MarvinSketch, penggunaannya untuk mengakses web page database

Niko P.

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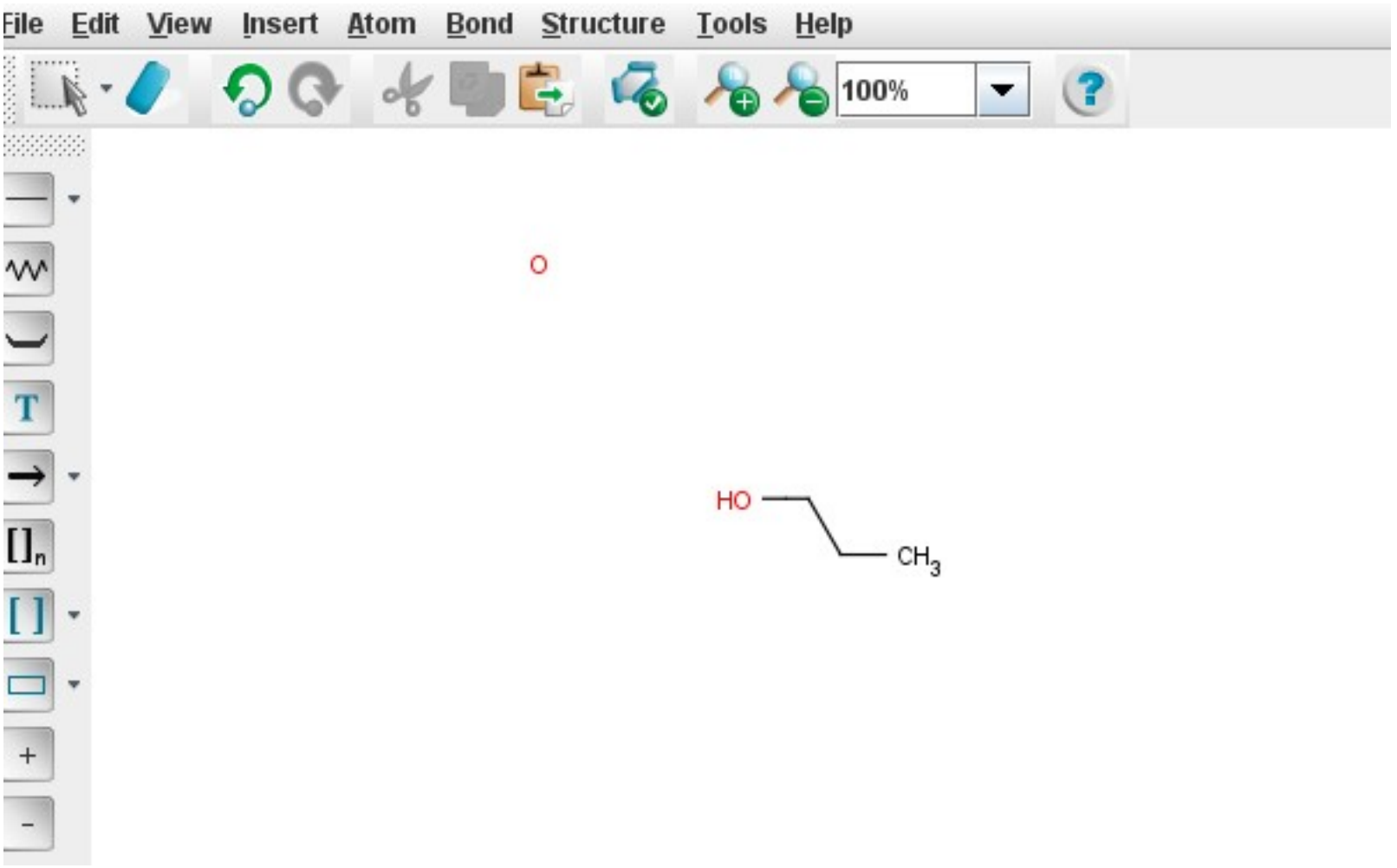
Neax502.wordpress.com

- **Kemoinformatika berkaitan dengan software dan database.**
- **Salah satu software yang dapat digunakan untuk mengakses data base/web page database adalah MarvinSketch.**
- **MarvinSketch adalah software buatan ChemAxon.**
- **Software ini dapat didownload secara bebas dari www.chemaxon.com.**
- **Meski demikian, kita bisa membeli lisensi untuk mengaktifkan plugin-plugin yang lebih banyak.**
- **MarvinSketch berjalan di atas 3 OS, yaitu: Microsoft Windows, Mac OS dan Linux**
- **Untuk menjalankannya harus menginstall Java.**

