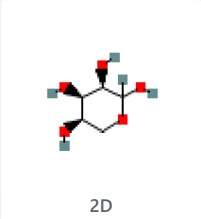
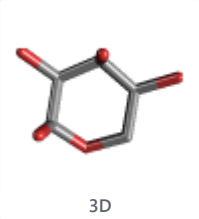
Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

PubChem

COMPOUND SUMMARY

# D-Ribose

| | |
|---|---|
| **PubChem CID** | 10975657 |
| **Structure** |  2D  3D<br>Find Similar Structures |
| **Molecular Formula** | $C_5H_{10}O_5$ |
| **Synonyms** | D-Rib<br>D-Ribopyranose<br>D-Ribopyranoside<br>D-Ribose<br>Rib<br>More... |
| **Molecular Weight** | 150.13 |
| **Dates** | Modify 2022-11-12<br>Create 2006-10-26 |

D-ribopyranose is a D-ribose and the D-enantiomer of ribopyranose. It is a ribopyranose and a D-ribose. It is an enantiomer of a L-ribopyranose.

ChEBI

D-Ribose is a natural product found in Tamarix aphylla, Streptomyces sporangiiformans, and Cannabis sativa with data available.

LOTUS - the natural products occurrence database

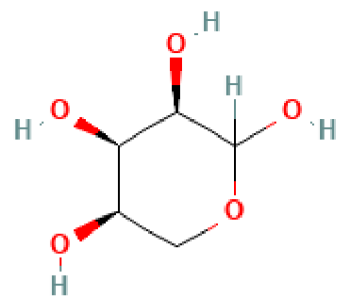
D-Ribose is a metabolite found in or produced by Saccharomyces cerevisiae.

- Yeast Metabolome Database (YMDB)

# 1 Structures

## 1.1 2D Structure

Chemical Structure Depiction



PubChem

## 1.2 3D Conformer

PubChem

## 2 Biologic Description

| | |
|---|---|
| **SVG Image** | |
| **IUPAC Condensed** | Rib |
| **LINUCS** | []{D-Ribp}{} |
| **IUPAC** | D-ribo-pentopyranose |
| **WURCS** | WURCS=2.0/1,1,0/[a222h-1x_1-5]/1/ |

PubChem

| | |
|---|---|
| **Permethylated Mass** | 206.11542378 |
| **Monosaccharide Composition** | $Xxx_1$ |

GlyGen

# 3 Names and Identifiers

## 3.1 Computed Descriptors

### 3.1.1 IUPAC Name

(3*R*,4*R*,5*R*)-oxane-2,3,4,5-tetrol

*Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)*

PubChem

### 3.1.2 InChI

InChI=1S/C5H10O5/c6-2-1-10-5(9)4(8)3(2)7/h2-9H,1H2/t2-,3-,4-,5?/m1/s1

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

PubChem

### 3.1.3 InChIKey

SRBFZHDQGSBBOR-SOOFDHNKSA-N

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

PubChem

### 3.1.4 Canonical SMILES

C1C(C(C(C(O1)O)O)O)O

*Computed by OEChem 2.3.0 (PubChem release 2021.05.07)*

PubChem

### 3.1.5 Isomeric SMILES

C1[C@H]([C@H]([C@H](C(O1)O)O)O)O

*Computed by OEChem 2.3.0 (PubChem release 2021.05.07)*

PubChem

## 3.2 Molecular Formula

C5H10O5

*Computed by PubChem 2.1 (PubChem release 2021.05.07)*

- PubChem

## 3.3 Other Identifiers

### 3.3.1 CAS

10257-32-6

- CAS Common Chemistry; ChemIDplus; EPA DSSTox; European Chemicals Agency (ECHA)

50-69-1

- DrugBank

### 3.3.2 European Community (EC) Number

700-481-3

- European Chemicals Agency (ECHA)

### 3.3.3 DSSTox Substance ID

DTXSID70450356

- EPA DSSTox

### 3.3.4 Wikidata

Q27120754

- Wikidata

### 3.3.5 GlyTouCan Accession

G75380KK

- GlyCosmos Glycoscience Portal; GlyTouCan Project

## 3.4 Synonyms

### 3.4.1 MeSH Entry Terms

D Ribose
D-Ribose
Ribose

- Medical Subject Headings (MeSH)

