Supplemental Information for:

Comparison of different fast gas chromatography - mass spectrometry techniques (Cold EI, MS/MS, and HRMS) for the analysis of pyrethroid insecticide residues in food

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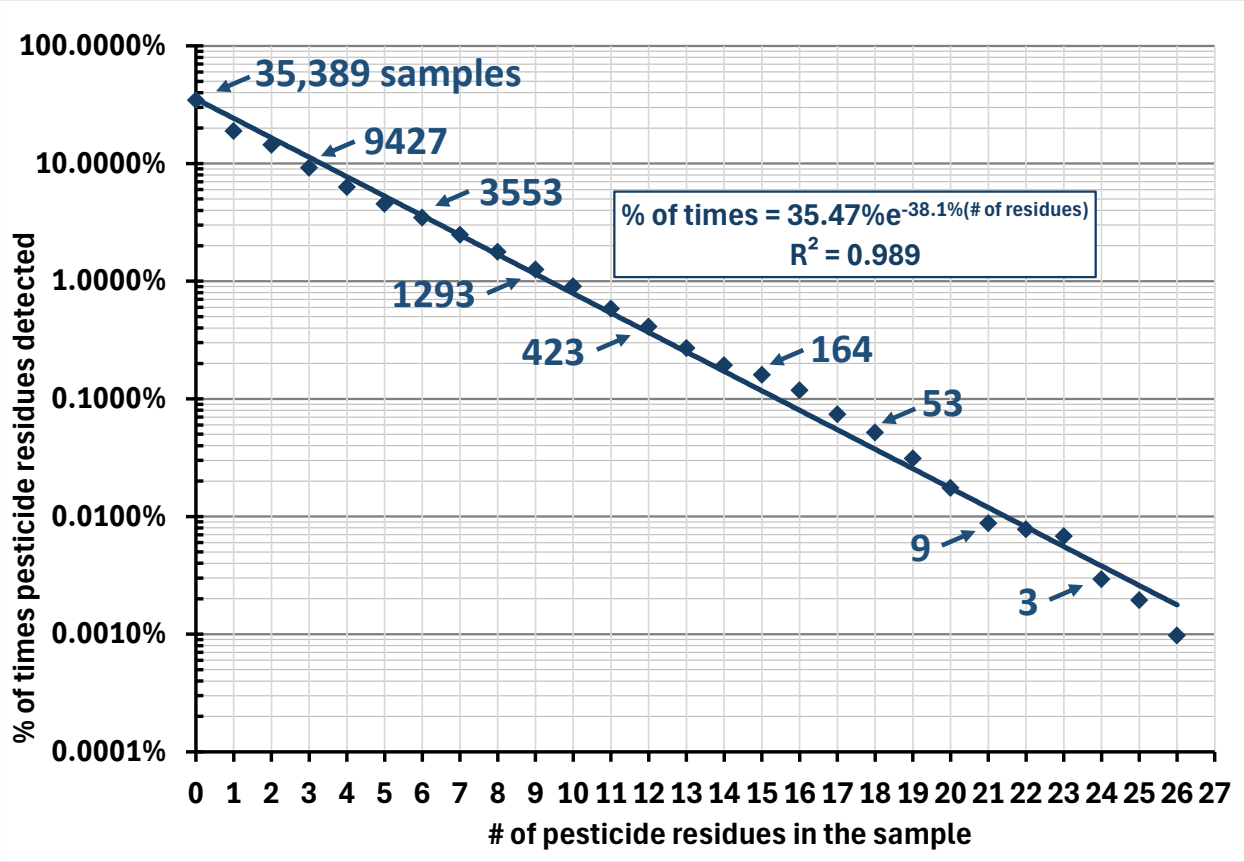

Figure S1. The percent (and number) of samples vs. number of different pesticide residues reported in each of 102,336 samples analyzed in the USDA Pesticide Data Program compiled from annual summary reports 2013-2022 (see: www.ams.usda.gov/datasets/pdp). Both GC and LC methods were used for analysis, typically using MS/MS for targeted detection and/or confirmation, but the number of false positives is unknown.

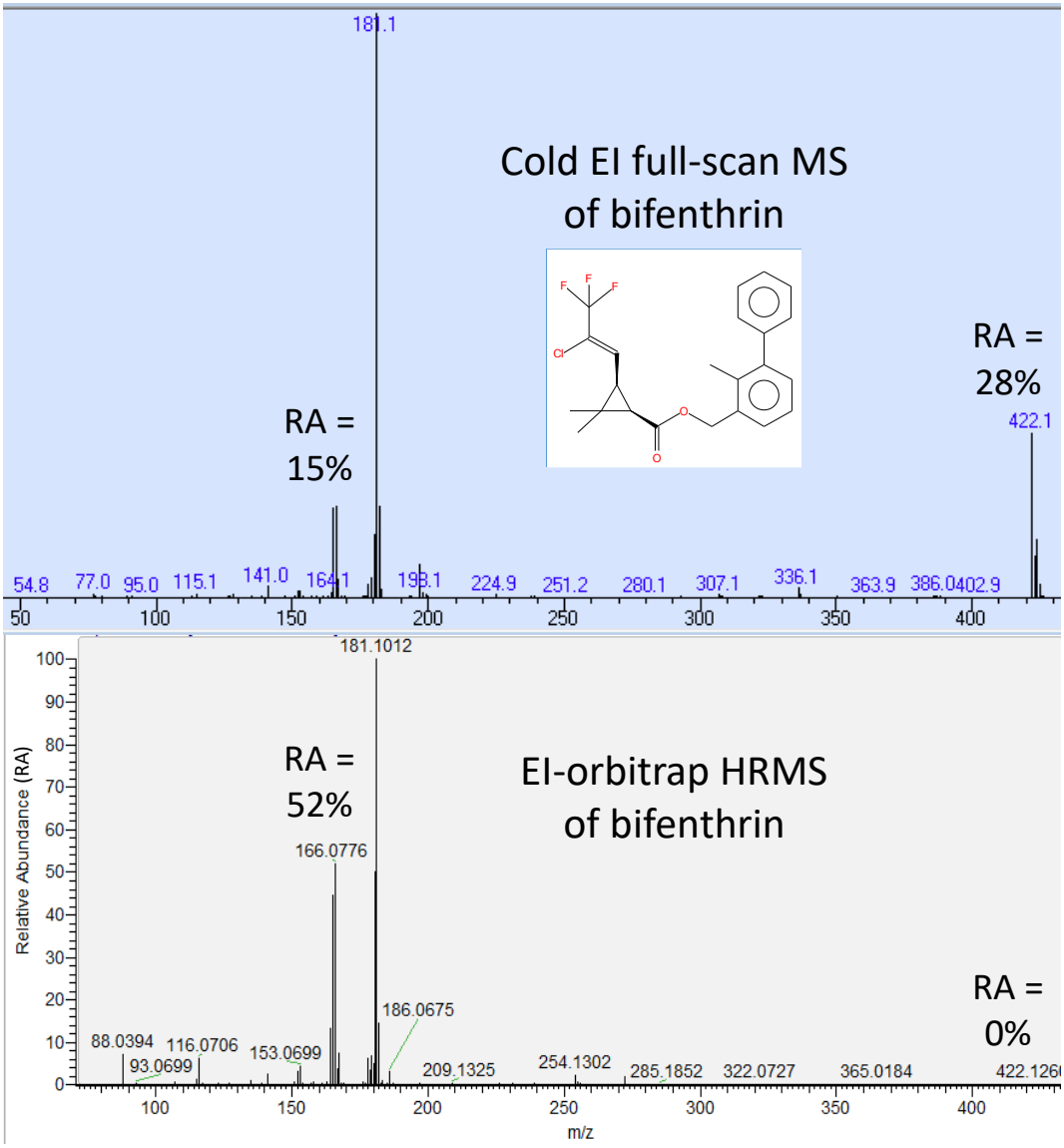

Figure S2. Comparison of the full-scan Cold EI and HRMS (orbitrap) spectra of bifenthrin. Note the shift of ions to higher masses, including enhanced M+ with 28% relative abundance, in Cold EI compared to standard EI.

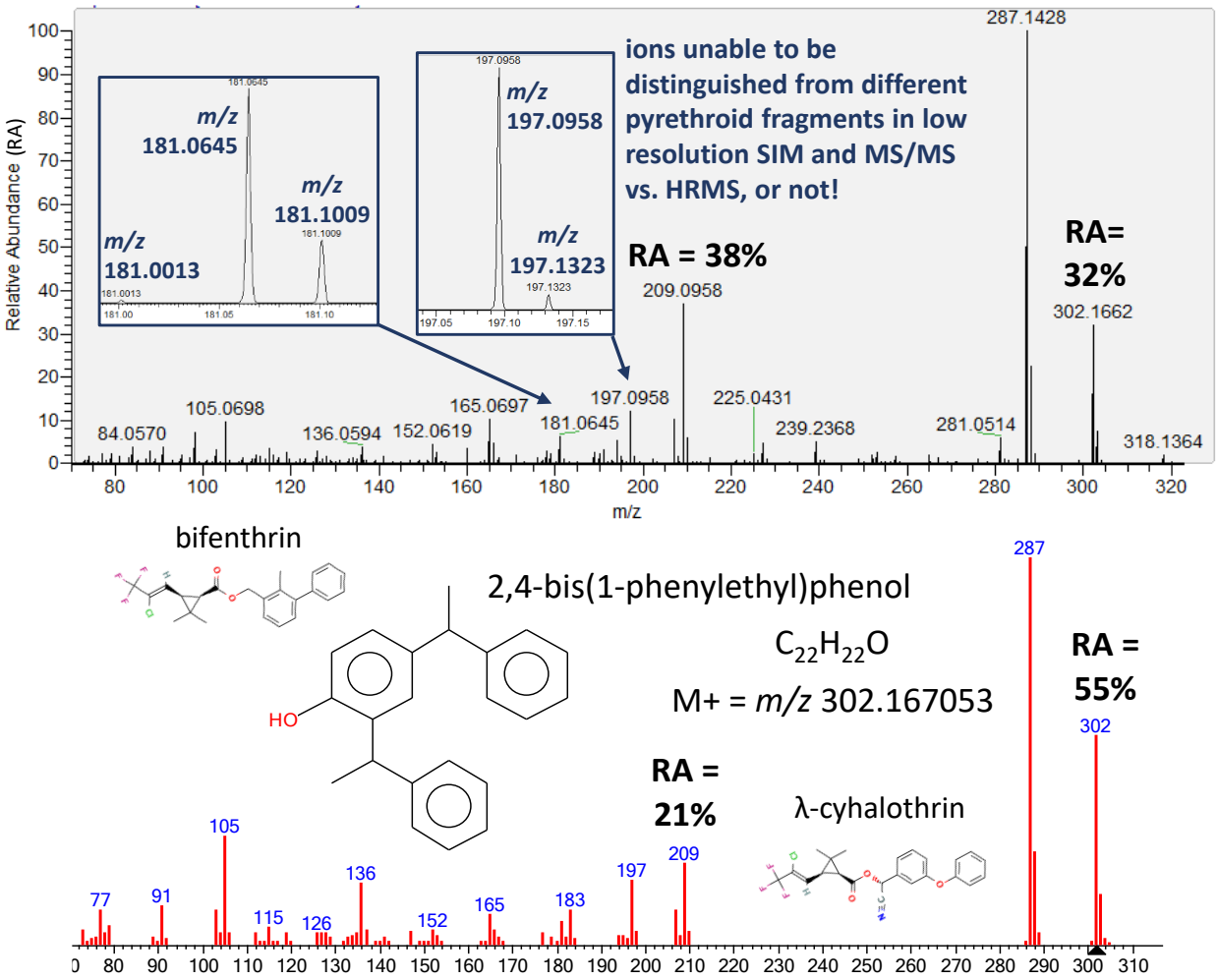

Figure S3. Background subtracted HRMS spectrum of the LPGC peak at 6.12 min in Figs. 4 and 5, and the top (88% probability) NIST library search hit, 2,4-bis(1-phenylethyl)phenol, with its chemical structure compared to bifenthrin and λ-cyhalothrin. The *m/z* 302.1662 HRMS ion has merely -2.8 ppm difference from the calculated monoisotopic mass of *m/z* 302.1671 for $C_{22}H_{22}O$. As in Figure S2 for Cold EI, the relative abundances of the ions in orbitrap were shifted to lower masses compared to the NIST spectrum.

