

Instructions for Searching the DTP Open Compound Collection by Exact Chemical Structure, Substructure or Similar Structure

The DTP Open Compound collection of ~250,000 structures can be searched by exact chemical structure or substructure using the resources at [NCBI PubChem](#). On the PubChem homepage click on Structure Search, then select the search mode (e.g. substructure). Once the search mode has been selected, open the Filters menu and select "DTP/NCI" as the Data Source. Enter the chemical structure by importing the appropriate file or launching and employing the PubChem drawing program. Once the desired structure has been entered click on the Search button. The search results should appear in an updated window.

In addition to chemical structures, the NSC number* can be obtained from this search. The NSC number can be used for additional searches within the DTP Data Search site or for ordering compounds from the [DTP Open Chemical Repository](#).

*NSC Number: Originally known as Cancer Chemotherapy National Service Center number, the NSC number is an identifying number assigned by DTP to an agent or product (e.g. small molecule or biological agent). Most structures have a unique NSC number but over the years a small percentage of structures or agents may have been assigned more than one NSC number. In the case of salts, different salt forms (e.g. HCl, HOAc) are designated with separate NSC numbers.