

Waters

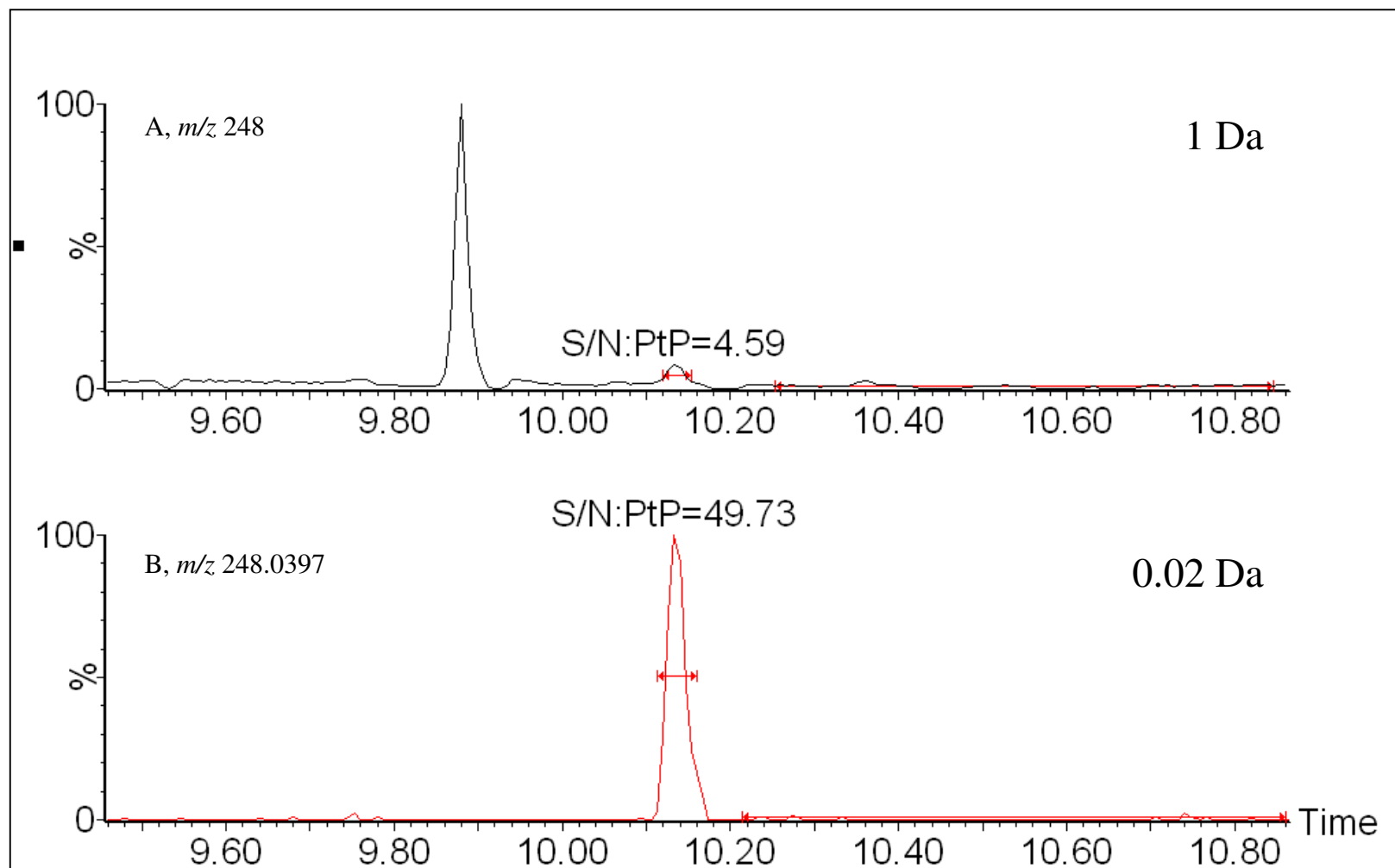
Jean-Marc Joumier
Business development Manager
GC-MS Europe

