

Detection of Anticoagulant Rodenticides by Direct Analysis in Real Time Time-of-Flight Mass Spectrometry: Novel Screening Techniques and Rapid Semi-Quantitative Determination Supplementary Data

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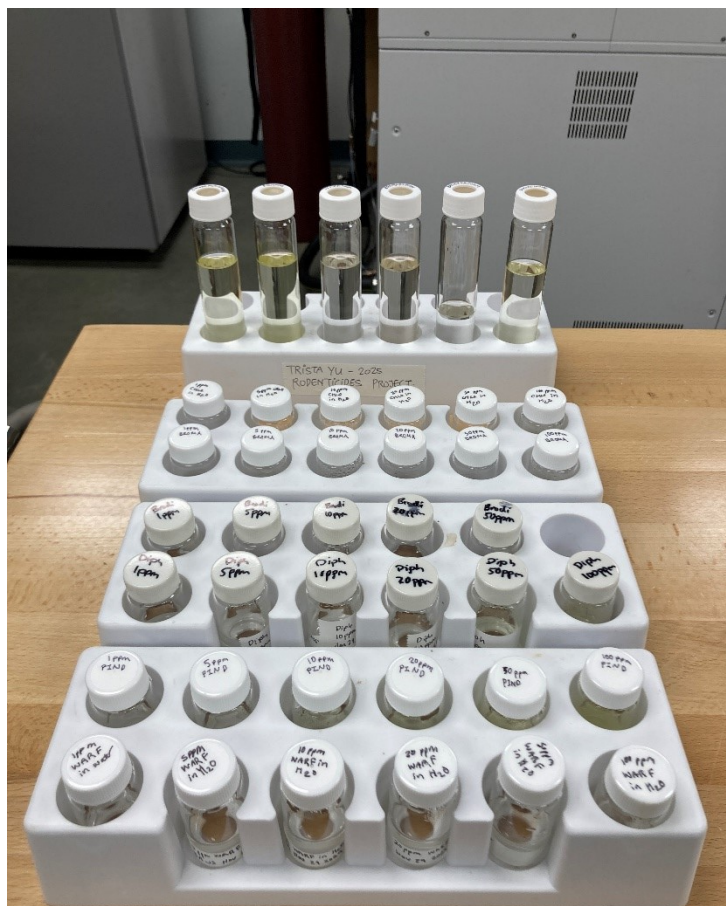


Figure S1: Rodenticide standards in ultra-high purity

from rodenticide standards in ultra-

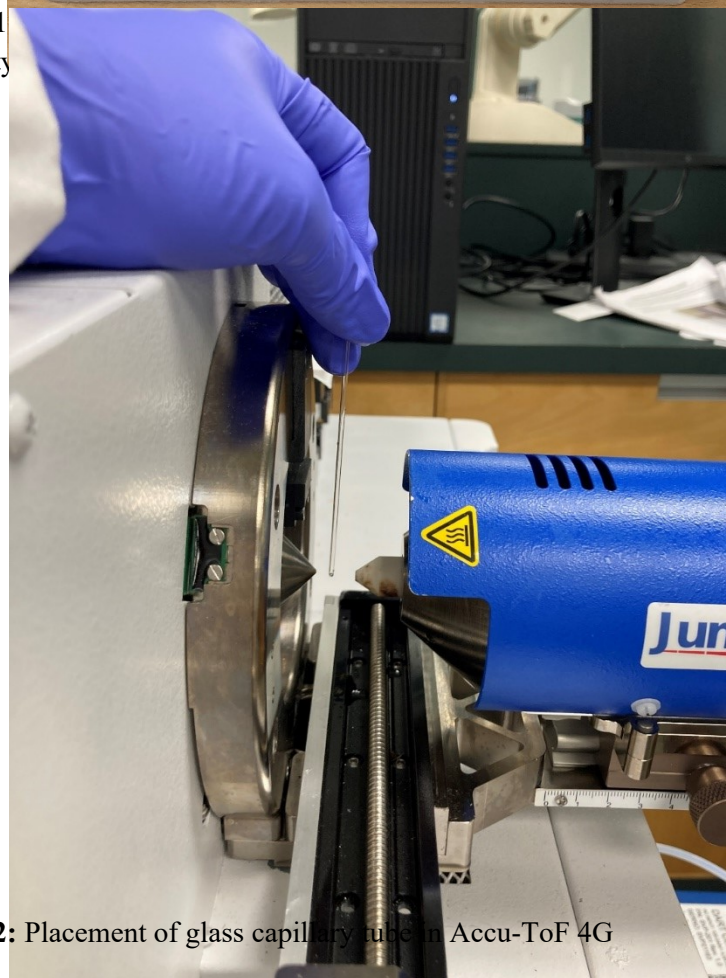
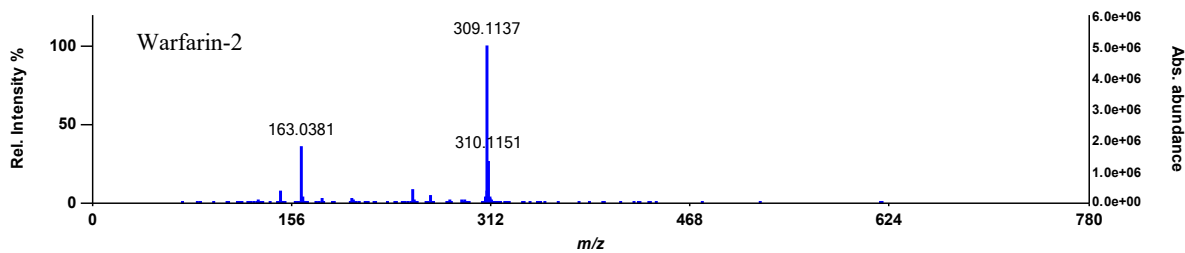
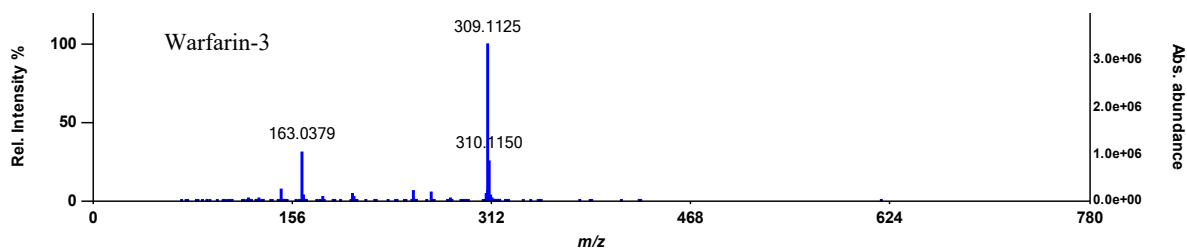


Figure S2: Placement of glass capillary tube in Accu-ToF 4G

Table S1: Summary of DART-ToF parameters

Parameter	NIST DIT	Positive mode testing for quantitation	Negative mode testing for quantitation
Ion mode	Positive	Positive	Negative
Heater temperature (°C)	400	350	350
Orifice temperature (°C)	120	120	150
Detector voltage (V)	2300	2300	2400
Orifice 1 voltage (V)	20, 30, 60, 90	20	-20
Orifice 2 voltage (V)	5	+5	-5
Ion guide voltage (V)	800	500	500
Sampling interval (ns)	0.25	0.25	0.25
Recording interval (s)	0.4	1	1

Low voltage (30V)**Figure S3:** Mass spectrum of warfarin replicate 2 at low voltage (30V)**Figure S4:** Mass spectrum of warfarin replicate 3 at low voltage (30V)

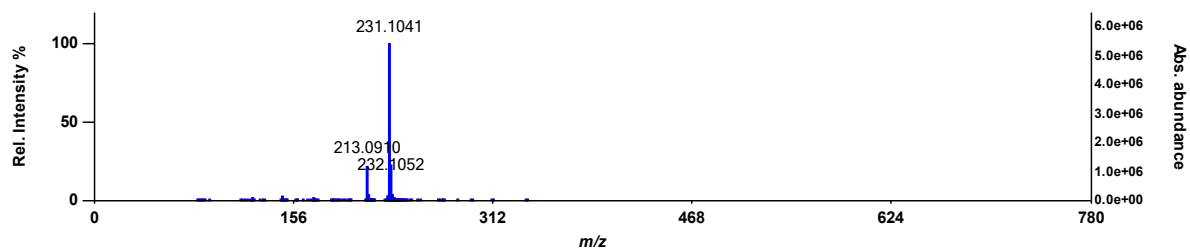


Figure S5: Mass spectrum of pindone replicate 2 at low voltage (30V)

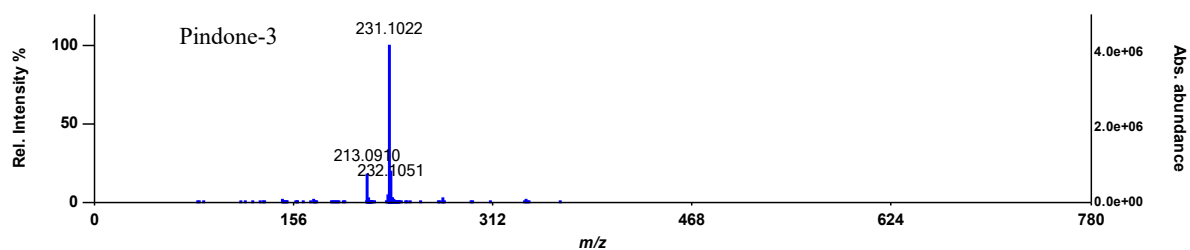


Figure S6: Mass spectrum of pindone replicate 3 at low voltage (30V)

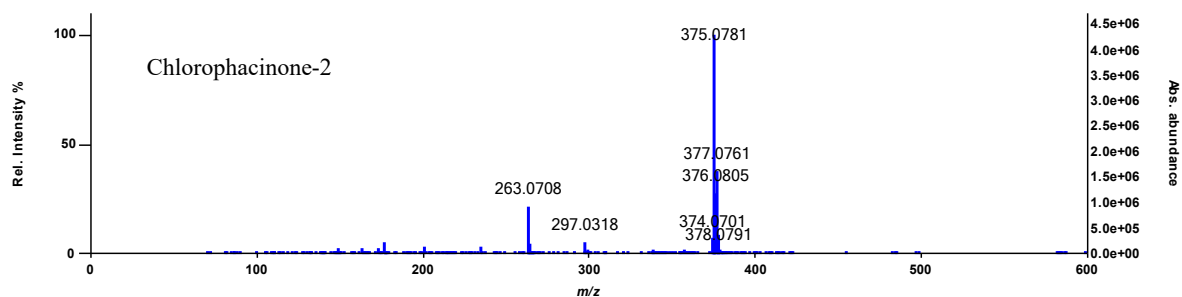


Figure S7: Mass spectrum of chlorophacinone replicate 2 at low voltage (30V)

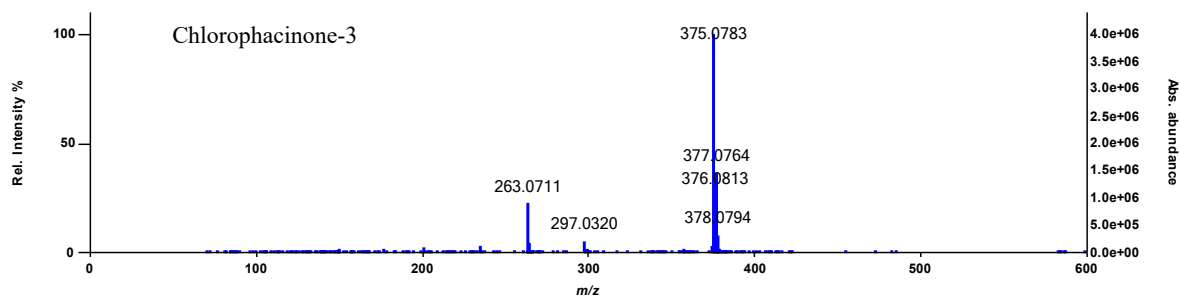


Figure S8: Mass spectrum of chlorophacinone replicate 3 at low voltage (30V)

Diphacinone-2

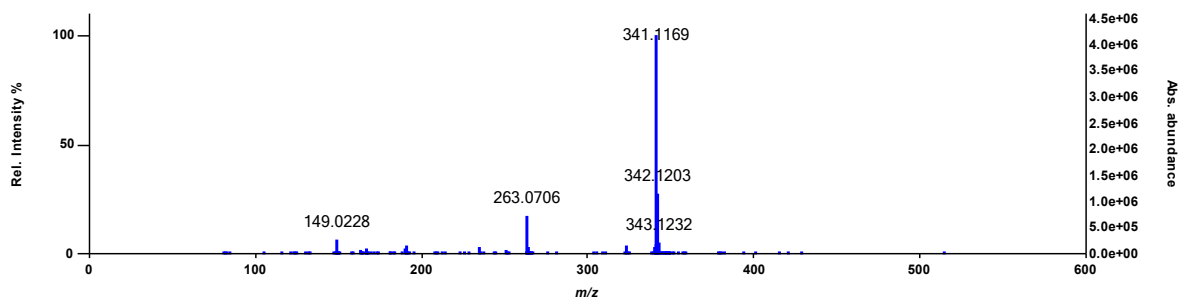


Figure S9: Mass spectrum of diphacinone replicate 2 at low voltage (30V)

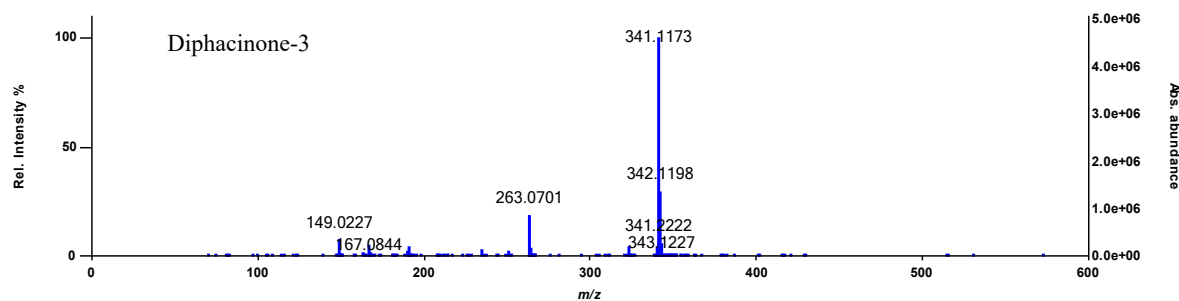


Figure S10: Mass spectrum of diphacinone replicate 3 at low voltage (30V)

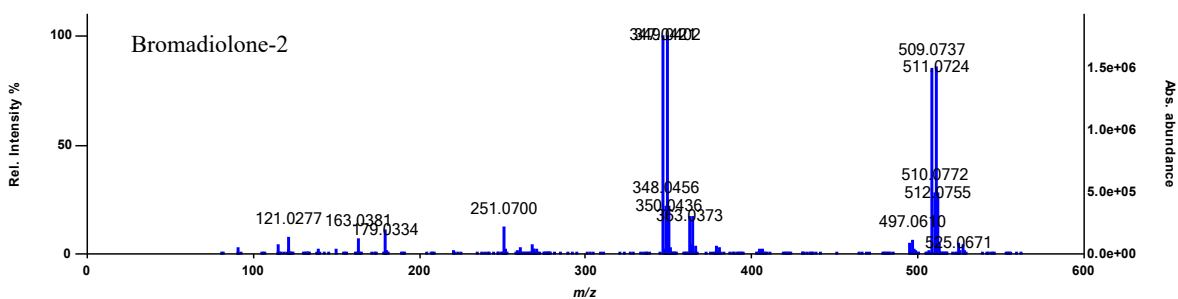


Figure S11: Mass spectrum of bromadiolone replicate 2 at low voltage (30V)

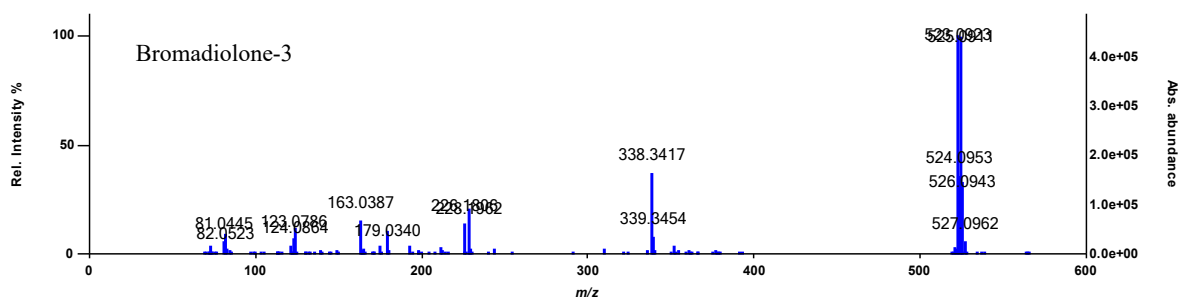


Figure S12: Mass spectrum of bromadiolone replicate 3 at low voltage (30V)

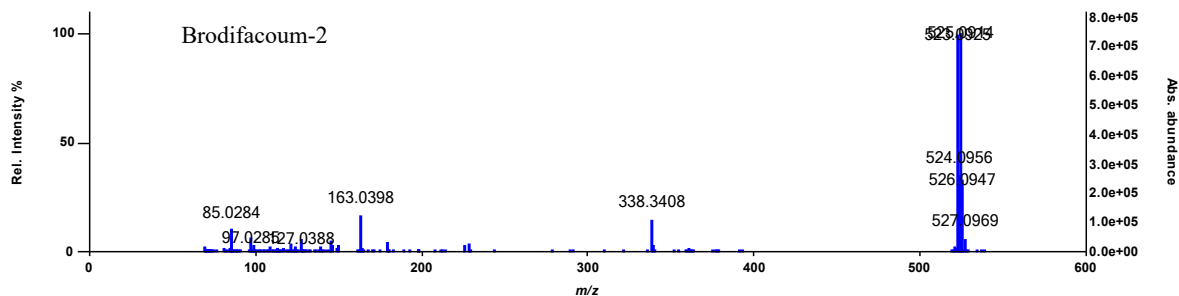


Figure S13: Mass spectrum of brodifacoum replicate 2 at low voltage (30V)

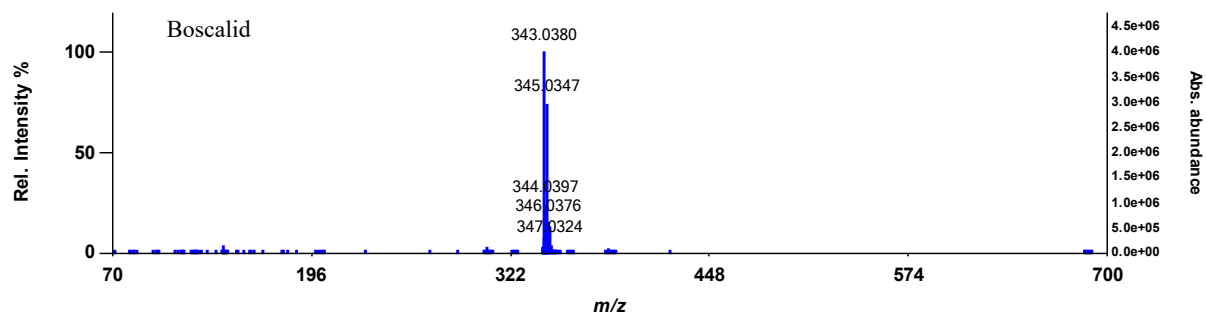


Figure S14: Mass spectrum of boscalid at low voltage (30V)

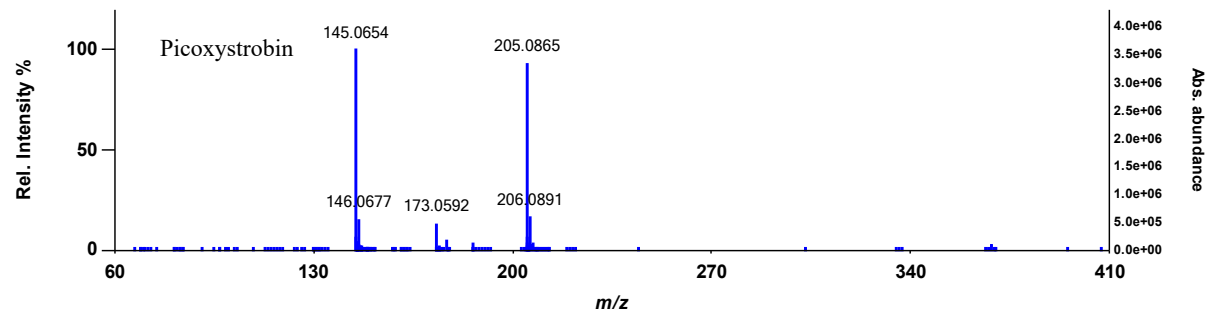


Figure S15: Mass spectrum of picoxystrobin at low voltage (30V)

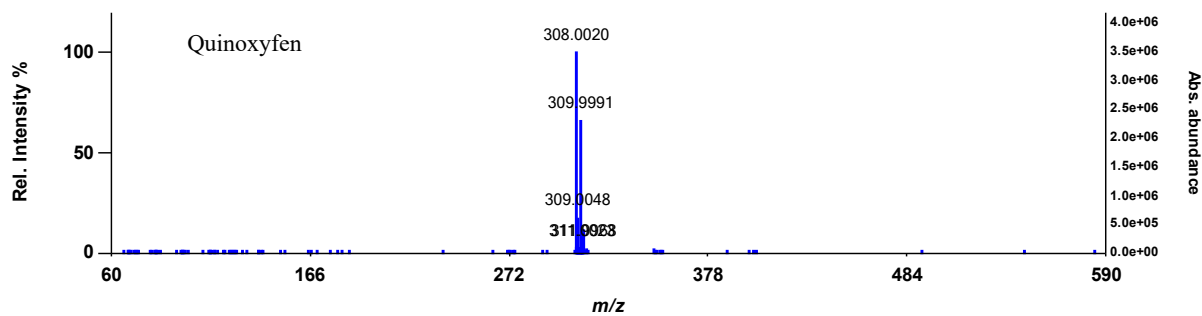


Figure S16: Mass spectrum of quinoxifyfen at low voltage (30V)

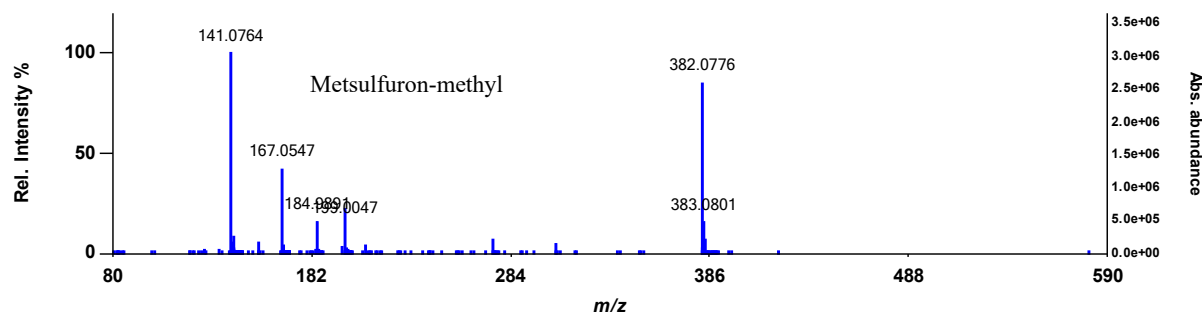


Figure S17: Mass spectrum of metsulfuron-methyl at low voltage (30V)

