Supporting Information C (SI-C) to:

New Relevant Pesticide Transformation Products in Groundwater Detected Using Target and Suspect Screening for Agricultural and Urban Micropollutants with LC-HRMS

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Tables SI-C 1 and 2 present the suspects, which were confirmed, tentatively identified or rejected using reference material or expert knowledge. The identification confidence is communicated using the classification method of Schymanski et al. 2014. Figure SI-C 1 summarises the identification confidence levels. We confirmed 19 transformation products (TPs) and one pesticide (Level 1) and rejected nine TPs and seven pesticides. Two TPs were identified as probable (Level 2, no reference standard), three TPs as tentative structure (Level 3), either because reference material was not available (2 TPs) or due to analytical problems (1 TPs), and three suspects remained unclear and could not be classified following Schymanski et al. (2014).

Extracted ion chromatograms (EICs) and MS/MS spectra of confirmed suspects (Level 1-3) are illustrated on page 18-45. In addition, EICs of the most intense fragments were plotted to avoid that background ions are mistakenly annotated as MS/MS fragments (see e.g. Fludioxonil−TP CGA 192155, Fluxapyroxad (BAS 700 F)−TP CSAA798670).

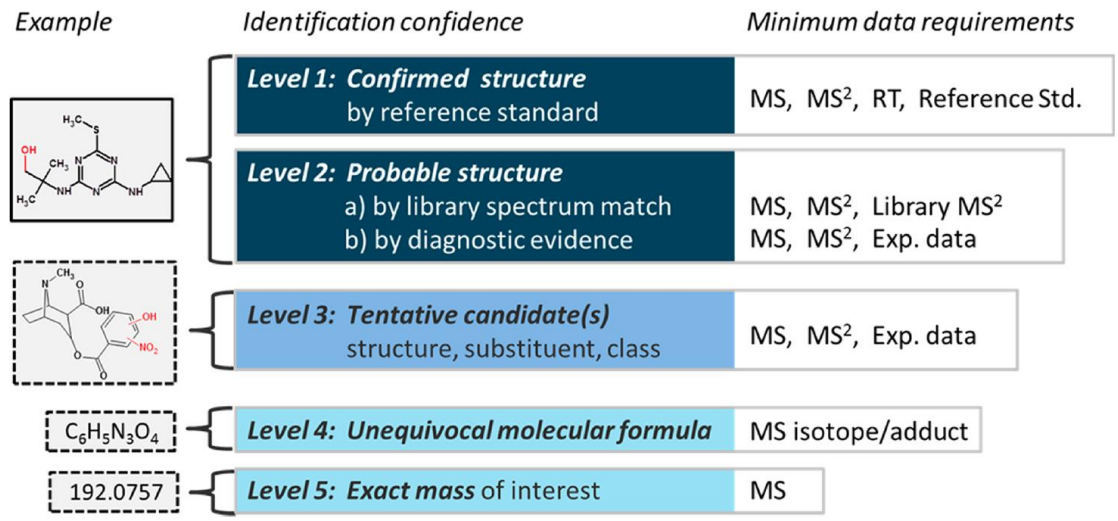


Figure SI-C 1: Identification confidence levels (Schymanski et al. 2014).

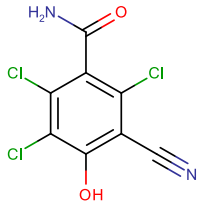
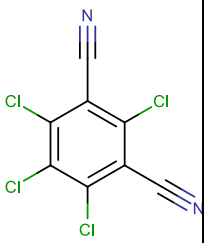
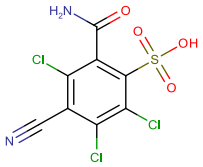
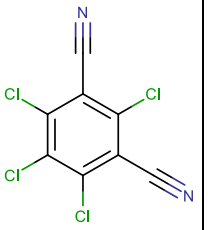
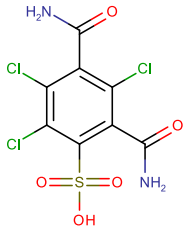
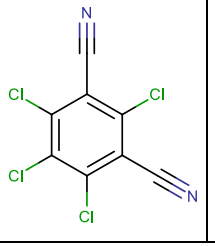
References

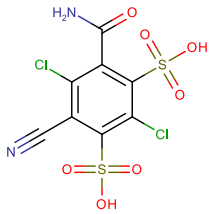
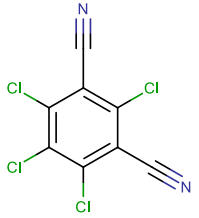
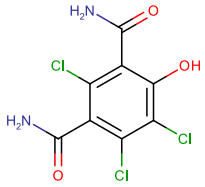
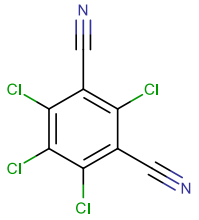
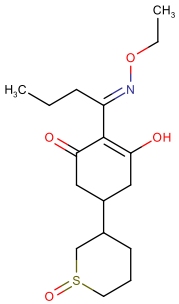
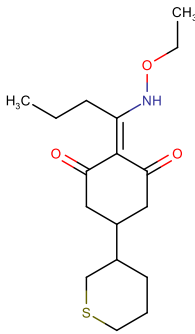
Schymanski, E.L., Jeon, J., Gulde, R., Fenner, K., Ruff, M., Singer, H.P. and Hollender, J. 2014. Identifying small molecules via high resolution mass spectrometry: communicating confidence. Environ Sci Technol 48(4), 2097-2098, 10.1021/es5002105.

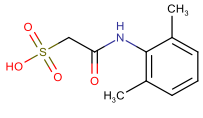
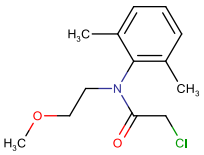
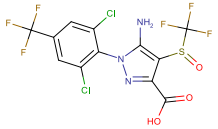
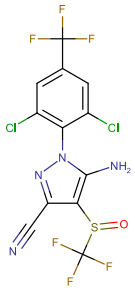
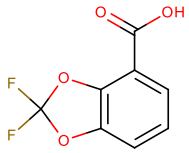
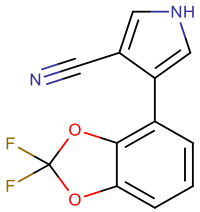
BLW, 2018. Sales per active ingredient (Verkaufsmengen je Pflanzenschutzmittel-Wirkstoff). Federal Office for the Agriculture. https://www.blw.admin.ch/blw/de/home/nachhaltige-produktion/pflanzenschutz/pflanzenschutzmittel/verkaufsmengen-der-pflanzenschutzmittel-wirkstoffe.html. Accessed: 18/01/2019.

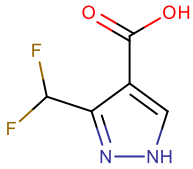
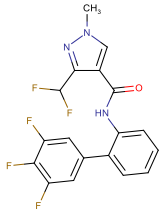
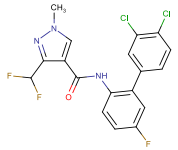
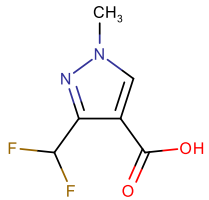
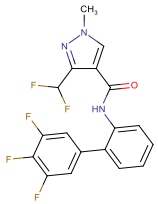
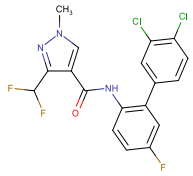
Reemtsma, T., Alder, L. and Banasiak, U., 2013. Emerging pesticide metabolites in groundwater and surface water as determined by the application of a multimethod for 150 pesticide metabolites. Water research 47(15), 5535-5545.

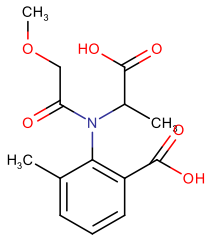
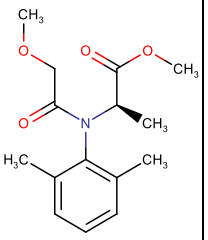
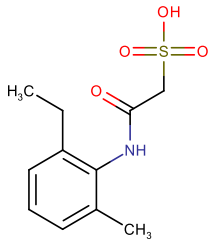
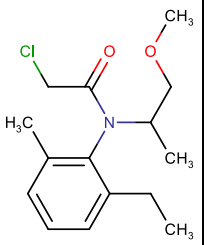
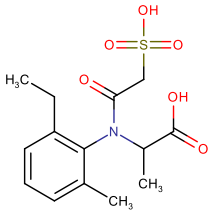
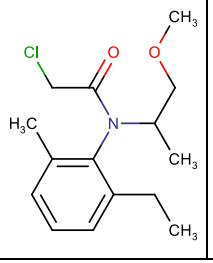
Table SI-C 1: Pesticide TPs

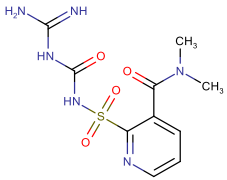
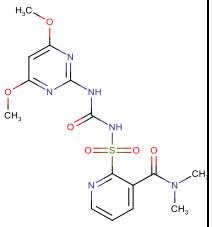
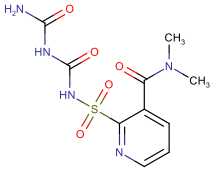
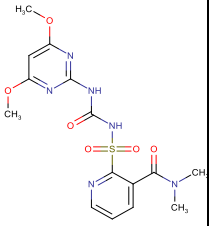
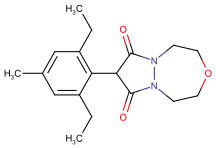
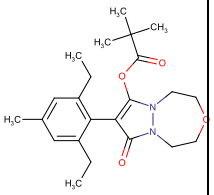
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Chlorothalonil-TP SYN507900 [M-H]- Level 1			30-50	0.4	12.9	Syngenta	Not included in study	13	150	1.3	• MS/MS okay • Biphenyl column: confirmed
Chlorothalonil-TP R417888 [M-H]- Level 1			30-50	-0.7	15.3	Syngenta	55	28	1300	1	• MS/MS okay • Biphenyl column: confirmed
Chlorothalonil-TP R471811 [M-H]- Level 1			30-50	-1.7	7.5	Syngenta	Not included in study	31	2700	3	• MS/MS okay • Biphenyl column: confirmed but RTs are not perfectly stable

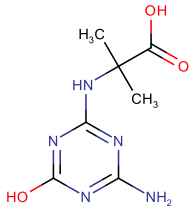
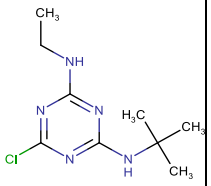
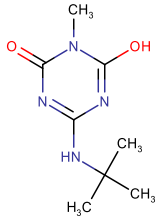
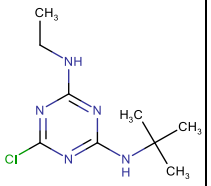
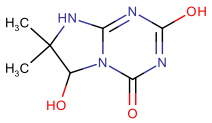
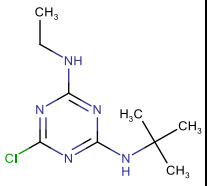
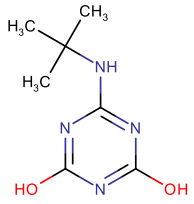
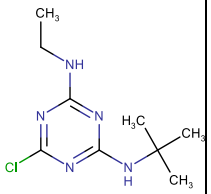
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Chlorothalonil-TP R419492 [M-2H]2- Level 1			30-50	-4.5	5	Syngenta	Not included in study	18	-	-	• Compound was detected later and could therefore not be confirmed and quantified in the here presented samples. Compound was confirmed (Level 1) in other groundwater samples.
Chlorothalonil-TP SYN548580 [M-H]- Level 1			30-50	0.0	10	Syngenta	Not included in study	13	-	-	• Compound was detected later and could therefore not be confirmed and quantified in the here presented samples. Compound was confirmed (Level 1) in other groundwater samples.
Cycloxydim-TP BH 517-TSO E/Z-isomer [M+H]+ Level 1			<1	-0.1	15.5 & 19	BASF	Not included in study	1	1.3	1	• 2 peaks in standard (RT 15.5 & 19 min); peak 19 min is more intense, different fragment ratios → E/Z isomers • MS/MS okay • Possibly, concentrations are overestimated as TP may be formed during LC by hydrolysis of cycloxydim: pH~3 →single injection of cycloxydim contains 5-10% of TP (estimation based on peak areas) • Biphenyl column: confirmed

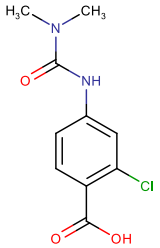
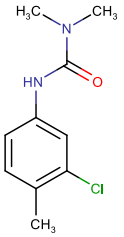
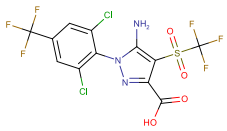
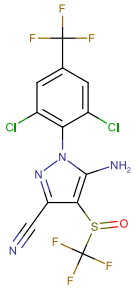
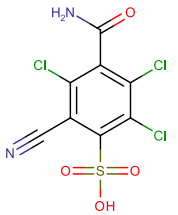
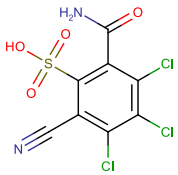
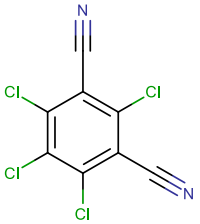
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Dimethachlor-TP CGA 369873 [M-H]- Level 1			5-10	-0.9	15	Syngenta	39	28	95	0.5	• MS/MS okay • Biphenyl column: confirmed
Fipronil-TP RPA 200761 [M+H]+ Level 1			<1	1.1	18.9	BASF	Not included in study	6	71	1	• MS/MS okay • Reference standard contains also fipronil-TP 106681 (intensity <1% relative to intensity of fipronil-TP RPA 200761) • reference standard: certificate of analysis is expired since May 2013 • Biphenyl column: TP is not in samples analysed with biphenyl column
Fludioxonil-TP CGA 192155 [M-H]- Level 1			1-5	-0.7	18	Syngenta	3	2	200	3	• MS/MS okay • Biphenyl column: confirmed

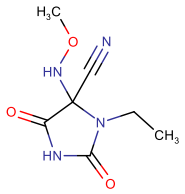
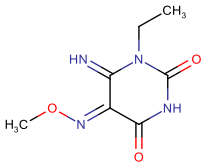
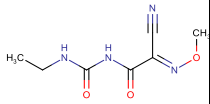
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Fluxapyroxad (BAS 700 F) & bixafen-TP CSCD465008 [M-H]- Level 1		 fluxapyroxad (BAS 700)  bixafen	1-5	-2.8	10.4	BASF	Not included in study	1	~60	15	• MS/MS okay • Shoulder peak in matrix sample possibly due to tautomerism or carboxylic acid (protonated / deprotonated form; predicted pKa 3.3) • concentrations are semiqantitative due to poor peak shape on Atlantis column • ChemSpider hit elutes 1.3 min later: 1-(Difluoromethyl)-1H-pyrazole-3-carboxylic acid • Biphenyl column: confirmed (better peak shape than on Atlantis column)
Fluxapyroxad (BAS 700 F)-TP CSAA798670 & bixafen-TP M42 [M+H]+ Level 1		 Fluxapyroxad (BAS 700)  bixafen	1-5	-2.7	12	BASF	Not included in study	1	13	10	• MS/MS okay • Shoulder peak in matrix sample possibly due to carboxylic acid (protonated / deprotonated form; predicted pKa 3.3) • Biphenyl column: confirmed

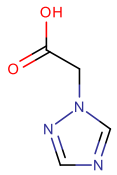
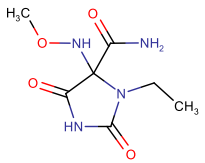
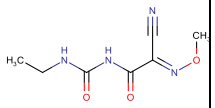
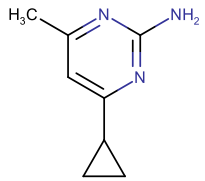
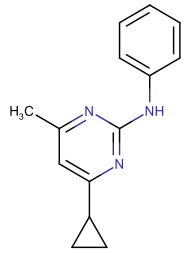
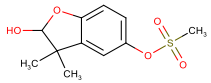
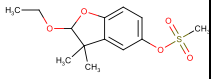
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Metalaxyl-M-TP CGA108906 [M+H]+ Level 1			1-5	-5	16	Syngenta	4	1	8.8	7	• MS/MS okay • Double peak possibly due to acid group (protonated / deprotonated form; predicted pKa 3.2) • Both peaks have same fragments • noisy -> high LOQ • according to MS/MS, compound is in several samples • Biphenyl column: TP is not in samples analysed with biphenyl column
Metolachlor-TP CGA 368208 / Acetochlor sulfonic acid [M-H]- Level 1			10-30	-0.5	17	Syngenta	9	20	150	1	• MS/MS okay • TP of metolachlor-ESA & acetochlor • Biphenyl column: confirmed
Metolachlor-TP NOA413173 [M-H]- Level 1			10-30	-3.6	22	Syngenta	290	22	430	1.7	• MS/MS okay • Double peak like metolachlor-ESA • TP of metolachlor-ESA • Biphenyl column: confirmed

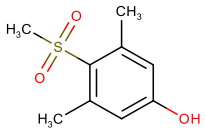
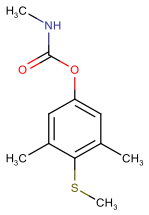
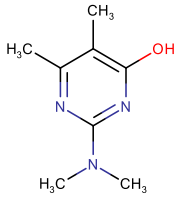
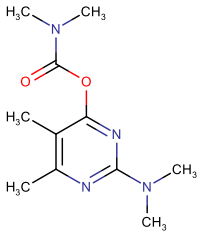
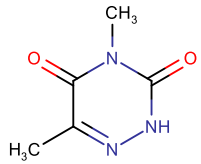
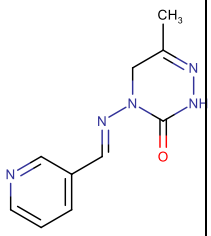
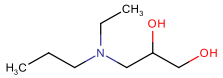
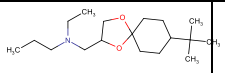
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Nicosulfuron-TP AUSN [M+H]+ Level 1			1-5	-1.6	8.5	Dupont	Not included in study	17	47	3	• MS/MS okay • Blind: up to 1 ng/L • Biphenyl column: confirmed
Nicosulfuron-TP UCSN [M+H]+ Level 1			1-5	-2.3	9.4	Dupont	Not included in study	27	75	0.2	• MS/MS okay • Biphenyl column: confirmed
Pinoxaden-TP NOA 407854 [M+H]+ Level 1			<1	2.1	18.2	Syngen ta	2	4	5.5	0.3	• Possibly, concentrations are overestimated as metabolite may be formed during LC by hydrolysis of pinoxaden: pH~3 →single injection of pinoxaden contains 10-20% of TP (estimation based on peak areas) • Noisy • Biphenyl column: confirmed

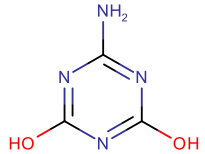
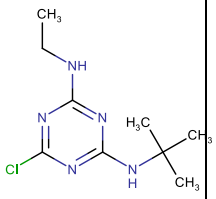
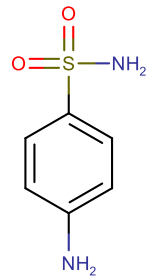
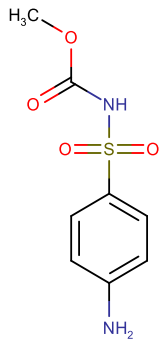
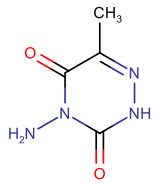
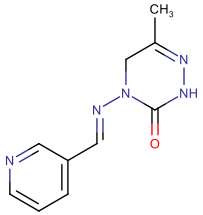
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Terbuthylazine-TP CSAA036479 [M+H]+ Level 1			30-50	-2.7	8	Syngenta	Not included in study	25	27	0.6	• MS/MS okay • Biphenyl column: confirmed
Terbuthylazine-TP CSCD648241 [M+H]+ Level 1			30-50	-2.5	14	Syngenta	Not included in study	29	190	0.5	• MS/MS okay • Biphenyl column: confirmed
Terbuthylazine-TP CSCD692760 [M+H]+ Level 1			30-50	-1.5	8.3	Syngenta	Not included in study	27	32	3	• MS/MS okay • Noisy • Biphenyl column: confirmed
Terbuthylazine-TP MT23-GS16984 [M+H]+ Level 1			30-50	1.8	12.7	Syngenta	Not included in study	29	78	0.5	• MS/MS okay • Many samples contain further isobaric peaks: RT 10.5, 11.8 min • Biphenyl column: confirmed

Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Chlorotoluron TP CGA 15140 [M-H]- Level 2a			10-30	-1.8	15		11	9	No STD	-	• **No standard** • Cl isotope pattern fits in samples with intense peaks • Fragments 197 & 152 detected (Reemtsma et al. 2013)
Fipronil-TP RPA 106681 [M+H]+ Level 2b			<1	1	19	BASF no STD synthet isized	Not included in study	11	120	-	• **No standard** • **semiquantitative**, same calibration model as for fipronil-TP RPA 200761; • standard RPA200761 seems to be not pure, i.e. contains as well RPA 106681 → fragments in standard & sample match perfectly
Chlorothalonil-TP 4-carbamoyl-2,3,5-trichloro-6-cyanobenzenes ulfonic acid / 2-carbamoyl-3,4,5-trichloro-6-cyanobenzenes ulfonic acid [M-H]- Level 3	 		30-50	-0.7 and -0.7	10.3 & 12		Not included in study	RT 10 min: 18 RT 12 min: 19	RT 10 min: 49 RT 12 min: 120	-	• Isomers of R417888 • **No standard** → **semi-quantitative,** conservative estimation, same calibration model as for chlorothalonil-TP R417888

Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Cymoxanil-TPs: IN-JX915 and IN-U3204 [M+H]+ Level 3	 TP IN-JX915 or  TP IN-U3204	 logD (pH7): 0.1	5-10	-2.3 and -0.3	11.5	Dupont	Not included in study	2	5.3	1	• Compounds are isobaric to cymoxanil **Cymoxanil:** • 2 peaks: 11.5, 15.3 min; highest intensity: 15.3 min **TP IN-JX915:** • 3 peaks (7.7, 11.5, 15.3 min); highest intensity: 11.5 min • Peak at 15.3 min is probably cymoxanil (cymoxanil is not stable during analysis → cymoxanil standard: 2 peaks (11.5 & 15.3 min) **TP IN-U3204:** • 2 peaks (7.7, 11.5); highest intensity: 11.5 min ➔ Equilibrium between 3 structures? According to logD (pH3): ○ 7.7 min: IN-JX915 ○ 11.5 min: IN-U3204 ○ 15.3 min: cymoxanil **Samples:** • Only peak at 11.5 min • Noisy • MS/MS okay Biphenyl column: concentration in samples was too low to be confirmed with biphenyl column

Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Azole-TP 1,2,4 triazole acetic acid [M+H]+ Rejected		Different azoles	5-10	-4.2	6	Bayer	Not included in study	0		10	• RT does not match • Biphenyl column: no clear peak in sample
Cymoxanil-TP IN-KQ960 [M+H]+ Rejected			5-10	-1.4	9.9	Dupont	Not included in study	0		15	• RT does not match • Noisy • Biphenyl column: rejected
Cyprodinil-TP CGA 249287 [M+H]+ Rejected			5-10	0.9	10	Syngen ta	Not included in study	0		5	• Noisy • Small peak (<5 ng/L) in 2 samples with similar RT as in standard, but fragment intensity ratios do not fit well in sample & standard • Spiked sample: double peak → probably different compound in sample • Biphenyl column: rejected (peak in sample elutes 0.5 min earlier)
Ethofumesate-2-hydroxy Rejected			10-30	1.3		Dr. Ehrenst orfer	Not included in study	0		Not deter mine d	• RT does not match • Low ionizability

Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Methiocarb-TP methiocarb sulfone phenol [M-H]- Rejected			1-5	1.5	14.5	Bayer	Not included in study	0		6	• RT does not match • Biphenyl column: rejected
Pirimicarb-desamido (R031805) [M+H]+ Rejected			1-5	1.8	8.5	Dr. Ehrenst orfer	Not included in study	0		0.5	• RT does not match • Biphenyl column: not tested
Pymetrozine-TP CGA371075 [M+H]+ Rejected			<1	-0.6	11	Syngen ta	Not included in study	0		-	• Reference standard: 2 peaks (10.7 & 11 min) • Samples: 1 peak (~10.8 min) • Different fragments • LOQ cannot be defined • Biphenyl column: no peak in STD
Spiroxamin aminodiol [M+H]+ Rejected			5-10	-2.3	7	Bayer	Not included in study	0		2	• RT does not match • • Biphenyl column: rejected

Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Terbuthylazine-TP MT24 G35713 [M+H]+ Rejected			30-50	0.5	3.8	Syngenta	Not included in study	0		Not determined	• RT does not match • Peak at 12.6 min in EIC is In-source fragment of Terbuthylazine-TP MT23-GS16984
Asulam-TP Sulfanilamide [M+NH4]+ Unclear			10-30	-0.2	7.5	LGC	Not included in study	3	14	10	• [M+H]+ and [M+NH4]+ of similar intensity • No MS/MS due to low intensity? • RT okay • Biphenyl column: concentration in samples was too low to be confirmed with biphenyl column
Pymetrozine-TP CGA294849 [M+H]+ Unclear			<1	-1.2	7.5	Syngenta	Not included in study	1	~LOQ	15	• No MS/MS in samples due to low intensity • noisy • low ionization efficiency • only in 1 sample with urban catchment • Standard was pursued due to later-eluting, more intense peaks • Biphenyl column: concentration in samples was too low to be confirmed with biphenyl column

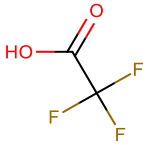
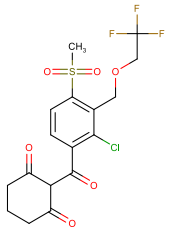
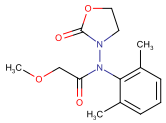
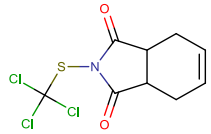
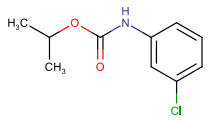
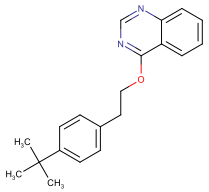
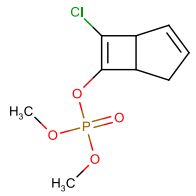
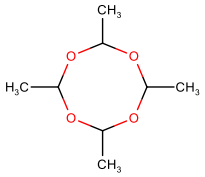
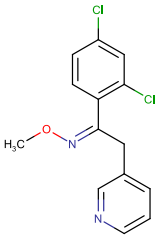
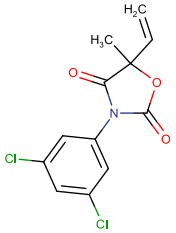
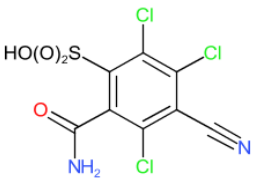
Suspect	Structure	Parent	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Trifluoroacetic-acid [M-H]- Unclear		 Tembotrione	<1	-2.6	5	Sigma-Aldrich	Not included in study	31		-	• in all samples • Only 1 fragment • Quantification not possible with applied LC method • Tembotrione is probably not the major source of trifluoroacetic acid • High background

Table SI-C 2: Pesticides

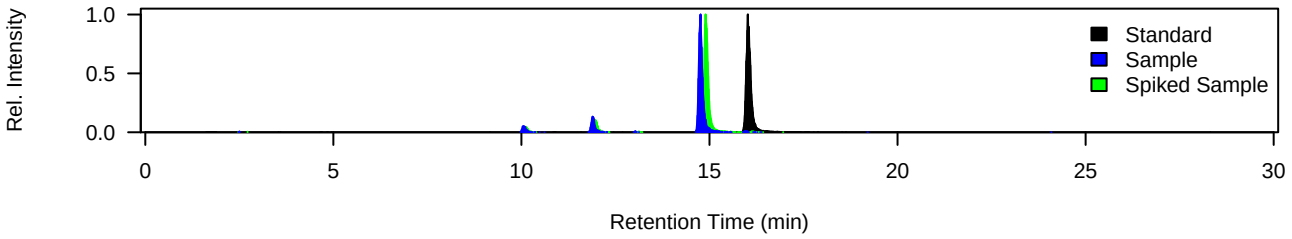
Suspect	Structure	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Oxadixyl [M+H]+ Level 1		No data	1.8	16	Riedel-de Haën	Not included in study	1	41	1	• MS/MS okay • Not approved as pesticide since 2011 • Biphenyl column: oxadixyl <LOQ in samples which were analysed with biphenyl column
Captan Rejected		30-50	3.2		Riedel-de Haën	Not included in study	0		-	• No ionization / not stable in water?
Chlorpropham (CIPC) [M+H]+ Rejected		1-5	3.2	20	Sigma-Aldrich	Not included in study	0		1000	• RT does not match • Low ionizability
Fenazaquin [M+H]+ Rejected		<1	5.4	24	Sigma-Aldrich	Not included in study	0		10	• RT does not match • Biphenyl column: no peaks in analysed samples
Heptenophos [M+H]+ Rejected		No data	1.1	18	Riedel-de Haën	Not included in study	0		50	• Ionization only in positive mode → no peak in samples

Suspect	Structure	Sales amount (t/a) (BLW 2018)	Log D (pH 7)	RT (min)	Refe-rence mate-rial from	Reemtsma et al. 2013: 75th percentile (ng/L)	Nr. Of Detects	Max. conc. (ng/L)	LOQ (ng/L)	Comment
Metaldehyde [M+NH4]+ Rejected		30-50	1.2	13.5	Dr. Ehrenstorfer	Not included in study	0		100	• High background • [M+NH4]+ more sensitive • Biphenyl column: rejected
Pyrifenox [M+H]+ Rejected		No data	3.7	18.5	Dr. Ehrenstorfer	Not included in study	0		3	• RT does not match • Biphenyl column: rejected
Vinclozolin [M+H]+ Rejected		No data	3.7	20.5	Dr. Ehrenstorfer		0		100	• RT does not match • Low ionizability

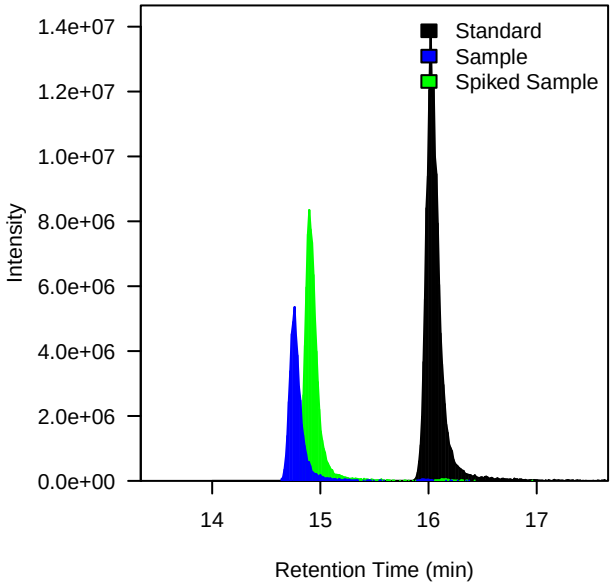
Chlorothalonil−TP R417888
Level 1
[M−H]− 326.88063
(STD 100 ng/L)



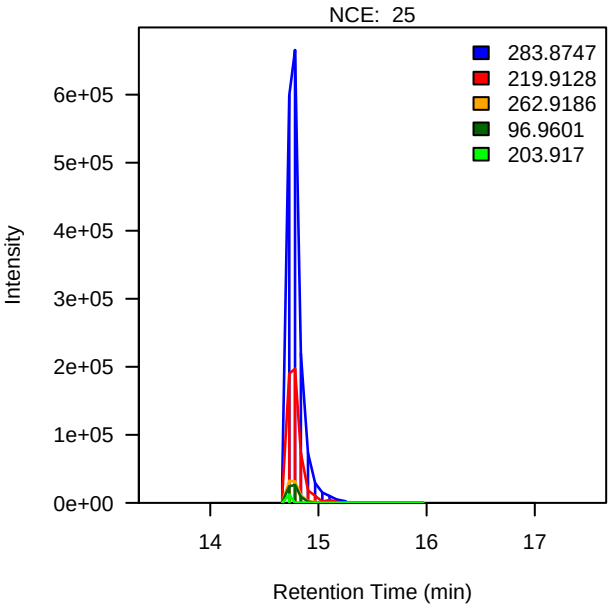
Normalized Extracted Ion Chromatogram (MS1)



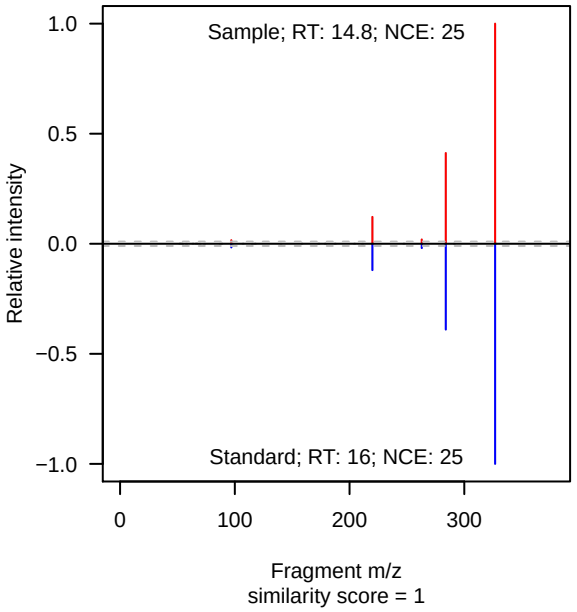
Extracted Ion Chromatogram (MS1)



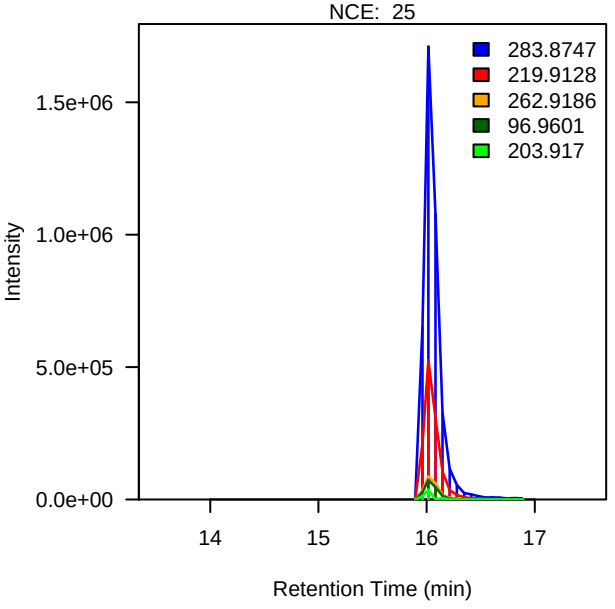
Most Intense Fragments in Sample



Most Intense MS2 Scan

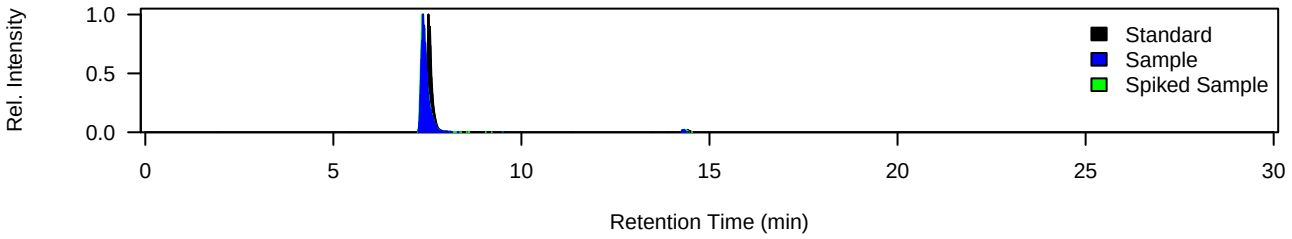


Most Intense Fragments in Standard

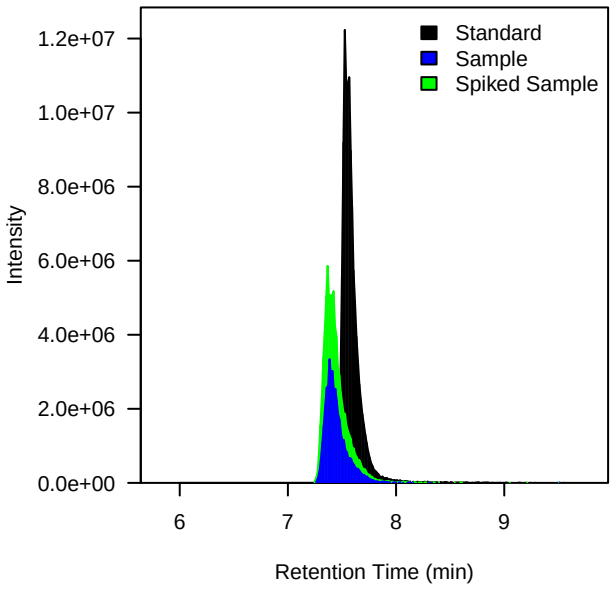


Chlorothalonil−TP R471811
Level 1
[M−H]− 344.8912
(STD 500 ng/L)

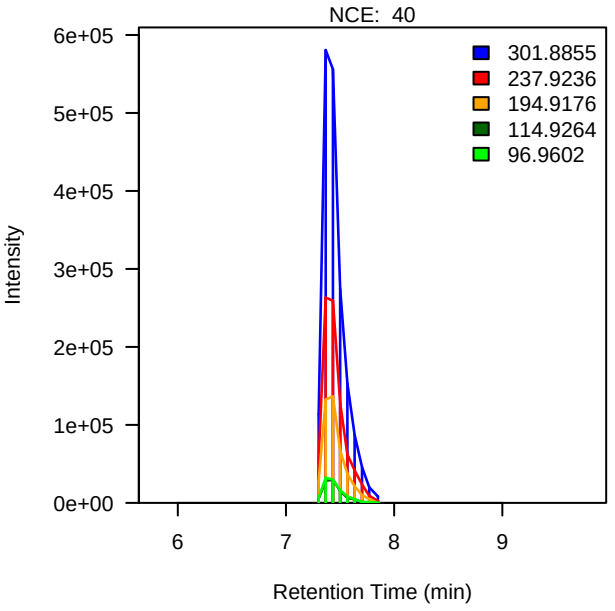
Normalized Extracted Ion Chromatogram (MS1)



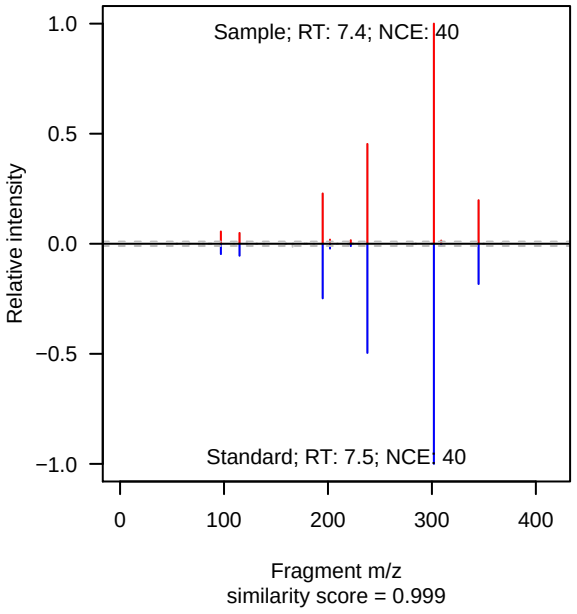
Extracted Ion Chromatogram (MS1)



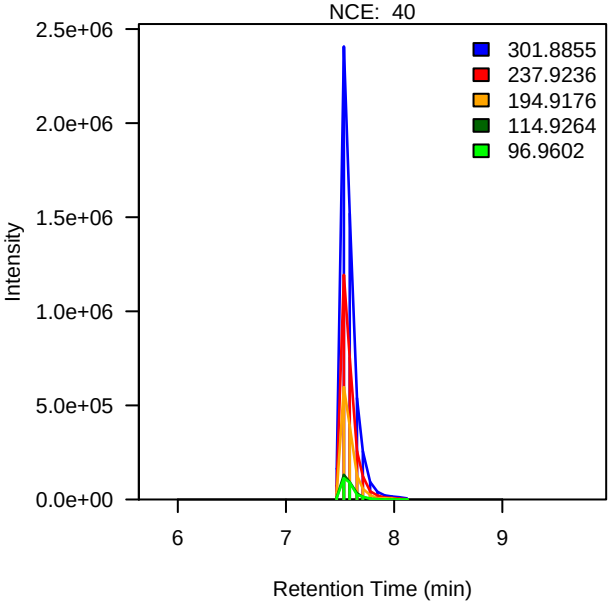
Most Intense Fragments in Sample



Most Intense MS2 Scan

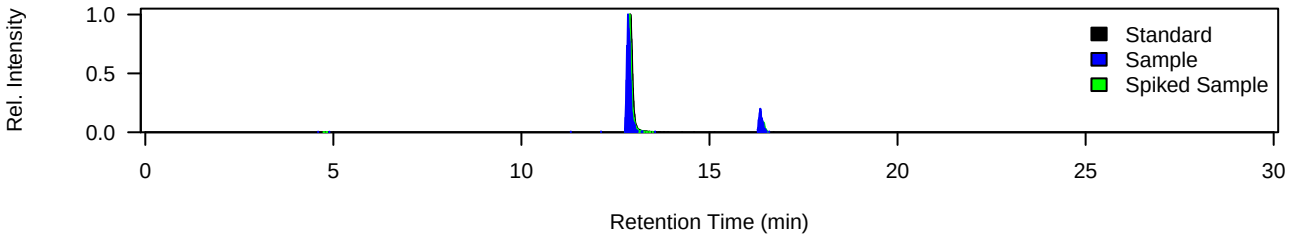


Most Intense Fragments in Standard

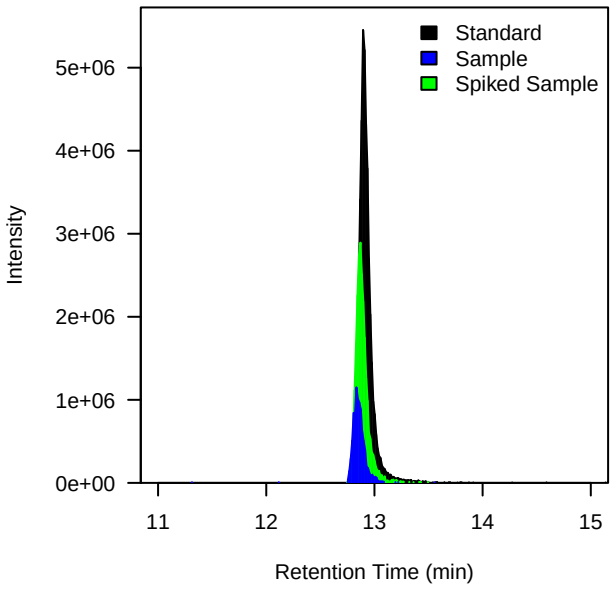


Chlorothalonil−TP SYN507900
Level 1
[M−H]− 262.91873
(STD 50 ng/L)

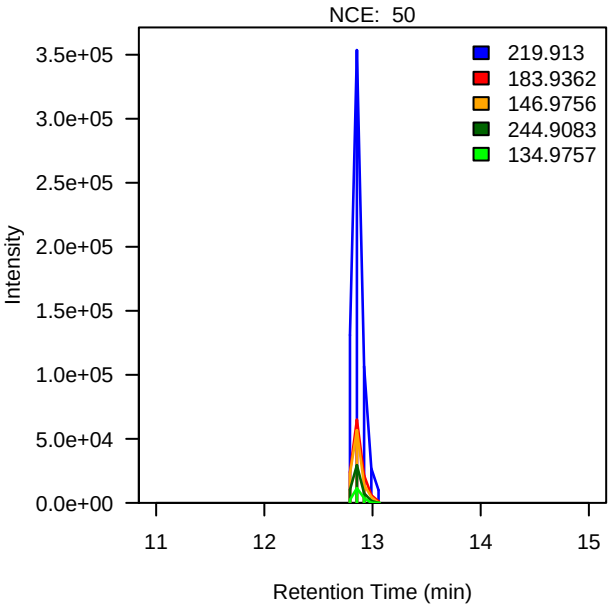
Normalized Extracted Ion Chromatogram (MS1)



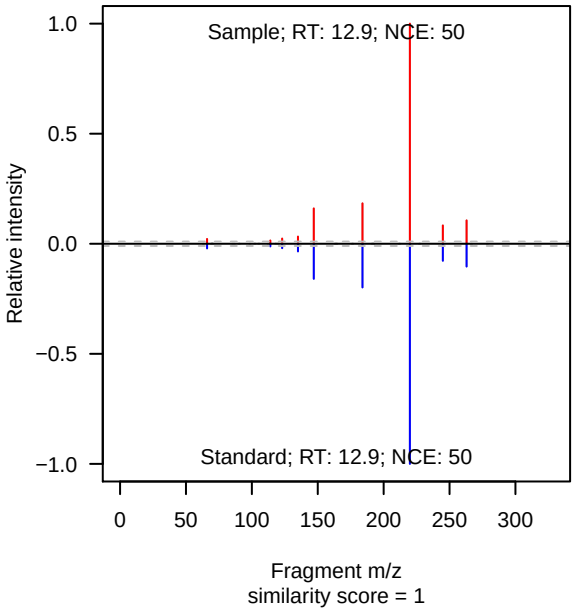
Extracted Ion Chromatogram (MS1)



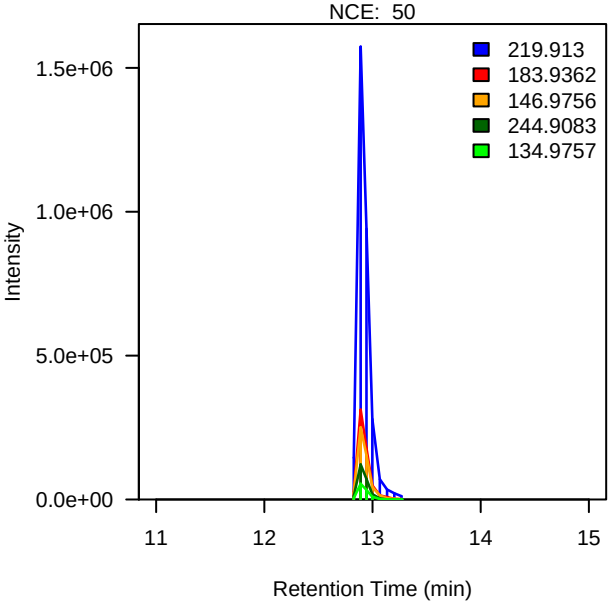
Most Intense Fragments in Sample



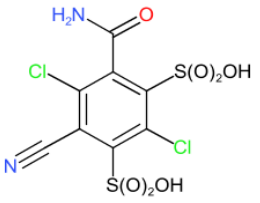
Most Intense MS2 Scan



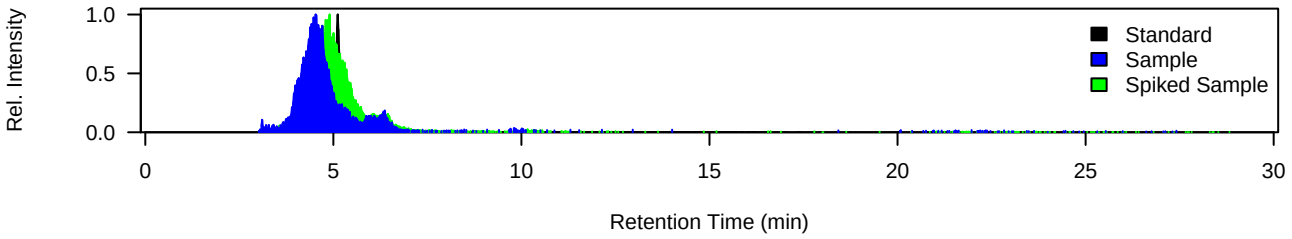
Most Intense Fragments in Standard



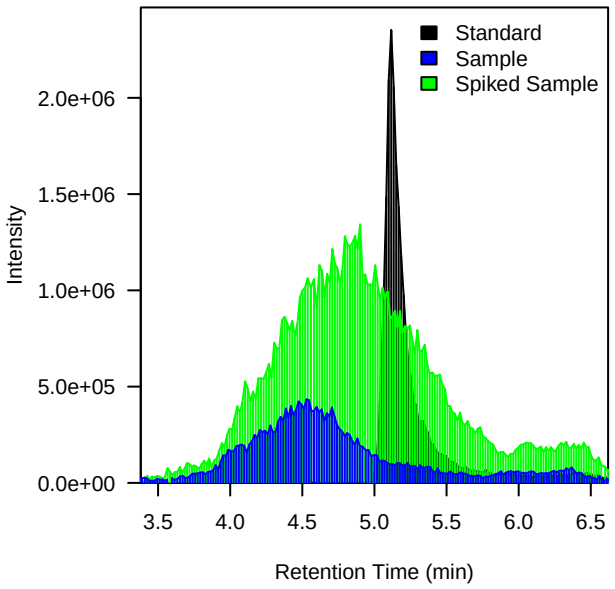
Chlorothalonil−TP R419492
Level 1
[M−2H]2− 185.934572
(STD 100 ng/L)



