

事務連絡
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〔特別区〕

厚生労働省医薬食品局食品安全部基準審査課

分析用ヘリウムの供給不足に伴う食品等に関する検査への対応について

昨今の世界的なヘリウムの供給不足により、検査機関の中には、ヘリウムの確保に支障が生じている機関もあるとの報告を受けているところです。

については、ヘリウム不足に対して、下記の点を踏まえ、検査への影響を最小限とするよう、対応方をお願いします。

記

1. ヘリウムの確保

ヘリウムの国内供給元が複数あることから、販売業者の供給元を確認しながら、ヘリウムの確保に努めること。

（参考）平成24年12月27日付け経済産業省製造産業局化学課長より、一般社団法人 日本産業・医療ガス協会会長宛て通知「ヘリウムの流通の安定化について」

<http://www2.jimga.or.jp/dl/kyokai/121227sangasukyokai-helium.pdf>

2. 試験法の変更について

上記1によるヘリウムの確保が困難な場合には、分析精度等を検証した上で、キャリアーガスを水素等に変更すること又は測定をLC-MSに変更することは差し支えない。農薬、飼料添加物及び動物用医薬品に関する試験法を変更する場合には、「食品中に残留する農薬等に関する試験法の妥当性評価ガイドラインの一部改正について」（平成22年12月24日食安発1224第1号厚生労働省医薬食品局食品安全部長通知）に従い適切に評価すること。また、別添のとおり、分析機器メーカーから提示されたLC-MSの測定条件を示すので参考とされたい。

A Rapid iMethod™ Application for Screening Pesticides V.2.2 for Cliquid® Software

Tools for routine testing labs for easy implementation of pesticide screening in food, water, and other consumer products

Overview

With more than 800 pesticides currently in use there is growing concern by government agencies about the effect of pesticide exposure on human health. As a result, the residue level of pesticides in food, water and other consumer products are highly regulated. While analytical techniques like GC or GC/MS have traditionally been used for pesticide analysis, LC/MS/MS has quickly become the technique of choice due to the ability to analyze a more diverse set of pesticides, faster with better sensitivity and less sample preparation.

The following description outlines the instrument requirements and expected results obtainable from the AB SCIEX iMethod™ Application for Pesticide Screening and Quantitation using an AB SCIEX 3200 QTRAP® system or API 3200™ system. This iMethod™ application consists of a pre-configured method to screen for 534 pesticides; a positive polarity method and a negative polarity method to screen for the analytes in EU MRL list; and individual quantitation methods for carbamate, phenyl urea, triazine, organophosphorus, and acidic pesticides.

All methods have also been verified for use on AB SCIEX 4000 QTRAP®, API 4000™, QTRAP® 5500 and AB SCIEX Triple Quad™ 5500 systems.

The iMethod™ Application also includes the *iDQuant™* Pesticide Standard Kit containing 204 compounds distributed in 10 vials for easy preparation of standards. See Tables 2 – 11 for a comprehensive list. More in-depth sample preparation, and instrument parameter information is included as part of the standard operating procedure provided with the method, as are the required analytical columns. Solvents, standards and any supplies required for sample preparation are not included. Please note that the use of QTRAP® system technology is recommended for use with the screening method provided and that the associated library is not included and may be purchased separately.

Experimental details

The pesticide screening method included in this iMethod™ application is for the routine screening of 534 pesticides from food samples using the QuEChERS extraction and cleanup technique. The method uses external calibration standards and matrix spike recoveries to correct for sample and instrument variability and is based upon the use of a 3200 QTRAP® LC/MS/MS system.

A suggested method for the extraction of pesticides from vegetable, nut and citrus plant materials is also provided and is based upon the use of widely available QuEChERS tubes. Separation is achieved using a simple methanol / water gradient with ammonium formate with a Phenomenex Synergi 2.5 µm Fusion 100 Å, 50 x 2 mm HPLC column that is included with this iMethod™ application. Table 1 provides representative recoveries, signal-to-noise ratios, and estimated detection limits for 130 selected pesticides spiked at 25 ng/mL in a cucumber matrix using QuEChERS sample processing technique.

Quantitation Methods

The following information outlines the list of standard compounds in each of the quantitation methods for each compound class listed above. The methodology presented below was developed to quantify each pesticide when run by compound class, at < 10 ppb in order to meet regulatory requirements. The 603-compound MRM catalogue provided can also be used to create new customized tests according to any combinations required.

Example sample preparation procedures are provided for fruits and vegetables, based upon a simple sample homogenization, centrifugation, extraction and dilution. These procedures may require additional optimization based upon the actual composition and consistency of the fruit or vegetable under investigation. Deuterated and/or C13-labeled internal standards of known concentrations are added during sample preparation to monitor sample recovery.

Figure 1: Chromatogram of a 303 pesticides mix on an API 3200™ LC/MS/MS system (10 ng/mL)

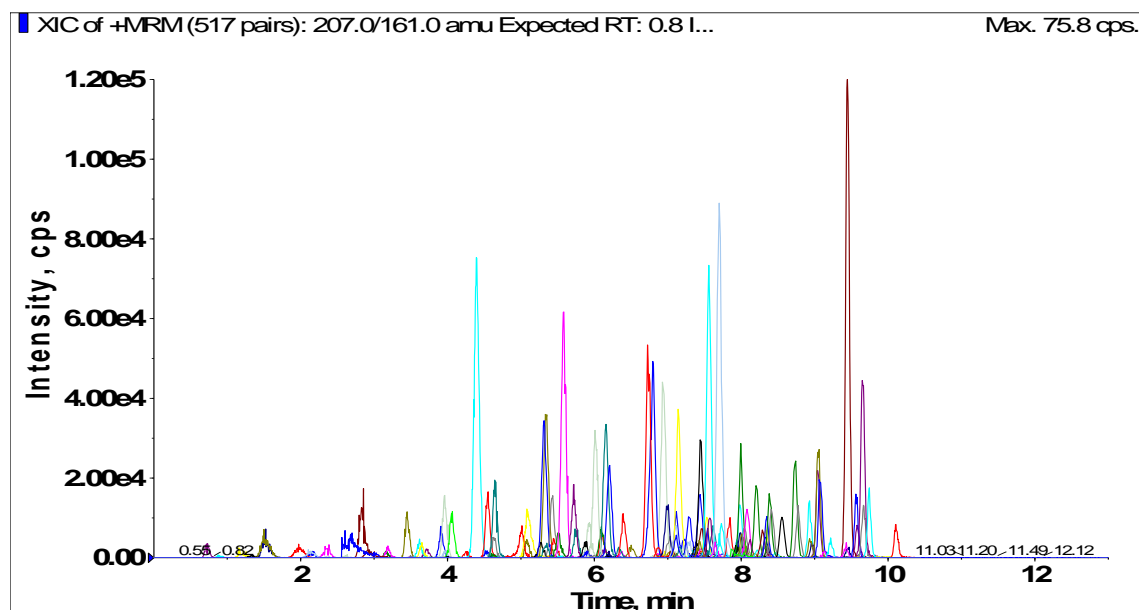


Table 1.

Representative recoveries, signal-to-noise ratios and estimated detection limits for 130 selected pesticides spiked at 25 ng/mL in a cucumber matrix using QuEChERS sample processing, as run on the 3200 QTRAP® LC/MS/MS system

Analyte	% Recovery	S/N*	% CV	Estimated detection limit (ng/mL)**
Aldicarb-sulfoxide	97.0%	26	4.2%	9.6
Aldoxycarb	96.4%	33.2	10.0%	7.5
Alloxydim	60.8%	32.2	7.5%	7.8
Aminocarb	84.2%	84	2.6%	3.0
Atrazine	65.1%	34	2.4%	7.4
Atrazine-2-hydroxy	79.9%	77.8	2.9%	3.2
Atrazine-desethyl-2-hydroxy	104.1%	38.8	1.9%	6.4
Benalaxyl	94.9%	39.5	18.1%	6.3
Bendiocarb	120.2%	33.1	16.2%	7.6
Benzoximate	119.9%	29.3	10.0%	8.5
Boscalid	15.3%	14.3	18.7%	17.5
Bromacil	99.0%	15.9	8.4%	15.7
Bupirimate	106.2%	43.8	9.0%	5.7
Butocarboxim-sulfoxid	102.2%	37.7	2.3%	6.6
Buturon	98.6%	20.4	4.1%	12.3
Carbaryl	98.4%	44.7	1.5%	5.6
Carbetamide	94.3%	58.8	4.9%	4.3
Chloridazon	111.1%	35.5	1.7%	7.0
Chlorotoluron	149.2%	38.1	2.4%	6.6
Chloroxuron	69.5%	24.7	11.0%	10.1
Cinosulfuron	88.6%	28.8	18.9%	8.7
Clomazone	107.2%	42.3	1.8%	5.9
Cloquintocet-mexyl	140.8%	95.8	10.1%	2.6
Coumaphos	120.8%	24.4	3.6%	10.2
Cyanazine	115.6%	22.1	20.1%	11.3
Cyproconazole	48.6%	24.6	7.1%	10.2
Cyprodinil	120.2%	11.3	7.6%	22.1

nalyte	% Recovery	S/N*	% CV	Estimated detection limit (ng/mL)**
<i>Demeton-S-methyl-sulfone</i>	90.0%	32.8	1.9%	7.6
<i>Diazinon</i>	100.5%	81.9	7.2%	3.1
<i>Diclobutrazol</i>	88.3%	26.3	7.6%	9.5
<i>Dicrotophos</i>	112.7%	58.1	19.1%	4.3
<i>Diethofencarb</i>	28.5%	16.2	8.0%	15.4
<i>Difenoxyuron</i>	104.0%	51	5.3%	5.0
<i>Dimefuron</i>	92.5%	20	6.6%	12.6
<i>Dimethachlor</i>	88.8%	13	11.8%	19.5
<i>Dimethenamide</i>	100.5%	39	2.7%	6.5
<i>Dimetilan</i>	106.0%	101	2.5%	2.5
<i>Dodemorph</i>	67.0%	107	3.0%	2.3
<i>Ethidimuron</i>	139.0%	28	6.5%	8.9
<i>Ethiofencarb-sulfon</i>	113.0%	59	14.7%	4.3
<i>Ethiofencarb-sulfoxid</i>	99.1%	119	3.6%	2.1
<i>Ethion</i>	113.9%	17	7.2%	14.8
<i>Ethirimol</i>	99.6%	42	4.9%	6.0
<i>Ethoprophos</i>	112.9%	16	14.1%	15.2
<i>Etrimfos</i>	93.3%	64	4.6%	3.9
<i>Fenbuconazole</i>	93.0%	21	2.2%	11.9
<i>Fenfuram</i>	98.0%	46	7.7%	5.5
<i>Fenhexamid</i>	47.9%	15	15.1%	17.0
<i>Fenoxaprop-P-ethyl</i>	113.9%	32	7.2%	7.8
<i>Fenpropimorph</i>	130.8%	152	4.2%	1.6
<i>Fenpyroximate</i>	161.6%	15	8.4%	16.8
<i>Fenuron</i>	102.8%	47	5.5%	5.3
<i>Flamprop-M-isopropyl</i>	104.1%	55	4.1%	4.5
<i>Flamprop-M-methyl</i>	90.2%	20	3.7%	12.4
<i>Flazasulfuron</i>	100.8%	74	7.5%	3.4
<i>Fluazifop-butyl</i>	144.5%	50	3.6%	5.0
<i>Flufenacet</i>	89.7%	22	12.8%	11.5
<i>Fluometuron</i>	120.9%	77	2.3%	3.2
<i>Fluridone</i>	68.4%	30	11.8%	8.4
<i>Flurtamone</i>	89.7%	20	5.2%	12.3
<i>Fuberidazole</i>	102.7%	125	6.2%	2.0
<i>Haloxyfop-P-methyl</i>	106.4%	15	3.2%	16.9
<i>Hexaconazole</i>	100.9%	23	2.1%	11.0
<i>Hexazinone</i>	106.3%	202	15.8%	1.2
<i>Imazalil</i>	117.7%	34	18.1%	7.3
<i>Isazofos</i>	74.9%	13	8.0%	19.1
<i>Isoprothiolane</i>	62.1%	77	1.2%	3.2
<i>Lenacil</i>	111.3%	43	6.1%	5.8
<i>Malaoxon</i>	44.7%	50	9.5%	5.0
<i>Malathion</i>	94.7%	30	5.9%	8.3
<i>Mepanipyrim</i>	79.5%	3	7.9%	80.6
<i>Metconazole</i>	118.2%	19	7.3%	13.4
<i>Methamidophos</i>	90.9%	33	6.5%	7.6
<i>Methfuroxam</i>	66.2%	96	1.1%	2.6
<i>Methidathion</i>	47.9%	35	4.2%	7.2
<i>Metobromuron</i>	116.1%	19	4.0%	12.9
<i>Metolachlor</i>	82.7%	22	2.6%	11.4
<i>Metosulam</i>	99.7%	51	2.7%	4.9
<i>Monuron</i>	100.3%	22	2.8%	11.6
<i>Napropamide</i>	103.7%	31	11.5%	8.1
<i>Oxasulfuron</i>	87.8%	78	6.6%	3.2

Analyte	% Recovery	S/N*	% CV	Estimated detection limit (ng/mL)**
Oxycarboxin	98.5%	110	5.3%	2.3
Paclobutrazol	105.4%	48	9.2%	5.2
Phosalone	102.9%	13	9.0%	18.9
Phosphamidon	95.2%	104	6.5%	2.4
Picoxystrobin	133.1%	104	3.8%	2.4
Pirimiphos-ethyl	129.7%	57	4.1%	4.4
Pirimiphos-methyl	105.1%	63	3.1%	4.0
Prometon	100.5%	105	6.0%	2.4
Prometryne	49.5%	14	19.5%	18.4
Propamocarb	106.5%	20	1.9%	12.8
Propazin-2-hydroxy	81.5%	19	3.6%	12.9
Propazine	72.8%	11	10.7%	22.5
Prosulfocarb	114.9%	145	6.1%	1.7
Pymetrozine	101.4%	115	2.6%	2.2
Pyraclostrobin	141.1%	24	9.6%	10.5
Pyrazophos	108.9%	55	4.8%	4.5
Pyridaben	102.8%	18	4.1%	14.1
Pyridaphenthion	88.6%	10	6.3%	25.3
Pyrimethanil	40.1%	18	5.8%	13.6
Pyriproxyfen	153.8%	51	4.3%	4.9
Quinalphos	124.9%	17	7.3%	14.8
Quinmerac	104.9%	116	1.3%	2.2
Sebuthylazine	56.9%	55	3.6%	4.6
Sebuthylazine-desethyl	88.6%	39	7.1%	6.5
Sethoxydim	82.5%	28	10.1%	8.9
Siduron	59.7%	14	5.3%	17.5
Simazine-2-hydroxy	105.5%	99	10.6%	2.5
Simetryn	95.7%	96	6.6%	2.6
Spiroxamine	97.1%	230	6.0%	1.1
Sulfometuron-methyl	98.2%	103	5.1%	2.4
Tebuconazol	87.3%	45	9.6%	5.5
Tebufenpyrad	125.2%	13	10.6%	18.8
Tebutam	87.2%	22	7.3%	11.4
Tebuthiuron	97.8%	61	14.4%	4.1
Terbufos	44.3%	4	20.3%	65.8
Terbutylazine	31.7%	18	3.3%	14.1
Terbutylazine-desethyl	88.7%	39	8.1%	6.5
Terbutryn	31.9%	119	6.0%	2.1
Tetraclorvinphos	101.3%	20	8.7%	12.5
Tetraconazole	82.1%	32	16.3%	7.8
Thifensulfuron-methyl	100.8%	74	4.2%	3.4
Triasulfuron	80.5%	35	7.5%	7.2
Triazophos	31.9%	19	9.9%	13.2
Tricyclazole	93.8%	72	1.9%	3.5
Trietazine	75.4%	12	13.6%	21.0
Trifloxystrobin	113.9%	83	5.8%	3.0
Triflumizole	122.4%	25	11.9%	10.1
Triticonazole	117.1%	24	5.8%	10.6
Uniconazole	66.5%	24	24.0%	10.6
Vamidothion	113.1%	36	13.9%	7.0

* Signal-to-noise obtained at three standard deviations on a 3200 QTRAP® System.

** Estimated detection limit based on estimated signal at 10 x the Signal-to-noise ratio.

Table 2. Content iDQuant™ Pesticide Standard A1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>3-Hydroxycarbofuran</i>	16655-82-6	<i>Formetanate HCL</i>	23422-53-9
<i>Acephate</i>	30560-19-1	<i>Fuberidazole</i>	3878-19-1
<i>Aldicarb sulfone</i>	1646-88-4	<i>Methamidophos</i>	10265-92-6
<i>Aldicarb sulfoxide</i>	1646-87-3	<i>Methomyl</i>	16752-77-5
<i>Aminocarb</i>	2032-59-9	<i>Mevinphos</i>	7786-34-7
<i>Butocarboxim</i>	34681-10-2	<i>Monocrotophos</i>	6923-22-4
<i>Butoxycarboxim</i>	34681-23-7	<i>Omethoate</i>	1113-02-6
<i>Carbendazim</i>	10605-21-7	<i>Oxamyl</i>	23135-22-0
<i>Cymoxanil</i>	57966-95-7	<i>Propamocarb</i>	24579-73-5
<i>Dicrotophos</i>	141-66-2	<i>Thiabendazole</i>	148-79-8
<i>Dimethoate</i>	60-51-5	<i>Tricyclazole</i>	41814-78-2
<i>Dioxacarb</i>	6988-21-2	<i>Formetanate HCL</i>	23422-53-9

Table 3. Content iDQuant™ Pesticide Standard B1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Aldicarb</i>	116-06-3	<i>Isoproc carb</i>	2631-40-5
<i>Bendiocarb</i>	22781-23-3	<i>Metalaxyl</i>	57837-19-1
<i>Carbaryl</i>	63-25-2	<i>Methiocarb</i>	2032-65-7
<i>Carbetamide</i>	16118-49-3	<i>Mexacarbate</i>	315-18-4
<i>Carbofuran</i>	1563-66-2	<i>Oxadixyl</i>	77732-09-3
<i>Carboxin</i>	5234-68-4	<i>Pirimicarb</i>	23103-98-2
<i>Clethodim</i>	99129-21-2	<i>Promecarb</i>	2631-37-0
<i>Desmedipham</i>	13684-56-5	<i>Propham</i>	122-42-9
<i>Diethofencarb</i>	87130-20-9	<i>Propoxur</i>	114-26-1
<i>Ethiofencarb</i>	29973-13-5	<i>Pyracarbolid</i>	24691-76-7
<i>Furalaxyl</i>	57646-30-7	<i>Thiofanox</i>	39196-18-4
<i>Iprovalicarb</i>	140923-17-7	<i>Thiophanate-methyl</i>	23564-05-8

Table 4. Content iDQuant™ Pesticide Standard C1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Alany carb</i>	83130-01-2	<i>Flufenacet</i>	142459-58-3
<i>Amitraz</i>	33089-61-1	<i>Furathiocarb</i>	65907-30-4
<i>Benalaxyl</i>	71626-11-4	<i>Indoxacarb</i>	144171-61-9
<i>Benfuracarb</i>	82560-54-1	<i>Mefenacet</i>	73250-68-7
<i>Benzoximate</i>	29104-30-1	<i>Mepronil</i>	55814-41-0
<i>Bifenazate</i>	149877-41-8	<i>Piperonyl butoxide</i>	51-03-6
<i>Cyazofamid</i>	120116-88-3	<i>Quinoxifen</i>	124495-18-7
<i>Fenamidone</i>	161326-34-7	<i>Spiroxamine</i>	118134-30-8
<i>Fenazaquin</i>	120928-09-8	<i>Thiobencarb</i>	28249-77-6
<i>Fenhexamid</i>	126833-17-8	<i>Zoxamide</i>	156052-68-5
<i>Fenoxycarb</i>	79127-80-3		

Table 5. Content iDQuant™ Pesticide Standard D1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Acetamiprid</i>	135410-20-7	<i>Metribuzin</i>	21087-64-9
<i>Acibenzolar-S-methyl</i>	135158-54-2	<i>Myclobutanil</i>	88671-89-0
<i>Bromucanazol</i>	116255-48-2	<i>Nitenpyram</i>	120738-89-8
<i>Clothianidin</i>	210880-92-5	<i>Nuarimol</i>	63284-71-9
<i>Cyproconazole</i>	113096-99-4	<i>Paclobutrazol</i>	76738-62-0
<i>Epoxiconazole</i>	135319-73-2	<i>Pyrimethanil</i>	53112-28-0
<i>Etaconazole</i>	60207-93-4	<i>Thiacloprid</i>	111988-49-9
<i>Fenarimol</i>	60168-88-9	<i>Thiamethoxam</i>	153719-23-4
<i>Flutriafol</i>	76674-21-0	<i>Triadimenol</i>	55219-65-3
<i>Imazalil</i>	35554-44-0	<i>Triticonazole</i>	131983-72-7
<i>Imidacloprid</i>	138261-41-3		

Table 6. Content iDQuant™ Pesticide Standard E1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Abamectin</i>	71751-41-2	<i>Flutolanil</i>	66332-96-5
<i>Bitertanol</i>	55179-31-2	<i>Hexaconazole</i>	79983-71-4
<i>Bupirimate</i>	41483-43-6	<i>Mepanipyrim</i>	110235-47-7
<i>Butafenacil</i>	134605-64-4	<i>Metconazole</i>	125116-23-6
<i>Clofentezine</i>	74115-24-5	<i>Methoxyfenozid</i>	161050-58-4
<i>Cyprodinil</i>	121552-61-2	<i>Penconazole</i>	66246-88-6
<i>Diclobutrazol</i>	75736-33-3	<i>Prochloraz</i>	67747-09-5
<i>Difenoconazole</i>	119446-68-3	<i>Propiconazole</i>	60207-90-1
<i>Diniconazol</i>	83657-24-3	<i>Rotenone</i>	83-79-4
<i>Ethofumesate</i>	26225-79-6	<i>Tebufozide</i>	112410-23-8
<i>Fenbuconazole</i>	114369-43-6	<i>Triflumizole</i>	68694-11-1
<i>Flusilazole</i>	85509-19-9		

Table 7. Content iDQuant™ Pesticide Standard F1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Carfentrazone-ethyl</i>	128639-02-1	<i>Mesotrione</i>	104206-82-8
<i>Doramectin</i>	117704-25-3	<i>Moxidectin</i>	113507-06-5
<i>Emamectin-benzoate</i>	155569-91-8	<i>Propargite</i>	2312-35-8
<i>Eprinomectin</i>	123997-26-2	<i>Spinosad</i>	168316-95-8
<i>Fluquinconazole</i>	136426-54-5	<i>Spirodiclofen</i>	148477-71-8
<i>Hexythiazox</i>	78587-05-0	<i>Spiromesifen</i>	283594-90-1
<i>Hydramethylnon</i>	67485-29-4	<i>Tebuconazol</i>	107534-96-3
<i>Ipconazole</i>	125225-28-7	<i>Tetraconazole</i>	112281-77-3
<i>Ivermectin</i>	70288-86-7		

Table 8. Content iDQuant™ Pesticide Standard G1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Chlortoluron</i>	15545-48-9	<i>Monolinuron</i>	1746-81-2
<i>Cycluron</i>	2163-69-1	<i>Prometon</i>	1610-18-0
<i>Diuron</i>	330-54-1	<i>Pymetrozine</i>	123312-89-0
<i>Fenuron</i>	101-42-8	<i>Secbumeton</i>	26259-45-0
<i>Fluometuron</i>	2164-17-2	<i>Simetryn</i>	1014-70-6
<i>Forchlorfenuron</i>	68157-60-8	<i>Sulfentrazone</i>	122836-35-5
<i>Isoproturon</i>	34123-59-6	<i>Tebuthiuron</i>	34014-18-1
<i>Methabenzthiazuron</i>	18691-97-9	<i>Terbumeton</i>	33693-04-8
<i>Methoprotryne</i>	841-06-5	<i>Thidiazuron</i>	51707-55-2
<i>Metobromuron</i>	3060-89-7	<i>Triadimefon</i>	43121-43-3

Table 9. Content iDQuant™ Pesticide Standard H1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Ametryn</i>	834-12-8	<i>Hexaflumuron</i>	86479-06-3
<i>Azoxystrobin</i>	131860-33-8	<i>Kresoxim-methyl</i>	143390-89-0
<i>Boscalid</i>	188425-85-6	<i>Linuron</i>	330-55-2
<i>Chloroxuron</i>	1982-47-4	<i>Neburon</i>	555-37-3
<i>Diflubenzuron</i>	35367-38-5	<i>Phenmedipham</i>	13684-63-4
<i>Dimethomorph</i>	110488-70-5	<i>Picoxystrobin</i>	117428-22-5
<i>Dimoxystrobin</i>	149961-52-4	<i>Prometryne</i>	7287-19-6
<i>Famoxadon</i>	131807-57-3	<i>Siduron</i>	1982-49-6
<i>Fipronil</i>	120068-37-3	<i>Terbutryne</i>	886-50-0
<i>Fludioxonil</i>	131341-86-1	<i>Triflumuron</i>	64628-44-0

Table 10. Content iDQuant™ Pesticide Standard J1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Buprofezin</i>	69327-76-0	<i>Lufenuron</i>	103055-07-8
<i>Chlorfluazuron</i>	71422-67-8	<i>Novaluron</i>	116714-46-6
<i>Ethiprole</i>	181587-01-9	<i>Prothioconazole</i>	178928-70-6
<i>Etoxazole</i>	153233-91-1	<i>Pyraclostrobin</i>	175013-18-0
<i>Fenpropimorph</i>	67564-91-4	<i>Pyridaben</i>	96489-71-3
<i>Fenpyroximate</i>	111812-58-9	<i>Pyriproxyfen</i>	95737-68-1
<i>Fluazinam</i>	79622-59-6	<i>Tebufenpyrad</i>	119168-77-3
<i>Flufenoxuron</i>	101463-69-8	<i>Teflubenzuron</i>	83121-18-0
<i>Fluoxastrobin</i>	361377-29-9	<i>Trifloxystrobin</i>	141517-21-7

Table 11. Content iDQuant™ Pesticide Standard K1

Pesticide Name	CAS Number	Pesticide Name	CAS Number
<i>Chlorantraniliprole</i>	500008-45-7	<i>Isocarboxiphos</i>	24353-61-5
<i>Cyromazine</i>	66215-27-8	<i>Mandipropamid</i>	374726-62-2
<i>Dinotefuran</i>	165252-70-0	<i>Metaflumizone</i>	139968-49-3
<i>Ethirimol</i>	23947-60-6	<i>Pencycuron</i>	66063-05-6
<i>Fenobucarb</i>	3766-81-2	<i>Spinetoram</i>	187166-40-1
<i>Flonicamid</i>	158062-67-0	<i>Spirotetramat</i>	203313-25-1
<i>Flubendimide</i>	272451-65-7	<i>Temephos</i>	3383-96-8
<i>Halofenozide</i>	112226-61-6	<i>Trichlorfon</i>	52-68-6

Table 12. List of triazine pesticides with retention times for each

Triazines	RT (Min)	Triazines	RT (Min)
<i>Atrazine</i>	8.5	<i>Prometon</i>	8.3
<i>Ametryn</i>	7.8	<i>Prometryn</i>	9.0
<i>Cyanazine</i>	6.7	<i>Propazine</i>	8.6
<i>Desisopropyl-atrazine</i>	5.4	<i>Sebutylazine</i>	8.4
<i>Desethyl-atrazine</i>	4.0	<i>Simazine</i>	6.9
<i>Hexazinon</i>	6.9	<i>Terbuthylazine</i>	8.6
<i>Metazoachlor</i>	7.8	<i>Terbutryn</i>	9.1
<i>Metolachlor</i>	9.2	<i>D5-atrazine (internal std)</i>	7.7
<i>Metribuzin</i>	7.4		

Figure 2: Chromatogram of a 300 pesticides mix spiked by API 3200™ LC/MS/MS system (100 ng/mL)

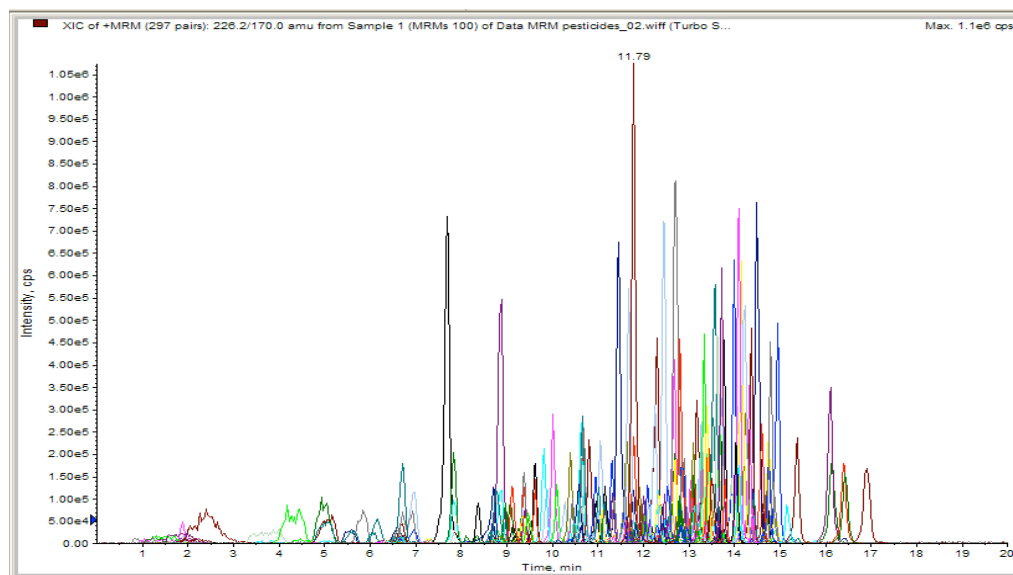
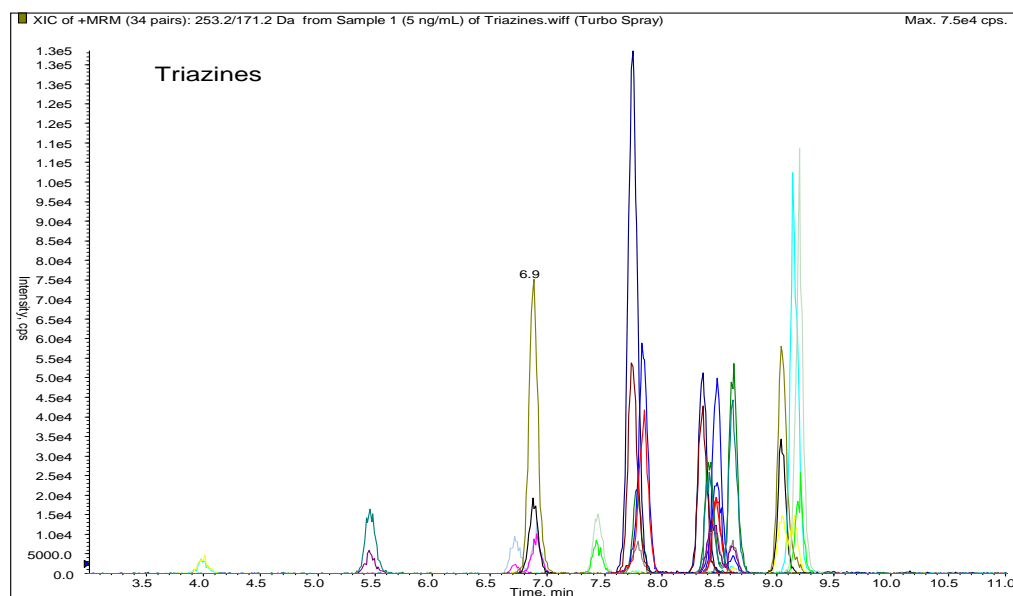


Figure 3: Chromatogram of triazine pesticides at 5 ng / mL



Get additional details on customizing a pesticide screen for your specific laboratory application by contacting AB SCIEX at support@absciex.com.

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A Rapid iMethod™ Application for Screening Pesticides V.2.4 for Cliquid® Software

Tools for routine testing labs for easy implementation of pesticide screening in food, water, and other consumer products for screening or quantitative analysis applications

Overview

With more than 800 pesticides currently in use there is growing concern by government agencies about the effect of pesticide exposure on human health. As a result, the residue level of pesticides in food, water and other consumer products are highly regulated. While analytical techniques like GC or GC/MS have traditionally been used for pesticide analysis, LC/MS/MS has quickly become the technique of choice due to the ability to analyze a more diverse set of pesticides faster and with better sensitivity and less sample preparation.

The following description outlines an overview of the AB SCIEX iMethod™ Application for Pesticide Screening and Quantitation using a 3200 Q TRAP® system, 4000 Q TRAP® system, or the QTRAP® 5500 LC/MS/MS system. This iMethod™ application consists of 9 pre-configured methods, designed for either quantitative analysis or for qualitative screening using QTRAP® technology. See Table 1 for the comprehensive list of tests included in this iMethod™ Application.

The iMethod™ application contains multiple sample preparation approaches, including EN 15662, AOAC Method 2007.01, and several others, instrument parameter information, and expected retention times for 3 different HPLC systems – the Shimadzu Prominence, the Agilent 1200, and the Eksigent ekspert™ ultraLC 100 and 100XL. The iMethod™ application also includes the required analytical columns for the analysis. Solvents, standards and any supplies required for sample preparation are not included.

Please note that the use of QTRAP® system technology is recommended for use with the screening method provided and that the associated library is not included and may be purchased separately. The compound library includes 603 pesticide compounds, and the catalogue can be used to create customized test methods according to any desired list of compounds.

Experimental details

The methods included in this iMethod™ application can be utilized for the routine screening of up to 535 pesticides or quantitative analysis of selected lists of pesticides from food samples using the QuEChERS extraction and cleanup technique, although several other sample preparation approaches, including one for the analysis of pesticides in water by direct injection, are provided within the method SOP. The methods use external calibration standards and matrix spike recoveries to correct for sample and instrument variability and are based upon the use of a 3200 Q TRAP® system, 4000 Q TRAP® system, or the QTRAP® 5500 LC/MS/MS system.

Quantitation Methods

Included below in Table 2 is an outline of the list of pesticide compounds included in the 5 quantitative analysis modules within this iMethod™ application. The methodology for this iMethod™ Application was developed to quantify each pesticide at < 10 ppb in order to meet regulatory requirements.

Example sample preparation procedures are provided for fruits and vegetables, based upon a simple sample homogenization, centrifugation, extraction and dilution. These procedures may require additional optimization based upon the actual composition and consistency of the fruit or vegetable under investigation. Deuterated and/or C13-labeled internal standards of known concentrations are added during sample preparation to monitor sample recovery. Additionally, iDQuant™ Standards kits, which contain 204 common pesticides in 10 easy-to-use and certified mixes, may also be used with this iMethod™ application to simplify standards preparation or for internal or external calibration.

