

Supporting Information

Selective and fast analysis of chlorinated paraffins in presence of chlorinated mono-, di- and tri-olefins with the R-based automated spectra evaluation routine (RASER)

Marco C. Knobloch ^{*1,2}, Flurin Mathis ^{1,3}, Oscar Mendo Diaz ^{1,2}, Urs Stalder ²,
Laurent Bigler ², Susanne Kern ³, Davide Bleiner ^{1,2}, Norbert V. Heeb ¹

¹Laboratory for Advanced Analytical Technologies, Swiss Federal Institute for Materials Science and Technology Empa, Überlandstrasse 129, 8600 Dübendorf, Switzerland

²Department of Chemistry, University of Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland

³Zürich University of Applied Sciences ZHAW, Einsiedlerstrasse 31, 8820 Wädenswil, Switzerland

* Corresponding author: marco.knobloch@empa.ch, +41 58 765 44 32, ORCID: 0000-0003-0197-4053

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1. Measured and reconstructed mass spectra of plastic material M2

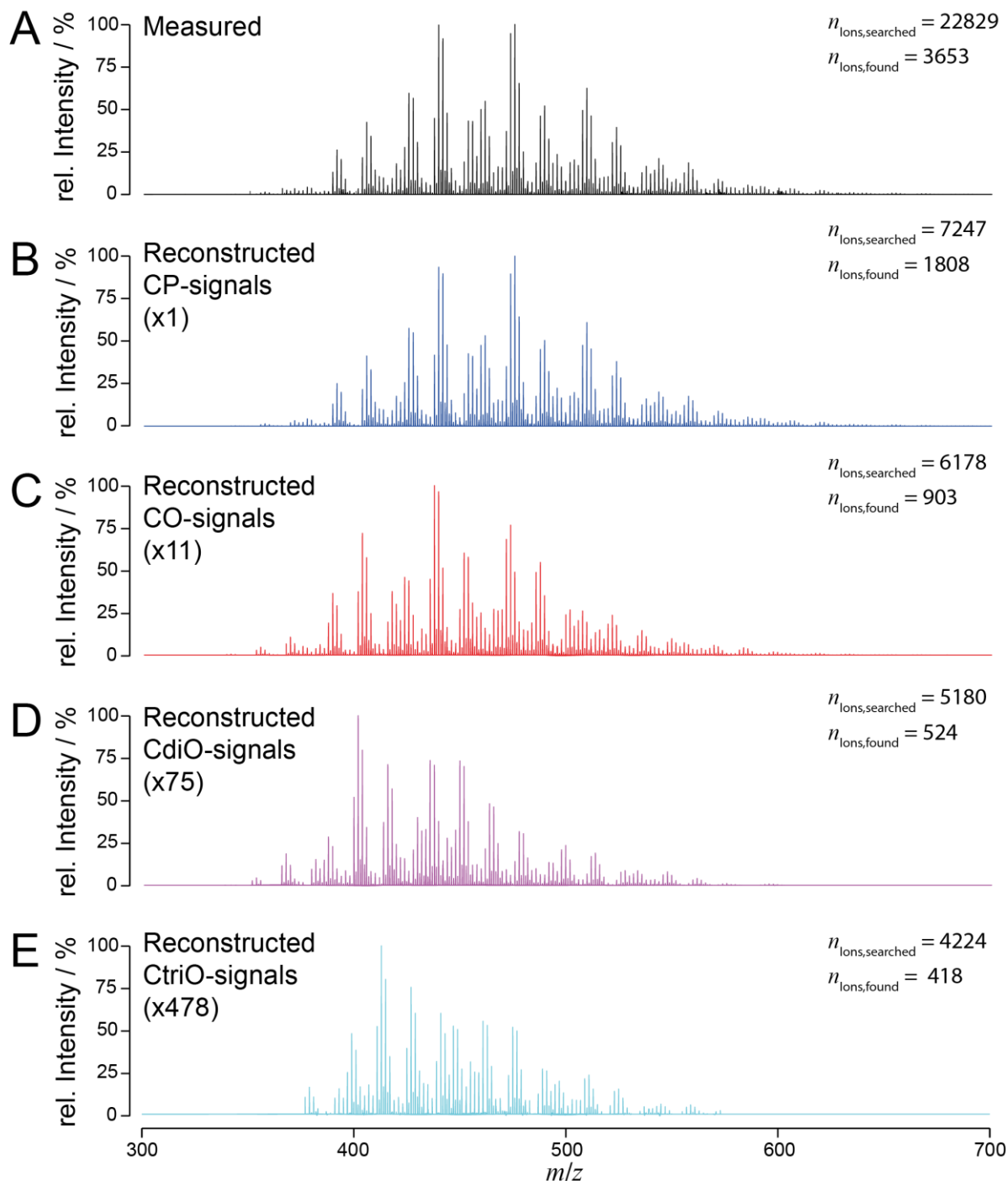


Figure S1. Measured (A) and reconstructed mass spectra (RMS) of CPs (B), COs (C), CdiOs (D) and CtriOs (E) as obtained from the extract of plastic material M1. The mass spectrum (A) was obtained by LC-APCI-Orbitrap-MS ($R \approx 140,000$). RASER was applied to extract and validate ions of specific isotope clusters of respective chloride-adduct $[M+Cl]^-$ ions of different CP-, CO-, CdiO- and CtriO-homologues. The total number of evaluated m/z values of the RMS and scaling factors in relation to the most abundant CP-ion are indicated.

2. Comparison of selected measured and simulated isotope clusters by RASER

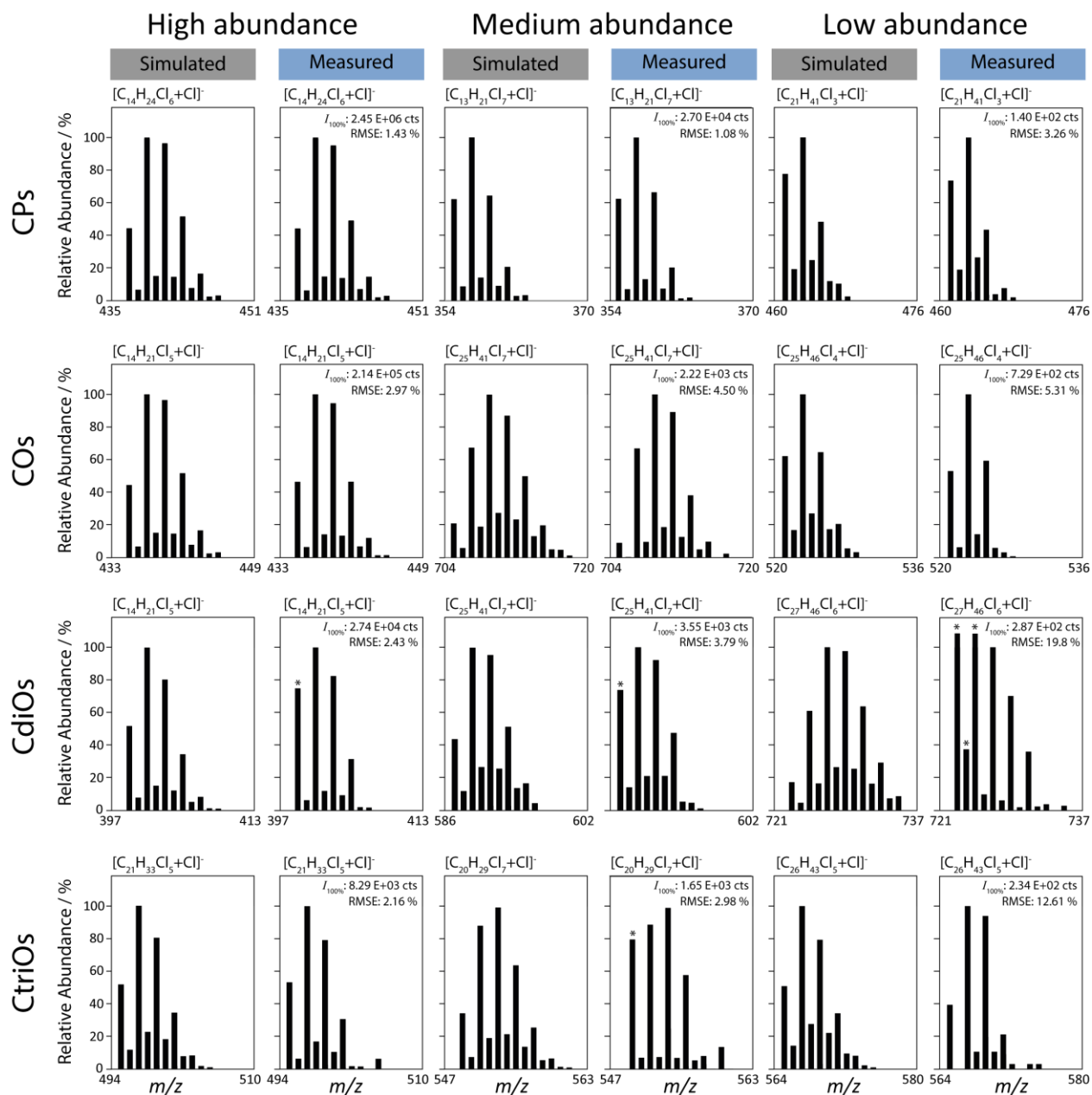


Figure S2. Measured and simulated isotope clusters of selected CP-, CO-, CdiO- and CtriO-homologues of M2 evaluated by RASER. Isotope clusters of homologues of high, medium and low abundance are displayed for each class of compounds. Respective $I_{100\%}$ signals differ by four orders of magnitude (10^2 to 10^6 cts). Deviations of the four most prominent isotopologues from the simulated and found isotope clusters are displayed as root mean square errors (RMSE). Signals not matching the isotope pattern are marked as interferences (*). Interfered signals were not used for the calculation of $I_{100\%}$ signals and RMSE.

