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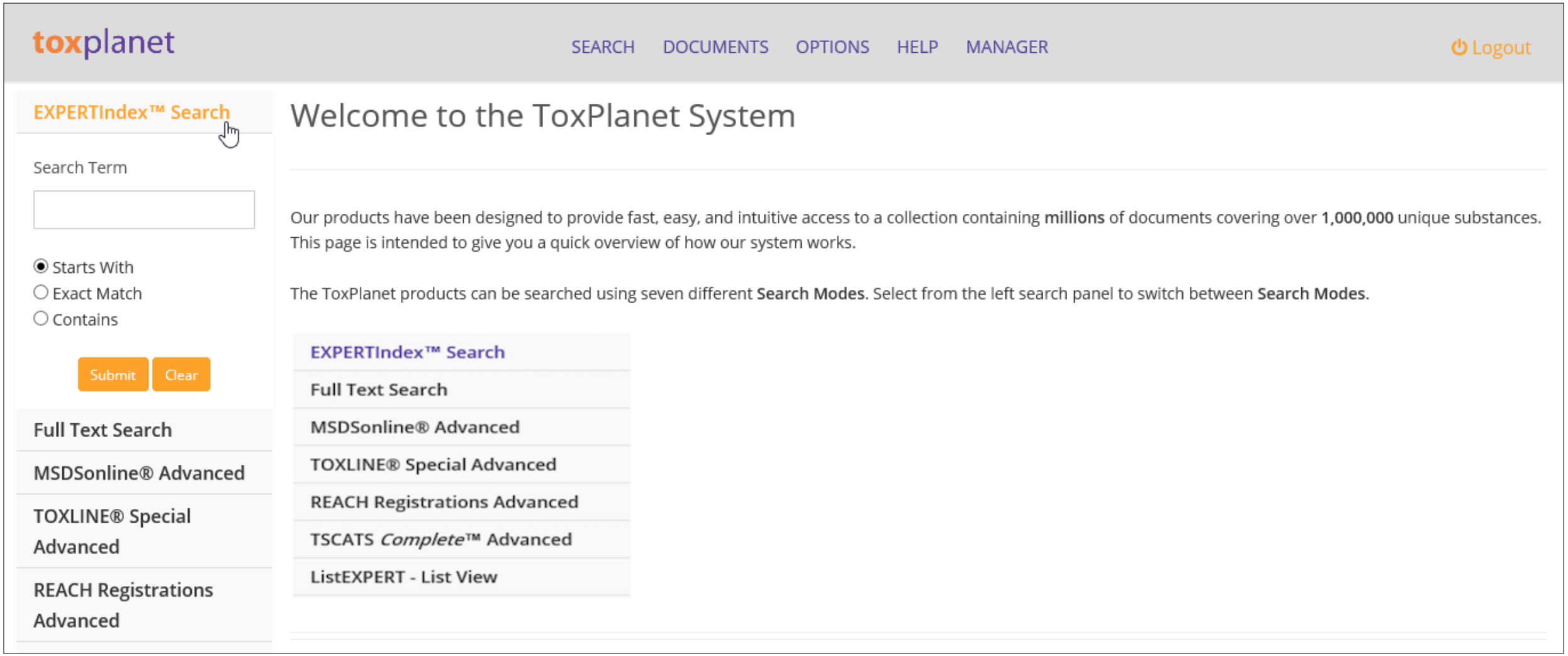
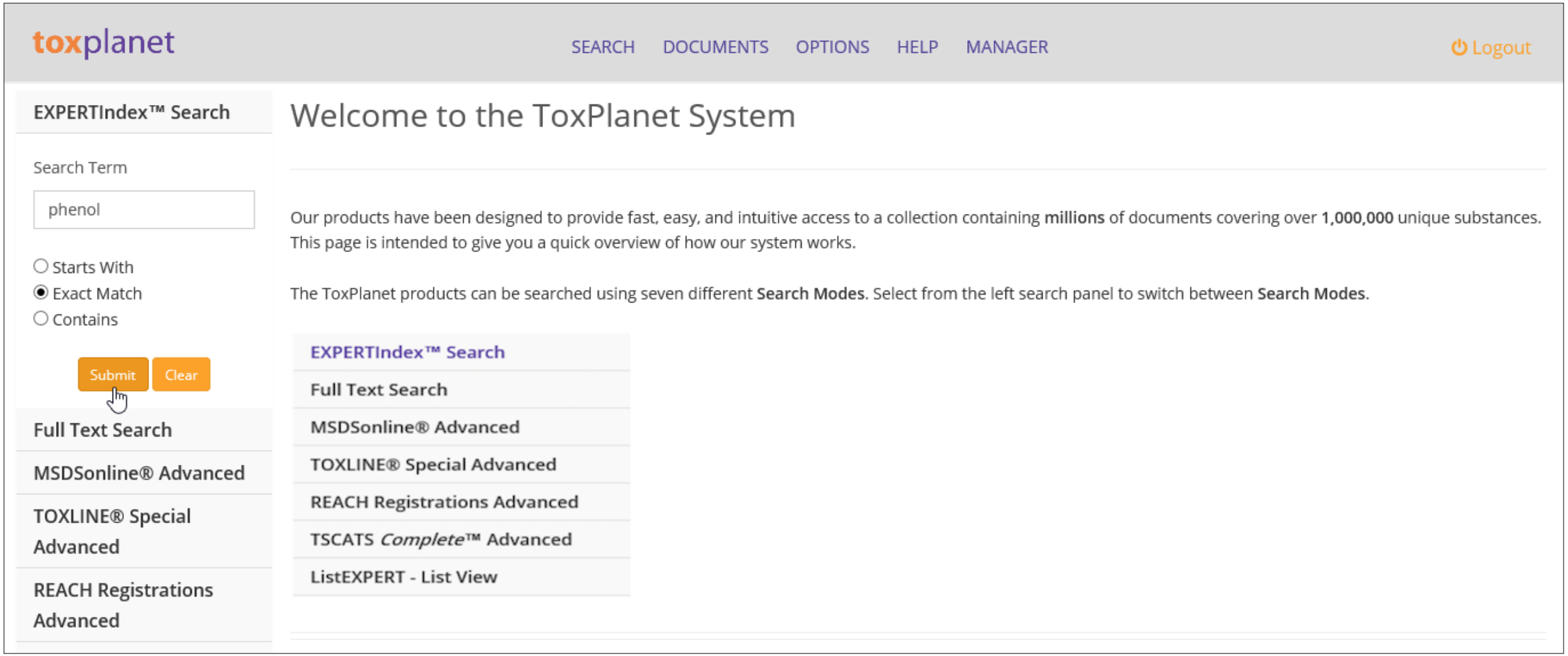
TUTORIAL