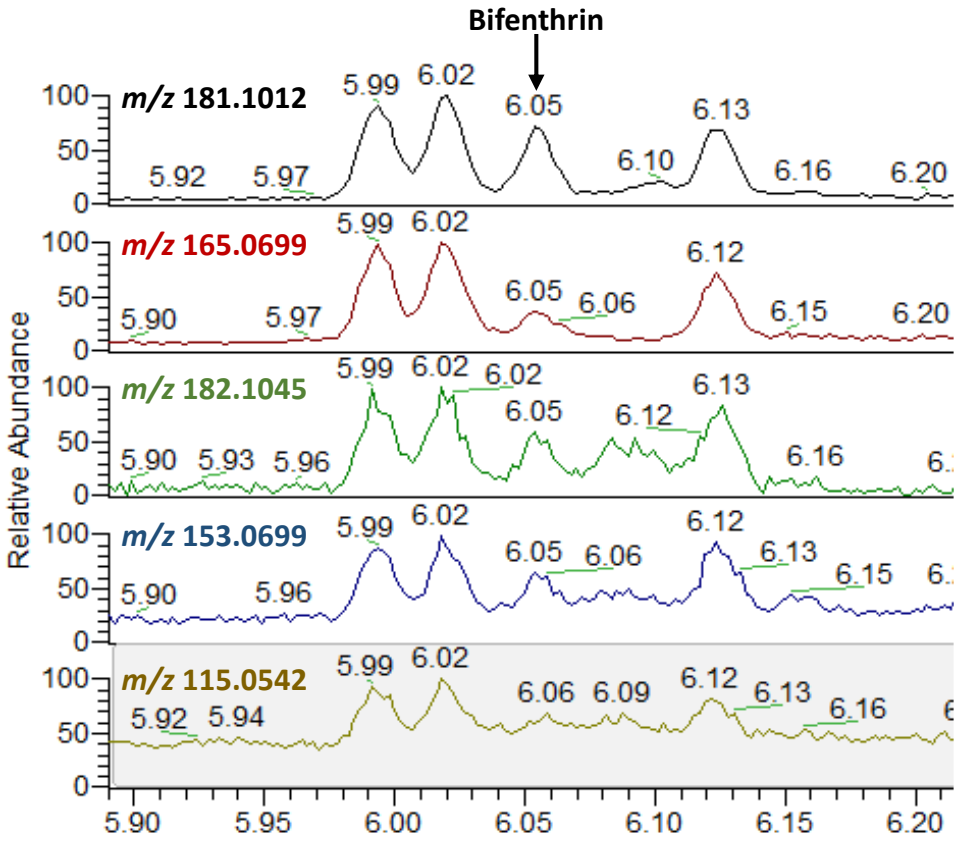

Figure S4. Because bifenthrin has the same exact mass fragments as bis(1-phenylethyl)phenol, no distinguishing fragment ion could be found, despite the increased selectivity of HRMS. However, Cold EI was able to sensitively detect the M+ and M+2 ions, and MS/MS relied on structural differences in the isotopes to better isolate bifenthrin from the chemical noise.

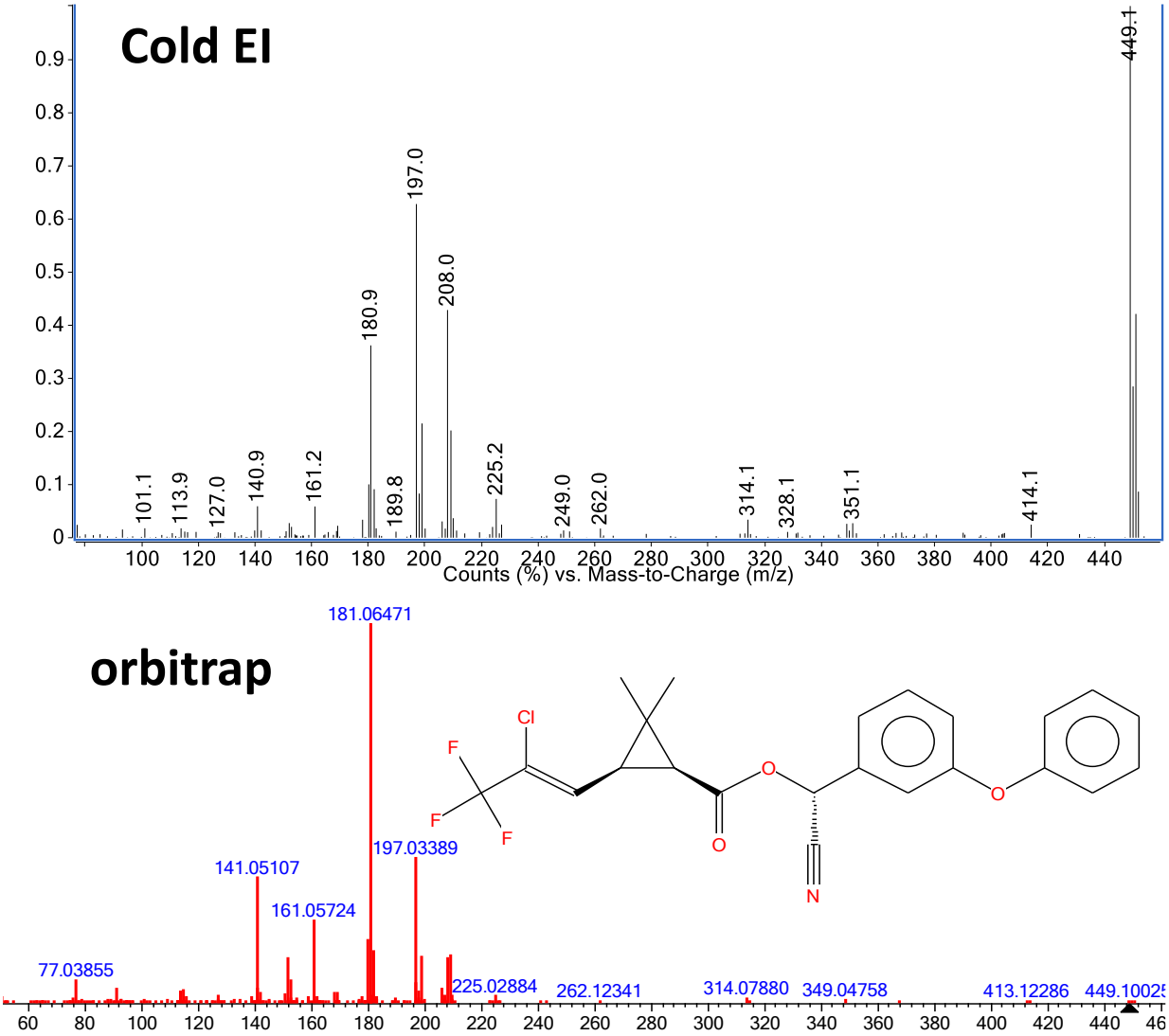

Figure S5. Comparison of the measured full-scan Cold EI and library HRMS (orbitrap) spectra of λ-cyhalothrin (co-elution with lactofen in the study did not yield a clean spectrum for display). The dramatic enhancement of the *m/z* 449 M+ ion in Cold EI led to it becoming the base peak from essentially 0% relative abundance in standard EI.