Table 1. Summary of the 9 tests included in the iMethod™ Application

Test	Application	Description
General pesticide screening	<i>QTRAP screening method</i>	Screening of 535 common pesticides in a single injection
EU MRL pesticide screening, positive ionization	<i>QTRAP screening method</i>	Screening of 352 pesticides regulated by the EU, using positive ESI
EU MRL pesticide screening, negative ionization	<i>QTRAP screening method</i>	Screening of 32 pesticides regulated by the EU, using negative ESI
Pesticide screening using iDQuant™ Standards Kit	<i>QTRAP screening method</i>	Screening of 214 pesticide compounds, all of which are included in the iDQuant™ Standards Kit
Acidic pesticides analysis	<i>Quantitative analysis method</i>	Method for the quantitative analysis of 19 acidic pesticide compounds
Carbamate pesticides analysis	<i>Quantitative analysis method</i>	Method for the quantitative analysis of 47 carbamate pesticide compounds
Organophosphorous pesticides analysis	<i>Quantitative analysis method</i>	Method for the quantitative analysis of 29 organophosphorous pesticide compounds
Phenyl urea compound analysis	<i>Quantitative analysis method</i>	Method for the quantitative analysis of 15 phenyl urea compounds
Triazine pesticides analysis	<i>Quantitative analysis method</i>	Method for the quantitative analysis of 16 triazine pesticide compounds

Figure 1: Sample chromatogram of a 300 pesticides mix spiked by API 3200™ LC/MS/MS system (100 ng/mL)

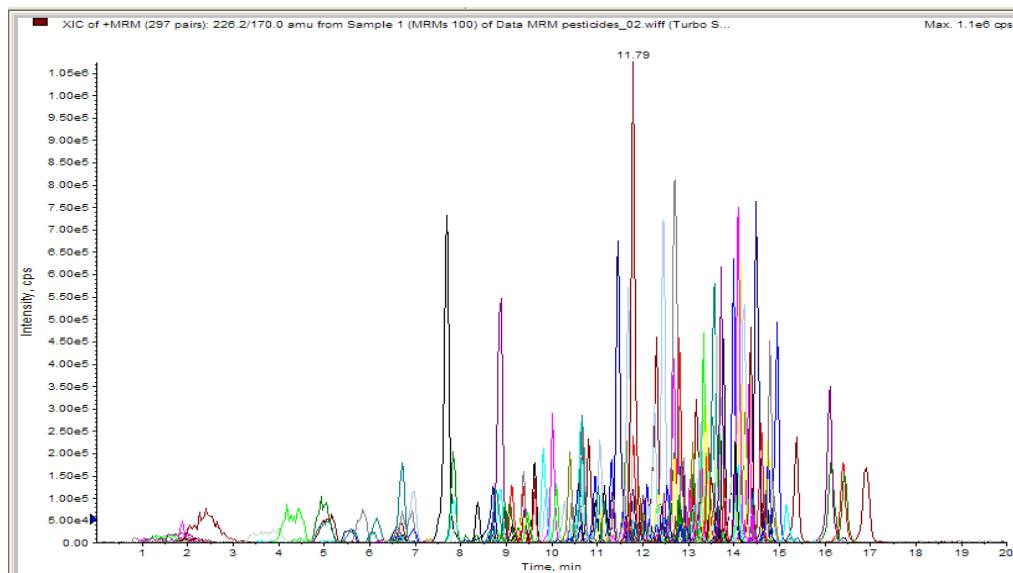


Table 2. Summary of the compounds included in the quantitative analysis test modules

Acidic pesticides	Carbamate Pesticides	Organophosphorous pesticides
2,4,5-T	3-Hydroxycarbofuran	Acephate
2,4,5-TP	Alanycarb	Azinphos methyl
2,4-D	Aldicarb	Azinphos-ethyl
2,4-DB	Aldicarb-sulfone	Chlorfenvinphos
2,4-DP	Aldicarb-sulfoxide	Chlorpyrifos
Bentazon	Aminocarb	Coumaphos
Bromoxynil	Bendiocarb	Demeton-S-methyl
Clopyralid	Benfuracarb	Demeton-S-methyl-sulfone
Dicamba	Benomyl	Diazinon
Dinoseb	Butocarboxim	Dichlorvos
Dinoterb	Butocarboxim-sulfoxide	Dicrotophos
Fluoxypyr	Butoxycarboxim	Dimethoate
Imazapyr	Carbaryl	EPTC

loxynil	Carbofuran	Famphur
MCPA	Carbosulfan	Fenthion
MCPB	Chloroprotham	Malathion
MCPD	Dimepiperate	Mevinphos
PCP	Dioxacarb	Naled
Triclopyr	EPTC	Parathion
	Esprocarb	Parathion-methyl
Phenyl urea compounds	Ethiofencarb	Phorate
Chlortoluron	Ethiofencarb-sulfone	Phorate sulfoxide
Diflubenzuron	Ethiofencarb-sulfoxide	Pirimiphos-ethyl
Diuron	Fenobucarb	Pirimiphos-methyl
Fenuron	Fenothiocarb	Sulfotep
Fluometuron	Fenoxycarb	Sulprofos
Isoproturon	Furathiocarb	Tetrachlorvinphos
Linuron	Iprovalicarb	Tokuthion
Methabenzthiazuron	Isoprocarb	Triazophos
Metobromuron	Methiocarb	
Metoxuron	Methiocarb-sulfone	Triazine pesticides
Monolinuron	Methomyl	Ametryn
Propanil	Oxamyl	Atrazine
Siduron	Phenmedipham	Cyanazine
Tebuthiuron	Pirimicarb	Desethyl-atrazine
Thidiazuron	Promecarb	Desisopropyl-atrazine
	Propamocarb	Hexazinone
	Propoxur	Metazachlor
	Pyributicarb	Metolachlor
	Terbucarb	Metribuzin
	Thiobencarb	Prometon
	Thiodicarb	Prometryn
	Thiofanox	Propazine
	Thiofanox-sulfone	Sebutylazine
	Thiuram	Simazine
	Triallate	Terbutylazine
	XMC	Terbutryn

Get additional details on customizing a pesticide screen for your specific laboratory application by contacting AB SCIEX at support@absciex.com.

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Publication number: 5460112-02

分析条件は、各化合物の分析条件はそれぞれのシートに記載しています。

農薬	英語名	シート 番号	備考	
EPN	EPN	1		
アセトクロール	Acetochlor			
クロルピリホス	Chlorpyrifos			
ジクロルボス	Dichlorvos			
ジコホール	Dicofol			
シペルメトリン	Cypermethrin			
テトラコナゾール	Tetraconazole			
トリアジメノール	Triadimenol			
トリアゾホス	Triazophos			
トリフルラリン	Trifluralin			
ピリメタニル	Pyrimethanil			
フェンバレレート	Fenvalerate			
フルキンコナゾール	Fluquinconazole			
フルシラゾール	Flusilazole			
ブピリメート	Bupirimate			
プロピコナゾール	Propiconazole			
プロメトリン	Prometryn			
ヘキサコナゾール	Hexaconazole			
ジフェノコナゾール	Difenoconazole		2	
シメコナゾール	Simeconazole			
テブフェノジド	Tebufenozide	Nega		
フェニトロチオン	Fenitrothion			
メタラキシル及びメフェ ノキサム	Metalaxyl and Mefenoxam	3		
アセフェート	Acephate			
イマザリル	Imazalil	4		
ハロキシホップ	Haloxifop		Q1、Q3、DP、CEのみ	
フルアジホップ	Fluazifop	5	Q1、Q3、DP、CEのみ	
モノクロトホス	Monocrotophos	6	Q1、Q3、DP、CEのみ	
エンドリン	Endrin	7	Q1、Q3、APCI	
ディルドリン(アルドリン を含む)	Dieldrin(include Aldrin)		Q1、Q3、APCI	
エポキシコナゾール	Epoxyconazole	8	Q1、Q3、DP、CEのみ	
エンドスルファン	Endosulfan	9	LC条件なし	
グリホサート	Glyphosate	10		
メタミドホス	Metamidophos	11		
メキシフェノジド	Methoxyfenozide	12		
メコナゾール	Metconazole	13	Q1、Q3のみ	
アメトリン	Ametryn	確認中		
ジニコナゾール	Diniconazole	確認中		
プロフェノホス	Profenofos	確認中		

Q1	Q3	time	ID	DP	EP	CE	CXP
270.0	224.0	50.0	Acetochlor	61	4.5	13	4
317.0	166.0	50.0	Bupirimate	71	9.5	35	4
352.0	200.0	50.0	Chlorpyrifos	61	4.5	29	30
416.0	191.0	50.0	Cypermethrin	71	4.5	57	6
221.0	127.0	50.0	Dichlorvos	96	3.5	21	4
369.0	205.0	50.0	Dicofol	71	4.5	57	2
324.0	157.0	50.0	EPN	66	4.5	31	4
420.0	167.0	50.0	Fenvalerate	56	3	27	2
376.0	307.0	50.0	Fluquinconazole	81	5	15	28
316.0	165.0	50.0	Flusilazole	71	7.5	37	4
314.0	159.0	50.0	Hexaconazole	56	10	43	4
242.0	158.0	50.0	Prometryn	66	4.5	33	4
342.0	159.0	50.0	Propiconazole	76	4.5	43	4
200.0	107.0	50.0	Pyrimethanil	81	10	33	4
372.0	159.0	50.0	Tetraconazole	76	10.5	45	4
296.0	70.0	50.0	Triadimenol	56	4	27	4
314.0	162.0	50.0	Triazophos	61	3.5	23	4
336.0	132.0	50.0	Trifluralin	71	6	49	4

HPLC system	Agilent 1100 series				
Column	100V (2.0mmΦ × 150mm, 5um)				
Mobile phase : A	0.1%半酸/2mM 酢酸アンモニウム水溶液				
: B	アセトニトリル				
Gradient					
Time [min.]	0	10	15	15.1	25
A [%]	95	0	0	95	95
B [%]	5	100	100	5	5
Flow rate (μL/min)	200				
Column temp. [°C]	60				
Sample cooler [°C]	8				
Injection volume [μL]	10				
Mass spectrometry	3200				
Ion source	Tuboion Spray [ESI]				
Mode	MRM				
Temperature [°C]	Positive Mode: 550		Negative Mode: 600		
Ion source voltage [V]	Positive Mode: 5500		Negative Mode: -4000		
Monitoring time [min.]	25				

Q1	Q3	time	ID	DP	EP	CE	CXP
406.1	251	50	Difenoconazole 1	75	9	40	5
408.1	253	50	Difenoconazole 2	75	9	40	5
294.1	73	50	Simeconazole 1	60	4	50	4
294.1	70	50	Simeconazole 2	60	4	45	4
278	109	50	Fenitrothion 1	60	10	27	4
280.1	220	50	Metalaxyl 1	50	10	20	5
280.1	192	50	Metalaxyl 2	50	10	26	4
351	149	50	Tebufoenozide 1	-80	-10	-28	-5
351	105	50	Tebufoenozide 2	-80	-10	-30	-5

<分析条件>

HPLC system	Shimadzu社製Prominence シリーズ UFLC						
Column	GLScience Inertsustin 粒径3 μ m (2.0mm Φ ×150mm)						
Mobile phase	A:	5mM 酢酸アンモニウム (酢酸アンモニウム:Aldorich >99.995%)					
	B:	メタノール (和光社製 LC/MS用メタノール)					
Flow rate(μ l/min)	250						
Gradient	Time(mi)	0	13	23	23.1	30	
	A(%)	80	10	10	80	80	
	B(%)	20	90	90	20	20	
Column temp.($^{\circ}$ C)	40						
Inj. Volume(μ L)	5						
Mass spectrometry	3200QTRAPTM System						
Ion source	Turbo V Ion Spray (ESI)						
Mode	MRM						
Turbo gas temp.($^{\circ}$ C)	350						
Spray voltage (V)	5500/-4500						
Polarity	Positive / Negative						

(ゴルフ場で使用される農薬による水質汚濁の防止に係る暫定指導指針に準拠)

イオン源パラメータ

CUR	CAD	IS	TEM	GS1	GS2
15/25	6	5500/-4500	350	70	60

Positive/Negative

Q1	Q3	time	ID	DP	EP	CE	CXP
184.0	143	50	Acephate 1	21	8	13	4
184.0	49.1	50	Acephate 2	21	8	31	4
297.0	158.9	50	Imazalil 1	26	4	31	4
297.0	41.1	50	Imazalil 2	26	4	43	4

HPLC system	Shimadzu Prominence-XR HPLCsystem								
Column	Shimadzu shimpack-XRODS 2mm × 75mm								
Mobile phase	5mM 酢酸アンモニウム含有超純水 5mM 酢酸アンモニウム含有メタノール								
: A									
: B									
Gradient									
Time [min.]	0	0.5	2.0	10	16	16.01	20		
A [%]	90	40	40	5	5	90	90		
B [%]	10	40	40	95	95	10	10		
Flow rate(μl/min)	250								
Column temp. [°C]	40°C								
サンプルクーラー	8°C								
Injection volume [uL]	1								

Mass spectrometry	5500QTRAP	
Ion source	Turboion Spray [ESI]	
Mode	MRM	
Temperature [°C]	350	
Polarity	Positive	Negative
Ion source voltage [V]	5500	4500
Monitoring time [min.]	20	

Q1	Q3	time	ID	DP	EP	CE	CXP
362	316	50	Haloxypop	126	-	23	-

HPLCシステム	Shimadzu UFLC XR						
カラム	AQUITY HSS T3 2.1 x 100mm 1.8um						
移動相							
: A	5mM ギ酸アンモニウム水溶液						
: B	5mM ギ酸アンモニウム/メタノール溶液 (1:9, v/v)						
グラジエント							
Time [min.]	0	1	15	18.3	18.4	20	
A [%]	95	95	15	5	5	95	
B [%]	5	5	98	98	95	5	
流速(μl/min)	300						
カラム温度[°C]	40						
サンプルクーラー[°C]	10						
注入量	2μL						
Mass Spectrometry	QTRAP5500 LC/MS/MS システム						
Ion Source	Turbo V™ Ion Source (ESI)						
Mode	MRM						
Temperature [°C]	400						
Polarity	Positive / Negative Switchng						

Q1	Q2	time	ID	DP	CE
328.1	282.2	50	Fluazifop	81	25

HPLC system	Shumadzu 20A					
Column	TSK-Gel ODS-80TsQA 5 μ (2.1mm Φ \times 150mm)					
Mobile phase	5mM HCOOH in H ₂ O:MeOH=8:2					
: A	5mM HCOOH in H ₂ O:MeOH=1:9					
: B						
Gradient						
Time [min.]	0	3	8	13	13.01	20
A [%]	30	30	0	0	30	30
B [%]	70	70	100	100	70	70
Flow rate(μ l/min)	200					
Column temp. [°C]	room temperature					
Injection volume [μ L]	10					
Mass spectrometry	3200QTRAP					
Ion source	Turbo Ion Spray (ESI)					
Mode	MRM					
Temperature [°C]	700					
Polarity	Positive					
Ionspray Voltage [V]	4500					
Monitoring time [min.]	20					

Q1	Q3	time	ID	DP	EP	CE	CXP
224.1	193.2	50	Monocrotophos	46	-	11	-

HPLC system	Agilent 1100 series					
Column	Develosil C30-UG-5 (2.0mmΦ×100mm)					
Mobile phase : A : B	0.1% 半酸および 10mM 半酸アンモニウムを含む 5%メタノール水溶液 メタノール					
Gradient Time [min.]	0	10	14	14.01	22	
A [%]	100	5	5	100	100	
B [%]	0	95	95	0	0	
Flow rate(μl/min)	200					
Column temp. [°C]	40°C					
サンプルクーラー	6°C					
Injection volume [μL]	5					
Mass spectrometry	API3000					
Ion source	Tuboion Spray [ESI]					
Mode	MRM					
Temperature [°C]	550					
Polarity	Positive					
Ion source voltage [V]	5500V					
Monitoring time [min.]	22					

Q1	Q3	time	ID	DP	EP	CE	CXP	
364.7	328.8	-	Aldrin	-	-	-	-	Posi
412	247	-	endrin	-	-	-	-	Nega
381	327	-	dieldrin	-	-	-	-	Posi

IonSource: APCI

Q1	Q3	time	ID	DP	EP	CE	CXP
330	121	50	Epoxyconazole	71	-	31	10

カラム Xterra MS C18(5um,2.1x150mm)
 温度 40°C
 流速 0.2mL/min
 移動相A 精製水
 移動相B メタノール
 グラジエント条件

	0	20	35
A	90	10	10
B	10	90	90

IS 5500
 TEM 500
 CAD 3

Q1	Q3	time	ID	DP	EP	CE	CXP
403.1	320.9	50	ENDOSULFAN	-40	-10	-20	-17

パラメーターのみ

Q1	Q3	time	ID	DP	EP	CE	CXP
168	63	50	Glyphosate 1	-70	-10	-30	-15
168	81	50	Glyphosate 2	-70	-10	-18	-16

HPLC system	Shimadzu UFLC					
Column	TOSOH TSKgel SUPER IC-AP 4.6mm×75mm					
Mobile phase : A : B	A: Water 50mM Formic acid ammonium B: Water					
Gradient Time min.	-6	0	5	28	29	30
A %	5	5	40	40	5	5
B %	95	95	60	60	95	95
Flow Rate(mL/min)	0.5					
Column Temp. [°C]	40					
Injection Volume [μl]	100					
Mass Spectrometry	AB SCIEX Triple Quad™ 5500 System					
Ion Source	TurboV™ (ESI)					
Mode	MRM					
Polarity	Negative					
Curtain Gas(CUR)	40					
Collision Gas(CAD)	10					
Ion Spray Voltage [V]	-4500					
Temperature [°C]	500					
Ion Source Gas1,	70					
Ion Source Gas2	60					
Monitoring Time [min]	30min					

Q1	Q3	time	ID	DP	EP	CE	CXP
142	94	50	Metamidophos 1	51	-	19	-
142	125	50	Metamidophos 2	51	-	17	-

HPLC system		Shimadzu社製Prominence				
Column		Inertsil-column ODS-SP、5 μ m、2.0 \times 150mm				
Mobile phase	A:	0.5mM 酢酸アンモニウム水溶液 (和光純薬工業 超純水 LC/MS用 / 1M酢酸アンモニウム水溶液 = 999.5/ 0.5 , v/v)				
	B:	0.5mM酢酸アンモニウムメタノール溶液 (MERCK社製LiChrosolv hypergrade (LC/MS)/ 1M酢酸アンモニウム水溶液 = 999.5/ 0.5 , v/v)				
Flow rate (μ l/min)		200				
Gradient	Time (min)	0	10	12.5	13	20
	A(%)	95	0	0	95	95
	B(%)	5	100	100	5	5
Column temp.($^{\circ}$ C)		40				
Inj. Volume (μ L)		2				
Mass spectrometry		3200 QTRAP LC/MS/MS システム				
Ion source		Turbo V Ion Spray (ESI)				
Mode		MRM				
Turbo gas temp.($^{\circ}$ C)		350				
Spray voltage (V)		5000				
Polarity		Positive				

Q1	Q3	time	ID	DP	EP	CE	CXP
369.2	149.1	5	Methoxyfenozide 1	51.0	10.0	23	4
369.2	91.1	5	Methoxyfenozide 2	51.0	10.0	65	4

HPLCシステム	SHIMADZU Prominence								
カラム	TOSOH TSKgel ODS-100V 2.0mmI.D.×15cm								
移動相:									
A	5mM酢酸アンモニウム水溶液								
B	5mM酢酸アンモニウムメタノール溶液								
グラジェント	0.0	1.0	3.5	6.0	8.0	17.5	30.0	30.1	43.0
Time [min.]									
A [%]	85	60	60	50	45	5	5	85	85
B [%]	15	40	40	50	55	95	95	15	15
流速 [μL/min]	200								
カラム温度 [°C]	40								
注入量 [μL]	10								
Mass Spectrometry	Applied Biosystems/MDS SCIEX API2000® LC/MS/MS システム								
Ion Source	TurbolonSpray®、(ESI)								
Mode	Scheduled MRM								
Temperature [°C]	350								
Polarity	Positive , Negative								
IonSpray Voltage [V]	5000 , -4500								
Monitoring Time [min.]	30								

Q1	Q3	time	ID	DP	EP	CE	CXP
320	70	50	Metconazole	-	-	-	-

HPLCシステム	SHIMADZU Prominence								
カラム	TOSOH TSKgel ODS-100V 2.0mmI.D.×15cm								
移動相:									
A	5mM酢酸アンモニウム水溶液								
B	5mM酢酸アンモニウムメタノール溶液								
グラジエント									
Time [min.]	0.0	1.0	3.5	6.0	8.0	17.5	30.0	30.1	43.0
A [%]	85	60	60	50	45	5	5	85	85
B [%]	15	40	40	50	55	95	95	15	15
流速 [μ L/min]	200								
カラム温度 [°C]	40								
注入量 [μ L]	10								
Mass Spectrometry	Applied Biosystems/MDS SCIEX API2000® LC/MS/MS システム								
Ion Source	TurbolonSpray®、(ESI)								
Mode	Scheduled MRM								
Temperature [°C]	350								
Polarity	Positive , Negative								
IonSpray Voltage [V]	5000 , -4500								
Monitoring Time [min.]	30								

■分析例 1

【システム】

- ・ LC ACQUITY UPLC I-Class システム(FTN)
- ・ MS Xevo TQ MS タンデム四重極型質量分析計
- ・ ソフトウェア MassLynx 4.1
TargetLynx アプリケーションマネージャ

【LC 条件】

- ・ サンプル温度 10℃
- ・ 注入量 5 uL
- ・ 洗浄溶媒 0.1%-ギ酸 in メタノール
- ・ カラム ACQUITY UPLC HSS C18 1.8 um, 2.1 x 100 mm
- ・ カラム温度 40℃
- ・ 流速 0.4 mL/min
- ・ 移動相 A 5mM-酢酸アンモニウム水溶液
- ・ 移動相 B 5mM-酢酸アンモニウム in MeOH
- ・ グラジエント
- ・ Run Time 17 分

【MS 条件】

MS Tune

- | | ESI ポジティブ | ESI ネガティブ |
|------------|-----------------|----------------|
| ・ イオン化モード | ESI ポジティブ | ESI ネガティブ |
| ・ キャピラリー電圧 | 0.75 kV (ポジティブ) | 0.5 kV (ネガティブ) |
| ・ 脱溶媒ガス | 1000 L/hr 450℃ | |
| ・ イオン源ヒーター | 150℃ | |

Abamectin	890.4	20	305.2	25	ES+
Abamectin	890.4	20	567.2	15	ES+
Acephate	184.1	8	143.0	8	ES+
Acephate	184.1	8	125.1	18	ES+
Acetamiprid	223.0	23	126.0	20	ES+
Acetamiprid	223.0	23	56.1	15	ES+
Acibenzolar_S_methyl	210.8	40	135.7	25	ES+
Acibenzolar_S_methyl	210.8	40	90.7	20	ES+
Acifluorfen	360.1	12	316.1	10	ES-
Acifluorfen	360.1	12	194.8	30	ES-
Alachlor	271.1	19	162.1	20	ES+
Alachlor	271.1	19	238.1	11	ES+
Aldicarb	207.9	10	88.7	15	ES+
Aldicarb	207.9	10	115.7	10	ES+
Allethrin	303.2	15	303.2	2	ES+
Allethrin	303.2	15	90.9	40	ES+
Ametryn	228.1	32	186.1	18	ES+
Ametryn	228.1	32	68.1	36	ES+
Anilofos	368.0	20	198.7	15	ES+
Anilofos	368.0	20	124.6	30	ES+
Atrazine	216.1	29	174.0	18	ES+
Atrazine	216.1	29	96.1	23	ES+
Azaconazole	300.0	25	159.0	28	ES+
Azaconazole	300.0	25	231.1	18	ES+
Azamethiphos	324.9	20	182.7	15	ES+
Azamethiphos	324.9	20	111.6	35	ES+
Azimsulfuron	425.0	26	182.0	20	ES+
Azimsulfuron	425.0	26	139.1	40	ES+
Azinphos_methyl	318.0	10	131.6	15	ES+
Azinphos_methyl	318.0	10	159.7	10	ES+
Azoxystrobin	404.1	20	371.9	15	ES+
Azoxystrobin	404.1	20	328.9	40	ES+
Benalaxyl	326.1	17	148.0	20	ES+
Benalaxyl	326.1	17	91.0	34	ES+
Bendiocarb	223.9	20	166.8	10	ES+
Bendiocarb	223.9	20	108.6	20	ES+
Benfluralin	336.0	25	57.0	18	ES+
Benfluralin	336.0	25	236.0	15	ES+
Benfuracarb	411.1	14	195.0	23	ES+
Benfuracarb	411.1	14	190.0	13	ES+
Bensulfuron_methyl	411.1	27	149.0	22	ES+
Bensulfuron_methyl	411.1	27	182.0	20	ES+
Bentazone	239.0	32	132.0	26	ES-
Bentazone	239.0	32	175.0	22	ES-
Benzofenap	431.0	40	104.6	35	ES+
Benzofenap	431.0	40	118.6	25	ES+
Bifenazate	301.1	7	198.0	10	ES+
Bifenazate	301.1	7	170.0	20	ES+
Bifenox	341.9	7	309.9	10	ES+
Bifenox	341.9	7	188.9	22	ES+
Bitertanol	338.1	12	99.1	16	ES+
Bitertanol	338.1	12	70.1	8	ES+
Bromacil	261.0	18	204.9	14	ES+
Bromacil	261.0	18	187.9	28	ES+
Bromoxynil	275.7	40	78.8	30	ES-
Bromoxynil	275.7	40	80.8	30	ES-
Bupirimate	317.0	31	166.0	28	ES+
Bupirimate	317.0	31	108.0	28	ES+
Buprofezin	306.1	22	201.0	12	ES+
Buprofezin	306.1	22	57.4	20	ES+

Butachlor	312.2	17	238.2	12	ES+
Butachlor	312.2	17	57.3	22	ES+
Butylate	218.1	19	57.2	17	ES+
Butylate	218.1	19	156.1	10	ES+
Carbaryl	201.9	20	144.7	10	ES+
Carbaryl	201.9	20	126.6	25	ES+
Carbendazim	192.1	24	160.1	18	ES+
Carbendazim	192.1	24	132.1	28	ES+
Carbetamide	237.0	11	192.0	9	ES+
Carbetamide	237.0	11	118.0	14	ES+
Carbofuran	221.9	20	164.8	15	ES+
Carbofuran	221.9	20	122.6	25	ES+
Carbosulfan	381.0	31	118.0	22	ES+
Carbosulfan	381.0	31	76.0	34	ES+
Carfentrazone-ethyl	412.0	29	346.0	24	ES+
Carfentrazone-ethyl	412.0	29	266.0	18	ES+
Carpropamid	334.0	20	138.6	25	ES+
Carpropamid	334.0	20	195.7	15	ES+
Chlorfenapyr	406.2	34	251.0	22	ES+
Chlorfenapyr	406.2	34	152.0	60	ES+
Chlorfenvinphos	358.9	18	155.0	12	ES+
Chlorfenvinphos	358.9	18	99.0	30	ES+
Chloridazon	221.9	40	91.6	25	ES+
Chloridazon	221.9	40	103.6	25	ES+
Chlorpropham	214.1	9	172.0	8	ES+
Chlorpropham	214.1	9	154.0	18	ES+
Chlorpyrifos	349.9	27	97.0	32	ES+
Chlorpyrifos	349.9	27	198.0	20	ES+
Chlorpyrifos-methyl	321.8	23	125.0	20	ES+
Chlorpyrifos-methyl	321.8	23	289.9	16	ES+
Chromafenozide	395.2	20	174.8	15	ES+
Chromafenozide	395.2	20	146.7	45	ES+
Clethodim	360.0	23	164.0	18	ES+
Clethodim	360.0	23	268.1	12	ES+
Clodinafop-propargyl	350.0	25	266.0	16	ES+
Clodinafop-propargyl	350.0	25	91.0	32	ES+
Clofentezine	303.0	20	137.9	15	ES+
Clofentezine	303.0	20	101.9	30	ES+
Clomazone	240.0	23	125.0	18	ES+
Clomazone	240.0	23	89.0	46	ES+
Clomeprop	324.0	30	119.6	25	ES+
Clomeprop	324.0	30	148.6	20	ES+
Cloprop_ES-	198.8	17	126.8	12	ES-
Cloprop_ES-	198.8	17	70.7	12	ES-
Cloransulam_methyl	430.1	27	398.1	15	ES+
Cloransulam_methyl	430.1	27	153.0	40	ES+
Clothianidin	249.9	20	131.6	20	ES+
Clothianidin	249.9	20	168.7	20	ES+
Cumyluron	303.1	25	184.9	15	ES+
Cumyluron	303.1	25	124.9	30	ES+
Cyanofenphos	304.0	25	157.0	22	ES+
Cyanofenphos	304.0	25	276.0	12	ES+
Cyazofamid	324.9	20	107.9	15	ES+
Cyazofamid	324.9	20	217.0	25	ES+
Cyclanilide	271.9	20	159.8	20	ES-
Cyclanilide	271.9	20	227.8	15	ES-
Cycloprothrin	499.0	20	181.0	30	ES+
Cycloprothrin	499.0	20	245.0	15	ES+
Cyclosulfamuron	422.2	37	261.1	15	ES+
Cyclosulfamuron	422.2	37	218.1	30	ES+

Cyflufenamid	413.0	30	240.8	25	ES+
Cyflufenamid	413.0	30	294.8	20	ES+
Cyproconazole	292.2	27	70.2	18	ES+
Cyproconazole	292.2	27	125.1	24	ES+
Cyprodinil	226.0	40	92.7	35	ES+
Cyprodinil	226.0	40	107.7	35	ES+
Daimuron	269.0	20	151.0	10	ES+
Daimuron	269.0	20	91.0	40	ES+
Deltamethrin	505.9	19	280.9	12	ES+
Deltamethrin	505.9	19	93.2	46	ES+
Desmedipham	301.0	25	136.0	22	ES+
Desmedipham	301.0	25	182.0	10	ES+
Dichlofluanid	333.0	19	123.0	24	ES+
Dichlofluanid	333.0	19	224.0	10	ES+
Dichlorprop	232.8	20	160.8	15	ES-
Dichlorprop	232.8	20	124.8	30	ES-
Dichlorvos	221.0	23	109.0	22	ES+
Dichlorvos	221.0	23	79.0	34	ES+
Diclobutrazol	328.0	25	70.0	20	ES+
Diclobutrazol	328.0	25	158.9	38	ES+
Diclomezine	255.0	49	140.8	30	ES+
Diclomezine	255.0	49	79.8	30	ES+
Diclosulam	406.1	37	161.0	30	ES+
Diclosulam	406.1	37	378.0	15	ES+
Diethofencarb	268.0	19	226.0	10	ES+
Diethofencarb	268.0	19	124.0	40	ES+
Difenoconazole	406.0	37	251.1	25	ES+
Difenoconazole	406.0	37	111.1	60	ES+
Dimepiperate	264.1	8	146.0	10	ES+
Dimepiperate	264.1	8	119.0	16	ES+
Dimethametryn	256.1	35	186.1	20	ES+
Dimethametryn	256.1	35	71.0	32	ES+
Dimethenamid	276.0	17	244.0	14	ES+
Dimethenamid	276.0	17	168.0	26	ES+
Dimethirimol	210.0	40	70.7	30	ES+
Dimethirimol	210.0	40	97.6	30	ES+
Dimethoate	230.1	12	199.0	10	ES+
Dimethoate	230.1	12	125.0	20	ES+
Dimethomorph_E	388.0	30	300.9	20	ES+
Dimethomorph_E	388.0	30	164.7	45	ES+
Dimethomorph_Z	388.0	30	300.9	20	ES+
Dimethomorph_Z	388.0	30	164.7	45	ES+
Dinotefuran	203.0	12	129.0	12	ES+
Dinotefuran	203.0	12	157.0	8	ES+
Disulfoton	274.9	14	89.0	20	ES+
Disulfoton	274.9	14	61.1	35	ES+
Dithiopyr	402.0	32	354.1	18	ES+
Dithiopyr	402.0	32	248.1	34	ES+
Edifenphos	311.0	23	109.0	32	ES+
Edifenphos	311.0	23	111.0	26	ES+
EPN	324.0	22	296.0	14	ES+
EPN	324.0	22	157.0	25	ES+
Epoxiconazole	330.0	30	120.6	25	ES+
Epoxiconazole	330.0	30	122.6	20	ES+
EPTC	190.0	17	128.1	11	ES+
EPTC	190.0	17	86.0	15	ES+
Esprocarb	266.1	21	91.0	22	ES+
Esprocarb	266.1	21	71.0	16	ES+
Ethiofencarb	226.1	16	107.0	17	ES+
Ethiofencarb	226.1	16	164.0	8	ES+

Ethiprole	414.1	12	396.9	9	ES+
Ethiprole	414.1	12	350.9	25	ES+
Ethofumesate	287.1	27	121.1	15	ES+
Ethofumesate	287.1	27	259.1	10	ES+
Ethoprophos	243.2	18	131.0	20	ES+
Ethoprophos	243.2	18	97.0	31	ES+
Ethoxyquin	218.2	37	148.1	22	ES+
Ethoxyquin	218.2	37	160.1	32	ES+
Ethoxysulfuron	398.9	25	261.0	16	ES+
Ethoxysulfuron	398.9	25	218.0	24	ES+
Etofenprox	394.3	17	177.0	15	ES+
Etofenprox	394.3	17	106.9	43	ES+
Etrimfos	293.1	29	125.0	26	ES+
Etrimfos	293.1	29	265.1	16	ES+
Famoxadone	392.2	12	331.1	10	ES+
Famoxadone	392.2	12	238.0	20	ES+
Fenamidone	312.0	20	91.6	25	ES+
Fenamidone	312.0	20	235.9	20	ES+
Fenamiphos	304.1	27	217.1	24	ES+
Fenamiphos	304.1	27	202.1	36	ES+
Fenarimol	331.0	37	268.0	22	ES+
Fenarimol	331.0	37	81.0	34	ES+
Fenbuconazole	337.0	29	125.0	36	ES+
Fenbuconazole	337.0	29	70.1	20	ES+
Fenitrothion	278.0	29	109.1	20	ES+
Fenitrothion	278.0	29	79.1	34	ES+
Fenobucarb	207.9	20	94.6	15	ES+
Fenobucarb	207.9	20	151.7	10	ES+
Fenoxaprop_ethyl	362.0	30	287.9	20	ES+
Fenoxaprop_ethyl	362.0	30	120.6	40	ES+
Fenoxycarb	302.0	20	87.6	25	ES+
Fenoxycarb	302.0	20	115.7	10	ES+
Fenpropathrin	350.1	15	125.0	14	ES+
Fenpropathrin	350.1	15	97.0	34	ES+
Fenpropimorph	304.2	41	147.1	28	ES+
Fenpropimorph	304.2	41	57.2	30	ES+
Fenpyroximate	422.1	30	365.9	20	ES+
Fenpyroximate	422.1	30	134.6	45	ES+
Fensulfothion	309.0	25	157.1	25	ES+
Fensulfothion	309.0	25	173.1	22	ES+
Fenthion	279.1	25	169.1	16	ES+
Fenthion	279.1	25	247.1	13	ES+
Ferimzone	255.0	40	90.7	35	ES+
Ferimzone	255.0	40	131.6	25	ES+
Flamprop-methyl	336.0	13	105.0	16	ES+
Flamprop-methyl	336.0	13	77.0	48	ES+
Florasulam	360.0	29	129.0	22	ES+
Florasulam	360.0	29	108.9	50	ES+
Fluazinam	464.8	23	373.0	26	ES+
Fluazinam	464.8	23	338.1	47	ES+
Fludioxonil	249.1	7	229.1	10	ES+
Fludioxonil	249.1	7	158.1	28	ES+
Flufenoxuron	489.0	30	157.9	30	ES+
Flufenoxuron	489.0	30	140.9	40	ES+
Flumetsulam	326.1	37	129.0	25	ES+
Flumetsulam	326.1	37	109.0	50	ES+
Flumioxazin	355.0	37	298.0	28	ES+
Flumioxazin	355.0	37	326.0	22	ES+
Fluridone	330.0	40	309.1	35	ES+
Fluridone	330.0	40	259.0	40	ES+

Fluroxypyr	254.9	19	208.8	16	ES+
Fluroxypyr	254.9	19	180.8	22	ES+
Flusilazole	316.0	27	247.0	18	ES+
Flusilazole	316.0	27	165.0	28	ES+
Flutolanil	324.1	23	262.1	18	ES+
Flutolanil	324.1	23	65.0	40	ES+
Flutriafol	302.1	23	70.2	18	ES+
Flutriafol	302.1	23	123.1	29	ES+
Fluvalinate	503.0	15	181.1	30	ES+
Fluvalinate	503.0	15	208.1	12	ES+
Fomesafen	437.0	50	221.9	30	ES-
Fomesafen	437.0	50	194.8	30	ES-
Fonofos	247.1	15	109.0	20	ES+
Fonofos	247.1	15	137.0	10	ES+
Forchlorfenuron	248.1	25	129.0	15	ES+
Forchlorfenuron	248.1	25	93.0	35	ES+
Fosthiazate	284.0	19	104.0	22	ES+
Fosthiazate	284.0	19	228.0	10	ES+
Furametpyr	334.0	30	156.7	30	ES+
Furametpyr	334.0	30	289.9	25	ES+
Furathiocarb	383.1	30	194.7	20	ES+
Furathiocarb	383.1	30	251.9	15	ES+
Gibberellic_acid	345.1	28	238.9	14	ES-
Gibberellic_acid	345.1	28	142.8	24	ES-
Haloxifop	362.0	27	315.8	18	ES+
Haloxifop	362.0	27	91.0	30	ES+
Hexaconazole	314.0	31	70.1	22	ES+
Hexaconazole	314.0	31	159.0	28	ES+
Hexaflumuron	459.0	26	439.0	12	ES-
Hexaflumuron	459.0	26	174.8	48	ES-
Hexazinone	253.1	23	171.1	16	ES+
Hexazinone	253.1	23	71.0	30	ES+
Hexythiazox	353.1	20	227.9	15	ES+
Hexythiazox	353.1	20	167.8	25	ES+
Imazalil	297.0	30	158.6	25	ES+
Imazalil	297.0	30	68.7	20	ES+
Imazapyr	262.2	27	69.2	26	ES+
Imazapyr	262.2	27	86.1	26	ES+
Imazaquin	312.2	29	267.2	20	ES+
Imazaquin	312.2	29	86.2	28	ES+
Imidacloprid	256.0	20	174.8	20	ES+
Imidacloprid	256.0	20	208.8	20	ES+
Indanofan	341.1	22	174.9	14	ES+
Indanofan	341.1	22	186.9	12	ES+
Indoxacarb	527.9	30	149.8	35	ES+
Indoxacarb	527.9	30	217.8	30	ES+
Ioxynil_ES-	369.7	31	126.8	26	ES-
Ioxynil_ES-	369.7	31	214.9	26	ES-
Iprobenphos	289.0	9	91.0	20	ES+
Iprobenphos	289.0	9	205.0	10	ES+
Iprovalicarb	321.2	20	118.7	20	ES+
Iprovalicarb	321.2	20	202.9	10	ES+
Isazophos	314.0	17	162.1	16	ES+
Isazophos	314.0	17	120.0	28	ES+
Isocarbofos	291.1	12	231.1	13	ES+
Isocarbofos	291.1	12	121.1	30	ES+
Isoprothiolane	291.1	17	188.8	22	ES+
Isoprothiolane	291.1	17	230.9	12	ES+
Isoxaflutole	360.0	30	251.0	15	ES+
Isoxaflutole	360.0	30	220.0	40	ES+

