

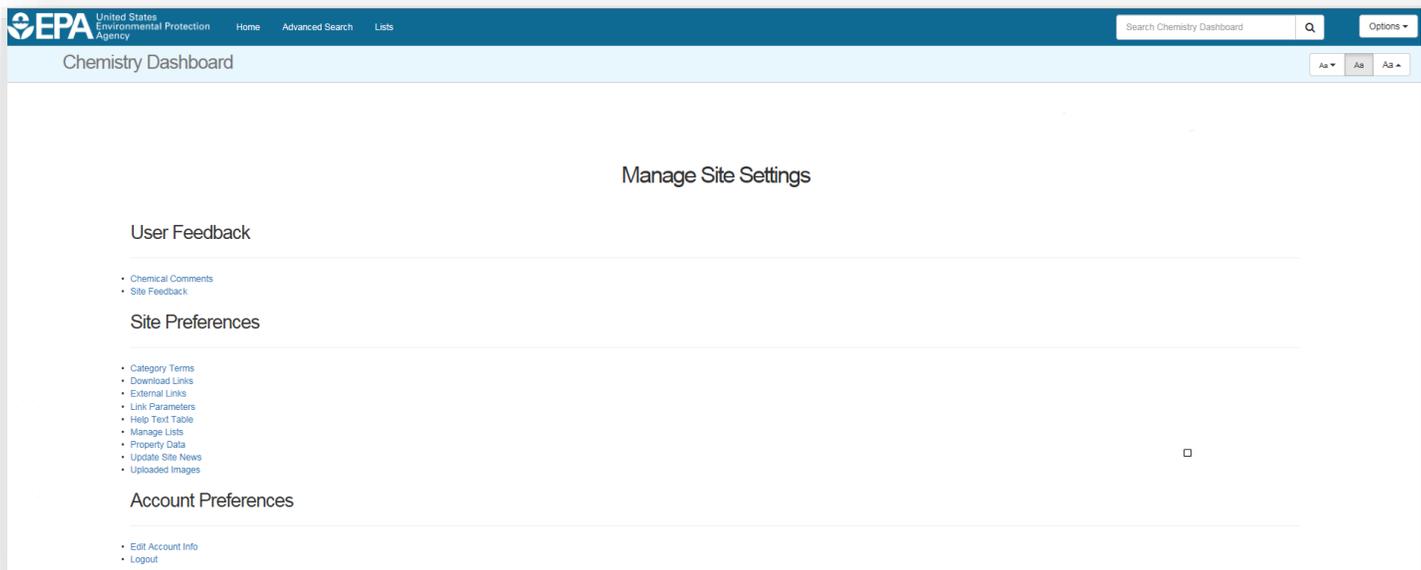
CompTox Chemistry Administration Dashboard

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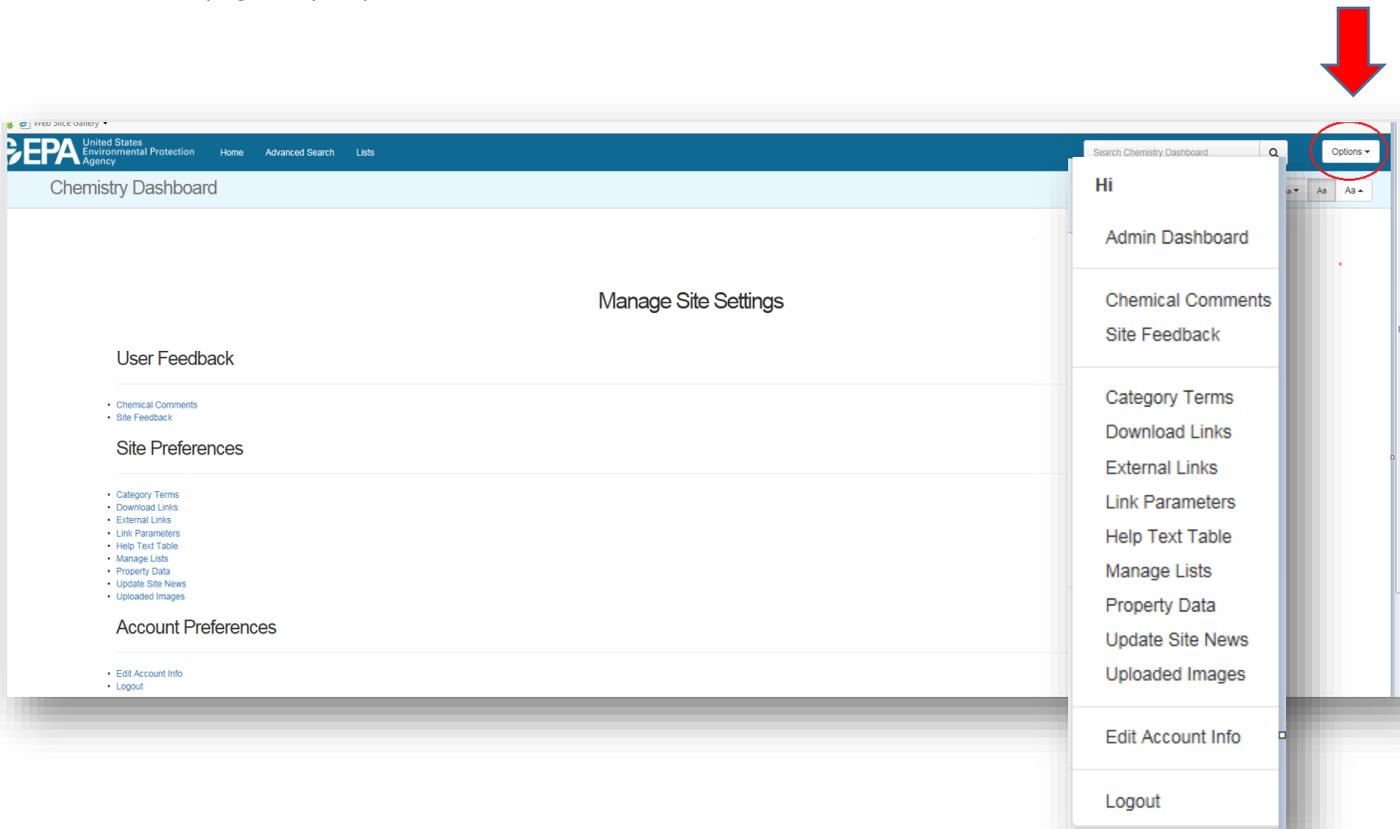
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Administration Home Page:

This is the Comptox Chemistry Dashboard administration “Home” page. This page provides links to all the available administrative tasks.



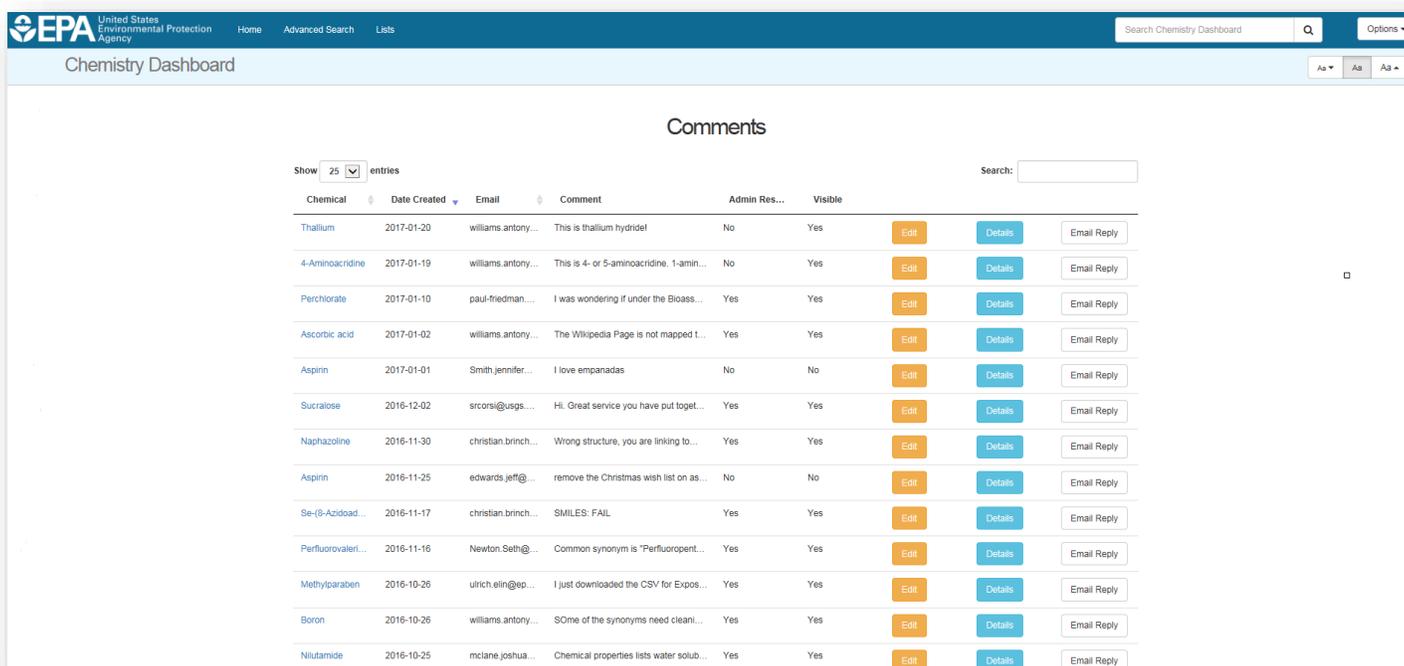
At any time in any page an administrator can select the “Options” drop down button in the upper right hand corner. (see red circle below) This provides options to return to this administration home page or allow a user to select any administration task page they require.



