MetaboAge User Guide

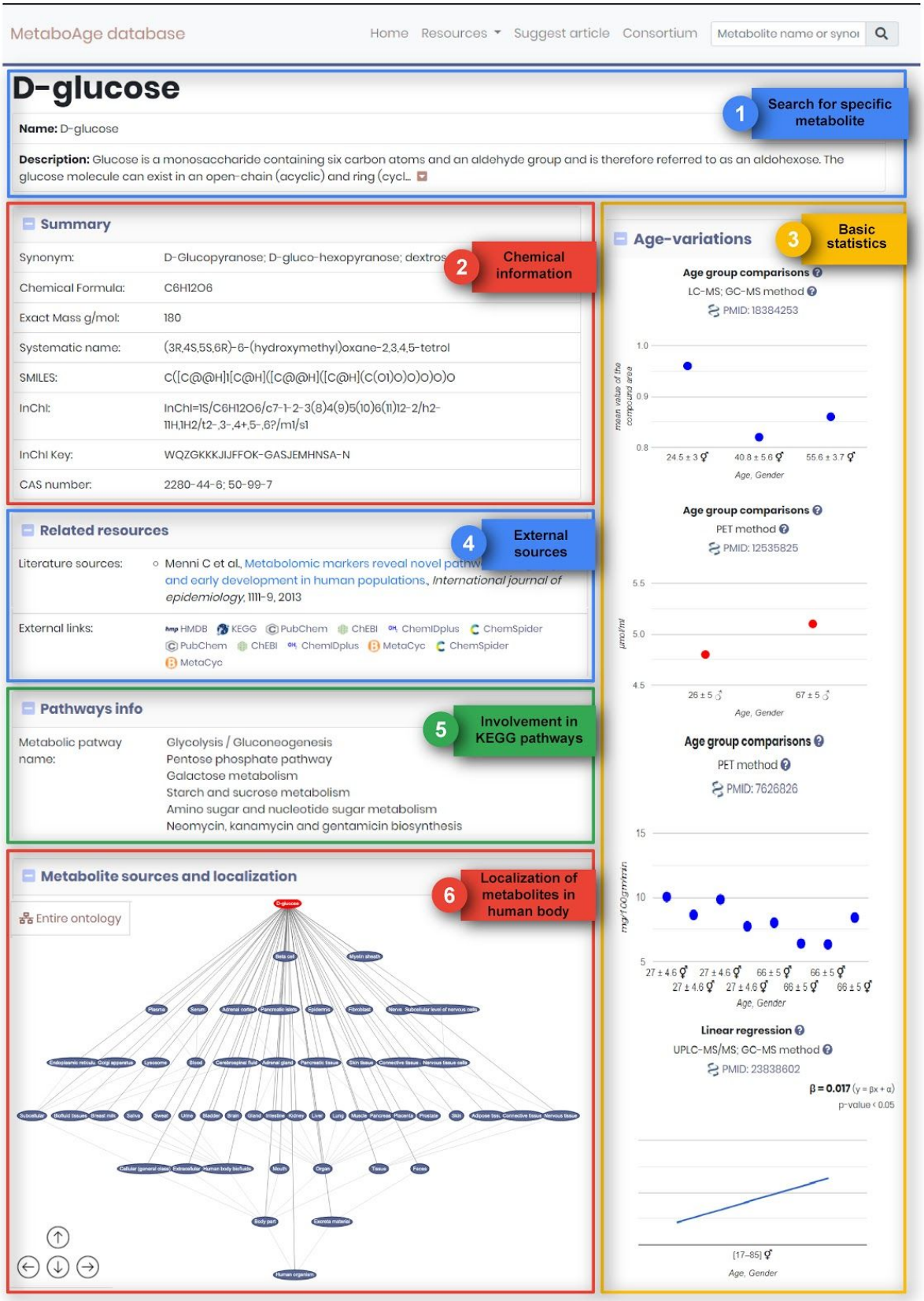
The database user guide covers every aspect of the MetaboAge database and informs the user on how to use each and every element of the database website. All the information about how to use the search function, ontology and how to interact with graphical representations of the database can be found in this user guide.

