



Adding more Power to your GC-MS Analysis through Deconvolution

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- Analytical training & consultancy services focusing on specialist subject fields of gas chromatography, mass spectrometry & periphery techniques
 - Scheduled and bespoke training from many industries & all levels of experience in techniques, hardware & software
 - Applications support to help choose the best techniques
 - Our consulting & instrument business areas to advise & support from assistance with method development to application support & technical authoring.
 - Teaching theory, hardware, software, method development, troubleshooting and maintenance and impart our knowledge and many years of experience in these subject areas
 - Customers from UK, to Middle East including PetroChemical companies like Saudi Aramco

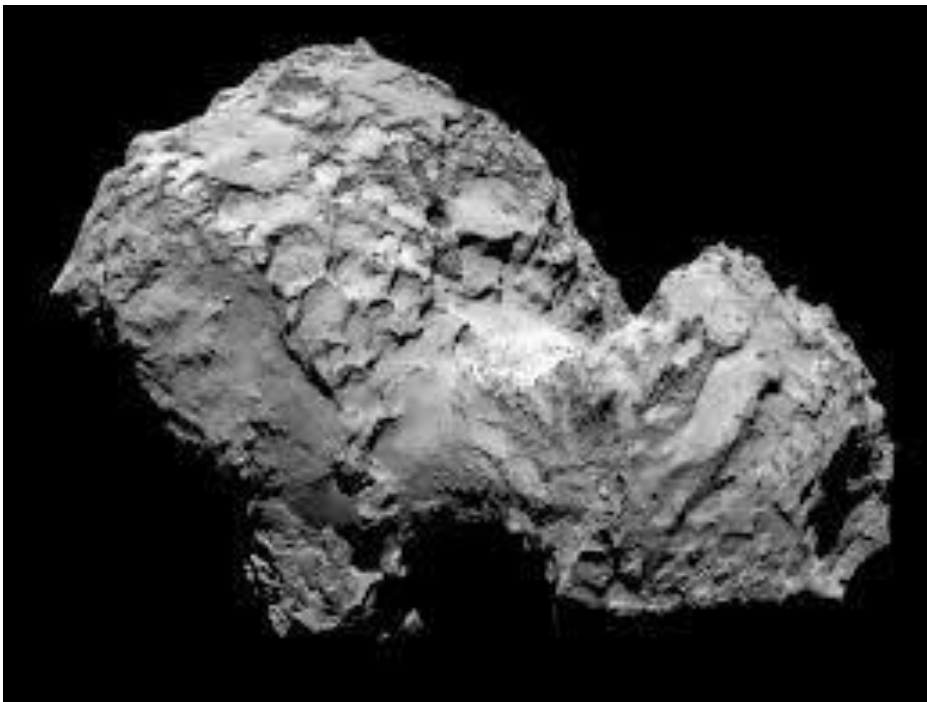


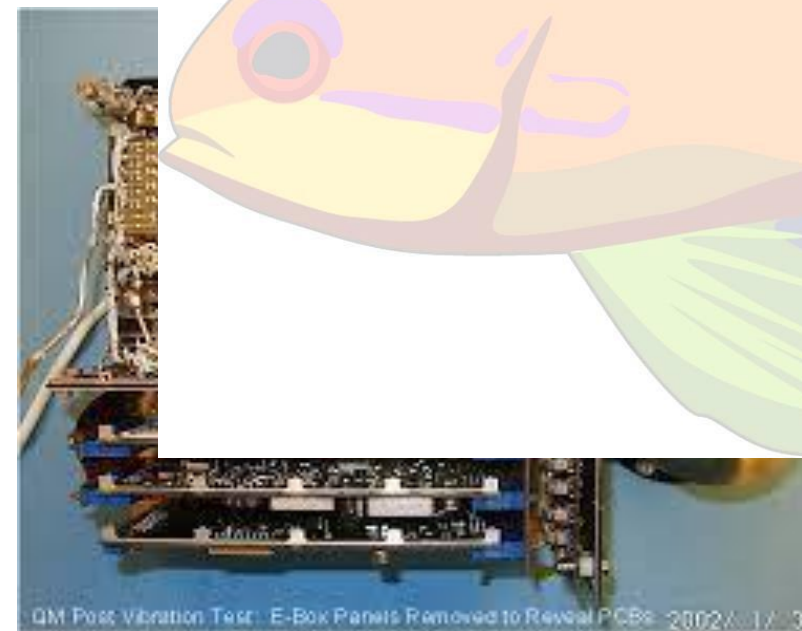
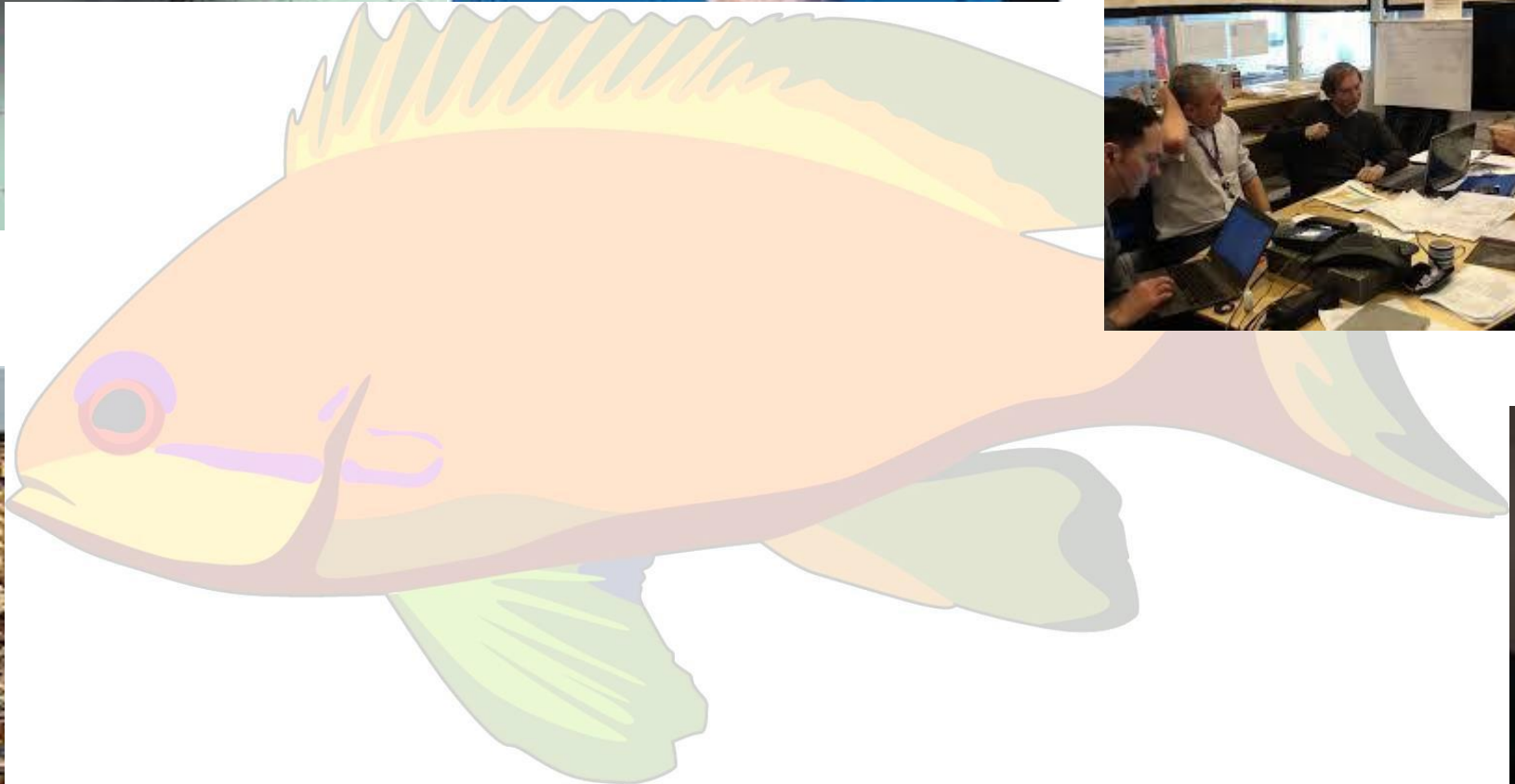
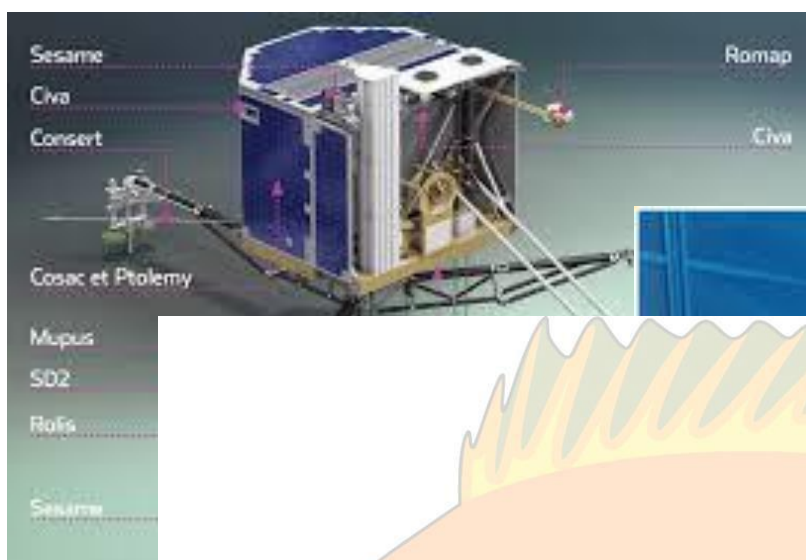
20+ training courses formally approved by Royal Society of Chemistry