### 3.4.2 Depositor-Supplied Synonyms

D-Rib
D-Ribopyranose
D-Ribopyranoside
D-Ribose
Rib
Ribopyranose
Ribopyranoside
Ribose
10257-32-6
Ribopyranose (7CI,8CI,9CI)
(3R,4R,5R)-Oxane-2,3,4,5-tetrol
(3R,4R,5R)-Tetrahydro-2H-pyran-2,3,4,5-tetraol
10257-33-7
(3R,4R,5R)-tetrahydro-2H-pyran-2,3,4,5-tetrol
Ribiose
EC 700-481-3
SCHEMBL339948
CHEBI:47006
DTXSID70450356
C21057
Q27120754
WURCS=2.0/1,1,0/[a222h-1x_1-5]/1/

- PubChem

# 4 Chemical and Physical Properties

## 4.1 Computed Properties

| Property Name | Property Value | Reference |
|---|---|---|
| Molecular Weight | 150.13 | Computed by PubChem 2.1 (PubChem release 2021.05.07) |
| XLogP3-AA | -2.5 | Computed by XLogP3 3.0 (PubChem release 2021.05.07) |
| Hydrogen Bond Donor Count | 4 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Hydrogen Bond Acceptor Count | 5 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Rotatable Bond Count | 0 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Exact Mass | 150.05282342 | Computed by PubChem 2.1 (PubChem release 2021.05.07) |
| Monoisotopic Mass | 150.05282342 | Computed by PubChem 2.1 (PubChem release 2021.05.07) |
| Topological Polar Surface Area | 90.2 $Å^2$ | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Heavy Atom Count | 10 | Computed by PubChem |
| Formal Charge | 0 | Computed by PubChem |
| Complexity | 117 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Isotope Atom Count | 0 | Computed by PubChem |
| Defined Atom Stereocenter Count | 3 | Computed by PubChem |
| Undefined Atom Stereocenter Count | 1 | Computed by PubChem |
| Defined Bond Stereocenter Count | 0 | Computed by PubChem |
| Undefined Bond Stereocenter Count | 0 | Computed by PubChem |
| Covalently-Bonded Unit Count | 1 | Computed by PubChem |
| Compound Is Canonicalized | Yes | Computed by PubChem (release 2021.05.07) |

PubChem

## 4.2 Experimental Properties

### 4.2.1 Collision Cross Section

135.3 $Å^2$ $[M+Na]^+$ [CCS Type: DT, Method: single field calibrated with Agilent tune mix (Agilent)]

*https://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b03091*

- CCSbase

135.2 $Å^2$ $[M+Na]^+$ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

*https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322*

- CCSbase

# 5 Spectral Information

## 5.1 Mass Spectrometry

### 5.1.1 LC-MS

Showing 2 of 5 View More

| | |
|---|---|
| **MoNA ID** | FiehnHILIC001489 |
| **MS Category** | Experimental |
| **MS Type** | LC-MS |
| **MS Level** | MS2 |
| **Precursor Type** | [M-H]- |
| **Precursor m/z** | 149.0447 |
| **Instrument** | Thermo Q Exactive HF |
| **Instrument Type** | LC-ESI-QFT |
| **Ionization Mode** | negative |
| **Collision Energy** | HCD (NCE 20-30-40%) |
| **Top 5 Peaks** | 59.01258 100<br>71.01237 46.88<br>148.90872 43.20<br>89.02288 9.99<br>130.89479 9.63 |
| **SPLASH** | splash10-0a4i-9300000000-5d6c40433d32873303f4 |
| **Thumbnail** | |

| | |
|---|---|
| **Submitter** | Megan Showalter, University of California, Davis |

MassBank of North America (MoNA)

| | |
|---|---|
| **MoNA ID** | FiehnHILIC001490 |
| **MS Category** | Experimental |
| **MS Type** | LC-MS |
| **MS Level** | MS2 |
| **Precursor Type** | [M-H]- |
| **Precursor m/z** | 149.0447 |
| **Instrument** | Thermo Q Exactive HF |
| **Instrument Type** | LC-ESI-QFT |
| **Ionization Mode** | negative |
| **Collision Energy** | HCD (NCE 20-30-40%) |
| **Top 5 Peaks** | 59.0126 100<br>148.90904 64.48<br>71.01237 49.01<br>89.0231 12.65<br>100.73466 8.02 |
| **SPLASH** | splash10-0a4j-9400000000-686f05ef692e6dafe9e1 |
| **Thumbnail** | |

| | |
|---|---|
| **Submitter** | Megan Showalter, University of California, Davis |

