

Designing a Master Pesticide Calibration Solution

Science
for a safer world



Outline



- Introduction to o2si, A LGC Standards Company
- Chemistry
- Stability
- Conclusion

Who Are We?



- Started in 1997
- Custom standards manufacturing
- Organic and inorganic reference materials as well as sample collection products
- Acquired by the LGC Group in November, 2016 as part of the Standards Group.

Who are we?

LGC Standards

- Is a division of the LGC Group
- The UK's designated *National Measurement Institute* for chemical and bioanalytical measurements
- An international leader in the laboratory services
 - Measurement Standards
 - Certified Reference Materials
 - Genomics
 - Proficiency testing





Who are we?

- US owned, headquartered in Teddington, Middlesex, UK
- LGC Standards has a network of dedicated sales offices extending across 20 countries in 5 continents and more than 30 years experience in the distribution of reference materials
- We have an unparalleled breadth of ISO 17034 accredited reference material production facilities at 4 sites across the US, the UK and Germany.
- Our portfolio of over 100,000 products and over 40 proficiency testing schemes supports a wide range of sectors including:

Food and beverage

Environmental

Pharmaceutical

Forensic

Clinical

Industrial

Life Science

Petrochemical










Why LGC?

- North American headquarters in Manchester, NH with a temperature controlled (-80° C to ambient) state of the art 13,000 ft² warehouse
 - Select materials warehoused upon request
- Over 100,000 reference materials, certified reference materials and SRMs including UK **NMI**, **NIST** and others
- Distributor of EU Joint Research Centre (JRC) RMs and CRMs including **IRMM**, **BCR**[®] and **ERM**[®] brands
- Exclusive distributor of ISO Guide 34 **CIFGA biotoxins**
- We also distribute for **Food Allergens Laboratory**, **MUVA kempten** and **Larodan**

LGC Standards Quality

Manufacturing capability for food, beverage and environmental testing



Site	Accreditation	Description
 Teddington	<ul style="list-style-type: none">ISO 9001 ✓ISO 17025 ✓ISO Guide 34 ✓	Production of reference materials as the UK National Measurement Institute for chemical and biochemical measurements
 Luckenwalde	<ul style="list-style-type: none">ISO 9001 ✓ISO 17025 ✓ISO Guide 34 ✓	Production of pharmaceutical impurities, clinical and forensic toxicology standards
 Manchester	<ul style="list-style-type: none">ISO 9001 ✓ISO 17025 ✓ISO 17034 ✓	Production of used and new oil reference standards, as well as inorganic aqueous standards. Distribution and warehousing.
 Augsburg	<ul style="list-style-type: none">ISO 9001 ✓ISO 17025 ✓ISO Guide 34 ✓	Production of RMs for residue analysis and custom synthesis.
 Charleston	<ul style="list-style-type: none">ISO 9001 ✓ISO 17025 ✓ISO 17034 ✓	Production of custom CRMs to support the food safety, environmental, chemical, petroleum, clinical, pharmaceutical and industrial hygiene industries.

What products can be used as part of your Quality Management System



CRMs

- Method Validation
- Calibration
- Measurement Uncertainty
- Ongoing Measurement Control - QC

Incurred Residues

- Independent Verification
- Demonstration of Competency
- Method Validation

Matrix materials

- Ongoing Measurement Control - QC
- Calibration
- Method Validation

Pure materials

- Calibration
- Preparation of In-House QC
- Internal Standard (Stable Isotopes)
- Second source / Independent Verification



Product Range

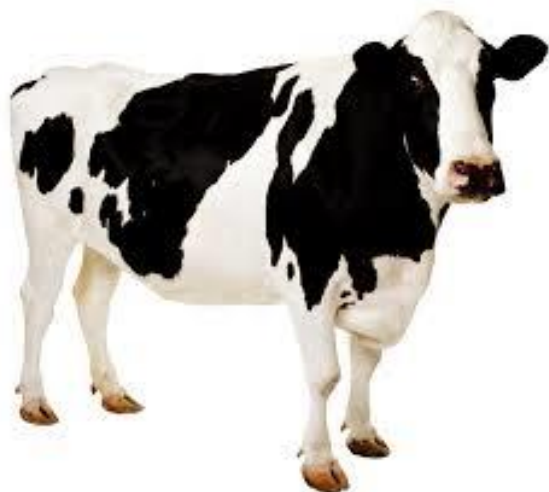
- LGC has an extensive range of CRMs to meet your requirements:
 - Over 7,000 neats, single solutions and mixes offered
 - All ISO 17034 custom mixture program made to your exact specifications
 - Isotopically labeled internal standards



Product Range – Pharmaceuticals & Veterinary Medicines



- LGC has an extensive range of products to meet your requirements:
 - Dr Ehrenstorfer reference standards – veterinary pharmaceuticals and metabolites available as neat, in solutions and mixtures
 - Isotope labeled internal standards from Dr Ehrenstorfer
 - RMs (matrix) from ERM and IRMM
 - New ISO 17034 Veterinary drug mixes by class



Dr Ehrenstorfer Products



Approximately 5,000 compounds / 7,000 products – key product ranges include;

- Pesticides/Metabolites
- Pharmaceuticals and Veterinary Medicines
- Dyes
- Nutritional components
- Deuterated/Carbon Labelled Compounds
- Odor Causing Compounds
- Food Packaging Contaminants
- PAH's
- And much more.....



Product Range – Allergens



- LGC is a major supplier of allergen reference materials
 - Extensive line of tree nut allergen reference materials
 - Many matrix materials available ie. eggs, milk, meat, crops, etc.

- LGC QC Kit - LGCQC101-KT
 - Blank and spiked matrix
 - EuroPrevall low dose threshold
 - Blank chocolate desert matrix



Product Range – Mycotoxins and Marine Biotoxins



- LGC has an extensive range of products to meet your mycotoxins requirements:
 - Reference Standards – available as neat, in solution and mixtures
 - Isotopically labeled standards (^{13}C and deuterated)
 - Matrix materials
- LGC – exclusive supplier of CIFGA
 - marine biotoxins available from stock
 - DSP, PSP, ASP
 - NRC materials also available



National Research
Council Canada

Product Range – Authenticity, Speciation and GMO



- Authenticity
 - Range of RMs in wine and sugar available
 - New product; ERM-AE672 Glycine – absolute carbon isotope ratio
- GMO
 - Range of RMs in cereals and food products
- Speciation
 - Range of matrix materials for different species - contamination levels (1% and 10%) and individual species



Product Range – Food nutritional



- LGC has an extensive range of products to meet your nutrient testing requirements
- Reference standards for
 - Food additives – antioxidants, sweeteners, colorings
 - Nutritional – elements, vitamins etc
 - Isotopically labeled internal standards
 - Matrix materials
 - Food packaging contaminants
- RMs and matrix materials
 - Meat products
 - Dairy products
 - Proximates, vitamins etc



A close-up photograph of a nutrition label on a food product. The label is titled 'Nutrition' and lists various nutrients with their typical values per 100ml and 250ml, and their percentage of the guideline daily amounts (GDA) for a typical adult. A finger is pointing to the 'Carbohydrate' row.

Typical values	100ml contains	250ml contains	%GDA*	Typical adult
Energy	199kJ 47kcal	500kJ 120kcal	6%	2000kcal
Protein	0.5g	1.3g		
Carbohydrate	10.5g	26.3g	2%	90g
of which sugars	10.5g	26.3g	2%	10g
Fat	trace	trace		
of which saturates	trace	trace		
Fibre	trace	trace		
Sodium	trace	trace		
Salt equivalent	trace	trace		

*Guideline daily amounts

Vitamins/Minerals

100ml contains (47% RDA) 62.5mg

Inorganic standards - VHG



Manufactured by LGC in Manchester, NH

- Aqueous inorganic standards for ICP, IC and AA
- Single element standards
- Multi element standards
- Ion Chromatography and Wet Chemistry Standards
- Speciation Standards
- Isotopic Standards
- All Single Solutions QC'd by The NIST High Performance Protocol



- NIST tested commercial standards and became concerned about claims of “NIST-Traceability.”
- In 1999, NIST and VHG developed HP-ICP-OES technique as the best instrument-based method to certify AA and ICP standards with direct traceability of assay and uncertainty to NIST SRMs.
- 4 samples of VHG standard, 4 samples of NIST SRM, internal reference spike, simultaneous comparisons , 6 hour run, 800 measurements, unbroken chain of measurements.
- VHG is the only CRM producer that spends 6 hours certifying one standard

LGC's Total Solution



A good quality control system requires many moving parts. With LGC's comprehensive portfolio we can help you fully reach all your food safety testing needs.





o2si Accreditations

- ISO 9001:2008 (NSF)
- ISO/IEC 17025:2005 (A2LA)
- ISO 17034:2016, RM and CRM (A2LA)



What We Make

- Manufacture single and multi component organic solutions (over 7,000 neat materials)
- Custom Solutions
- Catalog Solutions
- Approximately 400 solutions per week
- Approximately 100 of those are new solutions

QC Lab Accredited to Perform



- Atomic Fluorescence (AF)
- UV/Visible Spectroscopy (UV/Vis)
- Gas Chromatography (GC/FID) - 2
- Gas Chromatography/Mass Spectrometry (GC/MS) – 5
- Gas Chromatography/Vacuum Ultraviolet (GC/VUV)
- High Pressure Liquid Chromatography (HPLC/DAD/RID)
- High Pressure Liquid Chromatography High Resolution Accurate Mass Spectrometry (UPLC-HRAM)
- High Pressure Liquid Chromatography Triple Quad Mass Spectrometry (HPLC/MS/MS)
- Purge and Trap Gas Chromatography
- Ion Chromatography (IC)
- Enzymatic Analysis (EA)
- pH and Ion Selective Electrode (ISE)
- Wet Chemistry/Titrations
- Gravimetric Analysis

Solution Design – What Can Go Wrong?



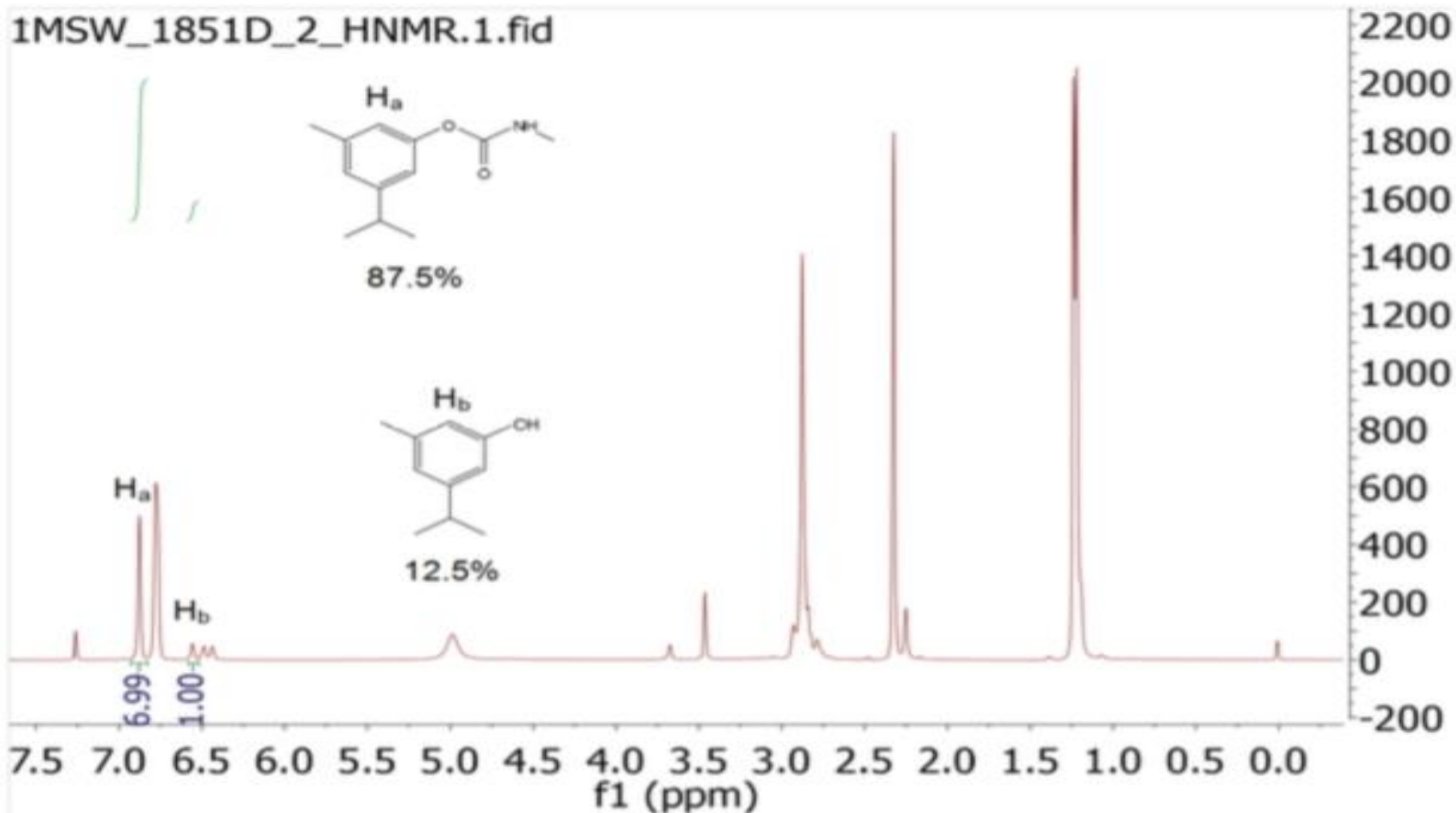
- The o2si company motto:

If you think something is easy, you just haven't found the problem yet.

