Supporting Information: Biodegradation kinetics testing of two hydrophobic UVCBs – potential for substrate toxicity supports testing at low concentrations.

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Supporting Information 1 – Details on passive dosing systems

Figure S1. Silicone loading kinetics. Mean value of n= 3 with standard error of mean.

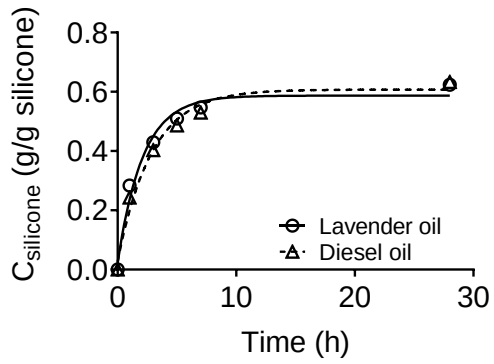


Figure S2. Passive dosing system with 20 g silicone in 100 mL bottle. In this study the rods were placed in 240 mL bottles.

Table S1. Dimensions and loading levels of the silicone rods used to set the initial mixture concentration and composition in the biodegradation experiment. Each passive dosing system consisted of a loaded silicone rod in a 240 mL gastight amber glass bottle. RSD = relative standard deviation.

Chemical	Test concentration	Mass of silicone rod (g)	Loading level (g oil/g silicone)	Loading level (% of saturation)
Diesel oil	low	20.0	0.010 (RSD 0.44 %)	1.6
	high	10.0	0.42 (RSD 3.3 %)	66
Lavender oil	low	30.0	0.010 (RSD 0.33 %)	1.6
	high	15.0	0.44 (RSD 4.2 %)	71

Supporting Information 2 – Characterization of surface water inoculum

Table S2. Characterization of surface water sample used as inoculum for biodegradation tests.

Parameter	**Value**
Water temperature	14 °C
Dissolved oxygen (DO)	8.7 mg/L
pH	7.96
conductivity	617 µS/cm
Nitrite-N	< 1 µg/L (average, n=3)
NO_x-N	97 µg/L (average, n=3)
Ammonia-N	23 µg/L (average, n=3)
Phosphate-P	23 µg/L (average, n=3)
Non-volatile organic carbon (NVOC)	9 mg/L (average, n=2, samples frozen prior to analysis)
Heterotrophic plate count (R2A agar)	$4.7*10^4$ CFU/mL

Table S3. Dissolved oxygen (and pH) during the biodegradation experiment measured with handheld probes. Test systems were opened to make the measurements, which may have introduced some uncertainty in the dissolved oxygen measurements.

	Day 10		**Day 21**		**Day 29**	
Test	pH	DO (mg/L)	pH	DO (mg/L)	pH	DO (mg/L)
Diesel low conc.	-	8.1	8.1	8.4	-	-
Diesel high conc.	-	8.3	8.0	8.6	-	8.0
Lavender low conc.	-	8.3	7.5	7.3	-	7.4
Lavender high conc.	-	8.1	7.3	8.1	-	8.0

Supporting Information S3 – List of mixture constituents and tentative identifications

Table S4: Diesel oil constituents. Tentative identification of constituents in diesel oil. Tentative identification is based on search and match in the spectral library NIST. For some constituents the identification was ambiguous and a comment is added.

Consti-tuent #	Retention time (min)	Quantifier ion (m/z)	Tentative identification/ compound name	Match factor	CAS#	Comment
1	15.82	91	Ethylbenzene	94.4	100-41-4	
2	16.11	91	p-Xylene	98.0	106-42-3	(or other dimethylbenzene)
3	16.15	91	o-Xylene	96.1	95-47-6	(or other dimethylbenzene)
4	16.84	91	Benzene, 1,3-dimethyl-	98.3	108-38-3	(or other dimethylbenzene)
5	17.85	105	Benzene, (1-methylethyl)-	84.7	98-82-8	
6	18.85	91	Benzene, propyl-	91.6	103-65-1	
7	19.10	105	Benzene, 1-ethyl-2-methyl-	97.4	611-14-3	(2-, 3- or 4- methyl-)
8	19.21	105	Benzene, 1-ethyl-2-methyl-	96.3	611-14-3	(2-, 3- or 4- methyl-)
9	19.38	105	1,3,5-trimethylbenzene	92.0	108-67-8	
10	19.71	105	Benzene, 1-ethyl-4-methyl-	96.0	622-96-8	(2-, 3- or 4- methyl-)
11	20.28	105	1,3,5-trimethylbenzene	98.6	108-67-8	(or 1,2,3- or 1,2,4-trimethyl-)
12	20.79	91	-			
13	20.86	105	Benzene, (1-methylpropyl)-	88.3	135-98-8	
14	21.21	119	-			
15	21.31	105	Benzene, 1,2,4-trimethyl-	96.0	95-63-6	
16	21.88	117	Indane	97.7	496-11-7	
17	22.29	119	Benzene, 1,4-diethyl-	82.2	105-05-5	(1,2- or 1,3- or 1,4 diethyl-)

Consti-tuent #	Retention time (min)	Quantifier ion (m/z)	Tentative identification/ compound name	Match factor	CAS#	Comment
18	22.44	105	Benzene, (1-methylpropyl)-	93.3	135-98-8	(or 1-methyl-3-propyl-)
19	22.67	91	Benzene, 1,4-diethyl-	93.7	105-05-5	
20	22.76	105	-			
21	23.06	105	Benzene, (1-methylpropyl)-	93.4	135-98-8	
22	23.48	119	1,3,8-p-Menthatriene	91.2	18368-95-1	
23	23.60	119	1,3,8-p-Menthatriene	92.4	18368-95-1	
24	23.81	132	Indan, 1-methyl-	81.7	767-58-8	
25	23.87	119	Benzene, 2-ethyl-1,4-dimethyl-	94.8	1758-88-9	(or other ethyl-dimethyl-)
26	24.01	117	1H-Indene, 2,3-dihydro-5-methyl-	90.0	874-35-1	
27	24.10	119	1-Pentanone, 1-(4-methylphenyl)-	86.0	1671-77-8	
28	24.64	119	Benzene, 1-methyl-4-(1-methylpropyl)-	80.4	1595-16-0	
29	24.77	119	Benzene, 1-ethyl-2,4-dimethyl-	81.6	874-41-9	
30	25.04	119	-			
31	25.35	119	Benzene, 1,2,3,5-tetramethyl-	82.2	527-53-7	(or other tetramethyl-)
32	25.53	119	Benzene, 1,2,4,5-tetramethyl-	95.1	95-93-2	(or other tetramethyl-)
33	26.23	119	-			
34	26.45	131	-			
35	26.57	117	1H-Indene, 2,3-dihydro-5-methyl-	92.2	874-35-1	
36	27.03	117	1H-Indene, 2,3-dihydro-5-methyl-	95.0	874-35-1	
37	27.11	119	Benzene, 1-ethyl-3,5-dimethyl-	87.8	934-74-7	(or other ethyl-dimethyl-)
38	27.35	91	-			
39	27.45	119	-			
40	27.62	131	-			
41	27.76	104	Naphthalene, 1,2,3,4-tetrahydro-	94.1	119-64-2	
42	28.25	119	-			
43	28.57	133	Indan, 1-methyl-	92.7	767-58-8	

Consti-tuent #	Retention time (min)	Quantifier ion (m/z)	Tentative identification/ compound name	Match factor	CAS#	Comment
44	28.89	131	-			
45	29.03	133	-			
46	29.10	131	1H-Indene, 2,3-dihydro-4,7-dimethyl-	87.1	6682-71-9	(or other dimethyl-)
47	29.31	131	-			
48	29.36	117	-			
49	29.46	133	-			
50	29.57	131	1H-Indene, 2,3-dihydro-1,1-dimethyl-	90.1	4912-92-9	(or other dimethyl-)
51	30.09	133	-			
52	30.61	133	-			
53	30.82	104	Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	91.2	3877-19-8	
54	31.00	133	-			
55	31.24	131	Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	86.4	1559-81-5	
56	31.66	117	-			
57	31.74	162	-			
58	31.99	119	-			(*)
59	32.10	133	-			
60	32.72	131	1H-Indene, 2,3-dihydro-4,7-dimethyl-	86.2	6682-71-9	(or other dimethyl-)
61	33.48	131	1H-Indene, 2,3-dihydro-4,7-dimethyl-	86.3	6682-71-9	(or other dimethyl-)
62	33.58	105	-			
63	33.80	131	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	95.6	1680-51-9	(or other methyl-tetralin)
64	34.30	119	-			
65	34.69	131	-			
66	35.02	145	-			
67	35.38	131	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	91.3	1680-51-9	(or other methyl-tetralin)
68	35.80	142	Naphthalene, 2-methyl-	94.8	91-57-6	
69	36.82	142	Naphthalene, 2-methyl-	88.1	91-57-6	