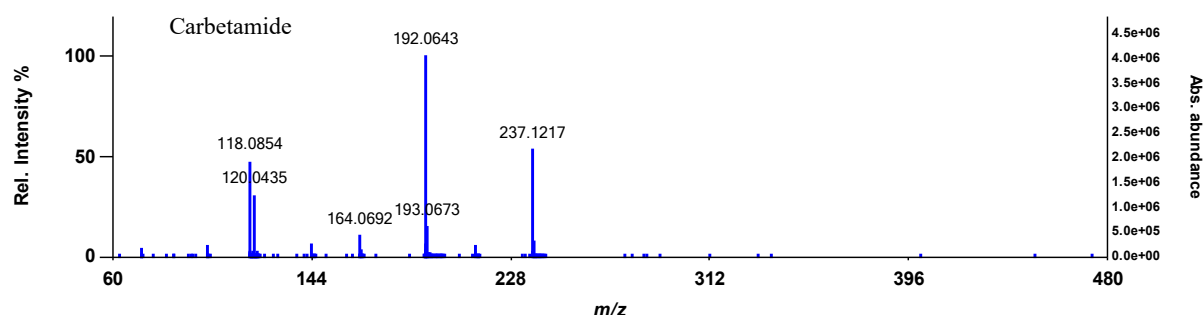


Figure S18: Mass spectrum of carbetamide at low voltage (30V)

MID (60V)

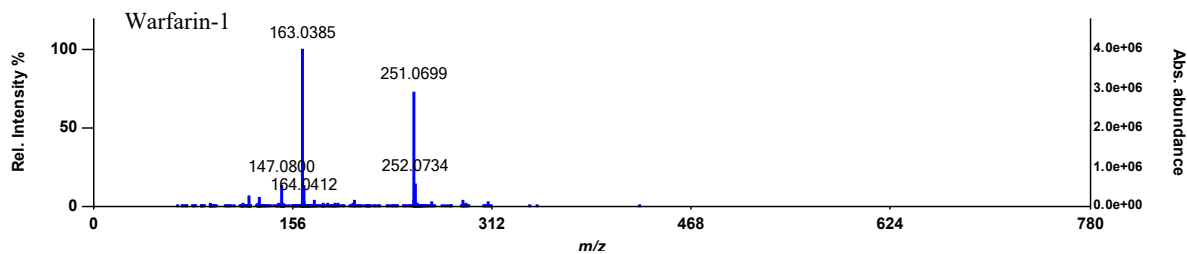


Figure S19: Mass spectrum of warfarin replicate 1 at mid voltage (60V)

Warfarin-2

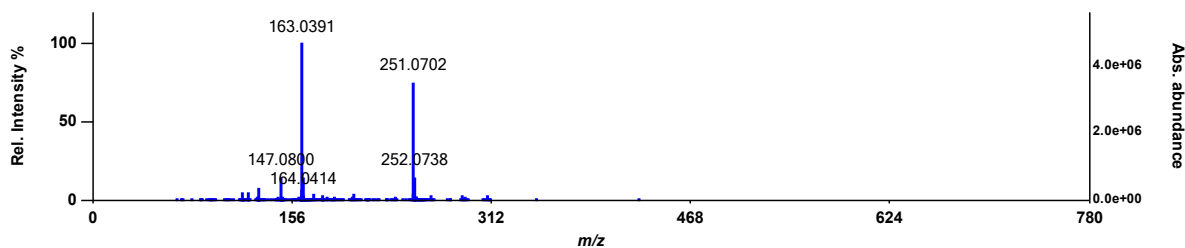


Figure S20: Mass spectrum of warfarin replicate 2 at mid voltage (60V)

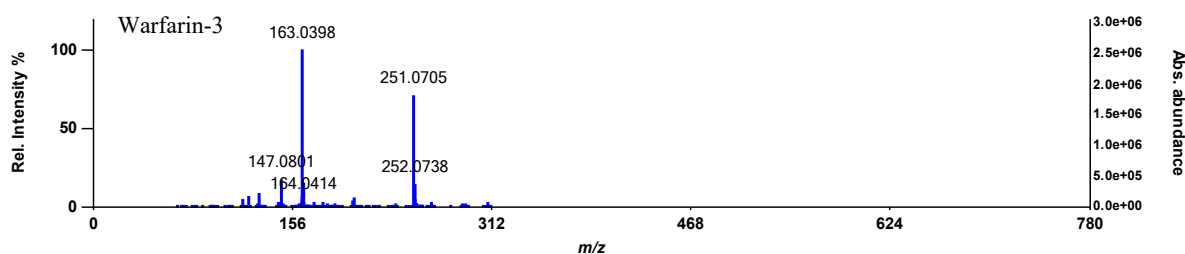


Figure S21: Mass spectrum of warfarin replicate 3 at mid voltage (60V)

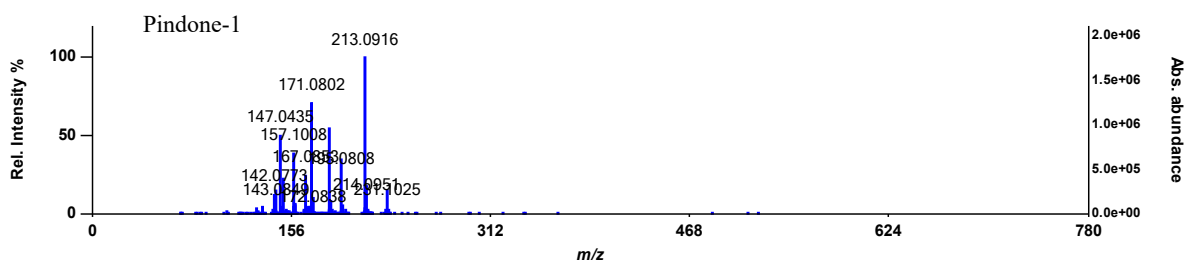


Figure S22: Mass spectrum of pindone replicate 1 at mid voltage (60V)

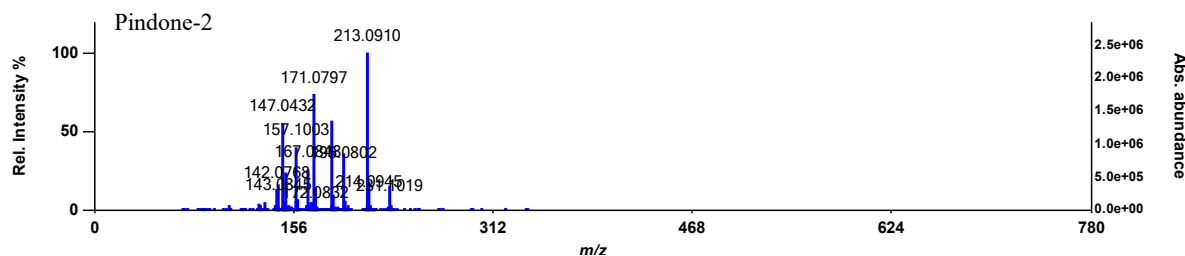


Figure S23: Mass spectrum of pindone replicate 2 at mid voltage (60V)

Pindone-3

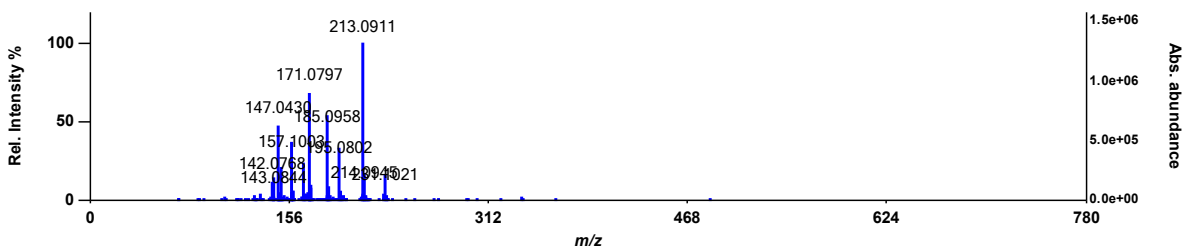


Figure S24: Mass spectrum of pindone replicate 3 at mid voltage (60V)

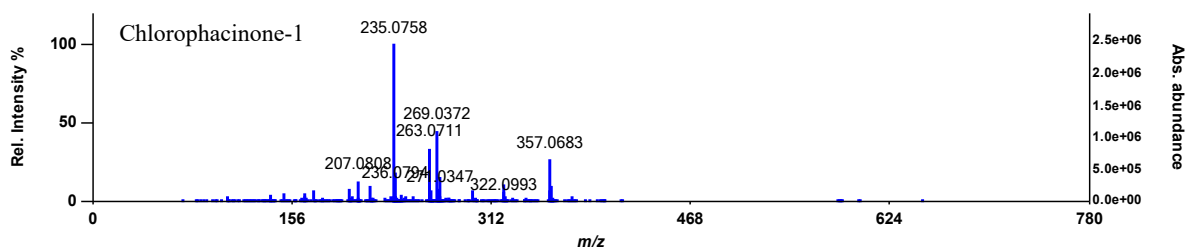


Figure S25: Mass spectrum of chlorophacinone replicate 1 at mid voltage (60V)

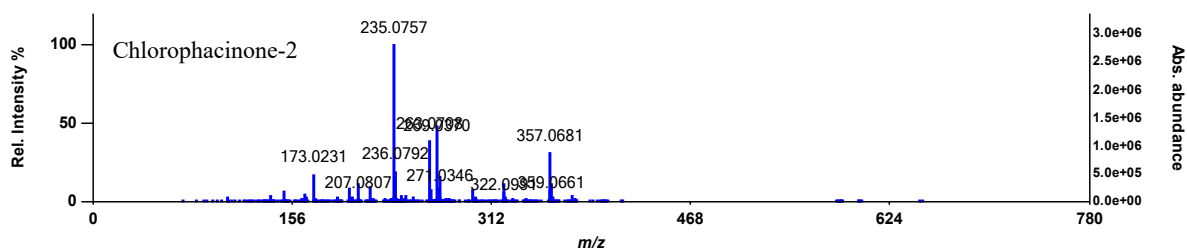


Figure S26: Mass spectrum of chlorophacinone replicate 2 at mid voltage (60V)

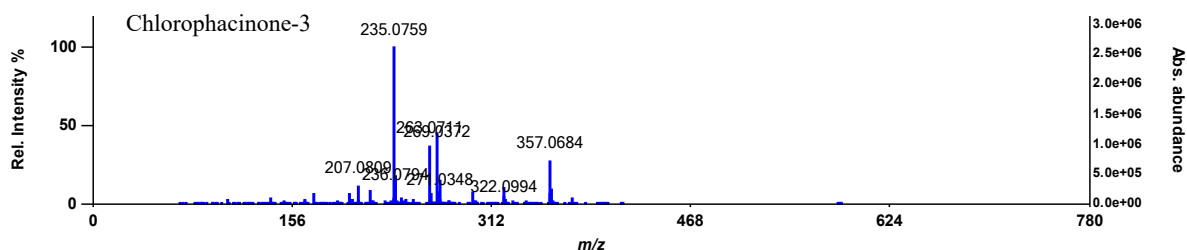


Figure S27: Mass spectrum of chlorophacinone replicate 3 at mid voltage (60V)

Diphacinone-1

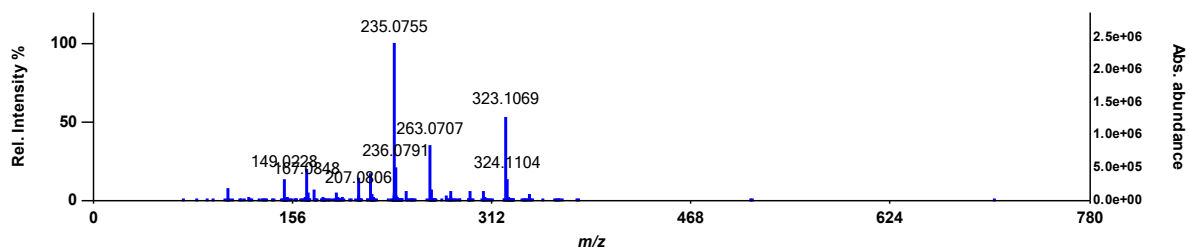


Figure S28: Mass spectrum of diphacinone replicate 1 at mid voltage (60V)

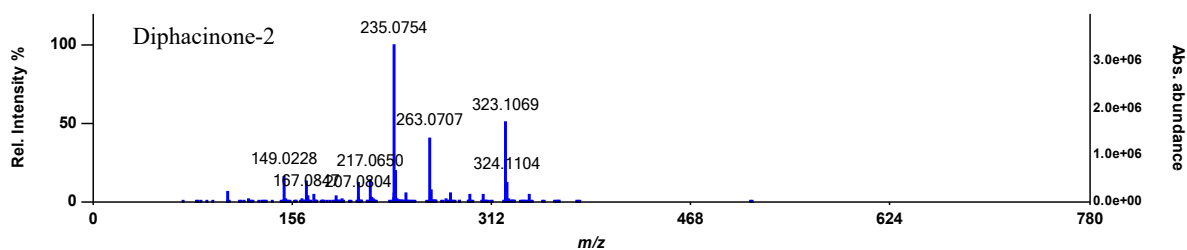


Figure S29: Mass spectrum of diphacinone replicate 2 at mid voltage (60V)

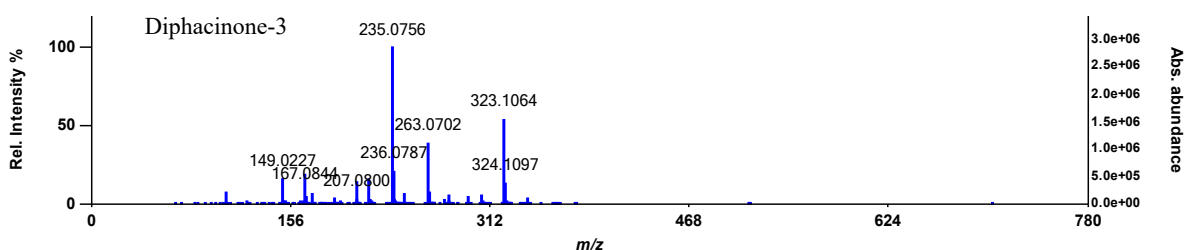


Figure S30: Mass spectrum of diphacinone replicate 3 at mid voltage (60V)

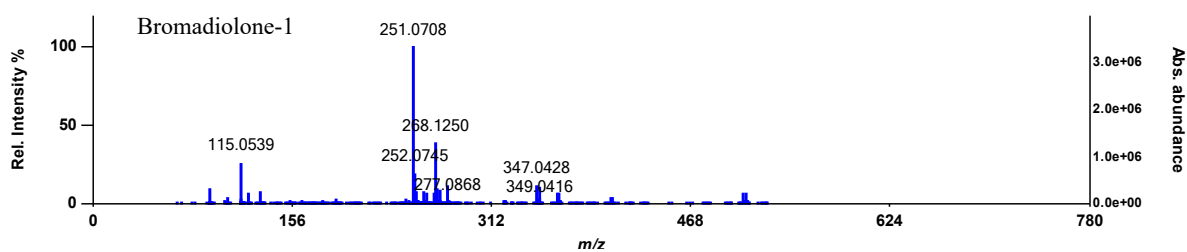


Figure S31: Mass spectrum of bromadiolone replicate 1 at mid voltage (60V)

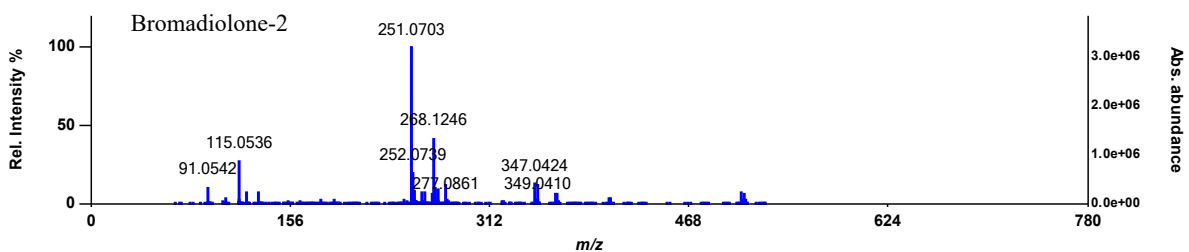


Figure S32: Mass spectrum of bromadiolone replicate 2 at mid voltage (60V)

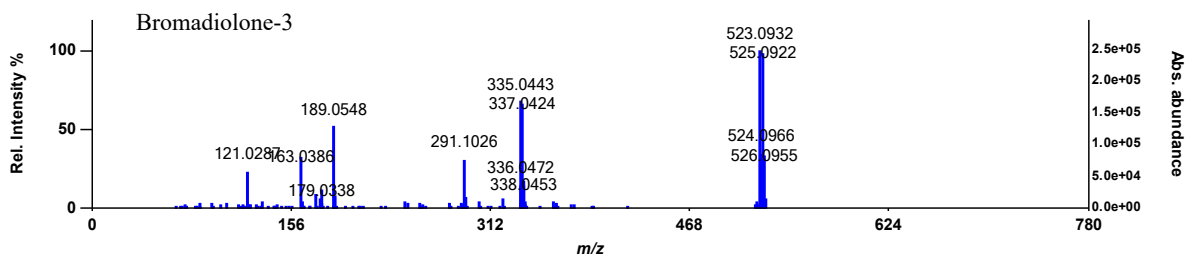


Figure S33: Mass spectrum of bromadiolone replicate 3 at mid voltage (60V)

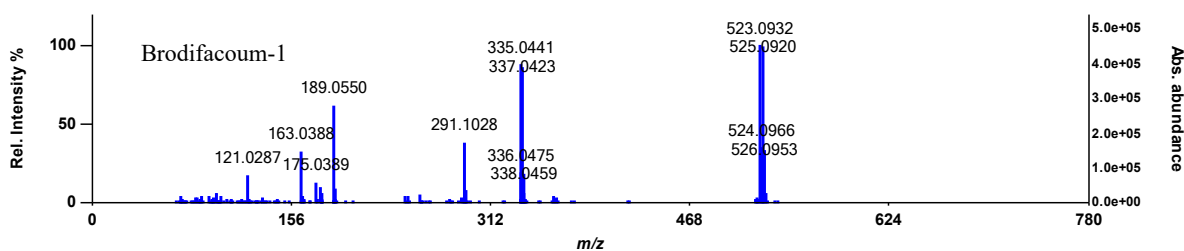


Figure S34: Mass spectrum of brodifacoum replicate 1 at mid voltage (60V)

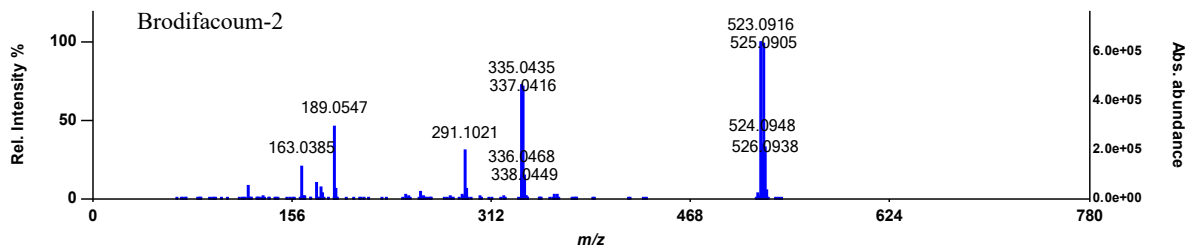


Figure S35: Mass spectrum of brodifacoum replicate 2 at mid voltage (60V)

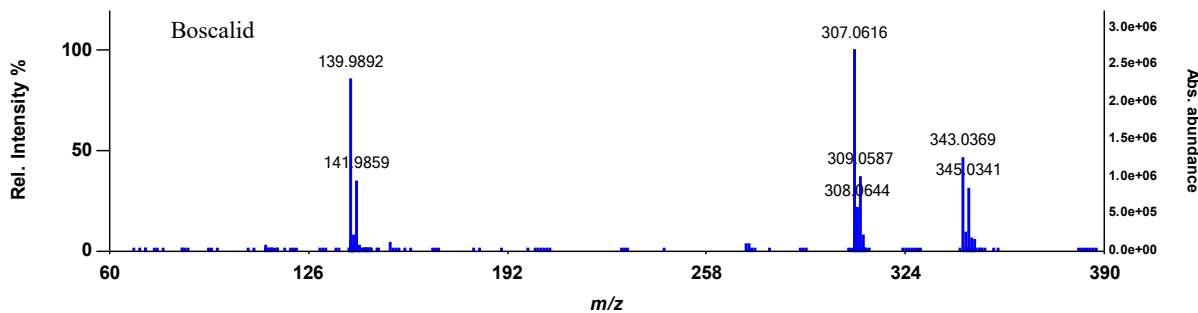


Figure S36: Mass spectrum of boscalid at mid voltage (60V)

Picoxystrobin

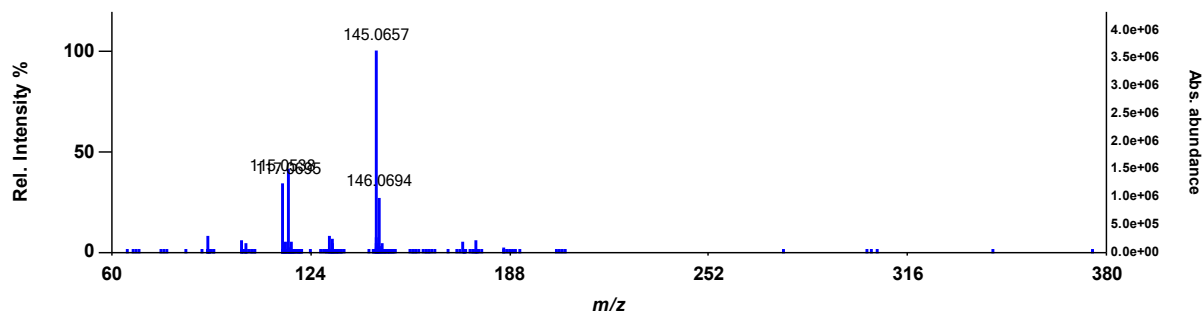


Figure S37: Mass spectrum of picoxystrobin at mid voltage (60V)

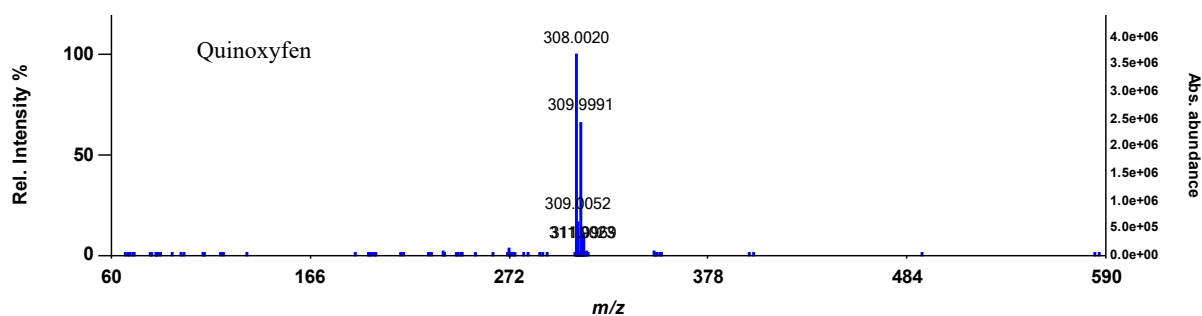


Figure S38: Mass spectrum of quinoxifen at mid voltage (60V)

