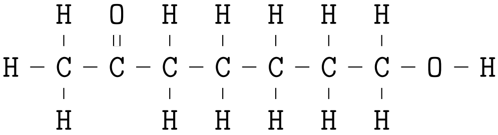
Analysing and Classifying Names of Chemical Compounds with CHEMorph

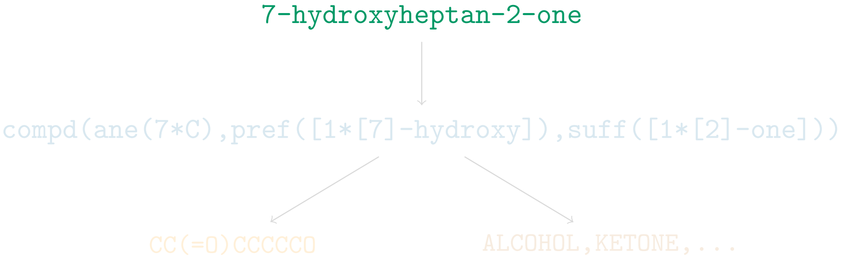
Stefanie Anstein   Gerhard Kremer

IMS, University of Stuttgart

April 11, 2006

Example Analysis





7-hydroxyheptan-2-one

compd(ane(7*C),pref([1*[7]-hydroxy]),suff([1*[2]-one]))

CC(=O)CCCCCO

ALCOHOL,KETONE,...

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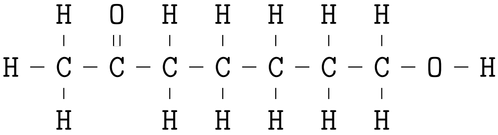

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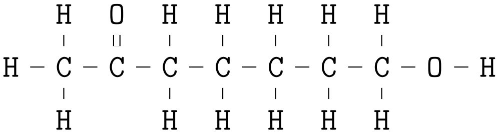

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↓

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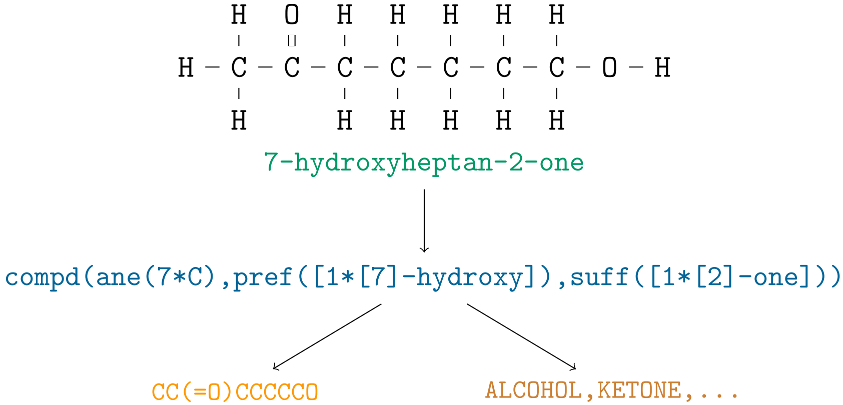

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Motivation & Background

- life sciences . . .

  and the amount of biomedical data

- terminology . . .

  and biochemical nomenclature

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Challenges

- term reference ▸
- coreferences ▸

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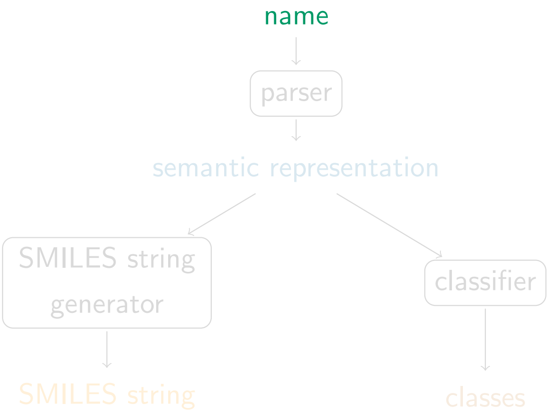
- R-0. 1.7.3 (IUPAC nomenclature of organic compounds):

