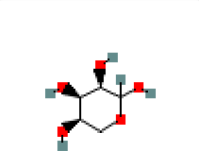
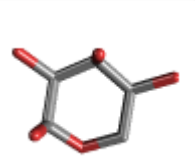
Case No.: IPR2023-00208
U.S. Patent No. 11,013,250

PubChem

COMPOUND SUMMARY

D-Ribose

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

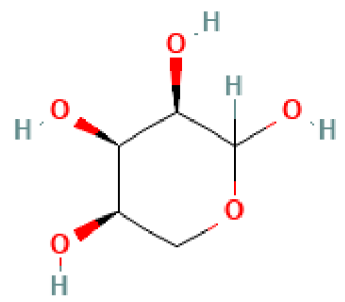
D-Ribose is a metabolite found in or produced by Saccharomyces cerevisiae.

- 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

Case No.: IPR2023-00208
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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

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- 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 71.01237 46.88 148.90872 43.20 89.02288 9.99 130.89479 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 100 148.90904 64.48 71.01237 49.01 89.0231 12.65 100.73466 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

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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.: IPR2023-00208
U.S. Patent No. 11,013,250

10 Associated Disorders and Diseases

- Comparative Toxicogenomics Database (CTD)

11 Literature

11.1 Coronavirus Studies

PubChem

11.2 NLM Curated PubMed Citations

Case No.: IPR2023-00208
U.S. Patent No. 11,013,250

PubChem

11.3 Springer Nature References

Springer Nature

11.4 Thieme References

Case No.: IPR2023-00208
U.S. Patent No. 11,013,250

- 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.: IPR2023-00208
U.S. Patent No. 11,013,250

PubChem

11.8 Chemical-Gene Co-Occurrences in Literature

PubChem

Case No.: IPR2023-00208
U.S. Patent No. 11,013,250

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)

Case No.: IPR2023-00208
U.S. Patent No. 11,013,250

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)**

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15 Classification

15.1 MeSH Tree

- Medical Subject Headings (MeSH)

15.2 ChEBI Ontology

ChEBI

15.3 ChemIDplus

ChemIDplus

15.4 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

15.5 CCSBase Classification

- CCSbase

15.6 EPA DSSTox Classification

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U.S. Patent No. 11,013,250

- 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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https://www.nlm.nih.gov/copyright.html

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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> 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

17. ## GlyTouCan Project

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18. ## GlyGen

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G75380KK

https://www.glygen.org/glycan/G75380KK

19. ## MassBank of North America (MoNA)

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Ribose
https://mona.fiehnlab.ucdavis.edu/spectra/browse?query=compound.metaData%3Dq%3D%27name%3D%3D%22InChIKey%22%20and%20value%3D%3D%22SRBFZHDQGSBBOR-SOOFDHNKSA-N%22%27

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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24. ## Wikidata

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

25. ## Medical Subject Headings (MeSH)

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> https://www.nlm.nih.gov/copyright.html

Ribose
https://www.ncbi.nlm.nih.gov/mesh/68012266

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