

Metabolomics: **Metabolite profiling and quantification from Mass Spectrometry data.**

Natalie J Stanford,
Catherine Winder,
Carole Goble.

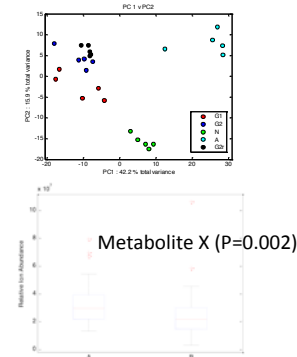
The Metabolomic Data Pipeline.



Sample coll.
and prep. →



Data analysis →



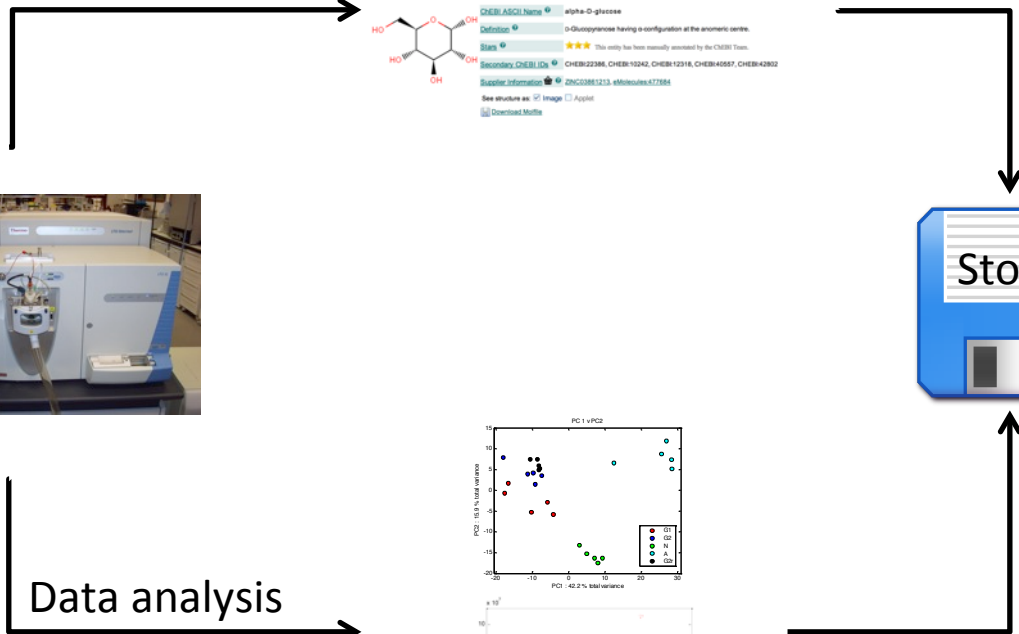
Metabolite ID. →

o-D-glucose (CHEBI:17925)

Main | CHEBI Ontology | Automatic Kebs

Search CHEBI term
Search for:

CHEBI Name: o-D-glucose
 CHEBI ID: CHEBI:17925
 CHEBI ASCII Name: alpha-D-glucose
 Definition: D-Glucopyranose having a configuration at the anomeric centre.
 Stars: ★★★ This entry has been manually annotated by the CHEBI Team.
 Secondary CHEBI IDs: CHEBI:22394, CHEBI:12242, CHEBI:12318, CHEBI:40587, CHEBI:42802
 Similar Information: ZINC13841213, eMolecules:677964
 See structure as: Image Applet
[Download Molfile](#)



The cost per metabolomic sample is ~£54.



Cost per sample is ~ £54.
1000 samples cost ~ £54k.



Metabolite ID.

o-D-glucose (CHEBI:17925)