Isoxathion	314.1	22	104.9	14	ES+
Isoxathion	314.1	22	96.9	35	ES+
Kresoxim-methyl	314.1	15	206.0	7	ES+
Kresoxim-methyl	314.1	15	116.0	12	ES+
Lenacil	235.2	18	153.1	16	ES+
Lenacil	235.2	18	136.1	32	ES+
Linuron	248.9	30	159.7	20	ES+
Linuron	248.9	30	181.8	15	ES+
Lufenuron	509.0	26	326.0	20	ES-
Lufenuron	509.0	26	174.8	36	ES-
Malathion	331.0	12	99.0	24	ES+
Malathion	331.0	12	127.0	12	ES+
Mecarbam	330.0	12	227.1	8	ES+
Mecarbam	330.0	12	97.0	35	ES+
Mecoprop	213.0	17	141.0	19	ES-
Mecoprop	213.0	17	71.0	12	ES-
Mefenacet	299.0	16	148.0	15	ES+
Mefenacet	299.0	16	120.0	25	ES+
Mepanipyrim	224.0	40	76.7	40	ES+
Mepanipyrim	224.0	40	105.7	30	ES+
Mepronil	270.1	27	119.0	28	ES+
Mepronil	270.1	27	91.0	44	ES+
Metalaxyl	280.1	15	220.1	13	ES+
Metalaxyl	280.1	15	192.1	17	ES+
Metamitron	203.1	28	175.1	16	ES+
Metamitron	203.1	28	104.0	22	ES+
Methabenzthiazuron	221.9	20	164.7	20	ES+
Methabenzthiazuron	221.9	20	149.7	35	ES+
Methamidophos	142.0	17	93.9	13	ES+
Methamidophos	142.0	17	124.9	13	ES+
Methidathion	303.0	10	145.0	10	ES+
Methidathion	303.0	10	85.1	20	ES+
Methiocarb	225.9	20	168.8	10	ES+
Methiocarb	225.9	20	120.7	20	ES+
Methomyl	162.7	10	87.6	10	ES+
Methomyl	162.7	10	105.6	10	ES+
Methoxyfenozide	369.1	20	148.7	20	ES+
Methoxyfenozide	369.1	20	313.0	10	ES+
Metolcarb	166.0	11	109.0	12	ES+
Metolcarb	166.0	11	94.1	27	ES+
Mevinphos	225.1	13	127.1	15	ES+
Mevinphos	225.1	13	193.1	8	ES+
Milbemectin_A3	546.2	10	511.1	10	ES+
Milbemectin_A3	546.2	10	112.7	15	ES+
Milbemectin_A4	525.2	25	109.0	20	ES+
Milbemectin_A4	525.2	25	160.9	25	ES+
Molinate	188.0	17	126.0	13	ES+
Molinate	188.0	17	55.0	24	ES+
Monocrotophos	224.1	15	127.1	16	ES+
Monocrotophos	224.1	15	98.1	12	ES+
Napropamide	272.1	21	129.1	16	ES+
Napropamide	272.1	21	171.1	18	ES+
Nitenpyram	271.1	22	125.9	25	ES+
Nitenpyram	271.1	22	224.9	12	ES+
Novaluron	493.0	30	157.7	20	ES+
Novaluron	493.0	30	140.6	45	ES+
Omethoate	214.1	16	125.1	22	ES+
Omethoate	214.1	16	183.1	11	ES+
Oryzalin	345.2	40	281.1	20	ES-
Oryzalin	345.2	40	77.5	35	ES-

Oxadixyl	279.0	31	219.0	10	ES+
Oxadixyl	279.0	31	132.0	34	ES+
Oxamyl	236.9	10	71.6	15	ES+
Oxamyl	236.9	10	89.6	10	ES+
Oxaziclomefone	376.0	20	189.8	15	ES+
Oxaziclomefone	376.0	20	160.7	30	ES+
Oxycarboxine	268.0	25	174.9	15	ES+
Oxycarboxine	268.0	25	146.9	25	ES+
Oxydemeton-methyl	247.0	18	168.8	14	ES+
Oxydemeton-methyl	247.0	18	108.9	25	ES+
Paclobutrazol	294.1	27	70.2	20	ES+
Paclobutrazol	294.1	27	125.1	38	ES+
Parathion	291.9	25	236.0	14	ES+
Parathion	291.9	25	110.0	33	ES+
Parathion-methyl	263.9	29	109.0	22	ES+
Parathion-methyl	263.9	29	79.0	36	ES+
Penconazole	284.0	25	70.1	16	ES+
Penconazole	284.0	25	159.0	34	ES+
Pencycuron	329.1	40	124.6	20	ES+
Pencycuron	329.1	40	217.9	15	ES+
Pendimethalin	282.2	12	212.2	10	ES+
Pendimethalin	282.2	12	194.1	17	ES+
Pentoxazone	371.0	10	285.7	15	ES+
Pentoxazone	371.0	10	185.6	35	ES+
Phenmedipham	318.0	20	167.7	15	ES+
Phenmedipham	318.0	20	135.6	30	ES+
Phorate	261.0	10	75.0	12	ES+
Phorate	261.0	10	97.0	32	ES+
Phosalone	367.9	12	181.9	14	ES+
Phosalone	367.9	12	110.9	42	ES+
Phosmet	318.0	19	160.0	22	ES+
Phosmet	318.0	19	77.0	46	ES+
Phosphamidon	300.1	17	174.1	14	ES+
Phosphamidon	300.1	17	127.1	25	ES+
Phoxim	299.0	12	129.0	13	ES+
Phoxim	299.0	12	153.0	7	ES+
Picolinafen	377.0	29	238.0	28	ES+
Picolinafen	377.0	29	359.0	21	ES+
Piperonyl butoxide	356.3	17	176.9	11	ES+
Piperonyl butoxide	356.3	17	119.0	37	ES+
Piperophos	354.1	22	171.0	22	ES+
Piperophos	354.1	22	143.0	32	ES+
Pirimicarb	239.0	30	71.6	20	ES+
Pirimicarb	239.0	30	181.8	20	ES+
Pirimiphos-methyl	306.1	25	164.1	22	ES+
Pirimiphos-methyl	306.1	25	108.1	32	ES+
Probenazole	224.0	13	196.1	13	ES+
Probenazole	224.0	13	41.5	10	ES+
Procloraz	376.0	13	70.1	34	ES+
Procloraz	376.0	13	307.1	16	ES+
Procymidone	284.1	33	67.1	28	ES+
Procymidone	284.1	33	256.1	17	ES+
Profenofos	372.9	25	302.6	20	ES+
Profenofos	372.9	25	127.9	40	ES+
Promecarb	208.1	17	151.0	9	ES+
Promecarb	208.1	17	109.0	15	ES+
Prometryn	242.0	27	158.0	24	ES+
Prometryn	242.0	27	200.1	17	ES+
Propachlor	212.1	22	170.1	14	ES+
Propachlor	212.1	22	94.1	25	ES+

Propamocarb	189.1	22	102.0	17	ES+
Propamocarb	189.1	22	144.0	12	ES+
Propanil	217.9	31	161.9	16	ES+
Propanil	217.9	31	127.0	22	ES+
Propazine	230.2	29	146.1	24	ES+
Propazine	230.2	29	188.1	18	ES+
Propetamphos	282.0	10	156.0	12	ES+
Propetamphos	282.0	10	138.0	20	ES+
Propham	180.0	5	138.0	8	ES+
Propham	180.0	5	120.0	16	ES+
Propiconazole	342.0	37	159.0	34	ES+
Propiconazole	342.0	37	69.0	22	ES+
Propoxur	210.0	12	111.0	16	ES+
Propoxur	210.0	12	168.0	10	ES+
Propoxycarbazone_sodium	399.0	17	199.0	19	ES+
Propoxycarbazone_sodium	399.0	17	116.0	32	ES+
Propyzamide	256.1	22	190.0	16	ES+
Propyzamide	256.1	22	173.0	23	ES+
Pyrazolynate	439.1	50	91.0	42	ES+
Pyrazolynate	439.1	50	172.9	20	ES+
Pyrazophos	374.0	33	222.1	22	ES+
Pyrazophos	374.0	33	194.0	32	ES+
Pyrazosulfuron_ethyl	415.0	22	182.0	20	ES+
Pyrazosulfuron_ethyl	415.0	22	82.9	45	ES+
Pyridaben	365.1	19	147.1	24	ES+
Pyridaben	365.1	19	309.1	12	ES+
Pyridaphenthion	341.0	31	189.0	22	ES+
Pyridaphenthion	341.0	31	92.0	34	ES+
Pyrifenox	295.0	29	93.1	22	ES+
Pyrifenox	295.0	29	67.2	60	ES+
Pyriproxifen	322.1	23	96.0	14	ES+
Pyriproxifen	322.1	23	227.1	14	ES+
Pyroquilon	174.0	32	132.0	23	ES+
Pyroquilon	174.0	32	117.0	30	ES+
Quinalphos	299.0	15	162.9	24	ES+
Quinalphos	299.0	15	96.9	30	ES+
Quinoxyfen	308.0	52	197.0	32	ES+
Quinoxyfen	308.0	52	161.9	44	ES+
Quizalofop_ethyl	373.0	30	298.8	25	ES+
Quizalofop_ethyl	373.0	30	90.6	35	ES+
Sethoxydim	328.0	25	178.0	22	ES+
Sethoxydim	328.0	25	282.0	10	ES+
Silafluofen	426.1	10	287.1	10	ES+
Silafluofen	426.1	10	168.0	35	ES+
Simazine	202.0	32	124.0	17	ES+
Simazine	202.0	32	96.0	22	ES+
Simeconazole	294.0	30	69.6	20	ES+
Simeconazole	294.0	30	72.6	30	ES+
Spinocyn_A	732.3	40	141.7	40	ES+
Spinocyn_A	732.3	40	97.9	45	ES+
Spinocyn_D	746.3	40	141.8	45	ES+
Spinocyn_D	746.3	40	97.8	45	ES+
Spirodiclofen	411.1	22	313.0	13	ES+
Spirodiclofen	411.1	22	71.2	13	ES+
Spiroxamine	298.0	27	144.0	20	ES+
Spiroxamine	298.0	27	100.0	32	ES+
Tebuconazole	308.0	31	70.1	22	ES+
Tebuconazole	308.0	31	125.0	40	ES+
Tebufenozide	353.1	10	297.0	10	ES+
Tebufenozide	353.1	10	132.7	20	ES+

Tebufenpyrad	334.0	43	117.0	34	ES+
Tebufenpyrad	334.0	43	145.0	28	ES+
Teflubenzuron	380.9	30	157.9	15	ES+
Teflubenzuron	380.9	30	140.9	30	ES+
Tepraloxymid	342.1	17	250.1	12	ES+
Tepraloxymid	342.1	17	166.1	20	ES+
Terbufos	289.0	12	103.0	8	ES+
Terbufos	289.0	12	57.2	22	ES+
Terbutryn	242.1	28	186.1	19	ES+
Terbutryn	242.1	28	91.0	28	ES+
Tetrachlorvinphos	366.8	30	126.5	15	ES+
Tetrachlorvinphos	366.8	30	240.7	25	ES+
Tetraconazole	372.0	32	159.0	30	ES+
Tetraconazole	372.0	32	70.1	20	ES+
Thiabendazole	201.8	40	174.7	30	ES+
Thiabendazole	201.8	40	130.6	35	ES+
Thiacloprid	252.9	30	125.6	20	ES+
Thiacloprid	252.9	30	89.6	35	ES+
Thiamethoxam	291.9	20	210.8	15	ES+
Thiamethoxam	291.9	20	131.5	25	ES+
Thiazopyr	397.1	27	377.1	23	ES+
Thiazopyr	397.1	27	317.1	25	ES+
Thidiazuron	221.0	28	101.9	15	ES+
Thidiazuron	221.0	28	93.9	13	ES+
Thiodicarb	354.9	20	87.6	20	ES+
Thiodicarb	354.9	20	107.6	15	ES+
Thiophanate-methyl	343.0	19	151.0	22	ES+
Thiophanate-methyl	343.0	19	93.0	46	ES+
Tralkoxydime	330.0	20	284.0	15	ES+
Tralkoxydime	330.0	20	138.0	20	ES+
Triadimefon	294.1	22	197.2	15	ES+
Triadimefon	294.1	22	69.3	20	ES+
Triadimenol	296.1	12	70.2	10	ES+
Triadimenol	296.1	12	99.1	15	ES+
Triallate	304.0	23	86.0	18	ES+
Triallate	304.0	23	142.9	28	ES+
Triazophos	314.1	22	161.9	18	ES+
Triazophos	314.1	22	118.9	35	ES+
Trichlorfon	257.0	22	109.0	17	ES+
Trichlorfon	257.0	22	79.0	30	ES+
Tricyclazole	190.0	32	163.0	22	ES+
Tricyclazole	190.0	32	136.0	27	ES+
Tridemorph	298.3	50	129.7	25	ES+
Tridemorph	298.3	50	97.7	30	ES+
Trifloxystrobin	409.0	25	186.0	16	ES+
Trifloxystrobin	409.0	25	145.0	40	ES+
Triflumizole	346.0	13	277.9	10	ES+
Triflumizole	346.0	13	60.0	10	ES+
Triflumuron	359.0	20	155.7	15	ES+
Triflumuron	359.0	20	138.7	30	ES+
Triticonazole	318.1	20	69.7	20	ES+
Triticonazole	318.1	20	124.5	45	ES+
Vamidothion	288.0	17	146.0	10	ES+
Vamidothion	288.0	17	118.0	28	ES+
Zoxamide	336.0	27	187.1	25	ES+
Zoxamide	336.0	27	159.0	38	ES+

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
3,4,5-Trimethacarb	2655-15-4	37874	Insecticide		C ₁₁ H ₁₅ NO ₂	193.1103	194.1	22	137.1	12	122.1	26	5.41	12	
Abamectin (B1a)	71751-41-2	46392	Insecticide/Acaricide				890.7	24	305.1	22	567.2	10	7.82		
Acephate	30560-19-1	45315	Insecticide		C ₄ H ₁₀ NO ₃ PS	183.0119	184.1	17	143.0	8	125.1	18	1.47	1	
Acetamiprid	135410-20-7	33674	Insecticide		C ₁₀ H ₁₁ ClN ₄	222.0672	223.0	34	126.0	20	56.1	15	3.41	4	
Acibenzolar-S-methyl	135158-54-2		Fungicide		C ₈ H ₆ N ₂ OS ₂	209.9922	210.9	50	135.9	30	69.0	52	5.78		14
Acitidone	66-81-9	46401	Fungicide	Cycloheximid	C ₁₅ H ₂₃ NO ₄	281.1627	282.1	26	264.1	11	246.1	14	4.28		5
Aclonifen	74070-46-5	36792	Herbicide		C ₁₂ H ₉ ClN ₂ O ₃	264.0302	265.0	30	248.0	18	182.1	32	6.51		
Acrinathrin	101007-06-1	46415	Insecticide/Acaricide		C ₂₆ H ₂₁ F ₆ NO ₅	541.1324	542.0	24	181.0	36	208.0	12	no		
Alachlor	15972-60-8	45316	Herbicide		C ₁₄ H ₂₀ ClNO ₂	269.1183	271.1	28	162.1	20	238.1	11	6.30		
Aldicarb	116-06-3	33386	Insecticide/Acaricide		C ₇ H ₁₄ N ₂ O ₂ S	190.0776	213.1	30	89.1	16	116.1	11	3.98	5	
Aldicarb sulfone	1646-88-4	33387	Metabolite	Aldoxycarb	C ₇ H ₁₄ N ₂ O ₄ S	222.0674	223.0	31	148.0	10	86.0	14	2.04	2	
Aldicarb sulfoxide	1646-87-3	36784	Metabolite		C ₇ H ₁₄ N ₂ O ₃ S	206.0725	207.0	22	89.0	14	132.0	10	1.91	2	
Ametryn	834-12-8	45321	Herbicide		C ₉ H ₁₇ N ₅ S	227.1205	228.1	38	186.1	18	68.1	36	4.88		8
Amidosulfuron	120923-37-7	33588	Herbicide		C ₉ H ₁₅ N ₅ O ₇ S ₂	369.0413	370.0	28	261.0	15	218.0	25	4.95		9
Aminocarb	2032-59-9	45322	Insecticide		C ₁₁ H ₁₆ N ₂ O ₂	208.1212	209.0	30	137.0	22	152.0	14	1.63		1
Amitraz	33089-61-1	45323	Acaricide		C ₁₉ H ₂₃ N ₃	293.1892	294.0	31	122.0	35	163.0	18	no		
Amitrole	61-82-5	45324	Herbicide		C ₂ H ₄ N ₄	84.0436	85.1	38	57.3	12	43.4	15	0.53	1	
Anilazine	101-05-3	45325	Fungicide		C ₉ H ₅ Cl ₃ N ₄	273.9580	274.9	46	153.0	26	178.0	24	5.98	16	
Anilofos	64249-01-0	37876	Herbicide		C ₁₃ H ₁₉ ClNO ₃ PS ₂	367.0233	367.9	30	124.9	34	198.9	15	6.57		21
Asulam	3337-71-1	45329	Herbicide		C ₈ H ₁₀ N ₂ O ₄ S	230.0361	230.9	22	155.9	12	92.0	22	1.82		1
Atraton	1610-17-9	36630	Herbicide	Atrazine-methoxy	C ₉ H ₁₇ N ₅ O	211.1433	212.0	40	170.1	18	100.0	28	3.96		4
Atrazine	1912-24-9	45330	Herbicide		C ₈ H ₁₄ ClN ₅	215.0938	216.1	39	174.1	18	96.1	23	5.20		10
Atrazine-desethyl	6190-65-4	36629	Metabolite		C ₆ H ₁₀ ClN ₅	187.0625	188.0	34	146.0	16	78.9	26	3.69		4
Atrazine-desisopropyl	1007-28-9	36628	Metabolite		C ₅ H ₈ ClN ₅	173.0468	174.0	40	96.0	18	78.9	18	2.85		2
Azaconazole	60207-31-0	34045	Fungicides		C ₁₂ H ₁₁ Cl ₂ N ₃ O ₂	299.0228	300.0	34	159.0	28	231.1	18	5.44	12	
Azafenidin	68049-83-2		Herbicide		C ₁₅ H ₁₃ Cl ₂ N ₃ O ₂	337.0385	338.1	56	264.1	29	299.1	20			
Azamethiphos	35575-96-3	45331	Insecticide		C ₉ H ₁₀ ClN ₂ O ₅ PS	323.9737	325.0	31	111.9	35	138.9	24	4.48	6	
Azimsulfuron	120162-55-2		Herbicide		C ₁₃ H ₁₆ N ₁₀ O ₅ S	424.1026	425.0	41	182.0	20	139.1	40			
Azinphos-ethyl	2642-71-9	45332	Insecticide/Acaricide		C ₁₂ H ₁₆ N ₃ O ₃ PS ₂	345.0371	346.0	16	132.0	16	77.1	36	6.20	18	
Azinphos-methyl	86-50-0	45333	Insecticide/Acaricide		C ₁₀ H ₁₂ N ₃ O ₃ PS ₂	317.0058	318.0	20	160.0	8	261.0	8	5.56	13	
Aziprotryne	4658-28-0	45334	Herbicide		C ₇ H ₁₁ N ₇ S	225.0797	226.0	26	156.0	16	68.0	30	5.95		15
Azobenzene	103-33-3	36689	Acaricide		C ₁₂ H ₁₀ N ₂	182.0844	183.0	32	76.9	18	51.0	40	5.36		11
Azoxystrobin	131860-33-8	46160	Fungicide		C ₂₂ H ₁₇ N ₃ O ₅	403.1168	404.0	28	372.0	15	329.0	30	5.73	14	
Benalaxyl	71626-11-4	36760	Fungicide		C ₂₀ H ₂₃ NO ₃	325.1678	326.1	26	148.0	20	91.0	34	6.62		21
Benazolin	3813-05-06	33380	Herbicide		C ₉ H ₆ ClNO ₃ S	242.9757	243.9	22	170.0	20	197.9	12	4.53	7	
Bendiocarb	22781-23-3	45336	Insecticide		C ₁₁ H ₁₃ NO ₄	223.0845	224.1	26	167.0	8	109.0	18	4.62	8	
Benfluralin	1861-40-1	45337	Herbicide		C ₁₃ H ₁₆ F ₃ N ₃ O ₄	335.1093	336.0	34	57.0	18	236.0	15	no		
Benfuracarb	82560-54-1	45759	Insecticide		C ₂₀ H ₃₀ N ₂ O ₅ S	410.1875	411.1	23	195.0	23	190.0	13	7.07		24
Benfuresate	68505-69-1	46088	Herbicide		C ₁₂ H ₁₆ O ₄ S	256.0769	257.0	28	163.0	12	121.0	22	5.43	12	
Benomyl	17804-35-2	45339	Fungicide		C ₁₄ H ₁₈ N ₄ O ₃	290.1379	291.0	22	160.0	28	192.0	16	5.50		
Bensulfuron methyl	83055-99-6	37897	Herbicide		C ₁₆ H ₁₈ N ₄ O ₇ S	410.0896	411.1	33	149.0	22	182.0	20	5.58	13	
Bensulide	741-58-2	45340	Herbicide		C ₁₄ H ₂₄ NO ₄ PS ₃	397.0605	398.0	18	157.9	24	313.9	10	6.44		19
Bentazone	25057-89-0	45341	Herbicide		C ₁₀ H ₁₂ N ₂ O ₃ S	240.0569	241.1	21	199.1	12	107.2	26	4.72		8
Benzofenap	82692-44-2		Herbicide		C ₂₂ H ₂₀ Cl ₂ N ₂ O ₃	430.0851	431.1	46	119.0	20	105.0	28			
Benzoximate	29104-30-1	33397	Acaricide		C ₁₈ H ₁₈ ClNO ₅	363.0874	364.0	18	199.1	8	105.0	26	6.77		22
Benzthiazuron	1929-88-0	36563	Herbicide		C ₉ H ₉ N ₃ OS	207.0466	208.0	28	151.0	16	109.0	36	4.61		7
Bifenazate	149877-41-8		Acaricide		C ₁₇ H ₂₀ N ₂ O ₃	300.1474	301.1	16	198.0	10	170.0	20	6.13	17	
Bifenox	42576-02-3	45345	Herbicide		C ₁₄ H ₉ Cl ₂ NO ₅	340.9858	341.9	16	309.9	10	188.9	22	no		
Bitertanol	55179-31-2	45349	Fungicide		C ₂₀ H ₂₃ N ₃ O ₂	337.1790	338.1	21	70.1	8	99.1	16	6.77		22

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Boscalid	188425-85-6	33875	Fungicide	Nicobifen	$C_{18}H_{12}Cl_2N_2O$	342.0327	342.9	41	307.0	20	139.9	20	5.90	15	
Bromacil	314-40-9	45350	Herbicide		$C_9H_{13}BrN_2O_2$	260.0160	261.0	22	204.9	14	187.9	28	4.58		7
Bromuconazole	116255-48-2	46094	Fungicide		$C_{13}H_{12}BrCl_2N_3O$	374.9541	376.0	41	158.9	35	70.1	25	6.10	17	
Bupirimate	41483-43-6	45360	Fungicide		$C_{13}H_{24}N_4O_3S$	316.1569	317.0	40	166.0	28	108.0	28	5.88	15	
Buprofezin	69327-76-0	37886	Insecticide		$C_{16}H_{23}N_3OS$	305.1562	306.1	31	201.0	12	57.4	20	6.96	24	
Butachlor	23184-66-9	37887	Herbicide		$C_{17}H_{26}ClNO_2$	311.1652	312.2	26	57.3	22	238.2	12	7.17		
Butocarboxim	34681-10-2	36121	Insecticide		$C_7H_{14}N_2O_2S$	190.0776	213.0	30	75.0	15	156.0	10	3.98		5
Butocarboxim sulfoxide	34681-24-8	45719	Fungicide		$C_7H_{14}N_2O_3S$	206.0725	207.0	23	74.9	12	132.0	6	1.83		1
Butoxycarboxim	34681-23-7	36122	Insecticide		$C_7H_{14}N_2O_4S$	222.0674	223.0	23	106.0	10	166.0	7	2.05	2	
Butralin	33629-47-9	36528	Herbicide		$C_{14}H_{21}N_3O_4$	295.1532	296.2	25	164.0	5	132.0	11	no		
Buturon	3766-60-7	36510	Herbicide		$C_{12}H_{13}ClN_2O$	236.0716	237.1	32	84.1	16	126.0	30	5.33		11
Butylate	2008-41-5	45363	Herbicide		$C_{11}H_{23}NOS$	217.1500	218.1	28	57.2	17	156.1	10	7.09		24
Cadusafos	95465-99-9		Insecticide/Nematicide		$C_{10}H_{23}O_2PS_2$	270.0877	271.1	28	159.0	16	131.0	22	6.88		23
Carbaryl	63-25-2	45367	Insecticide		$C_{12}H_{11}NO_2$	201.0790	202.0	28	145.0	22	117.0	28	4.86	9	
Carbendazim	10605-21-7	45368	Fungicide		$C_9H_9N_3O_2$	191.0695	192.1	33	160.1	18	132.1	28	2.20	2	
Carbetamide	16118-49-3	45369	Herbicide		$C_{12}H_{16}N_2O_3$	236.1161	237.0	20	192.0	9	118.0	14	4.32	6	
Carbofuran	1563-66-2	45370	Insecticide		$C_{12}H_{15}NO_3$	221.1052	222.1	34	165.1	16	123.0	16	4.63	8	
Carbofuran-3-hydroxy	16655-82-6	37896	Metabolite		$C_{12}H_{15}NO_4$	237.1001	238.0	34	181.0	10	163.0	16	3.40	4	
Carbofuran-3-keto	16709-30-1	37895	Metabolite		$C_{12}H_{13}NO_4$	235.0845	236.2	24	179.1	12	161.1	18	4.00	5	
Carbosulfan	55285-14-8	34300	Insecticide		$C_{20}H_{32}N_2O_3S$	380.2134	381.0	40	118.0	22	76.0	34	7.89	27	
Carboxin	5234-68-4	45371	Fungicide		$C_{12}H_{13}NO_2S$	235.0667	236.0	34	143.0	16	87.0	22	4.79	9	
Carfentrazone-ethyl	128639-02-1	34079	Herbicide		$C_{15}H_{14}Cl_2F_3N_3O_3$	411.0364	412.0	38	346.0	24	266.0	18	6.48	20	
Carpropamid	104030-54-8	46135	Fungicide		$C_{15}H_{18}Cl_3NO$	333.0454	334.0	31	138.9	18	103.0	40	6.59		
Chinomethionate	2439-01-2	45372	Acaricide/Fungicide		$C_{10}H_6N_2O_2S_2$	233.9922	234.9	28	207.0	16	163.0	28	no		
Chlorbromuron	13360-45-7	45377	Herbicide		$C_9H_{10}BrClN_2O_2$	291.9614	292.9	30	203.9	18	182.0	16	5.87	15	
Chlorfenvinphos	470-90-6	36551	Acaricide/Insecticide		$C_{12}H_{14}Cl_3O_4P$	357.9695	358.9	28	155.0	12	99.0	30	6.65		21
Chlorfluzaron	71422-67-8	36530	Insecticide		$C_{20}H_9Cl_3F_5N_3O_3$	538.9630	539.8	42	158.0	20	382.9	20	7.61		26
Chloridazon	1698-60-8	45385	Herbicide		$C_{10}H_8ClN_3O$	221.0356	222.0	56	92.0	30	77.0	30	3.43	4	
Chlorimuron ethyl	90982-32-4	PS1081	Herbicide		$C_{15}H_{15}ClN_4O_6S$	414.0401	415.1	46	186.0	15	83.0	40			
Chlormephos	24934-91-6	45386	Insecticide		$C_5H_{12}ClO_2PS_2$	233.9705	235.0	24	97.0	22	142.9	16	no		
Chloroxuron	1982-47-4	45389	Herbicide		$C_{15}H_{15}ClN_2O_2$	290.0822	291.1	41	72.0	25	164.1	15	6.15		17
Chlorpropham	101-21-3	45393	Herbicide		$C_{10}H_{12}ClNO_2$	213.0557	214.1	18	172.0	8	154.0	18	6.01		16
Chlorpyrifos	2921-88-2	45395	Insecticide		$C_9H_{11}Cl_3NO_3PS$	348.9263	349.9	36	97.0	32	198.0	20	7.35		25
Chlorpyrifos-methyl	5598-13-0	45396	Insecticide		$C_7H_7Cl_3NO_3PS$	320.8950	321.8	34	125.0	20	289.9	16	6.87		23
Chlorsulfuron	64902-72-3	34322	Herbicide		$C_{12}H_{12}ClN_5O_4S$	357.0299	358.0	30	141.0	16	167.0	18	4.93		9
Chlorthiophos	60238-56-4	36126	Insecticide		$C_{11}H_{15}Cl_2O_3PS_2$	359.9577	360.9	28	154.9	12	98.9	30	6.66		21
Chlortoluron	15545-48-9	45400	Herbicide		$C_{10}H_{13}ClN_2O$	212.0716	213.0	32	72.0	18	46.0	16	5.10	10	
Chromafenozide	143807-66-3		Insecticide		$C_{24}H_{30}N_2O_3$	394.2256	395.1	16	175.0	22	339.0	10			
Cinidon-ethyl	142891-20-1	46336	Herbicide		$C_{19}H_{17}Cl_2NO_4$	393.0535	394.0	34	348.0	18	107.0	28	7.18	25	
Cinosulfuron	94593-91-6	37893	Herbicide		$C_{15}H_{19}N_5O_7S$	413.1005	414.0	38	183.0	16	157.0	24	4.40	6	
Clethodim	99129-21-2	34190	Herbicide		$C_{17}H_{26}ClNO_3S$	359.1322	360.0	32	164.0	18	268.1	12	7.02	24	
Clodinafop	114420-56-3		Herbicide		$C_{14}H_{11}ClFNO_4$	311.0361	312.0	42	265.8	16	238.2	24			
Clodinafop-propargyl	105512-06-9	46122	Herbicide		$C_{17}H_{13}ClFNO_4$	349.0517	350.0	36	266.0	16	91.0	32	6.47	20	
Clofencet	129025-54-3		Growth Regulator		$C_{13}H_{11}ClN_2O_3$	278.0458	279.1	46	261.1	15	166.0	30			
Clofentezine	74115-24-5	36763	Acaricide		$C_{14}H_8Cl_2N_4$	302.0126	303.0	28	138.0	22	102.0	35	6.76		
Clomazone	81777-89-1	46120	Herbicide		$C_{12}H_{14}ClNO_2$	239.0713	240.0	32	125.0	18	89.0	46	5.60	13	
Clomeprop	84496-56-0		Herbicide		$C_{16}H_{15}Cl_2NO_2$	323.0480	324.1	41	120.1	20	203.1	15			
Clopyralid	1702-17-6	36758	Herbicide		$C_6H_3Cl_2NO_2$	190.9541	191.9	30	173.9	10	145.9	20	2.21	2	
Cloquintocet - mexyl	99607-70-2	46123	Herbicide		$C_{18}H_{22}ClNO_3$	335.1288	336.1	30	238.0	16	192.0	30	7.22		25
Cloransulam-methyl	147150-35-4		Herbicide		$C_{15}H_{13}ClFN_5O_5S$	429.0310	430.1	36	153.0	40	398.1	15			

