Supplementary Information:
Efficacy, Economics, and Sustainability of Bio-based Insecticides from Thermochemical Biorefineries

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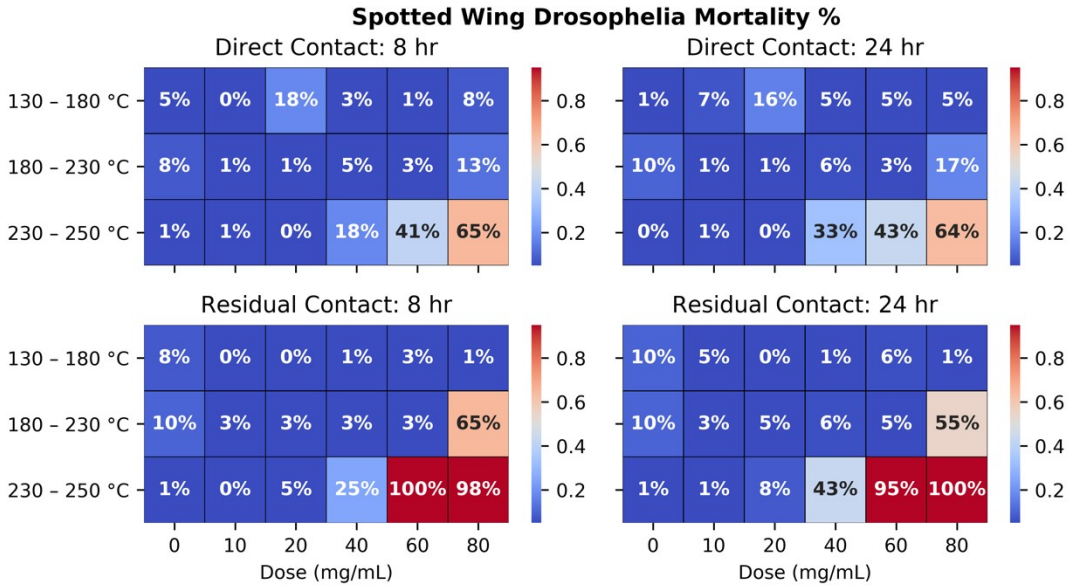
Supplementary Table 1: Physiochemical properties of bio-oil, Pt/TiO_2 CFP Oil, and the distillate resid remaining after distillation of bio-based insecticide fractions.

Parameter	PtTiO_2 CFP Oil	Distillate Resid	Units
Carbonyl Content	3.1±0.1	1.6±0.3	mol/kg
C	71[1]	74	%
H	7.5[1]	6.7	%
O	21[1]	20	%
Aluminum	ND	< 50	µg/g
Calcium	ND	< 50	µg/g
Chromium	ND	< 10	µg/g
Copper	ND	< 10	µg/g
Iron	ND	< 50	µg/g
Magnesium	ND	< 10	µg/g
Manganese	ND	< 2	µg/g
Nickel	ND	< 10	µg/g
Phosphorus	ND	< 100	µg/g
Potassium	ND	< 50	µg/g
Sodium	ND	< 50	µg/g
Sulfur	ND	< 100	µg/g
Vanadium	ND	< 2	µg/g
Zinc	ND	< 5	µg/g
Viscosity	<100[a]	>9300[b]	cP

[a] at 20 °C, [b] at 95 °C



Supplementary Figure 1: Annotated heat maps of spotting wing drosophelia mortality. Percentages represent the average number dead (n=60) as a function of candidate bio-based insecticide fraction dose (mg/mL), boiling point range of the candidate bio-based insecticide fraction, timepoint, and testing modality (i.e., direct or residual contact).

Supplementary Table 2: Table of calculated LC_{50} values for insect assays as a function of fraction, test modality, and insect model.

Fraction	Modality	Insect Model	LC_{50} (mg/mL)			LC_{50} p-value
130 – 180 °C	Diet	oriental fruit moth, *Grapholita molesta* (Herbst)			ND	
180 – 230 °C	Diet	oriental fruit moth, *Grapholita molesta* (Herbst)	13.1	±	1.08	<0.0001
230 – 250 °C	Diet	oriental fruit moth, *Grapholita molesta* (Herbst)	12.7	±	0.94	<0.0001
130 – 180 °C	Direct Contact	Spotted-wing drosophila, *Drosophila suzukii* (Matsumura)			ND	
180 – 230 °C	Direct Contact	Spotted-wing drosophila, *Drosophila suzukii* (Matsumura)	307.7	±	194.6	0.11
230 – 250 °C	Direct Contact	Spotted-wing drosophila, *Drosophila suzukii* (Matsumura)	62.46	±	3.94	<0.0001
130 – 180 °C	Residual Contact	Spotted-wing drosophila, *Drosophila suzukii* (Matsumura)			ND	
180 – 230 °C	Residual Contact	Spotted-wing drosophila, *Drosophila suzukii* (Matsumura)	102.23	±	14.13	<0.0001
230 – 250 °C	Residual Contact	Spotted-wing drosophila, *Drosophila suzukii* (Matsumura)	37.74	±	1.7	<0.0001

Supplementary Table 3: Compositional analysis of distillate fractions as determined by GC-MS/FID. Reported values are in weight percentages.

Class	130-180 °C	180-230 °C	230-250 °C
Phenol (0-carbon)	11.6	2.3	0.1
Phenol (1-carbon)	5.4	7.4	0.5
Phenol (2-carbon)	1.3	7.0	6.6
Phenol (3-carbon)	0.9	11.4	18.5
Phenol (4-carbon)	-	4.2	9.9
Phenol (+5-carbon)	-	2.5	3.1
Methoxyphenol	5	18.2	18.5
Acids	17.7	0.4	2.3
Cyclopentones	23.8	5.2	3.0
Other	31.0	39.9	36.8
Total Closure	**96.7**	**98.5**	**99.3**

Supplementary Table 4: Compositional analysis of distillate fractions as determined by GC-MS/FID. Reported values are in weight percentages.

