Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Hazard assessment of quinaldine-, alkylcarbazole-, benzene- and toluene-based liquid organic hydrogen carrier (LOHCs) systems

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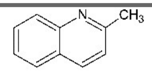
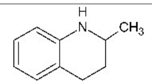
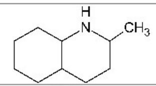
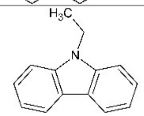
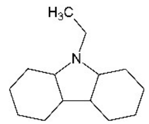
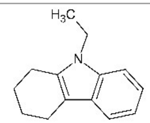
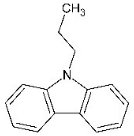
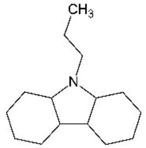
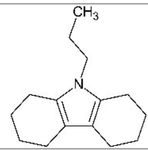
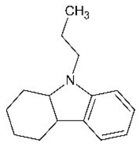
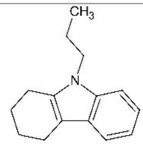
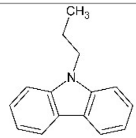
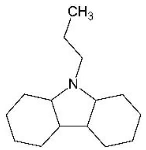
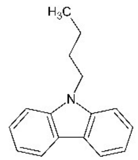
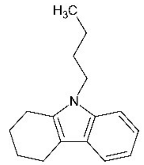
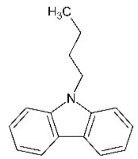
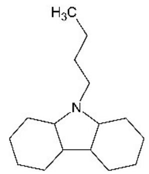
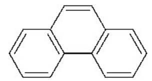
Supplementary information file

1. Analytical methods

Table SI 1. Details of analytical methods for quantification of LOHC chemicals using GC MS.Details of analytical methods for quantification of LOHC chemicals using GC MS.

Name	Abbreviation	Rt [min]	LOD/LOQ [mg L^{-1}]	Structure	Formula	Molecular weight [g mol^{-1}]	m/z*
2-methyl-quinoline (quinaldine)	Quin-2Me	4.02	0.08/0.23		$C_{10}H_9N$	143.2	**143**
1,2,3,4-tetrahydro-2-methyl-quinoline	Quin-2Me-ph	4.32	0.08/0.24		$C_{10}H_{13}N$	147.2	**147**
decahydro-2-methyl-quinoline	Quin-2Me-10H	3.14	0.32/0.96		$C_{10}H_{19}N$	153.3	**153**
9-ethyl-carbazole	Car2	5.85	0.04/0.11		$C_{14}H_{13}N$	195.3	180, **195**
9-ethyldodecahydro-carbazole	Car2-ph	4.58 (69.8%)	0.50/1.49		$C_{14}H_{25}N$	207.4	**164,** 192, 207
9-ethyltetrahydro-carbazole		5.81 (12.13%)			$C_{14}H_{17}N$	199.3	171, **199**

9-ethyldodecahydro-carbazole	Car2-H12	4.58	0.13/0.39		$C_{14}H_{25}N$	207.4	**164,** 192, 207
9-propyl-carbazole	Car3	6.09	0.04/0.13		$C_{15}H_{15}N$	209.3	**180**, 209
9-propyldodecahydro-carbazole	Car3-ph	4.92 (6.56 %)			$C_{15}H_{27}N$	221.4	**178,** 192, 221
9-propyloctahydro-carbazole		5.74 (6.79%)			$C_{15}H_{23}N$	217.3	188, **217**
9-propylhexahydro-carbazole		5.81 (5.24%)			$C_{15}H_{21}N$	215.3	171, 186, 199, **215**
9-propyltetrahydro-carbazole		6.06 (54.23%)	0.66/1.97		$C_{15}H_{19}N$	213.3	**184,** 213
9-propyl-carbazole		6.09 (11.02%)			$C_{15}H_{15}N$	209.3	**180,** 209
9-propyldodecahydro-carbazole	Car3-H12	4.92	0.76/2.27		$C_{15}H_{27}N$	221.4	178, **192**, 221

9-butyl-carbazole	Car4	6.38	0.04/0.12		$C_{16}H_{17}N$	223.3	180, **223**
9-butyltetrahydro-carbazole	Car4-ph	6.32 (53.6%)	0.54/1.63		$C_{16}H_{21}N$	227.3	**184,** 227
9-butyl-carbazole		6.38 (37.3%)			$C_{16}H_{17}N$	223.3	**180,** 223
9-butyldodecahydro-carbazole	Car4-H12	5.28	0.70/2.09		$C_{16}H_{29}N$	235.4	**192,** 235
phenanthrene	PHE (internal standard)	5.65	0.34/1.01		$C_{14}H_{10}$	178.2	178