**APPLICATION OF
HIGH RESOLUTION TOF-MS
FOR
MULTIRESIDUE ANALYSIS OF
PESTICIDES**

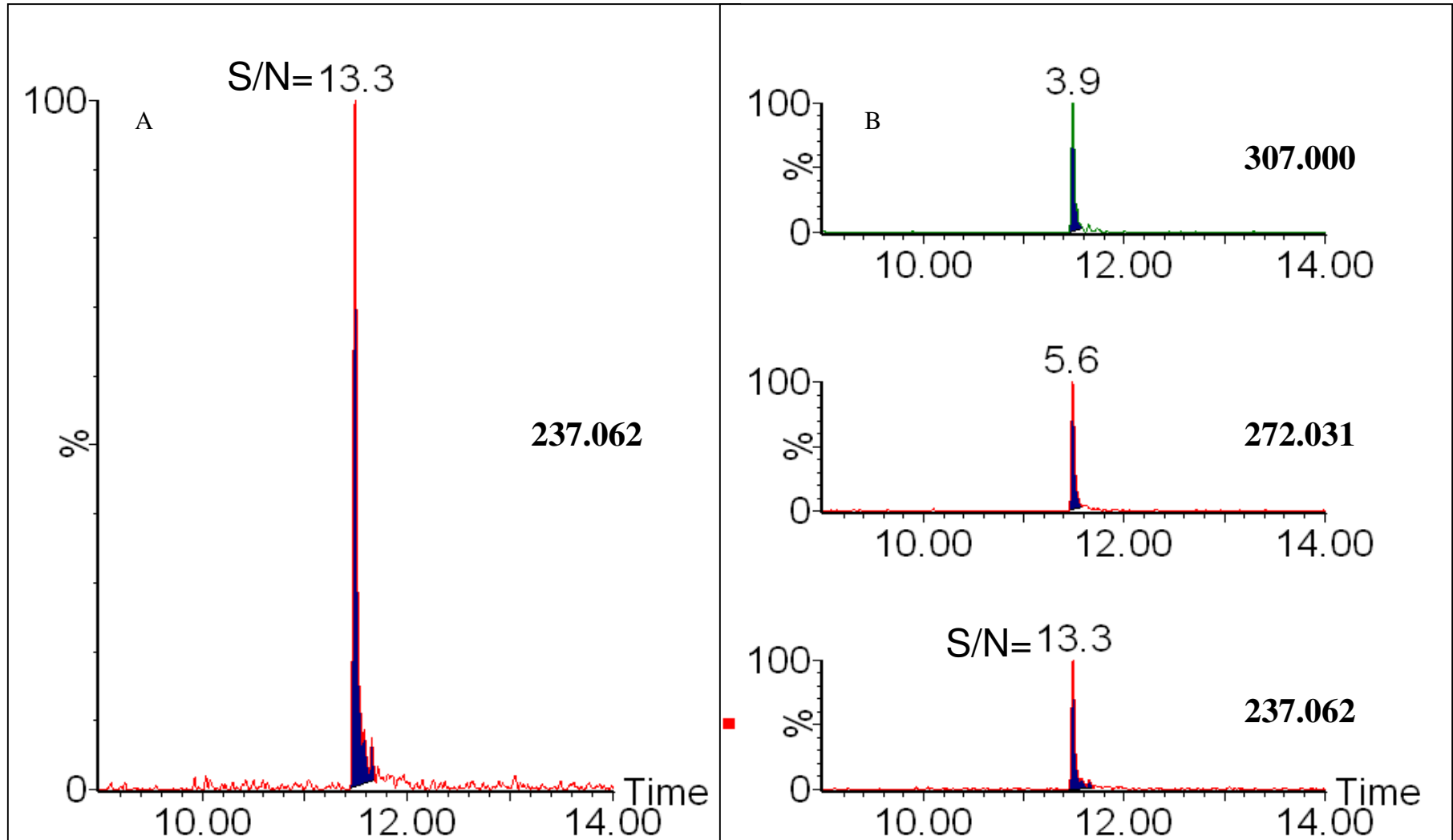
For Complete  Confidence

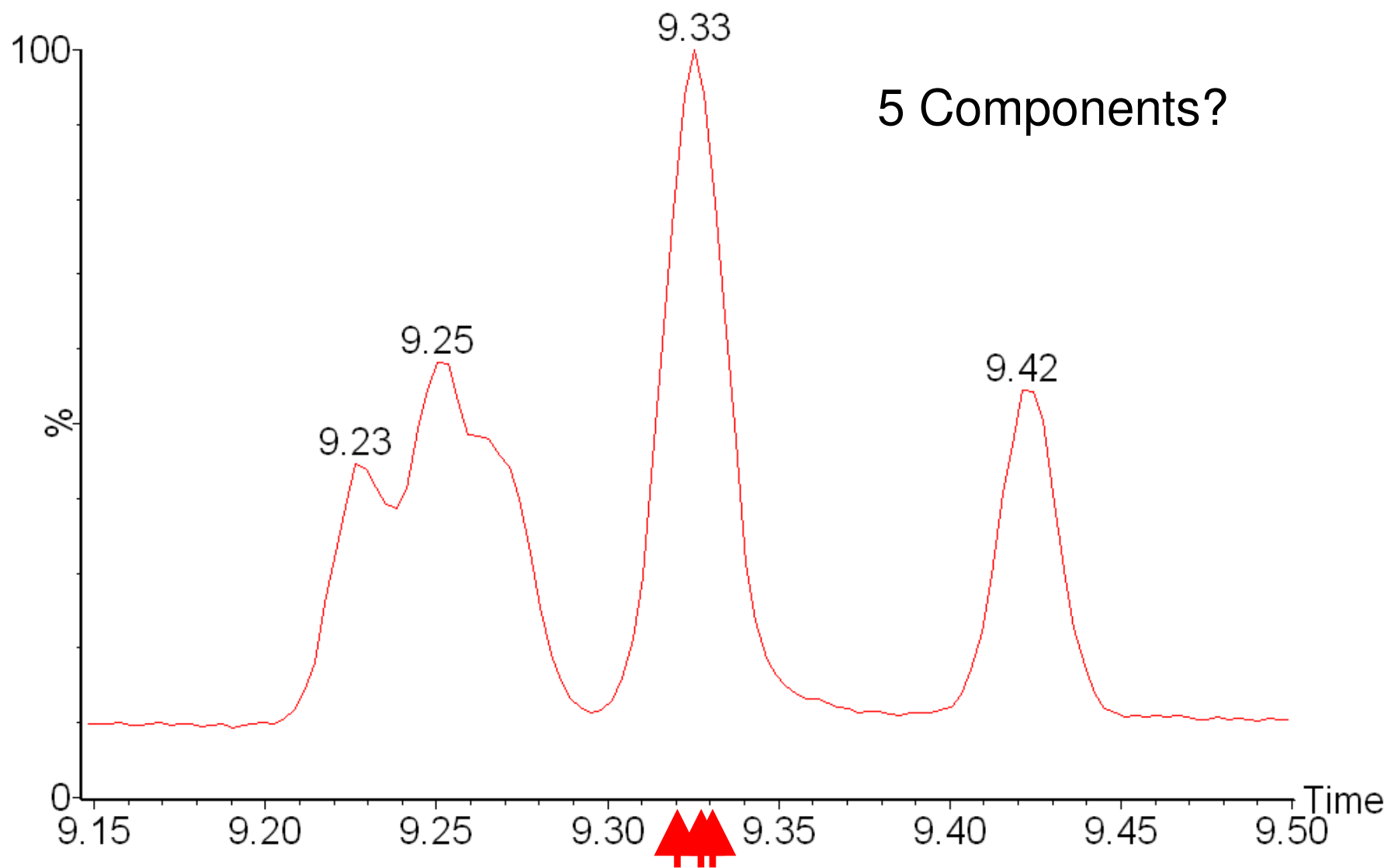
- **Pesticide residue analysis is inherently targeted (SIR-MRM). The post acquisition reprocessing and the discovery of unknown contaminants are difficult.**
- **Ion selective techniques are highly specific but discriminatory**
- **Exact mass TOF-MS is a full spectrum technique capable of both the targeted and the untargeted screening approaches. That methods can be extended to potentially unlimited numbers of residues without loss in sensitivity.**
- **No ion selection = no ion discrimination**