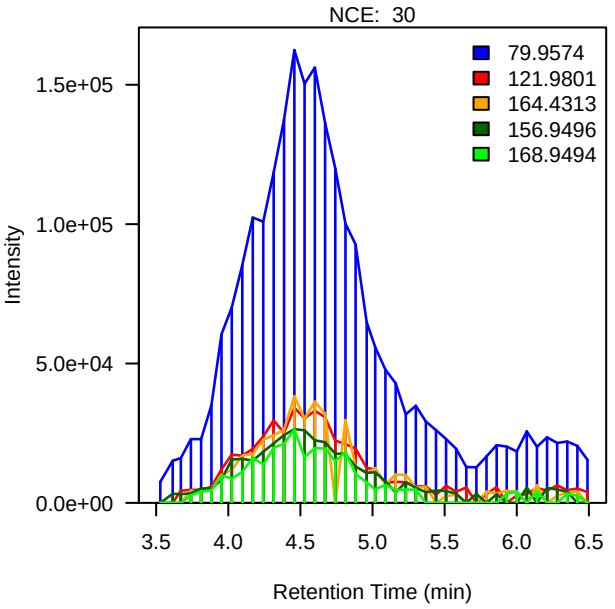
Normalized Extracted Ion Chromatogram (MS1)

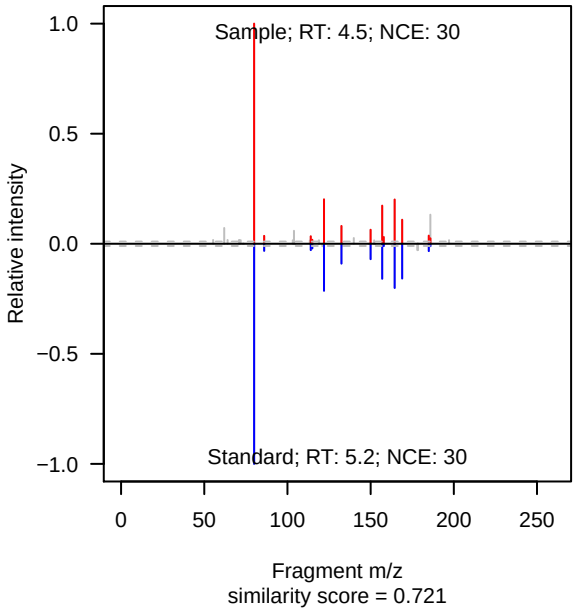


Extracted Ion Chromatogram (MS1)

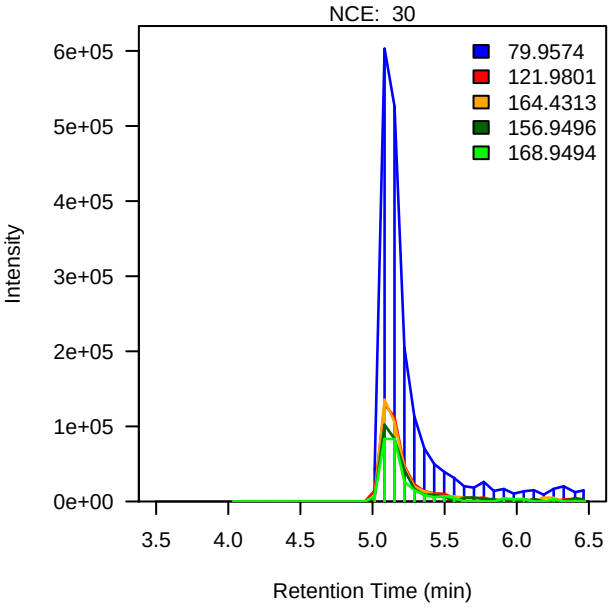


Most Intense Fragments in Sample

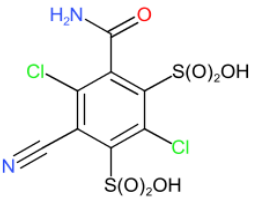




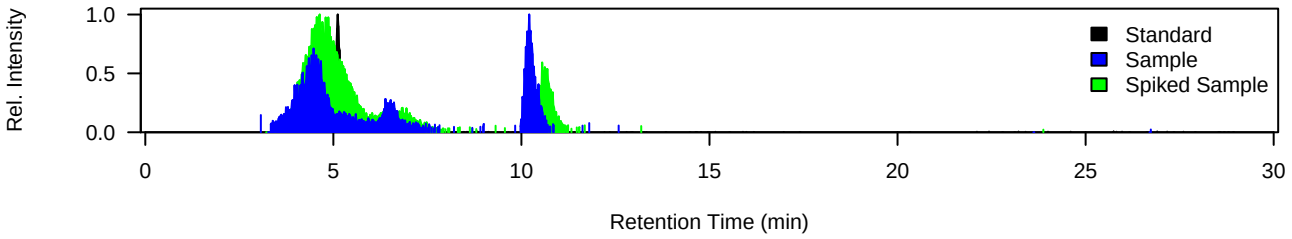
Most Intense Fragments in Standard



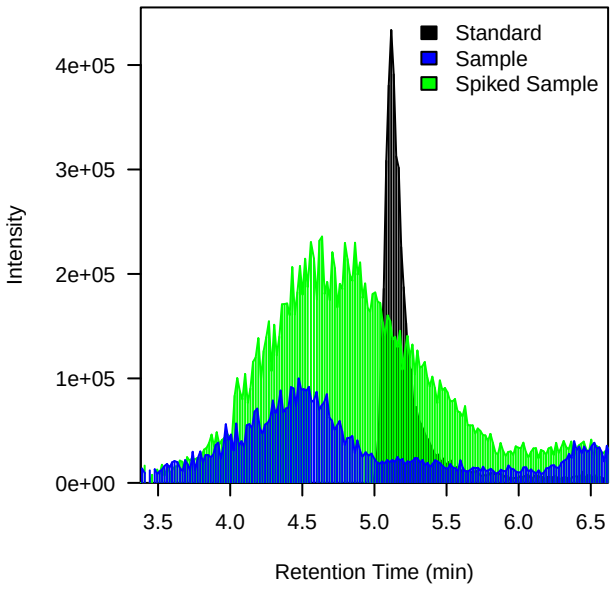
Chlorothalonil−TP R419492
Level 1
[M−H]− 372.87642
(STD 100 ng/L)



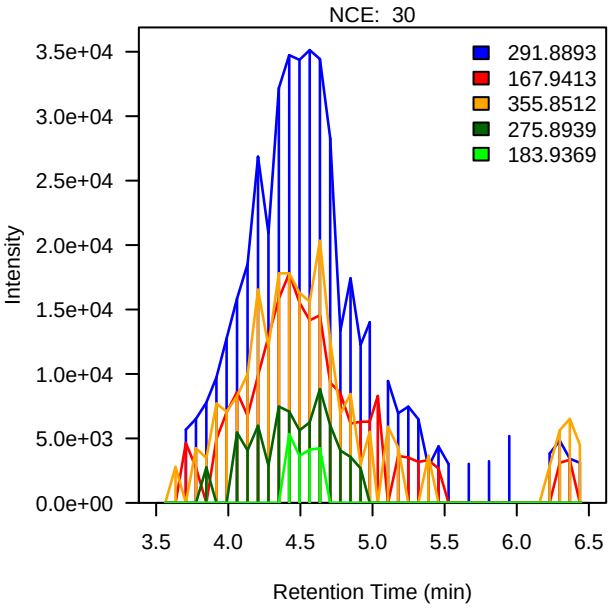
Normalized Extracted Ion Chromatogram (MS1)



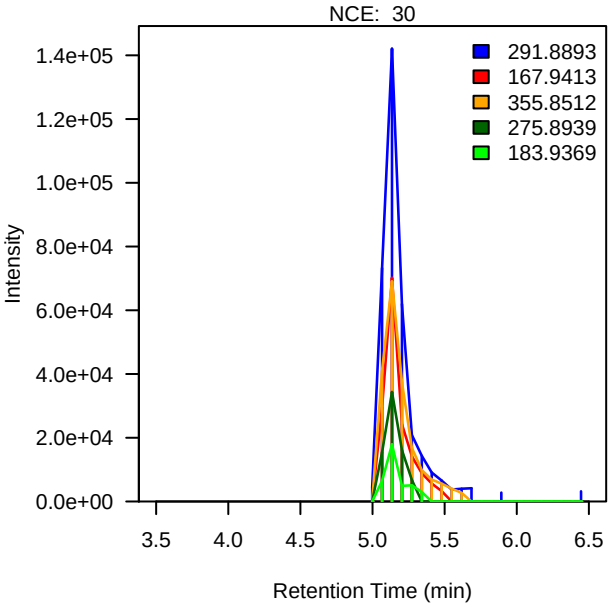
Extracted Ion Chromatogram (MS1)

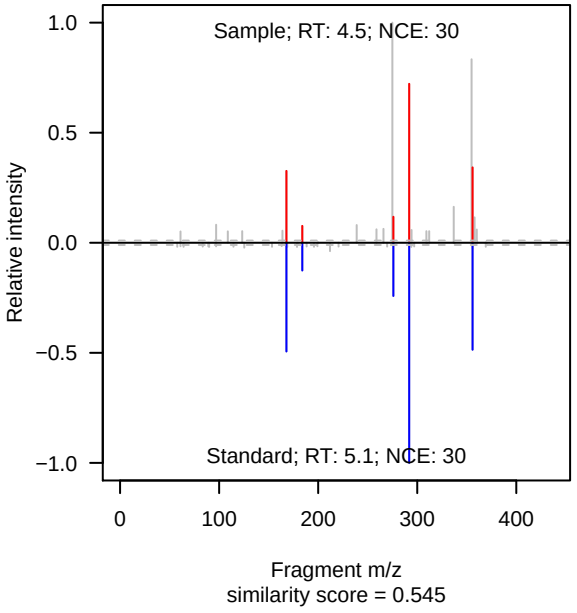


Most Intense Fragments in Sample

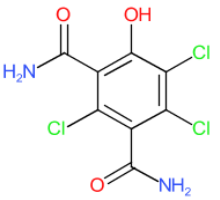


Most Intense Fragments in Standard

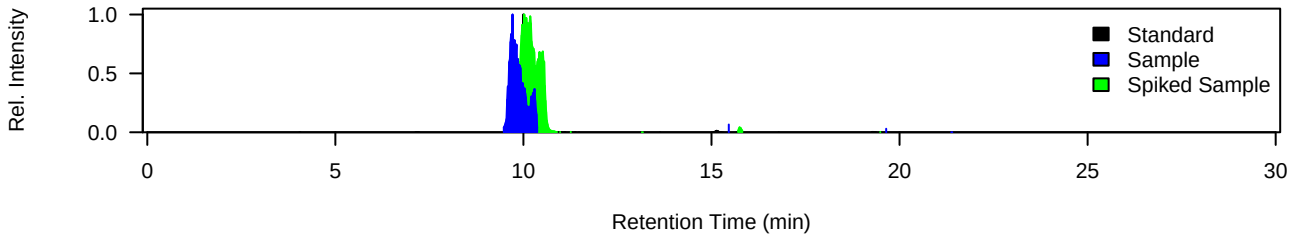




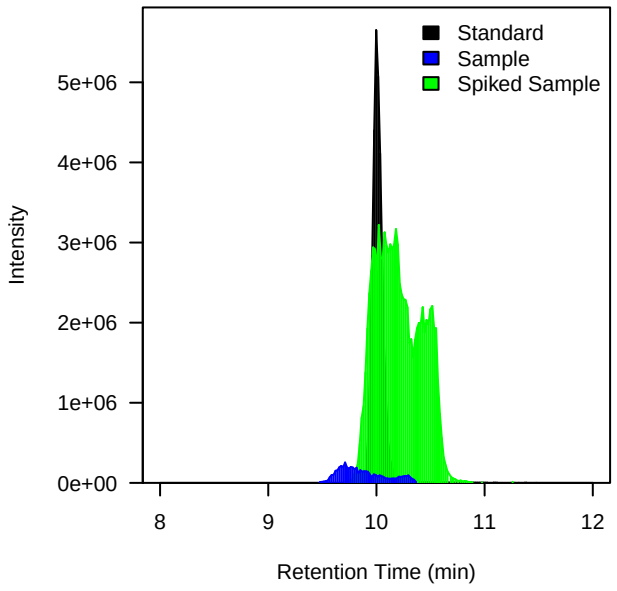
Chlorothalonil−TP SYN548580
Level 1
[M−H]− 280.9293
(STD 100 ng/L)



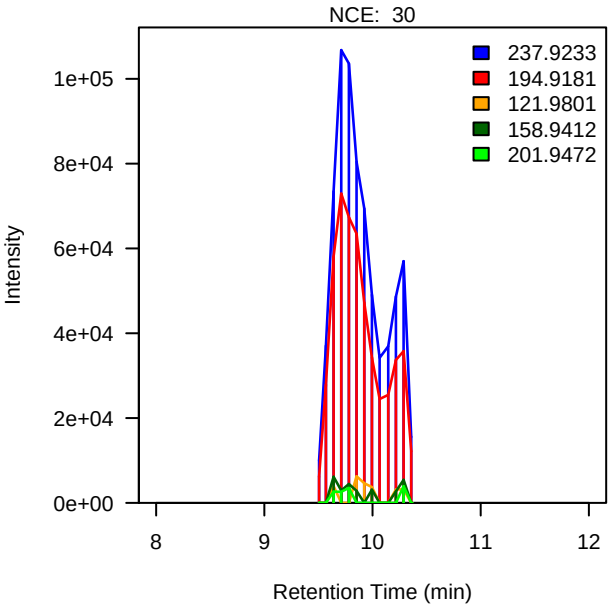
Normalized Extracted Ion Chromatogram (MS1)



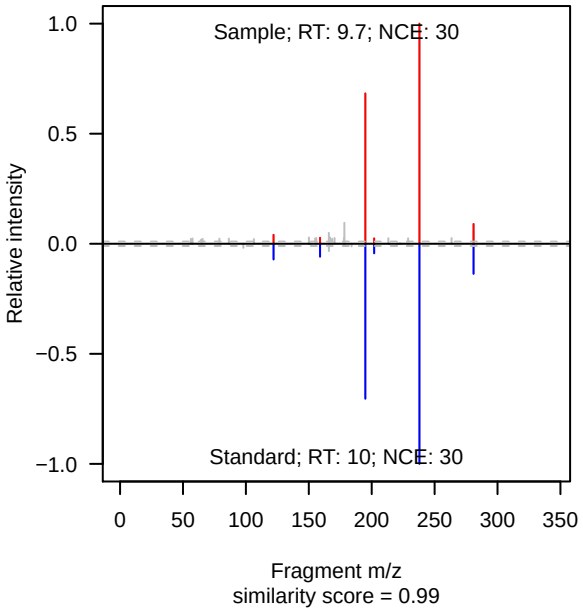
Extracted Ion Chromatogram (MS1)



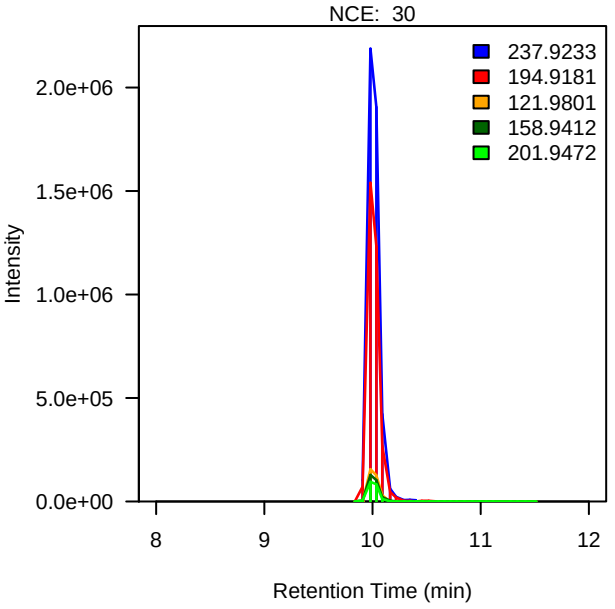
Most Intense Fragments in Sample



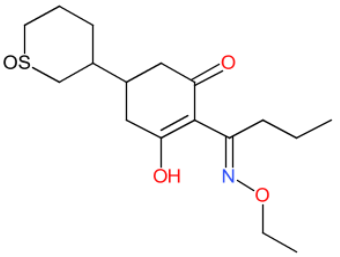
Most Intense MS2 Scan



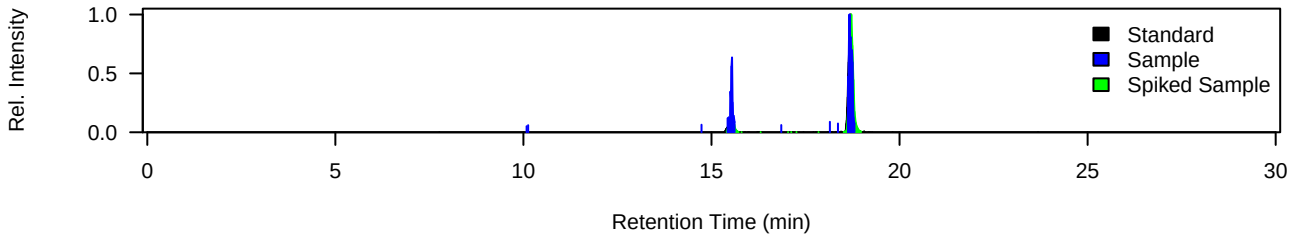
Most Intense Fragments in Standard



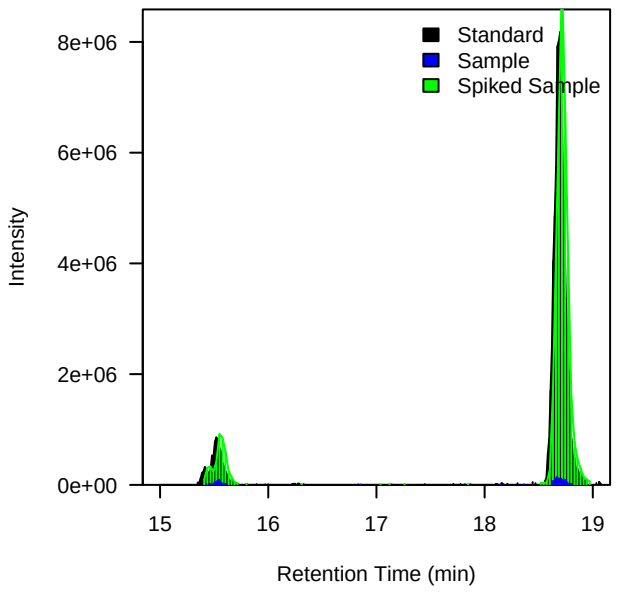
Cycloxydim−TP BH 517−TSO E/Z−isomer
Level 1
[M+H]+ 342.17336
(STD 25 ng/L)



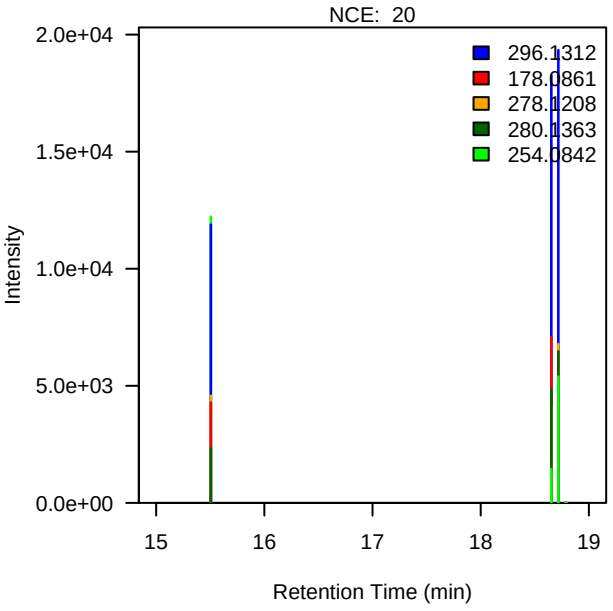
Normalized Extracted Ion Chromatogram (MS1)



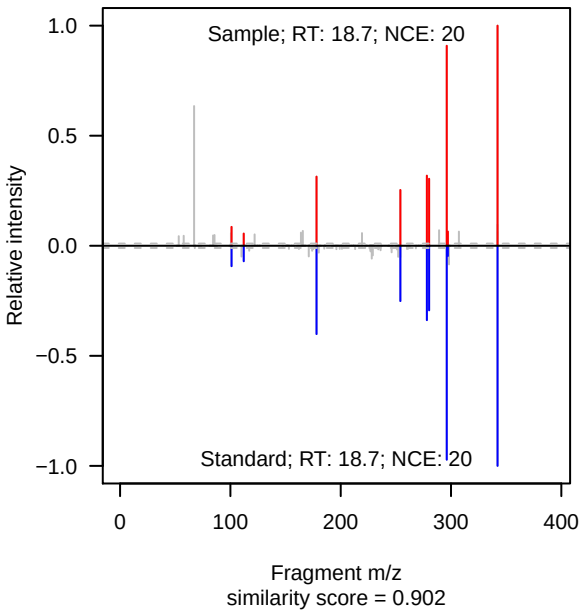
Extracted Ion Chromatogram (MS1)



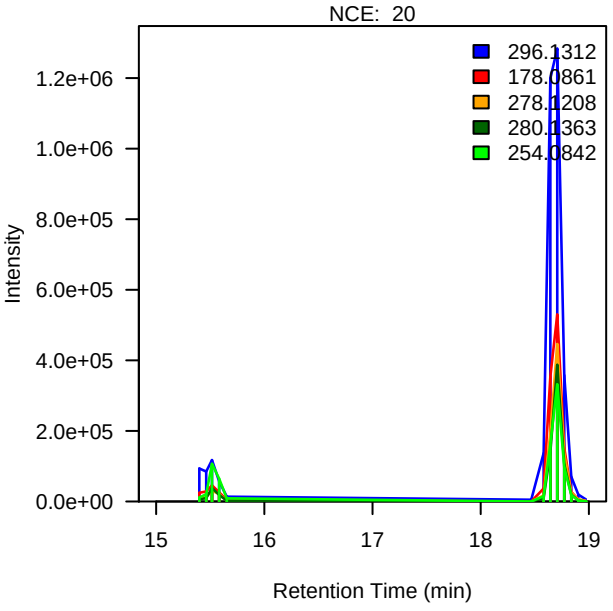
Most Intense Fragments in Sample



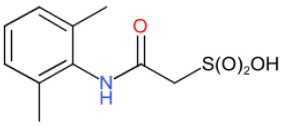
Most Intense MS2 Scan



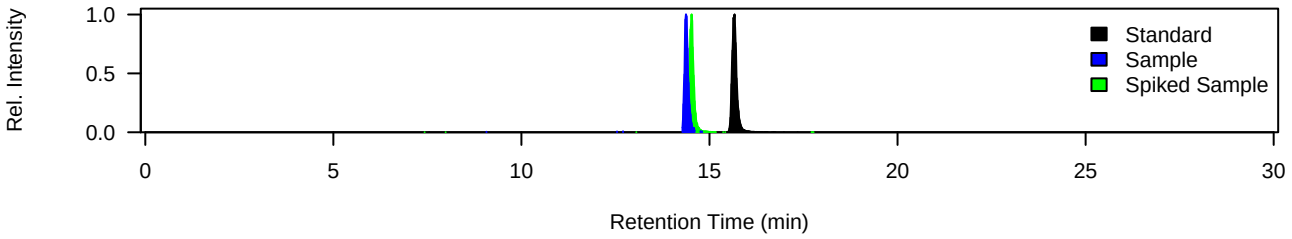
Most Intense Fragments in Standard



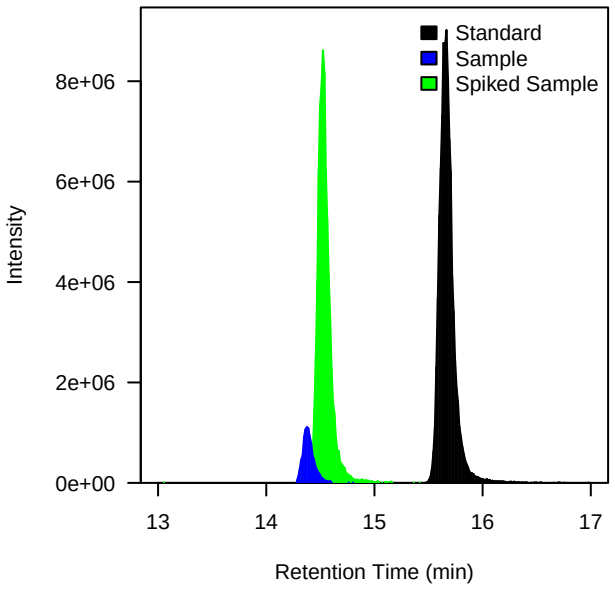
Dimethachlor−TP CGA 369873
Level 1
[M−H]− 242.04925
(STD 25 ng/L)



