

Scientific Lenses: Supporting Alternative Views of the Data

Alasdair J G Gray
University of Manchester

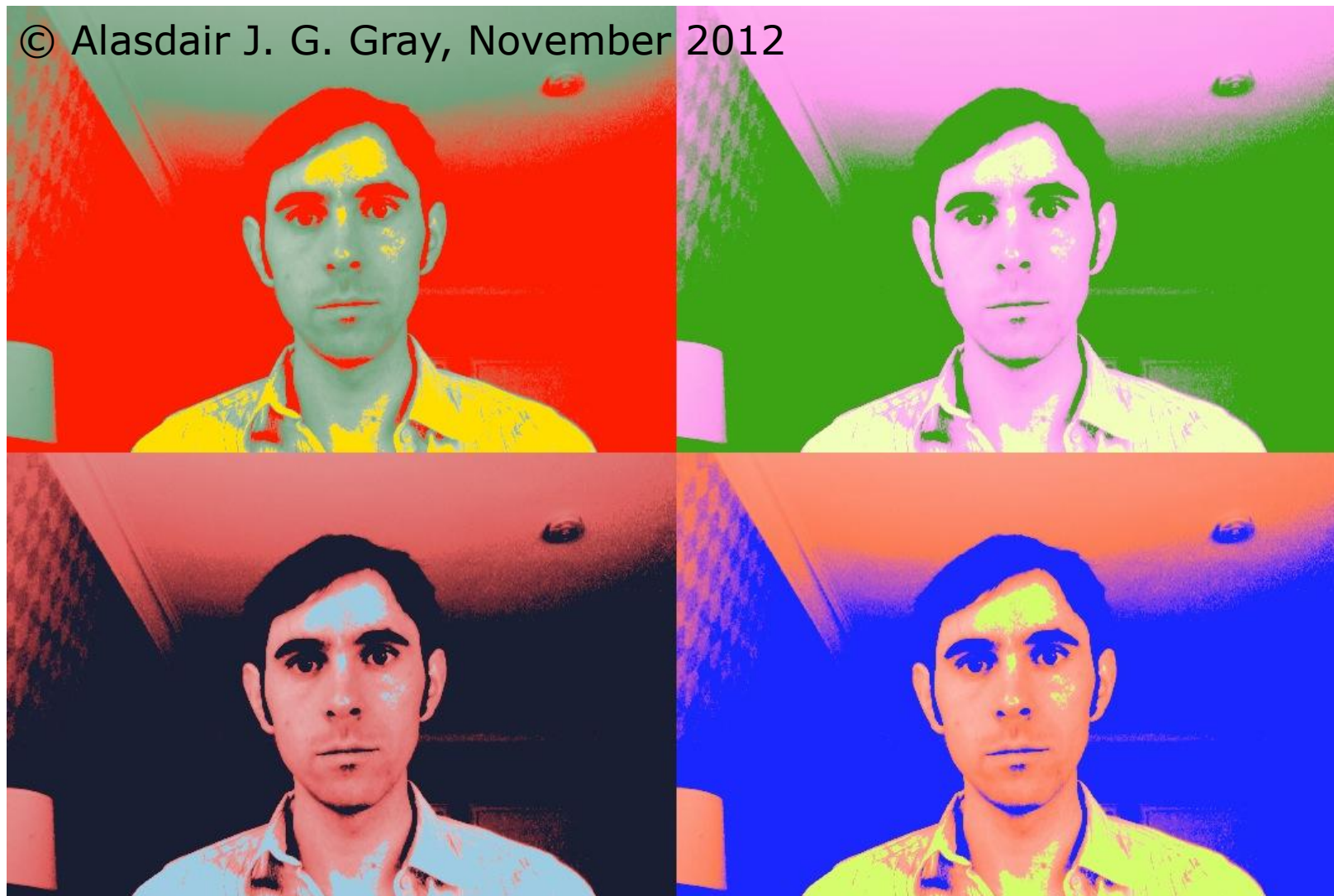
Authors:

Christian Y. A. Brenninkmeijer,
Chris Evelo, Carole Goble,
Alasdair J. G. Gray, Paul Groth,
Steve Pettifer, Robert Stevens,
Antony Williams and
Egon L. Willighagen