3. 2D-representations of CP-, CO-, CdiO- and CtriO-homologue distributions

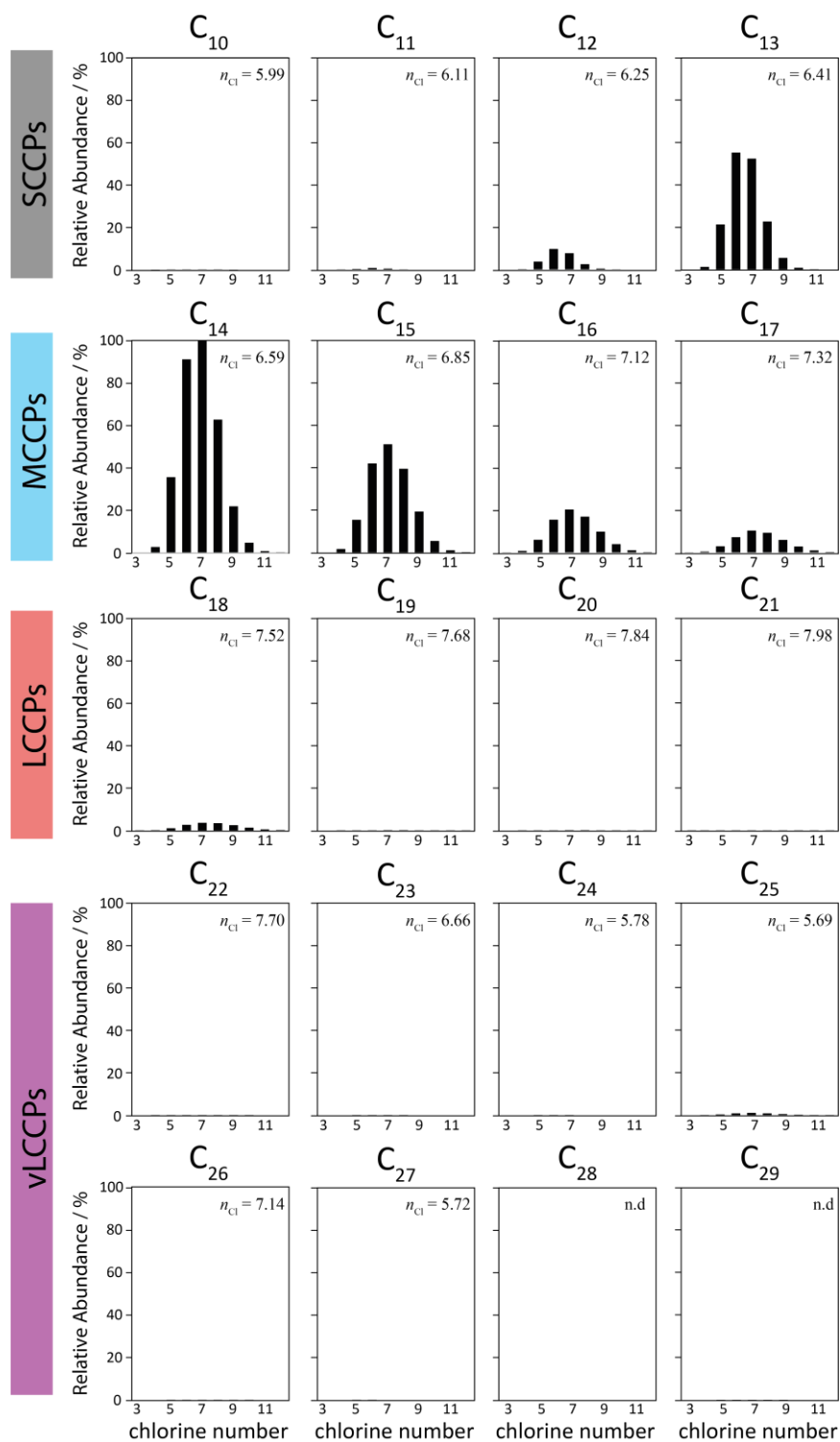


Figure S3. Relative abundances of C₁₀- to C₂₉-CP-homologues in M1. Abundances are normalized to the most abundant C₁₄Cl₇-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S1. Not detected C-homologues are indicated (n.d.).

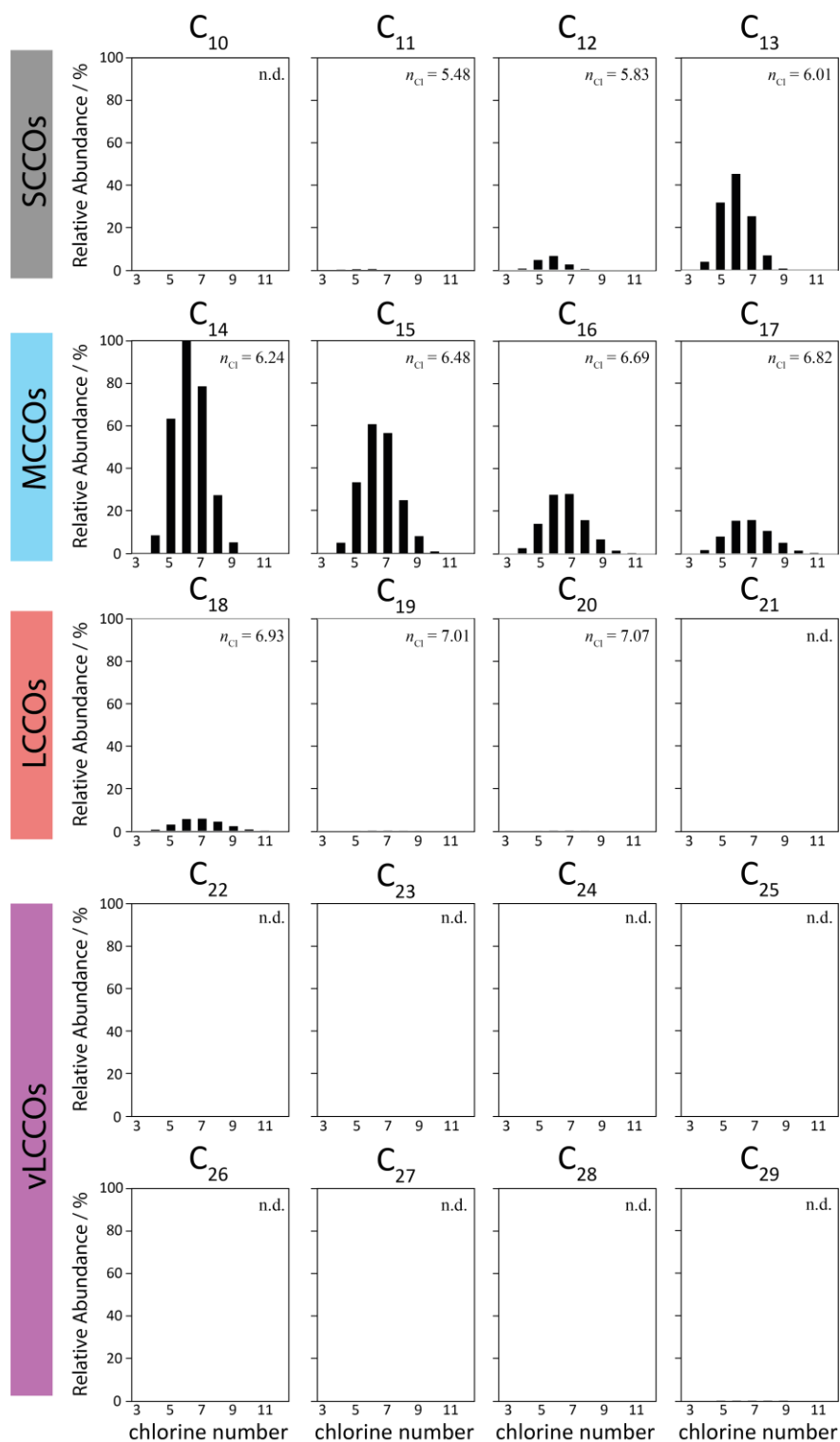


Figure S4. Relative abundances of C₁₀- to C₂₉-CO-homologues in M1. Abundances are normalized to the most abundant C₁₄Cl₆-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S2. Not detected C-homologues are indicated (n.d.).

