Literature-based cheminformatics for research in chemical toxicity

Nancy C. Baker

Leidos

Contractor to the US EPA

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

Acknowledgements

- Tom Knudsen
- 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)

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.

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

What is literature-based cheminformatics?

- Using computational methods on PubMed
  - Make the best use of this resource
  - Over 28 million records / citations
    - 100 years of research about chemicals and what they do in biological systems
  - Motivation – address shortcomings of PubMed
    - Fine-toothed comb
    - Bird's eye view
    - Collaborations
  - Bottom line – years of accumulated knowledge – we need it
- Deliver our methods to the public
  - Excel Abstract Sifter
  - EPA NCCT CompTox Chemistry Dashboard at comptox.epa.gov

Abstract Sifter in Excel

Strategy

Download to Excel

PubMed
Query results

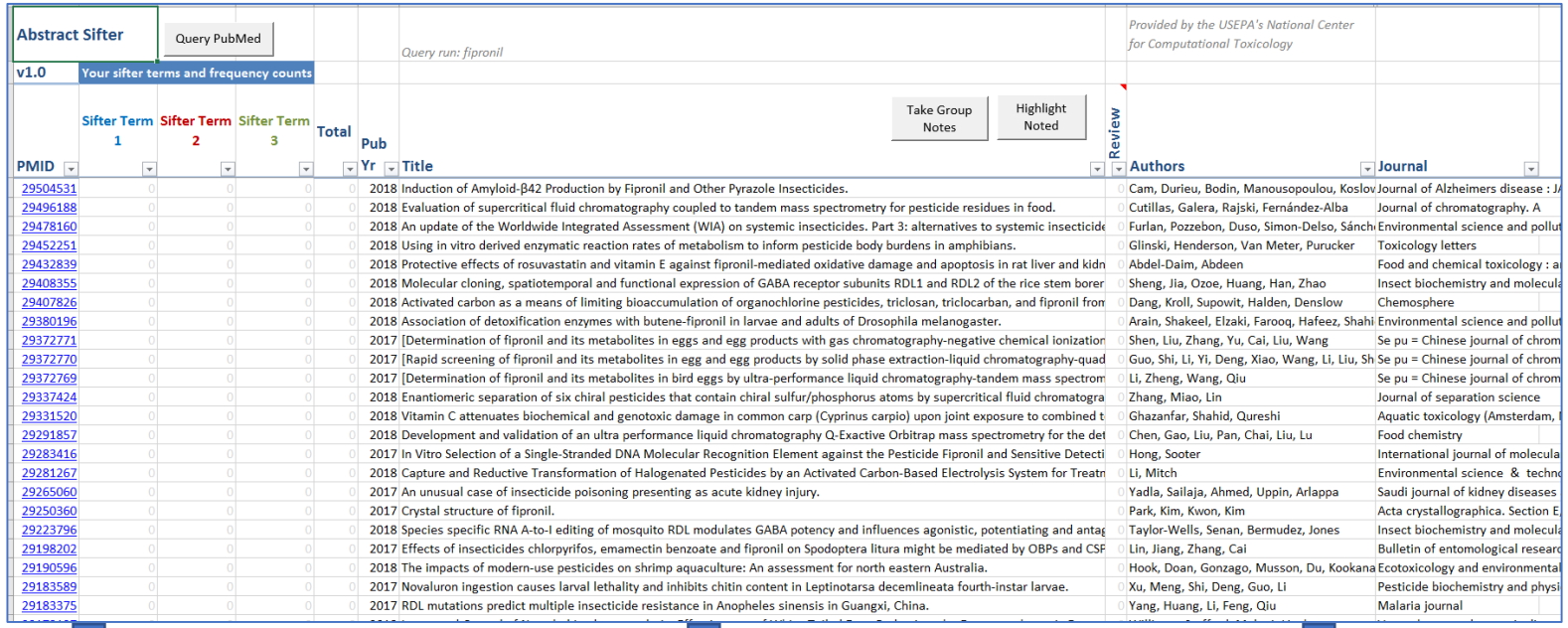
Abstract Sifter | Query PubMed | Query run: fipronil | Provided by the USEPA's National Center for Computational Toxicology

v1.0 | Your sifter terms and frequency counts | Take Group Notes | Highlight Noted

PMID	Sifter Term 1	Sifter Term 2	Sifter Term 3	Total	Pub Yr	Title	Review	Authors	Journal
29504531	0	0	0	0	2018	Induction of Amyloid-β42 Production by Fipronil and Other Pyrazole Insecticides.	0	Cam, Durieu, Bodin, Manousopoulou, Koslov	Journal of Alzheimers disease : J
29496188	0	0	0	0	2018	Evaluation of supercritical fluid chromatography coupled to tandem mass spectrometry for pesticide residues in food.	0	Cutillas, Galera, Rajski, Fernández-Alba	Journal of chromatography. A
29478160	0	0	0	0	2018	An update of the Worldwide Integrated Assessment (WIA) on systemic insecticides. Part 3: alternatives to systemic insecticide	0	Furlan, Pozzebon, Duso, Simon-Delso, Sánch	Environmental science and pollu
29452251	0	0	0	0	2018	Using in vitro derived enzymatic reaction rates of metabolism to inform pesticide body burdens in amphibians.	0	Glinski, Henderson, Van Meter, Purucker	Toxicology letters
29432839	0	0	0	0	2018	Protective effects of rosuvastatin and vitamin E against fipronil-mediated oxidative damage and apoptosis in rat liver and kidn	0	Abdel-Daim, Abdeen	Food and chemical toxicology : a
29408355	0	0	0	0	2018	Molecular cloning, spatiotemporal and functional expression of GABA receptor subunits RDL1 and RDL2 of the rice stem borer	0	Sheng, Jia, Ozoe, Huang, Han, Zhao	Insect biochemistry and molecula
29407826	0	0	0	0	2018	Activated carbon as a means of limiting bioaccumulation of organochlorine pesticides, triclosan, triclocarban, and fipronil from	0	Dang, Kroll, Supowit, Halden, Denslow	Chemosphere
29380196	0	0	0	0	2018	Association of detoxification enzymes with butene-fipronil in larvae and adults of Drosophila melanogaster.	0	Arain, Shakeel, Elzaki, Farooq, Hafeez, Shahi	Environmental science and pollu
29372771	0	0	0	0	2017	[Determination of fipronil and its metabolites in eggs and egg products with gas chromatography-negative chemical ionization	0	Shen, Liu, Zhang, Yu, Cai, Liu, Wang	Se pu = Chinese journal of chrom
29372770	0	0	0	0	2017	[Rapid screening of fipronil and its metabolites in egg and egg products by solid phase extraction-liquid chromatography-quad	0	Guo, Shi, Li, Yi, Deng, Xiao, Wang, Li, Liu, Sh	Se pu = Chinese journal of chrom
29372769	0	0	0	0	2017	[Determination of fipronil and its metabolites in bird eggs by ultra-performance liquid chromatography-tandem mass spectrom	0	Li, Zheng, Wang, Qiu	Se pu = Chinese journal of chrom
29337424	0	0	0	0	2018	Enantiomeric separation of six chiral pesticides that contain chiral sulfur/phosphorus atoms by supercritical fluid chromatogra	0	Zhang, Miao, Lin	Journal of separation science
29331520	0	0	0	0	2018	Vitamin C attenuates biochemical and genotoxic damage in common carp (Cyprinus carpio) upon joint exposure to combined t	0	Ghazanfar, Shahid, Qureshi	Aquatic toxicology (Amsterdam,
29291857	0	0	0	0	2018	Development and validation of an ultra performance liquid chromatography Q-Exactive Orbitrap mass spectrometry for the det	0	Chen, Gao, Liu, Pan, Chai, Liu, Lu	Food chemistry
29283416	0	0	0	0	2017	In Vitro Selection of a Single-Stranded DNA Molecular Recognition Element against the Pesticide Fipronil and Sensitive Detecti	0	Hong, Sooter	International journal of molecula
29281267	0	0	0	0	2018	Capture and Reductive Transformation of Halogenated Pesticides by an Activated Carbon-Based Electrolysis System for Treatn	0	Li, Mitch	Environmental science & techn
29265060	0	0	0	0	2017	An unusual case of insecticide poisoning presenting as acute kidney injury.	0	Yadla, Sailaja, Ahmed, Uppin, Arlappa	Saudi journal of kidney diseases
29250360	0	0	0	0	2017	Crystal structure of fipronil.	0	Park, Kim, Kwon, Kim	Acta crystallographica. Section E
29223796	0	0	0	0	2018	Species specific RNA A-to-I editing of mosquito RDL modulates GABA potency and influences agonistic, potentiating and antag	0	Taylor-Wells, Senan, Bermudez, Jones	Insect biochemistry and molecula
29198202	0	0	0	0	2017	Effects of insecticides chlorpyrifos, emamectin benzoate and fipronil on Spodoptera litura might be mediated by OBPs and CSF	0	Lin, Jiang, Zhang, Cai	Bulletin of entomological researc
29190596	0	0	0	0	2018	The impacts of modern-use pesticides on shrimp aquaculture: An assessment for north eastern Australia.	0	Hook, Doan, Gonzago, Musson, Du, Kookana	Ecotoxicology and environmental
29183589	0	0	0	0	2017	Novaluron ingestion causes larval lethality and inhibits chitin content in Leptinotarsa decemlineata fourth-instar larvae.	0	Xu, Meng, Shi, Deng, Guo, Li	Pesticide biochemistry and physi
29183375	0	0	0	0	2017	RDL mutations predict multiple insecticide resistance in Anopheles sinensis in Guangxi, China.	0	Yang, Huang, Li, Feng, Qiu	Malaria journal