Consti-tuent #	Retention time (min)	Quantifier ion (m/z)	Tentative identification/ compound name	Match factor	CAS#	Comment
70	37.32	118	Naphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-	86.7	7524-63-2	(or other dimethyl-)
71	37.41	160	-			
72	37.72	145	1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	81.2	2613-76-5	
73	38.02	104	-			
74	38.24	129	-			
75	38.43	131	-			
76	38.63	118	-			
77	38.90	160	-			
78	39.46	145	-			
79	39.89	131	-			
80	40.75	131	-			
81	41.15	130	-			
82	41.39	154	Acenaphthene	87.8	83-32-9	
83	42.16	145	Naphthalene, 1,2,3,4-tetrahydro-5,6-dimethyl-	90.4	20027-77-4	(or other dimethyl-)
84	42.42	145	-			
85	42.60	167	Benzene, 1,1',1'',1'''-(1,2-ethanediylidene)tetrakis-	85.9	632-50-8	
86	43.24	156	-			
87	43.37	155	-			
88	44.21	156	-			
89	44.51	156	Naphthalene, 1,6-dimethyl-	90.1	575-43-9	(or dimethyl-)
90	44.61	145	-			
91	45.55	132	-			
92	45.85	159	-			
93	45.98	159	-			
94	46.33	145	-			

Consti-tuent #	Retention time (min)	Quantifier ion (m/z)	Tentative identification/ compound name	Match factor	CAS#	Comment
95	47.53	159	-			
96	48.91	168	1,1'-Biphenyl, 4-methyl-	87.0	644-08-6	
97	49.35	167	-			
98	49.63	168	-			
99	51.42	144	-			
100	51.76	155	-			
101	54.78	144	-			
102	56.82	168	1,1'-Biphenyl, 4-methyl-	80.1	644-08-6	
103	57.28	182	-			
104	64.61	182	-			

Table S5: Lavender oil constituents. Tentative identification of constituents in lavender oil. Tentative identification is based on search and match in the spectral library NIST. For some constituents the identification was ambiguous and a comment is added.

Consti-tuent #	Retention time (min)	Quantifier ion (m/z)	Tentative identification/ compound name	Match factor	CAS#	Comment
1	19.82	99	3-Octanone	97.9	106-68-3	
2	20.00	93	.beta.-Myrcene	96.6	123-35-3	
3	20.16	89	Butanoic acid, butyl ester	97.8	109-21-7	
4	20.74	56	Acetic acid, hexyl ester	93.2	142-92-7	
5	20.83	93	3-Carene	90.3	13466-78-9	
6	21.41	119	o-Cymene	86.2	527-84-4	
7	21.61	68	D-Limonene	98.3	5989-27-5	
8	21.70	93	trans-.beta.-Ocimene	97.9	3779-61-1	
9	21.77	154	Eucalyptol (= 1,8-cineole)	97.8	470-82-6	
10	22.14	93	1,3,6-Octatriene, 3,7-dimethyl-, (Z)- (= cis-beta-ocimene)	97.7	3338-55-4	
11	23.95	121	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	95.1	586-62-9	
12	24.05	150	3-Methyl-2-(2-methyl-2-butenyl)-furan	95.7	15186-51-3	
13	24.48	121	Linalool	96.7	78-70-6	
14	27.06	95	(+)-2-Bornanone	97.1	464-49-3	
15	27.57	111	4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)- (= lavandulol)	85.9	498-16-8	

Consti-tuent #	Retention time (min)	Quantifier ion (m/z)	Tentative identification/ compound name	Match factor	CAS#	Comment
16	28.32	95	endo-Borneol	96.9	507-70-0	
17	28.73	111	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1.alpha.,2.beta.,5.alpha.)-	91.2	15537-55-0	
18	28.96	71	Butanoic acid, hexyl ester	96.2	2639-63-6	
19	29.07	96	1H-Pyrazole-1-carboximidamide, 3,5-dimethyl-	81.2	22906-75-8	
20	29.47	121	.alpha.-Terpineol	96.6	98-55-5	
21	32.44	93	Linalyl acetate	96.4	115-95-7	
22	34.52	93	4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, acetate (= lavandulyl acetate)	98.7	25905-14-0	
23	34.90	95	-			
24	37.62	101				
25	39.61	93	3-Carene	92.9	13466-78-9	
26	41.00	69	4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, acetate (= lavandulyl acetate)	96.1	25905-14-0	
27	44.26	94	Tricyclo[2.2.1.0(2,6)]heptane, 1,7-dimethyl-7-(4-methyl-3-pentenyl)-, (-)-	94.9	512-61-8	
28	44.45	133	Caryophyllene	98.5	87-44-5	
29	45.22	119	-			
30	46.50	69	cis-.beta.-Farnesene	96.1	28973-97-9	
31	46.98	147	-			
32	48.81	161	-			

Supporting Information 4 – mass balance calculations

Table S6. Mass balance calculations for diesel oil constituents. Distribution between water and air in the test systems (15 mL water, 5 mL headspace), and between water, air and silicone and silicone compartments in the passive dosing system used to set the initial concentration in the surface water inoculum (100 mL bottle with 18 mL (20 g) silicone rod and 65 mL ultrapure water). Calculations were done for the constituents where partition coefficients were available based on tentative identifications (table S-4). Partition coefficients ($LogK_{water/air}$ [L air / L water] and $LogK_{silicone/water}$ [L water / L PDMS]) are from the UFZ-LSER database (https://www.ufz.de/index.php?en=31698&contentonly=1&m=0&lserd_data[mvc]=Public/start).

			Governing partition coefficients		Mass balance – test systems		Mass balance – passive dosing systems		
Consti-tuent #	Rt	Target m/z	Log K_{wa}	Log K_{sw}	Water (%)	Air (%)	Water (%)	Air (%)	Silicone (%)
1	15.82	91	0.14	2.86	81	19	0.5	0.09	99.4
2	16.11	91	0.23	2.83	84	16	0.5	0.08	99.4
3	16.15	91	0.35	2.8	87	13	0.6	0.07	99.4
4	17.85	105	-0.07	3.3	72	28	0.2	0.06	99.8
5	18.85	91	-0.05	3.37	73	27	0.2	0.05	99.8
6	19.10	105	0.23	3.22	84	16	0.2	0.03	99.7
7	19.21	105	0.23	3.22	84	16	0.2	0.03	99.7
8	19.38	105	0.2	3.23	83	17	0.2	0.04	99.8
9	19.71	105	0.12	3.26	80	20	0.2	0.04	99.8
10	20.28	105	0.2	3.23	83	17	0.2	0.04	99.8
12	20.86	105	-0.28	3.8	61	39	0.1	0.03	99.9
14	21.31	105	0.33	3.21	87	13	0.2	0.03	99.8
15	21.42	119	-	-					
16	21.88	117	0.66	2.99	93	7	0.4	0.02	99.6
17	22.29	119	-0.08	3.78	71	29	0.1	0.02	99.9
18	22.44	105	-0.28	3.8	61	39	0.1	0.03	99.9
19	22.67	91	-0.08	3.78	71	29	0.1	0.02	99.9
21	23.06	105	-0.28	3.8	61	39	0.1	0.03	99.9
22	23.48	119	0.44	3.56	89	11	0.1	0.01	99.9
23	23.60	119	0.44	3.56	89	11	0.1	0.01	99.9
24	23.81	132	0.33	3.48	87	13	0.1	0.01	99.9
25	23.87	119	0.11	3.7	79	21	0.1	0.01	99.9
26	24.01	117	0.33	3.48	87	13	0.1	0.01	99.9
27	24.10	119	-	-					
28	24.64	119	-0.14	4.18	68	32	0.02	0.01	100.0
29	24.77	119	0.12	3.7	80	20	0.1	0.01	99.9
31	25.35	119	0.32	3.69	86	14	0.1	0.01	99.9