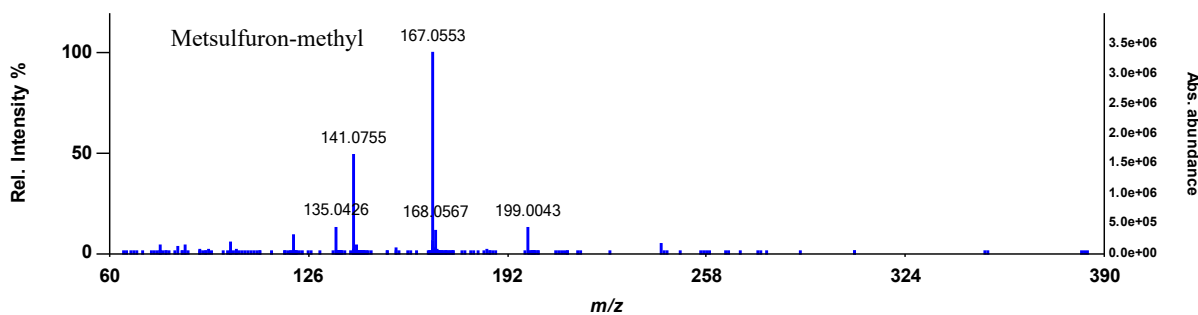


Figure S39: Mass spectrum of metsulfuron-methyl at mid voltage (60V)

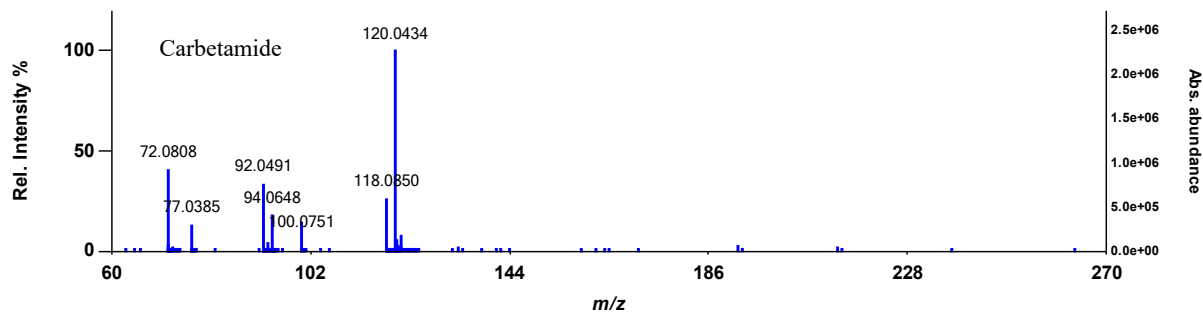


Figure S40: Mass spectrum of carbetamide at mid voltage (60V)

HIGH (90V)

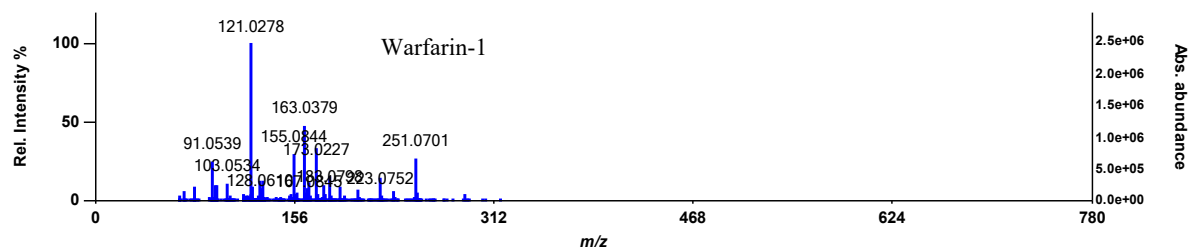


Figure S41: Mass spectrum of warfarin replicate 1 at high voltage (90V)

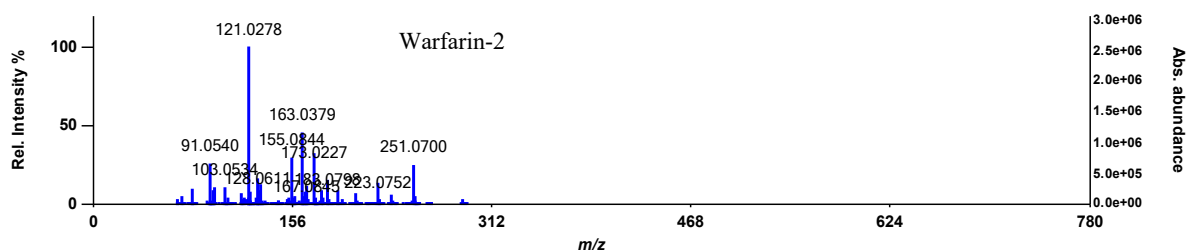


Figure S42: Mass spectrum of warfarin replicate 2 at high voltage (90V)

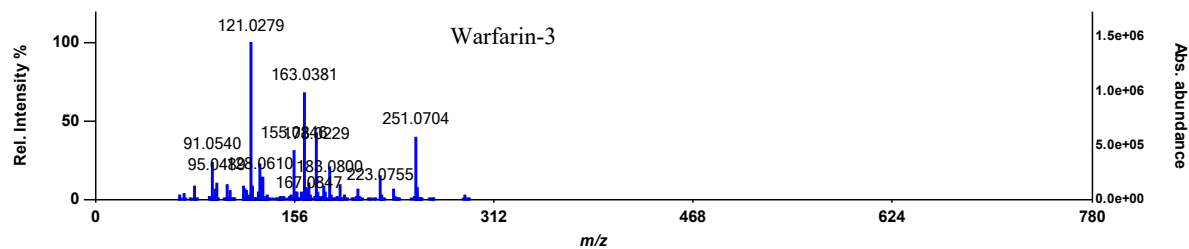


Figure S43: Mass spectrum of warfarin replicate 3 at high voltage (90V)

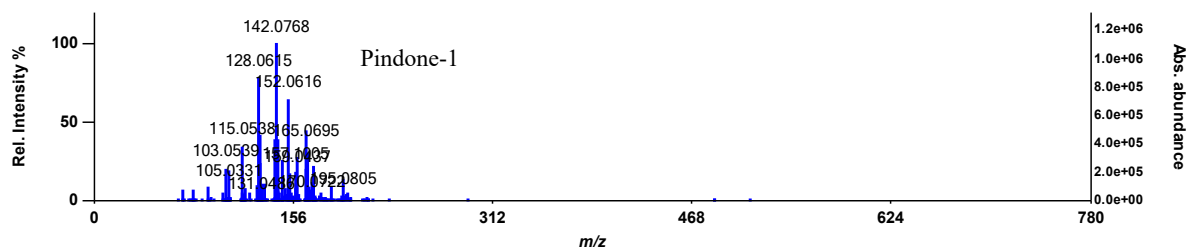


Figure S44: Mass spectrum of pindone replicate 1 at high voltage (90V)

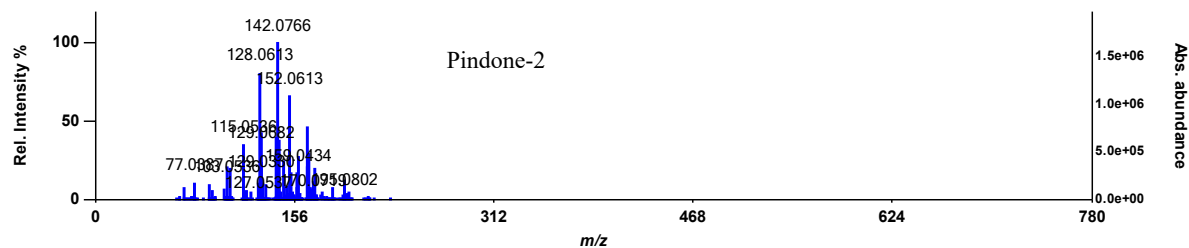


Figure S45: Mass spectrum of pindone replicate 2 at high voltage (90V)

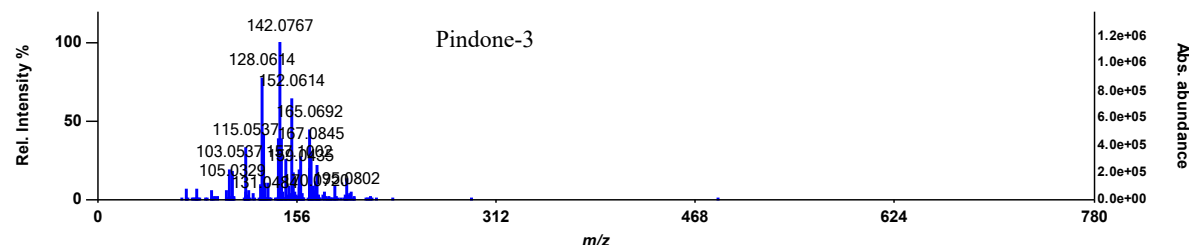


Figure S46: Mass spectrum of pindone replicate 3 at high voltage (90V)

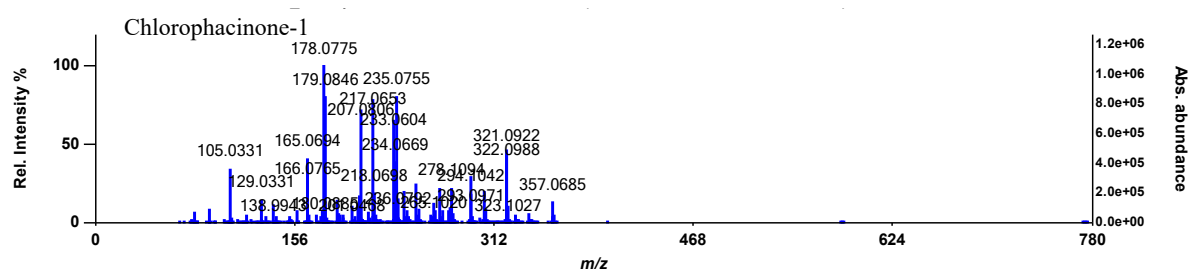


Figure S47: Mass spectrum of chlorophacinone replicate 1 at high voltage (90V)

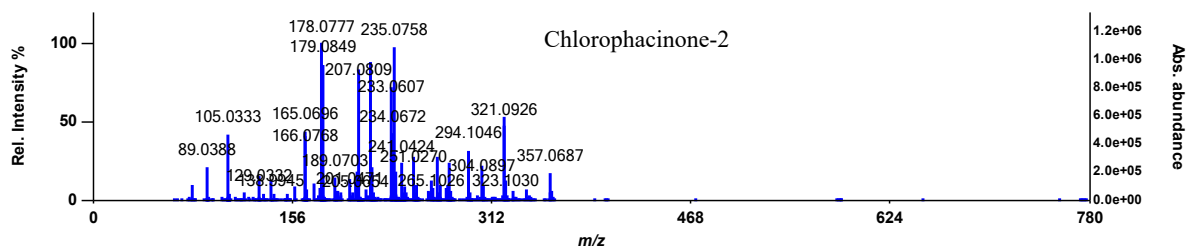


Figure S48: Mass spectrum of chlorophacinone replicate 2 at high voltage (90V)

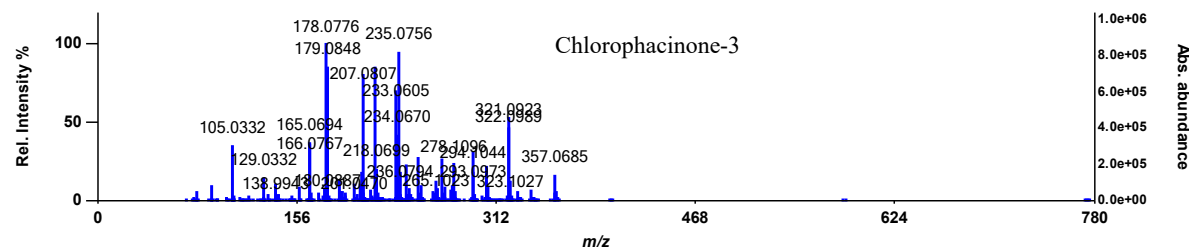


Figure S49: Mass spectrum of chlorophacinone replicate 3 at high voltage (90V)

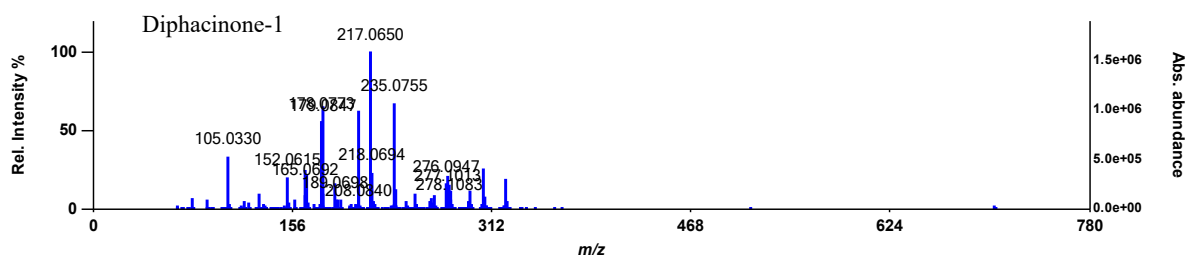


Figure S50: Mass spectrum of diphacinone replicate 1 at high voltage (90V)

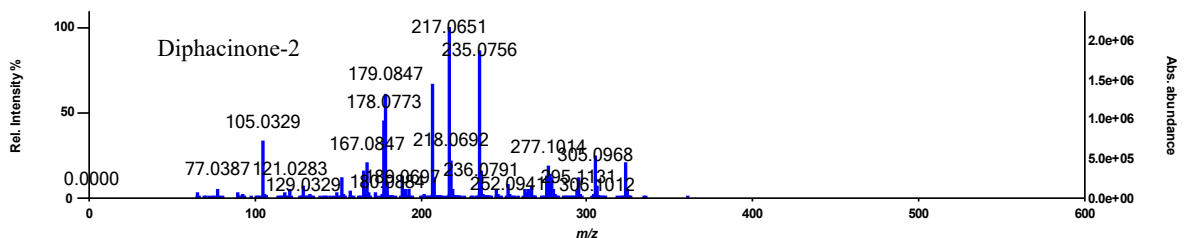


Figure S51: Mass spectrum of diphacinone replicate 2 at high voltage (90V)

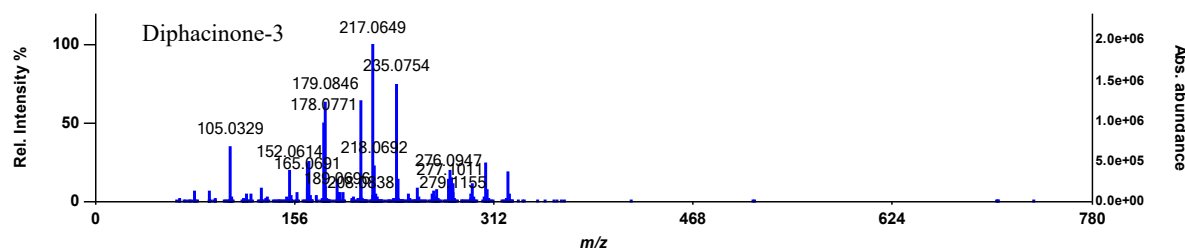


Figure S52: Mass spectrum of diphacinone replicate 3 at high voltage (90V)

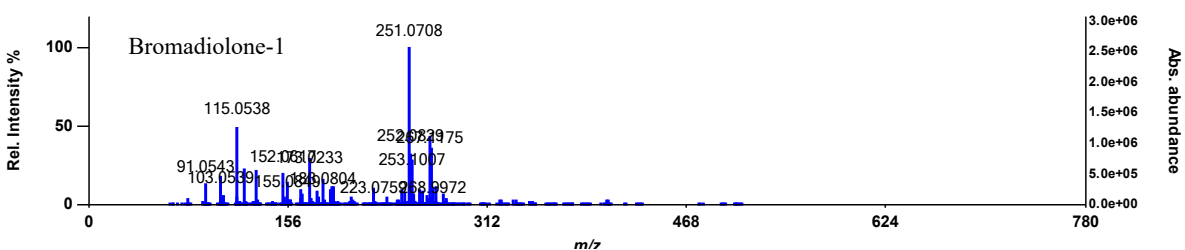


Figure S53: Mass spectrum of bromadiolone replicate 1 at high voltage (90V)

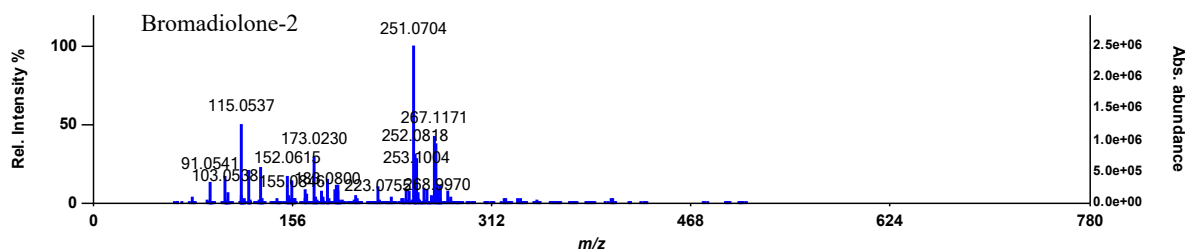


Figure S54: Mass spectrum of bromadiolone replicate 2 at high voltage (90V)

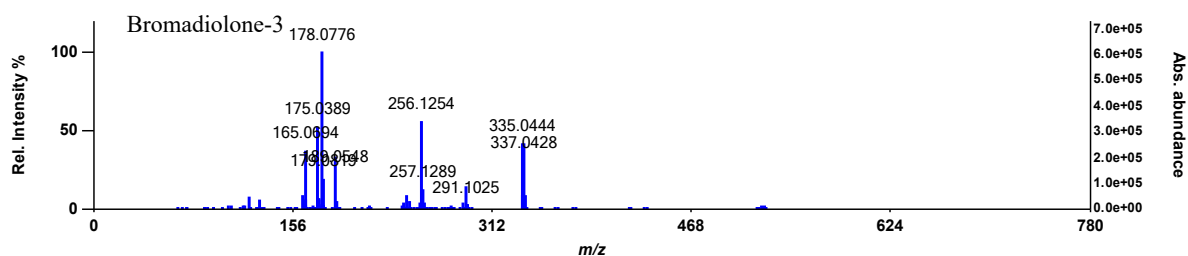


Figure S55: Mass spectrum of bromadiolone replicate 3 at high voltage (90V)

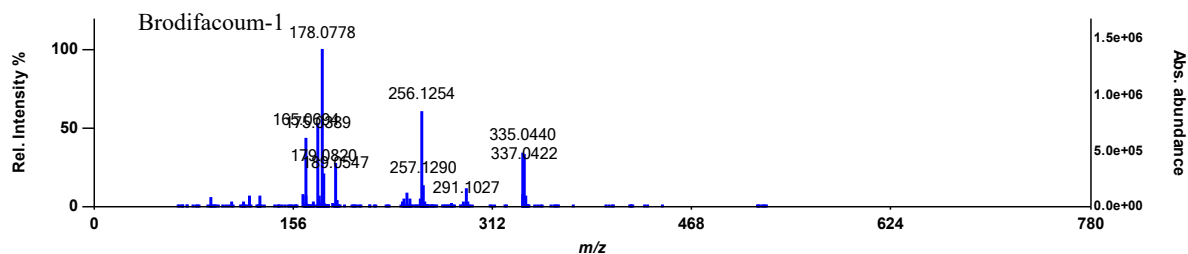


Figure S56: Mass spectrum of brodifacoum replicate 1 at high voltage (90V)

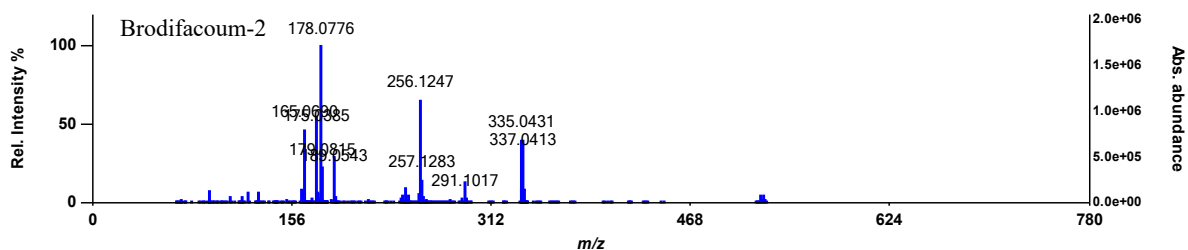


Figure S57: Mass spectrum of brodifacoum replicate 2 at high voltage (90V)

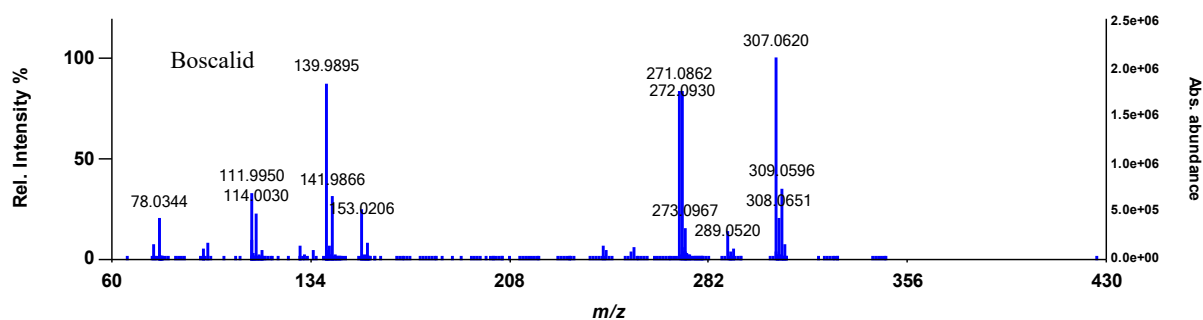


Figure S58: Mass spectrum of boscalid at high voltage (90V)

Picoxystrobin

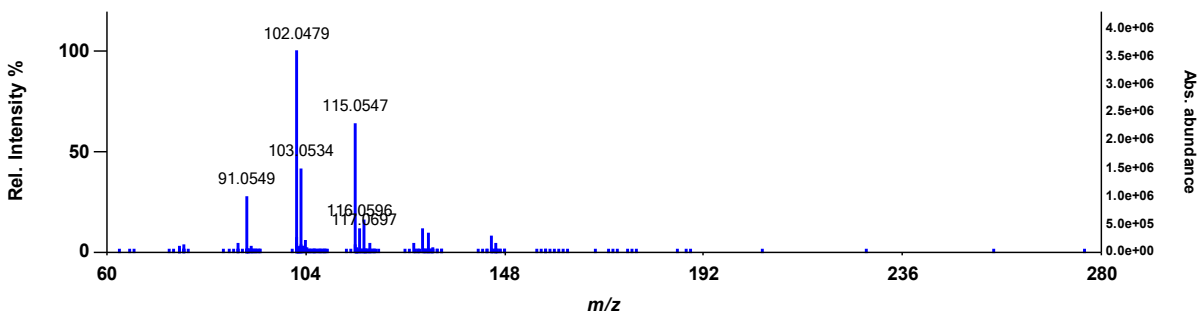


Figure S59: Mass spectrum of picoxystrobin at high voltage (90V)

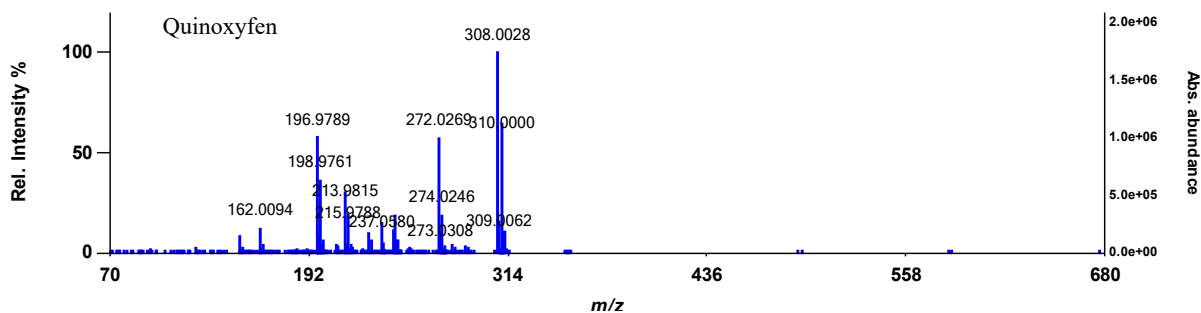


Figure S60: Mass spectrum of quinoxifen at high voltage (90V)

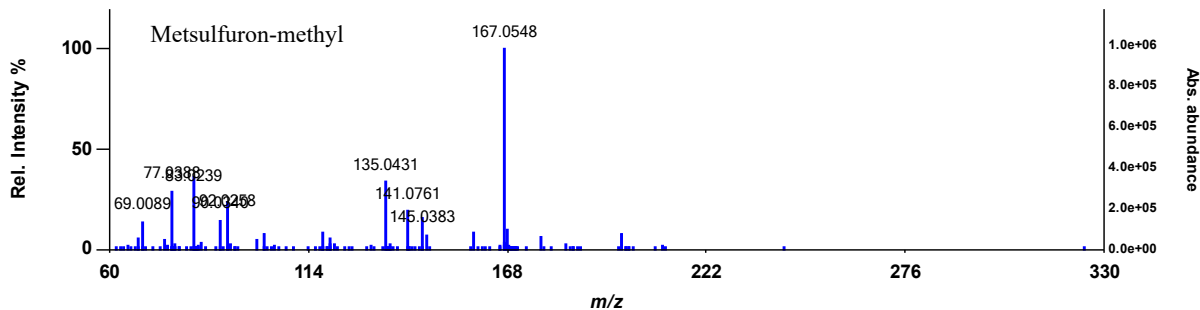


Figure S61: Mass spectrum of metsulfuron-methyl at high voltage (90V)

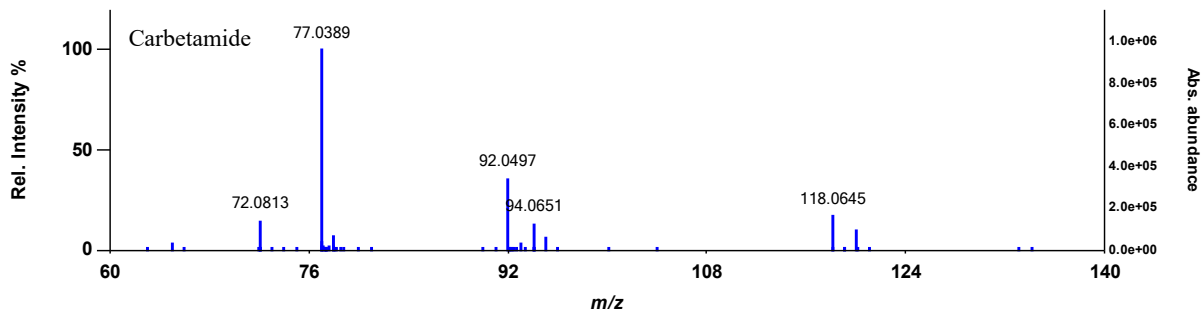


Figure S62: Mass spectrum of carbetamide at high voltage (90V)

Figures S4-S62: Mass spectra of library references in positive ion mode.