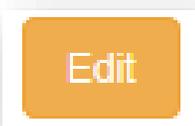
User Feedback:

Chemical Comments:

The chemical comments page is a report like page that shows a user entry for a suggested chemical that needs moderation. It shows the chemical in question, date the entry was created, email address of the user, the user comment, if an administrator has responded (Yes or No), and if the comment is visible (Yes or No). There is a search text box in the upper right corner, above the email reply button, that will allow an administrator to search on specific words. The chemical (highlighted in blue) can be selected and it will take the administrator directly to the chemical in question in the Comptox dashboard, in another browser tab. The show entries in the upper left hand side can be change to display either 25, 50, 75, or 100 entries on a page. The bottom right hand corner will show the number of pages and allows an administrator to go to the next page or skip to a desired page. There are also buttons that allow for additional functions.



Chemical	Date Created	Email	Comment	Admin Res...	Visible			
Thallium	2017-01-20	williams.antony...	This is thallium hydridel	No	Yes	Edit	Details	Email Reply
4-Aminoacridine	2017-01-19	williams.antony...	This is 4- or 5-aminoacridine. 1-amin...	No	Yes	Edit	Details	Email Reply
Perchlorate	2017-01-10	paul.friedman...	I was wondering if under the Bloass...	Yes	Yes	Edit	Details	Email Reply
Ascorbic acid	2017-01-02	williams.antony...	The Wikipedia Page is not mapped t...	Yes	Yes	Edit	Details	Email Reply
Aspirin	2017-01-01	Smith.jennifer...	I love empanadas	No	No	Edit	Details	Email Reply
Sucralose	2016-12-02	srcorsi@usgs...	Hi. Great service you have put toget...	Yes	Yes	Edit	Details	Email Reply
Naphazoline	2016-11-30	christian.brinch...	Wrong structure, you are linking to...	Yes	Yes	Edit	Details	Email Reply
Aspirin	2016-11-25	edwards.jeff@...	remove the Christmas wish list on as...	No	No	Edit	Details	Email Reply
Se-(8-Azidoa...	2016-11-17	christian.brinch...	SMILES: FAIL	Yes	Yes	Edit	Details	Email Reply
Perfluorvalent...	2016-11-16	Newton.Seth@...	Common synonym is "Perfluoropent...	Yes	Yes	Edit	Details	Email Reply
Methylparaben	2016-10-26	ulrich.elin@ep...	I just downloaded the CSV for Expos...	Yes	Yes	Edit	Details	Email Reply
Boron	2016-10-26	williams.antony...	SOME of the synonyms need cleani...	Yes	Yes	Edit	Details	Email Reply
Nitramide	2016-10-25	mciane.joshua...	Chemical properties lists water solub...	Yes	Yes	Edit	Details	Email Reply



Edit

The edit button displays a page that allows an administrator to reply to the users comment.

The visible check box allows for the response to be visible on the page to other users. The back button will return to the Comments home page. The Update Comment will post any response to the web page.

Reply to User Comment

User comment

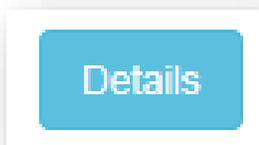
This is thallium hydride!

Response

Type your feedback here...

Visible

Back Update Comment



The details button shows a page that displays all the specific detailed information for this comment.

Comment Details

Comment For: Thallium (CID: 24830)

Comment Date: 2017-01-20

User Email:

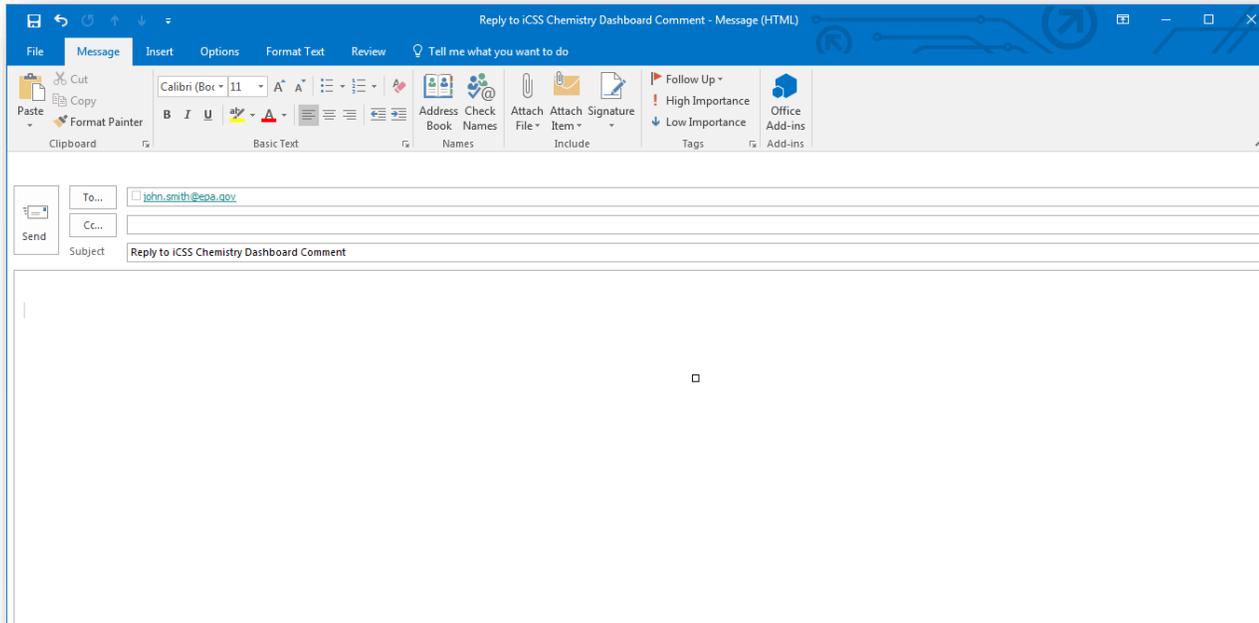
User Comment: This is thallium hydride!

Admin Reply: No one has replied to this comment yet.

Back

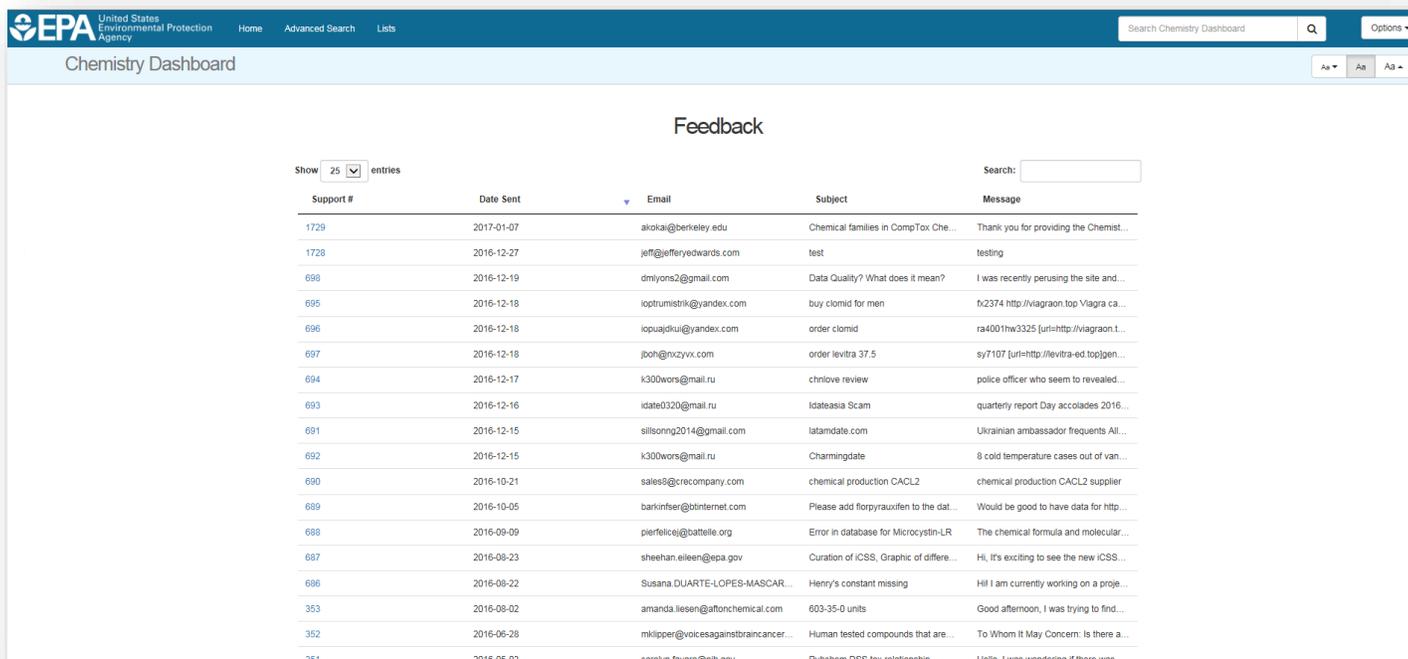
Email Reply

The email reply button will automatically launch outlook email message. The “To” will automatically be populated with the user’s email address and the subject line will automatically be populated “Reply to iCSS Chemistry Dashboard Comment”.