Add functionality Through VBA macro programming

What Excel allows us to do



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Take notes and tag articles

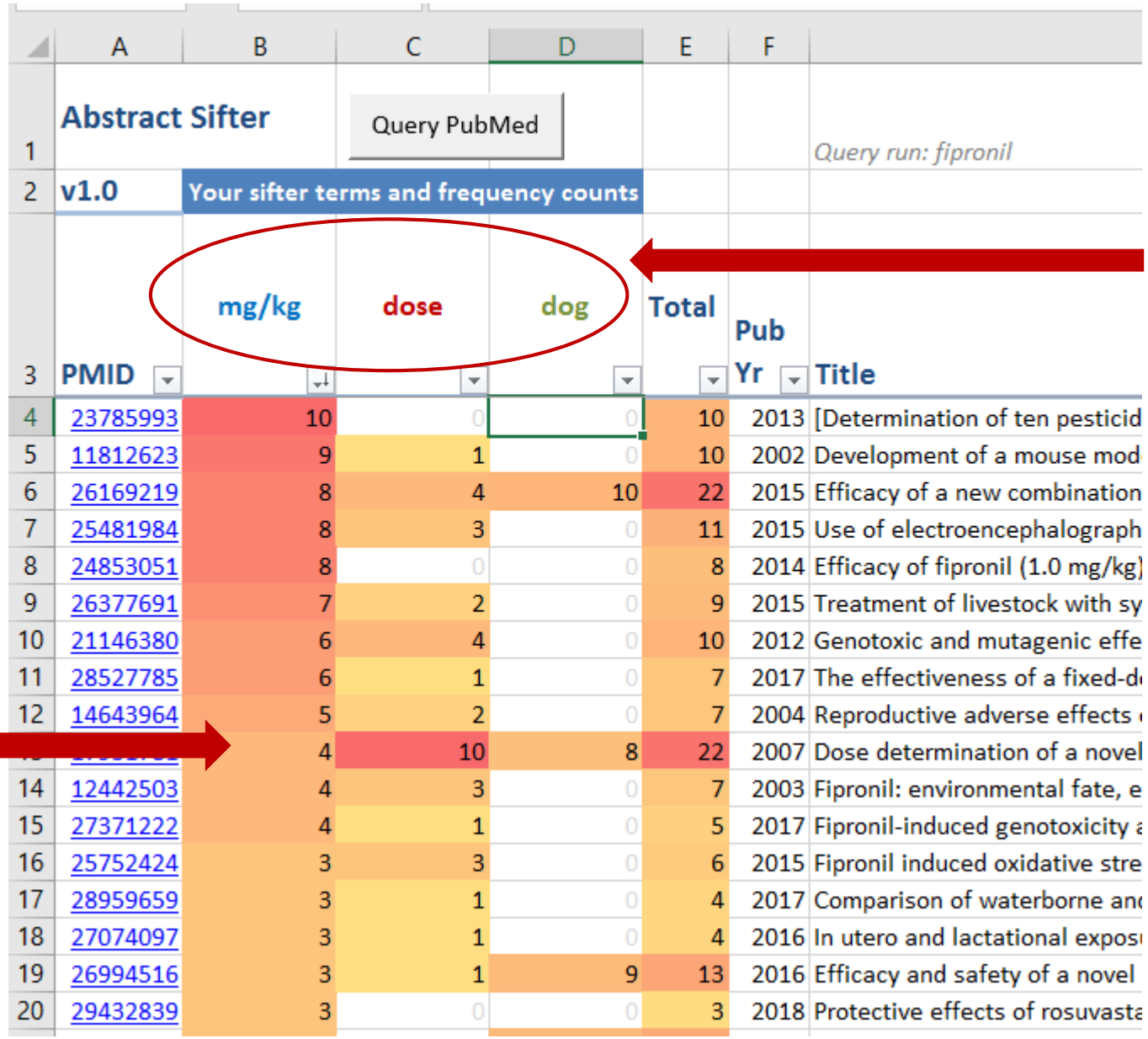
Find very specific text

Get an overview (Landscape)

Sifting

Key (and novel!) functionality

To see abstract, double-click on a cell



	A	B	C	D	E	F	
1	Abstract Sifter		Query PubMed				*Query run: fipronil*
2	v1.0	Your sifter terms and frequency counts					
3	PMID	mg/kg	dose	dog	Total	Pub Yr	Title
4	23785993	10	0	0	10	2013	[Determination of ten pesticid
5	11812623	9	1	0	10	2002	Development of a mouse mod
6	26169219	8	4	10	22	2015	Efficacy of a new combination
7	25481984	8	3	0	11	2015	Use of electroencephalograph
8	24853051	8	0	0	8	2014	Efficacy of fipronil (1.0 mg/kg)
9	26377691	7	2	0	9	2015	Treatment of livestock with sy
10	21146380	6	4	0	10	2012	Genotoxic and mutagenic effe
11	28527785	6	1	0	7	2017	The effectiveness of a fixed-d
12	14643964	5	2	0	7	2004	Reproductive adverse effects
		4	10	8	22	2007	Dose determination of a novel
14	12442503	4	3	0	7	2003	Fipronil: environmental fate, e
15	27371222	4	1	0	5	2017	Fipronil-induced genotoxicity a
16	25752424	3	3	0	6	2015	Fipronil induced oxidative stre
17	28959659	3	1	0	4	2017	Comparison of waterborne and
18	27074097	3	1	0	4	2016	In utero and lactational expos
19	26994516	3	1	9	13	2016	Efficacy and safety of a novel
20	29432839	3	0	0	3	2018	Protective effects of rosuvasta

Sifter terms

For each term, the number of occurrences in the title and abstract are counted.

View abstract and title with colorization

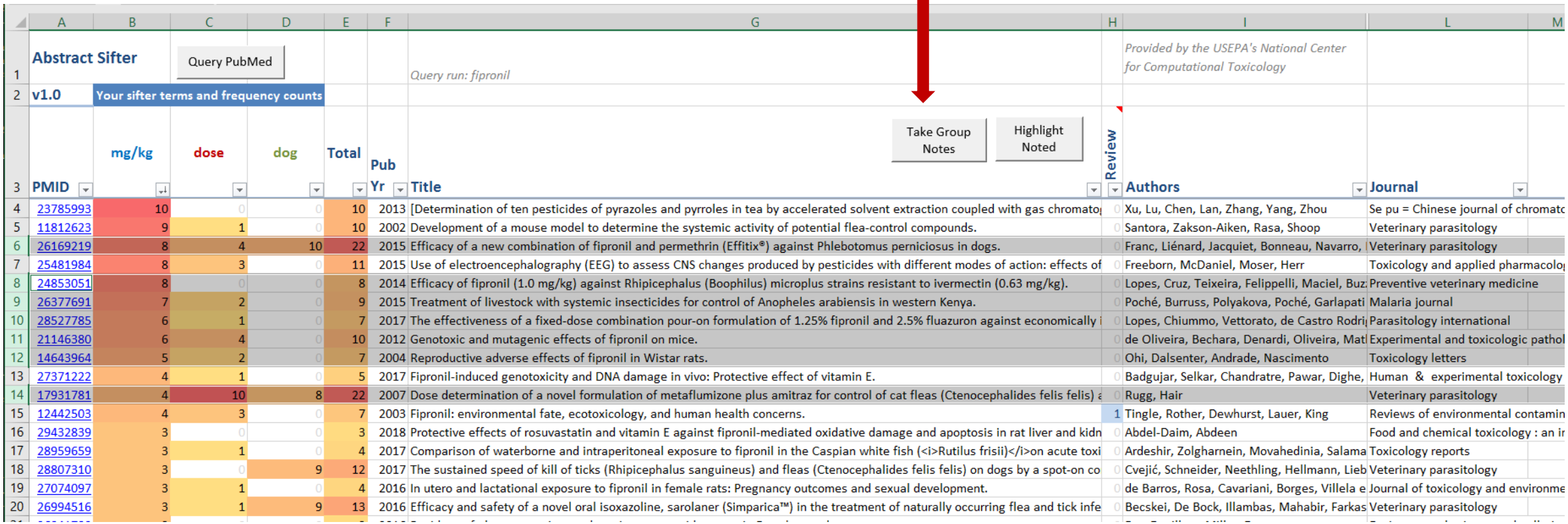
Abstract with highlights <-- Main Add Note See Notes ->

		PubYr	Authors
Article:	26169219		
Title:	Efficacy of a new combination of fipronil and permethrin (Effitix®) against Phlebotomus perniciosus in dogs.	2015	Franc, Liénard, Jacquiet, Bonneau, Navarro, Bouhsi
Title and Abstract:	Efficacy of a new combination of fipronil and permethrin (Effitix®) against Phlebotomus perniciosus in dogs. Abstract: Two controlled clinical trials were carried out to assess the anti-feeding and adulticidal effects of a spot-on combining fipronil and permethrin (Effitix(®), Virbac, Carros, France) against Phlebotomus perniciosus in dogs. The first study (Exp. A) was a dose-determination study in which 3 doses of permethrin (30 mg/kg, 60 mg/kg and 120 mg/kg) were compared. The second study (Exp. B) was an efficacy study using commercial dose of permethrin contained in Effitix(®) (the minimum dose of permethrin applied to dogs was 60 mg/kg). Twenty four and twelve Beagle dogs with equal sensitivity to sandflies were included in Exp. A and in Exp. B, respectively. Dogs were challenged with female sandflies (50 per dogs in Exp. A and 80 in Exp. B) for 60±5 min on Days - 7, 1, 7, 14, 21 and 28 (Day 0 being treatment day). Counts and engorgement determination of dead and alive sandflies were performed after each exposure to treated and untreated dogs. Dead sandflies were also counted 24 h after exposure. In Exp. A, the repellency induced by an administration of 30 mg/kg of permethrin to dogs was above 91% for the first two weeks and then dropped to 82.2, 83.1 and 81.1% on Days 14, 21 and 28, respectively. For dogs receiving 60 mg/kg of permethrin, the repellency was a bit higher with 95.8, 97.6, 92.1, 91.4, and 86.8%, for Days 1, 7, 14, 21 and 28, respectively. The repellency induced by 120 mg/kg of permethrin was significantly higher than that induced by 60 mg/kg of permethrin on Day 14 only. In Exp. B the anti-feeding effect of the spot-on formulation was 94.1, 97.8, 96.3, 90.8 and 87% on Days 1, 7, 14, 21 and 28, respectively. The mortality effect was 98.9, 99.1, 99.8, 97.0 and 89.7% on Days 1, 7, 14, 21 and 28, respectively. At each challenge point, the mortality and anti-feeding effects on sandflies were significantly different between control and treatment group (plt;0.05). The results indicate that a monthly administration of this new combination of permethrin and fipronil could be used as an effective sandfly control strategy in dogs and therefore recommended for use in an integrated leishmaniosis prevention program.		

