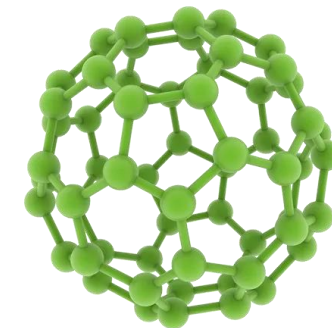
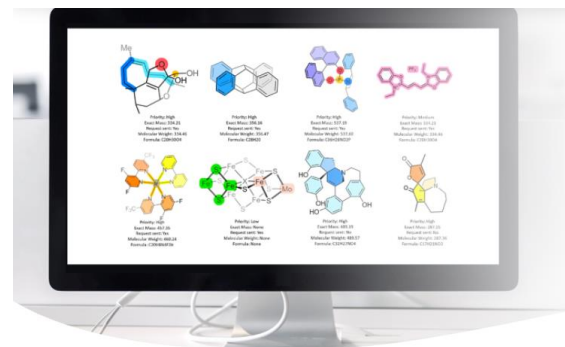


ChemDraw V23 Suite





Signal Research
Platform



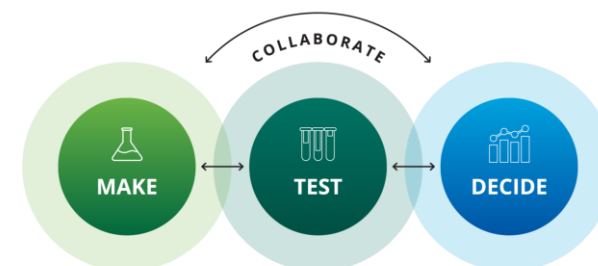
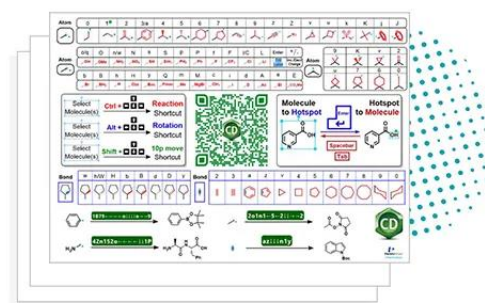
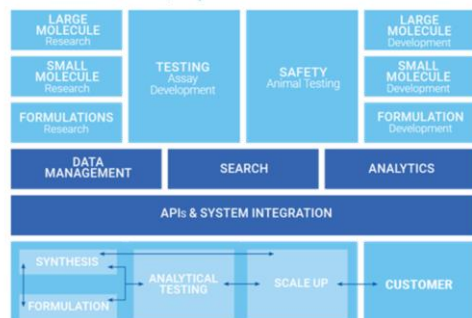
ChemDraw



E-Notebook
(ELN)