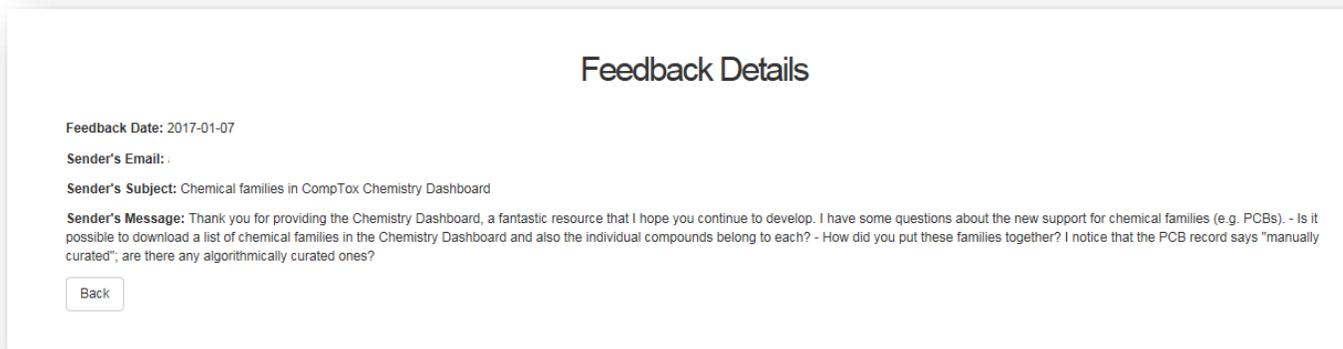
Site Feedback:

The site feedback page is a report listing of customer feedback to the CompTox Dashboard. This page shows Support #, date sent, email address, subject line and message. The Support number is a hyperlink (highlighted in blue) in which an administrator can click to get additional details on a specific message. There is a Feedback search text box in the upper right corner above the message column that will allow an administrator to search on specific words.



Support #	Date Sent	Email	Subject	Message
1729	2017-01-07	akoka@berkeley.edu	Chemical families in CompTox Che...	Thank you for providing the Chemist...
1728	2016-12-27	jeff@jeffreyedwards.com	test	testing
698	2016-12-19	dmyons2@gmail.com	Data Quality? What does it mean?	I was recently perusing the site and...
695	2016-12-18	ioptumstrik@yandex.com	buy clomid for men	fc2374 http://viagraon.top Viagra ca...
696	2016-12-18	iopujdkui@yandex.com	order clomid	ra4001hw3325 [url=http://viagraon.t...
697	2016-12-18	jboh@mszyv.com	order levitra 37.5	sy7107 [url=http://levitra-ed.top]gen...
694	2016-12-17	k300vors@mail.ru	chnlove review	police officer who seem to revealed...
693	2016-12-16	idate0320@mail.ru	ldateasia Scam	quarterly report Day accolades 2016...
691	2016-12-15	sillsong2014@gmail.com	latamdate.com	Ukrainian ambassador frequents All...
692	2016-12-15	k300vors@mail.ru	Charmingdate	8 cold temperature cases out of van...
690	2016-10-21	sales@crecompany.com	chemical production CAQL2	chemical production CAQL2 supplier
689	2016-10-05	barkinfser@btinternet.com	Please add forpyrauxifen to the dat...	Would be good to have data for http...
688	2016-09-09	perfelice@battelle.org	Error in database for Microcystin-LR	The chemical formula and molecular...
687	2016-08-23	sheehan.eileen@epa.gov	Curation of ICSS, Graphic of differe...	Hi, It's exciting to see the new ICSS...
686	2016-08-22	Susana DUARTE-LOPES-MASCAR...	Henry's constant missing	Hi! I am currently working on a proje...
353	2016-08-02	amanda.lesen@afonchemical.com	603-35-0 units	Good afternoon, I was trying to find...
352	2016-06-28	mkipper@voicesagainbraincancer...	Human tested compounds that are...	To Whom It May Concern: Is there a...
351	2016-05-03	carolyn.favaro@nih.gov	Pubchem DSS tox relationship	Hello. I was wonderino if there was...

Feedback Details: The feedback details page displays feedback date, sender's email, sender's subject, and sender's message.



Feedback Details

Feedback Date: 2017-01-07

Sender's Email:

Sender's Subject: Chemical families in CompTox Chemistry Dashboard

Sender's Message: Thank you for providing the Chemistry Dashboard, a fantastic resource that I hope you continue to develop. I have some questions about the new support for chemical families (e.g. PCBs). - Is it possible to download a list of chemical families in the Chemistry Dashboard and also the individual compounds belong to each? - How did you put these families together? I notice that the PCB record says "manually curated"; are there any algorithmically curated ones?

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The back button returns to the site feedback page.

Site Preferences:

Category Terms:

Category terms is a page that has four tabs that will allow administrators to customize drop down lists and input types at any time. There is a search text box for category terms in the upper right corner that will allow an administrator to search on specific words.

The screenshot displays the 'Category Terms' page within the EPA Chemistry Dashboard. The page features a navigation bar with the EPA logo and links for Home, Advanced Search, and Lists. A search box for the Chemistry Dashboard is located in the top right corner. Below the navigation bar, the 'Category Terms' section is titled, and there is a 'New Category' button. Four tabs are visible: Abstract Sifter, Batch Search, External Links, and Google Scholar. The 'Abstract Sifter' tab is selected, showing a table of 25 entries. The table has columns for Label, Parent, Rank, and Content. Each row includes 'Details', 'Edit', and 'Delete' buttons. The entries are:

Label	Parent	Rank	Content	Details	Edit	Delete
Hazard	-	1	(NOAEL or LOEL or RfD OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope fac...	Details	Edit	Delete
Fate and Transport	-	2	(degradation OR bioaccumulation OR sunlight OR bacteria OR breakdown OR transport[tiab])	Details	Edit	Delete
Metabolism/PK/PD	-	3	(metabolism OR metabolite or "tissue distribution"[tiab])	Details	Edit	Delete
Chemical Properties	-	4	(logp OR solubility OR equilibrium OR solute or "partition coefficient"[tiab] OR hydrophob OR hydrophil)	Details	Edit	Delete
Exposure	-	5	(exposure OR near-field OR far-field OR SHEDS[tiab] AND ENVIRONMENTAL MONITORING)	Details	Edit	Delete
Mixtures	-	6	(Drug synergism[mh] OR cocarcinogenesis OR pesticide synergists[mh] OR mixture[tiab] OR mixtures[tiab]...	Details	Edit	Delete

At the bottom of the table, it says 'Showing 1 to 6 of 6 entries'. There are also 'Previous', '1', and 'Next' navigation buttons.

Abstract Sifter – is found under the literature tab under the abstract sifter selection. It is used for specific queries against Pubmed articles using MeSH based searches and access to PubChem Patents. This panel allows administrators to add or remove pre-defined queries in the “Select Term” drop down list.

Batch Search – is found under the “Advanced Search” link that allows users to search on multiple chemicals and input types. This panel allows administrators to add or remove Input Types a user can search on and to place these types in a specific order.

External Links – is a panel that allows administrators to add, edit, or remove hyperlinks to external sites and order/sort these links.

Google Scholar – is found under the literature tab under the Google Scholar selection. Users can search for digital or physical copies of articles, whether online or in libraries. This panel allows administrators to add or remove selections for the drop down lists for items such as environmental, qualification, and non-targeted analysis search. These are appended into a search using the CAS Number and Preferred Name.

New Category

The new category button will allow an administrator to create a new category group, assign a parent and provide a label.