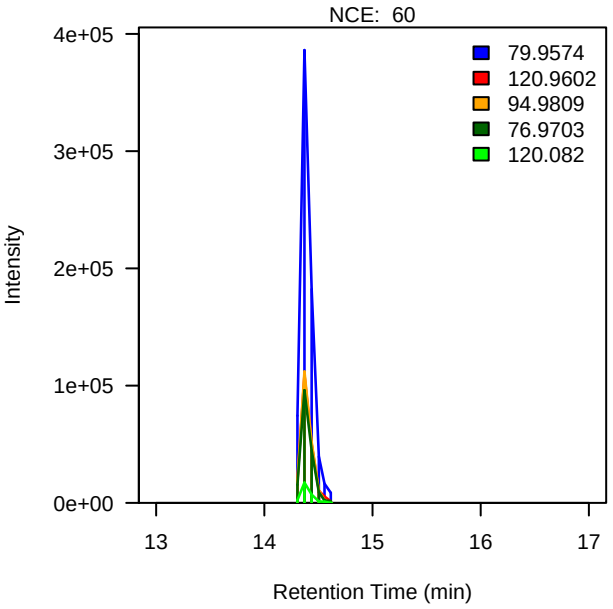
Normalized Extracted Ion Chromatogram (MS1)



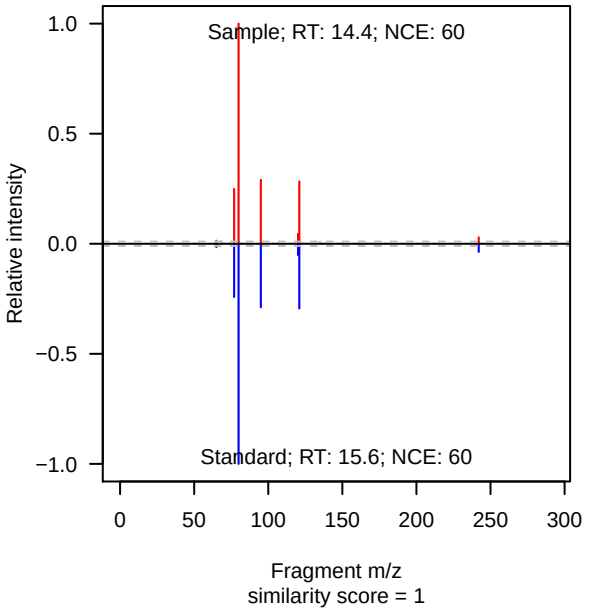
Extracted Ion Chromatogram (MS1)



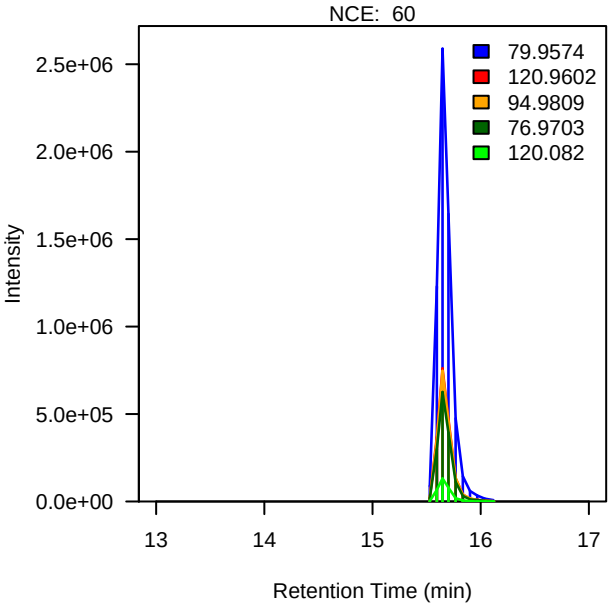
Most Intense Fragments in Sample



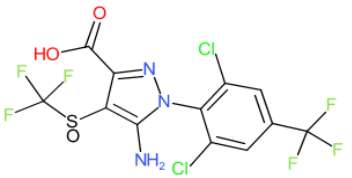
Most Intense MS2 Scan



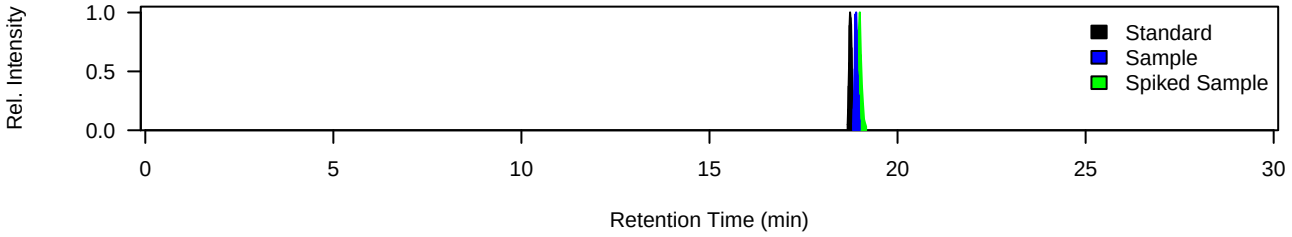
Most Intense Fragments in Standard



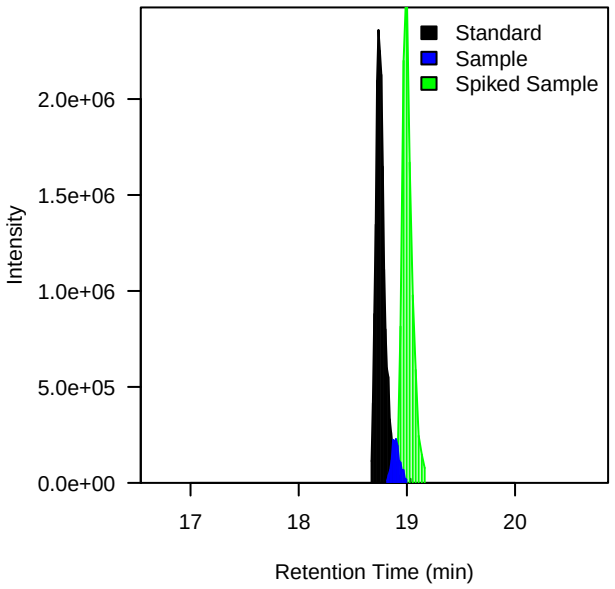
Fipronil−TP RPA 200761
Level 1
[M+H]+ 455.94056
(STD 25 ng/L)



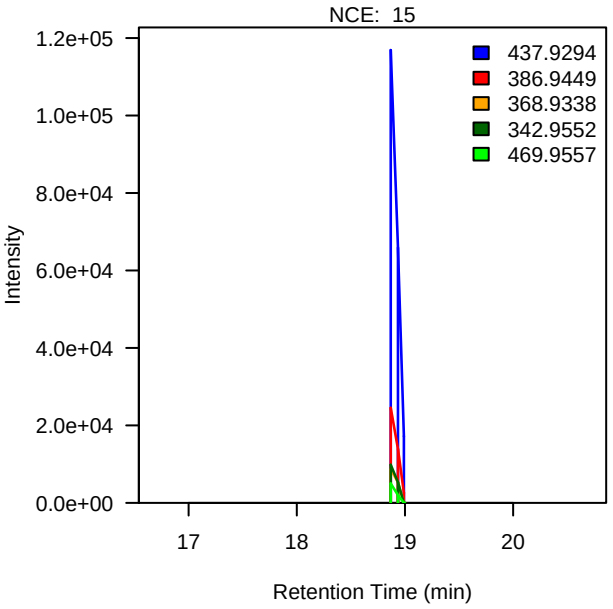
Normalized Extracted Ion Chromatogram (MS1)



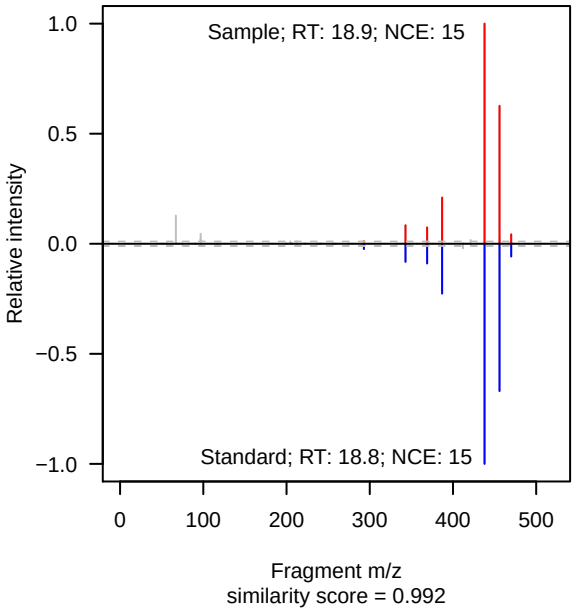
Extracted Ion Chromatogram (MS1)



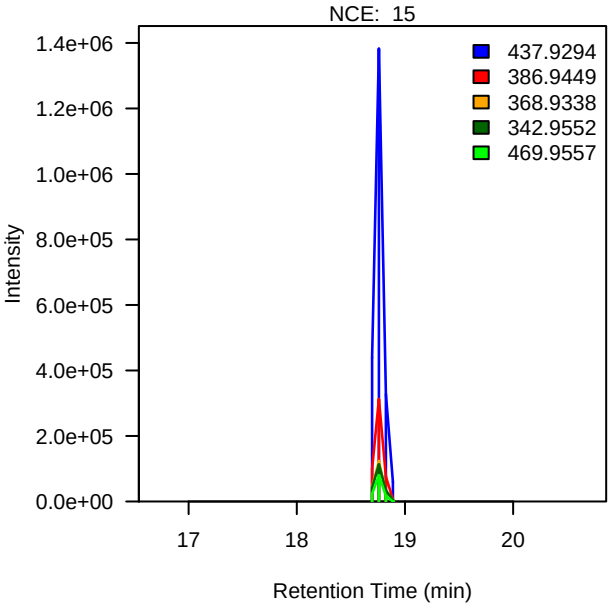
Most Intense Fragments in Sample



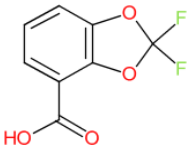
Most Intense MS2 Scan



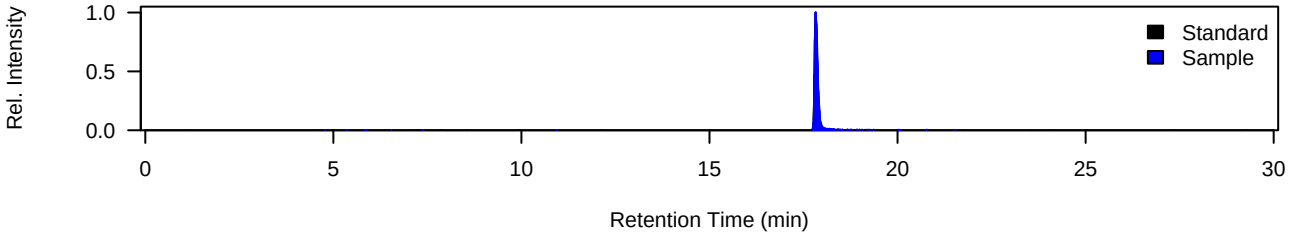
Most Intense Fragments in Standard



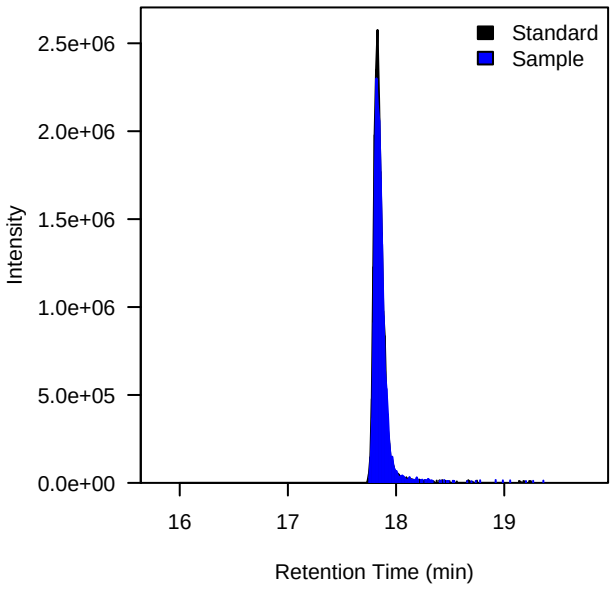
Fludioxonil−TP CGA 192155
Level 1
[M−H]− 201.00048
(STD 25 ng/L)



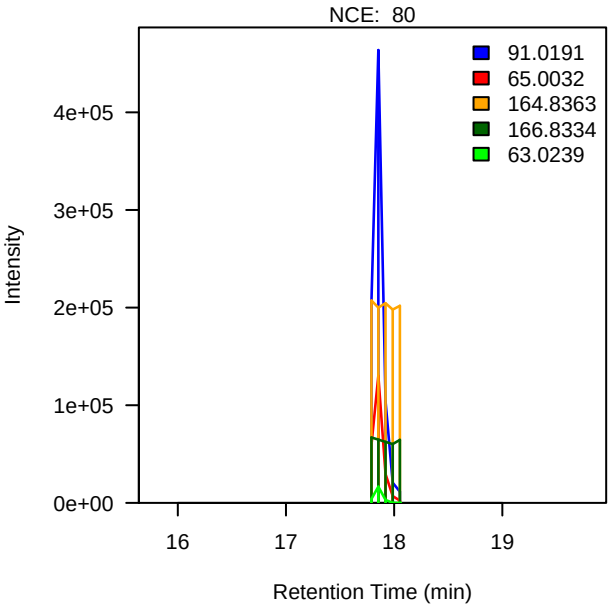
Normalized Extracted Ion Chromatogram (MS1)



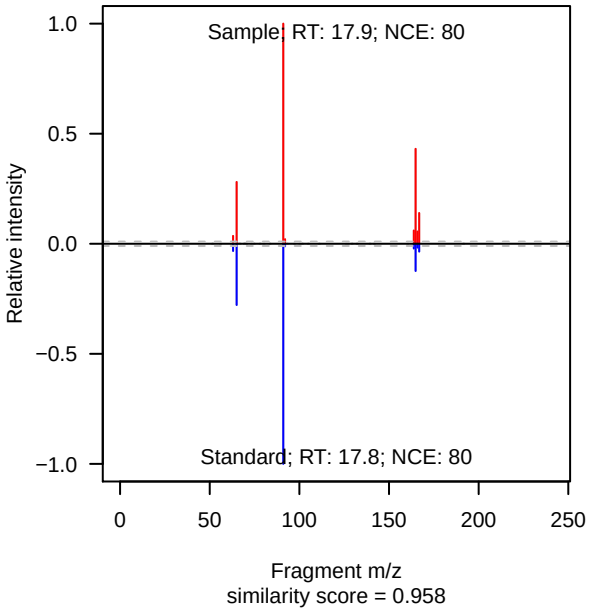
Extracted Ion Chromatogram (MS1)



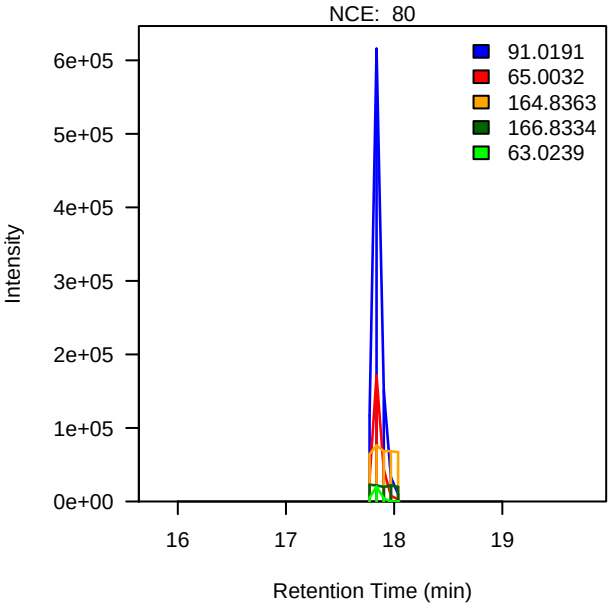
Most Intense Fragments in Sample



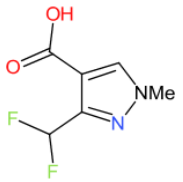
Most Intense MS2 Scan



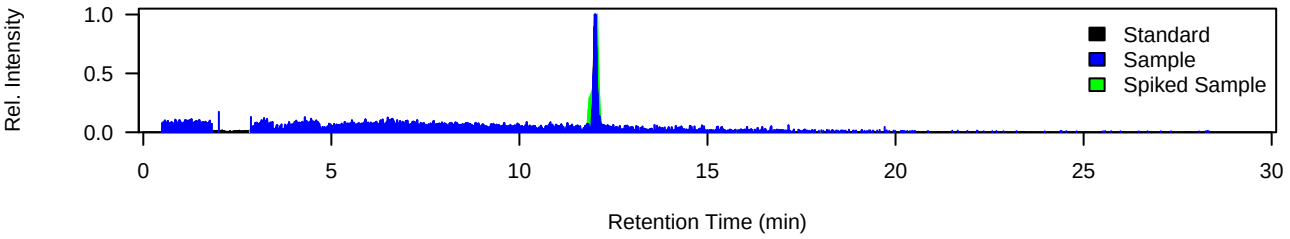
Most Intense Fragments in Standard



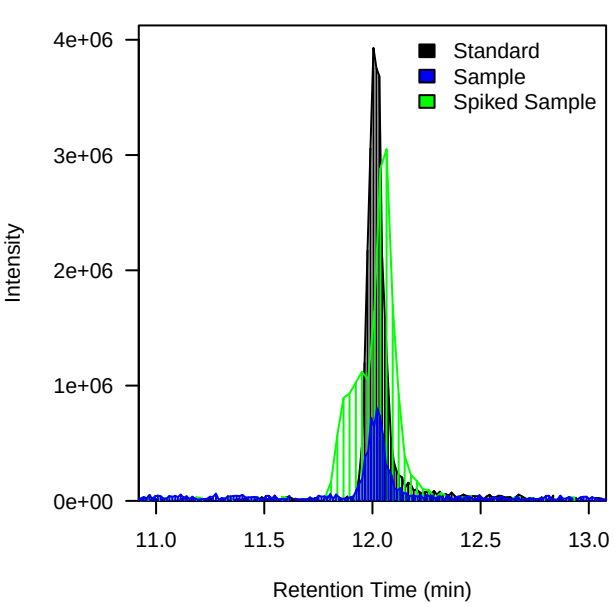
Fluxapyroxad (BAS 700 F)−TP CSAA798670
Level 1
[M+H]+ 177.04701
(STD 25 ng/L)



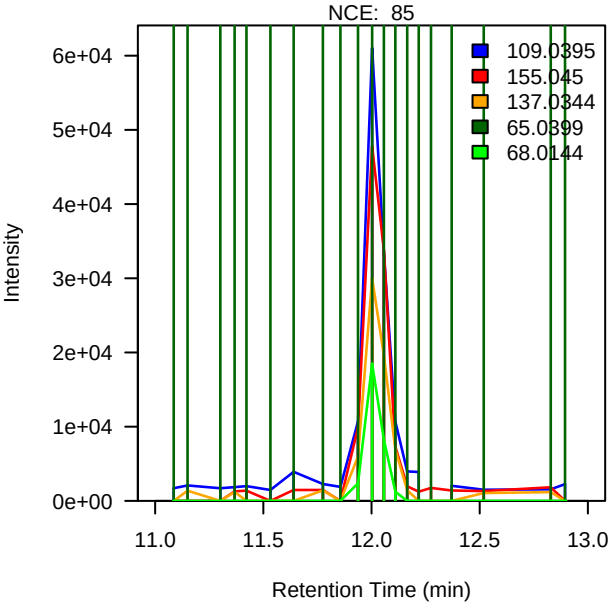
Normalized Extracted Ion Chromatogram (MS1)



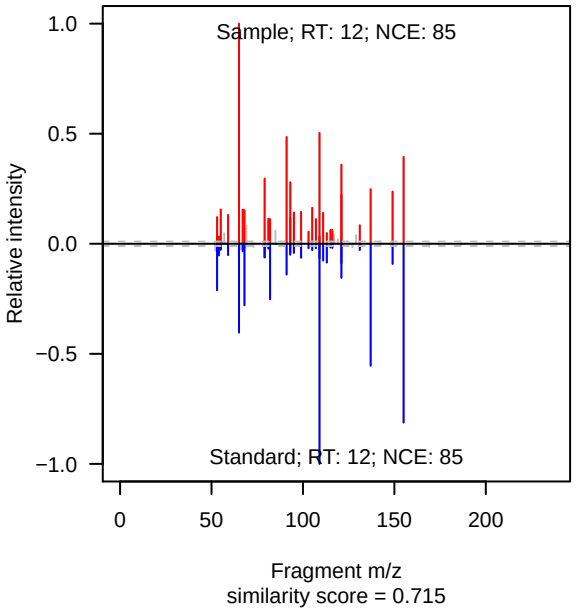
Extracted Ion Chromatogram (MS1)



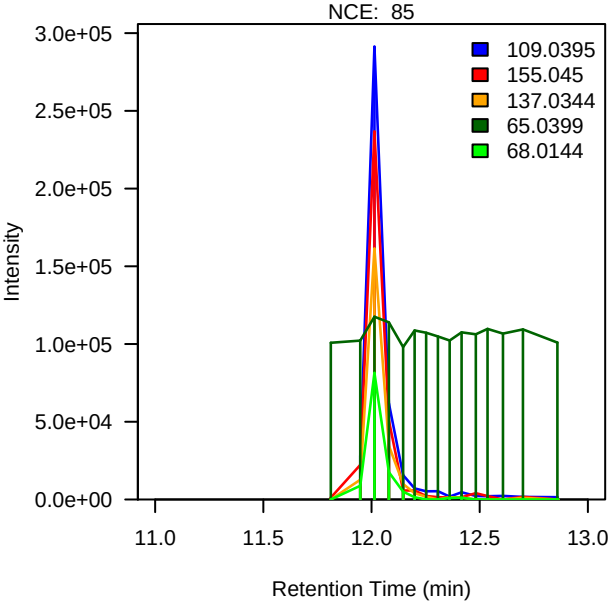
Most Intense Fragments in Sample



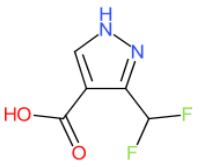
Most Intense MS2 Scan



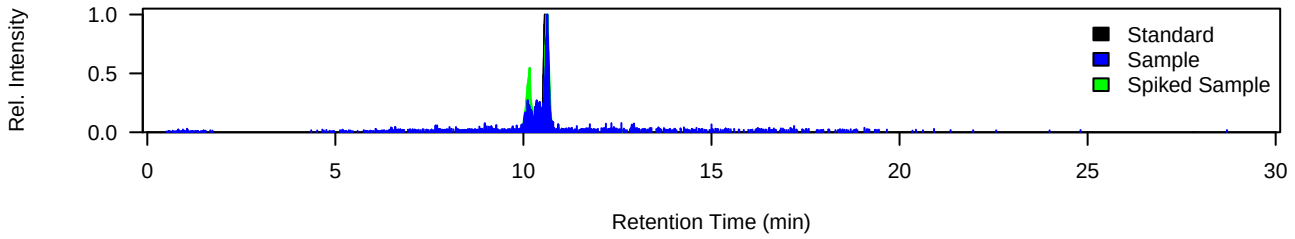
Most Intense Fragments in Standard



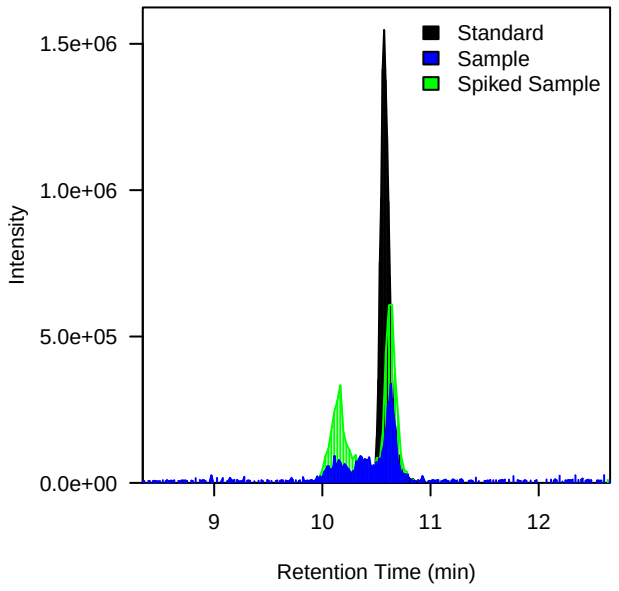
Fluxapyroxad (BAS 700 F)−TP CSCD465008
Level 1
[M−H]− 161.01681
(STD 25 ng/L)