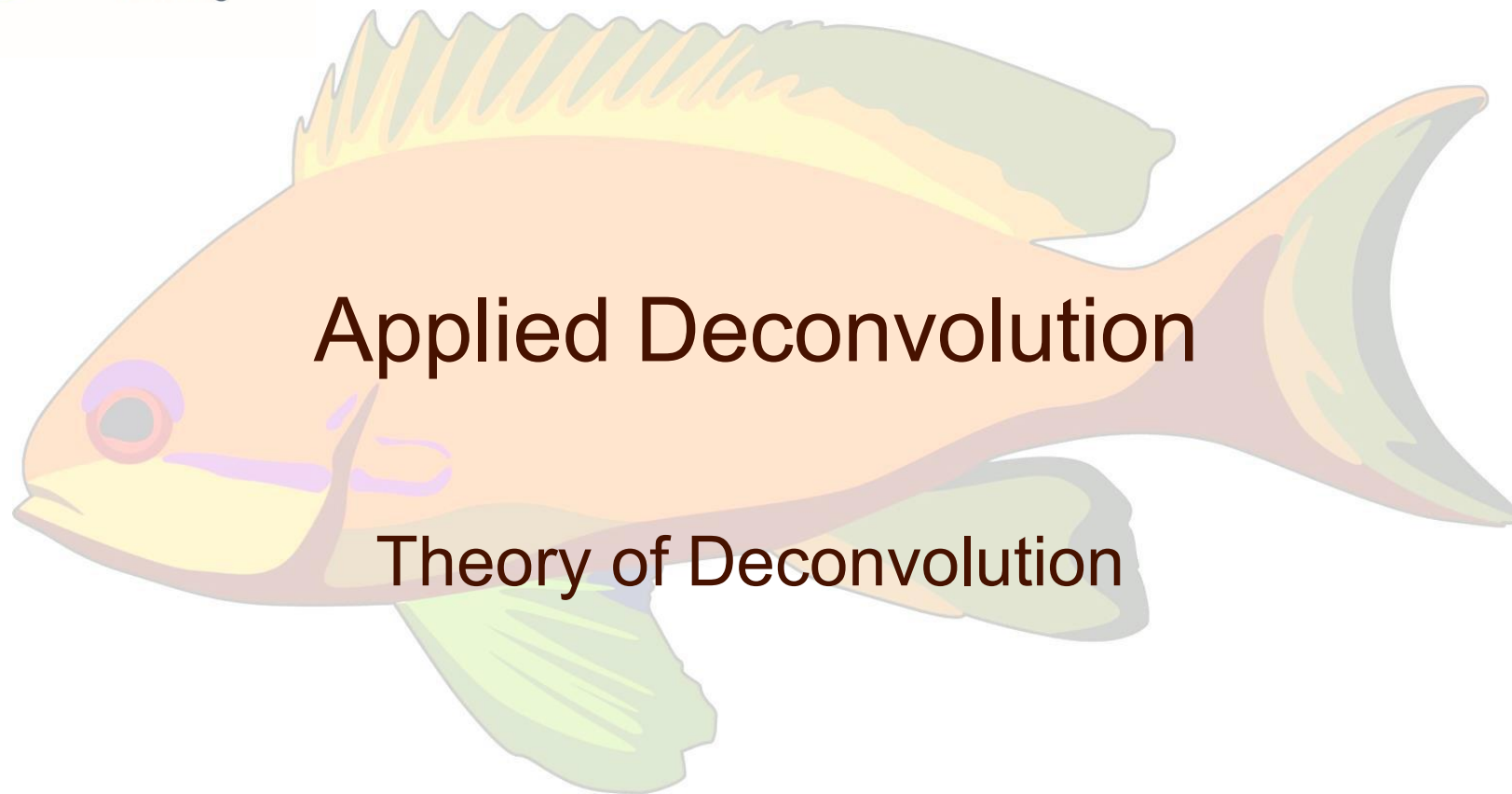
“The objectives of course approval are to highlight good quality training available to the community & encourage members’ continuing professional development (CPD)...The approval process is one of peer review, involving assessment against set criteria by members that are experts in their field”

Dr Andrea McGhee, RSC Accreditation Development Specialist

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- All practical scheduled courses take place here at Walton Hall, Milton Keynes, UK
 - Tailored training & consultancy services too
 - Distance learning and research university
 - The Open University ranks in top 3rd of UK universities for innovative research & development
 - Planetary & Space Department
 - Investigates the origin of the Solar System, evolution of the planets & the conditions for Life integrating use of spaceflight instrumentation with laboratory analyses and simulation
 - Instruments developed have been utilised for applications in health care, such as TB & cancer detection





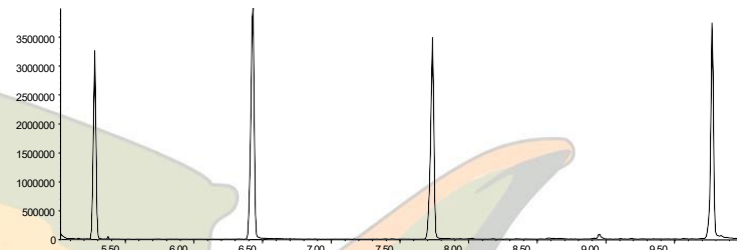


Applied Deconvolution

Theory of Deconvolution

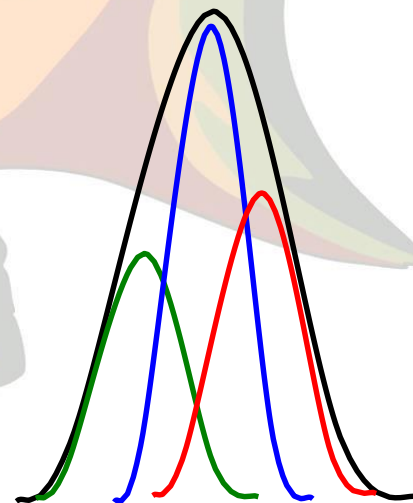
- Chromatographic resolution

Analytes are physically separated by their selective interaction with stationary phase of analytical column & elute at different retention times



- Analytical resolution

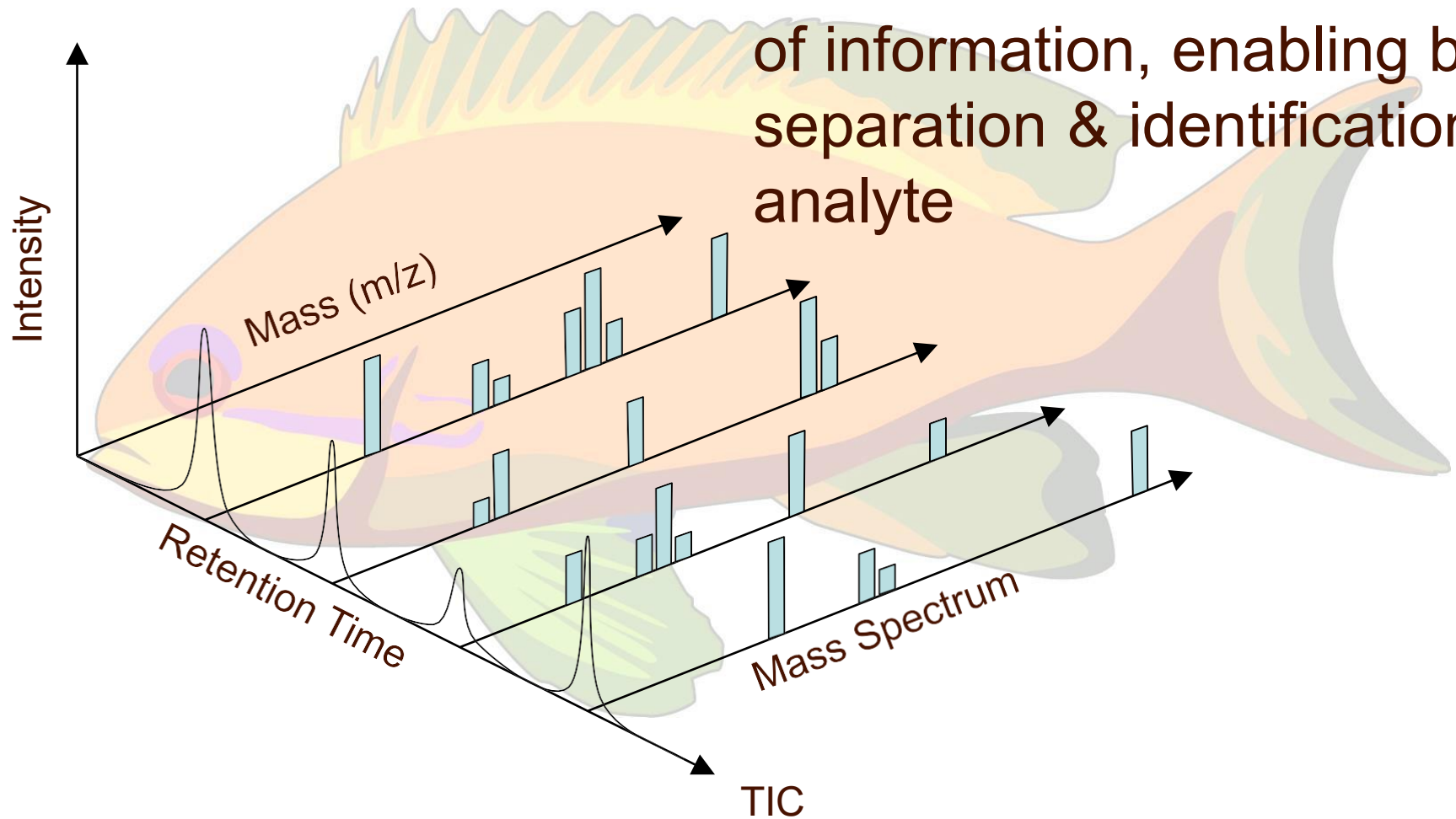
Analytes eluting at similar retention times are separated by their different (unique) masses