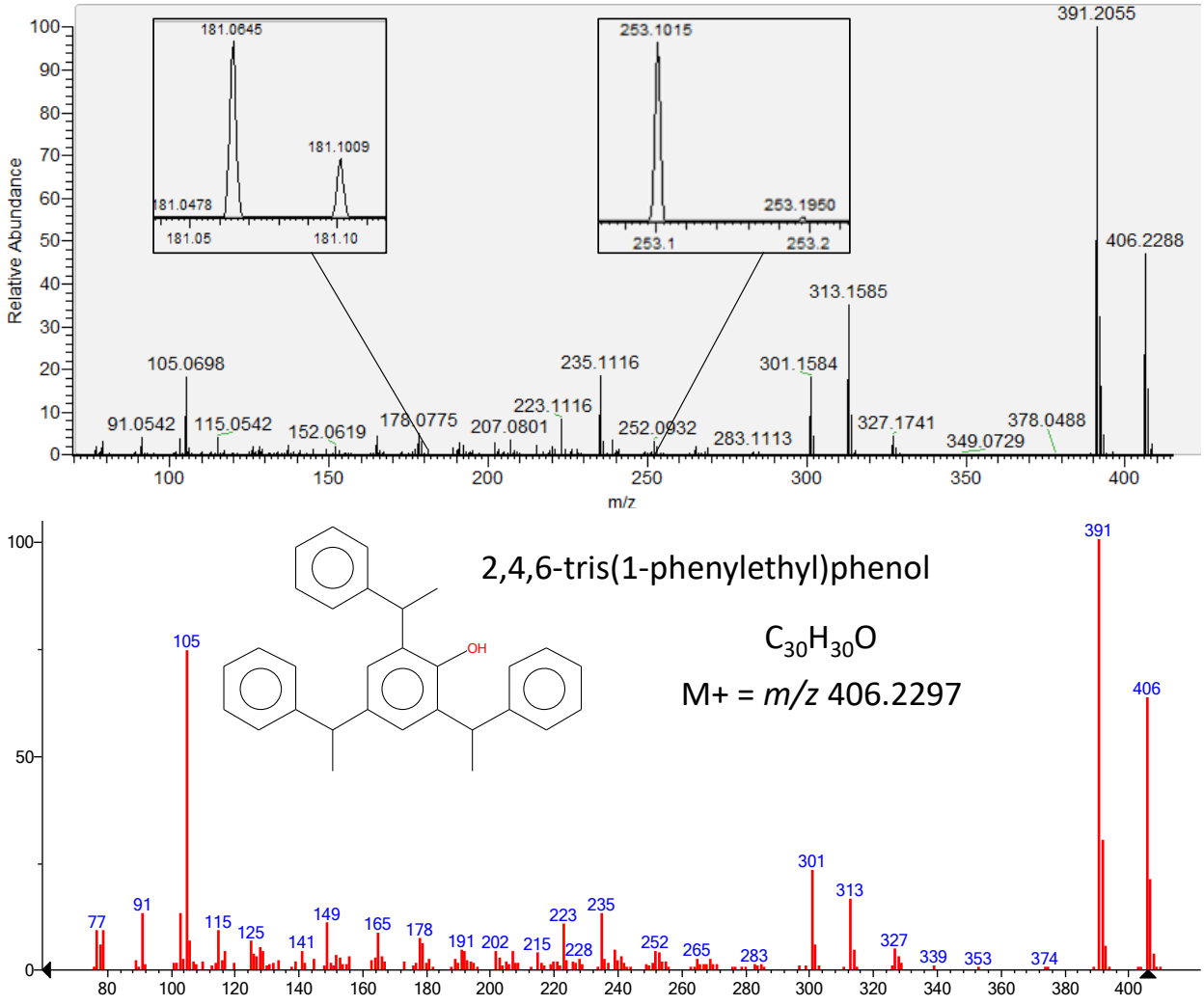

Figure S6. Background subtracted HRMS spectrum of the LPGC-MS/MS peak at 7.12 min in Figure 7 and the top NIST library search hit, 2,4,6-tris(1-phenylethyl)phenol, with 98% probability. The *m/z* 406.2288 HRMS ion has merely -2.2 ppm difference from the calculated monoisotopic mass for $C_{30}H_{30}O$. Despite the very high concentration of the interferants, the large mass defect of m/z 253 deltamethrin fragment ions containing Br avoided interferences, unlike non-halogenated ions from bifenthrin, λ-cyhalothrin, and fenpropathrin.

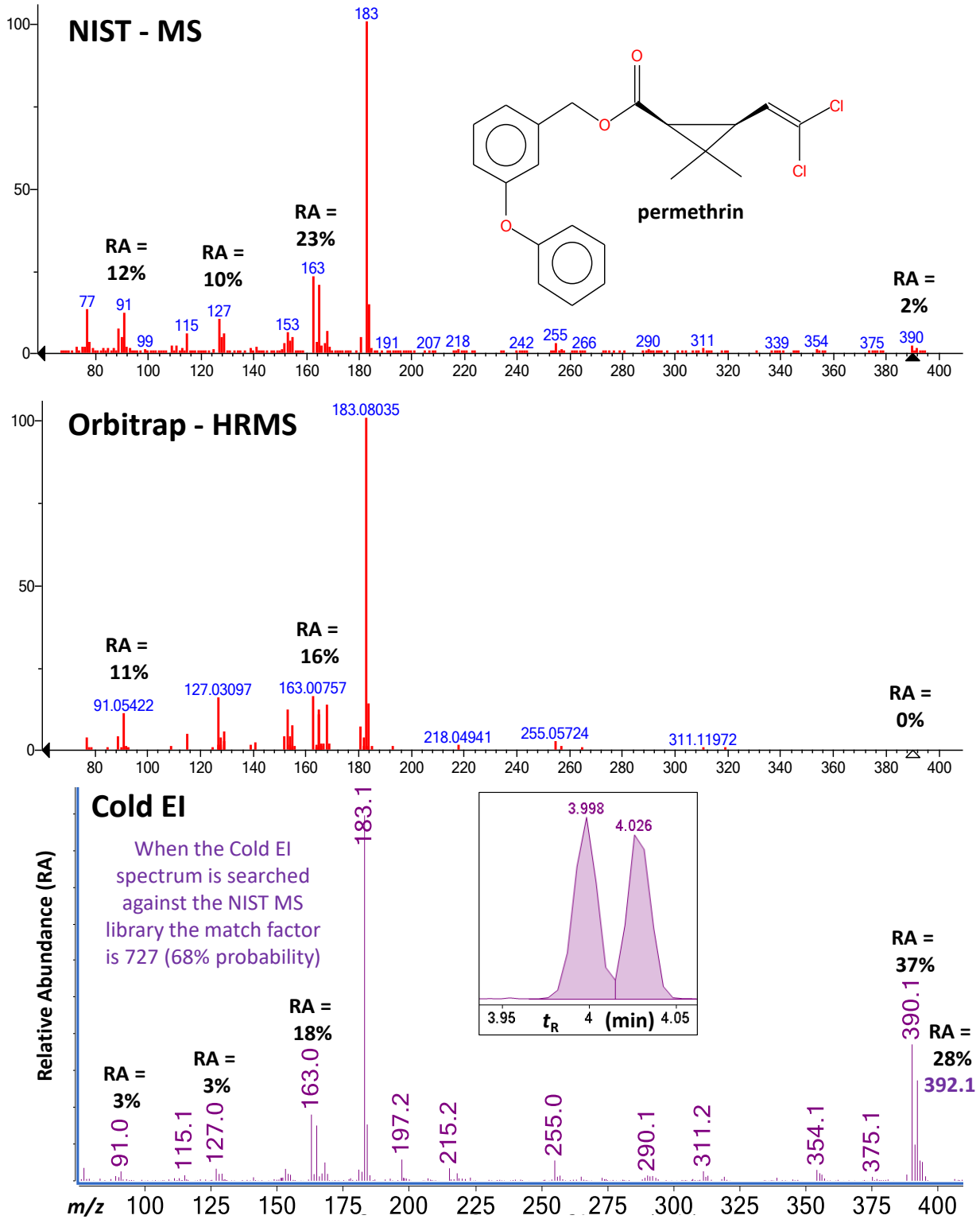

Figure S7. NIST and orbitrap library spectra of permethrin compared with the spectrum from Cold EI, demonstrating the significant enhancement of the M+ and reduction in the relative abundances of the low mass ions at *m/z* 91 and 127. Also, the fast-GC insert of *cis*/*trans*-permethrin in the 1/1 reference standard shows equal peak heights in Cold EI.

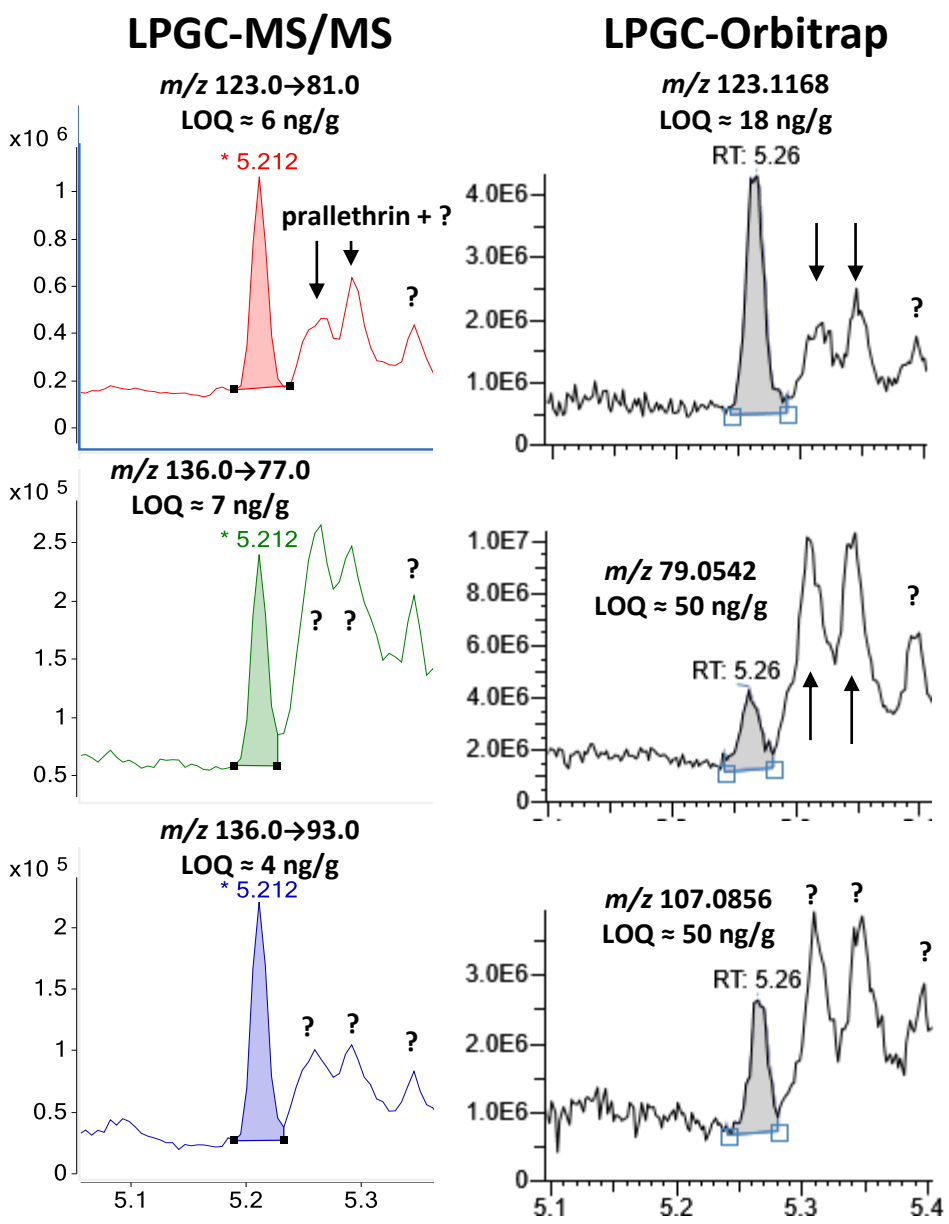

Figure S8. Comparison in the analysis of 100 ng/g (75 pg injected) allethrin in barley extract using the different LPGC- MS analyzers. Allethrin is fully separated from prallethrin and an unknown background component by the LPGC method with the usual 3-10 times lower LOQs in targeted MS/MS vs. non-targeted orbitrap HRMS detection. Fig. 13 shows that the m/z 136 and 107 ions are distinctive to allethrin, not prallethrin, which is why the chemical noise peak profiles change depending on the ions.