Website user guide:

MetaboAge website is available at http://metaboage.info/
On the home page is found the “Resources” drop-down list containing this user guide and the database download link.
The “Suggest article” page offers the user the possibility to recommend an age-related metabolomics article for our database collection feel free to fill in the form below.

On the website home, it can be found a search box for the metabolite entity of interest. You can search by hole name or part of it. From the query results, you can further filter the metabolites by endogenous or exogenous type.
This can be also done by clicking the button Browse Metabolites. You also can browse pathways by clicking the button Browse Pathways browse the localization-based ontology by clicking the button Browse Ontology.
After searching or browsing the metabolite you can enter into the metabolite page.

The metabolite page is divided into 5 sections, namely: 1) description of the searched metabolite, 2) chemical information, 3)basic statistics, 4)metabolite involvement in Homo sapiens pathways and 5) the metabolite localization-based ontology. These sections are represented in image 1.


MetaboAge database
Home
Resources
Suggest article
Consortium
Metabolite name or synor
D-glucose
Name: D-glucose
Description: Glucose is a monosaccharide containing six carbon atoms and an aldehyde group and is therefore referred to as an aldohexose. The glucose molecule can exist in an open-chain (acyclic) and ring (cycl...
1
Search for specific metabolite
Summary
Synonym: D-Glucopyranose; D-gluco-hexopyranose; dextros
2
Chemical information
Chemical Formula: C6H12O6
Exact Mass g/mol: 180
Systematic name: (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol
SMILES: C([C@@H]1[C@H]([C@@H]([C@H](C(O1)O)O)O)O)O
InChI: InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6?/m1/s1
InChI Key: WQZGKKKJIJFFOK-GASJEMHNSA-N
CAS number: 2280-44-6; 50-99-7
Related resources
4
External sources
Literature sources: Menni C et al., Metabolomic markers reveal novel pathw and early development in human populations., International journal of epidemiology, 1111-9, 2013
External links: HMDB KEGG PubChem ChEBI ChemIDplus ChemSpider PubChem ChEBI ChemIDplus MetaCyc ChemSpider MetaCyc
Pathways info
5
Involvement in KEGG pathways
Metabolic patway name: Glycolysis / Gluconeogenesis
Pentose phosphate pathway
Galactose metabolism
Starch and sucrose metabolism
Amino sugar and nucleotide sugar metabolism
Neomycin, kanamycin and gentamicin biosynthesis
Metabolite sources and localization
6
Localization of metabolites in human body
Entire ontology
Age-variations
3
Basic statistics
Age group comparisons
LC-MS; GC-MS method
PMID: 18384253
mean value of the compound area
24.5 ± 3
40.8 ± 5.6
55.6 ± 3.7
Age, Gender
Age group comparisons
PET method
PMID: 12535825
µmol/ml
26 ± 5
67 ± 5
Age, Gender
Age group comparisons
PET method
PMID: 7626826
mg/100g/min
Age, Gender
Linear regression
UPLC-MS/MS; GC-MS method
PMID: 23838602
β = 0.017 (y = βx + α)
p-value < 0.05
[17-85]
Age, Gender

Field Documentation:

Section 1).

FIELD	Description of the field
Name	This field represents the name of the metabolite as reported by the author (with some exception in the case of the misspelled names and when the name can be better assessed based on the scientific literature)
Description	This field holds the documentation of the aging-related metabolite

Section 2).