Solution Design – What Can Go Wrong

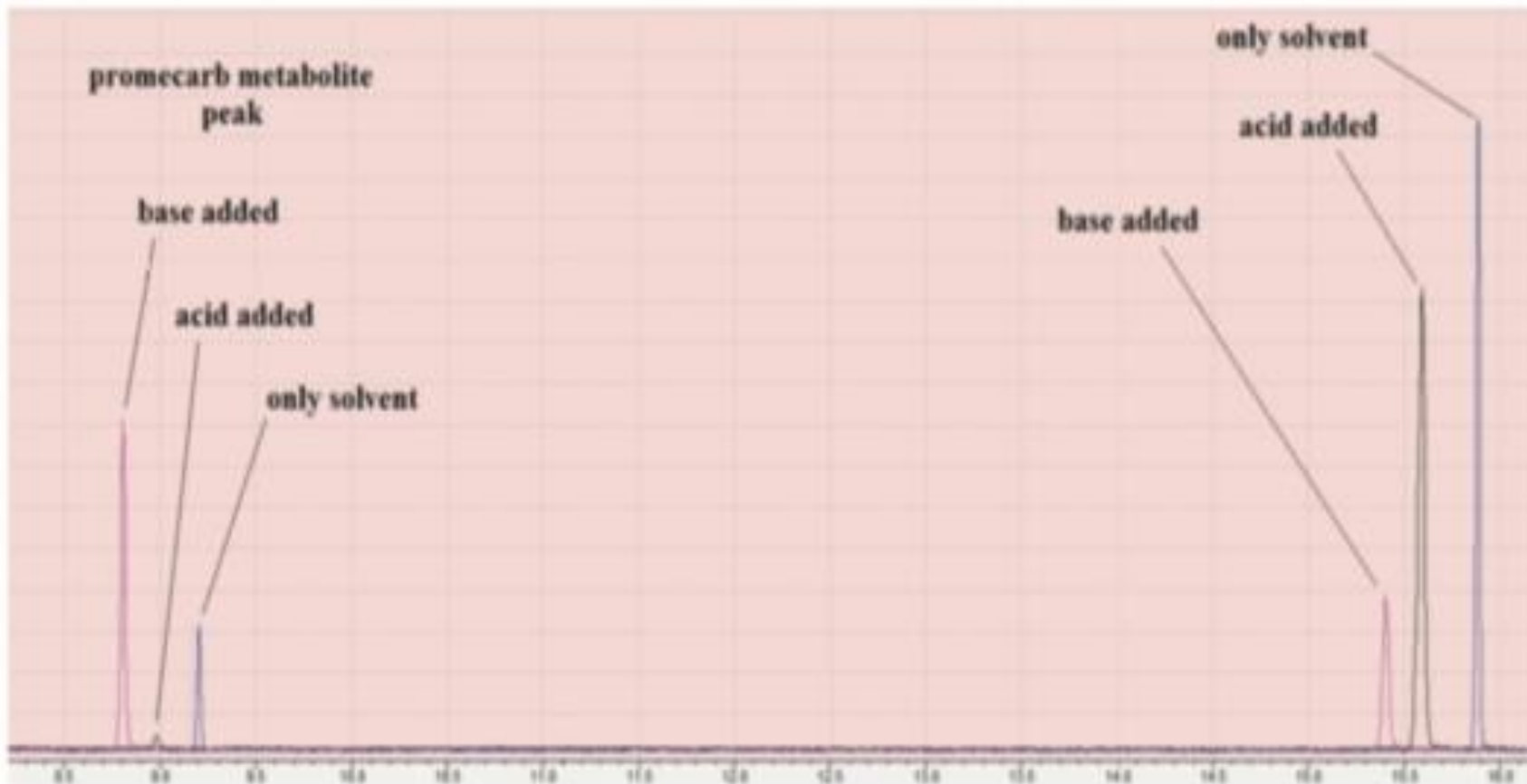
- Chemistry Issues
 - Solubility
 - Stability
 - Solvent-Analyte Interactions
 - Analyte-Analyte Interactions
 - Analyte-Analyte-Solvent Interactions
 - pH
- Packaging
 - Surface adsorption
 - Chemistry change

Solvent Instability of Carbamate Pesticides

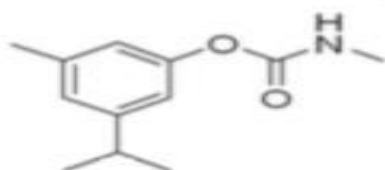


400MHz ^1H NMR collected data consistent with promecarb and 3-isopropyl-5-methylphenol.⁵

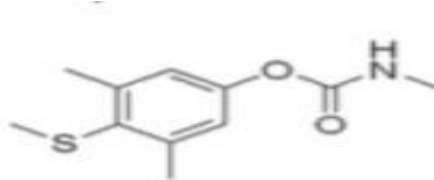
pH Dependence of Instability



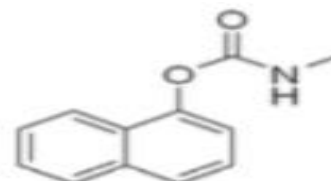
Degrade within Two Hours Under Basic Conditions (TLC)



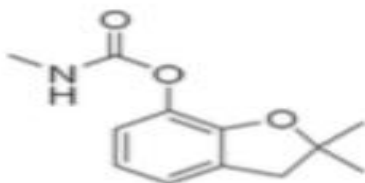
promecarb



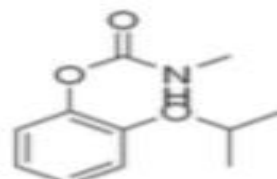
methiocarb



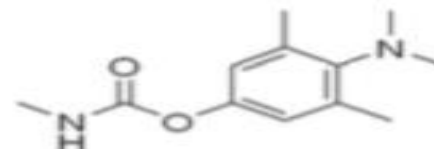
carbaryl



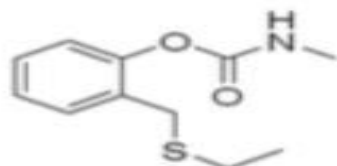
carbofuran



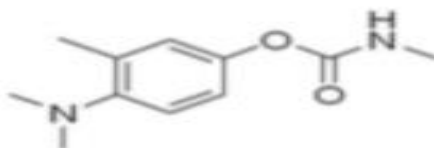
propoxur



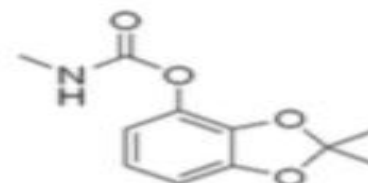
mexacarbamate



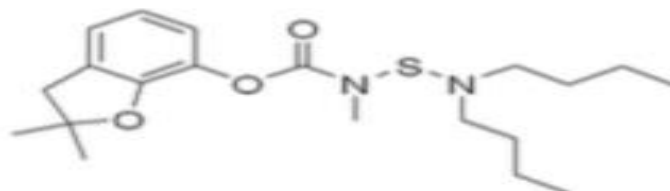
ethiofencarb



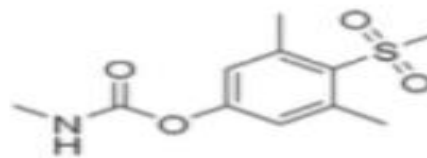
aminocarb



bendiocarb

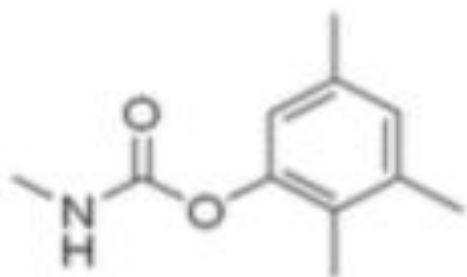


carbosulfan

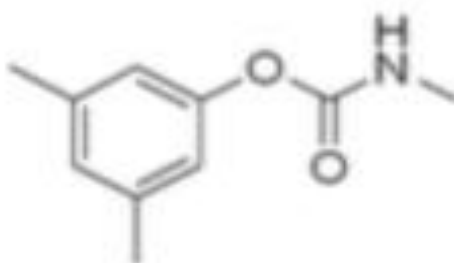


methiocarb sulfone

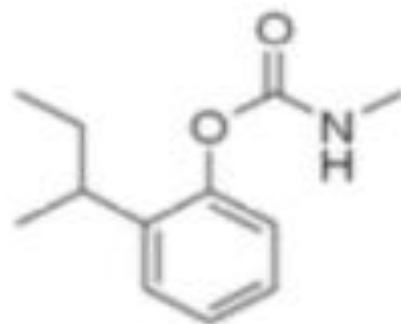
Degrade Within Twenty Hours Under Basic Conditions (TLC)