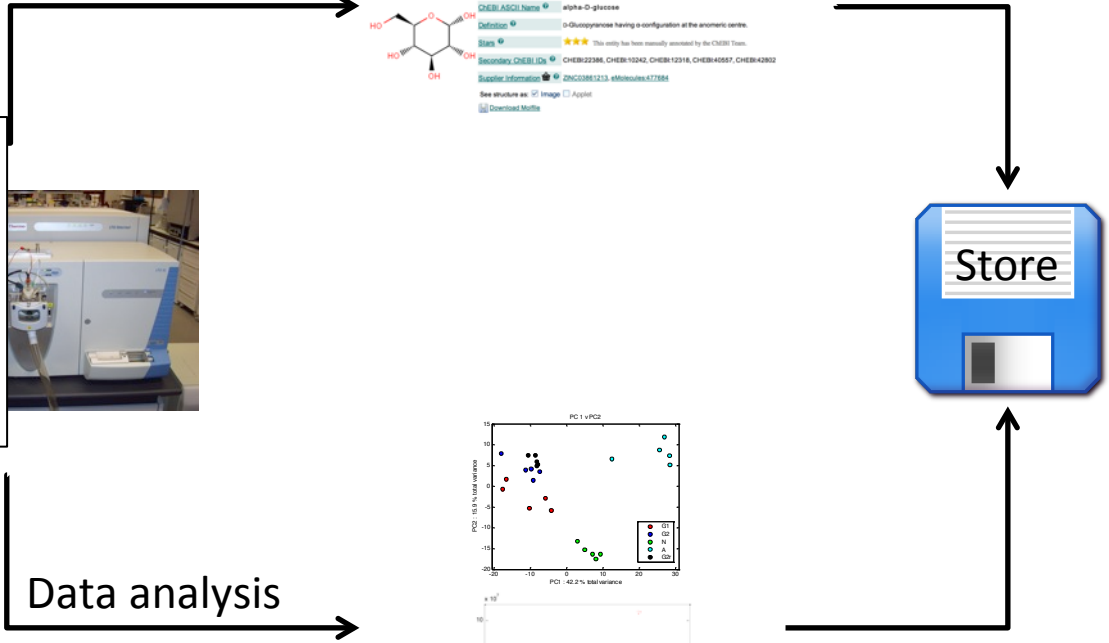
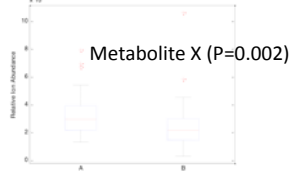
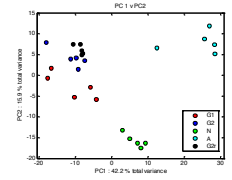
Main | CHEBI Ontology | Automatic Kebs

Search CHEBI here! Search for

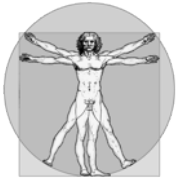
CHEBI Name o-D-glucose
CHEBI ID CHEBI:17925
CHEBI ASCII Name alpha-D-glucose
Definition D-Glucopyranose having a configuration at the anomeric centre.
Stars ★★★ This entry has been manually annotated by the CHEBI Team.
Secondary CHEBI IDs CHEBI:22394, CHEBI:12042, CHEBI:12318, CHEBI:40587, CHEBI:42802
Similar Information ZINC15841213 | eMolecules:677965
 See structure as: Image Applet
[Download Moltis](#)

OC[C@H]1O[C@H](O)[C@@H](O)[C@@H]1O

Data analysis



A single sample takes ~5min to turn from net.cdf format to .txt format.