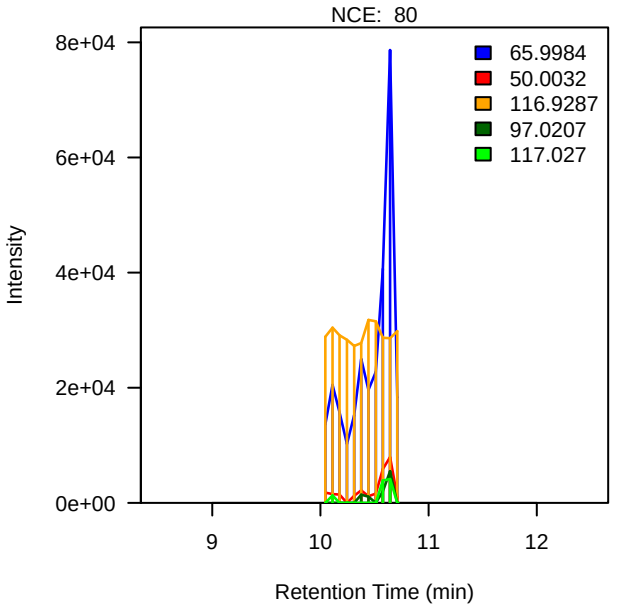
Normalized Extracted Ion Chromatogram (MS1)



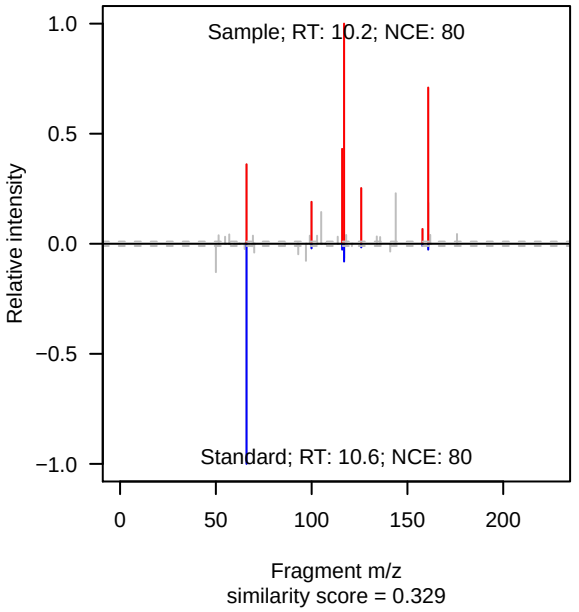
Extracted Ion Chromatogram (MS1)



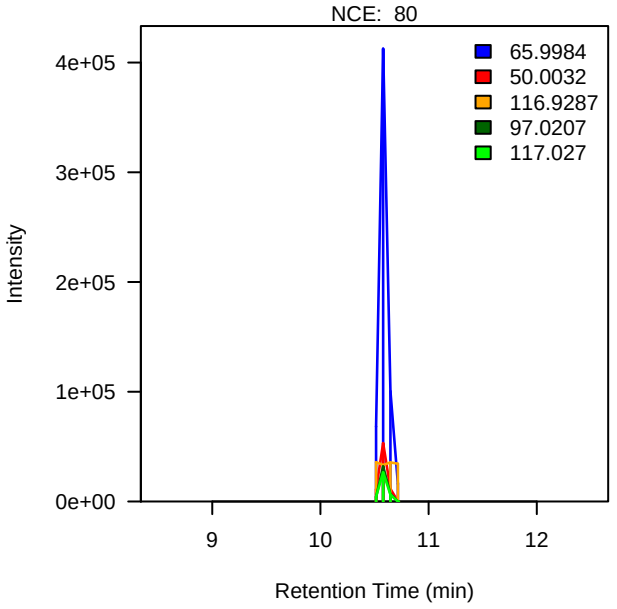
Most Intense Fragments in Sample



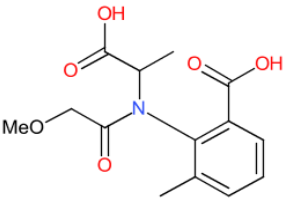
Most Intense MS2 Scan



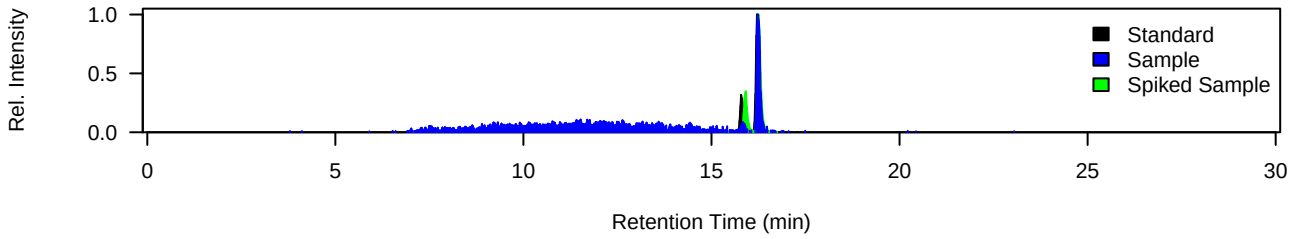
Most Intense Fragments in Standard



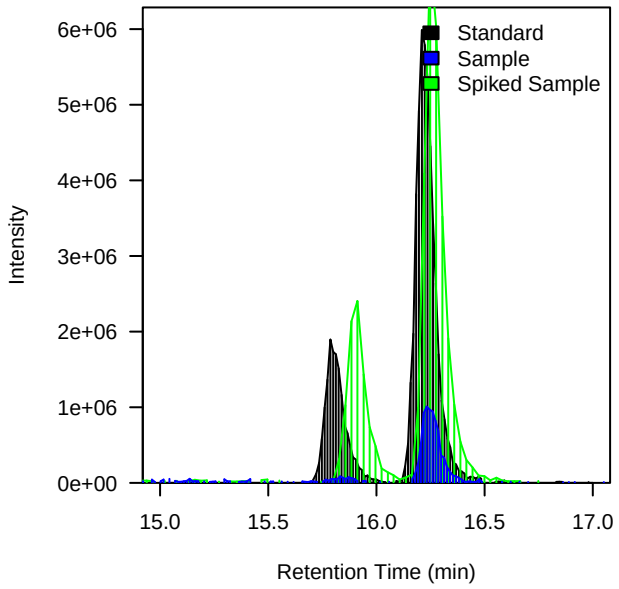
Metalaxyl−M−TP CGA108906
Level 1
[M+H]+ 296.11286
(STD 25 ng/L)



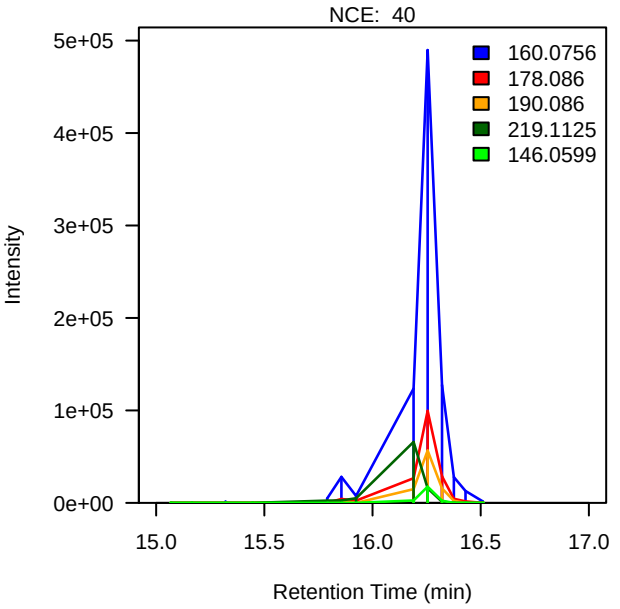
Normalized Extracted Ion Chromatogram (MS1)



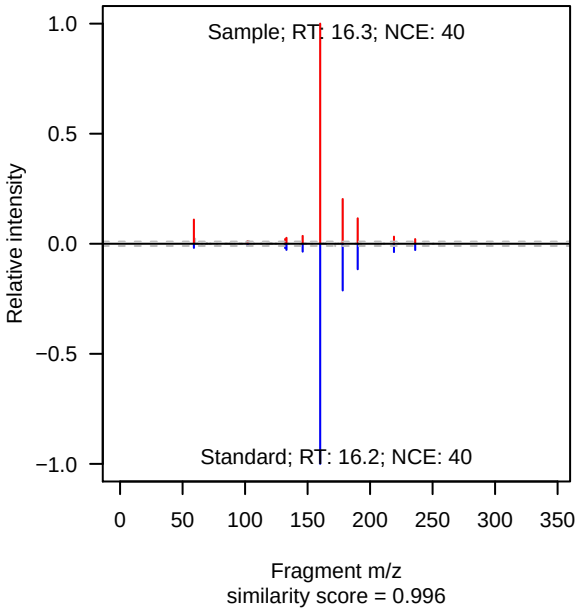
Extracted Ion Chromatogram (MS1)



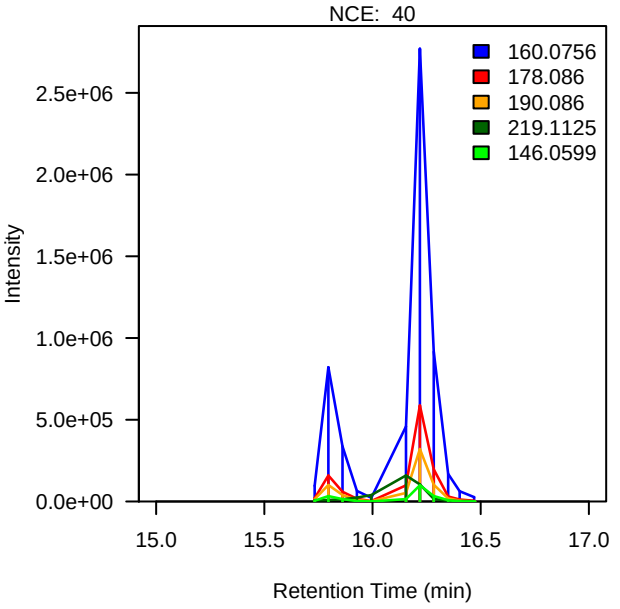
Most Intense Fragments in Sample



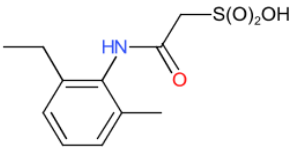
Most Intense MS2 Scan

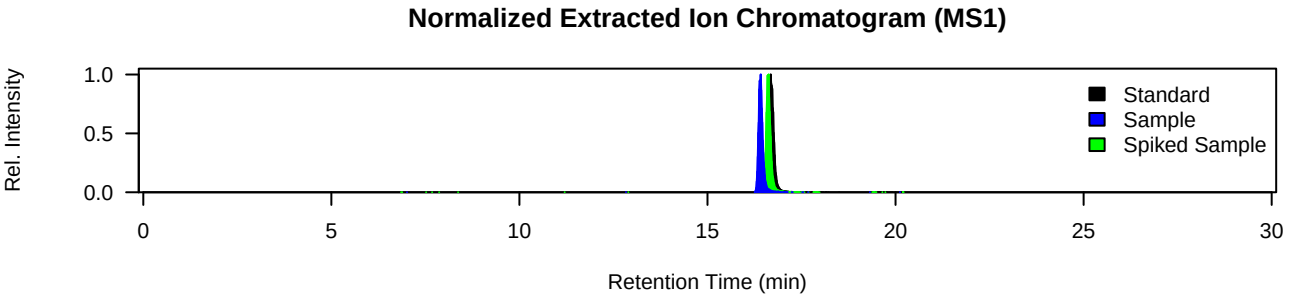


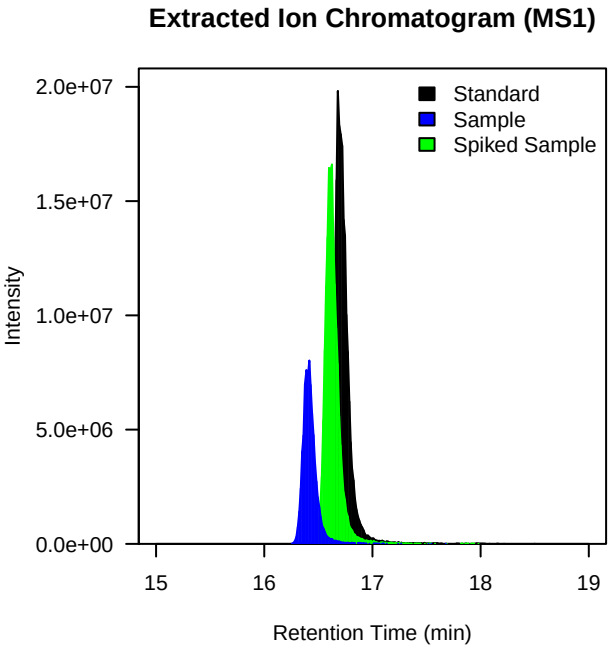
Most Intense Fragments in Standard

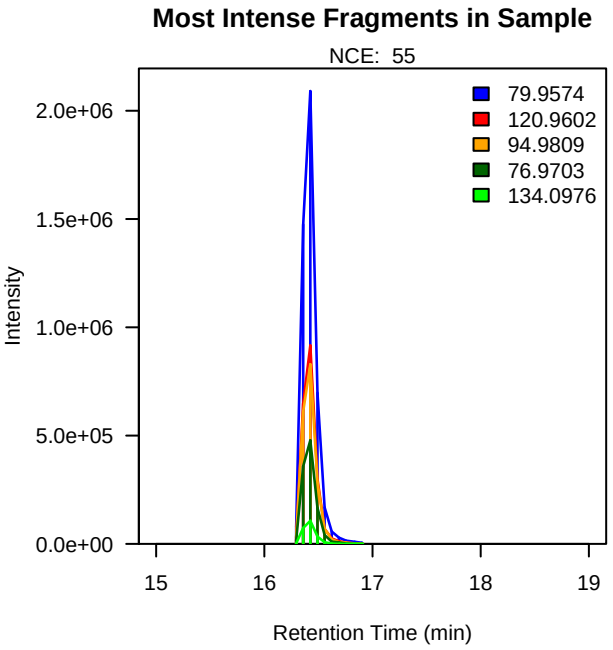


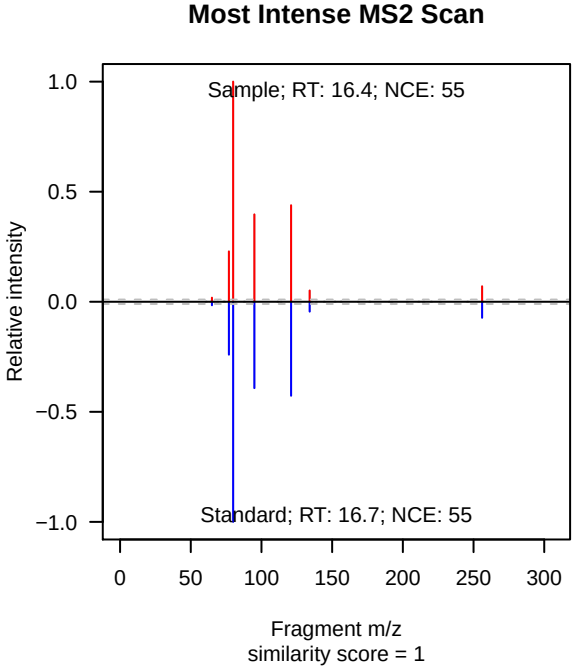
Metolachlor−TP CGA 368208 / Acetochlor sulfonic acid
Level 1
[M−H]− 256.0649
(STD 50 ng/L)

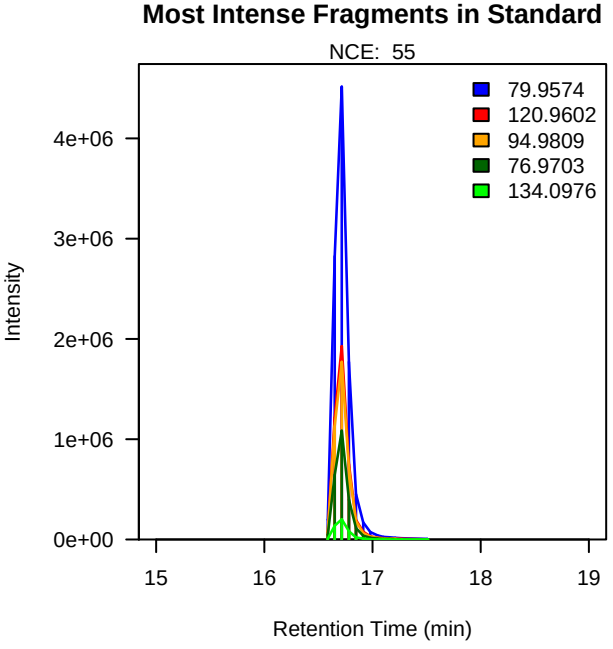




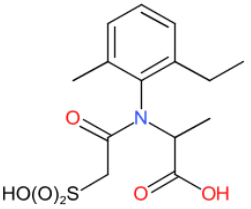




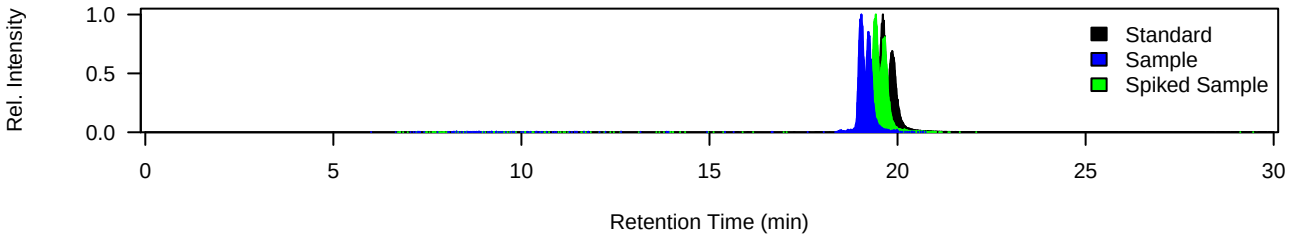




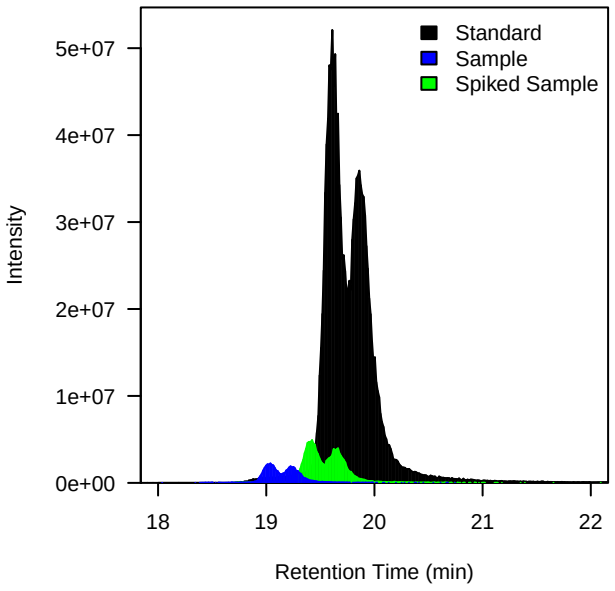
Metolachlor−TP NOA413173
Level 1
[M−H]− 328.08603
(STD 500 ng/L)



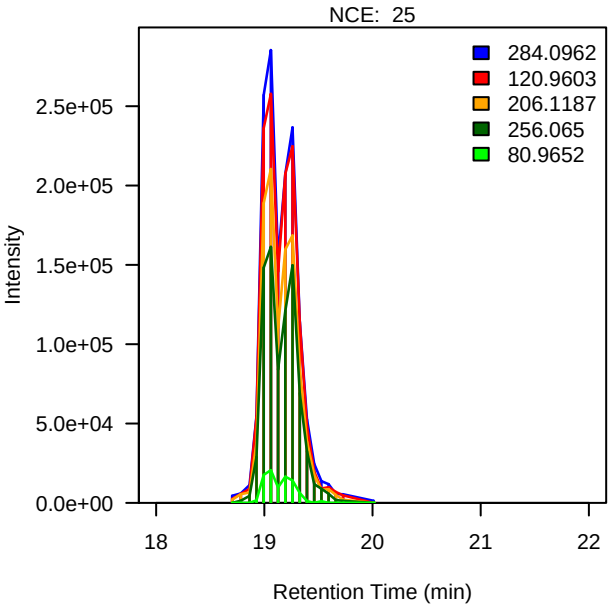
Normalized Extracted Ion Chromatogram (MS1)



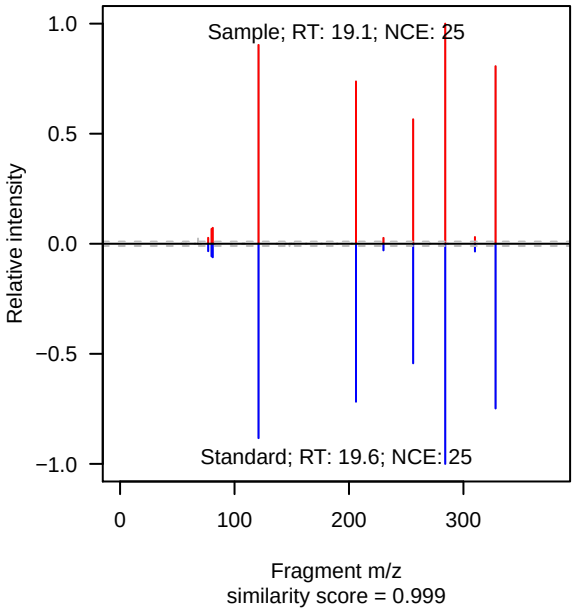
Extracted Ion Chromatogram (MS1)



