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Scientific Lenses: Supporting Alternative Views of the Data

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http://c745.r45.cf2.rackcdn.com/img/2009/lens_filter_coasters.jpg

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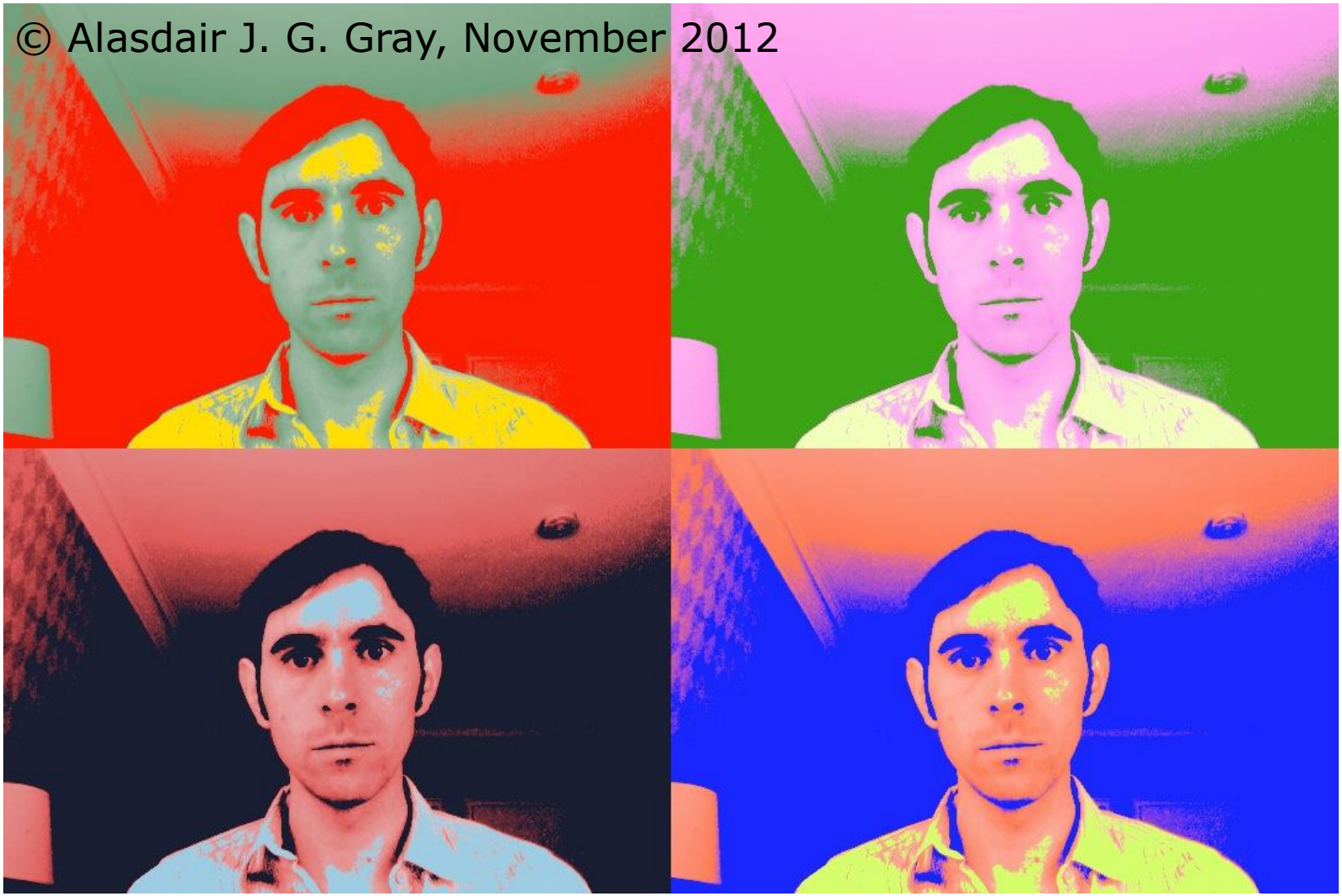
Filters Change our Perceptions

