

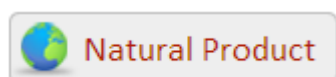
❖ Property Search

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?

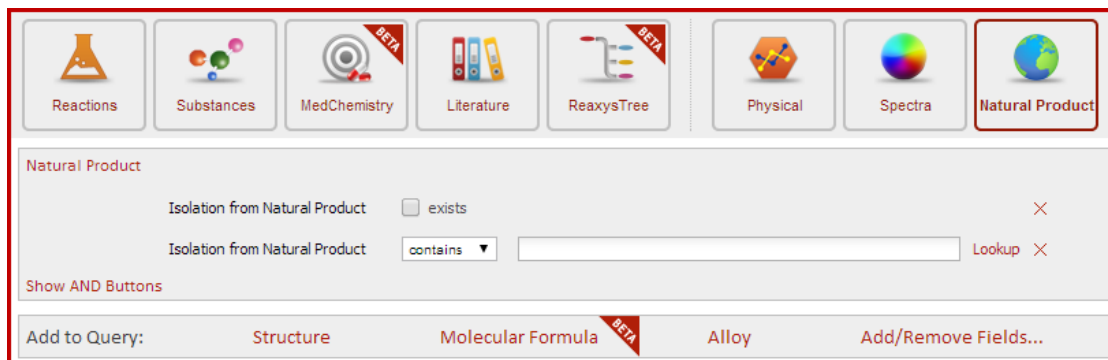
Strategy:

- 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.



The screenshot shows the REAXYS query interface. At the top, there is a row of theme buttons: Reactions, Substances, MedChemistry (marked BETA), Literature, ReaxysTree (marked BETA), Physical, Spectra, and Natural Product (which is highlighted with a red border). Below the themes, the 'Natural Product' form is displayed. It includes a search field with the text 'Isolation from Natural Product' and a dropdown menu set to 'contains'. There are also checkboxes for 'exists' and 'contains', and a 'Lookup' button. At the bottom, there is a section for 'Add to Query:' with buttons for 'Structure', 'Molecular Formula' (marked BETA), 'Alloy', and 'Add/Remove Fields...'. A 'Show AND Buttons' link is also visible.









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

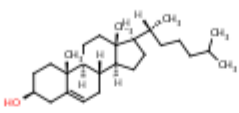
Spectroscopic Data

- ☒ 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>Chemical Name: cholest-5-en-3β-ol</p> <p>Reaxys Registry Number: 2060565 CAS Registry Number: 57-88-5 Type of Substance: isocyclic Molecular Formula: C₂₇H₄₆O Linear Structure Formula: HOC₁₇H₂₂(CH₃)₈ Molecular Weight: 386.662 InChI Key: HVYWMOMLDIMFJA-DPAQBDIFSA</p> |
| <p>Chemical Names and Synonyms cholest-5-en-3β-ol, Δ⁵,3β-hydroxysterol, cholest-5-en-3β-ol, 5-cholesten</p> <p>Hit Data Isolation from Natural Product (3 Hits out of 164 view all) Bioactivity Identification Physical Data Spectra Ecological Data Use/Application</p> | |

View the data:

Taxonomy

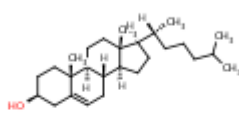
| Isolation from Natural Product | Reference |
|---|---|
| Xestospongia testudinaria (Petrosiidae), marine sponge; collected in coast of Sanya, north of South China Sea, Hainan, China | Lin, Xiuping; Liu, Yonghong; Yang, Bin; Yang, Xianwen; Zhou, Xuefeng; Lu, Yanan Chemistry and Physics of Lipids, 2011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





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

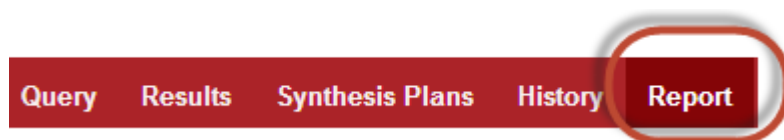
▲ UV/VIS Spectroscopy (5)

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

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.

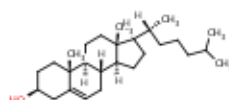
You can Save, Print, or Send the Report to colleagues from within Reaxys.

Xestospongia Report

Report Item: **IDE-XRN: 2060565**

Created: 2014-03-10 16:48 | Modified: 2014-03-10 16:48

Structure



Synthesize

Structure/Compound Data

Chemical Name :
cholest-5-en-3β-ol

Reaxys Registry Number: 2060565

CAS Registry Number : 57-88-5

Type of Substance: isocyclic

Molecular Formula : C₂₇H₄₆O

Linear Structure Formula : HOC

Molecular Weight : 386.662

InChI Key: HVYWMOMLDIMFJA-DP

Chemical Names and Synonyms

cholest-5-en-3β-ol, Δ⁵,3β-hydroxysterol, cholest-5-en-3β-ol, 5-cholesten-3β-ol, β-

Report Item: **IDE-XRN: 2060565**

Created: 2014-03-10 16:48 | Modified: 2014-03-10 16:48

Isolation from Natural Product

Isolation from Natural Product

Xestospongia testudinaria (Petrosiidae),
marine sponge; collected in coast of Sanya,
north of South China Sea, Hainan, China

Reference

Lin, Xiuping; Liu, Yonghong; Yang, Yong
Chemistry and Physics of Lipids, **2011**
[Title/Abstract](#) [Full Text](#) [View citation](#)

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 | ¹ H | chloroform-d ₁ | 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 | Kashimura, Kuroki, Ohtsuka, Tetrahedron, 2011, 67, 2259 Title/Abstract Full Text View citation |

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 ⁻¹ cm ⁻¹ | Akopyants, Russian Journal of Organic Chemistry, 2011, 48, 1270 Title/Abstract Full Text View citation |