New Category Term

Category group

Select a Category Group



Parent

Select a Parent



Label

Type the name of the category term as you would like it to appear

Back

Create Category

Details

The details button displays a page that administrators can modify the details associated to the category term properties currently set.

Category Term

Category Group: Abstract Sifter

Category Term Label: Hazard

Parent: N/A

Rank: 1

Content: (NOAEL or LOEL or Rfd OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

Admin:

Date Created: September 27, 2016

Date Updated: September 27, 2016

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Edit

The edit button displays a page that allows the administrator to modify the properties of the category term for category group, parent, label, content, and rank.

Edit Category Term

Category group

Abstract Sifter



Parent

None



Label

Hazard

Content

(NOAEL or LOEL or Rfd OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

Rank

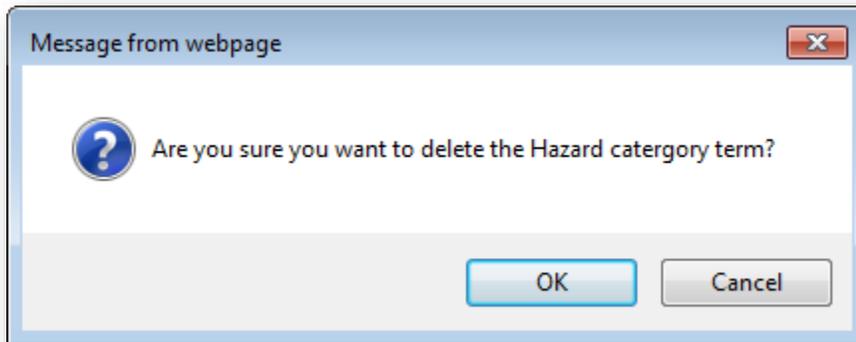
1

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Update Category



The delete button removes the download link from the page so that this link is no longer visible or available to the user.



Download Links:

Download link is found in the footer of the dashboard. This page displays links and descriptions that allows the EPA to distribute data as downloadable files. This panel allows administrators to add, remove, and edit these downloadable items.

The screenshot shows the EPA Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo and links for Home, Advanced Search, and Lists. A search bar is on the right. The main content area is titled 'Chemistry Dashboard' and 'Download Links'. Below the title is a 'New Download Link' button. A table lists existing download links with columns for Name, Label, URL, Description, and Admin Name. Each row includes 'Show', 'Edit', and 'Delete' buttons. A search bar is on the right side of the table. At the bottom left, it says 'Showing 1 to 8 of 8 entries'.

Name	Label	URL	Description	Admin Name			
DSSTox MS Ready Chemical Structures	DSSTox MS Ready Mapping File	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	The CompTox Chemistry Dashboard can...	Jennifer Smith	Show	Edit	Delete
Dsstox_CAS_number_name.xlsx	DSSTox identifiers mapped to CAS Numb...	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	The DSSTox Identifiers file is in Excel form...	Jennifer Smith	Show	Edit	Delete
DSSTox_Mapping_20160701	DSSTox Mapping File	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	The DSSTox mapping file contains mappi...	Jennifer Smith	Show	Edit	Delete
DSSTox_Predicted_NCCT_Model.zip	DSSTox Predicted Property Data	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	A number of property prediction models w...	Jennifer Smith	Show	Edit	Delete
DSSTox_SDF_File_20160720.sdf.gz	DSSTox SDF File	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	This zip file contains the entire chemical st...	Jennifer Smith	Show	Edit	Delete
DSSTox_Synonyms_20161018.zip	DSSTox Synonyms File	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	The DSSTox synonyms file is in SDF form...	Jennifer Smith	Show	Edit	Delete
PHYSPROP_Analysis	PHYSPROP Analysis File	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	The data associated with the publication <...	Jennifer Smith	Show	Edit	Delete
PubChem_DTXSID_mapping_file.bt	DSSTox Identifier to PubChem Identifier M...	ftp://newftp.epa.gov/COMPTOX/Sustainabl...	The DSSTox to PubChem Identifiers mapp...	Jennifer Smith	Show	Edit	Delete

New Download Link

a new download link.

The new download link button will display a page that allows administrators to create

New Download Link

Name

A more detailed name for internal use

Label

Name displayed to users

Uri

The URL must start with: `ftp://newftp.epa.gov/COMPTOX/Sustainable_Chemistry_Data/Chemistry_Dashboard/`

`ftp://newftp.epa.gov/COMPTOX/Sustainable_Chemistry_Data/Chemistry_Dashboard/...`

Description

Description shown to users

Back

Create Download link

Show

The show button will display a page that shows the administrator specific details associated to the download link properties currently set. In order to return to the download links home page, click the show all button. The show all button is similar to a back button.

News Item

Name: DSSTox MS Ready Chemical Structures

Label: DSSTox MS Ready Mapping File

Uri: `ftp://newftp.epa.gov/COMPTOX/Sustainable_Chemistry_Data/Chemistry_Dashboard/DSSTOX_MS_Ready_Chemical_Structures.zip`

Description: The CompTox Chemistry Dashboard can be used by mass spectrometrists for the purpose of structure identification. A normal formula search would search the exact formula associated with any chemical, whether it include solvents of hydration, salts or multiple components. However, mass spectrometry detects ionized chemical structures and molecular formulae searches should be based on desalted, and desolvated structures with stereochemistry removed. We refer to these as "MS ready structures" and the MS-ready mappings are delivered as Excel Spreadsheets containing the Preferred Name, CAS-RN, DTXSID, Formula, Formula of the MS-ready structure and associated masses, SMILES and InChI Strings/Keys.

	Preferred_Name	CAS-RN	DSSTox_Substance_ID	Formula	Formula (Desalted)	Monoisotopic Mass	Monoisotopic Mass (Desalted)
48	Pheniramine maleate	132-20-7	DTXSID0025866	C20H24N2O4	C16H20N2	356.1736073	240.1626487
49	Phenolphthalein glucuronide, sodium salt	6820-54-8	DTXSID9025871	C26H21NaO10	C26H22O10	516.1032412	494.1212969

Admin: Jennifer Smith

Edit

Show All



The edit button displays a page that allows the administrator to modify the download link's name, label, URL and description.

Edit Download Link

Name

Label

Uri

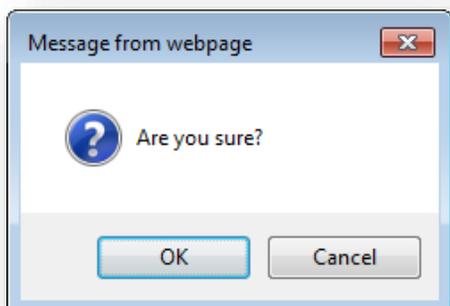
The URL must start with: `ftp://newftp.epa.gov/COMPTOX/Sustainable_Chemistry_Data/Chemistry_Dashboard/`

Description

The CompTox Chemistry Dashboard can be used by mass spectrometrists for the purpose of structure identification. A normal formula search would search the exact formula associated with any chemical, whether it include solvents of hydration, salts or multiple components. However, mass spectrometry detects ionized chemical structures and molecular formulae searches should be based on desalted, and desolvated structures with stereochemistry removed. We refer to these as "MS ready structures" and the MS-



The delete button removes the download link from the page so that this link is no longer visible or available to the user.



External Links:

External links is an administration page that will initially display a listing of all external links currently configured and available to the user. This page allows administrators to create a new link, view, edit and delete existing hyperlinks found under the external link tab on the dashboard.

The screenshot displays the 'External Links' section of the EPA Chemistry Dashboard. At the top, there is a search bar and an 'Add a new link' button. Below this is a table listing various external links. The table has four main columns: Name, URL, Parameter, and Category. Each row also includes three action buttons: Details, Edit, and Delete. The links listed include tools like 2D NMR HSQC/HMBC Prediction, ACToR, BioCaddie DataMed, Carbon-13 NMR Prediction, CCRIS, ChEMBL, ChemHat, Chemical Entities of Biological Interest (ChEBI), Chemical Vendors, ChemRTP Predictor, and Chempidder.