Table S2: Mass readings of rodenticide, herbicide and fungicide standards

	[M+H] ⁺ (m/z)						
Rodenticide	True mass	R1	R2	R3	Average	Standard Deviation	Relative Standard Deviation
Warfarin	309.112684	309.111554	309.113711	309.112511	309.112592	0.0010807788858	0.0003496392298%
Pindone	231.102119	231.103327	231.10411	231.102243	231.1032267	0.0009375352438	0.0004056781280%
Chlorophacinone	375.078797	375.078201	375.07812	375.078269	375.0781967	0.0000745944591	0.0000198877087%
Diphacinone	341.117769	341.117261	341.116928	341.117313	341.1171673	0.0002088931146	0.0000612379366%
Bromadiolone	527.085797	347.043007	347.04206	N/A	347.0425335	0.0006696301218	0.0001929533291%
Brodifacoum	523.090882	523.092357	523.092541	523.090182	523.0916933	0.0013120824415	0.0002508322075%
Boscalid	343.032668				343.038031		
Picoxystrobin	368.103143				368.109109		
Quinoxifen	308.00391				308.002003		
Metsulfuron-methyl	382.074304				382.077683		
Carbetamide	237.123113				237.121667		

NIST/NIJ DART-MS Data Interpretation Tool



Search Tool Libraries Scoring About

View:

☒ Interactive ☐ Reporting

Date...

Instrument ID...

Case No...

Item No...

Comments...

Load Presets

Download Presets

Restore Defaults

Query Spectra

Settings

Reference Library:

ECCC_Rodenticides_v05122025_forDITv3.f

Polarity: Positive

Source Gas: He

Select centroided mass spectrum (txt, jpg, csv)
measured at fragmentation levels of your choice.
Low (30 V) fragmentation required.

Browse...

1to1 warf diph 100ppm_3C

Upload complete

* required

Browse...

1to1 warf diph 100ppm_6C

Upload complete

Browse...

1to1 warf diph 100ppm_9C

Upload complete

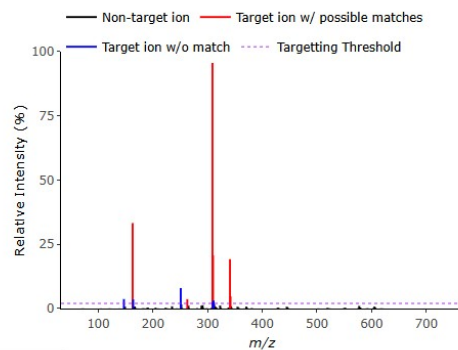
Search Library

Clear Search

References

Moorthy et. al. DOI:10.26434/chemrxiv-2022-s00s1

Low (30 V) Mid (60 V) High (90 V)



Show 10 entries

m/z	Relative Intensity	Target
309.0651	100.0	T1
163.0152	33.3	T2
310.0685	20.7	T3
341.0646	19.2	T4
251.0332	8.0	T5
342.0680	4.7	T6
147.0618	3.7	T7
263.0313	3.6	T8
164.0184	3.5	T9
311.0706	3.1	T10

Previous

1

2

3

4

5

...

15

Next

Target 1

Target 2

Target 3

Target 4

Target 5

Target 6

Target 7

Target 8

Target 9

Target 10

Target 11

Target 12

Measured m/z: 309.0651

Relative Intensity: 100.0 %

Potential matches:

Search:

	Compound	$\Delta m/z$	FPIE	RevMF	IRD	Match Type
1	Warfarin 1	-0.0475	0.946	0.984	0.001	Protonated Molecule
2	Warfarin 2	-0.0475	0.926	0.983	0.001	Protonated Molecule
3	Warfarin 3	-0.0475	0.901	0.962	0.001	Protonated Molecule

Figure S63: NIST/NIJ DART-MS DIT sample of results

Reference Library:

Trista_library_20250723_forDITv3.RDS

Show 25 entries

Previous 1 Next Search:

	Name	Formula	[M+H] ⁺	Synonyms	Base Peak
	All	All	All	All	All
1	Warfarin	C ₁₉ H ₁₆ O ₄	309.1127		NA
2	Pindone	C ₁₄ H ₁₄ O ₃	231.1021	2-Pivaloyl-1,3-indandione	NA
3	Chlorophacinone	C ₂₂ Cl ₁ H ₁₅ O ₃	375.0788		NA
4	Diphacinone	C ₂₃ H ₁₆ O ₃	341.1178	Diphenadione, difenacin, ratindan	NA
5	Bromadiolone	Br ₁ C ₂₀ H ₂₂ O ₄	527.0858	Broprodifacoum; Bromatrol	NA
6	Brodifacoum	Br ₁ C ₂₁ H ₂₂ O ₃	523.0909	Bromfenacoum	NA
7	Boscalid	C ₁₈ Cl ₂ H ₁₂ N ₂ O ₁	343.0405	BAS 510F, Nicobifen, Endura	343.0405
8	Picoxystrobin	C ₁₈ F ₃ H ₁₆ N ₁ O ₄	368.1110		NA
9	Quinoxifen	C ₁₅ Cl ₂ F ₁ H ₈ N ₁ O ₁	308.0045		308.0045
10	Metsulfuron Methyl	C ₁₄ H ₁₅ N ₃ O ₅ S ₁	382.0821		141.0776
11	Carbetamide	C ₁₂ H ₁₆ N ₂ O ₃	237.1239	Carbatamex, Carbethamide	192.0661

Figure S64: NIST/NIJ DART-MS DIT library contents

Table S3: Library metadata

Code	Canonical_SMILES	Name	Synonyms	IUPAC_Forma l_Nam e	Class
warfarin	<chem>CC(=O)CC(C\1=C(/O)c2ccccc2OC(=O)c3ccccc3</chem>	Warfarin		(R)-4-Hydroxy-3-(3-oxo-1-phenylbutyl)-2H-chromen-2-one	Coumarin
pindone	<chem>O=C2c1ccccc1C(=O)C2C(=O)C(C)(C)C</chem>	Pindone	2-Pivaloyl-1,3-indandione	2-(2,2-Dimethylpropanoyl)-1H-indene-1,3(2H)-dione	indadione
chlorophacinone	<chem>Clc1ccc(cc1)C(c2ccccc2)C(=O)C4C(=O)c3ccccc3C4=O</chem>	Chlorophacinone		2-[(4-Chlorophenyl)phenylacetyl]-1H-indene-1,3(2H)-dione	indadione
diphacinone	<chem>O=C2c1ccccc1C(=O)C2C(=O)C(c3ccccc3)c4ccccc4</chem>	Diphacinone	Diphenadione, difenacin, ratindan	2-(Diphenylacetyl)-1H-indene-1,3(2H)-dione	indadione
bromadiolone	<chem>Brc1ccc(cc1)c2ccc(cc2)C(O)CC(C\3=C(/O)c4ccccc4OC(=O)c5ccccc5</chem>	Bromadiolone	Broprodifacoum; Bromatrol	3-[3-[4-(4-Bromophenyl)phenyl]-3-hydroxy-1-phenylpropyl]-2-hydroxychromen-4-one	Coumarin
brodifacoum	<chem>Brc1ccc(cc1)c2ccc(cc2)C4Cc3ccccc3C(C4)C\5=C(/O)c6ccccc6OC(=O)c5ccccc5</chem>	Brodifacoum	Bromfenacoum	3-[3-[4-(4-Bromophenyl)phenyl]-1,2,3,4-tetrahydronaphthalen-1-yl]-2-hydroxychromen-4-one	Coumarin
boscalid	<chem>C1=CC=C(C(=C1)C2=CC=C(C(=C2)Cl)NC(=O)C3=C(N=CC=C3)Cl</chem>	Boscalid	BAS 510F, Nicobifen, Endura	2-chloro-N-(4'-chloro[1,1'-biphenyl]-2-yl)pyridine-3-carboxamide	biphenyl amide
picoxystrobin	<chem>CO/C=C(\C1=CC=CC=C1COC2=CC=CC(=N2)C(F)(F)F)/C(=O)OC</chem>	Picoxystrobin		methyl (E)-3-methoxy-2-[2-[[6-(trifluoromethyl)pyridin-2-yl]oxymethyl]phenyl]prop-2-enoate	biphenyl amide
quinoxifen	<chem>C1=CC(=CC=C1OC2=C3C(=CC(=CC3=NC=C2)Cl)Cl)F</chem>	Quinoxifen		5,7-dichloro-4-(4-fluorophenoxy)quinoli	biphenyl amide

				ne	
metsulfuron methyl	<chem>CC1=NC(=NC(=N1)OC)NC(=O)NS(=O)(=O)C2=CC=C(C=C2C(=O)OC</chem>	Metsulfuron Methyl		2-[[[4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]-oxomethyl]sulfamoyl}benzoic acid methyl ester	sulfonylurea
carbetamide	<chem>CCNC(=O)[C@H](C)OC(=O)NC1=CC=CC=C1</chem>	Carbetamide	Carbatamex, Carbethamide	[(2R)-1-(ethylamino)-1-oxopropan-2-yl] N-phenylcarbamate	carbanilate

