



インターネットセミナー

2014年5月の新機能

JAICI
化学情報協会

2014年5月

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本日はご紹介する内容

ついに実現！



- ChemBioDraw Ultra Version 14との連携
- Non-Java 作図ツールの強化

ChemBioDraw Ultra Version 14 との連携機能



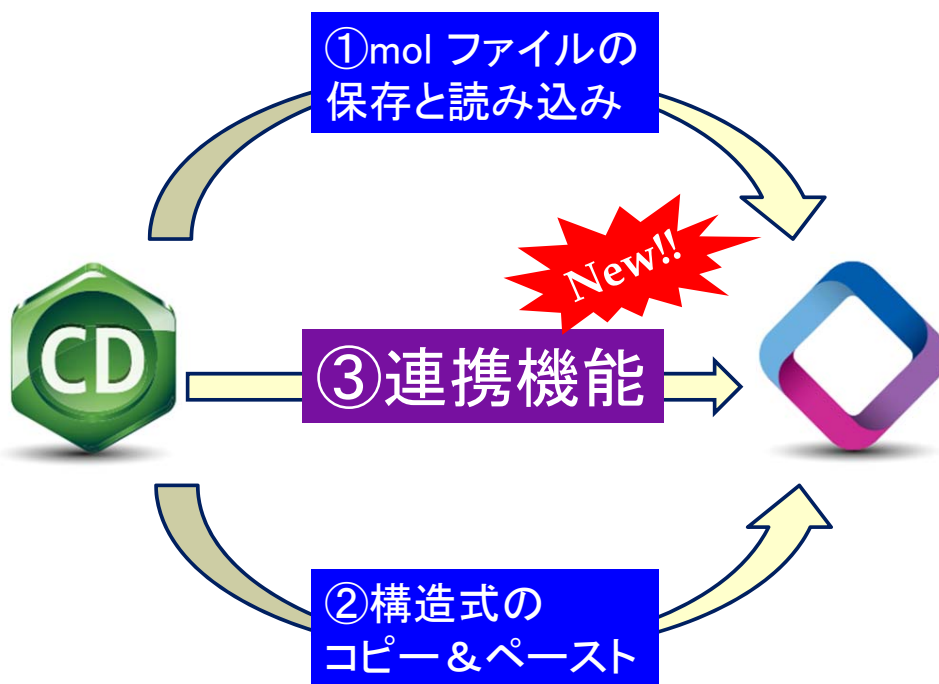
最も利用されている化学構造作図ツールから
SciFinder での検索がシームレスに行えます！

本日より有効です！

The screenshot shows the SciFinder search interface. On the left is a navigation menu with categories like REFERENCES, SUBSTANCES, and REACTIONS. The main area is titled 'SUBSTANCES: CHEMICAL STRUCTURE' and contains a 'Structure Editor' window, search options (Exact Structure, Substructure, Similarity), and a 'Search' button. A pink box highlights a new 'ChemDraw' button with the text: 'Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More'. On the right, there is a 'SAVED ANSWER SETS' section with a list of search results.

※ChemBioDraw Ultra Version 14 が必要です

ChemBioDraw から構造式を移す方法



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ついに実現！ ChemBioDraw との連携機能

ChemBioDraw Ultra

File Edit View Object Structure Text Curves Colors Search Window Help

Pomalyst.cdx*

Name: Pomalyst
Mode of Action: Antiangiogenesis agent
Indication: Multiple Myeloma

物質を選択

Search SciFinder

SciFinder®

Substance Search

Substructure

Exact Structure

Reaction Search (Substructure)

