Supporting Information

Carbon chain decomposition of short chain chlorinated paraffins (SCCPs) mediated by pumpkin and soybean seedlings

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Summary of the Supporting Information

Total Pages: 23; total text: 4; total tables: 6; total figures: 4

List of contents:

SCCPs (B) in different compartments of soybeans after 10 days exposure.

References

Text S1: Chemicals and regents

Florisil (60-100 mesh, Sigma−Aldrich, St. Louis, USA), silica gel (0.063-0.100 mm, Merk, Darmstadt, Germany) and anhydrous sodium sulfate (Na_2SO_4) were heated at 140 ^oC for 7 h, 550 ^oC for 12 h, and 660 ^oC for 6 h, respectively. Acid silica gel was a mixture of activated silica and concentrated H_2SO_4. Then, all of these were stored in a sealed desiccator. Pesticide grade hexane, dichloromethane, acetone and cyclohexane were purchased from J.T. Baker (Phillipsburg, NJ, USA). Ultrapure water (18.3 MΩ × cm) was obtained from a Milli-Q purification system (Millipore, Billerica, USA). All other chemicals and reagents were analytical grade or better.

Text S2: Extraction and clean up

The method for extraction and cleanup was the same as that in our previous research,[1] which was modified from the method developed by Zeng et al.[2] In brief, all samples were added with a surrogate standard (1 ng $^{13}C_{10}$-*trans*-chlordane) before extraction. Hydroponic solutions were extracted immediately with 15 mL of dichloromethane for three times consecutively after sampling. The volume of solutions of exposure groups and planted blank controls, and unplanted chemical controls was 22-32 mL, and 40 mL, respectively. The combined organic phase went through an anhydrous sodium sulfate (Na_2SO_4) column (5 g) to remove the remaining trace water and then concentrated to 2 mL. Ground-up plant samples were extracted by a mixture of n-hexane and dichloromethane (1:1, *v/v*) using an accelerated solvent extractor (ASE). The ASE parameters were set at a temperature of 100 ^{o}C, pressure of 1500 psi, thermal equilibration for 5 min, static extraction for three cycles (7 min per cycle), and a gaseous nitrogen purge for 100 s. The extract was shaken with the acid silica gel (44%, *w/w*), then passed through an anhydrous sodium sulfate column (5 g) and finally concentrated to 2 mL for further clean up.

All the extracts were cleaned-up by multilayer columns which were pre-cleaned by 50 mL of hexane. Columns contained 3 g florisil, 2 g activated silica gel, 5 g acid silica gel (30%, *w/w*), and 4 g anhydrous sodium sulfate from the bottom to the top. After impurities were rinsed by 35 mL of hexane, elution was carried out by adding 100 mL of dichloromethane/hexane (1:1, *v/v*). The eluent was dried, re-dissolved in 200 μL of cyclohexane and added with 10 ng injection standard for instrumental analysis.

Text S3 Instrumentation

The GC was equipped with a 7683B series injector and DB-5MSUI capillary column (30 m×0.25 mm×0.25 μm; Agilent, CA). Helium (≥ 99.999%) and methane (≥ 99.999%) were the carrier and moderating gases at constant flows of 2.0 and 0.40 mL/min, respectively. The column temperature was initially controlled at 100 °C, held for 1 min; then increased by 30 °C/min to 160 °C, held for 5 min; and finally increased to 300 °C at 30 °C /min and held for 12 min. The pulsed splitless mode injector, ion source and transfer line were set at 280 °C, 200 °C and 280 °C, respectively.

Text S4: Laboratory blanks/background contamination

Plants were grown in the cultivation chamber free of parent SCCPs exposure prior to the actual exposure experiment. All results subtracted the corresponding SCCP congener concentrations of the plant background. The calculation equation is shown as follow:

$C = C_{detected} - C_{plantbackground}$

in which C is the corrected concentration of SCCPs, $C_{detected}$ is the detected concentrations of SCCPs, and $C_{plantbackground}$ is the concentrations of the SCCPs in the plant background. No CPs were detected in the cultivation solution of the plant background.