Similar Compounds Searching

Similar Compounds is a powerful tool that fully automates the process of searching for chemical analogs. Using ToxPlanet's proprietary functionality, it allows for instant identification of structurally similar compounds. In this tutorial, we will look at how to search using Similar Compounds.



To search using Similar Compounds, begin by conducting an EXPERTIndex search. Start by clicking the EXPERTIndex™ Search button on the left side of the screen. This brings up a search box and several searching options (Starts With, Exact Match, and Contains). The "Starts With" radio button is enabled as it is the default setting.



Enter the desired search term in the search box (for example, "*phenol*"), select a search option (for example, "Exact Match"), and click the Submit button to execute the search.

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SEARCH DOCUMENTS OPTIONS HELP MANAGER Logout

EXPERTIndex™ Search

Search Term

phenol

- ○ Starts With
- ◉ Exact Match
- ○ Contains

Submit Clear

Full Text Search

MSDSonline® Advanced

TOXLINE® Special Advanced

REACH Registrations Advanced

Chemical Identity | ChemEXPERT™ | ReproEXPERT™ | ListEXPERT™ | PoisonEXPERT™ | REACH Registrations

C & L Inventory | DrugEXPERT™ | TOXLINE® Special | ECIS | TSCATS *Complete*™ | MSDSonline® | Similar Compounds

MyEXPERT™

Chemical Identity Search Results

Name of Substance

Phenol [USP:JAN]