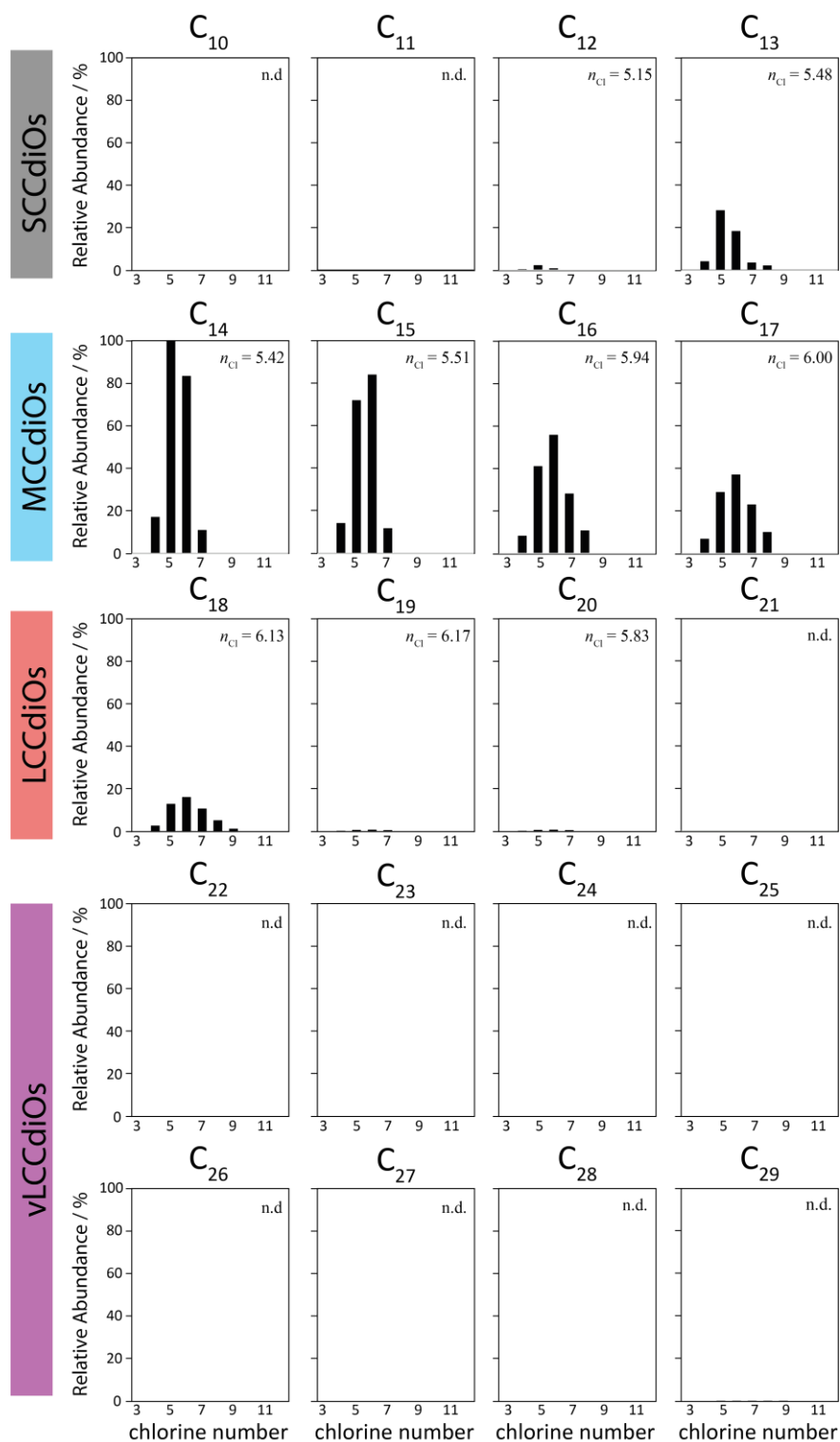


Figure S5. Relative abundances of C₁₀- to C₂₉-CdiO-homologues in M1. Abundances are normalized to the most abundant C₁₄Cl₅-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S3. Not detected C-homologues are indicated (n.d.).

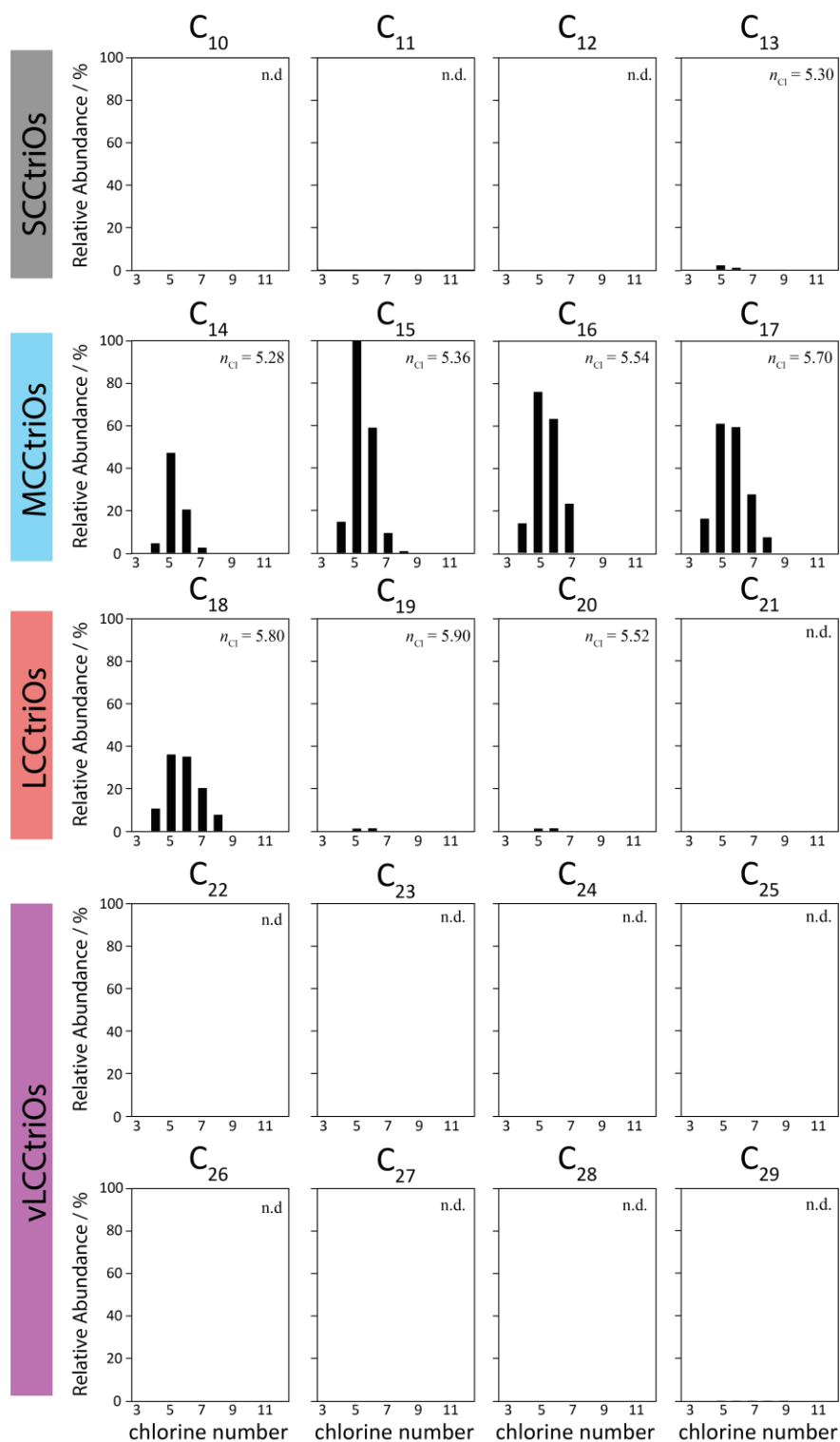


Figure S6. Relative abundances of C₁₀- to C₂₉-CtriO-homologues in M1. Abundances are normalized to the most abundant C₁₅Cl₅-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S4. Not detected C-homologues are indicated (n.d.).