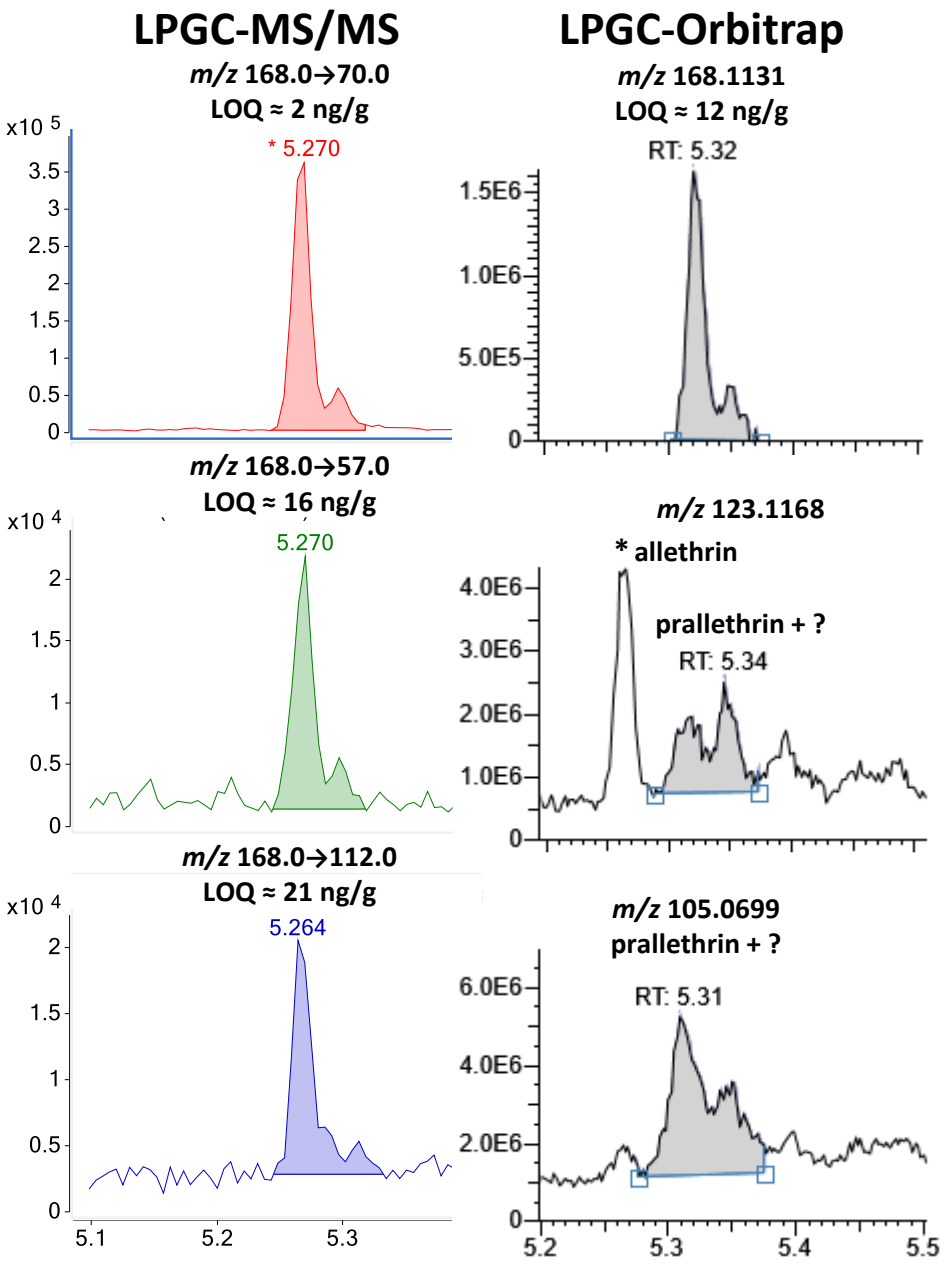

Figure S9. Comparison in the analysis of 100 ng/g (75 pg injected) triadimenol, easily confused with prallethrin, in barley extract using the different LPGC- MS analyzers. As shown in Fig. 13, the *m/z* 168 ion is shared by both prallethrin and allethrin, but it is even more prominent in co-eluting triadimenol. The Thermo/NIST HRMS library spectrum for m/z 168.1131shown in Fig. 13 looks to be incorrect. Unfortunately, prallethrin was still adversely impacted by the background interferant(s) at *m/z* 123.1168 and 105.0699, which is why the peak profiles are different.

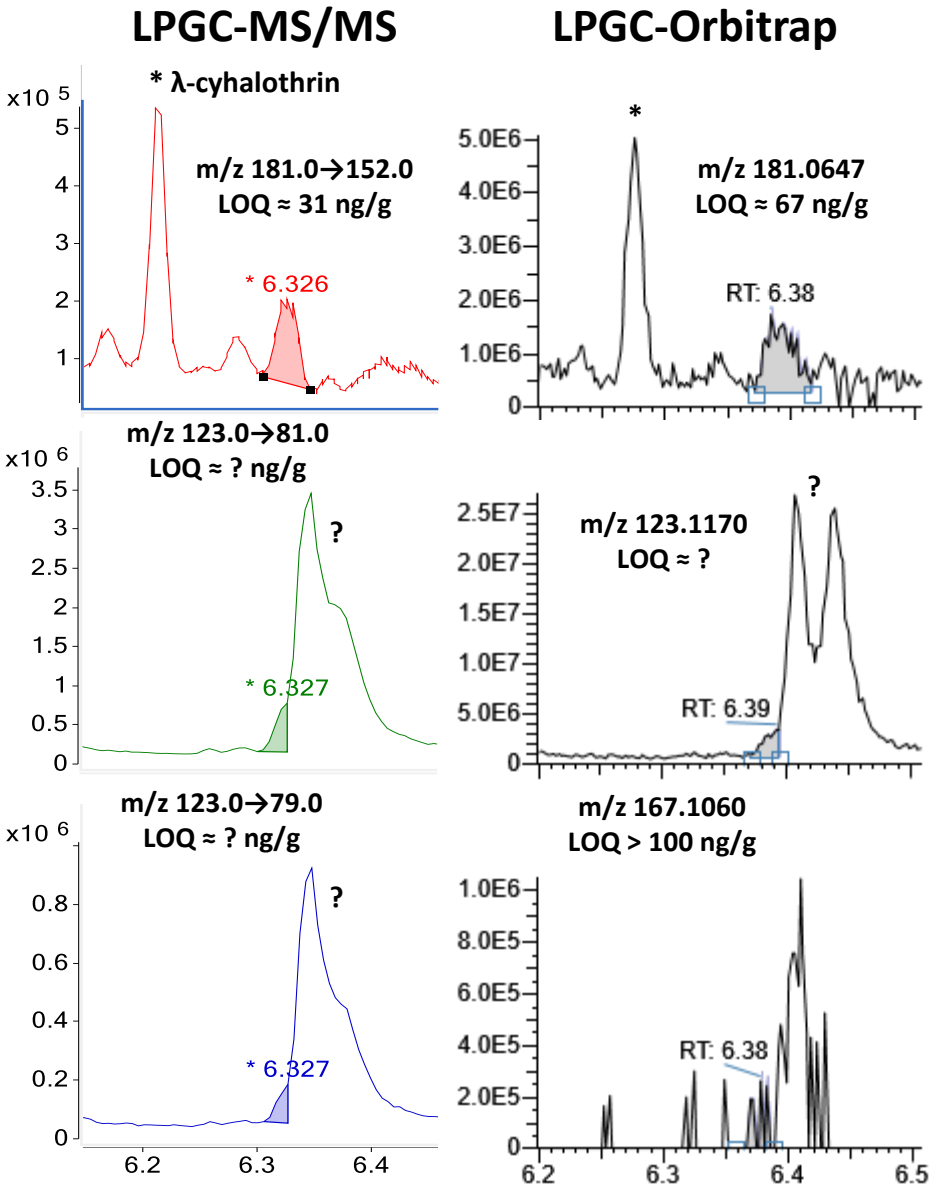

Figure S10. Comparison in the analysis of 100 ng/g (75 pg injected) cyphenothrin in barley extract using the different LPGC- MS analyzers. Unknown barley (first peak) and reagent matrix components interfered with the *m/z* 123 ion in both MS/MS and HRMS.

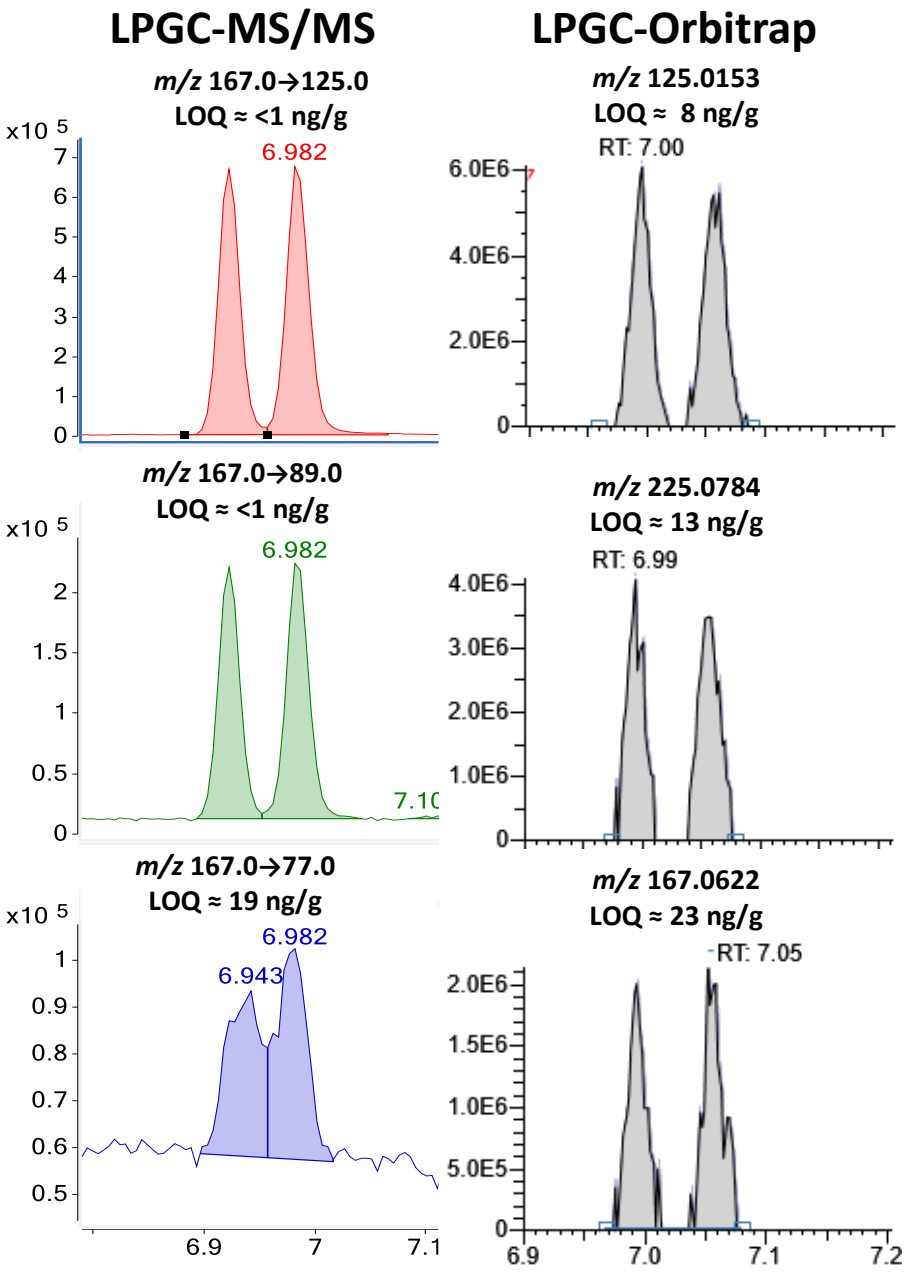

Figure S11. Comparison in the analysis of 100 ng/g (75 pg injected) es/fenvalerate in barley extract using the different LPGC- MS analyzers. The LOQs for the individual esfenvalerate and fenvalerate standards were about half of the reported LOQs for the summed pair.