•

- **MarvinSketch dapat digunakan untuk menggambar struktur, menampilkan nama dari struktur, menampilkan koefisien partisi, protonasi, analisis topologi dll.**
- **Dalam kaitannya dengan kemoinformatika, MarvinSketch dapat digunakan untuk mengakses database PubChem, ChemSpider dan chemicalize.**
- **Gambar dulu struktur yang diinginkan, kemudian baru mencari di database.**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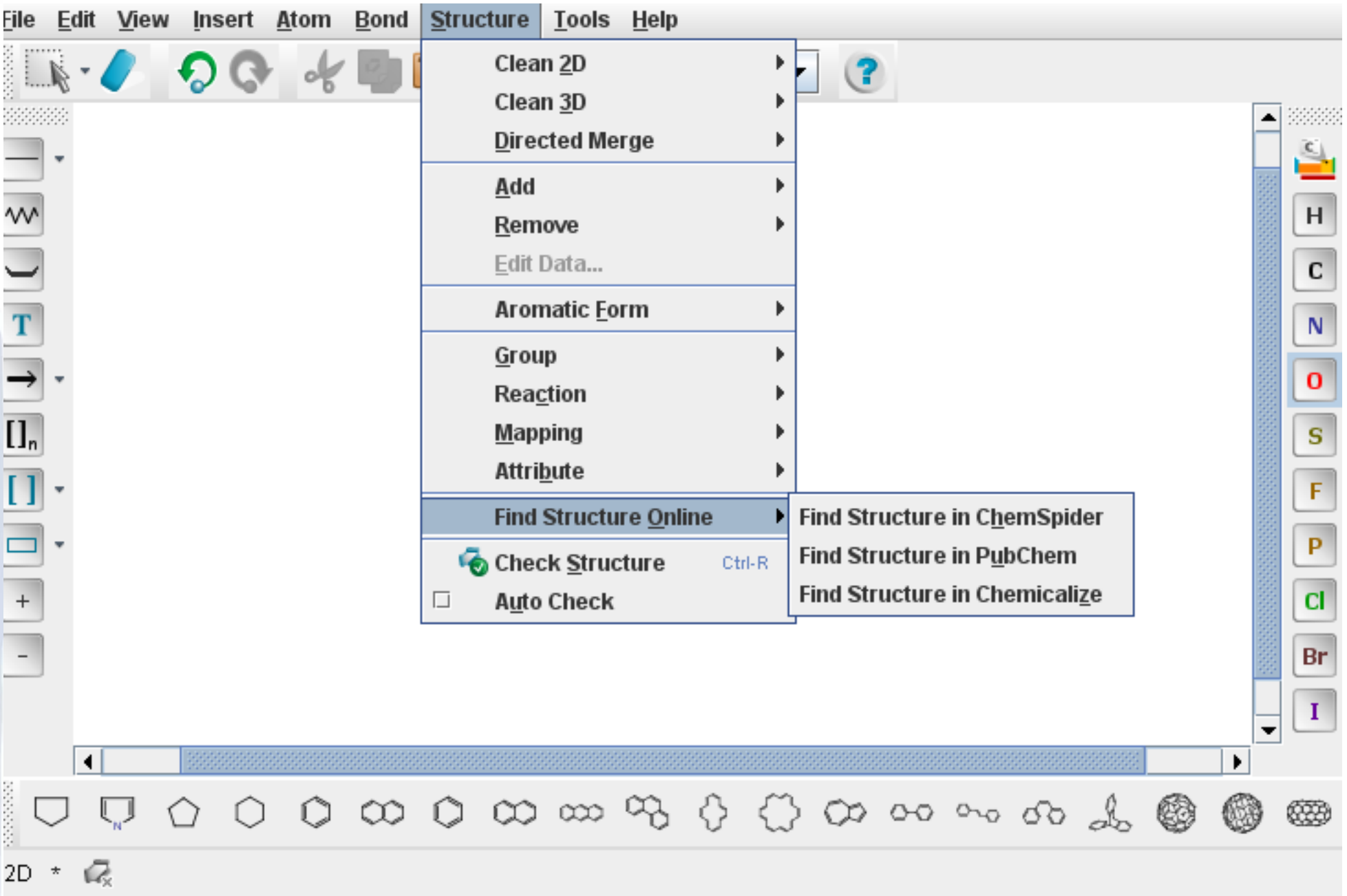
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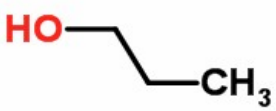