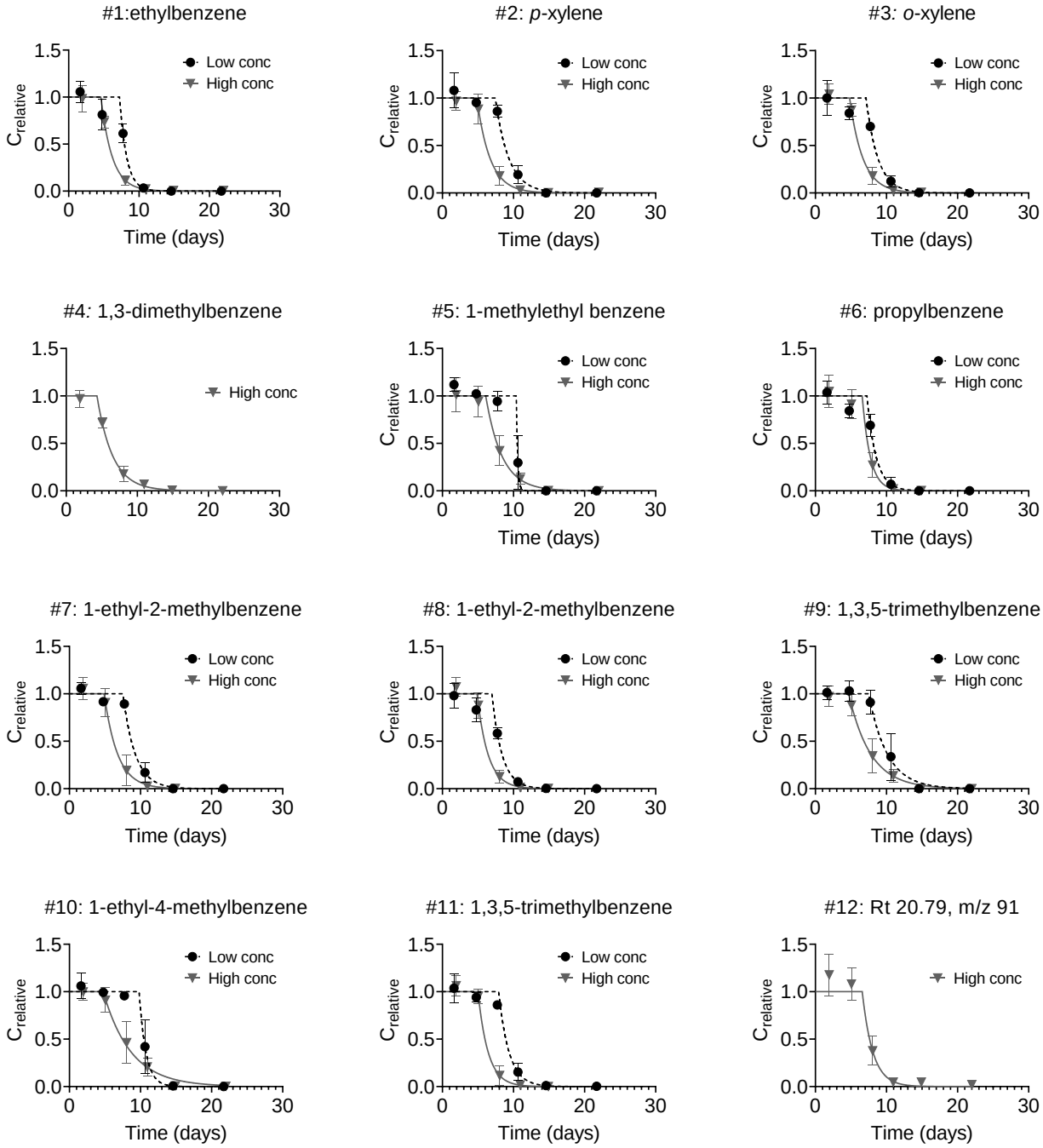
			Governing partition coefficients		Mass balance – test systems		Mass balance – passive dosing systems		
Consti-tuent #	Rt	Target m/z	Log K_{wa}	Log K_{sw}	Water (%)	Air (%)	Water (%)	Air (%)	Silicone (%)
32	25.53	119	0.29	3.69	85	15	0.1	0.01	99.9
35	26.57	117	0.47	3.56	90	10	0.1	0.01	99.9
36	27.03	117	0.47	3.56	90	10	0.1	0.01	99.9
37	27.11	119	0.02	3.72	76	24	0.1	0.02	99.9
41	27.76	104	0.61	3.5	92	8	0.1	0.01	99.9
46	29.10	131	-	-					
50	29.57	131	-	-					
53	30.82	104	-	-					
55	31.24	131	-	-					
60	32.72	131	-	-					
61	33.48	131	-	-					
63	33.80	131	-	-					
67	35.38	131	-	-					
68	35.80	142	1.32	3.23	98	2	0.2	< 0.01	99.8
69	36.82	142	1.32	3.23	98	2	0.2	< 0.01	99.8
70	37.32	118	-	-					
72	37.72	145	-	-					
82	41.39	154	1.93	3.36	99.6	0.4	0.2	< 0.01	99.8
83	42.16	145	-	-					
85	42.60	167	-	-					
89	44.51	156	1.36	3.79	99	1	0.1	< 0.01	99.9
96	48.91	168	1.53	3.86	99	1	0.05	< 0.01	99.9
102	56.82	168	1.53	3.86	99	1	0.05	< 0.01	99.9

Table S7. Mass balance calculations for lavender oil constituents. Distribution between water and air in the test systems (15 mL water, 5 mL headspace), and between water, air and silicone and silicone compartments in the passive dosing system used to set the initial concentration in the surface water inoculum (100 mL bottle with 27 mL (30 g) silicone rod and 65 mL ultrapure water). Calculations were done for the constituents where partition coefficients were available based on tentative identifications (table S-5). Partition coefficients ($LogK_{water/air}$ [L air / L water] and $LogK_{silicone/water}$ [L water / L PDMS]) are from the UFZ-LSER database (https://www.ufz.de/index.php?en=31698&contentonly=1&m=0&lserd_data[mvc]=Public/start).

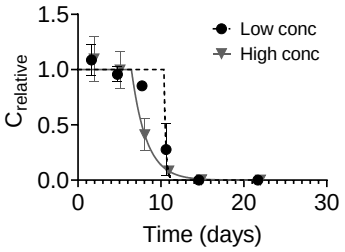
			Governing partition coefficients		Mass balance – test systems		Mass balance – passive dosing systems		
Consti-tuent #	Rt	Target m/z	Log K_{wa}	Log K_{sw}	Water (%)	Air (%)	Water (%)	Air (%)	Silicone (%)
1	19.82	99	1.65	2.02	99.3	0.7	2.2	0.01	97.7
2	20.00	93	-0.73	4.16	35.8	64.2	0.02	0.01	100.0
3	20.16	89	1.03	2.55	97.0	3.0	0.7	0.01	99.3
4	20.74	56	1.15	2.52	97.7	2.3	0.7	0.01	99.3
5	20.83	93	-1.03	4.44	21.9	78.1	0.01	0.01	100.0
6	21.41	119	0	3.65	75.0	25.0	0.1	0.01	99.9
7	21.61	68	-0.54	4.1	46.4	53.6	0.02	0.01	100.0
8	21.70	93	-0.58	4.26	44.1	55.9	0.01	0.01	100.0
9	21.77	154	1.89	1.99	99.6	0.4	2.4	< 0.01	97.6
10	22.14	93	-0.21	3.88	64.9	35.1	0.03	0.01	100.0
11	23.95	121	-0.43	4.2	52.7	47.3	0.02	0.01	100.0
12	24.05	150	-	-					
13	24.48	121	2.45	1.77	99.9	0.1	3.9	< 0.01	96.1
14	27.06	95	-	-					
15	27.57	111	-	-					
16	28.32	95	3.11	1.36	100.0	0.03	9.5	< 0.01	90.5
17	28.73	111	-	-					
18	28.96	71	0.71	3.58	93.9	6.1	0.1	< 0.01	99.9
19	29.07	96	-	-					
20	29.47	121	3	1.57	100.0	0.03	6.1	< 0.01	93.9
21	32.44	93	0.92	3.73	96.1	3.9	0.04	< 0.01	100.0
22	34.52	93	-	-					
25	39.61	93	-1.03	4.44	21.9	78.1	0.01	0.01	100.0
26	41.00	69	-	-					
27	44.26	94	-0.97	5.99	24.3	75.7	< 0.01	< 0.01	100.0
28	44.45	133	-1.31	6.36	12.8	87.2	< 0.01	< 0.01	100.0
30	46.50	69	-0.24	5.49	63.3	36.7	< 0.01	< 0.01	100.0

Supporting Information 5 – degradation curves and kinetics for diesel oil

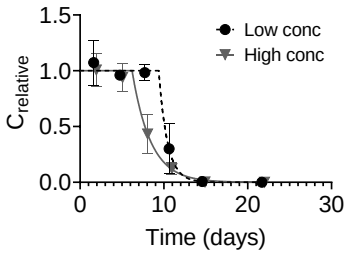
Figure S3. Degradation curves for individual constituents in diesel oil at low and high test concentration.