Table S1 Information on commercial standards of individual SCCP congeners.

Congener cod/CAS NO.	Formula	Name	Purity (%)	Concentration (μg/ mL)	Source
CP-3	$C_{10}H_{17}Cl_5$	1,2,5,6,9-pentachlorodecane	99.1[a]	10	E[b]
CP-4	$C_{10}H_{16}Cl_6$	1,2,5,6,9,10-hexachlorodecane	99.9	10	E
CP-6	$C_{10}H_{16}Cl_6$	1,2,4,5,9,10-hexachlorodecane	99.9	10	E
CP-7	$C_{10}H_{15}Cl_7$	1,2,4,5,6,9,10-heptachlorodecane	99.9	10	E
CP-8	$C_{10}H_{15}Cl_7$	1,2,5,5,6,9,10-heptachlorodecane	94.0	10	E
601523-23-3	$C_{10}H_{14}Cl_8$	1,1,1,3,8,10,10,10-octachlorodecane	96.4	100	C[c]
601523-28-8	$C_{11}H_{18}Cl_6$	1,1,1,3,10,11-hexachloroundecane	90.4	100	C
865306-23-6	$C_{13}H_{22}Cl_6$	1,1,1,3,12,13-hexachlorotridecane	95.0	100	C
865306-21-4	$C_9H_{14}Cl_6$	1,1,1,3,8,9- hexachlorononane	98.7	1000	C

[a] The concentrations of decane standard solutions from Ehrenstorfer GmbH have been adjusted according to the purity of the compounds as indicated. [b] Dr. Ehrensforfer GmbH, Germany. [c] Chiron, Norway.

Table S2 Water solubility and method detection limits (MDLs) of various parent individual SCCP congeners.

Congeners	Water solubility [a] (ng/mL)	MDLs	
		Plants (ng/g)	Solution (ng/mL)
1,2,5,6,9,10-HexCD	54.0	15.8 ± 6.3	0.27 ± 0.05
1,1,1,3,8,10,10,10-OctaCD	1.55	34.7 ± 5.3	0.32 ± 0.07
1,1,1,3,10,11-HexCU	4.80	213 ± 15	0.41 ± 0.03
1,1,1,3,12,13-HexCT	0.44	16.1 ± 7.2	0.25 ± 0.08

[a] Calculated value using the Estimation Programs Interface (EPI) Suite software.

Table S3 List of target chlorinated paraffins (CPs) and their SIM ions.

Short chain CPs			Medium chain CPs		
CP congener	Selected ions monitored		CP congener	Selected ions monitored	
	m/z_1 $[M-Cl]^-$	m/z_2 $[M-Cl]^-$		m/z_1 $[M-Cl]^-$	m/z_2 $[M-Cl]^-$
C_9Cl_5	264.9	262.9	$C_{14}Cl_5$	335.1	333.1
C_9Cl_6	298.9	300.9	$C_{14}Cl_6$	369.0	371.0
C_9Cl_7	332.9	334.9	$C_{14}Cl_7$	403.0	405.0
C_9C_8	366.9	368.9	$C_{14}Cl_8$	437.0	438.9
C_9C_9	402.8	400.8	$C_{14}Cl_9$	472.9	470.9
C_9C_{10}	436.8	434.8	$C_{14}Cl_{10}$	506.9	504.9
$C_{10}Cl_5$	279.0	277.0	$C_{15}Cl_5$	349.1	347.1
$C_{10}Cl_6$	313.0	315.0	$C_{15}Cl_6$	383.0	385.0
$C_{10}Cl_7$	346.9	348.9	$C_{15}Cl_7$	417.0	419.0
$C_{10}Cl_8$	380.9	382.9	$C_{15}Cl_8$	451.0	453.0
$C_{10}Cl_9$	416.8	414.8	$C_{15}Cl_9$	486.9	484.9
$C_{10}Cl_{10}$	450.8	448.8	$C_{15}Cl_{10}$	520.9	518.9
$C_{11}Cl_5$	293.0	291.0	$C_{16}Cl_5$	363.1	361.1
$C_{11}Cl_6$	327.0	329.0	$C_{16}Cl_6$	397.1	399.1
$C_{11}Cl_7$	360.9	362.9	$C_{16}Cl_7$	431.0	433.0
$C_{11}Cl_8$	394.9	396.9	$C_{16}Cl_8$	465.0	467.0
$C_{11}Cl_9$	430.9	428.9	$C_{16}Cl_9$	500.9	498.9
$C_{11}Cl_{10}$	464.8	462.8	$C_{16}Cl_{10}$	534.9	532.9