Exact mass chromatogram extraction: better selectivity, higher S/N



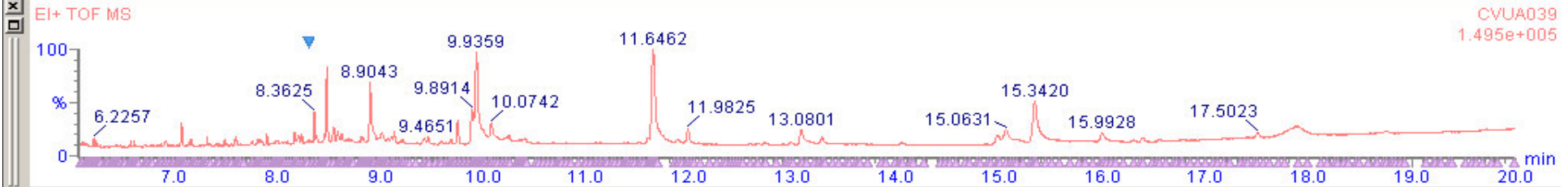
Increasing the ion extraction number doesn't affect the S/N



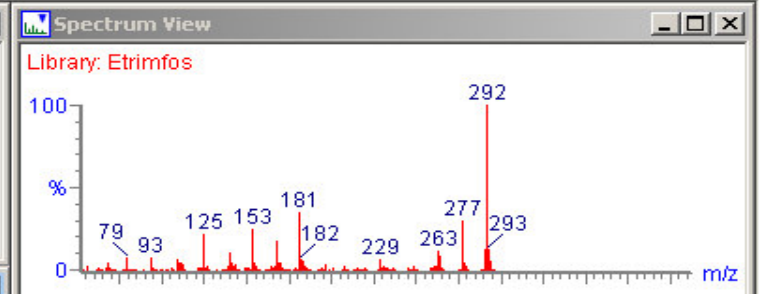
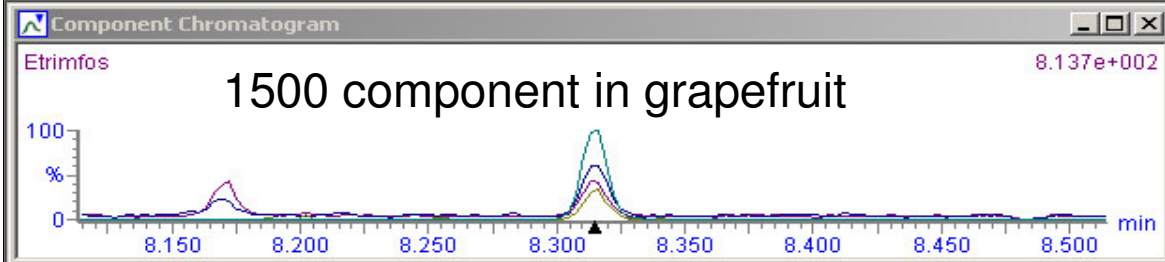