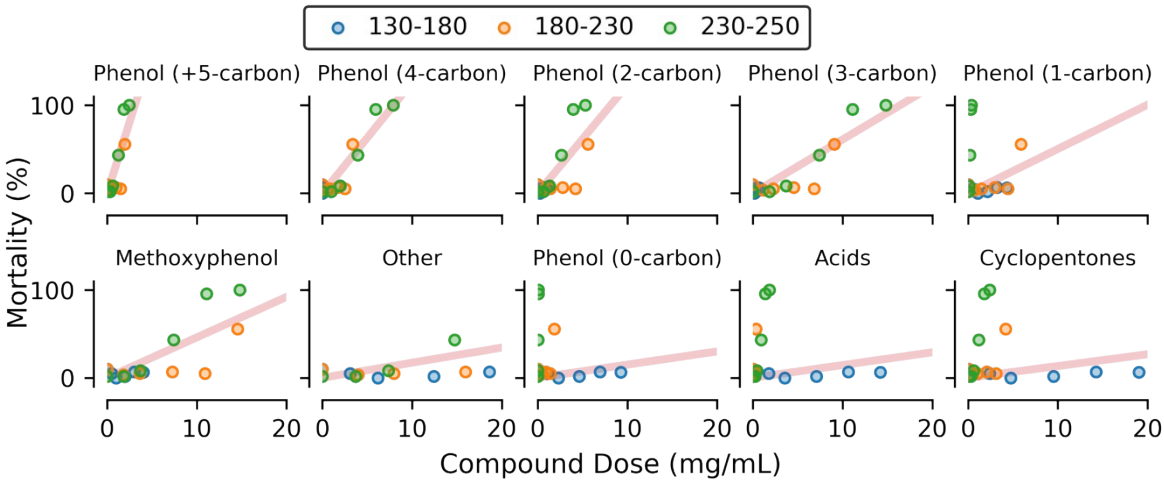
Class	Compound	130-180 °C	180-230 °C	230-250 °C
Phenol (0-carbon)	Phenol	11.6	2.3	0.1
Phenol (1-carbon)	Phenol, 2-methyl-	3.3	1.6	-
Phenol (1-carbon)	Phenol, 3-methyl-	2.1	5.7	0.5
Phenol (2-carbon)	Phenol, 2,3-dimethyl-	0.5	0.4	1
Phenol (2-carbon)	Phenol, 2-ethyl-	0.4	1	0.1
Phenol (2-carbon)	Phenol, 3,5-dimethyl-	-	-	0.2
Phenol (2-carbon)	Phenol, 3-ethyl-	0.5	5.6	5.2
Phenol (2-carbon)	Phenol, 4-ethyl-	-	-	0.2
Phenol (3-carbon)	Phenol, 2-ethyl-6-methyl-	0.6	3.5	6.1
Phenol (3-carbon)	Phenol, 2-propyl-	-	0.4	0.5
Phenol (3-carbon)	Phenol, 3,4,5-trimethyl-	0.1	0.2	0.7
Phenol (3-carbon)	Phenol, 3-propyl-	0.2	4.5	9.3
Phenol (3-carbon)	Phenol, 4-(2-propenyl)-	-	2.6	-
Phenol (3-carbon)	Phenol, 4-ethyl-2-methyl-	-	-	1.9
Phenol (3-carbon)	p-Hydroxyphenylacetone	-	-	-
Phenol (4-carbon)	2,5-Diethylphenol	-	1.4	2.3
Phenol (4-carbon)	2-(1-Methyl-2-propenyl)phenol	-	0.6	-
Phenol (4-carbon)	2-Allyl-4-methylphenol	-	-	0.3
Phenol (4-carbon)	4-Methyl-2-propylphenol	-	0.2	0.6
Phenol (4-carbon)	Phenol, 2,3,4,6-tetramethyl-	-	0.5	-
Phenol (4-carbon)	Phenol, 2,3,5,6-tetramethyl-	-	-	0.6
Phenol (4-carbon)	Phenol, 2-ethyl-4,5-dimethyl-	-	0.8	2.7
Phenol (4-carbon)	Phenol, 2-methyl-5-(1-methylethyl)-	-	-	0.1
Phenol (4-carbon)	Phenol, 2-methyl-6-(2-propenyl)-	-	0.1	0.1
Phenol (4-carbon)	Phenol, 3-methyl-6-propyl-	-	0.5	3
Phenol (4-carbon)	Phenol, 4-(2-methylpropyl)-	-	0.1	-
Phenol (4-carbon)	Phenol, p-(2-methylallyl)-	-	-	0.1
Phenol (+5-carbon)	2-Ethyl-5-n-propylphenol	-	1.4	2.4
Phenol (+5-carbon)	Phenol, 2,5-bis(1-methylethyl)-	-	0.4	0.7
Phenol (+5-carbon)	Phenol, 2-(2-penten-4-yl)-4-methyl-	-	0.7	-
Methoxyphenol	2-Methoxy-4-vinylphenol	-	0.6	0.2
Methoxyphenol	2-Methoxy-6-methylphenol	-	-	1.8
Methoxyphenol	2-Methyl-6-propylphenol	-	1	-
Methoxyphenol	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	-	-	0.2
Methoxyphenol	Creosol	-	3.9	-
Methoxyphenol	Eugenol	-	-	8.4
Methoxyphenol	Phenol, 2-methoxy-	4.1	2.2	0.2
Methoxyphenol	Phenol, 2-methoxy-3-(2-propenyl)-	-	3	-
Methoxyphenol	Phenol, 2-methoxy-4-(1-propenyl)-	-	4.9	3.7
Methoxyphenol	Phenol, 2-methoxy-4-propyl-	-	1.2	2.1
Methoxyphenol	Phenol, 4-ethyl-2-methoxy-	0.2	-	1.5
Methoxyphenol	Vanillin	-	-	0.2
Methoxyphenol	m-Guaiacol	-	-	0.1
Acids	3-Butenoic acid	0.4	-	-
Acids	4-n-Propylbenzoic acid	-	-	1.3
Acids	Acetic acid	6.6	0.4	-