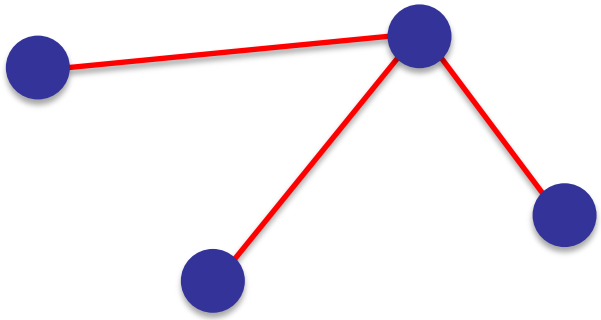


Resolving Multiple Identities

Multiple Points of View

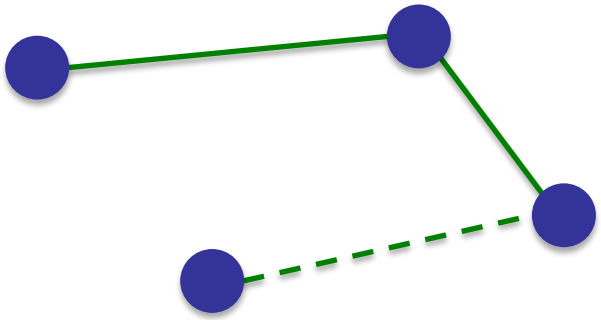
Chem-informatition

- Chemicals must be the same isomer
- Target can be gene or protein



Bio-informatition

- Chemicals can match only at structure
- Target is a protein, distinct from genes
- Sometimes I want to match across species



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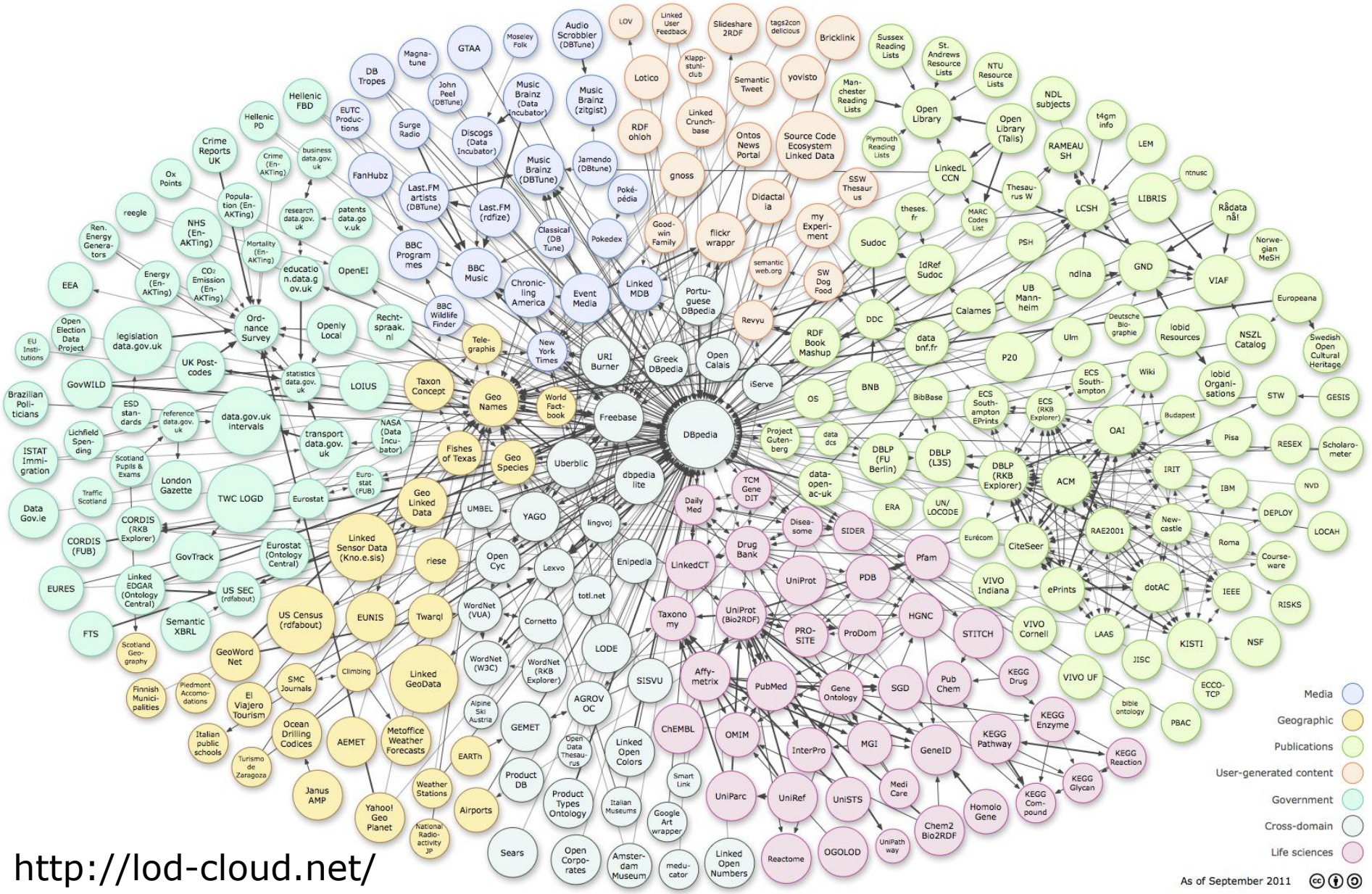
Linked Data Cloud