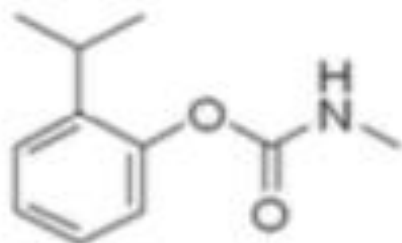
2,3,5-trimethacarb



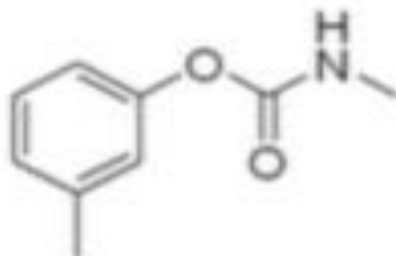
XMC



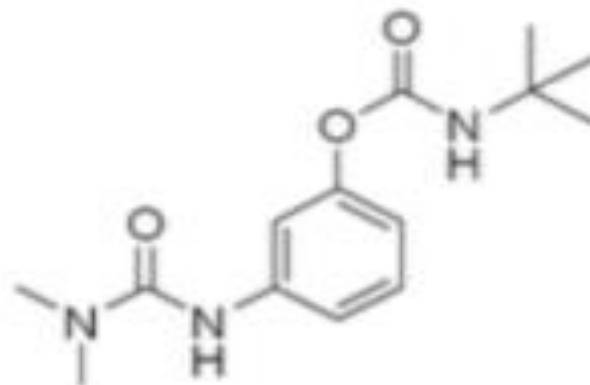
fenobucarb



isoprocarb

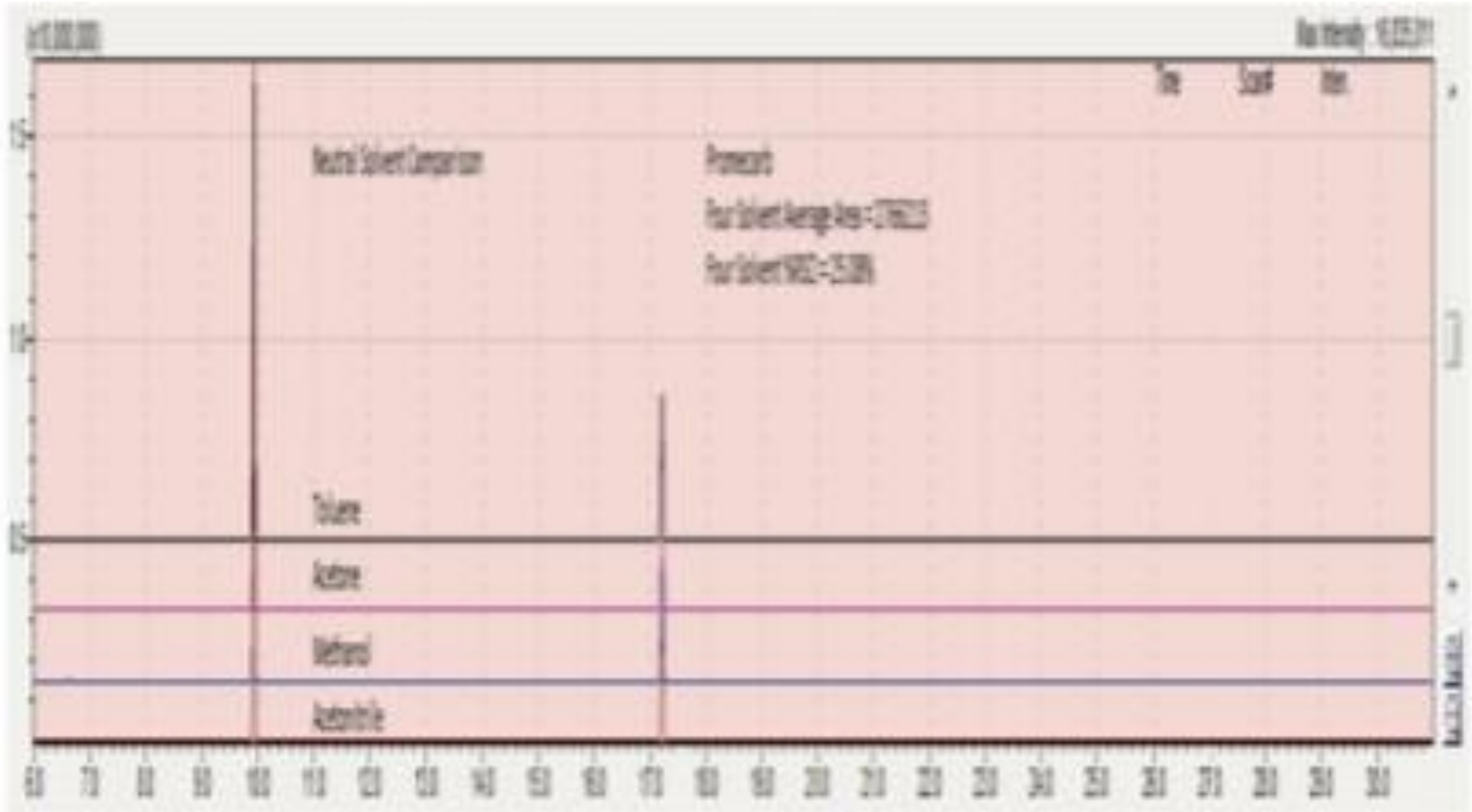


metolcarb

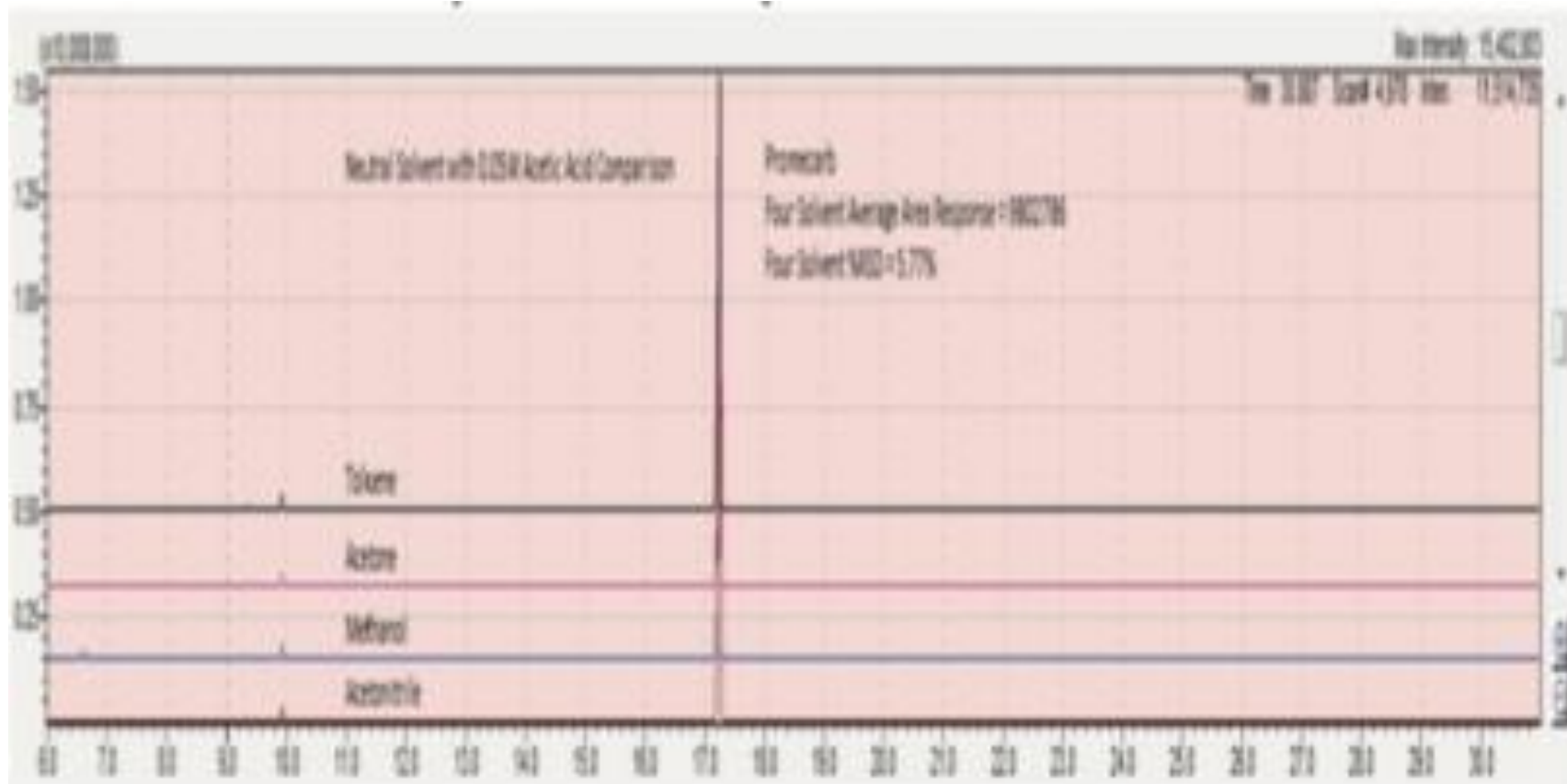


karbutilate

Neutral Conditions in GC Injection



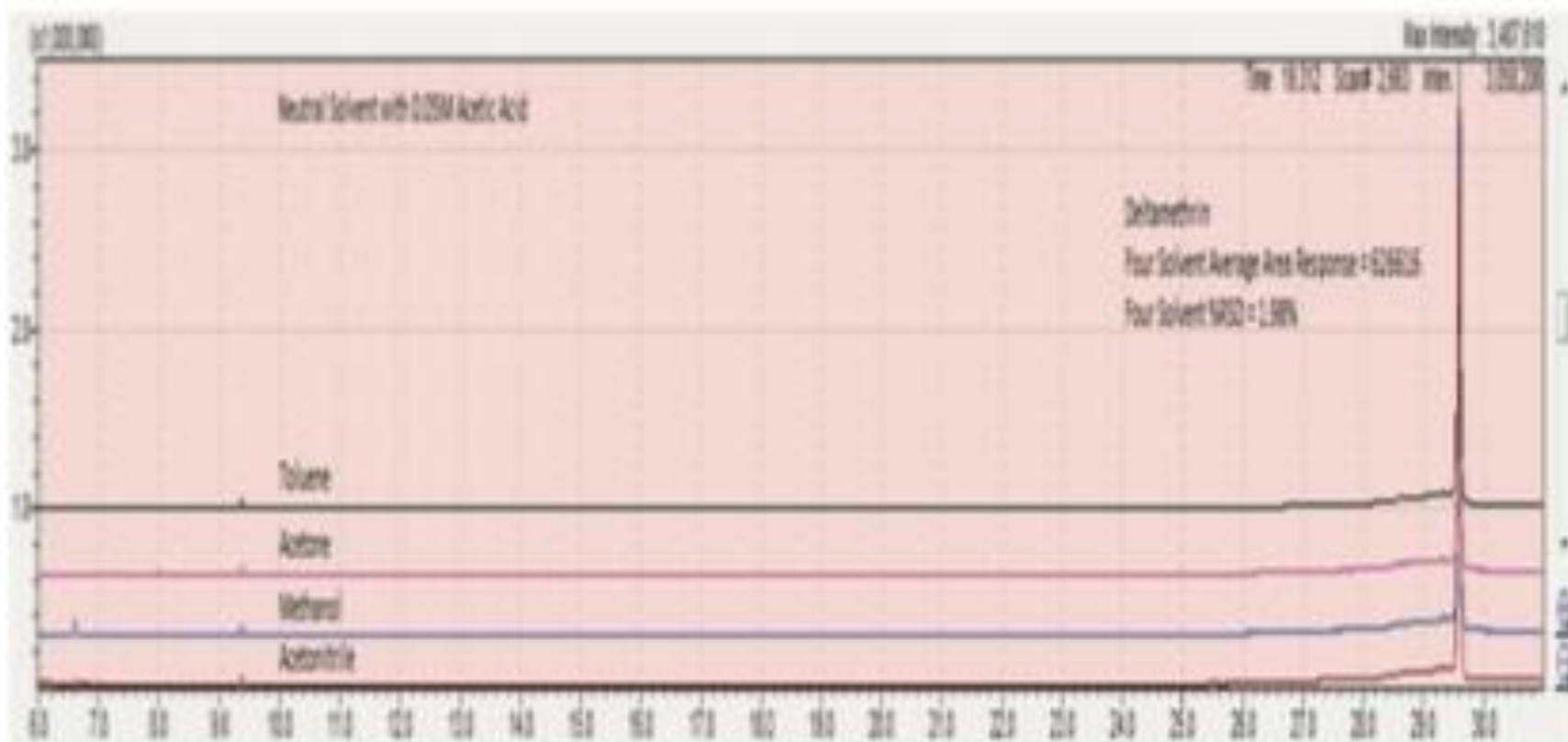
Acidic Conditions in GC Injection



Analyte Protection in GC Injection Port?



Acetic vs. Formic Acid – 20% higher area response

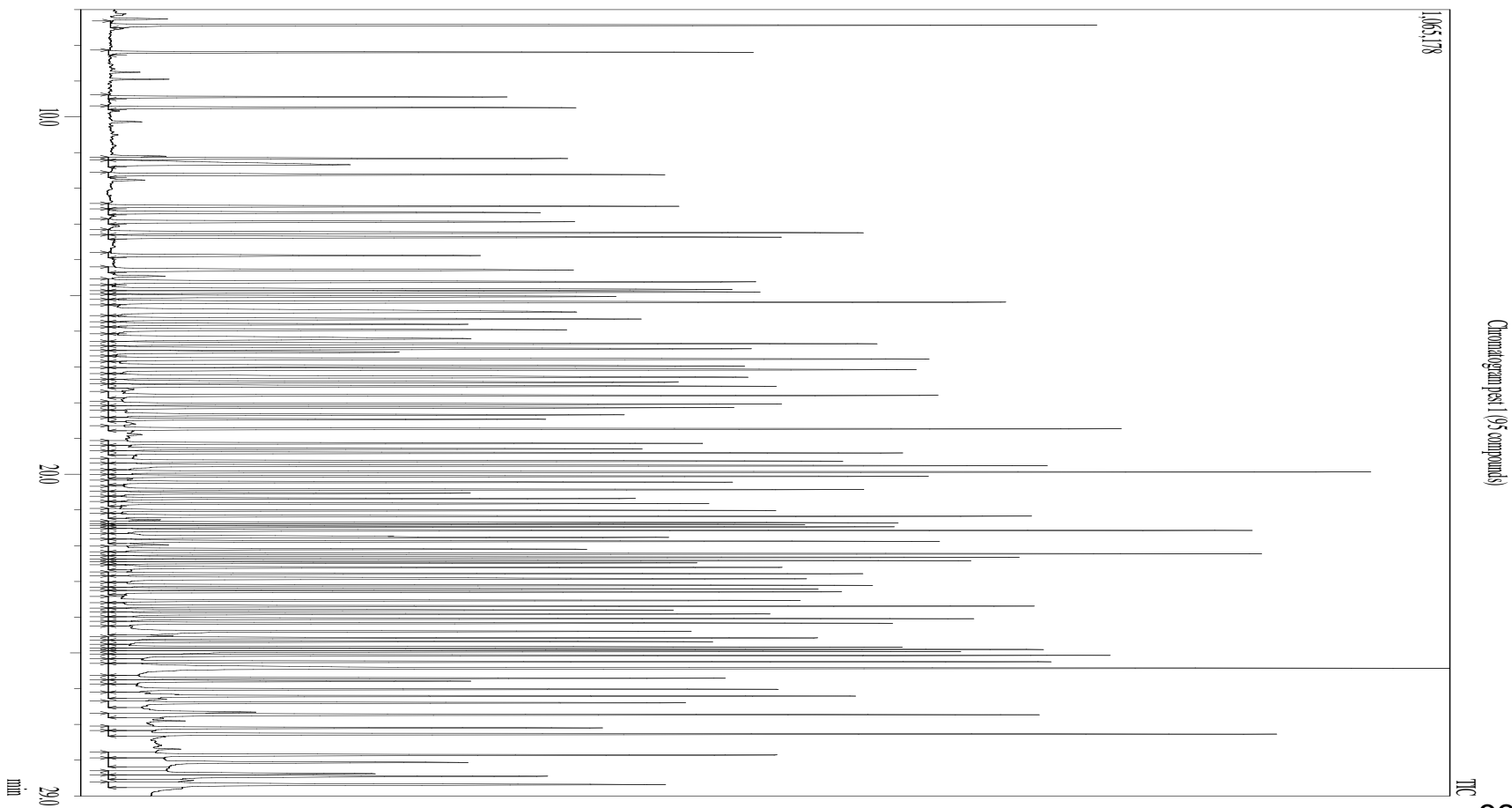




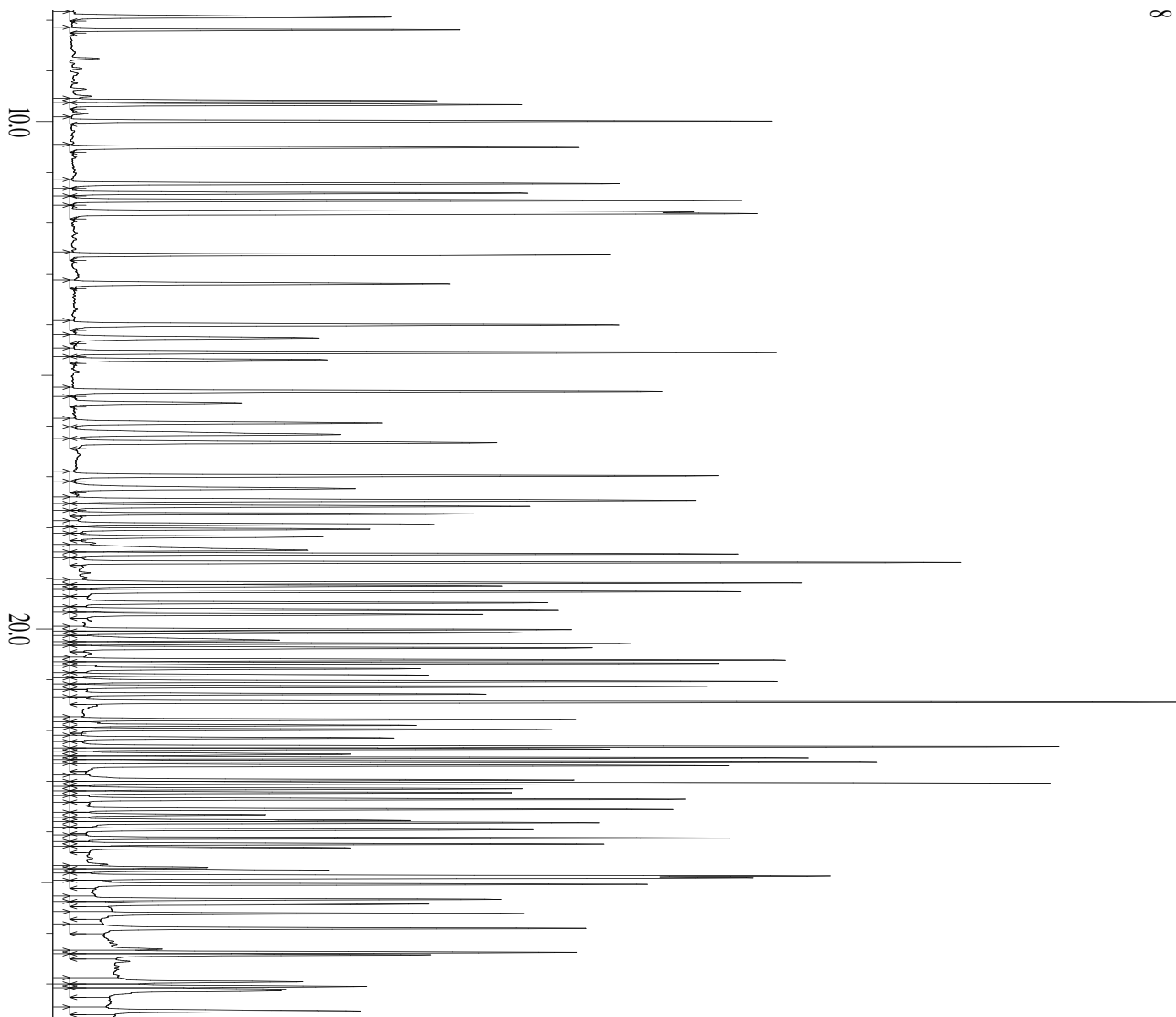
GC Pesticide Calibration Solutions

- Currently 346 analytes in four solutions
- Designed for minimal co-elution of analytes
- Use relative retention index from two internal standards
- Stability tested
 - Solutions 1-3 are stable for one year at -10 °C, 5 years at -70 °C
 - Less stable in solution 4