ChromaLynx Identify - Cucumber.ids

File Edit View Display Processing Window Help

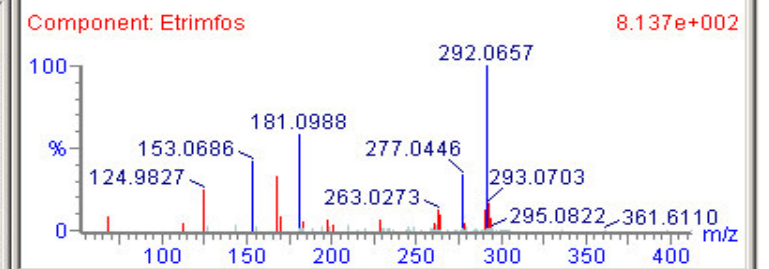


Scan	Function	Ret. Time	Rel. Ret. Time	Abundance	Rel. Abundance	Compound Name	Target Mass	Mass1	Mass2	Mass3
160	760	1	8.3144	8.3144	66	0.000	Etrinfos	153.0686	181.0988	277.0446
161	768	1	8.3360	8.3360	19	0.000	1-Formyl-2,6-dimethoxy-10-methyl-anthracene	70.0770	120.0775	280.3180
162	776	1	8.3625	8.3625	943	0.007	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	68.0590	82.0751	95.0838
163	779	1	8.3701	8.3701	4	0.000	Cyclohexanol, 2-(methylaminomethyl)-, trans-	59.9987	67.2889	72.0181
164	784	1	8.3857	8.3857	199	0.001	Pirimicarb	69.0697	70.0776	71.0860
165	795	1	8.4179	8.4179	9	0.000	Isothiourea, 2-methyl-1-(2,4-dimethylphenyl)-3-(1,1-dime...	69.0699	70.0773	84.0921



Library Match

Compound	Reverse Fit	292.0657 (mDa)	181.0988 (mDa)	153.0686 (mDa)
1 Etrinfos	809	1.0, C10H17N2O4PS	(1) 1.1, C9H13N2O2	(1) 0.5, C5H14O3P
2 Phosphorothioic acid, O-...	747	1.0, C10H17N2O4PS	(1) 1.1, C9H13N2O2	(1) 0.5, C5H14O3P
3 ETRIMFOS;(EKAMET),(S...	747	1.0, C10H17N2O4PS	(1) 1.1, C9H13N2O2	(1) 0.5, C5H14O3P
4 Phosphorothioic acid, O-...	854	1.0, C10H17N2O4PS	(1) 1.1, C9H13N2O2	(1) 0.5, C5H14O3P
5 Phosphorothioic acid, O-...	716	1.0, C10H17N2O4PS	(1) 1.1, C9H13N2O2	(1) 0.5, C5H14O3P
6 9H-Xanthen-9-one, 4-chl...	785			-1.8, C12H9
7 4,6-Di(4-methoxyphenyl)...	709		(1) 1.1, C9H13N2O2	(1) -1.8, C12H9



- **Methods is presented for the targeted analysis of pesticide residues in food commodities using both the GCT Premier and LCT Premier with TargetLynx.**
- **The residues can be analysed to concentration levels of 0.01 mg/kg or less in various matrices with the use of exact mass chromatograms.**
- **The methods can be extended to larger numbers of residues without loss in sensitivity due to the full spectrum approach provided by exact mass TOF instruments.**
- **The 1 run saved data files can also be used to screen for untargeted residues using ChromaLynx.**
- **ChromaLynx enables automatic peak detection, deconvolution, library searching and exact mass scoring.**

- The authors would like to thank Carmen Wauschkuhn, Diane Fuegel and Michelangelo Anastassiades at CVUA Stuttgart, Fellbach 70736, Germany for supplying the GCT Premier sample extracts.
- Thank you for your attention !

Waters

Jean-Marc Joumier
Business development Manager
GC-MS Europe

**APPLICATION OF
HIGH RESOLUTION TOF-MS
FOR
MULTIRESIDUE ANALYSIS OF
PESTICIDES**

For Complete  Confidence