ChemSpider ID: **1004**

Molecular Formula: C_3H_8O

Monoisotopic mass: 60.058 Da

Systematic name

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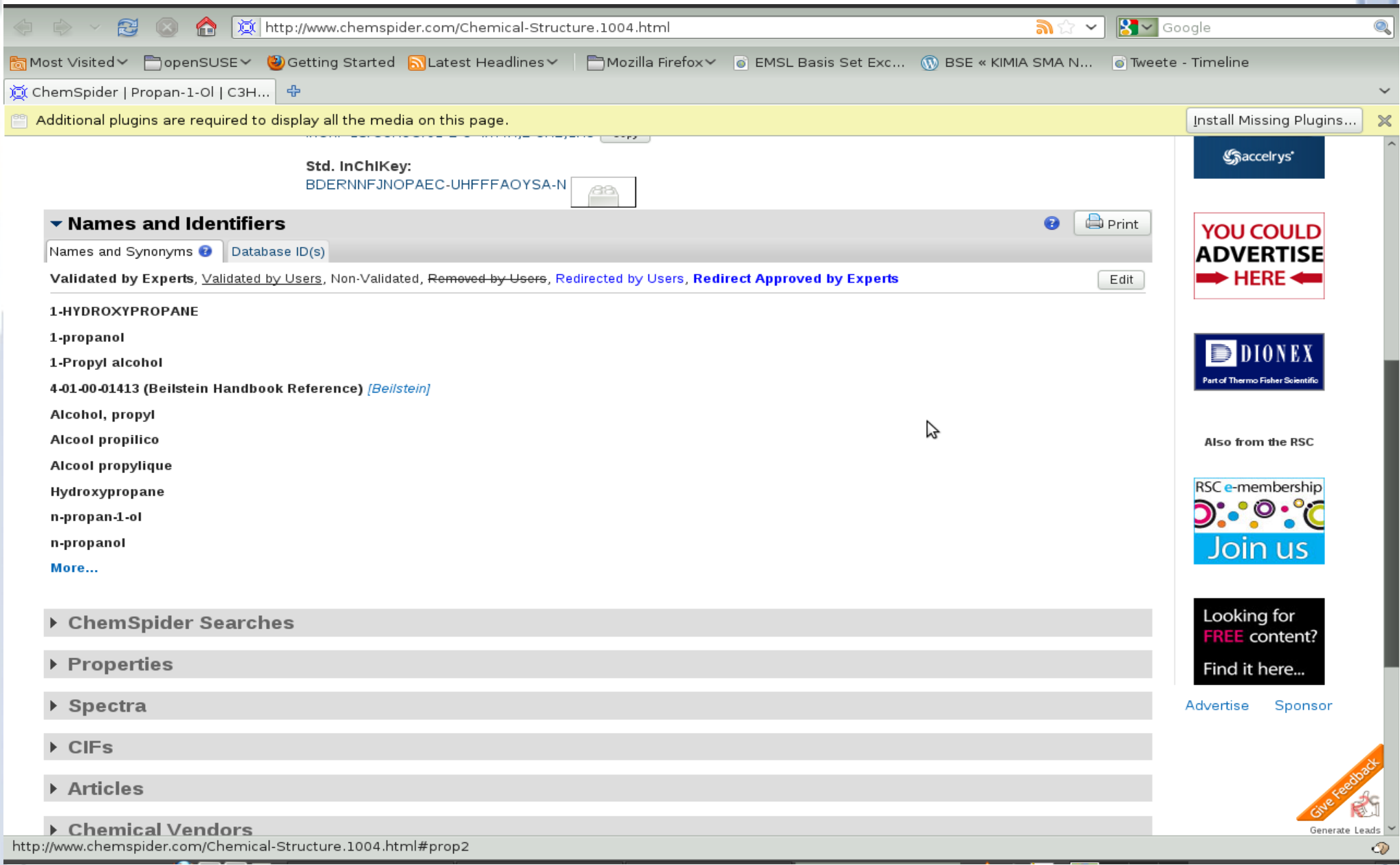
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