Pesticide Mix 1 Chromatogram (94)



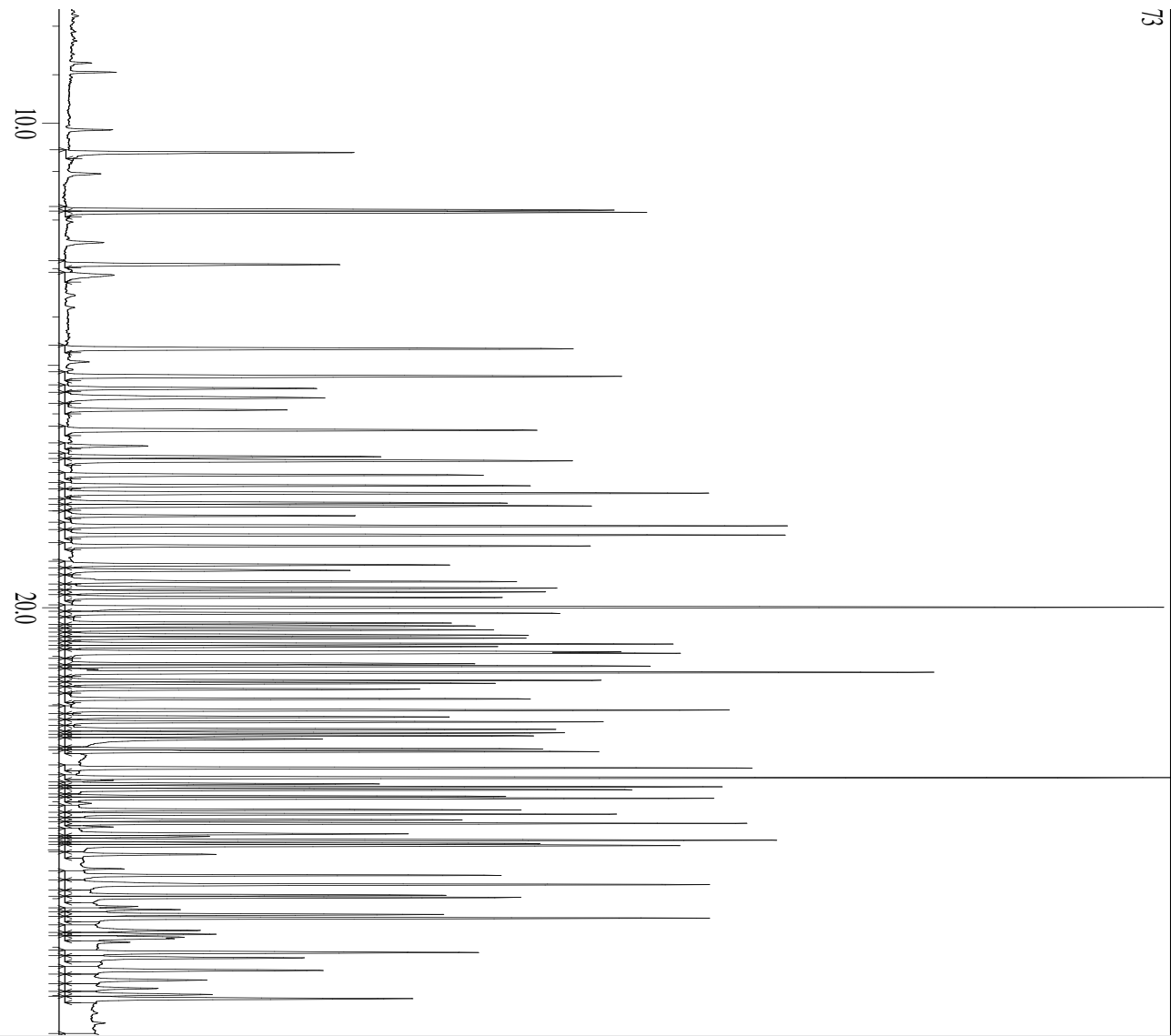
Pesticide Mix 2 Chromatogram (88)



Chromatogram pest 2 (89 compounds)

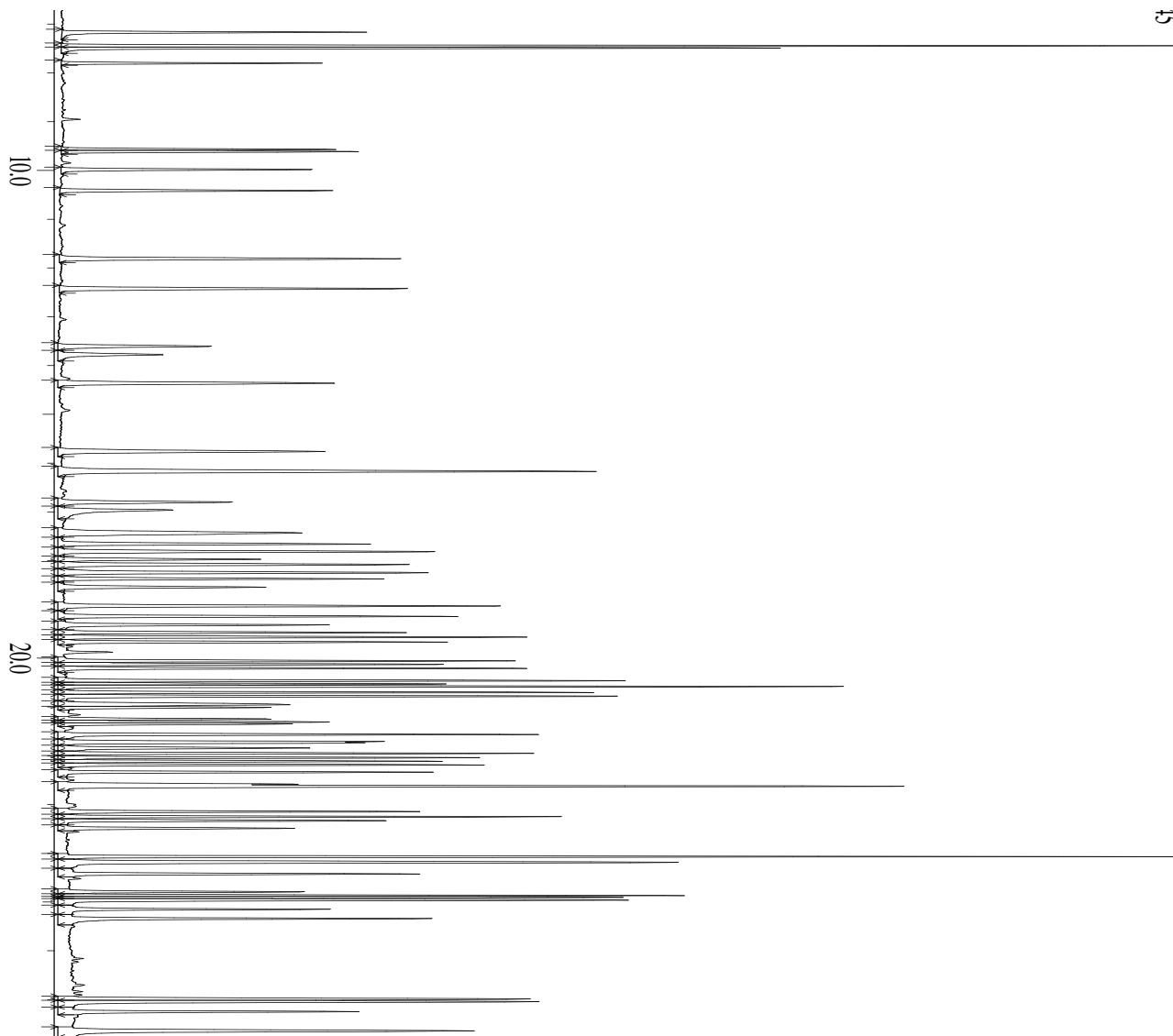


Pesticide Mix 3 Chromatogram (87)



Chromatogram pest 3 (87 compounds)

Pesticide Mix 4 Chromatogram (77)



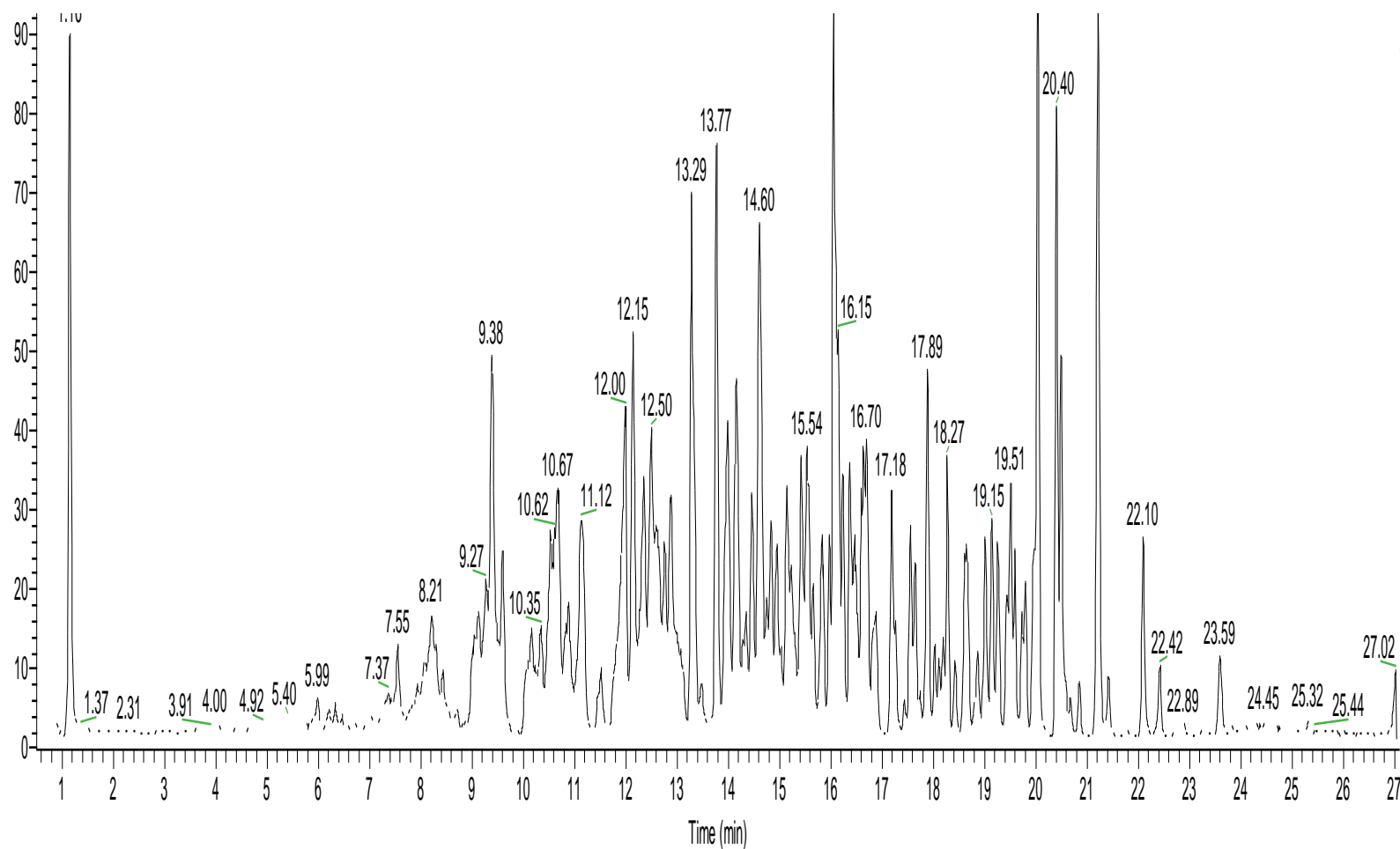
Chromatogram pest 4 (79 compounds)