Name	URL	Parameter	Category	Details	Edit	Delete
2D NMR HSQC/HMBC Prediction	http://www.nmrdb.org/service.php?name=hmbc-prediction&smiles=%s	smiles	Prediction	Details	Edit	Delete
ACToR	http://actor.epa.gov/actor/chemical.xhtml?casrn=%s	casrn	Toxicology	Details	Edit	Delete
ACToR PDF Report	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=%s	casrn	Toxicology	Details	Edit	Delete
BioCaddie DataMed	https://datamed.org/search.php?query=%s&searchtype=data	preferred_name	Publications	Details	Edit	Delete
Carbon-13 NMR Prediction	http://www.nmrdb.org/service.php?name=nmr-13c-prediction&smiles=%s	smiles	Prediction	Details	Edit	Delete
CCRIS	https://toxnet.nlm.nih.gov/cgi-bin/sis/search/2/?db=crris:@term+@r+++@rel+%s	casrn	Toxicology	Details	Edit	Delete
ChEMBL	https://www.ebi.ac.uk/chembl/compound/inspect/%s	chembl_id	General	Details	Edit	Delete
ChemHat: Hazards and Alternatives Toolbox	http://chemhat.org/en/chemical-finder/%s	casrn	General	Details	Edit	Delete
Chemical Entities of Biological Interest (ChEBI)	https://www.ebi.ac.uk/chebi/searchId.do?chebiId=ChEBI:%s	chebi_id	General	Details	Edit	Delete
Chemical Vendors	http://www.chemicalbook.com/Search_EN.aspx?keyword=%s	casrn	General	Details	Edit	Delete
ChemRTP Predictor	http://realtime.molinstincts.com/chemical-info.ce?ID=%s	inchi_key	Prediction	Details	Edit	Delete
Chempidder	http://www.chemspider.com/Chemical-Structure.%s.html	chemspider_id	General	Details	Edit	Delete

Add a new link

The add a new link button displays a page that allows administrators to enter information to create a new external link.

New External Link

Name

Type the name of the link as you would like it to appear

Please replace chemical identifier in the url with '%s'. Example: '...search?cas=50-00-0' would be '...search?cas=%s'



Url

Type the url for the link

Parameter

Select a Parameter



Do you need a parameter not on the list?

Add a new Parameter

Category

General



Icon

Select an Icon



Do you need to upload a new icon?

Add a new Icon

Description

Add a description of the site, service, or data for this link

Back

Create External link

Details

The details button displays a page that administrators can view the specific details associated to the hyperlink properties currently set.

Link Description

Link Name: 2D NMR HSQC/HMBC Prediction

URL: <http://www.nmrdb.org/service.php?name=hmbc-prediction&smiles=%s>

Parameter: smiles

Category: Prediction

Icon: ·

Description: 2D NMR predictions provided by NMRShiftDB.org

Preview of Link: · [2D NMR HSQC/HMBC Prediction](#)

Back

Edit

The edit button displays a page that allows the administrator to modify the hyperlink's name, URL, parameter, category, icon, upload a new icon, and description.

Edit Link

Name

Please replace chemical identifier in the url with '%s'. Example: '...search?cas=50-00-0' would be '...search?cas=%s' ✕

Uri

Parameter

Do you need a parameter not on the list?

Category

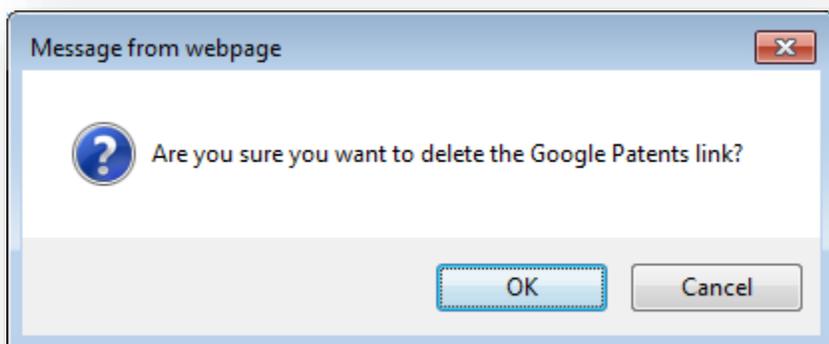
Icon

Do you need to upload a new icon?

Description

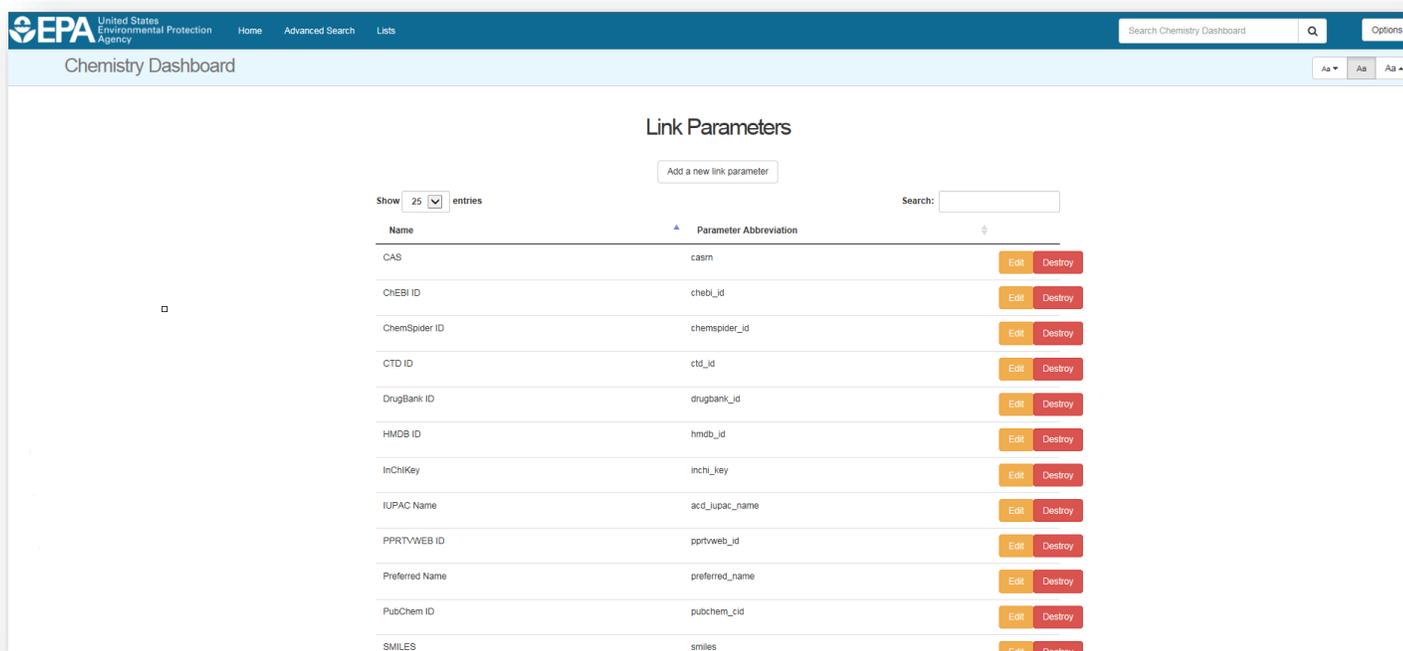


The delete button removes the download link from the page so that this link is no longer visible or available to the user.



Link Parameters:

Link parameters panel allows administrators to create, edit or delete a parameter that is required to be passed for external hyperlinks. Examples of possible parameters could be MeSH_ID or FDA registry number.



The screenshot shows the EPA Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo, "United States Environmental Protection Agency", and links for "Home", "Advanced Search", and "Lists". A search bar on the right contains "Search Chemistry Dashboard" and a magnifying glass icon. Below the navigation bar, the page title "Chemistry Dashboard" is displayed. The main content area is titled "Link Parameters" and features a button "Add a new link parameter". Below this, there is a "Show 25 entries" dropdown and a "Search:" input field. A table lists various link parameters with columns for "Name" and "Parameter Abbreviation". Each row includes "Edit" and "Destroy" buttons.

Name	Parameter Abbreviation		
CAS	casrn	Edit	Destroy
CHEBI ID	chebi_id	Edit	Destroy
ChemSpider ID	chemspider_id	Edit	Destroy
CTD ID	ctd_id	Edit	Destroy
DrugBank ID	drugbank_id	Edit	Destroy
HMDB ID	hmdb_id	Edit	Destroy
InChIKey	inchi_key	Edit	Destroy
IUPAC Name	acd_iupac_name	Edit	Destroy
PPRTVWEB ID	pprtweb_id	Edit	Destroy
Preferred Name	preferred_name	Edit	Destroy
PubChem ID	pubchem_cid	Edit	Destroy
SMILES	smiles	Edit	Destroy

Add a new link parameter

The add a new link parameter button displays a page that allows administrators to enter information to create a new link parameter.

New Link Parameter

Location in dsstox

Name

Parameter abbreviation

Create Link parameter

Back

An orange square button with the word "Edit" written in white text.

The edit button displays a page that allows the administrator to modify the properties of the link parameter select.

Editing Link Parameter

Location in dsstox

DSSTox Table



Name

CAS

Parameter abbreviation



Update Link parameter

Back

Destroy

The destroy button removes the link parameter from the page so that this link is no longer visible or available to the user.

Message from webpage



Are you sure?