Taking notes

First select the rows

Then click here



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11812623	9	1	0	10	2002	Development of a mouse model to determine the systemic activity of potential flea-control compounds.	0	Santora, Zakson-Aiken, Rasa, Shoop	Veterinary parasitology
26169219	8	4	10	22	2015	Efficacy of a new combination of fipronil and permethrin (Effitix®) against Phlebotomus perniciosus in dogs.	0	Franc, Liénard, Jacquiet, Bonneau, Navarro,	Veterinary parasitology
25481984	8	3	0	11	2015	Use of electroencephalography (EEG) to assess CNS changes produced by pesticides with different modes of action: effects of	0	Freeborn, McDaniel, Moser, Herr	Toxicology and applied pharmacolo
24853051	8	0	0	8	2014	Efficacy of fipronil (1.0 mg/kg) against Rhipicephalus (Boophilus) microplus strains resistant to ivermectin (0.63 mg/kg).	0	Lopes, Cruz, Teixeira, Felippelli, Maciel, Buz	Preventive veterinary medicine
26377691	7	2	0	9	2015	Treatment of livestock with systemic insecticides for control of Anopheles arabiensis in western Kenya.	0	Poché, Burruss, Polyakova, Poché, Garlapati	Malaria journal
28527785	6	1	0	7	2017	The effectiveness of a fixed-dose combination pour-on formulation of 1.25% fipronil and 2.5% fluazuron against economically i	0	Lopes, Chiummo, Vettorato, de Castro Rodri	Parasitology international
21146380	6	4	0	10	2012	Genotoxic and mutagenic effects of fipronil on mice.	0	de Oliveira, Bechara, Denardi, Oliveira, Mat	Experimental and toxicologic pathol
14643964	5	2	0	7	2004	Reproductive adverse effects of fipronil in Wistar rats.	0	Ohi, Dalsenter, Andrade, Nascimento	Toxicology letters
27371222	4	1	0	5	2017	Fipronil-induced genotoxicity and DNA damage in vivo: Protective effect of vitamin E.	0	Badgujar, Selkar, Chandratre, Pawar, Dighe,	Human & experimental toxicology
17931781	4	10	8	22	2007	Dose determination of a novel formulation of metaflumizone plus amitraz for control of cat fleas (Ctenocephalides felis felis) a	0	Rugg, Hair	Veterinary parasitology
12442503	4	3	0	7	2003	Fipronil: environmental fate, ecotoxicology, and human health concerns.	1	Tingle, Rother, Dewhurst, Lauer, King	Reviews of environmental contamin
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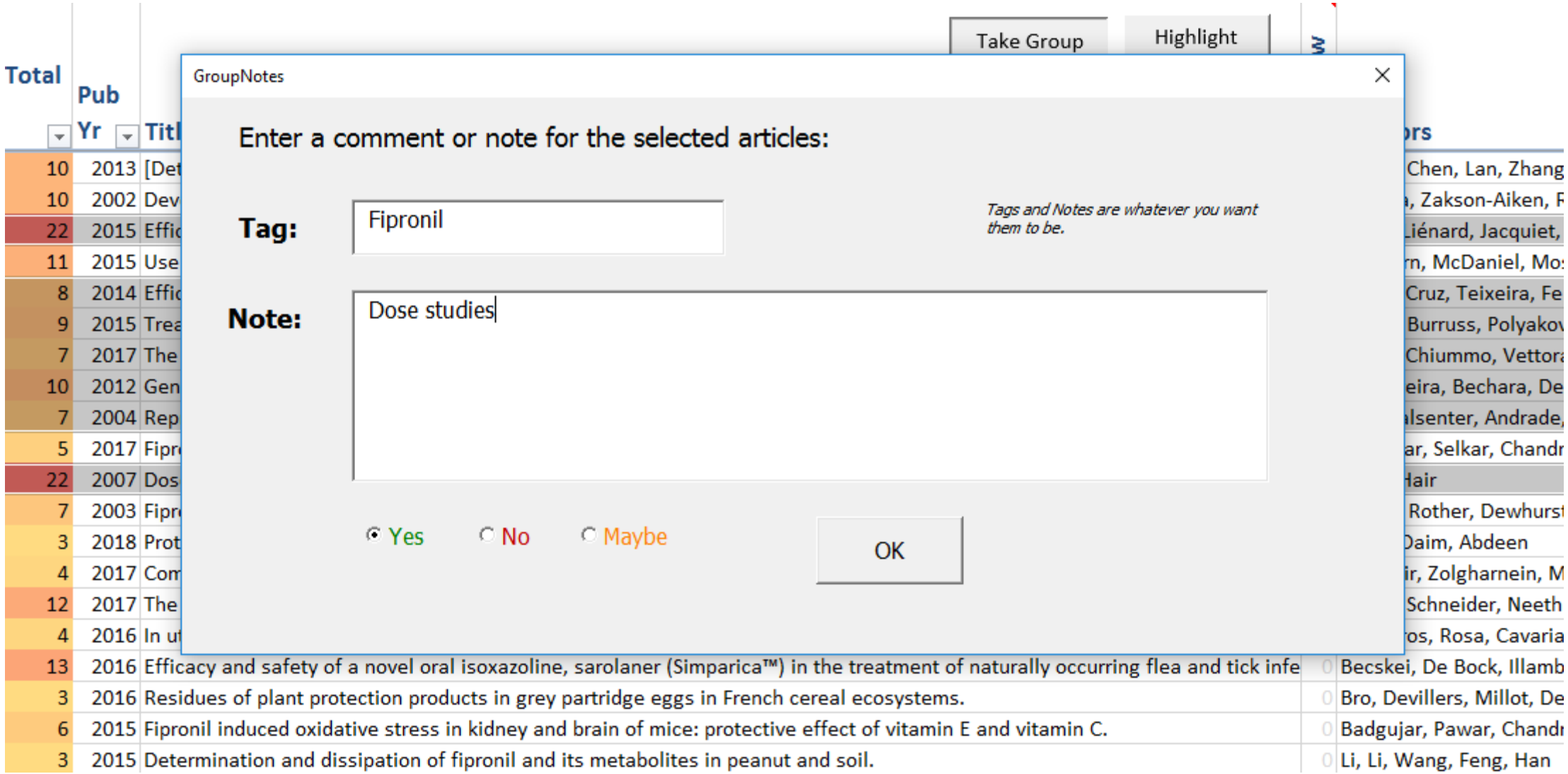
28959659	3	1	0	4	2017	Comparison of waterborne and intraperitoneal exposure to fipronil in the Caspian white fish (Rutilus frisii)on acute toxi	0	Ardeshir, Zolgharnein, Movahedinia, Salama	Toxicology reports
28807310	3	0	9	12	2017	The sustained speed of kill of ticks (Rhipicephalus sanguineus) and fleas (Ctenocephalides felis felis) on dogs by a spot-on co	0	Cvejić, Schneider, Neethling, Hellmann, Lieb	Veterinary parasitology
27074097	3	1	0	4	2016	In utero and lactational exposure to fipronil in female rats: Pregnancy outcomes and sexual development.	0	de Barros, Rosa, Cavariani, Borges, Villela e	Journal of toxicology and environme
26994516	3	1	9	13	2016	Efficacy and safety of a novel oral isoxazoline, sarolaner (Simparica™) in the treatment of naturally occurring flea and tick infe	0	Becskei, De Bock, Illambas, Mahabir, Farkas	Veterinary parasitology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Enter a comment or note for the selected articles:
Tag:
Fipronil
Tags and Notes are whatever you want them to be.
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10 2013 [Det Chen, Lan, Zhang
10 2002 Dev a, Zakson-Aiken, F
22 2015 Effic Liénard, Jacquiet,
11 2015 Use rn, McDaniel, Mos
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7 2017 The Chiummo, Vettora
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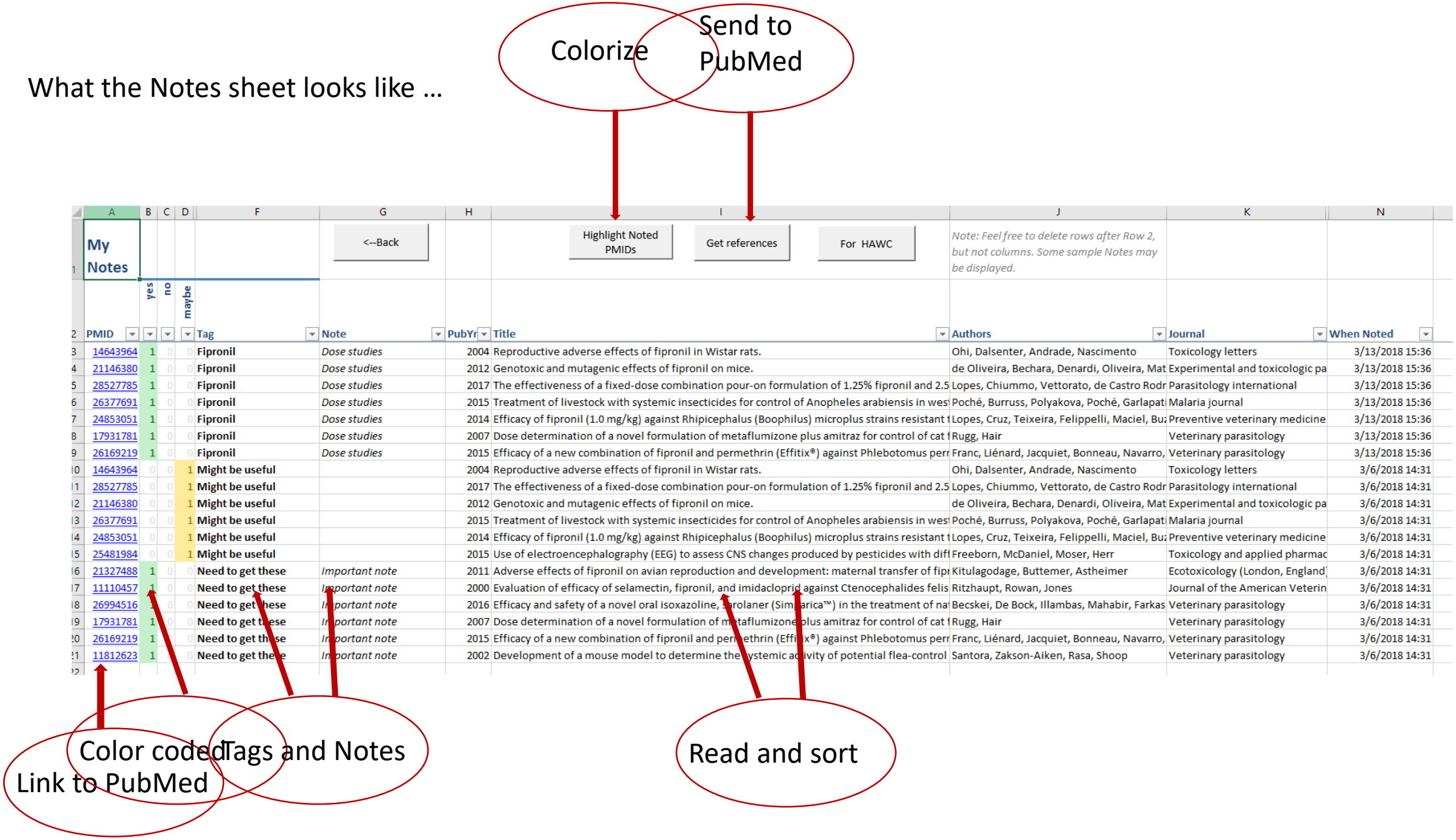
3 2016 Residues of plant protection products in grey partridge eggs in French cereal ecosystems. 0 Bro, Devillers, Millot, De
6 2015 Fipronil induced oxidative stress in kidney and brain of mice: protective effect of vitamin E and vitamin C. 0 Badgujar, Pawar, Chandr
3 2015 Determination and dissipation of fipronil and its metabolites in peanut and soil. 0 Li, Li, Wang, Feng, Han