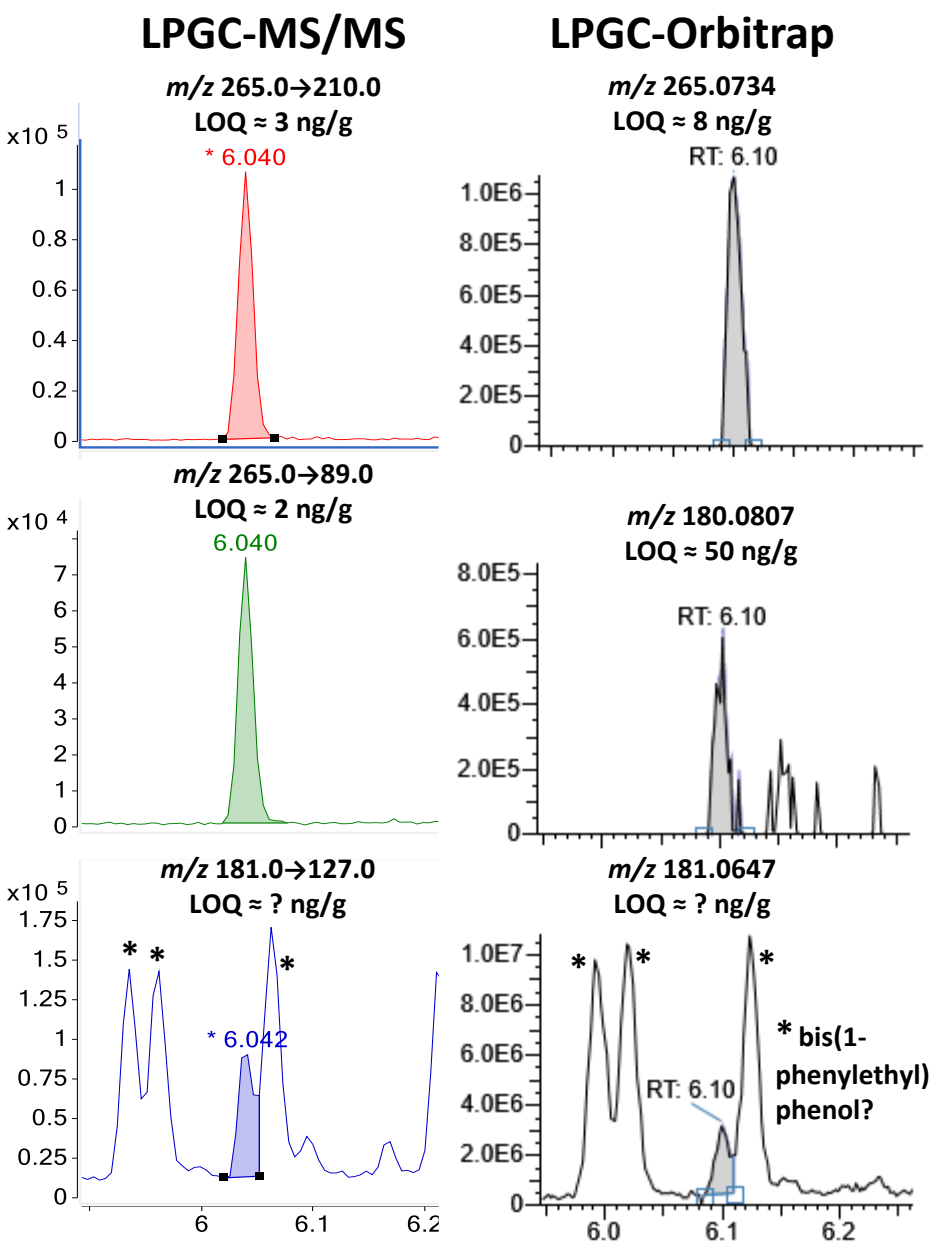

Figure S12. Comparison in the analysis of 100 ng/g (75 pg injected) fenpropathrin in barley extract using the different LPGC- MS analyzers. The bis(1-phenylethyl)phenol peaks interfered with the *m/z* 181 fragment / precursor ion as in the case of bifenthrin and λ-cyhalothrin in Figs. 4 and 5. Unfortunately, fenpropathrin partially co-eluted with one of the interferants, and since it originated from the exact same fragment, selective MS/MS conditions as used for bifenthrin were not possible.

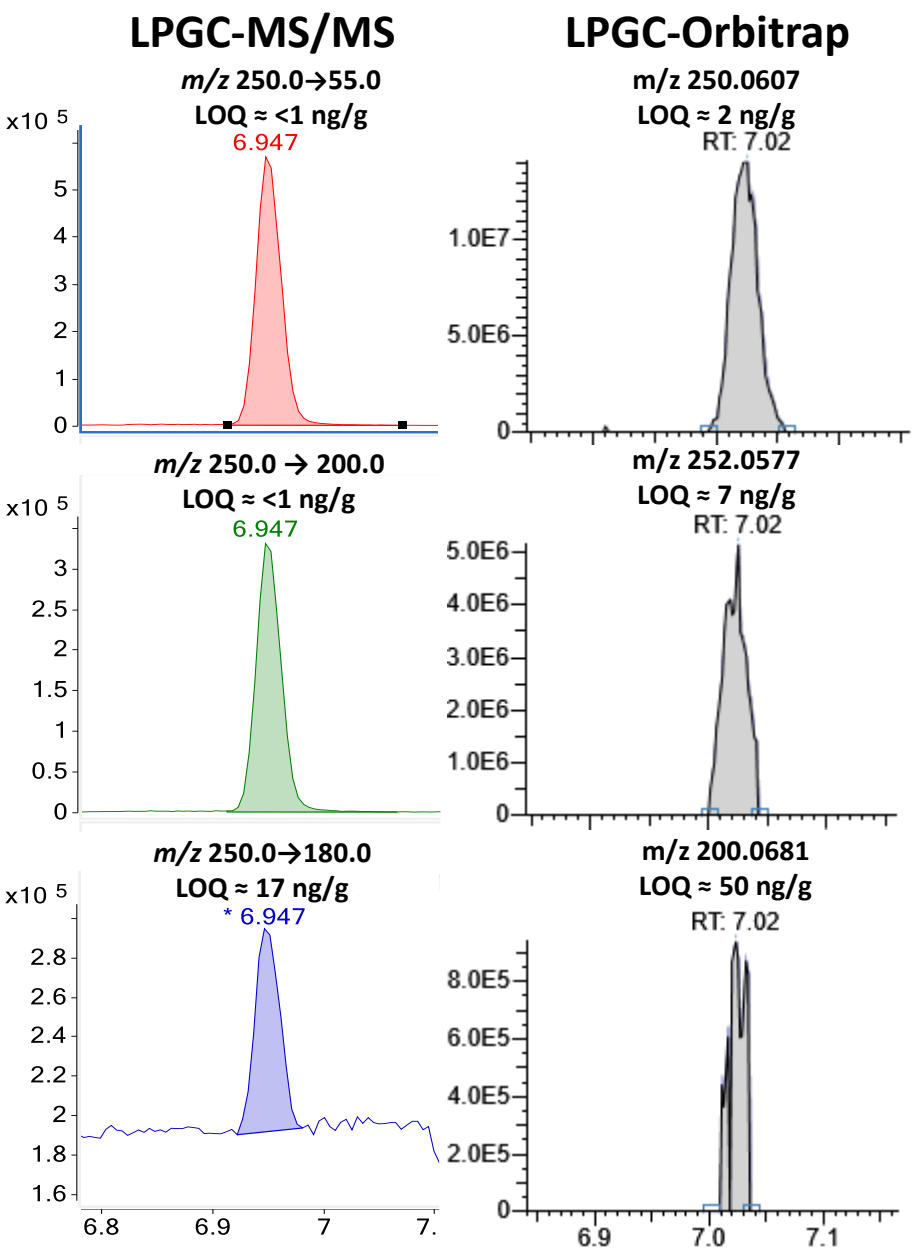

Figure S13. Comparison in the analysis of 100 ng/g (75 pg injected) fluvalinate in barley extract using the different LPGC- MS analyzers.