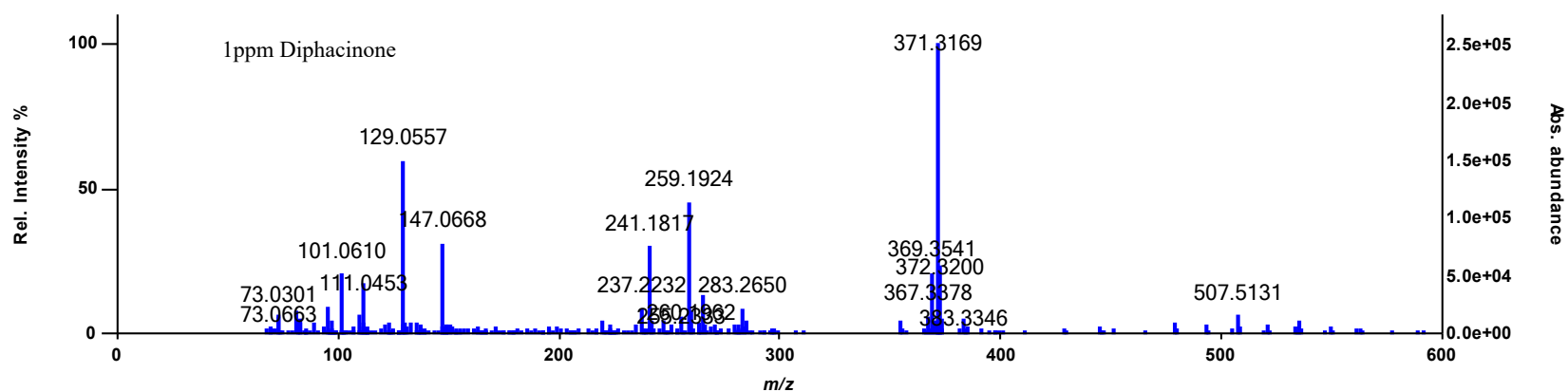


Figure S65: Mass spectrum of 1ppm diphacinone replicate 1

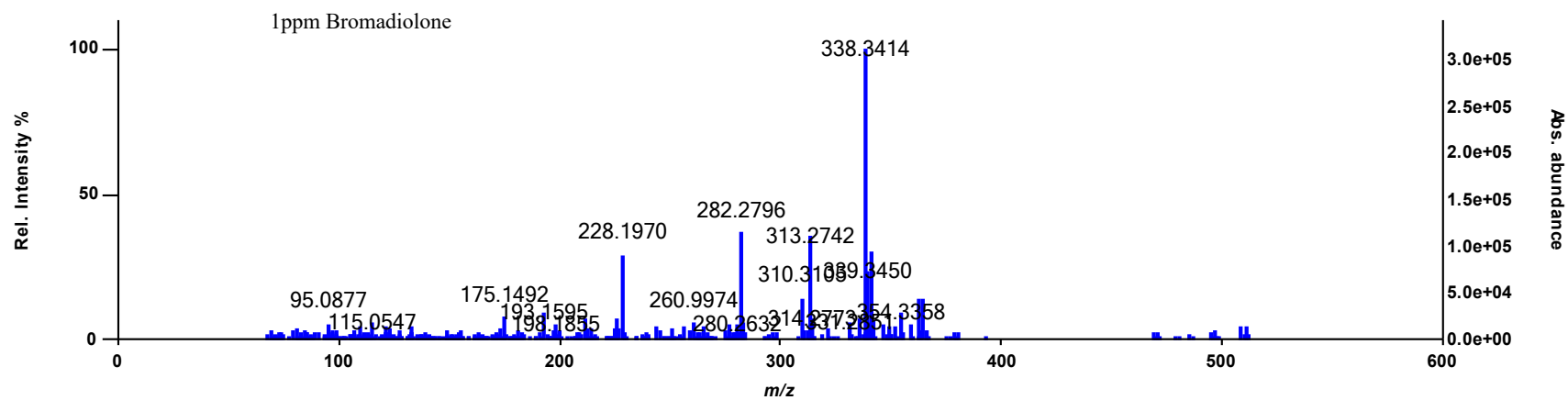


Figure S66: Mass spectrum of 1ppm bromadiolone replicate 1

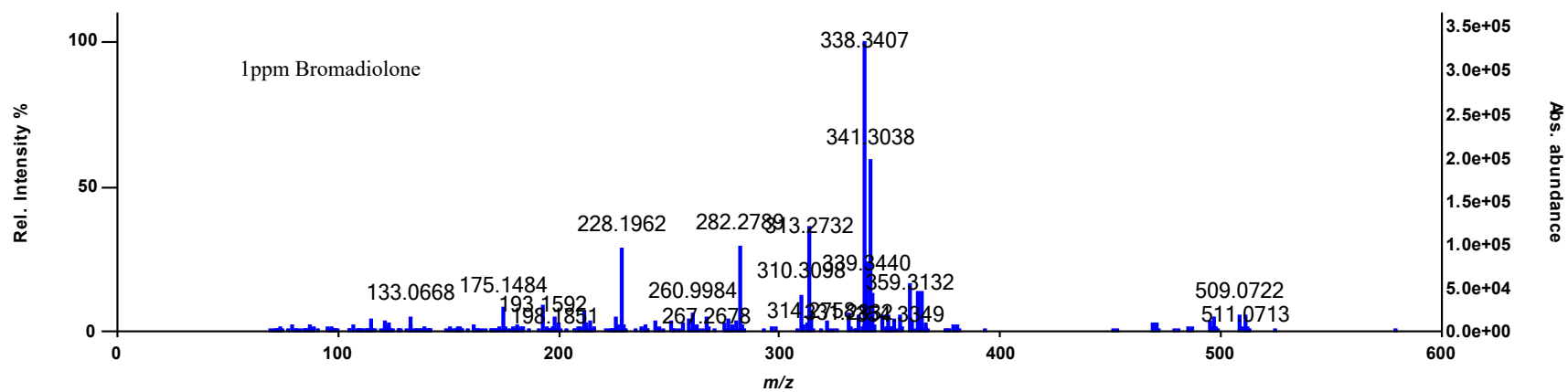


Figure S67: Mass spectrum of 1ppm bromadiolone replicate 2

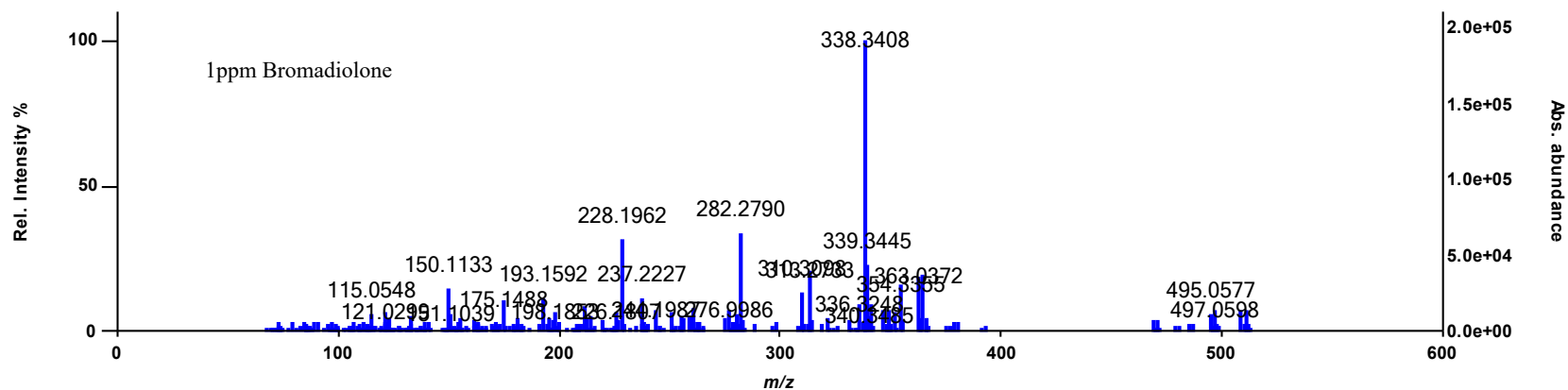


Figure S68: Mass spectrum of 1ppm bromadiolone replicate 3

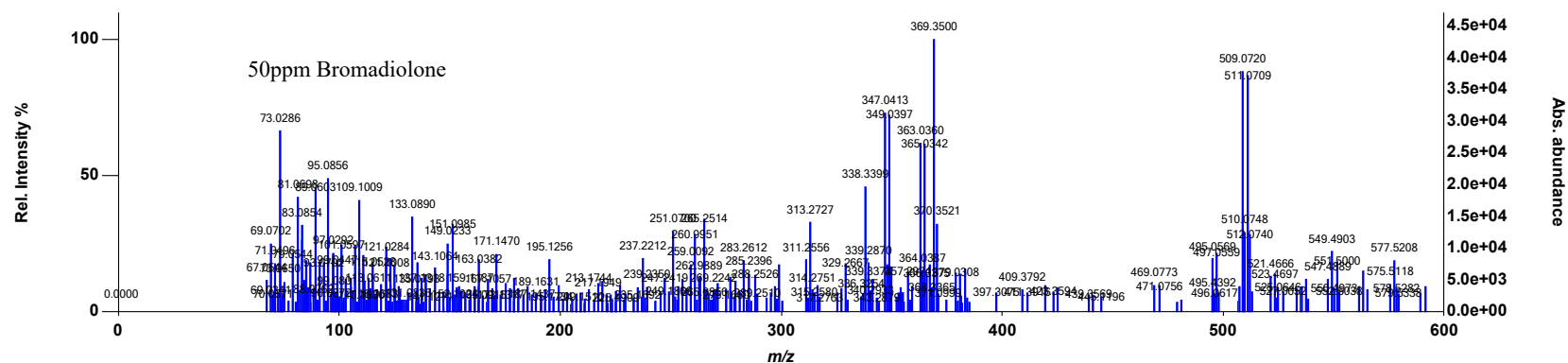


Figure S69: Mass spectrum of 50ppm bromadiolone replicate 3

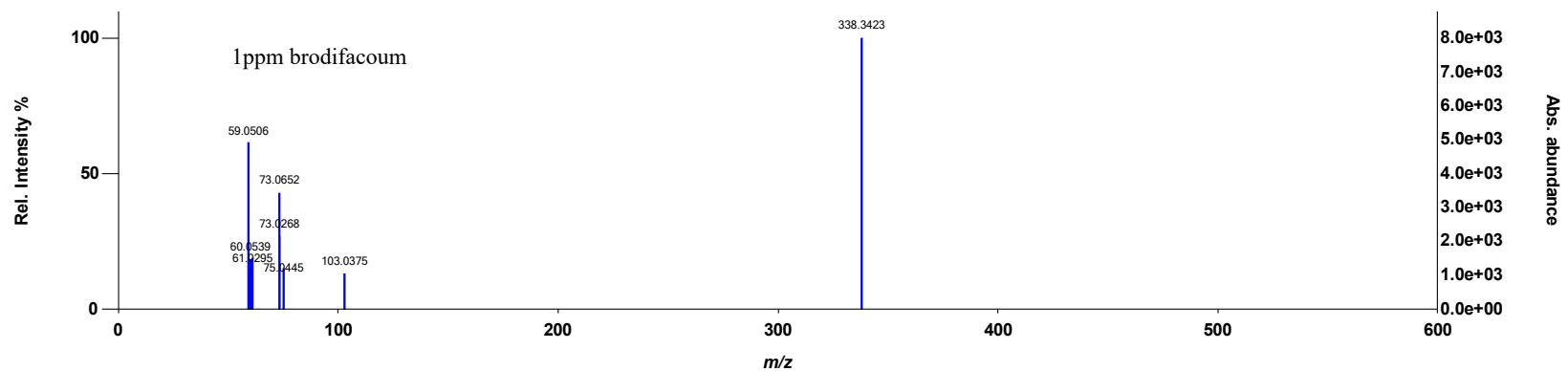


Figure S70: Mass spectrum of 1ppm brodifacoum replicate 2

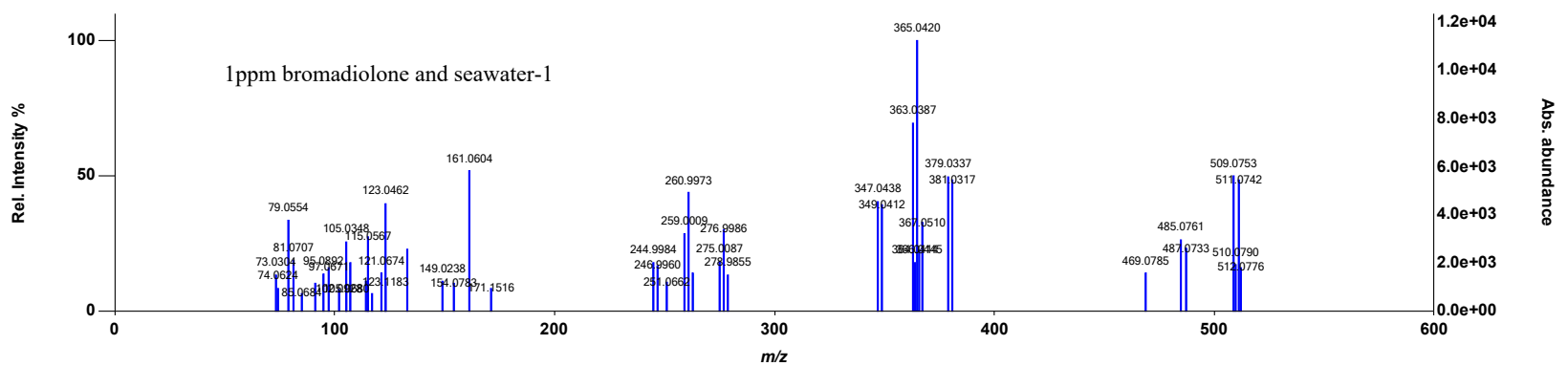


Figure S71: Mass spectrum of 1ppm bromadiolone and seawater replicate 1

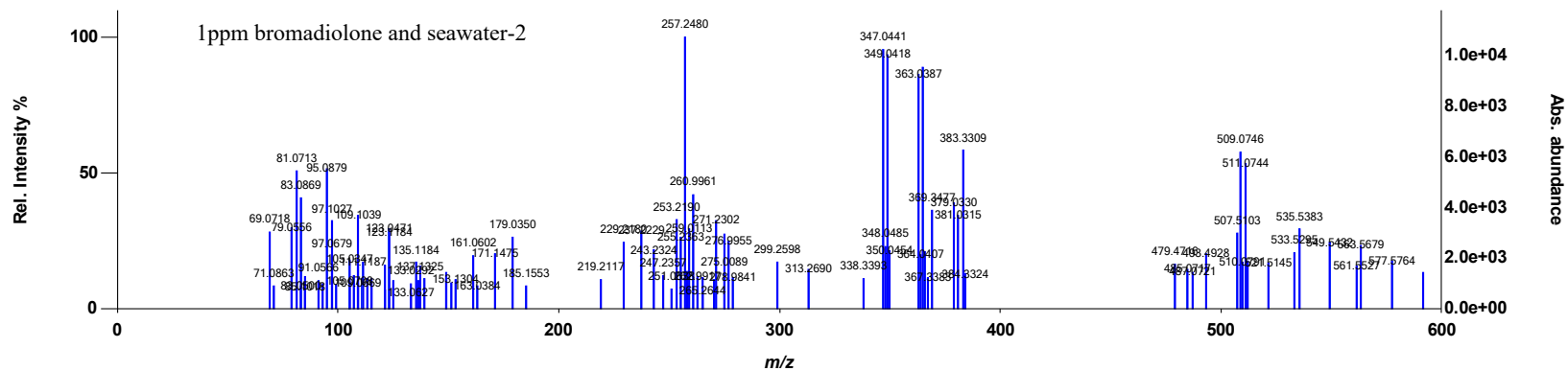


Figure S72: Mass spectrum of 1ppm bromadiolone and seawater replicate 2

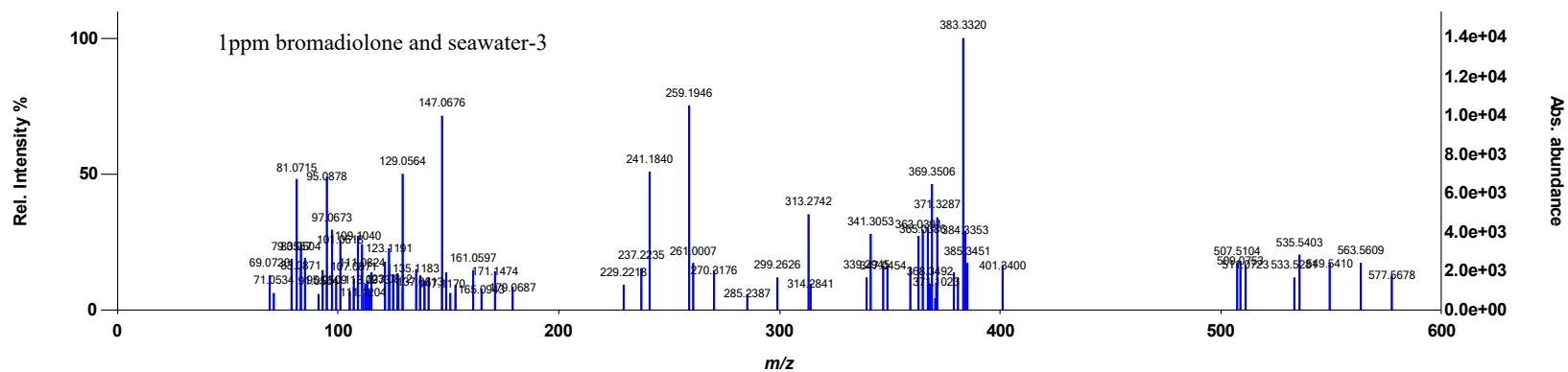


Figure S73: Mass spectrum of 1ppm bromadiolone and seawater replicate 3

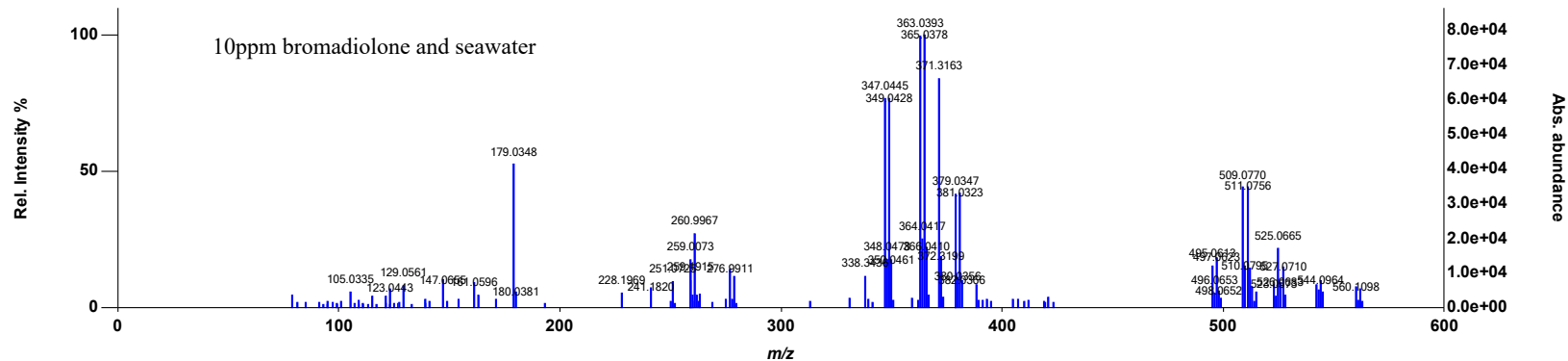


Figure S74: Mass spectrum of 10ppm bromadiolone and seawater replicate 1

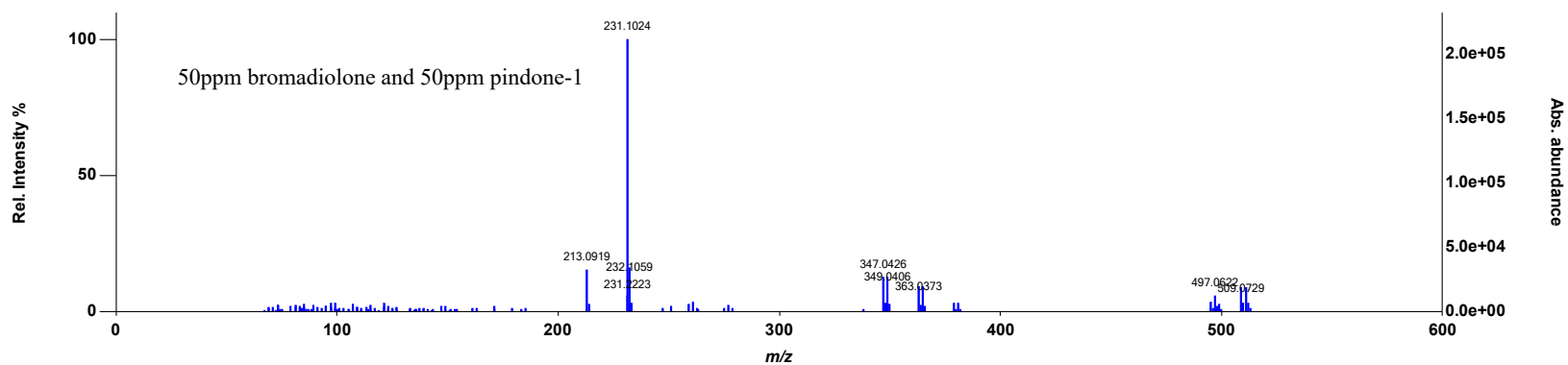


Figure S75: Mass spectrum of 50ppm bromadiolone and 50ppm pindone replicate 1

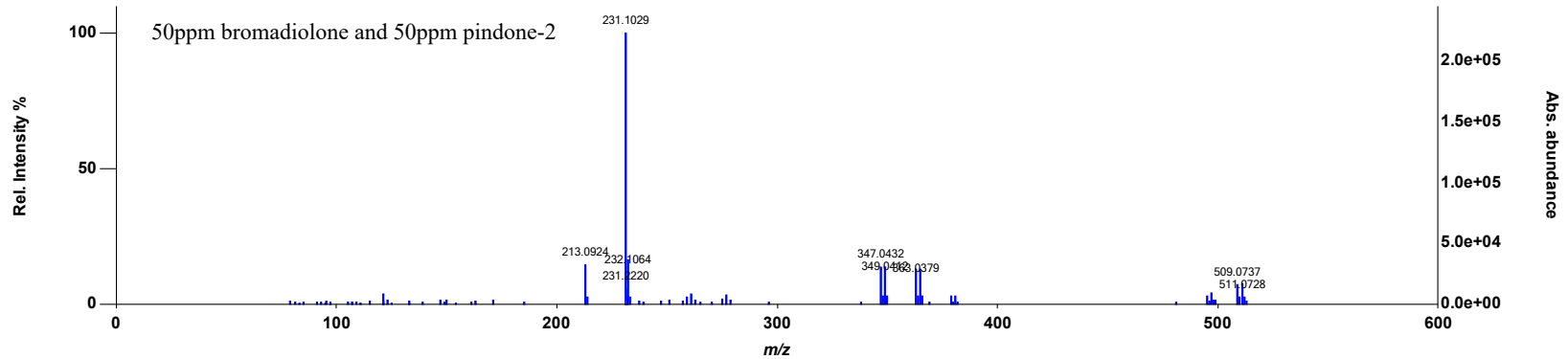
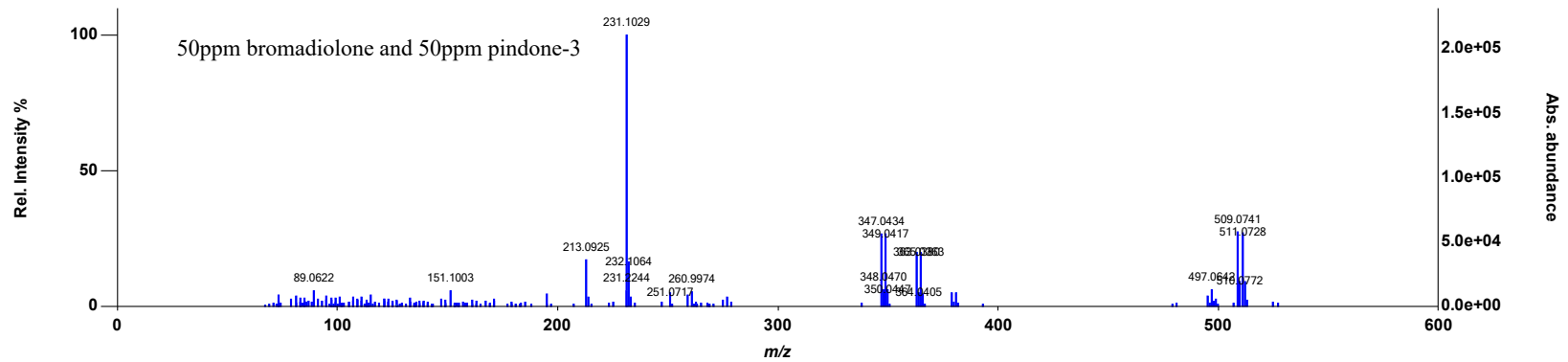


