

# Literature-based cheminformatics for research in chemical toxicity

Nancy C. Baker

Leidos

Contractor to the US EPA

2019 Spring ACS Annual Meeting

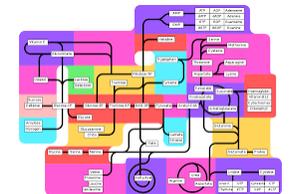
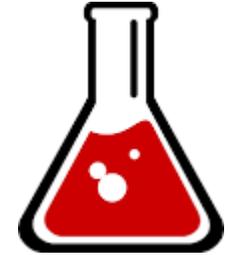
*DISCLAIMER: This presentation does not necessarily reflect U.S. EPA policy.*

# What is literature-based cheminformatics?

- Tools to optimize literature tasks
- Why?
  - Literature is the largest source of information about chemicals and what they do
- Existing tools are amazing but not optimized to many tasks

# Common chemical toxicity tasks

- One chemical
  - Deep dive – review literature for a chemical
  - Challenge: Can be thousands of articles, and only a few relevant
- Many chemicals
  - Overview to rank for prioritization
  - What do they have in common
- Mechanistic inquiry – by which mechanism (adverse outcome pathway) is a given chemical or set of chemicals acting
- Ad hoc quick lookup



# Technology: Abstract Sifter

- In two implementations
  - Excel
  - Web version – EPA Comptox Chemicals Dashboard
- Note
  - This presentation at high-level
  - Detailed documentation available
    - Including user guide
    - Video tutorials
- Both tools publicly available now

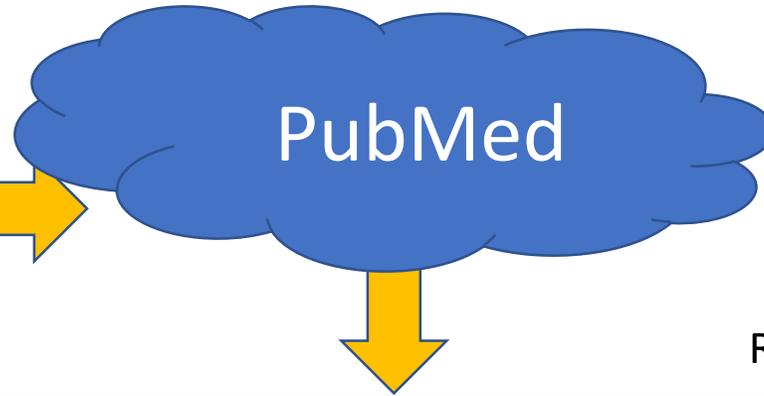
# Strategy

29 million citations

PubMed query

Enter your PubMed query and click on Submit.

tetrachloroethylene OR perchloroethylene



Results downloaded to Excel

Abstract	sifter	Query PubMed			Pub	Title	Authors	Journal
v3	Your sifter terms and frequency counts			Total	Yr			
PMID	sifter term 1	sifter term 2	sifter term 3	Total	Yr	Title	Authors	Journal
30856471	0	0	0	0	2019	A comparison of the electrolysis of soil washing wastes with active and non-active electrodes.	Karaçali, Muñoz-Morales, Kalkan, Kt	Chemosphere
30827336	0	0	0	0	2019	Environmental and Genetic Factors Influencing Kidney Toxicity.	Lash	Seminars in nephrology
30809199	0	0	0	0	2019	Functional Genes and Bacterial Communities During Organohalide Respiration of Chloroethenes in Microcosms of Multi-Ci	Hermon, Hellal, Denonfoux, Vuilleu	Frontiers in microbiology
30801570	0	0	0	0	2019	Perchloroethylene: acute occupational poisoning and a proposal for its replacement with other less toxic substances.	Sanz-Gallen, Sanz-Ribas, Marti-Ame	Medycyna pracy
30728999	0	0	0	0	2018	Comparative investigation of argon and argon/oxygen plasma performance for Perchloroethylene (PCE) removal from aqu	Karimaei, Shokri, Khani, Yaghmaeia	Journal of environmental health
30721169	0	0	0	0	2019	Extended Mortality Follow-up of a Cohort of Dry Cleaners.	Callahan, Stewart, Blair, Purdue	Epidemiology (Cambridge, Mass)
30691860	0	0	0	0	2019	Numerical modelling of the impact of surfactant partitioning on surfactant-enhanced aquifer remediation.	Babaei, Copty	Journal of contaminant hydrolog
30685665	0	0	0	0	2019	Degradation of tetra- and trichloroethylene under iron reducing conditions by Acidimicrobiaceae sp. A6.	Ge, Huang, Han, Jaffé	Environmental pollution (Barkin
30666385	0	0	0	0	2019	A Case Study of Natural Attenuation of Chlorinated Solvents Under Unstable Groundwater Conditions in Takahata, Japan.	Kawabe, Komai	Bulletin of environmental conta
30652270	0	0	0	0	2019	Elucidating the dechlorination mechanism of hexachloroethane by Pd-doped zerovalent iron microparticles in dissolved le	Rodrigues, Betelu, Colomano, Mas	Environmental science and poll
30637291	0	0	0	0	2019	ZnO Nanosheets Abundant in Oxygen Vacancies Derived from Metal-Organic Frameworks for ppb-Level Gas Sensing.	Yuan, Aljneibi, Yuan, Wang, Liu, Fan	Advanced materials (Deerfield B
30637211	0	0	0	0	2018	Aliphatic Halogenated Hydrocarbons: Report and Analysis of Liver Injury in 60 Patients.	Teschke	Journal of clinical and translati
30625652	0	0	0	0	2019	Groundwater diffuse pollution in functional urban areas: The need to define anthropogenic diffuse pollution background	Azzellino, Colombo, Lombi, Marche	The Science of the total environ
30623720	0	0	0	0	2018	Removal of non-aqueous phase liquids (NAPLs) from TPH-saturated sandy aquifer sediments using in situ air sparging com	Lee, Woo, Jeong	Journal of environmental scienc
30481679	0	0	0	0	2019	Acceleration of perchloroethylene dechlorination by extracellular secretions from Microbacterium in a mixed culture cont	Wan, Chen, Chen, Miao, Liu, Ye, Che	Environmental pollution (Barkin
30415115	0	0	0	0	2019	The aqueous solubility of common organic groundwater contaminants as a function of temperature between 5 and 70 °C.	Koproch, Dahmke, Köber	Chemosphere
30412867	0	0	0	0	2019	Intrusion of chlorinated hydrocarbons and their degradation products from contaminated soil. Measurement of indoor air	Scheepers, Graumans, van Dael, de	The Science of the total environ
30400949	0	0	0	0	2018	Modeled exposure to tetrachloroethylene-contaminated drinking water and the occurrence of birth defects: a case-contr	Aschengrau, Gallagher, Wintner, Butl	Environmental health : a global
30326388	0	0	0	0	2019	Multi-method assessment of the intrinsic biodegradation potential of an aquifer contaminated with chlorinated ethenes	Blázquez-Pallí, Rosell, Varias, Bosch	Environmental pollution (Barkin
30202895	0	0	0	0	2019	Modulation of Tetrachloroethylene-Associated Kidney Effects by Nonalcoholic Fatty Liver or Steatohepatitis in Male C57BL	Cichocki, Luo, Furuya, Venkatratnan	Toxicological sciences : an offic
30191930	0	0	0	0	2018	Reduction of PCE and TCE by magnetite revisited.	Culpepper, Scherer, Robinson, Neui	Environmental science. Process
30186333	0	0	0	0	2018	Preliminary Study: Environmental Assessment of Perchloroethylene in Dry-Cleaning Facilities in the UAE.	Habib, Ahmed, Al-Muhairi, Ziad	Journal of environmental and pu
30138882	0	0	0	0	2019	Combined use of ISCR and biostimulation techniques in incomplete processes of reductive dehalogenation of chlorinated	Herrero, Puigserver, Nijenhuis, Kun	The Science of the total environ
30096992	0	0	0	0	2018	Adsorption process of tetrachloroethylene (PCE) on network growth ring.	Huang, Zhong, Yuan, Ma, Yuan, Liu	Environmental technology
30060664	0	0	0	0	2018	Electric Field Deformation of Protein-Coated Droplets in Thin Channels.	Randall	Langmuir : the ACS journal of su
30058609	0	0	0	0	2018	Further examination of log Pow-based procedures to estimate biological occupational exposure limits.	Kawai, Sakurai, Ikeda	Journal of occupational health
30053492	0	0	0	0	2018	Comparative analysis of metabolism of trichloroethylene and tetrachloroethylene among mouse tissues and strains.	Luo, Hsieh, Soldatow, Chiu, Rusyn	Toxicology
30045527	0	0	0	0	2018	Combined chemical and microbiological degradation of tetrachloroethene during the application of Carbo-Iron at a contan	Vogel, Nijenhuis, Lloyd, Boothman,	The Science of the total environ
30014895	0	0	0	0	2018	Exposure to tetrachloroethylene-contaminated drinking water and time to pregnancy.	Wesselink, Hatch, Wise, Rothman,	Environmental research
29996414	0	0	0	0	2018	The change of representative elementary volume of DNAPL influenced by surface active agents during long-term remedia	Wu, Cheng, Qin, Lei, Wu, Wu, Hu, Li	The Science of the total environ
29989406	0	0	0	0	2018	Reductive Hexachloroethane Degradation by S2O8•- with Thermal Activation of Persulfate under Anaerobic Conditions.	Zhu, Zhu, Liu, Chen, Zhou, Fang, Ga	Environmental science & techn