LC Pesticide Calibration Solution

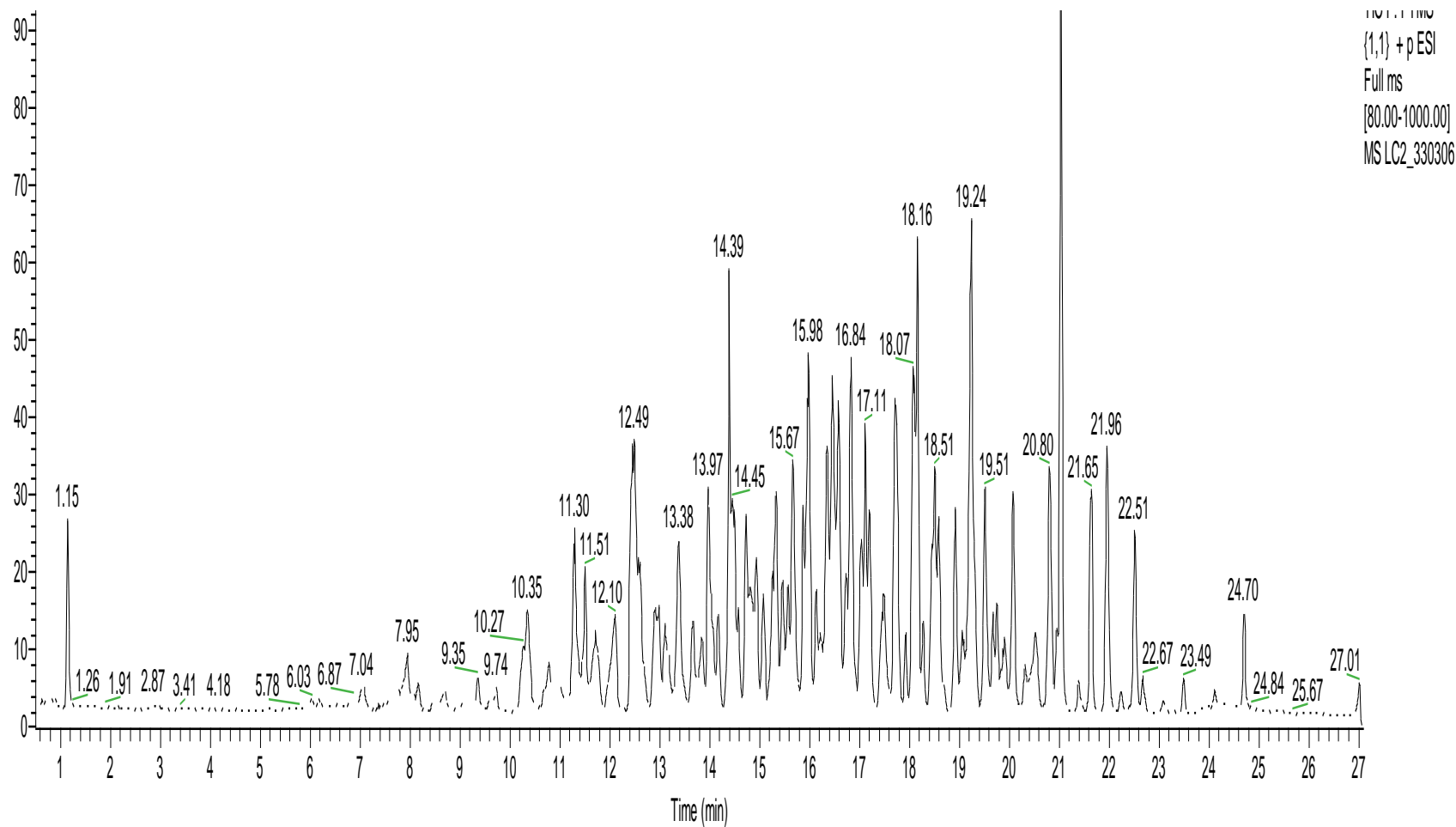
- Approximately 850 analytes in four solution
- Solutions designed for HRAMS to minimize structural isomer co-elution
- Currently doing stability testing on each of the four parent solutions individually and combined

LC Pesticide Mix 1 (246)

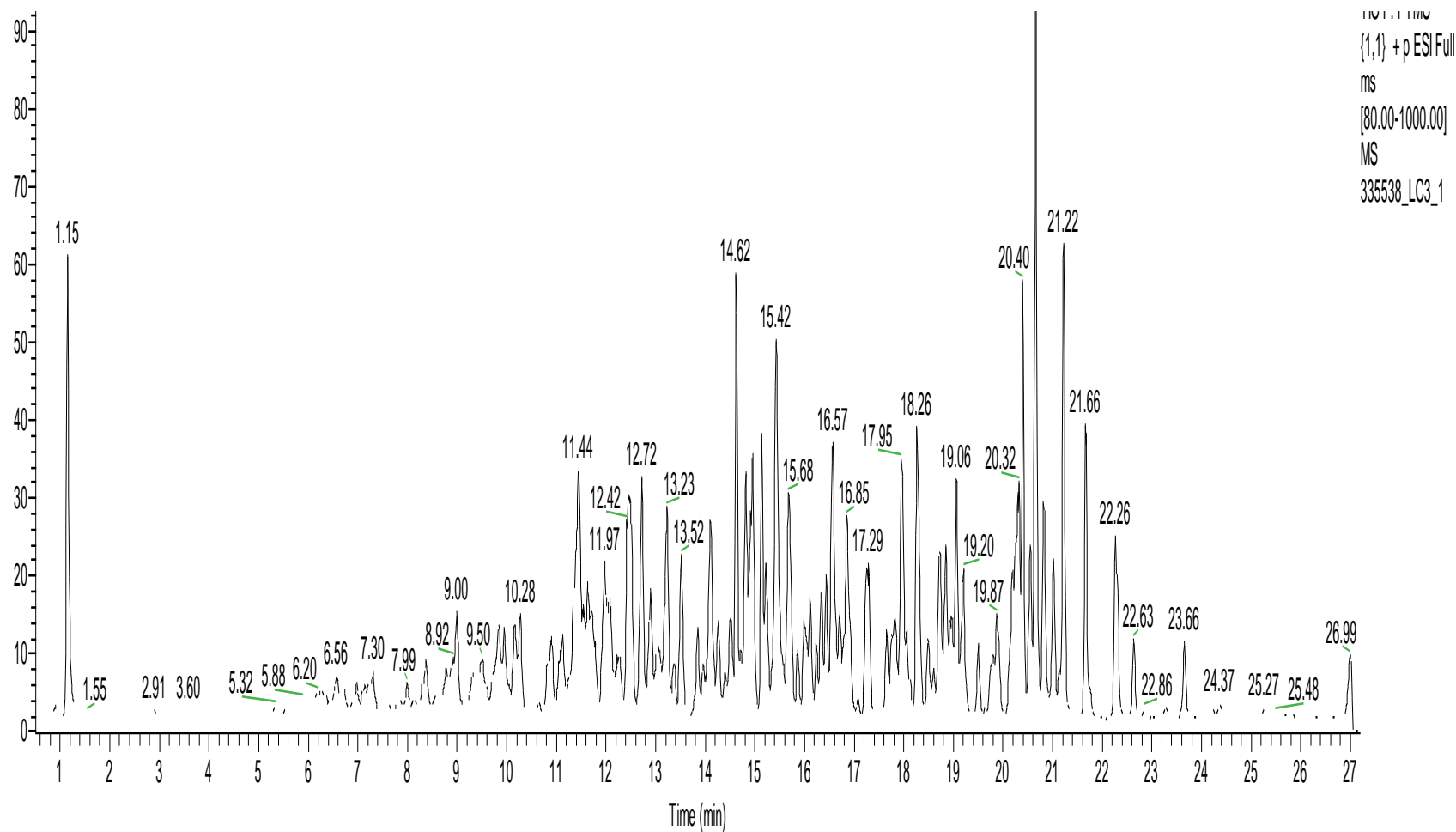


Full MS
{1,1} + p ESI
Full ms
[80.00-1000.00]
MS 329795_LC1

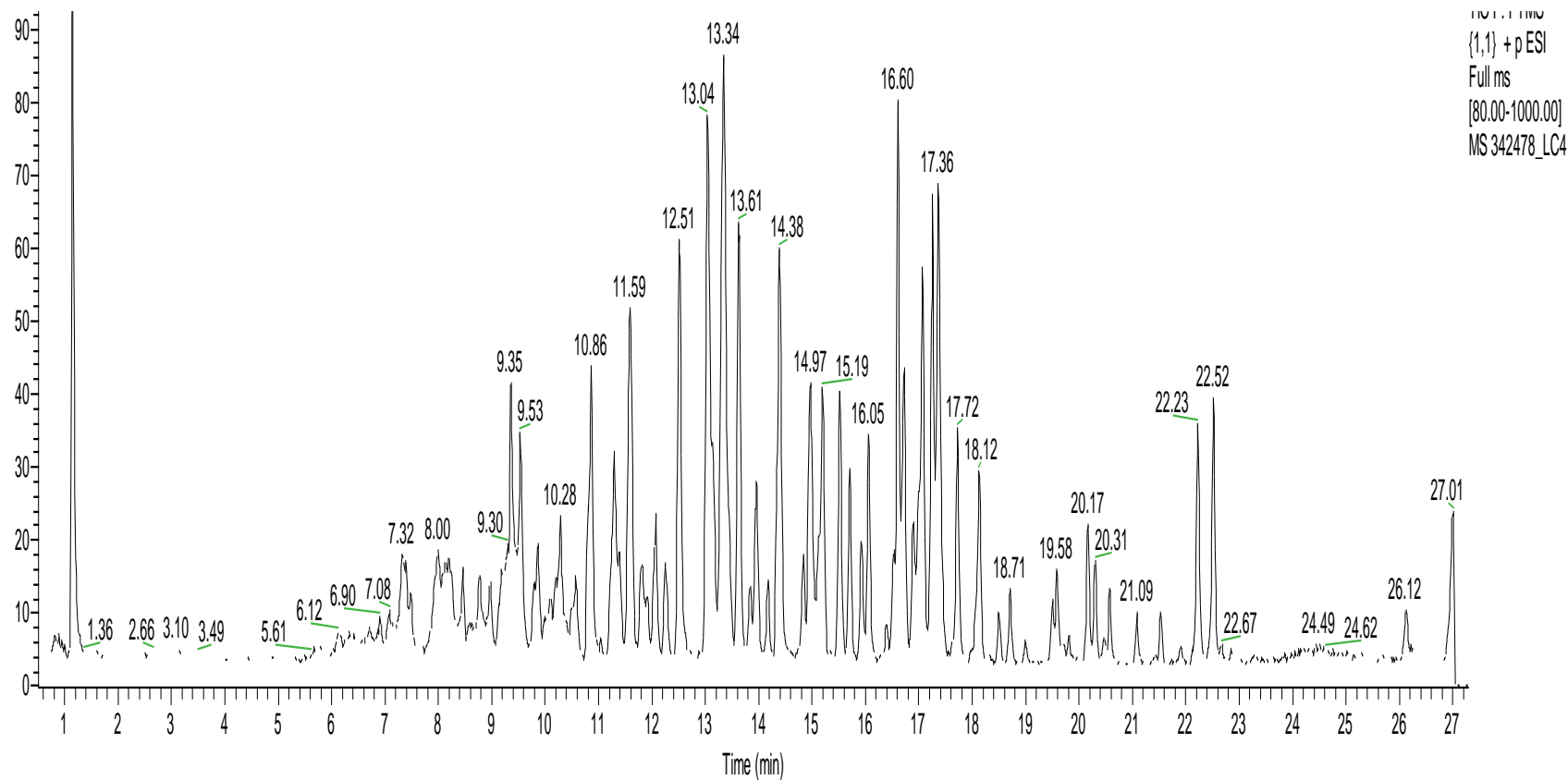
LC Pesticide Mix 2 (237)



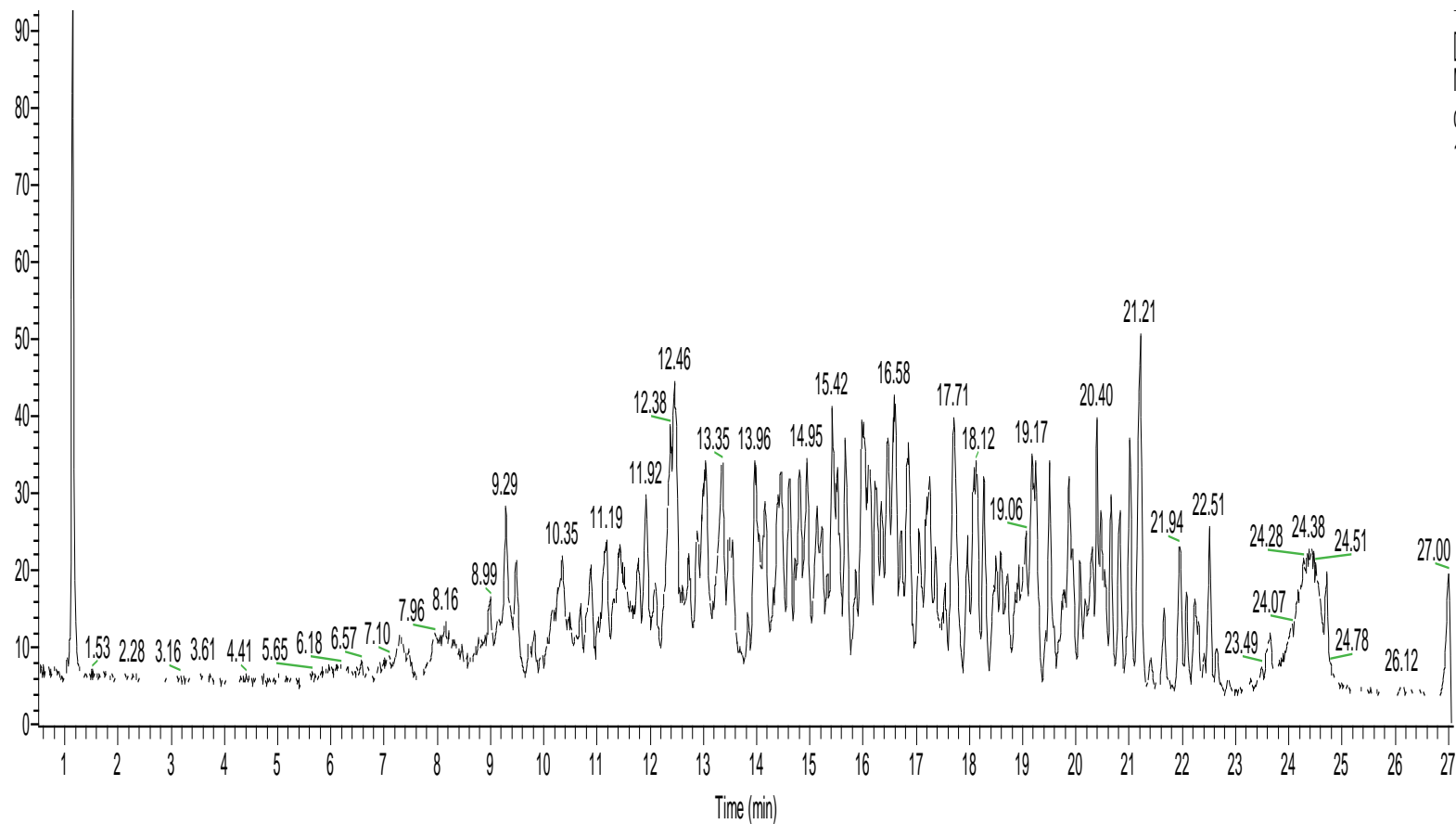
LC Pesticide Mix 3 (232)