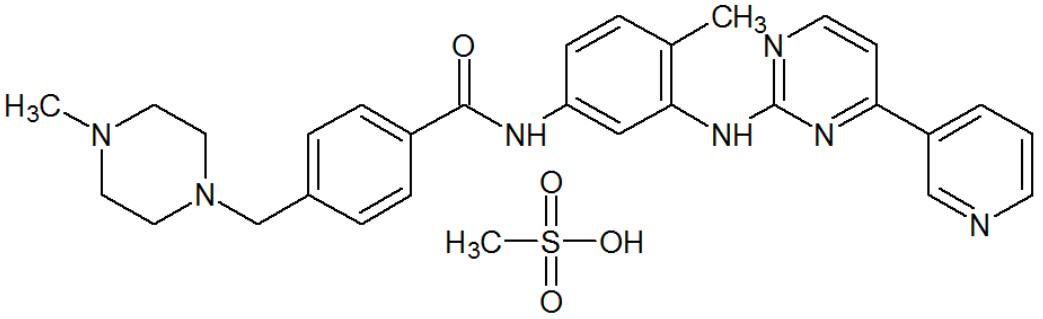


Media
Geographic
Publications
User-generated content
Government
Cross-domain
Life sciences

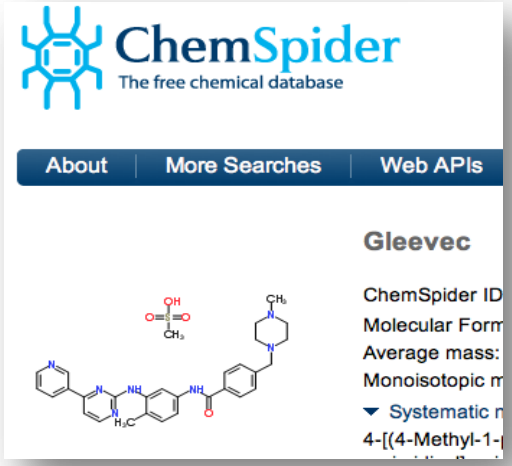
As of September 2011

http://lod-cloud.net/

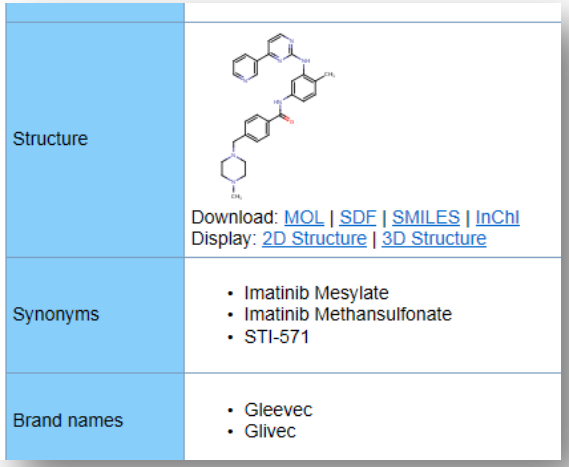
Gleevec® = Imatinib Mesylate



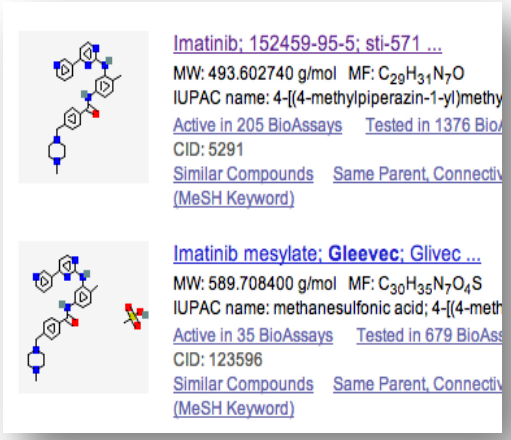
YLMAHDNUQAMNNX-UHFFFAOYSA-N



ChemSpider

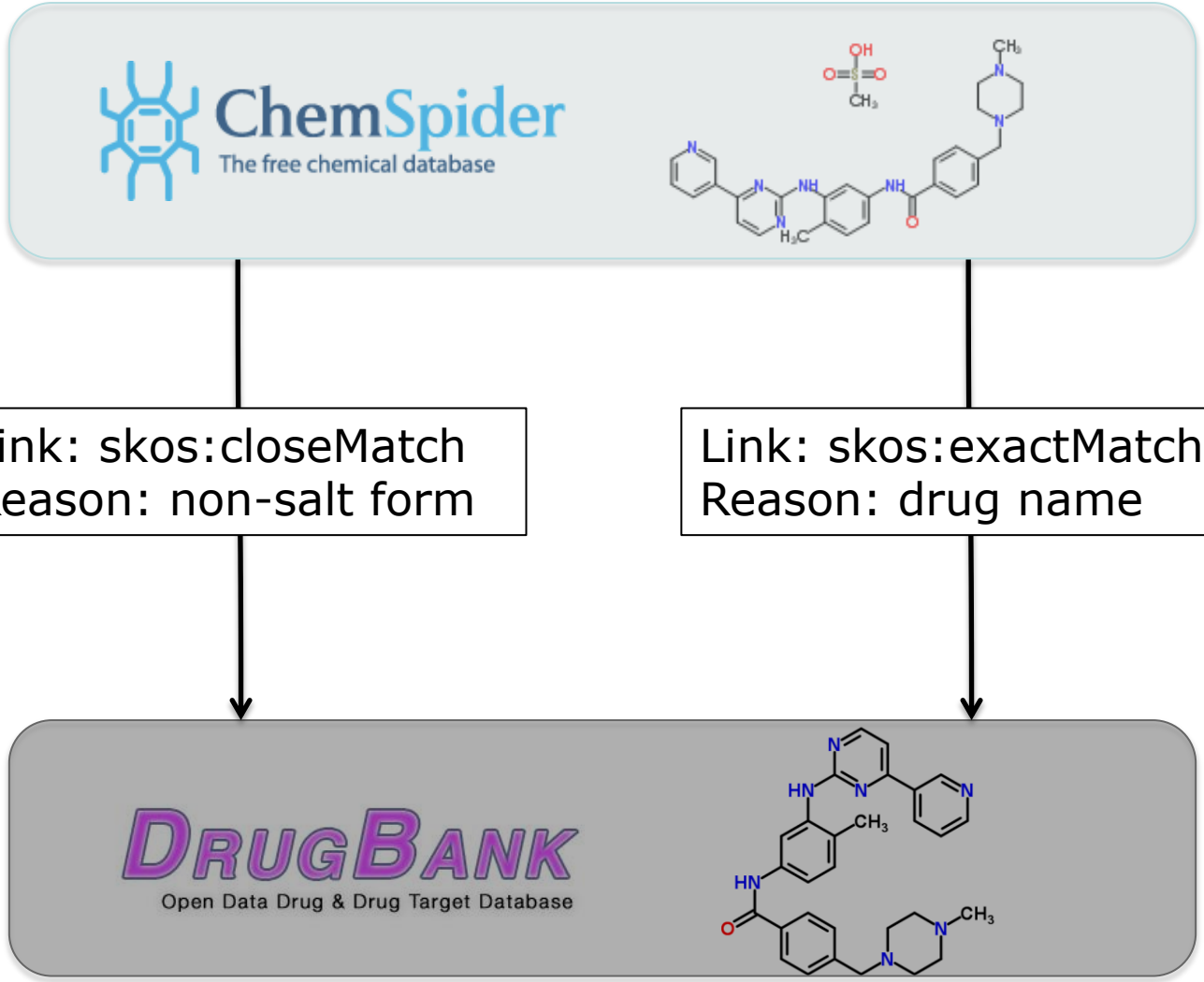


Drugbank



PubChem

Multiple Links: Different Reasons



Lenses: Operational Equivalence

```
InChI Key Match {
  chemspider:imantinib_mesylate  skos:exactMatch