- People like Excel
- Built-in functionality is rich
- Macros allow more functionality

What Excel allows us to do

The screenshot shows an Excel spreadsheet with the following data:

PMID	sifter term 1	sifter term 2	sifter term 3	Total	Pub	Title	Review	PMC	Authors	Journal
30856471	0	0	0	0	0	2019 A comparison of the electrolysis of soil washing wastes with active and non-active electrodes.	0	0	Karaçali, Muñoz-Morales, Kalkan, K...	Chemosphere
30827336	0	0	0	0	0	2019 Environmental and Genetic Factors Influencing Kidney Toxicity.	1	0	Lash	Seminars in nephrology
30809199	0	0	0	0	0	2019 Functional Genes and Bacterial Communities During Organohalide Respiration of Chloroethenes in Microcosms of Multi-C...	1	0	Hermon, Hellal, Denonfoux, Vuilleu	Frontiers in microbiology
30801570	0	0	0	0	0	2019 Perchloroethylene: acute occupational poisoning and a proposal for its replacement with other less toxic substances.	0	0	Sanz-Gallen, Sanz-Ribas, Marti-Ame	Medycyna pracy
30728999	0	0	0	0	0	2018 Comparative investigation of argon and argon/oxygen plasma performance for Perchloroethylene (PCE) removal from aqu...	1	0	Karimaei, Shokri, Khani, Yaghmaeia	Journal of environmental health s...
30721169	0	0	0	0	0	2019 Extended Mortality Follow-up of a Cohort of Dry Cleaners.	0	0	Callahan, Stewart, Blair, Purdue	Epidemiology (Cambridge, Mass.)
30691860	0	0	0	0	0	2019 Numerical modelling of the impact of surfactant partitioning on surfactant-enhanced aquifer remediation.	0	0	Babaei, Copty	Journal of contaminant hydrology
30685665	0	0	0	0	0	2019 Degradation of tetra- and trichloroethylene under iron reducing conditions by Acidimicrobiaceae sp. A6.	0	0	Ge, Huang, Han, Jaffé	Environmental pollution (Barking,
30666385	0	0	0	0	0	2019 A Case Study of Natural Attenuation of Chlorinated Solvents Under Unstable Groundwater Conditions in Takahata, Japan.	0	0	Kawabe, Komai	Bulletin of environmental contam
30652270	0	0	0	0	0	2019 Elucidating the dechlorination mechanism of hexachloroethane by Pd-doped zerovalent iron nanoparticles in dissolved le...	0	0	Rodrigues, Betelu, Colombano, Mas	Environmental science and polluti
30637791	0	0	0	0	0	2019 ZnO Nanosheets Abundant in Oxygen Vacancies Derived from Metal-Organic Frameworks for ppb-Level Gas Sensing.	0	0	Yuan, Aljneibi, Yuan, Wang, Liu, Fan	Advanced materials (Deerfield Be
30637211	0	0	0	0	0	2018 Aliphatic Halogenated Hydrocarbons: Report and Analysis of Liver Injury in 60 Patients.	1	0	Teschke	Journal of clinical and translationa
30625652	0	0	0	0	0	2019 Groundwater diffuse pollution in functional urban areas: The need to define anthropogenic diffuse pollution background l...	0	0	Azzellino, Colombo, Lombi, Marche	The Science of the total environm
30623720	0	0	0	0	0	2018 Removal of non-aqueous phase liquids (NAPLs) from TPH-saturated sandy aquifer sediments using in situ air sparging com...	0	0	Lee, Woo, Jeong	Journal of environmental science
30481679	0	0	0	0	0	2019 Acceleration of perchloroethylene dechlorination by extracellular secretions from Microbacterium in a mixed culture cont...	0	0	Wan, Chen, Chen, Miao, Liu, Ye, Che	Environmental pollution (Barking,
30415115	0	0	0	0	0	2019 The aqueous solubility of common organic groundwater contaminants as a function of temperature between 5 and 70 °C.	0	0	Koproch, Dahmke, Köber	Chemosphere
30412867	0	0	0	0	0	2019 Intrusion of chlorinated hydrocarbons and their degradation products from contaminated soil. Measurement of indoor air	0	0	Scheepers, Graumans, van Dael, de	The Science of the total environm
30400949	0	0	0	0	0	2018 Modeled exposure to tetrachloroethylene-contaminated drinking water and the occurrence of birth defects: a case-contrc...	1	0	Aschengrau, Gallagher, Winter, Butl	Environmental health : a global ac
30326388	0	0	0	0	0	2019 Multi-method assessment of the intrinsic biodegradation potential of an aquifer contaminated with chlorinated ethenes a...	0	0	Blázquez-Pallí, Rosell, Varias, Bosch	Environmental pollution (Barking,
30202895	0	0	0	0	0	2019 Modulation of Tetrachloroethylene-Associated Kidney Effects by Nonalcoholic Fatty Liver or Steatohepatitis in Male C57BL...	1	0	Cichocki, Luo, Furuya, Venkatratnan	Toxicological sciences : an official



Find very specific text through sifting (Main sheet)



Take notes and tag articles (Notes sheet)



Get an overview (Landscape sheet)

# Main sheet – query and get results

The image shows a spreadsheet with a PubMed query interface overlaid. The spreadsheet has columns for PMIDs and sifter terms. The query interface shows a search for 'tetrachloroethylene OR perchloroethylene' and a confirmation dialog for 2198 records.

