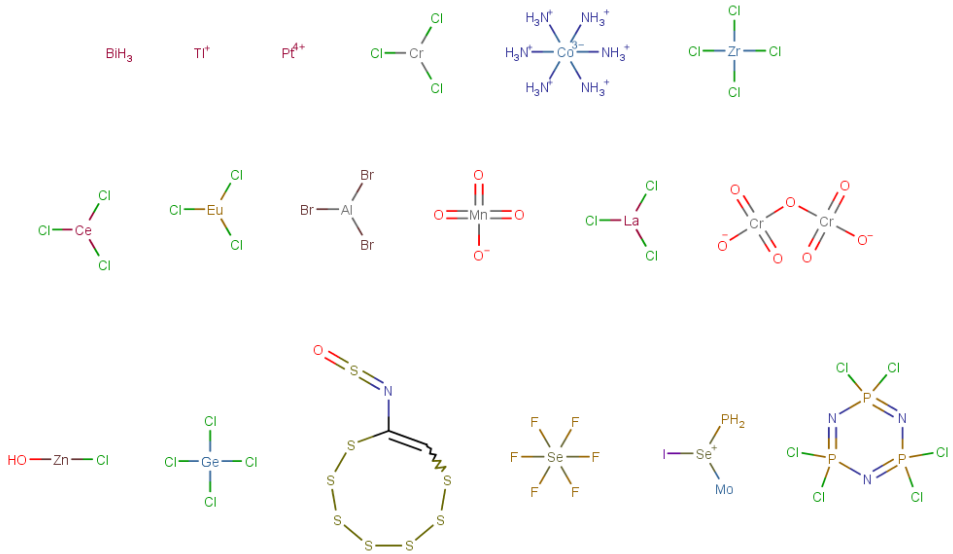


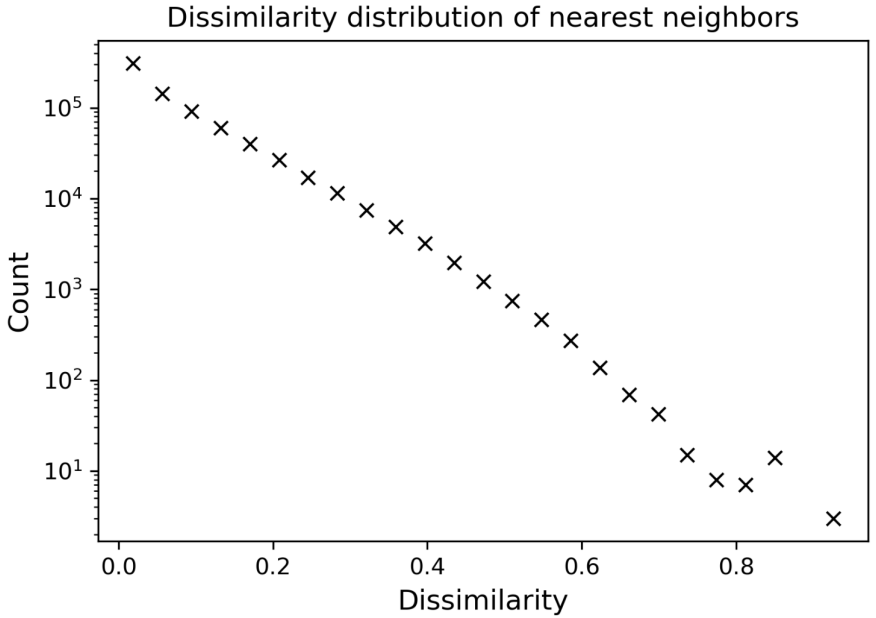




Chemical space - Structural similarity

- 50% of the molecules had its most similar pair within 0.05 dissimilarity;
- Molecules that are very different from their nearest neighbors:





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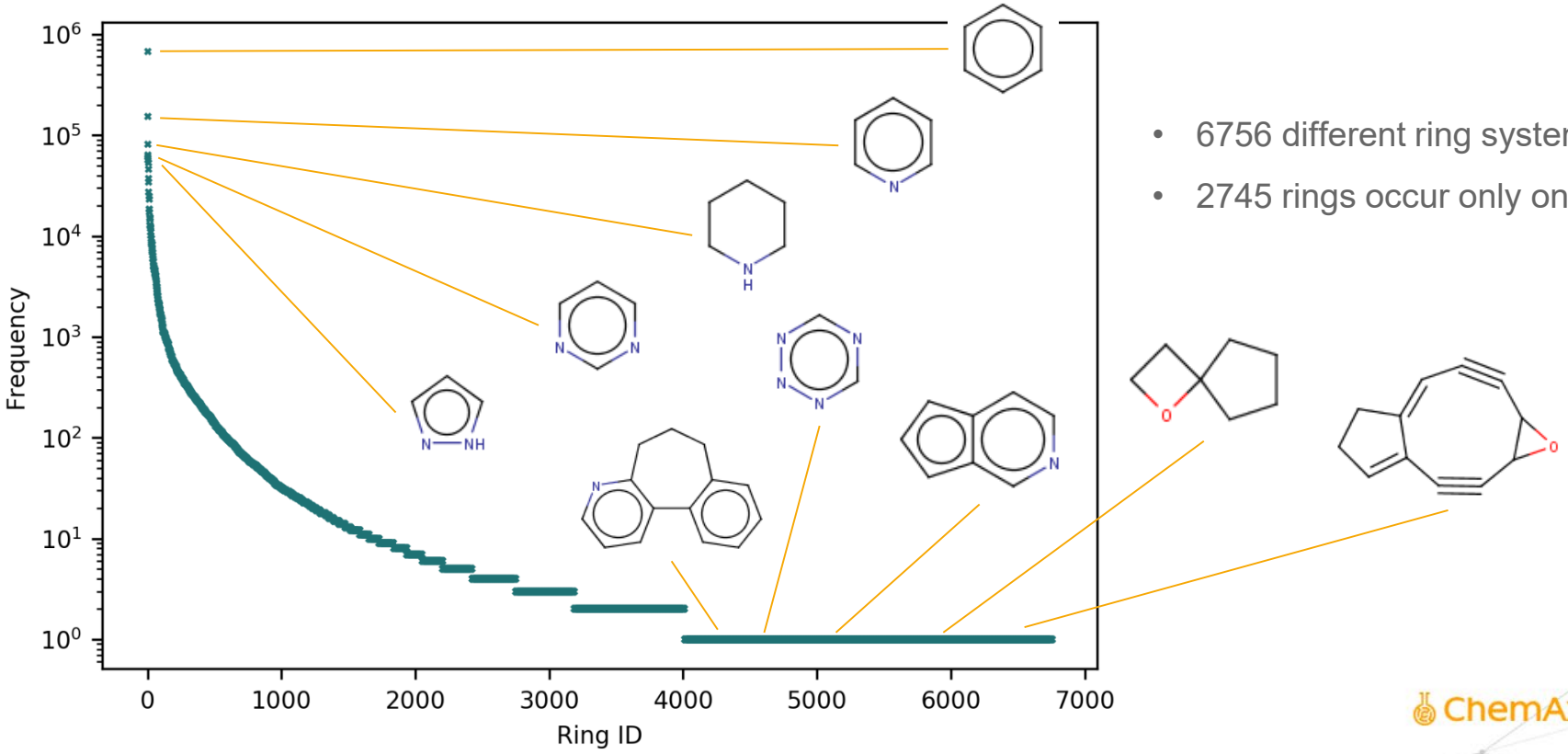
Chemical space - Typical ring systems



- 6756 different ring systems;
- 2745 rings occur only once;