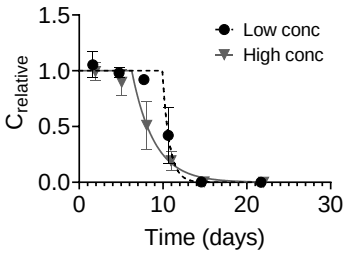
#13: 1-methylpropyl benzene



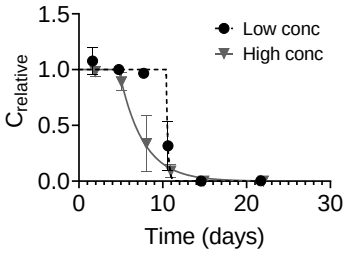
#14: Rt 21.21, m/z 119



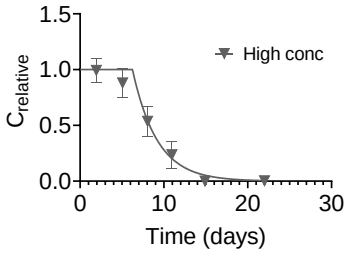
#15: 1,2,4-trimehylbenzene



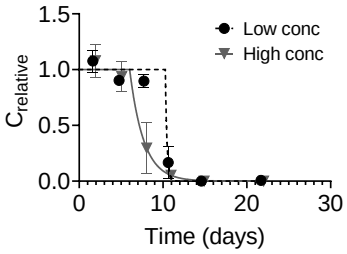
#16: Indane



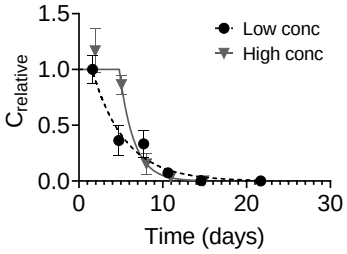
#17: 1,4-diethylbenzene



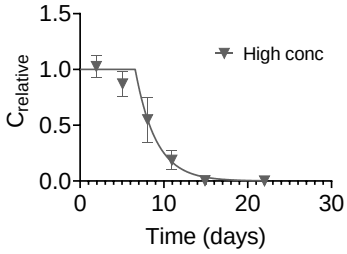
#18: 1-methylpropyl benzene



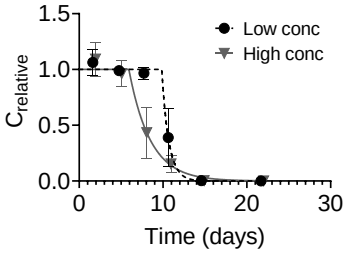
#19: 1,4-diethylbenzene



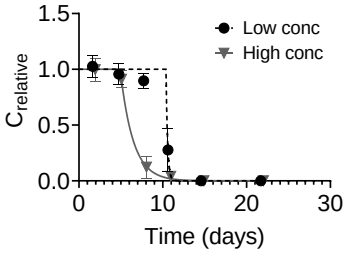
#19: Rt 22.76, m/z 105



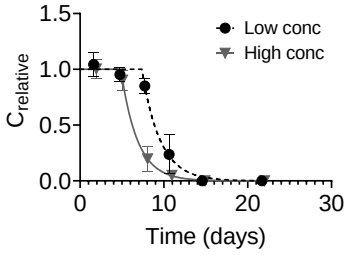
#21: 1-methylpropyl benzene



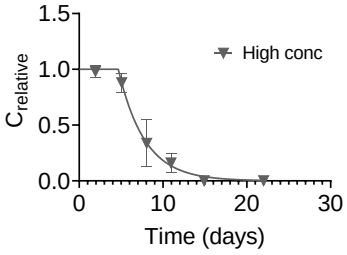
#22: 1,3,8-*p*-menthatriene



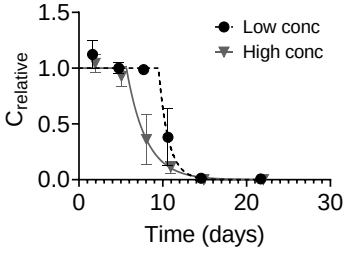
#23: 1,3,8-*p*-menthatriene



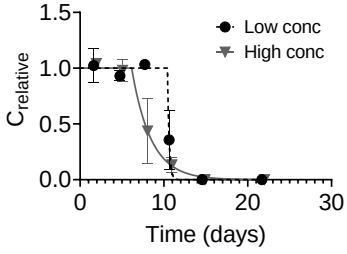
#24: 1-methyl indan



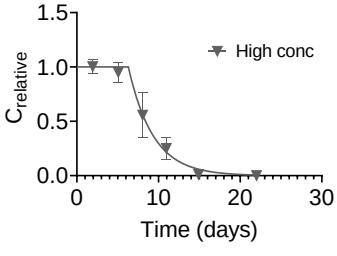
#25: 2-ethyl-1,4-dimethylbenzene



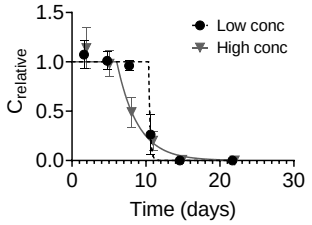
#26: 1-methyl indan



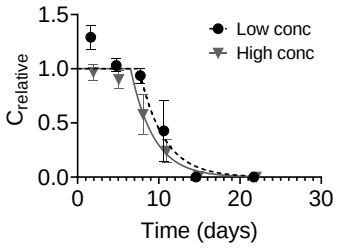
#27: 1-(4-methylphenyl)-1-pentanone



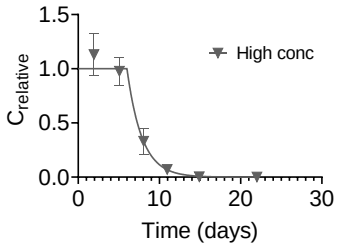
#28: 1-methyl-4-(1-methylpropyl)benzene



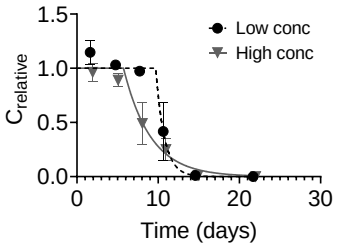
#29: 1-ethyl-2,4-dimethylbenzene



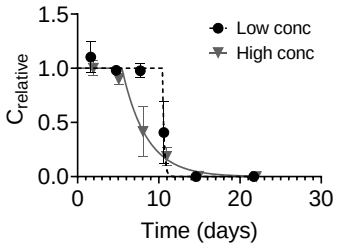
#30: Rt 25.04, m/z 119



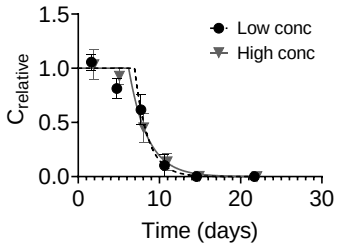
#31: 1,2,3,5-tetramethylbenzene



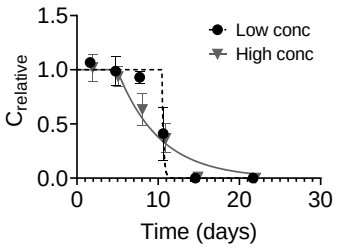
#32: 1,2,4,5-tetramethylbenzene



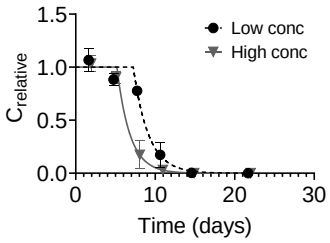
#33: Rt 26.23, m/z 119



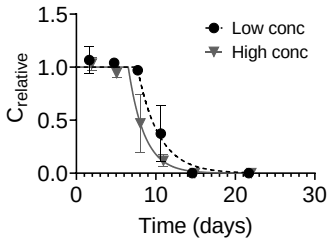
#34: Rt 26.45, m/z 131



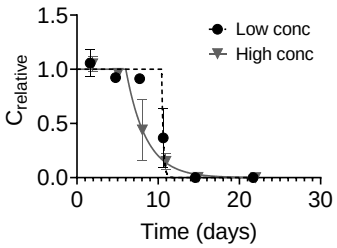
#35: 2,3-dihydro-5-methyl-1H-indene



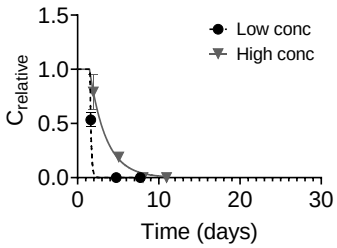
#36: 2,3-dihydro-5-methyl-1H-indene



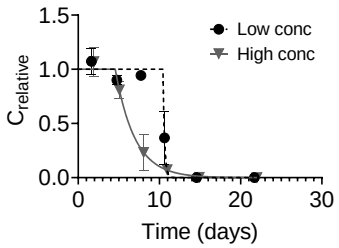
#37: 1-ethyl-3,5-dimethylbenzene



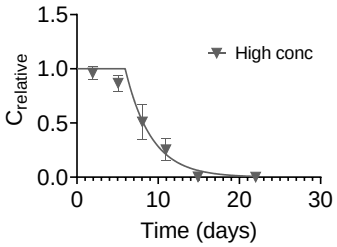
#38: Rt 27.35, m/z 91



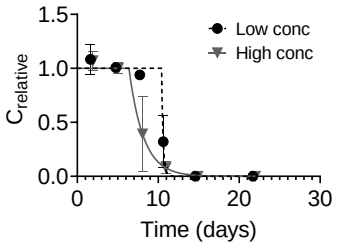
#39: Rt 27.45, m/z 119



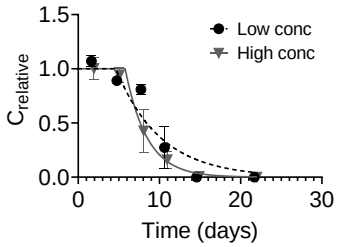
#40: Rt 27.62, m/z 131



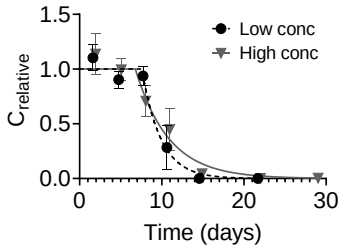
#41: 1,2,3,4-tetrahydronaphthalene



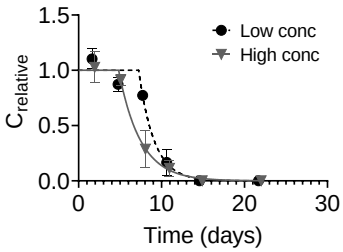
#42:Rt 28.25, m/z 119



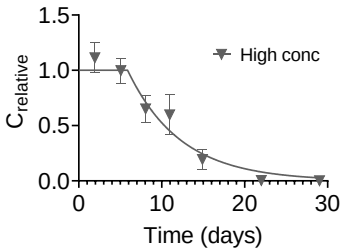