                                 chembl: imantinib_mesylate
}

Salt-forms {
  chemspider:imantinib_mesylate skos:closeMatch
                                drugbank:imatinib
}

Enantiomer {
  (+)Staurosporine skos:exactMatch
                                (-)Staurosporine
}
```

Lenses: P1 stereo-chemistry

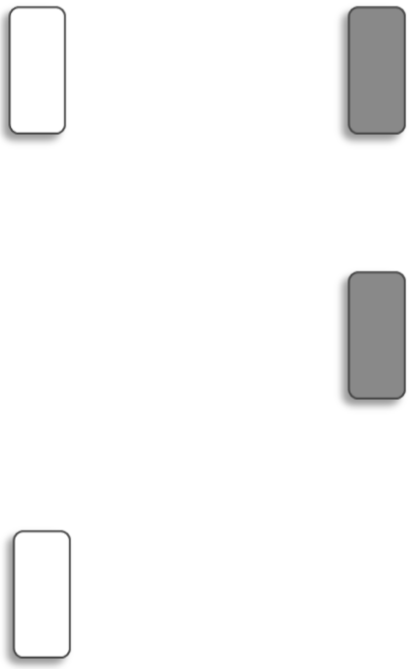
Profile P1
"Stereo"

```
InChI Key Match {
  chemspider:imantinib_mesylate  skos:exactMatch
                          chembl: imantinib_mesylate
}


Salt-forms {
  chemspider:imantinib_mesylate skos:closeMatch