What the Notes sheet looks like …



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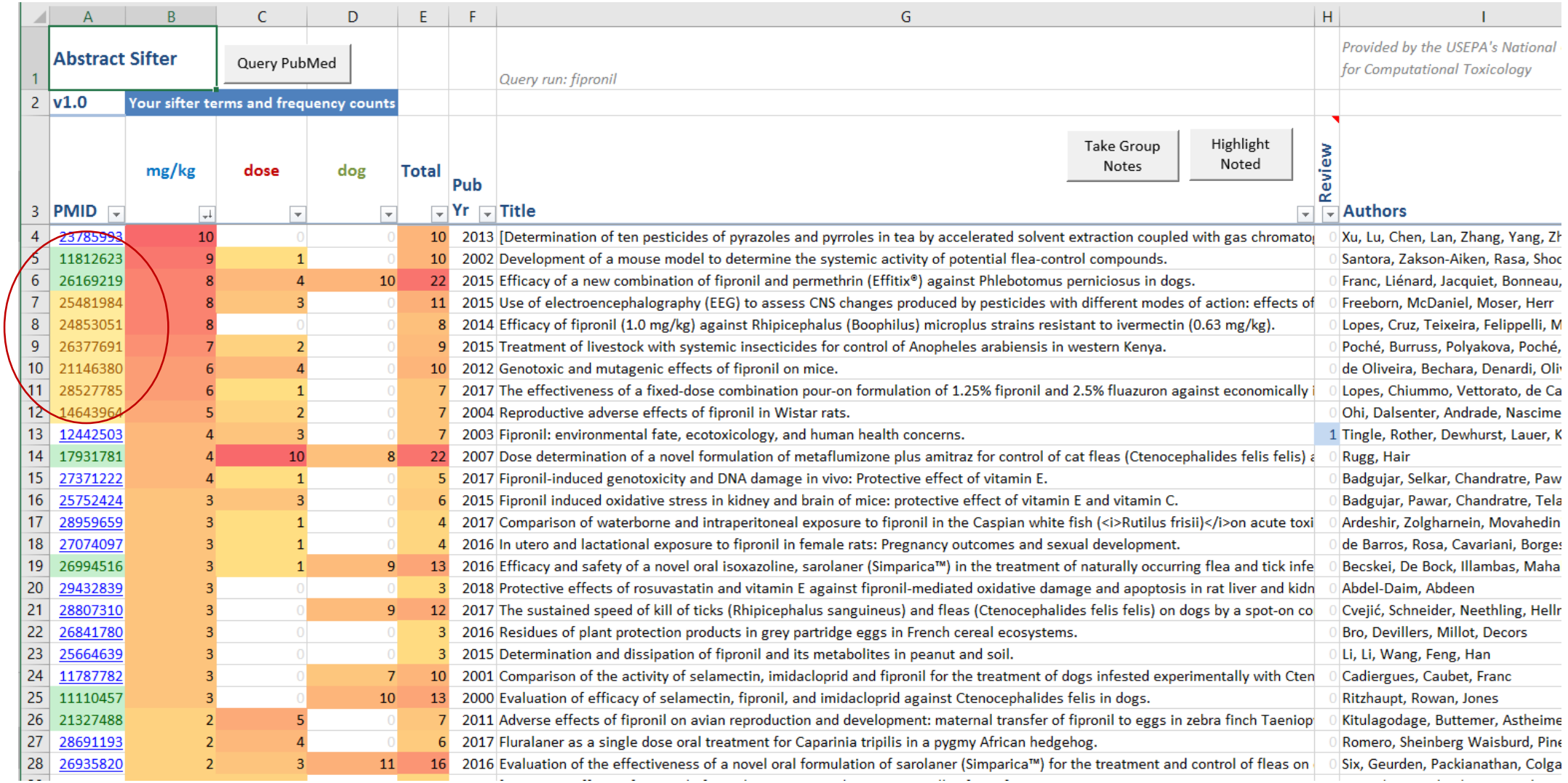

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15	27371222	4	1	0	5	2017	Fipronil-induced genotoxicity and DNA damage in vivo: Protective effect of vitamin E.	0	Badgujar, Selkar, Chandratre, Paw
16	25752424	3	3	0	6	2015	Fipronil induced oxidative stress in kidney and brain of mice: protective effect of vitamin E and vitamin C.	0	Badgujar, Pawar, Chandratre, Tela
17	28959659	3	1	0	4	2017	Comparison of waterborne and intraperitoneal exposure to fipronil in the Caspian white fish (Rutilus frisii)on acute toxi	0	Ardeshir, Zolgharnein, Movahedin
18	27074097	3	1	0	4	2016	In utero and lactational exposure to fipronil in female rats: Pregnancy outcomes and sexual development.	0	de Barros, Rosa, Cavariani, Borges
19	26994516	3	1	9	13	2016	Efficacy and safety of a novel oral isoxazoline, sarolaner (Simparica™) in the treatment of naturally occurring flea and tick infe	0	Becskei, De Bock, Illambas, Maha
20	29432839	3	0	0	3	2018	Protective effects of rosuvastatin and vitamin E against fipronil-mediated oxidative damage and apoptosis in rat liver and kidn	0	Abdel-Daim, Abdeen
21	28807310	3	0	9	12	2017	The sustained speed of kill of ticks (Rhipicephalus sanguineus) and fleas (Ctenocephalides felis felis) on dogs by a spot-on co	0	Cvejić, Schneider, Neethling, Hellr
22	26841780	3	0	0	3	2016	Residues of plant protection products in grey partridge eggs in French cereal ecosystems.	0	Bro, Devillers, Millot, Decors
23	25664639	3	0	0	3	2015	Determination and dissipation of fipronil and its metabolites in peanut and soil.	0	Li, Li, Wang, Feng, Han
24	11787782	3	0	7	10	2001	Comparison of the activity of selamectin, imidacloprid and fipronil for the treatment of dogs infested experimentally with Cten	0	Cadiergues, Caubet, Franc
25	11110457	3	0	10	13	2000	Evaluation of efficacy of selamectin, fipronil, and imidacloprid against Ctenocephalides felis in dogs.	0	Ritzhaupt, Rowan, Jones
26	21327488	2	5	0	7	2011	Adverse effects of fipronil on avian reproduction and development: maternal transfer of fipronil to eggs in zebra finch Taeniop	0	Kitulagodage, Buttemer, Astheime
27	28691193	2	4	0	6	2017	Fluralaner as a single dose oral treatment for Caparinia tripilis in a pygmy African hedgehog.	0	Romero, Sheinberg Waisburd, Pine
28	26935820	2	3	11	16	2016	Evaluation of the effectiveness of a novel oral formulation of sarolaner (Simparica™) for the treatment and control of fleas on	0	Six, Geurden, Packianathan, Colga

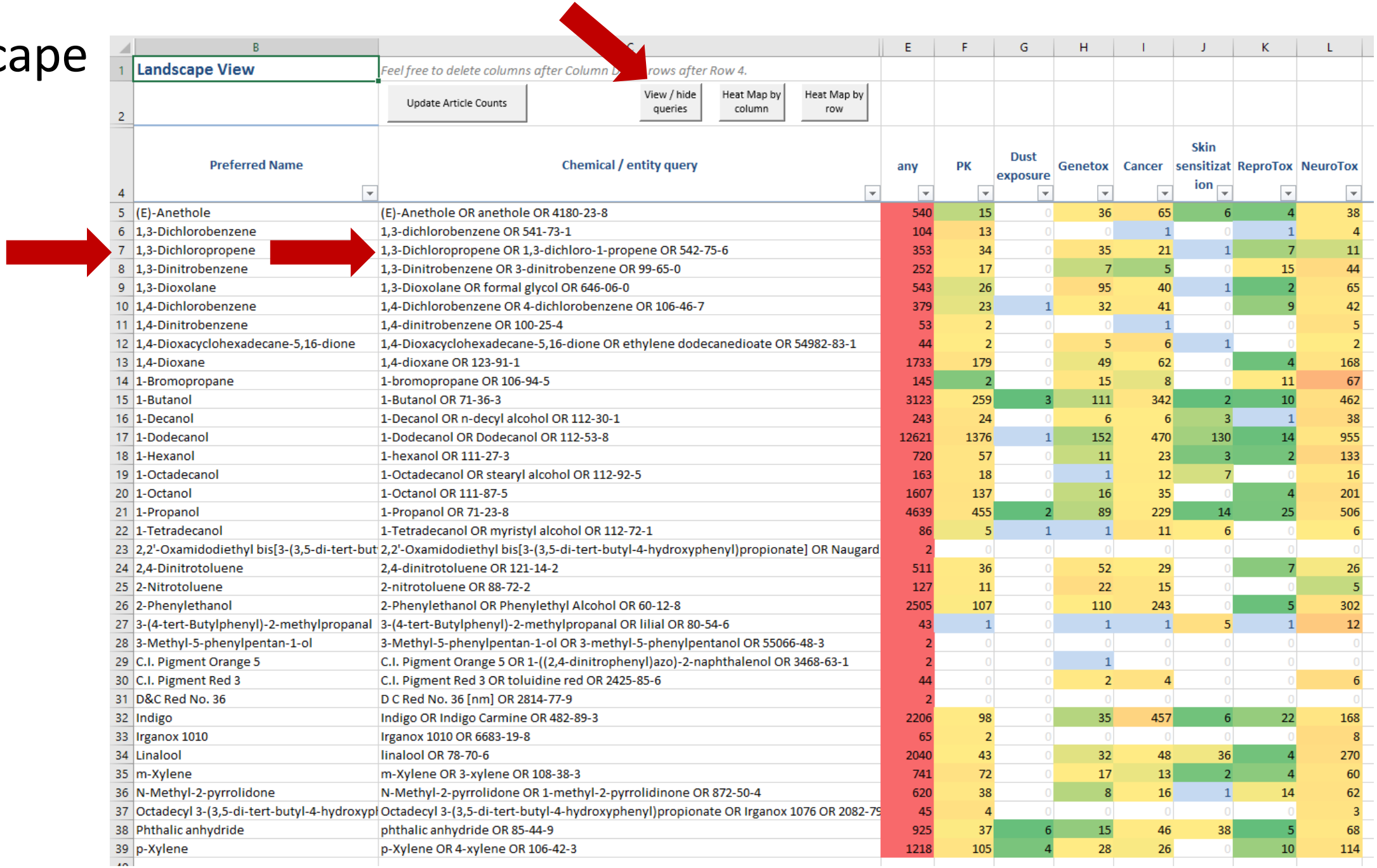
Helps with article triage: what have I evaluated … what did I think.