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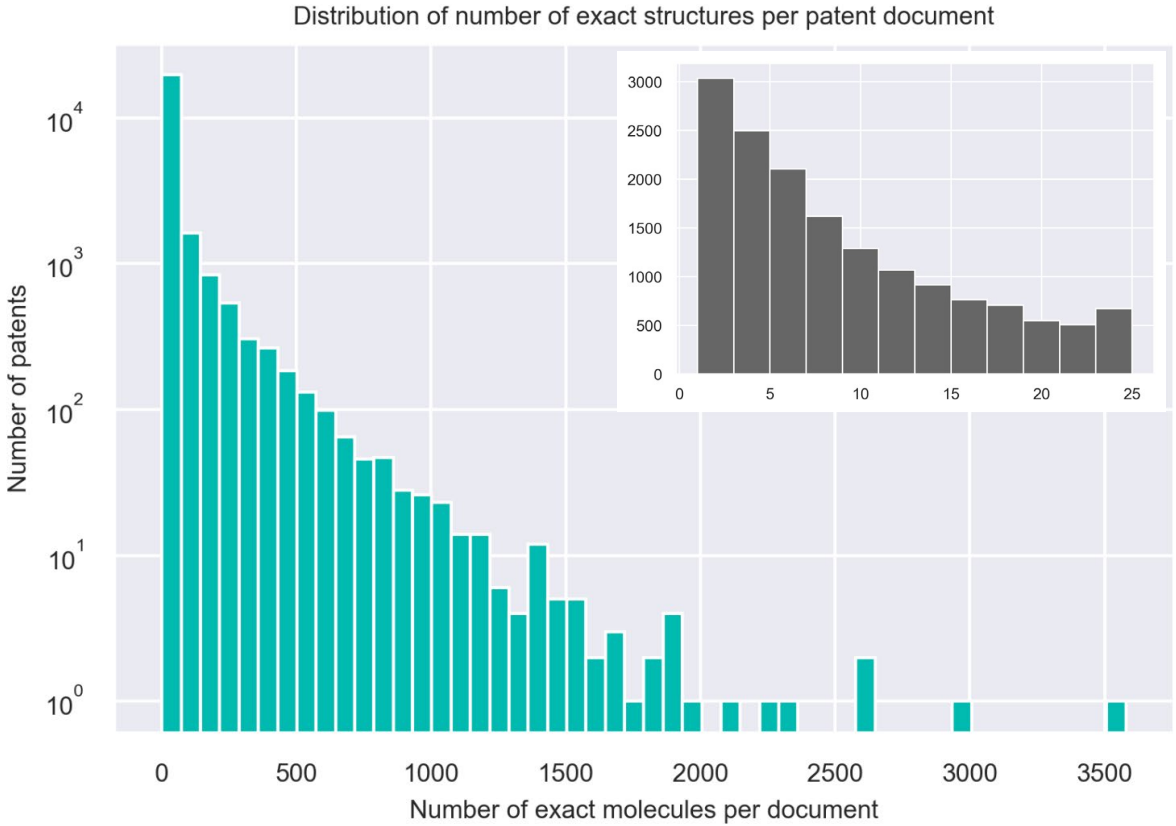
Chemical structures per document



- 1548 patents with a single exact molecule;
- Topics:
  - pharmaceutical preparation
  - pharmaceutical composition
  - method of treatment