MassBank of North America (MoNA)

# 6 Related Records

## 6.1 Related Compounds with Annotation

PubChem

## 6.2 Related Compounds

| | |
|---|---|
| Same Connectivity | 93 Records |
| Same Stereo | 14 Records |
| Same Isotope | 62 Records |
| Same Parent, Connectivity | 117 Records |
| Same Parent, Stereo | 14 Records |
| Same Parent, Isotope | 86 Records |
| Mixtures, Components, and Neutralized Forms | 10 Records |
| Similar Compounds | 1,410 Records |
| Similar Conformers | 1,906 Records |

PubChem

## 6.3 Substances

### 6.3.1 Related Substances

| | |
|---|---|
| All | 69 Records |
| Same | 57 Records |
| Mixture | 12 Records |

PubChem

### 6.3.2 Substances by Category

PubChem

## 6.4 Entrez Crosslinks

| | |
|---|---|
| PubMed | 4 Records |
| Taxonomy | 3 Records |
| Gene | 9 Records |

PubChem

## 7 Chemical Vendors

- PubChem

# 8 Drug and Medication Information

## 8.1 Clinical Trials

### 8.1.1 ClinicalTrials.gov

- ClinicalTrials.gov

# 9 Food Additives and Ingredients

## 9.1 FDA Generally Recognized as Safe - GRAS Notices

| | |
|---|---|
| **Substance** | D-Ribose |
| **GRN Number** | 243 |
| **Intended Use** | Ingredient in several food categories provided that D-ribose is used in conjunction with an additional carbohydrate energy source |
| **FDA Letter** | FDA has no questions |
| **Notifier** | Bioenergy, Inc. |
| **Date of Filing** | Feb 8, 2008 |
| **Date of Closure** | Nov 10, 2008 |

FDA Center for Food Safety and Applied Nutrition (CFSAN)

| | |
|---|---|
| **Substance** | D-Ribose |
| **GRN Number** | 100 |
| **Intended Use** | Use in food in general, including meat and poultry products, for multiple technical effects |
| **FDA Letter** | Notice does not provide a basis for a GRAS determination |
| **Notifier** | Bioenergy, Inc. |
| **Date of Filing** | Mar 14, 2002 |
| **Date of Closure** | Sep 3, 2002 |

FDA Center for Food Safety and Applied Nutrition (CFSAN)

Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

## 10 Associated Disorders and Diseases

- Comparative Toxicogenomics Database (CTD)

# 11 Literature

## 11.1 Coronavirus Studies

PubChem

## 11.2 NLM Curated PubMed Citations

Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

- PubChem

## 11.3 Springer Nature References

- Springer Nature

## 11.4 Thieme References

- Thieme Chemistry

## 11.5 Depositor Provided PubMed Citations

- PubChem

## 11.6 General References

Tromans et al. A biomimetic receptor for glucose. Nature Chemistry, doi: 10.1038/s41557-018-0155-z, published online 12 November 2018

- Nature Chemistry

## 11.7 Chemical Co-Occurrences in Literature

Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

PubChem

## 11.8 Chemical-Gene Co-Occurrences in Literature

PubChem

Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

## 11.9 Chemical-Disease Co-Occurrences in Literature

PubChem

# 12 Patents

## 12.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

## 12.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=SRBFZHDQGSBBOR-SOOFDHNKSA-N

- PATENTSCOPE (WIPO)

# 13 Interactions and Pathways

## 13.1 Chemical-Target Interactions

- Comparative Toxicogenomics Database (CTD)

## 14 Taxonomy

Ribose is a metabolite found in or produced by **Escherichia coli (strain K12, MG1655)**.

- **E. coli Metabolome Database (ECMDB)**

*Zebrafish Pathway Metabolite MetFrag Local CSV (Beta)* | ***DOI:10.5281/zenodo.3457553***

- **ECI Group, LCSB, University of Luxembourg**

*The LOTUS Initiative for Open Natural Products Research: frozen dataset union wikidata (with metadata)* | ***DOI:10.5281/zenodo.5794106***

- **LOTUS - the natural products occurrence database**

D-Ribose is a metabolite found in or produced by **Saccharomyces cerevisiae**.