Those analytes with same retention time AND all same masses cannot be separated

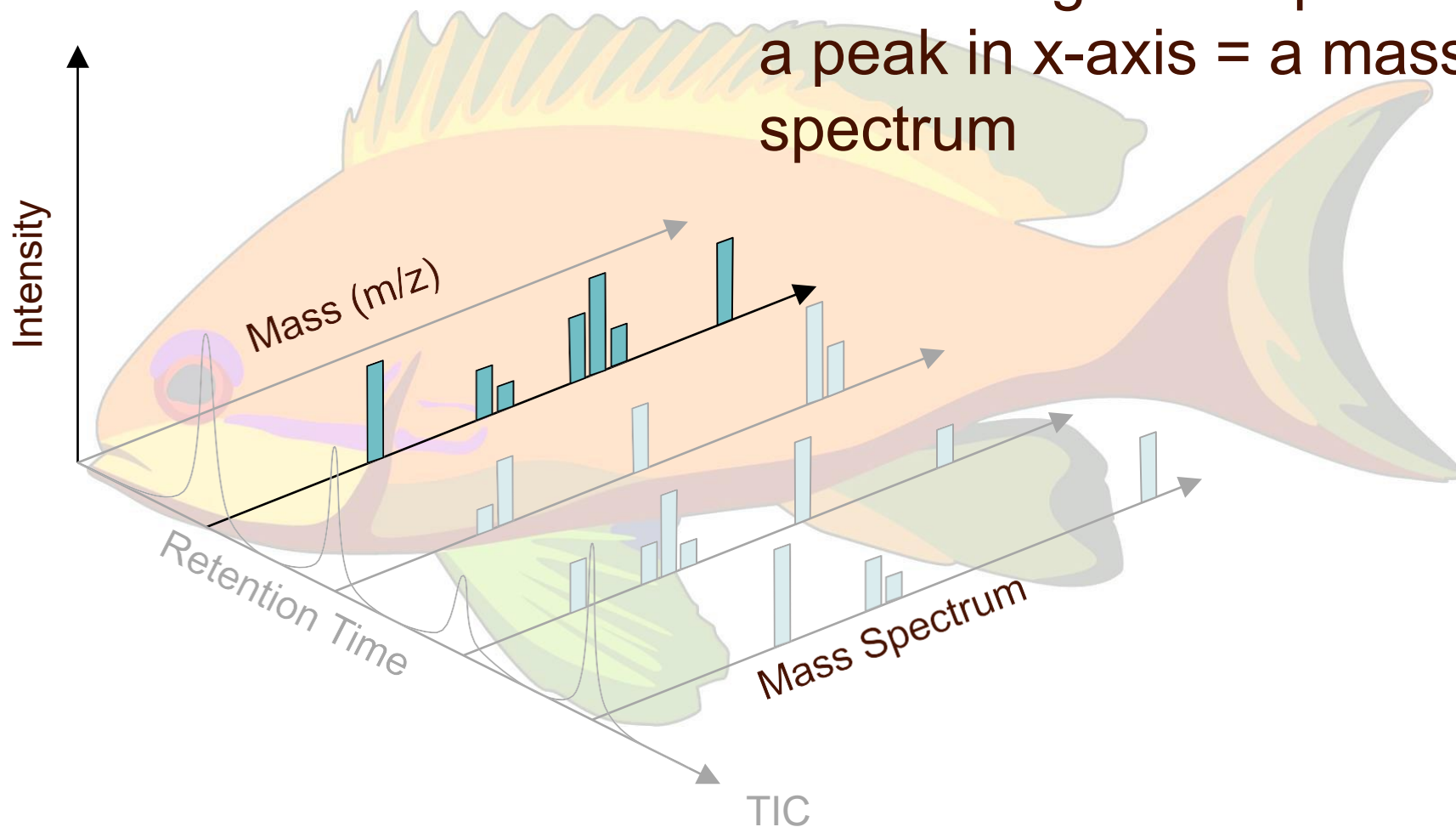
GC-MS = 3D data

MS adds another dimension of information, enabling both separation & identification of analyte