PMID	sifter term 1	sifter term 2	sifter term 3	Year	Title
<a href="#">30886018</a>	0	0			
<a href="#">30847966</a>	0	0			
<a href="#">30737695</a>	0	0			
<a href="#">30736927</a>	0	0			
<a href="#">30670843</a>	0	0			
<a href="#">30528580</a>	0	0			
<a href="#">30528216</a>	0	0			
<a href="#">30506962</a>	0	0			
<a href="#">30503062</a>	0	0		2018	Cytochemical patterns of the peripheral
<a href="#">30486750</a>	0	0		2018	The evil eye effect: vertical pupils are p
<a href="#">30486050</a>	0	0		2018	A new species of Crocodile Newt Tyloto
<a href="#">30486023</a>	0	0		2018	Systematic revision of the living African
<a href="#">30408484</a>	0	0		2019	Assessing impacts of precocious steroid
<a href="#">30362660</a>	0	0		2019	Scaling of major organs in hatchling fem

Query PubMed

Enter your PubMed query and click on Submit.

tetrachloroethylene OR perchloroethylene

Continue

Your query has found 2198 records. Do you wish to continue?

Yes No

When this form goes away, your query is done.

# Lots of rows – using Sifting to find what’s relevant

A	B	C	D	E	F	G	H	I	J		
Abstract Sifter	Query PubMed		Query run: tetrachloroethylene OR perchloroethylene							Provided by the USEPA's National Center for Computational Toxicology	
v3	Your sifter terms and frequency counts										
	sifter term 1	sifter term 2	sifter term 3	Total	Pub		Take Group Notes	Highlight Noted	Review	PMC	
PMID					Yr	Title			Authors	Journal	
<a href="#">30856471</a>	0	0	0	0	2019	A comparison of the electrolysis of soil washing wastes with active and non-active electrodes.	0	0	Karaçali, Muñoz-Morales, Kalkan, K	Chemosphe	
<a href="#">30827336</a>	0	0	0	0	2019	Environmental and Genetic Factors Influencing Kidney Toxicity.	1	0	Lash	Seminars in	
<a href="#">30809199</a>	0	0	0	0	2019	Functional Genes and Bacterial Communities During Organohalide Respiration of Chloroethenes in Microcosms of Multi-C	0	1	Hermon, Hellal, Denonfoux, Vuilleu	Frontiers in	
<a href="#">30801570</a>	0	0	0	0	2019	Perchloroethylene: acute occupational poisoning and a proposal for its replacement with other less toxic substances.	0	0	Sanz-Gallen, Sanz-Ribas, Martí-Ame	Medycyna p	
<a href="#">30728999</a>	0	0	0	0	2018	Comparative investigation of argon and argon/oxygen plasma performance for Perchloroethylene (PCE) removal from aqu	0	1	Karimaei, Shokri, Khani, Yaghmaeia	Journal of e	
<a href="#">30721169</a>	0	0	0	0	2019	Extended Mortality Follow-up of a Cohort of Dry Cleaners.	0	0	Callahan, Stewart, Blair, Purdue	Epidemiolo	
<a href="#">30691860</a>	0	0	0	0	2019	Numerical modelling of the impact of surfactant partitioning on surfactant-enhanced aquifer remediation.	0	0	Babaei, Copty	Journal of c	
<a href="#">30685665</a>	0	0	0	0	2019	Degradation of tetra- and trichloroethylene under iron reducing conditions by Acidimicrobiaceae sp. A6.	0	0	Ge, Huang, Han, Jaffé	Environmen	
<a href="#">30666385</a>	0	0	0	0	2019	A Case Study of Natural Attenuation of Chlorinated Solvents Under Unstable Groundwater Conditions in Takahata, Japan.	0	0	Kawabe, Komai	Bulletin of e	
<a href="#">30652270</a>	0	0	0	0	2019	Elucidating the dechlorination mechanism of hexachloroethane by Pd-doped zerovalent iron microparticles in dissolved le	0	0	Rodrigues, Betelu, Colombano, Mas	Environmen	
<a href="#">30637791</a>	0	0	0	0	2019	ZnO Nanosheets Abundant in Oxygen Vacancies Derived from Metal-Organic Frameworks for ppb-Level Gas Sensing.	0	0	Yuan, Aljneibi, Yuan, Wang, Liu, Fan	Advanced n	
<a href="#">30637211</a>	0	0	0	0	2018	Aliphatic Halogenated Hydrocarbons: Report and Analysis of Liver Injury in 60 Patients.	0	1	Teschke	Journal of c	
<a href="#">30625652</a>	0	0	0	0	2019	Groundwater diffuse pollution in functional urban areas: The need to define anthropogenic diffuse pollution background	0	0	Azzellino, Colombo, Lombi, Marche	The Science	
<a href="#">30623720</a>	0	0	0	0	2018	Removal of non-aqueous phase liquids (NAPLs) from TPH-saturated sandy aquifer sediments using in situ air sparging com	0	0	Lee, Woo, Jeong	Journal of e	
<a href="#">30481679</a>	0	0	0	0	2019	Acceleration of perchloroethylene dechlorination by extracellular secretions from Microbacterium in a mixed culture cont	0	0	Wan, Chen, Chen, Miao, Liu, Ye, Che	Environmen	
<a href="#">30415115</a>	0	0	0	0	2019	The aqueous solubility of common organic groundwater contaminants as a function of temperature between 5 and 70 °C.	0	0	Koproch, Dahmke, Köber	Chemosphe	
<a href="#">30412867</a>	0	0	0	0	2019	Intrusion of chlorinated hydrocarbons and their degradation products from contaminated soil. Measurement of indoor air	0	0	Scheepers, Graumans, van Dael, de	The Science	
<a href="#">30400949</a>	0	0	0	0	2018	Modeled exposure to tetrachloroethylene-contaminated drinking water and the occurrence of birth defects: a case-contr	0	1	Aschengrau, Gallagher, Winter, Butl	Environmen	

2198 citations downloaded  
in 35 seconds

# Sifter terms to find things fast

	A	B	C	D	E	F	G
1	Abstract Sifter		Query PubMed			Query ru	
2	v3	Your sifter terms and frequency counts					
		dose	mg/kg	ppm	total	Pub	
3	PMID				Yr	Title	
4	<a href="#">12778199</a>	35	2	0	37	1983 Carcinog	0-20-6)
5	<a href="#">12778204</a>	26	0	0	26	1983 Carcinog	-7) in F:
6	<a href="#">12748687</a>	20	4	1	25	1986 NTP Toxi	opane (
7	<a href="#">11803702</a>	17	13	0	30	1999 NTP tech	of chlor
8	<a href="#">12844153</a>	15	4	0	19	1977 Bioassay	
9	<a href="#">12209189</a>	10	0	11	21	1993 NTP tech	xture of
10	<a href="#">28973375</a>	10	2	0	12	2017 Editor's F	ver and
11	<a href="#">12748718</a>	9	0	11	20	1986 NTP Toxi	ylene (
12	<a href="#">17267091</a>	9	1	0	10	2007 Impact o	e in Sw
13	<a href="#">8870953</a>	8	3	0	11	1996 Bone ma	steine c
14	<a href="#">7783250</a>	8	3	0	11	1995 A multid	temict
15	<a href="#">16291521</a>	8	0	0	8	2005 Physiolo	dels in
16	<a href="#">24910396</a>	7	0	0	7	2014 Differen	rnosed

If looking for animal studies ... try:

Rats  
Mice  
Toxic  
Liver  
Hepato  
Brain  
Lung

Enter terms (strings of characters) of interest in the Sifter cells.

Automatically the Sifter counts the occurrences of that term in the title, abstract, and key words.

Here Excel built-in sorting and filtering is really useful!