FIELD	Description of the field
Synonyms	Alternative names of the metabolite (isomers and ionic forms of the acids are considered a separate metabolite entity in the database)
Description	This field holds the documentation of the aging-related metabolite
Chemical Formula	Chemical formula describing atomic or elemental composition
Exact Mass g/mol	The field represents the calculated mass from a molecular formula using known masses of specific isotopes with the appropriate number of decimal places. The exact mass is usually taken from the PubChem database
Systematic name	This field represents the systematic, IUPAC or chemical name of a metabolite.
CAS number	The chemical abstract service identification number.
SMILES	Isomeric SMILES string corresponding to metabolite structure

InChI	Standard InChI identifier
InChI Key	Standard InChI key
HMDB ID	Unique HMDB accession number consisting of a 4 letter prefix (HMDB) and a 5 number suffix.
KEGG ID	KEEG compound entry ID
Database IDs	Database compound identification numbers of the metabolite

Section 3).

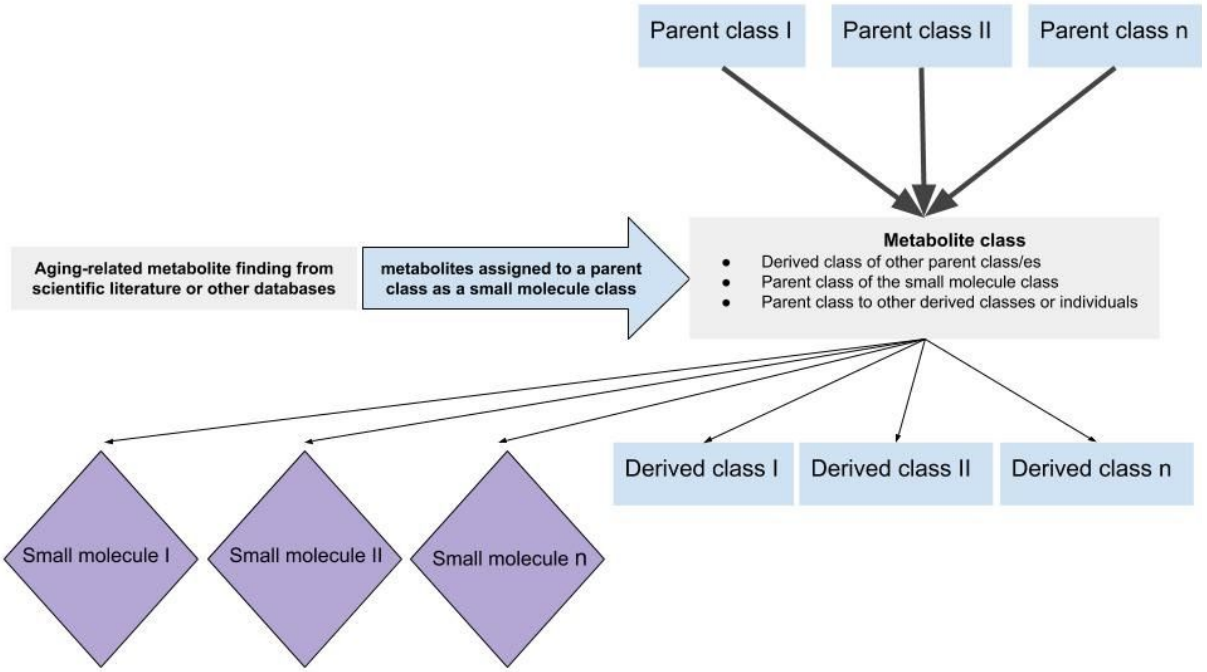
This section shows a graphical representation of the metabolite variation related to age in different age groups and according to different studies and methods.

Section 4)

FIELD	Description of the field
Metabolic pathway name	Name of the pathways from Homo sapiens species in which the metabolite is found according to KEGG database

Section 5)

Metabolite sources and localizations are integrated into an ontology. The way the ontology is structured is represented in the figure below.



In the metabolite page, you can browse the classes in which the metabolite is found by clicking on classes from the tree. By doing these you can see all the metabolites that are in these classes (see example in the image below).
You also have the option to browse the entire ontology bi clicking the upper left button of section 5):  .