* base ion (the most abundant ion in the spectrum) is marked in bold, structures are structures of corresponding molecular ions

2. AChE inhibition, cytotoxicity and mutagenicity – extended results table

Table SI 2. Results of acetylcholinesterase (AChE) inhibition test, cytotoxicity test using IPC-81 cell line, and mutagenicity (Salmonella typhimurium). EC_{50}/IC_{50} with 2.5%-97.5 % confidence intervals in brackets are given in µmol L^{-1} and mg L^{-1}.

Compound	***IC_{50} AChE***		***EC_{50} IPC-81***	
	µmol L^{-1}	mg L^{-1}	µmol L^{-1}	mg L^{-1}
Quin-2Me	427	61	2188	313

	(380–468)	(54–67)	(2042–2291)	(292–328)
Quin-2Me-ph	≥ 1000[a] (n.d.)	≥ 147[a] (n.d.)	≥ 3300[a] (n.d.)	≥ 480[a] (n.d.)
Quin-2Me-H10	589 (525–676)	90 (80–104)	5495 (4786–6457)	842 (734–990)
Car2	n.d.	n.d.	> 4.7[b]	> 0.92[b]
Car2-ph	n.d.	n.d.	n.a.	9.1[c] (8.3–10.0)
Car2-12H	n.d.	n.d.	291 (215–392)	60 (45–81)
Car3	n.d.	n.d.	> 1.14[b]	> 0.24[b]
Car3-ph	n.d.	n.d.	n.a.	0.78[d] (0.68–0.87)
Car3-12H	n.d.	n.d.	327 (280–385)	72 (62–85)
Car4	n.d.	n.d.	> 1.97[b]	> 0.44[b]
Car4-ph	n.d.	n.d.	n.a.	0.85[e] (0.78–0.94)
Car4-12H	n.d.	n.d.	251 (223–288)	59 (53–68)
Positive control	43 (40–46)[f]	9.8 (9.2–10.5)[f]	9.0 (8.3–9.8)[g]	0.33 (0.30–0.36)[g]

[a] The exact EC_{50} values could not be fitted since only approximately 50% effect was achieved at the highest tested concentration therefore the EC_{50} was reported as equal or higher than that concentration; [b] No effect was observed and no EC_{50} values were not obtained, the values are the averaged highest test concentrations corresponding to maximum solubility in test medium; [c] Quantified as Car2-12H (Table 2 and Table 3); [d] Quantified as Car3-4H (Table 2 and Table 3) ; [e] Quantified as Car4-4H (Table 2 and Table 3); [f] Octylmethylimidazolium chloride; [g] Carbendazim.