# Double-click on row to see the abstract

A	B	D
1	Abstract with highlights <span data-bbox="580 354 715 401">&lt;-- Main</span> <span data-bbox="774 354 894 401">Add Note</span> <span data-bbox="963 354 1174 401">See Notes -&gt;</span> <span data-bbox="1658 354 1837 401">Like this?</span>	
2	Article: <a href="#">12844153</a>	PubYr
4	Title: Bioassay of tetrachloroethylene for possible carcinogenicity.	1977
4	<b>Title and Abstract:</b> Bioassay of tetrachloroethylene for possible carcinogenicity. Abstract: Title: The bioassay of U.S.P.-grade tetrachloroethylene for possible carcinogenicity was conducted using Osborne-Mendel rats and B6C3F1 mice. Tetrachloroethylene in corn oil was administered by gavage at either of two dosages to groups of 50 male and 50 female animals of each species, 5 days a week, over a period of 78 weeks followed by an observation period of 32 weeks for rats and 12 weeks for mice. Initial dosage levels for the chronic bioassay were selected on the basis of a preliminary subchronic toxicity test. Subsequent dosage adjustments were made during the course of the chronic bioassay. The high and low time-weighted average dosages of tetrachloroethylene in the chronic study were 941 and 471 mg/kg/day for the male rats, 949 and 474 mg/kg/day for the female rats, 1,072 and 536 mg/kg/day for the male mice, and 772 and 386 mg/kg/day for the female mice. For each species, 20 animals of each sex were placed on test as vehicle controls. These animals were gavaged with corn oil at the same time that dosed animals were gavaged with tetrachloroethylene mixtures. Twenty animals of each sex were placed on test as untreated controls for each species. These animals received no gavage treatments. No significant increased incidence of neoplastic lesions was observed in treated rats. In both dosed and control rats, respiratory disease was observed with increasing frequency for the latter part of the first year until termination of the bioassay. Lesions indicative of pneumonia were observed in nearly all rats at necropsy. A high incidence of toxic nephropathy was observed in treated rats. Toxic nephropathy was noted in rats that died early in the study (as early as week 20 for male rats and week 28 for female rats). Mortality of rats was dose-related. Fifty percent of the high dose males had died by week 44 and 50 percent of the high dose females had died by week 66. In both male and female mice, administration of tetrachloroethylene was associated with a significantly increased incidence of hepatocellular carcinoma. Hepatocellular carcinomas were observed in 2/17 (12 percent) untreated control males, 2/20 (10 percent) vehicle control males, 32/49 (65 percent) low dose males, 27/48 (56 percent) high dose males, 2/20 (10 percent) untreated control females, 0/20 vehicle control females, 19/48 (40 percent) low dose females, and 19/48 (40 percent) high dose females. Hepatocellular carcinomas metastasized to the kidney in one untreated control male and to the lung in three low dose males, one low dose female, and one high dose female. Toxic nephropathy, similar to that observed in rats, was also observed in treated but not control mice. Fisher exact tests indicated a highly significant increased incidence of	

Colorization makes it easy to read.

# Sifting – to find things Not of interest

Abstract Sifter		Query PubMed		Query run: tetrachloroethylene OR perchloroethylene		
v3	Your sifter terms and frequency counts					
PMID	tetrachlo	dose	dechlor	Total	Pub	Title
10 10664879	13	0	2	15	1999	Tetrachloroethene-dehalogenating bacteria.
11 26766361	12	0	1	13	2016	The effects of co-contaminants and native wetland sediments on the
20 9385143	10	0	4	14	1997	Comparative studies on tetrachloroethene reductive dechlorination
27 23995945	9	0	2	11	2013	Functional genotyping of Sulfurospirillum spp. in mixed cultures allo
38 12831046	8	0	13	21	2003	Reductive dechlorination of carbon tetrachloride and tetrachloroethy
40 8663199	8	0	2	10	1996	Purification and characterization of tetrachloroethene reductive deh
60 15959725	7	0	5	12	2005	Biochemical and molecular characterization of a tetrachloroethene d
61 11995827	7	0	3	10	2001	Product distribution during transformation of multiple contaminants
62 11976751	7	0	1	8	2002	Tetrachloroethene reductive dehalogenase of Dehalospirillum multi
64 9082914	7	0	3	10	1996	Studies on tetrachloroethene respiration in Dehalospirillum multivoi
67 2403257	7	0	4	11	1990	Tetrachloroethene transformation to trichloroethene and cis-1,2-dicl
68 6859849	7	0	1	8	1983	Transformations of 1- and 2-carbon halogenated aliphatic organic con
76 10797233	6	0	5	11	2000	ATR-FTIR sensor development for continuous on-line monitoring of c
83 22961902	6	0	1	7	2012	Impact of vitamin B12 on formation of the tetrachloroethene reducti
84 22503214	6	0	1	7	2012	Successful microcosm demonstration of a strategy for biodegradator
85 22115467	6	0	12	18	2012	Dechlorination of chlorinated hydrocarbons by bimetallic Ni/Fe imm
86 21243405	6	0	8	14	2011	Reductive dechlorination of tetrachloroethene by a stepwise catalysi
92 16715399	6	0	3	9	2006	Anaerobic bioremediation of groundwater containing a mixture of 1,
93 15984786	6	0	5	11	2005	Enhanced dechlorination of chlorinated methanes and ethenes by ch
94 15746376	6	0	3	9	2005	Characterization of hydrogenase and reductive dehalogenase activiti
97 12708306	6	0	4	10	2003	[Degradation of volatile chlorinated aliphatics by zero-valent iron].
103 9171062	6	0	3	9	1997	Isolation of a bacterium that reductively dechlorinates tetrachloroeth

# Keeping track of what you find

- Notes
- Adds rows to the Notes sheet

# Taking notes

First select the rows

Then click here

	A	B	C	D	E	F	G	H	I	J
1	Abstract Sifter	Query PubMed				Query run: tetrachloroethylene OR perchloroethylene				Provided by the US Center for Computational Toxicology
2	v3	Your sifter terms and frequency counts								
		tetrachloro	dose	rat	Total	Pub				
3	PMID				Yr	Title		Review	PMC	Authors
4	12748718	25	9	20	54	1986	NTP Toxicology and Carcinogenesis Studies of Tetrachloroethylene (Perchloroethylene) (CAS No. 127-18-4) in F344/N Rats	0	0	
5	7131586	14	4	1	19	1982	Cardiopulmonary toxicity of tetrachloroethylene.	0	0	Kobayashi, Hutche
7	15147	13	1	1	15	1976	[Metabolism of tetrachloroethylene in guinea pigs (author's transl)].	0	0	Sakamoto
11	7726643	11	6	7	24	1995	Induction of rat liver drug-metabolizing enzymes by tetrachloroethylene.	0	0	Hanioka, Jinno, Toy
20	3296316	9	2	4	15	1986	Differences in rat liver enzyme-altered foci produced by chlorinated aliphatics and phenobarbital.	1	0	Story, Meierhenry,
21	6874093	9	1	0	10	1983	Health surveillance of workers exposed to tetrachloroethylene in dry-cleaning shops.	0	0	Lauwerys, Herbran
25	12778199	8	35	18	61	1983	Carcinogenesis Studies of 1,1,1,2-Tetrachloroethane (CAS: 630-20-6) in F344/N Rats and B6C3F1 Mice (Gavage Studies).	0	0	
26	12844153	8	15	15	38	1977	Bioassay of tetrachloroethylene for possible carcinogenicity.	0	0	
27	2361581	8	2	4	14	1990	Dose-dependent cytotoxicity of chlorinated hydrocarbons in isolated rat hepatocytes.	0	0	Dahlström-King, Cc
28	4057308	8	1	0	9	1985	Acute tetrachloroethylene poisoning--blood elimination kinetics during hyperventilation therapy.	0	0	Köppel, Arndt, Arei
29	6857689	8	1	5	14	1983	Tetrachloroethylene: balance and tissue distribution in male Sprague-Dawley rats by drinking-water administration.	0	0	Frantz, Watanabe
40	19892777	7	2	0	9	2010	DNA damage detected by the alkaline comet assay in the liver of mice after oral administration of tetrachloroethylene.	0	0	Cederberg, Henriks
41	8215591	7	1	1	9	1993	Cancer risk and tetrachloroethylene-contaminated drinking water in Massachusetts.	0	0	Aschengrau, Ozonc
42	4096155	7	1	1	9	1985	[Tetrachloroethylene: effect of low concentrations of 1,1,2-tetrachloroethylene (perchloroethylene) on organisms in the	0	0	Marth, Stünzner, Bi
55	3732662	6	6	8	20	1986	The subchronic toxicity of tetrachloroethylene (perchloroethylene) administered in the drinking water of rats.	0	0	Hayes, Condie, Bor
56	2586542	6	2	0	8	1989	Clastogenicity evaluation of seven chemicals commonly found at hazardous industrial waste sites.	0	0	Sandhu, Ma, Peng,
57	1828122	6	1	3	10	1991	Potentiating effects of chlorinated hydrocarbons on carbon tetrachloride toxicity in isolated rat hepatocytes and plasma m	0	0	Kefalas, Stacey
58	3113093	6	1	0	7	1987	Effects of trichloroethylene, tetrachloroethylene and dichloromethane on soil biomass and microbial counts.	0	0	Kanazawa, Filip
84	8459786	5	2	4	11	1993	Assessment of behavioral effects of tetrachloroethylene using a set of time-series analyses.	0	0	Motohashi, Miyaza
85	2124380	5	2	4	11	1990	Chronic inhalation effects of tetrachloroethylene on hepatic and renal microsomal electron transport components and del	0	0	Soni, Nomiya, N
86	12948058	5	1	0	6	2003	H2 consumption during the microbial reductive dehalogenation of chlorinated phenols and tetrachloroethene.	0	0	Mazur, Jones, Tebe
87	12868798	5	1	0	6	2002	Concordance across species in the reproductive and developmental toxicity of tetrachloroethylene.	1	0	Beliles

