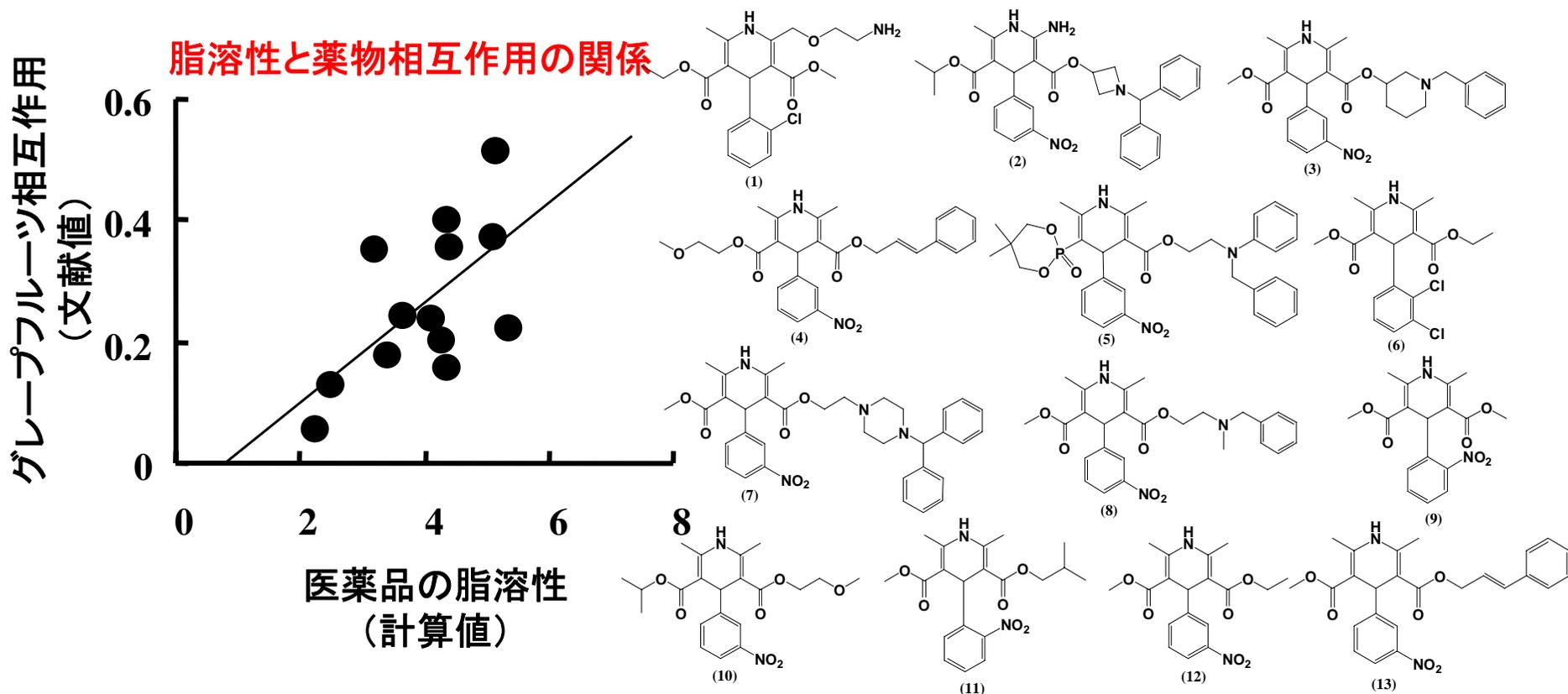


脂溶性 (LogP値) とは

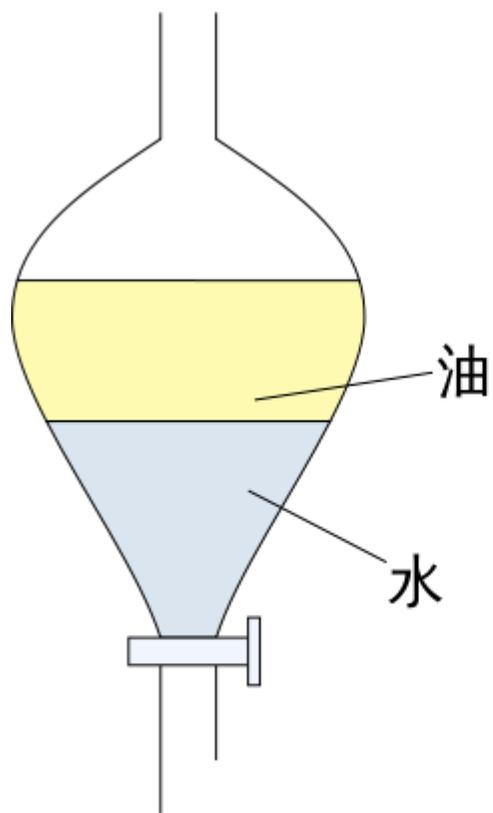
- 化合物の油に対する溶解しやすさの指標
- フラスコ振盪法などにより実験的に測定される。
- 化合物の生理活性や環境毒性を推定する上で最も重要な指標の一つ
- 構造式から脂溶性を推算する方法が、近年のIT技術の進展により多数利用可能
- **本発表では、ネット上のサービスを中心に様々な脂溶性推定法を紹介する**