- 25 documents with more than 1500 exact molecules;
- kinase inhibitors, H4 receptor inhibitors, glucokinase activators...

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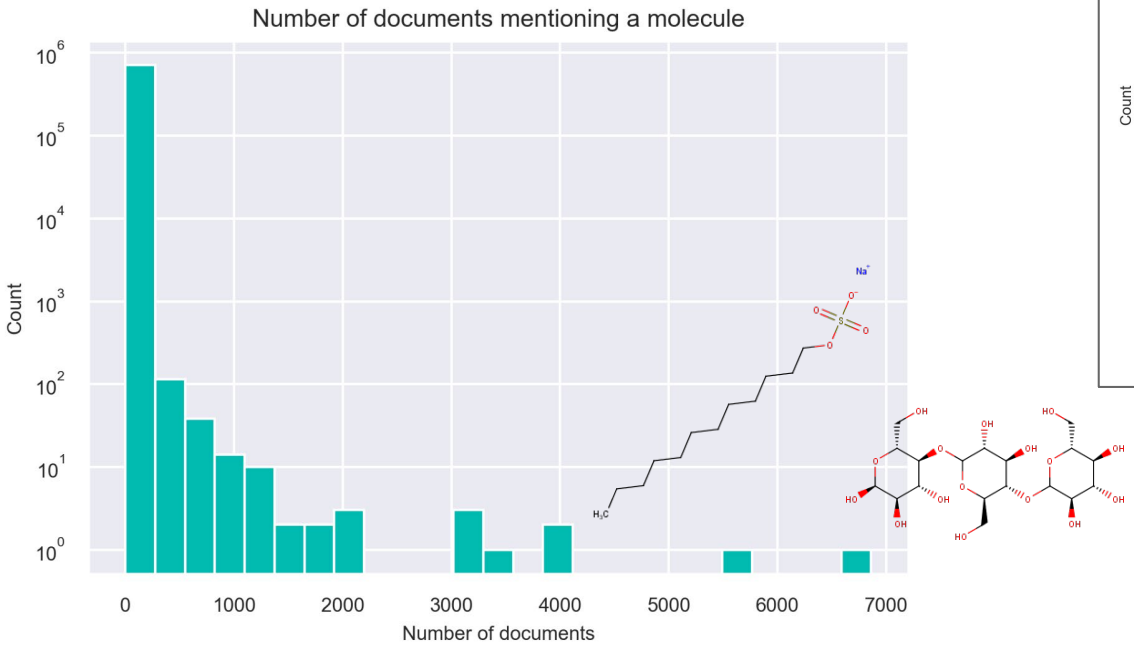
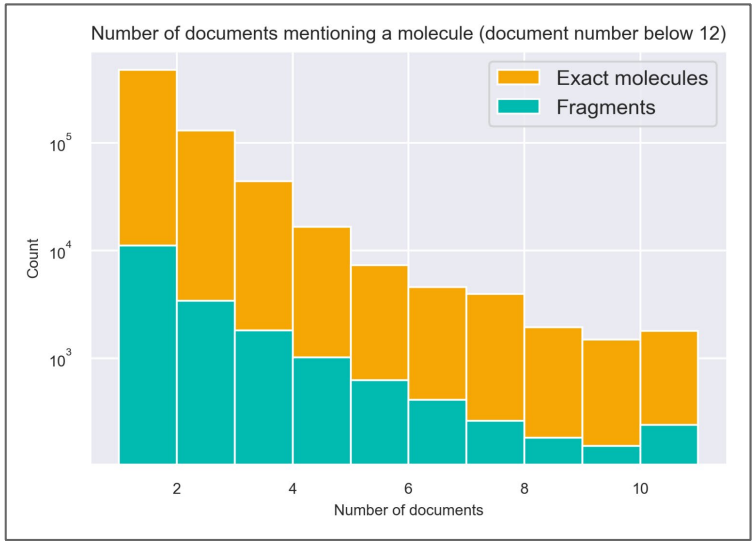
Frequency of chemical structures





