Metabolite signal identification in accurate mass metabolomics data with MZedDB, an interactive m/z annotation tool utilising predicted ionisation behaviour 'rules'

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Additional files

Additional file 1

File format: DOC

Title: Example MZedDB Metabolite Card

Description: This document shows an example MZedDB Metabolite Card entry for pipecolic acid.

Metabolite entry:

Database id	D22652 Adducts
Selected name	Pipecolic acid
Synonyms	Pipecolic acid;;L-pipecolate;;()-Piperidine-2-carboxylic acid;;(+/-)-2-Piperidinecarboxylate;;(+/-)-2-Piperidinecarboxylic acid;;(+/-)-Pipecolate;;(+/-)-Pipecolic acid;;(+/-)-Pipecolinate;;(+/-)-Pipecolinic acid;;(.+/-.)-2-Piperidinecarboxylic acid;;(RS)-2-Piperidinecarboxylate;;(RS)-2-Piperidinecarboxylic acid;;.alpha.-Pipecolinic acid;;2-Carboxypiperidine;;2-Pipecolinic acid;;2-Piperidinecarboxylate;;2-Piperidinecarboxylic acid;;2-Piperidinylcarboxylic acid;;a-Pipecolinate;;a-Pipecolinic acid;;acide pipecolique;;acide piperidine-carboxylique-2;;alpha-Pipecolinate;;alpha-Pipecolinic acid;;Dihydrobaikiane;;DL-2-Piperidinecarboxylate;;DL-2-Piperidinecarboxylic acid;;DL-Homoproline;;DL-Pipecolate;;DL-Pipecolic acid;;DL-Pipecolinate;;DL-Pipecolinic acid;;Hexahydro-2-picolinate;;Hexahydro-2-picolinic acid;;Hexahydropicolinate;;Hexahydropicolinic acid;;Homoproline;;pipecolate;;pipecolic acid;;Pipecolic acid free base;;Pipecolinate;;Pipecolinic acid;;piperidine-2-carboxylic acid;;Piperolinate;;Piperolinic acid
Accurate mass	129.078979
Molecular Formula	C6H11NO2 Search Isotope Adducts
Number of atoms	20
Number of stereocenters	0/1
Smiles	OC(=O)C1CCCCN1

Data source(s):

- HMDB: Pipecolic acid (HMDB00070)
- Metacyc: L-pipecolate (L-PIPECOLATE)

Known metabolic reactions:

- Metacyc: Small-Molecule-Reactions (RXN-8166)
  - Enzyme(s): 1.5.1.21
  - lysine degradation V (PWY-5283)
- Metacyc: Small-Molecule-Reactions;Chemical-Reactions (RXN-8161)
  - No associated enzyme
  - lysine degradation V (PWY-5283)
- Metacyc: L-pipecolate oxidase;Small-Molecule-Reactions (L-PIPECOLATE-OXIDASE-RXN)
  - Enzyme(s): 1.5.3.7
  - No associated pathway
- Metacyc: L-pipecolate dehydrogenase;Small-Molecule-Reactions (L-PIPECOLATE-DEHYDROGENASE-RXN)
  - Enzyme(s): 1.5.99.3
  - No associated pathway
- Metacyc: δ(1)-piperideine-2-carboxylate reductase;Small-Molecule-Reactions (1.5.1.21-RXN)
  - Enzyme(s): 1.5.1.21
  - No associated pathway

Related compound(s) with identical skeleton:

- D23128 - L-Pipecolic acid
- D23147 - D-Pipecolic acid

Related compound(s) with similarity >0.8:

- D23147 - D-Pipecolic acid - 1.000
- D23128 - L-Pipecolic acid - 1.000
- D22648 - d1-piperidine-dicarboxylate - 0.934
- D19675 - Homostachydrine - 0.882
- D23678 - 5-hydroxy-pipecolate - 0.864
- D13187 - (2S)-2-{[1-(R)-Carboxyethyl]amino}pentanoate - 0.827
- D5306 - (2S)-2-{[1-(R)-carboxyethyl]amino}pentanoate - 0.827