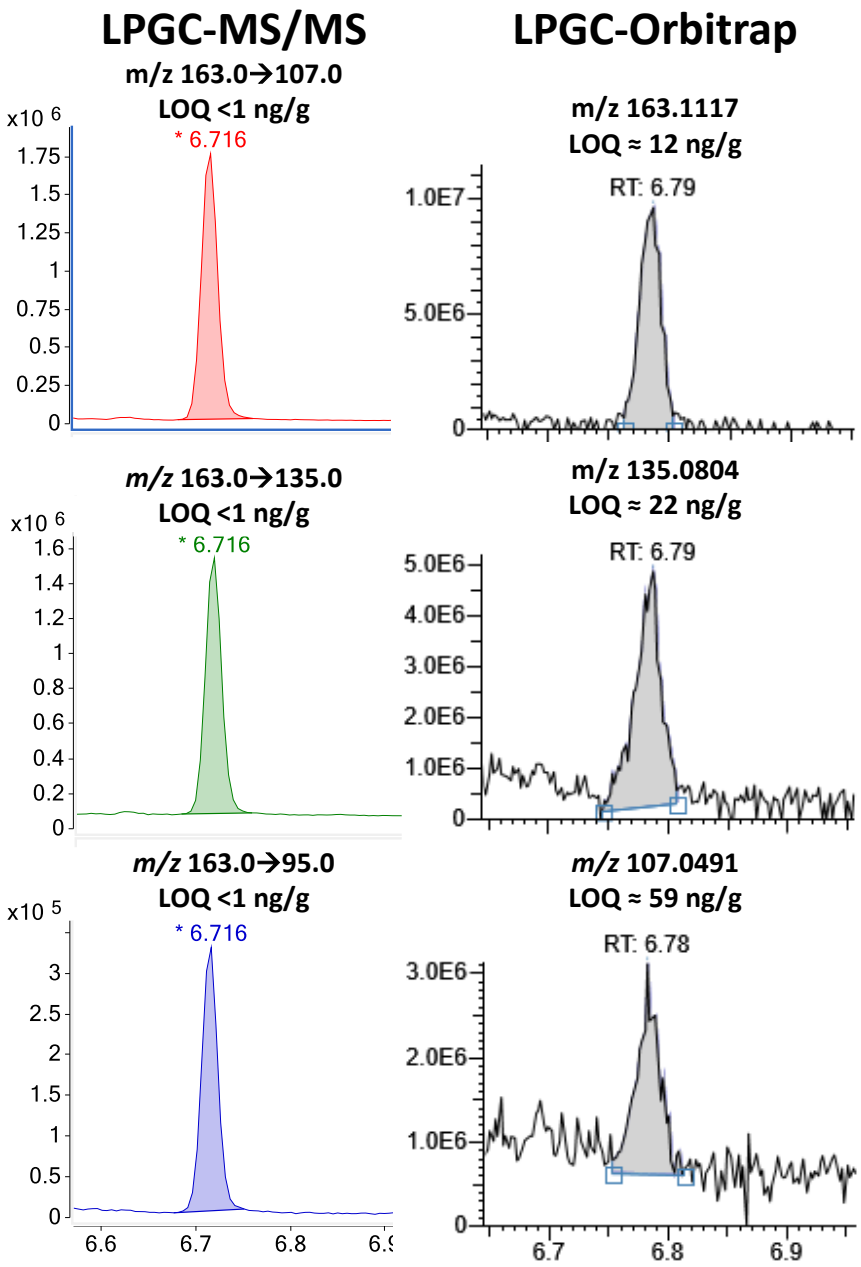

Figure S14. Comparison in the analysis of 100 ng/g (75 pg injected) etofenprox in barley extract using the different LPGC- MS analyzers.

Table S1. Listing of relative abundances (%) of all exact mass EI-HRMS ions (>5 ppm apart) with ≥1% relative abundance for which at least one pyrethroid in Thermo's orbitrap or NIST libraries. The pyrethroid analytes included in this study consist of: ale = allethrin; bif = bifenthrin; cyf = cyfluthrin; cyh = λ-cyhalothrin; cyf = cyfluthrin; cpe = cypermethrin; cph = cyphenothrin; del = deltamethrin; esf = es/fenvalerate; eto = etofenprox; fen = fenpropathrin; flu = fluvalinate; per = *cis*/*trans*-permethrins; phe = phenothrin; pra = prallethrin; res = resmethrin; tet = tetramethrin. Column headings: Mol. Form. = molecular formula; sum = sum of relative abundances (%) for the listed ion (red highlight for sum>10%); #pyr = no. of pyrethroids with relative ion abundance ≥1% for the listed ion (red highlight for #pyr>1). Base peaks for each analyte appear in bold text. Notes: empty cells = not done; isotopologues appear in bold purple text; "-" = not listed; "0" means <0.5% relative abundance; and ions rounded to the same *m/z* integer are boxed and highlighted in gold.

