



Chemaxon eUGM 2012

Budapest, May 2012

Ahmed Abdelaziz

About eADMET

- Established 2010, based in Munich, Germany
- Offer Online QSPR modeling platform (www.ochem.eu)
- AlogPS 3.0, DMSO, AMES CYP450 inhibition models
- Consulting services for QSAR, ADMET screening and early drug discovery



About OCHEM

- Web based solution with team management capabilities
- Integrates 3rd party descriptor packages: Chemaxon calculators, Dragon, ADRIANA.Code, ISIDA, and many others
- Integrates many machine learning algorithms: ANN, MLR, SVM, KNN, decision trees, and many others
- Available **free** online for academic use

ToxAlerts

 Structure alert browser
Here you can browse substructure alerts for various toxicological endpoints

FILTERS

Article:
All articles

Endpoint:
Skin sensitization

Name:

 Upload new alerts

 Screen compounds



1 - 100 of 161

100 items on page 1 of 2 >>



Acid halides

R = any atom/ group; X = F, Cl, Br

SMARTS: [CX3](=[OX1])[F,Cl,Br]

Endpoint: Skin sensitization

Barratt, MD

An expert system rulebase for identifying contact allergens...

Toxicol In Vitro 1994; 8 (5) 1053-60

16:52, 20 Feb 12 / 14:21, 14 Mar 12
midnighter 83 / SALMINA1987 83



Acid azides

R = any atom/ group

SMARTS: [CX3](=[OX1])\$([NX2]=[NX2+]=[NX1-]),\$(N=[NX2+]=N),\$([NX2-][NX2+]=[NX1])

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midnighter 83 / SALMINA1987 83



Sulphonyl halides

R = alkyl, aryl; X = Cl, Br

SMARTS: [CX4,alr0][Sv6X4](=[OX1])(=[OX1])[Cl,Br]

Endpoint: Skin sensitization

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Acid anhydrides

Filter Alerts

FILTERS

Article:

Endpoint:

Name:

- Article:
-
- All articles
 - 1988 Ashby
 - 1990 Hermens
 - 1992 Verhaar, H.J.M.
 - 1994 Payne
 - 1994 Barratt**
 - 2004 Gerner
 - 2005 Kazius
 - 2005 CheckMol
 - 2005 Kalgutkar
 - 2005 Bailey
 - 2008 Enoch
 - 2008 Benigni
 - 2011 Maybridge
 - 2011 Enamine
 - 2011 "Ontario"_filters
 - 2011 ChemDiv
 - 2011 Life_Chemicals
 - 2011 Enoch
 - 2012 Tetko, I.V.

- Endpoint:
-
- All endpoints
 - Acute Aquatic Toxicity -- to delete
 - Skin sensitization**
 - Non-genotoxic carcinogenicity
 - Genotoxic carcinogenicity, mutagenicity
 - Reactive, unstable, toxic
 - Potential electrophilic agents
 - Idiosyncratic toxicity (RM formation)
 - Custom filters
 - Functional groups

ToxAlerts

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[Upload new alerts](#)



[Screen compounds](#)



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All articles

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R = any atom/ group

SMARTS: [Sv6X4](=[OX1])(=[OX1])\$([CX4][NX2]=[NX2+]=[NX1-]),\$([CX4][NX2]=[NX2+]=N)

Endpoint: Skin sensitization

Barratt, MD

An expert system rulebase for identifying contact allergens...

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16:52, 20 Feb 12 / 18:35, 19 Apr 12
midnighter 83 / SALMINA1987 83

Acid anhydrides

Screen Compounds



Structure alert screening

Provide the compounds to screen against the substructure alerts

Choose a previously prepared set: [\[...\]](#)

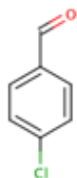
Select molecules by a tag: [\[...\]](#)

Upload compounds from a file
(SDF/MOL2/SMILES/Excel sheet)

Provide a Name/CAS-RN/SMILES

Draw Molecule

(click on depiction to the right to draw)