#43: Rt 28.57, m/z 133



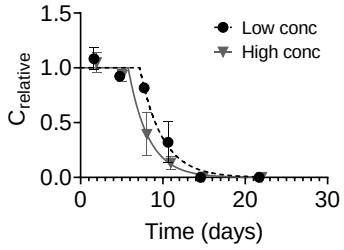
#44: Rt 28.89, m/z 131



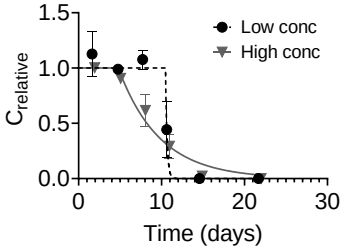
#45: Rt 29.03, m/z 133



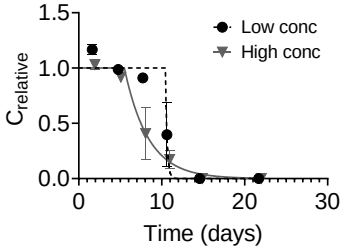
#46: 2,3-dihydro-4,7-dimethyl-1H-Indene



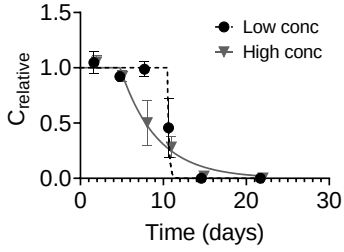
#47: Rt 29.31, m/z 131



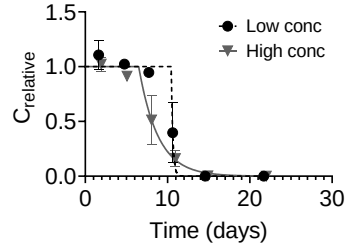
#48: Rt 29.36, m/z 117



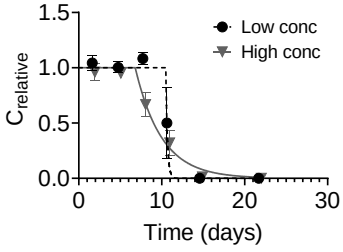
#49: Rt 29.45, m/z 133



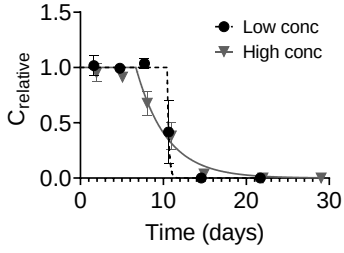
#50: 2,3-dihydro-1,1-dimethyl-1H-Indene



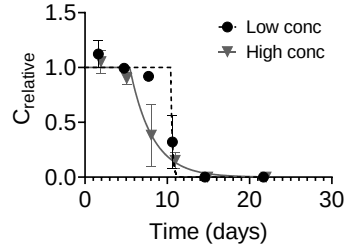
#51: Rt 30.09, m/z 133



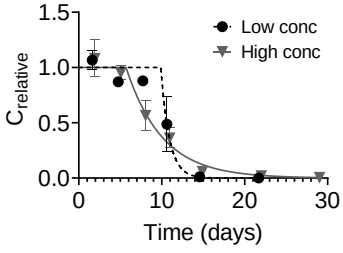
#52: Rt 30.61, m/z 133



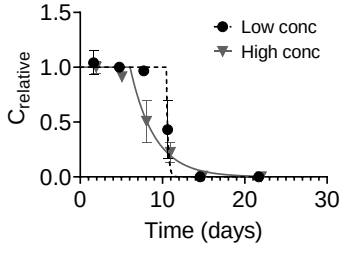
#53: 1,2,3,4-tetrahydro-2-methylnaphthalene



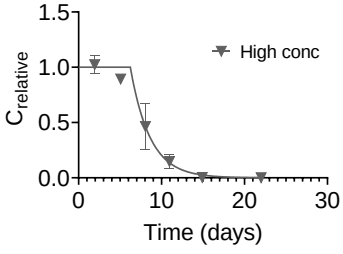
#54: Rt 31.00, m/z 133



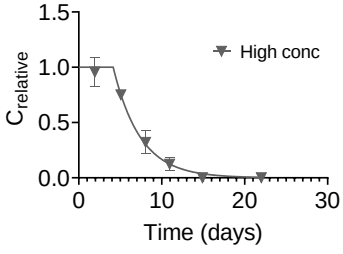
#55: 1,2,3,4-tetrahydro-1-methylnaphthalene



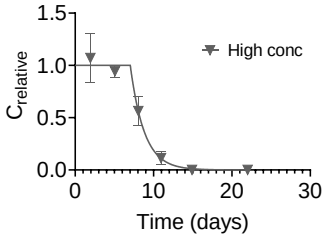
#56: Rt 31.66, m/z 117



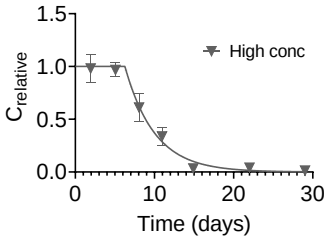
#57: Rt 31.74, m/z 162



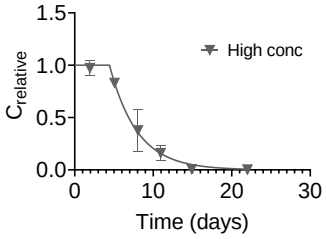
#58: Rt 31.99, m/z 119



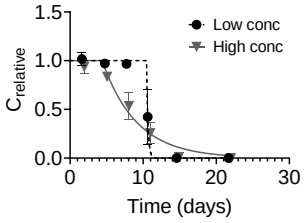
#59: Rt 32.10, m/z 133



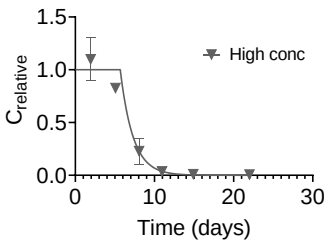
#60: 2,3-dihydro-4,7-dimethyl-1H-Indene



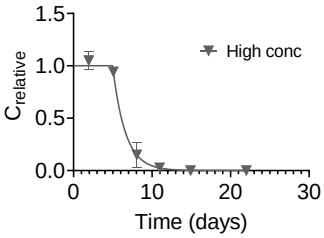
#61: 2,3-dihydro-4,7-dimethyl-1H-Indene



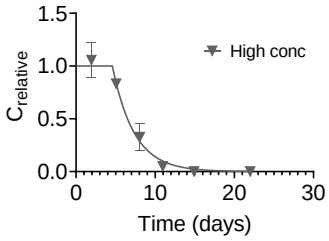
#62: Rt 33.58, m/z 105



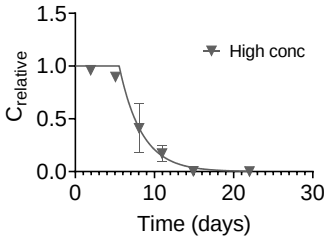
#63: 1,2,3,4-tetrahydro-6-methylnaphthalene



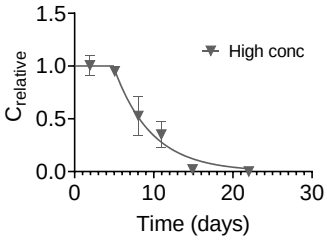
#64: Rt 34.30, m/z 119



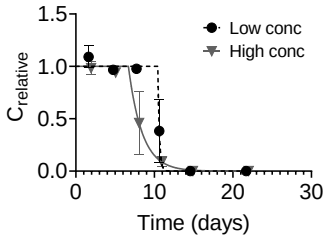
#65: Rt 34.69, m/z 131



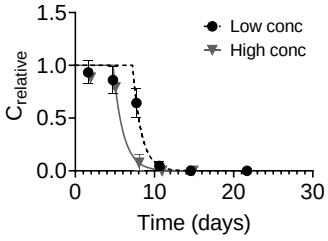
#66: Rt 35.02, m/z 145



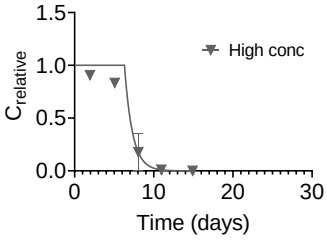
#67: 1,2,3,4-tetrahydro-6-methylnaphthalene



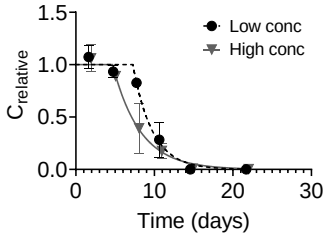
#68: 2-methyl-naphthalene



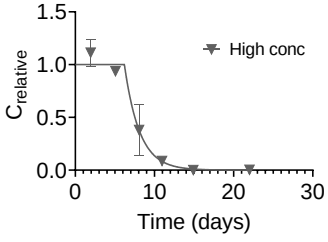
#69: 2-methyl-naphthalene



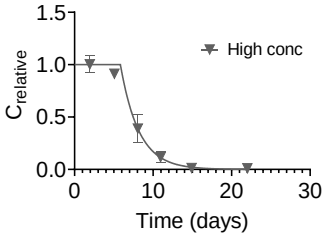
#70: 1,2,3,4-tetrahydro-2,6-dimethylnaphthalene



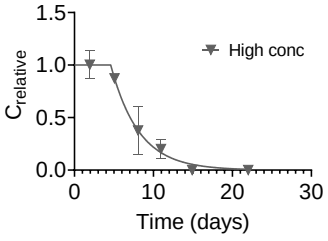
#71: Rt 37.41, m/z 160



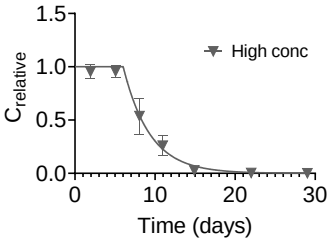
#72: 2,3-dihydro-1,1,3-trimethyl-1H-Indene