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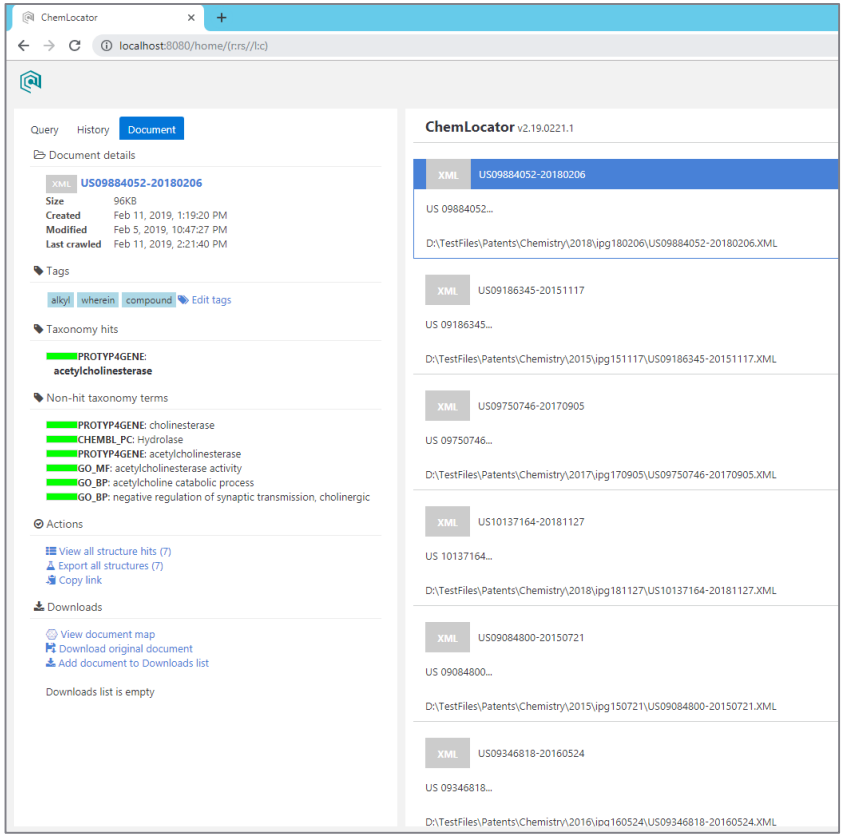
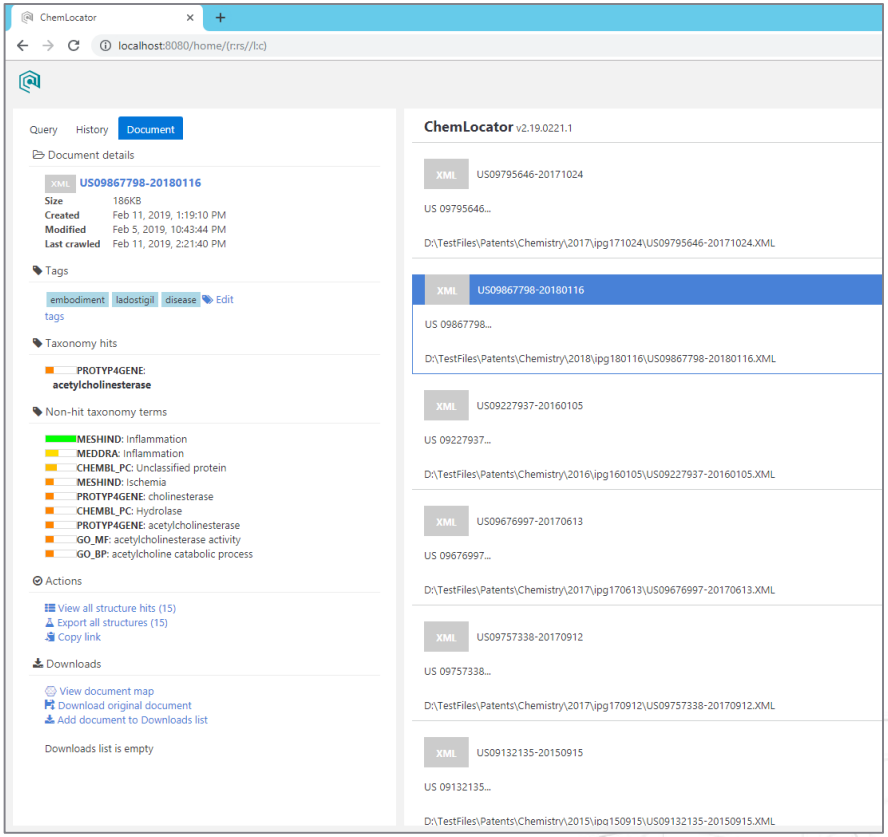
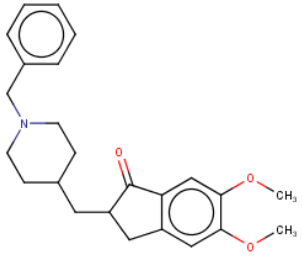
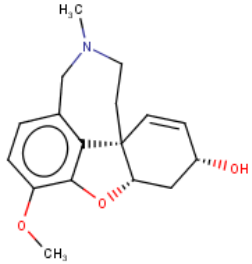
Chemical space overlap of two targets 1.

