Supplementary Information for

A fast gas chromatography coupled with electron capture negative ion mass spectrometry in selected ion monitoring mode screening method for short-chain and medium-chain chlorinated paraffins

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Tab. S1. Solutions of single-chain CP standards in *i*-octane used for quantification with respective chlorination degree (determined by EA) and concentration.

Chain length	Chlorine content	Concentration [ng/µL]
C_{10}-CPs	53.8%	11.0
	58.0%	9.5
	60.5%	10.2
	64.7%	13.2
C_{11}-CPs	51.2%	10.0
	56.2%	10.4
	62.6%	10.4
	68.5%	10.4
C_{12}-CPs	51.9%	10.0
	59.0%	9.9
	59.9%	9.9
	67.1%	9.6
C_{13}-CPs	50.3%	10.2
	54.4%	10.0
	59.6%	10.1
	66.4%	10.4
C_{14}-CPs	50.1%	10.1
	52.9%	10.0
	53.6%	9.8
	67.3%	10.3
C_{15}-CPs	50.9%	10.0
	53.5%	9.8
	55.0%	10.3
	68.5%	9.8
C_{16}-CPs	48.6%	9.9
	50.9%	9,5
	53.1%	10.1
	58.9%	9.7
C_{17}-CPs	50.3%	9.5
	54.9%	9.9
	61.3%	10.3

Tab. S2. Quantification (quantifier) and verification (qualifier) ions of the $[M-Cl]^-$ ions formed by the different compounds measured with the quantification method as well as their ratio (R). Repeatedly occurring nominal values are printed in bold.

Compound	*Quantifier* [*m/z*]	*Qualifier* [*m/z*]	R [%]	Compound	*Quantifier* [*m/z*]	*Qualifier* [*m/z*]	R [%]
$C_{10}H_{18}Cl_4$	243	245	96	$C_{14}H_{26}Cl_4$	299	301	96
$C_{10}H_{17}Cl_5$	279	277	78	$C_{14}H_{25}Cl_5$	335	333	78
$C_{10}H_{16}Cl_6$	**313**	**315**	64	$C_{14}H_{24}Cl_6$	369	371	64
$C_{10}H_{15}Cl_7$	**347**	**349**	80	$C_{14}H_{23}Cl_7$	403	405	80
$C_{10}H_{14}Cl_8$	381	**383**	96	$C_{14}H_{22}Cl_8$	437	439	96
$C_{10}H_{13}Cl_9$	**417**	415	89	$C_{14}H_{21}Cl_9$	473	471	89
$C_{10}H_{12}Cl_{10}$	**451**	449	78	$C_{14}H_{20}Cl_{10}$	507	505	78
$C_{10}H_{11}Cl_{11}$	**485**	**487**	87	$C_{14}H_{19}Cl_{11}$	541	543	87
$C_{10}H_{10}Cl_{12}$	**519**	**521**	98	$C_{14}H_{18}Cl_{12}$	575	577	98
$C_{11}H_{20}Cl_4$	257	259	96	$C_{14}H_{17}Cl_{13}$	611	609	92
$C_{11}H_{19}Cl_5$	293	291	78	$C_{14}H_{16}Cl_{14}$	645	643	84
$C_{11}H_{18}Cl_6$	**327**	**329**	64	$C_{15}H_{28}Cl_4$	**313**	**315**	96
$C_{11}H_{17}Cl_7$	**361**	**363**	80	$C_{15}H_{27}Cl_5$	**349**	**347**	78
$C_{11}H_{16}Cl_8$	395	**397**	96	$C_{15}H_{26}Cl_6$	**383**	385	64
$C_{11}H_{15}Cl_9$	**431**	429	89	$C_{15}H_{25}Cl_7$	**417**	419	80
$C_{11}H_{14}Cl_{10}$	**465**	463	78	$C_{15}H_{24}Cl_8$	**451**	453	96
$C_{11}H_{13}Cl_{11}$	**499**	**501**	87	$C_{15}H_{23}Cl_9$	**487**	**485**	89
$C_{11}H_{12}Cl_{12}$	537	**535**	98	$C_{15}H_{22}Cl_{10}$	**521**	**519**	78
$C_{12}H_{22}Cl_4$	271	273	96	$C_{15}H_{21}Cl_{11}$	555	557	87
$C_{12}H_{21}Cl_5$	307	305	78	$C_{15}H_{20}Cl_{12}$	589	591	98
$C_{12}H_{20}Cl_6$	**341**	**343**	64	$C_{15}H_{19}Cl_{13}$	625	623	92
$C_{12}H_{19}Cl_7$	**375**	**377**	80	$C_{15}H_{18}Cl_{14}$	659	657	84
$C_{12}H_{18}Cl_8$	409	**411**	96	$C_{16}H_{30}Cl_4$	**327**	**329**	96
$C_{12}H_{17}Cl_9$	**445**	443	89	$C_{16}H_{29}Cl_5$	**363**	**361**	78
$C_{12}H_{16}Cl_{10}$	**479**	477	78	$C_{16}H_{28}Cl_6$	**397**	399	64
$C_{12}H_{15}Cl_{11}$	**513**	**515**	87	$C_{16}H_{27}Cl_7$	**431**	433	80
$C_{12}H_{14}Cl_{12}$	**547**	**549**	98	$C_{16}H_{26}Cl_8$	**465**	467	96
$C_{12}H_{13}Cl_{13}$	**583**	581	92	$C_{16}H_{25}Cl_9$	**501**	**499**	89
$C_{13}H_{24}Cl_4$	285	287	96	$C_{16}H_{24}Cl_{10}$	**535**	533	78
$C_{13}H_{23}Cl_5$	321	319	78	$C_{16}H_{23}Cl_{11}$	569	567	68
$C_{13}H_{22}Cl_6$	355	357	64	$C_{16}H_{22}Cl_{12}$	603	605	98
$C_{13}H_{21}Cl_7$	389	391	80	$C_{16}H_{21}Cl_{13}$	639	637	92
$C_{13}H_{20}Cl_8$	423	425	96	$C_{16}H_{20}Cl_{14}$	671	673	84
$C_{13}H_{19}Cl_9$	459	457	89	$C_{17}H_{32}Cl_4$	**341**	**343**	96
$C_{13}H_{18}Cl_{10}$	493	491	78	$C_{17}H_{31}Cl_5$	**377**	**375**	78
$C_{13}H_{17}Cl_{11}$	527	529	87	$C_{17}H_{30}Cl_6$	**411**	413	64
$C_{13}H_{16}Cl_{12}$	561	563	98	$C_{17}H_{29}Cl_7$	**445**	447	80
$C_{13}H_{15}Cl_{13}$	597	595	92	$C_{17}H_{28}Cl_8$	**479**	481	96
$C_{13}H_{14}Cl_{14}$	631	629	84	$C_{17}H_{27}Cl_9$	**515**	**513**	89
				$C_{17}H_{26}Cl_{10}$	**549**	**547**	78
				$C_{17}H_{25}Cl_{11}$	**583**	585	69
				$C_{17}H_{24}Cl_{12}$	617	615	62
				$C_{17}H_{23}Cl_{13}$	651	653	62
				$C_{17}H_{22}Cl_{14}$	685	687	62