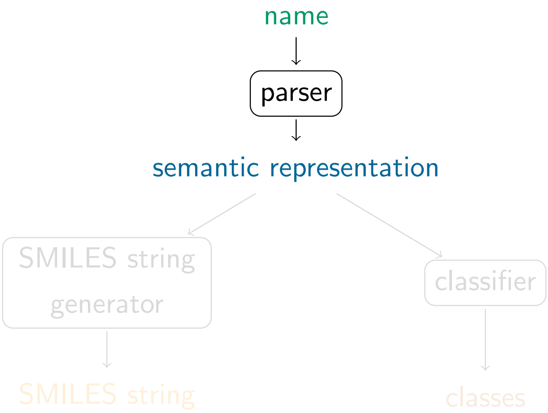
  Addition of the vowel “o”.

  For euphonic reasons, the vowel “o” is sometimes inserted between consonants.

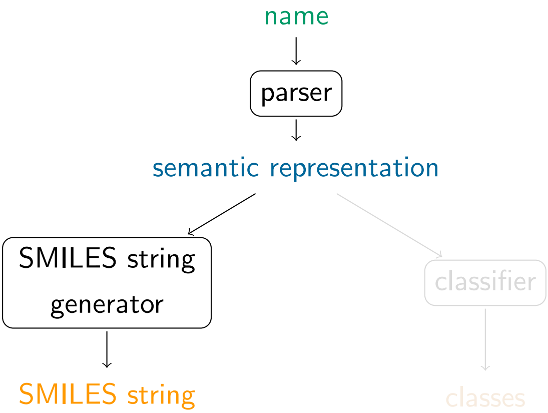
Modules Overview



Modules Overview



Modules Overview



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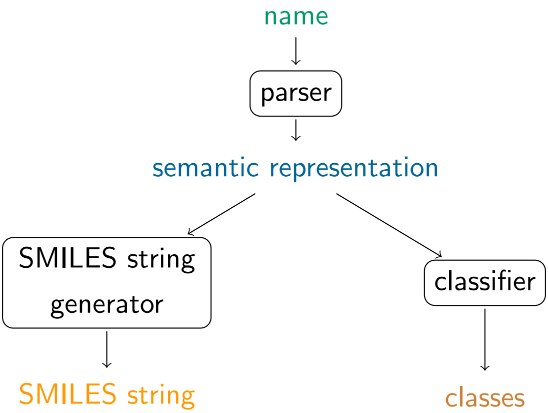

name

parser

semantic representation

SMILES string generator

classifier

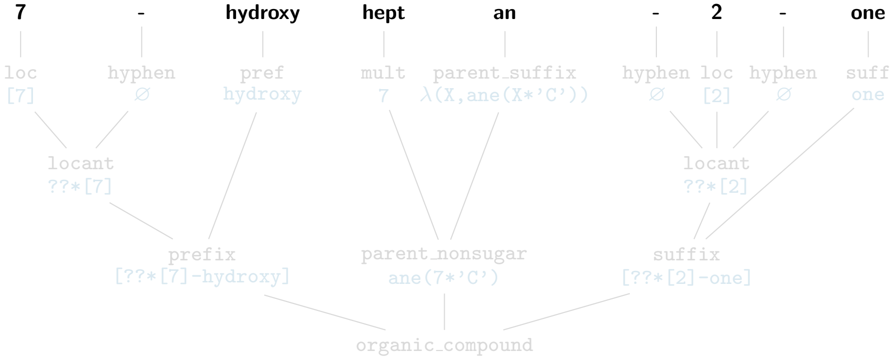
SMILES string

classes

Name Types

	fully specified	underspecified
systematic	7-hydroxyheptan-2-one	heptanone
trivial	benzene	∅
semi-systematic	benzene-1,3,5-triacetic acid	dihydrobenzene
class	∅	alcohol ▸
semi-systematic	∅	2-deoxysugar

Parser



7 **-** **hydroxy** **hept** **an** **-** **2** **-** **one**

loc [7] hyphen ∅ pref hydroxy mult 7 parent_suffix λ(X,ane(X*'C')) hyphen ∅ loc [2] hyphen ∅ suff one