SMARTER SCIENCE | Capabilities



■ 高效的化學繪圖應用套件

ChemDraw Prime



快速建立化學繪圖

ChemDraw Professional



快速連結科學資料庫

Singals ChemDraw



快速搜尋、製作化學報告

重要特性比較

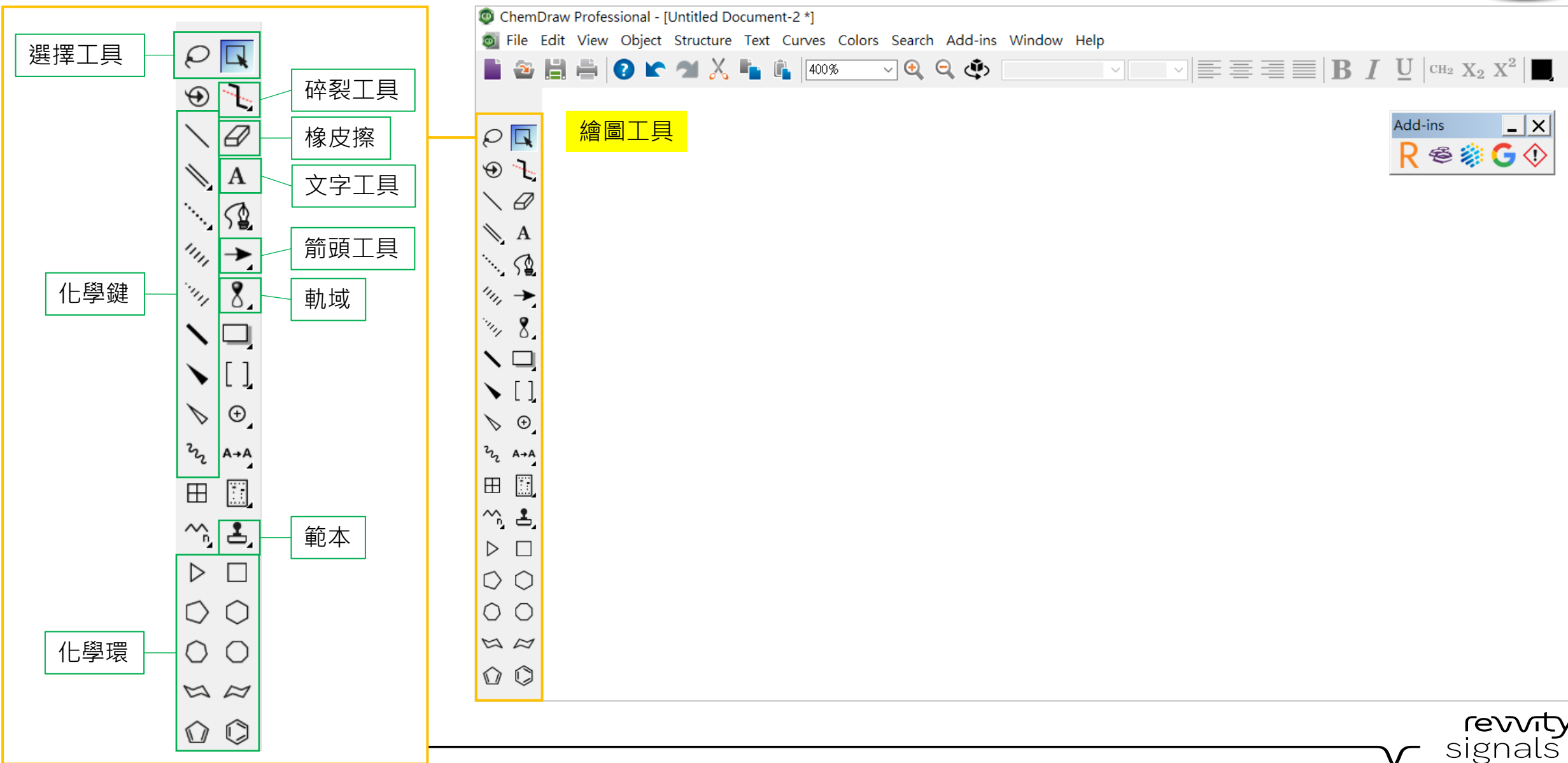
重要特性	功能	ChemDraw Prime	ChemDraw Professional	Singals ChemDraw
化學繪圖	完整的繪圖工具與範本	●	●	●
	熱鍵與快捷鍵	●	●	●
	化學結構整理	●	●	●
	智慧複製貼上(支持SMILES, InChI, HELM格式)	●	●	●
化學與生物的智慧分析	13C和1H的核磁共振(NMR)預測		●	●
	從CAS Number轉換成結構式		●	●
	化合物名稱和化學結構互換		●	●
	HELM(生物高分子)工具列		●	●
	從結構式取得分析和化學屬性	●	●	●
化學性質視覺化	3D 立體顯示		●	●
	2D 環狀結構填色/顏色標記原子與化學鍵		●	●
	支持3MF格式與3D顏色標記			●
外掛程式整合	ChemDraw for Excel		●	●
	連接SciFinder-n/Reaxys資料庫		●	●
	連接ChemACX資料庫/PubChem/Google Pattern			●
	連接3D計算軟體:GAMESS/Gaussian/Mopac/Autodoc/Conflex			●
	ChemFinder Ultra 化合物資料庫管理			●
雲端資料搜尋彙整	ChemOffice 雲端模組(>5)			●
	ChemDraw JS 嵌入(>5)			●
	Signals Notebook 電子實驗紀錄本(5-20)			●

■ 功能介紹

ChemDraw Prime



完整的繪圖工具與範本



The image displays the ChemDraw Professional software interface, highlighting the drawing tools and templates. The interface includes a menu bar (File, Edit, View, Object, Structure, Text, Curves, Colors, Search, Add-ins, Window, Help) and a toolbar with various drawing tools. The drawing area is labeled "繪圖工具" (Drawing Tools).

