

AI4NAMS - Deliverable 5

Draft case study report – Supplementary data

Case study 1

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1. Case Study Description

Table 1. List of pyrethrins and pyrethroids in scope of the case study including CAS numbers used in chemical batch search of structured databases.

Name	CAS
Permethrin	52645-53-1
Acrinathrin	101007-06-1
Alpha-cypermethrin (Alphamethrin)	67375-30-8
Bifenthrin	82657-04-3
(beta-)Cyfluthrin	68359-37-5
(zeta-)Cypermethrin	52315-07-8
Cyphenotrin (Zyphenothrin)	39515-40-7
d-Allethrin	231937-89-6; 584-79-2
Deltamethrin	52918-63-5
d-Tetramethrin	1166-46-7
Empenthrin	54406-48-3
Epsilon-momfluorothrin	1065124-65-3
Esbiothrin	260359-57-7
Esfenvalerate	66230-04-4
Etofenprox	80844-07-1
Imiprothrin	72963-72-5
Lambda-cyhalothrin	91465-08-6
Gamma-cyhalothrin	76703-62-3
Metofluthrin	240494-71-7
Prallethrin	23031-36-9
Tau-fluvalinate	102851-06-9
Tefluthrin	79538-32-2
Tetramethrin	7696-12-0
Transfluthrin	118712-89-3
1R-trans-phenothrin (D-phenothrin)	26046-85-5
Pyrethrin I	121-21-1
Pyrethrin II	121-29-9
Jasmolin I	4466-14-2
Jasmolin II	1172-63-0
Cinerin I	25402-06-6
Cinerin II	121-20-0
Bioresmethrin	28434-01-7

2. Search Strategy, Structured Data Sources

Table 2. Result of screening for data from structured data sources for pyrethroids in scope.

Name	CAS	ToxCast Assays	PubChem Assays
Permethrin	52645-53-1	1146	170
Acrinathrin	101007-06-1	0	43
Alpha-cypermethrin (Alphamethrin)	67375-30-8	271	50
Bifenthrin	82657-04-3	1142	97
(beta-)Cyfluthrin	68359-37-5	1142	202
(zeta-)Cypermethrin	52315-07-8	1180	59
Cyphenotrin (Zyphenothrin)	39515-40-7	237	10
d-Allethrin	231937-89-6; 584-79-2	1051	107
Deltamethrin	52918-63-5	705	101
d-Tetramethrin	1166-46-7	0	49
Empenthrin	54406-48-3	0	49
Epsilon-momfluorothrin	1065124-65-3	0	0
Esbiothrin	260359-57-7	0	5
Esfenvalerate	66230-04-4	1025	67
Etofenprox	80844-07-1	917	114
Imiprothrin	72963-72-5	79	50
Lambda-cyhalothrin	91465-08-6	695	69

Gamma-cyhalothrin	76703-62-3	493	69
Metofluthrin	240494-71-7	0	0
Prallethrin	23031-36-9	1143	46
Tau-fluvalinate	102851-06-9	441	67
Tefluthrin	79538-32-2	983	37
Tetramethrin	7696-12-0	998	87
Transfluthrin	118712-89-3	79	46
1R-trans-phenothrin (D-phenothrin)	26046-85-5	0	52
Pyrethrin I	121-21-1	0	36
Pyrethrin II	121-29-9	0	32
Jasmolin I	4466-14-2	0	26
Jasmolin II	1172-63-0	0	27
Cinerin I	25402-06-6	0	25
Cinerin II	121-20-0	0	27
Bioresmethrin	28434-01-7	237	52
Sum (containing duplicates)	2 w/o any data from structured data sources	13 w/o data	2 w/o data

3. Initial Data Collection, Unstructured Data Sources

Table 3. Search strings and number of hits received in PubMed for each pyrethroid in scope. The whole search string is presented for permethrin as an example. For further pyrethroids only the substance specific part is given.