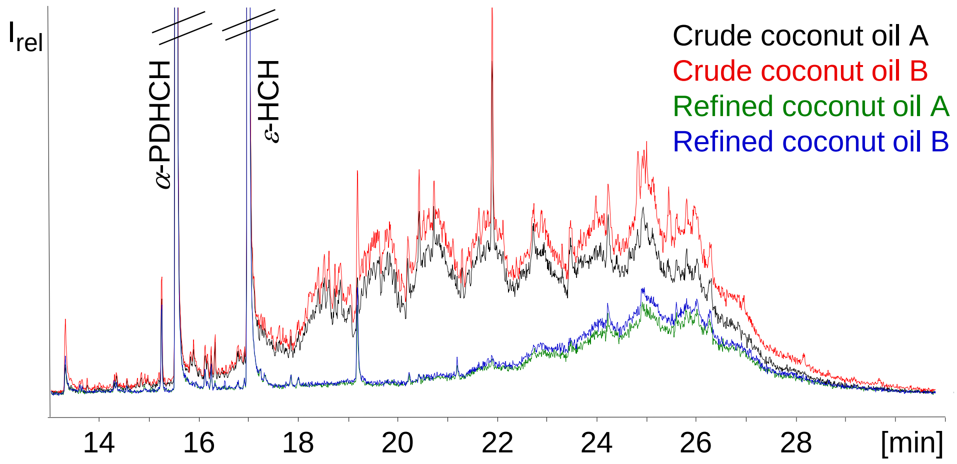

Fig. S1. GC/ECNI-MS-SIM total ion chromatograms of a crude and a refined coconut oil from the same batch analyzed in duplicate using the developed screening method.