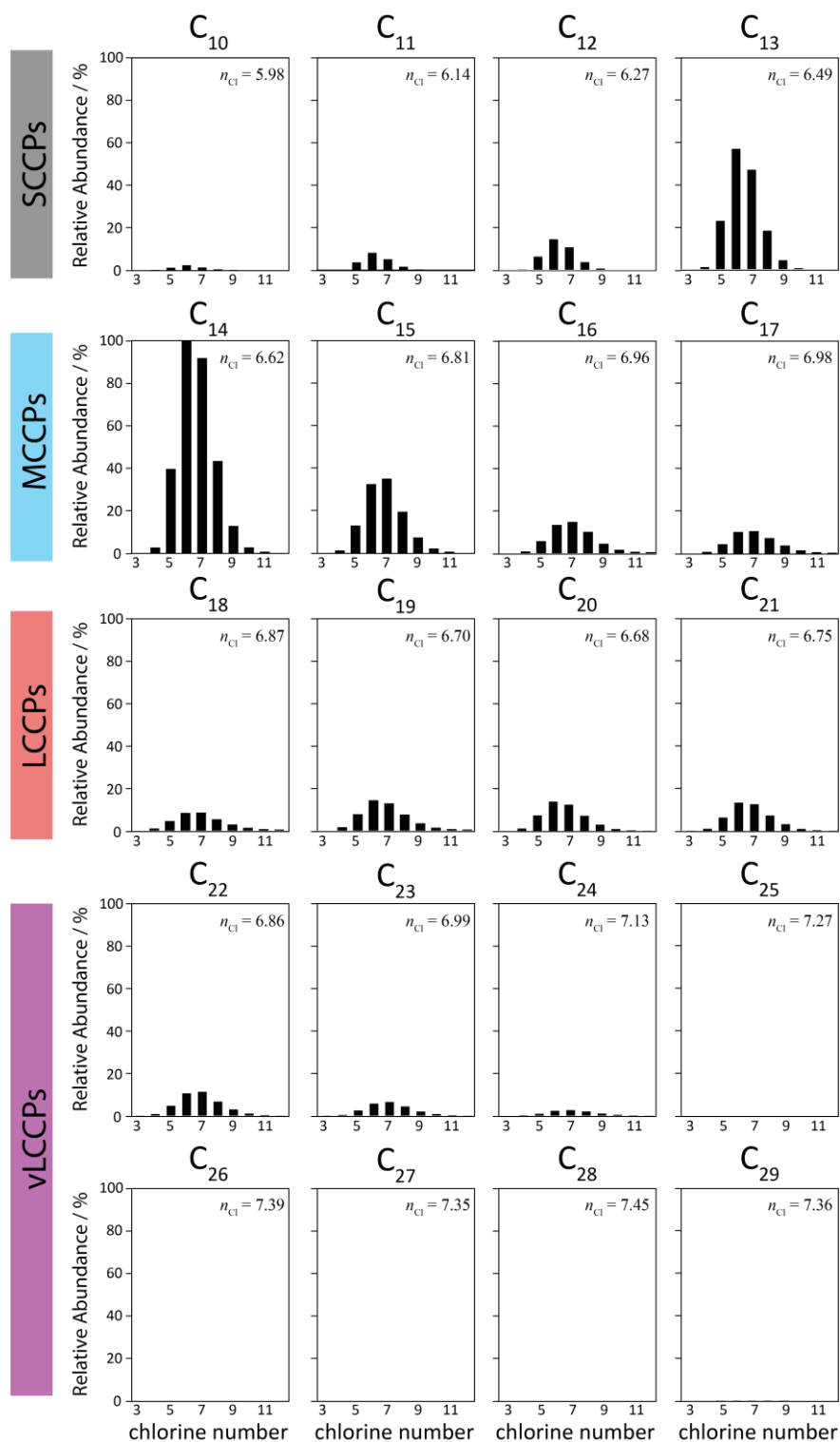


Figure S7. Relative abundances of C₁₀- to C₂₉-CP-homologues in M2. Abundances are normalized to the most abundant C₁₄Cl₆-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S5. Not detected C-homologues are indicated (n.d.).

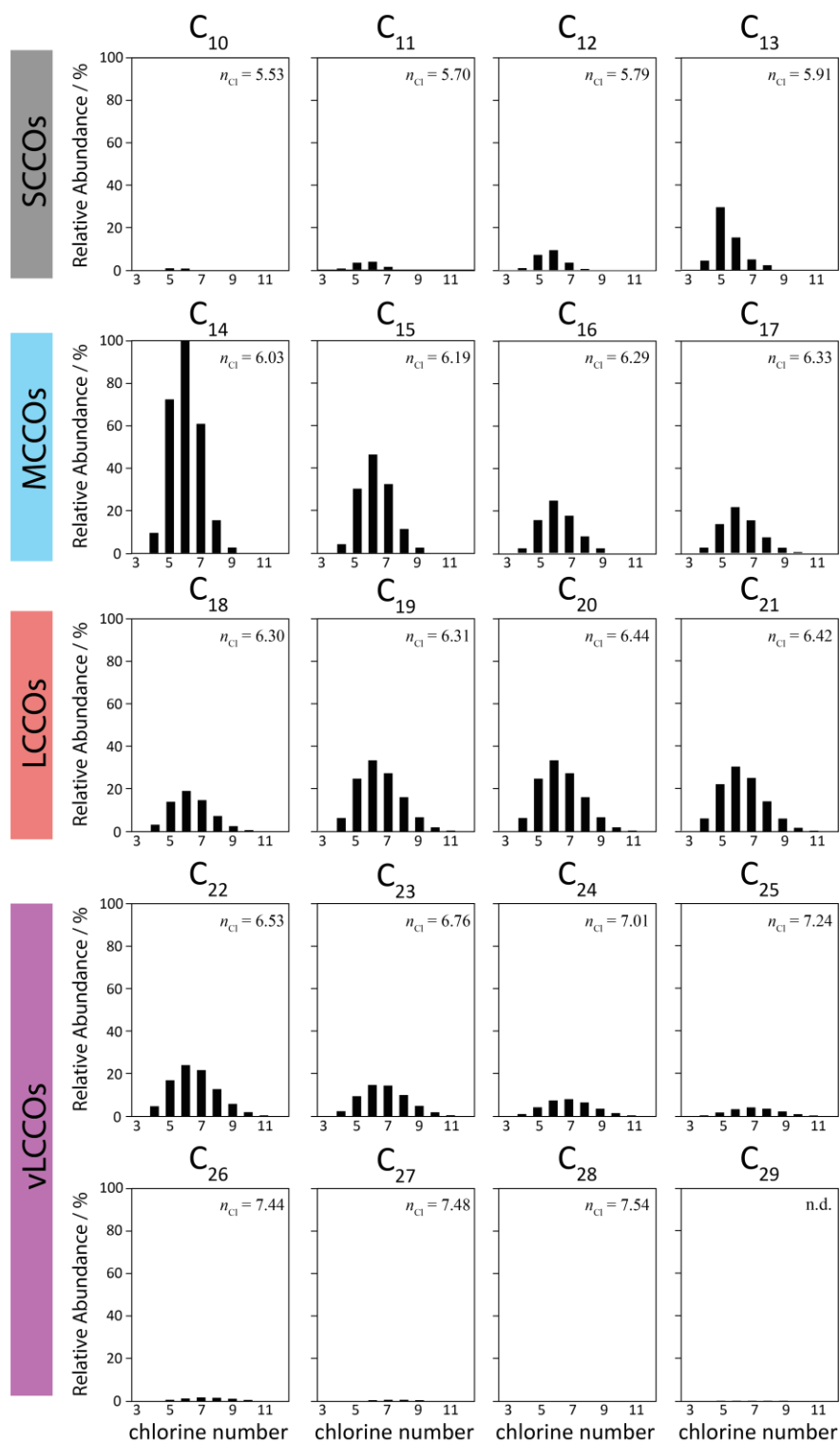


Figure S8. Relative abundances of C₁₀- to C₂₉-CO-homologues in M2. Abundances are normalized to the most abundant C₁₄Cl₆-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S6. Not detected C-homologues are indicated (n.d.).