LC Pesticide Mix 4 (136)



Combined LC1, LC2, LC3, LC4



TP LC11111111
[80.00-1000.00]
MS
combo_LCs_180514
111045

LC Pesticide Mix 1 Stability Problems



LC Master Solution Real Time Study

	#	LC1+FA 29795	#	LC1+FA 30294
< 90 days	2927	mesotrione	2927	mesotrione
	1369	chlorotoluron	1369	chlorotoluron
	331	fluometuron	331	fluometuron
	4023	amidosulfuron	4023	amidosulfuron
	1368	isoproturon	1368	isoproturon
	4402	difenoxurone		
	5106	chlorthion	5106	chlorthion
	1914	halosulfuron-methly	1914	halosulfuron-methly
	3142	azimsulfuron	3142	azimsulfuron
	3956	foramsulfuron	3956	foramsulfuron
	2997	nicosulfuron	2997	nicosulfuron
	2960	bifenazate		
	2119	carbosulfan		

LC Pesticide Mix 2 Stability Problems



LC Master Solution Real Time Study

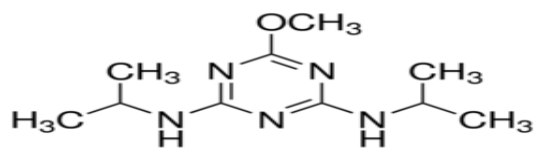
	#	LC2+FA 30306	#	LC2+FA 30368
< 90 days	2041	pymetrozine	2041	pymetrozine
	4421	Spirotetramat-enol	4421	Spirotetramat-enol
	4420	Spirotetramat-enol-glucoside	4420	Spirotetramat-enol-glucoside
	1862	thiophanate methyl	1862	thiophanate methyl
	2046	fenpropidin	2046	fenpropidin
			4019	propoxycarbazon sodium
	2555	dimefuron	Also in LC1	
	2948	emamectin benzoate	2948	emamectin benzoate



Current State of Master LC Solutions

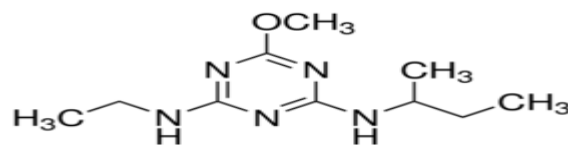
- Of the approximately 850 compounds, 40 compounds were not stable longer than 90-120 days with -70C storage in LC1 through LC4
- Future revisions will move those to a different (reactive) solution
- Currently evaluating stability of complete mixture, LC1 through LC4

Application - Discrimination of Isomers



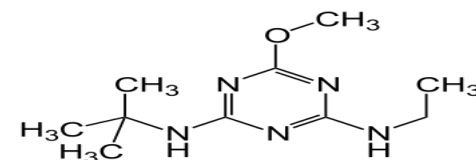
Prometon

RT = 8.94 min



Secbumeton

RT = 8.94 min



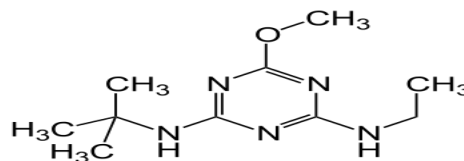
Terbumeton

RT = 9.14 min

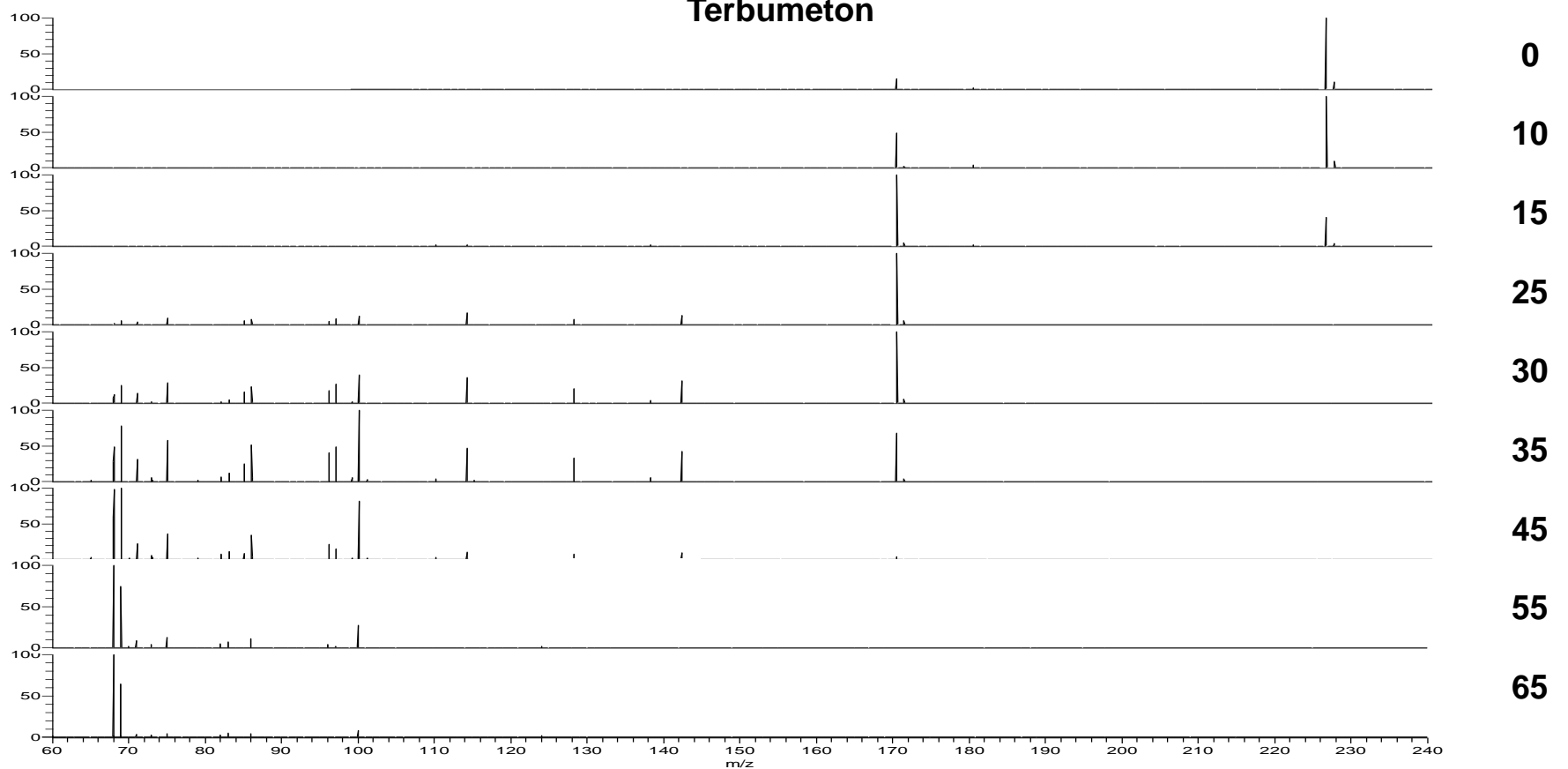
Different fragments

Different RT
Different RI

Collision Energy Profile

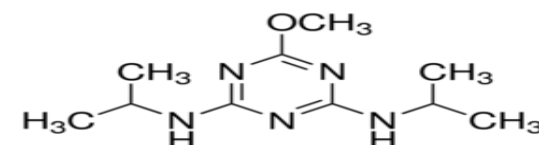
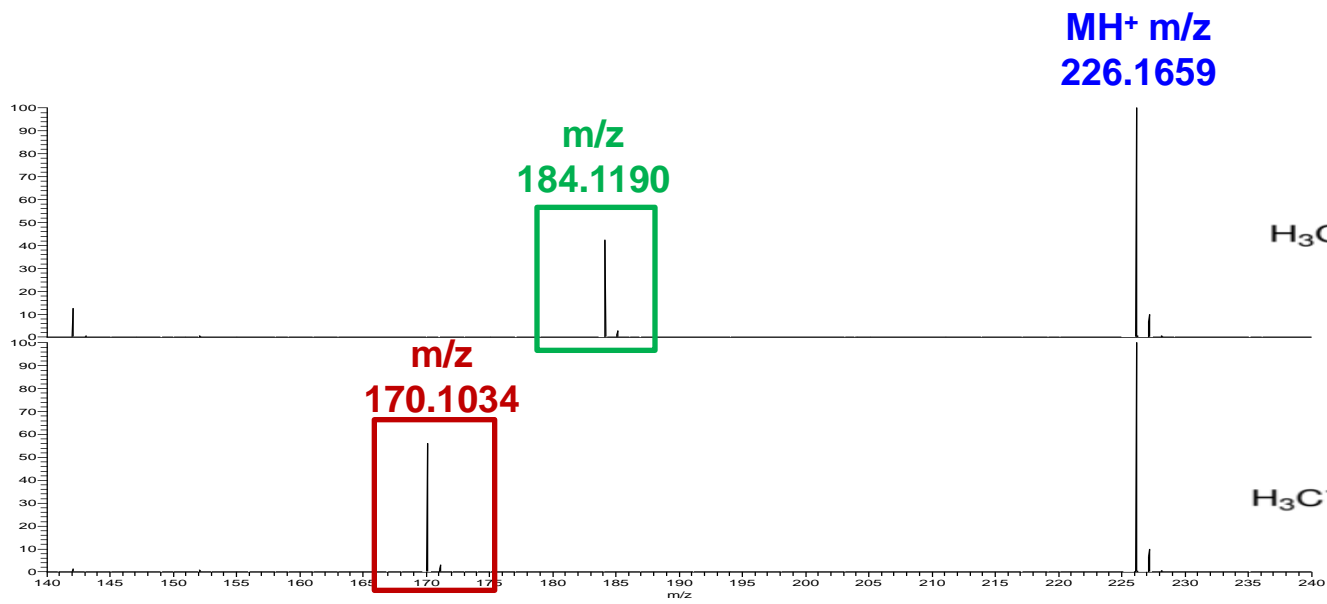


Terbumeton

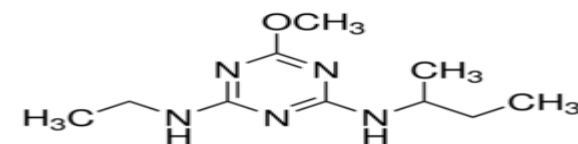


No significant change in MS pattern (collision energy: 65-105 eV)

Different Fragmentation Patterns



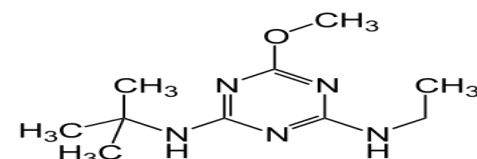
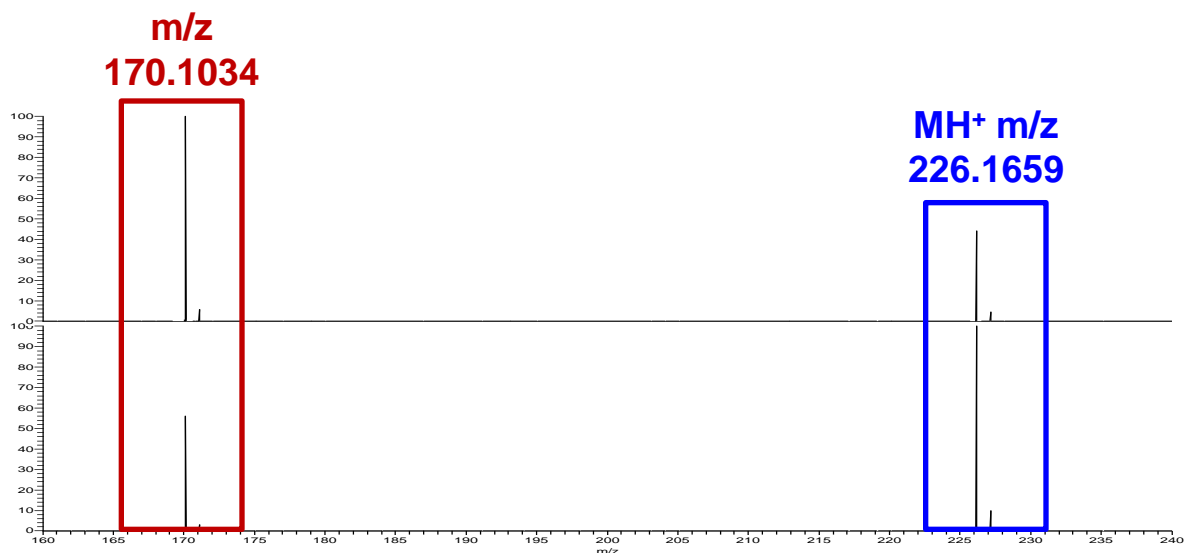
Prometon