Filters Change our Perceptions

© Alasdair J. G. Gray, November 2012



23 April 2013

Scientific Lenses – A. Gray

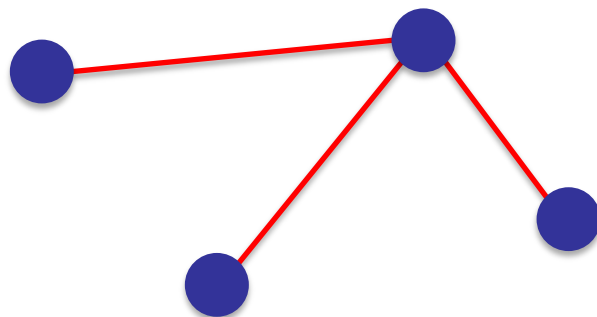
Resolving Multiple Identities



Multiple Points of View

Chem-informatition

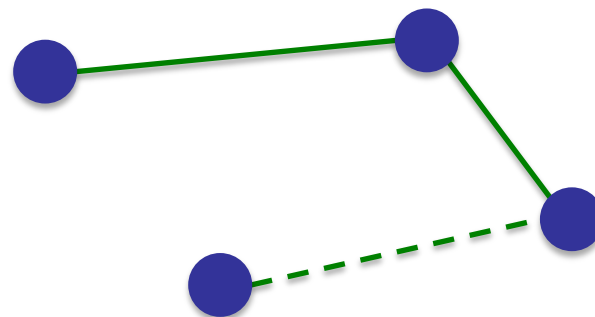
- Chemicals must be the same isomer
- Target can be gene or protein



23 April 2013

Bio-informatition

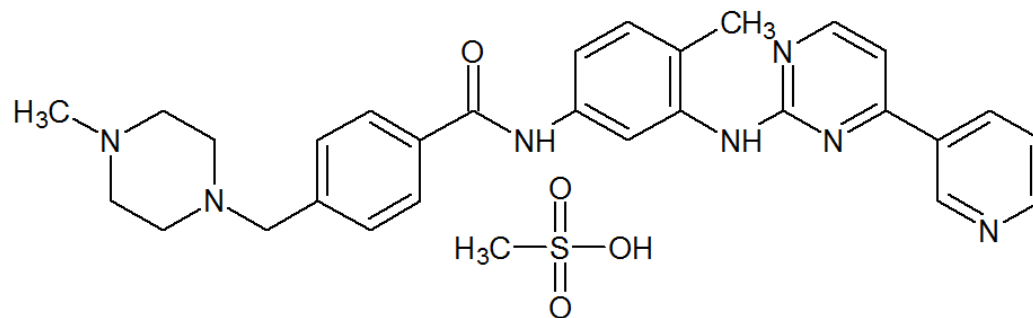
- Chemicals can match only at structure
- Target is a protein, distinct from genes
- Sometimes I want to match across species



Scientific Lenses – A. Gray

Gleevec® = Imatinib Mesylate

The University of Manchester



YLM AHDNUQAMNNX-UHFFFAOYSA-N

ChemSpider
The free chemical database

About | More Searches | Web APIs

Gleevec

ChemSpider ID: ...
Molecular Form: ...
Average mass: ...
Monoisotopic m: ...
Systematic n: 4-[[4-Methyl-1-

Structure	 Download: MOL SDF SMILES InChI Display: 2D Structure 3D Structure
Synonyms	<ul style="list-style-type: none"> Imatinib Mesylate Imatinib Methansulfonate STI-571
Brand names	<ul style="list-style-type: none"> Gleevec Glivec

[Imatinib; 152459-95-5; sti-571 ...](#)

MW: 493.602740 g/mol MF: C₂₉H₃₁N₇O
 IUPAC name: 4-[(4-methylpiperazin-1-yl)methyl]pyrimidin-2-amine
 CID: 5291
[Active in 205 BioAssays](#) [Tested in 1376 BioAssays](#)
[Similar Compounds](#) [Same Parent, Connectives](#)
[\(MeSH Keyword\)](#)

[Imatinib mesylate; Gleevec; Glivec ...](#)

MW: 589.708400 g/mol MF: C₃₀H₃₅N₇O₄S
 IUPAC name: methanesulfonic acid; 4-[(4-methylpiperazin-1-yl)methyl]pyrimidin-2-amine
 CID: 123596
[Active in 35 BioAssays](#) [Tested in 679 BioAssays](#)
[Similar Compounds](#) [Same Parent, Connectives](#)
[\(MeSH Keyword\)](#)