Web上の計算を用いた研究例



Uesawa Y and Mohri K,
Relationship between lipophilicities of 1,4-dihydropyridine derivatives and pharmacokinetic interaction strengths with grapefruit juice.
Yakugaku Zasshi 128(1):117-22(2008).

フラスコ振盪法



- ① 水とオクタノールを24時間以上混合して飽和する。
- ② 測定対象物質と共にフラスコに取り振盪する。
- ③ 遠心分離により相分離する。
- ④ 各相に含まれる対象物質を定量する。

PubChem

- <http://pubchem.ncbi.nlm.nih.gov/>

PubChem Compound
PubChem Compound
[Limits](#) [Advanced search](#)

Celiprolol - Compound Summary (CID 2663)



[» Links and Re](#)

A cardioselective beta-1 adrenergic antagonist that has intrinsic sympathomimetic activity. It is used in the management of ANGINA PECTORIS and HYPERTENSION.

Table of Contents

[Identification and Related Records](#)

[Pharmacology](#)

[Biomedical Effects and Toxicity](#)

[Safety and Handling](#)

[Literature](#)

[Biological Test Results](#)

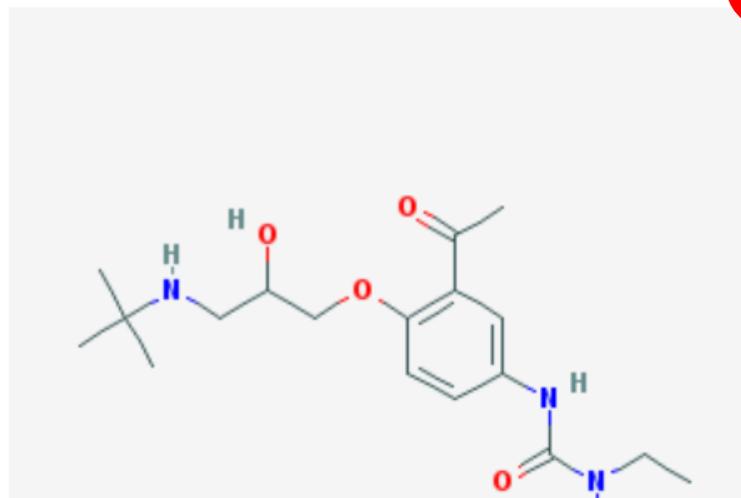
[Classification](#)

[Chemical and Physical Properties](#)

[Expand all contents](#)