CAS Registry Number

108-95-2

Molecular Formula

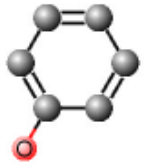
C6-H6-O

Other Registry Numbers

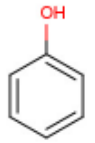
14534-23-7; 50356-25-7; 8002-07-1

SMILES

OC1=CC=CC=C1



Enlarge

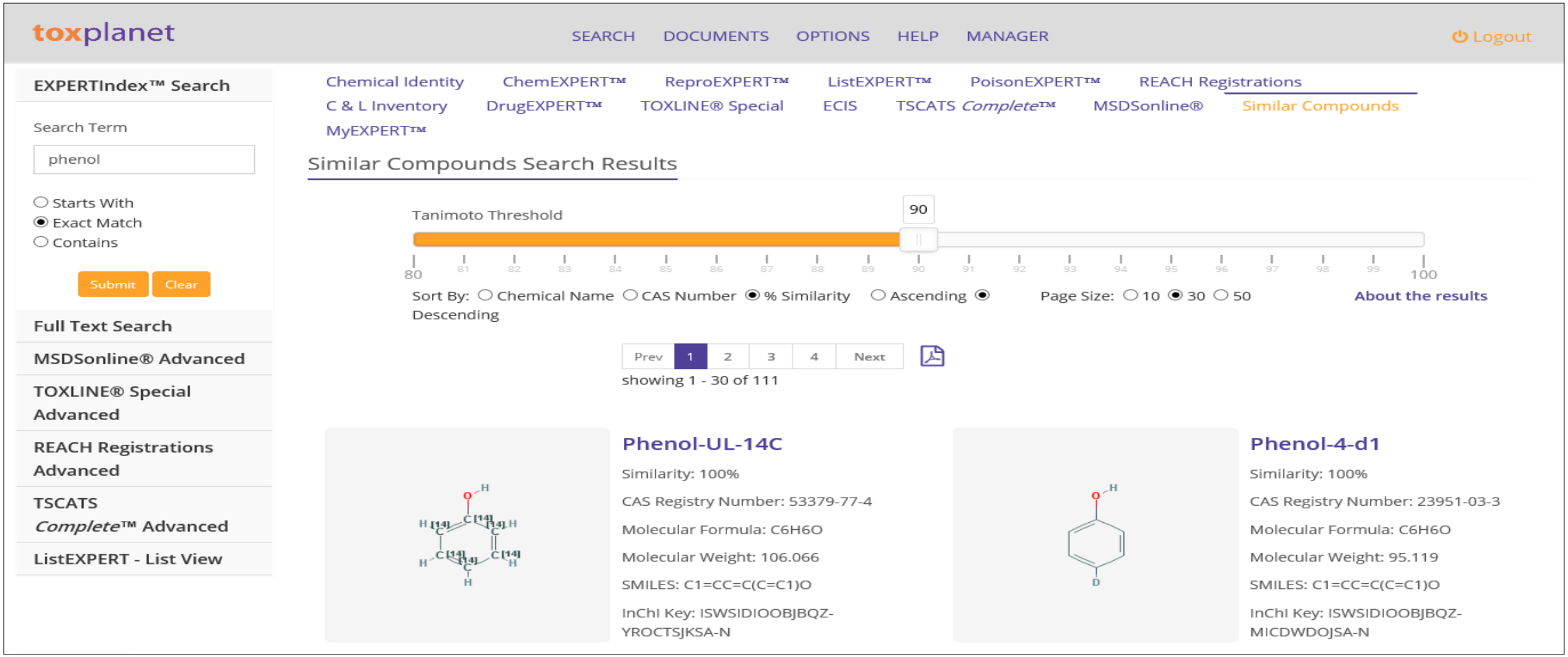


Enlarge

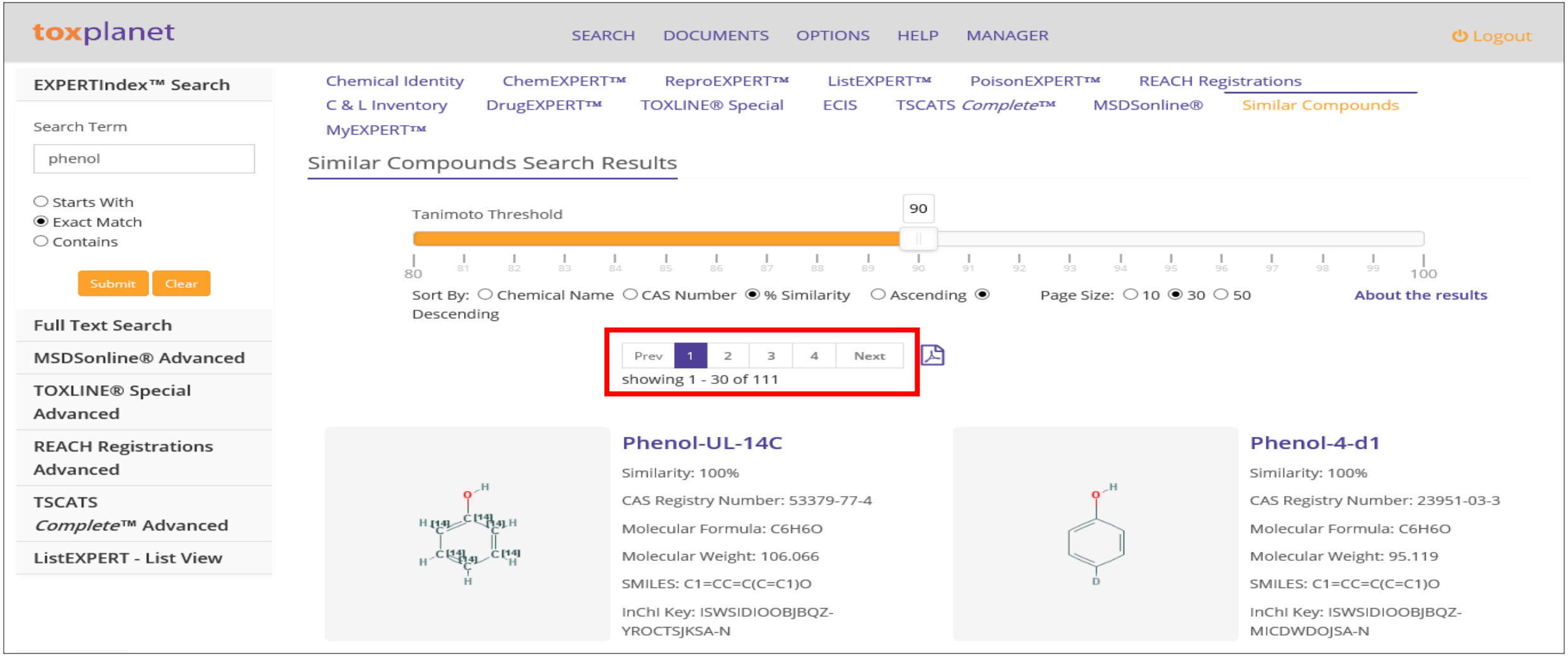
NFPA 704

View

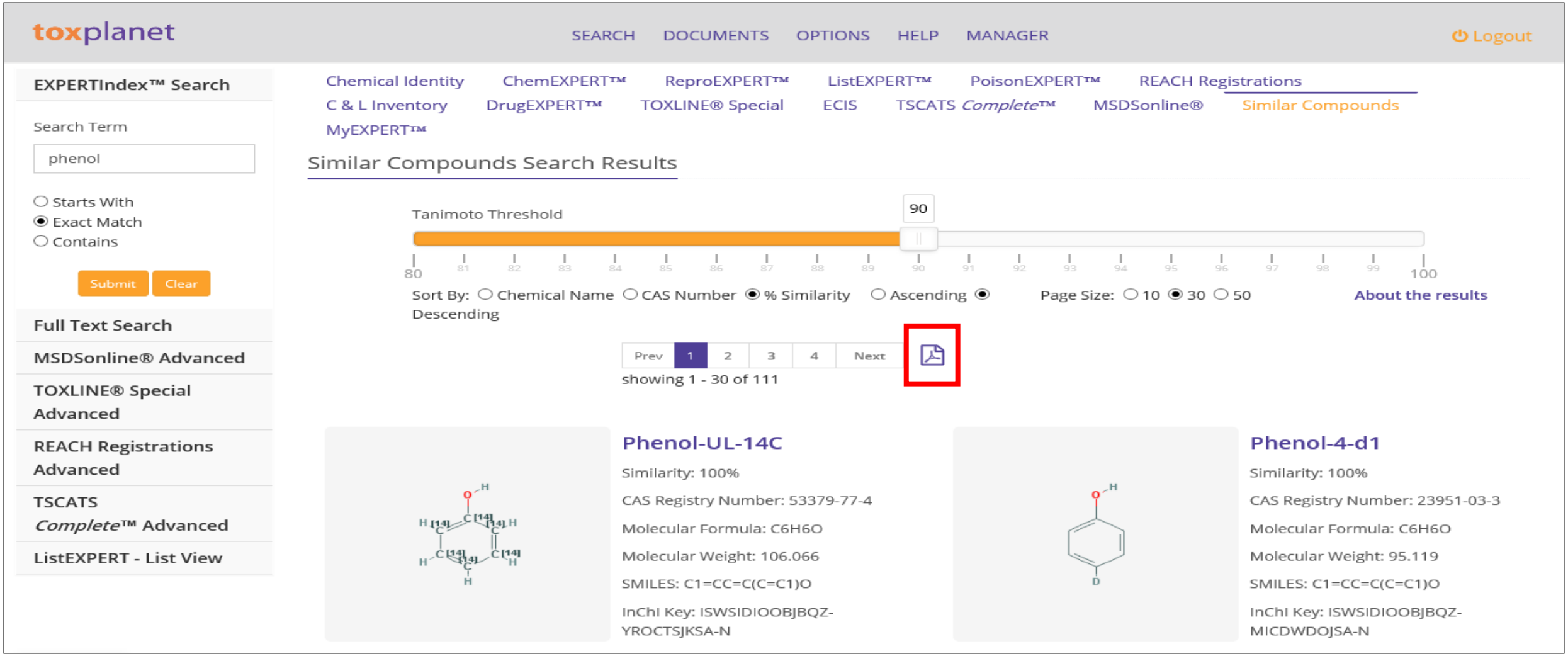
If there is an exact match in the EXPERTIndex, the system retrieves the Chemical Identity page for that substance.