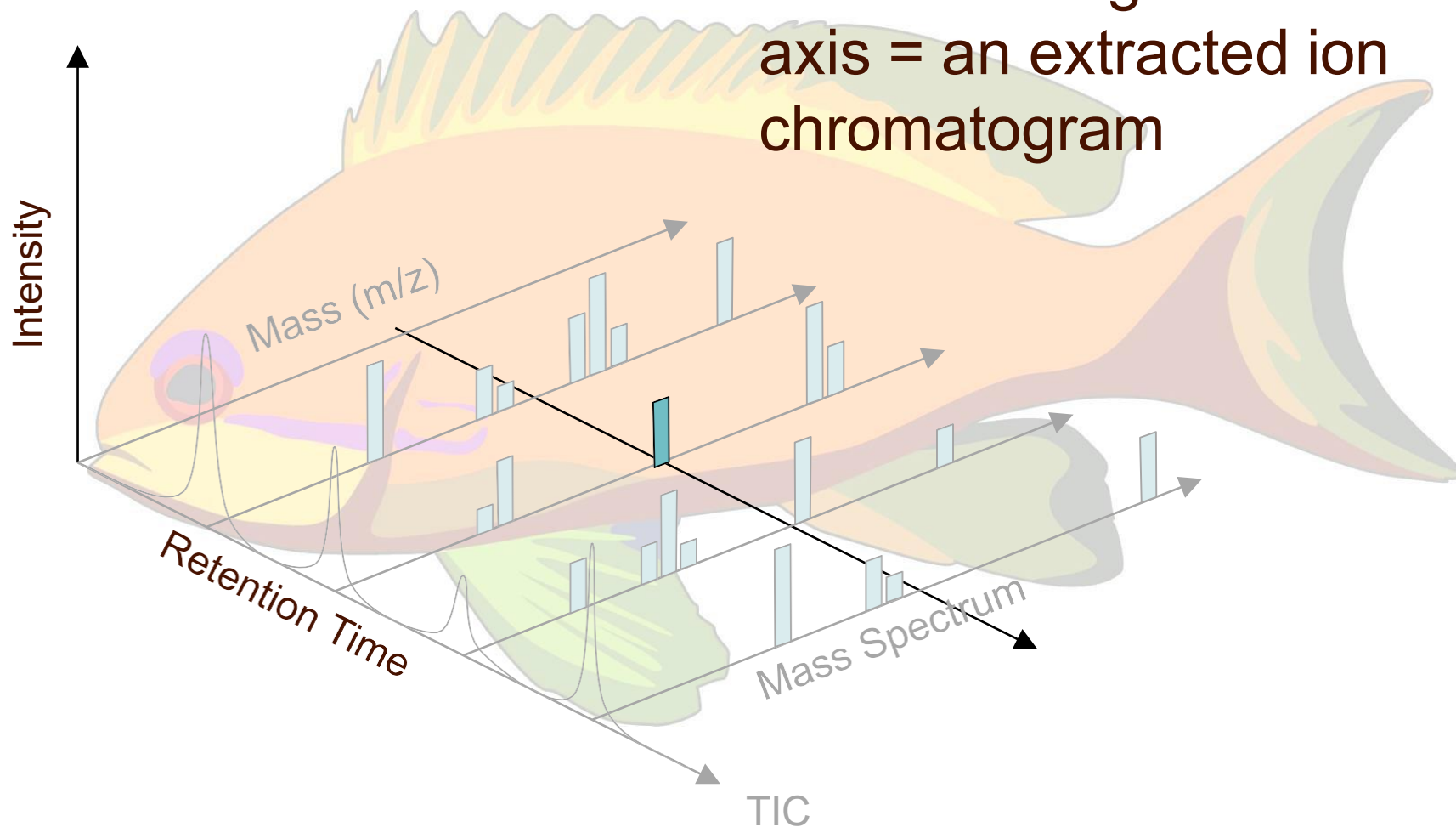
GC-MS = 3D data

Take a single data point on
a peak in x-axis = a mass
spectrum



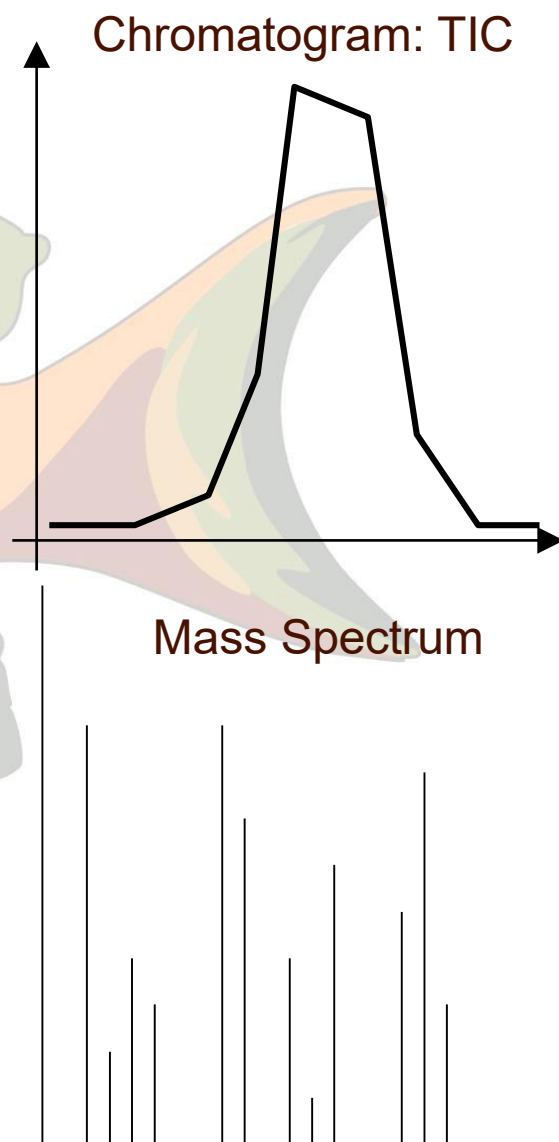
GC-MS = 3D data

Extract a single ion from z-axis = an extracted ion chromatogram

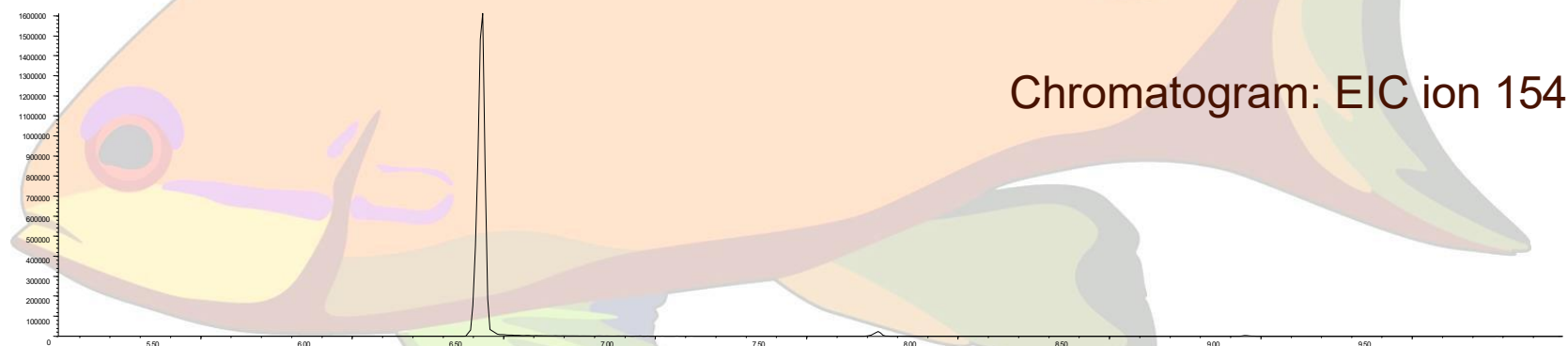
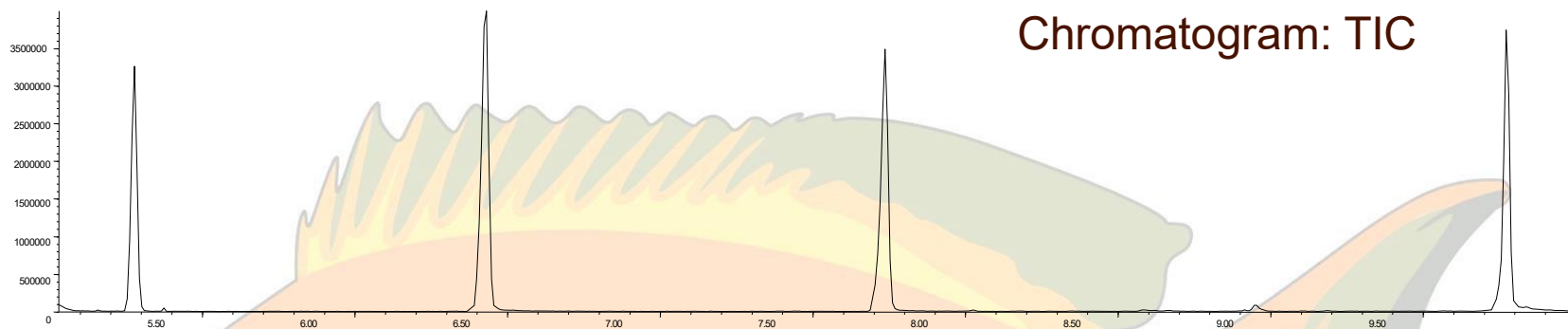


TIC

- Abundance of each mass at a particular data point is summed to produce a total ion current
- This is plotted for each data point (or scan)
- A 2D total ion chromatogram (TIC) is produced of retention time versus total ion current
- Selecting a single data point will then give a mass spectrum at that point in time
- If two peaks are co-eluting it will give a mixed mass spectrum of both peaks plus any background like column bleed



EIC



- Extracted ion chromatogram of 154 ion
 - Only peaks containing 154 ion can be seen
- Useful for looking for a particular known analyte
- Multiple ions can be extracted and summed if required

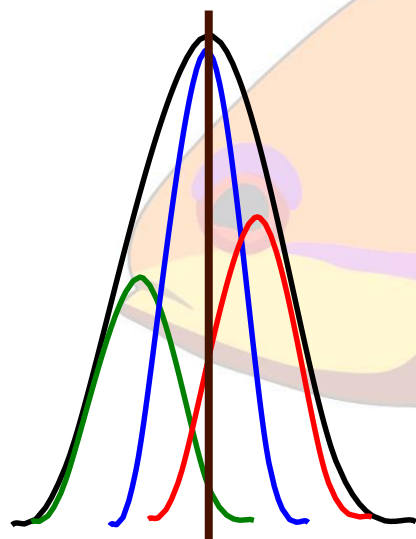
Why use deconvolution?