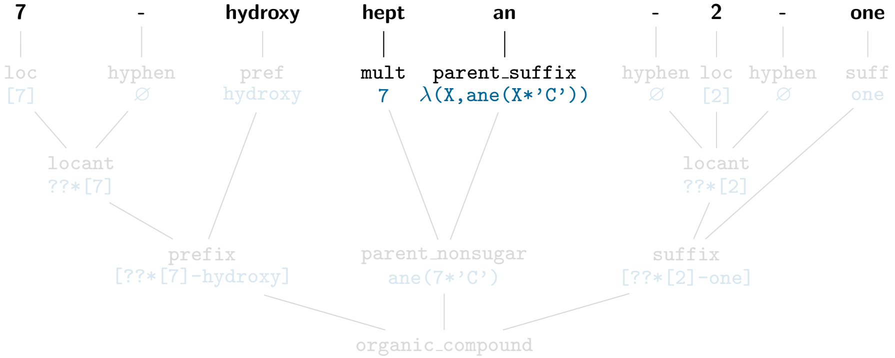
locant ??*[7] locant ??*[2]

prefix [??*[7]-hydroxy] parent_nonsugar ane(7*'C') suffix [??*[2]-one]

organic_compound

compd(ane(7*C) , pref([??*[7]-hydroxy]) ,
suff([??*[2]-one]))

Parser



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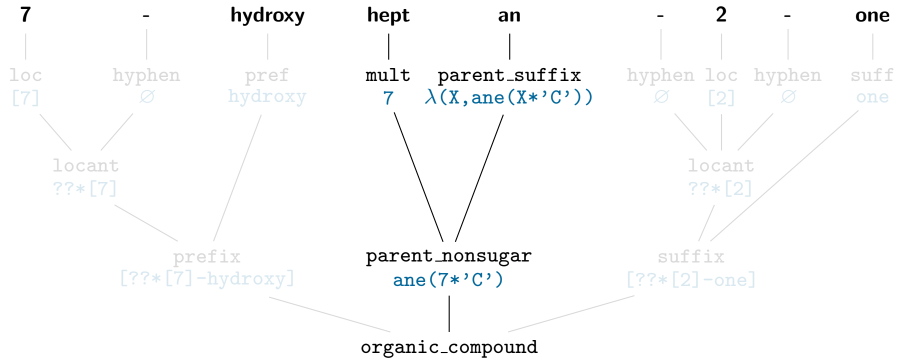

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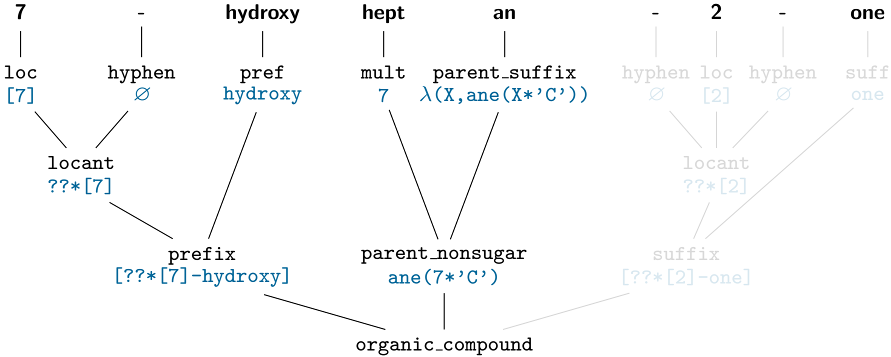
```
compd( ane(7*C) , pref( [??*[7]-hydroxy] ) ,
suff( [??*[2]-one] ) )
```

Parser



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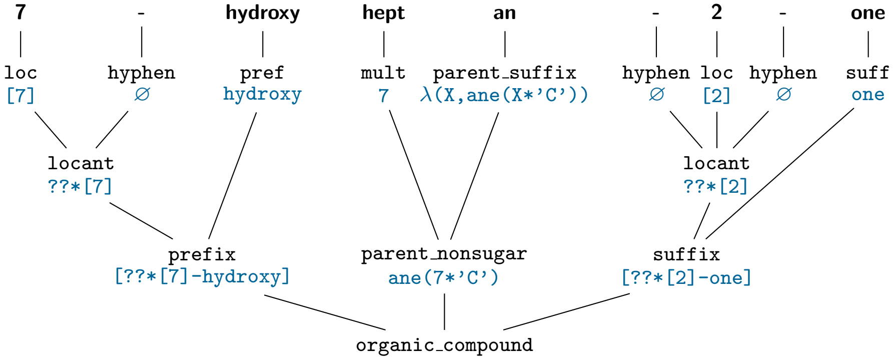