Sample coll. and prep. →

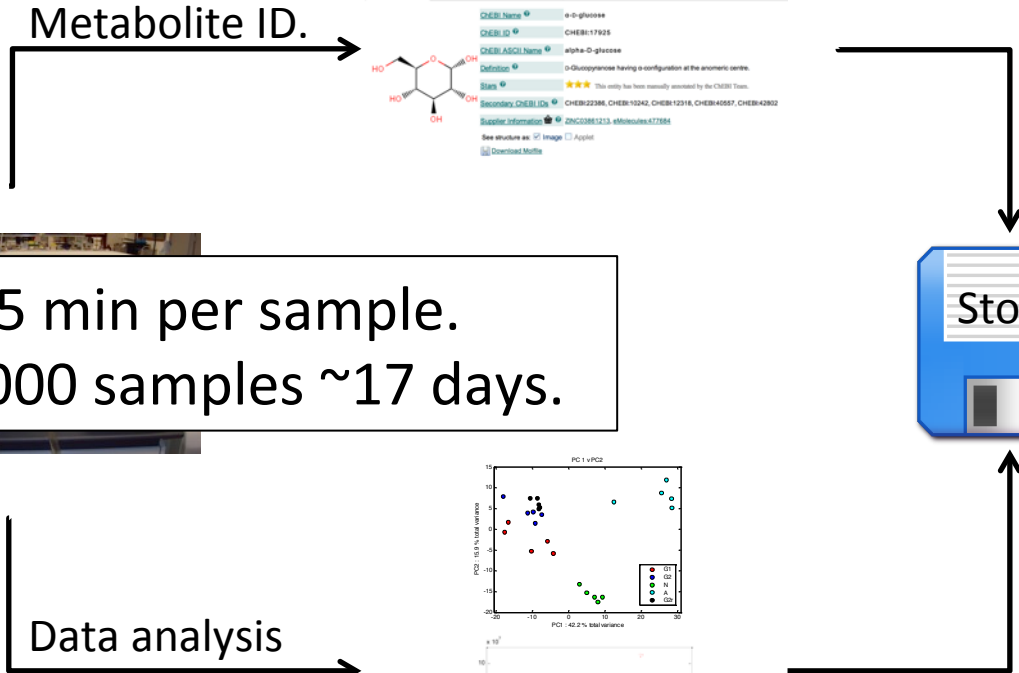
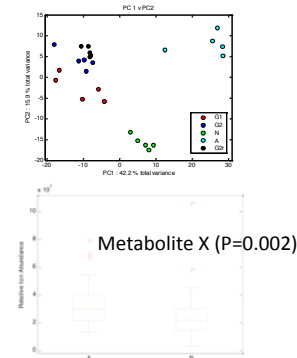
~ 5 min per sample.
1000 samples ~17 days.

Data analysis →

Metabolite ID. →

o-D-glucose (CHEBI:17925)

ChEMBL Name: alpha-D-glucose
ChEMBL ID: CHEBI:17925
ChEMBL ASCII Name: alpha-D-glucose
Definition: D-Glucopyranose having alpha-configuration at the anomeric centre.
Stars: ★★ This entry has been manually annotated by the ChEMBL Team.
Secondary ChEMBL IDs: CHEBI:22398, CHEBI:12242, CHEBI:12218, CHEBI:40587, CHEBI:42802
Similar Information: ZINC13841213, eMolecules:677968
See structure as: Image | Applet | Download Moltis



Volume of data.

Raw data:
~15mb per
single
Sample.

Batch ~1000
= ~15 gb.

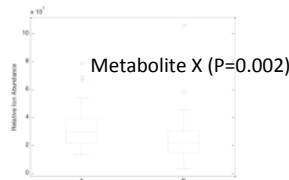
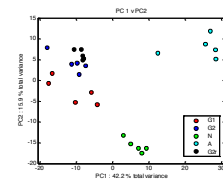


Metabolite ID.

o-D-glucose (CHEBI:17925)

ChEBI Name: o-D-glucose
ChEBI ID: CHEBI:17925
ChEBI ASCII Name: alpha-D-glucose
Definition: D-Glucopyranose having a configuration at the anomeric centre.
Status: This entry has been manually annotated by the ChEBI Team.
Secondary ChEBI IDs: CHEBI:22386, CHEBI:10242, CHEBI:12318, CHEBI:40587, CHEBI:42802
Supplier Information: ZINC0381213, eMolecules:47384

Data analysis



Derived
data:
~10kb per
Batch.

Variety of data: sources, forms, structures.



Sample coll. and prep.



Metabolite ID.

o-D-glucose (CHEBI:17925)