TIC

Mass 105

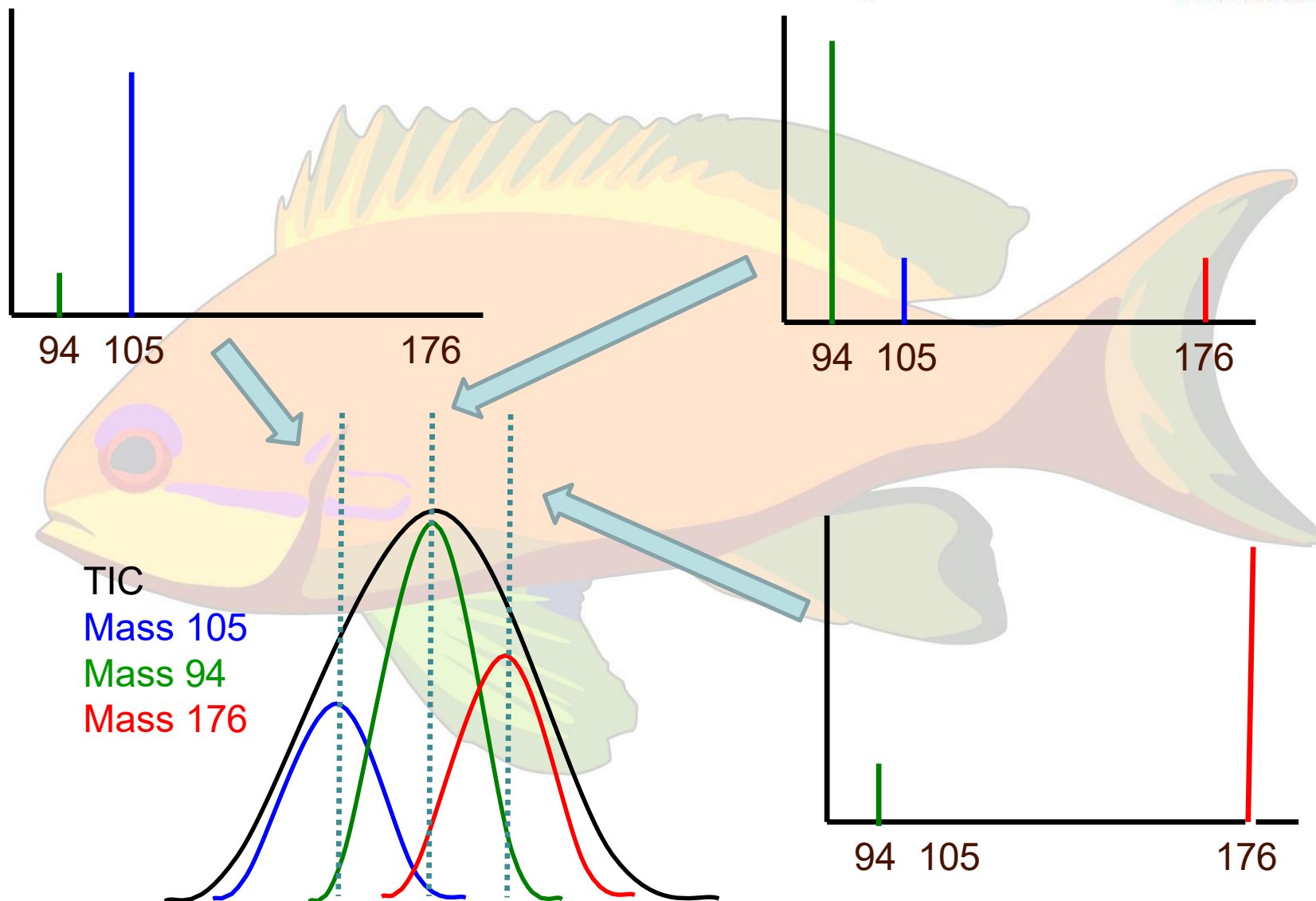
Mass 94

Mass 176



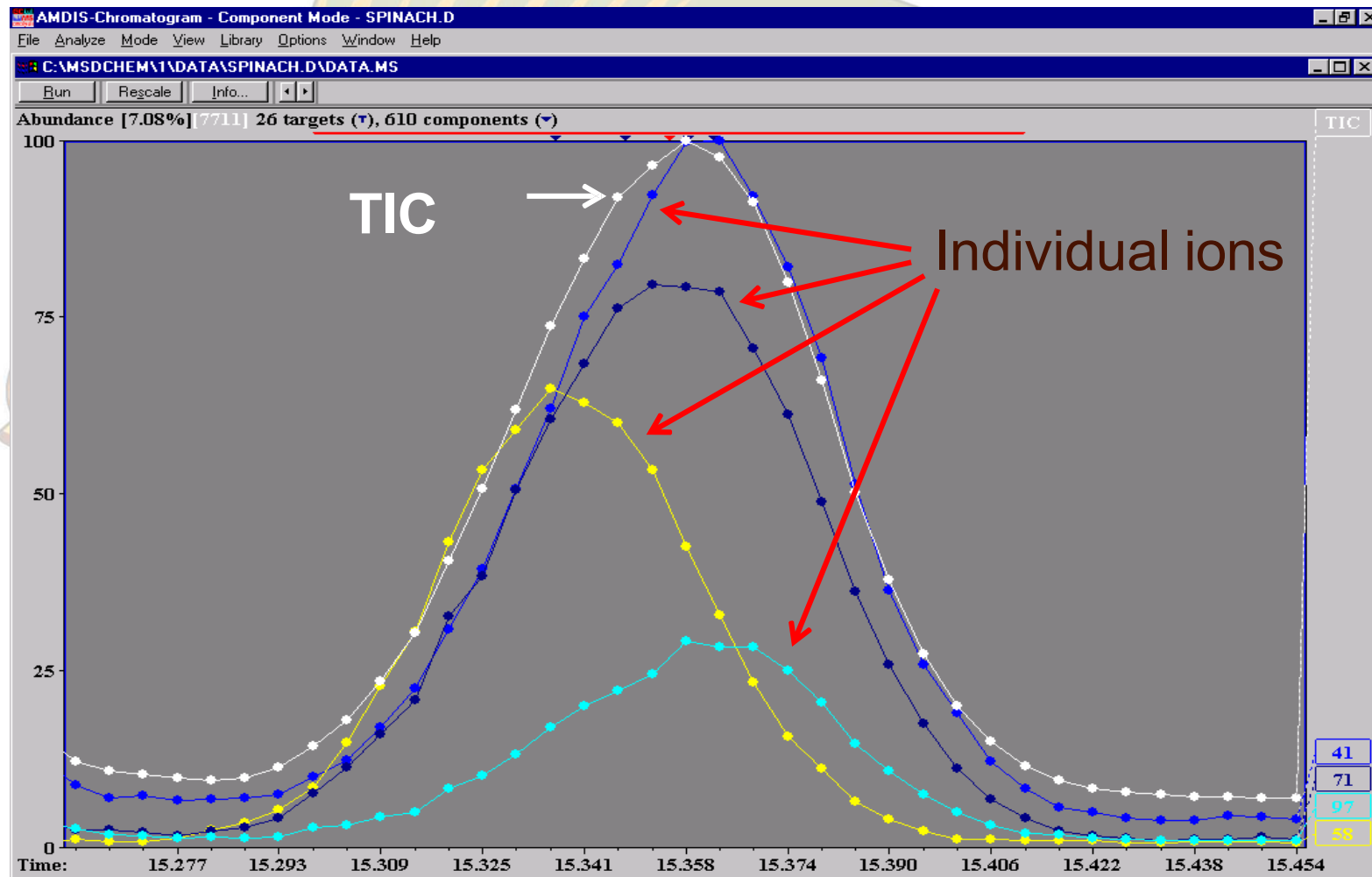
- If individual standards analysed – could get retention time & mass spectrum for each peak
- For target analysis where retention times & ions are known can identify & quantify analytes on unique masses
- For unknown samples:
 - Can you see if there are coelutions?
 - Can you get a high quality mass spectrum for library searching & identification?
- For target analytes, scan & SIM:
 - Coeluting peaks
 - Matrix interferences

Analytical resolution

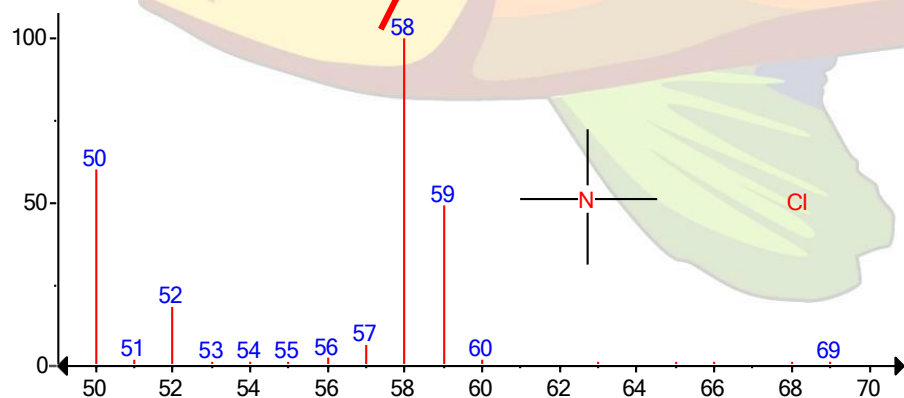
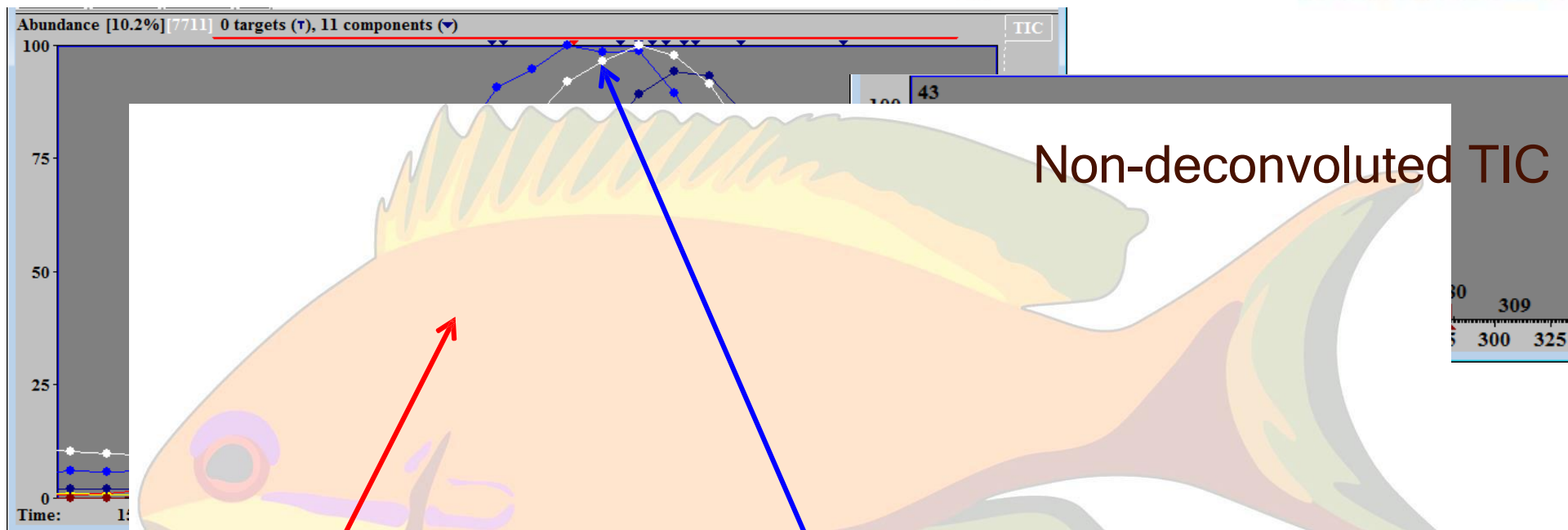


Deconvolution definition

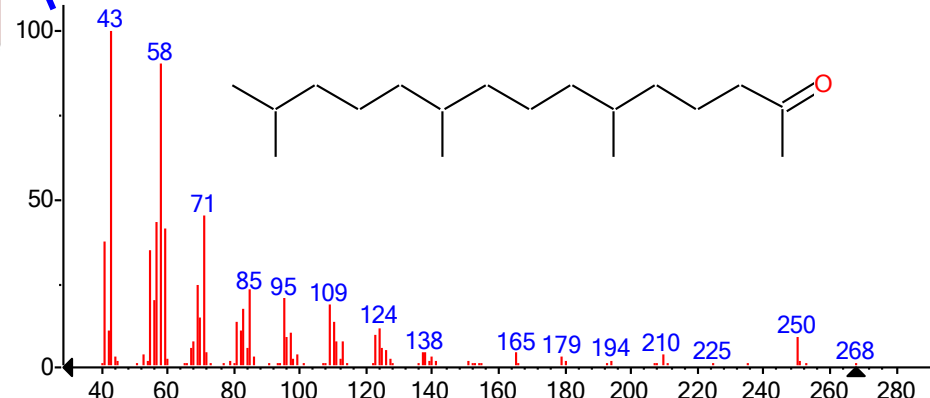
“...in the broad sense of extracting one signal from a complex mixture...” (From AMDIS)