Landscape sheet

This is where you get the bird’s eye view of …

a set of chemicals

Landscape Sheet

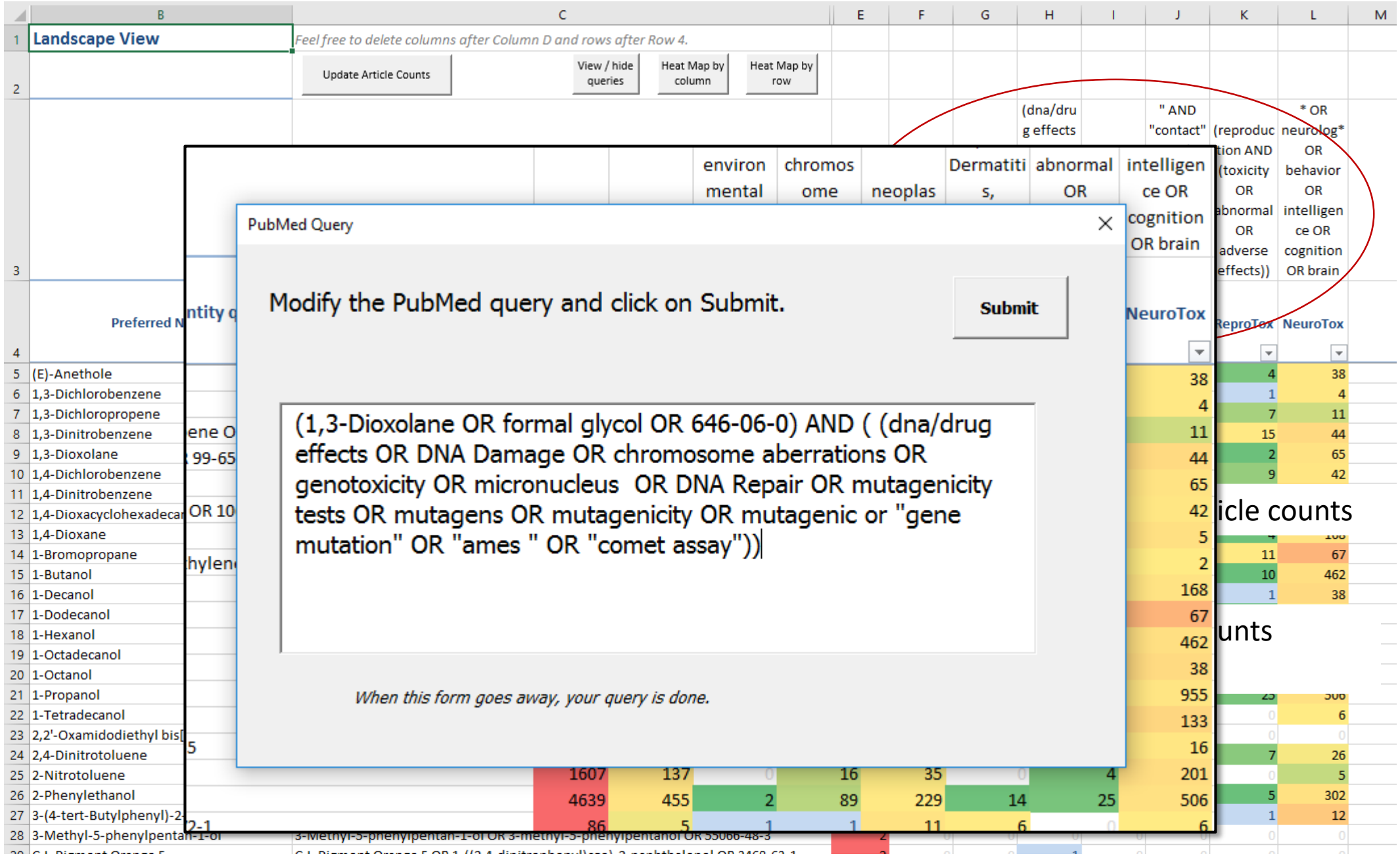


Landscape View

Feel free to delete columns after Column D ... rows after Row 4.

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

Preferred Name	Chemical / entity query	any	PK	Dust exposure	Genetox	Cancer	Skin sensitization	ReproTox	NeuroTox
(E)-Anethole	(E)-Anethole OR anethole OR 4180-23-8	540	15	0	36	65	6	4	38
1,3-Dichlorobenzene	1,3-dichlorobenzene OR 541-73-1	104	13	0	0	1	0	1	4
1,3-Dichloropropene	1,3-Dichloropropene OR 1,3-dichloro-1-propene OR 542-75-6	353	34	0	35	21	1	7	11
1,3-Dinitrobenzene	1,3-Dinitrobenzene OR 3-dinitrobenzene OR 99-65-0	252	17	0	7	5	0	15	44
1,3-Dioxolane	1,3-Dioxolane OR formal glycol OR 646-06-0	543	26	0	95	40	1	2	65
1,4-Dichlorobenzene	1,4-Dichlorobenzene OR 4-dichlorobenzene OR 106-46-7	379	23	1	32	41	0	9	42
1,4-Dinitrobenzene	1,4-dinitrobenzene OR 100-25-4	53	2	0	0	1	0	0	5
1,4-Dioxacyclohexadecane-5,16-dione	1,4-Dioxacyclohexadecane-5,16-dione OR ethylene dodecanedioate OR 54982-83-1	44	2	0	5	6	1	0	2
1,4-Dioxane	1,4-dioxane OR 123-91-1	1733	179	0	49	62	0	4	168
1-Bromopropane	1-bromopropane OR 106-94-5	145	2	0	15	8	0	11	67
1-Butanol	1-Butanol OR 71-36-3	3123	259	3	111	342	2	10	462
1-Decanol	1-Decanol OR n-decyl alcohol OR 112-30-1	243	24	0	6	6	3	1	38
1-Dodecanol	1-Dodecanol OR Dodecanol OR 112-53-8	12621	1376	1	152	470	130	14	955
1-Hexanol	1-hexanol OR 111-27-3	720	57	0	11	23	3	2	133
1-Octadecanol	1-Octadecanol OR stearyl alcohol OR 112-92-5	163	18	0	1	12	7	0	16
1-Octanol	1-Octanol OR 111-87-5	1607	137	0	16	35	0	4	201
1-Propanol	1-Propanol OR 71-23-8	4639	455	2	89	229	14	25	506
1-Tetradecanol	1-Tetradecanol OR myristyl alcohol OR 112-72-1	86	5	1	1	11	6	0	6
2,2'-Oxamidodiethyl bis[3-(3,5-di-tert-but	2,2'-Oxamidodiethyl bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate] OR Naugard	2	0	0	0	0	0	0	0
2,4-Dinitrotoluene	2,4-dinitrotoluene OR 121-14-2	511	36	0	52	29	0	7	26
2-Nitrotoluene	2-nitrotoluene OR 88-72-2	127	11	0	22	15	0	0	5
2-Phenylethanol	2-Phenylethanol OR Phenylethyl Alcohol OR 60-12-8	2505	107	0	110	243	0	5	302
3-(4-tert-Butylphenyl)-2-methylpropanal	3-(4-tert-Butylphenyl)-2-methylpropanal OR lilial OR 80-54-6	43	1	0	1	1	5	1	12
3-Methyl-5-phenylpentan-1-ol	3-Methyl-5-phenylpentan-1-ol OR 3-methyl-5-phenylpentanol OR 55066-48-3	2	0	0	0	0	0	0	0
C.I. Pigment Orange 5	C.I. Pigment Orange 5 OR 1-((2,4-dinitrophenyl)azo)-2-naphthalenol OR 3468-63-1	2	0	0	1	0	0	0	0
C.I. Pigment Red 3	C.I. Pigment Red 3 OR toluidine red OR 2425-85-6	44	0	0	2	4	0	0	6
D&C Red No. 36	D C Red No. 36 [nm] OR 2814-77-9	2	0	0	0	0	0	0	0
Indigo	Indigo OR Indigo Carmine OR 482-89-3	2206	98	0	35	457	6	22	168
Irganox 1010	Irganox 1010 OR 6683-19-8	65	2	0	0	0	0	0	8
Linalool	linalool OR 78-70-6	2040	43	0	32	48	36	4	270
m-Xylene	m-Xylene OR 3-xylene OR 108-38-3	741	72	0	17	13	2	4	60
N-Methyl-2-pyrrolidone	N-Methyl-2-pyrrolidone OR 1-methyl-2-pyrrolidinone OR 872-50-4	620	38	0	8	16	1	14	62
Octadecyl 3-(3,5-di-tert-butyl-4-hydroxypl	Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate OR Irganox 1076 OR 2082-79	45	4	0	0	0	0	0	3
Phthalic anhydride	phthalic anhydride OR 85-44-9	925	37	6	15	46	38	5	68
p-Xylene	p-Xylene OR 4-xylene OR 106-42-3	1218	105	4	28	26	0	10	114