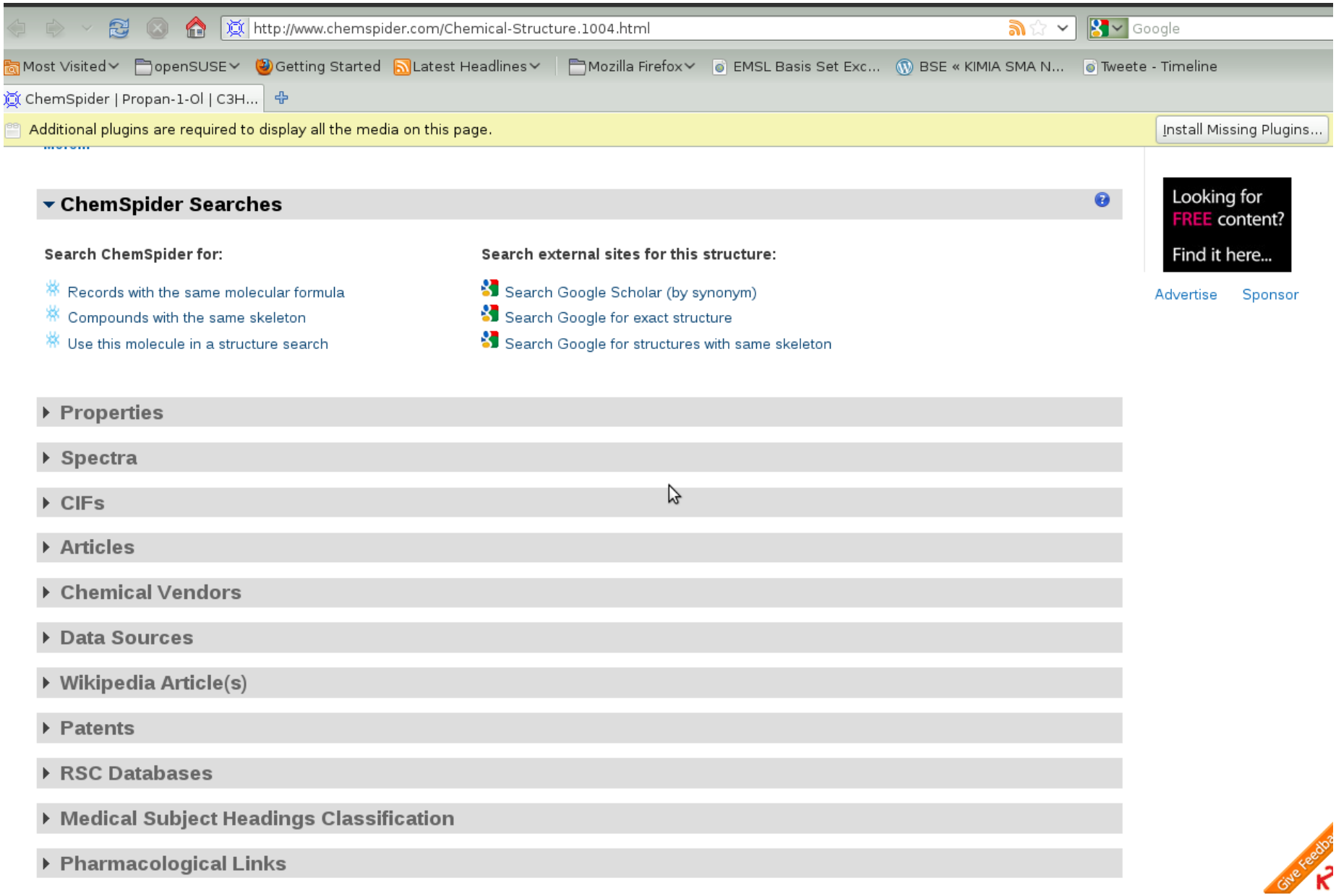
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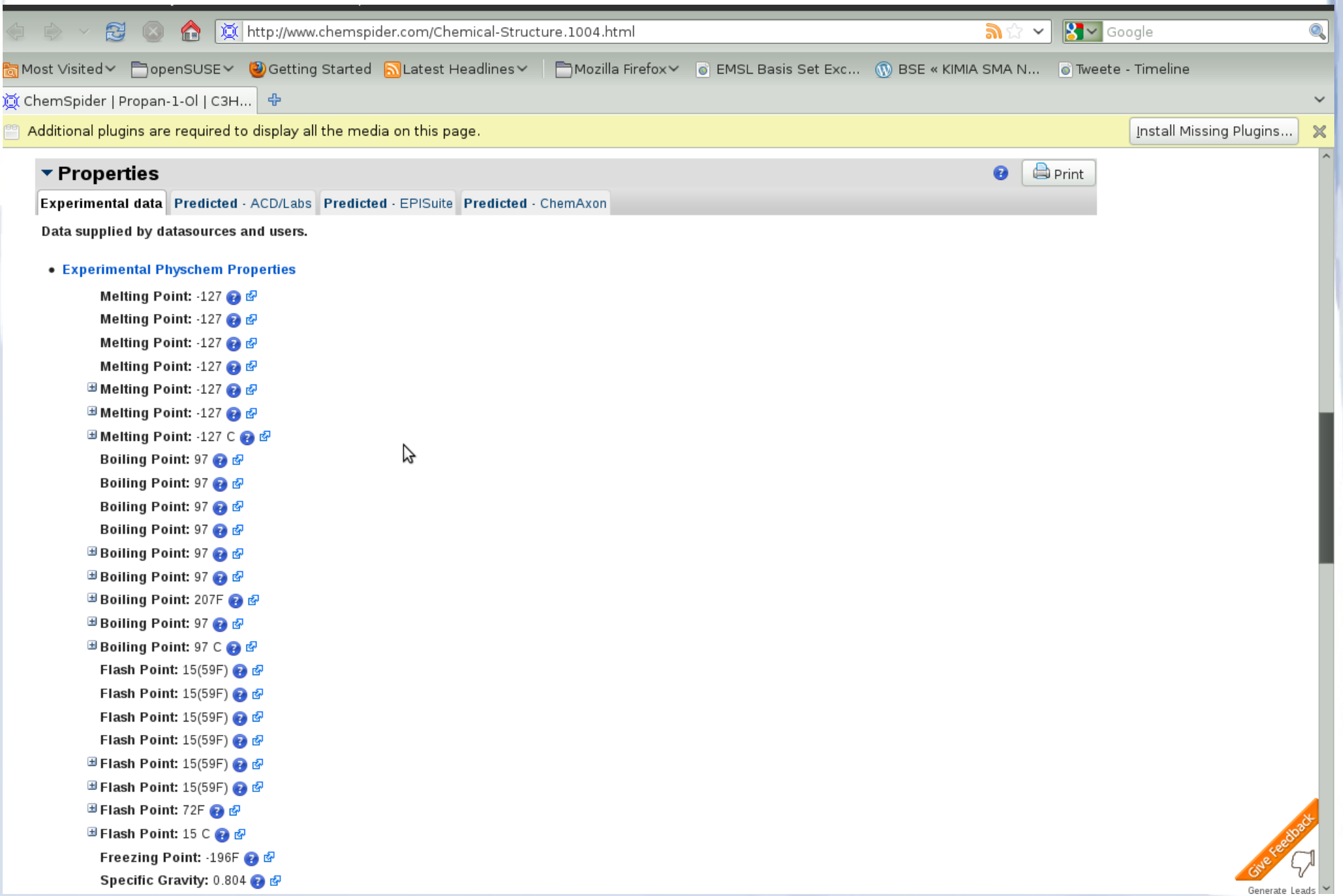
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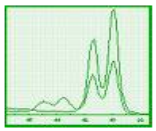

