Table S1 Phase I and Phase II Biotransformation Types in Meteor

Phase I

- Redox
  - Oxidation
    - Carboaliphatic Hydroxylation
    - Carboaromatic Hydroxylation
    - Heteroaromatic Hydroxylation
    - Epoxidation
    - Deamination
    - Dealkylation and Oxidative Ring-Opening
    - Oxidative Dehalogenation
    - Dehydrogenation
    - Oxidation of Aldehyde
    - Oxidation at Aliphatic and Aromatic Nitrogen
    - Oxidation at Aliphatic and Aromatic Sulphur
    - Oxidation at Other Heteroatoms
    - Miscellaneous Oxidative Ring Opening
    - Miscellaneous Oxidative Fragmentation
    - Miscellaneous Oxidative Coupling
    - Miscellaneous Other
  - Reduction
    - Carbonyl Reduction
    - Alkene Reduction
    - Alkyne Reduction
    - Reduction of Nitrogen-Containing Functional Groups
    - Reductive Bond Scission
- Non-Redox
  - Hydrolytic Reactions
    - Ester Hydrolysis
    - Amide Hydrolysis
    - Other Carboxylic Acid Derivatives
    - Other Unsaturated Functional Groups
    - Ether Hydrolysis
    - Hydrolytic Deamination
    - Hydrolytic Dehalogenation
    - Dehydration
  - Hydration
  - Hydrolytic Fragmentation or Ring-Opening
  - Non Hydrolytic Fragmentation or Ring-Opening
  - Ring-Closure Reactions
  - Other Elimination Reactions
  - Decarboxylation
  - Miscellanaeous
  - Rearrangement

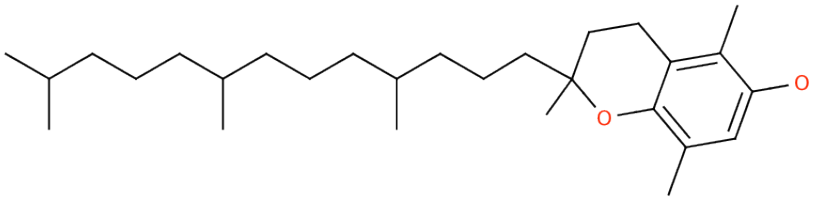
Phase II

- Glucuronidation
- Sulphonation
- Glutathione Conjugation
- Acetylation
- Methylation
- Conjugation with Amino Acids
- Conjugation with Other Acids
- Glucosidation

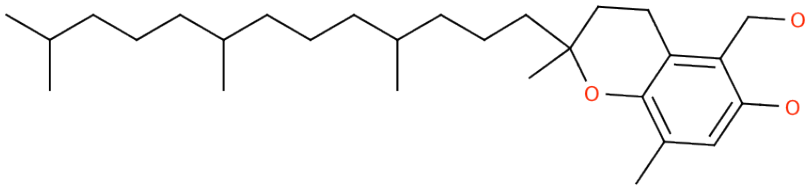
HMDB06335
Beta-tocopherol

Significant Differences in the Electrochemical Behavior of the α-, β-, γ-, and δ-Tocopherols (Vitamin E), Gregory J. Wilson,Ching Yeh Lin, and, and Richard D. Webster, *The Journal of Physical Chemistry B* **2006** *110* (23), 11540-11548

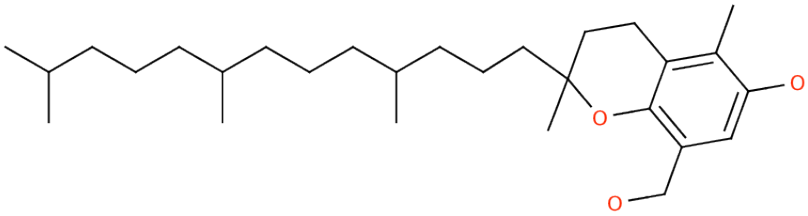
Parent Compound (HMDB06335)



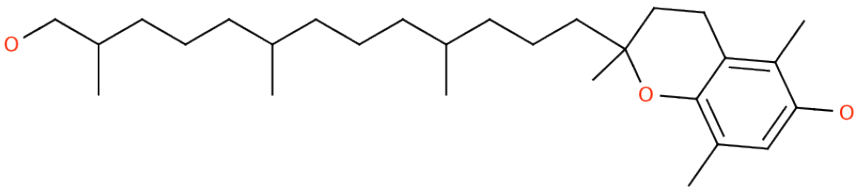
Meteor Generated Metabolites of HMDB06335