$C_{12}Cl_5$	307.0	305.0	$C_{17}Cl_5$	377.1	375.1
$C_{12}Cl_6$	341.0	343.0	$C_{17}Cl_6$	411.1	413.1
$C_{12}Cl_7$	375.0	377.0	$C_{17}Cl_7$	445.0	447.0
$C_{12}Cl_8$	408.9	410.9	$C_{17}Cl_8$	479.0	481.0
$C_{12}Cl_9$	444.9	442.9	$C_{17}Cl_9$	515.0	513.0
$C_{12}Cl_{10}$	478.8	476.8	$C_{17}Cl_{10}$	548.9	546.9
$C_{13}Cl_5$	321.1	319.1			
$C_{13}Cl_6$	355.0	357.0			
$C_{13}Cl_7$	389.0	391.0			
$C_{13}Cl_8$	422.9	424.9			
$C_{13}Cl_9$	458.9	456.9			
$C_{13}Cl_{10}$	492.9	490.9			

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Table S4 SCCPs of plant background (plants before exposure).

Plant species	Tissues	$C_{10}Cl_5$ (ng/g)	$C_{10}Cl_6$ (ng/g)	$C_{10}Cl_7$ (ng/g)	$C_{10}Cl_8$ (ng/g)	$C_{11}Cl_5$ (ng/g)	$C_{11}Cl_6$ (ng/g)	$C_{12}Cl_5$ (ng/g)	$C_{12}Cl_6$ (ng/g)	$C_{13}Cl_5$ (ng/g)	$C_{13}Cl_6$ (ng/g)
Background of pumpkin	Shoots	2790 ± 973[a]	1949 ± 476	624 ± 343	434 ± 324	2260 ± 887	1263 ± 234	444 ± 199	121 ± 47	502 ± 259	126 ± 58
	Stems	3218 ± 188	962 ± 242	248 ± 77	154 ± 47	3129 ± 349	805 ± 219	2756 ± 358	404 ± 118	2709 ± 463	421 ± 113
	Roots	4465 ± 1518	2038 ± 247	494 ± 38	239 ± 97	4329 ± 215	1694 ± 145	2895 ± 156	548 ± 34	2206 ± 39	546 ± 86
Background of soybean	Shoots	1492 ± 1227	1068 ± 976	438 ± 145	297 ± 112	2469 ± 562	1382 ± 333	1683 ± 289	160 ± 21	3093 ± 280	182 ± 103
	Stems	4773 ± 327	469 ± 43	194 ± 51	102 ± 86	5871 ± 388	570 ± 89	13621 ± 1889	237 ± 13	36787 ± 3336	265 ± 43
	Roots	8222 ± 614	322 ± 146	258 ± 117	61.8 ± 29.3	2655 ± 391	379 ± 128	5902 ± 761	482 ± 156	9747 ± 4084	398 ± 205

[a]Mean value ± standard deviation (n=3). No SCCPs detected in the cultivation solution for plant backgrounds.