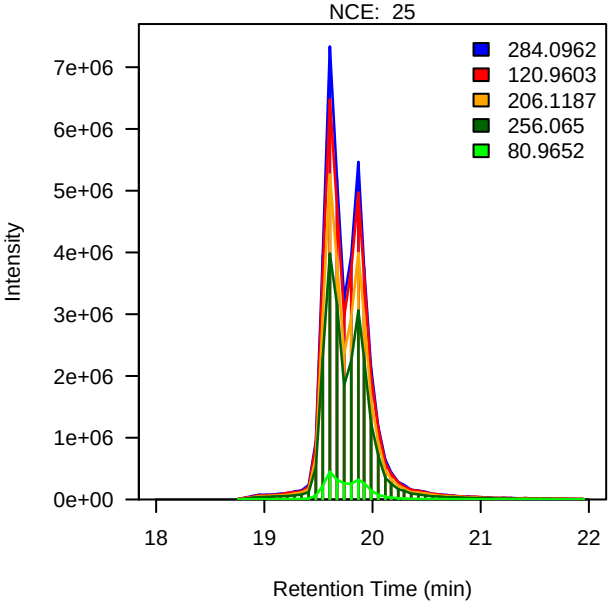
Most Intense Fragments in Sample



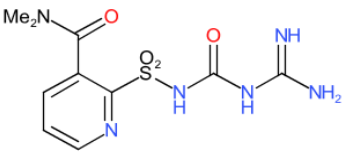
Most Intense MS2 Scan



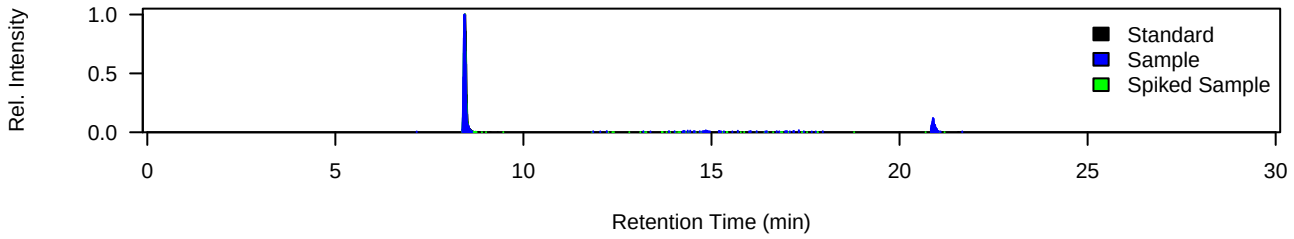
Most Intense Fragments in Standard



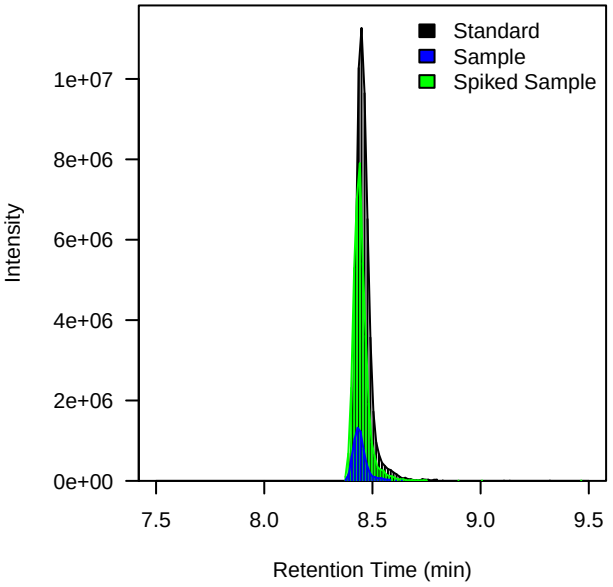
Nicosulfuron−TP AUSN
Level 1
[M+H]+ 315.087
(STD 50 ng/L)



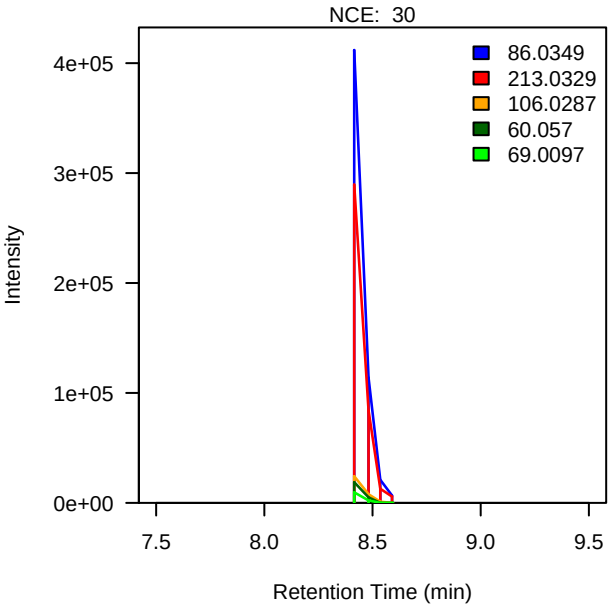
Normalized Extracted Ion Chromatogram (MS1)



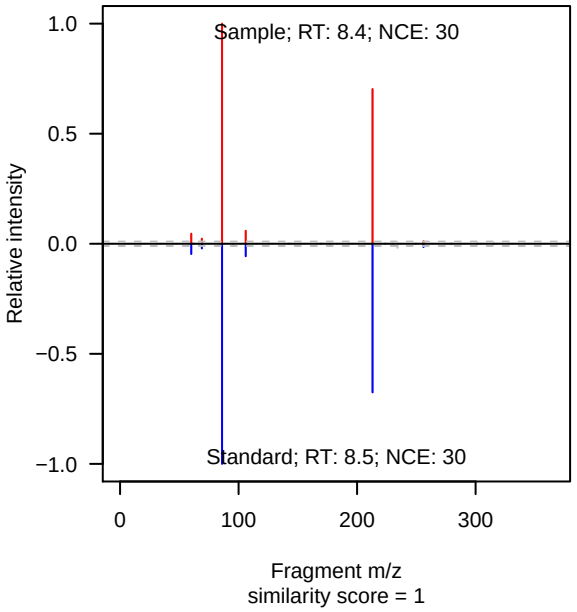
Extracted Ion Chromatogram (MS1)



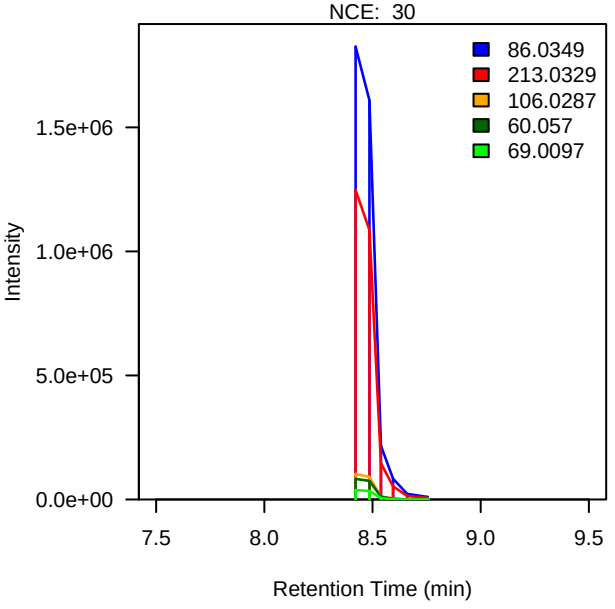
Most Intense Fragments in Sample



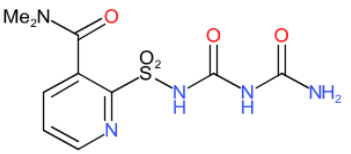
Most Intense MS2 Scan



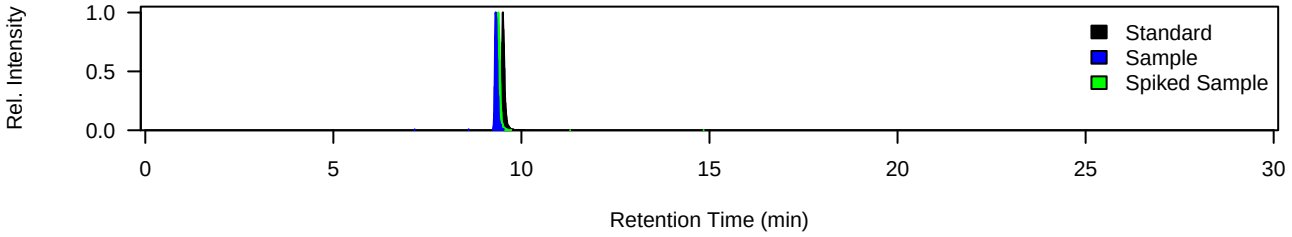
Most Intense Fragments in Standard



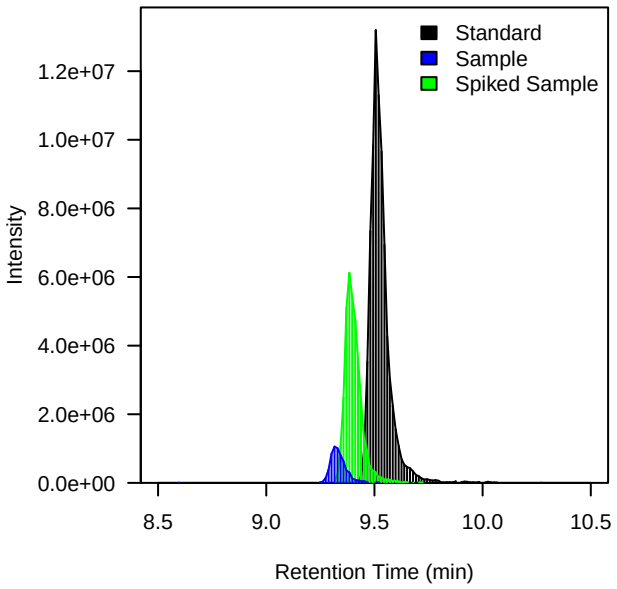
Nicosulfuron−TP UCSN
Level 1
[M+H]+ 316.07102
(STD 50 ng/L)



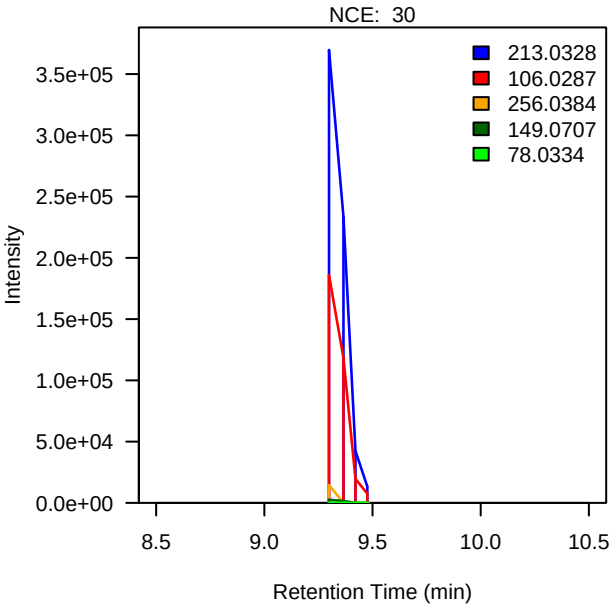
Normalized Extracted Ion Chromatogram (MS1)



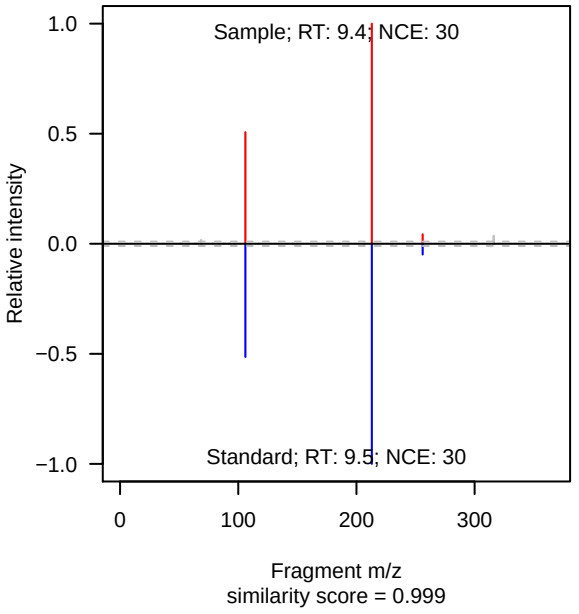
Extracted Ion Chromatogram (MS1)



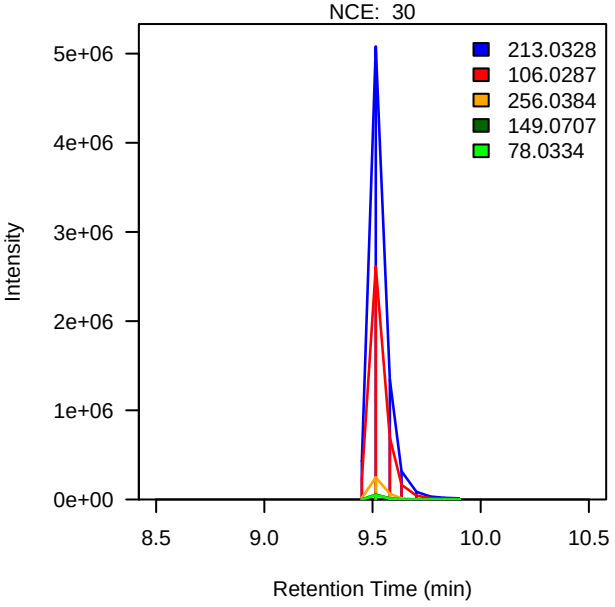
Most Intense Fragments in Sample



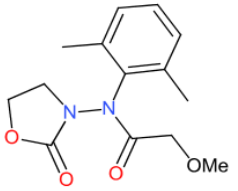
Most Intense MS2 Scan



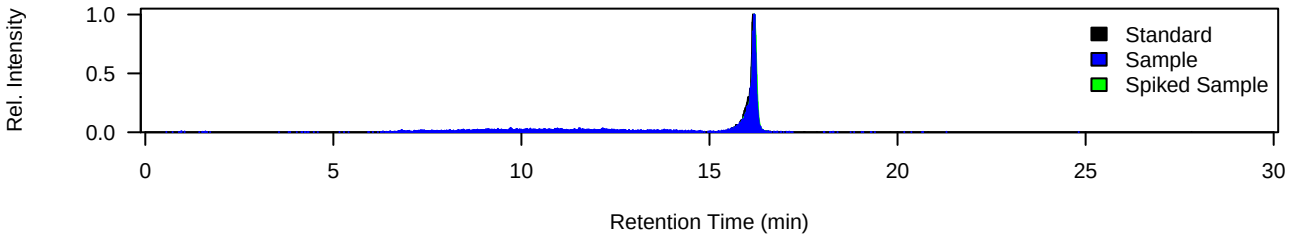
Most Intense Fragments in Standard



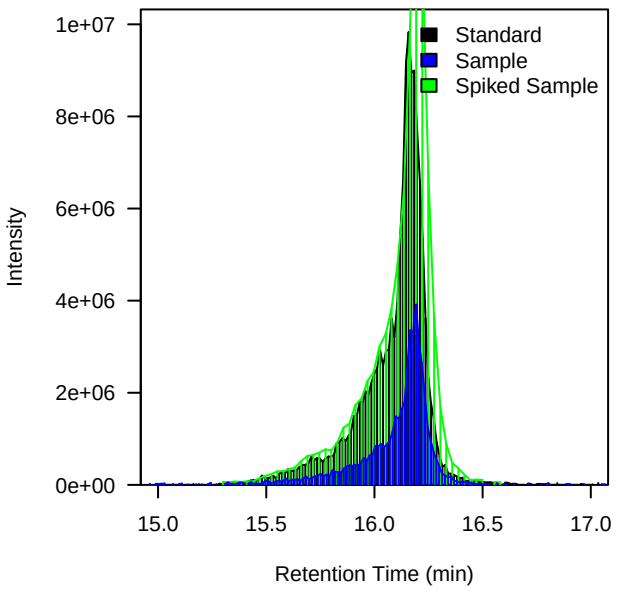
Oxadixyl
Level 1
[M+H]+ 279.13393
(STD 25 ng/L)



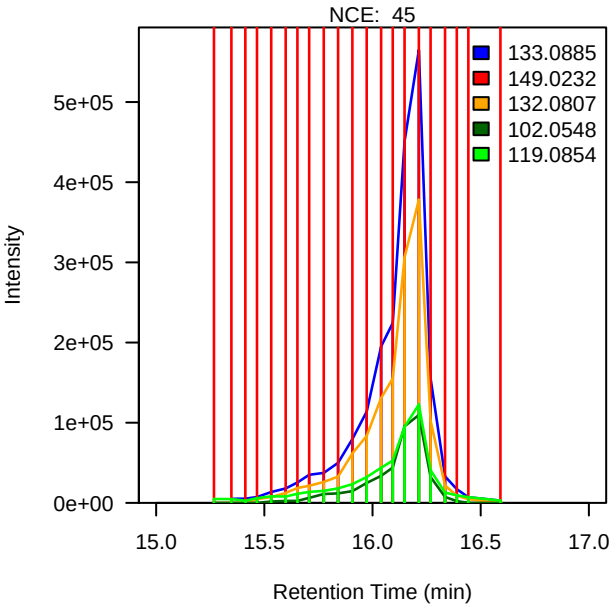
Normalized Extracted Ion Chromatogram (MS1)



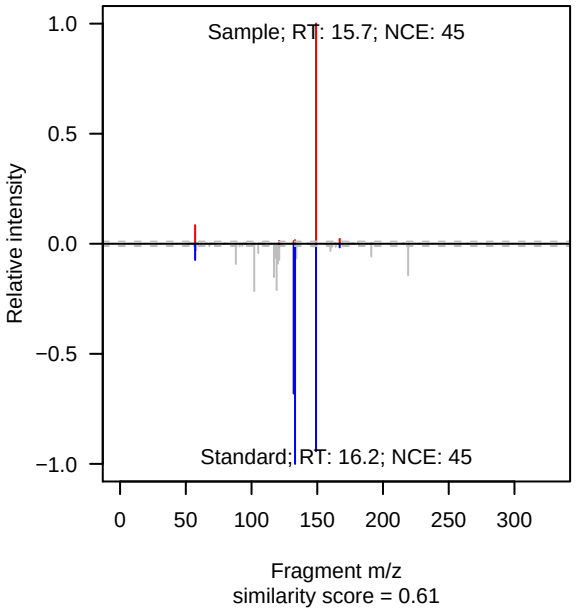
Extracted Ion Chromatogram (MS1)



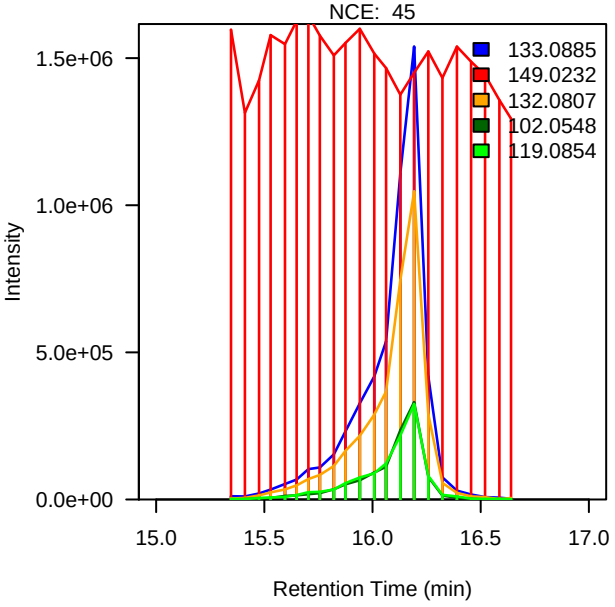
Most Intense Fragments in Sample



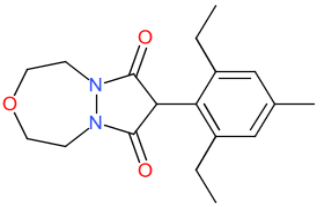
Most Intense MS2 Scan



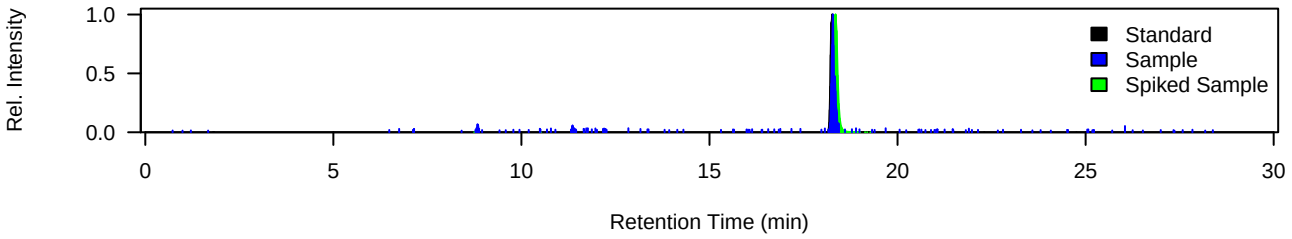
Most Intense Fragments in Standard



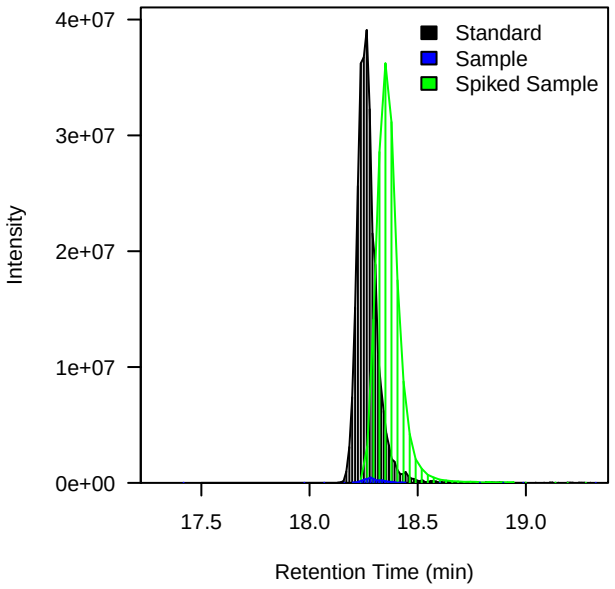
Pinoxaden−TP NOA 407854
Level 1
[M+H]+ 317.18597
(STD 25 ng/L)



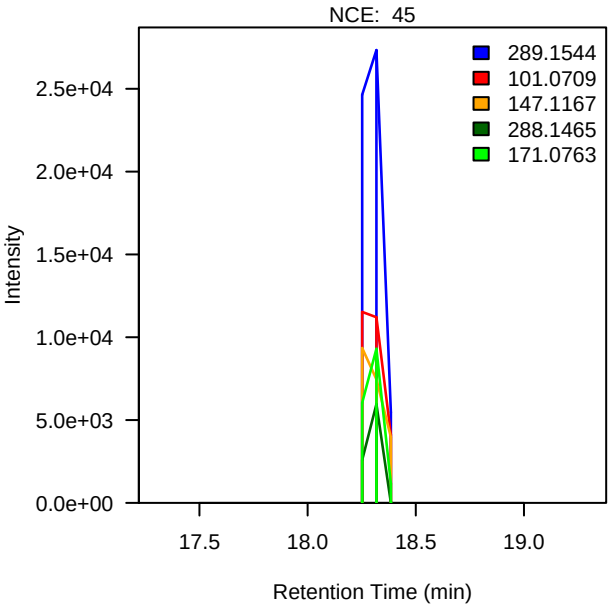
Normalized Extracted Ion Chromatogram (MS1)



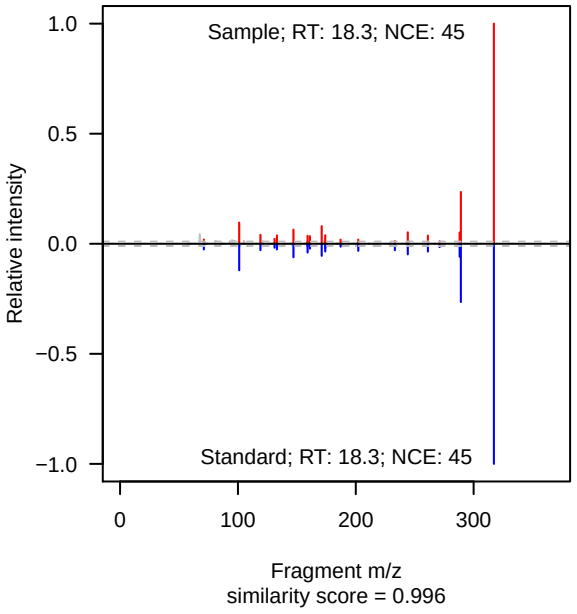
Extracted Ion Chromatogram (MS1)