Selected Structure(s) are Products

Selected Structure(s) are Reactants

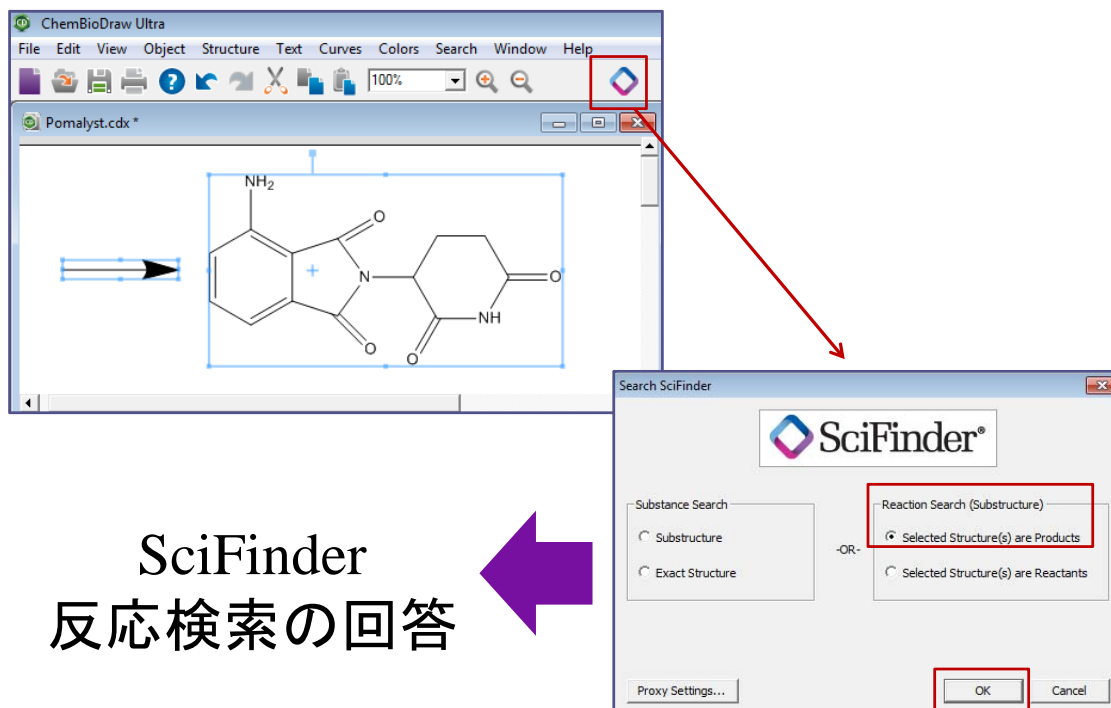
Proxy Settings...

OK Cancel

SciFinder
部分構造検索の回答

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ついに実現！ ChemBioDraw との連携機能



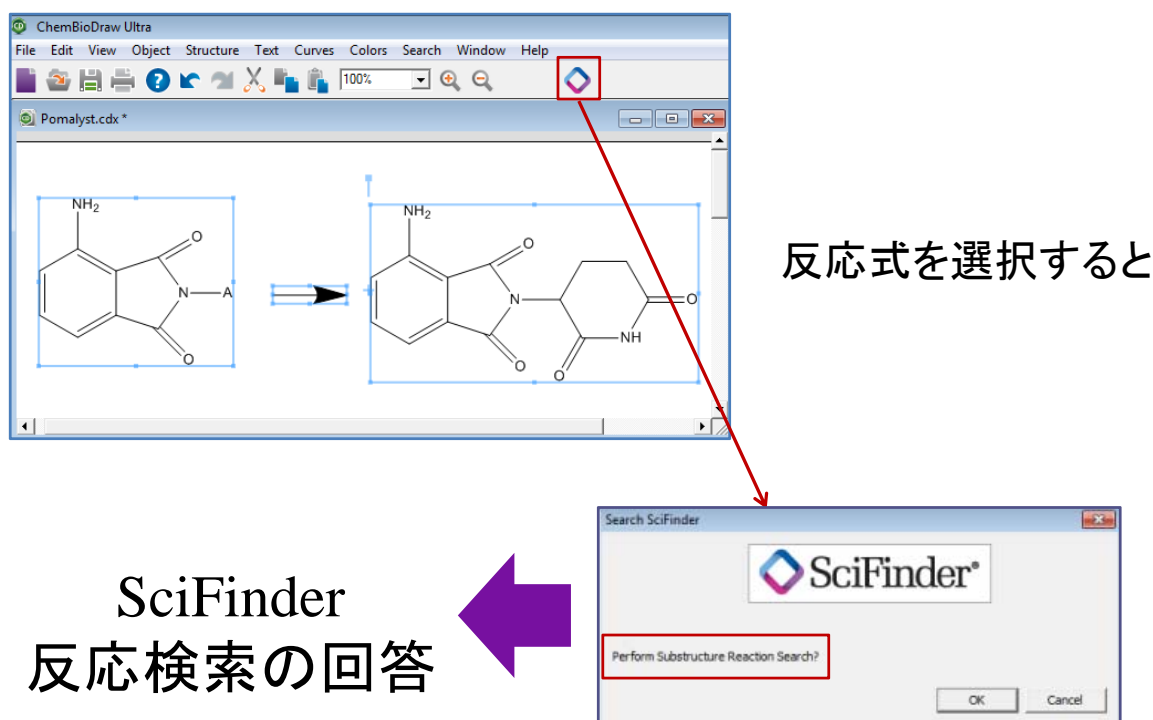
The image shows the ChemBioDraw Ultra interface with a chemical reaction scheme. A red box highlights the SciFinder icon in the top toolbar. A red arrow points from this icon to the SciFinder search dialog box. The dialog box has the following settings:

- Substance Search: Substructure, Exact Structure
- Reaction Search (Substructure): Selected Structure(s) are Products, Selected Structure(s) are Reactants
- Buttons: Proxy Settings..., OK, Cancel

SciFinder
反応検索の回答

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ついに実現！ ChemBioDraw との連携機能



The image shows the ChemBioDraw Ultra interface with a chemical reaction scheme. A red box highlights the SciFinder icon in the top toolbar. A red arrow points from this icon to the SciFinder search dialog box. The dialog box has the following settings:

- Perform Substructure Reaction Search?:
- Buttons: OK, Cancel

反応式を選択すると

SciFinder
反応検索の回答

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ついに実現！ ChemBioDraw との連携機能

SciFinder[®] Preferences | SciFinder Help | Sign Out

Explore | Saved Searches | SciPlanner Save Print Export

Reaction Structure substructure > reactions (9)

REACTIONS Get References Tools Send to SciPlanner

Analyze Refine

Analyze by: Reagent

H ₂	4
HCl	4
Et ₃ N	2
HOCH ₂ CH ₂ NH ₂	2
Dilimidazolyl ketone	1

Show More

Group by: No Grouping Sort by: Relevance

0 of 8 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

88%
~1

Overview

Steps/Stages	Notes
1.1 S: MeCN, rt → 45°C 1.2 R: Dilimidazolyl ketone, 4.5 h, reflux	alternative preparation shown, kilogram scale, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Processes for the preparation of 4-amino-2-(2,6-dioxo-3-piperidin-3-yl)isoindole-1,3-dione compounds
Quick View Full Text PDF
By Ge, Chuanshen et al
From U.S. Pat. Appl. Publ., 20070004920, 04 Jan 2007

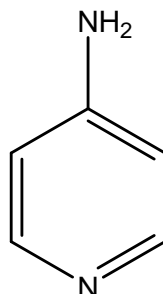
Experimental Procedure

Example 3 Preparation of 4-Amino-2-(2,6-dioxo-3-piperidinyl)isoindole-1,3-dione According to Scheme A [0086] A mixture of acetonitrile (42 L) and Example 2 (2120 g, 7.28 moles) was added to a round bottom flask equipped with a mechanical stirrer, a condenser, a nitrogen inlet and a heating mantle to form a solution.

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検索例 1

- CBD 上で以下の物質を作図し，そのまま SciFinder で部分構造検索を実行

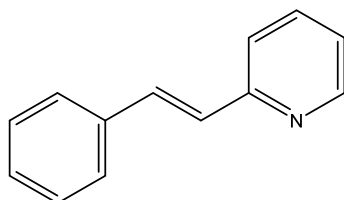


- 得られた回答で以下の絞込みを行う
 - 縮合環禁止 (Lock Rings)
 - R グループを使って限定

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検索例2

- CBD 上で以下の構造を作図し, そのまま**反応検索**を実行

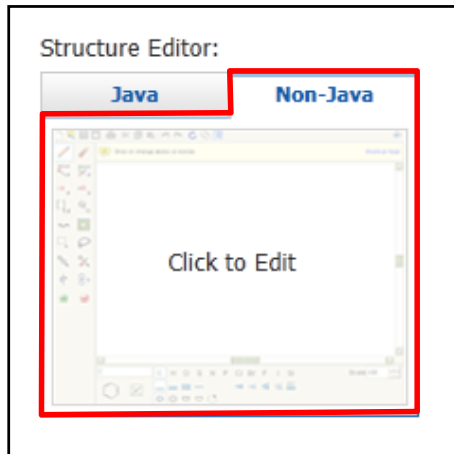


- 以下の絞込みを行う
 - 縮合環禁止 (Lock Rings)
 - Experimental Procedure が存在する反応
 - Heck 反応に限定