ChemSpider


23 April 2013

Drugbank

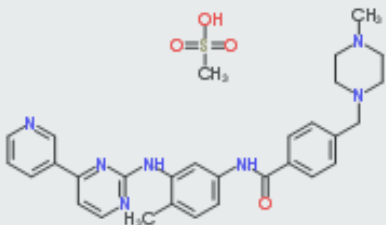
Scientific Lenses – A. Gray

PubChem

Multiple Links: Different Reasons



ChemSpider
The free chemical database



Link: skos:closeMatch
Reason: non-salt form

Link: skos:exactMatch
Reason: drug name



DRUGBANK
Open Data Drug & Drug Target Database



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"



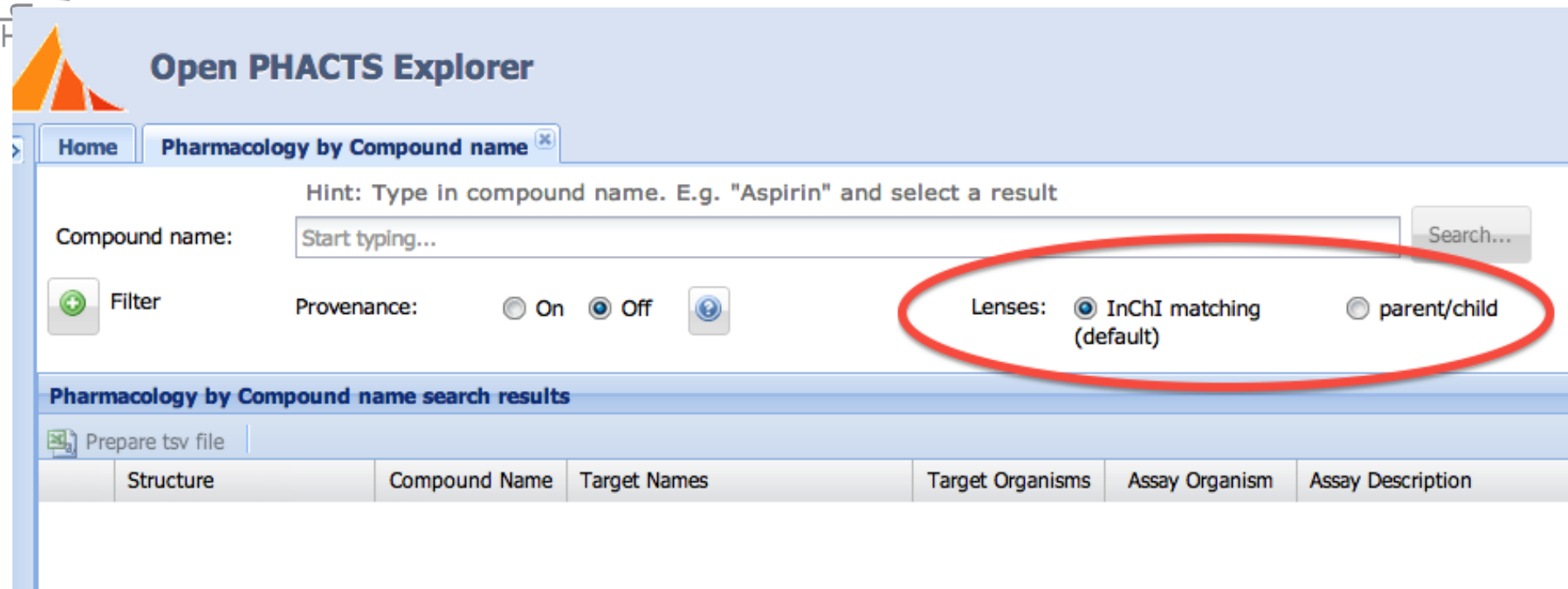
```
InChI Key Match {
  chemspider:imantinib_mesylate skos:exactMatch
  chembl: imantinib_mesylate
}
```

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

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

Lenses in the Explorer

The University
Manchester



Open PHACTS Explorer

Home | Pharmacology by Compound name

Hint: Type in compound name. E.g. "Aspirin" and select a result

Compound name:

Filter Provenance: On Off

Lenses: InChI matching (default) parent/child

Pharmacology by Compound name search results

Structure	Compound Name	Target Names	Target Organisms	Assay Organism	Assay Description
-----------	---------------	--------------	------------------	----------------	-------------------

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?

Alasdair.Gray@manchester.ac.uk

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.