Figure S76: Mass spectrum of 50ppm bromadiolone and 50ppm pindone replicate 2



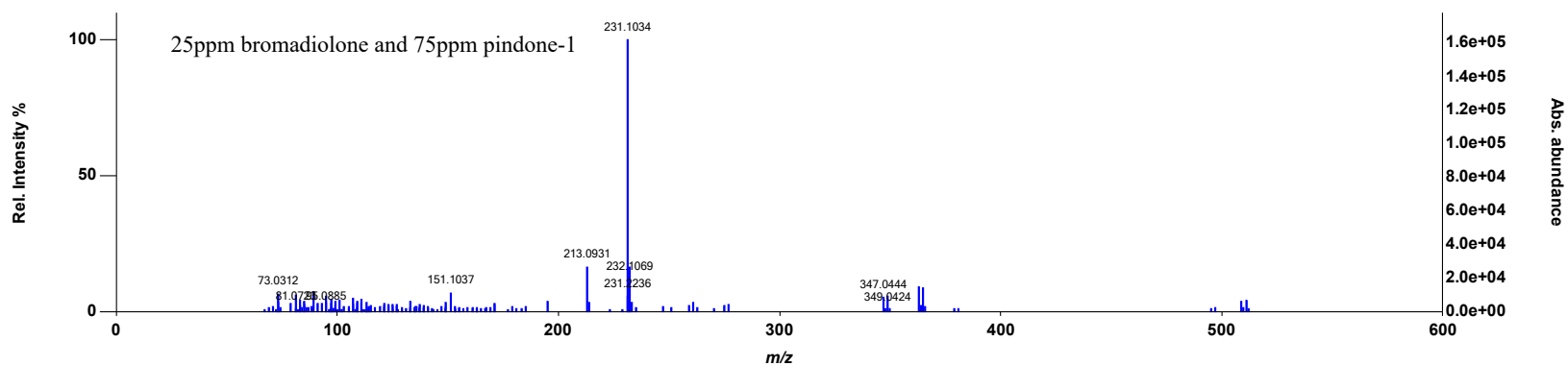


Figure S78: Mass spectrum of 25ppm bromadiolone and 75ppm pindone replicate 1

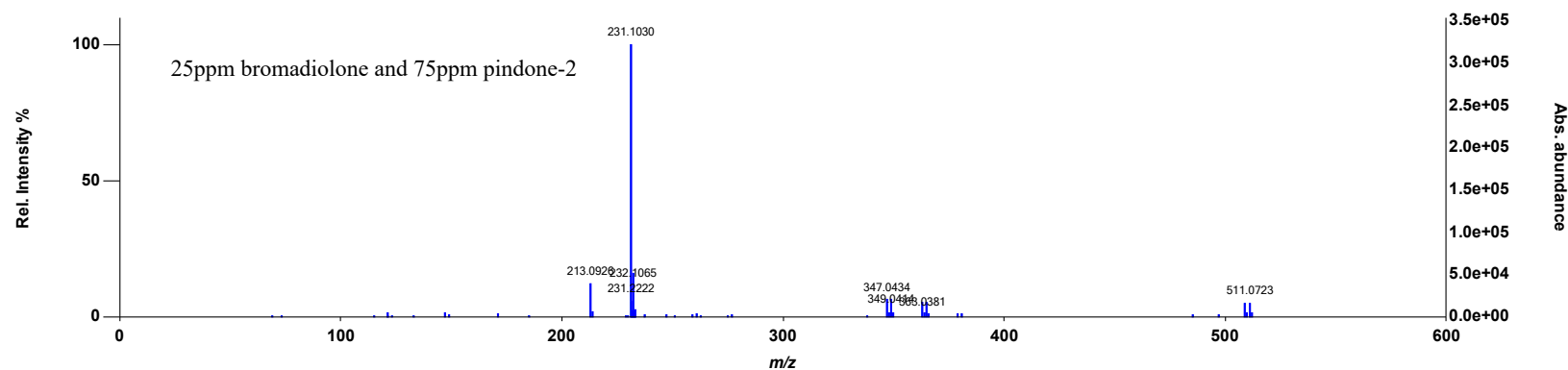


Figure S79: Mass spectrum of 25ppm bromadiolone and 75ppm pindone replicate 2

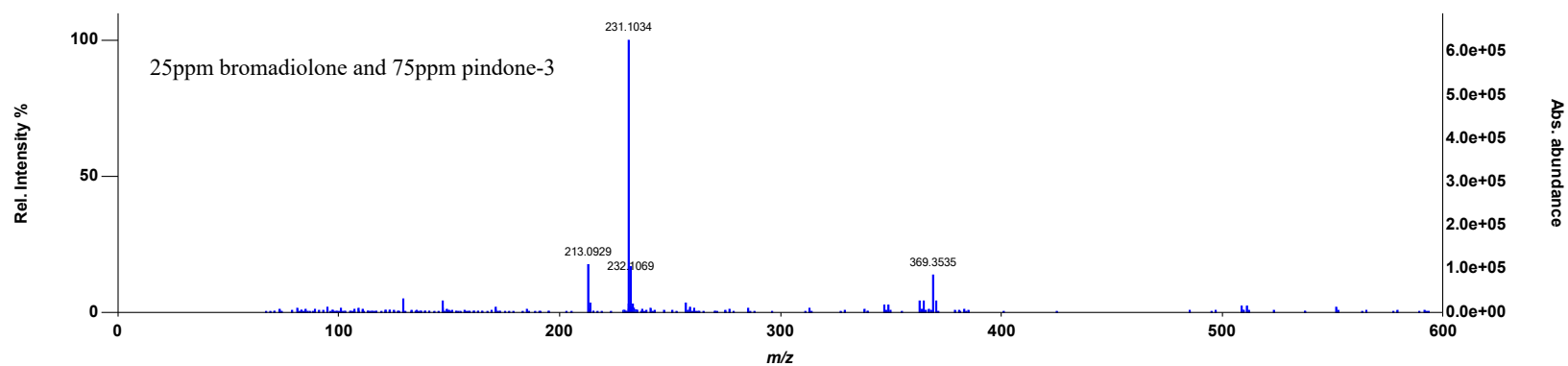


Figure S80: Mass spectrum of 25ppm bromadiolone and 75ppm pindone replicate 3

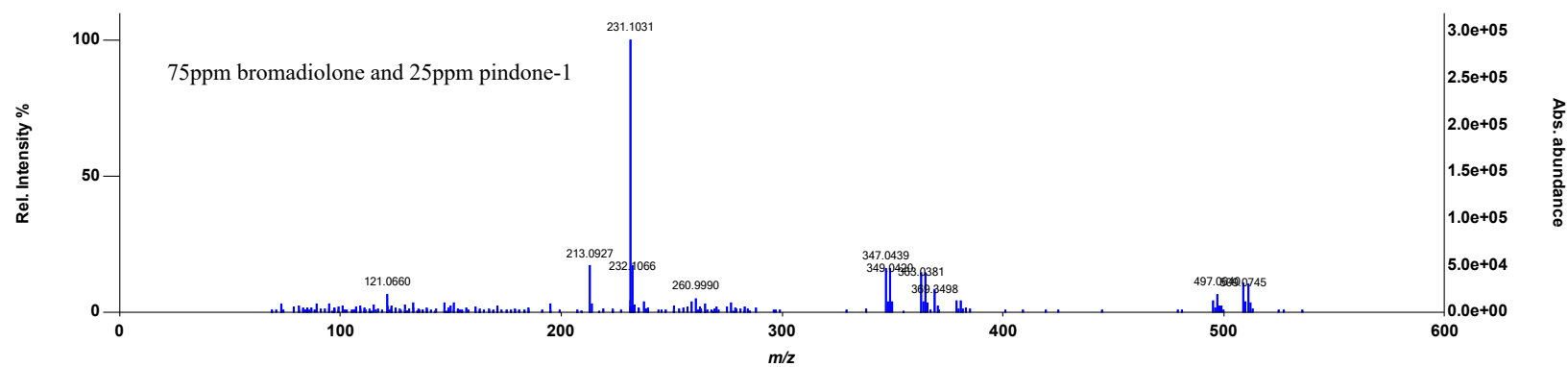


Figure S81: Mass spectrum of 75ppm bromadiolone and 25ppm pindone replicate 1

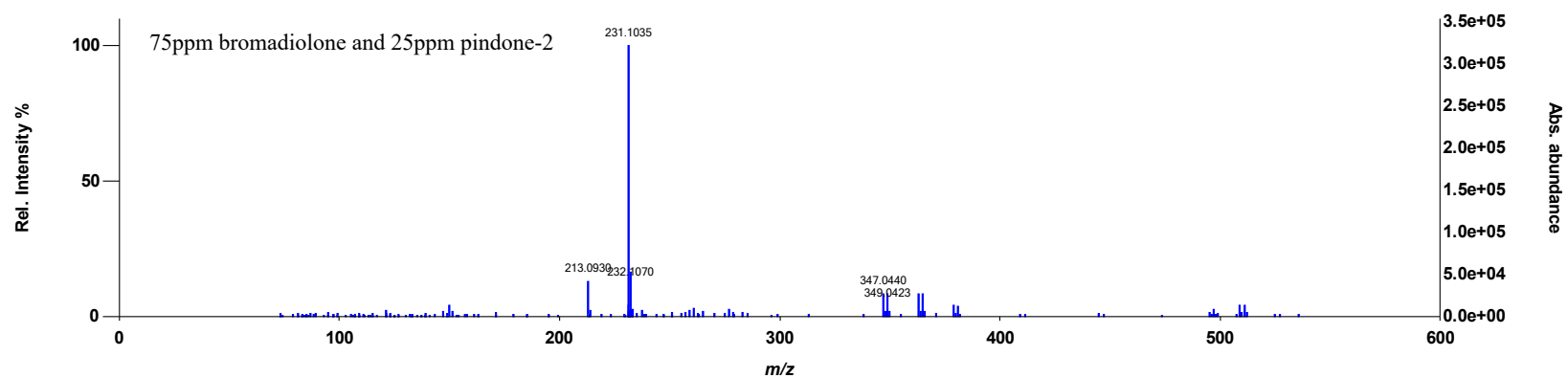


Figure S82: Mass spectrum of 75ppm bromadiolone and 25ppm pindone replicate 2

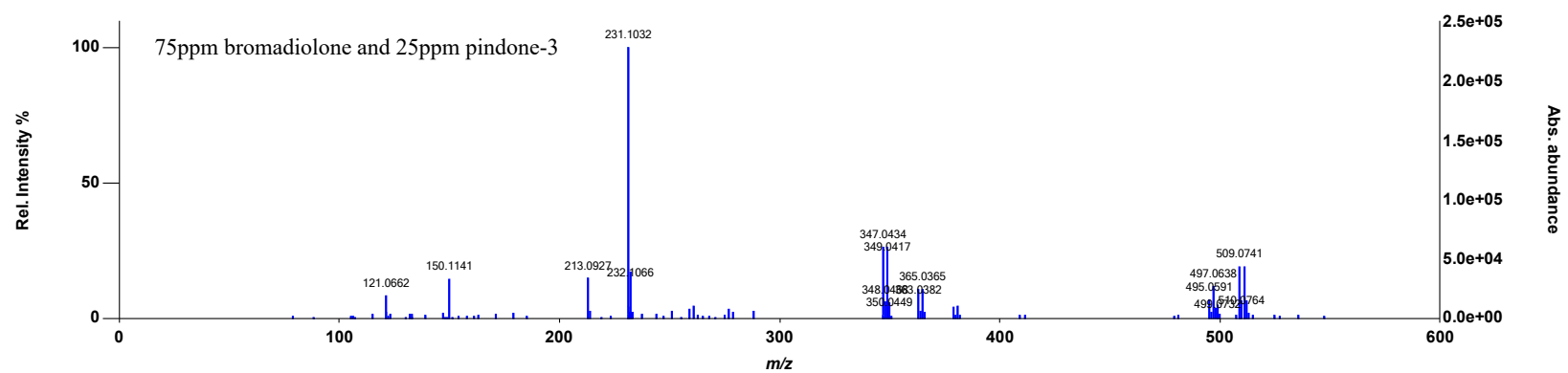


Figure S83: Mass spectrum of 75ppm bromadiolone and 25ppm pindone replicate 3

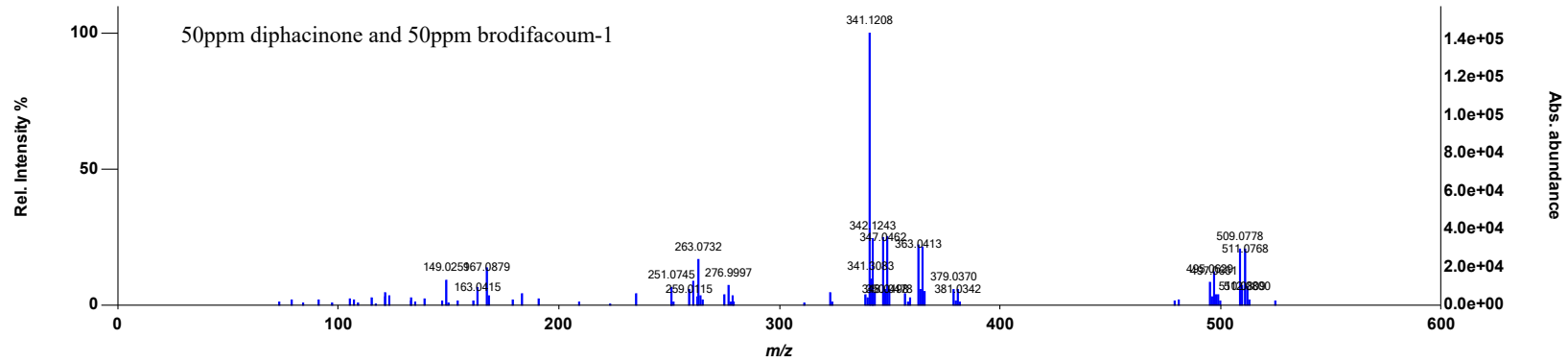


Figure S84: Mass spectrum of 50ppm diphacinone and 50ppm brodifacoum replicate 1

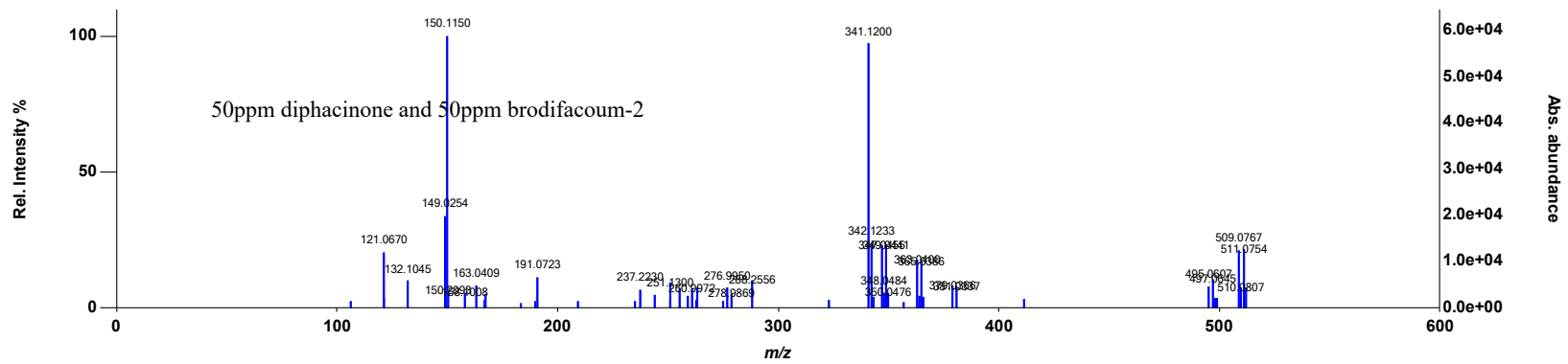


Figure S85: Mass spectrum of 50ppm diphacinone and 50ppm brodifacoum replicate 2

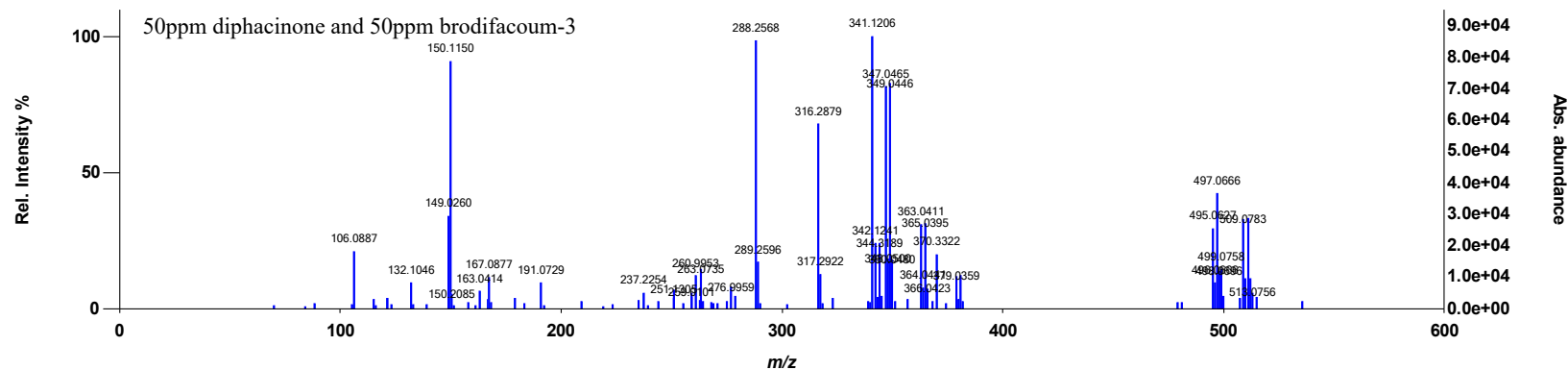


Figure S85: Mass spectrum of 50ppm diphacinone and 50ppm brodifacoum replicate 3

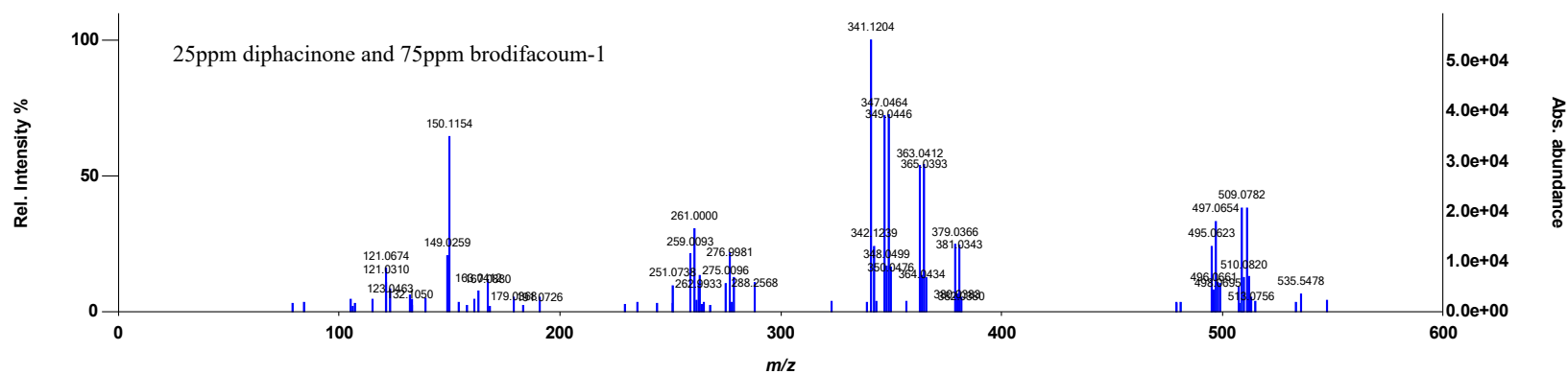


Figure S86: Mass spectrum of 25ppm diphacinone and 75ppm brodifacoum replicate 1

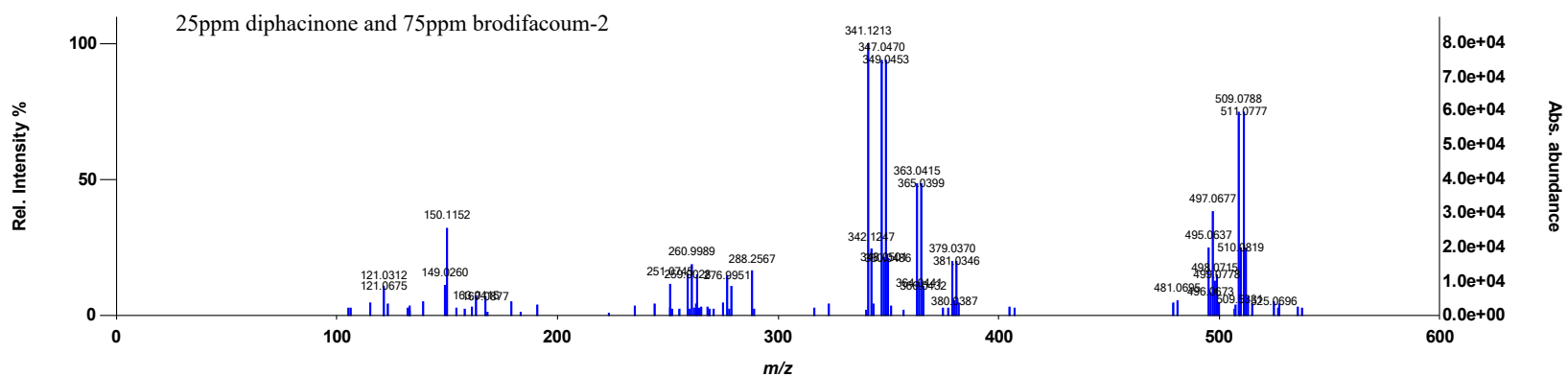


Figure S87: Mass spectrum of 25ppm diphacinone and 75ppm brodifacoum replicate 2

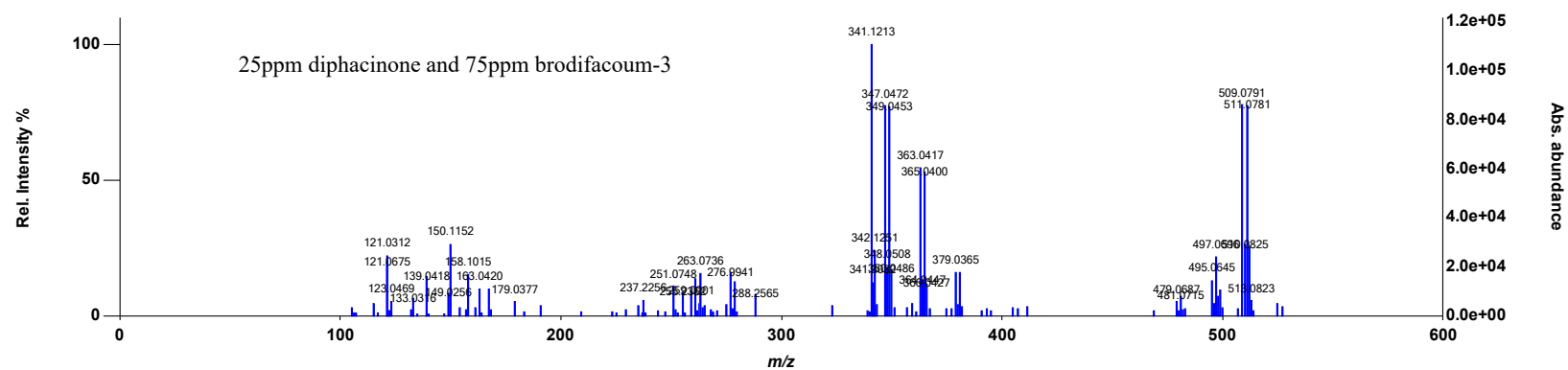


Figure S88: Mass spectrum of 25ppm diphacinone and 75ppm brodifacoum replicate 3

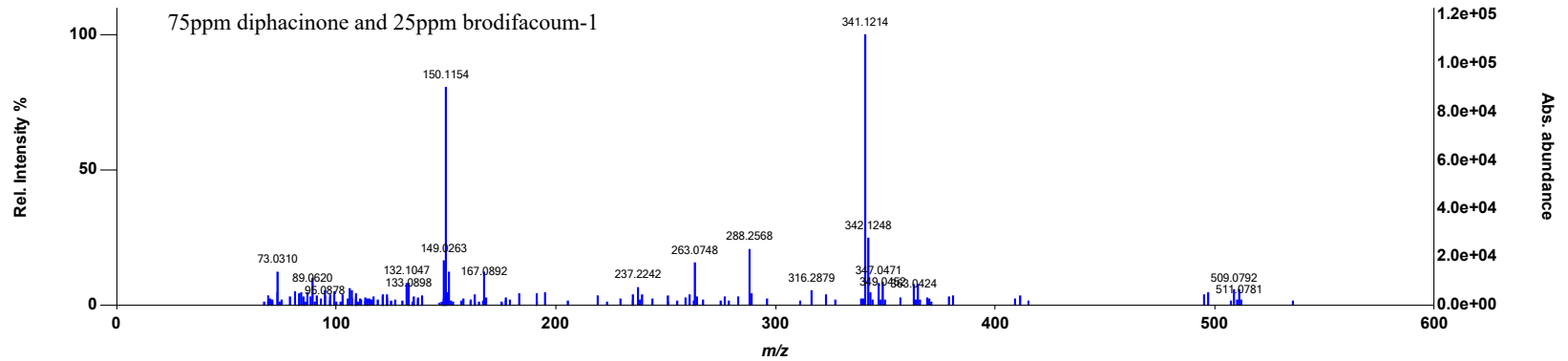
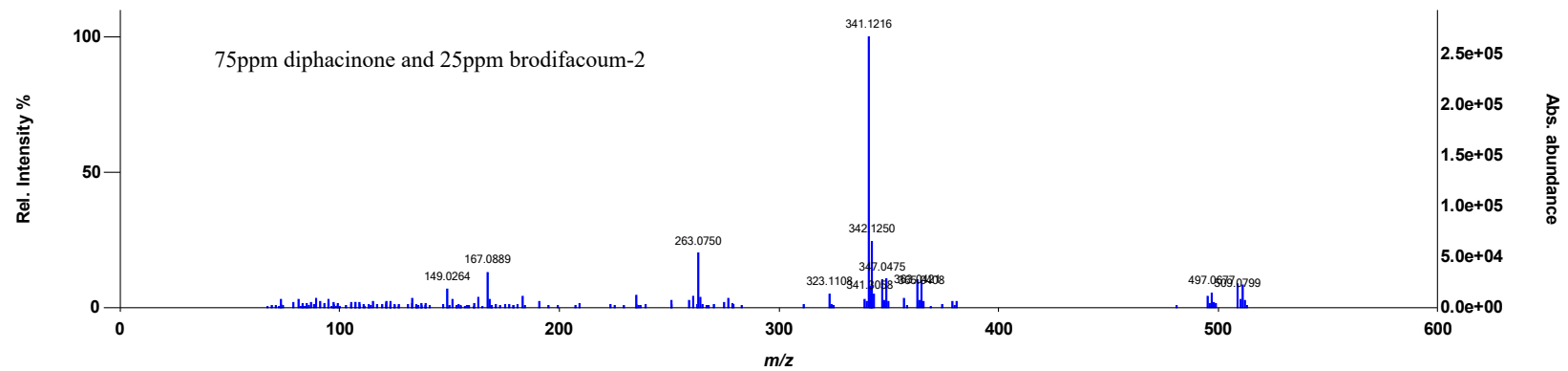


Figure S89: Mass spectrum of 75ppm diphacinone and 25ppm brodifacoum replicate 1



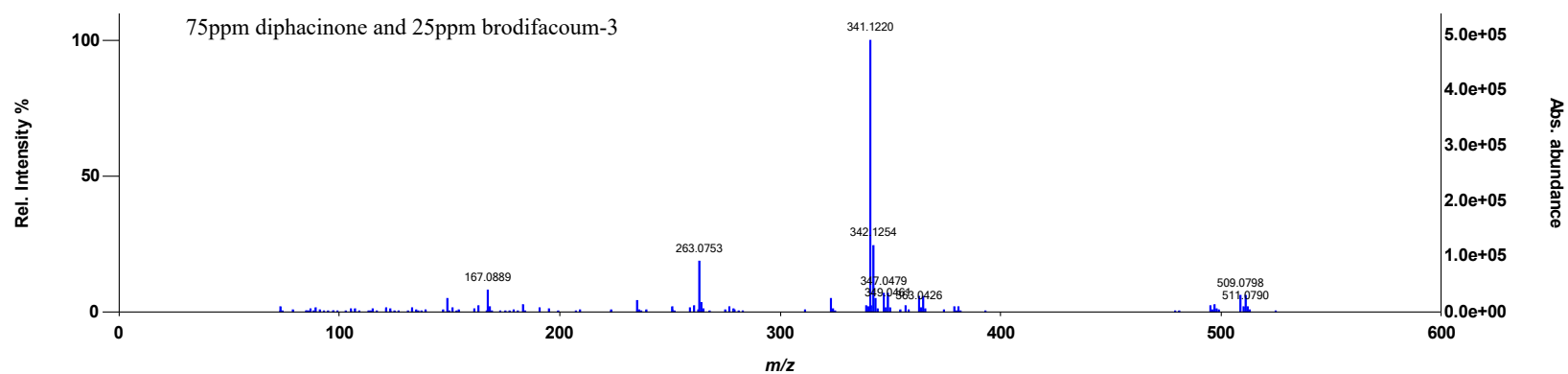


Figure S91: Mass spectrum of 75ppm diphacinone and 25ppm brodifacoum replicate 3

Figures S65-S91: Mass spectra of misidentified unknowns in positive ion mode at 30V.

NIST/NIJ DART-MS Data Interpretation Tool



Search Tool Libraries Scoring About

View:

☒ Interactive ☐ Reporting

Date...

Instrument ID...

Case No...

Item No...

Comments...

Load Presets

Download Presets

Restore Defaults

Query Spectra

Settings

Reference Library:

test-2.RDS

Polarity: Positive

Source Gas: NA

Select centroided mass spectrum (txt, jsp, csv)
measured at fragmentation levels of your choice.
Low (30 V) fragmentation required.

Browse... 30V_A1.1.txt

Upload complete

*required

Browse... 60V_A.1.1.txt

Upload complete

Browse... 90V_A1.1.txt

Upload complete

Search Library

Clear Search

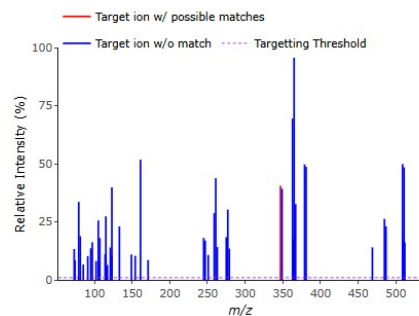
References

Moorthy et al. DOI:10.26434/chemrxiv-2022-s00s1

Moorthy & Sisco. DOI:10.1021/jasms.1c00097

Low (30 V) Mid (60 V) High (90 V)

Show 10 entries



m/z	Relative Intensity	Target
365.0420	100.0	T1
363.0387	69.5	T2
161.0604	51.8	T3
509.0753	49.9	T4
379.0337	49.7	T5
381.0317	48.7	T6
511.0742	48.5	T7
260.9973	43.8	T8
347.0438	40.5	T9
123.0462	39.8	T10

Previous 1 2 3 4 5 Next

Target 9

Measured m/z: 347.0438

Relative Intensity: 40.5 %

Potential matches:

Search:

Compound	$\Delta m/z$	FPIE	RevMF	IRD	Match Type
1 Bromadiolone	0.0553	0.683	0.616	NA	Protonated Molecule

Figure S92: Sample of DIT results using basic library search

Table S4: Basic library metadata

Code	Name	Target m/z
warfarin	Warfarin	309.1126
pindone	Pindone	231.1021
chlorophacinone	Chlorophacinone	375.0782
diphacinone	Diphacinone	341.1172
bromadiolone	Bromadiolone	347.0425
brodifacoum	Brodifacoum	523.0917
boscalid	Boscalid	343.0380
picoxystrobin	Picoxystrobin	368.1091
quinoxifen	Quinoxifen	308.0020
metsulfuron methyl	Metsulfuron Methyl	382.0777
carbetamide	Carbetamide	237.1212