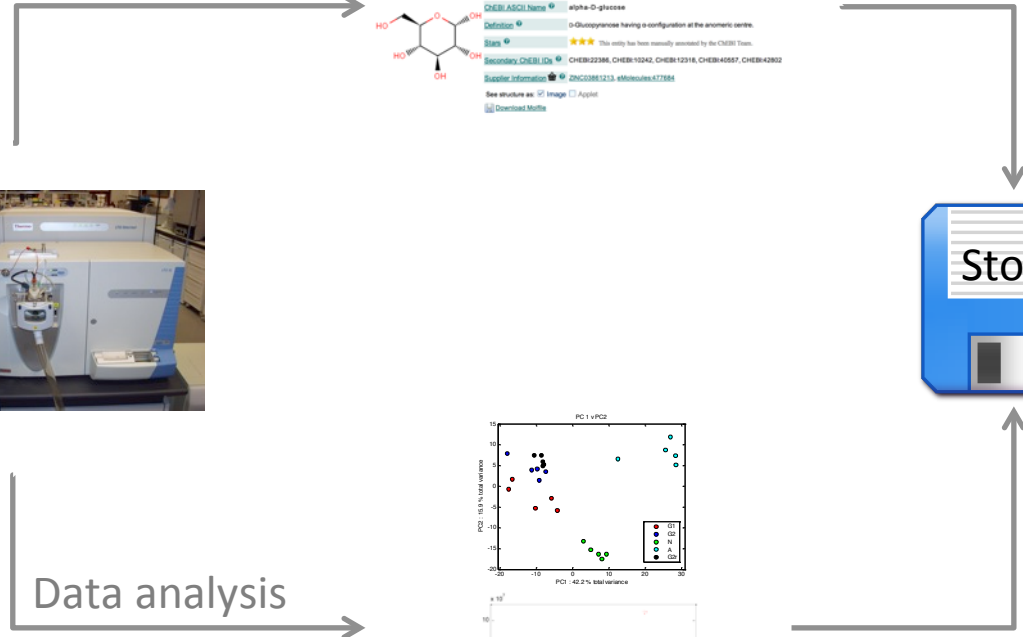
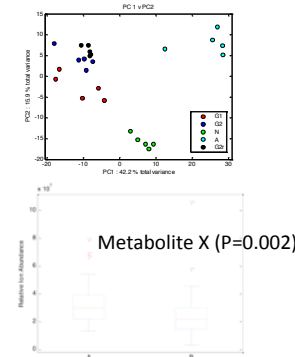
Main | CHEBI Ontology | Automatic Kebs

Search CHEBI term
Search for only

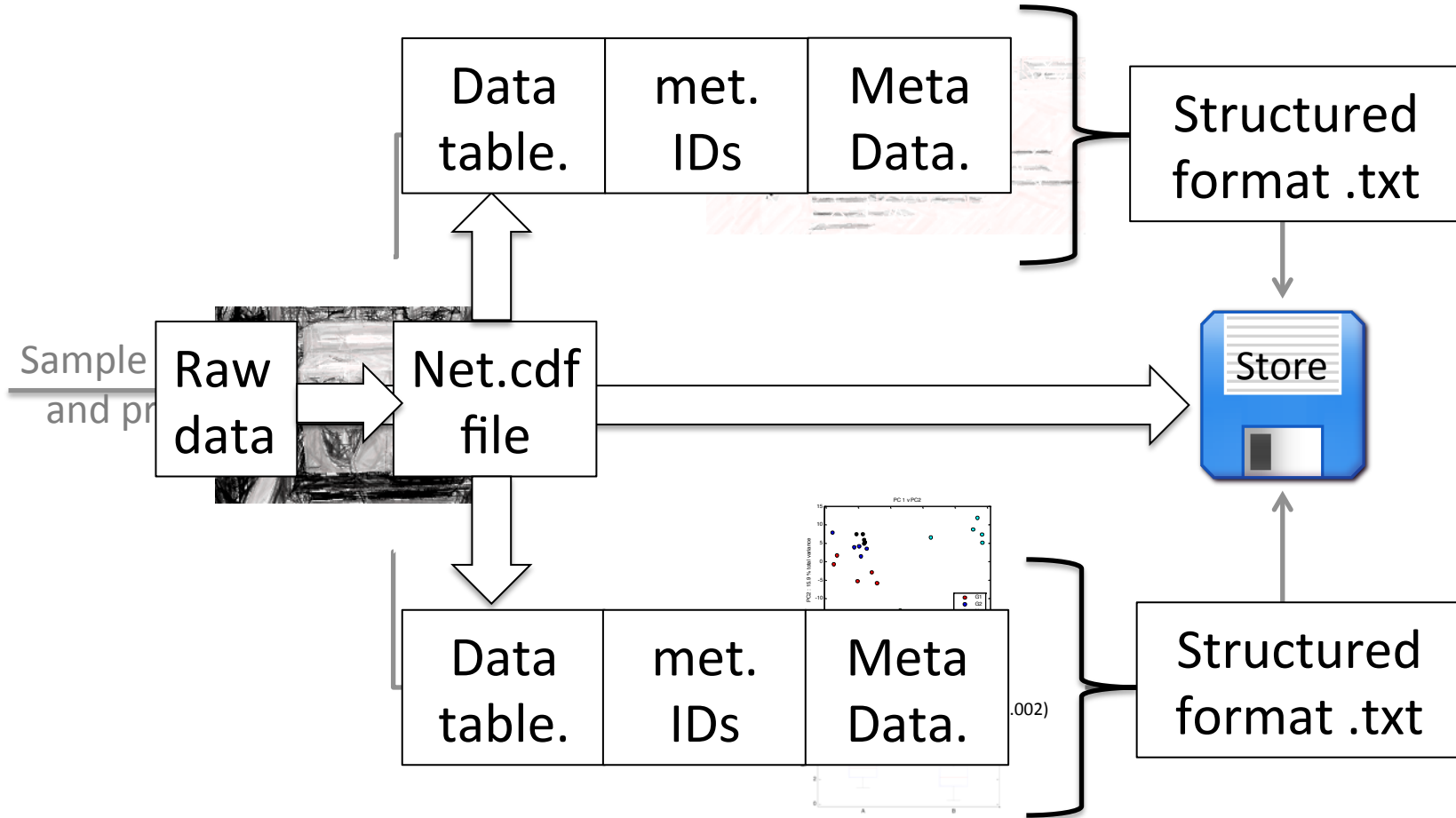
CHEBI Name o D-glucose
 CHEBI ID CHEBI:17925
 CHEBI ASCII Name alpha-D-glucose
 Definition D-Glucopyranose having a configuration at the anomeric centre.
 Stars ☆☆☆ This entry has been manually annotated by the CHEBI Team.
 Secondary CHEBI IDs CHEBI:22394, CHEBI:12042, CHEBI:12318, CHEBI:40587, CHEBI:42802
 Similar Information [ZINC15841213](#) [eMolecules:677965](#)
 See structure as: Image Applet
[Download Moltis](#)