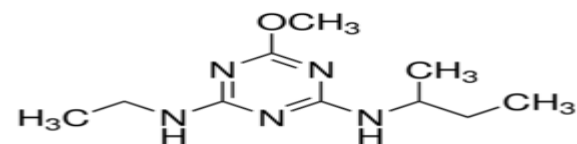
Secbumeton

Collision energy: 15 eV

Different Relative Intensities of Two Fragments



Terbumeton



Secbumeton

m/z	Terbumeton RI	Secbumeton RI
170.1034	226.91	56.24

Collision energy: 15 eV, RI refers to the ratio of the intensity of fragment ($m/z = 170.1034$) to the intensity of MH^+ ($m/z = 226.1659$)

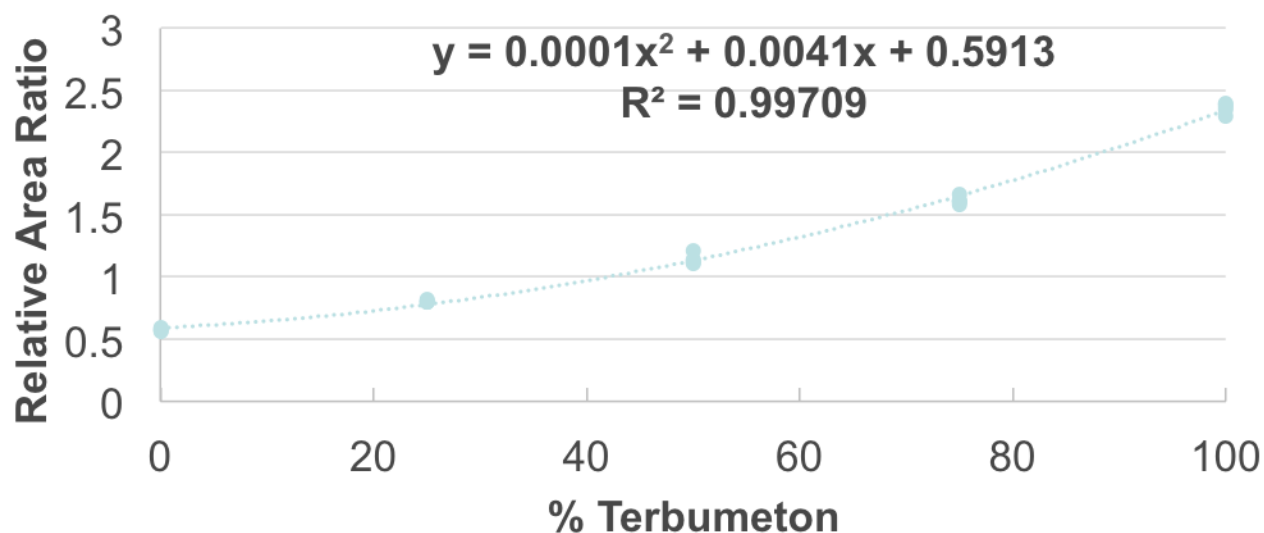


Method Verification

Trial	Terbumeton RI	Secbumeton RI
1	223.61	57.25
2	244.38	58.48
3	234.36	58.03
4	230.79	57.96
5	236.85	59.25

Collision energy: 15 eV, RI refers to the ratio of the intensity of fragment ($m/z = 170.1034$) to the intensity of MH^+ ($m/z = 226.1659$)

Quantification of Mixed Terbumeton and Secbumeton



Collision energy: 15 eV, relative area ratio refers to the ratio of the peak area of fragment (m/z = 170.1034) to the peak area of MH⁺ (m/z = 226.1659), 5 replicates



For further information or advice contact us:

LGC Standards

Adam Ross

Phone: 603-206-0759

Email: Adam.Ross@LGCGroup.com

Don Shelly

Phone: 603-206-0747

Email: Don.Shelly@LGCGrooup.com

Customer Service

Phone: 603-622-7660

GC Pesticide 1 Mix List (94)

Compound	RT	ISI -index	ISI ₂ -index	CAS	Compound	RT	ISI -index	ISI ₂ -index	CAS
1,2-dichloro-3-chloropropane	6.03	0.8175	0.2581	96-12-8	chlorpyrifos	20.46	2.6182	0.8254	2921-88-2
dichlorvos	8.21	1.0924	0.3448	62-73-7	chlorfenvinphos (dacthal)	20.56	2.6309	0.8305	1861-52-1
disulfoton silfoside	9.44	1.2604	0.3978	2997-07-6	hexaconazole	20.72	2.6455	0.8351	11291-17-3
Dibutyltin	9.77	1.2995	0.4102	11944-63-6	imazalil	20.85	2.6651	0.8413	33629-47-9
phosalone(TM) (mex-niphos)	11.19	1.4926	0.4680	7786-34-7	isopropanol	21.04	2.6878	0.8484	33828-53-0
acifluorfen	11.33	1.5005	0.4736	30560-19-1	cyprothiazole	21.21	2.7089	0.8551	12155-64-2
azelaole	11.66	1.5454	0.4878	2593-13-9	chlorfenvinphos (formers)	21.39	2.7311	0.8621	470-90-6
methidathion	12.25	1.6575	0.5232	62610-77-9	phenothiazine	21.43	2.7372	0.8640	947-40-4
chlorobenz	12.72	1.6799	0.5303	2675-77-6	phenothiazin	21.50	2.7457	0.8667	2597-03-7
2-phenylphenol	12.97	1.7166	0.5419	90-43-7	trifluralin (dalan)	21.60	2.7604	0.8713	55219-65-3
isoprocarb	13.38	1.7535	0.5535	2631-40-5	Bromophos ethyl	21.80	2.7822	0.8782	482-78-6
molinate	13.41	1.7749	0.5602	2212-67-1	pyrifentox	21.87	2.7988	0.8835	88283-41-4
Heptenophos	13.62	1.8368	0.5798	23560-59-0	cis-chlorothane	22.12	2.8261	0.8921	5103-71-9
acetazate	14.33	1.8897	0.5965	117-18-0	Hexaconazole	22.26	2.8390	0.8961	15299-99-7
propachlor	15.54	1.9322	0.6099	1918-16-7	profenofos	22.35	2.8512	0.9000	79938-71-4
2,4,5-trichloro-m-xylene	15.81	1.9619	0.6193	877-09-8	profenofos	22.45	2.8618	0.9033	41198-08-7
demeton-S-methyl	14.94	1.9697	0.6218	919-86-8	oxadiazon	22.51	2.8670	0.9050	19666-30-9
diphenylamine	15.07	1.9854	0.6267	122-39-4	flusilazole	22.63	2.8825	0.9099	85309-19-9
ediprophos (profos)	15.23	2.0056	0.6331	13194-84-4	chlorfenvinpr	22.82	2.9035	0.9165	122453-73-0
atazate dithiopyryl	15.46	2.0322	0.6415	1007-28-9	cyproconazole (formers)	22.94	2.9242	0.9231	94361-06-5
chlorpropham	15.70	2.0617	0.6508	101-21-3	chlorobenzilazole	23.13	2.9463	0.9300	510-15-6
iriflutrin	15.85	2.0738	0.6552	1582-09-8	diniconazole (formet)	24.11	2.9595	0.9342	70217-36-6
teracetyl dithiopyrophosphate	15.95	2.0977	0.6622	3689-24-5	p,p'-DDD	23.32	2.8689	0.9372	72-54-8
calusulfos	16.22	2.1274	0.6715	95465-99-9	triazophos	23.52	2.9969	0.9460	24017-47-8
phorate	16.40	2.1439	0.6768	298-40-2	benalaxyl	23.72	3.0183	0.9528	71626-11-4
β-BHC	16.53	2.1606	0.6820	319-84-6	Propiconazole (formers)	23.94	3.0480	0.9621	60207-90-1
hexachlorbenzene	16.63	2.1706	0.6852	118-74-1	hexazinon	24.07	3.0598	0.9658	51233-04-2
thionon	16.82	2.1923	0.6920	640-15-3	metenpyr-dithiyl	24.19	3.0767	0.9712	63284-71-9
dimethoate	17.02	2.2121	0.6983	60-51-5	Pyridaphenthion	24.42	3.1013	0.9789	135390-91-9
atrazin	17.10	2.2202	0.7008	1610-11-9	fenazoxin	24.61	3.1248	0.9864	119-12-0
simazine	17.94	2.2457	0.7033	122-34-9	terbufos	25.09	3.1865	1.0058	120928-09-8
proprazine	17.53	2.2740	0.7178	139-40-2	terbufos	25.27	3.2074	1.0124	116-39-0
terbufos	17.83	2.3085	0.7287	13071-79-9	pyriproxyfen	25.45	3.2291	1.0193	95737-68-1
diazinon	18.03	2.3325	0.7363	333-41-5	pyriproxyfen	25.73	3.2613	1.0295	13457-18-6
pyrimethanil	18.17	2.3459	0.7405	53112-28-0	imaza	25.82	3.2813	1.0358	2385-85-5
methyl parathion	18.34	2.3690	0.7478	950-35-6	fenoxaprop-P-ethyl	26.04	3.3013	1.0421	7102383-80-2
tefluthin	18.49	2.3800	0.7513	79358-32-2	fenoxaprop-P-ethyl	26.23	3.3278	1.0504	55179-31-2
iprodion	18.77	2.4173	0.7630	26087-47-8	bifenox (formers)	26.23	3.3278	1.0583	134426-54-5
dichlorfenon	19.17	2.4644	0.7779	97-17-6	fluquinconazole	26.42	3.3528	1.0726	114369-43-6
chlorpyrifos-methyl	19.29	2.4825	0.7836	5396-13-0	fenhexonazole	26.75	3.3981	1.0776	114369-43-6
vinlozolin	19.44	2.4945	0.7974	50471-44-8	flucythrinate	26.12	3.4515	1.0895	70124-77-5
heptachlor	19.67	2.5293	0.7984	76-44-8	ethiofentox	26.29	3.4727	1.0962	80844-07-1
prometrin	19.79	2.5367	0.8007	7287-19-6	fenvalerate (formers)	26.87	3.5588	1.1234	51636-38-1
prossulfocarb	20.30	2.5606	0.8083	52888-80-9	Diflucenazole	27.47	3.6457	1.1302	119446-68-3
terbufos	20.08	2.5735	0.8123	886-50-0	deltamethrin	27.70	3.6703	1.1366	52919-63-5
deltamethrin	20.25	2.5961	0.8195	1083-98-9					

GC Pesticide Mix 2 List (88)

Compound	RT	ISI-index	ISI ² -index	CAS	Compound	RT	ISI-index	ISI ² -index	CAS
O,O-dimethylphosphorothioate	7.50	0.9308	0.2937	126-68-1	imidation	20.71	2.697	0.3860	4312143-3
methidathion	7.96	1.0577	0.3337	1026592-6	kelthane ® (dicofol)	20.77	2.664	0.3806	115-32-2
dichlorvos	8.81	1.0924	0.3448	62-73-7	Bromophos methyl	20.90	2.6791	0.3853	2104-96-3
hexachlorocyclopentadiene	9.58	1.2618	0.4044	77-47-4	isofenphos-methyl	21.02	2.6930	0.3896	99675403-3
1-bromo-2-nitrobenzene	9.65	1.2907	0.4072	577-19-5	isodin	21.13	2.7129	0.3859	465-73-6
s-cis-1,2-dipropylthiocarbamate	10.94	1.3317	0.4201	759-94-4	peroxozonl	21.31	2.7224	0.3892	66268686-6
hiphenyl	10.49	1.4025	0.4425	92-52-4	heptachlor epoxide isomer A	21.43	2.7468	0.3866	28044483-9
chlorfenvos	11.21	1.4933	0.4711	2008-41-5	methidathion	21.82	2.7862	0.3790	990-37-8
fenitrothion	11.44	1.5182	0.4790	2493491-6	tetrachloro-pyrimfos (ISO)	21.89	2.7983	0.3829	2224879-9
vermidole	11.59	1.5363	0.4847	192977-7	disulfoton sulfone	22.01	2.8089	0.3862	2497406-5
2,4-dinitrotoluene	11.76	1.5633	0.4932	606-20-2	trans-nonachlor	22.18	2.8330	0.3938	39765300-5
penhale	11.86	1.5711	0.4957	111471-2	imazali	22.32	2.8495	0.3990	3555444-0
2,4-dichloro-1,4-methylphenol	12.61	1.6768	0.5290	128-37-0	isoprotoluene	22.39	2.8556	0.3910	5051235-1
2,4-dinitrotoluene	13.17	1.7455	0.5307	121-14-2	tricycloze	22.50	2.8704	0.3956	4181478-2
N,N-dimethyl-n-volumide	13.99	1.8355	0.5848	134-62-3	thibufos	22.57	2.8777	0.3979	78-48-8
nonheole	14.26	1.8870	0.5954	1113402-6	2,4-D ethylhexyl ester	22.60	2.8851	0.39103	1928-43-4
thionazie (etropfos)	14.53	1.9231	0.6067	29797-2	carboxime	22.68	2.8966	0.39139	5234-68-4
fenitroly phosphole	15.17	2.0192	0.6371	12673-8	Nitrofen	23.00	2.9315	0.39249	183675-5
difrom	15.52	2.0525	0.6476	30076-5	enlim	23.07	2.9441	0.39289	72-20-8
benidactol	15.92	2.0946	0.6609	2278123-3	fenasulfithion	23.18	2.9519	0.3913	115-90-2
monocrotophos	16.15	2.1154	0.6674	692522-4	fenitrothion-sulfone	23.22	2.9607	0.3941	3761-42-0
pronoxact	16.37	2.1382	0.6746	26137-0	acetonfen	23.34	2.9783	0.3997	7407046-5
Demeton OAS	16.96	2.2138	0.6985	806548-3	suprofos	23.54	3.0025	0.3973	3540043-2
carbofenon	17.21	2.2394	0.7065	156366-2	fenphur	23.65	3.0153	0.3913	52485-7
b-BHC	17.49	2.2618	0.7136	319485-7	norfluzon	23.76	3.0285	0.39549	2731413-2
Terbufoson	17.62	2.2806	0.7195	3369344-8	edifenphos	23.85	3.0368	0.39581	1710949-8
proflinon	17.77	2.2951	0.7241	2639936-0	p-p-DDT	23.98	3.0525	0.3951	50-29-3
propoxycarbide (promite)	17.97	2.3218	0.7325	2393658-5	fluoxypyr-ethyl	24.11	3.0702	0.3967	8140637-3
chlorobutanol	18.17	2.3457	0.7401	189745-6	triphenyl phosphole	24.23	3.0861	0.3737	115-86-6
triallele	18.56	2.3942	0.7354	230317-5	phosmet	24.75	3.1496	0.3937	732-11-6
tebuhydrinos	18.72	2.4112	0.7407	9618233-5	bifenox	24.86	3.1614	0.3974	3951541-8
phosphamidon	19.09	2.4615	0.7566	1317121-6	phosalone	25.06	3.1808	1.0036	42576402-3
dinosebuanid	19.18	2.4677	0.7386	8767468-8	Gardion®	25.45	3.2315	1.0195	86-500
aceochlor	19.31	2.4798	0.7324	3425682-1	acrinathin [SO]	25.60	3.2486	1.0249	101007406-1
alchlor	19.52	2.5065	0.7398	1597260-8	Gardion Ethyl	25.93	3.2905	1.0382	264271-9
carbaryl	19.65	2.5229	0.7360	63-25-2	comaphos	26.40	3.3509	1.0572	56-72-4
fenitrothios	19.71	2.5351	0.7398	299484-3	prochloraz	26.42	3.3583	1.0596	6774749-5
pirimiphos methyl	20.04	2.5678	0.8102	2923233-7	cypromethin (somers)	27.03	3.4452	1.0870	5231547-8
fenitrothion	20.07	2.5767	0.8129	122144-5	fluthione	27.51	3.5072	1.1065	59756604-4
homoxal	20.24	2.5898	0.8171	314404-9	tan-fluvalinate	28.01	3.5754	1.1280	102851406-9
metadiazin	20.28	2.6012	0.8207	12175-5	Indoxacarb (somers)	28.41	3.6325	1.1460	14417141-9
metdiazinor	20.41	2.6142	0.8248	5121845-2	dinethionoph	28.70	3.6794	1.1608	1499104-1
prozinon	20.64	2.6417	0.8334	5638-2		29.03	3.7286	1.1764	11048870-5