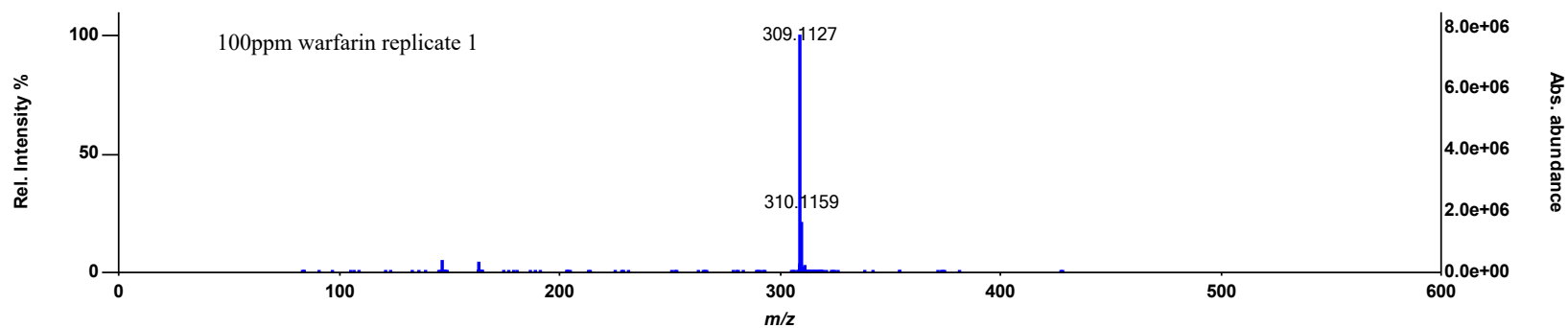


Figure S93: Mass spectrum of 100ppm warfarin replicate 1

100ppm warfarin replicate 2

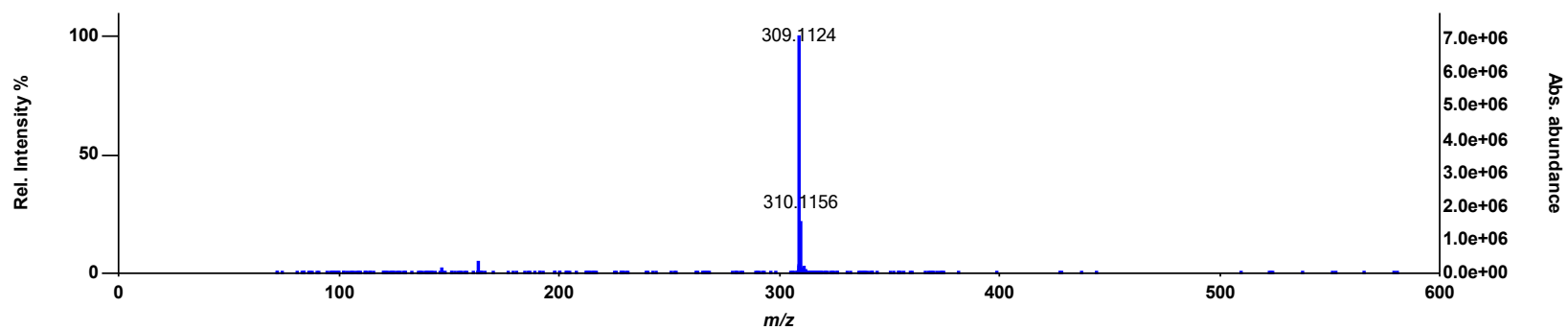


Figure S94: Mass spectrum of 100ppm warfarin replicate 2

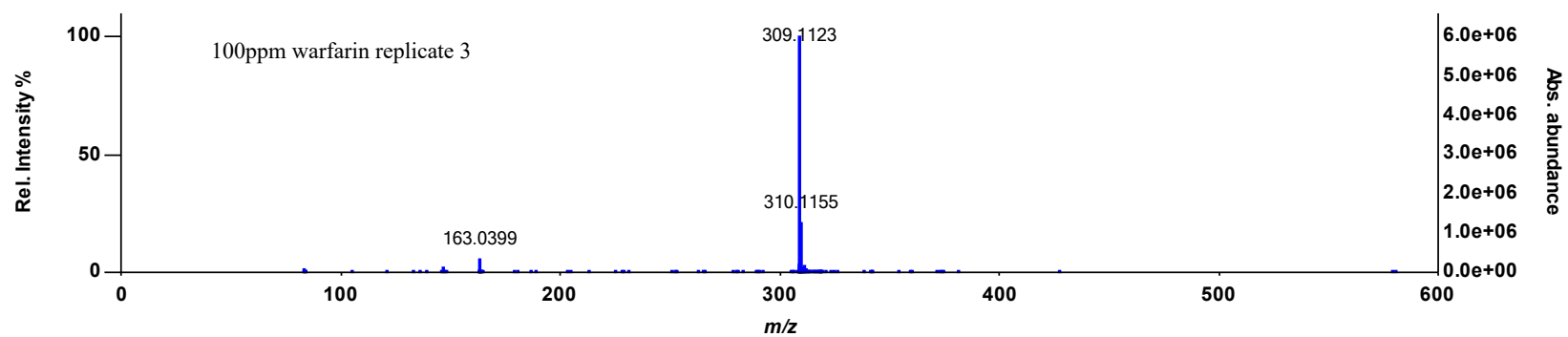


Figure S95: Mass spectrum of 100ppm warfarin replicate 3

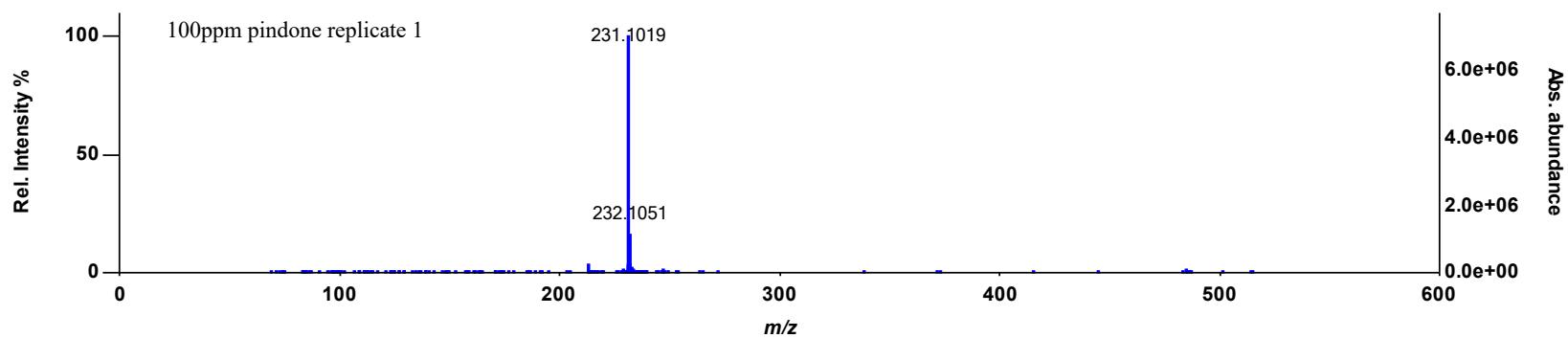


Figure S96: Mass spectrum of 100ppm pindone replicate 1

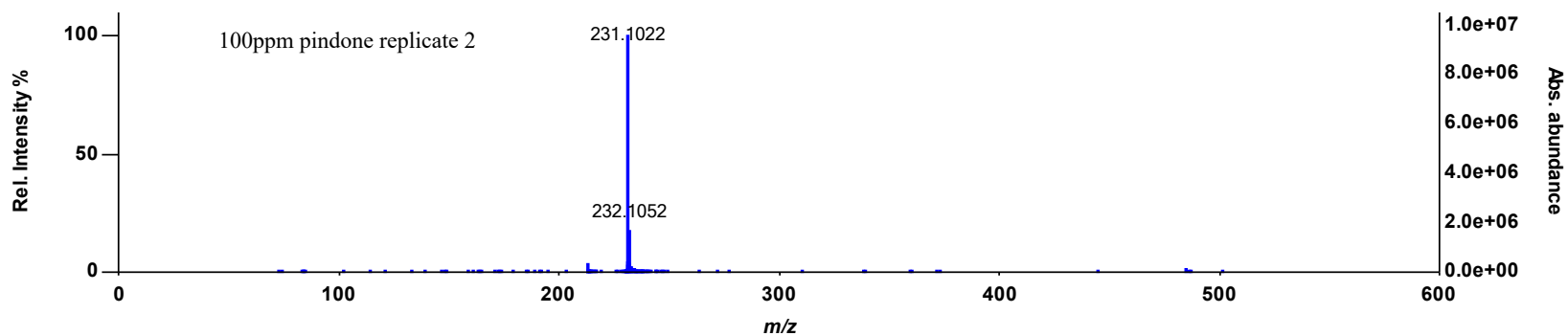


Figure S97: Mass spectrum of 100ppm pindone replicate 2

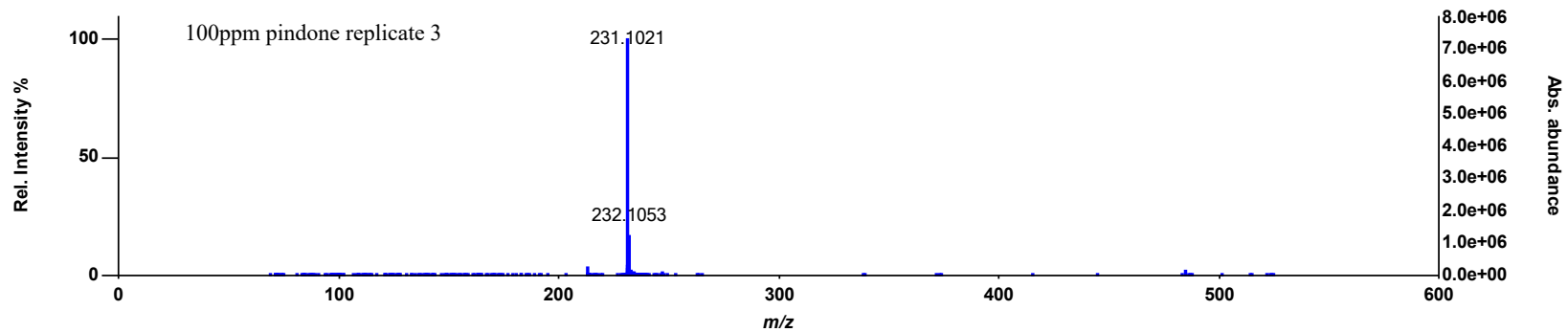


Figure S98: Mass spectrum of 100ppm pindone replicate 3

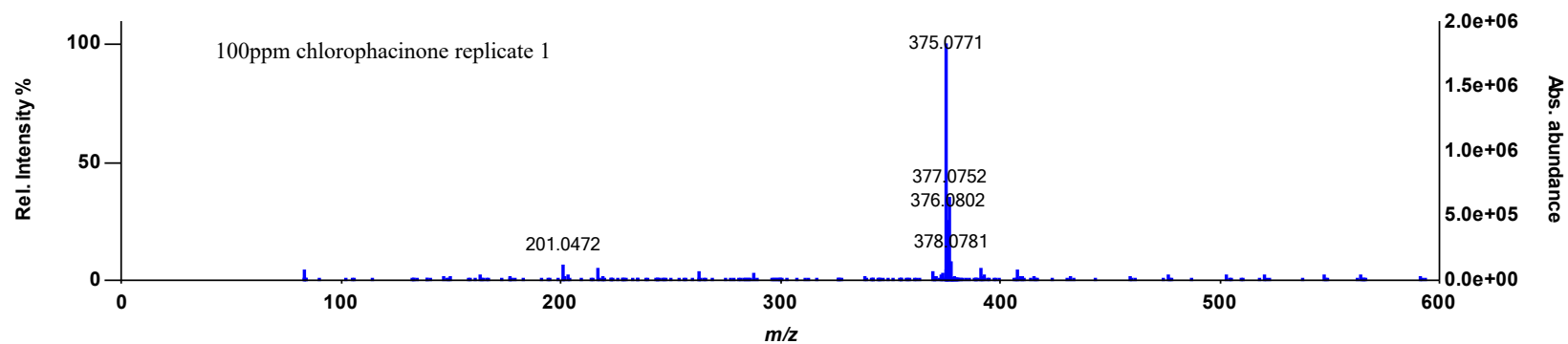


Figure S99: Mass spectrum of 100ppm chlorophacinone replicate 1

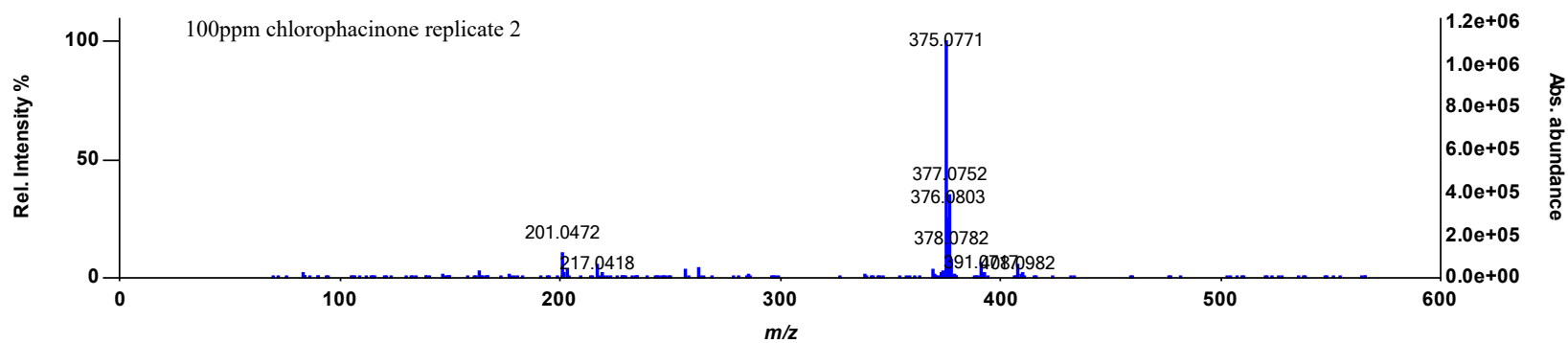


Figure S100: Mass spectrum of 100ppm chlorophacinone replicate 2

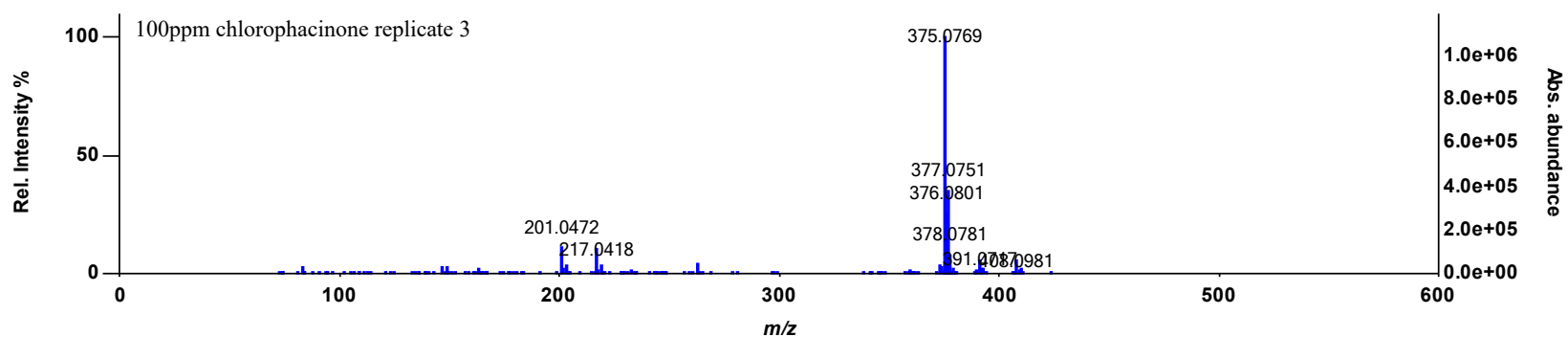


Figure S101: Mass spectrum of 100ppm chlorophacinone replicate 3

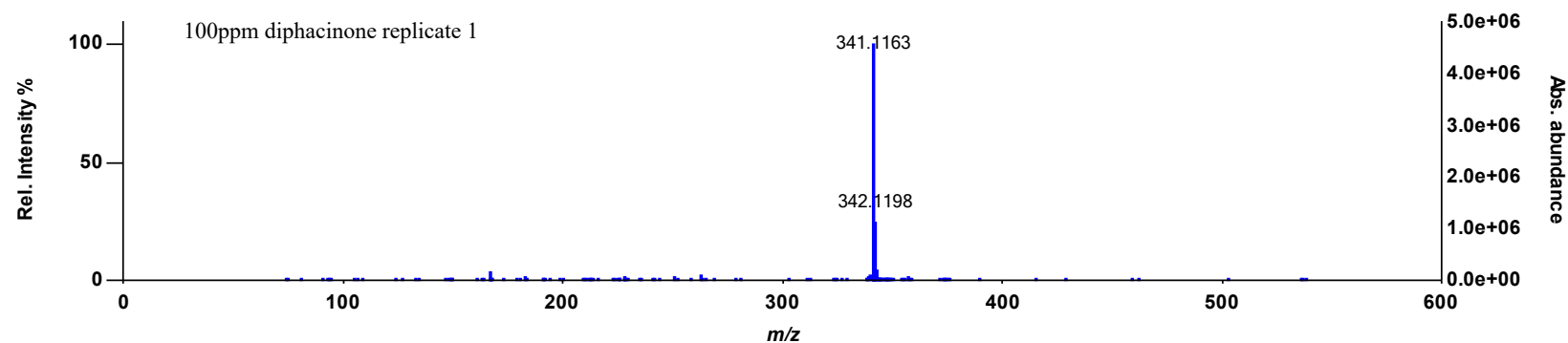


Figure S102: Mass spectrum of 100ppm diphacinone replicate 1

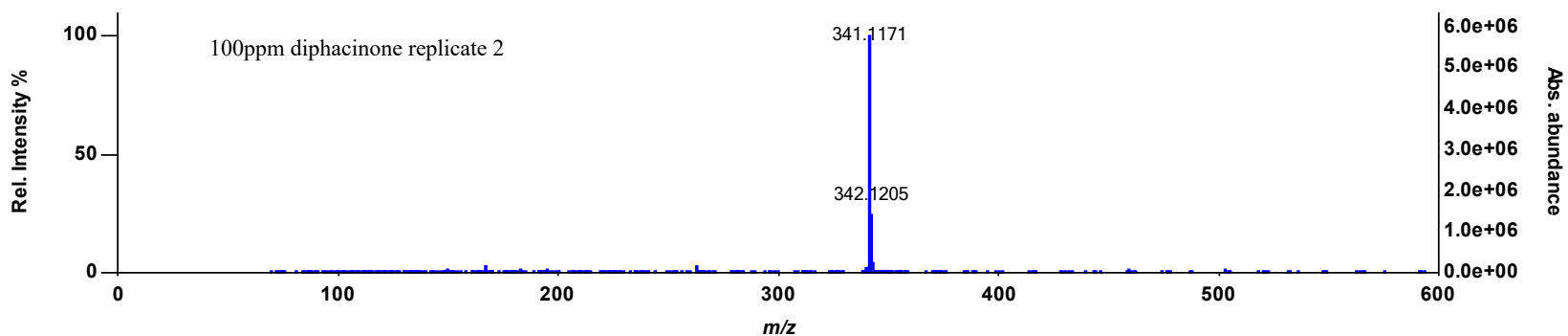


Figure S103: Mass spectrum of 100ppm diphacinone replicate 2

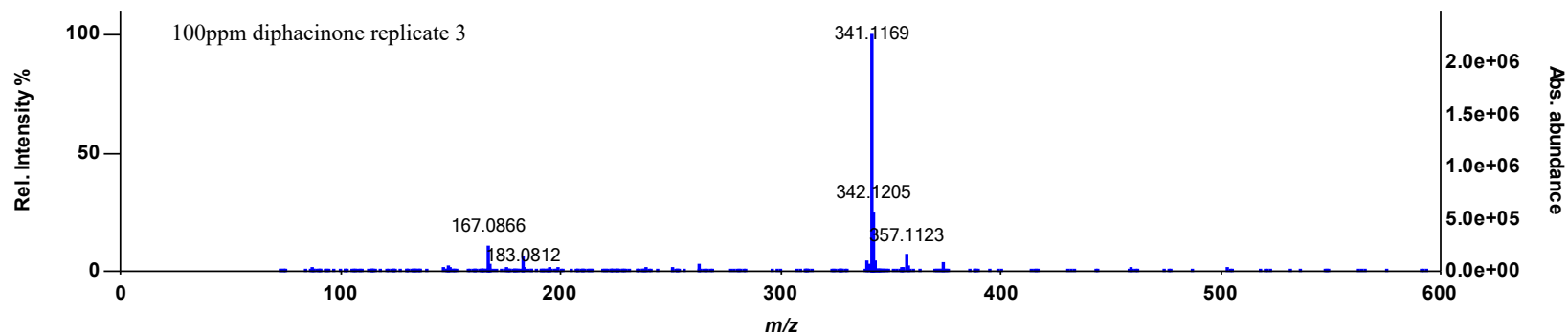


Figure S104: Mass spectrum of 100ppm diphacinone replicate 3

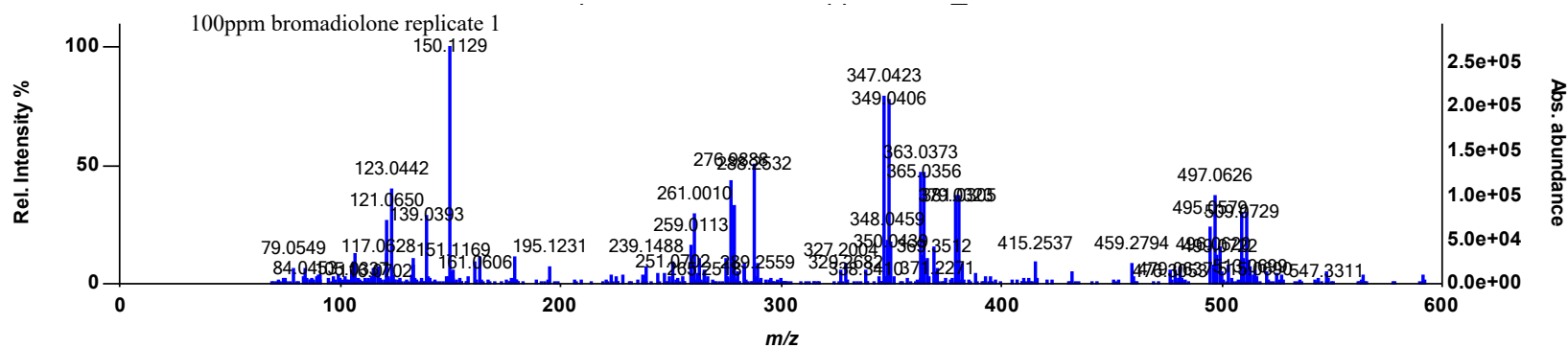


Figure S105: Mass spectrum of 100ppm bromadiolone replicate 1

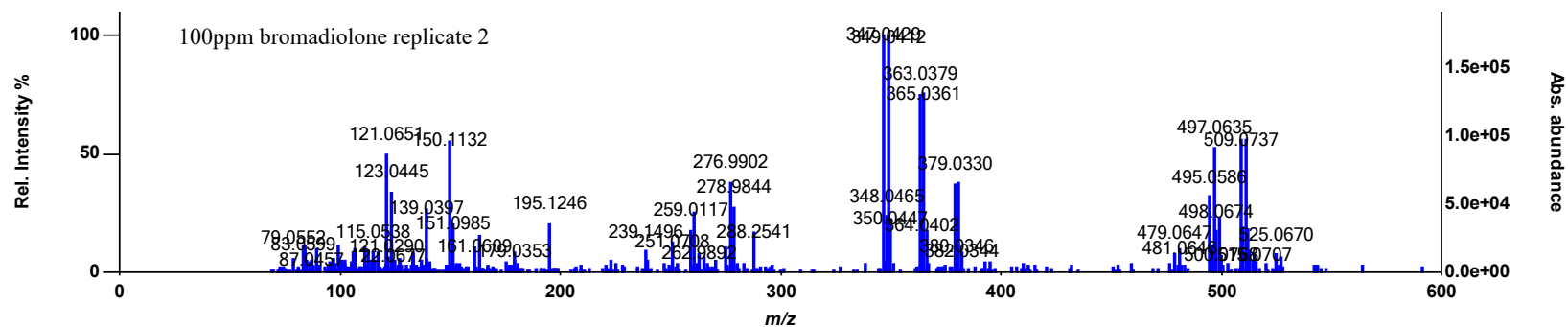


Figure S106: Mass spectrum of 100ppm bromadiolone replicate 2

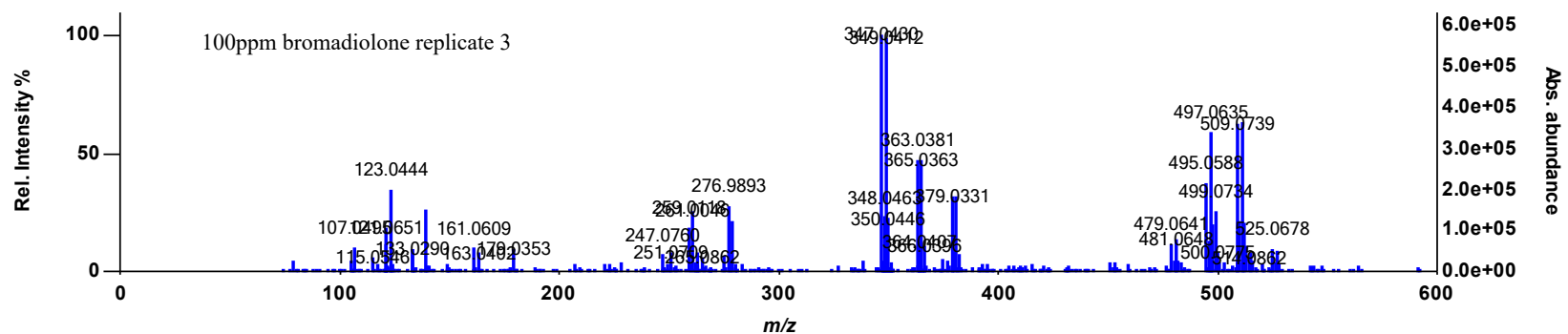


Figure S107: Mass spectrum of 100ppm bromadiolone replicate 3

Figure S108: Mass spectrum of 100ppm brodifacoum replicate 1

Figure S108: Mass spectrum of 100ppm brodifacoum replicate 1

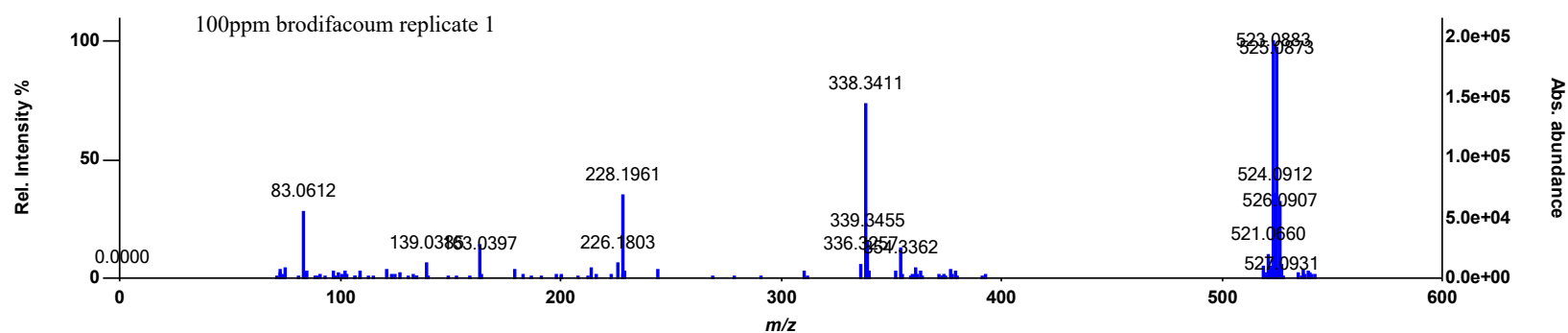


Figure S108: Mass spectrum of 100ppm brodifacoum replicate 1

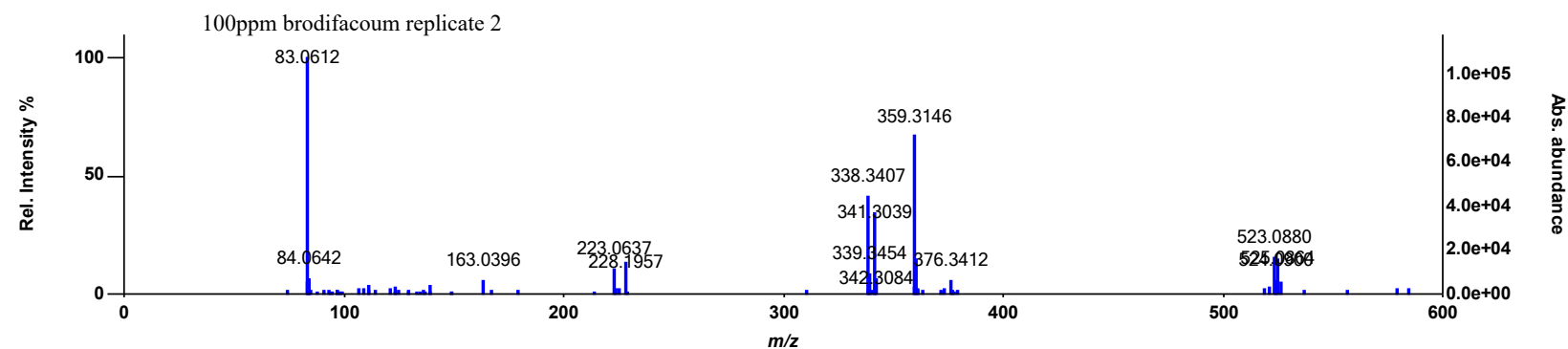


Figure S109: Mass spectrum of 100ppm brodifacoum replicate 2

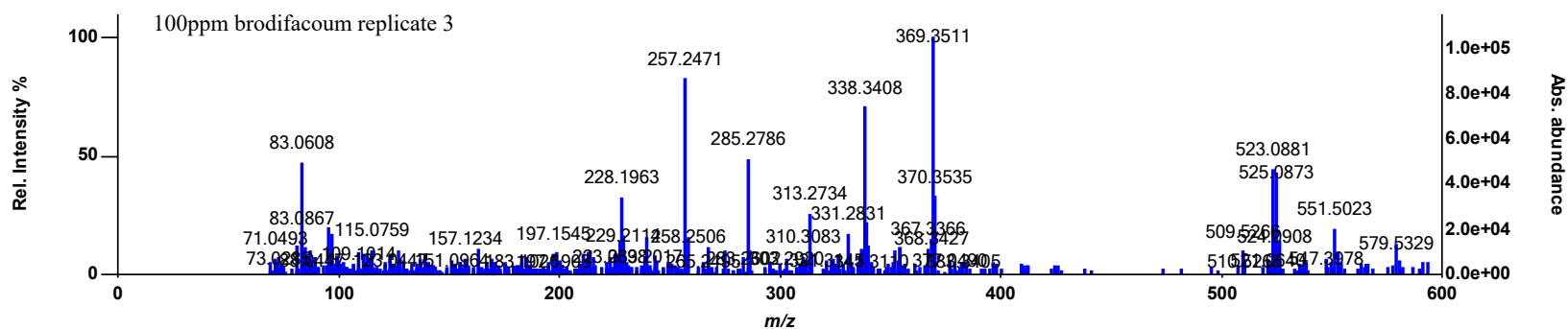


Figure S110: Mass spectrum of 100ppm brodifacoum replicate 3

Figures S92-110: Mass spectra of 100ppm rodenticides collected in positive ion mode.

Table S4: Average base peak intensities of positive ion mode-collected 100ppm rodenticides

Rodenticide	Base peak <i>m/z</i>	Peak intensity	Average <i>m/z</i>	Average intensity
Warfarin	309.1127	8,522,730	309.1124667	27,335,234
	309.1124	7,824,405		
	309.1123	65,658,567		
Pindone	231.1019	7,742,152	231.1020667	8,766,722
	231.1022	10,499,909		
	231.1021	8,058,104		
Chlorophacinone	375.0771	2,009,112	375.0770353	1,476,485
	375.0771	1,223,114		
	375.076906	1,197,229		
Diphacinone	341.1163	5,039,175	341.1167667	4,625,902
	341.1171	6,343,985		
	341.1169	2,494,545		
Bromadiolone	150.1129	294,074	347.0429245	412,033
	347.042949			

		191,343		
	347.0429	632,722		
Brodifacoum	523.08825	217,006	523.0880833	95,210
	523.0879	17,311		
	523.0881	51,314		

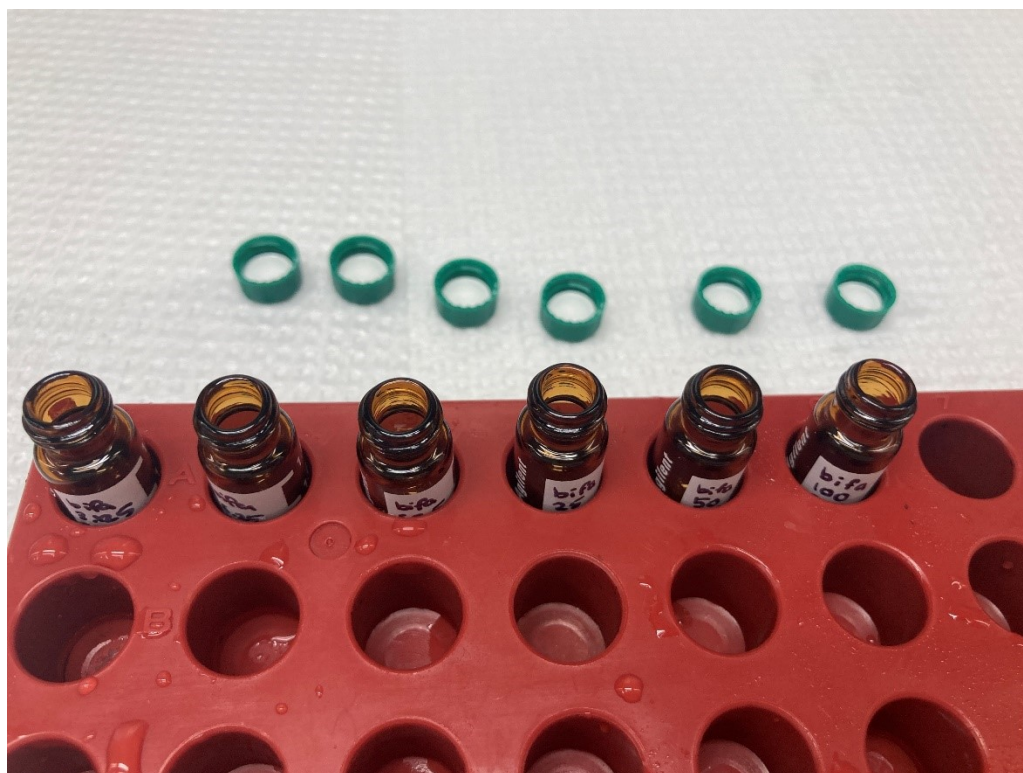


Figure S111: Gas chromatography (GC) vials used for serial dilution samples.

Table S5: Raw data for quantitation of brodifacoum using 20ppm N-(4-hydroxyphenyl-2,3,5,6-d4) acetamide-2,2,2-d3 internal standard

Rodenticide concentration (ppm)	Peak Intensity (<i>m/z</i>)		IS Response Ratio
	N-(4- hydroxyphenyl- 2,3,5,6-d4) acetamide- 2,2,2-d3 (157.1004)	Brodifacoum (523.0719)	
1.0625	7,299,827	-	0.000
	4,829,817	-	0.000
	4,242,402	-	0.000
	8,253,401	-	0.000
	3,054,227	-	0.000
	1,576,933	-	0.000
3.125	4,134,205	-	0.000
	1,478,714	-	0.000
	2,568,994	-	0.000
		-	0.000

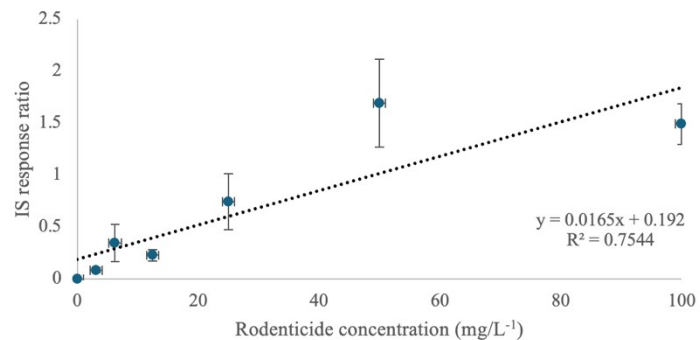
	5,977,933		
	5,168,943	-	0.000
	4,315,088	-	0.000
6.25	2,807,801	-	0.000
	2,216,883	-	0.000
	2,882,749	-	0.000
	2,281,865	-	0.000
	969,245	-	0.000
	2,258,852	-	0.000
12.5	1,554,247	342,542	0.220
	4,507,222	-	0.000
	4,587,944	-	0.000
	2,369,655	-	0.000
	3,975,371	-	0.000
	2,764,263	-	0.000
25	5,269,226	-	0.000
	3,522,722	-	0.000

	4,717,877	-	0.000
	3,969,887	-	0.000
	3,893,060	-	0.000
	5,364,030	-	0.000
50	3,240,051	-	0.000
	2,842,164	-	0.000
	2,034,954	365,912	0.180
	5,801,023	751,026	0.129
	1,410,008	224,959	0.160
	3,822,375	-	0.000

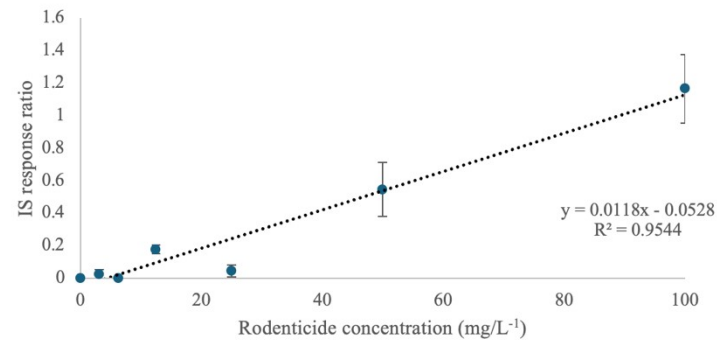
Table S6: Raw data for quantitation of bromadiolone using 100ppm N-(4-hydroxyphenyl-2,3,5,6-d4) acetamide-2,2,2-d3 internal standard

Concentration (mg/L ⁻¹)																	
3.125			6.25			12.5			25			50			100		
157.1	307.1	ratio	157.1	307.1	ratio	157.1	307.1	ratio	157.1	307.1	ratio	157.1	307.1	ratio	157.1	307.1	ratio
8,864,860	226,748	0.03	8,887,360	692,129	0.08	8,135,631	674,944	0.08	7,355,468	1,304,532	0.18	551,013	850,487	1.54	3,891,755	2,252,636	0.58