                                drugbank:imatinib
}


Enantiomer {
  (+)Staurosporine skos:exactMatch
                                (-)Staurosporine
}
```

Lenses: P2 salt-forms

Profile P1 "Stereo"

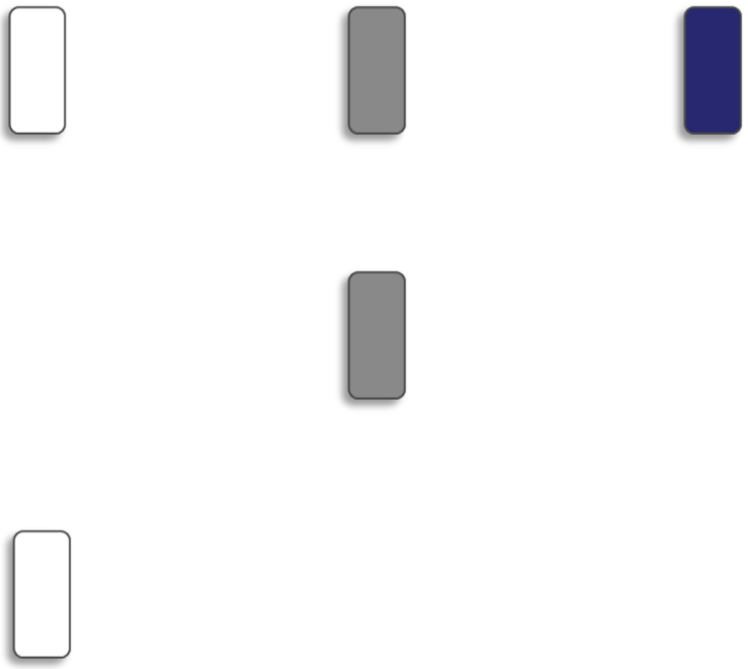
Profile P2 "Salts"



```
InChI Key Match {
  chemspider:imantinib_mesylate  skos:exactMatch
                          chembl: imantinib_mesylate
}


Salt-forms {
  chemspider:imantinib_mesylate skos:closeMatch
                              drugbank:imatinib
}


Enantiomer {
  (+)Staurosporine skos:exactMatch
                              (-)Staurosporine
}
```