Class	Compound	130-180 °C	180-230 °C	230-250 °C
Acids	Acetic acid ethenyl ester	0.5	-	-
Acids	Acetic acid, (acetyloxy)-	1.1	-	-
Acids	Acetic acid, oxo-, methyl ester	-	-	-
Acids	Butanoic acid	1.8	-	-
Acids	Crotonic acid	0.1	-	-
Acids	Hexanoic acid	0.4	-	-
Acids	Nonanoic acid	-	-	0.3
Acids	Octanoic acid	-	-	0.1
Acids	Pentanoic acid	1.5	-	-
Acids	Pentanoic acid, 2-methyl-	0.1	-	-
Acids	Pentanoic acid, 4-oxo-	-	-	0.6
Acids	Propanoic acid	4.8	-	-
Acids	Propanoic acid, 2-methyl-	0.4	-	-
Cyclopentones	1,2-Cyclopentanedione, 3-methyl-	-	1.2	0.8
Cyclopentones	2-Acetonylcyclopentanone	-	-	-
Cyclopentones	2-Butyl-2-cyclopentenone	-	0.2	-
Cyclopentones	2-Cyclopenten-1-one	13.2	0.2	0.1
Cyclopentones	2-Cyclopenten-1-one, 2,3-dimethyl-	1.5	0.4	0.2
Cyclopentones	2-Cyclopenten-1-one, 2-hydroxy-	0.7	0.4	-
Cyclopentones	2-Cyclopenten-1-one, 2-methyl-	5.5	0.1	-
Cyclopentones	2-Cyclopenten-1-one, 3,4-dimethyl-	0.2	-	-
Cyclopentones	2-Cyclopenten-1-one, 3-ethyl-	-	0.3	-
Cyclopentones	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	-	-	0.2
Cyclopentones	2-Cyclopenten-1-one, 3-methyl-	1	2.1	0.8
Cyclopentones	2-Ethyl-3-methylcyclopent-2-en-1-one	0.3	0.4	0.2
Cyclopentones	3-Ethenyl-3-methylcyclopentanone	-	-	-
Cyclopentones	3-Ethylcyclopentanone	0.1	-	-
Cyclopentones	Cyclopentanone	0.3	-	-
Cyclopentones	Cyclopentanone, 2-ethyl-	0.4	-	-
Cyclopentones	Cyclopentanone, 2-methyl-	0.7	-	-
Other	(1-Methylpenta-1,3-dienyl)benzene	-	-	-
Other	(S)-(+)-2',3'-Dideoxyribonolactone	-	0.2	-
Other	1(3H)-Isobenzofuranone	-	-	-
Other	1,1'-Biphenyl, 2-ethyl-	-	1.1	-
Other	1,1'-Biphenyl, 4-methyl-	-	0.2	-
Other	1,1'-Biphenyl, 4-methyl-	-	0.3	-
Other	1,2,3-Trimethylindene	-	0.4	-
Other	1,2-Dipropylcyclopropene	-	-	0.1
Other	1,2-Ethanediol	0.9	0.3	-
Other	1,3-Dioxolane, 2-(1-methylpropyl)-	0.2	0.2	-
Other	1,3-Pentadiene, 2-methyl-, (E)-	0.1	-	-
Other	1,4,5,8-Tetramethylnaphthalene	-	0.8	-
Other	1,4-Benzenediol, 2,3,5-trimethyl-	-	0.3	-
Other	1,4-Benzenediol, 2-methyl-	-	0.4	-
Other	1,4-Cyclohex-2-enedione	-	-	-
Other	1,4-Cyclohexanedione	-	-	0.1
Other	1,4-Dioxaspiro[4.5]decane	0.1	-	-
Other	1,4-Dioxin, 2,3-dihydro-	0.1	-	-
Other	1,4:3,6-Dianhydro-ν†-d-glucopyranose	-	0.4	-
Other	1-(p-Cumenyl)adamantane	-	0.3	-
Other	1-Hydroxy-2-butanone	0.7	-	-
Other	1-Isopropenylnaphthalene	-	0.3	-
Other	1-Methylcyclooctene	-	-	0.1
Other	1-Naphthalenol, 2-methyl-	-	0.6	-
Other	1-Propanone, 1-(5-methyl-2-furanyl)-	-	-	-
Other	1H-Inden-1-ol, 2,3-dihydro-	-	-	1.6
Other	1H-Inden-1-ol, 2,3-dihydro-	-	-	4.3
Other	1H-Inden-1-one, 2,3-dihydro-	-	0.2	0.1
Other	1H-Inden-1-one, 2,3-dihydro-2-methyl-	0.2	-	-
Other	1H-Inden-1-one, 2,3-dihydro-3,3-dimethyl-	-	0.1	-
Other	1H-Inden-5-ol, 2,3-dihydro-	-	1.8	0.4
Other	1H-Indene, 1-ethyl-2,3-dihydro-	0.1	-	-
Other	1H-Indene, 2,3-dihydro-1,2-dimethyl-	0.2	-	-
Other	1H-Indene, 2,3-dihydro-1,3-dimethyl-	0.1	-	-
Other	1H-Indene, 2,3-dihydro-1,6-dimethyl-	0.2	-	-

Class	Compound	130-180 °C	180-230 °C	230-250 °C
Other	1H-Indene, 2,3-dihydro-4-methyl-	0.3	-	-
Other	1H-Indene, 2,3-dimethyl-	0.2	0.2	-
Other	1H-Indene, 3-ethyl-1-(1-methylethyl)-	-	0.7	-
Other	1H-Indene, 3-methyl-	0.2	-	-
Other	1H-Indenol	-	-	0.2
Other	2(3H)-Benzofuranone, 3-methyl-	-	-	-
Other	2(3H)-Furanone, 5-acetyldihydro-	-	0.1	-
Other	2(3H)-Furanone, 5-methyl-	1.6	0.3	-
Other	2(3H)-Furanone, dihydro-3-methyl-	0.1	-	-
Other	2(3H)-Furanone, dihydro-5-methyl-	0.1	0.2	-
Other	2(3H)-Furanone, dihydro-5-propyl-	-	-	-
Other	2(5H)-Furanone	4.3	1.5	0.3
Other	2(5H)-Furanone, 3-methyl-	0.2	1.3	0.2
Other	2(5H)-Furanone, 5-ethyl-	-	0.1	-
Other	2(5H)-Furanone, 5-methyl-	-	0.1	-
Other	2,2'-Bi-1,3-dioxolane	-	0.2	-
Other	2,2-Dimethyl-3-heptanone	-	-	0.1
Other	2,3-Dimethyl-4-hydroxy-2-butenoic lactone	-	0.2	1.1
Other	2,3-Dimethylanisole	0.1	-	-
Other	2,4-Heptadienal, (E,E)-	-	-	0.6
Other	2,4-Hexadiene, 2,5-dimethyl-	-	-	0.1
Other	2,5-Furandione, 3-methyl-	-	-	-
Other	2,5-Furandione, dihydro-3-methyl-	-	-	0.1
Other	2,5-Hexanedione	-	0.1	-
Other	2-Butanone	-	-	-
Other	2-Cyclohexen-1-one	0.2	-	-
Other	2-Cyclohexen-1-one, 2-methyl-	0.2	-	-
Other	2-Cyclohexen-1-one, 3-methyl-	-	-	0.1
Other	2-Cyclohexen-1-one, 4-(1-methylethyl)-	-	-	0.2
Other	2-Ethylidenecyclohexanone	-	-	0.3
Other	2-Furancarboxaldehyde, 5-methyl-	2.1	0.1	-
Other	2-Furanmethanol, tetrahydro-	0.2	-	-
Other	2-Furanone, 2,5-dihydro-3,5-dimethyl	0.2	0.5	1.2
Other	2-Hepten-4-one, 2-methyl-	-	-	-
Other	2-Hexanone, 5-methyl-	-	-	-
Other	2-Hydroxy-gamma-butyrolactone	-	0.4	0.3
Other	2-Methylindene	0.2	-	-
Other	2-Naphthalenol	-	0.4	-
Other	2-Propanone, 1-hydroxy-	5.5	-	-
Other	2-Vinylfuran	0.2	-	-
Other	2H-Pyran-2-one	-	-	-
Other	2H-Pyran-2-one, tetrahydro-	-	0.6	1.5
Other	3,4-Anhydro-d-galactosan	-	0.3	-
Other	3,4-Dihydro-6-methyl-2H-pyran-2-one	-	0.1	-
Other	3,4-Dimethoxytoluene	-	0.1	0.1
Other	3-(p-Hydroxyphenyl)-1-propanol	-	-	0.1
Other	3-Ethylanisole	0.1	-	-
Other	3-Furaldehyde	0.1	0.1	-
Other	3-Hexen-2-one	0.1	-	-
Other	3-Methyl-3-cyclohexen-1-one	-	-	-
Other	3-Penten-2-one	-	-	-
Other	4-Hepten-3-one, 4-methyl-	-	0.1	0.1
Other	4-Hexen-2-one, 3-methyl-	-	-	0.2
Other	4-Hexen-3-one, 4,5-dimethyl-	-	-	0.1
Other	4-Methoxy-7-methylindan-1-one	-	0.6	-
Other	4-Methyl-5H-furan-2-one	-	1.3	4.1
Other	4H-Pyran-4-one	-	-	0.1
Other	5-methyl-2-(Z)-hepten-4-one	-	-	-
Other	6-Methoxy-1-indanone	-	-	0.2
Other	6-Methoxy-3-methylbenzofuran	-	-	0.2
Other	6-Methyl-4-indanol	-	-	0.5
Other	6-Oxabicyclo[3.1.0]hexan-2-one	-	-	-
Other	7-Hexadecene, (Z)-	-	0.2	-
Other	7-Methylindan-1-one	-	0.6	-
Other	Acenaphthene	-	0.4	0.3