Metabolite-1 (known-unknown) found in PubChem - CID 5347345



Metabolite-2 (unknown-unknown) not found in any current database

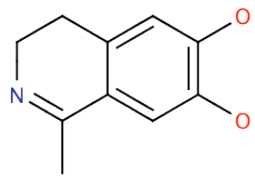


Metabolite-3 (unknown-unknown) not found in any current database

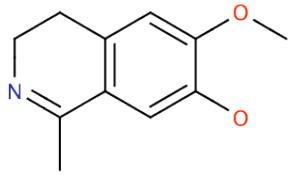
HMDB12490
1,2-Dehydrosalsolinol

Michael A. Collins, Bhe Y. Cheng, Oxidative decarboxylation of salsolinol-1-carboxylic acid to 1,2-dehydrosalsolinol: Evidence for exclusive catalysis by particulate factors in rat kidney, Archives of Biochemistry and Biophysics, Volume 263, Issue 1, 15 May 1988, Pages 86-95, ISSN 0003-9861, http://dx.doi.org/10.1016/0003-9861(88)90616-9.

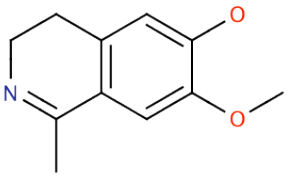
Parent Compound (HMDB12490)



Meteor Generated Metabolites of HMDB12490



Metabolite-1 (known-unknown) found in PubChem - CID 6056985



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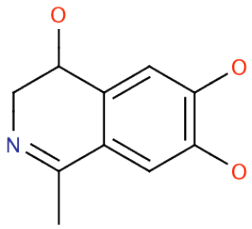
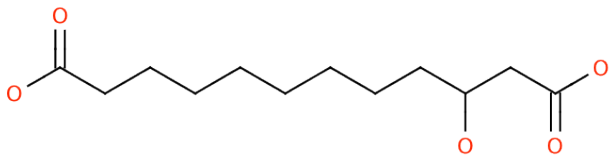


Metabolite-3 (unknown-unknown) not found in any current database

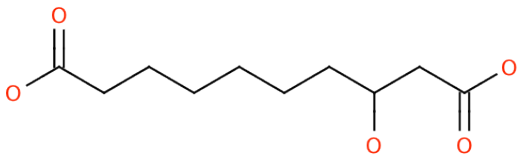
HMDB00413
3-Hydroxydodecanedioic acid

S.H. Korman, H. Mandel, and A. Gutman, Characteristic urine organic acid profile in peroxisomal biogenesis disorders, Journal of Inherited Metabolic Disease **23**, 425 (2000).

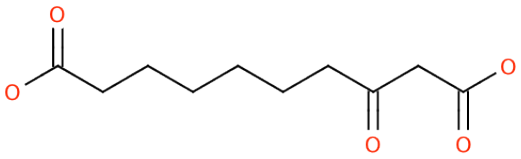
Parent Compound (HMDB00413)



Meteor Generated Metabolites of HMDB00413



Metabolite-1 (known-unknown) found in HMDB - HMDB00350



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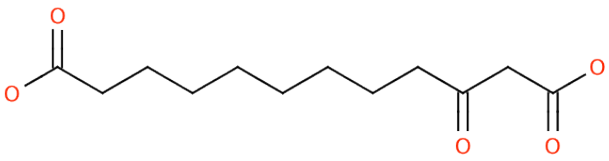

Metabolite-3 (unknown-unknown) not found in any current database

A step-by-step guide to viewing and converting structures

To view a single structure, copy and paste a SMILES string to the drawing area of any one of the following structure-drawing programs.

Chemaxon Marvin Sketch
ChemDraw
IsisDraw
ACD ChemSketch

Converting SMILES to SDF or Mol Format

1. Export the data in CSV format
2. Copy the column containing SMILES to a separate text file
3. Save the file with .smiles extension (e.g. strcutures.smiles)
4. Open the structures.smiles file with ChemAxon MarvinView
5. Click on File → Save All to save as an sd or mol file.