Select the alert set

Publication

Endpoint

Only **161** selected alerts

Screen Compounds

 Structure alert screening results

ENDPOINTS	
<input type="radio"/> Reactive, unstable, toxic	3697 compounds

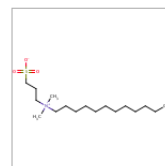
PUBLICATIONS	
<input type="radio"/> 2011 ChemDiv	1407 compounds
<input type="radio"/> 2011 Life_Chemicals	2735 compounds
<input type="radio"/> 2011 Enamine	2325 compounds

DETECTED ALERTS		
<input type="radio"/> Ammonium salts	2011 ChemDiv	86 compounds
<input type="radio"/> Sulphonic acids/esters	2011 Life_Chemicals	132 compounds
<input type="radio"/> Alkyl chains	2011 Life_Chemicals	288 compounds
<input type="radio"/> Aliphatic chain	2011 Enamine	188 compounds
<input type="radio"/> Activated halides (γ-halogen substituted N-heterocycles)	2011 Life_Chemicals	90 compounds
<input type="radio"/> o-Substituted phenols (2)	2011 Enamine	7 compounds
<input type="radio"/> Alkylhalides	2011 Life_Chemicals	82 compounds
<input type="radio"/> Alkyl halides	2011 Enamine	85 compounds
<input type="radio"/> Acyclic gem-dihalosubstituted carbon atom	2011 Life_Chemicals	20 compounds
<input type="radio"/> Halomethyl ethers	2011 ChemDiv	23 compounds
<input type="radio"/> Polyfluorinated compounds	2011 Enamine	10 compounds
<input type="radio"/> Carboxylic acid esters	2011 Enamine	317 compounds
<input type="radio"/> Aldimines and ketimines	2011 ChemDiv	159 compounds
<input type="radio"/> N-nitroso	2011 ChemDiv	4 compounds
<input type="radio"/> β-Haloamines	2011 ChemDiv	20 compounds
<input type="radio"/> N-N Single bond not in a ring	2011 Life_Chemicals	54 compounds
<input type="radio"/> Nitroso	2011 Life_Chemicals	14 compounds
<input type="radio"/> Singel acyclic N-N bonds	2011 Enamine	75 compounds

View records for the filtered compounds  Tag the 3697 filtered molecules

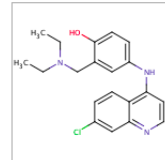
1 - 15 of 3697

15 items on page 1 of 247 > >>



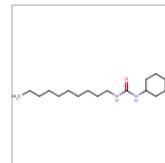
Ammonium salts (for Reactive, unstable, toxic in 2011 ChemDiv)
Sulphonic acids/esters (for Reactive, unstable, toxic in 2011 Life_Chemicals)
Alkyl chains (for Reactive, unstable, toxic in 2011 Life_Chemicals)
Aliphatic chain (for Reactive, unstable, toxic in 2011 Enamine)

MoleculeID: M4837



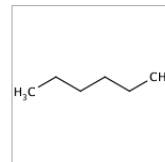
Activated halides (γ-halogen substituted N-heterocycles) (for Reactive, unstable, toxic in 2011 Life_Chemicals)
o-Substituted phenols (2) (for Reactive, unstable, toxic in 2011 Enamine)

MoleculeID: M8286



Alkyl chains (for Reactive, unstable, toxic in 2011 Life_Chemicals)
Aliphatic chain (for Reactive, unstable, toxic in 2011 Enamine)


MoleculeID: M6380



Aliphatic chain (for Reactive, unstable, toxic in 2011 Enamine)

MoleculeID: M11783

Upload alerts

 Structure alert upload

Alerts upload is under development!

Here you can upload substructure alerts from an Excel file.

Obligatory columns: SMARTS, ARTICLEID, PROPERTY, NAME.

Optional columns: DESCRIPTION, SMARTS_DESCRIPTION, COMMENT. You can provide additional consa-screen.xsltditions for each alert.

Please, select an Excel file:

Browse...

Submit

Want to know more?

How to handle a model with 250,000 compounds?

Secure computing and model sharing

Docking based approaches

www.ochem.eu



Thank you

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