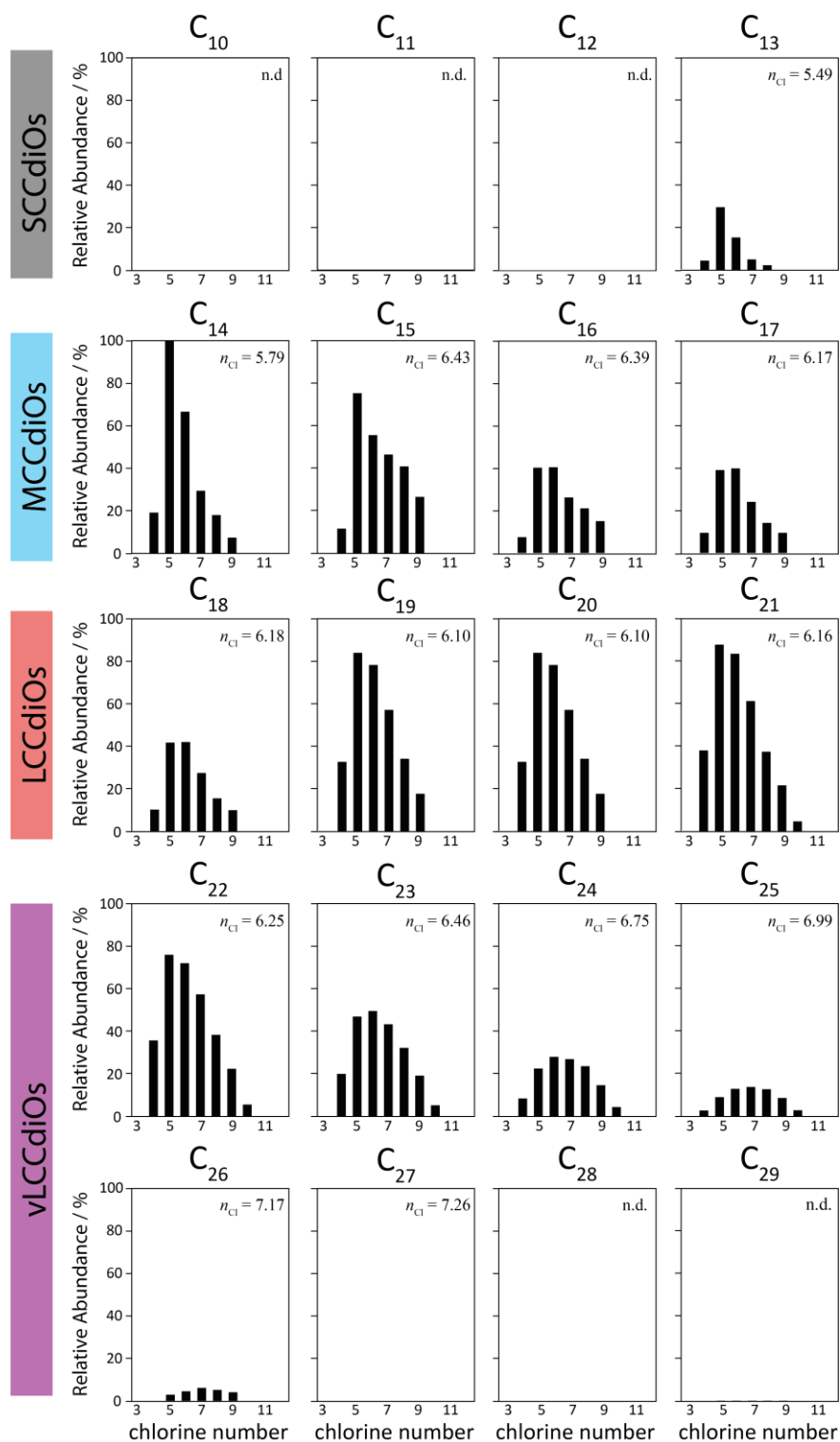


Figure S9. Relative abundances of C₁₀- to C₂₉-CdiO-homologues in M2. Abundances are normalized to the most abundant C₁₄Cl₅-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S7. Not detected C-homologues are indicated (n.d.).

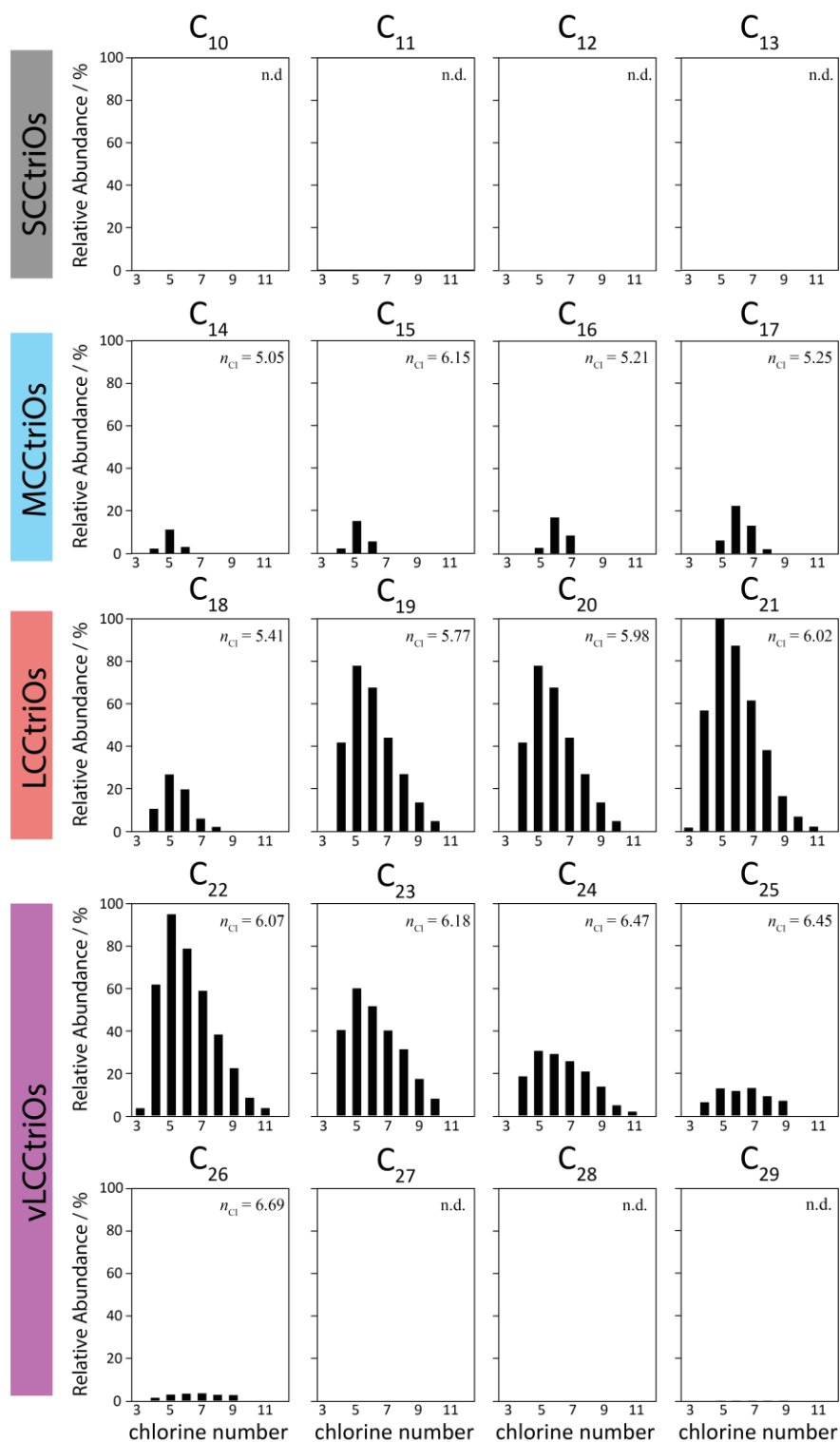


Figure S9. Relative abundances of C₁₀- to C₂₉-CtriO-homologues in M2. Abundances are normalized to the most abundant C₂₁Cl₅-homologue (100 %) and chlorine numbers (n_{Cl}) are indicated. Values of homologues not visible but still detectable are given in Table S8. Not detected C-homologues are indicated (n.d.).

