



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.

BUILT-IN CHEMICAL INTELLIGENCE

Both ChemDraw® Professional and ChemOffice Professional now include a Search SciFinder® button, enabling you to draw a structure or reaction query using your favorite drawing tool and then instantly send the query to SciFinder. With SciFinder built into ChemDraw, there's no need to open a separate browser window or bother with tedious steps of constant cutting and pasting. With a single click, you can access the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences. Results are displayed immediately in SciFinder, where you can use its rich set of tools to search, filter, and analyze the information.

HOW IT WORKS

Imagine you are looking at a newly approved drug, vilanterol, 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 ChemDraw, with minimal editing. The chemical intelligence built into the Search SciFinder function makes getting answers fast and easy.

Start by drawing vilanterol (Figure 1). If you draw or select the vilanterol structure and then click the Search SciFinder button [icon], 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.

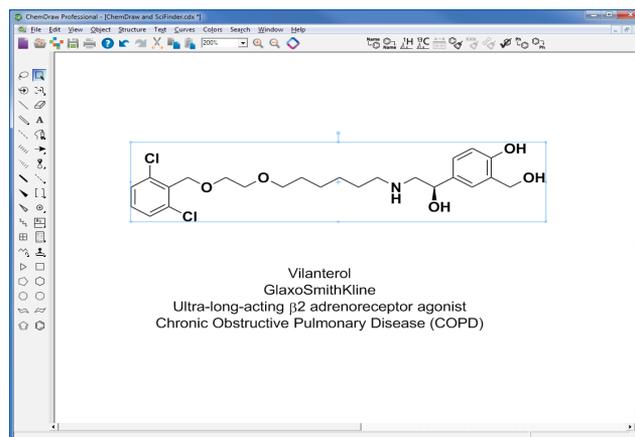


Figure 1: Vilanterol drawn in ChemDraw Professional.

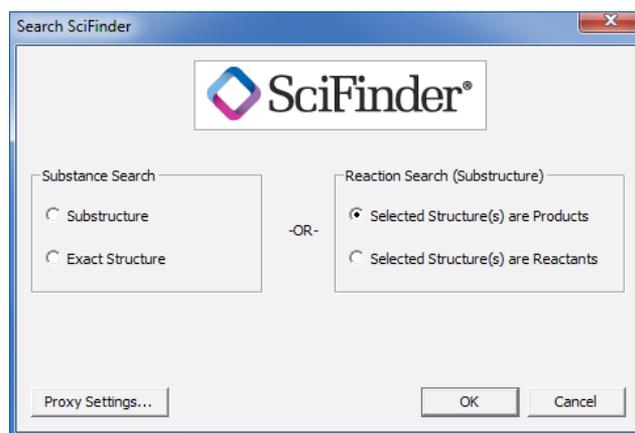


Figure 2: Substance Substructure Search.

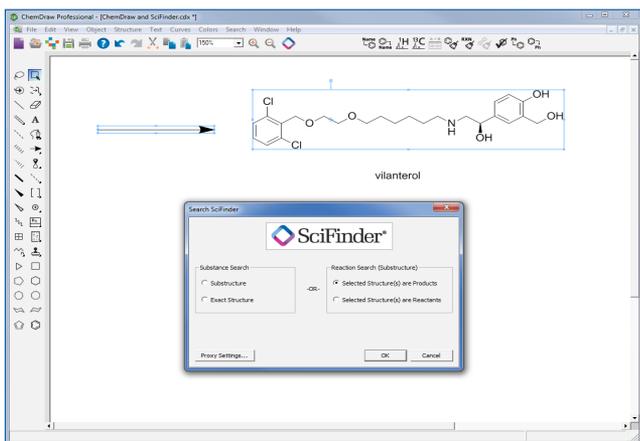


Figure 3: Reaction Search (Substructure): Selected Structure as Product.

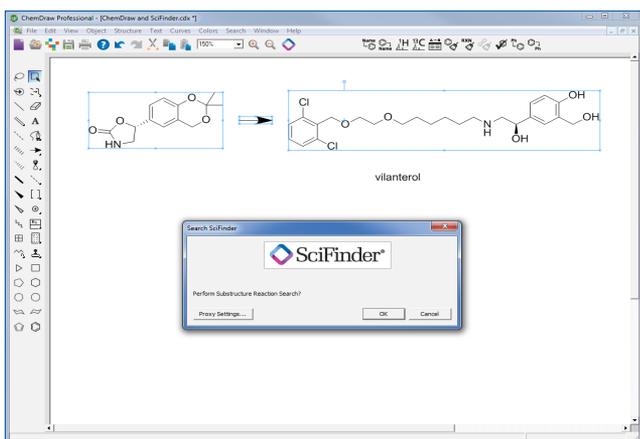


Figure 4: Substructure Reaction Search.

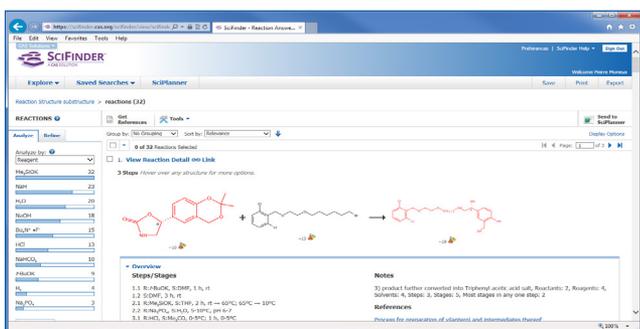


Figure 5: Results shown in SciFinder window from ChemDraw search.

EXPLORE SYNTHETIC PATHWAYS

If you want to explore synthetic pathways to vilanterol, you can draw a partial reaction query simply by adding a reaction arrow to the vilanterol structure in ChemDraw. When you click the Search SciFinder button [icon], the query type is automatically detected, and the Search SciFinder dialog box selection sets to "Reaction Search" (Substructure) > Selected Structure(s) are Products. (Figure 3).

SPECIFY 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 vilanterol structure in ChemDraw. When you click the Search SciFinder button [icon], the built-in intelligence sets the Search SciFinder query type to Substructure Reaction Search (Figure 4).

WORK SMARTER

In all cases, the query and search parameters are sent directly to SciFinder from ChemDraw, eliminating time-consuming steps of manually having to copy and paste. 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).

SciFinder's rich set of powerful tools enables you to quickly explore the search results to pinpoint the best answer to your questions. As a result, you'll be able to work faster, smarter, and more productively.