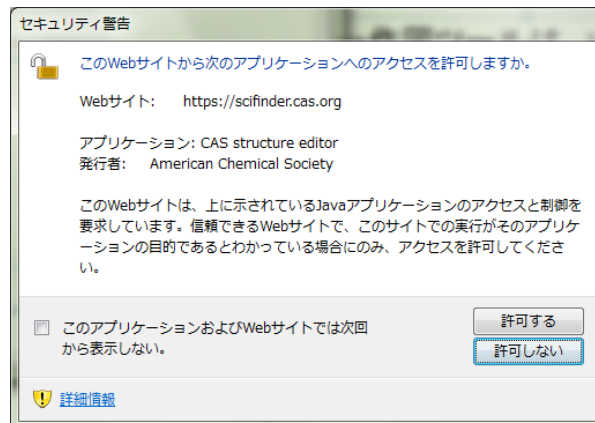
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Non-Java 作図ツールの強化

Java 構造作図ツール

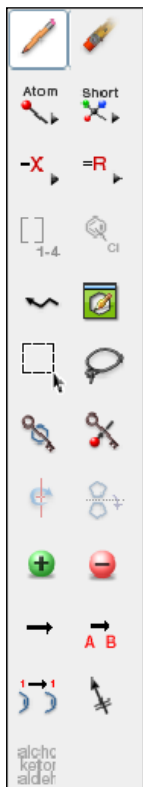


- Java作図ツールは, Java およびブラウザのセキュリティ方針変更が動作に影響
- セキュリティ警告が毎回表示される



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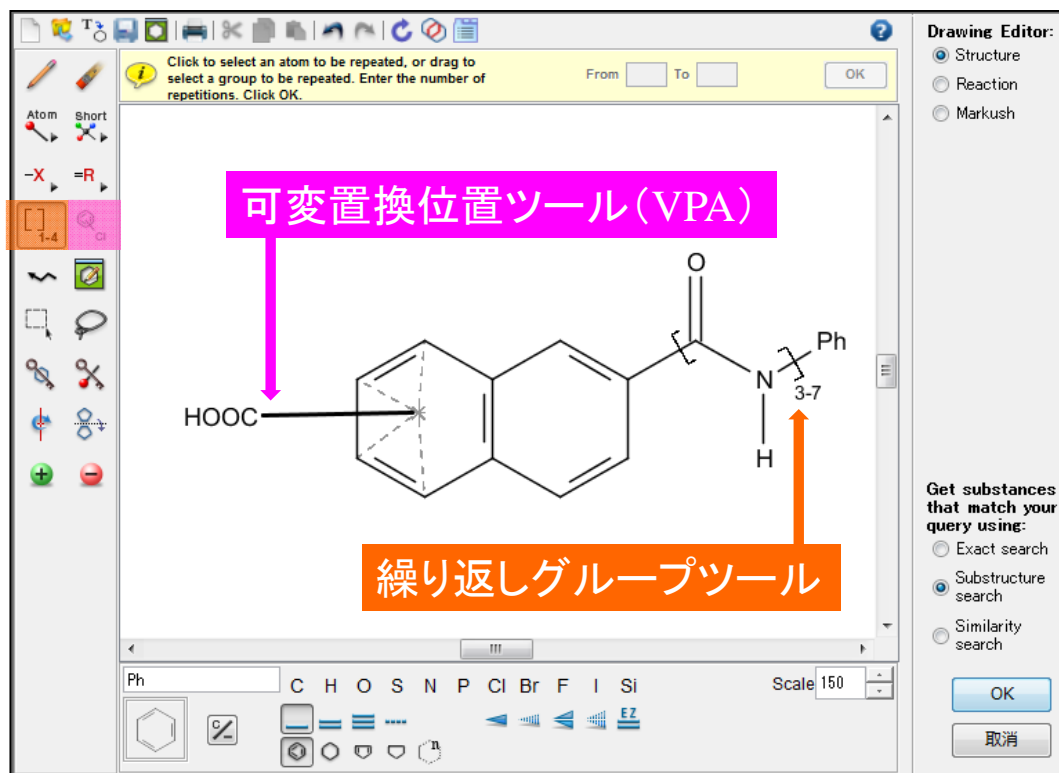
Non-Java構造作図ツールがますます便利に