Class	Compound	130-180 °C	180-230 °C	230-250 °C
Other	Acetaldehyde, hydroxy-	4	0.2	-
Other	Acetophenone	0.1	0.1	-
Other	Acetophenone, 4'-hydroxy-	-	0.1	-
Other	Anisole, o-(1-ethylvinyl)-	-	1.2	0.4
Other	Apocynin	-	0.7	-
Other	Benzene, (2-propenyloxy)-	-	-	0.1
Other	Benzene, (4,5,5-trimethyl-1,3-cyclopentadien-1-yl)-	-	-	0.2
Other	Benzene, (ethenyloxy)-	-	-	1
Other	Benzene, 1,2,4,5-tetraethyl-	-	0.7	-
Other	Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	-	-	-
Other	Benzene, 1,3-diethyl-5-methyl-	-	-	-
Other	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	0.1	-	-
Other	Benzene, 1-ethenyl-3-methoxy-	-	-	-
Other	Benzene, 1-ethoxy-4-ethyl-	-	-	0.2
Other	Benzene, 1-methoxy-3-methyl-	0.1	-	-
Other	Benzene, 1-methoxy-4-(1-methylpropyl)-	-	-	0.4
Other	Benzene, 1-methyl-4-(1-methylpropyl)-	-	-	-
Other	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-	-	-	1.6
Other	Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-	-	1.1	-
Other	Benzene, 4-ethyl-1,2-dimethoxy-	-	-	0.1
Other	Benzeneacetaldehyde, 2-methoxy-√†,5-dimethyl-	-	0.4	1
Other	Benzeneacetaldehyde, 2-methoxy-√†,5-dimethyl-	-	-	0.2
Other	Benzenemethanol, 4-(1,1-dimethylethyl)-	-	-	0.9
Other	Benzofuran	-	-	-
Other	Benzofuran, 2,3-dihydro-	0.1	-	-
Other	Benzofuran, 2,3-dihydro-	-	0.2	-
Other	Benzofuran, 2,3-dihydro-2-methyl-	-	0.4	-
Other	Benzofuran, 2-methyl-	0.1	-	-
Other	Benzofuran, 4,7-dimethyl-	0.2	-	-
Other	Benzofuran, 7-methoxy-	-	-	0.1
Other	Benzofuran, 7-methyl-	-	-	0.1
Other	Bicyclo[3.1.0]hexan-2-one	-	-	-
Other	Bicyclo[3.1.1]heptan-2-one	0.1	-	-
Other	Biphenyl	-	0.1	-
Other	Butyrolactone	1.6	1.4	0.1
Other	Catechol	-	0.7	0.4
Other	Cyclohexanone, 2-methyl-	0.1	-	-
Other	Cyclopentene, 3-ethenyl-	-	-	-
Other	Dehydromevalonic lactone	-	-	0.1
Other	Estragole	-	0.2	0.5
Other	Ethanone, 1-(2,5-dihydroxyphenyl)-	-	-	0.4
Other	Ethanone, 1-(2-furanyl)-	1.6	-	-
Other	Ethanone, 1-(2-methylcyclopropyl)-	-	0.1	-
Other	Ethanone, 1-cyclopentyl-	0.1	-	-
Other	Ethyl-2-benzofuran	0.1	-	-
Other	Furan, 2,3-dihydro-2,5-dimethyl-	-	-	-
Other	Furan, 2,3-dihydro-4-methyl-	0.1	-	-
Other	Furan, 2-ethyl-	0.6	-	-
Other	Furfural	1.4	-	-
Other	Heptadecane	-	0.1	0.1
Other	Hydroquinone	-	0.3	-
Other	Indan, 1-methyl-	0.1	-	-
Other	Indane	0.1	-	-
Other	Indene	0.1	-	-
Other	Maltol	-	0.1	-
Other	Methyl dehydroabietate	-	0.3	-
Other	Naphthalene	0.4	0.1	-
Other	Naphthalene, 1,2,3,4-tetramethyl-	-	0.2	0.2
Other	Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	-	-	0.1
Other	Naphthalene, 1,2-dihydro-2,5,8-trimethyl-	-	0.1	0.9
Other	Naphthalene, 1,2-dihydro-2-methyl-	0.2	-	-
Other	Naphthalene, 1,4,6-trimethyl-	-	-	0.4
Other	Naphthalene, 1,4,6-trimethyl-	-	2.8	0.2
Other	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	-	0.9	-
Other	Naphthalene, 1,7-dimethyl-	-	0.5	-

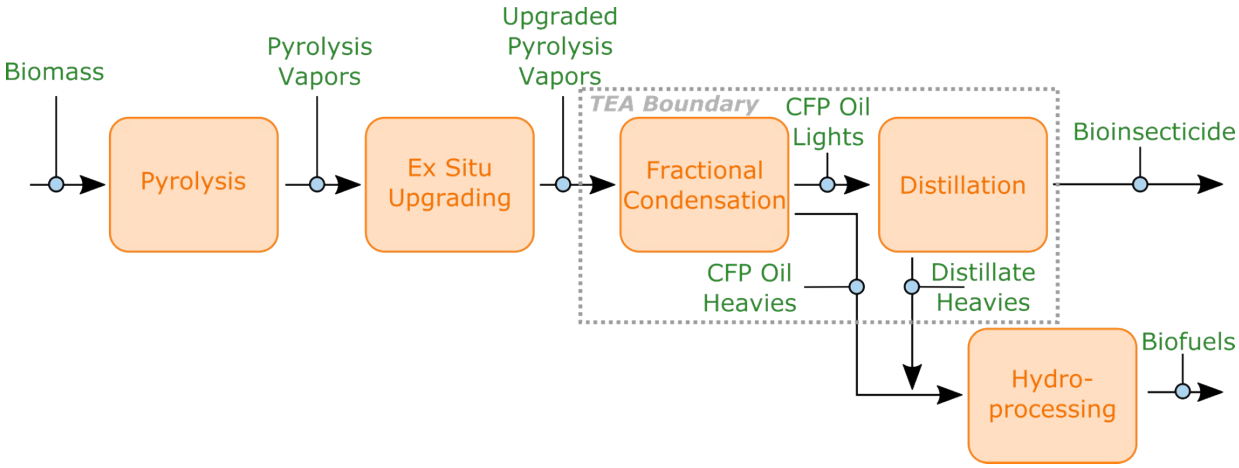
Class	Compound	130-180 °C	180-230 °C	230-250 °C
Other	Naphthalene, 1-ethyl-	-	0.2	-
Other	Naphthalene, 1-methyl-	0.2	-	-
Other	Naphthalene, 2,3-dimethyl-	-	0.2	0.9
Other	Naphthalene, 2-(1-methylethyl)-	-	0.4	-
Other	Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	-	-	-
Other	Pentadecane	-	-	-
Other	Phenanthrene	-	0.3	-
Other	Prenol	-	-	-
Other	Pyridine	-	-	-
Other	Succindialdehyde	0.2	-	-
Other	Toluene	-	-	-
Other	o-Cymene	-	-	-
Other	p-tert.-Butylcatechol	-	0.4	-