Name	CAS	No. hits	Search String
Permethrin	52645-53-1	43	((((in vitro) OR (chemico) OR (silico) OR (QSAR) OR (zebrafish) OR (danio rerio) OR (c. elegans) OR (transcriptom) OR (cell culture) OR (organ chip) OR (ex vivo) OR (cell line) OR (organoid) OR (Drosophila melanogaster)) AND ((neuron) OR (neurotox))) AND ('Permethrin'[Title/Abstract] OR '(m-Phenoxybenzyl)-cis,trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate'[Title/Abstract] OR '3-Phenoxybenzyl-(+)-cis,trans-2,2-dichlorovinyl-2,2-dimethylcyclopropylcarboxylic acid, ester'[Title/Abstract] OR '3-Phenoxybenzyl-cis,trans-(1RS)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate'[Title/Abstract] OR 'Ambush'[Title/Abstract] OR 'Cyclopropanecarboxylic Acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester'[Title/Abstract] OR 'Elimite'[Title/Abstract]))
Acrinathrin	101007-06-1	0	...AND ('2,2-dimethyl-3-(3-oxo-3-(2,2,2-trifluoro-1-(trifluoromethyl)ethoxy)-1-propenyl)cyano(3-phenoxyphenyl)cyclopropanecarboxylic acid, methyl ester'[Title/Abstract] OR 'acrinathrin'[Title/Abstract])
Alpha-cypermethrin (Alphamethrin)	67375-30-8	30	...AND ('alpha-cypermethrin'[Title/Abstract] OR 'alphacypermethrin'[Title/Abstract] OR 'alphamethrin'[Title/Abstract] OR 'beta-cipermetrina'[Title/Abstract] OR 'Cymbush'[Title/Abstract] OR 'cypermethrin'[Title/Abstract] OR 'Fastac 50EC'[Title/Abstract] OR 'Fendona'[Title/Abstract] OR 'NRDC 149'[Title/Abstract] OR 'supercypermethrin'[Title/Abstract] OR 'supermethrin'[Title/Abstract] OR 'WL 85871'[Title/Abstract])
Bifenthrin	82657-04-3	22	...AND ('bifenthrin'[Title/Abstract] OR '(2-methyl(1,1'-biphenyl)-3-yl)methyl (1R,3R)-3-((1Z)-2-chloro-3,3,3-trifluoroprop-1-en-1-yl)-2,2-dimethylcyclopropane-1-carboxylate'[Title/Abstract])
(beta-)Cyfluthrin	68359-37-5	11	...AND ('beta-cyfluthrin'[Title/Abstract] OR 'cyano(4-fluoro-3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane carboxylate'[Title/Abstract] OR 'cyfluthrin'[Title/Abstract] OR 'OMS 2012'[Title/Abstract])
(zeta)Cypermethrin	52315-07-8	0	...AND ('zeta-cypermethrin'[Title/Abstract])

Cyphenothrin (Zyphenothrin)	39515-40-7	1	...AND ('cis-cyphenothrin'[Title/Abstract] OR 'cyphenothrin'[Title/Abstract] OR 'zyphenothrin'[Title/Abstract])
d-Allethrin	231937-89-6; 584-79-2	8	...AND ('Allethrin'[Title/Abstract] OR 'Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl ester'[Title/Abstract] OR 'pallethrine'[Title/Abstract] OR 'bioallethrine'[Title/Abstract])
Deltamethrin	52918-63-5	55	...AND ('Deltamethrin'[Title/Abstract] OR 'Decamethrin'[Title/Abstract] OR 'Butox'[Title/Abstract] OR 'K-othrin'[Title/Abstract] OR 'Difexon'[Title/Abstract] OR 'NRDC 161'[Title/Abstract] OR 'OMS 1998'[Title/Abstract] OR 'alpha-cyano-3-phenoxybenzyl (1R,3R)-cis-3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate'[Title/Abstract])
d-Tetramethrin	1166-46-7	2	...AND ('d-Tetramethrin'[Title/Abstract] OR 'D-trans-Tetramethrin'[Title/Abstract] OR '(1R)-trans-Tetramethrin'[Title/Abstract] OR 'trans-Tetramethrin'[Title/Abstract] OR '(1,3,4,5,6,7-Hexahydro-1,3-dioxo-2H-isoindol-2-yl)methyl (1R-trans)-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate'[Title/Abstract] OR '(1,3-dioxo-4,5,6,7-tetrahydroisoindol-2-yl)methyl (1R,3R)-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropane-1-carboxylate'[Title/Abstract] OR '(+)-trans-Phthalthrin'[Title/Abstract] OR 'Cyclohexene-1,2-dicarboximido)methyl 2,2-dimethyl-'[Title/Abstract])
Empenthrin	54406-48-3	0	...AND ('empenthrin'[Title/Abstract] OR '1-ethynyl-2-methyl-2-pentenyl chrysanthemate'[Title/Abstract] OR 'Vaporthrin'[Title/Abstract] OR 'd-empenthrin'[Title/Abstract])
Epsilon-momfluorothrin	1065124-65-3	0	...AND ('epsilon-momfluorothrin'[Title/Abstract] OR 'Momfluorothrin, (Z,1R,3R)-'[Title/Abstract] OR 'Momfluorothrin, (Z,1R,3R)-'[Title/Abstract] OR '2,3,5,6-Tetrafluoro-4-(methoxymethyl)benzyl (1R,3R)-3-((Z)-2-cyanoprop-1-en-1-yl)-2,2-dimethylcyclopropane-1-carboxylate'[Title/Abstract])
Esbiothrin	260359-57-7	1	...AND ('esbiothrin'[Title/Abstract] OR 'depallethrin'[Title/Abstract] OR 'trans-allethrin'[Title/Abstract])
Esfenvalerate	66230-04-4	6	...AND ('alpha-cyano-3-phenoxybenzyl 2-(4-chlorophenyl)-3-methylbutyrate'[Title/Abstract] OR 'alpha-cyano-3-phenoxybenzyl alpha-isopropyl-4-chlorophenyl acetate'[Title/Abstract] OR 'Belmark'[Title/Abstract] OR 'esfenvalerate'[Title/Abstract] OR 'fenvalerate'[Title/Abstract] OR 'Pydrin'[Title/Abstract] OR 'Sumi-alpha'[Title/Abstract] OR 'Sumicidin'[Title/Abstract])