4. CO proportion in relation to respective CP-homologues

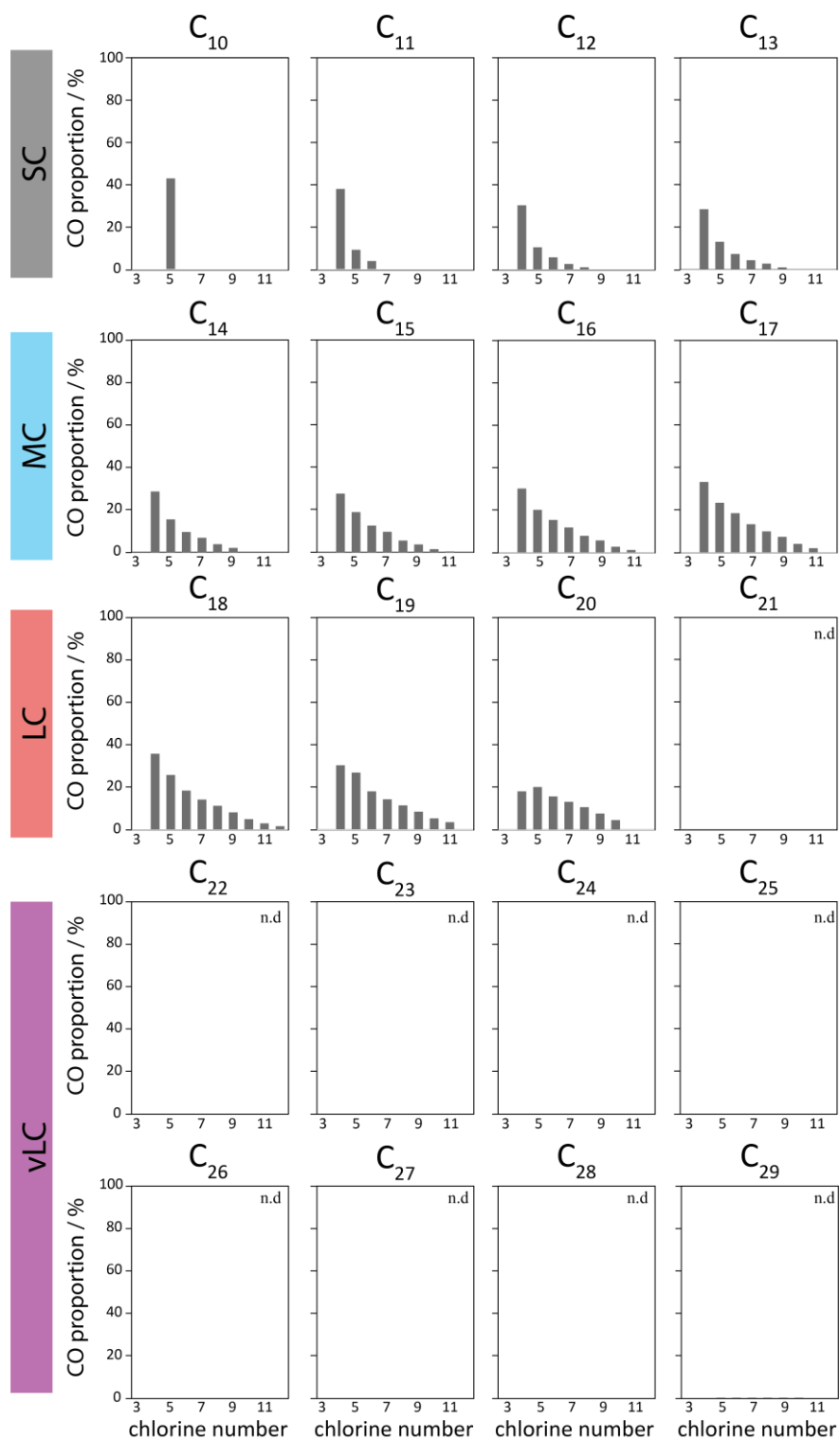


Figure S11. CO proportions relative to CPs of C₁₀- to C₂₉-homologues in material M1. CO-proportions were calculated based on the *I*_{100%}-signals of respective CPs and COs (Tables S1 and S2). Not detected C-homologues are indicated (n.d.).

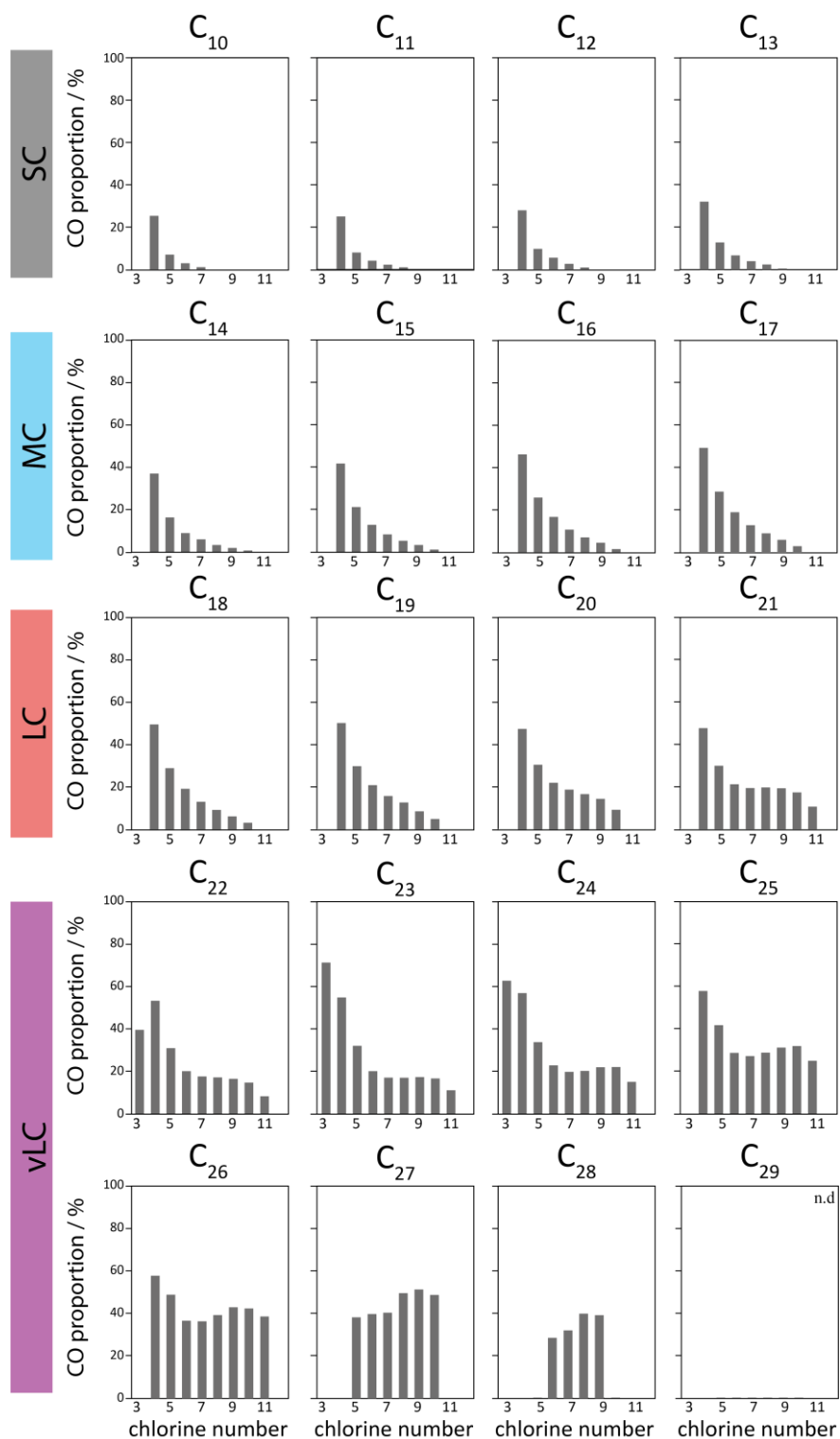


Figure S11. CO proportions relative to CPs of C₁₀- to C₂₉-homologues in material M2. CO-proportions were calculated based on the *I*_{100%}-signals of respective CPs and COs (Tables S5 and S6). Not detected C-homologues are indicated (n.d.).

5. Normalized $I_{100\%}$ -signals evaluated by RASER from Orbitrap-mass spectra of plastic material M1 and M2

Table S1. Normalized CP-signals ($I_{100\%}$) of plastic material M1. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{14}Cl_7$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue:		$C_{14}Cl_7$		$I_{100\%} / \text{cts}$ 7.57E+06		n_C 14.39		n_{Cl} 6.94		n_H 23.84						
$p_{VSC} / \%$ <1		$p_{SC} / \%$ 23		$p_{MC} / \%$ 75		$p_{LC} / \%$ 2		$p_{VLC} / \%$ <1								
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	<0.01	0.01	<0.01	-	-	-	-	-	-	-	-	-	-	C_9 5.99
C_{10}	-	-	0.02	0.06	0.03	<0.01	-	-	-	-	-	-	-	-	-	C_{10} 6.11
C_{11}	-	<0.01	0.24	0.66	0.42	0.09	-	-	-	-	-	-	-	-	-	C_{11} 6.25
C_{12}	-	0.13	3.69	9.66	7.63	2.46	0.39	<0.01	-	-	-	-	-	-	-	C_{12} 6.41
C_{13}	-	1.14	21.34	55.48	52.64	22.72	5.40	0.79	0.02	-	-	-	-	-	-	C_{13} 6.59
C_{14}	-	2.58	35.51	91.09	100.00	62.63	21.75	4.53	0.59	0.03	-	-	-	-	-	C_{14} 6.85
C_{15}	-	1.58	15.37	41.96	50.99	39.45	19.24	5.41	1.00	0.10	-	-	-	-	-	C_{15} 7.12
C_{16}	<0.01	0.70	5.95	15.38	20.27	16.86	9.76	3.86	0.99	0.16	0.01	-	-	-	-	C_{16} 7.32
C_{17}	<0.01	0.40	2.94	7.24	10.34	9.32	5.96	2.84	0.99	0.23	0.03	-	-	-	-	C_{17} 7.52
C_{18}	<0.01	0.15	1.01	2.67	3.58	3.43	2.47	1.30	0.55	0.18	0.04	-	-	-	-	C_{18} 7.68
C_{19}	-	0.04	0.22	0.61	0.84	0.78	0.60	0.36	0.18	0.08	0.02	-	-	-	-	C_{19} 7.84
C_{20}	-	0.01	0.04	0.09	0.13	0.13	0.10	0.06	0.04	0.02	0.01	-	-	-	-	C_{20} 7.98
C_{21}	-	<0.01	0.01	0.02	0.02	0.02	0.02	0.01	0.01	<0.01	-	-	-	-	-	C_{21} 7.70
C_{22}	-	<0.01	0.01	0.01	0.01	0.01	0.01	<0.01	-	-	-	-	-	-	-	C_{22} 6.66
C_{23}	-	-	0.01	0.01	<0.01	<0.01	-	-	-	-	-	-	-	-	-	C_{23} 5.78
C_{24}	-	-	0.01	0.01	<0.01	-	-	-	-	-	-	-	-	-	-	C_{24} 5.69
C_{25}	-	-	0.01	0.01	<0.01	-	-	-	-	-	-	-	-	-	-	C_{25} 5.98
C_{26}	-	-	<0.01	0.01	0.01	0.01	<0.01	<0.01	-	-	-	-	-	-	-	C_{26} 7.14
C_{27}	-	-	<0.01	<0.01	-	-	-	-	-	-	-	-	-	-	-	C_{27} 5.72
C_{28}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	C_{28} -
C_{29}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	C_{29} -
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	C_{30} -
n_C	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	
	17.20	14.54	14.14	14.14	14.30	14.58	14.98	15.48	16.14	16.93	17.83	-	-	-	-	