- 2013/10 リリース
- 2013/12 Lock Atoms, 鎖ツールの
- 2014/1 R グループツール, デフォルト化.
- 2014/3 mol ファイルインポート, ショートカットキー
- 2014/4 可変置換位置ツール(VPA), 官能基ツール
- 2014/5 繰り返しグループツール, SMILES, InChi 形式から構造呼び出し

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Non-Java構造作図ツールがますます便利に



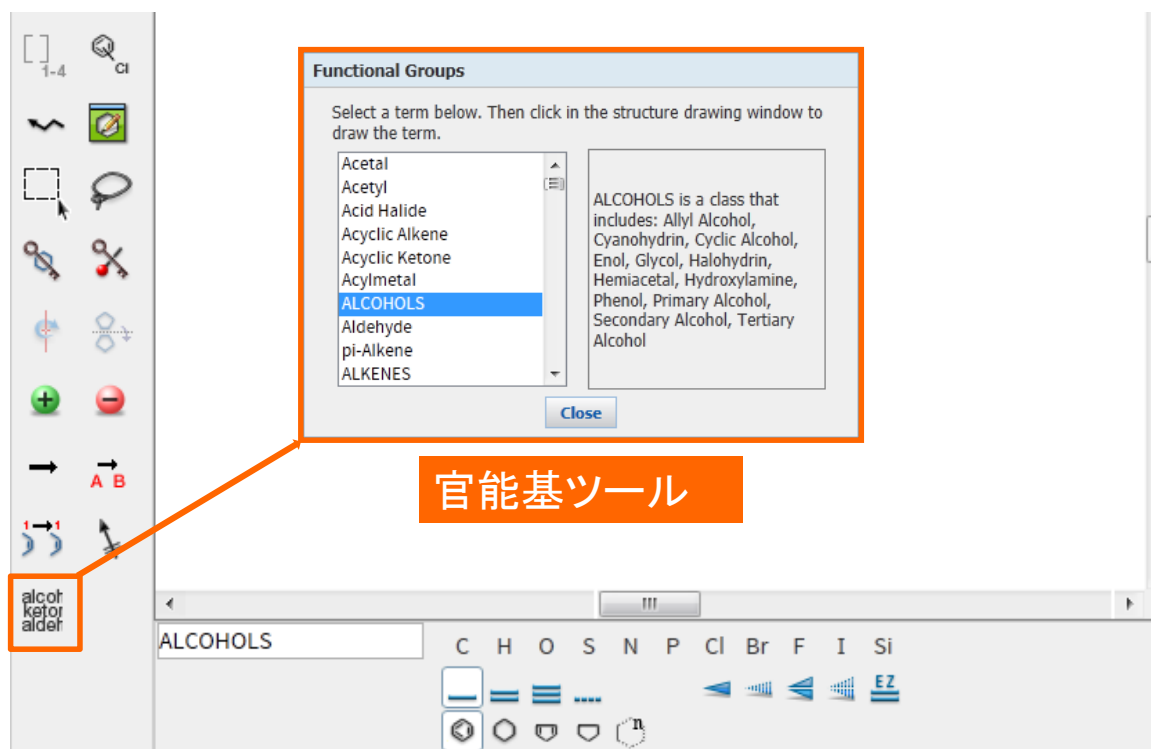
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Non-Java構造作図ツールがますます便利に

The screenshot shows the 'Structure Editor' window. The top toolbar has a button highlighted with a pink box. An orange arrow points from this button to an 'Import' dialog box, which is also highlighted with an orange box. The 'Import' dialog contains the text 'Only .cxf and .mol file formats are supported.' and a 'Cancel' button. A pink arrow points from the same toolbar button to an 'Add to Editor' dialog box, which is highlighted with a pink box. The 'Add to Editor' dialog contains a text input field for 'Enter CAS Registry Number:' with the value '33069-62-4', examples '50-00-0' and '50000', and 'OK' and 'Cancel' buttons. Below the 'Import' dialog is an orange box with the text 'mol ファイル インポート'. Below the 'Add to Editor' dialog is a pink box with the text 'CAS 登録番号 SMILES InChI 形式 からの構造呼び出し'.

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Non-Java構造作図ツールがますます便利に



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検索例

- 以下の官能基変換反応を実行

Carboxylate Ester → Aldehyde

- 以下の絞込みを行う
 - 構造式
 - VPA
 - 繰り返し構造

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