3. Bacterial reverse mutation test

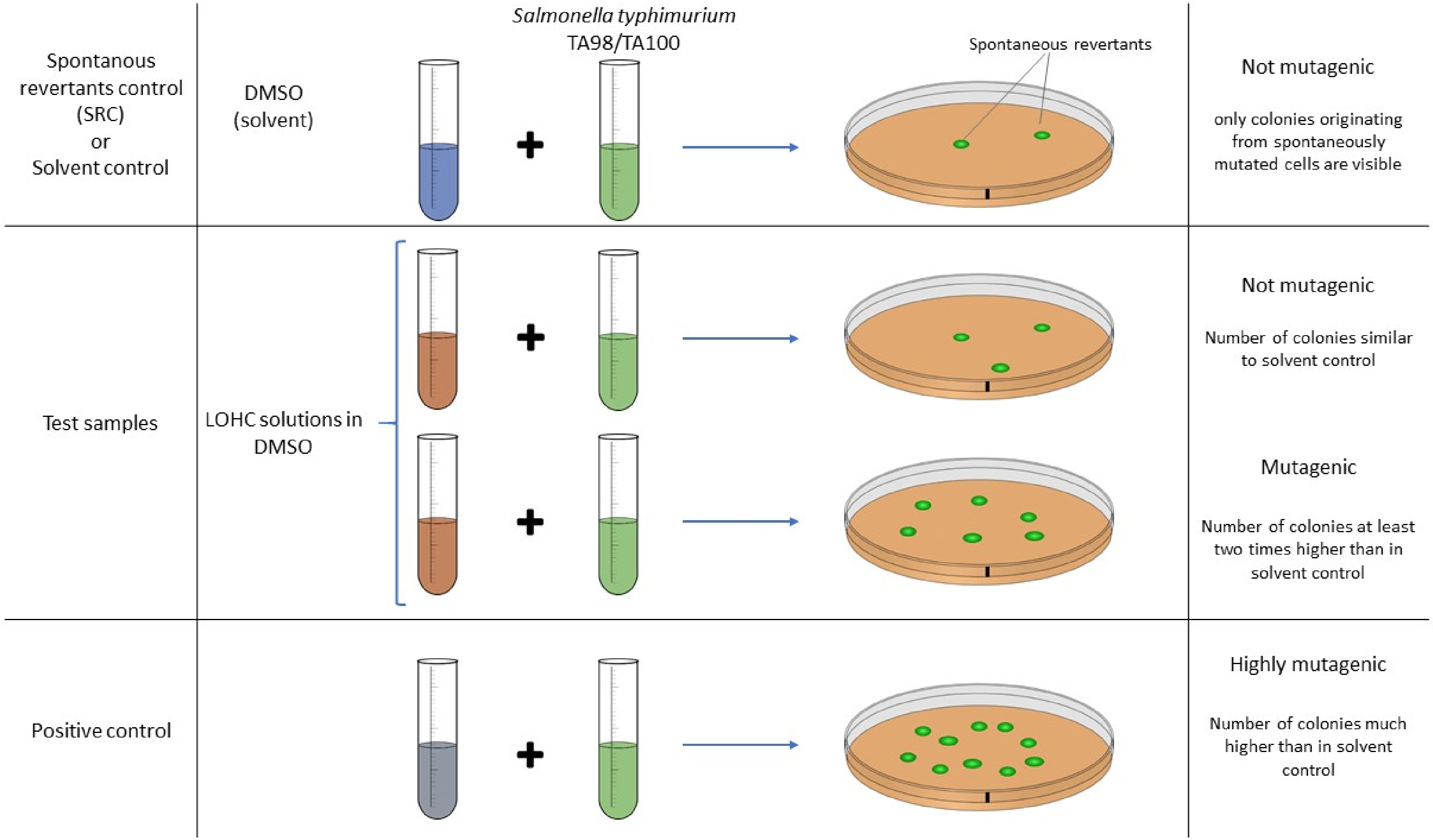


Figure SI 1: *Principle of the bacterial reverse mutation test (so called Ames test)*

4. Bacterial mutagenicity test – extended results table

Table SI 3: *Mutagenicity of LOHCs tested in the Ames test using Salmonella typhimurium strains TA98 and TA100.*

