

## ❖ Property Search

My research is on natural products and I often need to create reports on the identification of substances from specific marine life (for example, sponges of the genus *Xestospongia*). How do I find the taxonomy and geographic location of the samples collected as well as the spectra and other data for the isolated substances?

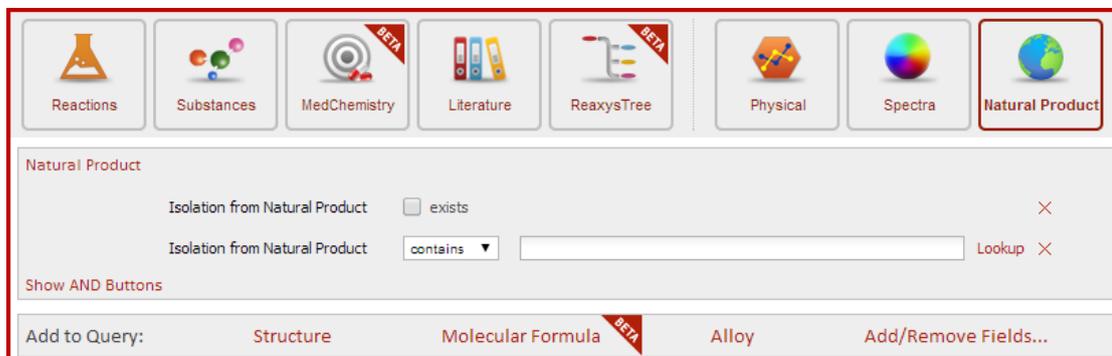
Strategy:

- Customize your search form to tailor it to your research needs.
- Search for *xestospongia* using the “Isolation from Natural Product” field.
- Filter your results.
- Select data for inclusion in a report.

## ❖ Customize the Query Page



Click the Natural Product theme button from the Start page. The Natural Product form is displayed.

A screenshot of the Reaxys search interface. At the top, there is a row of eight theme buttons: Reactions, Substances, MedChemistry (with a BETA badge), Literature, ReaxysTree (with a BETA badge), Physical, Spectra, and Natural Product (which is highlighted with a red border). Below this row is the "Natural Product" search form. It contains two search fields: "Isolation from Natural Product" with a checkbox labeled "exists" and a close button (X); and another "Isolation from Natural Product" field with a dropdown menu set to "contains", a text input box, and a "Lookup" button with a close button (X). Below the search fields is a "Show AND Buttons" link. At the bottom, there is a bar with "Add to Query:" followed by buttons for "Structure", "Molecular Formula" (with a BETA badge), "Alloy", and "Add/Remove Fields...".

Since this researcher will use the NP form most often, the query page can be customized to hide the other query themes.

Query Results Synthesis Plans History Report My Alerts **My Settings**

Click the Settings button.

Select **Modify Application Settings**. Then select **Query forms**. Uncheck the forms that you will use least. Scroll to the bottom of the page and click **Save**.

Use these options to disable queries you don't use, and place the most important ones first.

Visible

<input type="checkbox"/>	Reactions	
<input type="checkbox"/>	Substances	
<input type="checkbox"/>	MedChemistry	
<input checked="" type="checkbox"/>	Literature	
<input type="checkbox"/>	ReaxysTree	
<input type="checkbox"/>	Physical	
<input type="checkbox"/>	Spectra	
<input checked="" type="checkbox"/>	Natural Product	



Reset ↑

Back Save

## ❖ The Query

Select **Contains** from the dropdown menu. Click the **Lookup** link.

Isolation from Natural Product

contains ▼

is

starts with

ends with

contains

Lookup

Select index items and click 'Transfer'

Reaxys

Search for:

- xestophanesin (1)
- xestospongia (371)**
- xg (1)
- xg8d (3)
- xi (127)

Transfer

Look for xestospongia in the field index, select the term, and click the Transfer button. Click Search Substances.

Search Substances

## ❖ The Results

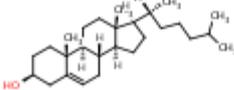
Spectroscopic Data

- NMR Spectroscopy 329
- IR Spectroscopy 232
- Mass Spectrometry 192
- UV/VIS Spectroscopy 178
- Fluorescence Spectroscopy 4
- Other Spectroscopic Methods 1
- Raman Spectroscopy 1

More

Limit to Exclude

Filter the results to display only the substances with NMR and UV data.