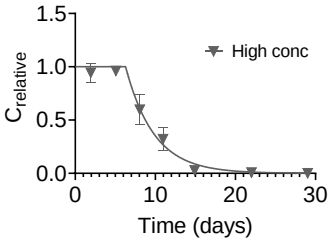
#73: Rt 38.02, m/z 104



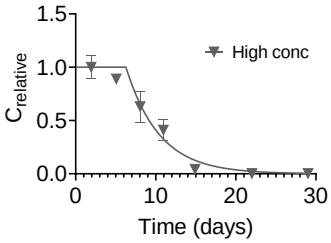
#74: Rt 38.24, m/z 129



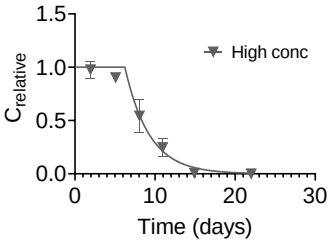
#75: Rt 38.43, m/z 131



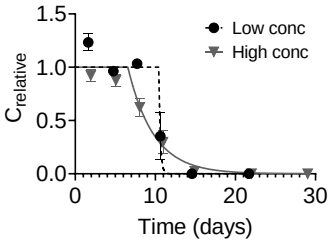
#76: Rt 38.63, m/z118



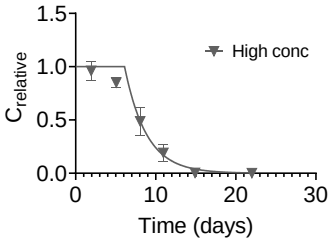
#77: Rt 38.90, m/z 160



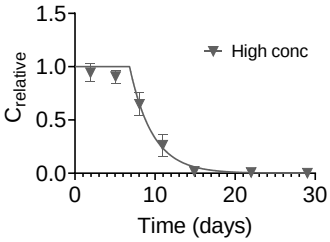
#78: Rt 39.46, m/z 145



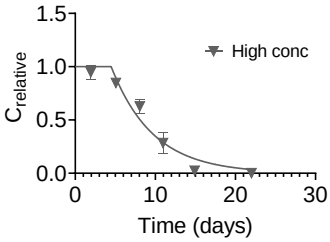
#79: Rt 39.89, m/z 131



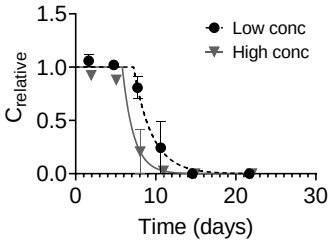
#80: Rt 40.75, m/z 131



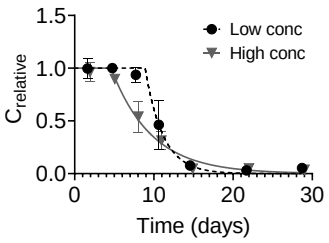
#81: Rt 41.15, m/z 130



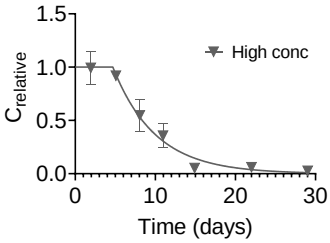
#82: Acenaphthene



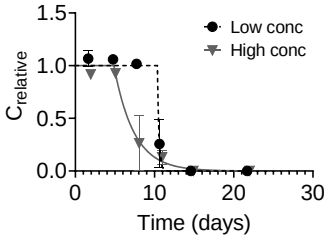
#83: 1,2,3,4-tetrahydro-5,6-dimethylnaphthalene



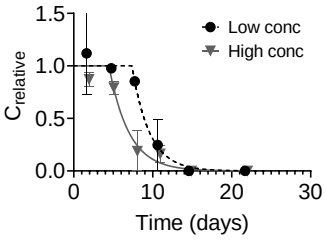
#84: Rt 42.42, m/z 145



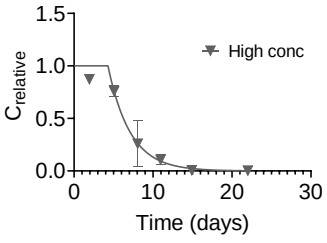
#85: 1,1',1",1"'-(1,2-ethanediylidene)tetrakis benzene



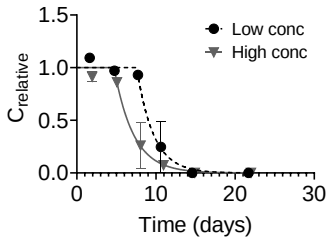
#86: Rt 43.24, m/z 156



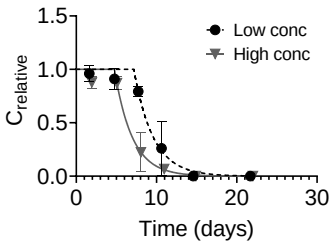
#87: Rt 43.37, m/z 155



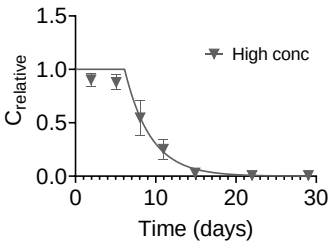
#88: Rt 44.21, m/z 156



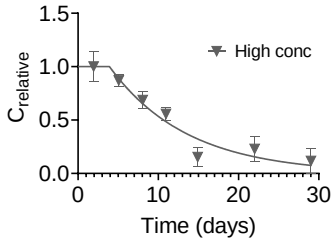
#89: 1,6-dimethylnaphthalene



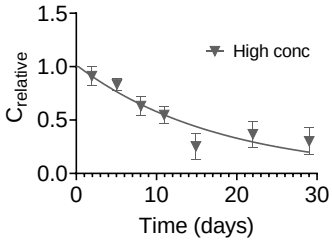
#90: Rt 44.61,m/z 145



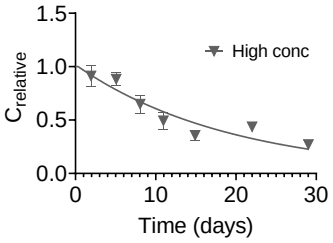
#91: Rt 45.55,m/z 132



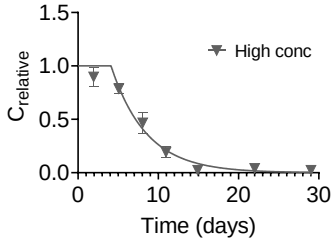
#92: Rt 45.85, m/z 159



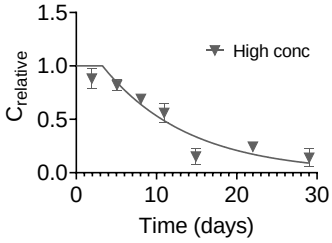
#93: Rt 45.98,m/z 159



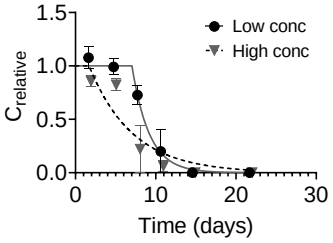
#94: Rt 46.33, m/z 145



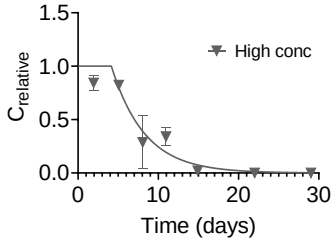
#95: Rt 47.53, m/z 159



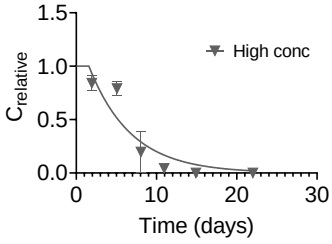
#96: 4-methyl-1,1'-biphenyl



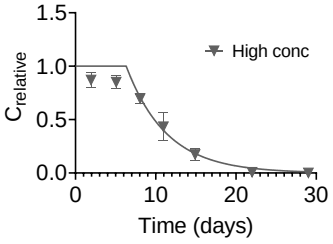
#97: Rt 49.35, m/z 167



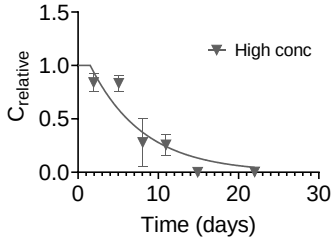
#98: Rt 49.63,m/z 168



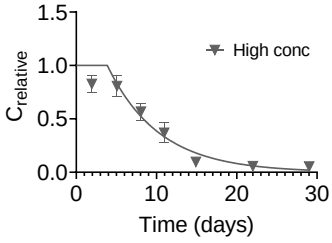
#99: Rt 51.42, m/z 144



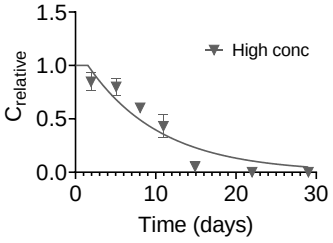
#100: Rt 51.76, m/z 155



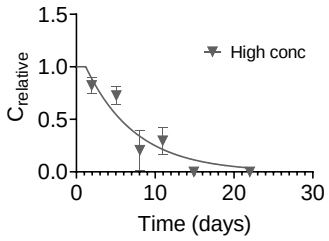
#101: Rt 54.78,m/z 144



#102: 4-methyl-1,1'-biphenyl



#103: Rt 57.28, m/z 182



#104: Rt 64.61, m/z 182

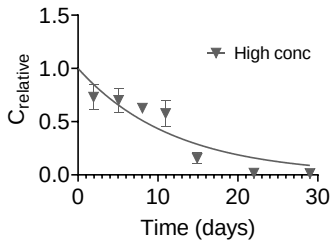


Table S8. Biodegradation kinetics from for diesel oil constituents; lag-phase, first-order degradation rate constant (k_{system}), first-order degradation half life ($T_{½}$) with 95% confidence intervals, and degradation half time (DT_{50}: lag-phase + one half-life). Lag phase and half life are only reported when at least two measurements were made during the visual degradation phase (10% < Crelative<90%) and $R^2 > 0.8$, otherwise only the DT_{50} is reported. A lag phase > 28 days means that degradation did not start within the test duration. *=lower limit set to zero when fit gave a negative value. ** = below limit of quantification. *** = R^2<0.8 or ambiguous fit.