Compound	Concentration [µg/plate]	TA98						Concentration [µg/plate]	TA100					
		-S9			+S9				-S9			+S9		
		Mean[a, b]	SD[b]	MA[c]	Mean[a, b]	SD[b]	MA[c]		Mean[a, b]	SD[b]	MA[c]	Mean[a, b]	SD[b]	MA[c]
Quin-2Me	**1.01**	11.3	1.2	**0.6**	11.3	1.5	**0.7**	**1.00**	80.0	1.0	**1.1**	78.7	3.2	**1.1**
	3.38	12.0	1.0	**0.7**	11.3	1.2	**0.7**	**3.35**	97.0	3.6	**1.4**	84.0	1.0	**1.1**
	10.13	11.3	1.5	**0.6**	13.7	0.6	**0.8**	**10.04**	**84.0[d]**	**4.2[d]**	**1.2**	85.0	2.0	**1.1**
	33.75	11.7	1.5	**0.7**	10.3	0.6	**0.6**	**33.45**	118.0	2.6	**1.7**	101.0	1.7	**1.4**
	101.25	11.3	0.6	**0.6**	12.3	0.6	**0.7**	**100.35**	137.3	2.5	**1.9**	115.0	5.0	**1.5**
	337.50	13.7	1.2	**0.8**	12.7	1.5	**0.8**	**334.50**	118.0	2.6	**1.7**	88.0	2.6	**1.2**
Quin-2Me-ph	**0.34**	12.0	1.7	**0.7**	12.7	1.5	**0.8**	**0.33**	70.3	0.6	**1.0**	80.0	4.4	**1.1**
	1.02	12.7	1.5	**0.7**	11.7	0.6	**0.7**	**1.00**	74.0	1.0	**1.0**	101.3	1.5	**1.4**
	3.39	12.0	1.0	**0.7**	11.3	2.3	**0.7**	**3.34**	73.3	2.9	**1.0**	97.7	2.5	**1.3**
	10.18	12.3	2.1	**0.7**	12.3	1.2	**0.7**	**10.03**	82.3	1.2	**1.2**	82.3	2.1	**1.1**
	33.93	11.3	1.2	**0.6**	11.3	1.2	**0.7**	**33.42**	95.0	2.0	**1.3**	74.3	4.0	**1.0**
	101.80	12.0	1.0	**0.7**	11.7	2.1	**0.7**	**100.25**	119.0	2.6	**1.7**	87.7	4.0	**1.2**
Quin-2Me-H10	**6.90**	11.3	0.6	**0.6**	12.0	1.0	**0.7**	**6.68**	84.3	3.1	**1.2**	65.7	2.1	**0.9**
	20.70	13.3	0.6	**0.8**	13.0	2.6	**0.8**	**20.05**	84.0	1.0	**1.2**	62.7	2.5	**0.8**
	69.00	12.0	1.7	**0.7**	12.0	1.0	**0.7**	**66.83**	111.7	2.9	**1.6**	71.0	2.6	**0.9**
	207.00	10.7	1.2	**0.6**	11.3	1.2	**0.7**	**200.50**	110.7	1.2	**1.6**	81.3	1.5	**1.1**
	690.00	12.0	1.7	**0.7**	11.0	1.0	**0.7**	**668.33**	95.0	2.6	**1.3**	96.0	2.6	**1.3**
	2070.00	11.3	0.6	**0.6**	11.7	1.5	**0.7**	**2005.00**	85.0	2.0	**1.2**	102.3	2.1	**1.4**
Car2	**0.71**	16.3	1.2	**0.9**	17.0	1.0	**1.0**	**0.68**	109.0	1.0	**1.5**	100.0	1.0	**1.3**
	2.14	18.0	1.0	**1.0**	18.0	1.0	**1.1**	**2.05**	109.7	0.6	**1.5**	137.0	2.0	**1.8**
	7.13	18.0	1.0	**1.0**	18.0	1.7	**1.1**	**6.82**	110.0	1.0	**1.5**	170.0	2.0	**2.3**
	21.40	17.3	0.6	**1.0**	17.3	2.1	**1.0**	**20.45**	100.0	1.0	**1.4**	182.3	0.6	**2.4**
	71.33	16.7	1.2	**0.9**	14.3	1.5	**0.9**	**68.17**	89.3	1.5	**1.3**	123.0	1.0	**1.6**
	214.00	17.7	1.5	**1.0**	14.7	0.6	**0.9**	**204.50[e]**	68.7	1.2	**1.0**	119.0	1.0	**1.6**
Car2-ph	**1.39**	16.3	0.6	**0.9**	17.3	1.5	**1.0**	**1.34**	109.0	1.0	**1.5**	109.0	1.0	**1.5**
	4.16	16.7	1.5	**0.9**	18.0	3.5	**1.1**	**4.02**	111.3	1.2	**1.6**	106.7	0.6	**1.4**
	13.87	16.3	1.5	**0.9**	17.7	0.6	**1.1**	**13.39**	109.7	0.6	**1.5**	109.7	0.6	**1.5**
	41.60	13.7	0.6	**0.8**	18.3	1.2	**1.1**	**40.16**	106.7	4.9	**1.5**	106.7	3.2	**1.4**