Etofenprox	80844-07-1	6	...AND ('2-(4-ethoxyphenyl)-2-methylpropyl-3-phenoxybenzyl ether'[Title/Abstract] OR 'ethofenprox'[Title/Abstract] OR 'etofenprox'[Title/Abstract] OR 'Trebon'[Title/Abstract])
Imiprothrin	72963-72-5	0	...AND ('imiprothrin'[Title/Abstract] OR 'pralle'[Title/Abstract] OR '(2,5-dioxo-3-prop-2-ynylimidazolidin-1-yl)methyl 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropane-1-carboxylate'[Title/Abstract] OR '(2,4-Dioxo-(2-propyn-1-yl)imidazolidin-3-yl)methyl(1R)-trans-chrysanthemate'[Title/Abstract])
Lambda-cyhalothrin	91465-08-6	9	...AND ('lambda-cyhalothrin'[Title/Abstract] OR 'lambdacycyhalothrin'[Title/Abstract] OR 'alpha-cyano-3-phenoxybenzyl 3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl cyclopropanecarboxylate'[Title/Abstract] OR 'cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester'[Title/Abstract])
Gamma-cyhalothrin	76703-62-3	9	...AND ('gammacyhalothrin'[Title/Abstract] OR 'gamma-cyhalothrin'[Title/Abstract] OR 'cyhalothrin'[Title/Abstract])
Metofluthrin	240494-71-7	0	...AND (('2,3,5,6-tetrafluoro-4-methoxymethylphenyl)methyl-2,2-dimethyl-3-(1-propenyl)cyclopropanecarboxylate'[Title/Abstract] OR 'metofluthrin'[Title/Abstract] OR 'epsilon-metofluthrin'[Title/Abstract] OR 'trans-(Z)-metofluthrin'[Title/Abstract])
Prallethrin	23031-36-9	1	...AND ('2-methyl-4-oxo-3-(2-propynyl)cyclopent-2-enyl chrysanthemate'[Title/Abstract] OR 'd,d-T80-prallethrin'[Title/Abstract] OR 'ETOC'[Title/Abstract] OR 'prallethrin'[Title/Abstract])
Tau-fluvalinate	102851-06-9	0	...AND ('Tau-fluvalinate'[Title/Abstract] OR 'Klartan'[Title/Abstract] OR 'cyano(3-phenoxyphenyl)methyl (2-chloro-4-(trifluoromethyl)phenyl)-D-valinate'[Title/Abstract] OR 'Fluvarol'[Title/Abstract] OR 'Fluwarol'[Title/Abstract] OR 'D-Valine, N-[2-chloro-4-(trifluoromethyl)phenyl]-,cyano(3-phenoxyphenyl)methyl ester'[Title/Abstract] OR '[cyano-(3-phenoxyphenyl)methyl] (2R)-2-[2-chloro-4-(trifluoromethyl)anilino]-3-methyl-butanoate'[Title/Abstract])
Tefluthrin	79538-32-2	16	...AND ('2,3,5,6-tetrafluoro-4-methylbenzyl (Z)-(1RS)-cis-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate'[Title/Abstract] OR 'tefluthrin'[Title/Abstract] OR 'tefluthrine'[Title/Abstract])
Tetramethrin	7696-12-0	13	...AND ('2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylic acid, ester with N-(hydroxymethyl)-1-cyclohexene 1,2-dicarboximide'[Title/Abstract] OR 'neopinamine'[Title/Abstract])

