

HARNESSING THE POWER OF TWO INDUSTRY-LEADING CHEMISTRY TOOLS



Chemical Abstracts Service and PerkinElmer have teamed up to make your life easier —by combining the familiarity and ease of ChemDraw® with the world's most comprehensive chemistry database: SciFinder®.

SEARCH SCIFINDER FEATURE

ChemBioDraw® Ultra v.14 software now includes a Search SciFinder button, so you can draw a structure or reaction query using your favorite drawing tool and then instantly send the query to SciFinder. There's no need to cut and paste. Results are displayed immediately in SciFinder, where you can use its rich set of tools to search, filter, and analyze the information.*

SAVE TIME AND HASSLES

This feature is a huge time-saver and a welcome convenience for users. In recent product demonstrations, users were delighted with the ease of use, the faster process, and the built-in chemical intelligence in the way the searches work.

HOW IT WORKS

Let's work through an example. Say you're looking at a newly approved drug, pomalyst, and want to find its close analogs and pathways to synthesize it. You can submit these structure and reaction searches in SciFinder, right from within ChemBioDraw Ultra, with minimal editing. The chemical intelligence built into the Search SciFinder function makes getting answers fast and easy.

BUILT-IN CHEMICAL INTELLIGENCE

Start by drawing pomalyst (Figure 1). If you draw or select the pomalyst structure and then click the Search SciFinder button , the Search SciFinder dialog box selection defaults to the most frequently used Substance Search > Substructure (other search options are also available) (Figure 2). This search will retrieve answers that contain the substructure query as drawn, as well as its analogs.

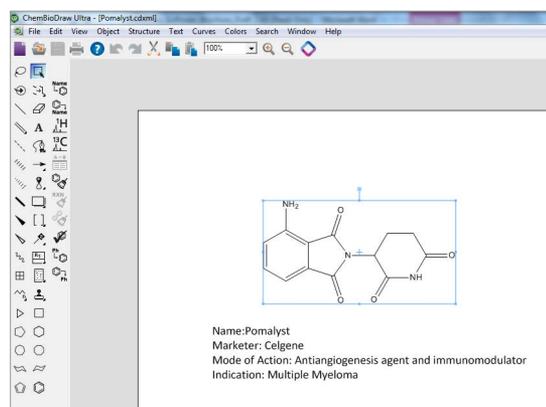


Figure 1 Pomalyst drawn in ChemBioDraw Ultra



Figure 2: Substance Substructure Search

PerkinElmer is collaborating with Chemical Abstracts Service to combine the power of two leading solutions: ChemBioDraw® and SciFinder®.



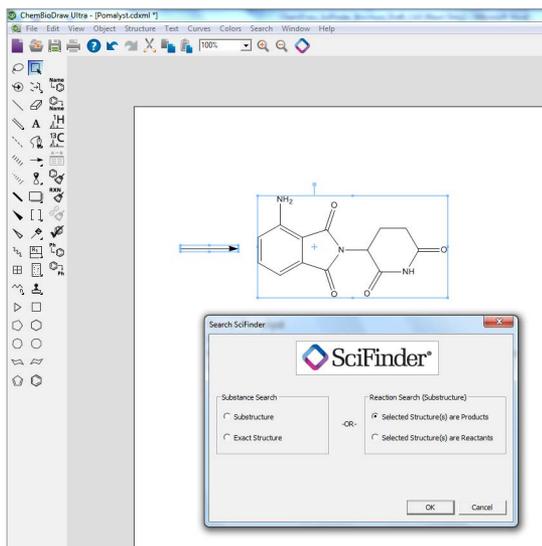


Figure 3 Reaction Search (Substructure): Selected Structure as Product

SPECIFYING POSSIBLE STRUCTURES

If you want to specify a possible structure for the starting material, you can draw a full reaction by copying and editing the pomalyst structure in ChemBioDraw software. When you click the Search SciFinder button , the built-in intelligence sets the Search SciFinder query type to Substructure Reaction Search (Figure 4).

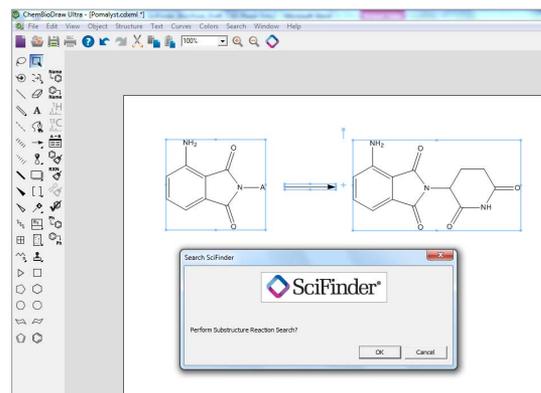


Figure 4 Substructure Reaction Search

A MUCH FASTER PROCESS

In all cases, the query and search parameters are sent directly to SciFinder from ChemBioDraw, with no time-consuming copying and pasting. And, as long as you're logged in to SciFinder, the search is run and the answer set is displayed in a new SciFinder window (Figure 5).

You can then use SciFinder's rich set of powerful tools to quickly explore the search results to pinpoint the best answer to your questions. As a result, you work faster, smarter, and more productively.

Analyze by:	Count
H ₂	4
HCl	4
Et ₃ N	2
HOCH ₂ CH ₂ NH ₂	2
Dimidazole ketone	1

Steps/Stages

- 1.1: S:MeCN, rt → 45°C
- 1.2: R:Dimidazole ketone, 4.5 h, reflux

Notes

alternative preparation shown, kilogram scale, Reactants: 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-dioxopiperidin-3-yl)indoline-1,3-dione compounds
 By Gu, Chuan-shen et al
 From U.S. Pat. Appl. Publ., 20070004620, 04 Jan 2007

Figure 5 SciFinder Search Results

*SciFinder® license required.

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