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Clothianidin	210880-92-5	33589	Insecticide		C ₆ H ₈ ClN ₅ O ₂ S	249.0087	250.0	24	169.0	12	132.0	18	3.10	3	
Coumaphos	56-72-4	45403	Insecticide		C ₁₄ H ₁₆ ClO ₅ PS	362.0145	363.0	32	307.0	16	289.0	24	6.60	21	
Cruformate	299-86-5		Insecticide	Ruelene	C ₁₂ H ₁₉ ClNO ₃ P	291.0791	292.0	40	108.1	28	236.1	18	6.45		19
Cumyruron	99485-76-4		Herbicide		C ₁₇ H ₁₉ ClN ₂ O	302.1186	303.2	46	185.1	15	125.0	30			
Cyanazine	21725-46-2	45407	Herbicide		C ₉ H ₁₃ ClN ₆	240.0890	241.0	41	214.0	17	96.0	25	4.39	6	
Cyanofenphos	13067-93-1	36509	Insecticide		C ₁₅ H ₁₄ NO ₂ PS	303.0483	304.0	34	157.0	22	276.0	12	6.57	21	
Cyazofamid	120116-88-3	33874	Fungicide		C ₁₃ H ₁₃ ClN ₄ O ₂ S	324.0448	325.0	26	107.9	20	261.0	10	6.30	19	
Cycloate	1134-23-2	45408	Herbicide		C ₁₁ H ₂₁ NOS	215.1344	216.1	32	83.1	18	55.2	28	6.91		23
Cyclosulfamuron	136849-15-5		Herbicide		C ₁₇ H ₁₉ N ₅ O ₆ S	421.1056	422.2	46	261.1	15	218.1	30			
Cycloxydim	101205-02-1	46071	Herbicide		C ₁₇ H ₂₇ NO ₃ S	325.1712	326.0	34	280.0	16	180.0	22	7.00	24	
Cycluron	2163-69-1	45409	Herbicide		C ₁₁ H ₂₂ N ₂ O	198.1732	199.0	32	89.1	14	69.2	22	5.42	12	
Cyflufenamid	180409-60-3		Fungicide		C ₂₀ H ₁₇ F ₅ N ₂ O ₂	412.1210	413.2	36	295.1	15	203.0	35	6.73	22	
Cymoxanil	57966-95-7	34326	Fungicide		C ₇ H ₁₀ N ₄ O ₃	198.0753	199.0	23	128.0	8	111.0	18	3.58		4
Cyproconazole	94361-06-5	46068	Fungicide		C ₁₅ H ₁₈ ClN ₃ O	291.1138	292.2	36	70.2	18	125.1	24	6.16		17
Cyprodinil	121552-61-2	34389	Fungicide		C ₁₄ H ₁₅ N ₃	225.1266	226.0	56	93.0	33	108.0	25	5.90	15	
Cyromazine	66215-27-8	45414	Insecticide		C ₆ H ₁₀ N ₆	166.0967	167.0	38	60.2	19	108.1	19	1.10	1	
Daminozide	1596-84-5	45418	Herbicide		C ₆ H ₁₂ N ₂ O ₃	160.0848	161.0	24	143.0	12	61.0	12	0.81	1	
Deltamethrin	52918-63-5	45423	Insecticide		C ₂₂ H ₁₉ Br ₂ NO ₃	502.9732	505.9	28	280.9	12	93.2	46	7.64		
Demeton O	298-03-3	34205	Acaricide/Insecticide		C ₈ H ₉ O ₃ PS ₂	258.0513	259.0	18	89.0	10	61.1	33	5.64		13
Demeton S	126-75-0	PS662	Acaricide/Insecticide		C ₈ H ₉ O ₃ PS ₂	258.0513	259.0	18	89.0	10	61.1	33	5.64		13
Demeton-O-sulfoxide			Metabolite		C ₈ H ₉ O ₄ PS ₂	274.0462	275.1	26	104.9	16	140.8	24	5.85		
Demeton-S-methyl	919-86-8	45304	Insecticide		C ₆ H ₁₅ O ₃ PS ₂	230.0200	231.1	16	89.1	10	61.2	30	4.68		8
Demeton-S-methyl-sulfon	17040-19-6	45424	Insecticide	Dioxydemeton-S-methyl	C ₆ H ₁₅ O ₅ PS ₂	262.0099	263.0	32	169.0	17	121.0	17	2.55		2
Desmedipham	13684-56-5	45426	Herbicide		C ₁₆ H ₁₆ N ₂ O ₄	300.1110	301.0	34	182.0	10	136.0	22	5.47		12
Desmethyl-formamidopirimicarb	27218-04-8	33887	Metabolite		C ₁₁ H ₁₆ N ₄ O ₃	252.1222	253.1	30	72.0	16	225.1	11	4.57		7
Desmethyl-pirimicarb	30614-22-3	33886	Metabolite		C ₁₀ H ₁₆ N ₄ O ₂	224.1273	225.1	32	72.0	20	168.1	16	2.71		2
Desmetryn	1014-69-3	45427	Herbicide		C ₈ H ₁₅ N ₅ S	213.1048	214.1	38	172.1	20	82.1	30	4.26		5
Dialifos	10311-84-9	36500	Acaricide/Insecticide		C ₁₄ H ₁₇ ClNO ₄ PS ₂	393.0025	394.0	18	187.0	8	208.0	16	6.82	23	
Diallate	2303-16-4	36501	Herbicide		C ₁₀ H ₁₇ Cl ₂ NOS	269.0408	270.1	29	86.1	15	128.1	11	6.98	24	
Diamuron	42609-52-9		Herbicide	Dymron	C ₁₇ H ₂₀ N ₂ O	268.1576	269.1	36	151.1	10	91.0	40			
Diazinon	333-41-5	45428	Insecticide		C ₁₂ H ₂₁ N ₂ O ₃ PS	304.1011	305.1	31	169.0	22	96.9	35	2.55		
Dibrom	300-76-5	45429	Insecticide/Nematicide	Naled	C ₄ H ₇ Br ₂ Cl ₂ O ₄ P	377.7826	378.7	24	127.0	16	109.0	36	5.45		12
Dichlofluanid	1085-98-9	45433	Fungicide		C ₉ H ₁₁ Cl ₂ FN ₂ O ₂ S ₂	331.9623	333.0	28	123.0	24	224.0	10	6.20	18	
Dichlorvos	62-73-7	45441	Acaricide/Insecticide		C ₄ H ₇ Cl ₂ O ₄ P	219.9459	221.0	34	109.0	22	79.0	34	4.53	7	
Diclobutrazol	75736-33-3	36764	Fungicide		C ₁₅ H ₁₉ Cl ₂ N ₃ O	327.0905	328.0	34	70.0	20	158.9	38	6.52		20
Diclomezine	62865-36-5		Fungicide		C ₁₁ H ₈ Cl ₂ N ₂ O	254.0014	255.0	58	79.8	30	140.8	30			
Diclosulam	145701-21-9	33968	Herbicide		C ₁₃ H ₁₀ Cl ₂ FN ₅ O ₃ S	404.9865	406.1	46	161.0	30	378.0	15			
Dicrotophos	141-66-2	45305	Insecticide		C ₈ H ₁₆ NO ₅ P	237.0766	238.0	28	112.0	10	193.0	10	2.97	3	
Diethofencarb	87130-20-9	34087	Fungicide		C ₁₄ H ₂₁ NO ₄	267.1471	268.0	28	226.0	10	124.0	40	5.71	14	
Difenoconazole	119446-68-3	36531	Fungicide		C ₁₉ H ₁₇ Cl ₂ N ₃ O ₃	405.0647	406.0	46	251.1	25	111.1	60	6.90		23
Difenoxuron	14214-32-5	45444	Herbicide		C ₁₆ H ₁₈ N ₂ O ₃	286.1317	287.0	38	72.0	20	123.0	20	5.38	12	
Diflubenzuron	35367-38-5	45446	Insecticide		C ₁₄ H ₉ ClF ₂ N ₂ O ₂	310.0321	311.1	32	227.0	8	269.0	8	6.39	20	
Dimefuron	34205-21-5	36788	Herbicide		C ₁₅ H ₁₉ ClN ₄ O ₃	338.1146	339.0	42	72.0	26	166.9	20	5.60		13
Dimepiperate	61432-55-1	33943	Herbicide		C ₁₅ H ₂₁ NOS	263.1344	264.1	14	146.0	10	119.0	16	6.95	24	
Dimethachlor	50563-36-5	45447	Herbicide		C ₁₃ H ₁₈ ClNO ₂	255.1026	256.2	29	148.2	25	224.2	15	5.50		12
Dimethametryn	22936-75-0	45448	Herbicide		C ₁₁ H ₂₁ N ₅ S	255.1518	256.1	42	186.1	20	71.0	32	5.92		14
Dimethenamid	87674-68-8	46385	Herbicide		C ₁₂ H ₁₈ ClNO ₂ S	275.0747	276.0	26	244.0	14	168.0	26	5.84		14
Dimethirimol	5221-53-4		Fungicide		C ₁₁ H ₁₉ N ₃ O	209.1528	210.1	46	71.1	30	140.0	21	3.57		4

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Dimethoate	60-51-5	45449	Acaricide/Insecticide		$C_5H_{12}NO_3PS_2$	228.9996	230.1	24	125.0	20	199.0	10	3.32		3
Dimethomorph	110488-70-5	46027	Fungicide		$C_{21}H_{22}ClNO_4$	387.1237	388.1	41	300.9	20	165.0	30	6.03		16
Dimetilan	644-64-4	45450	Insecticide		$C_{10}H_{16}N_4O_3$	240.1222	241.1	24	72.2	16	196.1	10	3.57		4
Dimoxystrobin	149961-52-4	33499	Fungicide		$C_{19}H_{22}N_2O_3$	326.1630	327.1	30	116.1	21	205.2	10	6.47	20	
Diniconazole	70217-36-6	46049	Fungicide		$C_{15}H_{17}Cl_2N_3O$	325.0749	326.1	46	70.2	25	159.0	34	6.87		23
Dioxacarb	6988-21-2	45454	Insecticide		$C_{11}H_{13}NO_4$	223.0845	224.1	20	123.1	16	167.1	8	3.39	4	
Diphenamid	957-51-7	45455	Herbicide		$C_{16}H_{17}NO$	239.1310	240.1	36	134.1	20	167.1	22	5.47		12
Diphenylamine	122-39-4	45456	Fungicide		$C_{12}H_{11}N$	169.0891	170.0	38	93.0	24	92.0	18	6.12	17	
Disulfoton	298-04-4	45460	Acaricide/Insecticide		$C_8H_{19}O_2PS_3$	274.0285	274.9	16	89.0	20	61.1	35	6.80		22
Disulfoton-sulfone	2497-06-5	45871	Metabolite		$C_8H_{19}O_4PS_3$	306.0183	307.1	24	97.1	28	153.1	12	5.16		10
Disulfoton-sulfoxide	2497-07-6	45897	Metabolite		$C_8H_{19}O_3PS_3$	290.0234	291.0	24	185.0	14	97.0	31	5.08		10
Ditalimfos	5131-24-8	45461	Fungicide		$C_{12}H_{14}NO_4PS$	299.0381	300.1	24	148.1	20	130.1	34	6.13		17
Dithiopyr	97886-45-8		Herbicide		$C_{15}H_{16}F_5NO_2S_2$	401.0543	402.0	41	354.1	18	248.1	34	6.99	24	
Diuron	330-54-1	45463	Herbicide		$C_9H_{10}Cl_2N_2O$	232.0170	233.0	34	72.1	18	46.3	14	5.37		11
DMSA			Metabolite	Dimethylphenylsulphamide	$C_8H_{12}N_2O_2S$	200.0619	201.0	31	92.0	17	137.0	9	4.14		
DMST	66840-71-9	34336	Metabolite	Dimethylaminosulfotoluidid	$C_9H_{14}N_2O_2S$	214.0776	215.0	26	106.0	15	79.1	29	4.79		8
Dodemorph	1593-77-7	45465	Fungicide		$C_{18}H_{35}NO$	281.2719	282.1	40	116.0	21	98.0	28	5.22	10	
Dodine	2439-10-3	45466	Fungicide		$C_{15}H_{33}N_3O_2$	287.2573	288.0	40	256.0	22	58.0	50	8.00		
Edifenphos	17109-49-8	45467	Fungicide		$C_{14}H_{15}O_2PS_2$	310.0251	311.0	32	109.0	32	111.0	26	6.56		20
Endothal	62059-43-2	35525	Herbicide		$C_8H_{10}O_5$	186.0528	187.0	12	169.0	6	123.0	14	1.75		
EPN	2104-64-5	36503	Acaricide/Insecticide		$C_{14}H_{14}NO_4PS$	323.0381	324.0	31	157.0	25	296.0	14	6.92		
Epoxiconazole	106325-08-0	36848	Fungicide		$C_{17}H_{13}ClF_3NO$	329.0731	330.0	34	121.0	22	101.0	50	6.27		18
EPTC	759-94-4	45469	Herbicide		$C_9H_{19}NOS$	189.1187	190.0	26	128.1	11	86.0	15	6.45		19
Esprocarb	85785-20-2	33898	Herbicide		$C_{15}H_{23}NOS$	265.1500	266.1	30	91.0	22	71.0	16	7.19	25	
Ethametsulfuron-methyl	97780-06-8		Herbicide		$C_{15}H_{18}N_6O_6S$	410.1009	411.2	46	168.1	30	196.1	15			
Ethidimuron	30043-49-3	45474	Herbicide		$C_7H_{12}N_4O_3S_2$	264.0351	265.0	34	208.1	14	114.0	20	3.14		3
Ethiofencarb	29973-13-5	45475	Insecticide		$C_{11}H_{15}NO_2S$	225.0824	226.1	25	107.0	17	164.0	8	4.98	10	
Ethiofencarb sulfone	53380-23-7	45810	Metabolite		$C_{11}H_{15}NO_4S$	257.0722	258.0	28	107.0	18	201.1	5	2.98	3	
Ethiofencarb sulfoxide	53380-22-6	45811	Metabolite		$C_{11}H_{15}NO_3S$	241.0773	242.1	28	107.1	18	185.1	8	3.08	3	
Ethion	563-12-2	45477	Acaricide		$C_9H_{22}O_4P_2S_4$	383.9876	284.9	25	199.1	10	97.0	46	5.22		
Ethiprole	181587-01-9	33976	Insecticide		$C_{13}H_9Cl_2F_3N_4OS$	395.9826	414.1	21	396.9	9	350.9	25	5.87		
Ethirimol	23947-60-6	45478	Fungicide		$C_{11}H_{19}N_3O$	209.1528	210.1	44	140.0	22	98.0	28	3.75		4
Ethofumesate	26225-79-6	45479	Herbicide		$C_{13}H_{18}O_5S$	286.0875	287.1	36	121.1	15	259.1	10	5.75	14	
Ethoprophos	13194-48-4	45306	Insecticide/Nematicide		$C_8H_{19}O_2PS_2$	242.0564	243.2	32	97.0	31	131.0	20	6.27		18
Ethoxyquin	91-53-2	45480	Fungicide/Herbicide		$C_{14}H_{19}NO$	217.1467	218.2	46	148.1	22	160.1	32	4.80	8	
Ethoxysulfuron	126801-58-9	46300	Herbicide		$C_{15}H_{18}N_4O_7S$	398.0896	398.9	32	261.0	16	218.0	24	5.99	16	
Etofenprox	80844-07-1	34094	Insecticide		$C_{25}H_{28}O_3$	376.2038	394.3	26	177.0	15	106.9	43	7.97	27	
Etrifos	38260-54-7	45481	Insecticide		$C_{10}H_{17}N_2O_4PS$	292.0647	293.1	38	125.0	26	265.1	16	6.58		
Famoxadone	131807-57-3	33495	Fungicide		$C_{22}H_{18}N_2O_4$	374.1267	392.2	21	331.1	10	238.0	20	6.67		
Famphur	52-85-7	34341	Insecticide		$C_{10}H_{16}NO_5PS_2$	325.0208	326.0	32	93.0	31	217.0	20	5.19		10
Fenamidone	161326-34-7	33965	Fungicide		$C_{17}H_{17}N_3OS$	311.1092	312.1	31	92.0	25	236.1	14	5.84		14
Fenamiphos	22224-92-6	45483	Nematicide		$C_{13}H_{22}NO_3PS$	303.1058	304.1	36	217.1	24	202.1	36	6.39	19	
Fenamiphos sulphone	31972-44-8	46292	Metabolite		$C_{13}H_{22}NO_5PS$	335.0956	336.1	34	266.1	20	188.2	28	4.83	9	
Fenamiphos sulphoxide	31972-43-7	46293	Metabolite		$C_{13}H_{22}NO_4PS$	319.1007	320.1	42	171.1	22	108.0	35	4.84	8	
Fenarimol	60168-88-9	45484	Fungicide		$C_{17}H_{12}Cl_2N_2O$	330.0327	331.0	46	268.0	22	81.0	34	6.26		18
Fenazaquin	120928-09-8	46087	Acaricide		$C_{20}H_{22}N_2O$	306.1732	307.2	36	57.2	25	161.0	19	7.70		26
Fenazox	495-48-7	45763	Insecticide		$C_{12}H_{10}N_2O$	198.0793	199.1	28	77.1	24	92.1	14	6.68	22	

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Fenbuconazole	114369-43-6	46096	Fungicide		C ₁₉ H ₁₇ ClN ₄	336.1142	337.0	38	70.1	20	125.0	36	6.37	19	
Fenfuram	24691-80-3	45486	Fungicide		C ₁₂ H ₁₁ NO ₂	201.0790	202.1	34	109.0	20	83.1	14	4.85	9	
Fenhexamid	126833-17-8	46278	Fungicide		C ₁₄ H ₁₇ Cl ₂ NO ₂	301.0636	302.1	41	97.2	22	55.3	38	6.22	18	
Fenitrothion	122-14-5	45487	Insecticide		C ₉ H ₁₂ NO ₅ PS	277.0174	278.0	38	109.1	20	79.1	34	6.06		
Fenobucarb	3766-81-2	45488	Insecticide		C ₁₂ H ₁₇ NO ₂	207.1259	208.0	22	94.9	14	152.0	8	5.72	14	
Fenoxaprop-ethyl	66441-23-4	45518	Herbicide		C ₁₈ H ₁₆ ClNO ₅	361.0717	362.1	46	288.1	20	121.1	25	no		
Fenoxycarb	72490-01-8	34343	Insecticide		C ₁₇ H ₁₉ NO ₄	301.1314	302.1	28	88.0	20	116.1	11	6.45	20	
Fenpiclonil	74738-17-3	36532	Fungicide		C ₁₁ H ₆ Cl ₂ N ₂	235.9908	236.9	44	202.0	20	140.0	38	5.66		13
Fenpropathrin	39515-41-8	36767	Insecticide		C ₂₂ H ₂₃ NO ₃	349.1678	350.1	24	125.0	14	97.0	34	7.51	26	
Fenpropidin	67306-00-7	46017	Fungicide		C ₁₉ H ₃₁ N	273.2457	274.2	56	147.1	28	86.1	28	5.44	11	
Fenpropimorph	67564-91-4	36772	Fungicide		C ₂₀ H ₃₃ NO	303.2562	304.2	50	147.1	28	57.2	30	5.53		11
Fenpyroximat	111812-58-9	46137	Acaricide		C ₂₄ H ₂₇ N ₃ O ₄	421.2002	422.2	32	366.1	15	138.1	32	7.53		26
Fensulfothion	115-90-2	45307	Insecticide/Nematicide		C ₁₁ H ₁₇ O ₄ PS ₂	308.0306	309.0	36	157.1	25	173.1	22	5.35		11
Fensulfothion oxon	6552-21-2		Metabolite		C ₁₁ H ₁₇ O ₅ PS	292.0534	293.0	34	237.0	19	265.0	14			
Fensulfothion oxon sulfone	6132-17-8		Metabolite		C ₁₁ H ₁₇ O ₆ PS	308.0483	309.0	33	253.0	16	175.0	27			
Fensulfothion sulfone	14255-72-2		Metabolite		C ₁₁ H ₁₇ O ₅ PS ₂	324.0255	325.0	32	269.0	16	297.0	11			
Fenthion	55-38-9	36552	Insecticide		C ₁₀ H ₁₅ O ₃ PS ₂	278.0200	279.1	36	169.1	16	247.1	13	6.57	21	
Fenthion-sulfone	3761-42-0	46023	Metabolite		C ₁₀ H ₁₅ O ₅ PS ₂	310.0099	311.0	38	125.0	22	109.0	28	4.94	10	
Fenthion-sulfoxide	3761-41-9	37885	Metabolite		C ₁₀ H ₁₅ O ₄ PS ₂	294.0149	295.0	38	109.0	32	280.0	18	4.82	9	
Fenuron	101-42-8	45494	Herbicide		C ₉ H ₁₂ N ₂ O	164.0950	165.0	28	71.9	16	45.9	14	3.21		3
Ferimzone	89269-64-7		Fungicide		C ₁₅ H ₁₈ N ₄	254.1531	255.2	46	132.1	20	91.0	30	no		
Flamprop-isopropyl	52756-22-6	45497	Herbicide		C ₁₉ H ₁₉ ClFNO ₃	363.1037	364.0	24	105.0	20	77.0	56	6.62		21
Flamprop-methyl	52756-25-9	45498	Herbicide		C ₁₇ H ₁₅ ClFNO ₃	335.0724	336.0	24	105.0	16	77.0	48	6.09		16
Flazasulfuron	104040-78-0	34052	Herbicide		C ₁₃ H ₁₂ F ₃ N ₅ O ₅ S	407.0511	408.1	26	181.9	20	138.9	44	5.55		
Florasulam	145701-23-1		Herbicide		C ₁₂ H ₈ F ₃ N ₅ O ₃ S	359.0300	360.0	40	129.0	22	108.9	50	6.62		
Fluazafop-P-butyl	79241-46-6	46276	Herbicide		C ₁₉ H ₂₀ F ₃ NO ₄	383.1344	384.1	38	282.1	22	328.1	16	7.11		24
Fluazifop	69335-91-7	36884	Herbicide		C ₁₅ H ₁₂ F ₃ NO ₄	327.0718	328.1	46	282.1	20	255.1	25	5.91		15
Fluazinam	79622-59-6	46316	Fungicide		C ₁₃ H ₄ Cl ₂ F ₆ N ₄ O ₄	463.9514	464.8	32	373.0	26	338.1	47	5.74		
Flucycloxuron	113036-88-7		Acaricide/Insecticide		C ₂₅ H ₂₀ ClF ₂ N ₃ O ₃	483.1161	484.0	24	132.1	40	289.1	12	7.42	26	
Flucythrinate	70124-77-5	33496	Acaricide/Insecticide		C ₂₆ H ₂₃ F ₂ NO ₄	451.1595	452.1	16	412.0	7	157.0	36	7.40		
Fludioxonil	131341-86-1	46102	Fungicide		C ₁₂ H ₆ F ₂ N ₂ O ₂	248.0397	249.1	16	158.1	28	229.1	10	5.90		
Flufenacet	142459-58-3	46327	Herbicide		C ₁₄ H ₁₃ F ₄ N ₃ O ₂ S	363.0665	364.0	22	152.1	20	194.1	11	6.22	18	
Flufenoxuron	101463-69-8	46069	Acaricide/Insecticide		C ₂₁ H ₁₁ ClF ₆ N ₂ O ₃	488.0362	489.1	40	158.0	22	141.0	46	7.47	26	
Flumetsulam	98967-40-9		Herbicide		C ₁₂ H ₉ F ₂ N ₅ O ₂ S	325.0445	326.1	46	129.0	25	109.0	50	no		
Flumioxazin	103361-09-7		Herbicide		C ₁₉ H ₁₅ FN ₂ O ₄	354.1016	355.0	46	326.0	22	298.0	28	no		
Fluomethuron	2164-17-2	45502	Herbicide		C ₁₀ H ₁₁ F ₃ N ₂ O	232.0823	233.2	34	72.2	18	46.4	18	5.02	10	
Fluoxastrobin	361377-29-9	33797	Fungicide		C ₂₁ H ₁₆ ClFN ₄ O ₅	458.0793	459.0	36	427.0	18	188.0	36	6.19	18	
Fluquinconazole	136426-54-5	46301	Fungicide		C ₁₆ H ₈ Cl ₂ FN ₅ O	375.0090	376.0	46	348.8	18	306.9	30	6.17		
Fluridon	59756-60-4	45511	Herbicide		C ₁₉ H ₁₄ F ₃ NO	329.1027	330.1	66	310.2	30	259.2	40	5.59		
Fluroxypyr	69377-81-7	45758	Herbicide		C ₇ H ₅ Cl ₂ FN ₂ O ₃	253.9661	254.9	28	208.8	16	180.8	22	4.42	6	
Fluroxypyr-meptyl	81406-37-3	36780	Herbicide		C ₁₅ H ₂₁ Cl ₂ FN ₂ O ₃	366.0913	367.0	21	254.9	11	181.0	32	7.44		26
Flurtamone	96525-23-4	46286	Herbicide		C ₁₈ H ₁₄ F ₃ NO ₂	333.0977	334.0	44	247.0	27	178.0	45	5.77	14	
Flusilazole	85509-19-9	45753	Fungicide		C ₁₆ H ₁₅ F ₂ N ₃ Si	315.1003	316.0	36	247.0	18	165.0	28	6.41	19	
Flutolanil	66332-96-5	PS2057	Fungicide		C ₁₇ H ₁₆ F ₃ NO ₂	323.1133	324.1	34	262.1	18	65.0	40	5.97	16	
Flutriafol	76674-21-0	34344	Fungicide		C ₁₆ H ₁₃ F ₂ N ₃ O	301.1027	302.1	32	70.2	18	123.1	29	5.24	11	
Fluvalinate	102851-06-9	46294	Acaricide/Insecticide		C ₂₆ H ₂₂ ClF ₃ N ₂ O ₃	502.1271	503.0	24	181.1	30	208.1	12	no		
Fonofos	944-22-9	45513	Insecticide		C ₁₀ H ₁₅ OPS ₂	246.0302	247.1	24	109.0	20	137.0	10	6.60	21	
Foramsulfuron	173159-57-4	33977	Herbicide		C ₁₇ H ₂₀ N ₆ O ₇ S	452.1114	453.0	35	182.0	22	272.0	14	4.92		9
Forchlorfenuron	68157-60-8	C2791	Growth Regulator	CPPU	C ₁₂ H ₁₀ ClN ₃ O	247.0512	248.1	36	129.0	15	93.0	35			

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Formetanate	22259-30-9	45514	Acaricide/Insecticide		C ₁₁ H ₁₅ N ₃ O ₂	221.1164	222.0	30	165.0	15	46.0	26	1.63		1
Fosthiazate	98886-44-3	34099	Nematicide		C ₉ H ₁₈ NO ₃ PS ₂	283.0466	284.0	28	228.0	10	104.0	22	5.04	10	
Fuberidazole	3878-19-1	45515	Fungicide		C ₁₁ H ₈ N ₂ O	184.0637	185.0	41	157.0	22	156.0	27	2.89	3	
Furametpyr	123572-88-3		Fungicide		C ₁₇ H ₂₀ ClN ₃ O ₂	333.1244	334.2	36	157.0	30	290.2	15			
Furathiocarb	65907-30-4	45517	Insecticide		C ₁₈ H ₂₆ N ₂ O ₅ S	382.1562	383.2	31	194.9	18	252.0	12	7.13	25	
Furmecyclox	60568-05-0	34347	Fungicide		C ₁₄ H ₂₁ NO ₃	251.1521	252.2	31	170.1	14	110.1	22	3.11		
Halofenozide	112226-61-6		Insecticide		C ₁₈ H ₁₉ ClN ₂ O ₂	330.1135	331.1	16	104.9	18	275.0	10	5.85		
Halosulfuron methyl	100784-20-1		Herbicide		C ₁₃ H ₁₅ ClN ₆ O ₇ S	434.0411	435.1	36	182.1	20	83.0	40	6.25		18
Haloxyfop	69806-34-4	45817	Herbicide		C ₁₅ H ₁₁ ClF ₃ NO ₄	361.0329	362.0	36	315.8	18	91.0	30	6.60		21
Haloxyfop-2-ethoxyethyl	87237-48-7	36778	Herbicide		C ₁₉ H ₁₉ ClF ₃ NO ₅	433.0904	434.0	34	91.0	34	316.0	20	7.10		24
Haloxyfop-methyl	69806-40-2	45820	Herbicide		C ₁₆ H ₁₃ ClF ₃ NO ₄	375.0485	376.0	36	91.1	32	316.1	18	6.90		23
Heptenophos	23560-59-0	45523	Insecticide		C ₉ H ₁₂ ClO ₄ P	250.0162	251.0	26	127.0	14	125.0	14	5.43	12	
Hexaconazole	79983-71-4	34348	Fungicide		C ₁₄ H ₁₇ Cl ₂ N ₃ O	313.0749	314.0	40	70.1	22	159.0	28	6.74	22	
Hexazinone	51235-04-2	36129	Herbicide		C ₁₂ H ₂₀ N ₄ O ₂	252.1586	253.1	35	171.1	16	71.0	30	4.66	8	
Hexythiazox	78587-05-0	33365	Acaricide		C ₁₇ H ₂₁ ClN ₂ O ₂ S	352.1012	353.0	30	168.1	26	228.1	14	7.37	26	
Imazalil	35554-44-0	36130	Fungicide		C ₁₄ H ₁₄ Cl ₂ N ₂ O	296.0483	297.0	40	159.0	22	69.0	22	5.03	9	
Imazapyr	81334-34-1	37877	Herbicide		C ₁₃ H ₁₅ N ₃ O ₃	261.1113	262.2	38	69.2	26	86.1	26	3.10	3	
Imazaquin	81335-37-7	37878	Herbicide		C ₁₇ H ₁₇ N ₃ O ₃	311.1270	312.2	40	86.2	28	267.2	20	4.64	8	
Imazosulfuron	122548-33-8		Herbicide		C ₁₄ H ₁₃ ClN ₆ O ₅ S	412.0357	413.0	16	155.9	18	152.8	12			
Imidacloprid	138261-41-3	37894	Insecticide		C ₉ H ₁₀ ClN ₅ O ₂	255.0523	256.1	34	175.1	20	209.1	15	3.08	3	
Indanofan	133220-30-1		Herbicide		C ₂₀ H ₁₇ ClO ₃	340.0866	341.1	21	186.9	12	174.9	14			
Indoxacarb	144171-61-9	33969	Insecticide		C ₂₂ H ₁₇ ClF ₃ N ₃ O ₇	527.0707	528.0	34	150.0	22	203.0	40	6.91	24	
Iodosulfuron methyl	144550-36-7	30317	Herbicide		C ₁₄ H ₁₄ IN ₅ O ₆ S	492.9553	508.1	31	167.1	25	141.1	25	5.58	13	
Iprobenphos	26087-47-8	45814	Fungicide		C ₁₃ H ₂₁ O ₃ PS	288.0949	289.0	18	91.0	20	205.0	10	6.47	20	
Iprodione	36734-19-7	36132	Fungicide		C ₁₃ H ₁₃ Cl ₂ N ₃ O ₃	329.0334	330.0	21	244.7	16	288.0	15	6.40		
Iprovalicarb	140923-17-7	33431	Fungicide		C ₁₈ H ₂₈ N ₂ O ₃	320.2100	321.1	28	119.1	16	203.1	10	6.15		17
Isazophos	42509-80-8	36133	Insecticide/Nematicide		C ₉ H ₁₇ ClN ₃ O ₃ PS	313.0417	314.0	26	120.0	28	162.1	16	6.10	17	
Isocarbamide	30979-48-7	36134	Herbicide		C ₈ H ₁₅ N ₃ O ₂	185.1164	186.1	27	87.1	16	130.1	12	3.67		4
Isocarbofos	24353-61-5	33857	Insecticide		C ₁₁ H ₁₆ NO ₄ PS	289.0538	291.1	21	121.1	30	231.1	13	5.39	12	
Isofenphos	25311-71-1	36135	Insecticide		C ₁₅ H ₂₄ NO ₄ PS	345.1164	346.1	16	245.1	12	217.0	22	6.75		22
Isomethiozin	57052-04-7	36136	Herbicide		C ₁₂ H ₂₀ N ₄ OS	268.1358	269.1	30	200.1	15	172.1	22	6.57	21	
Isonoruron	28805-78-9	33360	Herbicide		C ₁₃ H ₂₂ N ₂ O	222.1732	223.1	34	89.1	18	72.2	28	5.76	14	
Isoproc carb	2631-40-5	45541	Insecticide		C ₁₁ H ₁₅ NO ₂	193.1103	194.1	24	95.1	14	137.1	8	5.22	11	
Isopropalin	33820-53-0	36505	Herbicide		C ₁₅ H ₂₃ N ₃ O ₄	309.1689	310.2	34	226.2	19	268.2	15	7.65		26
Isoprothiolane	50512-35-1		Fungicide/Insecticide		C ₁₂ H ₁₈ O ₄ S ₂	290.0647	291.1	26	188.8	22	230.9	12	5.99		
Isoproturon	34123-59-6	36137	Herbicide		C ₁₂ H ₁₈ N ₂ O	206.1419	207.0	40	72.0	22	47.0	16	5.32		11
Isoxaben	82558-50-7	36138	Herbicide		C ₁₈ H ₂₄ N ₂ O ₄	332.1736	333.1	31	165.1	18	107.1	58	5.93		15
Isoxaflutole	141112-29-0	46437	Herbicide		C ₁₅ H ₁₂ F ₃ NO ₄ S	359.0439	360.0	31	250.9	14	219.9	40	5.35		
Isoxathion	18854-01-8		Insecticide		C ₁₃ H ₁₆ NO ₄ PS	313.0538	314.1	31	104.9	14	96.9	35	6.74		
Kresoxim-methyl	143390-89-0	37899	Fungicide		C ₁₈ H ₁₉ NO ₄	313.1314	314.1	24	116.0	12	206.0	7	6.50		20
Lenacil	2164-08-1	36140	Herbicide		C ₁₃ H ₁₈ N ₂ O ₂	234.1368	235.2	27	153.1	16	136.1	32	5.29	11	
Linuron	330-55-2	36141	Herbicide		C ₉ H ₁₀ Cl ₂ N ₂ O ₂	248.0119	249.1	31	160.1	18	181.1	16	5.75	14	
Malaaxon	1634-78-2	36142	Acaricide/Insecticide		C ₁₀ H ₁₉ O ₇ PS	314.0589	315.0	24	98.9	24	127.0	12	4.70		8
Malathion	121-75-5	36143	Acaricide/Insecticide		C ₁₀ H ₁₉ O ₆ PS ₂	330.0361	331.0	20	127.0	12	99.0	24	5.95		15
Mecarbam	2595-54-2	36515	Acaricide/Insecticide		C ₁₀ H ₂₀ NO ₅ PS ₂	329.0521	330.0	21	227.1	8	97.0	35	6.22	18	
Mefenacet	73250-68-7	36150	Herbicide		C ₁₆ H ₁₄ N ₂ O ₂ S	298.0776	299.0	25	148.0	15	120.0	25	6.09	17	
Mepanipyrim	110235-47-7	33970	Fungicide		C ₁₄ H ₁₃ N ₃	223.1109	224.1	46	106.0	25	77.0	40	6.12	17	
Mephosfolan	950-10-7	34352	Insecticide		C ₈ H ₁₆ NO ₃ PS ₂	269.0309	270.1	34	140.0	24	75.1	22	4.55	7	
Mepronil	55814-41-0	33361	Fungicide		C ₁₇ H ₁₉ NO ₂	269.1416	270.1	36	119.0	28	91.0	44	5.98	16	

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Mesosulfuron-methyl	208465-21-8	34178	Herbicide		C ₁₇ H ₂₁ N ₅ O ₉ S ₂	503.0781	504.0	38	182.0	24	82.9	60	5.23	11	
Mesotrione	104206-82-8	33855	Herbicide		C ₁₄ H ₁₃ NO ₇ S	339.0413	340.0	34	104.0	32	228.0	18	4.03	5	
Metalaxyl	57837-19-1	36153	Fungicide		C ₁₅ H ₂₁ NO ₄	279.1471	280.1	26	220.1	13	192.1	17	5.35		11
Metamitron	41394-05-2	36154	Herbicide		C ₁₀ H ₁₀ N ₄ O	202.0855	203.1	34	175.1	16	104.0	22	3.25		3
Metazachlor	67129-08-2	36155	Herbicide		C ₁₄ H ₁₆ ClN ₃ O	277.0982	278.0	22	134.1	22	210.0	10	5.27	11	
Metconazole	125116-23-6	37909	Fungicide		C ₁₇ H ₂₂ ClN ₃ O	319.1451	320.1	38	70.0	22	125.0	36	6.75		22
Methabenzthiazuron	18691-97-9	36156	Herbicide		C ₁₀ H ₁₁ N ₃ OS	221.0623	222.0	30	165.0	16	150.0	32	5.22	11	
Methacrifos	62610-77-9	45569	Acaricide/Insecticide		C ₇ H ₁₃ O ₅ PS	240.0221	241.1	20	125.0	20	209.1	8	5.47		12
Methamidophos	10265-92-6	33395	Acaricide/Insecticide		C ₂ H ₈ NO ₂ PS	141.0013	142.0	28	93.9	13	124.9	13	1.14	1	
Methfuroxam	28730-17-8	36157	Fungicide		C ₁₄ H ₁₅ NO ₂	229.1103	230.0	36	137.0	20	111.0	15	5.53	13	
Methidathion	950-37-8	36158	Insecticide		C ₆ H ₁₁ N ₂ O ₄ PS ₃	301.9619	303.0	18	85.1	20	145.0	10	5.45		12
Methiocarb	2032-65-7	PS543	Acaricide/Insecticide	Mercaptodimethur	C ₁₁ H ₁₅ NO ₂ S	225.0824	226.0	28	121.0	22	169.0	10	5.83		14
Methiocarb sulfone	2179-25-1	MET543A	Metabolite		C ₁₁ H ₁₅ NO ₄ S	257.0722	258.1	31	122.1	19	107.1	38	3.59		4
Methiocarb sulfoxide	2635-10-1	34177	Metabolite		C ₁₁ H ₁₅ NO ₃ S	241.0773	242.0	26	185.0	14	122.0	28	3.27		3
Methomyl	16752-77-5	36159	Insecticide		C ₅ H ₁₀ N ₂ O ₂ S	162.0463	163.0	26	88.0	10	106.0	10	2.34	2	
Methoprotrotryne	841-06-5	36160	Herbicide		C ₁₁ H ₂₁ N ₅ OS	271.1467	272.2	40	170.2	28	198.2	22	4.93		9
Methoxyfenozide	161050-58-4		Insecticide		C ₂₂ H ₂₈ N ₂ O ₃	368.2100	369.1	34	149.1	18	313.2	8	6.00		16
Metobromuron	3060-89-7	36162	Herbicide		C ₉ H ₁₁ BrN ₂ O ₂	258.0004	259.1	31	170.0	20	148.1	15	5.14		10
Metolachlor	51218-45-2	36163	Herbicide		C ₁₅ H ₂₂ ClNO ₂	283.1339	284.1	26	176.1	25	252.1	15	6.33	19	
Metolcarb	1129-41-5	33370	Insecticide		C ₉ H ₁₁ NO ₂	165.0790	166.0	20	109.0	12	94.1	27	4.29	6	
Metosulam	139528-85-1	46317	Herbicide		C ₁₄ H ₁₃ Cl ₂ N ₅ O ₄ S	417.0065	418.0	41	175.0	28	140.0	52	4.78		8
Metoxuron	19937-59-8	36164	Herbicide		C ₁₀ H ₁₃ ClN ₂ O ₂	228.0666	229.0	26	72.0	18	155.9	25	4.08		5
Metrafenone	220899-03-6		Fungicide		C ₁₉ H ₂₁ BrO ₅	408.0572	409.0	28	209.1	14	226.9	16	6.81	23	
Metribuzin	21087-64-9	36165	Herbicide		C ₈ H ₁₄ N ₄ OS	214.0888	215.0	41	131.0	18	89.0	20	4.53	7	
Metsulfuron methyl	74223-64-6	46432	Herbicide		C ₁₄ H ₁₅ N ₅ O ₆ S	381.0743	382.0	28	167.0	16	198.9	22	4.67	8	
Mevinphos	7786-34-7	36166	Acaricide/Insecticide		C ₇ H ₁₃ O ₆ P	224.0450	225.1	24	127.1	15	193.1	8	3.37	4	
Molinate	2212-67-1	36171	Herbicide		C ₉ H ₁₇ NOS	187.1031	188.0	26	126.0	13	55.0	24	6.04		16
Monocrotophos	6923-22-4	46159	Acaricide		C ₇ H ₁₄ NO ₅ P	223.0610	224.1	26	127.1	16	98.1	12	2.71		2
Monolinuron	1746-81-2	45590	Herbicide		C ₉ H ₁₁ ClN ₂ O ₂	214.0509	215.0	34	126.0	22	99.0	34	4.93		9
Monuron	150-68-5	36174	Herbicide		C ₉ H ₁₁ ClN ₂ O	198.0560	199.1	31	72.2	16	126.0	25	4.37		6
Myclobutanil	88671-89-0	34360	Fungicide		C ₁₅ H ₁₇ ClN ₄	288.1142	289.1	34	70.2	18	125.1	32	6.08		16
Naproanilide	52570-16-8		Herbicide		C ₁₉ H ₁₇ NO ₂	291.1259	292.2	36	171.1	15	120.1	25	no		
Napropamide	15299-99-7	36175	Herbicide		C ₁₇ H ₂₁ NO ₂	271.1572	272.1	30	129.1	16	171.1	18	6.28		18
Naptalam	132-66-1	33371	Herbicide		C ₁₈ H ₁₃ NO ₃	291.0895	292.1	20	144.1	9	149.1	22	4.69		8
Neburon	555-37-3	36176	Herbicide		C ₁₂ H ₁₆ Cl ₂ N ₂ O	274.0640	275.0	32	88.0	16	57.0	24	6.48		20
Nicosulfuron	111991-09-4	34210	Herbicide		C ₁₅ H ₁₈ N ₆ O ₆ S	410.1009	411.0	32	182.0	22	106.0	32	4.57		7
Nicotine	54-11-5	36733	Insecticide		C ₁₀ H ₁₄ N ₂	162.1157	163.1	36	130.1	18	132.1	15	0.74	1	
Nitenpyram	150824-47-8	46077	Insecticide		C ₁₁ H ₁₅ ClN ₄ O ₂	270.0884	271.1	31	125.9	25	224.9	12	2.15	2	
Nitralin	4726-14-1	36178	Herbicide		C ₁₃ H ₁₉ N ₃ O ₆ S	345.0995	346.1	31	304.1	16	262.1	20	6.41		19
Novaluron	116714-46-6		Insecticide		C ₁₇ H ₉ ClF ₈ N ₂ O ₄	492.0123	493.0	36	158.0	19	141.0	35			
Nuarimol	63284-71-9	36180	Fungicide		C ₁₇ H ₁₂ ClFN ₂ O	314.0622	315.0	46	81.1	28	252.0	22	5.80		14
Ofurace	58810-48-3	46143	Fungicide		C ₁₄ H ₁₆ ClNO ₃	281.0819	282.0	28	254.0	12	160.0	24	4.69		8
Omethoate	1113-02-6	36181	Acaricide/Insecticide		C ₅ H ₁₂ NO ₄ PS	213.0225	214.1	26	125.1	22	183.1	11	1.76		1
Orbencarb	34622-58-7	33362	Herbicide		C ₁₂ H ₁₆ ClNOS	257.0641	258.0	31	125.0	22	99.8	12	6.76		22
Oryzalin	19044-88-3	36182	Herbicide		C ₁₂ H ₁₈ N ₄ O ₆ S	346.0947	347.0	31	288.0	18	305.1	14	6.29		18
Oxadixyl	77732-09-3	34365	Fungicide		C ₁₄ H ₁₈ N ₂ O ₄	278.1267	279.0	40	219.0	10	132.0	34	4.32		
Oxamyl	23135-22-0	36184	Insecticide/Nematicide	Thioxamyl	C ₇ H ₁₃ N ₃ O ₃ S	219.0678	237.0	21	72.0	10	90.0	10	2.13	2	
Oxamyl-oxime	30558-43-1		Metabolite		C ₅ H ₁₀ N ₂ O ₂ S	162.0463	162.9	26	72.0	12	89.9	16	no		
Oxasulfuron	144651-06-9	46416	Herbicide		C ₁₇ H ₁₈ N ₄ O ₆ S	406.0947	407.0	31	150.1	20	107.1	50	4.40	6	