192 **Table S5 Concentrations of daughter SCCPs in shoots, stems and roots of exposed pumpkins and soybeans.**

Groups	Samples	$C_{10}Cl_5$ (ng/g)	$C_{10}Cl_6$ (ng/g)	$C_{10}Cl_7$ (ng/g)	$C_{10}Cl_8$ (ng/g)	$C_{11}Cl_5$ (ng/g)	$C_{11}Cl_6$ (ng/g)	$C_{12}Cl_5$ (ng/g)	$C_{12}Cl_6$ (ng/g)	$C_{13}Cl_5$ (ng/g)	$C_{13}Cl_6$ (ng/g)
Exposed pumpkin (1 day)	Shoots	n.d.[a]	n.d.	456 ± 424[b]	214 ± 178	1139 ± 921	692 ± 503	251 ± 211	83.0 ± 65.6	n.d.	82.2 ± 37.2
	Stems	n.d.	784 ± 670	255 ± 206	46.7 ± 56.2	n.d.	478 ± 372	n.d.	n.d.	n.d.	n.d.
	Roots	n.d.	894 ± 379	557 ± 199	62.7 ± 61.2	n.d.	592 ± 458	n.d.	n.d.	n.d.	n.d.
Exposed pumpkin (2 days)	Shoots	n.d.	3891 ± 2653	1437 ± 672	426 ± 256	699 ± 1067	668 ± 701	417 ± 268	144 ± 95	n.d.	131 ± 79
	Stems	n.d.	358 ± 289	210 ± 121	49.9 ± 37.4	n.d.	171 ± 174	n.d.	n.d.	n.d.	n.d.
	Roots	n.d.	558 ± 409	424 ± 109	99.4 ± 101	n.d.	400 ± 217	n.d.	n.d.	n.d.	n.d.

Exposed pumpkin (4 days)	Shoots	1735 ± 2262	6856 ± 5541	3188 ± 1978	1296 ± 838	n.d.	698 ± 844	1053 ± 772	297 ± 212	301 ± 302	299 ± 210
	Stems	n.d.	2074 ± 2757	818 ± 935	319 ± 320	n.d.	1076 ± 1149	n.d.	712 ± 1310	n.d.	570 ± 1135
	Roots	n.d.	959 ± 565	566 ± 134	192 ± 84	564 ± 429	1174 ± 1294	1475 ± 685	254 ± 166	727 ± 430	225 ± 140
Exposed pumpkin (6 days)	Shoots	n.d.	n.d.	954 ± 301	524 ± 133	n.d.	n.d.	811 ± 239	86.3 ± 23.0	863 ± 305	83.9 ± 30.0
	Stems	6096 ± 6112	232 ± 59	223 ± 136	61.3 ± 29.9	5550 ± 6186	71.6 ± 84.0	4666 ± 2381	304 ± 63	10720 ± 13972	345 ± 264
	Roots	6779 ± 6407	n.d.	81.8 ± 47.4	138 ± 65	18930 ± 6146	n.d.	21244 ± 8484	792 ± 215	16733 ± 8868	520 ± 225
Exposed	Shoots	n.d.	686 ±	820 ±	102 ±	n.d.	n.d.	490 ±	57.5 ±	139 ±	34.0 ±

pumpkin			718	128	76			140	22.9	96	9.8
(10 days)	Stems	1124 ± 1225	1840 ± 2144	1235 ± 1233	623 ± 814	n.d.	n.d.	910 ± 1034	871 ± 1706	2276 ± 1810	449 ± 903
	Roots	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	907 ± 1245	n.d.	1967 ± 2397	n.d.
Exposed	Shoots	n.d.	n.d.	1404 ± 130	1006 ± 78	n.d.	n.d.	2369 ± 603	141 ± 55	2382 ± 1507	145 ± 98
soybean											
(10 days)	Stems	13846 ± 11810	1344 ± 1478	1316 ± 1040	612 ± 903	12630 ± 6924	2020 ± 4343	7178 ± 8848	1162 ± 1923	41292 ± 32220	937 ± 883
	Roots	1727 ± 1124	844 ± 64	54.0 ± 30.6	256 ± 34	8530 ± 3627	552 ± 315	2463 ± 3155	549 ± 228	8291 ± 5378	235 ± 65

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194 [a] Non- detectable. [b] Mean value ± standard deviation (n = 5).