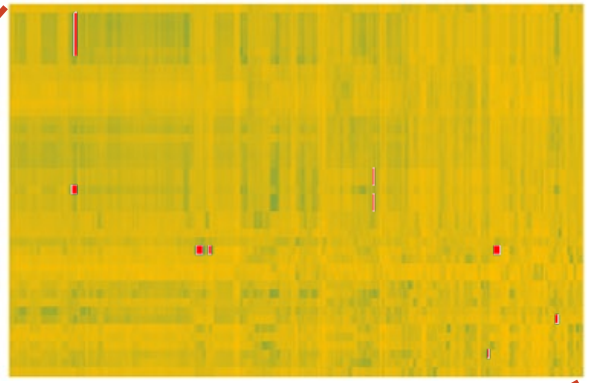


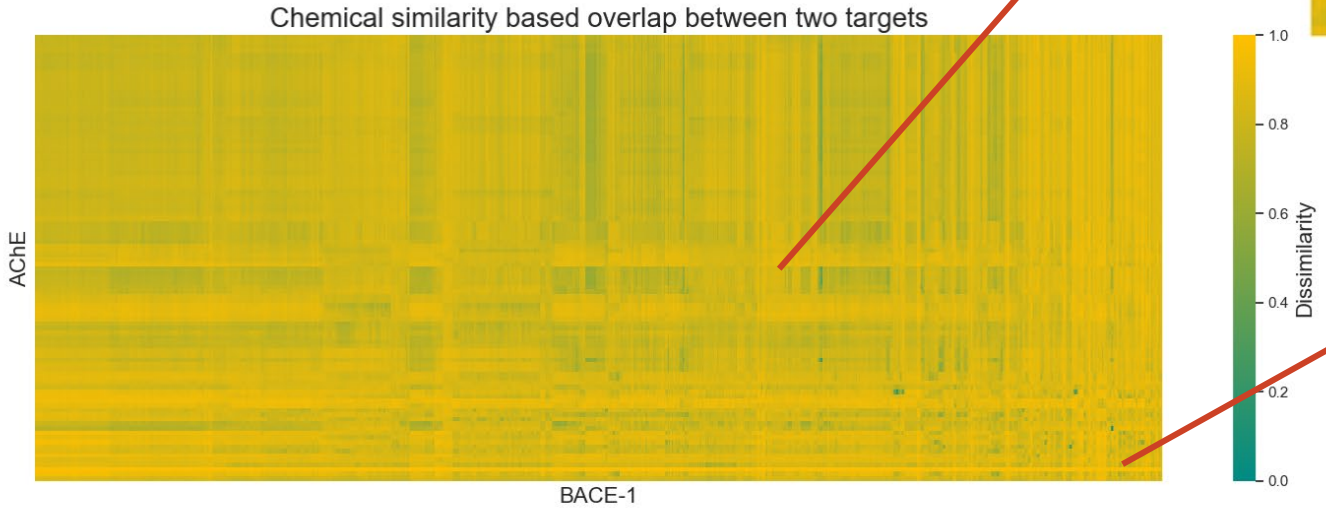


Chemical space overlap of two targets 2.









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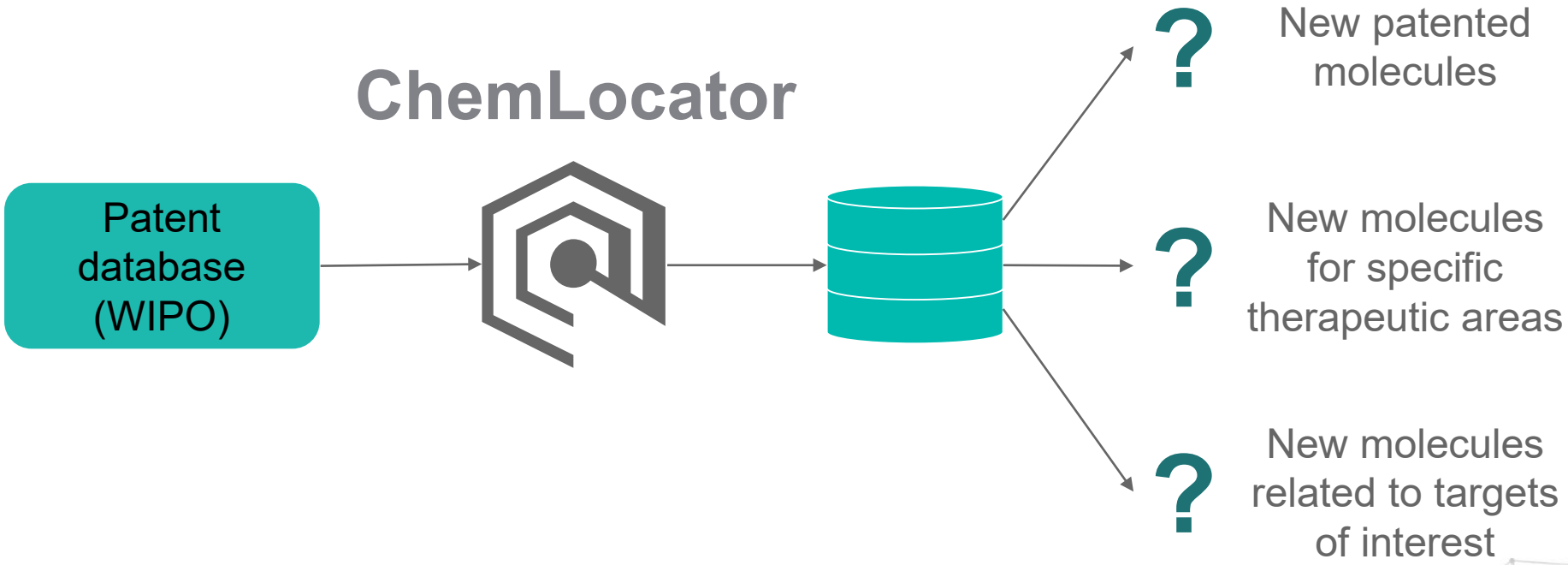

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THANK YOU!

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