- **Yeast Metabolome Database (YMDB)**

Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

# 15 Classification

## 15.1 MeSH Tree

- Medical Subject Headings (MeSH)

## 15.2 ChEBI Ontology

Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

ChEBI

## 15.3 ChemIDplus

ChemIDplus

## 15.4 NORMAN Suspect List Exchange Classification

Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

- NORMAN Suspect List Exchange

## 15.5 CCSBase Classification

- CCSbase

## 15.6 EPA DSSTox Classification

- EPA DSSTox

## 15.7 LOTUS Tree

- LOTUS - the natural products occurrence database

# 16 Information Sources

FILTER BY SOURCE ALL SOURCES

1. ## CAS Common Chemistry

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*D-Ribopyranose*
*https://commonchemistry.cas.org/detail?cas_rn=10257-32-6*

2. ## ChemIDplus

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*D-Ribopyranose*
*https://chem.nlm.nih.gov/chemidplus/sid/0010257326*

*ChemIDplus Chemical Information Classification*
*https://chem.nlm.nih.gov/chemidplus/*

3. ## DrugBank

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https://www.drugbank.ca/legal/terms_of_use

*Ribose*
*https://www.drugbank.ca/drugs/DB15073*

4. ## EPA DSSTox

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

*D-ribopyranose*
*https://comptox.epa.gov/dashboard/DTXSID70450356*

*CompTox Chemicals Dashboard Chemical Lists*
*https://comptox.epa.gov/dashboard/chemical-lists/*

5. ## European Chemicals Agency (ECHA)

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Case No.: IPR2023-00207
U.S. Patent No. 11,224,241

> https://echa.europa.eu/web/guest/legal-notice

*D-Ribopyranose*
*https://echa.europa.eu/substance-information/-/substanceinfo/100.225.002*

6. ## CCSbase

*D-Ribose*

*CCSbase Classification*
*https://ccsbase.net/*

7. ## ChEBI

*D-ribopyranose*
*http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:47006*

*ChEBI Ontology*
*http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology*

8. ## E. coli Metabolome Database (ECMDB)

> LICENSE
> ECMDB is offered to the public as a freely available resource.
> https://ecmdb.ca/citations

*https://ecmdb.ca/compounds/M2MDB000116*

9. ## LOTUS - the natural products occurrence database

> LICENSE
> The code for LOTUS is released under the GNU General Public License v3.0.
> https://lotus.nprod.net/

*LOTUS Tree*
*https://lotus.naturalproducts.net/*

10. ## West Coast Metabolomics Center-UC Davis

*Ribose*

11. ## Yeast Metabolome Database (YMDB)

> LICENSE
> YMDB is offered to the public as a freely available resource.
> http://www.ymdb.ca/downloads

*http://www.ymdb.ca/compounds/YMDB00253*

12. ## ClinicalTrials.gov

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> https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use

*https://clinicaltrials.gov/*

13. ## Comparative Toxicogenomics Database (CTD)

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http://ctdbase.org/about/legal.jsp

*https://ctdbase.org/detail.go?type=chem&acc=D012266*

14. ## ECI Group, LCSB, University of Luxembourg

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https://www.fda.gov/about-fda/about-website/website-policies#linking

*D-Ribose*

*https://www.cfsanappsexternal.fda.gov/scripts/fdcc/?set=GRASNotices&id=243*

*D-Ribose*

*https://www.cfsanappsexternal.fda.gov/scripts/fdcc/?set=GRASNotices&id=100*

16. ## GlyCosmos Glycoscience Portal

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*https://glycosmos.org/glycans/show/G75380KK*

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*https://glytoucan.org/Structures/Glycans/G75380KK*

18. ## GlyGen

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19. ## MassBank of North America (MoNA)

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*Ribose*
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20. ## Nature Chemistry
*https://pubchem.ncbi.nlm.nih.gov/substance/375892340*

21. ## PubChem
*https://pubchem.ncbi.nlm.nih.gov*

22. ## Springer Nature
*https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=10043502-138639178*

23. ## Thieme Chemistry

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*https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=10043502-138566307*

24. ## Wikidata

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*D-ribopyranose*
*https://www.wikidata.org/wiki/Q27120754*

25. ## Medical Subject Headings (MeSH)

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*MeSH Tree*
*http://www.nlm.nih.gov/mesh/meshhome.html*

26. ## NORMAN Suspect List Exchange

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*NORMAN Suspect List Exchange Classification*
*https://www.norman-network.com/nds/SLE/*

27. ## PATENTSCOPE (WIPO)

*SID 403525274*
*https://pubchem.ncbi.nlm.nih.gov/substance/403525274*