The tools are categorized into three groups, each highlighted with a green box and labeled with Chinese text:

- 選擇工具** (Selection Tools): Includes tools for selecting objects.
- 化學鍵** (Chemical Bonds): Includes tools for drawing single, double, and triple bonds, as well as aromatic bonds.
- 化學環** (Chemical Rings): Includes tools for drawing various chemical rings (triangles, squares, pentagons, hexagons, heptagons, octagons, and nonagons).

Other tools shown include:

- 碎裂工具** (Fragmentation Tool)
- 橡皮擦** (Eraser)
- 文字工具** (Text Tool)
- 箭頭工具** (Arrow Tool)
- 軌域** (Orbitals)
- 範本** (Templates)

The software interface also shows an "Add-ins" panel on the right side, containing icons for various add-ons like R, G, and a warning icon.

完整的繪圖工具與範本

人體圖

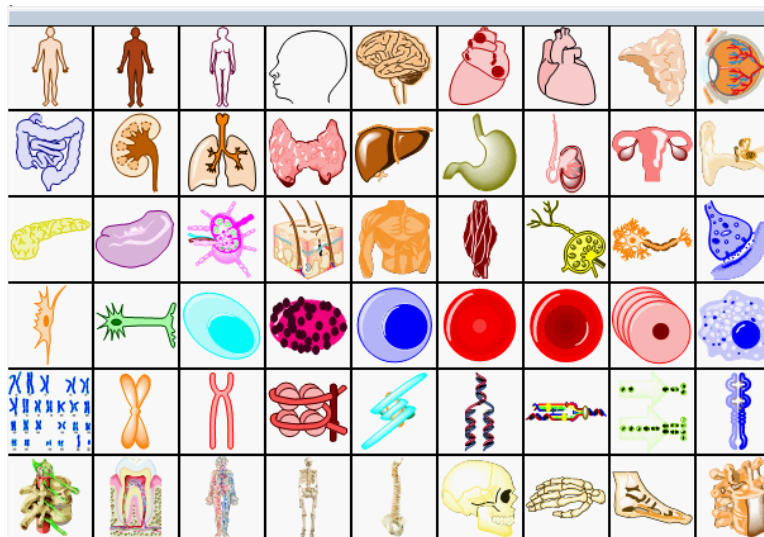
ChemDraw Prime



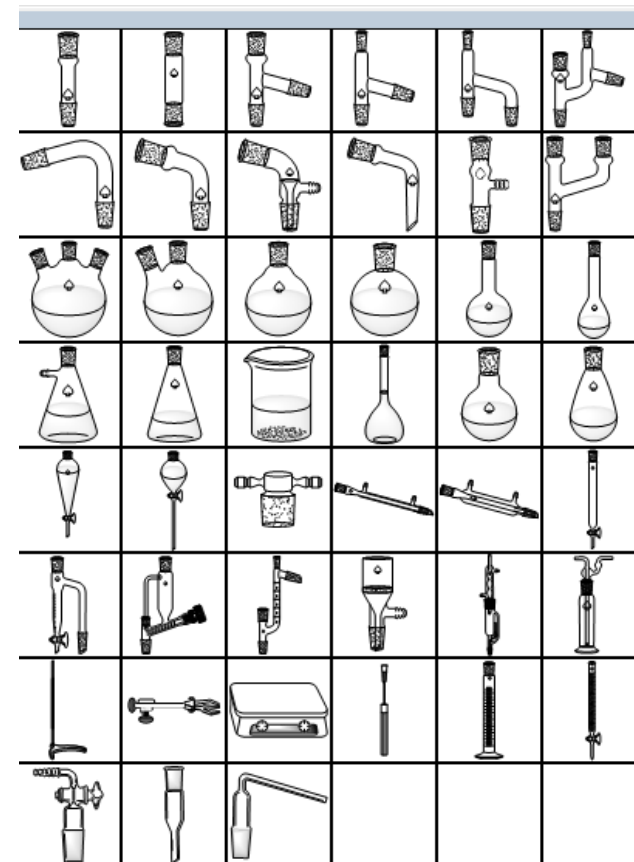
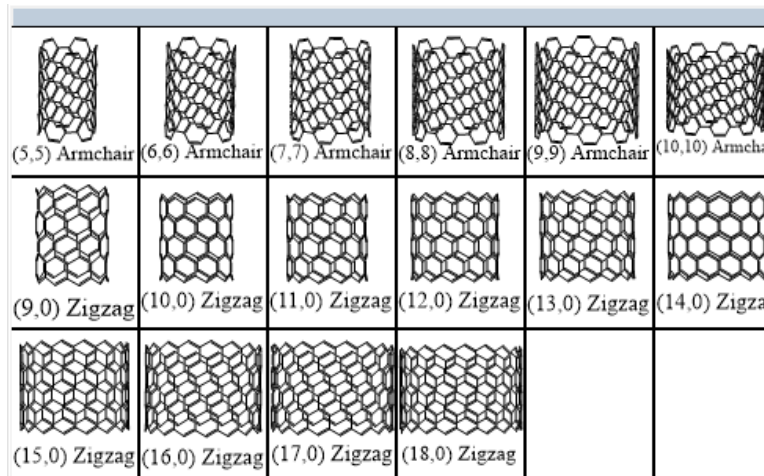
實驗室設備

範本

高級生物繪圖



奈米管



- Advanced BioDraw
- Amino Acid Side Chains
- Amino Acids
- Anatomy
- Animals
- Aromatics
- Bicyclics
- Bio Instruments
- BioArt
- Bugs
- Clipware, part 1
- Clipware, part 2
- Conformers
- Cp Rings
- Cycloalkanes
- DNA Templates
- Functional Groups
- Hexoses
- Metallocenes
- Microorganisms
- Nanotubes
- Organelles
- Ph Rings
- Polyhedra
- Polypeptides