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SMILES String Generator

- representation of single chain elements
- consistency check
- underspecification:

```
underspecified( CC(=O)CCCCC , [{1,3,4,5,6,7}-hydroxy] )
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Classifier

morpheme	class
`hydroxy- | -ol`	`ALCOHOL`
`cyclo- & -ane`	`CYCLOALKANE`

- compd(ane(7*C) , pref([1*[7]-hydroxy]) , suff([1*[2]-one]))

  → ALKANE, ALCOHOL, KETONE

- compd(ene(??*[??],ane(4*'C')) , pref([]) , suff([]))

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Results & Applications

- SMILES string and classification
- underspecification
- term reference
- coreference resolution ▸
- database curation and ontology acquisition ▸

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Conclusion & Outlook

- feasible, extendable and transferable approach

- extend grammar and lexicon
- elaborate SMILES and classification

- sophisticated linguistic analysis → database curation
- term identification → text processing applications

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Acknowledgements

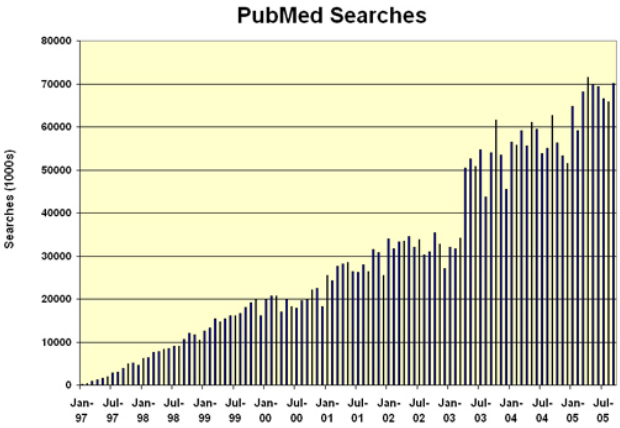
Stefanie Anstein

Uwe Reyle

Jasmin Šarić

EML Research gGmbH

Schönen Dank.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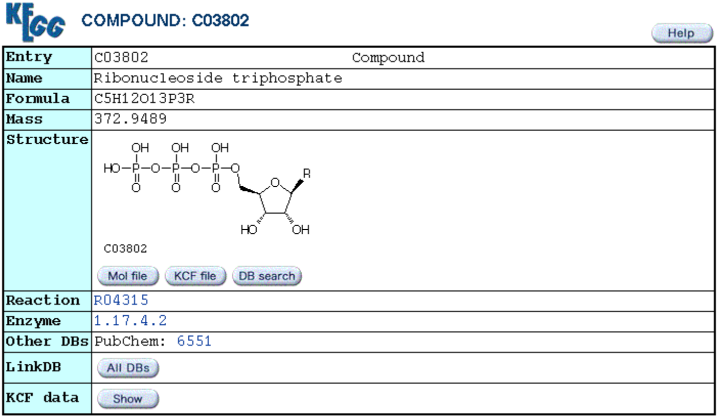
Jul-00
Jan-01
Jul-01
Jan-02
Jul-02
Jan-03
Jul-03
Jan-04
Jul-04
Jan-05
Jul-05

IUPAC Nomenclatures

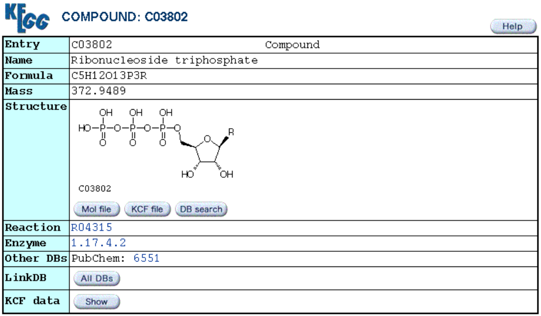
- Amino Acids and Peptides
- Biochemical thermodynamics
- Branched nucleic acids
- **Carbohydrates**
- Carotenoids
- Corrinoids (vitamin B12)