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
	421.1249	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	1	1
	420.1319	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	1	1
	419.1285	-	-	-	-	-	-	-	5	-	-	-	-	-	-	-	-	5	1
	417.2538	-	-	-	-	-	-	-	3	-	-	-	-	-	-	-	-	3	1
	376.2033	-	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	1	1
	349.1673	-	-	-	-	-	-	-	-	-	2	-	-	-	-	-	-	2	1
	338.1878	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
	334.1439	-	-	-	-	-	-	-	-	-	4	-	-	-	-	-	-	4	1
	327.9848	-	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	2	1
	323.1642	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
	314.0788	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	-	1	1
	304.1699	-	-	-	-	-	-	-	-	-	2	-	-	-	-	-	-	2	1
	303.1618	-	-	-	-	-	-	-	-	-	1	-	-	-	-	-	-	1	1
	298.8923	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	-	1	1
	296.8945	-	-	-	-	-	-	3	-	-	-	-	-	-	-	-	-	3	1
	294.8962	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	-	1	1
	294.1979	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
	293.0730	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	1	1
	290.1541	-	-	-	-	-	-	-	-	-	1	-	-	-	-	-	-	1	1
	280.9000	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	-	1	1
	279.1744	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3	-	3	1
	266.0767	-	-	-	-	-	-	-	-	-	5	-	-	-	-	-	-	5	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
$C_{16}H_{11}NO_3$	265.0734	-	-	-	-	-	-	-	-	-	29	-	-	-	-	-	-	29	1
	255.9060	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	-	2	1
$C_{16}H_{12}ClO$	255.0572	-	-	-	-	-	-	-	-	-	-	-	2	-	-	-	-	2	1
$C_7H_9{}^{81}Br_2$	254.9026	-	-	-	-	-	-	26	-	-	-	-	-	-	-	-	-	26	1
$C_6{}^{13}CH_9{}^{79}Br{}^{81}Br$	253.9081	-	-	-	-	-	-	4	-	-	-	-	-	-	-	-	-	4	1
$C_7H_9{}^{79}Br{}^{81}Br$	252.9046	-	-	-	-	-	-	53	-	-	-	-	-	-	-	-	-	53	1
$C_{19}H_8O$	252.0576	-	-	-	-	-	-	-	-	-	-	31	-	-	-	-	-	31	1
$C_6{}^{13}CH_9Br_2$	251.9102	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	-	2	1
$C_{18}H_5NO$	251.0369	-	-	-	-	-	-	-	-	-	-	11	-	-	-	-	-	11	1
$C_7H_9Br_2$	250.9067	-	-	-	-	-	-	27	-	-	-	-	-	-	-	-	-	27	1
$C_{16}H_{10}O_3$	250.0607	-	-	-	-	-	-	-	-	-	-	**100**	-	-	-	-	-	100	1
	247.1330	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
	247.0993	-	-	-	-	-	-	-	-	-	1	-	-	-	-	-	-	1	1
	239.1425	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4	-	4	1
	238.8525	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	-	2	1
	238.1354	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
	228.0780	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	-	1	1
$C_{14}H_{10}FNO$	227.0745	-	-	13	-	-	-	-	-	-	-	-	-	-	-	-	-	13	1
$C_{13}{}^{13}CH_{11}NO_2$	226.0818	-	-	-	-	-	-	-	7	-	-	-	-	-	-	-	-	7	1
$C_{14}H_9FNO$	226.0663	-	-	27	-	-	-	-	-	-	-	-	-	-	-	-	-	27	1
$C_{14}H_{11}NO_2$	225.0785	-	-	-	-	1	-	-	48	-	1	-	-	-	-	-	-	50	1
$C_{12}H_8ClF_2$	225.0288	-	0	-	2	-	-	-	-	-	-	-	-	-	-	-	-	2	1
	223.1109	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	-	1	1
	223.0629	-	-	-	0	1	-	-	1	-	-	-	-	-	-	-	-	2	1
	219.0680	-	-	-	-	-	-	-	0	-	2	-	-	-	-	-	-	2	1
	218.0494	-	-	-	-	-	-	-	-	-	-	-	1	-	-	-	-	1	1
	211.0709	-	-	-	0	-	-	-	-	-	1	-	-	-	-	-	-	1	1
	210.8574	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	-	2	1
	210.0869	-	-	-	2	3	-	3	2	-	2	-	-	-	-	-	-	12	5
	210.0678	-	-	-	1	-	-	-	0	-	8	-	-	-	-	-	-	10	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
$C_{14}H_{11}NO$	209.0836	-	-	-	13	21	-	19	10	-	17	-	-	-	-	-	-	79	5
$C_{14}H_{10}NO$	208.0760	-	-	-	12	6	-	6	3	-	9	-	-	-	-	-	-	36	5
$C_{11}H_3F_3O$	208.0135	-	-	-	-	-	-	-	-	-	-	2	-	-	-	-	-	2	1
$C_{14}H_9NO$	207.0683	-	-	-	2	3	-	3	1	-	2	-	-	-	-	-	-	12	5
$C_{13}{}^{13}CH_8NO$	207.0634	-	-	15	1	-	-	-	1	-	1	-	-	-	-	-	-	17	1
$C_8H_9Cl_2O_2$	206.9976	-	-	-	-	2	-	-	-	-	-	-	-	-	-	-	-	2	1
$C_{14}H_8NO$	206.0601	-	-	**100**	4	7	-	6	4	-	6	-	-	-	-	-	-	128	6
$C_{11}HF_3O$	205.9978	-	-	-	-	-	-	-	-	-	-	5	-	-	-	-	-	5	1
	203.1431	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
$C_{14}H_{17}O$	201.1274	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	-	1	1
$C_3H_3{}^{81}Br_2$	200.8555	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	-	2	1
$C_{10}H_9F_3N$	200.0681	-	-	-	-	-	-	-	-	-	-	6	-	-	-	-	-	6	1
$C_{10}H_{13}ClO_2$	200.0588	-	-	10	-	-	-	-	-	-	-	-	-	-	-	-	-	10	1
$C_{11}H_6NO_3$	200.0342	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	-	1	1
$C_{13}H_8FO$	199.0554	-	-	69	0	-	-	-	-	-	-	-	-	-	-	-	-	70	1
$C_8H_9{}^{37}ClF_3$	199.0310	-	0	-	12	-	-	-	-	-	-	-	-	-	-	-	-	12	1
$C_3H_3Br^{81}Br$	198.8575	-	-	-	-	-	-	4	0	-	-	-	-	-	-	-	-	5	1
$C_{12}{}^{13}CH_9O_2$	198.0676	-	-	-	1	3	-	2	3	0	2	-	-	-	-	-	-	12	5
$C_7{}^{13}CH_9ClF_3$	198.0372	-	-	-	3	-	-	-	-	-	-	-	-	-	-	-	-	3	1
$C_{13}H_9O_2$	197.0597	-	-	-	5	6	-	5	7	0	3	-	-	-	-	-	-	26	5
$C_8H_9ClF_3$	197.0339	-	0	-	38	-	-	-	-	-	-	-	-	-	-	-	-	38	1
$C_{12}H_5O_3$	197.0232	-	-	-	0	-	-	2	-	-	-	-	-	-	-	-	-	3	1
$C_3H_3Br_2$	196.8597	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	-	2	1
	190.0652	-	-	-	1	2	-	2	1	-	2	-	-	-	-	-	-	8	5
$C_{11}{}^{13}CH_{11}O$	184.0838	-	-	-	-	-	-	-	-	1	-	-	14	16	-	-	-	30	2
$C_{12}{}^{13}C_2H_{13}$	183.1080	-	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	1
$C_{13}H_{11}O$	183.0804	-	-	-	1	-	-	-	0	5	1	-	**100**	**100**	-	-	-	207	3
$C_6H_3ClF_3O$	182.9818	-	-	-	2	-	-	-	-	-	-	-	-	-	-	-	-	2	1
$C_{13}{}^{13}CH_{13}$	182.1045	-	15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	15	1
$C_{13}H_{10}O$	182.0727	-	-	-	-	-	-	-	-	1	-	-	3	-	-	-	-	4	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
$C_{12}{}^{13}CH_9O$	182.0682	-	-	-	14	14	-	14	7	0	14	-	1	-	-	-	-	63	5
$C_{14}H_{13}$	181.1011	-	**100**	-	-	-	-	-	-	-	-	-	-	-	-	-	-	100	1
$C_{13}H_{11}N$	181.0889	-	-	-	0	1	-	1	-	-	1	-	-	-	-	-	-	3	2
C_6H	181.0841	-	-	-	2	2	-	2	-	-	2	-	-	-	-	-	-	9	4
$C_{13}H_9O$	181.0648	-	-	-	**100**	**100**	20	**100**	47	2	**100**	18	7	-	-	-	-	493	9
$C_{14}H_{12}$	180.0933	-	7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	7	1
$C_{13}H_{10}N$	180.0808	-	-	-	17	16	-	17	8	-	17	-	-	-	-	-	-	75	5
	179.0855	-	7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	7	1
	179.0605	-	0	-	1	1	-	-	0	-	1	-	-	-	-	-	-	3	2
	178.0778	-	7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	7	1
	178.0651	-	-	-	2	2	-	2	1	-	2	-	-	-	-	-	-	10	5
	177.0576	-	-	-	1	1	-	1	1	-	1	-	-	-	-	-	-	4	2
	174.9940	-	-	-	-	-	-	5	-	-	-	-	-	-	-	-	-	5	1
	174.9896	-	-	-	-	-	-	4	-	-	-	-	-	-	-	-	-	4	1
$C_7H_9{}^{81}Br$	173.9862	-	-	-	-	-	-	58	-	-	-	-	-	-	-	-	-	58	1
	173.0908	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	-	1	1
	172.9961	-	-	-	-	-	-	5	-	-	-	-	-	-	-	-	-	5	1
	172.9917	-	-	-	-	-	-	4	-	-	-	-	-	-	-	-	-	4	1
	172.9783	-	-	-	-	-	-	6	-	-	-	-	-	-	-	-	-	6	1
$C_{12}H_{12}O$	172.0881	-	-	-	-	-	-	-	-	-	-	-	-	-	-	11	-	11	1
$C_{11}{}^{13}CH_{11}O$	172.0839	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6	-	6	1
C_7H_9Br	171.9882	-	-	-	-	-	-	58	-	-	-	-	-	-	-	-	-	58	1
$C_{12}H_{11}O$	171.0806	-	-	-	-	-	-	-	0	-	-	-	-	-	-	47	-	47	1
$C_8H_8ClO_2$	171.0207	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	1	1
$C_8H_6{}^{37}ClO_2$	171.0021	-	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	2	1
C_7H_8Br	170.9804	-	-	-	-	-	-	6	-	-	-	-	-	-	-	-	-	6	1
$C_{12}H_{10}O$	170.0727	-	-	-	0	-	-	-	1	-	0	-	-	-	-	5	-	6	1
$C_{12}H_7F$	170.0526	-	-	10	-	-	-	-	-	-	-	-	-	-	-	-	-	10	1
$C_8H_7ClO_2$	170.0129	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	1	1
C_7H_7Br	169.9725	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	-	2	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
$C_{12}H_9O$	169.0649	-	-	-	3	6	-	5	5	0	4	-	-	-	-	1	-	24	6
$C_{11}{}^{13}CH_8O$	169.0604	-	-	-	0	1	-	1	-	0	1	-	2	-	-	-	-	4	1
$C_{10}H_{12}{}^{37}Cl$	169.0593	-	-	-	-	-	-	-	11	-	-	-	-	-	-	-	-	11	1
$C_8H_6ClO_2$	169.0051	-	-	-	-	-	-	-	6	-	-	-	-	-	-	-	-	6	1
$C_8H_{16}O_2$	168.1145	4	-	-	-	-	-	-	-	-	-	-	-	-	4	-	-	4	1
$C_9{}^{13}CH_{12}Cl$	168.0656	-	-	-	-	-	-	-	4	-	-	-	-	-	-	-	-	4	1
$C_{12}H_8O$	168.0570	-	-	-	3	5	-	5	3	3	4	-	13	18	-	-	-	54	8
$C_{10}H_{15}O_2$	167.1067	1	-	-	-	-	7	-	-	-	-	-	-	-	1	-	-	8	1
$C_{13}H_{11}$	167.0855	-	1	-	-	-	-	0	1	0	0	-	-	-	-	-	-	2	1
$C_{12}{}^{13}CH_{10}$	167.0811	-	7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	7	1
$C_{10}H_{12}Cl$	167.0622	-	-	-	-	-	-	-	36	-	-	-	-	-	-	-	-	36	1
$C_7H_9{}^{37}Cl_2$	167.0017	-	-	-	-	8	-	-	-	-	-	-	2	-	-	-	-	9	2
$C_{10}H_{14}O_2$	166.0974	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6	-	6	1
$C_{13}H_{10}$	166.0778	-	49	-	-	-	-	-	0	-	0	-	-	-	-	-	-	49	1
$C_{12}{}^{13}CH_9$	166.0738	-	6	-	-	-	-	-	0	0	0	-	2	-	-	-	0	8	2
$C_6{}^{13}CH_9Cl{}^{37}Cl$	166.0080	-	-	-	-	4	-	-	-	-	-	-	1	-	-	-	-	4	1
$C_9{}^{13}C_2H_{15}O$	165.1187	-	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	1	1
$C_8{}^{13}CH_{10}NO_2$	165.0738	-		-	-	-	-	-	-	-	-	-	-	-	-	-	10	10	1
$C_{13}H_9$	165.0700	-	45	-	0	-	-	1	1	2	1	-	12	-	-	-	-	62	3
$C_7H_9Cl{}^{37}Cl$	165.0047	-	-	46	-	48	-	-	-	-	-	-	10	-	-	-	-	104	3
$C_{10}{}^{13}CH_{15}O$	164.1151	-	-	-	-	-	-	-	-	12	-	-	-	-	-	-	-	12	1
$C_9H_{10}NO_2$	164.0705	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	**100**	100	1
$C_{13}H_8$	164.0622	-	2	-	0	-	-	-	-	0	-	-	1	-	-	-	-	3	1
$C_5H_7ClNO_3$	164.0109	-	-	-	-	6	-	-	-	-	-	-	1	-	-	-	-	7	2
$C_{11}H_{15}O$	163.1117	-	-	-	-	-	-	-	-	**100**	-	-	-	-	-	-	-	100	1
$C_7H_9Cl_2$	163.0081	-	-	71	-	73	-	-	-	-	-	-	16	-	-	-	-	160	3
	162.1040	-	-	-	-	-	-	-	-	2	-	-	-	-	-	-	-	2	1
	162.0606	-	0	-	2	-	-	-	-	-	-	-	-	-	-	-	-	2	1
$C_8H_8F_3$	161.0572	-	1	-	22	-	-	-	-	-	-	-	-	-	-	-	-	22	1
	159.0416	-	0	-	2	-	-	-	-	-	-	-	-	-	-	-	-	2	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
	157.0648	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
	155.0855	-	-	-	0	-	-	-	-	1	-	-	7	-	-	-	-	8	1
	155.0605	-	0	-	-	1	-	-	0	0	1	-	1	-	-	6	-	10	2
	154.9870	-	0	-	1	-	-	-	-	-	-	-	-	-	-	-	-	1	1
	154.0778	-	0	-	0	-	-	0	0	1	0	-	4	-	-	-	-	6	1
	154.0734	-	1	-	1	1	-	1	1	0	1	-	1	-	-	-	-	7	4
	153.9994	-	-	-	-	-	-	-	7	-	-	-	-	-	-	-	-	7	1
$C_9H_{13}O_2$	153.0911	6	-	-	-	-	-	-	-	-	-	-	-	-	7	-	-	13	2
$C_{12}H_9$	153.0699	-	5	-	6	9	-	9	6	3	8	-	12	13	-	4	-	74	10
$C_{11}{}^{13}CH_8$	153.0656	-	0	-	1	3	-	2	1	0	2	-	-	-	-	-	-	11	5
C_8H_6ClO	153.0101	-	-	-	-	2	-	-	-	-	-	-	-	-	-	-	-	2	1
$C_7{}^{13}CH_5ClO$	153.0057	-	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	2	1
$C_{12}H_8$	152.0621	-	4	-	12	21	11	20	11	1	19	4	4	-	-	-	-	107	10
C_8H_5ClO	152.0024	-	-	-	-	-	-	-	22	-	-	-	-	-	-	-	-	22	1
	151.0543	-	1	-	2	4	-	4	3	0	4	-	-	-	-	-	-	17	5
	150.9526	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	1	1
	148.9557	-	-	-	-	2	-	-	-	-	-	-	-	-	-	-	-	2	1
	147.0806	-	-	-	-	-	-	-	-	0	-	-	-	-	-	2	0	2	1
	147.0316	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	1	1
	145.0648	-	-	-	0	-	-	-	-	-	0	-	-	-	-	2	-	2	1
$C_{10}{}^{13}CH_{11}$	144.0889	-	-	-	-	-	-	-	-	-	-	-	-	-	-	12	-	12	1
$C_{11}H_{11}$	143.0856	-	-	-	-	-	-	-	-	-	0	-	-	-	-	99	-	99	1
$C_7H_6{}^{37}ClO$	143.0073	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	1	1
	142.0778	-	-	-	0	-	-	-	0	-	0	-	-	-	-	5	-	5	1
	142.0734	-	0	-	0	1	-	1	1	0	1	-	-	-	-	3	-	7	2
	142.0544	-	0	-	3	-	-	-	-	-	-	-	-	-	-	-	-	3	1
$C_8H_{13}O_2$	141.0911	-	-	-	-	-	-	-	-	-	11	-	-	-	-	-	-	11	1
$C_{11}H_9$	141.0700	-	1	-	4	8	-	7	5	0	5	-	2	-	-	26	-	59	8
$C_8H_7F_2$	141.0511	-	3	-	33	-	-	-	-	-	-	-	-	-	-	-	-	36	2
$C_8H_8{}^{37}Cl$	141.0280	-	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	2	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
C_7H_6ClO	141.0103	-	-	-	-	-	-	-	4	-	-	-	-	-	-	-	-	4	1
	140.0496	-	-	-	1	1	-	1	1	-	1	-	-	-	-	-	-	5	2
	139.0544	-	1	-	2	3	-	3	2	0	3	-	1	-	-	2	-	17	7
C_8H_8Cl	139.0310	-	-	-	-	-	-	-	6	-	-	-	-	-	-	-	-	6	1
	137.0917	2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	1
	137.0599	-	-	-	-	1	-	2	-	-	-	-	-	-	-	-	-	2	1
$C_9H_{12}O$	136.0884	25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	25	1
$C_8{}^{13}CH_{11}O$	136.0839	-	-	-	-	-	-	-	-	3	-	-	-	-	-	-	-	3	1
$C_9H_{11}O$	135.0805	2	-	-	-	-	-	-	-	33	-	-	-	-	1	-	-	35	2
$C_8H_7O_2$	135.0441	-	-	-	-	-	-	-	0	-	-	-	-	-	-	-	7	7	1
	134.0728	1	-	-	-	-	-	-	-	1	-	-	-	-	9	-	-	11	2
	133.0649	2	-	-	-	-	-	-	-	1	-	-	-	-	6	-	-	9	2
	132.0571	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	-	2	1
	131.0492	-	-	-	-	-	-	-	-	0	-	-	-	-	2	-	-	2	1
	130.0314	-	-	-	-	2	-	-	-	-	-	-	-	-	-	-	-	2	1
$C_{10}H_9$	129.0700	-	0	-	-	-	-	-	-	1	0	-	2	-	-	4	-	7	2
$C_9{}^{13}CH_8$	129.0657	-	-	-	-	-	-	-	-	0	-	-	-	-	-	11	-	11	1
$C_7H_{10}Cl$	129.0467	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	1	1
$C_7H_8{}^{37}Cl$	129.0281	-	-	26	-	28	-	-	-	-	-	-	5	-	-	-	-	59	3
$C_{10}H_8$	128.0621	-	1	-	0	-	-	-	1	1	1	-	3	-	-	**100**	-	108	4
$C_{10}H_8$	128.0388	-	-	-	0	3	-	-	-	-	-	-	1	-	-	-	-	4	1
$C_5H_6NO_3$	128.0344	-	-	-	-	7	-	-	-	-	-	-	1	-	-	-	-	8	2
$C_6{}^{13}CH_6Cl$	128.0157	-	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	2	1
$C_{10}H_7$	127.0543	-	0	-	1	1	-	2	2	1	1	-	1	-	-	-	-	8	5
$C_7H_5F_2$	127.0355	-	1	-	2	-	-	-	-	-	-	-	-	-	-	-	-	3	1
C_7H_8Cl	127.0310	-	-	77	-	87	-	-	-	-	-	-	16	-	-	-	-	180	3
$C_7H_6{}^{37}Cl$	127.0124	-	-	-	-	1	-	-	32	-	-	-	-	-	-	-	-	33	1
$C_7{}^{13}CH_{13}O$	126.0995	-	-	-	-	-	-	-	-	-	2	-	-	-	-	-	-	2	1
$C_5H_4NO_3$	126.0187	-	-	-	-	-	-	-	7	-	-	-	-	-	-	-	-	7	1
$C_7H_5{}^{37}Cl$	126.0045	-	-	-	-	-	-	-	1	-	-	-	-	-	-	-	-	1	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
$C_8H_{13}O$	125.0962	0	-	-	-	-	-	-	-	-	28	-	-	-	1	-	-	29	1
$C_7H_9O_2$	125.0599	1	-	-	-	-	-	-	-	-	0	-	-	-	1	-	-	3	2
C_7H_6Cl	125.0154	-	-	-	-	3	-	-	**100**	-	-	-	1	-	-	-	-	103	2
$C_8{}^{14}CH_{15}$	124.1203	10	-	-	-	-	9	-	-	-	-	-	-	10	10	8	2	49	6
C_7H_5Cl	124.0075	-	-	-	-	-	-	-	5	-	-	-	-	-	-	-	-	5	1
C_9H_{15}	123.1169	**100**	-	-	-	-	**100**	-	-	-	-	-	-	96	**100**	85	16	497	6
$C_8H_{11}O$	123.0805	-	-	-	-	-	-	-	-	-	6	-	-	-	-	-	-	6	1
$C_4H_3Cl^{37}Cl$	122.9576	-	-	-	-	2	-	-	-	-	-	-	-	-	-	-	-	2	1
C_9H_{13}	121.1013	5	-	-	-	-	22	-	-	-	-	-	-	-	5	4	2	38	5
C_8H_9O	121.0649	3	-	-	-	-	-	-	-	0	-	-	-	-	1	1	0	6	1
$C_4H_3Cl_2$	120.9606	-	-	-	-	2	-	-	-	-	-	-	-	-	-	-	-	2	1
	119.0605	-	-	-	-	4	-	-	-	-	-	-	-	-	-	-	-	4	1
	119.0492	2	-	-	-	-	-	-	-	1	-	-	-	-	2	-	-	5	2
	118.9315	-	-	-	-	-	-	3	-	-	-	-	-	-	-	-	-	3	1
	117.0699	-	-	-	-	-	-	-	4	0	-	-	-	-	-	6	-	10	2
	116.9335	-	-	-	-	-	-	4	-	-	-	-	-	-	-	-	-	4	1
	116.0621	0	-	-	0	-	-	-	2	0	0	-	-	-	-	-	-	3	1
	116.0578	-	0	-	0	1	-	1	1	0	1	-	-	-	-	3	-	6	2
	116.0496	-	-	-	1	3	-	3	1	-	3	-	-	-	-	-	-	12	5
C_9H_7	115.0544	-	1	-	4	7	-	6	12	2	6	-	5	-	-	28	-	71	9
C_8H_5N	115.0418	-	-	-	1	1	-	1	1	-	1	-	-	-	-	-	-	5	3
C_6H_8Cl	115.0310	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	1	1
	114.0339	-	-	-	3	5	-	5	3	-	5	-	-	-	-	-	-	20	5
	113.0962	-	-	-	-	-	-	-	-	-	2	-	-	-	-	-	-	2	1
	113.0917	-	-	-	-	-	-	-	2	-	-	-	-	-	-	-	-	2	1
	113.0153	-	-	-	0	1	-	-	2	-	-	-	-	-	-	-	-	3	2
	110.9577	-	-	-	-	3	-	-	-	-	-	-	-	-	-	-	-	3	1
	110.1091	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	2	1
	109.0649	1	-	-	-	1	-	2	-	-	1	-	-	-	1	1	0	8	4
	108.9609	-	-	-	-	5	-	-	-	-	-	-	1	-	-	-	-	6	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
	108.0934	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	1
	108.0889	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	1
	108.0571	6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	6	1
	108.0525	-	-	-	-	-	-	-	-	1	-	-	-	-	-	-	1	2	1
C_8H_{11}	107.0856	11	-	-	-	-	-	-	-	0	-	-	-	-	4	3	2	19	4
C_7H_7O	107.0492	1	-	-	-	-	-	-	-	17	-	-	-	-	-	-	9	27	3
	106.0777	0	-	-	-	-	-	-	-	0	-	-	-	-	2	-	-	2	1
	106.0733	1	-	-	-	-	-	-	-	-	-	-	-	-	2	-	-	3	1
C_8H_9	105.0700	9	-	-	-	-	-	-	-	1	-	-	-	-	19	2	1	32	3
	104.0621	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-	-	2	1
	104.0577	-	-	-	-	-	-	0	-	-	-	-	-	-	1	-	-	1	1
C_8H_7	103.0544	2	-	-	-	-	-	2	-	0	-	-	-	-	12	1	-	18	4
	103.0417	-	-	-	0	1	-	1	-	-	1	-	-	-	-	-	-	3	1
	102.0465	-	0	-	0	-	-	0	-	0	0	-	-	-	1	1	-	3	1
	98.9997	-	-	-	-	1	-	1	-	-	-	-	-	-	-	-	-	2	1
	98.1046	-	-	-	-	-	-	-	-	-	3	-	-	-	-	-	-	3	1
C_7H_{13}	97.1012	-	-	-	-	-	-	-	-	-	47	-	-	-	-	-	-	47	1
C_7H_{11}	95.0856	10	-	-	-	-	10	-	-	-	9	-	-	-	11	11	2	52	6
C_6H_7O	95.0492	1	-	-	0	1	-	1	-	3	1	-	-	-	1	-	0	8	4
C_7H_{10}	94.0778	0	-	-	-	-	-	9	-	-	-	-	-	-	-	-	-	10	1
$C_6{}^{13}CH_9$	94.0733	1	-	-	-	-	-	2	-	-	-	-	-	-	-	-	0	4	2
C_7H_9	93.0700	17	0	-	1	5	-	31	-	0	1	-	1	-	-	4	4	63	5
C_7H_8	92.0621	1	-	-	-	-	-	10	-	-	-	-	-	-	1	-	-	12	2
$C_6{}^{13}CH_7$	92.0577	2	0	-	0	4	-	2	-	0	-	-	1	-	1	1	0	12	4
C_7H_7	91.0543	33	1	47	4	56	3	25	-	2	1	-	11	10	10	17	3	220	12
	89.0387	0	1	-	1	2	-	2	8	2	1	-	4	-	1	2	-	24	7
	88.0308	-	0	-	1	2	-	1	1	-	1	-	-	-	-	-	-	6	2
	86.9996	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	1	1
	84.9839	-	-	-	-	2	-	-	-	-	-	-	1	-	-	-	-	3	1
	84.0934	-	-	-	-	-	-	-	-	-	5	-	-	-	-	-	-	5	1