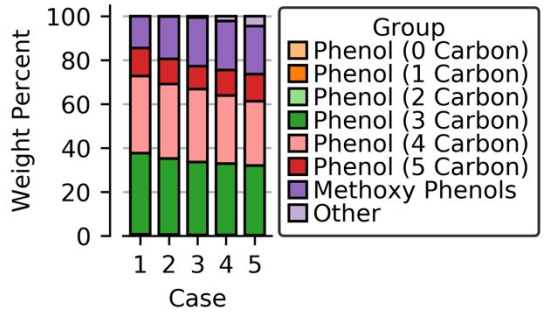
Supplementary Figure 2: Scatter plots showing mortality as a function of the compound dose (mg/mL), compound classification, and boiling point range of the candidate bio-based insecticide fraction. Compound dose is equal to the dose of the fraction multiplied by the weight percent for the specific compound. Blue lines represent linear regression with intercept fixed at zero.

Supplementary Table 5: Ordinary least squared regression results from linear fits to mortality vs. dose. *n* represents the number of data points. *Slope* is the linear coefficient from the regression. Slope error is the 95% confidence interval of the slope. *Intercept* was set to zero. R^2 is the coefficient of determination. *P-value* is the probability that the slope is non-zero.

classify	n	Slope			Intercept	R-squared	P-value
Phenol (+5-carbon)	12	32.3	±	10.3	0	0.81	<0.001
Phenol (4-carbon)	18	12.6	±	1.6	0	0.91	<0.001
Phenol (2-carbon)	18	12.3	±	4.0	0	0.71	<0.001
Phenol (3-carbon)	18	6.1	±	1.2	0	0.87	<0.001
Phenol (1-carbon)	18	5.0	±	7.5	0	0.10	0.178
Methoxyphenol	18	4.6	±	1.4	0	0.73	<0.001
Other	18	1.7	±	0.8	0	0.57	<0.001
Phenol (0-carbon)	18	1.5	±	6.1	0	0.02	0.612
Acids	18	1.4	±	4.0	0	0.03	0.455
Cyclopentones	18	1.3	±	2.8	0	0.05	0.340



Supplementary Figure 3: Block flow diagram for process model. Dashed-grey line indicates analysis boundary for the bio-based insecticide. In this model catalytic fast pyrolysis oil is treated as a feedstock with associated cost. The bio-based insecticide is isolated from the oil and the remaining oil is sent to hydro-processing for fuel production.



Supplementary Figure 4: Resulting bio-based insecticide composition, grouped by compound class, for each case considered in the technoeconomic model.

Supplementary Table 6: Categories (CAT.) and subcategories (SUB CAT.) for the toxicological and environmental risk assessment of each compound in the candidate bio-based insecticide fractions. A brief description, the criteria that a compound was assessed against, and the data sources that were used as the basis for the assessment are provided.

CAT.	SUB CAT.	DESCRIPTION	CRITERIA	DATA SOURCE
Acute Toxicity	Who 1a	Extremely hazardous (Class 1a) according to WHO	LD_{50} for rats is <5 or <50 mg/kg for rat for oral or dermal, respectively	2,3
	Who 1b	Highly hazardous (Class 1b) according to WHO	LD_{50} for rats is 5-50 or 50-200 mg/kg for rat for oral or dermal, respectively	2,3
	Inhalation Hazard (H330)	Fatal if inhaled. Hazard classification according to the GHS	Will have hazard code H330	4
Long Term Effects	EPA Carcinogen	Human carcinogen according to EPA	Listed as group A in the EPA's Risk Assessment for Carcinogenic Effects	5
	EPA Probably Carcinogen	Probable/ Likely carcinogen according to EPA	Listed as group b in the EPA's Risk Assessment for Carcinogenic Effects	5
	IARC (WHO) Carcinogen	Human carcinogen according to IARC (WHO)	Labeled as group 1 in Agents Classified by the IARC Monographs, Volumes 1–127	6
	IARC (WHO) Probable Carcinogen	Probable carcinogen according to IARC (WHO)	Labeled as group 2a in Agents Classified by the IARC Monographs, Volumes 1–127	6
	EU GHS (1A, 1B) Carcinogen	Known or presumed human carcinogens according to EU GHS Regulation 1272/2008/EC	Will have hazard code H350	3,4
	EU GHS (1A, 1B) Mutagen	Known or presumed mutagen ccording to EU Regulation 1272/2008/EC	Will have hazard code H340	3,4
	EU GHS (1A, 1B) Reproductive Toxicant	Known or presumed reproductive toxicant according to EU GHS Regulation 1272/2008/EC	Will have hazard code H360	4
	EU Potential Endocrine Disruptor	Endocrine disruptor or potential endocrine disruptor according to EU	Listed Annex 10 of EU endocrine disruption strategy as Category 1	7
Environmental Toxicity	High Bioaccumulation	Compound will accumulate in the environment.	Bioaccumulation Factor (BCF) >5000 or Kow logP >5 (BCF values supersede Kow logP data)	2,3
	Very environmentally persistent	Very persistent in water. Soils, or sediments.	Half-life in water > 60 days. Half-life in soil or sediment > 180 days	8
	Very toxic to aqueous organisms	Has high toxicity to aquatic life	LC_{50} or EC_{50} <0.1 mg/L for Daphnia species	3
	Highly toxic to bees	Hazard to ecosystem services – Highly toxic to bees	LD50 <2 µg/bee as defined by EPA guidance	-
International Conventions	Montreal Protocol	Ozone depleting chemical according to the Montreal Protocol	Listed in Montreal Protocol as ozone depleting chemical	9
	PIC	Identified as a severely hazardous pesticide and industrial chemical	Listed in Annex III of the Rotterdam Convention	10
	POP	Identified as a persistent organic pollutant.	Listed in Annex III of the Stockholm Convention	11

Supplementary Table 7: Results for toxicological and environmental risk assessment of each compound in the candidate bio-based insecticide fractions.