Table S2. Normalized CO-signals ($I_{100\%}$) of plastic material M1. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{14}Cl_6$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue:		$C_{14}Cl_6$	$I_{100\%}$ / cts	n_C	n_{Cl}	n_H										
			6.58E+05	14.68	6.38	22.98										
	p_{VSC} / %	n.d.	p_{SC} / %	16	p_{MC} / %	80	p_{LC} / %	4	p_{VLC} / %	n.d.						
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{10}	-	-	0.09	-	-	-	-	-	-	-	-	-	-	-	-	5.00
C_{11}	-	0.02	0.25	0.29	-	-	-	-	-	-	-	-	-	-	-	5.48
C_{12}	-	0.44	4.47	6.44	2.36	0.31	-	-	-	-	-	-	-	-	-	5.83
C_{13}	-	3.71	31.79	45.41	25.30	6.73	0.48	-	-	-	-	-	-	-	-	6.01
C_{14}	-	8.51	63.43	100.00	78.70	27.43	5.19	-	-	-	-	-	-	-	-	6.24
C_{15}	-	5.04	33.48	60.86	56.72	25.05	8.13	0.91	0.04	-	-	-	-	-	-	6.48
C_{16}	-	2.46	13.95	27.58	27.98	15.67	6.58	1.28	0.16	-	-	-	-	-	-	6.69
C_{17}	-	1.52	7.93	15.41	15.76	10.61	4.99	1.30	0.22	-	-	-	-	-	-	6.82
C_{18}	-	0.62	2.99	5.62	5.77	4.37	2.26	0.72	0.18	0.03	-	-	-	-	-	6.93
C_{19}	-	0.14	0.69	1.25	1.36	1.01	0.57	0.21	0.07	-	-	-	-	-	-	7.01
C_{20}	-	0.01	0.09	0.17	0.20	0.16	0.09	0.03	-	-	-	-	-	-	-	7.07
C_{21}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{22}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{23}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{24}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{25}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{26}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{27}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{28}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{29}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	
n_C	-	14.58	14.37	14.51	14.75	15.14	15.70	16.58	17.11	18.00	-	-	-	-	-	

Table S3. Normalized CdiO-signals ($I_{100\%}$) of plastic material M1. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{14}Cl_5$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue:		$C_{14}Cl_5$	$I_{100\%} / \text{cts}$	n_C	n_{Cl}	n_H										
			8.61E+04	15.30	5.68	22.91										
$p_{VSC} / \%$		n.d.														
$p_{SC} / \%$		8														
$p_{MC} / \%$		84														
$p_{LC} / \%$		8														
$p_{VLC} / \%$		n.d.														
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{10}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{11}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{12}	-	0.18	2.08	0.59	-	-	-	-	-	-	-	-	-	-	-	5.15
C_{13}	-	3.97	28.20	18.28	3.35	1.94	-	-	-	-	-	-	-	-	-	5.48
C_{14}	-	16.90	100.00	83.31	10.74	-	-	-	-	-	-	-	-	-	-	5.42
C_{15}	-	14.03	71.91	83.96	11.60	-	-	-	-	-	-	-	-	-	-	5.51
C_{16}	-	8.05	40.85	55.61	27.92	10.57	-	-	-	-	-	-	-	-	-	5.94
C_{17}	-	6.63	28.71	37.03	22.83	9.82	-	-	-	-	-	-	-	-	-	6.00
C_{18}	-	2.54	12.74	16.00	10.56	5.05	1.07	-	-	-	-	-	-	-	-	6.13
C_{19}	-	0.94	2.76	4.01	4.21	1.36	-	-	-	-	-	-	-	-	-	6.17
C_{20}	-	0.07	0.51	0.58	0.39	-	-	-	-	-	-	-	-	-	-	5.83
C_{21}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{22}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{23}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{24}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{25}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{26}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{27}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{28}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{29}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
n_C	-	15.14	14.96	15.25	16.16	16.63	18.00	-	-	-	-	-	-	-	-	-

Table S4. Normalized CtriO-signals ($I_{100\%}$) of plastic material M1. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{15}Cl_5$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue: $C_{15}Cl_5$																
		$I_{100\%} / \text{cts}$		n_C		n_{Cl}		n_H								
		1.22E+04		16.17		5.56		22.79								
		$p_{VSC} / \%$		$p_{SC} / \%$		$p_{MC} / \%$		$p_{LC} / \%$		$p_{VLC} / \%$						
		n.d.		<1		82		18		n.d.						
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{10}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{11}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{12}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{13}	-	-	2.02	0.87	-	-	-	-	-	-	-	-	-	-	-	5.30
C_{14}	-	4.47	47.20	20.44	2.47	-	-	-	-	-	-	-	-	-	-	5.28
C_{15}	-	14.68	100.00	59.12	9.37	0.82	-	-	-	-	-	-	-	-	-	5.36
C_{16}	-	13.94	76.01	63.24	23.19	-	-	-	-	-	-	-	-	-	-	5.54
C_{17}	-	16.15	61.21	59.60	27.68	7.33	-	-	-	-	-	-	-	-	-	5.70
C_{18}	-	9.44	32.26	31.36	18.12	6.81	-	-	-	-	-	-	-	-	-	5.80
C_{19}	-	2.65	9.78	10.20	6.23	2.80	-	-	-	-	-	-	-	-	-	5.90
C_{20}	-	-	0.98	1.07	-	-	-	-	-	-	-	-	-	-	-	5.52
C_{21}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{22}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{23}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{24}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{25}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{26}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{27}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{28}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{29}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
n_C	-	16.32	15.87	16.22	16.78	17.61	-	-	-	-	-	-	-	-	-	-

Table S5. Normalized CP-signals ($I_{100\%}$) of plastic material M2. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{14}Cl_6$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue:		$C_{14}Cl_6$	$I_{100\%}$ / cts	n_C	n_{Cl}	n_H										
			2.45E+06	15.67	6.68	26.65										
p_{VSC} / %		<1														
p_{SC} / %		23														
p_{MC} / %		52														
p_{LC} / %		17														
p_{VLC} / %		8														
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	0.09	0.21	0.08	-	-	-	-	-	-	-	-	-	-	5.98
C_{10}	-	0.03	1.07	2.25	1.21	0.29	0.02	-	-	-	-	-	-	-	-	6.14
C_{11}	-	0.14	3.57	8.04	5.09	1.51	0.24	-	-	-	-	-	-	-	-	6.27
C_{12}	-	0.27	6.32	14.47	10.72	3.67	0.68	-	-	-	-	-	-	-	-	6.37
C_{13}	-	1.11	23.00	57.03	47.16	18.34	4.34	0.61	0.03	-	-	-	-	-	-	6.49
C_{14}	-	2.24	39.32	100.00	91.60	43.03	12.39	2.26	0.26	-	-	-	-	-	-	6.62
C_{15}	-	0.86	12.62	32.18	34.74	19.11	6.97	1.79	0.29	-	-	-	-	-	-	6.81
C_{16}	-	0.41	5.24	12.90	14.33	9.66	4.04	1.19	0.27	0.02	-	-	-	-	-	6.96
C_{17}	-	0.43	4.08	9.83	10.23	6.94	3.42	1.15	0.31	0.05	-	-	-	-	-	6.98
C_{18}	-	0.54	4.06	7.92	8.09	4.92	2.43	0.91	0.27	0.05	-	-	-	-	-	6.87
C_{19}	-	0.81	5.24	9.35	8.64	5.01	2.12	0.77	0.21	0.04	-	-	-	-	-	6.70
C_{20}	-	1.16	7.31	13.85	12.39	7.15	2.99	0.93	0.25	0.04	-	-	-	-	-	6.68
C_{21}	0.01	1.00	6.30	13.32	12.58	7.25	3.20	0.97	0.26	0.03	-	-	-	-	-	6.75
C_{22}	0.01	0.73	4.62	10.48	11.17	6.56	2.91	0.96	0.26	0.04	-	-	-	-	-	6.86
C_{23}	0.01	0.35	2.42	5.63	6.40	4.31	1.92	0.70	0.20	0.04	-	-	-	-	-	6.99
C_{24}	-	0.14	0.86	2.24	2.57	1.94	0.96	0.38	0.11	0.02	-	-	-	-	-	7.13
C_{25}	-	0.05	0.30	0.77	0.97	0.77	0.44	0.18	0.06	0.01	-	-	-	-	-	7.27
C_{26}	-	0.01	0.10	0.25	0.34	0.28	0.18	0.07	0.03	-	-	-	-	-	-	7.39
C_{27}	-	-	0.03	0.08	0.11	0.09	0.06	0.02	-	-	-	-	-	-	-	7.35
C_{28}	-	-	0.01	0.03	0.04	0.04	0.02	0.01	-	-	-	-	-	-	-	7.45
C_{29}	-	-	-	0.01	0.02	0.01	0.01	-	-	-	-	-	-	-	-	7.36
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
n_C	21.71	17.11	15.48	15.30	15.55	16.06	16.80	17.72	18.69	20.05	-	-	-	-	-	