7,394,683	297,808	0.04	8,324,171	948,452	0.11	4,891,490	2,935,451	0.60	8,652,508	1,541,743	0.18	5,726,661	2,546,354	0.44	4,389,282	4,834,648	1.10
8,232,393	332,542	0.04	5,435,769	1,187,376	0.22	4,247,890	151,943	0.04	4,750,541	1,287,749	0.27	4,161,293	3,494,537	0.84	3,193,838	2,231,000	0.70
6,322,632	102,650	0.02	5,335,333	121,753	0.02	8,306,895	1,873,713	0.23	6,290,119	744,832	0.12	2,977,929	2,408,969	0.81	1,618,821	4,076,111	2.52
3,920,411	269,583	0.07	10,672,626	1,207,815	0.11	3,370,655	474,939	0.14	9,514,019	1,746,674	0.18	2,585,208	1,577,409	0.61	1,764,507	829,884	0.47
3,590,835	233,242	0.06	10,605,748	1,225,293	0.12	2,972,000	761,929	0.26	5,177,194	1,232,684	0.24	1,297,446	962,066	0.74	2,240,086	2,582,165	1.15
		0.04			0.11			0.22			0.19			0.83			1.09
		49%			58%			90%			27%			45%			69%

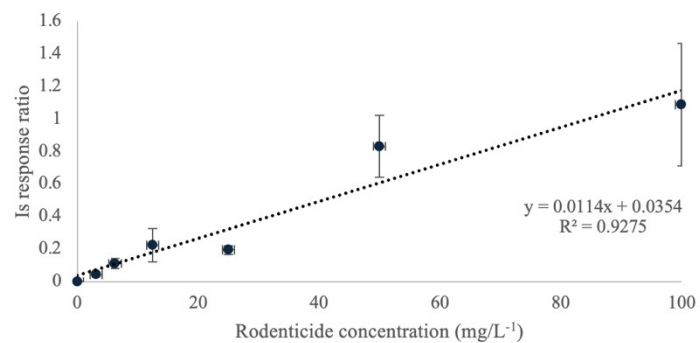
A Internal Standard Response - Diphacinone + 20ppm
Deuterated Acetaminophen



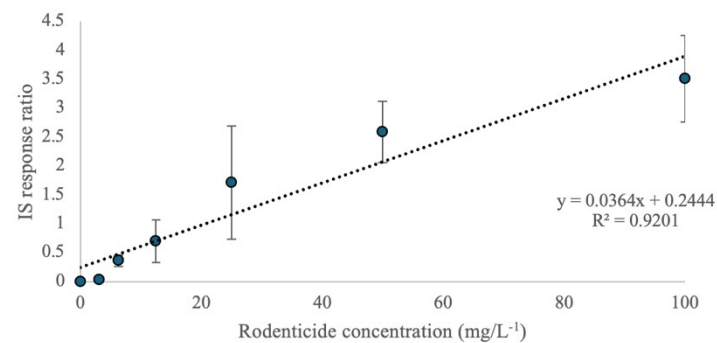
B Internal Standard Response - Diphacinone + 20ppm
Decanoic d3 acid



C Internal Standard Response - Warfarin + 100ppm
Deuterated Acetaminophen



D Internal Standard Response - Warfarin + 20ppm Decanoic
d3 acid



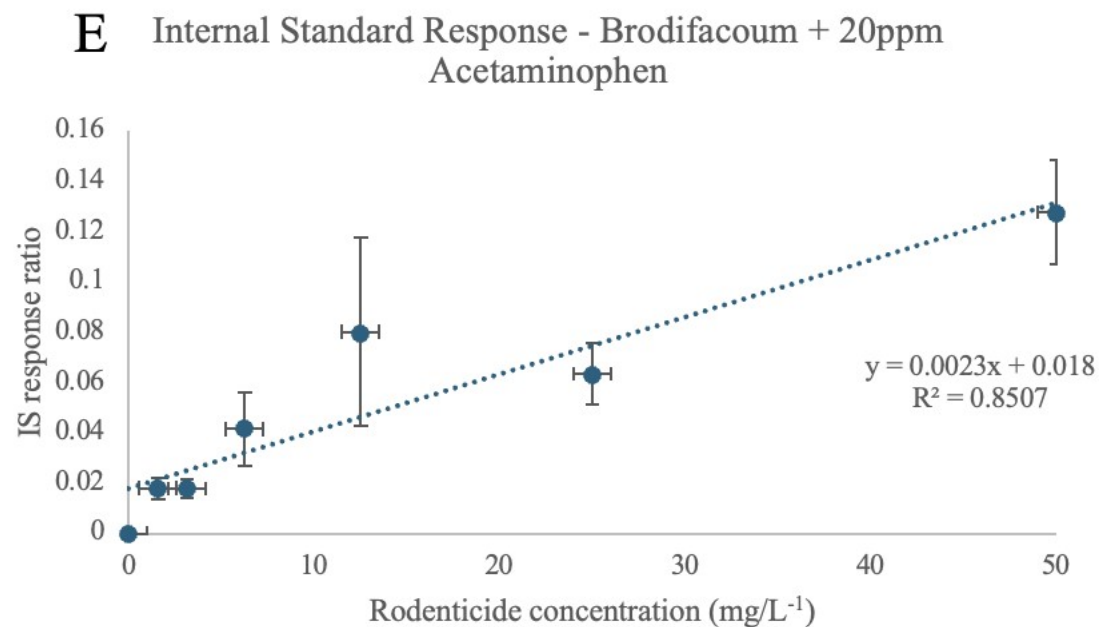


Figure S112: Linear regression plots of internal standard response for rodenticides where $R^2 < 0.98$.

Table S7: Statistical analysis of QA quantitation tests – Method 1 (As described in Methods)

METHOD		1							
IS peak height	1	Warfarin	Pindone	Chlorophacinone	Bromadiolone	Warfarin	Pindone	Chlorophacinone	Bromadiolone
	1	2,287,600	2,258,198	2,104,230	8,605,299	3,229,049	1,827,932	3,575,326	6,914,558
	2	3,272,029	2,737,530	2,929,150	4,425,090	4,566,189	2,562,232	5,408,561	4,825,366
	3	2,152,608	1,739,740	2,130,259	2,503,665	3,668,084	3,231,595	1,287,707	5,648,076
	4	1,357,619	3,080,175	1,345,684	3,132,592	6,202,833	1,776,489	5,327,064	6,347,392
	5	2,038,831	1,880,368	3,363,878	7,294,861	5,111,439	3,097,159	5,108,005	3,512,670

	6	1,989,887	994,868	1,075,728	6,562,460	4,265,681	1,647,419	4,797,396	2,035,982
Rodenticide ion peak height	1	3,661,150	4,451,590	184,834	6,914,558	901,222	10,536,614	266,700	45,311
	2	3,914,268	3,268,578	83,009	4,825,366	1,260,191	16,264,953	86,999	61,874
	3	1,649,390	1,718,188	411,154	5,648,076	672,949	15,451,717	1,850	39,169
	4	2,994,289	2,793,665	310,957	6,347,392	2,152,746	16,990,064	15,635	30,907
	5	2,229,338	2,524,202	393,700	3,512,670	613,824	14,686,311	207,727	64,520
	6	4,352,063	745,785	611,272	2,035,982	1,353,497	9,431,092	87,444	11,594
IS response ratio	1	1.6004	1.9713	0.0878	0.8035	0.2791	5.7642	0.0746	0.0066
	2	1.1963	1.1940	0.0283	1.0905	0.2760	6.3480	0.0161	0.0128
	3	0.7662	0.9876	0.1930	2.2559	0.1835	4.7815	0.0014	0.0069
	4	2.2055	0.9070	0.2311	2.0262	0.3471	9.5638	0.0029	0.0049
	5	1.0934	1.3424	0.1170	0.4815	0.1201	4.7419	0.0407	0.0184
	6	2.1871	0.7496	0.5682	0.3102	0.3173	5.7248	0.0182	0.0057
Average		1.50817	1.19199	0.20426	1.16132	0.25383	6.15402	0.02566	0.00921
SD		0.59591	0.43558	0.19258	0.80817	0.08566	1.78207	0.02782	0.00530
ax		0.386	0.0819	0.0691	0.0004	0.386	0.0819	0.0691	0.0004
b		-0.0424	0.3761	-0.3135	-0.0008	-0.0424	0.3761	-0.3135	-0.0008
Guess concentration		4.02	9.96	7.49	2905.30	0.77	70.55	4.91	25.02
SD converted		1.65	0.73	7.32	2022.44	0.33	17.17	4.94	15.25
True concentration		50	10.000	20	10	10	100	5.00	20.00
Uncertainty		1.65	0.73	7.32	2022.44	0.33	17.17	4.94	15.25
Standard Error		0.68	0.30	2.99	825.66	0.14	7.01	2.02	6.22
Test statistic (t)		-68.11	-0.13	-4.18	3.51	-68.17	-4.20	-0.05	0.81

Table S8: Statistical analysis of QA quantitation tests – Method 2 (As described in Methods)**METHOD 2**

	Warfarin	Pindone	Chlorophacinone	Bromadiolone	Warfarin	Pindone	Chlorophacinone	Bromadiolone
IS Peak height avg	2,183,096	2,115,146	2,158,155	5,420,661	4,507,213	2,357,138	4,250,676	4,880,674
SD (IS)	622,443	747,018	881,322	2,436,946	1,062,062	703,603	1,598,031	1,835,408
Rodenticide ion peak height average	3,133,417	2,583,668	332,487	4,880,674	1,159,071	13,893,458	111,059	42,229
SD (Rod)	1,040,421	1,275,362	185,559	1,835,408	571,929	3,144,864	105,582	19,841
Ratio	1.4353	1.2215	0.1541	0.9004	0.2572	5.8942	0.0261	0.0087
SD (ratio)	0.48	0.60	0.09	0.34	0.13	1.33	0.02	0.00
Guess concentration	3.83	10.32	6.77	2252.96	0.78	67.38	4.92	23.63
SD (concentration)	1.34	2.77	5.78	848.49	0.44	11.70	4.90	12.16
Standard Error	0.55	1.13	2.36	346.39	0.18	4.78	2.00	4.97
Test statistic (t)	-84.12	0.29	-5.61	6.48	-51.52	-6.83	-0.04	0.73