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- Volha Vetokhina, Michał Kijak, Gabriela Wiosna-Sałyga, Randolph P. Thummel, Jerzy Herbich and Jacek Waluk. On the origin of fluorescence quenching of pyridylindoles by hydroxylic solvents, *Photochem. Photobiol. Sci.*, *2010*, *9*, *923*. [DOI: 10.1039/c0pp00043d]
- Jonghyun Choi, Kyung Min Lee, Ryszard Wycisk, Peter N. Pintauro and Patrick T. Mather. Nanofiber composite membranes with low equivalent weight perfluorosulfonic acid polymers, *J. Mater. Chem.*, *2010*, *20*, *6282*. [DOI: 10.1039/c0jm00441c]
- Ana G. Maldonado and Gadi Rothenberg. Predictive modeling in homogeneous catalysis: a tutorial, *Chem. Soc. Rev.*, *2010*, *39*, *1891*. [DOI: 10.1039/b921393g]
- Shuxun Cui. The possible roles of water in the prebiotic chemical evolution of DNA, *Phys. Chem. Chem. Phys.*, *2010*, *12*, *10147*. [DOI: 10.1039/c002414g]
- Costas Tsioptsias, Ioannis TsivintzelisCurrent address: Department of Chemical and Biochemical Engineering, Technical University of Denmark. and Costas Panayiotou. Equation-of-state modeling of mixtures with ionic liquids, *Phys. Chem. Chem. Phys.*, *2010*, *12*, *4843*. [DOI: 10.1039/c000208a]
- Jeong Woo Lee, Woo Chul Choi and Jong-Duk Kim. Size-controlled layered zinc hydroxide intercalated with dodecyl sulfate: effect of alcohol type on dodecyl sulfate template, *CrystEngComm*, *2010*, *12*, *3249*. [DOI: 10.1039/c002296a]
- John McMurtrie and Ian Dance. Alternative metal grid structures formed by [M(terpy)2]2+ and [M(terpyOH)] complexes with small and large tetrahedral dianions, and by [Ru(terpy)], *CrystEngComm*, *2010*, *12*, *2700*. [DOI: 10.1039/b926074a]
- Lik H. Wee, Sneha R. Bajpe, Nikki Janssens, Ive Hermans, Kristof Houthoofd, Christine E. A. Kirschhock and Johan A. Martens. Convenient synthesis of Cu3(BTC)2 encapsulated Keggin heteropolyacid nanomaterial for application in catalysis, *Chem. Commun.*, *2010*, *46*, *8186*. [DOI: 10.1039/c0cc01447h]
- Jennifer Hannant, Joseph H. Hedley, Jonathan Pate, Adam Walli, Said A. Farha Al-Said, Miguel A. Galindo, Bernard A. Connolly, Benjamin R. Horrocks, Andrew Houlton and Andrew R. Pike. Modification of DNA-templated conductive polymer nanowires via click chemistry, *Chem. Commun.*, *2010*, *46*, *5870*. [DOI: 10.1039/c0cc00693a]
- Xiaoxiao Guo, Fazhi Zhang, David G. Evans and Xue Duan. Layered double hydroxide films: synthesis, properties and applications, *Chem. Commun.*, *2010*, *46*, *5197*. [DOI: 10.1039/c0cc00313a]