2D

3D



Properties

Compound ID: 2663

Molecular Weight: 379

Molecular Formula: C₂

XLogP3: 1.9

H-Bond Donor: 3

H-Bond Acceptor: 5

BioActivity Da

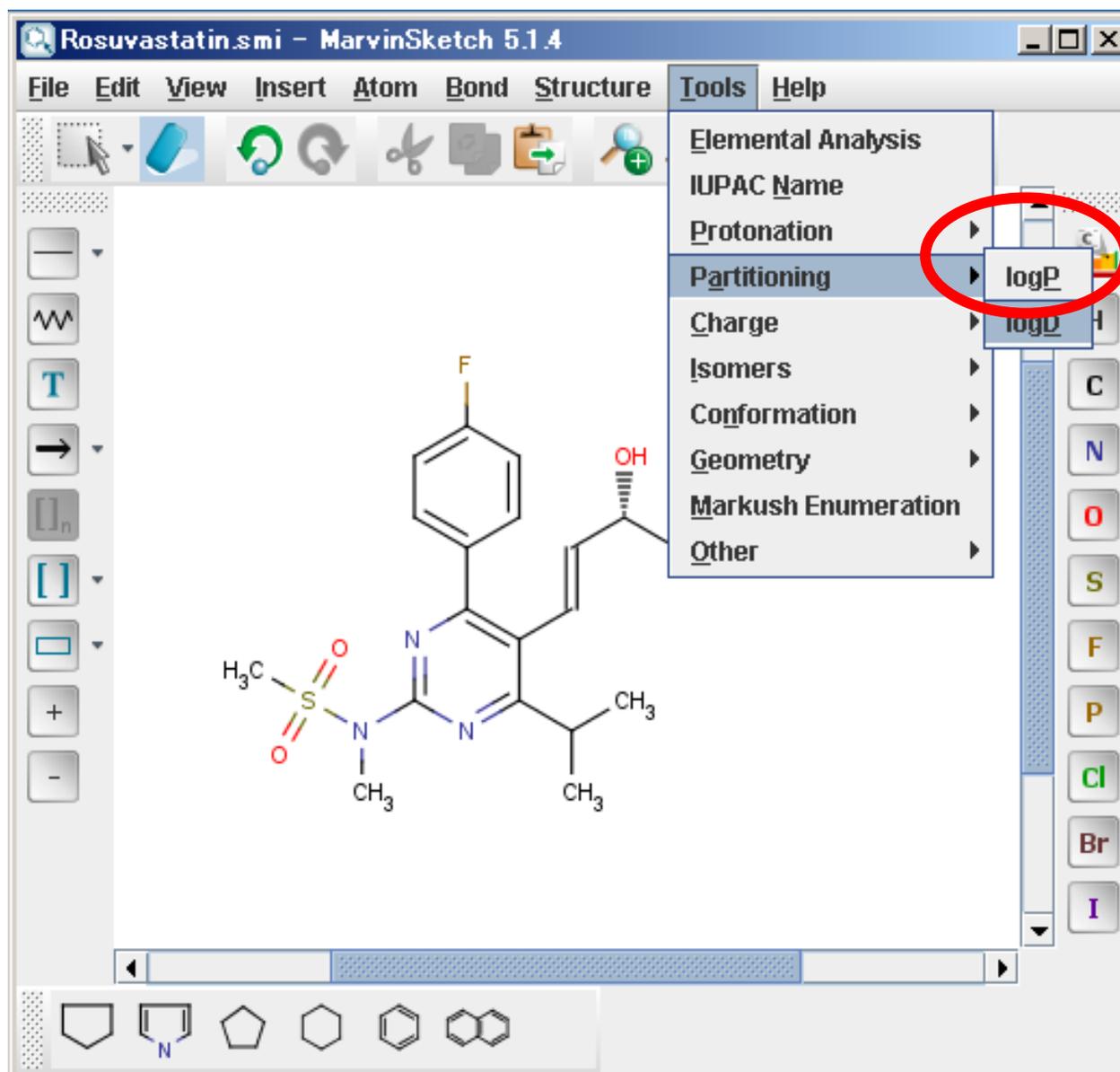
[This Compound](#)

[with Similar Compoun](#)