Landscape View
Feel free to delete columns after Column D and rows after Row 4.
Update Article Counts
View / hide queries
Heat Map by column
Heat Map by row
PubMed Query
Modify the PubMed query and click on Submit.
Submit
(1,3-Dioxolane OR formal glycol OR 646-06-0) AND ((dna/drug effects OR DNA Damage OR chromosome aberrations OR genotoxicity OR micronucleus OR DNA Repair OR mutagenicity tests OR mutagens OR mutagenicity OR mutagenic or "gene mutation" OR "ames " OR "comet assay"))
When this form goes away, your query is done.
environmental
chromosome
neoplas
Dermatitis,
abnormal OR
intelligence OR cognition OR brain
" AND "contact"
(dna/drug effects
(reproduction AND (toxicity OR abnormal OR adverse effects))
* OR neurolog* OR behavior OR intelligence OR cognition OR brain
Preferred N
NeuroTox
ReproTox
NeuroTox
(E)-Anethole
1,3-Dichlorobenzene
1,3-Dichloropropene
1,3-Dinitrobenzene
1,3-Dioxolane
1,4-Dichlorobenzene
1,4-Dinitrobenzene
1,4-Dioxacyclohexadecar
1,4-Dioxane
1-Bromopropane
1-Butanol
1-Decanol
1-Dodecanol
1-Hexanol
1-Octadecanol
1-Octanol
1-Propanol
1-Tetradecanol
2,2'-Oxamidodiethyl bis[
2,4-Dinitrotoluene
2-Nitrotoluene
2-Phenylethanol
3-(4-tert-Butylphenyl)-2-
3-Methyl-5-phenylpentan-1-ol
3-Methyl-5-phenylpentan-1-ol OR 3-methyl-5-phenylpentanol OR 55066-48-3
38 4 38
4 1 4
11 7 11
44 15 44
65 2 65
42 9 42
5
2 11 67
168 10 462
67 1 38
462
38
955
133 6
16
201 7 26
506 0 5
6 5 302
1 12
1607 137 16 35 4
4639 455 2 89 229 14 25
86 5 1 1 11 6
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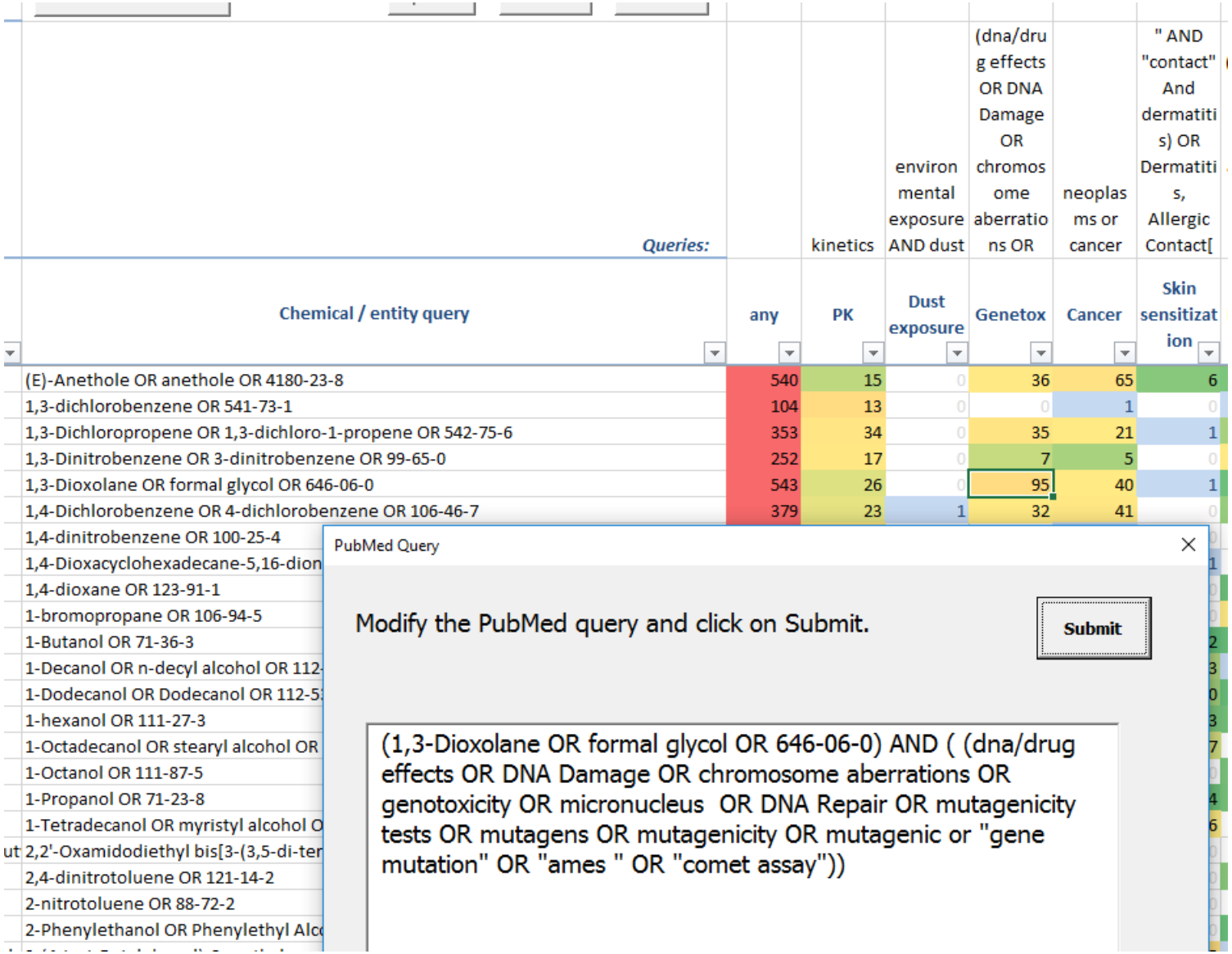
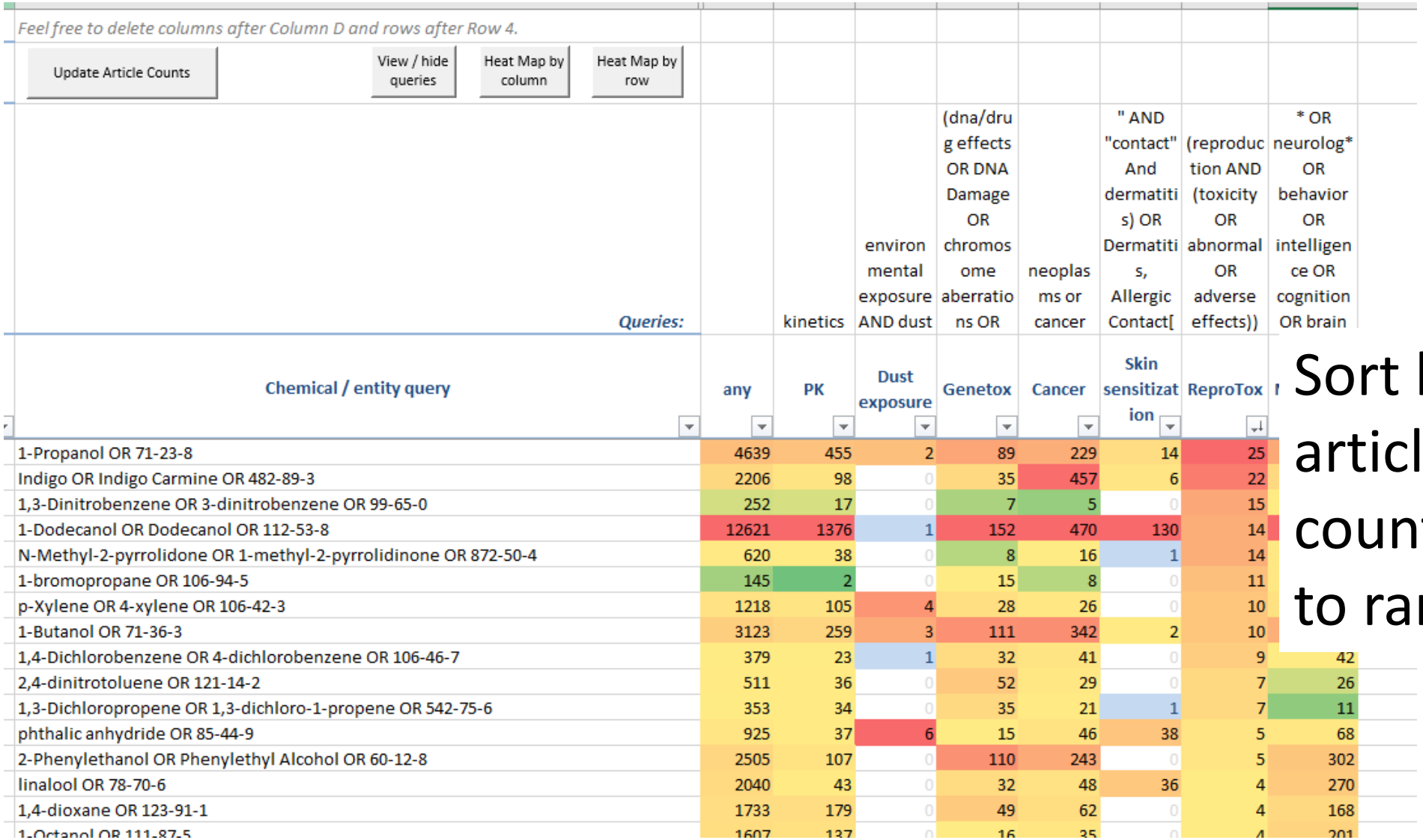
unts

Double-clicking on a cell causes a query to be composed from the chemical part of the query and the subject matter part.



Take advantage of the bird's eye view



Feel free to delete columns after Column D and rows after Row 4.