- Cyclitols
- Electron transport proteins
- Enzyme kinetics
- Enzyme nomenclature
  - EC 1 Oxidoreductases
  - EC 2 Transferases
  - EC 3 Hydrolases
  - EC 4 Lyases
  - EC 5 Isomerases
  - EC 6 Ligases
- Folic acid
- Glycolipids
- Glycoproteins
- myo-Inositol numbering
- Lignan Nomenclature
- Lipid Nomenclature
- Multienzymes
- Multiple forms of enzymes
- Nucleic acid constituents
- Nucleic acid sequence
- **Organic Chemistry**
- Peptide hormones
- Phosphorus containing compds
- Polymerized amino acids
- Polypeptide conformation
- Polynucleotide conformation
- Polysaccharide conformation
- Prenol nomenclature
- Pyridoxal (vitamin B6)
- Quinones w. an Isoprenoid Chain
- Retinoids
- Steroids
- Tetrapyrroles
- Tocopherols (vitamin E)
- Translation Factors
- Vitamin D



COMPOUND: C03802

Entry	C03802 Compound
Name	Ribonucleoside triphosphate
Formula	C5H12O13P3R
Mass	372.9489
Structure	C03802
Reaction	R04315
Enzyme	1.17.4.2
Other DBs	PubChem: 6551
LinkDB	All DBs
KCF data	Show

KEGG: Kyoto Encyclopedia of Genes and Genomes



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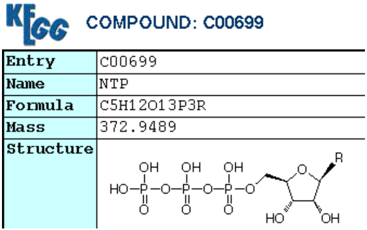
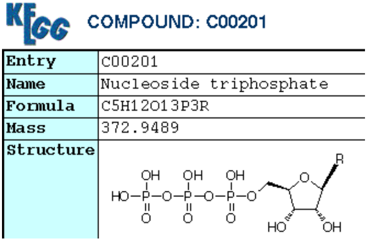


COMPOUND: C00699

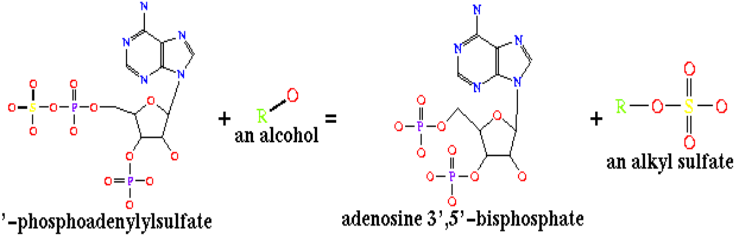
Entry	C00699
Name	NTP
Formula	C5H12O13P3R
Mass	372.9489
Structure	



COMPOUND: C00201

Entry	C00201
Name	Nucleoside triphosphate
Formula	C5H12O13P3R
Mass	372.9489
Structure	

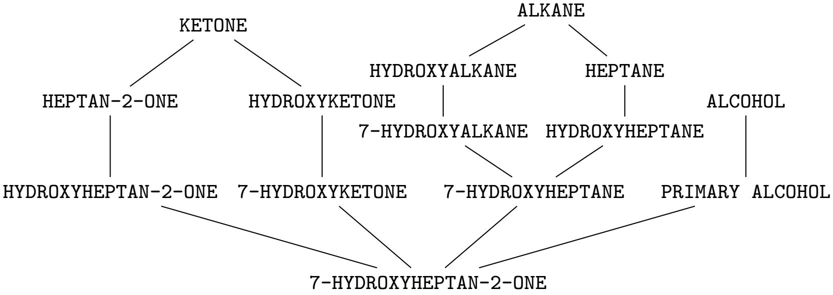
Reaction: *3′-phosphoadenylyl sulfate + an alcohol = adenosine 3′,5′-bisphosphate + an alkyl sulfate.*