Passes Criteria	Passes Criteria, reason for additional concern	Insufficient data to make determination	Fails Criteria

Category	Acute Toxicity			Long Term Effects								Environmental Toxicity				International Conventions		
Subcategory	Who 1a	Who 1b	Inhalation Hazard (H330)	EPA Carcinogen	EPA Probably Carcinogen	IARC (WHO) Carcinogen	IARC (WHO) Probable Carcinogen	EU GHS (1A, 1B) Carcinogen	EU GHS (1A, 1B) Mutagen	EU GHS (1A, 1B) Reproductive Tox.	EU Potential Endocrine Disruptor	High Bioaccumulation	Verry persistent	Very tox to aq. Organism	Highly Toxic bees	Montreal Prot.	PIC	POP
(1-Methylpenta-1,3-dienyl)benzene 116669-49-9																		
1,2,3-Trimethylindene 4773-83-5																		
1,2-Dipropylcyclopropene 10306-92-0																		
1,4-Cyclohexanedione 637-88-7																		
1,4:3,6-Dianhydro-à-d-glucopyranose NA																		
1-Methylcyclooctene 933-11-9																		
1H-Inden-1-ol, 2,3-dihydro- 501-92-8																		
1H-Inden-1-one, 2,3-dihydro- 83-33-0																		
1H-Indenol 56631-57-3																		
2(3H)-Furanone, 5-acetyldihydro- 29393-32-6																		
2(5H)-Furanone, 3-methyl- 22122-36-7																		
2(5H)-Furanone, 5-ethyl- 2407-43-4																		
2,2-Dimethyl-3-heptanone 19078-97-8																		
2,3-Dimethyl-4-hydroxy-2-butenoic lactone 1575-46-8																		
2,4-Heptadienal, (E,E)- 4313-03-5																		
2,4-Hexadiene, 2,5-dimethyl-																		

Category	Acute Toxicity			Long Term Effects								Environmental Toxicity				International Conventions		
Subcategory	Who 1a	Who 1b	Inhalation Hazard (H330)	EPA Carcinogen	EPA Probably Carcinogen	IARC (WHO) Carcinogen	IARC (WHO) Probable Carcinogen	EU GHS (1A, 1B) Carcinogen	EU GHS (1A, 1B) Mutagen	EU GHS (1A, 1B) Reproductive Tox.	EU Potential Endocrine Disruptor	High Bioaccumulation	Verry persistent	Very tox to aq. Organism	Highly Toxic bees	Montreal Prot.	PIC	POP
764-13-6																		
2,5-Diethylphenol 876-20-0																		
2,5-Furandione, dihydro-3-methyl- 4100-80-5																		
2-(1-Methyl-2-propenyl)phenol 18272-63-4																		
2-Acetonylcyclopentanone 60415-94-3																		
2-Allyl-4-methylphenol 6628-06-4																		
2-Butyl-2-cyclopentenone 5561-05-7																		
2-Cyclohexen-1-one, 3-methyl- 1193-18-6																		
2-Cyclohexen-1-one, 4-(1-methylethyl)- 500-02-7																		
2-Cyclopenten-1-one 930-30-3																		
2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- 21835-01-8																		
2-Ethyl-3-methylcyclopent-2-en-1-one NA																		
2-Ethylidenecyclohexanone 1122-24-3																		
2-Furanone, 2,5-dihydro-3,5-dimethyl 5584-69-0																		
2-Hepten-4-one, 2-methyl- 22319-24-0																		
2-Hydroxy-gamma-butyrolactone 19444-84-9																		
2-Methoxy-6-methylphenol 2896-67-5																		
2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- 2503-46-0																		
2H-Pyran-2-one, tetrahydro- 542-28-9																		

Category	Acute Toxicity			Long Term Effects								Environmental Toxicity				International Conventions		
Subcategory	Who 1a	Who 1b	Inhalation Hazard (H330)	EPA Carcinogen	EPA Probably Carcinogen	IARC (WHO) Carcinogen	IARC (WHO) Probable Carcinogen	EU GHS (1A, 1B) Carcinogen	EU GHS (1A, 1B) Mutagen	EU GHS (1A, 1B) Reproductive Tox.	EU Potential Endocrine Disruptor	High Bioaccumulation	Verry persistent	Very tox to aq. Organism	Highly Toxic bees	Montreal Prot.	PIC	POP
3,4-Dimethoxytoluene 494-99-5																		
3-(p-Hydroxyphenyl)-1-propanol 10210-17-0																		
3-Ethenyl-3-methylcyclopentanone 49664-66-6																		
3-Methyl-2-propylcyclopent-2-en-1-one 50397-91-6																		
3-Methyl-3-cyclohexen-1-one 3524-87-6																		
4-Hepten-3-one, 4-methyl- 22319-31-9																		
4-Hexen-2-one, 3-methyl- 72189-24-3																		
4-Hexen-3-one, 4,5-dimethyl- 17325-90-5																		
4-Methyl-2-propylphenol 4074-46-8																		
4-n-Propylbenzoic acid 2438-05-3																		
4H-Pyran-4-one 108-97-4																		
5-methyl-2-(Z)-hepten-4-one 24608-84-2																		
6-Methoxy-1-indanone 13623-25-1																		
6-Methoxy-3-methylbenzofuran 29040-52-6																		
6-Oxabicyclo[3.1.0]hexan-2-one 6705-52-8																		
Acenaphthene 83-32-9																		
Anisole, o-(1-ethylvinyl)- 18272-74-7																		
Benzene, (2-propenyloxy)- 1746-13-0																		
Benzene, (4,5,5-trimethyl-1,3-cyclopentadien-1-yl)-																		

Category	Acute Toxicity			Long Term Effects								Environmental Toxicity				International Conventions		
Subcategory	Who 1a	Who 1b	Inhalation Hazard (H330)	EPA Carcinogen	EPA Probably Carcinogen	IARC (WHO) Carcinogen	IARC (WHO) Probable Carcinogen	EU GHS (1A, 1B) Carcinogen	EU GHS (1A, 1B) Mutagen	EU GHS (1A, 1B) Reproductive Tox.	EU Potential Endocrine Disruptor	High Bioaccumulation	Verry persistent	Very tox to aq. Organism	Highly Toxic bees	Montreal Prot.	PIC	POP
33930-85-7																		
Benzene, (ethenyloxy)- 766-94-9																		
Benzene, 1,2,4-trimethyl-5-(1-methylethyl)- 10222-95-4																		
Benzene, 1-ethoxy-4-ethyl- 1585-06-4																		
Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)- 6379-73-3																		
Benzene, 4-ethyl-1,2-dimethoxy- 5888-51-7																		
2-(2-Methoxy-5-methylphenyl)propanal 53155-90-1																		
Benzenemethanol, 4-(1,1-dimethylethyl)- 877-65-6																		
Benzofuran, 7-methoxy- 7168-85-6																		
Benzofuran, 7-methyl- 17059-52-8																		
Butyrolactone 96-48-0																		
Catechol 120-80-9																		
Cyclopentene, 3-ethenyl- 26727-45-7																		
Dehydromevalonic lactone 2381-87-5																		
Estragole 140-67-0																		
Ethanone, 1-(2,5-dihydroxyphenyl)- 490-78-8																		
Furan, 2,3-dihydro-2,5-dimethyl- 17108-52-0																		
Naphthalene, 1,2,3,4-tetramethyl- 3031-15-0																		
Naphthalene, 1,2-dihydro-1,5,8-trimethyl- 4506-36-9																		

