

## Aberystwyth University

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

Draper, John; Enot, David Pierre Louis; Parker, David A; Beckmann, Manfred; Snowdon, Stuart; Lin, Wanchang; Zubair, Hassan

*Published in:*  
BMC Bioinformatics

*DOI:*  
[10.1186/1471-2105-10-227](https://doi.org/10.1186/1471-2105-10-227)

*Publication date:*  
2009

*Citation for published version (APA):*

Draper, J., Enot, D. P. L., Parker, D. A., Beckmann, M., Snowdon, S., Lin, W., & Zubair, H. (2009). Metabolite signal identification in accurate mass metabolomics data with MZedDB, an interactive m/z annotation tool utilising predicted ionisation behaviour 'rules'. *BMC Bioinformatics*, 10(227), Article 227. <https://doi.org/10.1186/1471-2105-10-227>

#### **Document License** CC BY

#### **General rights**

Copyright and moral rights for the publications made accessible in the Aberystwyth Research Portal (the Institutional Repository) are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the Aberystwyth Research Portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the Aberystwyth Research Portal

#### **Take down policy**

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

tel: +44 1970 62 2400  
email: [is@aber.ac.uk](mailto:is@aber.ac.uk)

## Additional files

Additional file 1

File format: DOC

Title: Example MZedDB Metabolite Card

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

### Metabolite entry:

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

### Data source(s):

- HMDB: Pipercolic 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:  $\delta(1)$ -piperidine-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