Data analysis



Variety of data: sources, forms, structures.



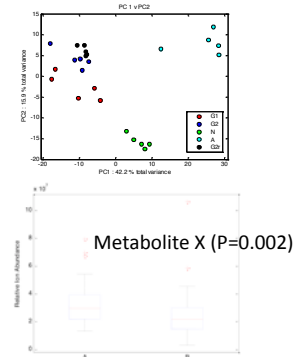
Varacity of data: noise, bias, reproducibility.



Sample coll. and prep. →



Data analysis →



Metabolite ID. →

o-D-glucose (CHEBI:17925)

Main CHEBI Ontology Automatic Kebs Search CHEBI term Search for ★★ ★ only

CHEBI Name o-D-glucose
 CHEBI ID CHEBI:17925
 CHEBI ASCII Name alpha-D-glucose
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 Secondary CHEBI IDs CHEBI:22398, CHEBI:10242, CHEBI:12318, CHEBI:40587, CHEBI:42802
 Similar Information ZINC13841213 eMolecules:677968
 See structure as: Image Applet Download Mofds



Varacity of data: noise, bias, reproducibility.

SOPs are used throughout the pipeline. QA/QC is used to e.g. check instrument drift.



Sample coll. and prep.

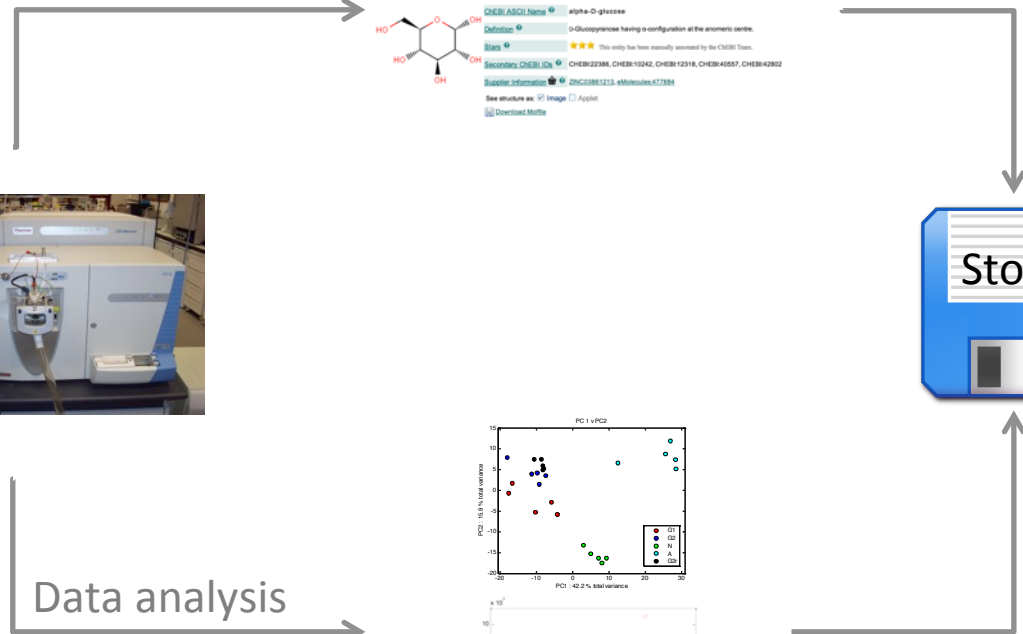
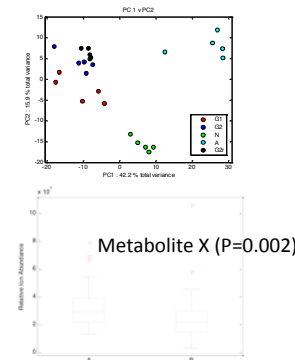


Metabolite ID.

alpha-D-glucose (CHEBI:17925)