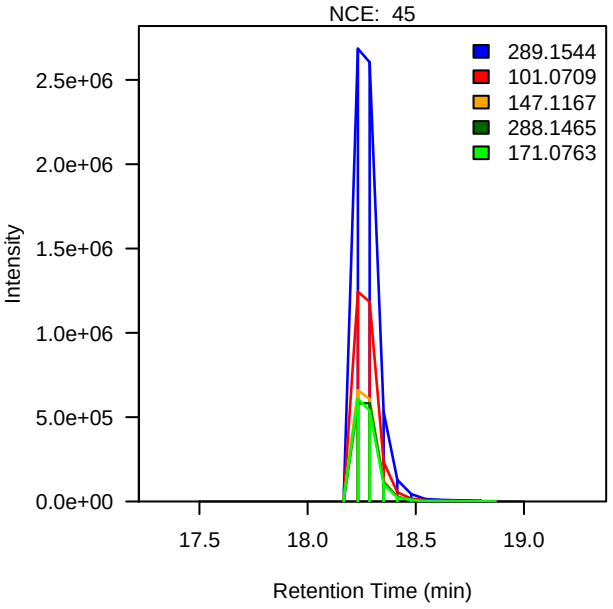
Most Intense Fragments in Sample



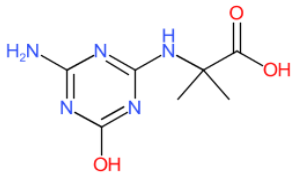
Most Intense MS2 Scan



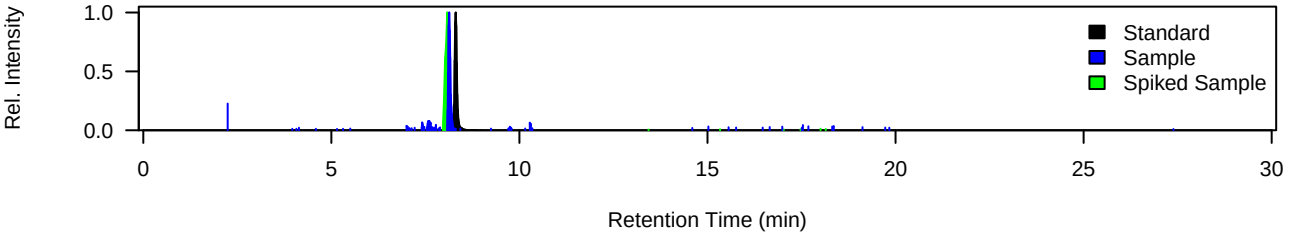
Most Intense Fragments in Standard



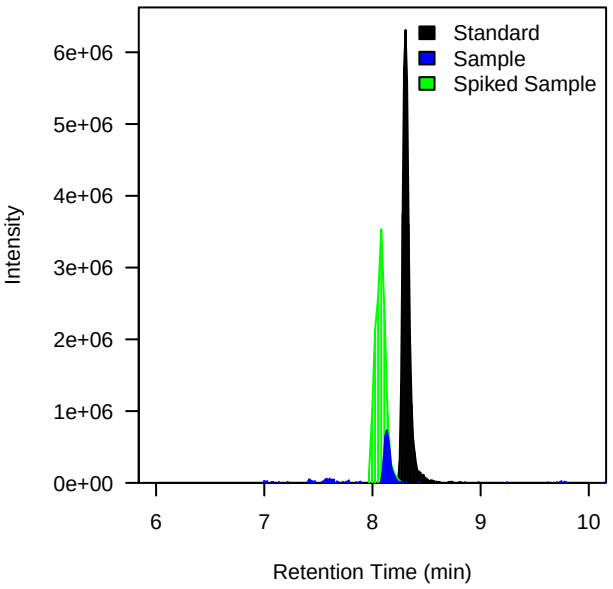
Terbuthylazine−TP CSAA036479
Level 1
[M+H]+ 214.09347
(STD 25 ng/L)



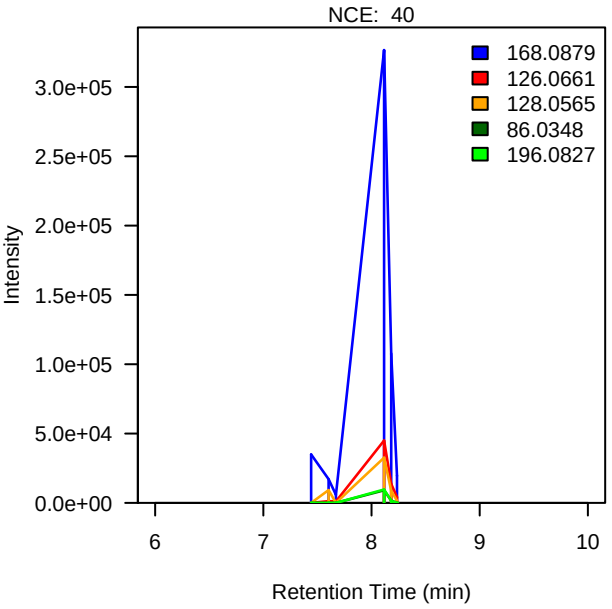
Normalized Extracted Ion Chromatogram (MS1)



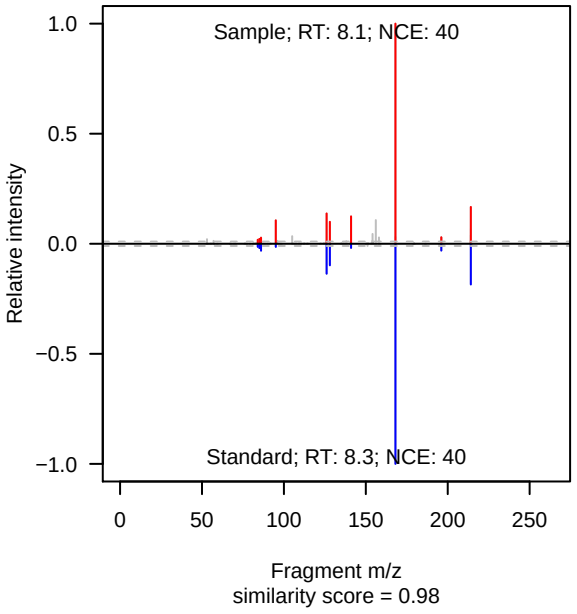
Extracted Ion Chromatogram (MS1)



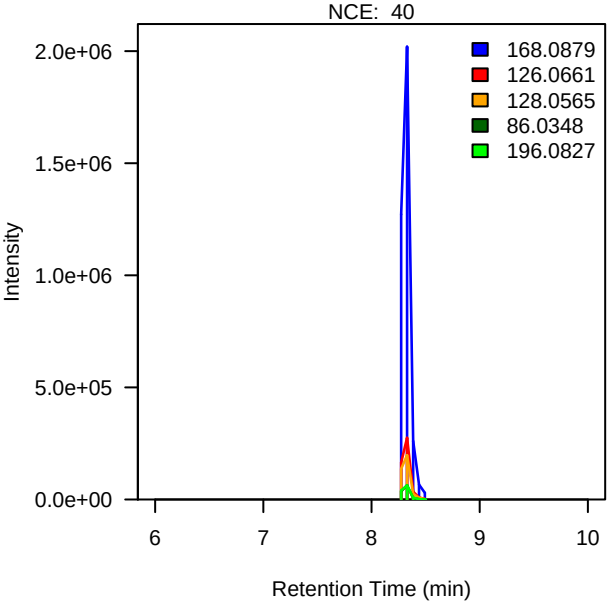
Most Intense Fragments in Sample



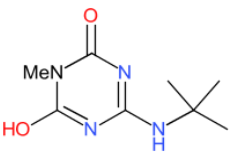
Most Intense MS2 Scan



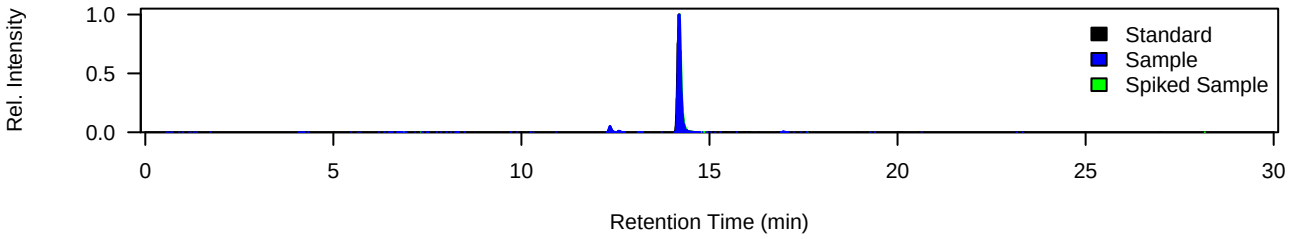
Most Intense Fragments in Standard



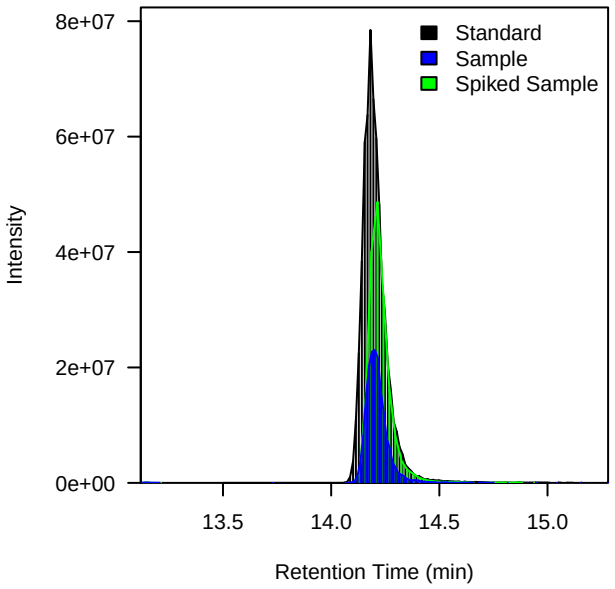
Terbuthylazine−TP CSCD648241
Level 1
[M+H]+ 199.11895
(STD 100 ng/L)



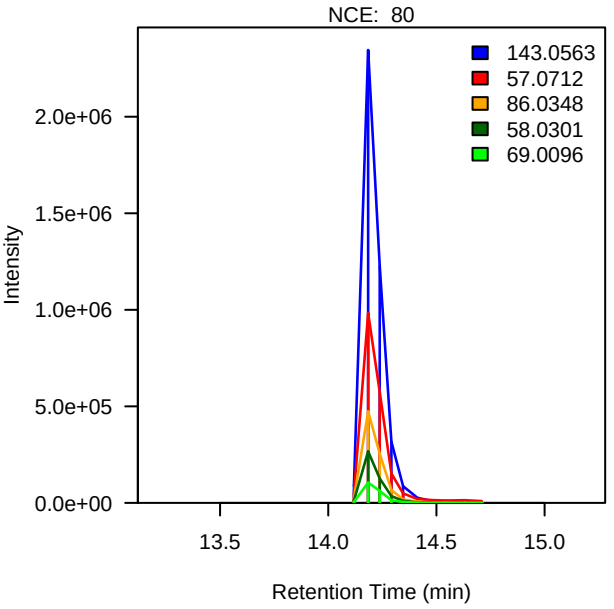
Normalized Extracted Ion Chromatogram (MS1)



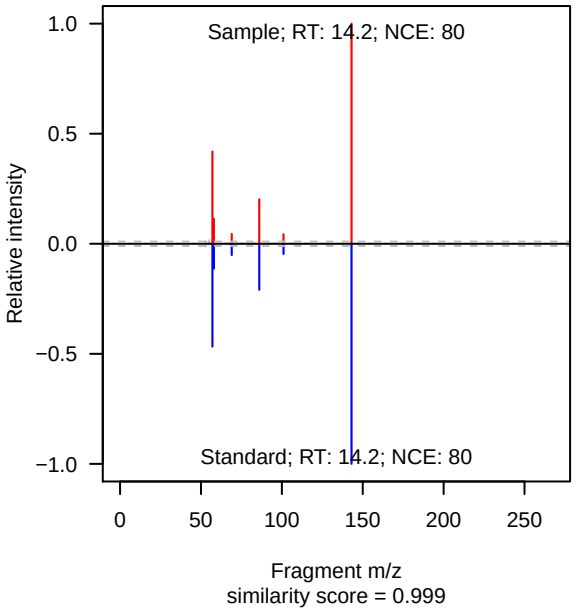
Extracted Ion Chromatogram (MS1)



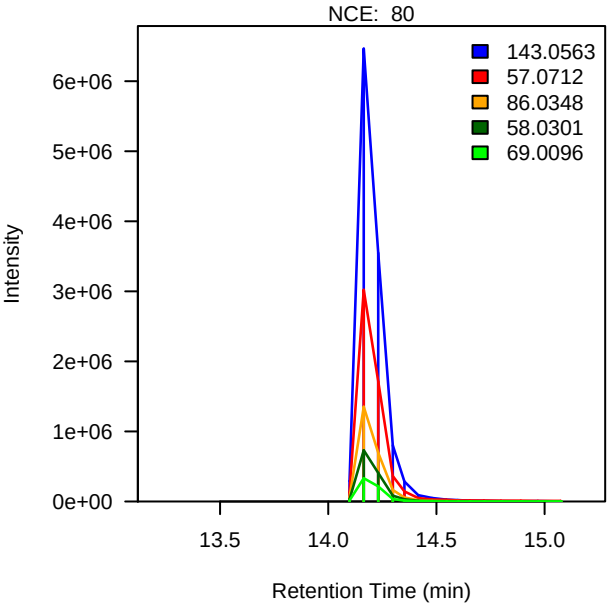
Most Intense Fragments in Sample



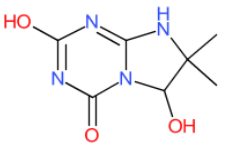
Most Intense MS2 Scan



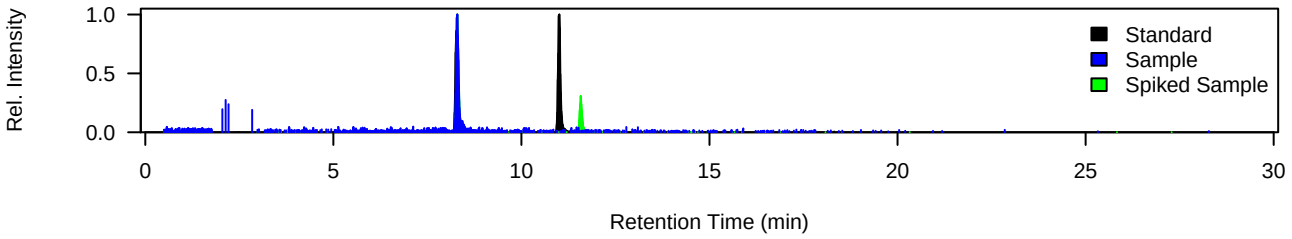
Most Intense Fragments in Standard



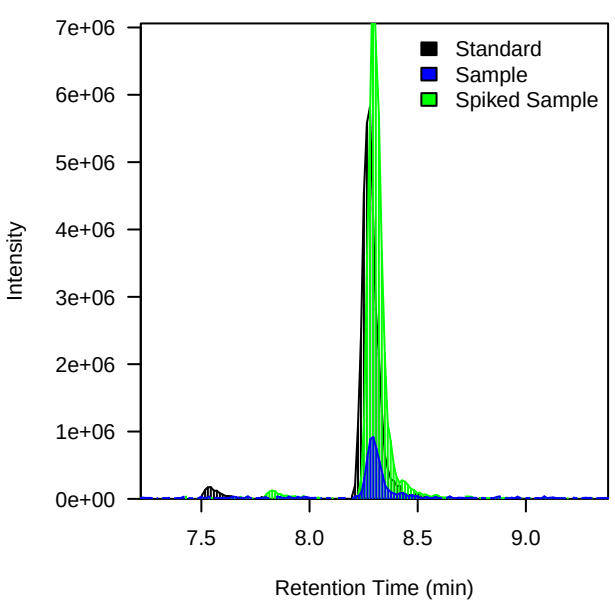
Terbuthylazine−TP CSCD692760
Level 1
[M+H]+ 199.08257
(STD 25 ng/L)



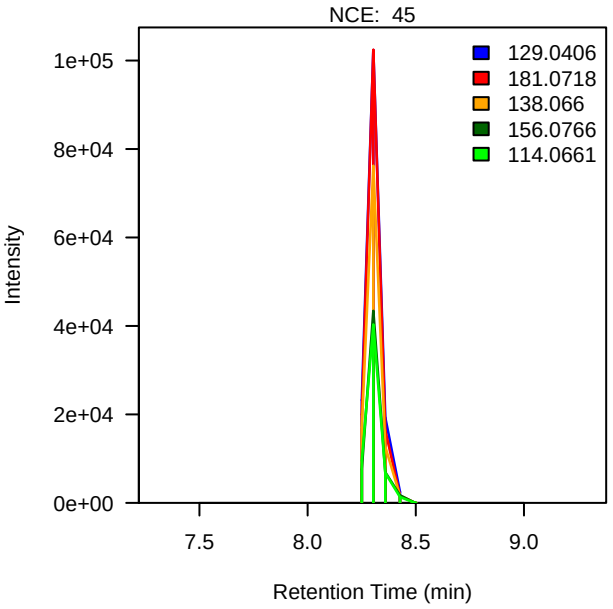
Normalized Extracted Ion Chromatogram (MS1)



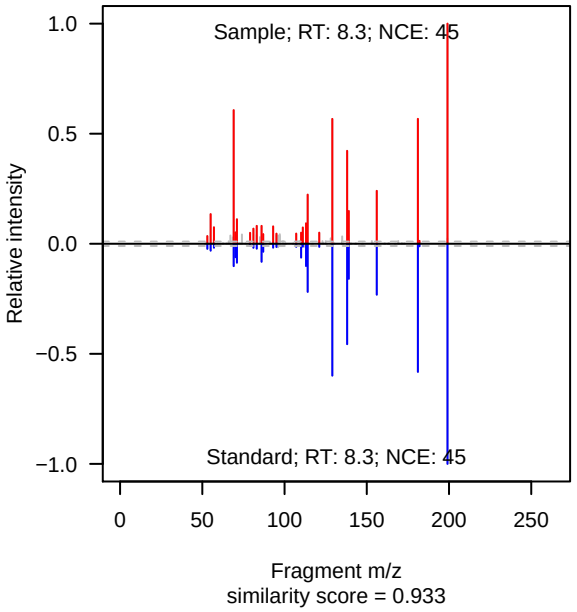
Extracted Ion Chromatogram (MS1)



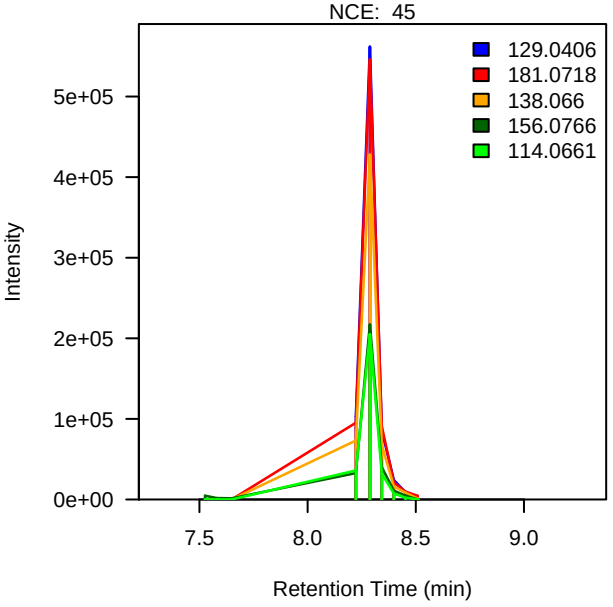
Most Intense Fragments in Sample



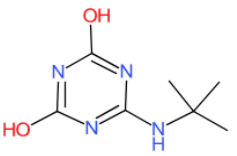
Most Intense MS2 Scan



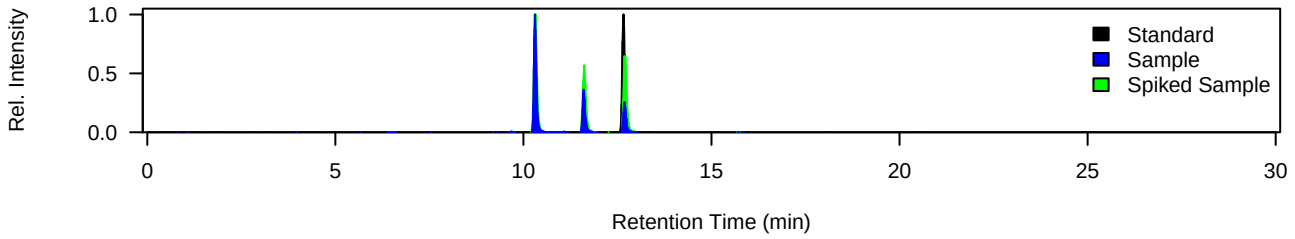
Most Intense Fragments in Standard



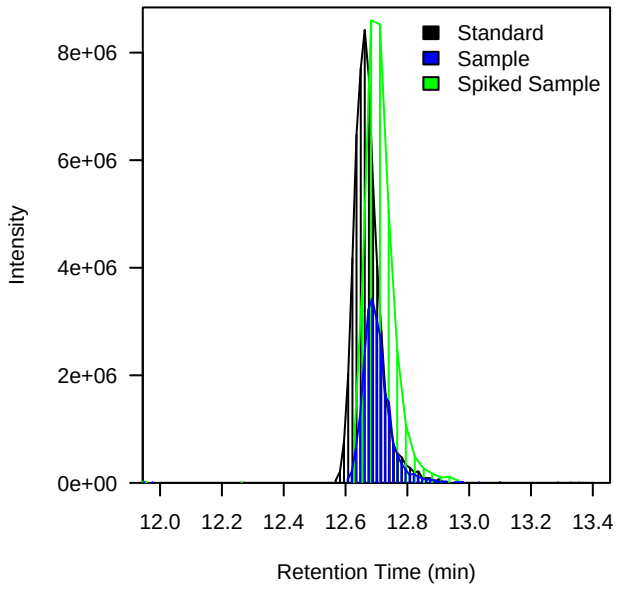
Terbuthylazine−TP MT23_GS16984
Level 1
[M+H]+ 185.1033
(STD 25 ng/L)



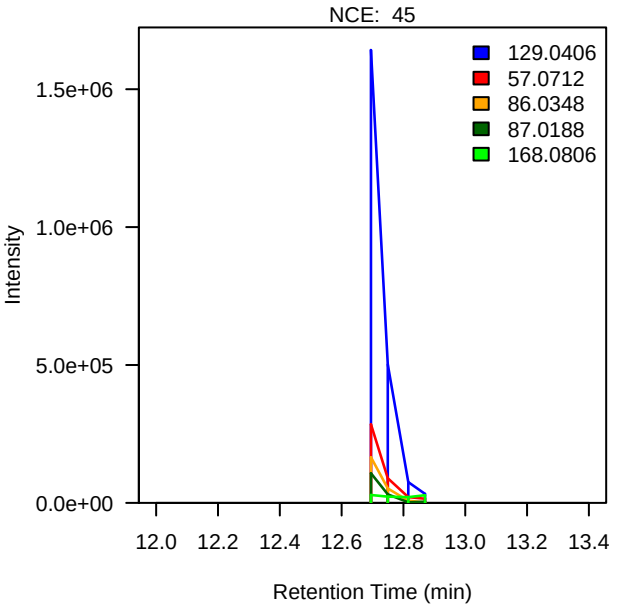
Normalized Extracted Ion Chromatogram (MS1)



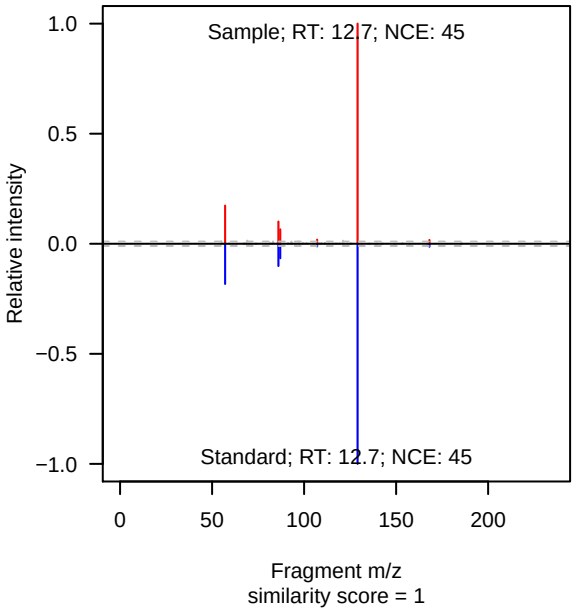
Extracted Ion Chromatogram (MS1)