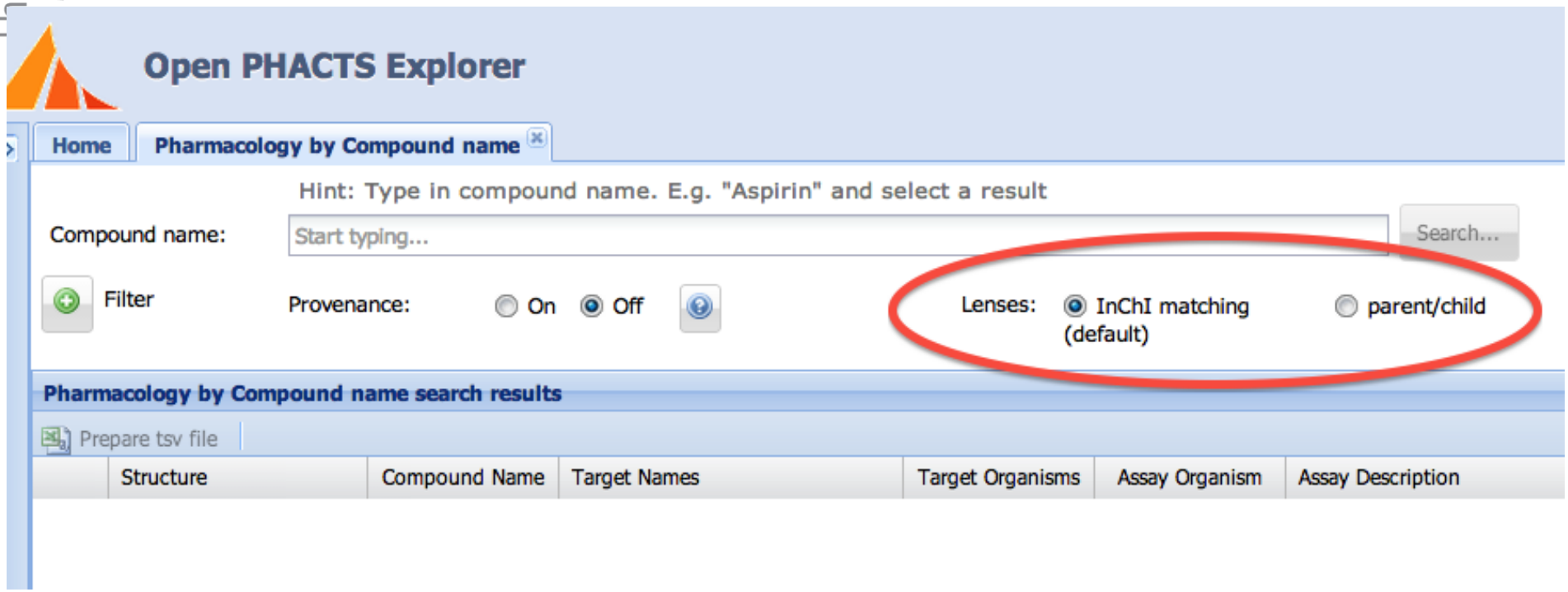
Lenses: P3 strict equivalence

Profile P1 "Stereo" | Profile P2 "Salts" | Profile P3 "Strict"



```
InChI Key Match {
  chemspider:imantinib_mesylate  skos:exactMatch
                          chembl: imantinib_mesylate
}

Salt-forms {
  chemspider:imantinib_mesylate skos:closeMatch
                                drugbank:imatinib
}

Enantiomer {
  (+)Staurosporine skos:exactMatch
                                (-)Staurosporine
}
```

Lenses in the Explorer



Lenses Support Dynamic Equality

Strict — Relaxed

Analysing — Browsing

- Tuneable
  (same data, different questions)
- Data & entity specific
- User driven
- Traceable

OPS Lenses

- Compound Drugs
- Salt-form Drugs
- Parent/child Chemical Relationships
- Genes/proteins

Ideas for other lenses?

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Thank you

- Alasdair.Gray@manchester.ac.uk
- Paper:

  Christian Y. A. Brenninkmeijer, Chris Evelo, Carole Goble, Alasdair J. G. Gray, Paul Groth, Steve Pettifer, Robert Stevens, Antony Williams, and Egon L. Willighagen. Scientific Lenses over Linked Data: An approach to support task specific views of the data. A vision. In 2nd International Workshop on Linked Science 2012—Tackling Big Data (LISC2012) co-located with 11th International Semantic Web Conference (ISWC2012), Boston, MA, USA, November 2012.