 Main | CHEBI Ontology | Automatic Kecls | Search CHEBI term | Search for:

- CHEBI Name** alpha-D-glucose
- CHEBI ID** CHEBI:17925
- CHEBI ASCII Name** alpha-D-glucose
- Definition** D-Glucopyranose having a configuration at the anomeric centre.
- Stars** ★★★ This entry has been manually annotated by the CHEBI Team.
- Secondary CHEBI IDs** CHEBI:22394, CHEBI:12242, CHEBI:12218, CHEBI:40587, CHEBI:42802
- Similar Information** [ZINC1281213](#) [Pubmed/PMID:627968](#)
- See structure as: Image Applet
- [Download Moltis](#)

Data analysis



Varacity of data: noise, bias, reproducibility.

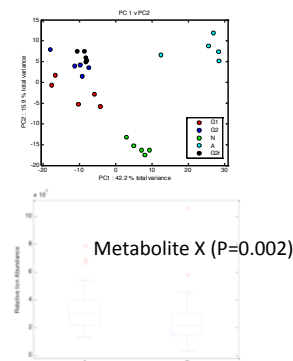
Metadata are added to the data tables.



Metabolite ID.



Data analysis



Volatility of data: change, relevance, preservation.



Sample coll. and prep.



Metabolite ID.

o-D-glucose (CHEBI:17925)

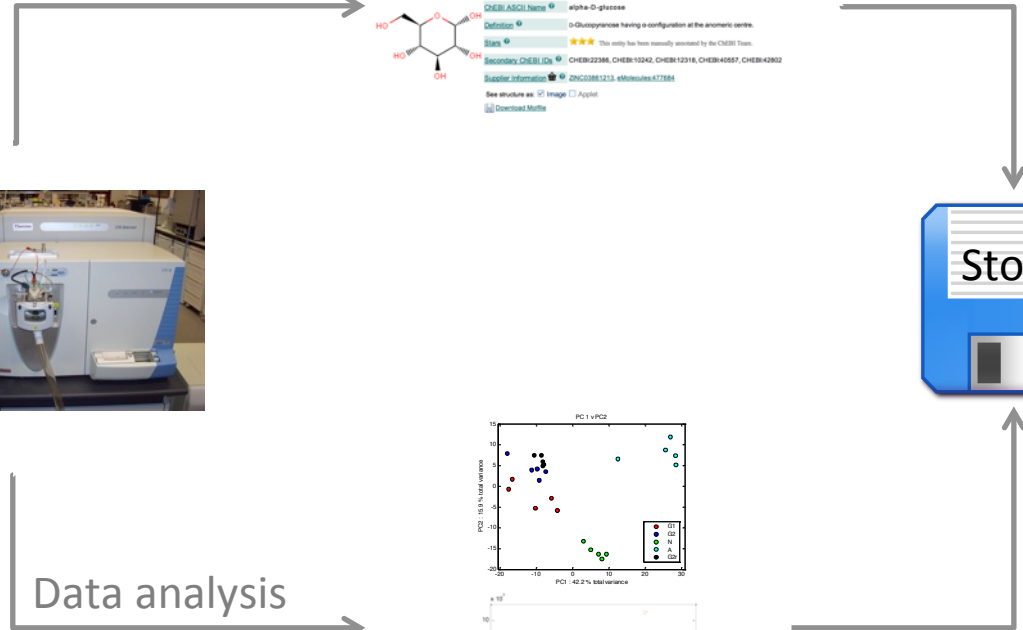
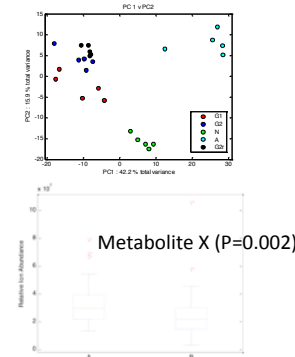
Main CHEBI Ontology Automatic Kebs