- RNA Templates
- Shapes
- Stereocenters
- Supramolecules
- New Templates...

熱鍵與快捷鍵



ChemDraw 22 Hotkeys Cheat Sheet - located in Help > Hotkeys Cheat Sheet Menu

1

Atom	0	1	2	3/a	4	5	6	7	8	9	z	Z	v	u	k	K	j	J
Atom	o/q	O	n/w	N	s	S	P	P	f	F	I/C	L	Enter	+/-				
	b	B	h	H	y	Q	m	M	c	i	d	A	e	E				

Atom	9	K	v	2
	u	7	6	0

2

Select Molecule(s) → Ctrl + → Reaction Shortcut

Select Molecule(s) → Alt + → Rotation Shortcut

Select Molecule(s) → Shift + → 10 px move Shortcut

Atom **g** "grabs atom/bond" from hotspot to atom selection

Bond **g** from hotspot to bond selection

Select Molecule(s) → Shift + Alt + → 3D Rotation Shortcut

Molecule to Hotspot → Enter → Hotspot to Molecule

Spacebar

Tab

1

Bond	w	h/W	H	b	B	d	D	y	Bond	2	3	a	z	v	4	5	6	7	8	9	0	

	1B79←←←←o!!!o→→9			2o1n1←5←2↓↓→2	
	42n152o←←←←!!!1P			az!!!n1y	

熱鍵與快捷鍵

ChemDraw Prime



Located in Help > Shortcuts Cheat Sheet Menu

ChemDraw Shortcuts Cheat Sheet

1 **Ctrl + Shift + Click & Drag** (with hand icon) → **2-Click to select** (with mouse icon) → **Ctrl + Click & Drag** (with hand icon) →

2 **Ctrl + Shift + Alt + H** → **Ctrl + Shift + Alt + L (Left)** → **Ctrl + Shift + Alt + C (Center)** → **Ctrl + Shift + Alt + R (Right)** → **Horizontal alignment: Ctrl + Shift + Alt + T (Top) + M (Middle) + B (Bottom)**