Patents

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Process for ammoxidation of 1-propanol

US Pat. 4138430 - Sep 28, 1977 - E. I. Du Pont de Nemours and Company

PROCESS FOR AMMOXIDATION OF **1-PROPANOL** CROSS REFERENCE TO RELATED APPLICATIONS This application is a continuation-in-part application of our copending **...**

Amino-Propanol Derivatives

US Pat. App 11568645 - May 25, 2005

27, 2007 (54) AMINO-**PROPANOL** DERIVATIVES Publication Classification (76) Inventors: Klaus Hinterding, Wittlingen (DE); Klemens Hogenauer, Wien (AT); **...**

ISOPROPYL-Z-PROPANOL

US Pat. 3873618 - Jul 18, 1969

Representative of the compounds disclosed are l-(5-propionamidonaphth-l-yloxy)-3 -t-butylamino-2- **propanol** and l-[4-(4-acetamidophenyl)phenoxy]-3- **...**

DISUBSTITUTED-L-PROPANOL CAR-

US Pat. 3081341 - Mar 10, 1958 - Sterling Drug Inc

More particularly, it concerns 3-halo-2,2-disubstituied-l-**propanol** carbamates and their preparation. Carbamates of alkanols are known. **...**

Z-METHYLAMIBTO-PROPANOL-L

US Pat. 1865880 - Jul 19, 1930

469265 a process is described for the production of the normal 1- (paraaminophenyl) -2- methylamino-**propanol-1**. According to the A present invention it has **...**

2-(3-Phenoxyphenyl) propanol

US Pat. 4062895 - Feb 14, 1977 - Eli Lilly and Company

13, 1977 [54] 2-(3-PHENOXYPHENYL) **PROPANOL** [75] Inventor: Winston S. Marshall, Indianapolis, Ind. [73] Assignee: Eli Lilly and

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US Pat. App 10526760 - Sep 12, 2003
27, 2006 (54) AMINO-**PROPANOL** DERIVATIVES Publication Classification (51) Int. Cl . A61K 31/66 (2006.01) A61K 31/137 (2006.01) C07F 9/02 (2006.01) (52) US Cl **...**

PRINTING INK COMPRISING PROPANOL
US Pat. 3034997 - Oct 02, 1959 - Intercaemical Cor
Primary among these deficiencies was the reactivity of the 1:1 **n-propanol**/ aliphatic hydrocarbon solvent with natural rubber plates and rollers normally used **...**