Enter tag, note, color flag. Notes and tags are whatever you want them to be.

Abstract Sifter Query PubMed Query run: tetrachloroethylene OR perchloroethylene

v3 Your sifter terms and frequency counts

tetrachloro dose rat Total Pub

PMID	tetrachloro	dose	rat	Total	Pub Yr	Title
12748718	25	9	20	54	1986	NTP Toxicology
7131586	14	4	1	19	1982	Cardiopulmona
15147	13	1	1	15	1976	[Metabolism o
7726643	11	6	7	24	1995	Induction of ra
3296316	9	2	4	15	1986	Differences in
6874093	9	1	0	10	1983	Health surveill
12778199	8	35	18	61	1983	Carcinogenesis
12844153	8	15	15	38	1977	Bioassay of tet
2361581	8	2	4	14	1990	Dose-depende
4057308	8	1	0	9	1985	Acute tetrachl
6857689	8	1	5	14	1983	Tetrachloroeth
19892777	7	2	0	9	2010	DNA damage d
8215591	7	1	1	9	1993	Cancer risk and
4096155	7	1	1	9	1985	[Tetrachloroet
3732662	6	6	8	20	1986	The subchronic
2586542	6	2	0	8	1989	Clastogenicity
1828122	6	1	3	10	1991	Potentiating et
3113093	6	1	0	7	1987	Effects of trich
8459786	5	2	4	11	1993	Assessment of
2124380	5	2	4	11	1990	Chronic inhalation effects of tetrachloroethylene on hepatic and renal microsomal electron transport components and del
12948058	5	1	0	6	2003	H2 consumption during the microbial reductive dehalogenation of chlorinated phenols and tetrachloroethene.

Take Group Notes Highlight Noted view MC

GroupNotes

Enter a comment or note for the selected articles:

Tag:  *Tags and Notes are whatever you want them to be.*

Note:

Yes  No  Maybe

OK

Soni, Nomiya, Nomiya. Mazur, Jones, Tebes-Steven

# What the Notes sheet looks like ...

A	B	C	D	F	G	H	I	J	K	N
My Notes					<--Back		Highlight Noted PMIDs	Export	Note: Feel free to delete rows after Row 2, but not columns. Some sample Notes may be displayed.	
	yes	no	maybe							
PMID			Tag	Note	PubYr	Title	Authors	Journal	When Noted	
<a href="#">3732662</a>	1	0	0	Rat dose studies	1986	The subchronic toxicity of tetrachloroethylene (perchloroethylene) administered in the drinking water	Hayes, Condie, Borzelleca	Fundamental and applied toxicology	3/19/2019 15:03	
<a href="#">8459786</a>	1	0	0	Rat dose studies	1993	Assessment of behavioral effects of tetrachloroethylene using a set of time-series analyses.	Motohashi, Miyazaki, Takano	Neurotoxicology and teratology	3/19/2019 15:03	
<a href="#">2124380</a>	1	0	0	Rat dose studies	1990	Chronic inhalation effects of tetrachloroethylene on hepatic and renal microsomal electron transport	Soni, Nomiyama, Nomiyama	Toxicology letters	3/19/2019 15:03	
<a href="#">12778199</a>	1	0	0	Rat dose studies	1983	Carcinogenesis Studies of 1,1,1,2-Tetrachloroethane (CAS: 630-20-6) in F344/N Rats and B6C3F1 Mice (Gavage Studies).		National Toxicology Program technical report	3/19/2019 15:03	
<a href="#">12844153</a>	1	0	0	Rat dose studies	1977	Bioassay of tetrachloroethylene for possible carcinogenicity.		National Cancer Institute carcinogenesis studies	3/19/2019 15:03	

	A	B	C	D	E	F	G	H	I
1	Abstract Sifter		Query PubMed				Query run: tetrachloroethylene OR perchloroethylene		Provided by Center for C Toxicology
2	v3	Your sifter terms and frequency counts							
		tetrachloro	dose	dry-clean	Total	Pub		Take Group Notes	Highlighted Noted
3	PMID				Yr	Title		Review	PMC
4	11911491	1	7	0	8	2002 Chronic toxicity of a mixture of chlorinated alkanes and alkenes in ICR mice.		0	0
5	19464572	2	6	0	8	2009 Contribution of trichloroacetic acid to liver tumors observed in perchloroethylene (perc)-exposed mice.		0	0
6	30202895	2	5	0	7	2019 Modulation of Tetrachloroethylene-Associated Kidney Effects by Nonalcoholic Fatty Liver or Steatohepatitis in Male C57Bl		1	0
7	19101834	1	2	0	3	2008 Final report on the safety assessment of Trichloroethane.		0	0
8	28148637	4	1	0	5	2017 Impact of Nonalcoholic Fatty Liver Disease on Toxicokinetics of Tetrachloroethylene in Mice.		0	1
9	12778199	8	35	0	43	1983 Carcinogenesis Studies of 1,1,1,2-Tetrachloroethane (CAS: 630-20-6) in F344/N Rats and B6C3F1 Mice (Gavage Studies).		0	0
10	12844153	8	15	0	23	1977 Bioassay of tetrachloroethylene for possible carcinogenicity.		0	0
11	2361581	8	2	0	10	1990 Dose-dependent cytotoxicity of chlorinated hydrocarbons in isolated rat hepatocytes.		0	0
12	3732662	6	6	0	12	1986 The subchronic toxicity of tetrachloroethylene (perchloroethylene) administered in the drinking water of rats.		0	0
13	8459786	5	2	0	7	1993 Assessment of behavioral effects of tetrachloroethylene using a set of time-series analyses.		0	0
14	2124380	5	2	0	7	1990 Chronic inhalation effects of tetrachloroethylene on hepatic and renal microsomal electron transport components and del		0	0
15	7992032	2	0	11	13	1994 Indoor exposure to perchloroethylene (PCE) in individuals living with dry-cleaning workers.		0	0
16	11843196	2	0	10	12	2002 An evaluation of retrofit engineering control interventions to reduce perchloroethylene exposures in commercial dry-clea		0	0
17	28085652	0	0	9	9	1999 Residual Perchloroethylene in Dry-Cleaned Acetate: The Effect of Pressing and Extent of Inter-Dry-Cleaner Variability.		0	0
18	22538166	2	0	8	10	2012 Colloidal interactions in liquid CO2--a dry-cleaning perspective.		1	0
19	1824329	10	0	7	17	1991 Effect of dry-cleaned clothes on tetrachloroethylene levels in indoor air, personal air, and breath for residents of several N		0	0
20	19298226	5	0	7	12	2009 A first French assessment of population exposure to tetrachloroethylene from small dry-cleaning facilities.		0	0
21	11843197	2	0	7	9	2002 Effects of retrofit emission controls and work practices on perchloroethylene exposures in small dry-cleaning shops.		0	0
22	2924758	4	0	6	10	1989 Residual tetrachloroethylene in dry-cleaned clothes.		0	0
23	9353538	14	0	5	19	1996 Internal and external tetrachloroethene exposure of persons living in differently polluted areas of Northrhine-Westphalia		0	0
24	30186333	2	0	5	7	2018 Preliminary Study: Environmental Assessment of Perchloroethylene in Dry-Cleaning Facilities in the UAE.		1	0
25	21898565	2	0	5	7	2011 Quantification of perchloroethylene residues in dry-cleaned fabrics.		0	0
26	23898811	0	1	5	6	2000 Kidney and liver biomarkers in female dry-cleaning workers exposed to perchloroethylene.		0	0