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197 **Table S6 Concentrations of daughter SCCPs in shoots, stems and roots of planted blank controls of pumpkin (PBCP) and soybean (PBCS).**

Groups	Samples	$C_{10}Cl_5$ (ng/g)	$C_{10}Cl_6$ (ng/g)	$C_{10}Cl_7$ (ng/g)	$C_{10}Cl_8$ (ng/g)	$C_{11}Cl_5$ (ng/g)	$C_{11}Cl_6$ (ng/g)	$C_{12}Cl_5$ (ng/g)	$C_{12}Cl_6$ (ng/g)	$C_{13}Cl_5$ (ng/g)	$C_{13}Cl_6$ (ng/g)
PBCP (1 day)	Shoots	n.d.[a]	n.d.	300 ± 40[b]	53.9 ± 25.9	245 ± 166	106 ± 94	91.0 ± 65.8	27.2 ± 7.7	n.d.	13.9 ± 2.3
	Stems	n.d.	440 ± 527	182 ± 141	76.1 ± 44.0	n.d.	246 ± 245	n.d.	n.d.	n.d.	n.d.
	Roots	n.d.	878 ± 785	330 ± 195	74.5 ± 33.5	n.d.	706 ± 583	n.d.	n.d.	n.d.	n.d.
PBCP (2 days)	Shoots	n.d.	2753 ± 549	1071 ± 108	283 ± 5	599 ± 35	678 ± 77	353 ± 30	167 ± 92	n.d.	117 ± 32
	Stems	n.d.	601 ± 115	245 ± 41	78.1 ± 3.7	n.d.	153 ± 11	n.d.	n.d.	n.d.	n.d.
	Roots	n.d.	826 ± 824	387 ± 296	89.5 ± 78.5	n.d.	538 ± 455	n.d.	n.d.	n.d.	n.d.

PBCP (4 days)	Shoots	n.d.	4726 ± 865	2180 ± 206	693 ± 80	n.d.	215 ± 153	564 ± 128	179 ± 24	n.d.	166 ± 27
	Stems	n.d.	n.d.	54.9 ± 7.2	31.9 ± 39.7	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Roots	n.d.	n.d.	165 ± 270	79.5 ± 106	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PBCP (6 days)	Shoots	n.d.	n.d.	912 ± 665	589 ± 473	n.d.	n.d.	2207 ± 864	174 ± 122	449 ±604	148 ± 107
	Stems	n.d.	n.d.	n.d.	n.d.	2146 ± 2397	n.d.	6490 ± 7484	113 ± 120	13353 ± 14185	116 ± 174
	Roots	1193 ± 1030	n.d.	n.d.	n.d.	875 ± 508	n.d.	9771 ± 9301	391 ± 330	3817 ± 2652	47.7 ± 30.7
PBCP	Shoots	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	460 ±	n.d.	443 ±	n.d.

(10 days)								565		541	
	Stems	3002 ± 3090	455 ± 629	145 ± 120	65.8 ± 8.2	1163 ± 1560	n.d.	3145 ± 3207	92.9 ± 85.0	441 ± 539	254 ± 327
	Roots	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	921 ± 420	n.d.	287 ± 66	n.d.
PBCS	Shoots	1945 ± 138	n.d.	2291 ± 2548	1345 ± 1490	2711 ± 1847	n.d.	2893 ± 1930	177 ± 150	n.d.	224 ± 320
(10 days)	Stems	64171 ± 56413	707 ± 284	2378 ± 1778	271 ± 51	8745 ± 8417	803 ± 1243	n.d.	1018 ± 851	n.d.	596 ± 392
	Roots	n.d.	176 ±168	808 ± 1010	108 ± 30	4824 ± 4166	379 ± 515	2042 ± 3079	n.d.	n.d.	146 ± 125

[a] Non-detectable. [b] Mean value ± standard deviation (n = 3).