	138.67	17.0	1.0	**1.0**	15.0	1.7	**0.9**	**133.87**	130.0	1.0	**1.8**	109.3	1.2	**1.5**
	416.00	20.0	1.0	**1.1**	17.3	0.6	**1.0**	**401.60**	43.3	3.5	**0.6**	109.3	0.6	**1.5**
Car2-H12	**2.27**	15.7	2.3	**0.9**	18.3	0.6	**1.1**	**1.67**	109.7	1.2	**1.5**	109.3	0.6	**1.5**
	6.82	16.3	2.9	**0.9**	14.7	1.2	**0.9**	**5.01**	108.7	0.6	**1.5**	109.7	0.6	**1.5**
	22.73	15.7	1.5	**0.9**	16.7	0.6	**1.0**	**16.69**	110.7	1.2	**1.6**	130.0	1.0	**1.7**
	68.20	15.0	2.6	**0.8**	15.3	0.6	**0.9**	**50.08**	109.7	1.2	**1.5**	131.7	0.6	**1.8**
	227.33	18.0	1.7	**1.0**	18.3	1.2	**1.1**	**166.92**	82.3	1.5	**1.2**	125.0	1.0	**1.7**
	682.00	17.3	1.5	**1.0**	16.0	1.0	**1.0**	**500.75**	75.0	1.0	**1.1**	74.3	1.5	**1.0**
Car3	**2.07**	20.7	2.1	**1.2**	18.0	1.0	**1.1**	**2.00**	94.0	1.0	**1.3**	100.3	1.5	**1.3**
	6.88	20.0	1.7	**1.1**	16.7	1.5	**1.0**	**6.66**	98.0	1.0	**1.4**	97.7	0.6	**1.3**
	20.65	15.0	1.7	**0.8**	16.3	2.1	**1.0**	**19.99**	97.7	1.2	**1.4**	143.0	2.0	**1.9**
	68.83	14.7	1.2	**0.8**	13.0	1.7	**0.8**	**66.63**	109.3	0.6	**1.5**	154.7	1.2	**2.1**
	206.50	15.0	1.7	**0.8**	14.3	2.3	**0.9**	**199.90**	104.7	0.6	**1.5**	141.0	1.7	**1.9**
	688.33	14.7	1.5	**0.8**	12.3	1.5	**0.7**	**666.33**	82.7	1.5	**1.2**	72.3	1.2	**1.0**
Car3-ph	**0.64**	12.7	1.5	**0.7**	16.0	2.6	**1.0**	**0.51**	104.0	3.6	**1.5**	96.3	1.5	**1.3**
	2.13	12.7	1.5	**0.7**	17.0	1.0	**1.0**	**1.70**	100.3	1.5	**1.4**	94.7	0.6	**1.3**
	6.39	12.3	1.2	**0.7**	17.0	1.7	**1.0**	**5.10**	102.3	0.6	**1.4**	104.3	0.6	**1.4**
	21.30	15.3	3.1	**0.9**	15.7	4.0	**0.9**	**17.00**	100.7	0.6	**1.4**	90.0	1.0	**1.2**
	63.90	17.3	0.6	**1.0**	16.7	0.6	**1.0**	**51.00**	87.7	1.2	**1.2**	88.0	1.0	**1.2**
	213.00	15.7	1.5	**0.9**	14.3	2.9	**0.9**	**170.00**	74.0	1.0	**1.0**	84.0	1.0	**1.1**
Car3-H12	**0.06**	12.3	0.6	**0.7**	14.3	2.1	**0.9**	**0.06**	67.0	2.0	**0.9**	99.3	1.5	**1.3**
	0.19	12.3	1.2	**0.7**	14.0	1.0	**0.8**	**0.19**	65.7	0.6	**0.9**	100.0	1.0	**1.3**
	0.56	12.3	1.2	**0.7**	13.7	2.1	**0.8**	**0.58**	64.7	0.6	**0.9**	97.7	0.6	**1.3**
	1.87	12.7	1.2	**0.7**	15.7	3.2	**0.9**	**1.92**	81.0	1.0	**1.1**	103.3	4.2	**1.4**
	5.60	12.3	1.5	**0.7**	12.0	1.0	**0.7**	**5.75**	96.7	2.5	**1.4**	100.7	1.2	**1.3**
	18.67	11.7	1.2	**0.7**	13.7	3.1	**0.8**	**19.17**	69.0	1.0	**1.0**	101.7	1.5	**1.4**
Car4	**2.00**	14.7	1.5	**0.8**	12.7	0.6	**0.8**	**2.00**	126.0	2.6	**1.8**	81.0	2.6	**1.1**
	6.67	15.0	1.0	**0.8**	13.3	1.5	**0.8**	**6.67**	156.3	4.6	**2.2**	96.7	1.5	**1.3**
	20.00	14.7	2.1	**0.8**	13.0	1.0	**0.8**	**20.00**	165.3	2.5	**2.3**	73.7	2.1	**1.0**
	66.67	15.0	1.0	**0.8**	13.0	1.0	**0.8**	**66.67**	151.3	1.5	**2.1**	70.0	1.0	**0.9**
	200.00	18.3	1.2	**1.0**	14.0	2.0	**0.8**	**200.00**	148.7	0.6	**2.1**	67.0	1.7	**0.9**
	666.67	18.7	0.6	**1.1**	13.7	1.2	**0.8**	**666.67**	135.7	2.1	**1.9**	65.0	1.0	**0.9**
Car4-ph	**0.50**	10.7	0.6	**0.6**	13.0	1.7	**0.8**	**0.50**	110.7	1.2	**1.6**	75.0	5.2	**1.0**
	1.66	10.7	1.2	**0.6**	13.3	1.5	**0.8**	**1.67**	130.0	1.7	**1.8**	102.0	1.0	**1.4**
	4.97	10.7	0.6	**0.6**	12.3	1.5	**0.7**	**5.00**	132.7	0.6	**1.9**	104.0	1.0	**1.4**
	16.57	12.0	1.0	**0.7**	14.0	1.0	**0.8**	**16.67**	137.0	3.5	**1.9**	102.7	0.6	**1.4**