OK

Cancel

Help Text Table:

The help text model is used to keep the information about help texts for the different sections of the application. For example, the section that relates to the author text of an AOP would have the id reference to the author heading with the content of what should be contained in the author section. This panel provides a way for administrators to define the position (top, bottom, left, right) edit or delete content associated with it

The screenshot shows the EPA Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo, 'United States Environmental Protection Agency', and links for 'Home', 'Advanced Search', and 'Lists'. A search bar is located on the right side of the dashboard. Below the navigation bar, the page title 'Chemistry Dashboard' is displayed. The main content area is titled 'Help and Info Text Table'. At the top of this section, there is a button labeled 'Add a new help text'. Below the button, there is a table with columns for 'Icon Type', 'Text', 'Location', 'Popover Pos...', 'Admin Name', and 'Created At'. The table contains eight rows of data, each representing a help text entry. Each row has an 'Edit' button (orange) and a 'Delete' button (red) to the right of the 'Created At' column. The table also includes a search bar and a 'Show 25 entries' dropdown menu.

Icon Type	Text	Location	Popover Pos...	Admin Name	Created At		
Information	The Centers for Disease Control (CDC) Nation...	SR NHANES Ta...	right	Antony Williams	2016-12-12	Edit	Delete
Information	In Figure 4 of the 2014 publication "High Throu...	SR Exposure Rank	right	Antony Williams	2016-12-12	Edit	Delete
Information	In the 2014 publication "High Throughput Heurt...	SR Expo Pred. T...	right	Antony Williams	2016-12-12	Edit	Delete
Information	Here, women of "reproductive age" are defined...	SR Exposure Re...	bottom	Antony Williams	2016-12-13	Edit	Delete
Information	This search is based on what we refer to as &q...	AS MS Ready F...	right	Antony Williams	2016-12-13	Edit	Delete
Information	CPCat (Chemical and Product Categories) is a...	SR CPCat Graph	left	Antony Williams	2016-08-23	Edit	Delete
Information	This graph shows chemical screening data fro...	SR ToxCast Graph	left	Antony Williams	2016-08-23	Edit	Delete
Information	The DTXSID is the DSSTOX substance identifi...	SR DTXSID	right	Antony Williams	2016-08-23	Edit	Delete

Add a new help text

The add a new help text button displays a page that allows administrators to enter information to create new help text.

New Help Text

Type

Please select the type of text



Location

Please select the type of text



Popover position

Please select the position of the popover



Text

Type the help text here...

Links may be added using html. (Ex. Here is a `link`)

Back

Create Help text

Edit

The edit button displays a page that allows the administrator to modify the properties of the help text selected.

Edit Help Text

Type

Information



Location

SR NHANES Table



Popover position

right



Text

The Centers for Disease Control (CDC) National Health and Nutrition Examination Survey (NHANES) is a program of studies designed to assess the health and nutritional status of adults and children in the United States (link). As part of the NHANES, the CDC Links may be added using html. (Ex. Here is a link)



Back

Update Help text

Delete

The delete button removes the help text from the page so that this link is no longer visible or available to the user.

Message from webpage



Are you sure you want to delete this Information text?

OK

Cancel

Manage Lists:

In the top upper left hand corner of the Comptox Dashboard, there is a List link. This page displays all the preloaded chemical lists available to the users. The administration list panel allows administrators to create, edit and make these lists visible to the public. The lists that come from DSSTOX an administrator will find that they cannot change the properties. These list reside in the DSSTOX table and must be changed in the table. However, application created lists can be created, modified and deleted from the admin panel. Accessibility column displays the groups that segregate who gets to see which lists and which lists will remain private.

Label	Abbreviation	DSSTOX Chemical Li...	Short Description	List Owner	Accessibility	Visible		
All chemicals in ChemTrack	COASUMMARIES	240	All chemicals in ChemTrack	Antony Williams	EPA	true	Show	Edit
EDSP	EDSPU	272	EDSP Superset of all EDSP Lists	Antony Williams	EPA	true	Show	Edit
EPAHERO	HEROMAP	318	HERO: Health and Environmental Research Online	Antony Williams	EPA	true	Show	Edit
GENRA	GENRA		This is the set of chemicals associated with the GENRA prototype application development	Antony Williams	EPA	true	Show	Edit
IRIS Assessments	IRIS	303	Each IRIS assessment can cover a chemical, a group of related chemicals,	Antony Williams	EPA	true	Show	Edit
Jennifer's List	JENNIFER		test list	Jennifer Smith	PUBLIC	true	Show	Edit
Joshua Hamill's HTRR_MCF7 List	HTRRMCF7	283	A list of chemicals which will be run in the HTRR Pilot Screen in MCF7 cells by Joshua Hamill's laboratory	Antony Williams	EPA	true	Show	Edit
OLEM Case Study List_V2	OLEMV2		26 chemicals covering a wide range of chemical space, differing levels of data availability, and highlighting different types of compounds that are of particular interest to OLEM.	Antony Williams	EPA	true	Show	Edit
OLEM RapidTox Chemicals	OLEMCI	198	OLEM RapidTox Chemicals	Jennifer Smith	EPA	true	Show	Edit
OPP Inerts List for RapidTox	OPPINERTS	199	OPP Inerts List for RapidTox	Jennifer Smith	EPA	true	Show	Edit
OPPT Brominated Phthalates	BRPHTHAL	265	A list of flame retardant brominated phthalates of interest to OPPT	Antony Williams	EPA	true	Show	Edit
BEASToGrace	BEASGRACE	117	A list of polychlorinated chemicals of interest to Grace Patlewicz	Antony Williams	EPA	true	Show	Edit

Add a New List

The add a new list button displays a page that allows administrators to enter information to create a new list.

New List

Select List Type

Label

Warning: List abbreviations must be unique, cannot contain special characters or spaces, and cannot be edited after list creation.

Abbreviation

Short Description

Chemicals

Please enter line separated DXTSIDs.

Check List

Show List?

Choose tabs to be displayed on the single results page.

- Select All
- Links
- Properties
- Synonyms

Show

The show button will display a page that shows the administrator specific details associated to the list properties currently set.

Label: First 10 TSCA Chemicals

Abbreviation: 10TSCA

Short Description: Requested list of chemicals from TSCA List submitted by Richard

Number of Chemicals: 10

List Owner: Antony Williams

Visible: true

Visible Tabs (in order):

- Properties
- Similar Molecules
- Synonyms
- Exposure
- Bioassays
- Product Composition
- Comments
- Links
- Literature
- Predicted Hazards

[View All Lists](#)



The edit button displays a page that allows the administrator to modify the properties of the list selected.

Edit List

Label

First 10 TSCA Chemicals

Warning: List abbreviations must be unique, cannot contain special characters or spaces, and cannot be edited after list creation. ✕

Abbreviation

10TSCA

Short Description

Requested list of chemicals from TSCA List submitted by Richard

Chemicals

DTXSID4020533
DTXSID6021874
DTXSID4023888
DTXSID8020250
DTXSID4023233

Check List

Show List?

Choose tabs to be displayed on the single results page.

Select All

Links

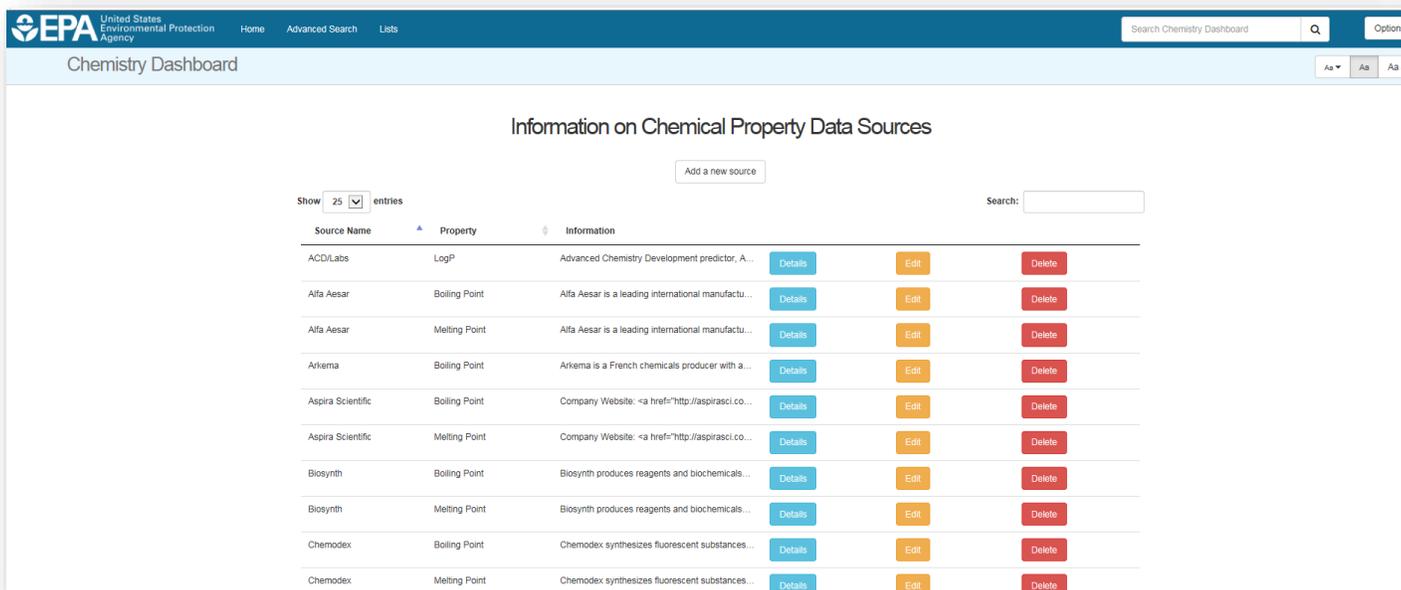
Properties

Synonyms

Exposure

Property Data:

For chemical properties there are five forms of predicted property data available. These include data from EPISuite, from OPERA models, from NICEATM models, from the Toxicity Estimation Software Tool models and harvested from the Open PHACTS project as predicted by ACD/Labs. The Information on Chemical Property Data Sources panel allows an administrator to create a new data source, view and edit an existing source or delete a source.