			OR 'neopynamin'[Title/Abstract] OR 'tetramethrin'[Title/Abstract])
Transfluthrin	118712-89-3	1	...AND ('2,3,5,6-tetrafluorobenzyl (+)-(1R-trans)-2,2-dimethyl-3-(2,2-dichlorovinyl)cyclopropanecarboxylate'[Title/Abstract] OR 'transfluthrin'[Title/Abstract])
1R-trans-phenothrin (D-phenothrin)	26046-85-5	2	...AND (('3-phenoxyphenyl)methyl cis,trans-(+)-2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate'[Title/Abstract] OR 'd-phenothrin'[Title/Abstract] OR 'phenothrin'[Title/Abstract] OR 'Sumithrin'[Title/Abstract])
Pyrethrin I	121-21-1	2	...AND ('pyrethrin I'[Title/Abstract] OR 'pyrethrin II'[Title/Abstract] OR 'Chrysanthemum monocarboxylic acid pyrethrolone ester'[Title/Abstract] OR '[(1S)-2-methyl-4-oxo-3-[(2Z)-penta-2,4-dienyl]cyclopent-2-en-1-yl] (1R,3R)-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropane-1-carboxylate'[Title/Abstract] OR '(1S)-2-methyl-4-oxo-3-[(2Z)-penta-2,4-dien-1-yl]cyclopent-2-en-1-yl (1R,3R)-3-[(1E)-3-methoxy-2-methyl-3-oxoprop-1-en-1-yl]-2,2-dimethylcyclopropanecarboxylate'[Title/Abstract] OR '(+)-Pyrethronyl (+)-pyrethrate'[Title/Abstract] OR 'Chrysanthemumdicarboxylic acid monomethyl ester pyrethrolone ester'[Title/Abstract] OR 'Pyrethrolone ester of chrsanthemumdicarboxylic acid monomethyl ester'[Title/Abstract] OR 'pyrethrin'[Title/Abstract] OR 'pyrethrine'[Title/Abstract])
Pyrethrin II	121-29-9		
Jasmolin I	4466-14-2	0	...AND ('jasmolin I'[Title/Abstract] OR 'jasmolin II'[Title/Abstract] OR 'jasmolin'[Title/Abstract])
Jasmolin II	1172-63-0		
Cinerin I	25402-06-6	0	...AND ('cinerin I'[Title/Abstract] OR 'cinerin II'[Title/Abstract] OR 'cinerin'[Title/Abstract] OR 'cinerine'[Title/Abstract])
Cinerin II	121-20-0		
Bioresmethrin	28434-01-7	1	...AND ('bioresmethrin'[Title/Abstract] OR 'trans-resmethrin'[Title/Abstract] OR 'Biobenzofuroline'[Title/Abstract] OR '(+)-trans-Resmethrin'[Title/Abstract] OR '1R-trans-Resmethrin'[Title/Abstract] OR '(1RS)-trans-Resmethrin'[Title/Abstract] OR 'Resbuthrin'[Title/Abstract] OR 'Isathrine'[Title/Abstract] OR 'Isatrin'[Title/Abstract] OR 'd-trans-Resmethrin'[Title/Abstract] OR '5-Benzyl-3-furylmethyl (1R)-trans-chrysanthemate'[Title/Abstract] OR 'Bioresmethrinum'[Title/Abstract] OR 'd-trans-Chrysron'[Title/Abstract] OR 'Chrysanthemate'[Title/Abstract])
Sum (containing duplicates)		239	