3 **2-Click on Arrow selects reaction** (with mouse icon) → **Ctrl + Shift + X Reaction Clean-up** →

4

H ₂ SO ₄ (cat.)	+ b Bold
C ₆ H ₅ CH ₃ , 60°C, 48h	+ i italic
Ctrl + f	+ u underlined
H ₂ SO ₄ (cat.)	+ L Aligned Left
C ₆ H ₅ CH ₃ , 60°C, 48h	+ R Aligned Right
Ctrl + Shift + C	+ J Justified
H ₂ SO ₄ (cat.)	
C ₆ H ₅ CH ₃ , 60°C, 48h	

Ctrl + Shift + K →

5 **Ctrl + Shift + H** → **Ctrl + Shift + V** →

6 **Ctrl + Alt + N** → **Ctrl + Shift + N** →

7 **Alt + D** → **Ctrl + Shift + D** →

8 **Ctrl + Shift + K** →

9 **Shift + Click then Ctrl + J** (works with bonds) →

10 **Alt + K** →

*** = requires ChemDraw Professional licence**

■ 功能介紹

ChemDraw Professional



13C和1H的核磁共振(NMR)預測

ChemDraw Professional



ChemDraw Professional | Structure | File | Edit | View | Object | Text | Curves | Colors | Search | Add-ins | Window | Help

Atom Properties...
Bond Properties...
Bracket Properties...
Check Structure
Clean Up Structure Shift+Ctrl+K
Clean Up Reaction Shift+Ctrl+X
Clean Up Biopolymer
Expand Label
Contract Label
Expand Generic Structure
Add Multi-Center Attachment
Add Variable Attachment
R-Logic Query...
Add 3D Property
Enhanced Stereochemistry
Map Reaction Atoms
Clear Reaction Map
Analyze Stoichiometry
Autonumber Reaction
Clear Reaction Numbers
Predict 1H-NMR Shifts
Predict 13C-NMR Shifts
Make Spectrum-Structure Assignment
Add Structure to Dictionary...
Define Nicname...
Convert Name to Structure Shift+Ctrl+N
Convert Structure to Name Alt+Ctrl+N

ChemNMR 1H Estimation

Estimation quality is indicated by color: good, medium, rough

Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
OH	8,09	4,20	alcohol
		4,80	1 -C*R
		-0,91	general corrections
NH	11,50	7,00	sec. amide
		?	1 unknown substituent(s)
		0,70	1 -1'C*C*C*C*C*1 from sec. amideC
		?	1 unknown substituent(s) from sec amine
		?	1 unknown substituent(s) from amine
		3,80	general corrections
CH	7,13	7,26	1-benzene
		-0,38	1 -O-C
		0,00	1 -O-C
		-0,10	1 -N=C
		0,18	1 -C(=O)N
		0,17	general corrections
CH	7,49	7,26	1-benzene
		0,00	1 -O-C
		-0,38	1 -O-C
		0,00	1 -N=C
		0,69	1 -C(=O)N
		-0,08	general corrections
CH	7,47	7,62	benzylidenimin
		0,00	1 -1'C*C*C*C*C*1
		-0,17	1 -O from 1-benzene

Predict 1H-NMR Shifts
Predict 13C-NMR Shifts

Display a calculated 1H NMR spectrum for the selected structure

ChemDraw for Excel

ChemDraw Professional



ChemDraw for Excel Add-In

ChemDraw for Excel 插件

Chemically active structure

化學活性結構

Substructure search available utilizing ChemDraw toolbar

使用Chemdraw 工具列 可進行分子結構搜索

Structure	MolfileName	PUBCHEM_ATOM	IPUBCHEM_ATOM	IPUBCHEM_BOND	PUBCHEM_BOND	IPUBCHEM_CACTVS	PUBCHEM_CACTVS	PUBCHEM_CACT
$C_{12}H_{13}NO_2S$								
$C_{21}H_{21}F_4N_2O$	3233846							



外掛程式	功能
Reaxys	全球最大物質理化性質、事實反應資料庫和藥物化學資料庫
Sci-Finder n	全世界最大、最全面的化學和科學資訊資料庫。透過網路直接查看「化學文摘」