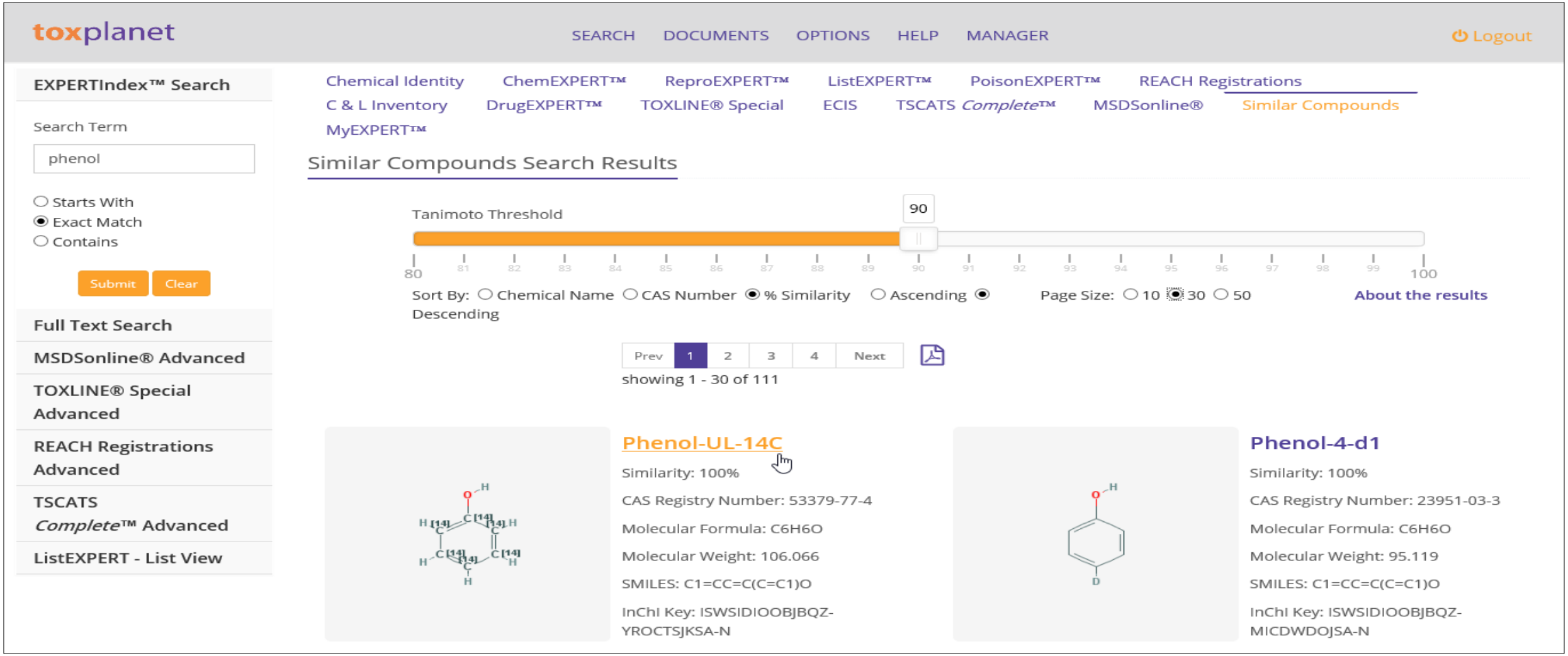
Clicking the Similar Compounds tab returns a list of chemical compounds similar to the compound in your initial search. This display also provides additional information, including Similarity %, CAS Registry Number, Molecular Formula, Molecular Weight, SMILES Notation, InChI Key, as well as the number of compounds in the results list.