1 2 3 4 5 6 7 8

RSC Databases

Medical Subject Headings Classification

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Descriptor Data | Chemical Classification | Supplemental

MeSH Heading	1-Propanol	
Concept 1 (Preferred)	1-Propanol	
	Scope Note	A colorless liquid made by oxidation of aliphatic hydrocarbons that is used as a solvent and chemical intermediate.
	Term	1-Propanol
	Term	n-Propanol
	Term	Propanol
	Term	Alcohol, Propyl
Allowable Qualifiers	ADAEANAIBLCFCSCLDUECHIIMIPMEPKPDPORESTSDTUTOURCHCTAG	
Registry Number	71-23-8	

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1-Propanol - Compound Summary (CID 1031)

A colorless liquid made by oxidation of aliphatic hydrocarbons that is used as a solvent and chemical intermediate.

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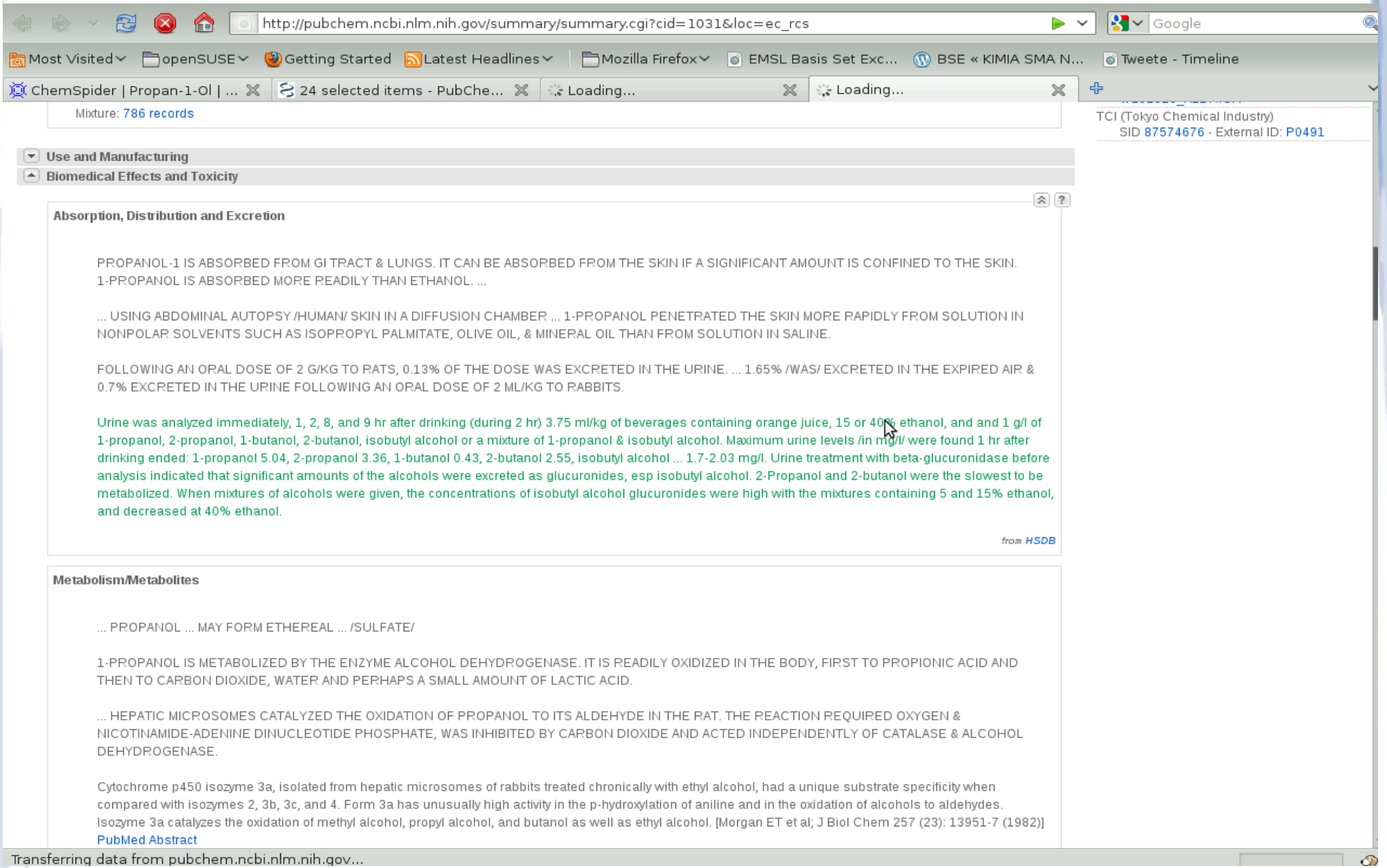
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Mixture: 786 records
TCI (Tokyo Chemical Industry)
SID 87574676 - External ID: P0491
Use and Manufacturing
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Absorption, Distribution and Excretion
PROPANOL-1 IS ABSORBED FROM GI TRACT & LUNGS. IT CAN BE ABSORBED FROM THE SKIN IF A SIGNIFICANT AMOUNT IS CONFINED TO THE SKIN. 1-PROPANOL IS ABSORBED MORE READILY THAN ETHANOL. ...
... USING ABDOMINAL AUTOPSY /HUMAN/ SKIN IN A DIFFUSION CHAMBER ... 1-PROPANOL PENETRATED THE SKIN MORE RAPIDLY FROM SOLUTION IN NONPOLAR SOLVENTS SUCH AS ISOPROPYL PALMITATE, OLIVE OIL, & MINERAL OIL THAN FROM SOLUTION IN SALINE.
FOLLOWING AN ORAL DOSE OF 2 G/KG TO RATS, 0.13% OF THE DOSE WAS EXCRETED IN THE URINE. ... 1.65% /WAS/ EXCRETED IN THE EXPIRED AIR & 0.7% EXCRETED IN THE URINE FOLLOWING AN ORAL DOSE OF 2 ML/KG TO RABBITS.