Constituent #	Conc. level	Lag phase (d)	k (d^{-1})	$T_{½}$ (d)	$CI_{95\%}$ for $T_{½}$ (d)	DT_{50} (d)
1	L					7.9
	H	4.6	0.62	1.1	0* – 1.8	5.7
2	L	7.4	0.53	1.3	0.52 – 2.2	8.8
	H	4.8	0.54	1.3	0.58 – 2.0	6.1
3	L	7.1	0.60	1.2	0* – 2.4	8.3
	H	4.8	0.54	1.3	0.71 – 1.9	6.1
4	L**					
	H	4.3	0.45	1.5	0.97 – 2.2	5.9
5	L					10.5***
	H	6.1	0.44	1.6	1.3 – 3.7	7.7
6	L	7.2	0.79	0.9	0* – 1.9	8.1
	H					7.4
7	L	7.5	0.58	1.2	0.74 – 1.7	8.7
	H					6.2
8	L	7.0	0.71	1.0	0* – 2.3	7.9
	H	4.9	0.65	1.1	0* – 1.8	5.9
9	L					9.3
	H	4.7	0.32	2.1	1.3 – 3.4	6.8
10	L					10.5
	H	4.8	0.26	2.7	1.6 – 4.4	7.4
11	L	7.9	0.69	1.0	0* – 2.3	8.9
	H					6.0
12	L**					
	H					7.6
13	L					10.5***
	H	6.4	0.56	1.2	0* – 3.2	7.7
14	L					10.1
	H	6.2	0.45	1.5	1.4 – 3.5	7.7
15	L					10.5
	H	6.3	0.37	1.9	1.8 – 4.5	8.1
16	L					10.5***
	H	4.8	0.35	2.0	1.1 – 3.3	6.7
17	L**					
	H	6.3	0.34	2.0	0.67 – 4.8	8.3
18	L					10.4***
	H	6.0	0.60	1.2	0* – 3.0	7.2
19	L	1.6	0.25	2.7	1.4 – 4.0	4.3
	H	4.8	0.58	1.2	0* – 2.4	6.0

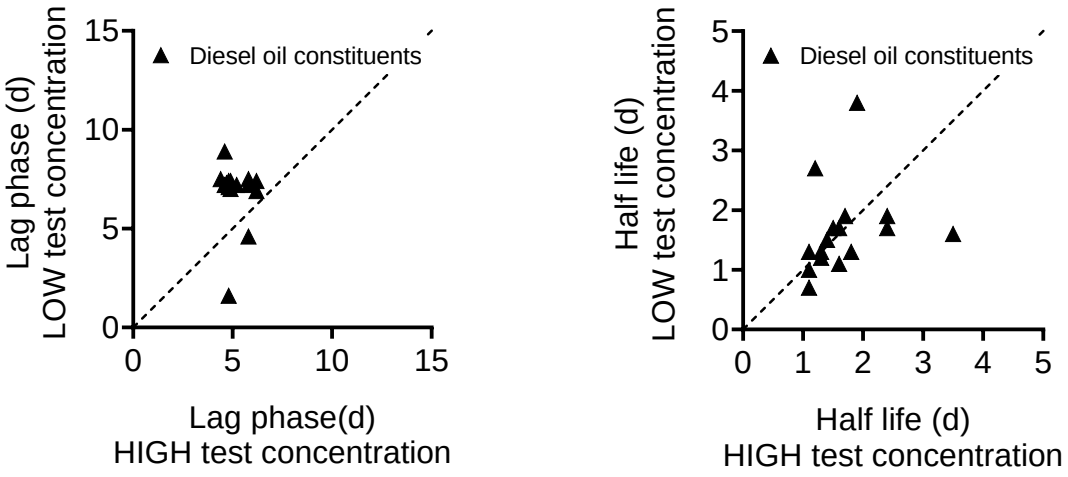
Constituent #	Conc. level	Lag phase (d)	k (d^{-1})	$T_{½}$ (d)	$CI_{95\%}$ for $T_{½}$ (d)	DT_{50} (d)
20	L**					
	H	6.6	0.40	1.7	0* – 4.6	8.3
21	L					10
	H	5.9	0.39	1.8	0* – 3.8	7.7
22	L					11***
	H					6.0
23	L	7.4	0.46	1.5	0.75 – 2.5	8.9
	H	4.9	0.51	1.4	0.83 – 2.0	6.2
24	L**					
	H	4.7	0.32	2.2	1.3 – 3.5	6.8
25	L					10
	H	5.7	0.43	1.6	0* – 3.3	7.3
26	L					11***
	H	6.2	0.44	1.6	0* – 3.7	7.7
27	L**					
	H	6.3	0.33	2.1	0.80 – 4.3	8.4
28	L					11***
	H	6.1	0.35	2.0	0* – 4.2	8.0
29	L					9.7
	H	6.5	0.35	2.0	0.75 – 4.5	8.5
30	L**					
	H	6.0	0.54	1.3	0* – 2.9	7.3
31	L					10
	H	5.7	0.30	2.3	0.84 – 4.8	8.0
32	L					11***
	H	5.5	0.33	2.1	0* – 4.2	7.5
33	L	6.9	0.62	1.1	0* – 2.6	8.1
	H	6.2	0.43	1.6	0* – 3.5	7.8
34	L					11***
	H	4.9	0.19	3.6	1.1 – 5.5	8.6
35	L	7.2	0.53	1.3	0.59 – 2.2	8.6
	H	5.2	0.61	1.1	0* – 2.0	6.3
36	L					9.5
	H	6.5	0.50	1.4	0* – 3.6	7.9
37	L					11***
	H	6.0	0.40	1.7	0* – 3.8	7.7
38	L					1.6***
	H	1.5	0.49	1.4	0.58 – 2.3	2.9
39	L					11***
	H	4.6	0.42	1.7	0.83 – 2.8	6.2

Constituent #	Conc. level	Lag phase (d)	k (d^{-1})	$T_{½}$ (d)	$CI_{95\%}$ for $T_{½}$ (d)	DT_{50} (d)
40	L**					
	H	5.9	0.31	2.2	0.91 – 4.9	8.2
41	L					11***
	H	6.4	0.56	1.2	0* – 3.5	7.6
42	L	4.6	0.18	3.8	0* – 5.8	8.4
	H	5.8	0.37	1.9	0* – 3.6	7.6
43	L					9.2
	H	6.8	0.25	2.8	0* – 5.5	9.6
44	L	7.2	0.54	1.3	0.48 – 2.2	8.5
	H	4.8	0.38	1.8	1.1 – 2.8	6.6
45	L**					
	H	5.9	0.16	4.4	2.5 – 7.4	10.3
46	L	7.2	0.37	1.9	1.1 – 3.1	9.1
	H	5.8	0.41	1.7	1.4 – 3.3	7.5
47	L					11***
	H	4.8	0.20	3.5	2.5 – 4.8	8.2
48	L					11***
	H	5.5	0.35	2.0	0* – 3.9	7.5
49	L					11***
	H	4.8	0.23	3.1	2.1 – 4.6	7.8
50	L					11***
	H	6.5	0.43	1.6	0* – 3.9	8.1
51	L					11***
	H	6.8	0.31	2.2	1.3 – 3.6	9.0
52	L					11***
	H	6.7	0.27	2.6	1.6 – 4.0	9.3
53	L					11***
	H	5.4	0.36	1.9	0* – 4.2	7.3
54	L					10.6
	H	5.7	0.23	3.0	1.6 – 5.1	8.7
55	L					11***
	H	6.1	0.33	2.1	0.77 – 4.2	8.1
56	L	7.4	0.40	1.7	0.91 – 3.0	9.2
	H	6.2	0.42	1.6	0* – 3.9	7.9
57	L**					
	H	4.2	0.31	2.3	1.5 – 3.3	6.4
58	L**					
	H	7.0	0.56	1.2	0* – 3.5	8.3
59	L**					
	H	6.3	0.27	2.6	1.5 – 4.5	8.9