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Oxaziclomefone	153197-14-9		Herbicide		C ₂₀ H ₁₉ Cl ₂ NO ₂	375.0793	376.1	36	190.1	15	161.1	30			
Oxycarboxin	<u>5259-88-1</u>	36185	Fungicide		C ₁₂ H ₁₃ NO ₄ S	267.0565	268.1	26	174.8	16	146.9	25	3.69		4
Oxydemeton-methyl	<u>301-12-2</u>	PS641	Metabolite	Demeton-S-methyl sulfoxide	C ₆ H ₁₅ O ₄ PS ₂	246.0149	247.0	26	168.8	14	108.9	25	2.35		2
Paclobutrazol	<u>76738-62-0</u>	46046	Growth Regulator		C ₁₅ H ₂₀ ClN ₃ O	293.1295	294.1	36	125.1	38	70.2	20	5.95	16	
Paraoxon-methyl	<u>950-35-6</u>	46192	Metabolite		C ₈ H ₁₀ NO ₆ P	247.0246	248.0	36	90.0	25	202.0	19	4.19		5
Parathion	<u>56-38-2</u>	45607	Acaricide/Insecticide		C ₁₀ H ₁₄ NO ₅ PS	291.033	291.9	36	236.0	14.0	110.0	33	6.44		19
Parathion-methyl	<u>298-00-0</u>	36187	Insecticide		C ₈ H ₁₀ NO ₅ PS	263.0017	263.9	38	109.0	22	79.0	36	5.71		
Pebulat	<u>1114-71-2</u>	36188	Herbicide		C ₁₀ H ₂₁ NOS	203.1344	204.1	26	57.2	16	128.0	11	6.83	23	
Penconazole	<u>66246-88-6</u>	36189	Fungicide		C ₁₃ H ₁₅ Cl ₂ N ₃	283.0643	284.0	34	70.1	16	159.0	34	6.58	21	
Pencycuron	<u>66063-05-6</u>	36190	Fungicide		C ₁₉ H ₂₁ ClN ₂ O	328.1342	329.1	40	125.0	40	125.1	22	6.84	23	
Pendimethalin	<u>40487-42-1</u>	36191	Herbicide		C ₁₃ H ₁₉ N ₃ O ₄	281.1376	282.2	21	212.2	10	194.1	17	7.40	26	
Penoxsulam	219714-96-2		Herbicide		C ₁₆ H ₁₄ F ₅ N ₅ O ₅ S	483.0636	484.2	51	195.1	30	164.1	40			
Pentoxazone	110956-75-7		Herbicide		C ₁₇ H ₁₇ ClFNO ₄	353.0830	354.0	28	285.9	14	185.9	26			
Phenmedipham	<u>13684-63-4</u>	36192	Herbicide		C ₁₆ H ₁₆ N ₂ O ₄	300.1110	301.0	34	168.0	10	136.0	22	5.57	13	
Phenthoate	<u>2597-03-7</u>	46079	Insecticide		C ₁₂ H ₁₇ O ₄ PS ₂	320.0306	321.0	18	163.0	12	135.0	20	6.47	20	
Phorate	<u>298-02-2</u>	33388	Insecticide		C ₇ H ₁₇ O ₂ PS ₃	260.0128	261.0	17	75.0	12	97.0	32	6.74		22
Phorate sulfone	<u>2588-04-7</u>	46031	Metabolite		C ₇ H ₁₇ O ₄ PS ₃	292.0027	293.0	24	96.9	30	115.0	24	5.20		10
Phorate sulfoxide	<u>2588-03-6</u>	45762	Metabolite		C ₇ H ₁₇ O ₃ PS ₃	276.0077	277.0	24	96.9	32	143.0	20	5.13		10
Phosalone	<u>2310-17-0</u>	36194	Acaricide/Insecticide		C ₁₂ H ₁₅ ClNO ₄ PS ₂	366.9869	367.9	22	181.9	14	110.9	42	6.75		22
Phosfolan	947-02-4	PS842	Insecticide		C ₇ H ₁₄ NO ₃ PS ₂	255.0153	256.0	26	140.0	20	168.0	20	4.03		
Phosmet	<u>732-11-6</u>	36195	Insecticide	PMP	C ₁₁ H ₁₂ NO ₄ PS ₂	316.9945	318.0	28	160.0	22	77.0	46	4.22		
Phosmet-oxon	3735-33-9	MET65 3A	Metabolite		C ₁₁ H ₁₂ NO ₅ PS	301.0174	302.0	28	160.0	16	77.0	50	no		
Phosphamidon	<u>13171-21-6</u>	45622	Insecticide/Nematicide		C ₁₀ H ₁₉ ClNO ₅ P	299.0689	300.1	28	174.1	14	127.1	25	4.40	6	
Phoxim	<u>14816-18-3</u>	36197	Insecticide		C ₁₂ H ₁₅ N ₂ O ₃ PS	298.0541	299.0	22	129.0	13	153.0	7	6.69	22	
Picloram	<u>1918-02-1</u>	36774	Herbicide		C ₆ H ₃ Cl ₃ N ₂ O ₂	239.9260	241.0	26	195.0	21	168.0	30	2.79		2
Picolinafen	<u>137641-05-5</u>	37912	Herbicide		C ₁₉ H ₁₂ F ₄ N ₂ O ₂	376.0835	377.0	38	238.0	28	359.0	21	7.19	25	
Picoxystrobin	<u>117428-22-5</u>	33658	Fungicide		C ₁₈ H ₁₆ F ₃ NO ₄	367.1031	368.0	20	145.1	22	205.1	10	6.41		19
Piperonyl butoxide	<u>51-03-6</u>	45626	Antiparasiticide/Synergist		C ₁₉ H ₃₀ O ₅	338.2093	356.3	26	176.9	11	119.0	37	7.24		25
Piperophos	<u>24151-93-7</u>	46011	Herbicide		C ₁₄ H ₂₈ NO ₃ PS ₂	353.1248	354.1	31	171.0	22	143.0	32	6.89		23
Pirimicarb	<u>23103-98-2</u>	45627	Insecticide		C ₁₁ H ₁₈ N ₄ O ₂	238.1430	239.1	34	72.0	18	182.1	15	3.55		3
Pirimiphos-ethyl	<u>23505-41-1</u>	45628	Insecticide		C ₁₃ H ₂₄ N ₃ O ₃ PS	333.1276	334.1	42	198.1	23	182.1	25	7.09		24
Pirimiphos-methyl	<u>29232-93-7</u>	45629	Insecticide		C ₁₁ H ₂₀ N ₃ O ₃ PS	305.0963	306.1	36	164.1	22	108.1	32	6.58	21	
Primisulfuron-methyl	<u>86209-51-0</u>	46010	Herbicide		C ₁₅ H ₁₂ F ₄ N ₄ O ₇ S	366.9869	469.0	16	254.0	20	199.0	20	6.02		
Probenazole	27605-76-1		Fungicide		C ₁₀ H ₉ NO ₃ S	223.0303	224.0	22	41.5	10	196.1	13	4.38		
Procloraz	<u>67747-09-5</u>	45631	Fungicide		C ₁₅ H ₁₆ Cl ₃ N ₃ O ₂	375.0308	376.0	22	307.1	16	70.1	34	6.53		20
Procymidone	<u>32809-16-8</u>	36640	Fungicide		C ₁₃ H ₁₁ Cl ₂ NO ₂	283.0167	284.1	42	67.1	28	256.1	17	no		
Profenofos	<u>41198-08-7</u>	45632	Insecticide		C ₁₁ H ₁₅ BrClO ₃ PS	371.9351	372.9	36	302.6	20	127.9	40	7.12		24
Promecarb	<u>2631-37-0</u>	45634	Insecticide		C ₁₂ H ₁₇ NO ₂	207.1259	208.1	26	151.0	9	109.0	15	5.94		15
Prometon	<u>1610-18-0</u>	45635	Herbicide		C ₁₀ H ₁₉ N ₅ O	225.1590	226.0	38	86.3	28	184.3	18	4.57		6
Prometryn	<u>7287-19-6</u>	45636	Herbicide		C ₁₀ H ₁₉ N ₅ S	241.1361	242.0	26	158.0	25	200.1	17	5.44	12	
Propachlor	<u>1918-16-7</u>	45637	Herbicide		C ₁₁ H ₁₄ ClNO	211.0764	212.1	31	170.1	14	94.1	25	5.31		11
Propamocarb	<u>24579-73-5</u>	45638	Herbicide		C ₉ H ₂₀ N ₂ O ₂	188.1525	189.1	31	102.0	17	144.0	12	1.82		1
Propanil	<u>709-98-8</u>	45639	Herbicide		C ₉ H ₉ Cl ₂ NO	217.0061	217.9	40	161.9	16	127.0	22	5.79		14
Propaquizafop	<u>111479-05-1</u>	46007	Herbicide		C ₂₂ H ₂₂ ClN ₃ O ₅	443.1248	444.2	36	100.0	20	163.1	60	7.18	25	
Propargite	<u>2312-35-8</u>	45310	Acaricide		C ₁₉ H ₂₆ O ₄ S	350.1552	351.1	14	231.1	5	57.0	20	no		
Propazine	<u>139-40-2</u>	45640	Herbicide		C ₉ H ₁₆ ClN ₅	229.1094	230.2	40	146.1	24	188.1	18	5.75	14	
Propetamphos	<u>31218-83-4</u>	34371	Insecticide		C ₁₀ H ₂₀ NO ₄ PS	281.0851	282.0	17	138.0	20	156.0	12	6.07		16
Propham	<u>122-42-9</u>	45641	Herbicide		C ₁₀ H ₁₃ NO ₂	179.0946	180.0	14	138.0	8	120.0	16	5.15		10

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Propiconazole	60207-90-1	45642	Fungicide		C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	341.0698	342.0	46	69.0	22	159.0	34	6.65		21
Propoxur	114-26-1	45644	Insecticide		C ₁₁ H ₁₅ NO ₃	209.1052	210.0	21	111.0	16	168.0	10	4.58		7
Propyzamide	23950-58-5	45645	Herbicide		C ₁₂ H ₁₁ Cl ₂ NO	255.0218	256.1	31	190.0	16	173.0	23	5.98	16	
Prosulfocarb	52888-80-9	36520	Herbicide		C ₁₄ H ₂₁ NOS	251.1344	252.0	29	90.9	22	127.9	13	7.04		24
Prosulfuron	94125-34-5	46104	Herbicide		C ₁₅ H ₁₆ F ₃ N ₅ O ₄ S	419.0875	420.0	32	141.0	20	167.0	20	5.80		14
Prothioconazole	178928-70-6	34232	Fungicide		C ₁₄ H ₁₅ Cl ₂ N ₃ OS	343.0313	344.0	22	326.0	12	189.0	20	6.71		
Pymetrozine	123312-89-0	46119	Insecticide		C ₁₀ H ₁₁ N ₅ O	217.0964	218.0	38	105.0	20	79.0	30	1.43	1	
Pyracarbolid	24691-76-7	45646	Fungicide		C ₁₃ H ₁₅ NO ₂	217.1103	218.1	32	125.1	18	97.1	28	4.66	8	
Pyraclostrobin	175013-18-0	33696	Fungicide		C ₁₉ H ₁₈ ClN ₃ O ₄	387.0986	388.1	31	163.0	25	193.9	12	6.70	22	
Pyrazolynate	58011-68-0		Herbicide	Pyrazolate	C ₁₉ H ₁₆ Cl ₂ N ₂ O ₄ S	438.0208	439.1	34	91.0	42	172.9	20			
Pyrazophos	13457-18-6	45648	Fungicide		C ₁₄ H ₂₀ N ₃ O ₅ PS	373.0861	374.0	44	222.1	22	194.0	32	6.75		22
Pyrazosulfuron-ethyl	93697-74-6	46323	Herbicide		C ₁₄ H ₁₈ N ₆ O ₇ S	414.0958	415.0	28	182.0	20	82.9	45	6.16		17
Pyridaben	96489-71-3	46047	Acaricide/Insecticide		C ₁₉ H ₂₅ ClN ₂ OS	364.1376	365.1	28	147.1	24	309.1	12	7.71		26
Pyridafol	40020-01-7		Metabolite	6-chloro-4-hydroxy-3-phenylpyridazin	C ₁₀ H ₇ ClN ₂ O	206.0247	207.0	46	103.9	22	77.0	30	4.03		5
Pyridaphenthion	119-12-0	36895	Insecticide		C ₁₄ H ₁₇ N ₂ O ₄ PS	340.0647	341.0	40	189.0	22	92.0	34	6.07		16
Pyridate	55512-33-9	45312	Herbicide		C ₁₉ H ₂₃ ClN ₂ O ₂ S	378.1169	379.0	28	207.0	18	351.1	10	7.88		26
Pyrifenoxy	88283-41-4	45737	Fungicide		C ₁₄ H ₁₂ Cl ₂ N ₂ O	294.0327	295.0	38	93.1	22	67.2	60	5.60		12
Pyrifthalid	135186-78-6	33694	Herbicide		C ₁₅ H ₁₄ N ₂ O ₄ S	318.0674	319.1	51	139.1	25	179.1	30			
Pyrimethanil	53112-28-0	46039	Fungicide		C ₁₂ H ₁₃ N ₃	199.1109	200.0	51	107.0	24	82.0	24	5.03	9	
Pyriproxifen	95737-68-1	34174	Growth Regulator		C ₂₀ H ₁₉ NO ₃	321.1365	322.1	32	96.0	14	227.1	14	7.27		25
Pyroquilon	57369-32-1	45650	Fungicide		C ₁₁ H ₁₁ NO	173.0841	174.0	41	132.0	23	117.0	30	4.49	7	
Quinalphos	13593-03-8	45651	Acaricide/Insecticide		C ₁₂ H ₁₅ N ₂ O ₃ PS	298.0541	299.0	24	162.9	24	96.9	30	6.47	20	
Quinmerac	90717-03-6	36522	Herbicide		C ₁₁ H ₈ ClNO ₂	221.0244	222.2	28	204.2	15	141.1	30	3.36	4	
Quinoxifen	124495-18-7	46439	Fungicide		C ₁₅ H ₈ Cl ₂ FNO	306.9967	308.0	61	197.0	32	161.9	44	7.33		25
Quizalofop-ethyl	76578-14-8	34306	Herbicide		C ₁₉ H ₁₇ ClN ₂ O ₄	372.0877	373.0	40	299.1	18	91.1	32	7.08		24
Quizalofop-methyl	76578-13-7		Herbicide		C ₁₈ H ₁₅ ClN ₂ O ₄	358.0720	359.0	40	299.1	18	91.1	28	6.84	23	
Quizalofop-p-tefuryl	200509-41-7	33942	Herbicide		C ₂₂ H ₂₁ ClN ₂ O ₅	428.1139	429.1	34	299.0	22	147.1	27			
Rabenzazol	40341-04-6	45654	Fungicide		C ₁₂ H ₁₂ N ₄	212.1062	213.1	40	172.1	20	118.1	35	5.16		10
Rimsulfuron	122931-48-0	46097	Herbicide		C ₁₄ H ₁₇ N ₅ O ₇ S ₂	431.0569	431.9	34	325.1	14	182.1	22	4.94		
Rotenone	83-79-4	45656	Insecticide		C ₂₃ H ₂₂ O ₆	394.1416	395.0	46	213.1	24	192.1	24	6.39	19	
Sebuthylazin	7286-69-3	36785	Herbicide		C ₉ H ₁₆ ClN ₅	229.1094	230.0	36	174.0	18	96.0	26	5.70	15	
Sebuthylazin-desethyl	37019-18-4	36511	Metabolite		C ₇ H ₁₂ ClN ₅	201.0781	202.2	36	146.1	17	79.2	25	4.37	6	
Secbumeton	26259-45-0	45658	Herbicide		C ₁₀ H ₁₉ N ₅ O	225.1590	226.2	36	170.2	19	100.2	28	4.39	6	
Sethoxydim	74051-80-2	36795	Herbicide		C ₁₇ H ₂₉ NO ₃ S	327.1868	328.0	34	178.0	22	282.0	10	7.16	25	
Siduron	1982-49-6	34373	Herbicide		C ₁₄ H ₂₀ N ₂ O	232.1576	233.0	36	93.8	25	137.0	17	5.76	14	
Simazine	122-34-9	45659	Herbicide		C ₇ H ₁₂ ClN ₅	201.0781	202.0	40	124.0	16	96.0	22	4.57		7
Simeconazole	149508-90-7		Fungicide		C ₁₄ H ₂₀ FN ₃ OSi	293.1360	294.1	32	70.1	22	141.0	25	5.99		15
Simetryn	1014-70-6	45660	Herbicide		C ₈ H ₁₅ N ₅ S	213.1048	214.0	41	124.0	20	95.9	25	4.27		5
Spinosad A	131929-60-7		Insecticide		C ₄₁ H ₆₅ NO ₁₀	731.4608	732.6	56	142.0	31	98.1	59	6.43		18
Spinosad D	131929-63-0		Insecticide		C ₄₂ H ₆₇ NO ₁₀	745.4765	746.5	51	142.0	31	98.1	53	6.61		19
Spirodiclofen	148477-71-8	33654	Acaricide		C ₂₁ H ₂₄ Cl ₂ O ₄	410.1052	411.1	31	71.2	13	313.0	13	7.57		
Spiromesifen	283594-90-1	33599	Insecticide		C ₂₃ H ₃₀ O ₄	370.2144	371.1	16	273.1	10	255.1	24	7.43	26	
Spiroxamine	118134-30-8	46443	Fungicide		C ₁₈ H ₃₅ NO ₂	297.2668	298.0	38	144.0	20	100.0	32	5.44	13	
Sulcotrione	99105-77-8	46318	Herbicide		C ₁₄ H ₁₃ ClO ₅ S	328.0172	329.0	36	139.1	18	69.2	38	4.42	6	
Sulfallate	95-06-7	45663	Herbicide		C ₈ H ₁₄ CINS ₂	223.0256	224.0	22	116.0	12	87.9	20	6.54		20
Sulfaquinoxaline	59-40-5	45662	Rodenticide		C ₁₄ H ₁₂ N ₄ O ₂ S	300.0681	301.1	32	156.1	16	92.2	30	3.91	5	
Sulfentrazone	122836-35-5		Herbicide		C ₁₁ H ₁₀ Cl ₂ F ₂ N ₄ O ₃ S	385.9819	387.0	36	307.0	20	145.8	46			
Sulfometuron-methyl	74222-97-2	34224	Metabolite		C ₁₅ H ₁₆ N ₄ O ₅ S	364.0841	365.0	30	150.0	18	107.0	43	4.65	8	
Sulfosulfuron	141776-32-1	33307	Herbicide		C ₁₆ H ₁₈ N ₆ O ₇ S ₂	470.0678	471.0	29	211.0	13	261.0	18	5.69		13

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Sulfotep	3689-24-5	45664	Insecticide		C ₈ H ₂₀ O ₅ P ₂ S ₂	322.0227	323.0	28	97.0	32	171.0	15	6.51		20
Tebuconazole	107534-96-3	36565	Fungicide		C ₁₆ H ₂₂ ClN ₃ O	307.1451	308.0	40	70.1	22	125.0	40	6.58	21	
Tebufenozide	112410-23-8	46095	Insecticide		C ₂₂ H ₂₈ N ₂ O ₂	352.2151	353.1	19	133.0	20	297.1	8	6.43		19
Tebufenpyrad	119168-77-3	46438	Acaricide/Insecticide		C ₁₈ H ₂₄ ClN ₃ O	333.1608	334.0	52	117.0	34	145.0	28	7.19	25	
Tebupirimfos	96182-53-5	46075	Insecticide		C ₁₃ H ₂₃ N ₂ O ₃ PS	318.1167	319.0	29	153.0	29	277.0	15	7.21		25
Tebutam	35256-85-0	36566	Herbicide		C ₁₅ H ₂₃ NO	233.1780	234.1	33	91.0	18	192.1	18	6.31	19	
Tebuthiuron	34014-18-1	45671	Herbicide		C ₉ H ₁₆ N ₄ OS	228.1045	229.0	36	172.0	18	116.0	26	4.75		8
Teflubenzuron	83121-18-0	45756	Insecticide		C ₁₄ H ₆ Cl ₂ F ₄ N ₂ O ₂	379.9742	380.9	26	158.0	20	140.9	40	7.29		
Temephos	3383-96-8	45673	Insecticide		C ₁₆ H ₂₀ O ₆ P ₂ S ₃	465.9897	466.8	38	125.0	38	418.9	22	7.20	25	
TEPP	107-49-3	36567	Acaricide/Insecticide	Tetraethyl diphosphate	C ₈ H ₂₀ O ₇ P ₂	290.0684	291.0	34	179.0	22	99.0	34			
Tepraloxymid	149979-41-9	46331	Herbicide		C ₁₇ H ₂₄ ClNO ₄	341.1394	342.1	26	250.1	12	166.1	20	6.13		17
Terbufos	13071-79-9	45313	Insecticide		C ₉ H ₂₁ O ₂ PS ₃	288.0441	289.0	18	103.0	8	57.2	22	7.16		24
Terbufos-sulfone	56070-16-7	46043	Metabolite		C ₉ H ₂₁ O ₄ PS ₃	320.0340	321.0	20	97.0	40	171.0	12	5.65		13
Terbufos-sulfoxide	10548-10-4	46044	Metabolite		C ₉ H ₂₁ O ₃ PS ₃	304.0390	305.0	20	187.0	11	97.0	40	5.66		13
Terbumeton	33693-04-8	45676	Herbicide		C ₁₀ H ₁₉ N ₅ O	225.1590	226.1	21	170.1	15	114.1	25	4.55	6	
Terbumeton-desethyl	30125-64-5	36514	Metabolite		C ₈ H ₁₅ N ₅ O	197.1277	198.2	32	142.1	16	86.1	24	3.35	4	
Terbutylazine	5915-41-3	45678	Herbicide		C ₉ H ₁₆ ClN ₅	229.1094	230.0	34	174.0	16	96.0	28	5.82		14
Terbutylazine-2-hydroxy	66753-07-9	46019	Metabolite		C ₉ H ₁₇ N ₅ O	211.1433	212.2	30	156.1	15	86.1	24	3.26		3
Terbutylazine-desethyl	30125-63-4	36769	Metabolite		C ₇ H ₁₂ ClN ₅	201.0781	202.1	30	146.1	16	79.1	26	4.78		8
Terbutryn	886-50-0	45677	Herbicide		C ₁₀ H ₁₉ N ₅ S	241.1361	242.1	40	186.1	20	91.0	28	5.49		11
Tetrachlorvinphos	22248-79-9	45679	Insecticide		C ₁₀ H ₉ Cl ₄ O ₄ P	363.8993	364.8	32	127.0	16	238.9	20	6.47	20	
Tetraconazole	112281-77-3		Fungicide		C ₁₃ H ₁₁ Cl ₂ F ₄ N ₃ O	371.0215	372.0	41	70.1	20	159.0	30	6.25		18
Thiabendazole	148-79-8	45684	Fungicide		C ₁₀ H ₇ N ₃ S	201.0361	202.0	51	175.0	25	131.0	30	2.66		2
Thiacloprid	111988-49-9	37905	Insecticide		C ₁₀ H ₉ ClN ₄ S	252.0236	253.0	41	126.0	20	90.1	40	3.76	5	
Thiamethoxam	153719-23-4	37924	Insecticide		C ₈ H ₁₀ ClN ₅ O ₃ S	291.0193	292.0	28	211.2	12	132.0	22	2.56		2
Thiazafuron	25366-23-8	45685	Herbicide		C ₆ H ₇ F ₃ N ₄ OS	240.0293	241.0	27	184.0	15	73.9	32	4.71		8
Thiazopyr	117718-60-2		Herbicide		C ₁₆ H ₁₇ F ₅ N ₂ O ₂ S	396.0931	397.1	36	377.1	23	317.1	25			
Thidiazuron	51707-55-2	45686	Herbicide		C ₉ H ₈ N ₄ OS	220.0419	221.0	28	101.9	15	93.9	13	4.63	8	
Thifensulfuron methyl	79277-27-3	46028	Herbicide		C ₁₂ H ₁₃ N ₅ O ₆ S ₂	387.0307	388.0	36	167.0	15	56.0	40	4.54	7	
Thiodicarb	59669-26-0	34375	Insecticide		C ₁₀ H ₁₈ N ₄ O ₄ S ₃	354.0490	355.0	26	87.9	16	107.9	16	5.01	10	
Thiofanox	39196-18-4	45314	Insecticide		C ₉ H ₁₈ N ₂ O ₂ S	218.1089	219.0	16	57.0	12	76.0	8	5.05	10	
Thiofanox-sulfone	39184-59-3	45764	Metabolite		C ₉ H ₁₈ N ₂ O ₄ S	250.0987	251.1	18	57.2	10	76.1	6	3.26	4	
Thiometon sulfoxide	39184-27-5	45765	Metabolite		C ₆ H ₁₅ O ₃ PS ₃	261.9921	263.0	26	124.8	25	92.9	30	no		
Thiophanate	23564-06-9	PS223	Fungicide		C ₁₄ H ₁₈ N ₄ O ₄ S ₂	370.0769	371.0	28	151.0	22	93.1	50	5.37		11
Thiophanate-methyl	23564-05-8	45688	Fungicide		C ₁₂ H ₁₄ N ₄ O ₄ S ₂	342.0456	343.0	28	151.0	22	93.0	46	4.58		7
Thiuram	137-26-8	45689	Fungicide	Tetramethylthiuram disulfide	C ₆ H ₁₂ N ₂ S ₄	239.9883	241.0	19	87.9	11	119.9	16	no		
Tolcofos methyl	57018-04-9	36641	Fungicide		C ₉ H ₁₁ Cl ₂ O ₃ PS	299.9544	301.1	41	125.0	17	174.9	29	no		
Tolyfluanid	731-27-1	45690	Fungicide		C ₁₀ H ₁₃ Cl ₂ FN ₂ O ₂ S ₂	345.9780	347.0	25	137.0	28	238.0	10	6.53		20
Topramezone	210631-68-8	34225	Herbicide		C ₁₆ H ₁₇ N ₃ O ₅ S	363.0889	364.0	31	334.0	16	125.0	29	3.17		3
Tralkoxidym	87820-88-0	36536	Herbicide		C ₂₀ H ₂₇ NO ₃	329.1991	330.2	31	138.1	19	284.3	13	7.37	26	
Triadimefon	43121-43-3	45693	Fungicide		C ₁₄ H ₁₆ ClN ₃ O ₂	293.0931	294.1	31	69.3	20	197.2	15	5.94		16
Triadimenol	55219-65-3	46138	Fungicide		C ₁₄ H ₁₈ ClN ₃ O ₂	295.1088	296.1	21	70.2	10	99.1	15	6.15		17
Triallate	2303-17-5	45695	Herbicide		C ₁₀ H ₁₆ Cl ₃ NOS	303.0018	304.0	32	86.0	18	142.9	28	7.41	26	
Triasulfuron	82097-50-5	33383	Herbicide		C ₁₄ H ₁₆ ClN ₅ O ₅ S	401.0561	402.0	31	167.1	17	141.0	20	4.54	7	
Triasulfuron methyl	126535-15-7		Herbicide		C ₁₃ H ₁₄ ClN ₅ O ₅ S	387.0404	388.2	26	167.2	20	141.1	20			
Triazophos	24017-47-8	45696	Acaricide/Neematicide		C ₁₂ H ₁₆ N ₃ O ₃ PS	313.0650	314.1	31	161.9	18	118.9	35	6.12	17	
Triazoxid	72459-58-6	33373	Fungicide		C ₁₀ H ₆ ClN ₅ O	247.0261	248.0	48	68.1	28	95.0	26	4.39		6
Tribenuron methyl	101200-48-0	46013	Herbicide		C ₁₅ H ₁₇ N ₅ O ₆ S	395.0900	396.1	24	154.9	14	180.9	22	no		

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Method 1 Function	Method 2 Function
Trichlorfon	52-68-6	45698	Insecticide		C ₄ H ₈ Cl ₃ O ₄ P	255.9226	257.0	28	109.0	18	79.0	30	3.31		3
Tricyclazole	41814-78-2	45808	Fungicide		C ₉ H ₇ N ₃ S	189.0361	190.0	41	163.0	22	136.0	27	3.94	5	
Tridemorph	24602-86-6	36199	Fungicide		C ₁₉ H ₃₉ NO	297.3032	298.1	52	57.0	28	98.0	34	no		
Trietazine	1912-26-1	46086	Herbicide		C ₉ H ₁₆ ClN ₅	229.1094	230.0	41	98.9	23	70.9	30	6.21	18	
Trifloxystrobin	141517-21-7	46447	Fungicide		C ₂₀ H ₁₉ F ₃ N ₂ O ₄	408.1297	409.0	34	186.0	16	145.0	40	6.93	24	
Trifloxysulfuron	199119-58-9	33672	Herbicide		C ₁₄ H ₁₄ F ₃ N ₅ O ₆ S	437.0617	438.0	30	182.0	20	139.0	45	5.26	11	
Triflumizole	99387-89-0		Fungicide		C ₁₅ H ₁₅ ClF ₃ N ₃ O	345.0856	346.0	22	277.9	10	60.0	10	6.87		23
Triflumuron	64628-44-0	35029	Insecticide		C ₁₅ H ₁₀ ClF ₃ N ₂ O ₃	358.0332	359.0	31	156.1	16	139.1	35	6.71	22	
Triflurosulfuron-methyl	126535-15-7	46326	Herbicide		C ₁₇ H ₁₉ F ₃ N ₆ O ₆ S	492.1039	493.2	34	264.0	18	96.0	45	5.87	15	
Triticonazole	131983-72-7	34172	Fungicide		C ₁₇ H ₂₀ ClN ₃ O	317.1295	318.1	31	70.1	16	124.9	35	2.56		2
Tritosulfuron	142469-14-5	33873	Herbicide		C ₁₃ H ₉ F ₆ N ₅ O ₄ S	445.0279	446.0	36	195.0	18	145.0	34	no		
Vamidothion	2275-23-2	37914	Acaricide/Insecticide		C ₈ H ₁₈ NO ₄ PS ₂	287.0415	288.0	28	146.0	10	118.0	28	3.38	4	
Vamidothion sulfone	70898-34-9		Metabolite		C ₈ H ₁₈ NO ₆ PS ₂	319.0313	320.0	36	177.9	14	86.0	25	2.55		
Vamidothion sulfoxide	20300-00-9		Metabolite		C ₈ H ₁₈ NO ₅ PS ₂	303.0364	304.2	38	201.0	15	169.0	15			
Vernolat	1929-77-7	45704	Herbicide		C ₁₀ H ₂₁ NOS	203.1344	204.1	28	128.1	11	86.1	14	6.83	23	
Zoxamide	156052-68-5		Fungicide		C ₁₄ H ₁₆ Cl ₃ NO ₂	335.0247	336.0	38	187.1	25	159.0	38	6.67		21