Mol. Form.	ion *(m/z)*	ale	bif	cyf	cyh	cpe	cph	del	esf	eto	fen	flu	per	phe	pra	res	tet	sum	#pyr
C_6H_{11}	83.0856	-	-	-	-	-	-	-	-	0	1	-	-	-	-	-	-	1	1
C_5H_7O	83.0492	1	-	-	1	2	-	2	-	-	13	-	-	-	1	-	-	19	4
$CHCl_2$	82.9449	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	1	1
	82.0733	4	-	-	-	-	-	-	1	-	0	-	-	-	3	3	1	12	3
	81.9236	-	-	-	-	-	-	4	-	-	-	-	-	-	-	-	-	4	1
C_6H_9	81.0699	56	-	-	-	-	46	-	-	-	3	-	-	38	52	50	10	256	7
	80.0621	-	-	-	0	-	-	1	-	-	0	-	-	-	-	-	-	1	1
	80.0576	3	-	-	-	-	-	1	-	0	0	-	-	-	2	1	1	7	2
	79.9256	-	-	-	-	-	-	3	-	-	-	-	-	-	-	-	-	3	1
C_6H_7	79.0543	49	0	-	1	-	8	-	-	1	3	-	1	-	23	11	7	103	6
	78.0465	2	-	-	1	-	-	-	-	1	1	-	1	-	3	1	0	9	3
	78.0420	-	-	-	0	1	-	-	1	0	1	-	-	-	1	-	0	4	1
C_6H_5	77.0387	16	1	-	6	15	-	19	8	4	9	-	3	13	16	5	4	118	13
	76.0309	-	1	-	1	2	-	-	1	0	2	-	-	-	-	-	-	8	4
	75.0230	-	0	-	1	2	-	-	1	-	1	-	-	-	-	-	-	4	1
	74.9810	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	1	1
	72.9841	-	-	-	0	3	-	-	0	-	-	-	-	-	-	-	-	3	1