Constituent #	Conc. level	Lag phase (d)	k (d^{-1})	$T_{½}$ (d)	$CI_{95\%}$ for $T_{½}$ (d)	DT_{50} (d)
60	L	7.5	0.37	1.9	0.98 – 3.2	9.4
	H	4.4	0.28	2.4	1.6 – 3.7	6.9
61	L					11***
	H	4.4	0.21	3.3	2.3 – 4.7	7.7
62	L**					
	H	5.7	0.62	1.1	0* – 3.4	6.8
63	L**					
	H					6.1
64	L**					
	H	4.6	0.36	1.9	1.2 – 2.9	6.5
65	L**					
	H	5.5	0.35	2.0	0* – 4.0	7.5
66	L**					
	H	4.9	0.21	3.3	0* – 4.9	8.2
67	L					11***
	H	6.7	0.57	1.2	0* – 3.6	7.9
68	L					8.0
	H	4.8	0.79	0.9	0* – 1.3	5.6
69	L					8.8
	H	6.3	0.99	0.7	0* – 2.7	7.0
70	L	7.3	0.40	1.7	0.96 – 2.8	9.0
	H	4.7	0.29	2.4	1.4 – 4.0	7.1
71	L**					
	H	6.2	0.52	1.3	0* – 3.3	7.5
72	L	7.5	0.41	1.7	0.94 – 2.8	9.2
	H	5.8	0.43	1.6	1.5 – 3.1	7.5
73	L**					
	H	4.6	0.28	2.5	1.4 – 4.1	7.1
74	L**					
	H	6.0	0.30	2.3	1.2 – 4.0	8.3
75	L**					
	H	6.3	0.28	2.5	1.5 – 4.2	8.8
76	L**					
	H	6.3	0.24	2.9	1.7 – 5.5	9.2
77	L**					
	H	6.2	0.33	2.1	1.0 – 4.2	8.3
78	L					11***
	H	6.6	0.31	2.2	1.4 – 3.6	8.8
79	L**					
	H	6.1	0.37	1.9	0.66 – 4.5	8.0
80	L**					
	H	6.8	0.35	2.0	1.2 – 3.3	8.8
81	L**					
	H	4.5	0.19	3.6	2.7 – 4.9	8.1
82	L	7.2	0.44	1.6	0.61 – 3.0	8.8
	H					6.8

Constituent #	Conc. level	Lag phase (d)	k (d^{-1})	$T_{½}$ (d)	$CI_{95\%}$ for $T_{½}$ (d)	DT_{50} (d)
83	L	8.9	0.44	1.6	0* – 3.9	11
	H	4.6	0.20	3.5	2.6 – 4.8	8.1
84	L					
	H	4.7	0.19	3.7	2.6 – 5.3	8.4
85	L					11***
	H	4.9	0.40	1.8	0.85 – 3.0	6.6
86	L					8.9***
	H	4.5	0.40	1.7	0.72 – 3.2	6.2
87	L					
	H	4.3	0.35	2.0	0.99 – 3.4	6.2
88	L					9.0
	H	4.7	0.41	1.7	0.92 – 2.7	6.4
89	L	7.2	0.41	1.7	0.63 – 2.3	8.8
	H	4.8	0.45	1.5	0.81 – 2.4	6.3
90	L					
	H	6.1	0.31	2.3	1.1 – 4.7	8.4
91	L					
	H	3.9	0.10	6.7	3.5 – 11	11
92	L					
	H	0.3	0.06	12.3	7.4 - 17	13
93	L					
	H					14***
94	L					
	H	4.1	0.23	3.1	2.3 – 4.2	7.2
95	L					
	H	3.3	0.09	7.4	5.0 – 12	11
96	L	7.0	0.46	1.5	0-31 – 3.0	8.5
	H					5.5***
97	L					
	H					7.0***
98	L					
	H					5.2***
99	L					
	H	6.3	0.20	3.5	2.2 – 6.8	9.8
100	L					
	H					6.1***
101	L					
	H	3.9	0.15	4.5	3.2 – 6.5	8.3
102	L					
	H	1.6	0.11	6.3	0* – 8.6	7.9
103	L					
	H					5.6***
104	L					
	H					8.3***

Figure S4. Comparison of biodegradation kinetics (lag phase and half life) for diesel oil constituents at low and high concentration based on the kinetic data in table S7.



Supporting Information 6 – degradation curves and kinetics for lavender oil

Figure S5. Degradation curves for individual constituents in lavender oil at low and high test concentration.

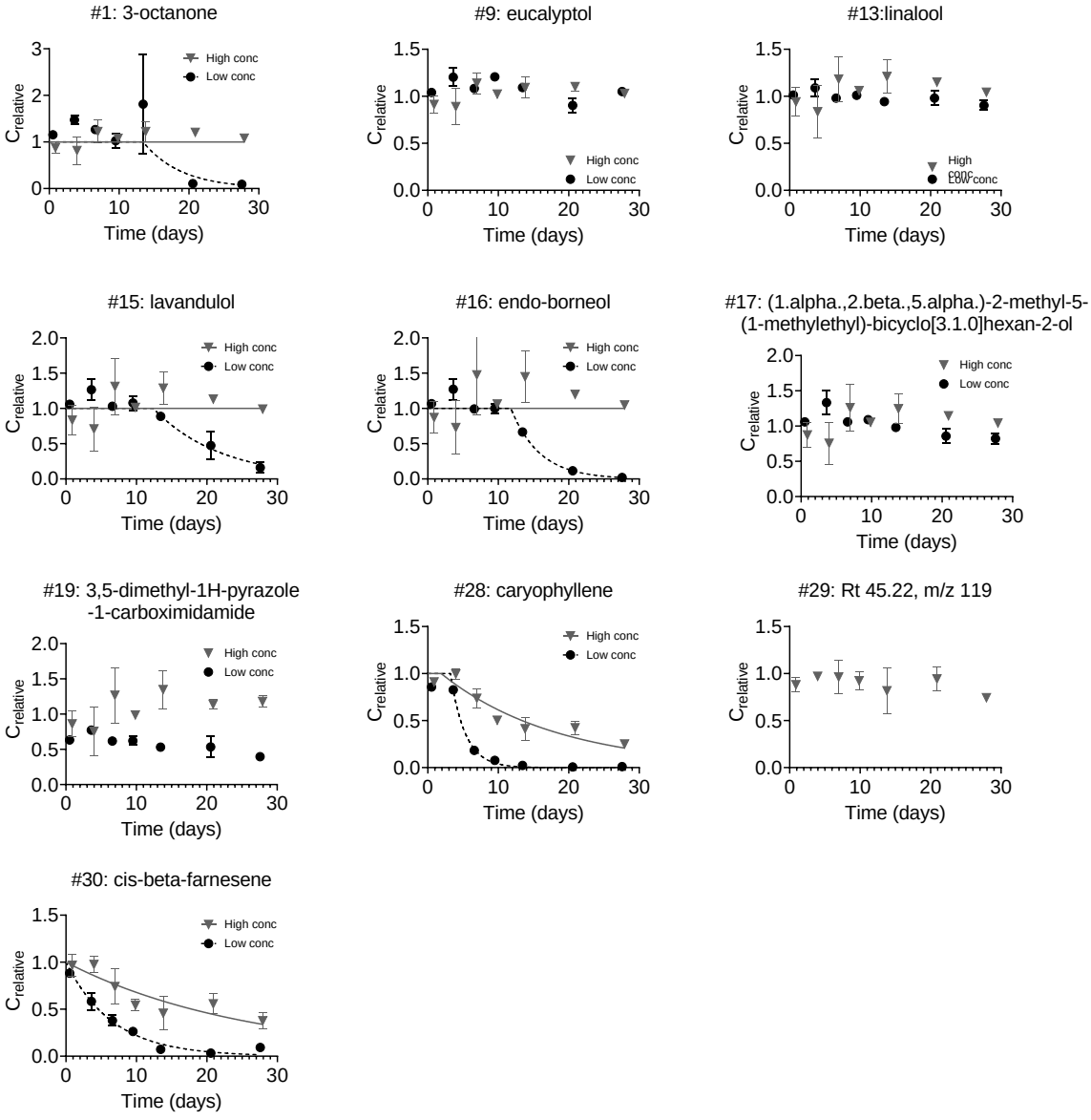


Table S9. Biodegradation kinetics for lavender oil constituents; lag-phase, first-order degradation rate constant (k_{system}), first-order degradation half life (T½) with 95% confidence intervals ($CI_{95\%}$), and degradation half time (DT50: lag-phase + one half-life). Lag phase, k and $T_{½}$ are only reported when at least two measurements were made during the visual degradation phase (10% < Crelative<90%) and R^2 > 0.8, otherwise only the DT_{50} is reported. A lag phase > 28 days means that degradation did not start within the test duration. * = derived from fit with R^2<0.8 or from ambiguous fit. **= lower limit set to zero when fit gave a negative value. *** = below limit of quantification.

Constituent #	Conc. level	Lag phase (d)	k (d^{-1})	$T_{½}$ (d)	$CI_{95\%}$ for T½	DT_{50} (d)
1	L					17*
	H	> 28				
9	L	> 28				
	H	> 28				
13	L	> 28				
	H	> 28				
15	L					19*
	H	> 28				
16	L	12	0.26	2.8	0** – 5.7	15
	H	> 28				
17	L	> 28				
	H	> 28				
19	L	> 28				
	H	> 28				
28	L	3.2	0.48	1.5	1.1 – 1.9	4.7
	H					13*
29	L***					
	H	> 28				
30	L	0.0	0.15	4.7	3.9-5.3	4.7
	H					18*

Supporting Information 7 – Figure 2 and 3 with R^2 values

Figure S6. Figure 2 and 3 with R^2 values of the fitted biodegradation kinetic curves (to low concentration data) in the two figures.