Highlighted:

Helps with article triage: what have I evaluated ... what did I think.

# Demo Case study

- (Pretend) use case was to identify rodent dose studies and categorize all

Summary : fast and easy way to triage and organize the literature on a chemical.

- Pivot table built from Notes sheet to summarize

	A	B	C	D	E
1	Tetrachloroethylene/perchloroethylene triage				
2					
3	<b>Tag</b>	<b>Maybe</b>	<b>No</b>	<b>Yes</b>	
4	Breathing/air	8	0	0	
5	Chemistry	0	142	0	
6	Cytotox	7	0	0	
7	Dechlorination	0	99	0	
8	Degradation	0	348	0	
9	Dry cleaning	0	227	0	
10	Embryotoxicity	1	0	0	
11	Exposure	0	123	0	
12	General effects	4	0	0	
13	Groundwater	0	45	0	
14	Identification	0	10	0	

22	Not English	0	249	0	
23	Occupational	0	106	0	
24	PBPK	10	0	0	
25	Rats	0	0	127	
26	Rats/mice	0	0	1	
27	Remediation	0	85	0	
28	Soil	0	16	0	
29	Testing	1	0	0	
30	Ther use	0	7	0	
31	Various	0	75	0	
32	Water	2	0	0	
33	<b>Grand Total</b>	<b>89</b>	<b>1866</b>	<b>243</b>	<b>2198</b>
34					

# Common chemical toxicity tasks

- One chemical
  - Deep dive – review literature for a chemical
  - Challenge: Can be thousands of articles, and only a few relevant
- **Many chemicals**
  - Overview to rank for prioritization
  - What do they have in common
- Mechanistic inquiry – by which mechanism (adverse outcome pathway) is a given chemical or set of chemicals acting
- Ad hoc quick lookup

# Landscape Sheet

	B	C	I	J
1	Landscape View			
2		<input type="button" value="Update Article Counts"/> <input type="button" value="View / hide queries"/> <input type="button" value="Heat Map by column"/> <input type="button" value="Heat Map by row"/>		
3			zebrafish AND behavior	occupational exposure
4			<i>Subject queries:</i>	
5	Preferred Name	Chemical / Entity query	zebrafish / behavior	occ expo
6	PERC/PCE/perchloroethylene	Tetrachloroethylene[majr]	0	13
7	Tripropylene glycol	Tripropylene glycol OR 24800-44-0	0	5
8	Tetrachlorophthalic anhydride	Tetrachlorophthalic anhydride	0	8
9	Phthalic anhydride	Phthalic anhydride		
10	Linalool	Linalool		
11	Toluene 2,4-Diisocyanate	Toluene 2,4-Diisocyanate	0	361
12	TBBPA	Tetrabromobisphenol A OR TBBPA	9	21
13	TPHP	Triphenyl phosphate	5	17
14	BDE-100	2,2',4,4',6-Pentabromodiphenyl ether OR BDE-100 OR 18904-64-8	8	31
15				

(Toluene 2,4-Diisocyanate) AND (occupational exposure)

# Sample queries sheet

	A	B	D
1	<b>Sample Queries</b>		<a href="#">Send queries to Landscape</a>
2			
3	<b>Category</b>	<b>Heading</b>	<b>Query (double-click to see how the query looks to PubMed)</b>
4	Ecological	Algae	"algal bloom" OR eutrophication OR algae)
5	Epidemiology	Epi	epidemiology
6	Exposure	Dust exposure	environmental exposure AND dust
7	Exposure	Food exposure	environmental exposure AND food
8	Exposure	Water exposure	environmental exposure AND (water OR groundwater OR drinking water)
9	Emergency/disaster	Emergency / disaster	(emergency OR spill OR disaster or hurricane OR flood OR explosion OR forest fire OR wildfire OR climate ch
10	Mechanism	Oxidative stress	"oxidative stress" OR "free radicals" OR "reactive oxygen species" OR peroxides
11	Metabolism	Metabolism	(metabolism OR metabolite OR tissue distribution OR pharmacokinetics OR pharmacodynamics)
12	Methods	Analytical chemistry	"Chemistry Techniques, Analytical" OR analytical chemistry
13	Methods	Statistical	Statistics as Topic[mh] OR statistics OR statistical
14	Methods	In vitro	In Vitro Techniques[mh] OR cell culture or "in vitro"
15	Mixtures	Mixtures	(Drug synergism[mh] OR cocarcinogenesis OR pesticide synergists[mh] OR mixture[tiab] OR mixtures[tiab]
16	Medicine	Clinical trials	((clinical[Title/Abstract] AND trial[Title/Abstract]) OR clinical trial[Publication Type] )
17	Medicine	Clinical trials in children	((children OR child OR infants) AND human) AND ((clinical[Title/Abstract] AND trial[Title/Abstract]) OR clini
18	Medicine	Obesity	(obesity OR obese OR adipose OR overweight Or adipogenesis OR adipose tissue)
19	Toxicity	Genetox	(dna/drug effects OR DNA Damage OR chromosome aberrations OR genotoxicity OR micronucleus OR DNA
20	Toxicity	Cancer	neoplasms or cancer
21	Toxicity	ReproTox	(reproduction AND (toxicity OR abnormal OR adverse effects))
22	Toxicity	NeuroTox	(neurotoxicity OR (Nervous system diseases and chemically induced) OR ((neurons OR brain OR behavior) A
23	Toxicity	DevTox	(toxicity OR congenital abnormalities OR Prenatal Exposure Delayed Effects) AND (fetus OR embryo OR emb
24	Toxicity	Skin sensitization	("allergic" AND "contact" And dermatitis) OR Dermatitis, Allergic Contact[mh]
25	Toxicity	Respiratory sensitisation	(Respiratory hypersensitivity OR respiratory sensitization OR Bronchial Hyperreactivity OR Respiration Diso
26	Use	Pharmaceutical	"therapeutic use" OR "therapeutic use"[subheading]" OR pharmacologic actions[mh] OR drug therapy
27	Use	Pesticide	pesticide OR insecticide OR rodenticide OR fungicide