■ 功能介紹

Singals ChemDraw





外掛程式	功能
Google Patents	Google 搜尋引擎 add-in
Pubchem	安全性/有機小分子生物活性數據
ChemACX	屬性/來源/安全性
Mnova for ChemDraw Edition	一維計算
GAMESS	3D 計算軟體/量子化學
Gaussian	3D 計算軟體/量子化學
Mopac	3D 計算軟體/半經驗分子軌道程式包 (分子結構和化學反應)
Autodock	3D 計算軟體/分子模擬
Conflex	3D 計算軟體/構象搜尋與分析
ChemFinder	化合物資料庫管理



SignalsNotebook Quick Find 🔍 📄 📁 🗑️ 🔗 🌐 🔬 🌟 👤 🏠

Add New ▾ 0🔔 Ben Bracke ▾

◀ Back BB-001 ▶ BB-001-CHEM554 One pot Synthesis of 5-methyl-3,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one

🌟 0🗨️ ACTIVE ▾ NOT SHARED 🔍 ChemACX

📄 Contents 🗨️ Comments ➕ Add Content ▾

📄 Properties 🕒 History 🖋️ Signing 📄 Sharing 🔄 Related ⚙️

Experiment Contents

📄 Main Page ▾

- ⚙️ Reaction
- 📄 Samples
- 📄 Preparation
- 📄 Discussion
- 📄 Conclusion
- 📄 Materials Table
- 📄 Variety Table

📄 Supporting Materials ▾

- 📄 HCLGenerator Equipment Setup.JPG
- 📄 Equipment used in this experiment
- 📄 ViscosityCalculatorModels.xls
- 📄 coshrra.docx

📄 Analytical Evidence ▾

- 📄 1H-NMR-FNMR002374.PDF

📄 Reference Material ▾

- 📄 pale crystalline powder 500x500.jpg
- 📄 My ToDo List - Copy.xlsx

Reaction

Reactants

Rxn ID	Reactant	MF	MW	EM	Limit?	Eq	Sample Mass	Moles	Molarity	Vol	d	% Wt	CAS Number	Supplier	Lot Number
I	2-cyanoacetamide	C ₃ H ₄ N ₂ O	84.08	84.03236		1.0	66 g	0.78 mol		70 mL	0.936 g/mL				
II	2-(2-oxopropyl)isoindoline-1,3-dione	C ₁₁ H ₉ NO ₃	203.20	203.05824	✓	1	156 g	766 mmol		236 mL	.6598 g/mL				
III	lithium hydroxide	HLiO	23.95	24.01874		1	36.7 g	766 mmol		138 mL	0.2658 g/mL	50 %	1310-65-2	Alfa Aesar	13407
IV	tetrahydrofuran	C ₄ H ₈ O	72.11	72.05751		1	55.3 g	766 mmol		95 mL	0.58 g/mL		24979-97-3	ABCR	MP-9478
V	methanol	CH ₄ O	32.04	32.02621		3	73.7 g	2.30 mol		161 mL	.4589 g/mL		67-56-1	VWR International	EM1.09259.0250
VI	sodium methanolate	CH ₃ NaO	54.02	54.00816		1	63.7 g	766 mmol		63.6 mL	1.002 g/mL	65 %	124-41-4		
VII	sodium methanolate	CH ₃ NaO	54.02	54.00816		1	41.4 g	766 mmol		41.3 mL	1.002 g/mL		124-41-4		
VIII	ethyl formate	C ₃ H ₆ O ₂	74.08	74.03678		2.5	142 g	1.92 mol					109-94-4	Aldrich	W243418

Total Volume: 925 mL Reaction Molarity: 829 mmolar

Products

Rxn ID	Product ID	Product	MF	MW	EM	Theo Mass	Actual Mass	Purity	Yield	Theo Mol	Actual Mol	Internal ID
IX	P1	5-methyl-3,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one	C ₇ H ₇ N ₃ O	149.15	149.05891	114 g	100 g	98.6 %	86.3 %	766 mmol	661 mmol	PH10298

Solvents

Solvent	Ratio	Volume
2,2,2-Trifluoroethanol		120 mL

Main Page Supporting Materials Analytical Evidence Reference Material

企業客戶





Thank you!