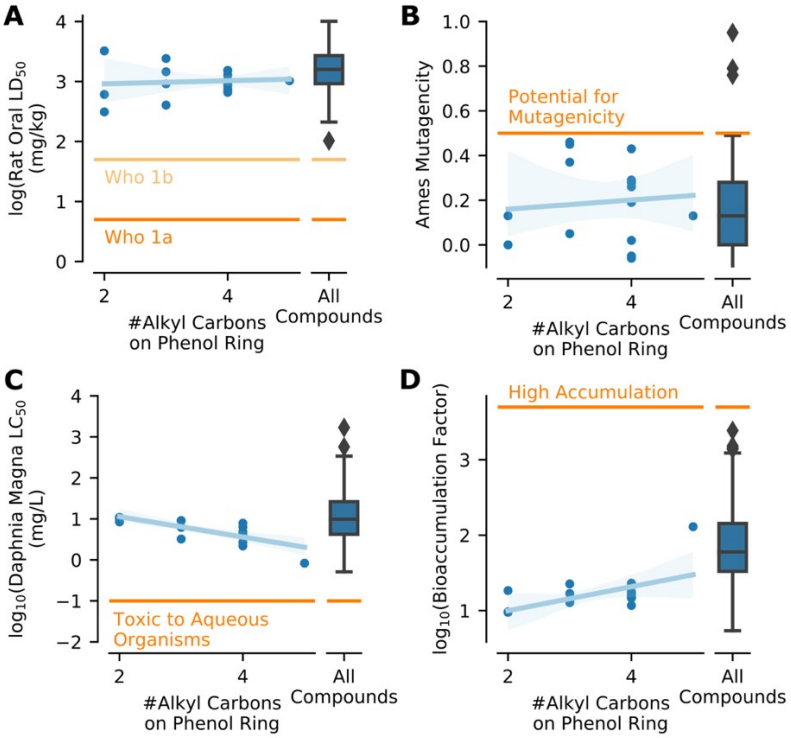
Category	Acute Toxicity			Long Term Effects								Environmental Toxicity				International Conventions		
Subcategory	Who 1a	Who 1b	Inhalation Hazard (H330)	EPA Carcinogen	EPA Probably Carcinogen	IARC (WHO) Carcinogen	IARC (WHO) Probable Carcinogen	EU GHS (1A, 1B) Carcinogen	EU GHS (1A, 1B) Mutagen	EU GHS (1A, 1B) Reproductive Tox.	EU Potential Endocrine Disruptor	High Bioaccumulation	Verry persistent	Very tox to aq. Organism	Highly Toxic bees	Montreal Prot.	PIC	POP
Naphthalene, 1,2-dihydro-2,5,8-trimethyl- 30316-23-5																		
Naphthalene, 1,4-dihydro-2,5,8-trimethyl- 30316-19-9																		
Naphthalene, 2,3-dimethyl- 581-40-8																		
Nonanoic acid 112-05-0																		
Octanoic acid 124-07-2																		
Pentanoic acid, 4-oxo- 123-76-2																		
Phenol, 2,3,5,6-tetramethyl- 527-35-5																		
Phenol, 2,5-bis(1-methylethyl)- 35946-91-9																		
Phenol, 2-ethyl- 90-00-6																		
Phenol, 2-ethyl-4,5-dimethyl- 2219-78-5																		
Phenol, 2-ethyl-6-methyl- 1687-64-5																		
Phenol, 2-methoxy-4-(1-propenyl)- 97-54-1																		
Phenol, 2-methyl-6-(2-propenyl)- 3354-58-3																		
Phenol, 3,4,5-trimethyl- 527-54-8																		
Phenol, 3,5-dimethyl- 108-68-9																		
Phenol, 3-methyl-6-propyl- 31143-55-2																		
Phenol, 3-propyl- 621-27-2																		
Phenol, 4-ethyl- 123-07-9																		
Phenol, 4-ethyl-2-methyl-																		

Category	Acute Toxicity			Long Term Effects								Environmental Toxicity				International Conventions		
Subcategory	Who 1a	Who 1b	Inhalation Hazard (H330)	EPA Carcinogen	EPA Probably Carcinogen	IARC (WHO) Carcinogen	IARC (WHO) Probable Carcinogen	EU GHS (1A, 1B) Carcinogen	EU GHS (1A, 1B) Mutagen	EU GHS (1A, 1B) Reproductive Tox.	EU Potential Endocrine Disruptor	High Bioaccumulation	Verry persistent	Very tox to aq. Organism	Highly Toxic bees	Montreal Prot.	PIC	POP
2219-73-0																		
Phenol, p-(2-methylallyl)- 33641-78-0																		
Vanillin 121-33-5																		
m-Guaiacol 150-19-6																		
Phenol, 2-propyl- 644-35-9																		
Eugenol 97-53-0																		
Phenol, 3-ethyl- 620-17-7																		
1H-Inden-5-ol, 2,3-dihydro-																		
2-Ethyl-5-n-propylphenol 72386-20-0																		
4-Methyl-5H-furan-2-one 6124-79-4																		
Phenol, 4-ethyl-2-methoxy- 2785-89-9																		
Phenol, 2-methyl-5-(1-methylethyl)- 89-83-8																		
1,2-Cyclopentanedione, 3-methyl- 765-70-8																		
2(5H)-Furanone 497-23-4																		
2-Cyclopenten-1-one, 2,3-dimethyl- 1121-05-7																		
2-Cyclopenten-1-one, 3-methyl- 2758-18-1																		
2-Methoxy-4-vinylphenol 7786-61-0																		
6-Methyl-4-indanol 20294-32-0																		
Benzene, 1-methoxy-4-(1-methylpropyl)- 4917-90-2																		
Heptadecane																		

Category	Acute Toxicity			Long Term Effects								Environmental Toxicity				International Conventions		
Subcategory	Who 1a	Who 1b	Inhalation Hazard (H330)	EPA Carcinogen	EPA Probably Carcinogen	IARC (WHO) Carcinogen	IARC (WHO) Probable Carcinogen	EU GHS (1A, 1B) Carcinogen	EU GHS (1A, 1B) Mutagen	EU GHS (1A, 1B) Reproductive Tox.	EU Potential Endocrine Disruptor	High Bioaccumulation	Verry persistent	Very tox to aq. Organism	Highly Toxic bees	Montreal Prot.	PIC	POP
544-76-3																		
Naphthalene, 1,4,6-trimethyl- 0-00-0																		
Phenol 108-95-2																		
Phenol, 2,3-dimethyl- 526-75-0																		
Phenol, 2-methoxy- 90-05-1																		
Phenol, 2-methoxy-4-propyl- 2785-87-7																		
Phenol, 3-methyl- 108-39-4																		

Supplementary Table 8: Table summarizing results from toxicological and environmental risk assessment. Explanation for indication is provided.