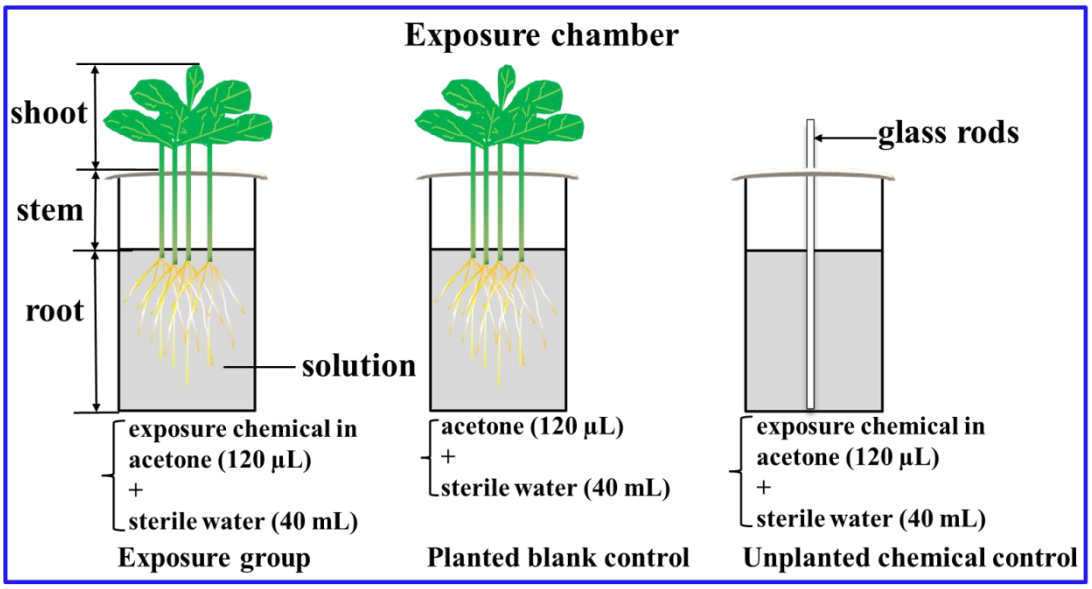
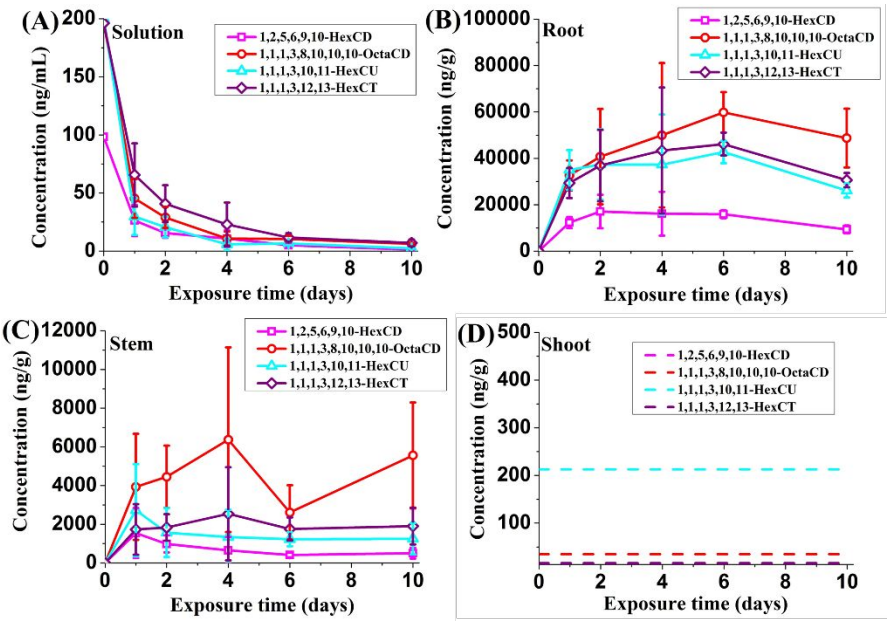