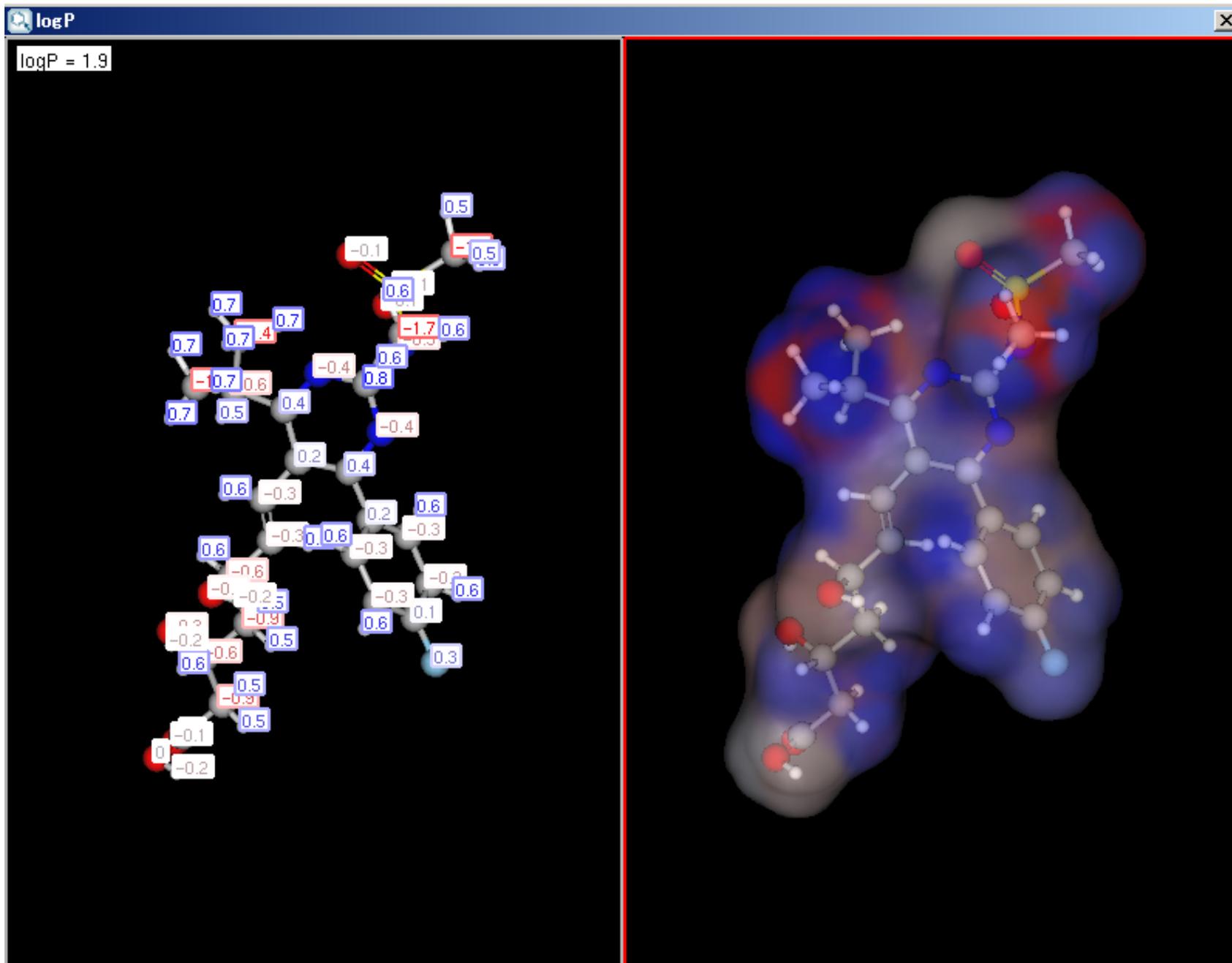
[with Similar Conforme](#)

Marvin Sketch

- <http://www.chemaxon.com/marvin/sketch/index.php>



Marvin SketchによるLogP値の推算



ALOGPS

<http://www.vcclab.org/lab/alogps/>

Provide CAS RN or SMILES of a molecule and press the "submit" button © VCCLAB 2006

Upload a file with molecule(s) in 48 formats

[CAS RN](#) 56980-93-9 [formula](#) C20H33N3O4 [MW](#) 379.56

[SMILES](#) OC(CNC(C)(C)C)COC1=C(C(C)=O)C=C(NC(N(CC)CC)=O)C=C1

logP (exp) :	1.92	logS (exp) :	
ALOGPs	2.29 <+0.37>	ALOGpS	-3.34 (0.17 g/l)
IA_logP	1.39 <-0.53>	IA_logS	-2.37 (1.62 g/l)
AB/LogP	2.27 <+0.35>	AB/logS	-3.48 (0.13 g/l)
QlogP	2.49 <+0.57>	QlogS	-5.50 (1.20 mg/l)
COSMOFrag	4.78 <+2.86>	Average logS	-3.67(+/-1.31)
miLogP	2.65 <+0.73>		
KOWWIN	1.93 <+0.01>	AB/pKa (Base)	9.40
XLOGP	1.90 <-0.02>	AB/pKa (Acid)	
Average logP	2.46(+/-1.02) <+0.54>	PhysProp ref	
		Sangster's ref	