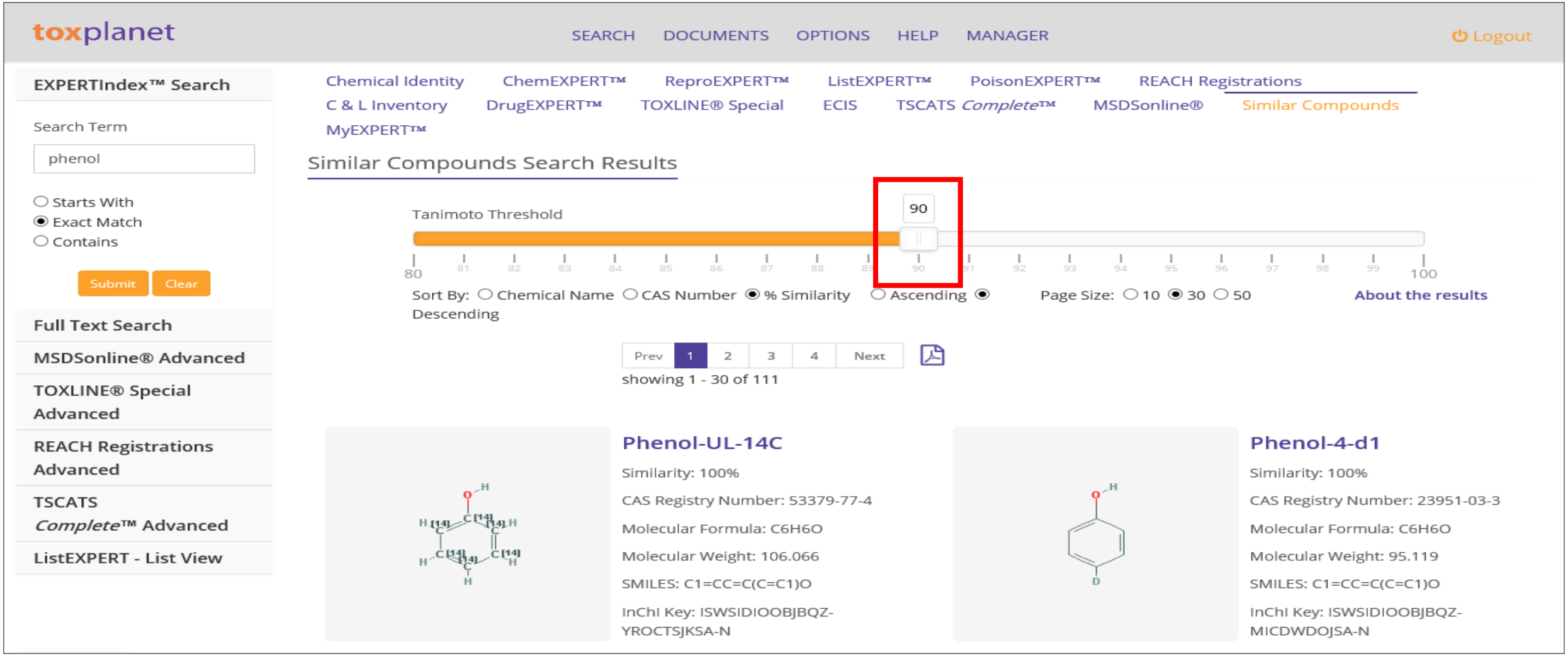
You can navigate the results pages using the page number buttons, or by clicking “Prev” or “Next".