The screenshot shows the EPA Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo and links for Home, Advanced Search, and Lists. A search bar is located on the right side of the dashboard. The main content area is titled "Information on Chemical Property Data Sources" and features a table of data sources. Above the table, there is a "Show 25 entries" dropdown menu and a search box. A button labeled "Add a new source" is positioned above the table. The table has three columns: "Source Name", "Property", and "Information". Each row represents a data source and includes "Details", "Edit", and "Delete" buttons.

Source Name	Property	Information	Details	Edit	Delete
ACD/Labs	LogP	Advanced Chemistry Development predictor, A...	Details	Edit	Delete
Alfa Aesar	Boiling Point	Alfa Aesar is a leading international manufactu...	Details	Edit	Delete
Alfa Aesar	Melting Point	Alfa Aesar is a leading international manufactu...	Details	Edit	Delete
Arkema	Boiling Point	Arkema is a French chemicals producer with a...	Details	Edit	Delete
Aspira Scientific	Boiling Point	Company Website: <a href="http://aspirasci.co...	Details	Edit	Delete
Aspira Scientific	Melting Point	Company Website: <a href="http://aspirasci.co...	Details	Edit	Delete
Biosynth	Boiling Point	Biosynth produces reagents and biochemicals...	Details	Edit	Delete
Biosynth	Melting Point	Biosynth produces reagents and biochemicals...	Details	Edit	Delete
Chemodex	Boiling Point	Chemodex synthesizes fluorescent substances...	Details	Edit	Delete
Chemodex	Melting Point	Chemodex synthesizes fluorescent substances...	Details	Edit	Delete

Add a new source

The add a new source button displays a page that allows administrators to enter information to create a new data source.

New Data Source

The Physchem Database is not available right now. Please try again later.

[Back](#)

[Details](#)

The details button displays a page that administrators can view the specific details associated to the data source properties currently set.

Data Source Description

Source Name: ACD/Labs

Property: LogP

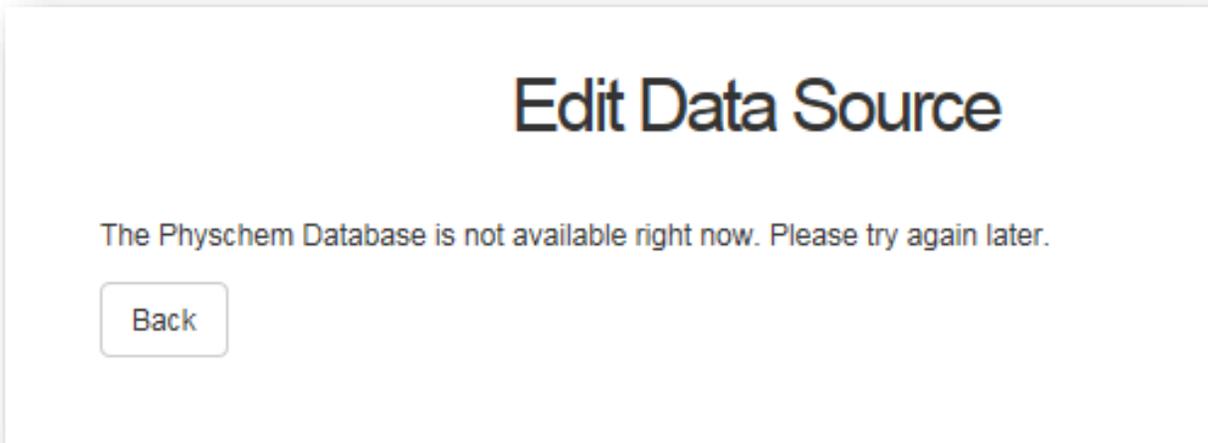
Information: Advanced Chemistry Development predictor, ACD/Labs (<http://www.acdlabs.com/products/percepta/predictors/logp>). The logP prediction model incorporates two different predictive approaches—Classic and GALAS (Global, Adjusted Locally According to Similarity). A Consensus logP based on these two models is also available.

Preview of Source: [ACD/Labs](#)

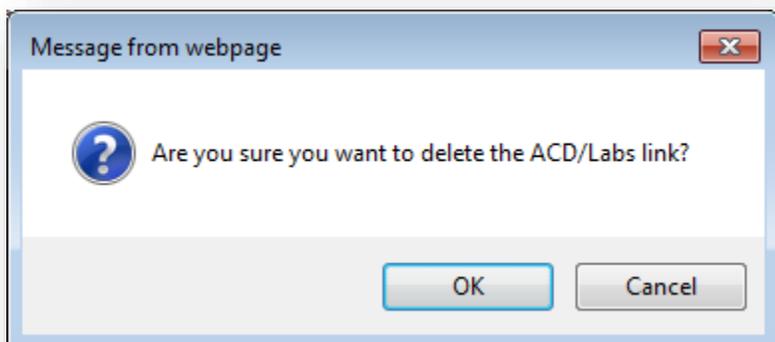
[Back](#)



The edit button displays a page that allows the administrator to modify the properties of the data source selected for the chemical property.

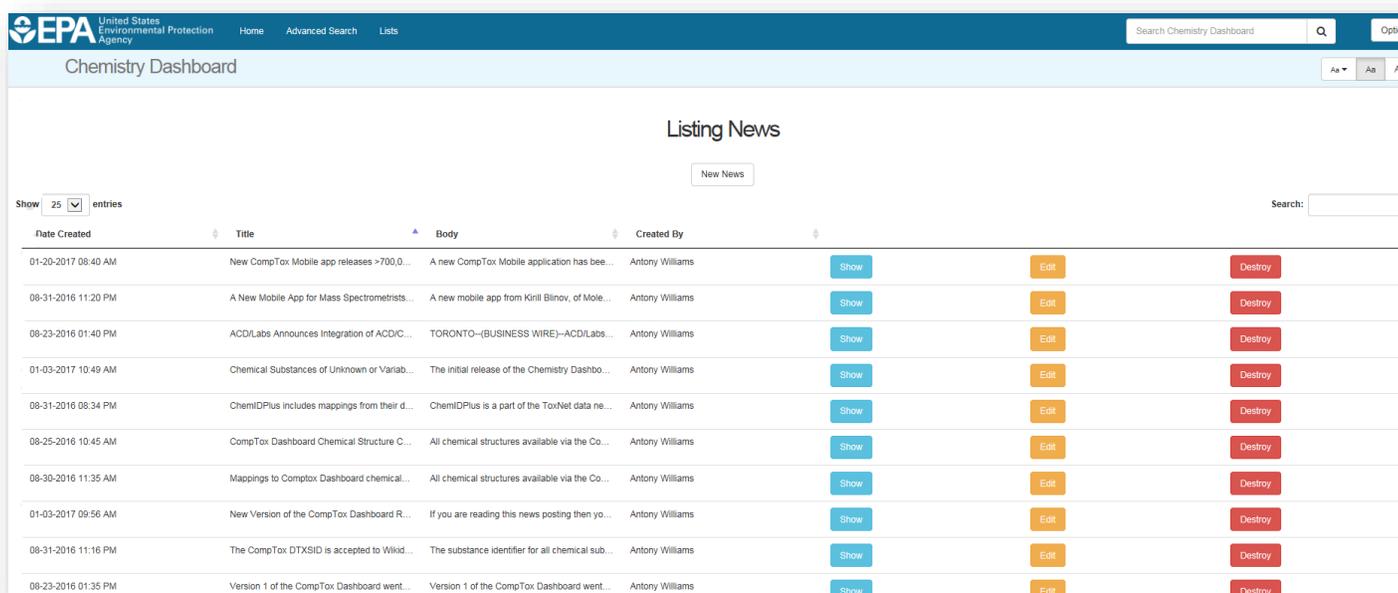


The delete button removes the data source from the page so that this link is no longer visible or available to the user.



Update Site News:

This administration panel displays all the existing news items. A news item is important content/information we want to share with our users. It is submitted by an administrator that will be posted to the home page automatically. It allows an administrator to see the details of an existing entry, edit an entry, create a new entry, and delete an entry.