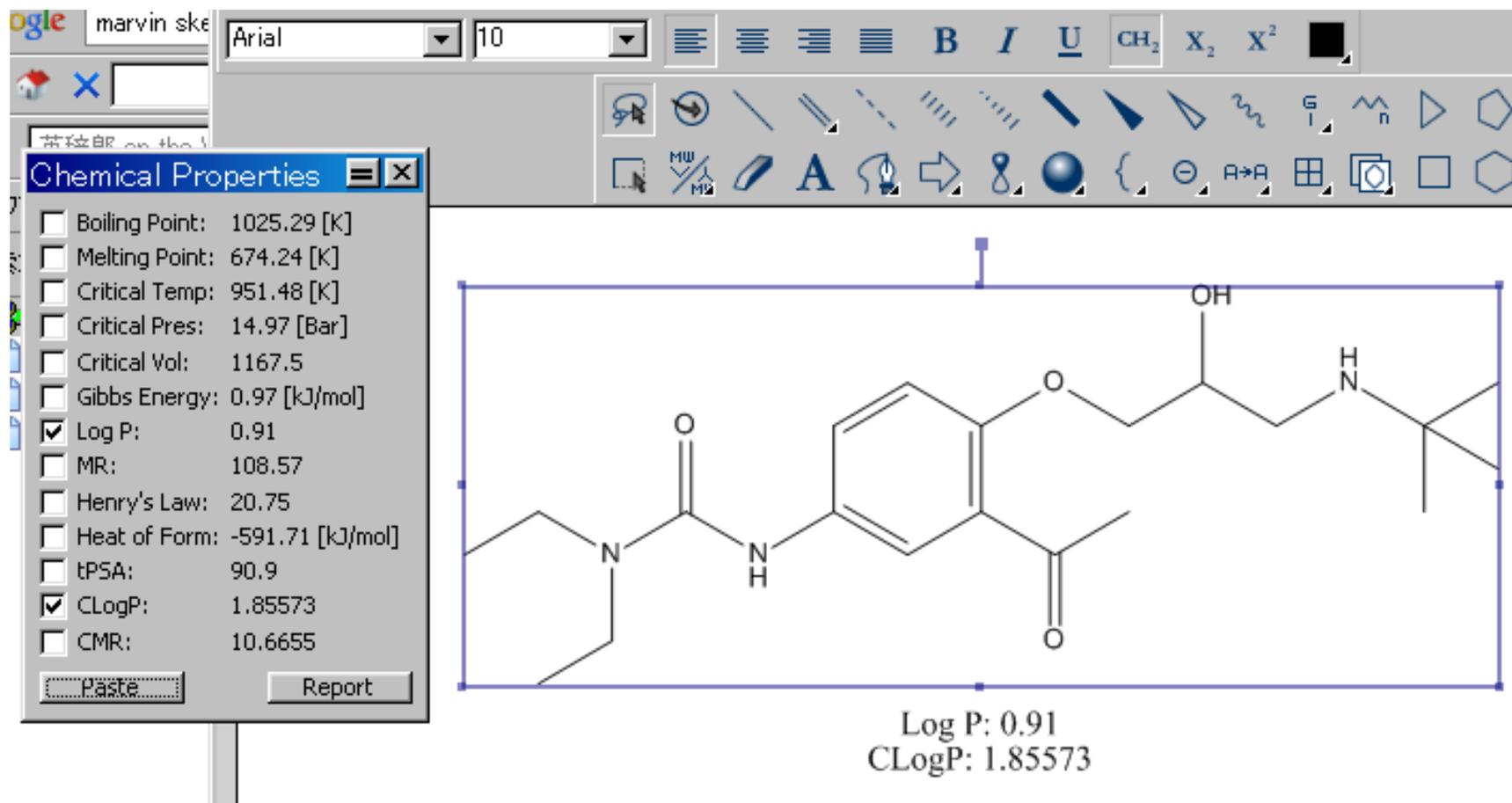
User's [LogP LIBRARY](#) User's [LogS LIBRARY](#)