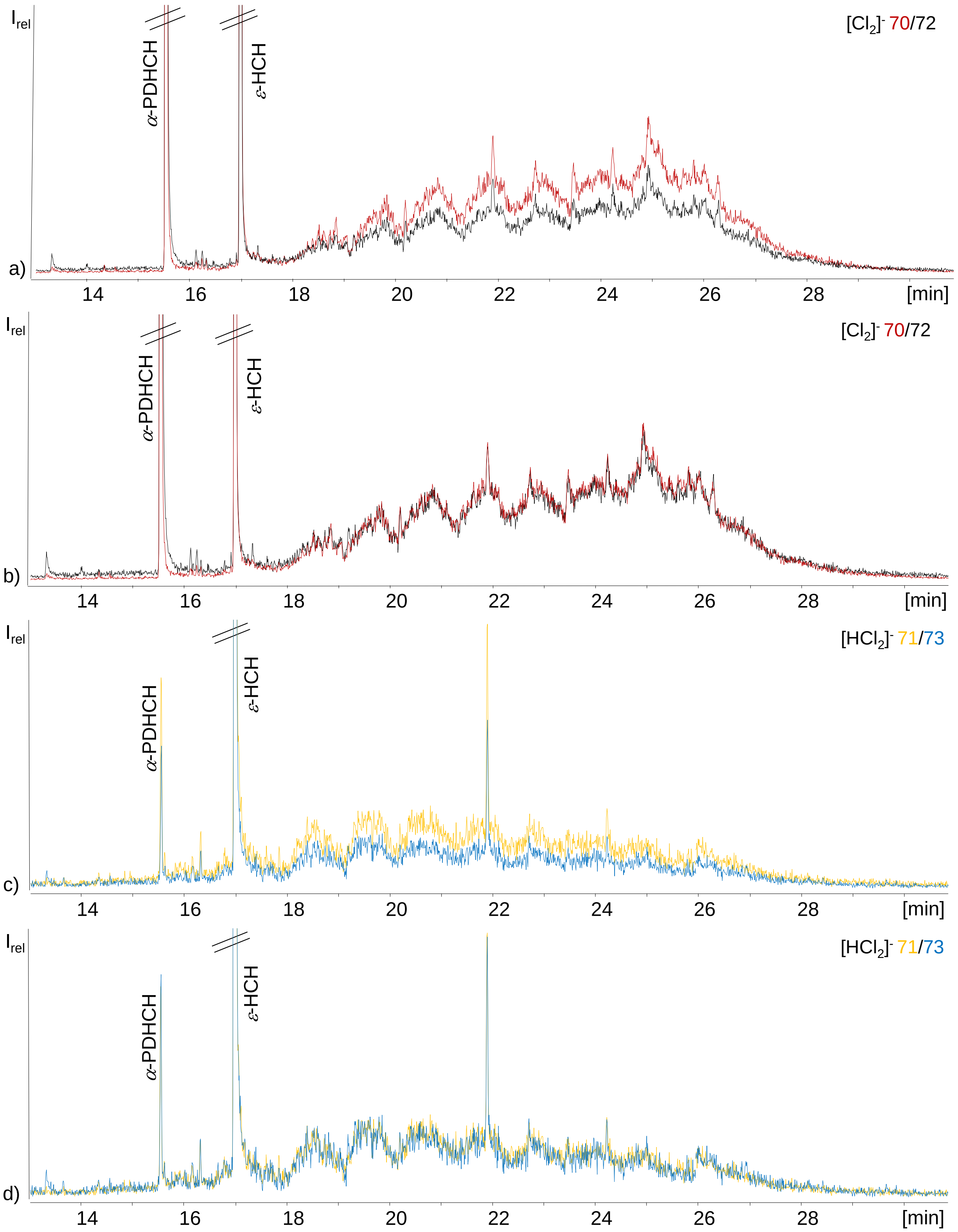

Fig. S2. Comparison of (**a**) *m/z* 70 to *m/z* 72 of Cl_2^- as well as (**c**) *m/z* 71 to *m/z* 73 of HCl_2^- as measured and after normalization of (**b**) *m/z* 70 to equal abundance of *m/z* 72 as well as (**d**) *m/z* 71 to equal abundance of *m/z* 73 formed by the crude coconut oil ($C1_C$) analyzed with the developed screening method.