Figure S1 Schematic of the hydroponic exposure experiments and sampling. Bottles were wrapped with aluminum foil. Pumpkins and soybeans were separately exposed to parent SCCPs.



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216 **Figure S2** Concentrations of parent SCCPs in the solutions (A), roots (B), stems (C), and shoots

217 (D) when pumpkin plants were exposed to SCCPs over time. No parent SCCPs were detected

218 in the shoots (lower than the method detection limits (MDLs) as the dashed lines show).

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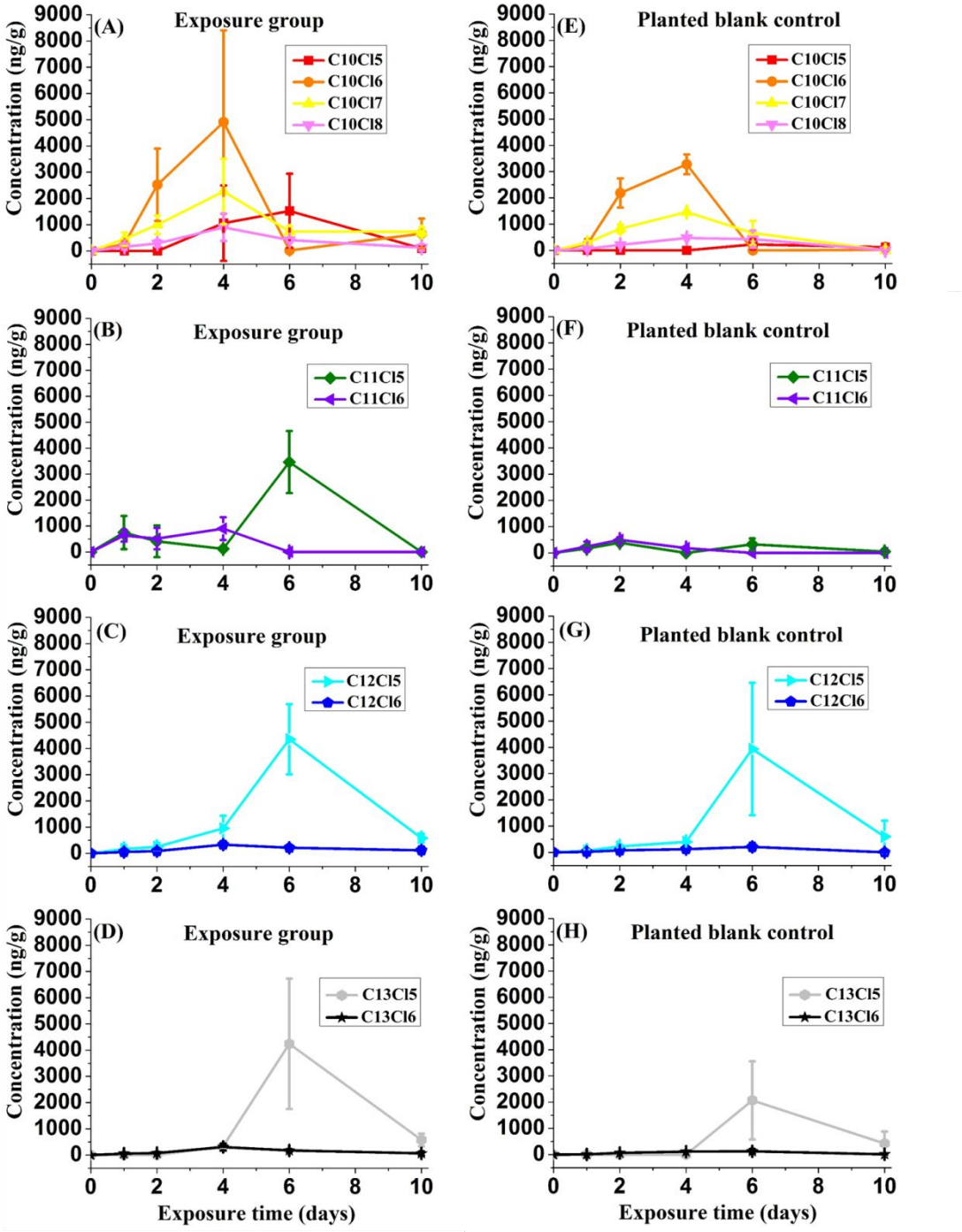