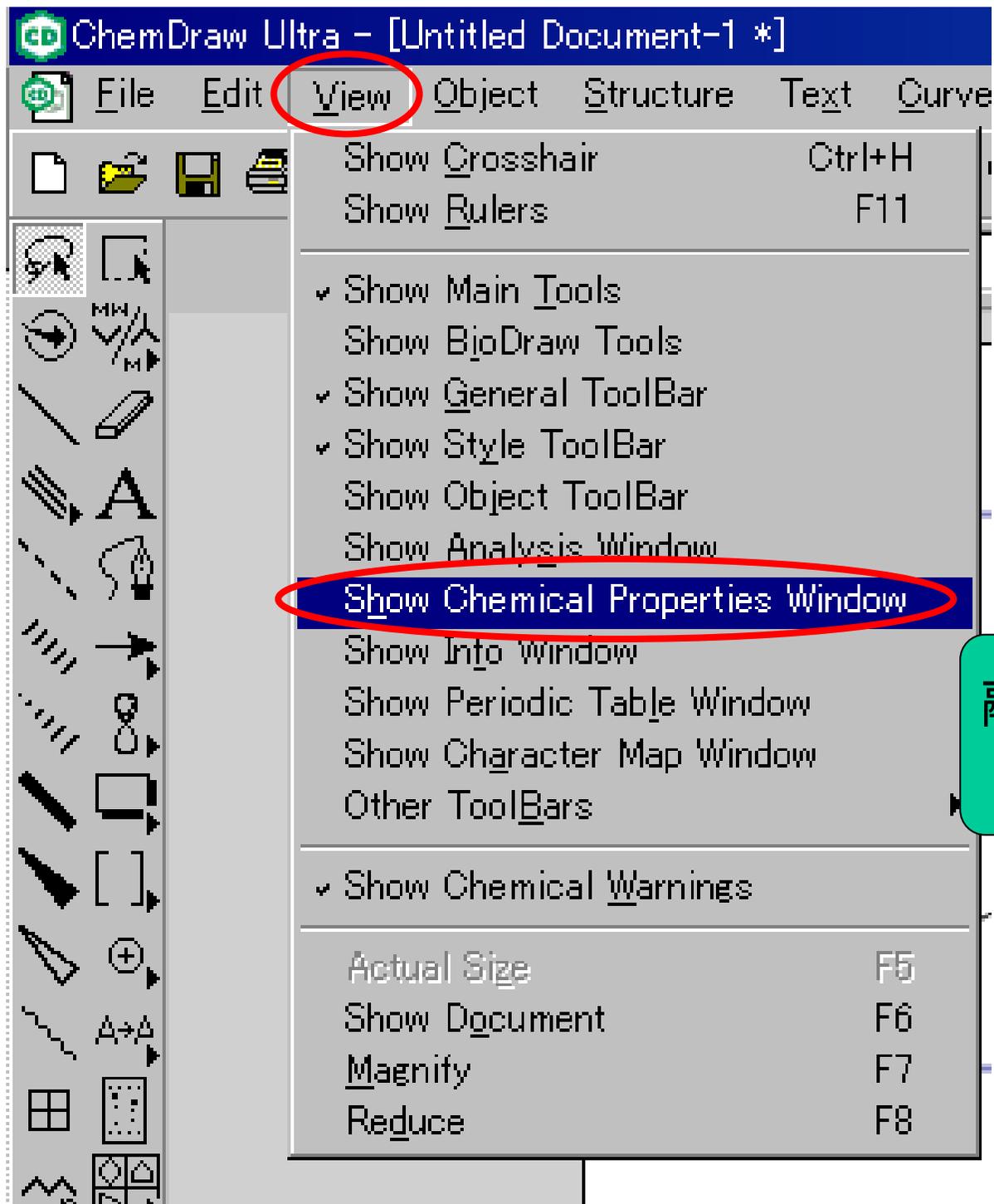
各種LogP推算值

水溶性予測値

pKa
予測値

ChemBioDraw





融点や脂溶性(logP値)
の予測

SPARC on line calculator

<http://sparc.chem.uga.edu/sparc/>

プログラムの選択(この画面)

The screenshot shows the SPARC online calculator interface. On the left is a vertical navigation menu with buttons for Reference, Home, SMILES, Calculate, Search DB, Search CAS, Options, and Help. The main area features the SPARC logo and a grid of 15 calculation buttons: pKa, Gas pKa, NonAq pKa, Solid pKa, Kinetics, Properties, Henry(pH), Reduction Potential, Tautomers, LogD, Alpha/Beta, Hydrolysis, Hydration, Heat of Formation, and Ions. The LogD button is circled in red. At the bottom, a message reads: "Current type is not set Press buttons above to choose type."

Reference

SPARC Performs Automated Reasoning in Chemistry

Home

SMILES

Calculate

Search DB

Search CAS

Options

Help

SPARC PERFORMS AUTOMATED REASONING IN CHEMISTRY v4.1

WELCOME TO THE SPARC ON LINE CALCULATOR

pKa

Gas pKa

NonAq pKa

Solid pKa

Kinetics

Properties

Henry(pH)

Reduction Potential

Tautomers

LogD

$\alpha\beta$ Alpha/Beta

Hydrolysis

Hydration

Heat of Formation

Ions

Current type is not set Press buttons above to choose type.

構造式の入力

計算の実行

脂溶性



SPARCによるLogD値の推算

SPARC Property Plot