# To use sample queries

	A	B	D
1	<b>Sample Queries</b>		<i>Note: these are starting points ... please expand and customize</i>
2			
3	<b>Category</b>	<b>Heading</b>	<b>Query (double-click to see how the query looks to PubMed)</b>
16	Medicine	Clinical trials	((clinical[Title/Abstract] AND trial[Title/Abstract]) OR clinical trial[Publication Type] )
17	Medicine	Clinical trials in children	((children OR child OR infants) AND human) AND ((clinical[Title/Abstract] AND trial[Title/Abstract]) OR clinical trial[Publication Type] )
18	Medicine	Obesity	(obesity OR obese OR adipose OR overweight Or adipogenesis OR adipose tissue)
19	Toxicity	Genetox	(dna/drug effects OR DNA Damage OR chromosomal damage OR DNA Repair OR mutagenesis)
20	Toxicity	Cancer	neoplasms or cancer
21	Toxicity	ReproTox	(reproduction AND (toxicity OR abnormal OR adverse effects))
22	Toxicity	NeuroTox	(neurotoxicity OR (Nervous system diseases and chemical effects)) AND drug effects)
23	Toxicity	DevTox	(toxicity OR congenital abnormalities OR Prenatal Effects) AND embryonic development
24	Toxicity	Skin sensitization	("allergic" AND "contact" And dermatitis) OR Dermatitis
25	Toxicity	Respiratory sensitisation	(Respiratory hypersensitivity OR respiratory sensitization OR Bronchial Hyperreactivity OR Respiration Disorders OR Respiratory Diseases)
26	Use	Pharmaceutical	"therapeutic use" OR "therapeutic use"[subheading]" OR pharmacologic actions[mh] OR drug therapy
27	Use	Pesticide	pesticide OR insecticide OR rodenticide OR fungicide
28	Use	Cosmetics	cosmetics OR beauty
29	Use	Explosive Agents	Explosive Agents OR explosive OR explosives
30	Use	Food	food OR diet OR beverage OR nutrition
31	Use	Surface-acting	Antifoaming OR Anti-foaming OR detergent OR detergents OR soap OR detergent OR surfactant
32	Use	Dye/coloring	dye OR "coloring agent" OR pigment OR pigments
33	Use	Fertilizer	fertilizer OR fertilize
34	Use	Solvents	solvents OR solvent
35			

Send queries to Landscape

First select rows of interest, then click on this button.



The queries will be inserted into row 3. Select the intersection region and click on Update Article Counts.

		Genetox	Cancer	ReproTox	NeuroTox	DevTox	Skin sensitization
<div style="display: flex; justify-content: space-between; border-bottom: 1px solid black;"> <span>Update Article Counts</span> <span>View / hide queries</span> <span>Heat Map by column</span> <span>Heat Map by row</span> </div>							
<i>Subject queries:</i> effects OR DNA Damage OR chromosome aberrations OR genotoxicity OR micronuclei		neoplasms or cancer		(reproduction AND (toxicity OR abnormal OR adverse effects))	city OR (Nervous system diseases and chemically induced) OR ((neurons OR brain OR	OR congenital abnormalities OR Prenatal Exposure Delayed Effects) AND (fetus OR embryo	("allergic" AND "contact" And dermatitis ) OR Dermatitis , Allergic Contact[mh])
Chemical / Entity query		Genetox	Cancer	ReproTox	NeuroTox	DevTox	Skin sensitization
<input type="text" value="Tetrachloroethylene[majr]"/>							
<input type="text" value="Tripropylene glycol OR 24800-44-0"/>							
<input type="text" value="Tetrachlorophthalic anhydride"/>							
<input type="text" value="Phthalic anhydride"/>							
<input type="text" value="Linalool"/>							
<input type="text" value="Toluene 2,4-Diisocyanate"/>							
<input type="text" value="Tetrabromobisphenol A OR TBBPA"/>							
<input type="text" value="Triphenyl phosphate"/>							
<input type="text" value="2,2',4,4',6-Pentabromodiphenyl ether OR BDE-100 OR 189084-64-8"/>							



# Get the article counts

... then click here->

Update Article Counts

View / hide queries

Heat Map by column

Heat Map by row

effects OR DNA Damage OR chromosome aberrations OR genotoxicity OR micronucleus OR neoplasms or cancer (reproduction AND (toxicity OR abnormal OR adverse effects)) city OR (Nervous system diseases and chemically induced) OR ((neurons OR brain OR OR embryonic OR congenital abnormalities OR Prenatal Exposure Delayed Effects) AND (fetus OR embryo)) ("allergic" AND "contact" And dermatitis ) OR Dermatitis , Allergic Contact[mh]

*Subject queries:*

Chemical / Entity query

Genetox

Cancer

ReproTox

NeuroTox

DevTox

Skin sensitization

Tetrachloroethylene[majr]						
Tripropylene glycol OR 24800-44-0						
Tetrachlorophthalic anhydride						
Phthalic anhydride						
Linalool						
Toluene 2,4-Diisocyanate						
Tetrabromobisphenol A OR TBBPA						
Triphenyl phosphate						
2,2',4,4',6-Pentabromodiphenyl ether OR BDE-100 OR 189084-64-8						

First select the cells of interest ...

# Queries built and counts retrieved

Update Article Counts   View / hide queries   Heat Map by column   Heat Map by row

effects OR DNA Damage OR chromosome  
city OR (Nervous system diseases and  
OR congenital abnormalities OR Prenatal  
("allergic" AND "contact" AND

Summary : fast and easy way to get a bird's eye view of a set of chemicals and their effects.

Chemical / Entity query	Genetox	Cancer	ReproTox	NeuroTox	DevTox	Skin sensitization
Tetrachloroethylene[majr]	42	75	38	68	14	0
Tripropylene glycol OR 24800-44-0	4	3	0	0	0	5
Tetrachlorophthalic anhydride	1	0	0	1	0	0
Phthalic anhydride	16	50	4	36	6	40
Linalool	40	52	5	153	22	47
Toluene 2,4-Diisocyanate	62	33	6	40	2	44
Tetrabromobisphenol A OR TBBPA	15	46	44	75	53	0
Triphenyl phosphate	8	11	20	25	24	3
2,2',4,4',6-Pentabromodiphenyl ether OR BDE-100 OR 189084-64-8	10	28	74	82	58	0

# Common chemical toxicity tasks

- One chemical
  - Deep dive – review literature for a chemical
  - Challenge: Can be thousands of articles, and only a few relevant
- Many chemicals
  - Overview to rank for prioritization
  - What do they have in common
- Mechanistic inquiry – by which mechanism (adverse outcome pathway) is a given chemical or set of chemicals acting
- Ad hoc quick lookup



Let's review what's there ...

Update Article Counts	View / hide queries	Heat Map by column	Heat Map by row									
OR congenital abnormalities OR Prenatal Exposure Delayed Effects) AND (fetus	(Pregnane X Receptor OR NR112 protein) AND (activate OR activation	((thyroid hormone OR t3 OR t4) AND (brain or cortex or	hormone OR t3 OR t4) AND (serum or blood or plasma) and (decrease OR inhibition	(glucuronyltransferase AND upregulation OR agonism	glucuronides) AND (increase OR upregulation) AND (bile OR biliary OR urine OR excrete	((hippocampus AND (anatomy) and	((hippocampus AND (physiology) and	AND drug effects) OR (ear AND drug effects) OR (Neurons, Afferent OR auditory hair cells				

Summary : fast and easy way to get a bird's eye view of a set of chemicals and by which mechanisms and pathways they may act.