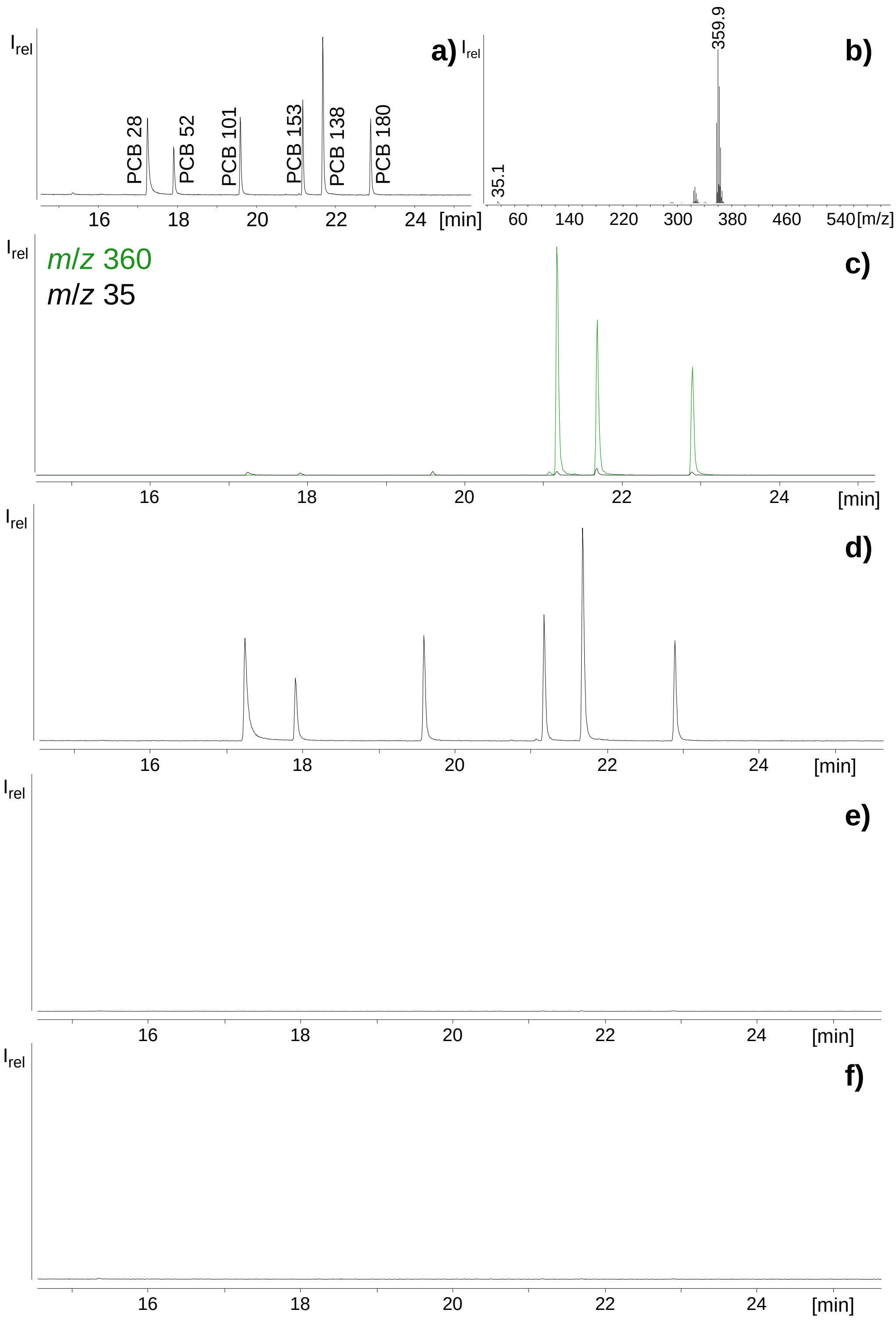

Fig. S3. (**a**) GC/ECNI-MS-SIM total ion chromatogram of the PCB mix acquired with the screening method, as well as the (**b**) mass spectrum of the PCB 153 (fourth peak in **a**) acquired with GC/ECNI-MS in full scan mode. Additionally, (**c**) ion traces *m/z* 360 and *m/z* 35 extracted from the GC/ECNI-MS full scan chromatogram and response to (**d**) *m/z* 35, (**e**) *m/z* 70, and (**f**) *m/z* 71 by the PCBs measured with the developed GC/ECNI-MS-SIM screening method.