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

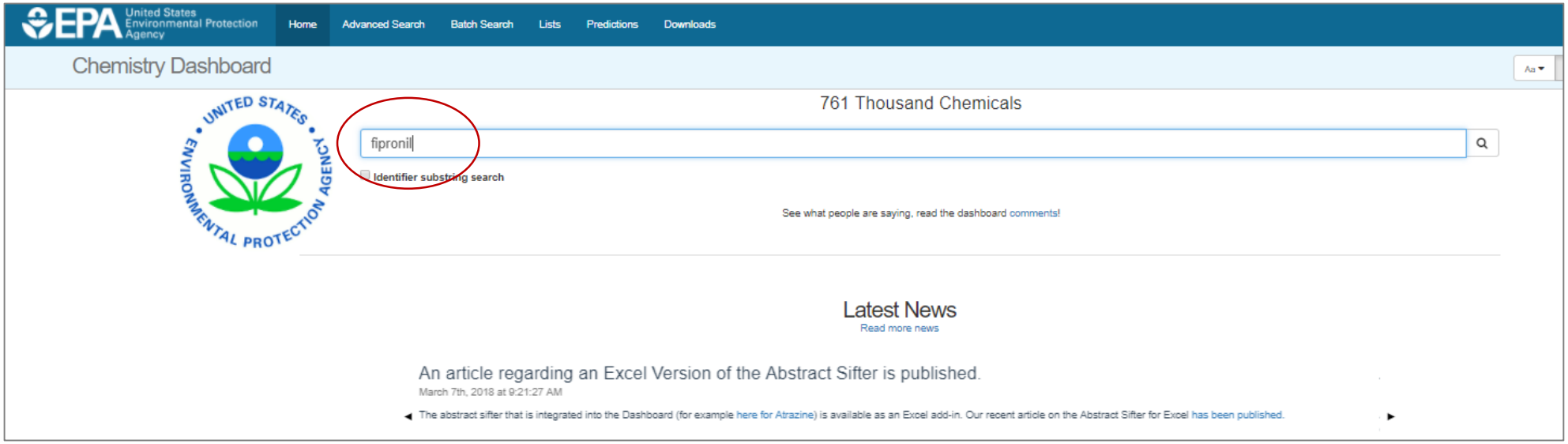
Queries:		kinetics	environmental exposure AND dust	(dna/drug effects OR DNA Damage OR chromosome aberrations OR	neoplasms or cancer	" AND "contact" And dermatitis) OR Dermatitis, Allergic Contact[	(reproduction AND (toxicity OR abnormal OR adverse effects))	* OR neurolog* OR behavior OR intelligence OR cognition OR brain
Chemical / entity query	**any**	**PK**	**Dust exposure**	**Genetox**	**Cancer**	**Skin sensitization**	**ReproTox**	
1-Propanol OR 71-23-8	4639	455	2	89	229	14	25	
Indigo OR Indigo Carmine OR 482-89-3	2206	98	0	35	457	6	22	
1,3-Dinitrobenzene OR 3-dinitrobenzene OR 99-65-0	252	17	0	7	5	0	15	
1-Dodecanol OR Dodecanol OR 112-53-8	12621	1376	1	152	470	130	14	
N-Methyl-2-pyrrolidone OR 1-methyl-2-pyrrolidinone OR 872-50-4	620	38	0	8	16	1	14	
1-bromopropane OR 106-94-5	145	2	0	15	8	0	11	
p-Xylene OR 4-xylene OR 106-42-3	1218	105	4	28	26	0	10	
1-Butanol OR 71-36-3	3123	259	3	111	342	2	10	
1,4-Dichlorobenzene OR 4-dichlorobenzene OR 106-46-7	379	23	1	32	41	0	9	42
2,4-dinitrotoluene OR 121-14-2	511	36	0	52	29	0	7	26
1,3-Dichloropropene OR 1,3-dichloro-1-propene OR 542-75-6	353	34	0	35	21	1	7	11
phthalic anhydride OR 85-44-9	925	37	6	15	46	38	5	68
2-Phenylethanol OR Phenylethyl Alcohol OR 60-12-8	2505	107	0	110	243	0	5	302
linalool OR 78-70-6	2040	43	0	32	48	36	4	270
1,4-dioxane OR 123-91-1	1733	179	0	49	62	0	4	168
1-Octanol OR 111-87-5	1607	137	0	16	35	0	4	201

Sort by article count to rank

EPA’s other implementation of the sifter technology

EPA’s Comptox Chemistry Dashboard

https://comptox.epa.gov/dashboard



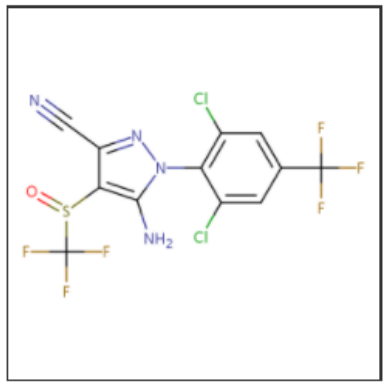
EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Search All Data

Chemistry Dashboard | Submit Comment | Share | Copy | Aa

Fipronil

120068-37-3 | DTXSID4034609

Searched by Approved Name: Found 1 result for 'fipronil'.



Wikipedia

Fipronil is a broad-spectrum insecticide that belongs to the phenylpyrazole chemical family. Fipronil disrupts the insect central nervous system by blocking GABA-gated chloride channels and glutamate-gated chloride (GluCl) channels. This causes hyperexcitation of contaminated insects' nerves and muscles. Fipronil's specificity towards insects is believed to be due to its greater affinity to the GABA receptor in insects relative to mammals and its effect on GluCl channels, which do not exist...Read more

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Executive Summary (Beta) | Chemical Properties | Env. Fate/Transport | Hazard | ADME (Beta) | Exposure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links | Comments

Google Scholar

PubMed Abstract Sifter

PubChem Articles

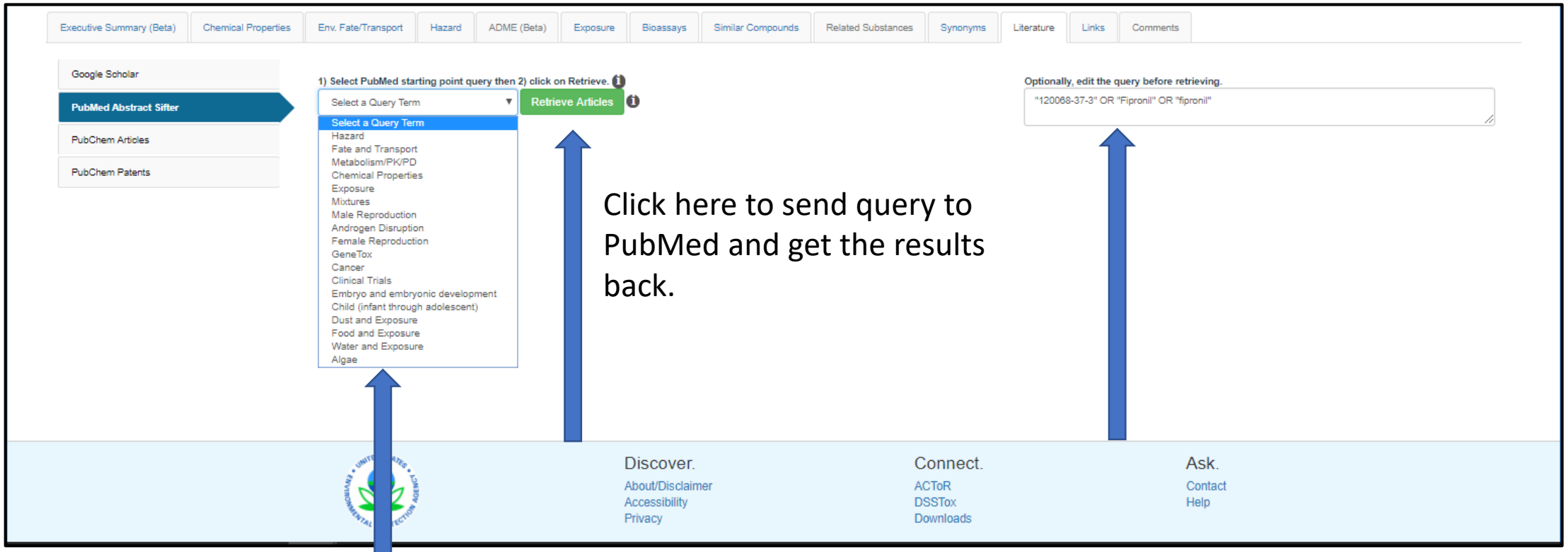
PubChem Patents

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

Select a Query Term | Retrieve Articles

Optionally, edit the query before retrieving.

"120068-37-3" OR "Fipronil" OR "fipronil"



Click here to send query to PubMed and get the results back.

Some queries are already constructed for use as starting points.

You can also compose your own query.

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

Mixtures

Retrieve Articles

70 of 70 articles loaded...

Optionally, edit the query before retrieving.

("120068-37-3" OR "Fipronil" OR "fipronil") AND (Drug synergism[mh] OR cocarcinogenesis OR pesticide synergists[mh] OR mixture[tiab] OR mixtures[tiab] OR Drug Antagonism[mh] OR Drug Interactions[mh] OR drug agonism)

To find articles quickly, enter terms to sift abstracts.

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PMID	Year	Title	Authors	Journal	Rev
29407826	2018	Activated carbon as a means of limiting bioaccumulation of organochlorine pesticides, triclosan, tri...	Dang; Kroll; Supowit; Halden; Denslow	Chemosphere	
29380196	2018	Association of detoxification enzymes with butene-fipronil in larvae and adults of Drosophila melan...	Arain; Shakeel; Elzaki; Farooq; Hafeez; Shahid; Sh...	Environmental science and pollution research intern...	
29372769	2018	[Determination of fipronil and its metabolites in bird eggs by ultra-performance liquid chromatograp...	Li; Zheng; Wang; Qiu	Se pu = Chinese journal of chromatography	
29291857	2018	Development and validation of an ultra performance liquid chromatography Q-Exactive Orbitrap m...	Chen; Gao; Liu; Pan; Chai; Liu; Lu	Food chemistry	
29190596	2017	The impacts of modern-use pesticides on shrimp aquaculture: An assessment for north eastern Au...	Hook; Doan; Gonzago; Musson; Du; Kookana; Sell...	Ecotoxicology and environmental safety	
28991419	2017	Synergistic interactions between a variety of insecticides and an ergosterol biosynthesis inhibitor f...	Raimets; Karise; Mänd; Kaart; Ponting; Song; Cres...	Pest management science	
28991164	2017	Differential Expression Profile of lncRNAs from Primary Human Hepatocytes Following DEET and ...	Mitchell; Wallace; Hodgson; Roe	International journal of molecular sciences	
28802893	2017	Complex mixtures of dissolved pesticides show potential aquatic toxicity in a synoptic study of Mid...	Nowell; Moran; Schmidt; Norman; Nakagaki; Shoda...	The Science of the total environment	
28786535	2017	Enantiomer-specific measurements of current-use pesticides in aquatic systems.	Ulrich; TenBrook; McMillan; Wang; Lao	Environmental toxicology and chemistry	
28158628	2017	Study of Synergism, Antagonism, and Resistance Mechanisms in Insecticide-Resistant Oxycarenu...	Ullah; Ejaz; Ali Shad	Journal of economic entomology	
28122816	2017	Effectiveness of Fipronil as a Systemic Control Agent Against Xenopsylla cheopis (Siphonaptera: ...	Rajonhson; Miarinjara; Rahelinirina; Rajerison; Boyer	Journal of medical entomology	
28011991	2016	Hair analysis for the biomonitoring of pesticide exposure: comparison with blood and urine in a rat ...	Appenzeller; Hardy; Grova; Chata; Faÿs; Briand; Sc...	Archives of toxicology	

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

Mixtures

Retrieve Articles

70 of 70 articles loaded...

Optionally, edit the query before retrieving.