Toluene 2,4-Diisocyanate	2	0	0	0	0	0	0	0	0	40
Tetrabromobisphenol A OR TBBPA	53	0	17	4	0	0	1	1	3	
Triphenyl phosphate	24	2	1	1	0	0	0	0	0	
2,2',4,4',6-Pentabromodiphenyl ether OR BDE-100 OR 189084-64-8	58	2	11	6	3	0	0	5	2	

Overview of Devtox

Developmental ototoxicity via AOP8?

# Common chemical toxicity tasks

- One chemical
  - Deep dive – review literature for a chemical
  - Challenge: Can be thousands of articles, and only a few relevant
- Many chemicals
  - Overview to rank for prioritization
  - What do they have in common
- Mechanistic inquiry – by which mechanism (adverse outcome pathway) is a given chemical or set of chemicals acting
- Ad hoc quick lookup

# EPA's other implementation of the sifter technology

## EPA's Comptox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>

The screenshot shows the EPA Comptox Chemicals Dashboard. The browser address bar displays <https://comptox.epa.gov/dashboard>. The EPA logo and navigation menu are visible at the top. The dashboard header indicates "875 Thousand Chemicals". A search bar is highlighted with a red circle, containing the text "tetrachloroethylene". Below the search bar, the results list "Tetrachloroethylene" with the DTXSID2021319 and "Tetrachloroethylene-13C1".

United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

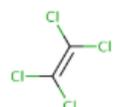
875 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

tetrachloroethylene

Tetrachloroethylene  
DTXSID2021319

Tetrachloroethylene-13C1



# Tetrachloroethylene

127-18-4 | DTXSID2021319

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ▶ ADME
- ▶ EXPOSURE
- ▶ BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- ▼ LITERATURE
  - GOOGLE SCHOLAR
  - PUBMED ABSTRACT SIFTER**
  - PUBCHEM ARTICLES
  - PUBCHEM PATENTS
  - PPRTV
  - IRIS
- LINKS
- COMMENTS

1) Select PubMed starting point query then 2) click on Retrieve. 

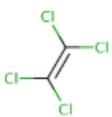
Select a Query Term  Retrieve Articles

- Select a Query Term
- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Cancer
- Clinical Trials
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure
- Food and Exposure
- Water and Exposure
- Algae
- Disaster / Emergency

## Abstract Sifter

Optionally, edit the query before retrieving.

"127-18-4" OR "Tetrachloroethylene"



Tetrachloroethylene  
127-18-4 | DTXSID2021319  
Searched by DSSTox Substance Id.

## Abstract Sifter

1) Select PubMed starting point query then 2) click on Retrieve.

Exposure

Retrieve Articles

99 of 99 articles loaded...

Optionally, edit the query before retrieving.

("127-18-4" OR "Tetrachloroethylene") AND (exposure OR near-field OR far-field OR SHEDS[tiab] AND ENVIRONMENTAL MONITORING)



To find articles quickly, enter terms to sift abstracts.

occup worker expos vapor visual  Clear Terms

Download / Send to... Download Sifter for Excel

Summary : fast and easy way to find specific literature about a chemical.

Clear Terms

	occup	worker	expos	vapor	visual	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	0	3	0	0	0	3					and public health	
<input type="checkbox"/>	2	0	0	0	0	2						
<input type="checkbox"/>	0	0	0	0	0	0						
<input type="checkbox"/>	0	0	0	0	0	0						
<input type="checkbox"/>	4	0	0	0	0	4						
<input type="checkbox"/>	0	0	0	0	0	0						
<input type="checkbox"/>	0	0	0	0	0	0						
<input type="checkbox"/>	0	0	0	0	0	0						
<input type="checkbox"/>	0	0	0	0	0	0						
<input type="checkbox"/>	1	0	3	0	0	4	30186333	2018	Preliminary Study: Environmental Assessment of Perchloroethylene in Dry-Cleaning Facilities in the UA			
<input type="checkbox"/>	1	2	1	0	0	4	30058609	2018	Further examination of log Pow-based procedures to estimate biological occupational exposure limits.			
<input type="checkbox"/>	0	1	1	0	0	2	25323406	2014	Measurements of chlorinated volatile organic compounds emitted from office printers and photocopiers.	Kowalska; Szewczyńska; Pośniak	Environmental science and pollution research inter...	
<input type="checkbox"/>	0	0	4	3	0	7	24195534	2013	Short duration needle trap sampling with gas chromatography analysis to determine nearly instantaneous concentrations of selec...	Strating; Juarez; Stevens; White; Smith	Journal of occupational and environmental hygiene	
<input type="checkbox"/>	3	7	6	0	0	16	24116666	2013	Biomonitoring study of dry cleaning workers using cytogenetic tests and the comet assay.	Everatt; Slapšytė; Mierauskienė; Dedonytė; Bakiėnė	Journal of occupational and environmental hygiene	

[Early effects of PCE exposure on visual function among dry cleaning workers].

**BACKGROUND:** A number of studies have shown a possible correlation between exposure to perchlorethylene (PCE) in dry cleaning workers and impairment of colour perception.

**OBJECTIVES:** to ascertain the possible presence of alterations in visual function in a group of workers exposed to current limit value levels of PCE.

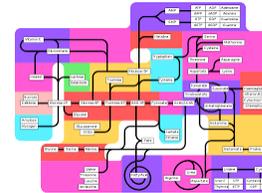
**METHODS:** The study was conducted on 38 workers exposed to PCE in 21 dry cleaning establishments in the district of Modena and 60 controls selected according to criteria of comparability. We measured exposure to PCE among the dry cleaning workers using environmental monitoring (mean exposure 16.9 mg/m3). Both groups then answered a medical history questionnaire and underwent the Ishihara test for evaluating exclusion criteria followed by Lanthony D15d and Visual Acuity in Contrast Reduced (VCS) tests to evaluate changes in visual function. The results of Lanthony's test were expressed using Index Confusion Chromatic (ICC).

**RESULT:** In the cases the average value of ICC was 1.28 (DS 0.21) and in the controls 1.15 (SD 0.21); the difference was statistically significant (p <0.01). The values of ICC tended to be worse in subjects engaged only in the washing phase, who also had higher levels of exposure to PCE (mean exposure 26.8 mg/m3). The values VCS for each frequency did not show, however, significant differences between the two groups.

**CONCLUSIONS:** On this basis, our data indicate that occupational exposure to PCE well below the current limit values may still be able to induce impairment of colour perception and that such levels are therefore not adequately protective, at least against these effects.

# Summary: Common chemical toxicity tasks

- One chemical
- Many chemicals
- Mechanistic inquiry
- Ad hoc quick lookup



# Things I didn't talk about

- Importing
- Exporting
- Log sheet
- Like this
- What's coming
  - Beyond PubMed
  - Pdf retrieval
  - Pie charts
  - Dashboard enhancements
  - More video tutorials

# Availability

- The tools presented today are PUBLICLY AVAILABLE at this very moment.

<https://comptox.epa.gov/dashboard>

- Fastest way to get the Excel Abstract Sifter

<https://comptox.epa.gov/dashboard/downloads>

# Acknowledgements

- Tom Knudsen and VTM group
- Antony Williams
- NCCT programming staff

## Publications

Baker N, Knudsen T and Williams A. **Abstract Sifter: a comprehensive front-end system to PubMed** [version 1; referees: 2 approved]. *F1000Research* 2017, **6**(Chem Inf Sci):2164  
(doi: [10.12688/f1000research.12865.1](https://doi.org/10.12688/f1000research.12865.1))

Williams AJ, Grulke CM, Edwards J, McEachran AD, Mansouri K, Baker NC, Patlewicz G, Shah I, Wambaugh JF, Judson RS, Richard AM: **The Comptox chemistry dashboard: A community data resource for environmental chemistry.** *Journal of cheminformatics* (2017) **9**(1):61.

Questions?

Thank you!