Urine was analyzed immediately, 1, 2, 8, and 9 hr after drinking (during 2 hr) 3.75 ml/kg of beverages containing orange juice, 15 or 40% ethanol, and and 1 g/l of 1-propanol, 2-propanol, 1-butanol, 2-butanol, isobutyl alcohol or a mixture of 1-propanol & isobutyl alcohol. Maximum urine levels /in mg/l/ were found 1 hr after drinking ended: 1-propanol 5.04, 2-propanol 3.36, 1-butanol 0.43, 2-butanol 2.55, isobutyl alcohol ... 1.7-2.03 mg/l. Urine treatment with beta-glucuronidase before analysis indicated that significant amounts of the alcohols were excreted as glucuronides, esp isobutyl alcohol. 2-Propanol and 2-butanol were the slowest to be metabolized. When mixtures of alcohols were given, the concentrations of isobutyl alcohol glucuronides were high with the mixtures containing 5 and 15% ethanol, and decreased at 40% ethanol.
from HSDB
Metabolism/Metabolites
... PROPANOL ... MAY FORM ETHEREAL ... /SULFATE/
1-PROPANOL IS METABOLIZED BY THE ENZYME ALCOHOL DEHYDROGENASE. IT IS READILY OXIDIZED IN THE BODY, FIRST TO PROPIONIC ACID AND THEN TO CARBON DIOXIDE, WATER AND PERHAPS A SMALL AMOUNT OF LACTIC ACID.
... HEPATIC MICROSOMES CATALYZED THE OXIDATION OF PROPANOL TO ITS ALDEHYDE IN THE RAT. THE REACTION REQUIRED OXYGEN & NICOTINAMIDE-ADENINE DINUCLEOTIDE PHOSPHATE, WAS INHIBITED BY CARBON DIOXIDE AND ACTED INDEPENDENTLY OF CATALASE & ALCOHOL DEHYDROGENASE.
Cytochrome p450 isozyme 3a, isolated from hepatic microsomes of rabbits treated chronically with ethyl alcohol, had a unique substrate specificity when compared with isozymes 2, 3b, 3c, and 4. Form 3a has unusually high activity in the p-hydroxylation of aniline and in the oxidation of alcohols to aldehydes. Isozyme 3a catalyzes the oxidation of methyl alcohol, propyl alcohol, and butanol as well as ethyl alcohol. [Morgan ET et al; J Biol Chem 257 (23): 13951-7 (1982)]
PubMed Abstract
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Kesimpulan :

kombinasi antara MarvinSketch dengan web pages database dapat digunakan secara efektif untuk mencari sifat-sifat dari senyawa yang pada akhirnya nanti akan memberikan informasi yang berharga bagi kita

SEKIAN DAN TERIMA KASIH