Deconvolution example

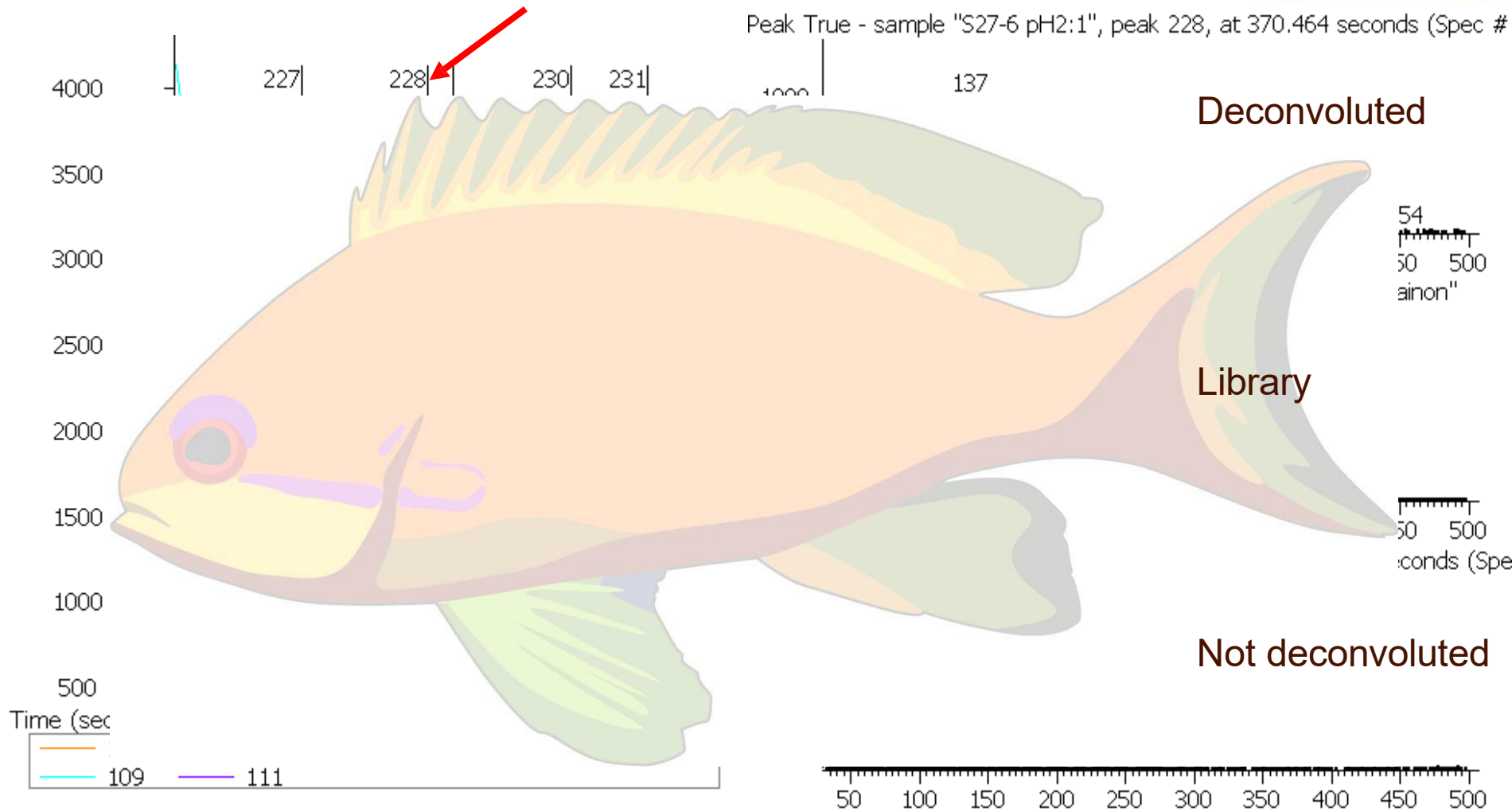


Tetramethylammonium chloride

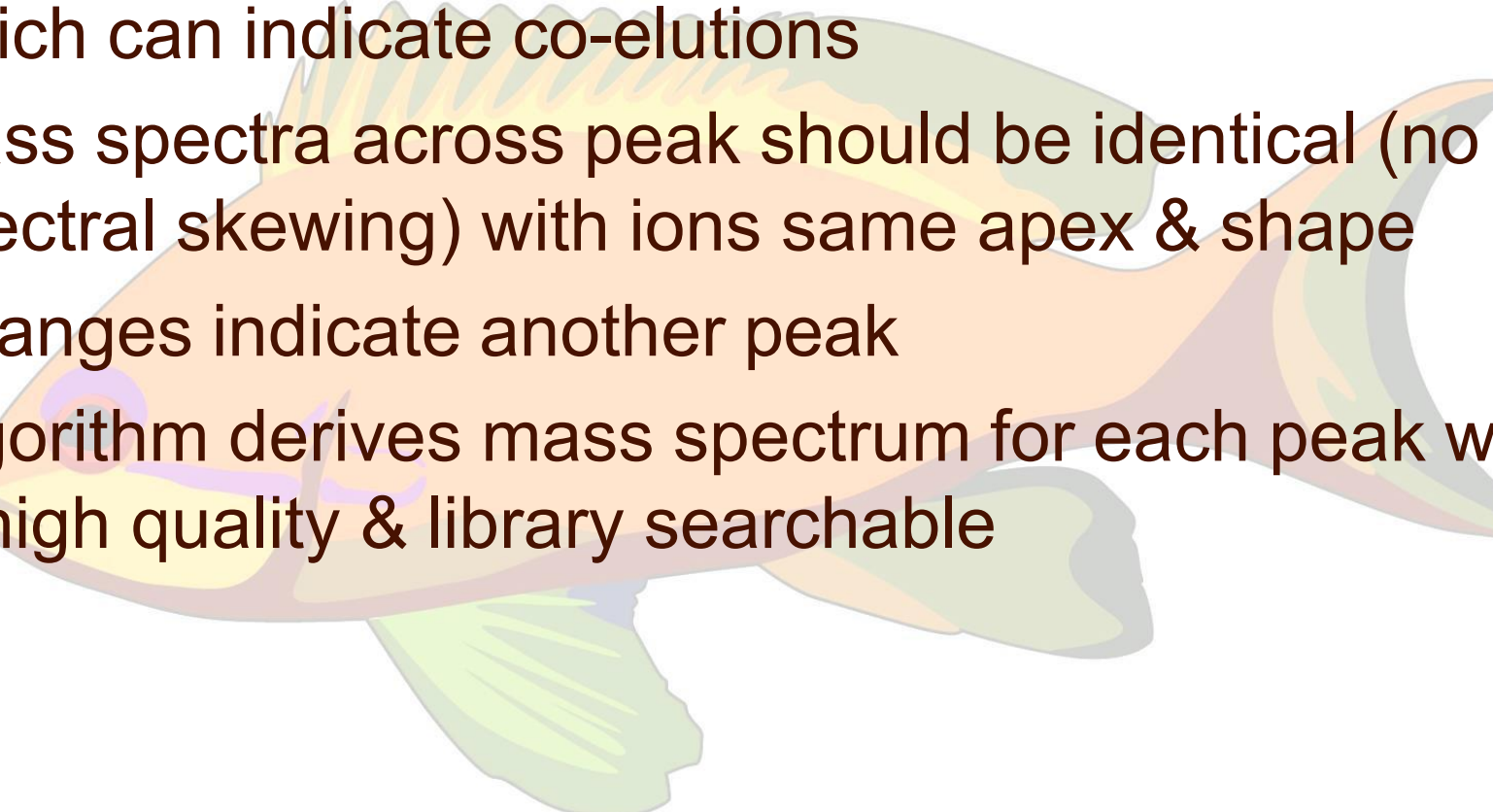


Perhydrofarnesyl acetone

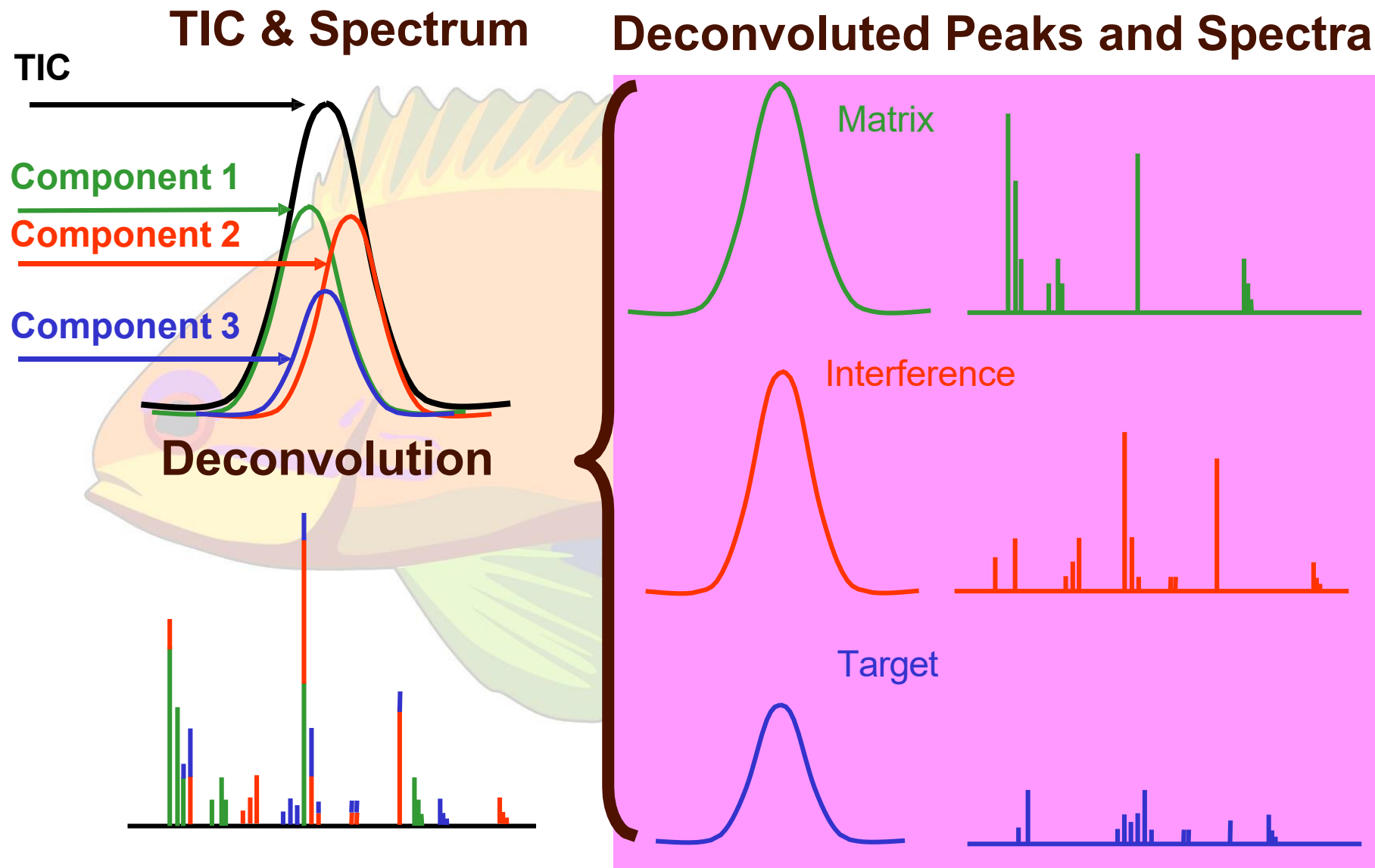
Deconvolution



Courtesy of Leco Instruments

- Detects differences in mass spectra across a peak which can indicate co-elutions