Search CHEBI term
Search for in only

CHEBI Name o-D-glucose
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 CHEBI ASCII Name alpha-D-glucose
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 Similar Information ZINC13841213 eMolecules:677968
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OC[C@H]1O[C@H](O)[C@@H](O)[C@@H]1O

Data analysis



Volatility of data: change, relevance, preservation.

As technology advances much of the data needs to be replaced.



Sample coll. and prep. →



Metabolite ID. →

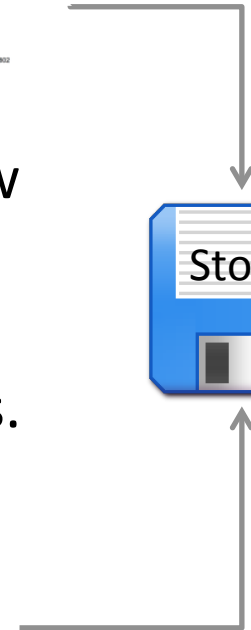
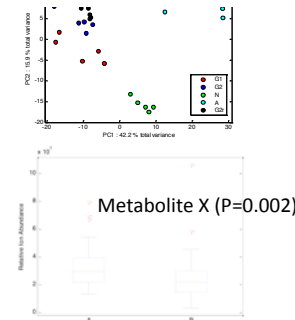
o-D-glucose (CHEBI:17925)

Main | CHEBI Ontology | Automatic Kebs

CHEBI Name: α-D-glucose
 CHEBI ID: CHEBI:17925
 CHEBI ASCII Name: alpha-D-glucose
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 Stars: ★★ This entry has been manually annotated by the CHEBI Team.
 Secondary CHEBI IDs: CHEBI:22398, CHEBI:12042, CHEBI:12318, CHEBI:40587, CHEBI:42802
 Synonym Information: ZINC3841213, wikipedia:α-D-glucose
 See structure as: Image | Applet | Download Moltis

Can re-analyse raw data in many different ways for different purposes.

Data analysis →



Velocity of data: flow, scale, stream.

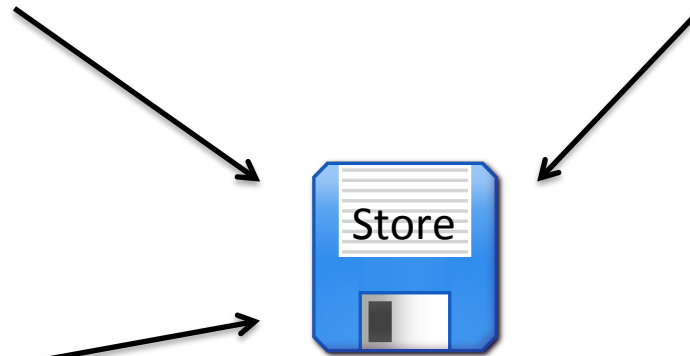


Velocity of data: flow, scale, stream.

Instrumentation becomes more powerful in detection

Databases allow more metabolites to be identified per study.

There are ~ 20 listed database resources for metabolomics data.



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