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233 **Figure S3** Concentrations of daughter SCCP congeners in exposure groups (A-D) and planted

234 blank controls (E-H) of pumpkin seedlings over time. No C_9 daughter congeners were detected

235 in plants tissues and solutions of exposure groups and planted blank controls.

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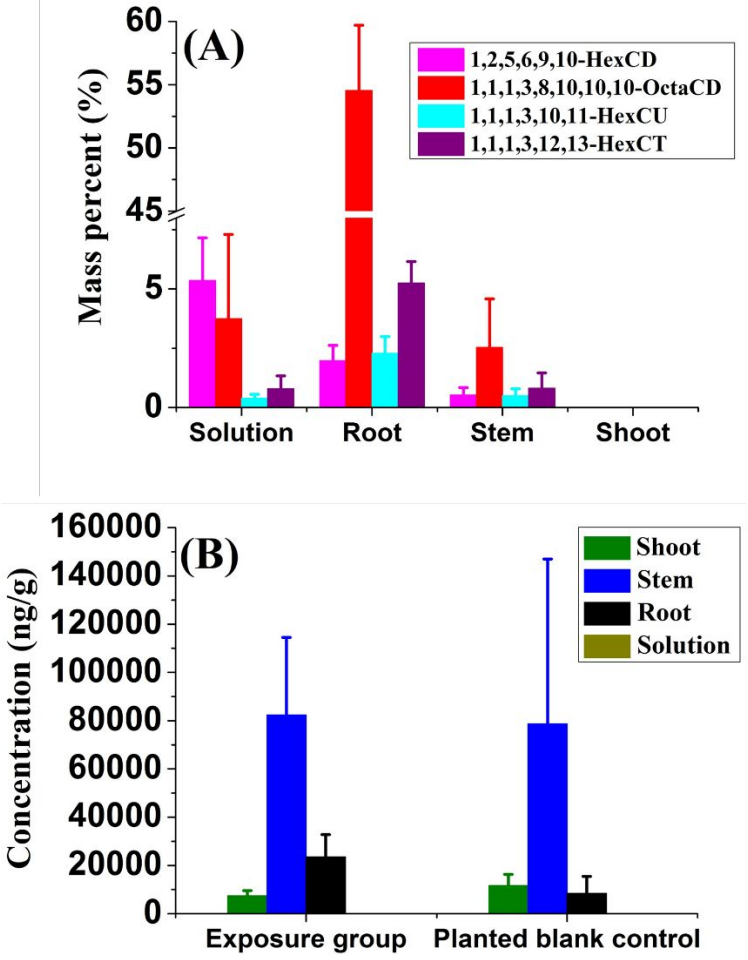

Figure S4 Mass percent of individual parent SCCPs (A) and concentrations of total daughter SCCPs (B) in different compartments of soybeans after 10 days exposure. No parent SCCPs were found in the shoots of the exposure group, and no daughter SCCPs were found in solution of the exposure group or the planted blank control.

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