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
3,4,5-Trimethacarb	2655-15-4	37874	Insecticide		$C_{11}H_{15}NO_2$	193.1103	194.1	16	137.1	12	122.1	26	5.41	1.98E+06	12	
Abamectin (B1a)	71751-41-2	46392	Insecticide/Acaricide				890.7	18	305.1	22	567.2	10	7.82	1.17E+03		
Acephate	30560-19-1	45315	Insecticide		$C_4H_{10}NO_3PS$	183.0119	184.1	11	143.0	8	125.1	18	1.47	3.62E+06	1	
Acetamiprid	135410-20-7	33674	Insecticide		$C_{10}H_{11}ClN_4$	222.0672	223.0	28	126.0	20	56.1	15	3.41	4.43E+06	4	
Acibenzolar-S-methyl	135158-54-2		Fungicide		$C_8H_6N_2OS_2$	209.9922	210.9	44	135.9	30	69.0	52	5.78	1.82E+05		14
Acitidone	66-81-9	46401	Fungicide	Cycloheximid	$C_{15}H_{23}NO_4$	281.1627	282.1	20	264.1	11	246.1	14	4.28	1.94E+05		5
Aclonifen	74070-46-5	36792	Herbicide		$C_{12}H_9ClN_2O_3$	264.0302	265.0	24	248.0	18	182.1	32	6.51	4.46E+03		
Acrinathrin	101007-06-1	46415	Insecticide/Acaricide		$C_{26}H_{21}F_6NO_5$	541.1324	542.0	18	181.0	36	208.0	12	no	no		
Alachlor	15972-60-8	45316	Herbicide		$C_{14}H_{20}ClNO_2$	269.1183	271.1	22	162.1	20	238.1	11	6.30	2.33E+05		
Aldicarb	116-06-3	33386	Insecticide/Acaricide		$C_7H_{14}N_2O_2S$	190.0776	213.1	24	89.1	16	116.1	11	3.98	1.73E+07	5	
Aldicarb sulfone	1646-88-4	33387	Metabolite	Aldoxycarb	$C_7H_{14}N_2O_4S$	222.0674	223.0	25	148.0	10	86.0	14	2.04	5.29E+05	2	
Aldicarb sulfoxide	1646-87-3	36784	Metabolite		$C_7H_{14}N_2O_3S$	206.0725	207.0	16	89.0	14	132.0	10	1.91	2.54E+06	2	
Ametryn	834-12-8	45321	Herbicide		$C_9H_{17}N_5S$	227.1205	228.1	32	186.1	18	68.1	36	4.88	9.73E+07		8
Amidosulfuron	120923-37-7	33588	Herbicide		$C_9H_{15}N_5O_7S_2$	369.0413	370.0	22	261.0	15	218.0	25	4.95	2.08E+06		9
Aminocarb	2032-59-9	45322	Insecticide		$C_{11}H_{16}N_2O_2$	208.1212	209.0	24	137.0	22	152.0	14	1.63	2.14E+07		1
Amitraz	33089-61-1	45323	Acaricide		$C_{19}H_{23}N_3$	293.1892	294.0	25	122.0	35	163.0	18	no	no		
Amitrole	61-82-5	45324	Herbicide		$C_2H_4N_4$	84.0436	85.1	32	57.3	12	43.4	15	0.53	1.34E+06	1	
Anilazine	101-05-3	45325	Fungicide		$C_9H_5Cl_3N_4$	273.9580	274.9	40	153.0	26	178.0	24	5.98	3.62E+05	16	
Anilofos	64249-01-0	37876	Herbicide		$C_{13}H_{19}ClNO_3PS_2$	367.0233	367.9	24	124.9	34	198.9	15	6.57	7.59E+06		21
Asulam	3337-71-1	45329	Herbicide		$C_8H_{10}N_2O_4S$	230.0361	230.9	16	155.9	12	92.0	22	1.82	8.38E+05		1
Atraton	1610-17-9	36630	Herbicide	Atrazine-methoxy	$C_9H_{17}N_5O$	211.1433	212.0	34	170.1	18	100.0	28	3.96	4.46E+07		4
Atrazine	1912-24-9	45330	Herbicide		$C_8H_{14}ClN_5$	215.0938	216.1	33	174.1	18	96.1	23	5.20	2.08E+07		10
Atrazine-desethyl	6190-65-4	36629	Metabolite		$C_6H_{10}ClN_5$	187.0625	188.0	28	146.0	16	78.9	26	3.69	6.87E+06		4
Atrazine-desisopropyl	1007-28-9	36628	Metabolite		$C_5H_8ClN_5$	173.0468	174.0	34	96.0	18	78.9	18	2.85	8.57E+05		2
Azaconazole	60207-31-0	34045	Fungicides		$C_{12}H_{11}Cl_2N_3O_2$	299.0228	300.0	28	159.0	28	231.1	18	5.44	6.65E+07	12	
Azafenidin	68049-83-2		Herbicide		$C_{15}H_{13}Cl_2N_3O_2$	337.0385	338.1	50	264.1	29	299.1	20				
Azamethiphos	35575-96-3	45331	Insecticide		$C_9H_{10}ClN_2O_5PS$	323.9737	325.0	25	111.9	35	138.9	24	4.48	3.46E+06	6	
Azimsulfuron	120162-55-2		Herbicide		$C_{13}H_{16}N_{10}O_5S$	424.1026	425.0	35	182.0	20	139.1	40				
Azinphos-ethyl	2642-71-9	45332	Insecticide/Acaricide		$C_{12}H_{16}N_3O_3PS_2$	345.0371	346.0	10	132.0	16	77.1	36	6.20	2.35E+06	18	
Azinphos-methyl	86-50-0	45333	Insecticide/Acaricide		$C_{10}H_{12}N_3O_3PS_2$	317.0058	318.0	14	160.0	8	261.0	8	5.56	1.66E+06	13	
Aziprotryne	4658-28-0	45334	Herbicide		$C_7H_{11}N_7S$	225.0797	226.0	20	156.0	16	68.0	30	5.95	2.28E+06		15
Azobenzene	103-33-3	36689	Acaricide		$C_{12}H_{10}N_2$	182.0844	183.0	26	76.9	18	51.0	40	5.36	7.68E+05		11
Azoxystrobin	131860-33-8	46160	Fungicide		$C_{22}H_{17}N_3O_5$	403.1168	404.0	22	372.0	15	329.0	30	5.73	1.55E+07	14	
Benalaxyl	71626-11-4	36760	Fungicide		$C_{20}H_{23}NO_3$	325.1678	326.1	20	148.0	20	91.0	34	6.62	2.37E+07		21
Benazolin	3813-05-06	33380	Herbicide		$C_9H_6ClNO_3S$	242.9757	243.9	16	170.0	20	197.9	12	4.53	1.82E+05	7	
Bendiocarb	22781-23-3	45336	Insecticide		$C_{11}H_{13}NO_4$	223.0845	224.1	20	167.0	8	109.0	18	4.62	8.29E+06	8	
Benfluralin	1861-40-1	45337	Herbicide		$C_{13}H_{16}F_3N_3O_4$	335.1093	336.0	28	57.0	18	236.0	15	no	no		
Benfuracarb	82560-54-1	45759	Insecticide		$C_{20}H_{30}N_2O_5S$	410.1875	411.1	17	195.0	23	190.0	13	7.07	1.39E+06		24
Benfuresate	68505-69-1	46088	Herbicide		$C_{12}H_{16}O_4S$	256.0769	257.0	22	163.0	12	121.0	22	5.43	5.36E+04	12	
Benomyl	17804-35-2	45339	Fungicide		$C_{14}H_{18}N_4O_3$	290.1379	291.0	16	160.0	28	192.0	16	5.50	4.28E+03		
Bensulfuron methyl	83055-99-6	37897	Herbicide		$C_{16}H_{18}N_4O_7S$	410.0896	411.1	27	149.0	22	182.0	20	5.58	3.59E+06	13	
Bensulide	741-58-2	45340	Herbicide		$C_{14}H_{24}NO_4PS_3$	397.0605	398.0	12	157.9	24	313.9	10	6.44	3.15E+05		19
Bentazone	25057-89-0	45341	Herbicide		$C_{10}H_{12}N_2O_3S$	240.0569	241.1	15	199.1	12	107.2	26	4.72	7.61E+04		8
Benzofenap	82692-44-2		Herbicide		$C_{22}H_{20}Cl_2N_2O_3$	430.0851	431.1	40	119.0	20	105.0	28				
Benzoximate	29104-30-1	33397	Acaricide		$C_{18}H_{18}ClNO_5$	363.0874	364.0	12	199.1	8	105.0	26	6.77	1.73E+05		22
Benzthiazuron	1929-88-0	36563	Herbicide		$C_9H_9N_3OS$	207.0466	208.0	22	151.0	16	109.0	36	4.61	3.83E+06		7
Bifenazate	149877-41-8		Acaricide		$C_{17}H_{20}N_2O_3$	300.1474	301.1	10	198.0	10	170.0	20	6.13	9.06E+04	17	
Bifenox	42576-02-3	45345	Herbicide		$C_{14}H_9Cl_2NO_5$	340.9858	341.9	10	309.9	10	188.9	22	no	no		
Bitertanol	55179-31-2	45349	Fungicide		$C_{20}H_{23}N_3O_2$	337.1790	338.1	15	70.1	8	99.1	16	6.77	6.86E+04		22
Boscalid	188425-85-6	33875	Fungicide	Nicobifen	$C_{18}H_{12}Cl_2N_2O$	342.0327	342.9	35	307.0	20	139.9	20	5.90	3.62E+06	15	
Bromacil	314-40-9	45350	Herbicide		$C_9H_{13}BrN_2O_2$	260.0160	261.0	16	204.9	14	187.9	28	4.58	1.15E+06		7
Bromuconazole	116255-48-2	46094	Fungicide		$C_{13}H_{12}BrCl_2N_3O$	374.9541	376.0	35	158.9	35	70.1	25	6.10	1.03E+07	17	

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Bupirimate	41483-43-6	45360	Fungicide		C ₁₃ H ₂₄ N ₄ O ₃ S	316.1569	317.0	34	166.0	28	108.0	28	5.88	3.92E+07	15	
Buprofezin	69327-76-0	37886	Insecticide		C ₁₆ H ₂₃ N ₃ OS	305.1562	306.1	25	201.0	12	57.4	20	6.96	7.17E+07	24	
Butachlor	23184-66-9	37887	Herbicide		C ₁₇ H ₂₆ ClNO ₂	311.1652	312.2	20	57.3	22	238.2	12	7.17	4.95E+03		
Butocarboxim	34681-10-2	36121	Insecticide		C ₇ H ₁₄ N ₂ O ₂ S	190.0776	213.0	24	75.0	15	156.0	10	3.98	1.97E+07		5
Butocarboxim sulfoxide	34681-24-8	45719	Fungicide		C ₇ H ₁₄ N ₂ O ₃ S	206.0725	207.0	17	74.9	12	132.0	6	1.83	2.20E+06		1
Butoxycarboxim	34681-23-7	36122	Insecticide		C ₇ H ₁₄ N ₂ O ₄ S	222.0674	223.0	17	106.0	10	166.0	7	2.05	1.38E+06	2	
Butralin	33629-47-9	36528	Herbicide		C ₁₄ H ₂₁ N ₃ O ₄	295.1532	296.2	19	164.0	5	132.0	11	no	no		
Buturon	3766-60-7	36510	Herbicide		C ₁₂ H ₁₃ ClN ₂ O	236.0716	237.1	26	84.1	16	126.0	30	5.33	1.12E+06		11
Butylate	2008-41-5	45363	Herbicide		C ₁₁ H ₂₃ NOS	217.1500	218.1	22	57.2	17	156.1	10	7.09	3.74E+06		24
Cadusafos	95465-99-9		Insecticide/Nematicide		C ₁₀ H ₂₃ O ₂ PS ₂	270.0877	271.1	22	159.0	16	131.0	22	6.88	1.33E+07		23
Carbaryl	63-25-2	45367	Insecticide		C ₁₂ H ₁₁ NO ₂	201.0790	202.0	22	145.0	22	117.0	28	4.86	3.12E+06	9	
Carbendazim	10605-21-7	45368	Fungicide		C ₉ H ₉ N ₃ O ₂	191.0695	192.1	27	160.1	18	132.1	28	2.20	7.93E+06	2	
Carbetamide	16118-49-3	45369	Herbicide		C ₁₂ H ₁₆ N ₂ O ₃	236.1161	237.0	14	192.0	9	118.0	14	4.32	1.18E+06	6	
Carbofuran	1563-66-2	45370	Insecticide		C ₁₂ H ₁₅ NO ₃	221.1052	222.1	28	165.1	16	123.0	16	4.63	1.05E+07	8	
Carbofuran-3-hydroxy	16655-82-6	37896	Metabolite		C ₁₂ H ₁₅ NO ₄	237.1001	238.0	28	181.0	10	163.0	16	3.40	2.24E+06	4	
Carbofuran-3-keto	16709-30-1	37895	Metabolite		C ₁₂ H ₁₃ NO ₄	235.0845	236.2	18	179.1	12	161.1	18	4.00	4.91E+06	5	
Carbosulfan	55285-14-8	34300	Insecticide		C ₂₀ H ₃₂ N ₂ O ₃ S	380.2134	381.0	34	118.0	22	76.0	34	7.89	1.22E+05	27	
Carboxin	5234-68-4	45371	Fungicide		C ₁₂ H ₁₃ NO ₂ S	235.0667	236.0	28	143.0	16	87.0	22	4.79	1.76E+07	9	
Carfentrazone-ethyl	128639-02-1	34079	Herbicide		C ₁₅ H ₁₄ Cl ₂ F ₃ N ₃ O ₃	411.0364	412.0	32	346.0	24	266.0	18	6.48	2.77E+05	20	
Carpropamid	104030-54-8	46135	Fungicide		C ₁₅ H ₁₈ Cl ₃ NO	333.0454	334.0	25	138.9	18	103.0	40	6.59	1.64E+05		
Chinomethionate	2439-01-2	45372	Acaricide/Fungicide		C ₁₀ H ₆ N ₂ O ₂ S ₂	233.9922	234.9	22	207.0	16	163.0	28	no	no		
Chlorbromuron	13360-45-7	45377	Herbicide		C ₉ H ₁₀ BrClN ₂ O ₂	291.9614	292.9	24	203.9	18	182.0	16	5.87	4.67E+05	15	
Chlorfenvinphos	470-90-6	36551	Acaricide/Insecticide		C ₁₂ H ₁₄ Cl ₃ O ₄ P	357.9695	358.9	22	155.0	12	99.0	30	6.65	8.34E+06		21
Chlorfluzaron	71422-67-8	36530	Insecticide		C ₂₀ H ₉ Cl ₃ F ₅ N ₃ O ₃	538.9630	539.8	36	158.0	20	382.9	20	7.61	4.00E+04		26
Chloridazon	1698-60-8	45385	Herbicide		C ₁₀ H ₈ ClN ₃ O	221.0356	222.0	50	92.0	30	77.0	30	3.43	2.27E+06	4	
Chlorimuron ethyl	90982-32-4	PS1081	Herbicide		C ₁₅ H ₁₅ ClN ₄ O ₆ S	414.0401	415.1	40	186.0	15	83.0	40				
Chlormephos	24934-91-6	45386	Insecticide		C ₅ H ₁₂ ClO ₂ PS ₂	233.9705	235.0	18	97.0	22	142.9	16	no	no		
Chloroxuron	1982-47-4	45389	Herbicide		C ₁₅ H ₁₅ ClN ₂ O ₂	290.0822	291.1	35	72.0	25	164.1	15	6.15	1.32E+07		17
Chlorpropham	101-21-3	45393	Herbicide		C ₁₀ H ₁₂ ClNO ₂	213.0557	214.1	12	172.0	8	154.0	18	6.01	2.25E+05		16
Chlorpyrifos	2921-88-2	45395	Insecticide		C ₉ H ₁₁ Cl ₃ NO ₃ PS	348.9263	349.9	30	97.0	32	198.0	20	7.35	2.22E+05		25
Chlorpyrifos-methyl	5598-13-0	45396	Insecticide		C ₇ H ₇ Cl ₃ NO ₃ PS	320.8950	321.8	28	125.0	20	289.9	16	6.87	1.34E+05		23
Chlorsulfuron	64902-72-3	34322	Herbicide		C ₁₂ H ₁₂ ClN ₅ O ₄ S	357.0299	358.0	24	141.0	16	167.0	18	4.93	6.96E+05		9
Chlorthiophos	60238-56-4	36126	Insecticide		C ₁₁ H ₁₅ Cl ₂ O ₃ PS ₂	359.9577	360.9	22	154.9	12	98.9	30	6.66	8.04E+05		21
Chlortoluron	15545-48-9	45400	Herbicide		C ₁₀ H ₁₃ ClN ₂ O	212.0716	213.0	26	72.0	18	46.0	16	5.10	7.23E+04	10	
Chromafenozide	143807-66-3		Insecticide		C ₂₄ H ₃₀ N ₂ O ₃	394.2256	395.1	10	175.0	22	339.0	10				
Cinidon-ethyl	142891-20-1	46336	Herbicide		C ₁₉ H ₁₇ Cl ₂ NO ₄	393.0535	394.0	28	348.0	18	107.0	28	7.18	6.82E+05	25	
Cinosulfuron	94593-91-6	37893	Herbicide		C ₁₅ H ₁₉ N ₅ O ₇ S	413.1005	414.0	32	183.0	16	157.0	24	4.40	2.71E+06	6	
Clethodim	99129-21-2	34190	Herbicide		C ₁₇ H ₂₆ ClNO ₃ S	359.1322	360.0	26	164.0	18	268.1	12	7.02	6.71E+05	24	
Clodinafop	114420-56-3		Herbicide		C ₁₄ H ₁₁ ClFNO ₄	311.0361	312.0	36	265.8	16	238.2	24				
Clodinafop-propargyl	105512-06-9	46122	Herbicide		C ₁₇ H ₁₃ ClFNO ₄	349.0517	350.0	30	266.0	16	91.0	32	6.47	9.91E+05	20	
Clofencet	129025-54-3		Growth Regulator		C ₁₃ H ₁₁ ClN ₂ O ₃	278.0458	279.1	40	261.1	15	166.0	30				
Clofentezine	74115-24-5	36763	Acaricide		C ₁₄ H ₈ Cl ₂ N ₄	302.0126	303.0	22	138.0	22	102.0	35	6.76	7.28E+04		
Clomazone	81777-89-1	46120	Herbicide		C ₁₂ H ₁₄ ClNO ₂	239.0713	240.0	26	125.0	18	89.0	46	5.60	7.40E+06	13	
Clomeprop	84496-56-0		Herbicide		C ₁₆ H ₁₅ Cl ₂ NO ₂	323.0480	324.1	35	120.1	20	203.1	15				
Clopyralid	1702-17-6	36758	Herbicide		C ₆ H ₃ Cl ₂ NO ₂	190.9541	191.9	24	173.9	10	145.9	20	2.21	4.74E+04	2	
Cloquintocet - mexyl	99607-70-2	46123	Herbicide		C ₁₈ H ₂₂ ClNO ₃	335.1288	336.1	24	238.0	16	192.0	30	7.22	4.05E+06		25
Cloransulam-methyl	147150-35-4		Herbicide		C ₁₅ H ₁₃ ClFNO ₅ S	429.0310	430.1	30	153.0	40	398.1	15				
Clothianidin	210880-92-5	33589	Insecticide		C ₆ H ₈ ClN ₅ O ₂ S	249.0087	250.0	18	169.0	12	132.0	18	3.10	8.85E+05	3	
Coumaphos	56-72-4	45403	Insecticide		C ₁₄ H ₁₆ ClO ₅ PS	362.0145	363.0	26	307.0	16	289.0	24	6.60	1.37E+06	21	
Cruformate	299-86-5		Insecticide	Ruelene	C ₁₂ H ₁₉ ClNO ₃ P	291.0791	292.0	34	108.1	28	236.1	18	6.45	2.10E+06		19
Cumyruron	99485-76-4		Herbicide		C ₁₇ H ₁₉ ClN ₂ O	302.1186	303.2	40	185.1	15	125.0	30				
Cyanazine	21725-46-2	45407	Herbicide		C ₉ H ₁₃ ClN ₆	240.0890	241.0	35	214.0	17	96.0	25	4.39	2.27E+07	6	

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Cyanofenphos	13067-93-1	36509	Insecticide		C ₁₅ H ₁₄ NO ₂ PS	303.0483	304.0	28	157.0	22	276.0	12	6.57	3.69E+05	21	
Cyazofamid	120116-88-3	33874	Fungicide		C ₁₃ H ₁₃ ClN ₄ O ₂ S	324.0448	325.0	20	107.9	20	261.0	10	6.30	6.32E+06	19	
Cycloate	1134-23-2	45408	Herbicide		C ₁₁ H ₂₁ NOS	215.1344	216.1	26	83.1	18	55.2	28	6.91	2.80E+06		23
Cyclosulfamuron	136849-15-5		Herbicide		C ₁₇ H ₁₉ N ₅ O ₆ S	421.1056	422.2	40	261.1	15	218.1	30				
Cycloxydim	101205-02-1	46071	Herbicide		C ₁₇ H ₂₇ NO ₃ S	325.1712	326.0	28	280.0	16	180.0	22	7.00	9.87E+05	24	
Cycluron	2163-69-1	45409	Herbicide		C ₁₁ H ₂₂ N ₂ O	198.1732	199.0	26	89.1	14	69.2	22	5.42	6.42E+06	12	
Cyflufenamid	180409-60-3		Fungicide		C ₂₀ H ₁₇ F ₅ N ₂ O ₂	412.1210	413.2	30	295.1	15	203.0	35	6.73	1.41E+05	22	
Cymoxanil	57966-95-7	34326	Fungicide		C ₇ H ₁₀ N ₄ O ₃	198.0753	199.0	17	128.0	8	111.0	18	3.58	1.18E+06		4
Cyproconazole	94361-06-5	46068	Fungicide		C ₁₅ H ₁₈ ClN ₃ O	291.1138	292.2	30	70.2	18	125.1	24	6.16	1.36E+05		17
Cyprodinil	121552-61-2	34389	Fungicide		C ₁₄ H ₁₅ N ₃	225.1266	226.0	50	93.0	33	108.0	25	5.90	1.44E+07	15	
Cyromazine	66215-27-8	45414	Insecticide		C ₆ H ₁₀ N ₆	166.0967	167.0	32	60.2	19	108.1	19	1.10	3.21E+04	1	
Daminozide	1596-84-5	45418	Herbicide		C ₆ H ₁₂ N ₂ O ₃	160.0848	161.0	18	143.0	12	61.0	12	0.81	3.65E+05	1	
Deltamethrin	52918-63-5	45423	Insecticide		C ₂₂ H ₁₉ Br ₂ NO ₃	502.9732	505.9	22	280.9	12	93.2	46	7.64	3.53E+04		
Demeton O	298-03-3	34205	Acaricide/Insecticide		C ₈ H ₁₉ O ₃ PS ₂	258.0513	259.0	12	89.0	10	61.1	33	5.64	7.66E+05		13
Demeton S	126-75-0	PS662	Acaricide/Insecticide		C ₈ H ₁₉ O ₃ PS ₂	258.0513	259.0	12	89.0	10	61.1	33	5.64	4.51E+06		13
Demeton-O-sulfoxide			Metabolite		C ₈ H ₁₉ O ₄ PS ₂	274.0462	275.1	20	104.9	16	140.8	24	5.85	3.36E+05		
Demeton-S-methyl	919-86-8	45304	Insecticide		C ₆ H ₁₅ O ₃ PS ₂	230.0200	231.1	10	89.1	10	61.2	30	4.68	1.94E+06		8
Demeton-S-methyl-sulfon	17040-19-6	45424	Insecticide	Dioxydemeton-S-methyl	C ₆ H ₁₅ O ₅ PS ₂	262.0099	263.0	26	169.0	17	121.0	17	2.55	5.79E+06		2
Desmedipham	13684-56-5	45426	Herbicide		C ₁₆ H ₁₆ N ₂ O ₄	300.1110	301.0	28	182.0	10	136.0	22	5.47	7.46E+05		12
Desmethyl-formamido-pirimicarb	27218-04-8	33887	Metabolite		C ₁₁ H ₁₆ N ₄ O ₃	252.1222	253.1	24	72.0	16	225.1	11	4.57	7.68E+06		7
Desmethyl-pirimicarb	30614-22-3	33886	Metabolite		C ₁₀ H ₁₆ N ₄ O ₂	224.1273	225.1	26	72.0	20	168.1	16	2.71	1.83E+07		2
Desmetryn	1014-69-3	45427	Herbicide		C ₈ H ₁₅ N ₅ S	213.1048	214.1	32	172.1	20	82.1	30	4.26	8.00E+07		5
Dialifos	10311-84-9	36500	Acaricide/Insecticide		C ₁₄ H ₁₇ ClNO ₄ PS ₂	393.0025	394.0	12	187.0	8	208.0	16	6.82	2.68E+04	23	
Diallate	2303-16-4	36501	Herbicide		C ₁₀ H ₁₇ Cl ₂ NOS	269.0408	270.1	23	86.1	15	128.1	11	6.98	4.09E+04	24	
Diamuron	42609-52-9		Herbicide	Dymron	C ₁₇ H ₂₀ N ₂ O	268.1576	269.1	30	151.1	10	91.0	40				
Diazinon	333-41-5	45428	Insecticide		C ₁₂ H ₂₁ N ₂ O ₃ PS	304.1011	305.1	25	169.0	22	96.9	35	2.55	4.11E+03		
Dibrom	300-76-5	45429	Insecticide/Nematocide	Naled	C ₄ H ₇ Br ₂ Cl ₂ O ₄ P	377.7826	378.7	18	127.0	16	109.0	36	5.45	3.23E+05		12
Dichlofluanid	1085-98-9	45433	Fungicide		C ₉ H ₁₁ Cl ₂ FN ₂ O ₂ S ₂	331.9623	333.0	22	123.0	24	224.0	10	6.20	1.67E+06	18	
Dichlorvos	62-73-7	45441	Acaricide/Insecticide		C ₄ H ₇ Cl ₂ O ₄ P	219.9459	221.0	28	109.0	22	79.0	34	4.53	3.09E+06	7	
Diclobutrazol	75736-33-3	36764	Fungicide		C ₁₅ H ₁₉ Cl ₂ N ₃ O	327.0905	328.0	28	70.0	20	158.9	38	6.52	8.01E+06		20
Diclomezine	62865-36-5		Fungicide		C ₁₁ H ₈ Cl ₂ N ₂ O	254.0014	255.0	52	79.8	30	140.8	30				
Diclosulam	145701-21-9	33968	Herbicide		C ₁₃ H ₁₀ Cl ₂ FN ₅ O ₃ S	404.9865	406.1	40	161.0	30	378.0	15				
Dicrotophos	141-66-2	45305	Insecticide		C ₈ H ₁₆ NO ₅ P	237.0766	238.0	22	112.0	10	193.0	10	2.97	1.85E+07	3	
Diethofencarb	87130-20-9	34087	Fungicide		C ₁₄ H ₂₁ NO ₄	267.1471	268.0	22	226.0	10	124.0	40	5.71	6.40E+06	14	
Difenoconazole	119446-68-3	36531	Fungicide		C ₁₉ H ₁₇ Cl ₂ N ₃ O ₃	405.0647	406.0	40	251.1	25	111.1	60	6.90	6.67E+06		23
Difenoxyuron	14214-32-5	45444	Herbicide		C ₁₆ H ₁₈ N ₂ O ₃	286.1317	287.0	32	72.0	20	123.0	20	5.38	3.50E+06	12	
Diflubenzuron	35367-38-5	45446	Insecticide		C ₁₄ H ₉ ClF ₂ N ₂ O ₂	310.0321	311.1	26	227.0	8	269.0	8	6.39	9.45E+05	20	
Dimefuron	34205-21-5	36788	Herbicide		C ₁₅ H ₁₉ ClN ₄ O ₃	338.1146	339.0	36	72.0	26	166.9	20	5.60	2.19E+06		13
Dimepiperate	61432-55-1	33943	Herbicide		C ₁₅ H ₂₁ NOS	263.1344	264.1	8	146.0	10	119.0	16	6.95	2.14E+06	24	
Dimethachlor	50563-36-5	45447	Herbicide		C ₁₃ H ₁₈ ClNO ₂	255.1026	256.2	23	148.2	25	224.2	15	5.50	6.36E+06		12
Dimethametryn	22936-75-0	45448	Herbicide		C ₁₁ H ₂₁ N ₅ S	255.1518	256.1	36	186.1	20	71.0	32	5.92	4.64E+07		14
Dimethenamid	87674-68-8	46385	Herbicide		C ₁₂ H ₁₈ ClNO ₂ S	275.0747	276.0	20	244.0	14	168.0	26	5.84	6.19E+06		14
Dimethirimol	5221-53-4		Fungicide		C ₁₁ H ₁₉ N ₃ O	209.1528	210.1	40	71.1	30	140.0	21	3.57	9.22E+06		4
Dimethoate	60-51-5	45449	Acaricide/Insecticide		C ₅ H ₁₂ NO ₃ PS ₂	228.9996	230.1	18	125.0	20	199.0	10	3.32	2.06E+06		3
Dimethomorph	110488-70-5	46027	Fungicide		C ₂₁ H ₂₂ ClNO ₄	387.1237	388.1	35	300.9	20	165.0	30	6.03	7.91E+06		16
Dimetilan	644-64-4	45450	Insecticide		C ₁₀ H ₁₆ N ₄ O ₃	240.1222	241.1	18	72.2	16	196.1	10	3.57	4.34E+07		4
Dimoxystrobin	149961-52-4	33499	Fungicide		C ₁₉ H ₂₂ N ₂ O ₃	326.1630	327.1	24	116.1	21	205.2	10	6.47	5.36E+06	20	
Diniconazole	70217-36-6	46049	Fungicide		C ₁₅ H ₁₇ Cl ₂ N ₃ O	325.0749	326.1	40	70.2	25	159.0	34	6.87	4.36E+05		23
Dioxacarb	6988-21-2	45454	Insecticide		C ₁₁ H ₁₃ NO ₄	223.0845	224.1	14	123.1	16	167.1	8	3.39	3.62E+05	4	
Diphenamid	957-51-7	45455	Herbicide		C ₁₆ H ₁₇ NO	239.1310	240.1	30	134.1	20	167.1	22	5.47	4.92E+07		12

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Diphenylamine	122-39-4	45456	Fungicide		C ₁₂ H ₁₁ N	169.0891	170.0	32	93.0	24	92.0	18	6.12	2.19E+06	17	
Disulfoton	298-04-4	45460	Acaricide/Insecticide		C ₈ H ₁₉ O ₂ PS ₃	274.0285	274.9	10	89.0	20	61.1	35	6.80	1.88E+06		22
Disulfoton-sulfone	2497-06-5	45871	Metabolite		C ₈ H ₁₉ O ₄ PS ₃	306.0183	307.1	18	97.1	28	153.1	12	5.16	9.24E+06		10
Disulfoton-sulfoxide	2497-07-6	45897	Metabolite		C ₈ H ₁₉ O ₃ PS ₃	290.0234	291.0	18	185.0	14	97.0	31	5.08	9.61E+06		10
Ditalimfos	5131-24-8	45461	Fungicide		C ₁₂ H ₁₄ NO ₄ PS	299.0381	300.1	18	148.1	20	130.1	34	6.13	6.86E+06		17
Dithiopyr	97886-45-8		Herbicide		C ₁₅ H ₁₆ F ₅ NO ₂ S ₂	401.0543	402.0	35	354.1	18	248.1	34	6.99	1.25E+05	24	
Diuron	330-54-1	45463	Herbicide		C ₉ H ₁₀ Cl ₂ N ₂ O	232.0170	233.0	28	72.1	18	46.3	14	5.37	4.16E+05		11
DMSA			Metabolite	Dimethylphenylsulphamide	C ₈ H ₁₂ N ₂ O ₂ S	200.0619	201.0	25	92.0	17	137.0	9	4.14	4.66E+04		
DMST	66840-71-9	34336	Metabolite	Dimethylaminosulfotoluidid	C ₉ H ₁₄ N ₂ O ₂ S	214.0776	215.0	20	106.0	15	79.1	29	4.79	1.74E+05		8
Dodemorph	1593-77-7	45465	Fungicide		C ₁₈ H ₃₅ NO	281.2719	282.1	34	116.0	21	98.0	28	5.22	9.36E+07	10	
Dodine	2439-10-3	45466	Fungicide		C ₁₅ H ₃₃ N ₃ O ₂	287.2573	288.0	34	256.0	22	58.0	50	8.00	2.85E+03		
Edifenphos	17109-49-8	45467	Fungicide		C ₁₄ H ₁₅ O ₂ PS ₂	310.0251	311.0	26	109.0	32	111.0	26	6.56	1.97E+06		20
Endothal	62059-43-2	35525	Herbicide		C ₈ H ₁₀ O ₅	186.0528	187.0	6	169.0	6	123.0	14	1.75	2.40E+04		
EPN	2104-64-5	36503	Acaricide/Insecticide		C ₁₄ H ₁₄ NO ₄ PS	323.0381	324.0	25	157.0	25	296.0	14	6.92	1.00E+03		
Epoxiconazole	106325-08-0	36848	Fungicide		C ₁₇ H ₁₃ ClFN ₃ O	329.0731	330.0	28	121.0	22	101.0	50	6.27	2.43E+07		18
EPTC	759-94-4	45469	Herbicide		C ₉ H ₁₉ NOS	189.1187	190.0	20	128.1	11	86.0	15	6.45	1.06E+06		19
Esprocarb	85785-20-2	33898	Herbicide		C ₁₅ H ₂₃ NOS	265.1500	266.1	24	91.0	22	71.0	16	7.19	4.75E+06	25	
Ethametsulfuron-methyl	97780-06-8		Herbicide		C ₁₅ H ₁₈ N ₆ O ₆ S	410.1009	411.2	40	168.1	30	196.1	15				
Ethidimuron	30043-49-3	45474	Herbicide		C ₇ H ₁₂ N ₄ O ₃ S ₂	264.0351	265.0	28	208.1	14	114.0	20	3.14	7.19E+06		3
Ethiofencarb	29973-13-5	45475	Insecticide		C ₁₁ H ₁₅ NO ₂ S	225.0824	226.1	19	107.0	17	164.0	8	4.98	5.22E+06	10	
Ethiofencarb sulfone	53380-23-7	45810	Metabolite		C ₁₁ H ₁₅ NO ₄ S	257.0722	258.0	22	107.0	18	201.1	5	2.98	4.61E+06	3	
Ethiofencarb sulfoxide	53380-22-6	45811	Metabolite		C ₁₁ H ₁₅ NO ₃ S	241.0773	242.1	22	107.1	18	185.1	8	3.08	3.98E+06	3	
Ethion	563-12-2	45477	Acaricide		C ₉ H ₂₂ O ₄ P ₂ S ₄	383.9876	284.9	19	199.1	10	97.0	46	5.22	3.85E+03		
Ethiprole	181587-01-9	33976	Insecticide		C ₁₃ H ₉ Cl ₂ F ₃ N ₄ OS	395.9826	414.1	15	396.9	9	350.9	25	5.87	1.00E+04		
Ethirimol	23947-60-6	45478	Fungicide		C ₁₁ H ₁₉ N ₃ O	209.1528	210.1	38	140.0	22	98.0	28	3.75	9.54E+06		4
Ethofumesate	26225-79-6	45479	Herbicide		C ₁₃ H ₁₈ O ₅ S	286.0875	287.1	30	121.1	15	259.1	10	5.75	3.31E+06	14	
Ethoprophos	13194-48-4	45306	Insecticide/Nematicide		C ₈ H ₁₉ O ₂ PS ₂	242.0564	243.2	26	97.0	31	131.0	20	6.27	4.16E+06		18
Ethoxyquin	91-53-2	45480	Fungicide/Herbicide		C ₁₄ H ₁₉ NO	217.1467	218.2	40	148.1	22	160.1	32	4.80	9.32E+05	8	
Ethoxysulfuron	126801-58-9	46300	Herbicide		C ₁₅ H ₁₈ N ₄ O ₇ S	398.0896	398.9	26	261.0	16	218.0	24	5.99	1.40E+07	16	
Etofenprox	80844-07-1	34094	Insecticide		C ₂₅ H ₂₈ O ₃	376.2038	394.3	20	177.0	15	106.9	43	7.97	2.05E+05	27	
Etrimfos	38260-54-7	45481	Insecticide		C ₁₀ H ₁₇ N ₂ O ₄ PS	292.0647	293.1	32	125.0	26	265.1	16	6.58	2.85E+03		
Famoxadone	131807-57-3	33495	Fungicide		C ₂₂ H ₁₈ N ₂ O ₄	374.1267	392.2	15	331.1	10	238.0	20	6.67	6.69E+03		
Famphur	52-85-7	34341	Insecticide		C ₁₀ H ₁₆ NO ₅ PS ₂	325.0208	326.0	26	93.0	31	217.0	20	5.19	2.04E+06		10
Fenamidone	161326-34-7	33965	Fungicide		C ₁₇ H ₁₇ N ₃ OS	311.1092	312.1	25	92.0	25	236.1	14	5.84	2.02E+07		14
Fenamiphos	22224-92-6	45483	Nematicide		C ₁₃ H ₂₂ NO ₃ PS	303.1058	304.1	30	217.1	24	202.1	36	6.39	1.40E+07	19	
Fenamiphos sulphone	31972-44-8	46292	Metabolite		C ₁₃ H ₂₂ NO ₅ PS	335.0956	336.1	28	266.1	20	188.2	28	4.83	6.84E+06	9	
Fenamiphos sulphoxide	31972-43-7	46293	Metabolite		C ₁₃ H ₂₂ NO ₄ PS	319.1007	320.1	36	171.1	22	108.0	35	4.84	9.76E+04	8	
Fenarimol	60168-88-9	45484	Fungicide		C ₁₇ H ₁₂ Cl ₂ N ₂ O	330.0327	331.0	40	268.0	22	81.0	34	6.26	1.05E+07		18
Fenazaquin	120928-09-8	46087	Acaricide		C ₂₀ H ₂₂ N ₂ O	306.1732	307.2	30	57.2	25	161.0	19	7.70	1.62E+05		26
Fenazox	495-48-7	45763	Insecticide		C ₁₂ H ₁₀ N ₂ O	198.0793	199.1	22	77.1	24	92.1	14	6.68	4.87E+06	22	
Fenbuconazole	114369-43-6	46096	Fungicide		C ₁₉ H ₁₇ ClN ₄	336.1142	337.0	32	70.1	20	125.0	36	6.37	8.98E+05	19	
Fenfuram	24691-80-3	45486	Fungicide		C ₁₂ H ₁₁ NO ₂	201.0790	202.1	28	109.0	20	83.1	14	4.85	2.63E+07	9	
Fenhexamid	126833-17-8	46278	Fungicide		C ₁₄ H ₁₇ Cl ₂ NO ₂	301.0636	302.1	35	97.2	22	55.3	38	6.22	1.02E+06	18	
Fenitrothion	122-14-5	45487	Insecticide		C ₉ H ₁₂ NO ₅ PS	277.0174	278.0	32	109.1	20	79.1	34	6.06	2.92E+03		
Fenobucarb	3766-81-2	45488	Insecticide		C ₁₂ H ₁₇ NO ₂	207.1259	208.0	16	94.9	14	152.0	8	5.72	6.17E+06	14	
Fenoxaprop-ethyl	66441-23-4	45518	Herbicide		C ₁₈ H ₁₆ ClNO ₅	361.0717	362.1	40	288.1	20	121.1	25	no	no		
Fenoxycarb	72490-01-8	34343	Insecticide		C ₁₇ H ₁₉ NO ₄	301.1314	302.1	22	88.0	20	116.1	11	6.45	7.77E+06	20	
Fenpiclonil	74738-17-3	36532	Fungicide		C ₁₁ H ₆ Cl ₂ N ₂	235.9908	236.9	38	202.0	20	140.0	38	5.66	1.01E+05		13
Fenpropathrin	39515-41-8	36767	Insecticide		C ₂₂ H ₂₃ NO ₃	349.1678	350.1	18	125.0	14	97.0	34	7.51	3.91E+04	26	
Fenpropidin	67306-00-7	46017	Fungicide		C ₁₉ H ₃₁ N	273.2457	274.2	50	147.1	28	86.1	28	5.44	6.66E+07	11	