	49.70	15.0	1.0	**0.8**	13.3	2.3	**0.8**	**50.00**	138.3	3.8	**1.9**	81.3	0.6	**1.1**
	165.67	16.7	0.6	**0.9**	13.7	1.5	**0.8**	**166.67**	128.7	0.6	**1.8**	81.3	1.5	**1.1**
Car4-H12	**0.19**	12.0	2.6	**0.7**	12.7	2.9	**0.8**	**0.17**	128.0	1.0	**1.8**	110.3	1.5	**1.5**
	0.56	12.0	1.0	**0.7**	12.7	1.2	**0.8**	**0.51**	132.0	1.0	**1.9**	119.3	1.5	**1.6**
	1.87	12.7	1.5	**0.7**	14.0	1.0	**0.8**	**1.71**	129.0	1.0	**1.8**	121.3	1.5	**1.6**
	5.60	13.0	2.0	**0.7**	12.3	0.6	**0.7**	**5.14**	119.0	1.0	**1.7**	107.7	4.0	**1.4**
	18.67	13.7	0.6	**0.8**	13.3	1.2	**0.8**	**17.13**	109.0	1.0	**1.5**	101.3	2.3	**1.4**
	56.00	12.7	2.1	**0.7**	15.0	1.0	**0.9**	**51.40**	98.7	1.2	**1.4**	96.7	2.3	**1.3**
SRC[f]	**-**	17.1	1.6	**1.0**	17.0	1.7	**1.0**	**-**	76.0	2.9	**1.1**	**75.7[h]**	**3.2[h]**	**1.0**
SC[g]	**-**	17.7	3.0	**1.0**	16.8	1.5	**1.0**	**-**	71.0	2.3	**1.0**	**74.8[h]**	**2.4[h]**	**1.0**
4-N-PD[i]	**5**	459.6	12.2	**26.0**	-	-	**-**	**-**	-	-	**-**	-	-	**-**
NaN_3[j]	**-**	-	-	**-**	-	-	**-**	**5**	212.7	6.1	**3.0**	-	-	**-**
B[*a*]P[k]	**5**	-	-	**-**	469.0	13.7	**28.0**	**5**	-	-	**-**	459.9	6.4	**6.2**

[a] Revertants/plate

[b] Mean and SD of a triplicate determination of one experiment (n = 1)

[c] Mutagenic activity [fold of solvent ctrl.]

[d] Due to a technical error, the mean and SD of only two plates is given

[e] This concentration slightly changed the morphology of the bacterial background lawn (only TA100 -S9)

[f] Spontaneous revertant control (buffer only); mean and SD of a triplicate determination of three independent experiments (n = 3)

[g] Solvent control (7.7 % DMSO); mean and SD of a triplicate determination of three independent experiments (n = 3). These means were used as reference for the calculation of the MAs of TA98 - and +S9 as well as TA100 -S9

[h] Mean and SD of a triplicate determination of three independent experiments (n = 3); two of the three control experiments were performed separately from the experiments assaying the LOHCs (only TA100 +S9). Since the revertant values of those two data sets matched those of the sole experiment performed concomitantly with one LOHC batch, they were deemed valid for the calculation of the mean used as reference for the calculation of all MAs of TA100 +S9