("120068-37-3" OR "Fipronil" OR "fipronil") AND (Drug synergism[mh] OR cocarcinogenesis OR pesticide synergists[mh] OR mixture[tiab] OR mixtures[tiab] OR Drug Antagonism[mh] OR Drug Interactions[mh] OR drug agonism)

To find articles quickly, enter terms to sift abstracts.

flea | tick | dog | | Clear Terms

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flea	tick	dog	Total	PMID	Year	Title	Authors	Journal	Rev
1	1	3	5	24649911	2014	Prediction of formulation effects on dermal absorption of topically appli...	Riviere; Brooks; Collard; Deng; de Rose; Mahabir; ...	Journal of veterinary pharmacology and therapeutics	
0	5	0	5	21243407	2011	Synergy between fipronil and amitraz in a Rhipicephalus sanguineus ti...	Prullage; Cawthorne; Le Hir de Fallois; Timmons	Experimental & applied acarology	
0	4	0	4	27717758	2016	Multiple resistance to acaricides in field populations of Rhipicephalus ...	Klafke; Webster; Dall Agnol; Pradel; Silva; de La Ca...	Ticks and tick-borne diseases	
0	4	0	4	21777731	2011	The combined mode of action of fipronil and amitraz on the motility of ...	Prullage; Tran; Timmons; Harriman; Chester; Powell	Veterinary parasitology	
1	0	0	1	28122816	2017	Effectiveness of Fipronil as a Systemic Control Agent Against Xenops...	Rajonhson; Miarinjara; Rahelinirina; Rajerison; Boyer	Journal of medical entomology	
0	1	0	1	22235587	2012	[Prevention of tick borne diseases].	Bouman	Tijdschrift voor diergeneeskunde	
0	0	1	1	18322939	2008	Metabolic interactions of agrochemicals in humans.	Hodgson; Rose	Pest management science	✓
0	0	1	1	15135087	2004	In vitro metabolism of fipronil by human and rat cytochrome P450 and ...	Tang; Amin Usmani; Hodgson; Rose	Chemico-biological interactions	
0	0	0	0	29407826	2018	Activated carbon as a means of limiting bioaccumulation of organochl...	Dang; Kroll; Supowit; Halden; Denslow	Chemosphere	
0	0	0	0	29380196	2018	Association of detoxification enzymes with butene-fipronil in larvae an...	Arain; Shakeel; Elzaki; Farooq; Hafeez; Shahid; Sh...	Environmental science and pollution research intern...	
0	0	0	0	29372769	2018	[Determination of fipronil and its metabolites in bird eggs by ultra-perfo...	Li; Zheng; Wang; Qiu	Se pu = Chinese journal of chromatography	
0	0	0	0	29291857	2018	Development and validation of an ultra performance liquid chromatogr...	Chen; Gao; Liu; Pan; Chai; Liu; Lu	Food chemistry	

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

Mixtures

Retrieve Articles

70 of 70 articles loaded...

Optionally, edit the query before retrieving.

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To find articles quickly, enter terms to sift abstracts.

flea | tick | dog | | Clear Terms

Download / Send to... | Download Sifter for Excel

flea	tick	dog	Total	PMID	Year	Title	Authors	Journal	Rev
1	1	3	5	24649911	2014	Prediction of formulation effects on dermal absorption of topically appli...	Riviere; Brooks; Collard; Deng; de Rose; Mahabir; ...	Journal of veterinary pharmacology and therapeutics	
0	5	0	5	21243407	2011	Synergy between fipronil and amitraz in a Rhipicephalus sanguineus ti...	Prullage; Cawthorne; Le Hir de Fallois; Timmons	Experimental & applied acarology	
0	4	0	4	27717758	2016	Multiple resistance to acaricides in field populations of Rhipicephalus ...	Klafke; Webster; Dall Agnol; Pradel; Silva; de La Ca...	Ticks and tick-borne diseases	
0	4	0	4	21777731	2011	The combined mode of action of fipronil and amitraz on the motility of ...	Prullage; Tran; Timmons; Harriman; Chester; Powell	Veterinary parasitology	
1	0	0	1	28122816	2017	Effectiveness of Fipronil as a Systemic Control Agent Against Xenops...	Rajonhson; Miarinjara; Rahelinirina; Rajerison; Boyer	Journal of medical entomology	
0	1	0	1	22235587	2012	[Prevention of tick borne diseases].	Bouman	Tijdschrift voor diergeneeskunde	
0	0	1	1	18322939	2008	Metabolic interactions of agrochemicals in humans.	Hodgson; Rose	Pest management science	✓
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0	0	0	0	29380196	2018	Association of detoxification enzymes with butene-fipronil in larvae an...	Arain; Shakeel; Elzaki; Farooq; Hafeez; Shahid; Sh...	Environmental science and pollution research intern...	
0	0	0	0	29372769	2018	[Determination of fipronil and its metabolites in bird eggs by ultra-perfo...	Li; Zheng; Wang; Qiu	Se pu = Chinese journal of chromatography	
0	0	0	0	29291857	2018	Development and validation of an ultra performance liquid chromatogr...	Chen; Gao; Liu; Pan; Chai; Liu; Lu	Food chemistry	

Prediction of formulation effects on dermal absorption of topically applied ectoparasiticides dosed in vitro on canine and porcine skin using a mixture-adjusted quantitative structure permeability relationship.

Topical application of ectoparasiticides for flea and tick control is a major focus for product development in animal health. The objective of this work was to develop a quantitative structure permeability relationship (QSPeR) model sensitive to formulation effects for predicting absorption and skin deposition of five topically applied drugs administered in six vehicle combinations to porcine and canine skin in vitro. Saturated solutions (20 μL) of (14) C-labeled demiditraz, fipronil, permethrin, imidacloprid, or sisapronil were administered in single or binary (50:50 v/v) combinations of water, ethanol, and transcutol (6 formulations, n = 4-5 replicates per treatment) nonoccluded to 0.64 cm(2) disks of dermatomed pig or dog skin mounted in flow-through diffusion cells. Perfusate flux over 24 h and skin deposition at termination were determined. Permeability (logKp), absorption, and penetration endpoints were modeled using a four-term Abrahams and Martin (hydrogen-bond donor acidity and basicity, dipolarity/polarizability, and excess molar refractivity) linear free energy QSPeR equation with a mixture factor added to compensate for formulation ingredient interactions. Goodness of fit was judged by r(2) , cross-validation coefficient, coefficients (q(2) s), and Williams Plot to visualize the applicability domain. Formulation composition was the primary determinant of permeation. Compounds generally penetrated dog skin better than porcine skin. The vast majority of permeated penetrant was deposited within the dosed skin relative to transdermal flux, an attribute for ectoparasiticides. The best QSPeR logKp model for pig skin permeation (r(2) = 0.86, q(2) s = 0.85) included log octanol/water partition coefficient as the mixture factor, while for dogs (r(2) = 0.91, q(2) s = 0.90), it was log water solubility. These studies clearly showed that the permeation of topical ectoparasiticides could be well predicted using QSPeR models that account for both the physical-chemical properties of the penetrant and formulation components.

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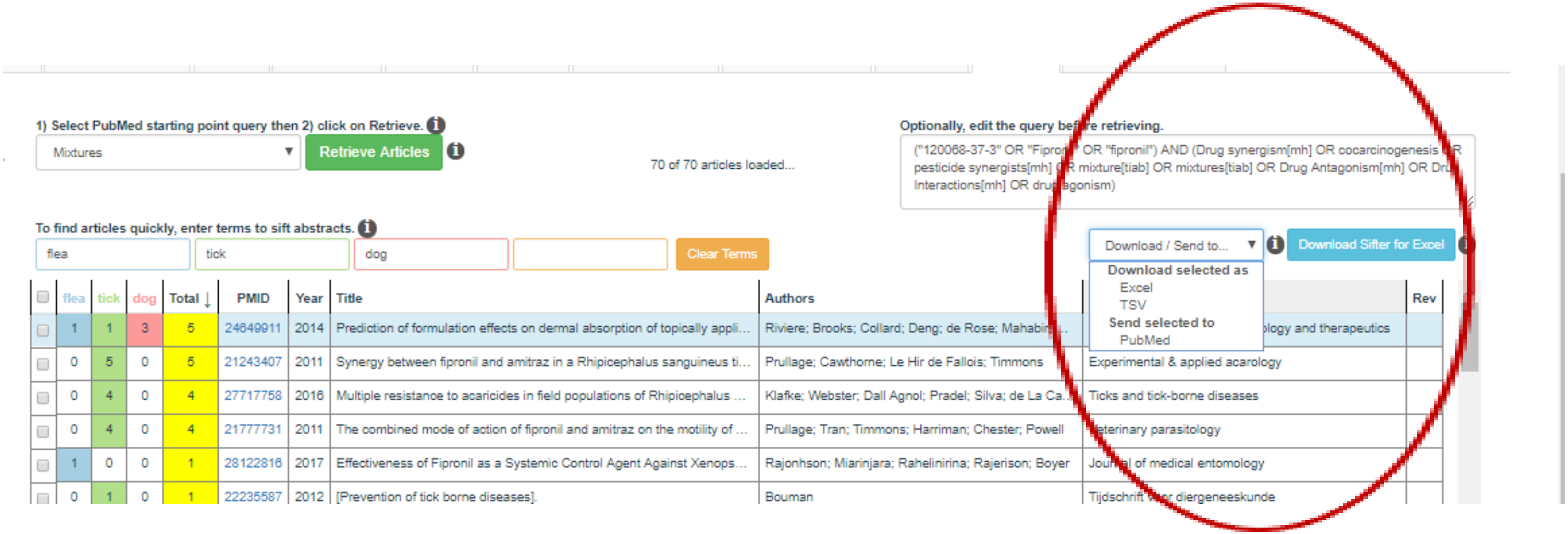

flea	tick	dog	Total	PMID	Year	Title	Authors		Rev
1	1	3	5	24649911	2014	Prediction of formulation effects on dermal absorption of topically appli...	Riviere; Brooks; Collard; Deng; de Rose; Mahabir...	...logy and therapeutics	
0	5	0	5	21243407	2011	Synergy between fipronil and amitraz in a Rhipicephalus sanguineus ti...	Prullage; Cawthorne; Le Hir de Fallois; Timmons	Experimental & applied acarology	
0	4	0	4	27717758	2016	Multiple resistance to acaricides in field populations of Rhipicephalus ...	Klafke; Webster; Dall Agnol; Pradel; Silva; de La Ca...	Ticks and tick-borne diseases	
0	4	0	4	21777731	2011	The combined mode of action of fipronil and amitraz on the motility of ...	Prullage; Tran; Timmons; Harriman; Chester; Powell	...eterinary parasitology	
1	0	0	1	28122816	2017	Effectiveness of Fipronil as a Systemic Control Agent Against Xenops...	Rajonhson; Miarinjara; Rahelinirina; Rajerison; Boyer	Jou...l of medical entomology	
0	1	0	1	22235587	2012	[Prevention of tick borne diseases].	Bouman	Tijdschrift voor diergeneeskunde	

What's coming

- More documentation including video tutorials
- More integration between the Dashboard and the Excel version of the Sifter

Stay tuned!

And be part of the conversation…
Comment on the F1000 article or comment via the Dashboard

Thank you!

Questions?