The screenshot shows the EPA Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo and links for Home, Advanced Search, and Lists. A search bar is located on the right. Below the navigation bar, the page title is 'Chemistry Dashboard'. The main content area is titled 'Listing News' and features a 'New News' button. Below this, there is a table with the following columns: Date Created, Title, Body, and Created By. Each row in the table has three buttons: 'Show', 'Edit', and 'Destroy'. The table contains 10 rows of news items, all created by 'Antony Williams'.

Date Created	Title	Body	Created By	Show	Edit	Destroy
01-20-2017 08:40 AM	New CompTox Mobile app releases >700,0...	A new CompTox Mobile application has bee...	Antony Williams	Show	Edit	Destroy
09-31-2016 11:20 PM	A New Mobile App for Mass Spectrometrists...	A new mobile app from Kirill Blinov, of Mole...	Antony Williams	Show	Edit	Destroy
09-23-2016 01:40 PM	ACDLabs Announces Integration of ACD/IC...	TORONTO--(BUSINESS WIRE)--ACDLabs...	Antony Williams	Show	Edit	Destroy
01-03-2017 10:49 AM	Chemical Substances of Unknown or Variab...	The initial release of the Chemistry Dashbo...	Antony Williams	Show	Edit	Destroy
09-31-2016 08:34 PM	ChemIDPlus includes mappings from their d...	ChemIDPlus is a part of the ToxNet data ne...	Antony Williams	Show	Edit	Destroy
09-25-2016 10:45 AM	CompTox Dashboard Chemical Structure C...	All chemical structures available via the Co...	Antony Williams	Show	Edit	Destroy
09-30-2016 11:35 AM	Mappings to CompTox Dashboard chemical...	All chemical structures available via the Co...	Antony Williams	Show	Edit	Destroy
01-03-2017 09:56 AM	New Version of the CompTox Dashboard R...	If you are reading this news posting then yo...	Antony Williams	Show	Edit	Destroy
09-31-2016 11:16 PM	The CompTox DTXSID is accepted to Wikid...	The substance identifier for all chemical sub...	Antony Williams	Show	Edit	Destroy
09-23-2016 01:35 PM	Version 1 of the CompTox Dashboard went...	Version 1 of the CompTox Dashboard went...	Antony Williams	Show	Edit	Destroy



The add a new news button displays a page that allows administrators to enter information to create a new news.

New News

Title

Body

Back

Create News

Show

The show button will display a page that shows the administrator specific details associated to the news item currently set.

News Item

Date Posted: January 20, 2017

Title: New CompTox Mobile app releases >700,000 chemicals on iPhone and iPad

Body: A new CompTox Mobile application has been released that puts the content associated with the dashboard onto an iPad or iPhone in your hand. The data are searchable by name, by CAS Number and link through directly to the dashboard pages. Also included is the ability to search by mass and predicted NMR shifts. The link to the iTunes download page is here: <https://itunes.apple.com/us/app/comp-tox-mobile/id1179517689?is=1&mt=8>

Shortened Body (visible on home page): A new CompTox Mobile application has been released that puts the content associated with the dashboard onto an iPad or iPhone in your hand. The data are searchable by name, by CAS Number and link t...

Show All News

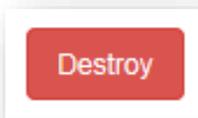


The edit button displays a page that allows the administrator to modify the properties of an existing news item selected.

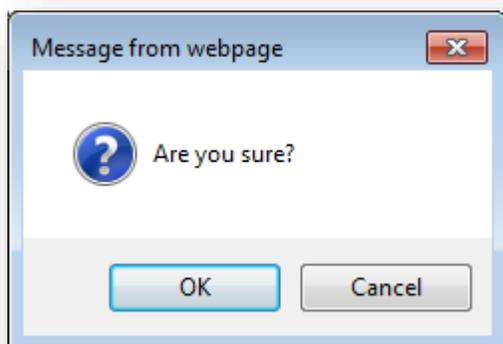
Editing News Item

Title

Body

https://itunes.apple.com/us/app/comptox-mobile/id1179517689?ls=1&mt=8"/>

The destroy button removes the news item from the page so that this link is no longer visible or available to the user.



Upload Images:

Upload images is a panel that allows administrators to upload new images, edit existing images or delete images. These images can be references throughout the entire Comptox dashboard.

The screenshot shows the 'Uploaded Images' section of the EPA Chemistry Dashboard. The page header includes the EPA logo and navigation links. The main content area features a table of uploaded images. The table has the following columns: Name, Image Type, Edit, and Delete. The table lists 11 items, all of which are 'Link Icon' type. Each item has an orange 'Edit' button and a red 'Delete' button. Above the table, there is a search bar and a 'Show 25 entries' dropdown. A 'Add a new image' button is located above the table.

Name	Image Type	Edit	Delete
Search	Link Icon	Edit	Delete
Chemicalize	Link Icon	Edit	Delete
Chempidder	Link Icon	Edit	Delete
CTDbase	Link Icon	Edit	Delete
DrugBank	Link Icon	Edit	Delete
DrugInfo	Link Icon	Edit	Delete
ChEBI	Link Icon	Edit	Delete
eChemPortal	Link Icon	Edit	Delete
EPA	Link Icon	Edit	Delete
For Ident	Link Icon	Edit	Delete

Add a new image

The add a new image button displays a page that allows administrators to enter information to upload a new image.

Upload New Image

Name

Type the name of the icon as you would like it to appear

Image type

Select an Image Type



Browse...

Back

Create Uploaded image

Edit

selected.

The edit button displays a page that allows the administrator to modify the properties of the image

Edit Image

Name

Image type



The delete button removes the image from the page so that this link is no longer visible or available to the user.

Message from webpage

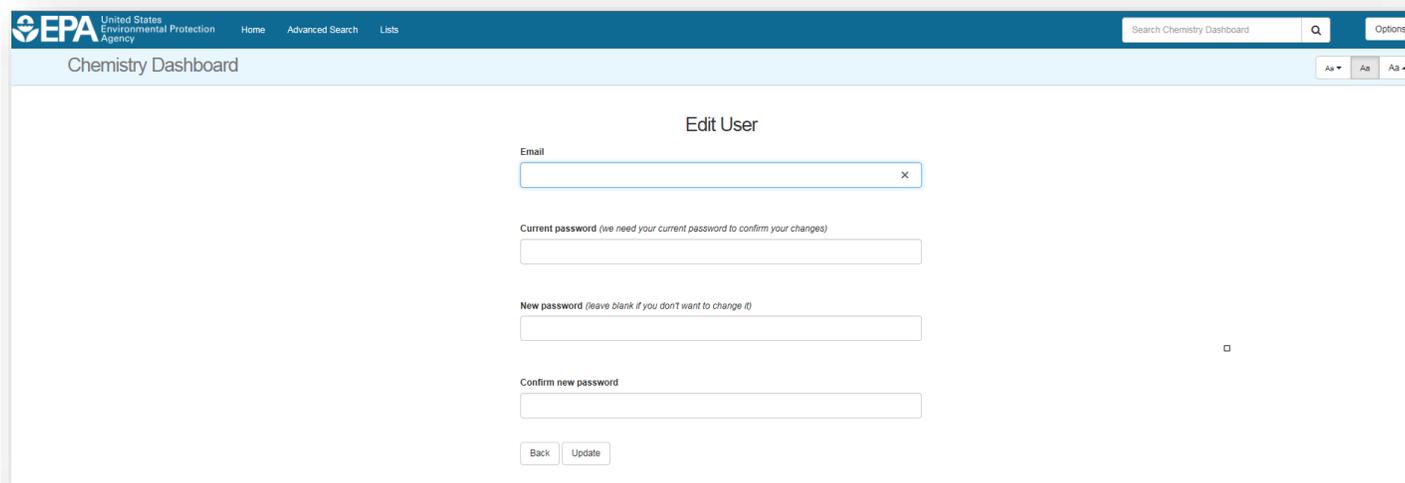


Are you sure?

Account Preferences:

Edit Account Info:

This panel allows an administrator to update their existing password or another admin's password.



The screenshot shows the 'Edit User' form within the EPA Chemistry Dashboard. The dashboard header includes the EPA logo, 'United States Environmental Protection Agency', and navigation links for 'Home', 'Advanced Search', and 'Lists'. A search bar for 'Chemistry Dashboard' and an 'Options' menu are also visible. The form itself is titled 'Edit User' and contains the following fields:

- Email:** A text input field with a clear 'x' button.
- Current password (we need your current password to confirm your changes):** A text input field.
- New password (leave blank if you don't want to change it):** A text input field.
- Confirm new password:** A text input field.

At the bottom of the form are two buttons: 'Back' and 'Update'.

Logout:

The logout link will log the administrator out of the administrator dashboard.