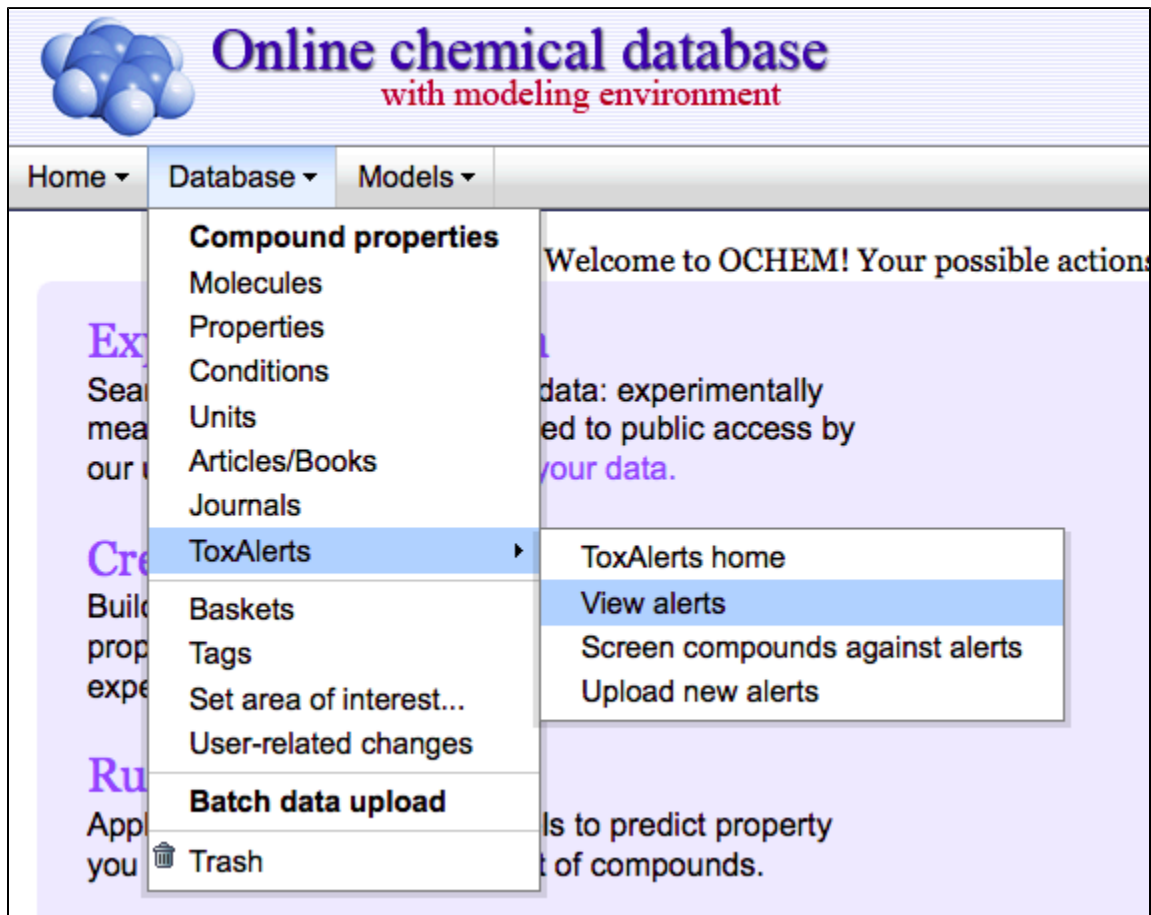


Browsing available alerts

The available alerts can be accessed from the alerts browser accessible via **Database > ToxAlerts > View alerts** menu item:



Similarly to other OCHEM browsers, the alerts browser displayed on the figure below has filters area (on the left) and the content area (on the right).

The filters include:

- filters by scientific publication
- filters by toxicological endpoint
- filters by name of an alert

The content area displays the alerts matching the current filters. For each alert, the following information is shown:

- Name of the alert
- Depiction of an alert (if available)
- SMARTS pattern
- Endpoint
- Scientific publication
- User who introduced this alert

Article:
1988 Ashby

Endpoint:
All endpoints

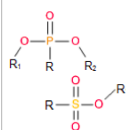
Name:

☐ Show only approved alerts [Upload new alerts](#)

 Screen compounds

 Awaiting approval

1 - 17 of 17



Alkyl esters of phosphonic or sulphonic acids

R = aliphatic carbon or any aromatic atom; R1 = aliphatic carbon; R2 = H, aliphatic carbon

SMARTS: [S]([CX4,a][Sv6X4])(=[OX1])(=[OX1])[OX2][CX4),[S]([CX4,a][Pv5X4])(=[OX1])([OX2][#1,CX4])[OX2][CX4)]

Endpoint: Genotoxic carcinogenicity, mutagenicity

Ashby, J
Chemical structure, Salmonella mutagenicity and extent of ca...
Mutat. Res. 1988; 204 (1) 17-115

16:52, 20 Feb 12 / 11:46, 6 Dec 12
midnighter ✉ / SALMINA1987 ✉



Aromatic nitro groups

Ar = any aromatic/heteroaromatic ring; chemicals with ortho-disubstitution, or with an ortho carboxylic acid substituent to the nitrogen substituent are excluded

SMARTS: [a!r0]\$(([NX3+](=[OX1])[O-]),\$([NX3](=[OX1])=[OX1]);!\$([NX3]a(a-[!#1])a-[!#1]);!\$([NX3]aa-C(=[OX1])[OH]))

Endpoint: Genotoxic carcinogenicity, mutagenicity

Ashby, J
Chemical structure, Salmonella mutagenicity and extent of ca...
Mutat. Res. **1988**; 204 (1) 17-115

16:52, 20 Feb 12 / 18:54, 19 Apr 12
midnighter ✉ / SALMINA1987 ✉



Aromatic azo groups

Ar = any aromatic/heteroaromatic atom; chemicals with sulfonic acid group at both ring systems connected to the aromatic azo group are excluded

SMARTS: [\$([NX2]([a!r0])=[NX2][a!r0]);!\$([NX2](aaS(=O)(=O)[OH])=[NX2]aaS(=O)(=O)[OH]);!\$ [show full SMARTS](#)

Endpoint: Genotoxic carcinogenicity, mutagenicity

Ashby, J

Chemical structure, Salmonella m
Mutat. Res. 1988; 204 (1) 17-115

16:52, 20 Feb 12
midnighter ✉