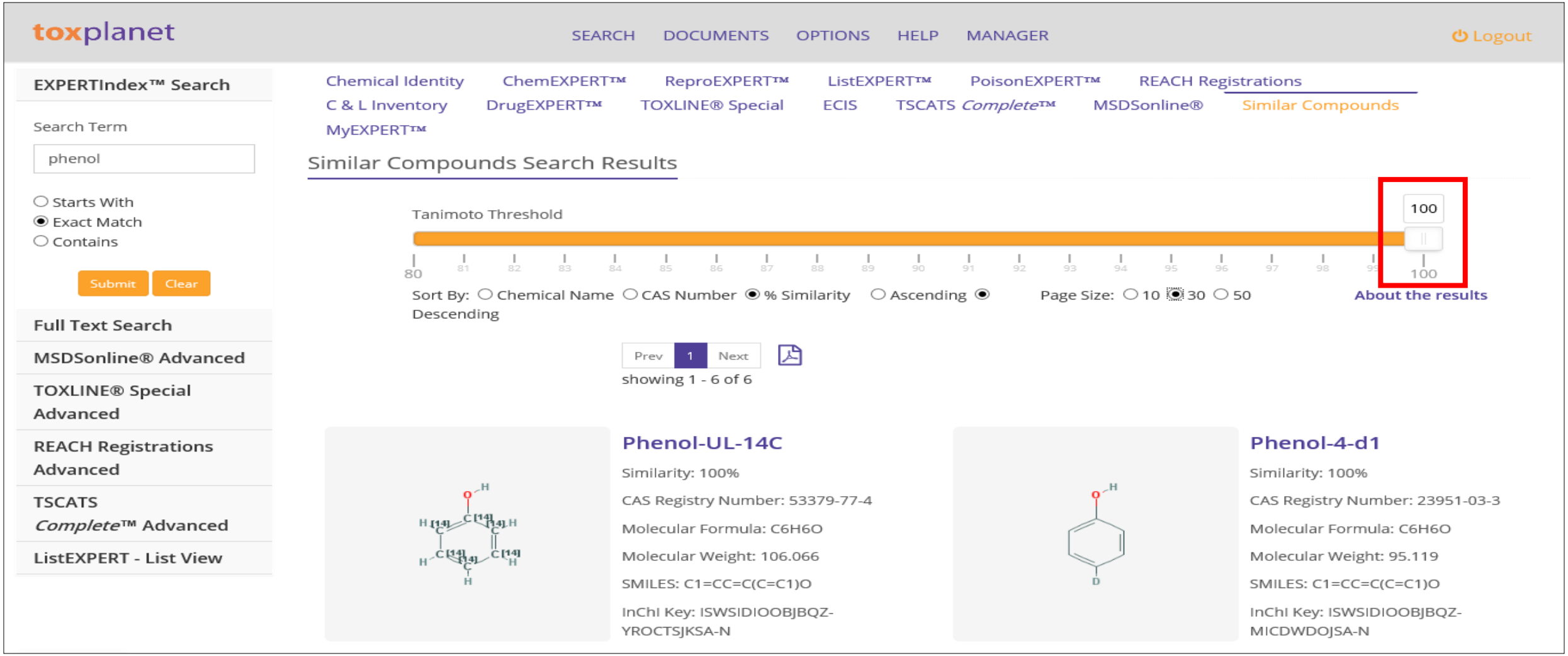
You can also print current page results by clicking the purple PDF icon.



By clicking on a compound in the results list, you will be able to view its Chemical Identity page (when available) and access all full-text documents available for that compound.



Similar Compounds utilizes the Tanimoto coefficient, which mathematically calculates the degree of similarity between structures. By default, the level of similarity in the results is set at 90% (meaning the results shown are those with 90% structural similarity or greater). The level of similarity (and, in turn, the number of results) can be adjusted using the slide bar. You can also adjust the sort order and page size for the results using the corresponding radio buttons.



Adjusting the threshold with the slide bar allows you to narrow or broaden your search requirements. In this example, changing the threshold from 90% to 100% displays only those compounds that are 100% similar to the chemical in the original search. There are fewer results (6 results at 100% vs. 111 results at 90%) due to increased specificity.

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For more information, visit our website

www.toxplanet.com