[i] 4-Nitro-*o*-phenylenediamine (positive control TA98 -S9); mean and SD of a triplicate determination of three independent experiments (n = 3)

[j] Sodium azide (positive control TA100 -S9); mean and SD of a triplicate determination of three independent experiments (n = 3)

[k] Benzo[*a*]pyrene (positive control TA98 and TA100 +S9); mean and SD of a triplicate determination of three independent experiments (n = 3)

5. Aquatic toxicity – extended results table

Table SI 4.Results of acute aquatic ecotoxicity test with green algae (Raphidocelis subcapitata), duckweed (Lemna minor) and water flea (Daphnia magna). EC50 in µmol L-1and mg L-1¬with 2.5% and 97.5 %confidence intervals are given

Compound	*Vibrio fischeri*		*Raphidocelis subcapitata*		*Lemna minor*		*Daphnia magna*	
	µmol L^{-1}	mg L^{-1}	µmol L^{-1}	mg L^{-1}	µmol L^{-1}	mg L^{-1}	µmol L^{-1}	mg L^{-1}
Quin-2Me	133 (113–156)	19 (16–22)	301 (-)	43 (-)	291 (254–334)	42 (36–48)	393 (375–411)	56 (54–59)
Quin-2Me-ph	50 (42–61)	7.4 (6.2–8.9)	118 (98–137)	17 (14–20)	348 (303–400)	51 (46–59)	18 (16–22)	2.7 (2.3–3.2)
Quin-2Me-H10	> 1998	> 306	339 (323 – 355)	52 (50 – 55)	~6524	~1000	1011 (784–1243)	155 (120–191)
Car2	> 1.8[a]	> 0.36[a]	n.d.	n.d.	> 3.33 [a]	> 0.65[a]	> 1.96 [a]	> 0.38[a]
Car2-ph	n.a.	2.5[b] (2.09–2.82)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Car2-12H	> 2079[a]	> 431[a]	n.d.	n.d.	1242 (1225–1266)	258 (254–263)	291 (242–366)	60 (50–76)
Car3	> 0.29[a]	> 0.06[a]	n.d.	n.d.	> 1.89 [a]	> 0.40[a]	> 1.72 [a]	> 0.36[a]
Car3-ph	n.a.	4.3[c] (3.8 – 4.8)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Car3-12H	> 1987	> 440[a]	n.d.	n.d.	> 1084	> 240	46 (38–57)	10.2 (8.3–12.6)
Car4	> 0.15[a]	> 0.03[a]	n.d.	n.d.	> 0.56 [a]	> 0.063[a]	> 0.72 [a]	> 0.16[a]
Car4-ph	n.a.	> 2.9[a,d]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Car4-12H	> 1945[a]	> 457[a]	n.d.	n.d.	478 (n.d.)	112 (n.d.)	41 (32–50)	9.6 (7.7–11.8)
Reference	See below[e]	See below[e]	9.9[f] (7.9–11.8)	1.6[f] (1.3–1.9)	17 [g] (12–26)[c]	6.6[g] (4.5–10.2)	3.6 [h] (3.2–4.0)	1.1 [h] (0.96–1.17)
Diesel oil	-	-	-	22-78[i]	-	-	-	13-210[i]
Benzene	-	-	371[k]	29.0[k]	-	-	128–220[l]	10.0–17.2[l]
Cyclohexane	-	-	42[m]	3.4[m]	-	-	11–47[n]	0.9–3.8[n]
Toluene	-	-	136–2247[o]	12.5–207[o]	-	-	41–162[p]	3.8–14.9[p]
Methylcyclohexane	-	-	1.3[r]	0.13[r]	-	-	3.4[s]	0.33[s]