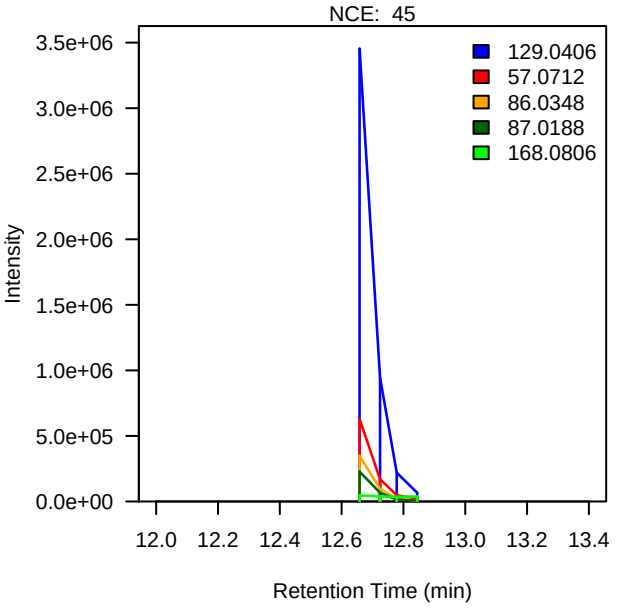
Most Intense Fragments in Sample



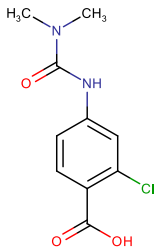
Most Intense MS2 Scan

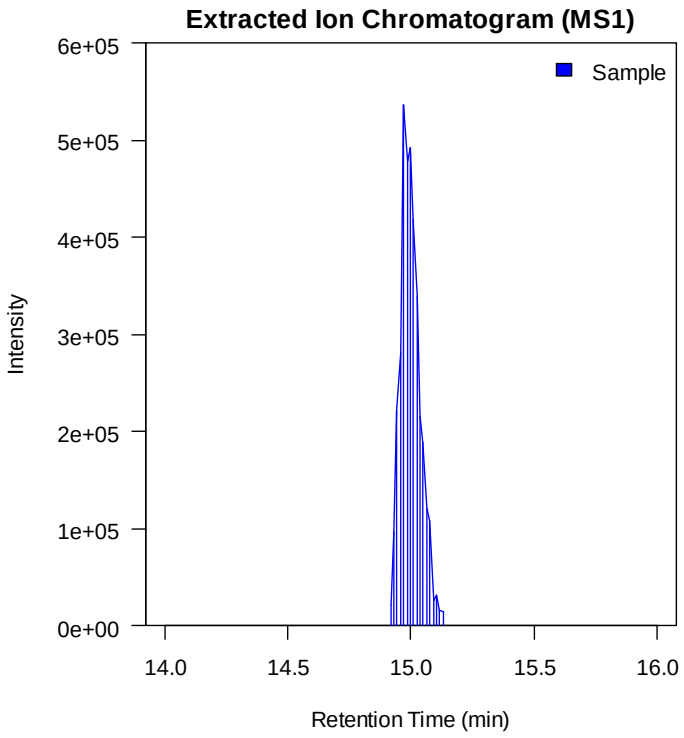


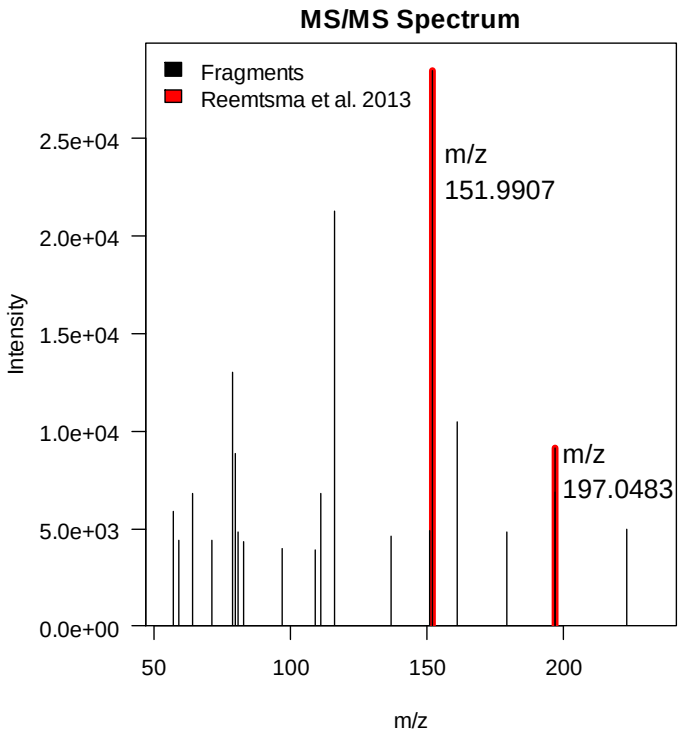
Most Intense Fragments in Standard



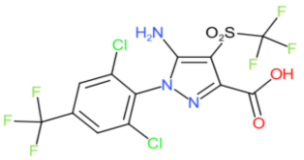
Chlorotoluron-TP CGA 15140
Level 2a
[M-H]- 241.038543

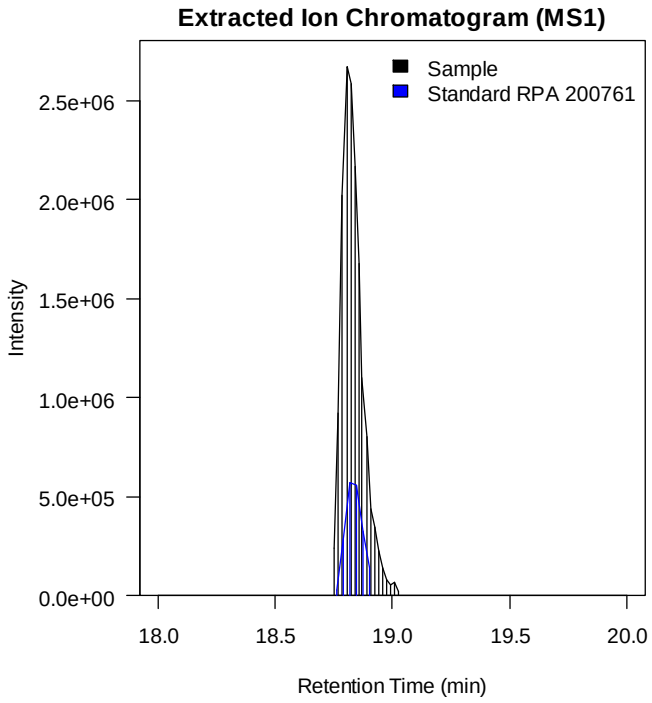


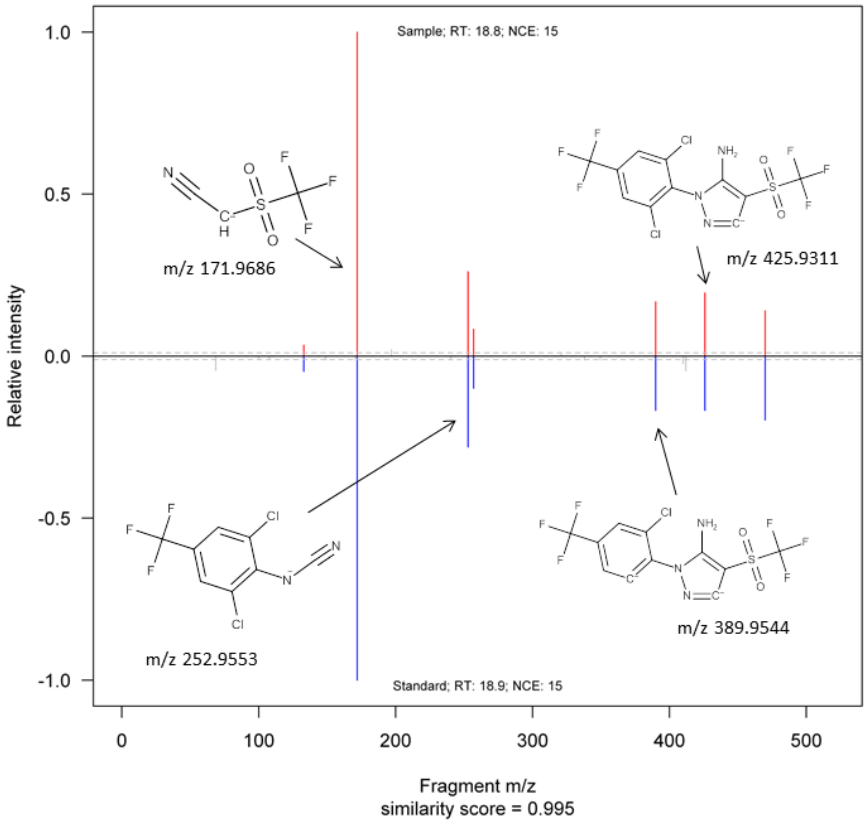




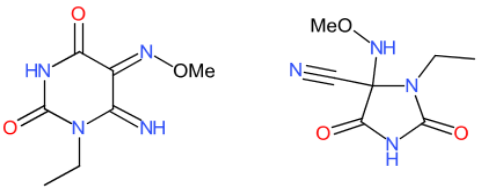
Fipronil-TP RPA 106681
Level 2b
[M-H]- 469.920924
Standard RPA 200761



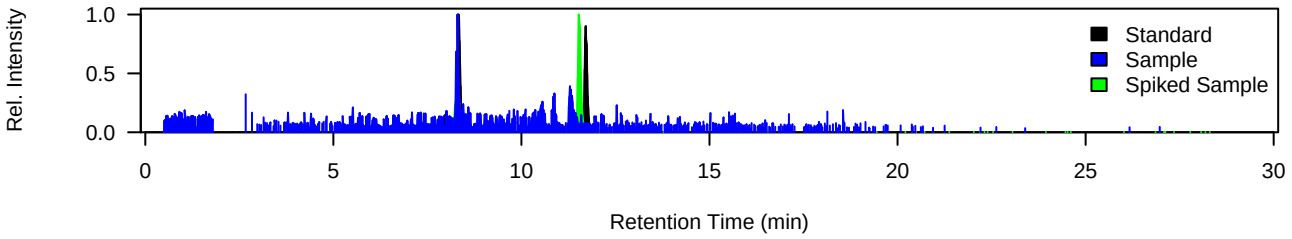




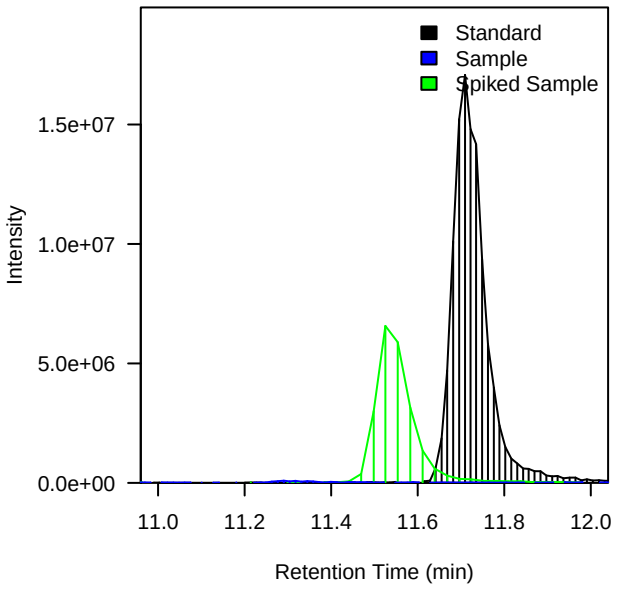
Cymoxanil−TP IN−JX915 / U3204
Level 3
[M+H]+ 199.08257
(STD 50 ng/L)



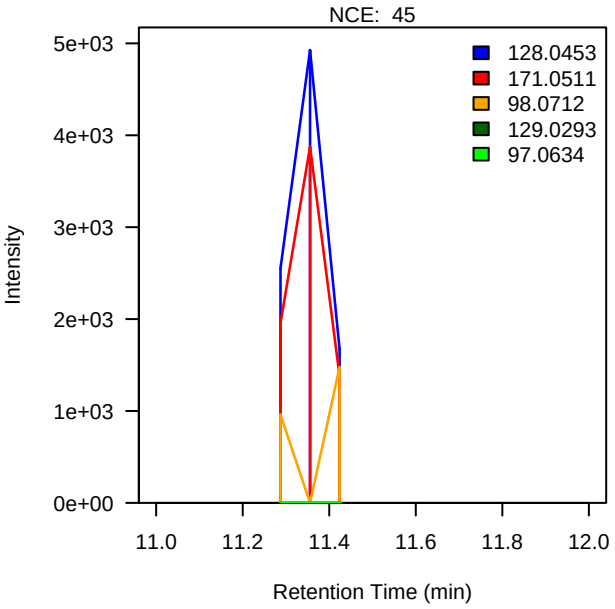
Normalized Extracted Ion Chromatogram (MS1)



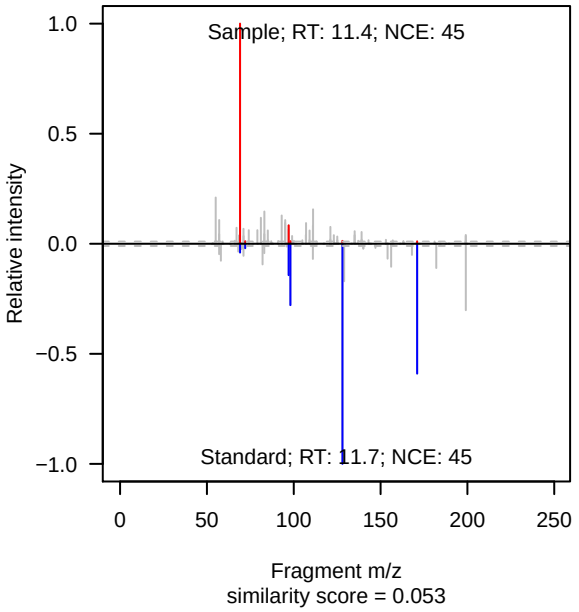
Extracted Ion Chromatogram (MS1)



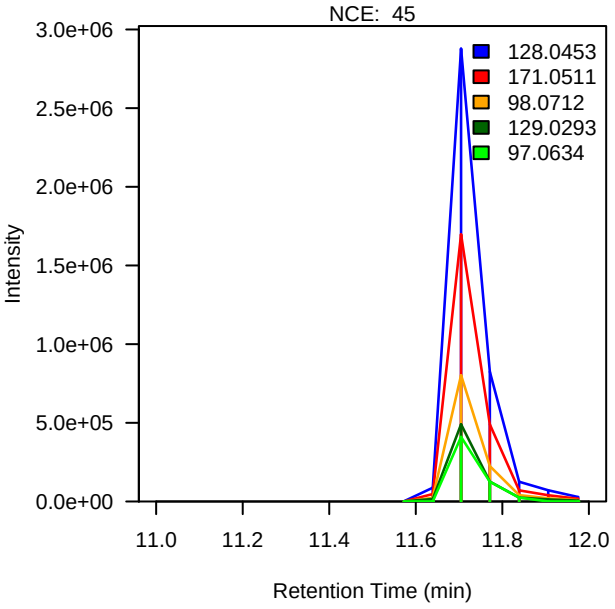
Most Intense Fragments in Sample



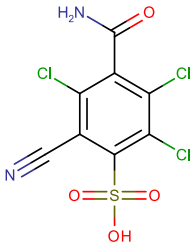
Most Intense MS2 Scan

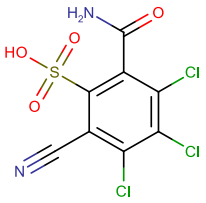


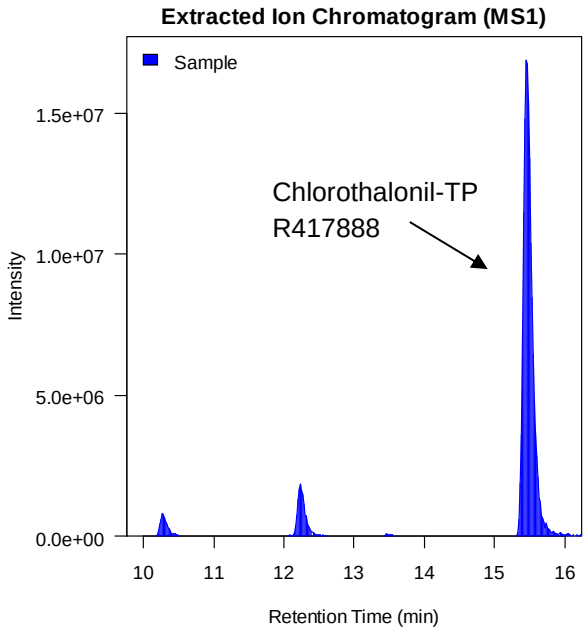
Most Intense Fragments in Standard

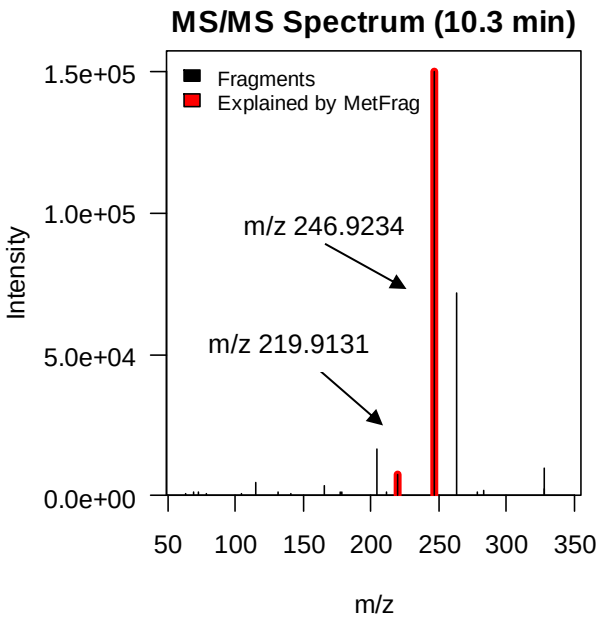


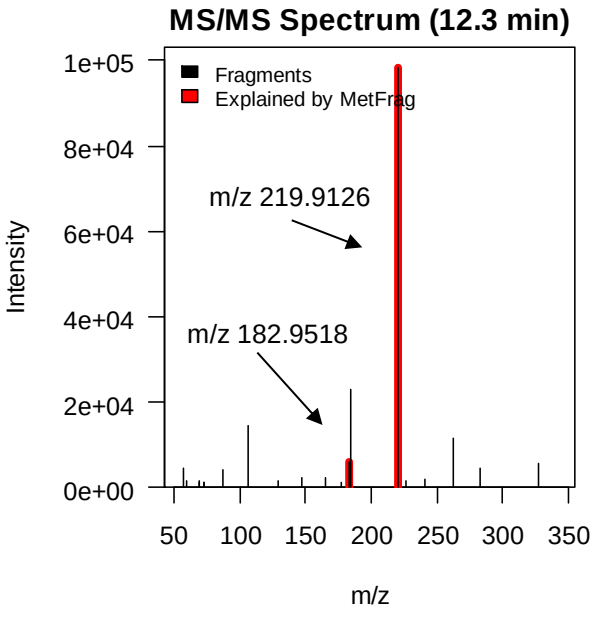
Chlorothalonil-TPs
4-carbamoyl-2,3,5-trichloro-6-cyanobenzenesulfonic acid &
2-carbamoyl-3,4,5-trichloro-6-cyanobenzenesulfonic acid
Level 3
[M-H]- 326.88063



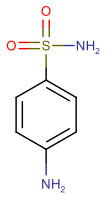


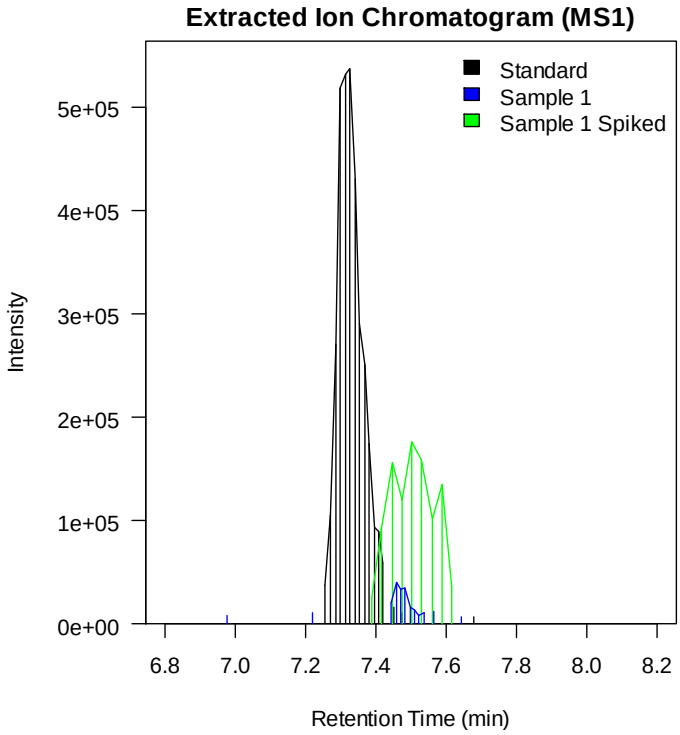


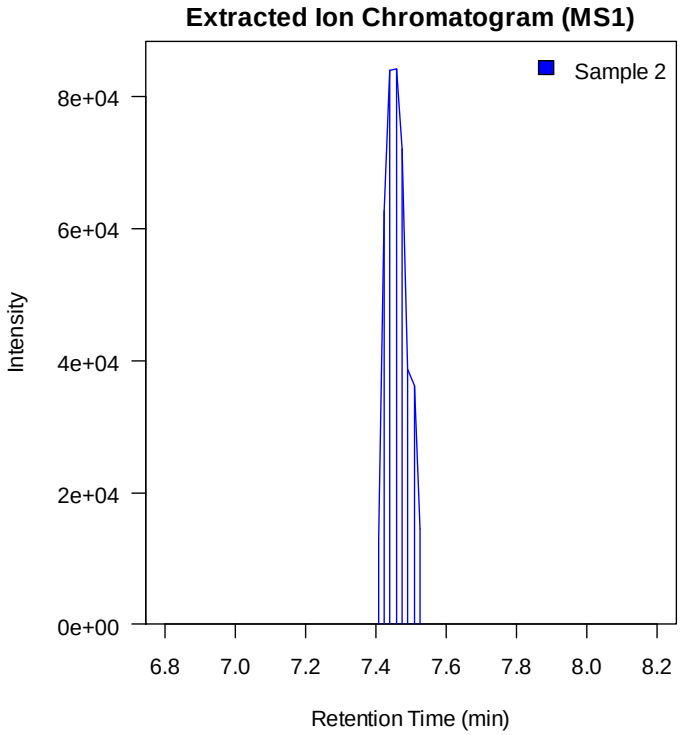




Asulam-TP Sulfanilamide
Unclear
[M+NH4]+ 190.06447
STD 25 ng/L

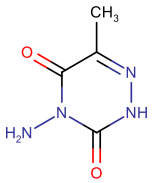


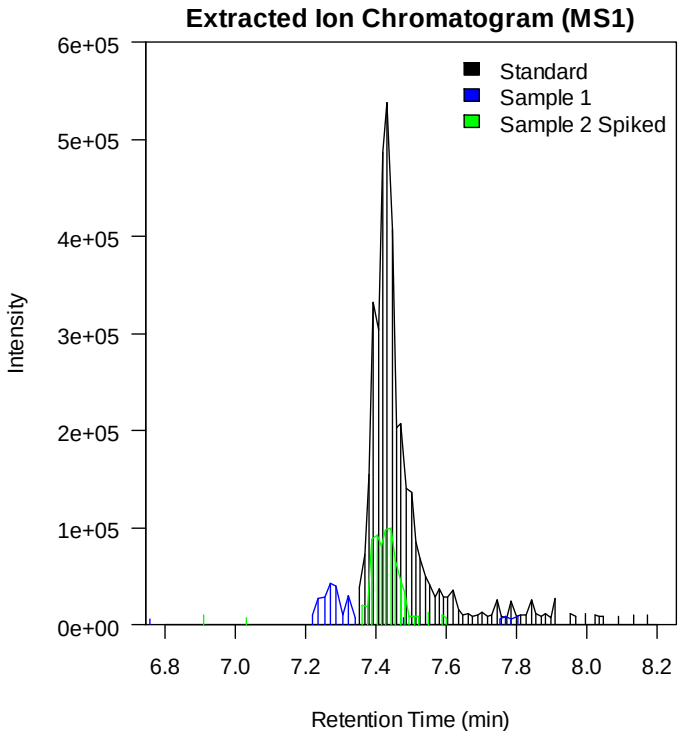




Remark: Sample 2 was not measured in the same sequence as standard, sample 1 and sample 1 spiked.

Pymetrozine-TP CGA294849
Unclear
[M+H]+ 143.05635
STD 100 ng/L





Remark: Sample 1 was not measured in the same sequence as standard & sample 2 spiked; no peak in sample 2.