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Fenpropimorph	67564-91-4	36772	Fungicide		C ₂₀ H ₃₃ NO	303.2562	304.2	44	147.1	28	57.2	30	5.53	5.56E+07		11
Fenpyroximat	111812-58-9	46137	Acaricide		C ₂₄ H ₂₇ N ₃ O ₄	421.2002	422.2	26	366.1	15	138.1	32	7.53	1.57E+07		26
Fensulfothion	115-90-2	45307	Insecticide/Nematicide		C ₁₁ H ₁₇ O ₄ PS ₂	308.0306	309.0	30	157.1	25	173.1	22	5.35	1.01E+07		11
Fensulfothion oxon	6552-21-2		Metabolite		C ₁₁ H ₁₇ O ₅ PS	292.0534	293.0	28	237.0	19	265.0	14				
Fensulfothion oxon sulfone	6132-17-8		Metabolite		C ₁₁ H ₁₇ O ₆ PS	308.0483	309.0	27	253.0	16	175.0	27				
Fensulfothion sulfone	14255-72-2		Metabolite		C ₁₁ H ₁₇ O ₅ PS ₂	324.0255	325.0	26	269.0	16	297.0	11				
Fenthion	55-38-9	36552	Insecticide		C ₁₀ H ₁₅ O ₃ PS ₂	278.0200	279.1	30	169.1	16	247.1	13	6.57	4.78E+05	21	
Fenthion-sulfone	3761-42-0	46023	Metabolite		C ₁₀ H ₁₅ O ₅ PS ₂	310.0099	311.0	32	125.0	22	109.0	28	4.94	5.65E+06	10	
Fenthion-sulfoxide	3761-41-9	37885	Metabolite		C ₁₀ H ₁₅ O ₄ PS ₂	294.0149	295.0	32	109.0	32	280.0	18	4.82	4.05E+06	9	
Fenuron	101-42-8	45494	Herbicide		C ₉ H ₁₂ N ₂ O	164.0950	165.0	22	71.9	16	45.9	14	3.21	2.81E+06		3
Ferimzone	89269-64-7		Fungicide		C ₁₅ H ₁₈ N ₄	254.1531	255.2	40	132.1	20	91.0	30	no	no		
Flamprop-isopropyl	52756-22-6	45497	Herbicide		C ₁₉ H ₁₉ ClFNO ₃	363.1037	364.0	18	105.0	20	77.0	56	6.62	1.51E+06		21
Flamprop-methyl	52756-25-9	45498	Herbicide		C ₁₇ H ₁₅ ClFNO ₃	335.0724	336.0	18	105.0	16	77.0	48	6.09	1.51E+06		16
Flazasulfuron	104040-78-0	34052	Herbicide		C ₁₃ H ₁₂ F ₃ N ₅ O ₅ S	407.0511	408.1	20	181.9	20	138.9	44	5.55	1.70E+05		
Florasulam	145701-23-1		Herbicide		C ₁₂ H ₈ F ₃ N ₅ O ₃ S	359.0300	360.0	34	129.0	22	108.9	50	6.62	1.30E+03		
Fluazafop-P-butyl	79241-46-6	46276	Herbicide		C ₁₉ H ₂₀ F ₃ NO ₄	383.1344	384.1	32	282.1	22	328.1	16	7.11	6.11E+06		24
Fluazifop	69335-91-7	36884	Herbicide		C ₁₅ H ₁₂ F ₃ NO ₄	327.0718	328.1	40	282.1	20	255.1	25	5.91	2.96E+06		15
Fluazinam	79622-59-6	46316	Fungicide		C ₁₃ H ₄ Cl ₂ F ₆ N ₄ O ₄	463.9514	464.8	26	373.0	26	338.1	47	5.74	4.86E+03		
Flucycloxuron	113036-88-7		Acaricide/Insecticide		C ₂₅ H ₂₀ ClF ₂ N ₃ O ₃	483.1161	484.0	18	132.1	40	289.1	12	7.42	2.45E+05	26	
Flucythrinate	70124-77-5	33496	Acaricide/Insecticide		C ₂₆ H ₂₃ F ₂ NO ₄	451.1595	452.1	10	412.0	7	157.0	36	7.40	1.59E+03		
Fludioxonil	131341-86-1	46102	Fungicide		C ₁₂ H ₆ F ₂ N ₂ O ₂	248.0397	249.1	10	158.1	28	229.1	10	5.90	2.12E+04		
Flufenacet	142459-58-3	46327	Herbicide		C ₁₄ H ₁₃ F ₄ N ₃ O ₂ S	363.0665	364.0	16	152.1	20	194.1	11	6.22	4.60E+06	18	
Flufenoxuron	101463-69-8	46069	Acaricide/Insecticide		C ₂₁ H ₁₁ ClF ₆ N ₂ O ₃	488.0362	489.1	34	158.0	22	141.0	46	7.47	2.63E+06	26	
Flumetsulam	98967-40-9		Herbicide		C ₁₂ H ₉ F ₂ N ₅ O ₂ S	325.0445	326.1	40	129.0	25	109.0	50	no	no		
Flumioxazin	103361-09-7		Herbicide		C ₁₉ H ₁₅ FN ₂ O ₄	354.1016	355.0	40	326.0	22	298.0	28	no	no		
Fluomethuron	2164-17-2	45502	Herbicide		C ₁₀ H ₁₁ F ₃ N ₂ O	232.0823	233.2	28	72.2	18	46.4	18	5.02	3.35E+05	10	
Fluoxastrobin	361377-29-9	33797	Fungicide		C ₂₁ H ₁₆ ClFN ₄ O ₅	458.0793	459.0	30	427.0	18	188.0	36	6.19	6.01E+05	18	
Fluquinconazole	136426-54-5	46301	Fungicide		C ₁₆ H ₈ Cl ₂ FN ₅ O	375.0090	376.0	40	348.8	18	306.9	30	6.17	2.47E+06		
Fluridon	59756-60-4	45511	Herbicide		C ₁₉ H ₁₄ F ₃ NO	329.1027	330.1	60	310.2	30	259.2	40	5.59	1.22E+03		
Fluroxypyr	69377-81-7	45758	Herbicide		C ₇ H ₅ Cl ₂ FN ₂ O ₃	253.9661	254.9	22	208.8	16	180.8	22	4.42	4.85E+05	6	
Fluroxypyr-meptyl	81406-37-3	36780	Herbicide		C ₁₅ H ₂₁ Cl ₂ FN ₂ O ₃	366.0913	367.0	15	254.9	11	181.0	32	7.44	2.16E+05		26
Flurtamone	96525-23-4	46286	Herbicide		C ₁₈ H ₁₄ F ₃ NO ₂	333.0977	334.0	38	247.0	27	178.0	45	5.77	6.05E+06	14	
Flusilazole	85509-19-9	45753	Fungicide		C ₁₆ H ₁₅ F ₂ N ₃ Si	315.1003	316.0	30	247.0	18	165.0	28	6.41	7.44E+07	19	
Flutolanil	66332-96-5	PS2057	Fungicide		C ₁₇ H ₁₆ F ₃ NO ₂	323.1133	324.1	28	262.1	18	65.0	40	5.97	8.69E+06	16	
Flutriafol	76674-21-0	34344	Fungicide		C ₁₆ H ₁₃ F ₂ N ₃ O	301.1027	302.1	26	70.2	18	123.1	29	5.24	1.35E+05	11	
Fluvalinate	102851-06-9	46294	Acaricide/Insecticide		C ₂₆ H ₂₂ ClF ₃ N ₂ O ₃	502.1271	503.0	18	181.1	30	208.1	12	no	no		
Fonofos	944-22-9	45513	Insecticide		C ₁₀ H ₁₅ OPS ₂	246.0302	247.1	18	109.0	20	137.0	10	6.60	5.59E+05	21	
Foramsulfuron	173159-57-4	33977	Herbicide		C ₁₇ H ₂₀ N ₆ O ₇ S	452.1114	453.0	29	182.0	22	272.0	14	4.92	1.58E+06		9
Forchlorfenuron	68157-60-8	C2791	Growth Regulator	CPPU	C ₁₂ H ₁₀ ClN ₃ O	247.0512	248.1	30	129.0	15	93.0	35				
Formetanate	22259-30-9	45514	Acaricide/Insecticide		C ₁₁ H ₁₅ N ₃ O ₂	221.1164	222.0	24	165.0	15	46.0	26	1.63	1.67E+06		1
Fosthiazate	98886-44-3	34099	Nematicide		C ₉ H ₁₈ NO ₃ PS ₂	283.0466	284.0	22	228.0	10	104.0	22	5.04	8.52E+06	10	
Fuberidazole	3878-19-1	45515	Fungicide		C ₁₁ H ₈ N ₂ O	184.0637	185.0	35	157.0	22	156.0	27	2.89	1.05E+07	3	
Furametpyr	123572-88-3		Fungicide		C ₁₇ H ₂₀ ClN ₃ O ₂	333.1244	334.2	30	157.0	30	290.2	15				
Furathiocarb	65907-30-4	45517	Insecticide		C ₁₈ H ₂₆ N ₂ O ₅ S	382.1562	383.2	25	194.9	18	252.0	12	7.13	7.39E+06	25	
Furmecycloz	60568-05-0	34347	Fungicide		C ₁₄ H ₂₁ NO ₃	251.1521	252.2	25	170.1	14	110.1	22	3.11	5.65E+03		
Halofenozide	112226-61-6		Insecticide		C ₁₈ H ₁₉ ClN ₂ O ₂	330.1135	331.1	10	104.9	18	275.0	10	5.85	7.42E+04		
Halosulfuron methyl	100784-20-1		Herbicide		C ₁₃ H ₁₅ ClN ₆ O ₇ S	434.0411	435.1	30	182.1	20	83.0	40	6.25	5.11E+06		18
Haloxypyr	69806-34-4	45817	Herbicide		C ₁₅ H ₁₁ ClF ₃ NO ₄	361.0329	362.0	30	315.8	18	91.0	30	6.60	1.07E+06		21
Haloxypyr-2-ethoxyethyl	87237-48-7	36778	Herbicide		C ₁₉ H ₁₉ ClF ₃ NO ₅	433.0904	434.0	28	91.0	34	316.0	20	7.10	3.29E+06		24
Haloxypyr-methyl	69806-40-2	45820	Herbicide		C ₁₆ H ₁₃ ClF ₃ NO ₄	375.0485	376.0	30	91.1	32	316.1	18	6.90	5.10E+06		23

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Heptenophos	23560-59-0	45523	Insecticide		C ₉ H ₁₂ ClO ₄ P	250.0162	251.0	20	127.0	14	125.0	14	5.43	1.73E+07	12	
Hexaconazole	79983-71-4	34348	Fungicide		C ₁₄ H ₁₇ Cl ₂ N ₃ O	313.0749	314.0	34	70.1	22	159.0	28	6.74	3.11E+06	22	
Hexazinone	51235-04-2	36129	Herbicide		C ₁₂ H ₂₀ N ₄ O ₂	252.1586	253.1	29	171.1	16	71.0	30	4.66	1.50E+07	8	
Hexythiazox	78587-05-0	33365	Acaricide		C ₁₇ H ₂₁ ClN ₂ O ₂ S	352.1012	353.0	24	168.1	26	228.1	14	7.37	3.07E+06	26	
Imazalil	35554-44-0	36130	Fungicide		C ₁₄ H ₁₄ Cl ₂ N ₂ O	296.0483	297.0	34	159.0	22	69.0	22	5.03	7.25E+06	9	
Imazapyr	81334-34-1	37877	Herbicide		C ₁₃ H ₁₅ N ₃ O ₃	261.1113	262.2	32	69.2	26	86.1	26	3.10	2.17E+07	3	
Imazaquin	81335-37-7	37878	Herbicide		C ₁₇ H ₁₇ N ₃ O ₃	311.1270	312.2	34	86.2	28	267.2	20	4.64	2.64E+07	8	
Imazosulfuron	122548-33-8		Herbicide		C ₁₄ H ₁₃ ClN ₆ O ₅ S	412.0357	413.0	10	155.9	18	152.8	12				
Imidacloprid	138261-41-3	37894	Insecticide		C ₉ H ₁₀ ClN ₅ O ₂	255.0523	256.1	28	175.1	20	209.1	15	3.08	1.35E+06	3	
Indanofan	133220-30-1		Herbicide		C ₂₀ H ₁₇ ClO ₃	340.0866	341.1	15	186.9	12	174.9	14				
Indoxacarb	144171-61-9	33969	Insecticide		C ₂₂ H ₁₇ ClF ₃ N ₃ O ₇	527.0707	528.0	28	150.0	22	203.0	40	6.91	8.52E+05	24	
Iodosulfuron methyl	144550-36-7	30317	Herbicide		C ₁₄ H ₁₄ IN ₅ O ₆ S	492.9553	508.1	25	167.1	25	141.1	25	5.58	7.90E+06	13	
Iprobenphos	26087-47-8	45814	Fungicide		C ₁₃ H ₂₁ O ₃ PS	288.0949	289.0	12	91.0	20	205.0	10	6.47	4.40E+06	20	
Iprodione	36734-19-7	36132	Fungicide		C ₁₃ H ₁₃ Cl ₂ N ₃ O ₃	329.0334	330.0	15	244.7	16	288.0	15	6.40	5.96E+03		
Iprovalicarb	140923-17-7	33431	Fungicide		C ₁₈ H ₂₈ N ₂ O ₃	320.2100	321.1	22	119.1	16	203.1	10	6.15	1.06E+07		17
Isazophos	42509-80-8	36133	Insecticide/Nematicide		C ₉ H ₁₇ ClN ₃ O ₃ PS	313.0417	314.0	20	120.0	28	162.1	16	6.10	2.48E+07	17	
Isocarbamide	30979-48-7	36134	Herbicide		C ₈ H ₁₅ N ₃ O ₂	185.1164	186.1	21	87.1	16	130.1	12	3.67	1.84E+07		4
Isocarbofos	24353-61-5	33857	Insecticide		C ₁₁ H ₁₆ NO ₄ PS	289.0538	291.1	15	121.1	30	231.1	13	5.39	2.04E+04	12	
Isofenphos	25311-71-1	36135	Insecticide		C ₁₅ H ₂₄ NO ₄ PS	345.1164	346.1	10	245.1	12	217.0	22	6.75	1.17E+07		22
Isomethiozin	57052-04-7	36136	Herbicide		C ₁₂ H ₂₀ N ₄ OS	268.1358	269.1	24	200.1	15	172.1	22	6.57	8.31E+07	21	
Isonoruron	28805-78-9	33360	Herbicide		C ₁₃ H ₂₂ N ₂ O	222.1732	223.1	28	89.1	18	72.2	28	5.76	4.34E+06	14	
Isoprocab	2631-40-5	45541	Insecticide		C ₁₁ H ₁₅ NO ₂	193.1103	194.1	18	95.1	14	137.1	8	5.22	1.87E+06	11	
Isopropalin	33820-53-0	36505	Herbicide		C ₁₅ H ₂₃ N ₃ O ₄	309.1689	310.2	28	226.2	19	268.2	15	7.65	8.90E+05		26
Isoprothiolane	50512-35-1		Fungicide/Insecticide		C ₁₂ H ₁₈ O ₄ S ₂	290.0647	291.1	20	188.8	22	230.9	12	5.99	4.27E+05		
Isoproturon	34123-59-6	36137	Herbicide		C ₁₂ H ₁₈ N ₂ O	206.1419	207.0	34	72.0	22	47.0	16	5.32	1.52E+07		11
Isoxaben	82558-50-7	36138	Herbicide		C ₁₈ H ₂₄ N ₂ O ₄	332.1736	333.1	25	165.1	18	107.1	58	5.93	3.81E+07		15
Isoxaflutole	141112-29-0	46437	Herbicide		C ₁₅ H ₁₂ F ₃ NO ₄ S	359.0439	360.0	25	250.9	14	219.9	40	5.35	3.97E+04		
Isoxathion	18854-01-8		Insecticide		C ₁₃ H ₁₆ NO ₄ PS	313.0538	314.1	25	104.9	14	96.9	35	6.74	4.03E+05		
Kresoxim-methyl	143390-89-0	37899	Fungicide		C ₁₈ H ₁₉ NO ₄	313.1314	314.1	18	116.0	12	206.0	7	6.50	1.63E+06		20
Lenacil	2164-08-1	36140	Herbicide		C ₁₃ H ₁₈ N ₂ O ₂	234.1368	235.2	21	153.1	16	136.1	32	5.29	2.81E+05	11	
Linuron	330-55-2	36141	Herbicide		C ₉ H ₁₀ Cl ₂ N ₂ O ₂	248.0119	249.1	25	160.1	18	181.1	16	5.75	1.27E+06	14	
Malaoxon	1634-78-2	36142	Acaricide/Insecticide		C ₁₀ H ₁₉ O ₇ PS	314.0589	315.0	18	98.9	24	127.0	12	4.70	7.10E+06		8
Malathion	121-75-5	36143	Acaricide/Insecticide		C ₁₀ H ₁₉ O ₆ PS ₂	330.0361	331.0	14	127.0	12	99.0	24	5.95	4.46E+06		15
Mecarbam	2595-54-2	36515	Acaricide/Insecticide		C ₁₀ H ₂₀ NO ₅ PS ₂	329.0521	330.0	15	227.1	8	97.0	35	6.22	6.45E+06	18	
Mefenacet	73250-68-7	36150	Herbicide		C ₁₆ H ₁₄ N ₂ O ₂ S	298.0776	299.0	19	148.0	15	120.0	25	6.09	5.31E+06	17	
Mepanipyrim	110235-47-7	33970	Fungicide		C ₁₄ H ₁₃ N ₃	223.1109	224.1	40	106.0	25	77.0	40	6.12	1.11E+07	17	
Mephosfolan	950-10-7	34352	Insecticide		C ₈ H ₁₆ NO ₃ PS ₂	269.0309	270.1	28	140.0	24	75.1	22	4.55	1.93E+07	7	
Mepronil	55814-41-0	33361	Fungicide		C ₁₇ H ₁₉ NO ₂	269.1416	270.1	30	119.0	28	91.0	44	5.98	5.35E+06	16	
Mesosulfuron-methyl	208465-21-8	34178	Herbicide		C ₁₇ H ₂₁ N ₅ O ₉ S ₂	503.0781	504.0	32	182.0	24	82.9	60	5.23	2.10E+06	11	
Mesotrione	104206-82-8	33855	Herbicide		C ₁₄ H ₁₃ NO ₇ S	339.0413	340.0	28	104.0	32	228.0	18	4.03	2.27E+05	5	
Metalaxyl	57837-19-1	36153	Fungicide		C ₁₅ H ₂₁ NO ₄	279.1471	280.1	20	220.1	13	192.1	17	5.35	1.25E+07		11
Metamitron	41394-05-2	36154	Herbicide		C ₁₀ H ₁₀ N ₄ O	202.0855	203.1	28	175.1	16	104.0	22	3.25	2.79E+05		3
Metazachlor	67129-08-2	36155	Herbicide		C ₁₄ H ₁₆ ClN ₃ O	277.0982	278.0	16	134.1	22	210.0	10	5.27	2.35E+06	11	
Metconazole	125116-23-6	37909	Fungicide		C ₁₇ H ₂₂ ClN ₃ O	319.1451	320.1	32	70.0	22	125.0	36	6.75	5.76E+06		22
Methabenzthiazuron	18691-97-9	36156	Herbicide		C ₁₀ H ₁₁ N ₃ OS	221.0623	222.0	24	165.0	16	150.0	32	5.22	9.92E+06	11	
Methacrifos	62610-77-9	45569	Acaricide/Insecticide		C ₇ H ₁₃ O ₅ PS	240.0221	241.1	14	125.0	20	209.1	8	5.47	3.02E+06		12
Methamidophos	10265-92-6	33395	Acaricide/Insecticide		C ₂ H ₈ NO ₂ PS	141.0013	142.0	22	93.9	13	124.9	13	1.14	1.13E+06	1	
Methfuroxam	28730-17-8	36157	Fungicide		C ₁₄ H ₁₅ NO ₂	229.1103	230.0	30	137.0	20	111.0	15	5.53	4.18E+06	13	
Methidathion	950-37-8	36158	Insecticide		C ₆ H ₁₁ N ₂ O ₄ PS ₃	301.9619	303.0	12	85.1	20	145.0	10	5.45	5.94E+04		12

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Methiocarb	2032-65-7	PS543	Acaricide/Insecticide	Mercaptodimethur	C ₁₁ H ₁₅ NO ₂ S	225.0824	226.0	22	121.0	22	169.0	10	5.83	4.31E+06		14
Methiocarb sulfone	2179-25-1	MET543A	Metabolite		C ₁₁ H ₁₅ NO ₄ S	257.0722	258.1	25	122.1	19	107.1	38	3.59	6.19E+06		4
Methiocarb sulfoxide	2635-10-1	34177	Metabolite		C ₁₁ H ₁₅ NO ₃ S	241.0773	242.0	20	185.0	14	122.0	28	3.27	1.97E+07		3
Methomyl	16752-77-5	36159	Insecticide		C ₅ H ₁₀ N ₂ O ₂ S	162.0463	163.0	20	88.0	10	106.0	10	2.34	1.05E+06	2	
Methoprotrotryne	841-06-5	36160	Herbicide		C ₁₁ H ₂₁ N ₅ OS	271.1467	272.2	34	170.2	28	198.2	22	4.93	6.35E+07		9
Methoxyfenozide	161050-58-4		Insecticide		C ₂₂ H ₂₈ N ₂ O ₃	368.2100	369.1	28	149.1	18	313.2	8	6.00	7.04E+06		16
Metobromuron	3060-89-7	36162	Herbicide		C ₉ H ₁₁ BrN ₂ O ₂	258.0004	259.1	25	170.0	20	148.1	15	5.14	7.30E+05		10
Metolachlor	51218-45-2	36163	Herbicide		C ₁₅ H ₂₂ ClNO ₂	283.1339	284.1	20	176.1	25	252.1	15	6.33	1.45E+07	19	
Metolcarb	1129-41-5	33370	Insecticide		C ₉ H ₁₁ NO ₂	165.0790	166.0	14	109.0	12	94.1	27	4.29	4.60E+06	6	
Metosulam	139528-85-1	46317	Herbicide		C ₁₄ H ₁₃ Cl ₂ N ₅ O ₄ S	417.0065	418.0	35	175.0	28	140.0	52	4.78	1.46E+06		8
Metoxuron	19937-59-8	36164	Herbicide		C ₁₀ H ₁₃ ClN ₂ O ₂	228.0666	229.0	20	72.0	18	155.9	25	4.08	1.43E+06		5
Metrafenone	220899-03-6		Fungicide		C ₁₉ H ₂₁ BrO ₅	408.0572	409.0	22	209.1	14	226.9	16	6.81	2.12E+05	23	
Metribuzin	21087-64-9	36165	Herbicide		C ₈ H ₁₄ N ₄ OS	214.0888	215.0	35	131.0	18	89.0	20	4.53	3.93E+05	7	
Metsulfuron methyl	74223-64-6	46432	Herbicide		C ₁₄ H ₁₅ N ₅ O ₆ S	381.0743	382.0	22	167.0	16	198.9	22	4.67	3.16E+06	8	
Mevinphos	7786-34-7	36166	Acaricide/Insecticide		C ₇ H ₁₃ O ₆ P	224.0450	225.1	18	127.1	15	193.1	8	3.37	2.87E+06	4	
Molinate	2212-67-1	36171	Herbicide		C ₉ H ₁₇ NOS	187.1031	188.0	20	126.0	13	55.0	24	6.04	2.99E+06		16
Monocrotophos	6923-22-4	46159	Acaricide		C ₇ H ₁₄ NO ₅ P	223.0610	224.1	20	127.1	16	98.1	12	2.71	1.46E+06		2
Monolinuron	1746-81-2	45590	Herbicide		C ₉ H ₁₁ ClN ₂ O ₂	214.0509	215.0	28	126.0	22	99.0	34	4.93	5.46E+05		9
Monuron	150-68-5	36174	Herbicide		C ₉ H ₁₁ ClN ₂ O	198.0560	199.1	25	72.2	16	126.0	25	4.37	1.34E+05		6
Myclobutanil	88671-89-0	34360	Fungicide		C ₁₅ H ₁₇ ClN ₄	288.1142	289.1	28	70.2	18	125.1	32	6.08	3.01E+05		16
Naproanilide	52570-16-8		Herbicide		C ₁₉ H ₁₇ NO ₂	291.1259	292.2	30	171.1	15	120.1	25	no	no		
Napropamide	15299-99-7	36175	Herbicide		C ₁₇ H ₂₁ NO ₂	271.1572	272.1	24	129.1	16	171.1	18	6.28	3.30E+06		18
Naptalam	132-66-1	33371	Herbicide		C ₁₈ H ₁₃ NO ₃	291.0895	292.1	14	144.1	9	149.1	22	4.69	4.75E+06		8
Neburon	555-37-3	36176	Herbicide		C ₁₂ H ₁₆ Cl ₂ N ₂ O	274.0640	275.0	26	88.0	16	57.0	24	6.48	2.06E+06		20
Nicosulfuron	111991-09-4	34210	Herbicide		C ₁₅ H ₁₈ N ₆ O ₆ S	410.1009	411.0	26	182.0	22	106.0	32	4.57	1.03E+05		7
Nicotine	54-11-5	36733	Insecticide		C ₁₀ H ₁₄ N ₂	162.1157	163.1	30	130.1	18	132.1	15	0.74	8.67E+06	1	
Nitenpyram	150824-47-8	46077	Insecticide		C ₁₁ H ₁₅ ClN ₄ O ₂	270.0884	271.1	25	125.9	25	224.9	12	2.15	1.25E+06	2	
Nitralin	4726-14-1	36178	Herbicide		C ₁₃ H ₁₉ N ₃ O ₆ S	345.0995	346.1	25	304.1	16	262.1	20	6.41	1.01E+06		19
Novaluron	116714-46-6		Insecticide		C ₁₇ H ₉ ClF ₈ N ₂ O ₄	492.0123	493.0	30	158.0	19	141.0	35				
Nuarimol	63284-71-9	36180	Fungicide		C ₁₇ H ₁₂ ClFN ₂ O	314.0622	315.0	40	81.1	28	252.0	22	5.80	2.49E+05		14
Ofurace	58810-48-3	46143	Fungicide		C ₁₄ H ₁₆ ClNO ₃	281.0819	282.0	22	254.0	12	160.0	24	4.69	8.84E+05		8
Omethoate	1113-02-6	36181	Acaricide/Insecticide		C ₅ H ₁₂ NO ₄ PS	213.0225	214.1	20	125.1	22	183.1	11	1.76	1.41E+06		1
Orbencarb	34622-58-7	33362	Herbicide		C ₁₂ H ₁₆ ClNOS	257.0641	258.0	25	125.0	22	99.8	12	6.76	2.65E+06		22
Oryzalin	19044-88-3	36182	Herbicide		C ₁₂ H ₁₈ N ₄ O ₆ S	346.0947	347.0	25	288.0	18	305.1	14	6.29	8.11E+05		18
Oxadixyl	77732-09-3	34365	Fungicide		C ₁₄ H ₁₈ N ₂ O ₄	278.1267	279.0	34	219.0	10	132.0	34	4.32	2.10E+06		
Oxamyl	23135-22-0	36184	Insecticide/Nematicide	Thioxamyl	C ₇ H ₁₃ N ₃ O ₃ S	219.0678	237.0	15	72.0	10	90.0	10	2.13	1.44E+06	2	
Oxamyl-oxime	30558-43-1		Metabolite		C ₅ H ₁₀ N ₂ O ₂ S	162.0463	162.9	20	72.0	12	89.9	16	no	no		
Oxasulfuron	144651-06-9	46416	Herbicide		C ₁₇ H ₁₈ N ₄ O ₆ S	406.0947	407.0	25	150.1	20	107.1	50	4.40	2.11E+07	6	
Oxaziclomefone	153197-14-9		Herbicide		C ₂₀ H ₁₉ Cl ₂ NO ₂	375.0793	376.1	30	190.1	15	161.1	30				
Oxycarboxin	5259-88-1	36185	Fungicide		C ₁₂ H ₁₃ NO ₄ S	267.0565	268.1	20	174.8	16	146.9	25	3.69	2.04E+06		4
Oxydemeton-methyl	301-12-2	PS641	Metabolite	Demeton-S-methyl sulfoxide	C ₆ H ₁₅ O ₄ PS ₂	246.0149	247.0	20	168.8	14	108.9	25	2.35	1.94E+06		2
Paclobutrazol	76738-62-0	46046	Growth Regulator		C ₁₅ H ₂₀ ClN ₃ O	293.1295	294.1	30	125.1	38	70.2	20	5.95	4.92E+05	16	
Paraoxon-methyl	950-35-6	46192	Metabolite		C ₈ H ₁₀ NO ₆ P	247.0246	248.0	30	90.0	25	202.0	19	4.19	6.07E+05		5
Parathion	56-38-2	45607	Acaricide/Insecticide		C ₁₀ H ₁₄ NO ₅ PS	291.033	291.9	30.0	236.0	14.0	110.0	33	6.44	1.05E+06		19
Parathion-methyl	298-00-0	36187	Insecticide		C ₈ H ₁₀ NO ₅ PS	263.0017	263.9	32	109.0	22	79.0	36	5.71	5.49E+03		
Pebulat	1114-71-2	36188	Herbicide		C ₁₀ H ₂₁ NOS	203.1344	204.1	20	57.2	16	128.0	11	6.83	1.48E+07	23	
Penconazole	66246-88-6	36189	Fungicide		C ₁₃ H ₁₅ Cl ₂ N ₃	283.0643	284.0	28	70.1	16	159.0	34	6.58	1.89E+06	21	
Pencycuron	66063-05-6	36190	Fungicide		C ₁₉ H ₂₁ ClN ₂ O	328.1342	329.1	34	125.0	40	125.1	22	6.84	8.96E+06	23	
Pendimethalin	40487-42-1	36191	Herbicide		C ₁₃ H ₁₉ N ₃ O ₄	281.1376	282.2	15	212.2	10	194.1	17	7.40	1.22E+05	26	