GC Pesticide Mix 3 List (87)

Compound	RT	ISI-index	IS2-index	CAS	Compound	RT	ISI-index	IS2-index	CAS
propiconcarb	11.24	1.4099	0.4453	24579-73-5	captan	21.55	2.7566	0.8707	133-06-2
propham	11.83	1.5642	0.4941	122-42-9	Folpet	22.59	2.7707	0.8752	133-07-3
metolcarb	11.88	1.5700	0.4959	1129-41-5	o,p'-DDE	21.90	2.7946	0.887	342-482-6
pentachlorobenzene	12.95	1.7141	0.5414	608-93-5	endosulfan I	22.14	2.8265	0.8928	959-98-8
oxamyl	13.16	1.7333	0.5475	23135-22-0	flutolanil	22.24	2.8358	0.8957	66332-96-5
propoxur	14.69	1.9329	0.6105	114-26-1	perflachlor	22.38	2.8494	0.9000	51218-49-6
Cyflate	15.27	2.0097	0.6348	1134-23-2	p,p'-DDE	22.53	2.8701	0.9066	72-55-9
ethalfenalin	15.46	2.0342	0.6425	55283-68-6	Systeme TM	22.61	2.8771	0.9088	88671-89-0
desethyl atrazine	15.65	2.0586	0.6502	6190-65-4	o,p'-DDD	22.67	2.8871	0.9119	53-19-0
Benfluramin (Benflin)	15.95	2.0859	0.6589	1861-40-1	dichlorazotol (isomers)	22.73	2.8958	0.9147	75736-33-3
di-allylate (isomers)	16.32	2.1392	0.6757	2303-16-4	fluzaricop-propargyl	22.94	2.9158	0.9210	79241-46-6
2,4-D-isopropyl	16.87	2.1985	0.6944	94-11-1	Perthane (TM)	22.99	2.9260	0.9242	72-56-0
Dichloran	17.00	2.2101	0.6981	99-30-9	chlorothipfos	23.33	2.9661	0.9369	60238-56-4
prometon	17.30	2.2396	0.7074	1610-18-0	cis-nomachlor	23.34	2.9713	0.9385	5103-73-1
Command (dimethazone)	17.51	2.2692	0.7167	81777-89-1	meprotil	23.49	2.9902	0.9445	55814-41-0
g-BHC	17.67	2.2893	0.7231	58-89-9	endim aldehyde	23.54	2.9959	0.9463	7421-93-4
terbuflylazine	17.87	2.3073	0.7288	5915-41-3	carfentazone-ethyl	23.67	3.0045	0.9490	12869-02-1
dyfonate (TM)	17.94	2.3188	0.7324	9444-22-9	trifloxystrobin	23.72	3.0105	0.9509	141517-21-7
fluchloralin	18.13	2.3348	0.7375	33245-39-5	carbophenothion	23.74	3.0234	0.9550	786-19-6
disulfoton	18.35	2.3654	0.7471	298-04-4	clodinafop-propargyl	23.88	3.0364	0.9591	105512-06-9
erimfos	18.49	2.3843	0.7531	38260-54-7	endosulfan sulfate	23.92	3.0475	0.9626	1031-407-8
Primicarb	18.76	2.4104	0.7614	23103-98-2	dichlorop-methyl	24.20	3.0718	0.9703	51338-27-3
dioxacarb	19.16	2.4581	0.7764	6988-21-2	Caprafol	24.42	3.1010	0.9795	2425-06-1
Propanil	19.28	2.4702	0.7803	709-98-8	spromesifen	24.44	3.1068	0.9813	283594-90-1
methyl parathion	19.46	2.5008	0.7899	298-00-0	acetamiprid	24.69	3.1326	0.9895	135410-20-7
simetryn	19.62	2.5149	0.7944	1014-70-6	bromconazole (isomer)	24.71	3.1408	0.9921	116255-48-2
metalaxyl-m	19.82	2.5377	0.8016	3111-45-5	fenoxycarb	24.78	3.1473	0.9941	72490-01-8
paraoxon ethyl	19.98	2.5654	0.8103	67306-00-7	methoxychlor	24.85	3.1569	0.9971	72-43-5
fenpropiadin	20.14	2.5774	0.8141	2032-65-7	lambda-cyhalothrin	25.35	3.2341	1.0215	91465-08-6
methiocarb	20.34	2.6002	0.8213	117718-60-2	ipconazole	25.74	3.2612	1.0301	125225-28-7
bithiazopyr	20.36	2.6107	0.8246	87392-12-9	ametoctradin	25.92	3.2866	1.0381	865318-97-4
S-metolachlor	20.46	2.6197	0.8275	2388-04-7	pyraclofos	25.99	3.2934	1.0403	77458-01-6
phorate-sulfone	20.55	2.6288	0.8304	21725-46-2	permethrin (isomer)	26.35	3.3403	1.0551	52645-53-1
bladex	20.62	2.6367	0.8329	142459-58-3	pyridaben	26.45	3.3525	1.0589	96489-71-3
flufenacet	20.74	2.6514	0.8375	16118-49-3	baytroid (isomer)	26.76	3.3942	1.0721	68359-37-5
carbenthanil	20.83	2.6624	0.8410	327-98-0	boscalid	27.10	3.4482	1.0892	188425-85-6
trichlorate	20.89	2.6708	0.8436	23305-41-1	flumorph	27.21	3.4611	1.0932	211867-47-9
Primiphos-ethyl	20.97	2.6780	0.8459	957-51-7	praziclostrobin	27.46	3.5252	1.1056	2051-24-3
difepramid	21.14	2.7032	0.8539	40487-42-1	esfenvalerate	28.05	3.5802	1.1309	66230-04-4
metazachlor	21.20	2.7247	0.8666	25311-71-1	zoxystrobin	28.85	3.6928	1.1664	131860-33-8
Isotepfos	21.33	2.7325	0.8631	27304-13-8	fenoxadone	29.14	3.7337	1.1800	131807-57-3
oxyclofandane	21.49	2.7464	0.8675	13593-03-8					



GC Pesticide Mix 4 List (77)

2,6-dimethylphenol	6.20	0.8417	0.2651	576-26-1	fenpropimorph	20.57	2.6574	0.8320	67306-03-
2,4-dichlorophenol	7.15	0.9626	0.3030	120-83-2	isocyanophos	20.69	2.6583	0.8363	2433-19-
3,4-dimethylphenol	7.43	0.9958	0.3133	95-65-8	nitrothal isopropyl	20.77	2.6582	0.8385	10652-74-
naphthalene	7.48	1.0058	0.3168	91-20-3	isobenzan	20.77	2.6706	0.8411	297-78-9
hexachlorobutadiene	7.79	1.0444	0.3286	87-68-3	benzozon	20.91	2.6781	0.8448	25857-89-
1,2,3,5-tetrachlorobenzene	9.55	1.2783	0.4026	634-90-2	fenchazate	21.05	2.6914	0.8467	98886-44-
1,2,4,5-tetrachlorobenzene	9.60	1.2842	0.4044	95-94-3	trifluralin	21.27	2.7137	0.8560	120068-37
2,6-trichlorophenol	9.97	1.3314	0.4191	88-06-2	chlorzoxime	21.30	2.7247	0.8595	84332-86-
1,2,3,4-tetrachlorobenzene	10.40	1.3902	0.4378	634-66-2	heptachlor epoxide isomer B	21.39	2.7365	0.8632	1024-57-3
acranaphthylene	11.79	1.5744	0.4959	208-96-8	procymidone	21.59	2.7576	0.8699	32809-16-
acranaphthene	12.40	1.6537	0.5208	83-32-9	pralsetrin	21.76	2.7795	0.8744	23031-36-
2,3,4,6-tetrachlorophenol	13.60	1.8031	0.5676	58-90-2	trans-chlordane	21.88	2.7955	0.8818	5103-74-2
methomyl	13.77	1.8204	0.5727	16752-77-5	butachlor	21.98	2.8039	0.8845	23184-66-
fluorene	13.34	1.9043	0.5997	86-73-7	picoxystrobin	22.02	2.8180	0.8871	117428-22
dicrotophos	15.74	2.0751	0.6528	141-66-2	imazamfos	22.10	2.8239	0.8908	36335-67-
bonminal	16.13	2.1206	0.6675	1689-84-5	fenamiphos	22.22	2.8312	0.8931	22224-92-
tebutam	16.15	2.1255	0.6691	35256-85-0	Takathion®	22.35	2.8329	0.8999	34643-46-
pentachloroanisole	16.84	2.1990	0.6918	1825-21-4	oxyfluorfen	22.57	2.8781	0.9079	42874-03-
desmethopram	17.21	2.2057	0.6958	13684-56-5	kraxoxim methyl	22.61	2.8923	0.9099	143390-89
dimehpinin	17.47	2.2628	0.7138	55290-64-7	dieldrin	22.66	2.8941	0.9129	60-57-1
pentachloronitrobenzene	17.49	2.2696	0.7159	82-68-8	fenitroth sulfoxide	23.13	2.9578	0.9311	3761-41-9
aminocarb	17.64	2.2893	0.7221	2032-59-9	ethion	23.28	2.9720	0.9350	563-12-2
cyanophos	17.81	2.3089	0.7283	2666-26-2	o,p'-DDT	23.36	2.9767	0.9390	789-02-6
Dioxoth	17.96	2.3269	0.7340	142040-1	desmethyl nordiazon	23.47	2.9976	0.9436	22576-34-
phenanthrene	18.06	2.3477	0.7394	85-01-8	bis(2-ethylhexyl)cadipate	24.08	3.0670	0.9657	103-23-1
chloridene	18.29	2.3663	0.7464	3734-48-3	diflufenican	24.14	3.0802	0.9696	83164-33-
isazophos	18.36	2.3777	0.7480	42509-80-8	tebuconazol (Folicur)	24.23	3.0806	0.9718	107534-96
d-BHC	18.38	2.3930	0.7549	319-86-8	epoxiconazole (ISQ)	24.45	3.1080	0.9804	133855-98
ethioncarb	18.92	2.4340	0.7697	29973-13-5	homompropylate	24.82	3.1334	0.9947	18181-80-
dimehachlor	19.18	2.4659	0.7779	50563-36-5	fenpropaflin	24.85	3.1607	0.9970	64257-84-
methidiazin	19.36	2.4856	0.7841	21087-64-9	chrysene	24.95	3.1817	1.0020	218-01-9
tolclofos-methyl	19.47	2.5062	0.7906	57018-04-9	flurimone	25.14	3.2008	1.0076	96525-23-
cymiazole	19.55	2.5177	0.7942	61676-87-7	trifloxazole	25.37	3.2211	1.0161	131983-72
metaxyl	19.71	2.5277	0.7973	57837-19-1	benzoflufenanthene	26.97	3.4441	1.0847	205-99-2
terbutryne	20.95	2.5735	0.8123	886-50-0	benzoflufenanthene	27.02	3.4519	1.0871	207-08-9
ethionfosate	20.11	2.5815	0.8143	26225-79-6	acequinocyl	27.23	3.4786	1.0944	57960-19-
di-n-butyl phthalate	20.19	2.5957	0.8171	84-74-2	benzoflapyrene	27.62	3.5348	1.1133	50-32-8
thiobenzach	20.49	2.6248	0.8280	28248-77-6					