Structure	Structure/Compound Data
 <p>Synthesize   Hide Details</p>	<p><b>Chemical Name:</b> cholest-5-en-3β-ol</p> <p><b>Reaxys Registry Number:</b> 2060565  <b>CAS Registry Number:</b> 57-88-5  <b>Type of Substance:</b> isocyclic  <b>Molecular Formula:</b> C<sub>27</sub>H<sub>46</sub>O  <b>Linear Structure Formula:</b> HOC<sub>17</sub>H<sub>22</sub>(CH<sub>3</sub>)<sub>8</sub>  <b>Molecular Weight:</b> 386.662  <b>InChI Key:</b> HVYWMOMLDIMFJA-DPAQBDIFSA</p>
<p><b>Chemical Names and Synonyms</b> cholest-5-en-3β-ol, Δ<sup>5</sup>,3β-hydroxysterol, cholest-5-en-3β-ol, 5-cholesten</p> <p><b>Hit Data</b></p> <ul style="list-style-type: none"> <li><input checked="" type="checkbox"/> Isolation from Natural Product ( 3 Hits out of 164 view all )</li> <li><input type="checkbox"/> Bioactivity</li> <li><input type="checkbox"/> Identification</li> <li><input type="checkbox"/> Physical Data</li> <li><input checked="" type="checkbox"/> Spectra</li> <li><input type="checkbox"/> Ecological Data</li> <li><input type="checkbox"/> Use/Application</li> </ul>	

View the data:

**Taxonomy**

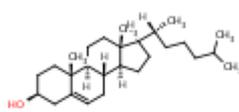
Isolation from Natural Product	Reference
<p><a href="#">Xestospongia testudinaria</a> (Petrosiidae), marine sponge; collected in coast of Sanya, north of South China Sea, Hainan, China</p>	<p><b>Lin, Xiuping; Liu, Yonghong; Yang, Bin; Yang, Xianwen; Zhou, Xuefeng; Lu, Yanan</b>            Chemistry and Physics of Lipids, <b>2011</b>, vol. 164, # 7 p. 703 - 706  <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a></p>

**Location**

## ❖ The Report

Select the individual data points that you want to add to your report by moving your mouse over the data until you see a red page curl and then selecting the appropriate option.

Structure



Synthesize | Hide Details

**Copy to Reaxys Report:**

- Structure only
- Structure and Header Data

▲ UV/VIS Spectroscopy (5)

Description	Solvent	Absorption Maxima	Ext./Abs. Coefficient	Reference
Absorption maxima	hexane	212 nm	1270 l·mol <sup>-1</sup> ·cm <sup>-1</sup>	<b>Akopova; Giricheva</b> Russian Journal of General Chemistry, <b>1997</b> , vol. 67, # 3 p. 470 - 473 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">citing articles</a>

Copy to Reaxys Report:

- This fact
- This fact and the structure
- This fact, the structure and header data

View the report:

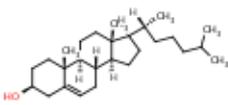


Click the Report button.

You can Save, Print, or Send the Report to colleagues from within Reaxys.

### Xestospongia Report

Report Item: **IDE-XRN: 2060565** Created: 2014-03-10 16:48 | Modified: 2014-03-10 16:48

Structure	Structure/Compound Data
  Synthesize	<b>Chemical Name :</b> cholest-5-en-3β-ol  <b>Reaxys Registry Number:</b> 2060565 <b>CAS Registry Number :</b> 57-88-5 <b>Type of Substance:</b> isocyclic <b>Molecular Formula :</b> C <sub>27</sub> H <sub>46</sub> O <b>Linear Structure Formula :</b> HOC <b>Molecular Weight :</b> 386.662 <b>InChI Key :</b> HVYWMOMLDMFJA-DF

#### Chemical Names and Synonyms

cholest-5-en-3β-ol, Δ<sup>5</sup>,3β-hydroxysterol, cholest-5-en-3β-ol, 5-cholesten-3β-ol, β-

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#### Isolation from Natural Product

Isolation from Natural Product	Reference
Xestospongia testudinaria (Petrosiidae), marine sponge; collected in coast of Sanya, north of South China Sea, Hainan, China	<b>Lin, Xiuping; Liu, Yonghong; Yang</b> Chemistry and Physics of Lipids, <b>2011</b> <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citation</a>

Report Item: **IDE-XRN: 2060565** Created: 2014-03-10 16:48 | Modified: 2014-03-10 16:48

#### NMR Spectroscopy

Description	Nucleus	Solvents	Frequency	Signals	Kind of signal	Reference
Chemical shifts	<sup>1</sup> H	chloroform-d <sub>1</sub>	300 MHz	7.38 - 7.45 ppm 7.26 - 7.31 ppm 7.08 - 7.13 ppm 5.44 ppm	m, 2H m, 1H m, 2H br d, 1H, J=5.1 Hz	<b>Kas</b> <b>Kuro</b> <b>Ohts</b> Tetra 2259 <a href="#">Title/Abstract</a> <a href="#">Show</a>

Report Item: **IDE-XRN: 2060565** Created: 2014-03-10 16:49 | Modified: 2014-03-10 16:49

#### UV/VIS Spectroscopy

Description	Solvent	Absorption Maxima	Ext./Abs. Coefficient	Reference
Absorption maxima	hexane	212 nm	1270 l·mol <sup>-1</sup> ·cm <sup>-1</sup>	<b>Akopo</b> Russian <a href="#">Title/Abstract</a>