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Penoxsulam	219714-96-2		Herbicide		C ₁₆ H ₁₄ F ₅ N ₅ O ₅ S	483.0636	484.2	45	195.1	30	164.1	40				
Pentoxazone	110956-75-7		Herbicide		C ₁₇ H ₁₇ ClFNO ₄	353.0830	354.0	22	285.9	14	185.9	26				
Phenmedipham	13684-63-4	36192	Herbicide		C ₁₆ H ₁₆ N ₂ O ₄	300.1110	301.0	28	168.0	10	136.0	22	5.57	9.69E+05	13	
Phenthoate	2597-03-7	46079	Insecticide		C ₁₂ H ₁₇ O ₄ PS ₂	320.0306	321.0	12	163.0	12	135.0	20	6.47	3.01E+05	20	
Phorate	298-02-2	33388	Insecticide		C ₇ H ₁₇ O ₂ PS ₃	260.0128	261.0	11	75.0	12	97.0	32	6.74	1.14E+06		22
Phorate sulfone	2588-04-7	46031	Metabolite		C ₇ H ₁₇ O ₄ PS ₃	292.0027	293.0	18	96.9	30	115.0	24	5.20	6.83E+05		10
Phorate sulfoxide	2588-03-6	45762	Metabolite		C ₇ H ₁₇ O ₃ PS ₃	276.0077	277.0	18	96.9	32	143.0	20	5.13	1.31E+05		10
Phosalone	2310-17-0	36194	Acaricide/Insecticide		C ₁₂ H ₁₅ ClNO ₄ PS ₂	366.9869	367.9	16	181.9	14	110.9	42	6.75	1.91E+05		22
Phosfolan	947-02-4	PS842	Insecticide		C ₇ H ₁₄ NO ₃ PS ₂	255.0153	256.0	20	140.0	20	168.0	20	4.03	4.56E+05		
Phosmet	732-11-6	36195	Insecticide	PMP	C ₁₁ H ₁₂ NO ₄ PS ₂	316.9945	318.0	22	160.0	22	77.0	46	4.22	4.04E+03		
Phosmet-oxon	3735-33-9	MET653A	Metabolite		C ₁₁ H ₁₂ NO ₅ PS	301.0174	302.0	22	160.0	16	77.0	50	no	no		
Phosphamidon	13171-21-6	45622	Insecticide/Nematicide		C ₁₀ H ₁₉ ClNO ₅ P	299.0689	300.1	22	174.1	14	127.1	25	4.40	1.95E+07	6	
Phoxim	14816-18-3	36197	Insecticide		C ₁₂ H ₁₅ N ₂ O ₃ PS	298.0541	299.0	16	129.0	13	153.0	7	6.69	5.74E+05	22	
Picloram	1918-02-1	36774	Herbicide		C ₆ H ₃ Cl ₃ N ₂ O ₂	239.9260	241.0	20	195.0	21	168.0	30	2.79	1.29E+06		2
Picolinafen	137641-05-5	37912	Herbicide		C ₁₉ H ₁₂ F ₄ N ₂ O ₂	376.0835	377.0	32	238.0	28	359.0	21	7.19	6.87E+05	25	
Picoxystrobin	117428-22-5	33658	Fungicide		C ₁₈ H ₁₆ F ₃ NO ₄	367.1031	368.0	14	145.1	22	205.1	10	6.41	7.81E+06		19
Piperonyl butoxide	51-03-6	45626	Antiparasiticide/Synergist		C ₁₉ H ₃₀ O ₅	338.2093	356.3	20	176.9	11	119.0	37	7.24	3.09E+07		25
Piperophos	24151-93-7	46011	Herbicide		C ₁₄ H ₂₈ NO ₃ PS ₂	353.1248	354.1	25	171.0	22	143.0	32	6.89	2.10E+07		23
Pirimicarb	23103-98-2	45627	Insecticide		C ₁₁ H ₁₈ N ₄ O ₂	238.1430	239.1	28	72.0	18	182.1	15	3.55	3.71E+07		3
Pirimiphos-ethyl	23505-41-1	45628	Insecticide		C ₁₃ H ₂₄ N ₃ O ₃ PS	333.1276	334.1	36	198.1	23	182.1	25	7.09	1.14E+08		24
Pirimiphos-methyl	29232-93-7	45629	Insecticide		C ₁₁ H ₂₀ N ₃ O ₃ PS	305.0963	306.1	30	164.1	22	108.1	32	6.58	8.77E+07	21	
Primisulfuron-methyl	86209-51-0	46010	Herbicide		C ₁₅ H ₁₂ F ₄ N ₄ O ₇ S	366.9869	469.0	10	254.0	20	199.0	20	6.02	3.01E+04		
Probenazole	27605-76-1		Fungicide		C ₁₀ H ₉ NO ₃ S	223.0303	224.0	16	41.5	10	196.1	13	4.38	3.88E+05		
Prochloraz	67747-09-5	45631	Fungicide		C ₁₅ H ₁₆ Cl ₃ N ₃ O ₂	375.0308	376.0	16	307.1	16	70.1	34	6.53	1.08E+04		20
Procymidone	32809-16-8	36640	Fungicide		C ₁₃ H ₁₁ Cl ₂ NO ₂	283.0167	284.1	36	67.1	28	256.1	17	no	no		
Profenofos	41198-08-7	45632	Insecticide		C ₁₁ H ₁₅ BrClO ₃ PS	371.9351	372.9	30	302.6	20	127.9	40	7.12	2.70E+06		24
Promecarb	2631-37-0	45634	Insecticide		C ₁₂ H ₁₇ NO ₂	207.1259	208.1	20	151.0	9	109.0	15	5.94	1.20E+07		15
Prometon	1610-18-0	45635	Herbicide		C ₁₀ H ₁₉ N ₅ O	225.1590	226.0	32	86.3	28	184.3	18	4.57	3.54E+07		6
Prometryn	7287-19-6	45636	Herbicide		C ₁₀ H ₁₉ N ₅ S	241.1361	242.0	20	158.0	25	200.1	17	5.44	2.56E+07	12	
Propachlor	1918-16-7	45637	Herbicide		C ₁₁ H ₁₄ ClNO	211.0764	212.1	25	170.1	14	94.1	25	5.31	2.37E+07		11
Propamocarb	24579-73-5	45638	Herbicide		C ₉ H ₂₀ N ₂ O ₂	188.1525	189.1	25	102.0	17	144.0	12	1.82	2.42E+07		1
Propanil	709-98-8	45639	Herbicide		C ₉ H ₉ Cl ₂ NO	217.0061	217.9	34	161.9	16	127.0	22	5.79	4.69E+05		14
Propaquizafop	111479-05-1	46007	Herbicide		C ₂₂ H ₂₂ ClN ₃ O ₅	443.1248	444.2	30	100.0	20	163.1	60	7.18	5.07E+06	25	
Propargite	2312-35-8	45310	Acaricide		C ₁₉ H ₂₆ O ₄ S	350.1552	351.1	8	231.1	5	57.0	20	no	no		
Propazine	139-40-2	45640	Herbicide		C ₉ H ₁₆ ClN ₅	229.1094	230.2	34	146.1	24	188.1	18	5.75	4.90E+07	14	
Propetamphos	31218-83-4	34371	Insecticide		C ₁₀ H ₂₀ NO ₄ PS	281.0851	282.0	11	138.0	20	156.0	12	6.07	6.09E+05		16
Propham	122-42-9	45641	Herbicide		C ₁₀ H ₁₃ NO ₂	179.0946	180.0	8	138.0	8	120.0	16	5.15	5.49E+05		10
Propiconazole	60207-90-1	45642	Fungicide		C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	341.0698	342.0	40	69.0	22	159.0	34	6.65	7.10E+06		21
Propoxur	114-26-1	45644	Insecticide		C ₁₁ H ₁₅ NO ₃	209.1052	210.0	15	111.0	16	168.0	10	4.58	9.36E+06		7
Propyzamide	23950-58-5	45645	Herbicide		C ₁₂ H ₁₁ Cl ₂ NO	255.0218	256.1	25	190.0	16	173.0	23	5.98	2.73E+06	16	
Prosulfocarb	52888-80-9	36520	Herbicide		C ₁₄ H ₂₁ NOS	251.1344	252.0	23	90.9	22	127.9	13	7.04	4.89E+06		24
Prosulfuron	94125-34-5	46104	Herbicide		C ₁₅ H ₁₆ F ₃ N ₅ O ₄ S	419.0875	420.0	26	141.0	20	167.0	20	5.80	1.75E+06		14
Prothioconazole	178928-70-6	34232	Fungicide		C ₁₄ H ₁₅ Cl ₂ N ₃ OS	343.0313	344.0	16	326.0	12	189.0	20	6.71	7.12E+04		
Pymetrozine	123312-89-0	46119	Insecticide		C ₁₀ H ₁₁ N ₅ O	217.0964	218.0	32	105.0	20	79.0	30	1.43	5.86E+06	1	
Pyracarbolid	24691-76-7	45646	Fungicide		C ₁₃ H ₁₅ NO ₂	217.1103	218.1	26	125.1	18	97.1	28	4.66	3.58E+07	8	
Pyraclostrobin	175013-18-0	33696	Fungicide		C ₁₉ H ₁₈ ClN ₃ O ₄	387.0986	388.1	25	163.0	25	193.9	12	6.70	5.14E+06	22	
Pyrazolynate	58011-68-0		Herbicide	Pyrazolate	C ₁₉ H ₁₆ Cl ₂ N ₂ O ₄ S	438.0208	439.1	28	91.0	42	172.9	20				
Pyrazophos	13457-18-6	45648	Fungicide		C ₁₄ H ₂₀ N ₃ O ₅ PS	373.0861	374.0	38	222.1	22	194.0	32	6.75	4.51E+05		22
Pyrazosulfuron-ethyl	93697-74-6	46323	Herbicide		C ₁₄ H ₁₈ N ₆ O ₇ S	414.0958	415.0	22	182.0	20	82.9	45	6.16	4.15E+06		17
Pyridaben	96489-71-3	46047	Acaricide/Insecticide		C ₁₉ H ₂₅ ClN ₂ OS	364.1376	365.1	22	147.1	24	309.1	12	7.71	5.01E+06		26

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Pyridafol	40020-01-7		Metabolite	6-chloro-4-hydroxy-3-phenylpyridazin	C ₁₀ H ₇ ClN ₂ O	206.0247	207.0	40	103.9	22	77.0	30	4.03	2.51E+04		5
Pyridaphenthion	119-12-0	36895	Insecticide		C ₁₄ H ₁₇ N ₂ O ₄ PS	340.0647	341.0	34	189.0	22	92.0	34	6.07	1.82E+07		16
Pyridate	55512-33-9	45312	Herbicide		C ₁₉ H ₂₃ ClN ₂ O ₂ S	378.1169	379.0	22	207.0	18	351.1	10	7.88	2.16E+05		26
Pyrifenoxy	88283-41-4	45737	Fungicide		C ₁₄ H ₁₂ Cl ₂ N ₂ O	294.0327	295.0	32	93.1	22	67.2	60	5.60	5.63E+07		12
Pyrifthalid	135186-78-6	33694	Herbicide		C ₁₅ H ₁₄ N ₂ O ₄ S	318.0674	319.1	45	139.1	25	179.1	30				
Pyrimethanil	53112-28-0	46039	Fungicide		C ₁₂ H ₁₃ N ₃	199.1109	200.0	45	107.0	24	82.0	24	5.03	6.34E+06	9	
Pyriproxifen	95737-68-1	34174	Growth Regulator		C ₂₀ H ₁₉ NO ₃	321.1365	322.1	26	96.0	14	227.1	14	7.27	5.58E+07		25
Pyroquilon	57369-32-1	45650	Fungicide		C ₁₁ H ₁₁ NO	173.0841	174.0	35	132.0	23	117.0	30	4.49	1.42E+06	7	
Quinalphos	13593-03-8	45651	Acaricide/Insecticide		C ₁₂ H ₁₅ N ₂ O ₃ PS	298.0541	299.0	18	162.9	24	96.9	30	6.47	1.85E+06	20	
Quinmerac	90717-03-6	36522	Herbicide		C ₁₁ H ₈ ClNO ₂	221.0244	222.2	22	204.2	15	141.1	30	3.36	5.11E+06	4	
Quinoxifen	124495-18-7	46439	Fungicide		C ₁₅ H ₈ Cl ₂ FNO	306.9967	308.0	55	197.0	32	161.9	44	7.33	1.40E+06		25
Quizalofop-ethyl	76578-14-8	34306	Herbicide		C ₁₉ H ₁₇ ClN ₂ O ₄	372.0877	373.0	34	299.1	18	91.1	32	7.08	5.93E+06		24
Quizalofop-methyl	76578-13-7		Herbicide		C ₁₈ H ₁₅ ClN ₂ O ₄	358.0720	359.0	34	299.1	18	91.1	28	6.84	5.43E+06	23	
Quizalofop-p-tefuryl	200509-41-7	33942	Herbicide		C ₂₂ H ₂₁ ClN ₂ O ₅	428.1139	429.1	28	299.0	22	147.1	27				
Rabenzazol	40341-04-6	45654	Fungicide		C ₁₂ H ₁₂ N ₄	212.1062	213.1	34	172.1	20	118.1	35	5.16	6.74E+07		10
Rimsulfuron	122931-48-0	46097	Herbicide		C ₁₄ H ₁₇ N ₅ O ₇ S ₂	431.0569	431.9	28	325.1	14	182.1	22	4.94	5.77E+03		
Rotenone	83-79-4	45656	Insecticide		C ₂₃ H ₂₂ O ₆	394.1416	395.0	40	213.1	24	192.1	24	6.39	8.29E+05	19	
Sebuthylazin	7286-69-3	36785	Herbicide		C ₉ H ₁₆ ClN ₅	229.1094	230.0	30	174.0	18	96.0	26	5.70	2.22E+07	15	
Sebuthylazin-desethyl	37019-18-4	36511	Metabolite		C ₇ H ₁₂ ClN ₅	201.0781	202.2	30	146.1	17	79.2	25	4.37	5.50E+07	6	
Secbumeton	26259-45-0	45658	Herbicide		C ₁₀ H ₁₉ N ₅ O	225.1590	226.2	30	170.2	19	100.2	28	4.39	1.02E+08	6	
Sethoxydim	74051-80-2	36795	Herbicide		C ₁₇ H ₂₉ NO ₃ S	327.1868	328.0	28	178.0	22	282.0	10	7.16	8.21E+06	25	
Siduron	1982-49-6	34373	Herbicide		C ₁₄ H ₂₀ N ₂ O	232.1576	233.0	30	93.8	25	137.0	17	5.76	3.71E+06	14	
Simazine	122-34-9	45659	Herbicide		C ₇ H ₁₂ ClN ₅	201.0781	202.0	34	124.0	16	96.0	22	4.57	2.85E+07		7
Simeconazole	149508-90-7		Fungicide		C ₁₄ H ₂₀ FN ₃ OSi	293.1360	294.1	26	70.1	22	141.0	25	5.99	2.31E+06		15
Simetryn	1014-70-6	45660	Herbicide		C ₈ H ₁₅ N ₅ S	213.1048	214.0	35	124.0	20	95.9	25	4.27	2.10E+07		5
Spinosad A	131929-60-7		Insecticide		C ₄₁ H ₆₅ NO ₁₀	731.4608	732.6	50	142.0	31	98.1	59	6.43	1.47E+06		18
Spinosad D	131929-63-0		Insecticide		C ₄₂ H ₆₇ NO ₁₀	745.4765	746.5	45	142.0	31	98.1	53	6.61	1.47E+05		19
Spirodiclofen	148477-71-8	33654	Acaricide		C ₂₁ H ₂₄ Cl ₂ O ₄	410.1052	411.1	25	71.2	13	313.0	13	7.57	1.16E+05		
Spiromesifen	283594-90-1	33599	Insecticide		C ₂₃ H ₃₀ O ₄	370.2144	371.1	10	273.1	10	255.1	24	7.43	1.47E+05	26	
Spiroxamine	118134-30-8	46443	Fungicide		C ₁₈ H ₃₅ NO ₂	297.2668	298.0	32	144.0	20	100.0	32	5.44	9.12E+07	13	
Sulcotrione	99105-77-8	46318	Herbicide		C ₁₄ H ₁₃ ClO ₅ S	328.0172	329.0	30	139.1	18	69.2	38	4.42	8.10E+06	6	
Sulfallate	95-06-7	45663	Herbicide		C ₈ H ₁₄ CINS ₂	223.0256	224.0	16	116.0	12	87.9	20	6.54	1.69E+05		20
Sulfaquinoxaline	59-40-5	45662	Rodenticide		C ₁₄ H ₁₂ N ₄ O ₂ S	300.0681	301.1	26	156.1	16	92.2	30	3.91	2.08E+07	5	
Sulfentrazone	122836-35-5		Herbicide		C ₁₁ H ₁₀ Cl ₂ F ₂ N ₄ O ₃ S	385.9819	387.0	30	307.0	20	145.8	46				
Sulfometuron-methyl	74222-97-2	34224	Metabolite		C ₁₅ H ₁₆ N ₄ O ₅ S	364.0841	365.0	24	150.0	18	107.0	43	4.65	8.77E+06	8	
Sulfosulfuron	141776-32-1	33307	Herbicide		C ₁₆ H ₁₈ N ₆ O ₇ S ₂	470.0678	471.0	23	211.0	13	261.0	18	5.69	1.07E+06		13
Sulfotep	3689-24-5	45664	Insecticide		C ₈ H ₂₀ O ₅ P ₂ S ₂	322.0227	323.0	22	97.0	32	171.0	15	6.51	3.29E+06		20
Tebuconazole	107534-96-3	36565	Fungicide		C ₁₆ H ₂₂ ClN ₃ O	307.1451	308.0	34	70.1	22	125.0	40	6.58	3.56E+06	21	
Tebufenozide	112410-23-8	46095	Insecticide		C ₂₂ H ₂₈ N ₂ O ₂	352.2151	353.1	13	133.0	20	297.1	8	6.43	6.33E+06		19
Tebufenpyrad	119168-77-3	46438	Acaricide/Insecticide		C ₁₈ H ₂₄ ClN ₃ O	333.1608	334.0	46	117.0	34	145.0	28	7.19	1.92E+05	25	
Tebupirimfos	96182-53-5	46075	Insecticide		C ₁₃ H ₂₃ N ₂ O ₃ PS	318.1167	319.0	23	153.0	29	277.0	15	7.21	1.25E+07		25
Tebutam	35256-85-0	36566	Herbicide		C ₁₅ H ₂₃ NO	233.1780	234.1	27	91.0	18	192.1	18	6.31	1.57E+07	19	
Tebuthiuron	34014-18-1	45671	Herbicide		C ₉ H ₁₆ N ₄ OS	228.1045	229.0	30	172.0	18	116.0	26	4.75	1.92E+07		8
Teflubenzuron	83121-18-0	45756	Insecticide		C ₁₄ H ₆ Cl ₂ F ₄ N ₂ O ₂	379.9742	380.9	20	158.0	20	140.9	40	7.29	1.35E+03		
Temephos	3383-96-8	45673	Insecticide		C ₁₆ H ₂₀ O ₆ P ₂ S ₃	465.9897	466.8	32	125.0	38	418.9	22	7.20	1.98E+06	25	
TEPP	107-49-3	36567	Acaricide/Insecticide	Tetraethyl diphosphate	C ₈ H ₂₀ O ₇ P ₂	290.0684	291.0	28	179.0	22	99.0	34				
Tepraloxymid	149979-41-9	46331	Herbicide		C ₁₇ H ₂₄ ClNO ₄	341.1394	342.1	20	250.1	12	166.1	20	6.13	3.59E+06		17
Terbufos	13071-79-9	45313	Insecticide		C ₉ H ₂₁ O ₂ PS ₃	288.0441	289.0	12	103.0	8	57.2	22	7.16	2.28E+06		24
Terbufos-sulfone	56070-16-7	46043	Metabolite		C ₉ H ₂₁ O ₄ PS ₃	320.0340	321.0	14	97.0	40	171.0	12	5.65	5.84E+06		13
Terbufos-sulfoxide	10548-10-4	46044	Metabolite		C ₉ H ₂₁ O ₃ PS ₃	304.0390	305.0	14	187.0	11	97.0	40	5.66	1.78E+07		13

Pesticide	CAS	Sigma	Application	Synonyms	Formula	Monoisotopic mass	Parent	CV (V)	Product 1	CE (eV)	Product 2	CE (eV)	RT	Sensitivity	Method 1 Function	Method 2 Function
Terbumeton	33693-04-8	45676	Herbicide		$C_{10}H_{19}N_5O$	225.1590	226.1	15	170.1	15	114.1	25	4.55	3.47E+07	6	
Terbumeton-desethyl	30125-64-5	36514	Metabolite		$C_8H_{15}N_5O$	197.1277	198.2	26	142.1	16	86.1	24	3.35	1.06E+08	4	
Terbutylazine	5915-41-3	45678	Herbicide		$C_9H_{16}ClN_5$	229.1094	230.0	28	174.0	16	96.0	28	5.82	9.42E+07		14
Terbutylazine-2-hydroxy	66753-07-9	46019	Metabolite		$C_9H_{17}N_5O$	211.1433	212.2	24	156.1	15	86.1	24	3.26	1.00E+08		3
Terbutylazine-desethyl	30125-63-4	36769	Metabolite		$C_7H_{12}ClN_5$	201.0781	202.1	24	146.1	16	79.1	26	4.78	8.64E+07		8
Terbutryn	886-50-0	45677	Herbicide		$C_{10}H_{19}N_5S$	241.1361	242.1	34	186.1	20	91.0	28	5.49	3.53E+07		11
Tetrachlorvinphos	22248-79-9	45679	Insecticide		$C_{10}H_9Cl_4O_4P$	363.8993	364.8	26	127.0	16	238.9	20	6.47	8.80E+05	20	
Tetraconazole	112281-77-3		Fungicide		$C_{13}H_{11}Cl_2F_4N_3O$	371.0215	372.0	35	70.1	20	159.0	30	6.25	6.54E+05		18
Thiabendazole	148-79-8	45684	Fungicide		$C_{10}H_7N_3S$	201.0361	202.0	45	175.0	25	131.0	30	2.66	1.45E+07		2
Thiacloprid	111988-49-9	37905	Insecticide		$C_{10}H_9ClN_4S$	252.0236	253.0	35	126.0	20	90.1	40	3.76	4.04E+06	5	
Thiamethoxam	153719-23-4	37924	Insecticide		$C_8H_{10}ClN_5O_3S$	291.0193	292.0	22	211.2	12	132.0	22	2.56	6.66E+05		2
Thiazafluron	25366-23-8	45685	Herbicide		$C_6H_7F_3N_4OS$	240.0293	241.0	21	184.0	15	73.9	32	4.71	2.53E+06		8
Thiazopyr	117718-60-2		Herbicide		$C_{16}H_{17}F_5N_2O_2S$	396.0931	397.1	30	377.1	23	317.1	25				
Thidiazuron	51707-55-2	45686	Herbicide		$C_9H_8N_4OS$	220.0419	221.0	22	101.9	15	93.9	13	4.63	1.57E+06	8	
Thifensulfuron methyl	79277-27-3	46028	Herbicide		$C_{12}H_{13}N_5O_6S_2$	387.0307	388.0	30	167.0	15	56.0	40	4.54	8.72E+05	7	
Thiodicarb	59669-26-0	34375	Insecticide		$C_{10}H_{18}N_4O_4S_3$	354.0490	355.0	20	87.9	16	107.9	16	5.01	3.70E+06	10	
Thiofanox	39196-18-4	45314	Insecticide		$C_9H_{18}N_2O_2S$	218.1089	219.0	10	57.0	12	76.0	8	5.05	7.19E+04	10	
Thiofanox-sulfone	39184-59-3	45764	Metabolite		$C_9H_{18}N_2O_4S$	250.0987	251.1	12	57.2	10	76.1	6	3.26	2.36E+04	4	
Thiometon sulfoxide	39184-27-5	45765	Metabolite		$C_6H_{15}O_3PS_3$	261.9921	263.0	20	124.8	25	92.9	30	no	no		
Thiophanate	23564-06-9	PS223	Fungicide		$C_{14}H_{18}N_4O_4S_2$	370.0769	371.0	22	151.0	22	93.1	50	5.37	8.65E+06		11
Thiophanate-methyl	23564-05-8	45688	Fungicide		$C_{12}H_{14}N_4O_4S_2$	342.0456	343.0	22	151.0	22	93.0	46	4.58	1.02E+07		7
Thiuram	137-26-8	45689	Fungicide	Tetramethylthiuram disulfide	$C_6H_{12}N_2S_4$	239.9883	241.0	13	87.9	11	119.9	16	no	no		
Tolcofos methyl	57018-04-9	36641	Fungicide		$C_9H_{11}Cl_2O_3PS$	299.9544	301.1	35	125.0	17	174.9	29	no	no		
Tolyfluanid	731-27-1	45690	Fungicide		$C_{10}H_{13}Cl_2FN_2O_2S_2$	345.9780	347.0	19	137.0	28	238.0	10	6.53	1.45E+06		20
Topramezone	210631-68-8	34225	Herbicide		$C_{16}H_{17}N_3O_5S$	363.0889	364.0	25	334.0	16	125.0	29	3.17	3.17E+05		3
Tralkoxidym	87820-88-0	36536	Herbicide		$C_{20}H_{27}NO_3$	329.1991	330.2	25	138.1	19	284.3	13	7.37	1.26E+07	26	
Triadimefon	43121-43-3	45693	Fungicide		$C_{14}H_{16}ClN_3O_2$	293.0931	294.1	25	69.3	20	197.2	15	5.94	2.46E+07		16
Triadimenol	55219-65-3	46138	Fungicide		$C_{14}H_{18}ClN_3O_2$	295.1088	296.1	15	70.2	10	99.1	15	6.15	6.99E+04		17
Triallate	2303-17-5	45695	Herbicide		$C_{10}H_{16}Cl_3NOS$	303.0018	304.0	26	86.0	18	142.9	28	7.41	5.03E+05	26	
Triasulfuron	82097-50-5	33383	Herbicide		$C_{14}H_{16}ClN_5O_5S$	401.0561	402.0	25	167.1	17	141.0	20	4.54	3.73E+05	7	
Triasulfuron methyl	126535-15-7		Herbicide		$C_{13}H_{14}ClN_5O_5S$	387.0404	388.2	20	167.2	20	141.1	20				
Triazophos	24017-47-8	45696	Acaricide/Ne-matocide		$C_{12}H_{16}N_3O_3PS$	313.0650	314.1	25	161.9	18	118.9	35	6.12	2.94E+06	17	
Triazoxid	72459-58-6	33373	Fungicide		$C_{10}H_6ClN_5O$	247.0261	248.0	42	68.1	28	95.0	26	4.39	1.03E+07		6
Tribenuron methyl	101200-48-0	46013	Herbicide		$C_{15}H_{17}N_5O_6S$	395.0900	396.1	18	154.9	14	180.9	22	no	no		
Trichlorfon	52-68-6	45698	Insecticide		$C_4H_8Cl_3O_4P$	255.9226	257.0	22	109.0	18	79.0	30	3.31	1.49E+06		3
Tricyclazole	41814-78-2	45808	Fungicide		$C_9H_7N_3S$	189.0361	190.0	35	163.0	22	136.0	27	3.94	3.12E+07	5	
Tridemorph	24602-86-6	36199	Fungicide		$C_{19}H_{39}NO$	297.3032	298.1	46	57.0	28	98.0	34	no	no		
Trietazine	1912-26-1	46086	Herbicide		$C_9H_{16}ClN_5$	229.1094	230.0	35	98.9	23	70.9	30	6.21	1.89E+07	18	
Trifloxystrobin	141517-21-7	46447	Fungicide		$C_{20}H_{19}F_3N_2O_4$	408.1297	409.0	28	186.0	16	145.0	40	6.93	1.10E+07	24	
Trifloxysulfuron	199119-58-9	33672	Herbicide		$C_{14}H_{14}F_3N_5O_6S$	437.0617	438.0	24	182.0	20	139.0	45	5.26	3.36E+06	11	
Triflumizole	99387-89-0		Fungicide		$C_{15}H_{15}ClF_3N_3O$	345.0856	346.0	16	277.9	10	60.0	10	6.87	1.60E+07		23
Triflumuron	64628-44-0	35029	Insecticide		$C_{15}H_{10}ClF_3N_2O_3$	358.0332	359.0	25	156.1	16	139.1	35	6.71	3.54E+06	22	
Triflusulfuron-methyl	126535-15-7	46326	Herbicide		$C_{17}H_{19}F_3N_6O_6S$	492.1039	493.2	28	264.0	18	96.0	45	5.87	1.11E+06	15	
Triticonazole	131983-72-7	34172	Fungicide		$C_{17}H_{20}ClN_3O$	317.1295	318.1	25	70.1	16	124.9	35	2.56	1.07E+06		2
Tritosulfuron	142469-14-5	33873	Herbicide		$C_{13}H_9F_6N_5O_4S$	445.0279	446.0	30	195.0	18	145.0	34	no	no		
Vamidothion	2275-23-2	37914	Acaricide/Insecticide		$C_8H_{18}NO_4PS_2$	287.0415	288.0	22	146.0	10	118.0	28	3.38	3.49E+07	4	
Vamidothion sulfone	70898-34-9		Metabolite		$C_8H_{18}NO_6PS_2$	319.0313	320.0	30	177.9	14	86.0	25	2.55	2.32E+05		
Vamidothion sulfoxide	20300-00-9		Metabolite		$C_8H_{18}NO_5PS_2$	303.0364	304.2	32	201.0	15	169.0	15				
Vernolat	1929-77-7	45704	Herbicide		$C_{10}H_{21}NOS$	203.1344	204.1	22	128.1	11	86.1	14	6.83	1.20E+07	23	
Zoxamide	156052-68-5		Fungicide		$C_{14}H_{16}Cl_3NO_2$	335.0247	336.0	32	187.1	25	159.0	38	6.67	4.02E+06		21

Mobile phase A 98:2 Water/Methanol + 0.1% FA
Mobile phase B Methanol + 0.1% FA

Gradient	Time	Flow	%A	%B	Curve
	Initial	0.45	95.0	5.0	Initial
	0.25	0.45	95.0	5.0	6
	7.75	0.45	0.0	100.0	6
	8.50	0.45	0.0	100.0	6
	8.51	0.45	95.0	5.0	6
	10.00	0.45	95.0	5.0	6

Column ACQUITY BEH C18, 2.1 x 100 mm, 1.7 μ m
Column temperature 40 °C

Waters part number: 186002352

Injection mode Full loop
Injection volume 20 μ L
Sample temperature 10 °C

Capillary	1.0
Extractor	4.0
RF Lens	0.0
Source temperature	120.0
Desolvation temperature	450.0
Desolvation flow rate	1000.0
Cone gas flow rate	50.0
LM Res 1	13.5
HM Res 2	13.5
Ion energy 1	0.7
Entrance	0.0
Exit	0.0
LM Res 2	13.5
HM Res 2	13.5
Ion energy 2	1.0
PM	670.0
Collision gas pressure	3.50E-03
Ion counting	30.0

TQD should be calibrated using peg neo to help get accurate mass measurement at the lower end of the mass scale. Use NaICs for work that has fragments above 132da in size.

Capillary	1.0
Extractor	4.0
RF Lens	0.0
Source temperature	120.0
Desolvation temperature	450.0
Desolvation flow rate	1000.0
Cone gas flow rate	50.0
LM Res 1	13.5
HM Res 2	13.5
Ion energy 1	0.7
Entrance	0.0
Exit	0.0
LM Res 2	13.5
HM Res 2	13.5
Ion energy 2	1.0
PM	670.0
Collision gas pressure	3.50E-03
Ion counting	30.0

QPXE should be calibrated using peg neo to help get accurate mass measurement at the lower end of the mass scale. Use NaICs for work that has fragments above 132da in size.

■分析例 3

【システム】

- ・ SFC ACQUITY UPC² システム
- ・ MS Xevo TQD タンデム四重極型質量分析計
- ・ ソフトウェア MassLynx 4.1
TargetLynx アプリケーションマネージャ

【UPC²条件】

- ・ サンプル温度 10°C
- ・ 注入量 2 uL
- ・ 洗浄溶媒 メタノール/イソプロパノール=70/30
- ・ カラム ACQUITY UPC² HSS C18 SB, 1.8 um, 3.0 ×100 mm
- ・ カラム温度 60°C
- ・ 流速 2.0 mL/min
- ・ 移動相 超臨界二酸化炭素
- ・ Modifier MeOH/MeCN = 50/50
- ・ グラジエント
- ・ Run Time 4.5 分
- ・ Make Up MeOH 0.3mL/min
- ・ Convergence 2000 psi

【MS条件】

MS Tune

- ・ イオン化モード APCI ポジティブ APCI ネガティブ
- ・ コロナ電流 1.5 kV(ポジティブ) 15 kV(ネガティブ)
- ・ 脱溶媒ガス 1100 L/hr 350°C
- ・ イオン源ヒーター 150°C

SIM

化合物	APCI	フレイカーイオン	フレイカーイオン (<i>m/z</i>)	Dwell Time	イオン電圧 (V)
Methoxychlor	+	(M-CCl ₃) ⁺	227.1	0.03	60
Etridiazol	+	(M+H) ⁺	246.8	0.03	26
Dicofol	+	(M-CCl ₃) ⁺	250.9	0.03	22
Ethalfuralin	+	(M+H) ⁺	333.9	0.039	24
Trifluralin	+	(M+H) ⁺	335.9	0.039	28
Benfluralin	+	(M+H) ⁺	335.9	0.039	26
Fenpropathrin	+	(M+H) ⁺	350.0	0.054	22
Tecnazene	-	(M-Cl+O) ⁻	239.8	0.039	42
HCB	-	(M-Cl+O) ⁻	264.7	0.047	50
Quintozene	-	(M-Cl+O) ⁻	275.7	0.047	42
A-BHC	-	(M+H) ⁻	288.8	0.03	10
B-BHC	-	(M+H) ⁻	288.8	0.03	25
D-BHC	-	(M+H) ⁻	288.8	0.054	15
Tetradiphon	-	(M-Cl+O) ⁻	336.8	0.03	58
Heptachlor epoxideA	-	(M-Cl+O) ⁻	368.7	0.099	22
Heptachlor epoxideB	-	(M-Cl+O) ⁻	368.7	0.099	22
Endrin	-	(M+H) ⁻	380.7	0.03	15
Dieldrin	-	(M+H) ⁻	380.7	0.03	15
cis Chlordane	-	(M+H) ⁻	388.7	0.03	18
trans Chlordane	-	(M+H) ⁻	388.7	0.03	18

■ジコホール

分析条件

装置 Waters 2695 セパレーションモジュール
Quattro *micro* API タンデムマス検出器

HPLC カラム Waters Atlantis dC18 (3.0 μ m 2.1 x 150mm) 40°C
移動相 A:10mM 酢酸アンモニウム
B:メタノール
C:10% ギ酸

グラジエント

Time(min)	A%	B%	C%	Curve
0.0	84	15	1	1
10.0	29	70	1	6
25.0	4	95	1	6
30.0	84	15	1	11

流速 0.20 ml/min

注入量 10 μ L

試料調製 検量線用試料は、標準溶液 1000ppm を 10% アセトニトリルで混合希釈し、HPLC/MS 注入用試料としました。

また実試料は、乾燥野菜抽出液に標準混合溶液を 500ppb, 10ppb になるよう添加したものと、それを 10%アセトニトリルで 10 倍、100 倍、1000 倍したものを HPLC/MS 注入用試料としました。

MS ESI モード
キャピラリー電圧 0.75 kv
脱溶媒ガス 750 L /hr(450°C)
コーンガス 50 L/hr
イオン源ヒーター 120°C

MS データ取り込み条件(MRM)

	サンプル名	Mass	Dwell 時間	コーン電圧	コリジョンエネルギー	取り込み時間
1	イミダクロプリド	256.1>175.1	0.3sec	20V	20eV	10~13min
2	イプロジオン	330.0>245.0	0.5sec	25V	15eV	13~21.5min
3	イプロジオン代謝物	330.0>100.8	0.3sec	30V	25eV	21.5~30min
4	クロルフルアズロン	541.8>384.8	0.3sec	30V	25eV	21.5~30min
5	チオファネートメチル	343.0>150.9	0.5sec	20V	20eV	13~21.5min
6	バミドチオン	288.0>146.0	0.3sec	20V	15eV	10~13min
7	メタミドホス	142.0>111.8	0.5sec	25V	15eV	0~5min
8	モノクロトホス	224.1>126.8	0.5sec	20V	15eV	5~10.2min
9	トリクロルホン	257.0>126.8	0.3sec	20V	15eV	10~13min
*10	ジコホール	251.1>138.9	0.3sec	20V	20eV	21.5~30min

【システム】
 LC : ACQUITY UPLC® BSM (バイナリーソルベントマネージャー),
 SM (サンプルマネージャー)
 MS : Xevo™ TQ MS
 ソフトウェア : MassLynx™ ソフトウェア

【LC条件】

・サンプル温度 5°C
 ・注入量(注入方法) 5 µL (パーシャルループ)
 ・弱洗浄溶媒 10%-アセトニトリル水溶液 600 µL
 ・強洗浄溶媒 アセトニトリル 200 µL
 ・カラム ACQUITY UPLC BEH C18 (2.1×100 mm, 1.7 µm)
 ・移動相
 A: 5 mM-酢酸アンモニウム水溶液
 B: 5 mM-酢酸アンモニウム/メタノール
 ・カラム温度 40°C
 ・流速 0.4 mL/min
 ・グラジエント

時間 (min)	A (%)	B (%)	Curve
0.0	85	15	Initial
1.1	60	40	6
2.0	60	40	6
2.8	50	50	6
4.0	45	55	6
8.0	10	90	6
8.5	10	90	6
8.6	5	95	6
10.0	85	15	11

・分析時間 12 min

【MS条件】

MS Tune
 ・イオン化モード: ESIポジティブ/ESIネガティブ
 ・キャピラリー電圧: 0.5 kV(ポジティブ)、0.5 kV(ネガティブ)
 ・脱溶媒ガス: 1200 L/hr (550 °C)
 ・コーンガス: 50 L/hr
 ・イオン源ヒーター: 150 °C
 ・コリジョンガス流量 0.15 mL/min

No.	Compound	Ion	アーカーサイオン (m/z)	プロダクトイオン (m/z)	トウエルタイム (sec)	コソ電圧 (V)	コリソエネルギー (eV)	取り込み時間
51	Pyraclostrobin	+	1 st	388.1	194.0	0.018	16	6.97 - 7.39
			2 nd	388.1	163.0	0.018	16	
52	Pyrazolynate	+	1 st	439.0	90.9	0.018	28	7.13 - 7.55
			2 nd	439.0	173.0	0.018	28	
53	Pyrifthalid	+	1 st	319.1	139.1	0.050	40	5.22 - 5.64
			2 nd	319.1	179.0	0.050	40	
54	Simeconazole	+	1 st	294.1	69.7	0.010	22	6.28 - 6.70
			2 nd	294.1	135.1	0.010	22	

【システム】

・LC	ACQUITY UPLC H-Class システム(FTN)
・MS	Xevo TQ-S タンデム四重極型質量分析計
・ソフトウェア	MassLynx 4.1 TargetLynx アプリケーションマネージャ

【LC条件】

・サンプル温度	10°C
・注入量	50 uL
・洗浄溶媒	水
・カラム	TOSOH TKSgel SUPER IC-AP 4.6 x 75 mm
・カラム温度	40°C
・流速	0.5 mL/min
・移動相A	50mM-ギ酸アンモニウム水溶液
・移動相B	水
・グラジエント	

Time(min)	A%	B%	Curve
0.0	5	95	Initial
5.0	40	60	6
28.0	40	60	6
29.0	5	95	6
40.0	5	95	6

・Run Time	40分
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【MS条件】

MS Tune

・イオン化モード	ESIポジティブ/ESIネガティブ
・キャピラリー電圧	0.5 kV(ポジティブ) 0.5 kV(ネガティブ)
・脱溶媒ガス	1000 L/hr 650°C
・イオン源ヒーター	150°C

MRM

化合物	極性	プレークライオン (<i>m/z</i>)	プロダクトイオン (<i>m/z</i>)	Dwell Time	コーン電圧 (V)	コリジョンエネルギー (eV)
Glyphosate	ESI+	170.2	88.2	3.985	2	8
Glyphosate	ESI-	168.1	81.1	3.985	16	14
Glufosinate	ESI-	180.2	85.1	1.126	30	18