[a] Not more than 40 % luminescence inhibition was recorded for Quin-2Me-10H at the highest attainable concentration. Therefore, the EC_{50} value was reported as higher than this concentration; [b] Averaged maximum solubility in the test medium; [c] Quantified as Car2-12H (Table 2 and Table 3); [d] Quantified as Car3-4H (Table 2 and Table 3); [e] Quantified as Car4-4H (Table 2 and Table 3); [f] 7.5 % (w/w) NaCl (luminescence inhibition between 40 and 60 % is expected); [g] 3,5-dichlorophenol; [h] Benzalkonium chloride; [i] Potassium dichromate; [j] American Petroleum Institute (API) for automotive diesel oil CAS 68334-30-573; [k] short-term EC_{50} for *Raphidocelis subcapitata*[74]; [l] short-term EC_{50} for *Daphnia magna* or *Ceriodaphnia dubia*[75,76]; [m] short-term EC_{50} for *Raphidocelis subcapitata*[77]; [n] short-term EC_{50} for *Daphnia magna*[77]; [o] short-term EC_{50} for *Raphidocelis subcapitata, Chlamydomonas angulosa* or *Chlorella vulgaris*[74,78]; [p] short-term EC_{50} for *Daphnia magna* or *Ceriodaphnia dubia*[75,76,79,80]; [r] short-term EC_{50} for *Raphidocelis subcapitata* taken from[81]; [s] short-term EC_{50} for *Daphnia magna* taken from[81]; n.d.: value not determined; n.a.: not applicable, because the substance is a mixture and it is therefore not possible to calculate molar concentration.

6. Details regarding treatment of the data

The eco(toxicity) tests were performed at least three times unless no effect was observed in the first two tests. The results of each experiment were inspected for violations of quality criteria given in the corresponding guidelines (e.g. mortality in controls, growth rates in controls, response in positive controls, standard deviation of response etc.). Tests which did not match quality criteria where discarded and the test was repeated. The data of each experiment were log-normal transformed and plotted together. Subsequently probit, logit or linlogit models were fitted using the drfit package (version 3.1.0) for R (version 3.4; http://www.r-project.org) to obtain the EC_{50} value with confidence intervals. The data was visually inspected to see if the model adequately represented the data.

The comparison between EC_{50} values of different LOHC chemicals was done using hypothesis testing. First, each set of data was tested for normality using the Shapiro-Wilk test. Then, the two sets of data to be compared were checked for homogeneity of variance using the F-test. For normally distributed data with homogenous variance, a student's *t*-test was performed, while data which were not normally distributed were subjected to a Wilcoxon-Mann-Whitney test. All statistical analyses were based on a significance level of $\alpha = 0.05$. The results of Wilcoxon-Mann-Whitney tests are presented below.

Compound	*p*-value
Test system: IPC-81	
Quin-2Me vs. Quin-2Me-H10	0.146
Car2-ph vs. Car3-ph	0.1175
Car2-ph vs. Car4-ph	0.0005012
Car3-ph vs. Car4-ph	0.05591
Car2-H12 vs. Car3-H12	0.3444
Car2-H12 vs. Car4-H12	0.0003275
Car3-H12 vs. Car4-H12	0.002155
Test system: AChE	
Quin-2Me vs. Quin-2Me-H10	0.06505
Test system: *Vibrio fischeri*	
Quin-2Me vs Quin-2Me-ph	0.3334
Quin-2Me vs- Car2	0.05228
Quin-2Me-ph vs Car2	0.2446
Test system: *Raphidocelis subcapitata*	
Quin-2Me vs Quin-2Me-ph	0.1929
Quin-2Me vs. Quin-2Me-H10	0.6805
Quin-2Me-ph vs. Quin-2Me-H10	0.4659

Test system: *Lemna minor*	
Quin-2Me vs Quin-2Me-ph	0.01815
Car2-H12 vs Car4-H12	0.2858
Quin-2Me vs Car2-H12	6.59E-14
Quin-2Me-ph vs Car2-H12	1.83E-09
Quin-2Me vs Car4-H12	1.13E-10
Quin-2Me-ph vs Car4-H12	4.47E-07
Test system: *Daphnia magna*	
Quin-2Me vs. Quin-2Me-ph	1.81E-05
Quin-2Me vs. Quin-2Me-H10	0.5876
Quin-2Me-ph vs. Quin-2Me-H10	4.63E-08
Car2-H12-Car3-H12A	2.21E-13
Car2-H12-Car4-H12A	7.27E-14
Car3-H12-Car4-H12A	0.0003391
Quin-2Me vs. Car2-H12	0.3268
Quin-2Me-ph vs. Car2-H12	3.82E-09
Quin-2Me-H10 vs. Car2-H12	0.5636
Quin-2Me vs. Car3-H12	0.0002729
Quin-2Me-ph vs. Car3-H12	0.007247
Quin-2Me-H10 vs. Car3-H12	1.45E-10
Quin-2Me vs. Car4-H12	1.90E-08
Quin-2Me-ph vs. Car4-H12	0.2918
Quin-2Me-H10 vs. Car4-H12	3.66E-12