

Table. 2 Detected SCCPs and their relative standard deviations (RSDs) of repeated injections (n = 5) for each concentration level

Compositional formula	m/z	5.8 ppm	12 ppm	29 ppm	58 ppm
C ₁₀ H ₁₇ Cl ₅	279.0	2.9	3.5	1.6	2.3
C ₁₁ H ₁₉ Cl ₅	293.0	3.5	3.2	2.0	2.7
C ₁₀ H ₁₆ Cl ₆	312.9	3.0	3.2	1.7	3.2
C ₁₁ H ₁₈ Cl ₆	327.0	4.0	4.0	1.1	3.0
C ₁₂ H ₂₀ Cl ₆	341.0	3.4	4.1	1.7	3.2
C ₁₀ H ₁₅ Cl ₇	346.9	3.5	3.8	1.9	3.1
C ₁₁ H ₁₇ Cl ₇	360.9	3.8	4.2	2.1	3.3
C ₁₂ H ₁₉ Cl ₇	374.9	3.7	4.6	2.5	2.7
C ₁₂ H ₁₈ Cl ₈	408.9	3.3	5.3	2.2	2.8

Table. 3 Method quantification limits (MQL) of the detected SCCPs

Compositional formula	MQL- Σ SCCPs (ppm) ¹	MQL-individual (ppm) ²
C ₁₀ H ₁₇ Cl ₅	1.67	0.075
C ₁₁ H ₁₉ Cl ₅	2.01	0.35
C ₁₀ H ₁₆ Cl ₆	1.71	0.053
C ₁₁ H ₁₈ Cl ₆	2.34	0.19
C ₁₂ H ₂₀ Cl ₆	2.00	0.17
C ₁₀ H ₁₅ Cl ₇	2.01	0.027
C ₁₁ H ₁₇ Cl ₇	2.23	0.14
C ₁₂ H ₁₉ Cl ₇	2.15	0.22
C ₁₂ H ₁₈ Cl ₈	1.90	0.085

¹ Based on the total SCCP conversion of the technical mixture (58%)

² Based on the analytical value of the individual m/z of SCCPs (analyzed by GC–Orbitrap–MS)

Table. 4 Comparisons of method quantification limits (MQL) with other published methods (ppb)

	This study	GC-HRMS ¹	GC-NCI-QToFMS ¹	GC-Orbitrap-MS ¹
MQL (ppb)	27-350	0.50-58	2.5-40	0.10–6.7
Target SCCPs (Individual)	Individual SCCPs (C10-13, C15-9)	C10-13, C15-9	C10-13, C15-9	C10-13, C15-9
References		3	6	7
	This study	GC-APCI-QToFMS ¹	GC-NCI-QToFMS ¹	LC-Orbitrap-MS ¹
MQL (ppb)	1700	330-3300	79-270	13-90
Target SCCPs (Total)	Total SCCPs	49, 60, 70%Cl	52, 56, 63%Cl	52, 56, 63%Cl
References		4	6	8

¹ Based on 3.3 times the instrumental detection limit