Table S6. Normalized CO-signals ($I_{100\%}$) of plastic material M2. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{14}Cl_6$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue:		$C_{14}Cl_6$	$I_{100\%}$ / cts	n_C	n_{Cl}	n_H										
			2.15E+05	17.41	6.29	28.54										
	$p_{VSC} / \%$	n.d.	$p_{SC} / \%$	11	$p_{MC} / \%$	43	$p_{LC} / \%$	30	$p_{VLC} / \%$	16						
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{10}	-	0.09	0.86	0.78	0.16	-	-	-	-	-	-	-	-	-	-	5.53
C_{11}	-	0.41	3.14	3.59	1.18	0.13	-	-	-	-	-	-	-	-	-	5.70
C_{12}	-	0.87	7.10	9.34	3.42	0.46	-	-	-	-	-	-	-	-	-	5.79
C_{13}	-	4.06	33.69	43.43	21.30	5.03	0.24	-	-	-	-	-	-	-	-	5.91
C_{14}	-	9.43	72.37	100.00	60.87	15.39	2.51	0.15	-	-	-	-	-	-	-	6.03
C_{15}	-	4.08	30.29	46.38	32.41	11.25	2.49	0.20	-	-	-	-	-	-	-	6.19
C_{16}	-	2.13	15.45	24.63	17.48	7.76	2.10	0.21	-	-	-	-	-	-	-	6.29
C_{17}	-	2.44	13.53	21.60	15.35	7.34	2.43	0.42	-	-	-	-	-	-	-	6.33
C_{18}	-	3.10	13.91	19.02	14.67	7.18	2.39	0.51	-	-	-	-	-	-	-	6.30
C_{19}	-	4.43	18.37	23.65	18.64	9.59	3.52	0.82	-	-	-	-	-	-	-	6.31
C_{20}	-	6.27	24.82	33.42	27.39	16.06	6.60	1.85	0.31	-	-	-	-	-	-	6.44
C_{21}	0.07	6.06	22.19	30.50	25.13	14.14	6.00	1.61	0.24	-	-	-	-	-	-	6.42
C_{22}	0.09	4.58	16.88	23.98	21.64	12.67	5.73	1.82	0.32	-	-	-	-	-	-	6.53
C_{23}	0.04	2.26	9.31	14.60	14.37	9.91	4.79	1.75	0.34	-	-	-	-	-	-	6.76
C_{24}	-	0.92	4.08	7.32	7.97	6.39	3.42	1.39	0.32	-	-	-	-	-	-	7.01
C_{25}	-	0.34	1.65	3.22	4.02	3.46	2.15	0.88	0.26	-	-	-	-	-	-	7.24
C_{26}	-	0.09	0.51	1.16	1.63	1.45	1.04	0.46	0.10	-	-	-	-	-	-	7.44
C_{27}	-	-	0.13	0.35	0.51	0.51	0.33	0.12	-	-	-	-	-	-	-	7.48
C_{28}	-	-	-	0.10	0.16	0.19	0.11	-	-	-	-	-	-	-	-	7.54
C_{29}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
n_C	21.86	17.76	16.70	16.81	17.57	18.92	20.27	21.50	22.70	-	-	-	-	-	-	-

Table S7. Normalized CdiO-signals ($I_{100\%}$) of plastic material M2. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{14}Cl_5$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue:		$C_{14}Cl_5$	$I_{100\%} / \text{cts}$	n_C	n_{Cl}	n_H										
			2.74E+04	19.22	6.24	30.21										
	$p_{VSC} / \%$	n.d.	$p_{SC} / \%$	2	$p_{MC} / \%$	30	$p_{LC} / \%$	38	$p_{VLC} / \%$	29						
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{10}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{11}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{12}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{13}	-	4.42	29.63	15.35	4.98	2.27	-	-	-	-	-	-	-	-	-	5.49
C_{14}	-	19.04	100.00	66.56	29.32	17.86	7.18	-	-	-	-	-	-	-	-	5.79
C_{15}	-	11.44	75.32	55.53	46.35	40.78	26.42	-	-	-	-	-	-	-	-	6.43
C_{16}	-	7.40	40.18	40.38	26.13	21.04	15.00	-	-	-	-	-	-	-	-	6.39
C_{17}	-	9.47	39.05	39.85	24.05	14.17	9.46	-	-	-	-	-	-	-	-	6.17
C_{18}	-	10.18	41.73	42.00	27.44	15.46	9.89	-	-	-	-	-	-	-	-	6.18
C_{19}	-	19.84	55.45	53.16	38.01	21.19	11.52	-	-	-	-	-	-	-	-	6.10
C_{20}	-	32.69	84.10	78.33	57.20	34.13	17.64	-	-	-	-	-	-	-	-	6.10
C_{21}	0.81	38.06	87.91	83.61	61.37	37.47	21.59	4.61	-	-	-	-	-	-	-	6.16
C_{22}	-	35.78	76.17	72.22	57.53	38.41	22.45	5.54	-	-	-	-	-	-	-	6.25
C_{23}	-	20.06	47.03	49.68	43.41	32.29	19.18	5.23	-	-	-	-	-	-	-	6.46
C_{24}	-	8.47	22.51	28.06	26.99	23.64	14.67	4.36	-	-	-	-	-	-	-	6.75
C_{25}	-	2.75	9.04	12.96	13.86	12.81	8.68	2.85	-	-	-	-	-	-	-	6.99
C_{26}	-	0.61	2.88	4.50	6.12	5.17	4.05	0.95	-	-	-	-	-	-	-	7.17
C_{27}	-	-	0.50	1.05	1.62	1.61	0.97	-	-	-	-	-	-	-	-	7.26
C_{28}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{29}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
n_C	21.00	19.64	18.51	19.05	19.61	19.71	19.80	22.92	-	-	-	-	-	-	-	-

Table S8. Normalized CtriO-signals ($I_{100\%}$) of plastic material M2. Respective chloride-adduct ions were extracted from APCI-mass spectra by RASER. Signals were normalized to the most abundant homologue (MAH, $C_{21}Cl_5$, 100 %), which is indicated together with the respective $I_{100\%}$ intensity (cts). Homologues not detected are reported as dashes. Calculated mean chlorine numbers (n_{Cl}) and mean carbon numbers (n_C) per homologue class are also given. Proportions of very short- (p_{VSC}), short- (p_{SC}), medium- (p_{MC}), long- (p_{LC}) and very long- (p_{VLC}) chain homologues are given.

Most abundant homologue:		$C_{21}Cl_5$	$I_{100\%} / \text{cts}$	n_C	n_{Cl}	n_H										
			8.29E+03	21.16	6.01	32.32										
	$p_{VSC} / \%$	n.d.	$p_{SC} / \%$	n.d.	$p_{MC} / \%$	6	$p_{LC} / \%$	47	$p_{VLC} / \%$	47						
	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}	n_{Cl}
C_9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{10}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{11}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{12}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{13}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{14}	-	2.22	11.23	3.01	-	-	-	-	-	-	-	-	-	-	-	5.05
C_{15}	-	2.28	15.28	5.66	-	-	-	-	-	-	-	-	-	-	-	5.15
C_{16}	-	2.59	16.94	8.41	-	-	-	-	-	-	-	-	-	-	-	5.21
C_{17}	-	6.08	22.43	13.02	1.99	-	-	-	-	-	-	-	-	-	-	5.25
C_{18}	-	10.49	26.70	19.67	5.89	1.97	-	-	-	-	-	-	-	-	-	5.41
C_{19}	-	21.08	47.12	35.29	19.91	11.65	4.76	-	-	-	-	-	-	-	-	5.77
C_{20}	-	41.76	77.94	67.63	44.01	26.87	13.48	4.72	-	-	-	-	-	-	-	5.98
C_{21}	1.65	56.85	100.00	87.42	61.59	38.16	16.49	6.84	2.09	-	-	-	-	-	-	6.02
C_{22}	3.35	61.67	94.84	78.63	58.74	38.12	22.24	8.36	3.42	-	-	-	-	-	-	6.07
C_{23}	-	40.26	59.91	51.48	40.01	31.17	17.19	7.91	-	-	-	-	-	-	-	6.18
C_{24}	-	18.42	30.46	28.93	25.57	20.69	13.56	4.76	1.75	-	-	-	-	-	-	6.47
C_{25}	-	6.22	12.76	11.49	12.88	9.08	6.86	-	-	-	-	-	-	-	-	6.45
C_{26}	-	1.29	2.82	3.23	3.40	2.69	2.57	-	-	-	-	-	-	-	-	6.69
C_{27}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{28}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{29}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C_{30}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
n_C	21.67	21.17	20.56	20.96	21.64	21.87	22.18	22.04	22.19	-	-	-	-	-	-	-