Molecule diagrams generated from .mol files obtained from the KEGG ftp site.

Other name(s): *Hydroxysteroid sulfotransferase.*

Comments: *Primary and secondary alcohols, including aliphatic alcohols, ascorbate, chloramphenicol, ephedrine and hydroxysteroids, but not phenolic steroids, can act as acceptors (cf. Ec 2.8.2.15).*



ALKANE

KETONE

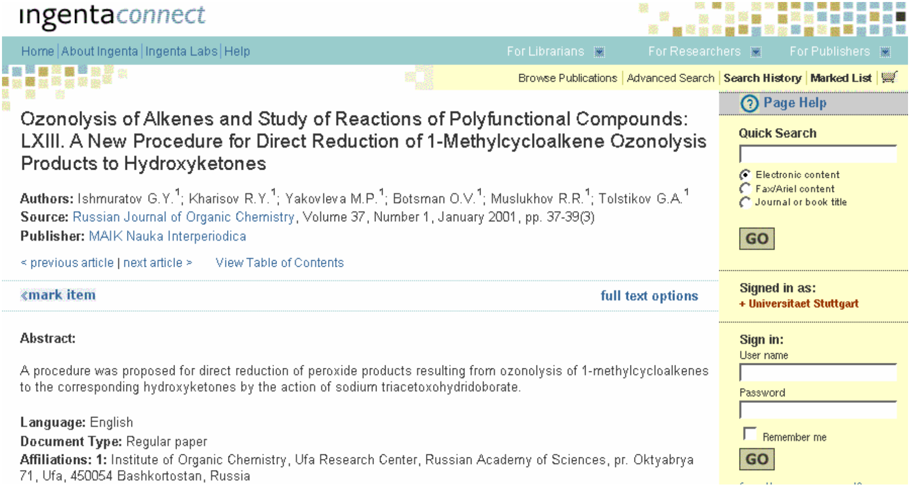
HYDROXYALKANE HEPTANE

HEPTAN-2-ONE HYDROXYKETONE ALCOHOL

7-HYDROXYALKANE HYDROXYHEPTANE

HYDROXYHEPTAN-2-ONE 7-HYDROXYKETONE 7-HYDROXYHEPTANE PRIMARY ALCOHOL

7-HYDROXYHEPTAN-2-ONE



Ozonolysis of Alkenes and Study of Reactions of Polyfunctional Compounds: LXIII. A New Procedure for Direct Reduction of 1-Methylcycloalkene Ozonolysis Products to Hydroxyketones

Authors: Ishmuratov G.Y.[1]; Kharisov R.Y.[1]; Yakovleva M.P.[1]; Botsman O.V.[1]; Muslukhov R.R.[1]; Tolstikov G.A.[1]

Source: Russian Journal of Organic Chemistry, Volume 37, Number 1, January 2001, pp. 37-39(3)

Publisher: MAIK Nauka Interperiodica

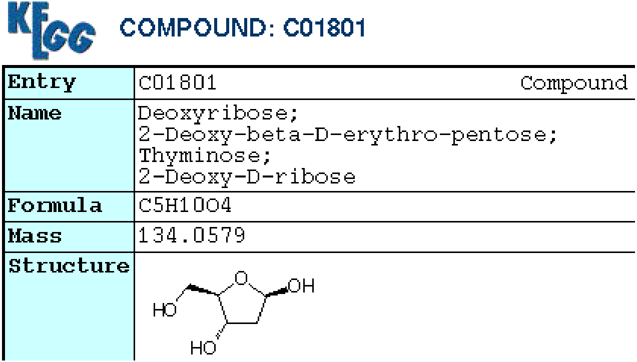
Abstract:

A procedure was proposed for direct reduction of peroxide products resulting from ozonolysis of 1-methylcycloalkenes to the corresponding hydroxyketones by the action of sodium triacetoxohydridoborate.

Language: English

Document Type: Regular paper

Affiliations: 1: Institute of Organic Chemistry, Ufa Research Center, Russian Academy of Sciences, pr. Oktyabrya 71, Ufa, 450054 Bashkortostan, Russia



COMPOUND: C01801

Entry	C01801	Compound

Name	Deoxyribose;
	2-Deoxy-beta-D-erythro-pentose;
	Thyminose;
	2-Deoxy-D-ribose	

Formula	C5H10O4	
Mass	134.0579	
Structure		