COMPOUND CAS	SUB CAT.	MEETS CRITERIA OR REASON FOR CONCERN	DESCRIPTION
4H-Pyran-4-one 108-97-4	Who 1b	Meets criteria	EPA TEST estimated oral rat LD_{50} to be 100 mg/kg. If experimental data supported this estimate, this compound would meet the criteria for acute toxicity label Who 1b.
Catechol 120-80-9	EU GHS (1A, 1B) Carcinogen	Meets criteria	Known or presumed human carcinogens according to EU GHS Regulation 1272/2008/EC.
Phenol 108-95-2	Inhalation Hazard (H330)	Reason for concern	Does not have H330 label. Has been labeled H331 - toxic if inhaled.
	EU GHS (1A, 1B) Mutagen	Reason for concern	Has been labeled as GHS Category 2 (H341). Suspected of causing genetic defects.
Phenol, 3-methyl- 108-39-4	EU GHS (1A, 1B) Reproductive Tox.	Reason for concern	Has H361 label, suspected of damaging fertility or unborn child



Supplementary Figure 5: Toxicity and environment outcomes as a function of alkyl carbons pendent to the phenol ring. Whisker plot insets use all compounds within the candidate bio-based insecticides to show data for both alkyl substituted phenols and other components found in the bio-based insecticide. **(A)** Shows the log-linear correlation between rat oral LD_{50} and number of alkyl carbons pendant to the phenol ring. Rat oral LD_{50} is used as a representative metric for acute toxicity. **(B)** Shows the linear correlation between the probability a compound will fail the Ames mutagenicity assay and alkyl carbons on phenol ring. The is used as a representative metric for mutagenic and cariogenic propensity. **(C)** Shows the log-linear correlation between Daphnia Magna LC_{50} and number of alkyl carbons pendant to the phenol ring. The LC_{50} value for is used as a representative metric for aqueous organism toxicity. **(D)** Shows the log-linear correlation between bioaccumulation factor and number of alkyl carbons pendant to the phenol ring. Bioaccumulation factor measures the degree to which a compound will accumulate in organisms. It is the ratio of the compound's concentration in an organism to the concentration in the environment and accounts for uptake via ingestion and respiration.

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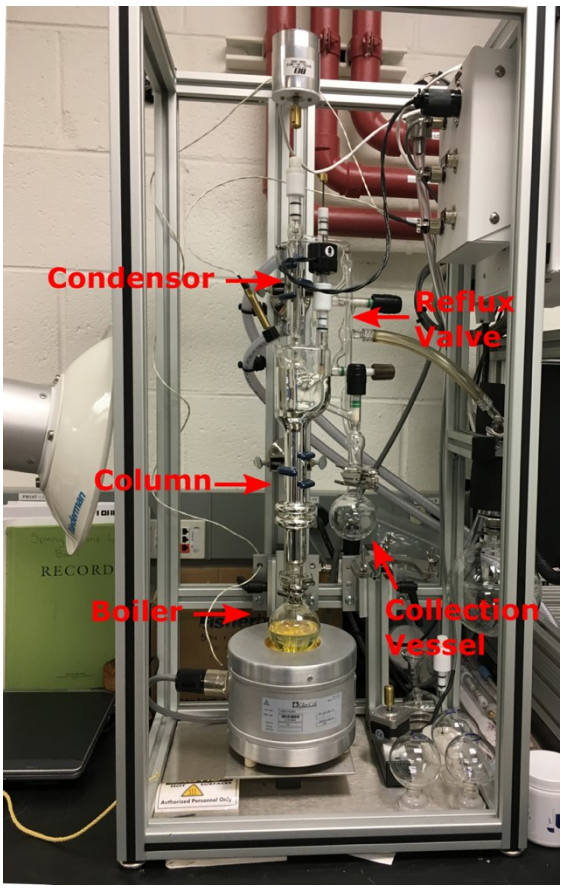

Supplementary Figure 6: Spinning band distillation column used to isolate bio-based insecticides from catalytic fast pyrolysis oils.

Supplementary Table 9: GC×GC method parameters.

Column			
Primary	Rxi-17Sil, 20 m x 180 µm x 0.18 µm		
Secondary	ZB-5HT Inferno, 1.5 m x 180 µm x 0.10 µm		
Injector			
1.0 µL injection, split 200:1	300°C		
Oven			
Primary	35°C, hold 5 min, ramp 5°C/min to 325°C, hold 1 min		
Secondary	15°C offset from primary		
Modulator	15°C offset from secondary		
Modulator cycle timing	modulator period, sec	hot pulse time, sec	cold time, sec
	8	3.0	1.0
Mass Spectrometer			
Transfer line	350°C		
TOF mass range	m/z 29-600		
TOF acquisition rate	200 spectra/sec		
Solvent delay	65 s		
FID			
Transfer line	350°C		
H_2 Flow	40 sccm		
Air Flow	300 scccm		
N_2 Makeup Flow	25 sccm		

SI References

1 R. J. French, K. Iisa, K. A. Orton, M. B. Griffin, E. Christensen, S. Black, K. Brown, S. E. Palmer, J. A. Schaidle, C. Mukarakate and T. D. Foust, *ACS Sustain. Chem. Eng.*, 2021, **9**, 1235–1245.

2 S. Kim, J. Chen, T. Cheng, A. Gindulyte, J. He, S. He, Q. Li, B. A. Shoemaker, P. A. Thiessen, B. Yu, L. Zaslavsky, J. Zhang and E. E. Bolton, *Nucleic Acids Res.*, 2019, **47**, D1102–D1109.

3 T. Martin, P. Harten and D. Young, *U.S. Environ. Prot. Agency, Washington, DC, EPA/600/C-12/006*.

4 European Chemicals Agency, ECHA Database - Information on Chemicals, https://echa.europa.eu/home, (accessed 20 December 2020).

5 United States Environmental Protection Agency, *Risk Assessment for Carcinogenic Effects (1986-Present)*, 2018.

6 IARC, List of Classifications – IARC Monographs on the Identification of Carcinogenic Hazards to Humans, https://monographs.iarc.fr/list-of-classifications, (accessed 20 December 2020).

7 European Commission, Chemicals - Environment - European Commission, https://ec.europa.eu/environment/chemicals/endocrine/strategy/substances_en.htm, (accessed 20 December 2020).

8 A. J. Williams, C. M. Grulke, J. Edwards, A. D. McEachran, K. Mansouri, N. C. Baker, G. Patlewicz, I. Shah, J. F. Wambaugh, R. S. Judson and A. M. Richard, *J. Cheminform.*, 2017, **9**, 1–27.

9 S. A. Montzka, S. Reimann, A. Engel, K. Krüger, S. O'Doherty, W. T. Sturges, D. Blake, M. Dorf, P. Fraser, L. Froidevaux, K. Jucks, K. Kreher, M. J. Kurylo, A. Mellouki, J. Miller, O.-J. Nielsen, V. L. Orkin, R. G. Prinn, R. Rhew, M. L. Santee, A. Stohl and D. Verdonik, *Sci. Assess. Ozone Deplet. 2010*, 2011, Chapter 1.

10 Rotterdam Convention, Annex III Chemicals, http://www.pic.int/TheConvention/Chemicals/AnnexIIIChemicals, (accessed 20 December 2020).

11 United Nations Environment Programme, Listing of POPs in the Stockholm Convention, http://chm.pops.int/TheConvention/ThePOPs/ListingofPOPs, (accessed 20 December 2020).