 - Mass spectra across peak should be identical (no spectral skewing) with ions same apex & shape
 - Changes indicate another peak
 - Algorithm derives mass spectrum for each peak which is high quality & library searchable
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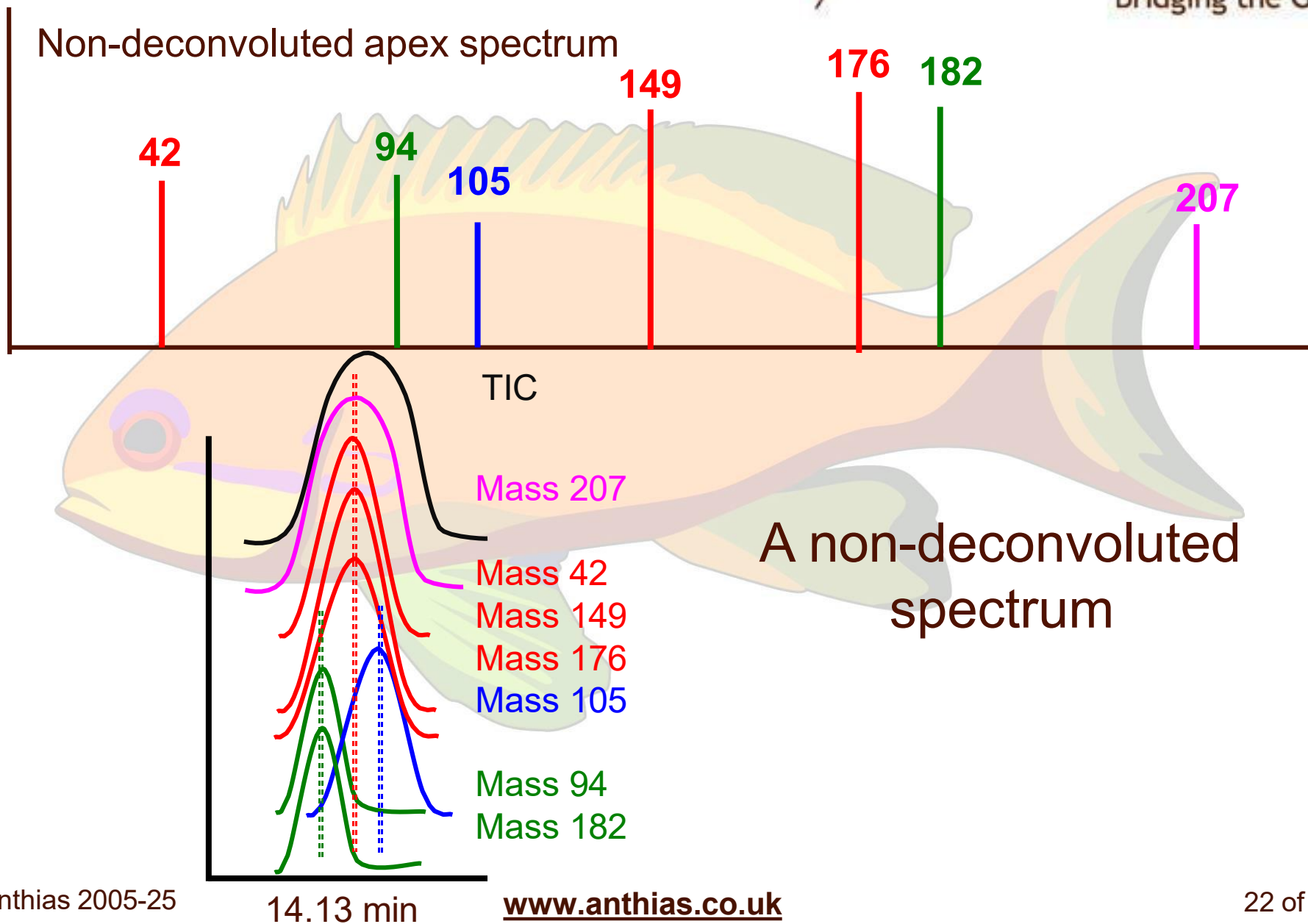
Deconvolution example



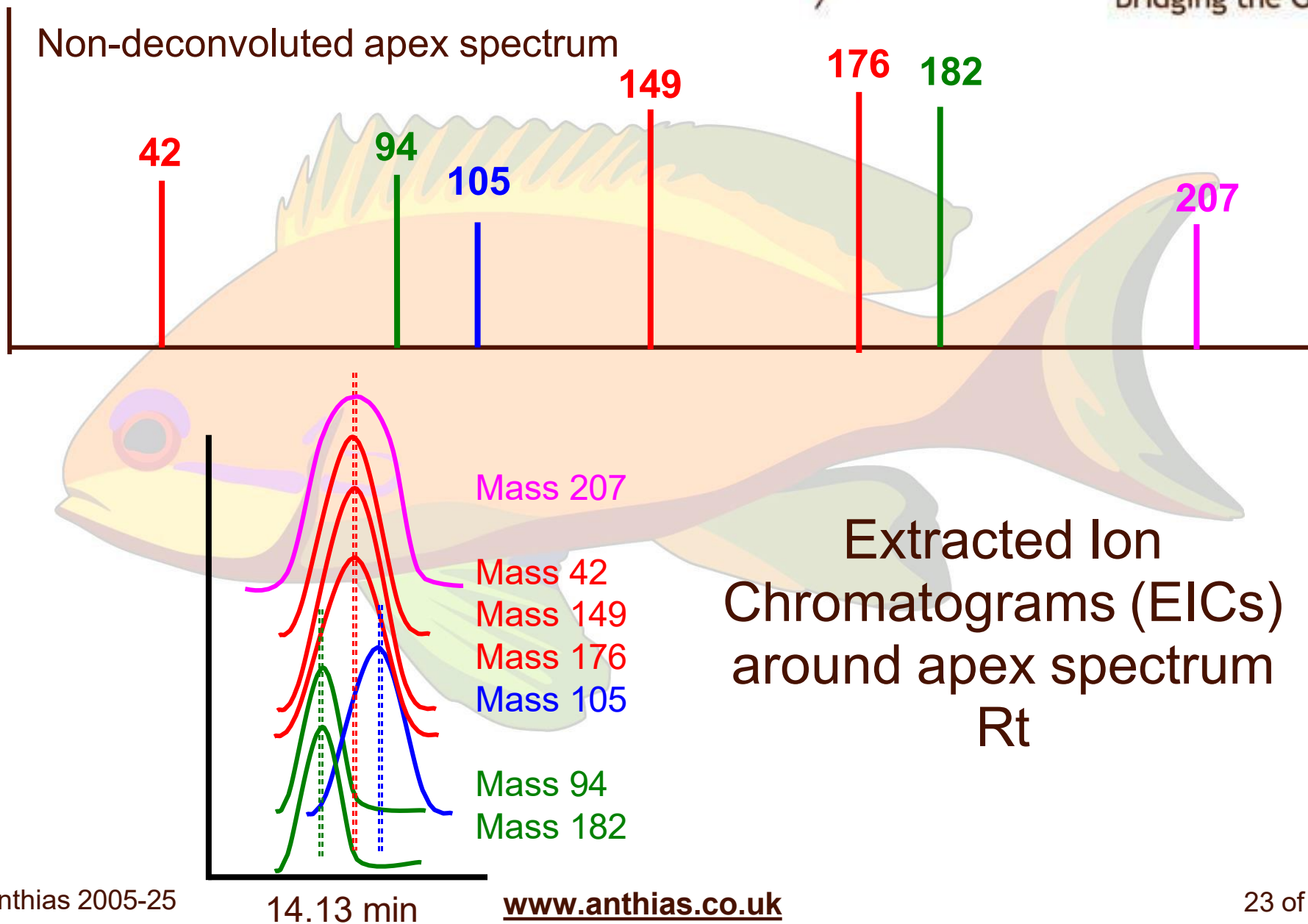
Exact steps dependent on deconvolution software:

- Noise is defined & compensated for
- Scan skew is corrected
- True peak maximum found for each ion
- Ion profiles are tracked, rate of rise/fall
- Ions present in mass spectrum of that peak should have
 - Same apex
 - Rise up & fall together (have same shape)
- Deconvoluted mass spectrum produced for each peak found according to settings/integration parameters
- Deconvoluted mass spectra can be library searched
- Retention index can be used as a qualifier to check correct isomer identified

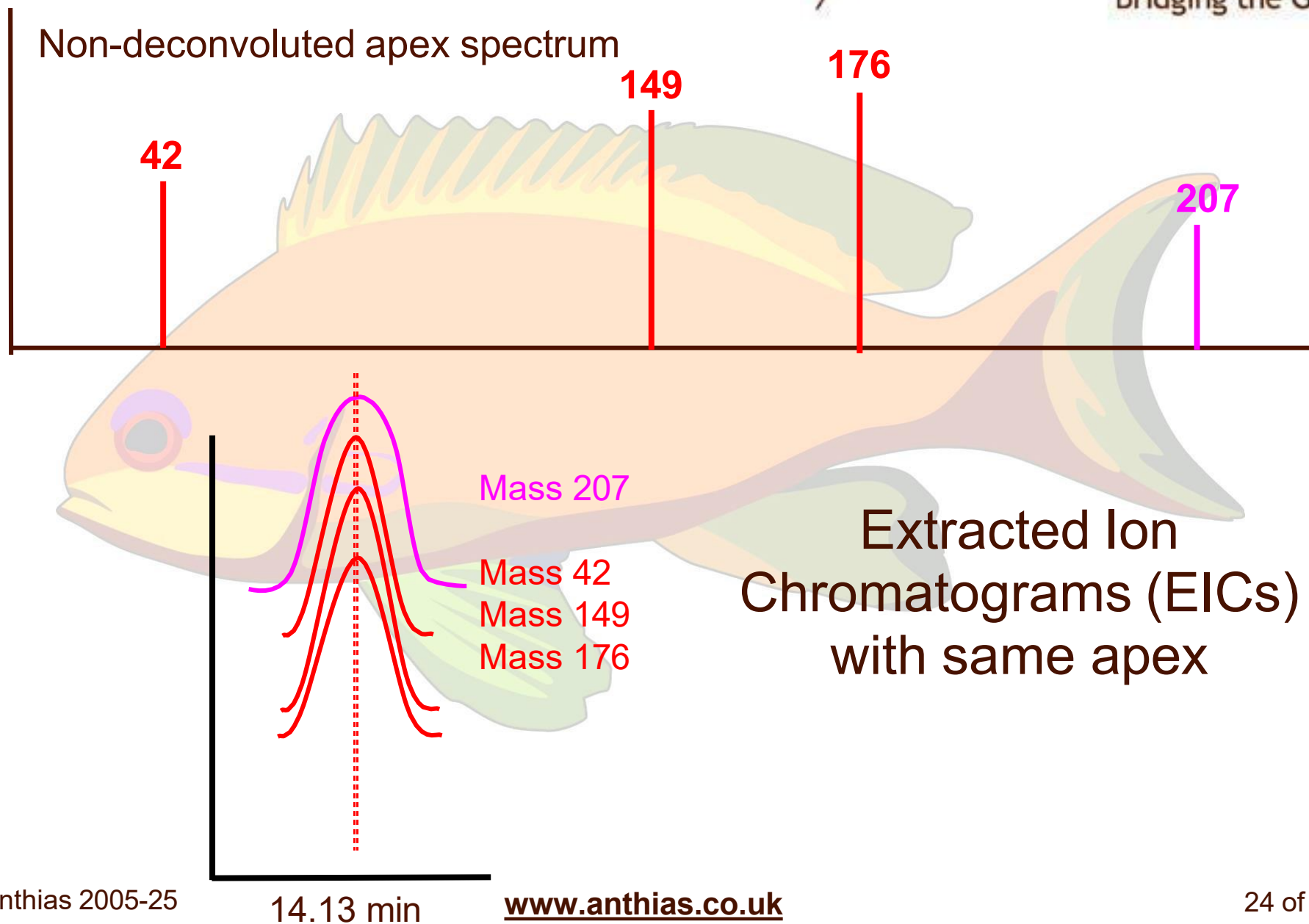
Deconvolution process

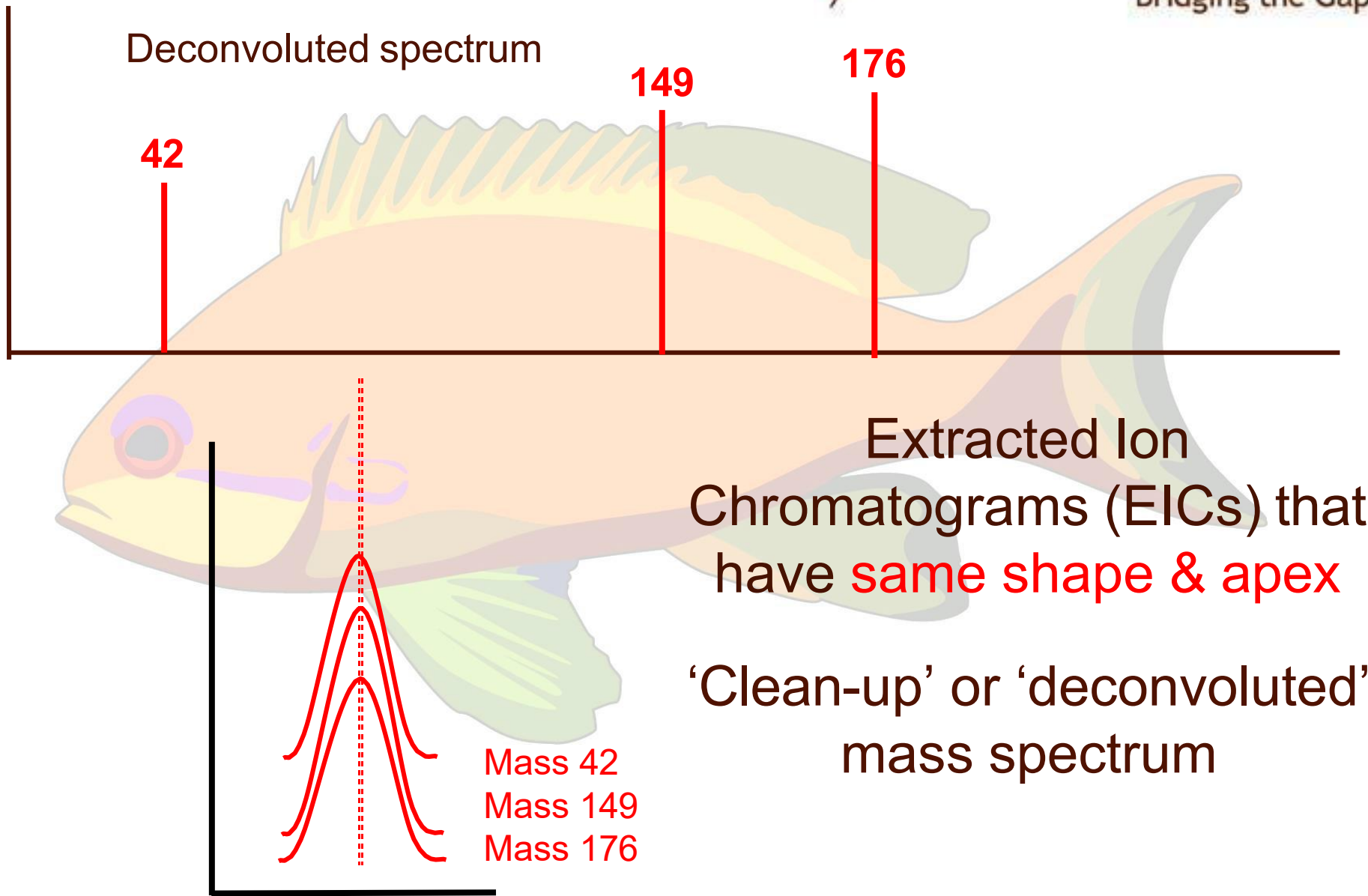


Deconvolution process



Eliminate ions: different apex





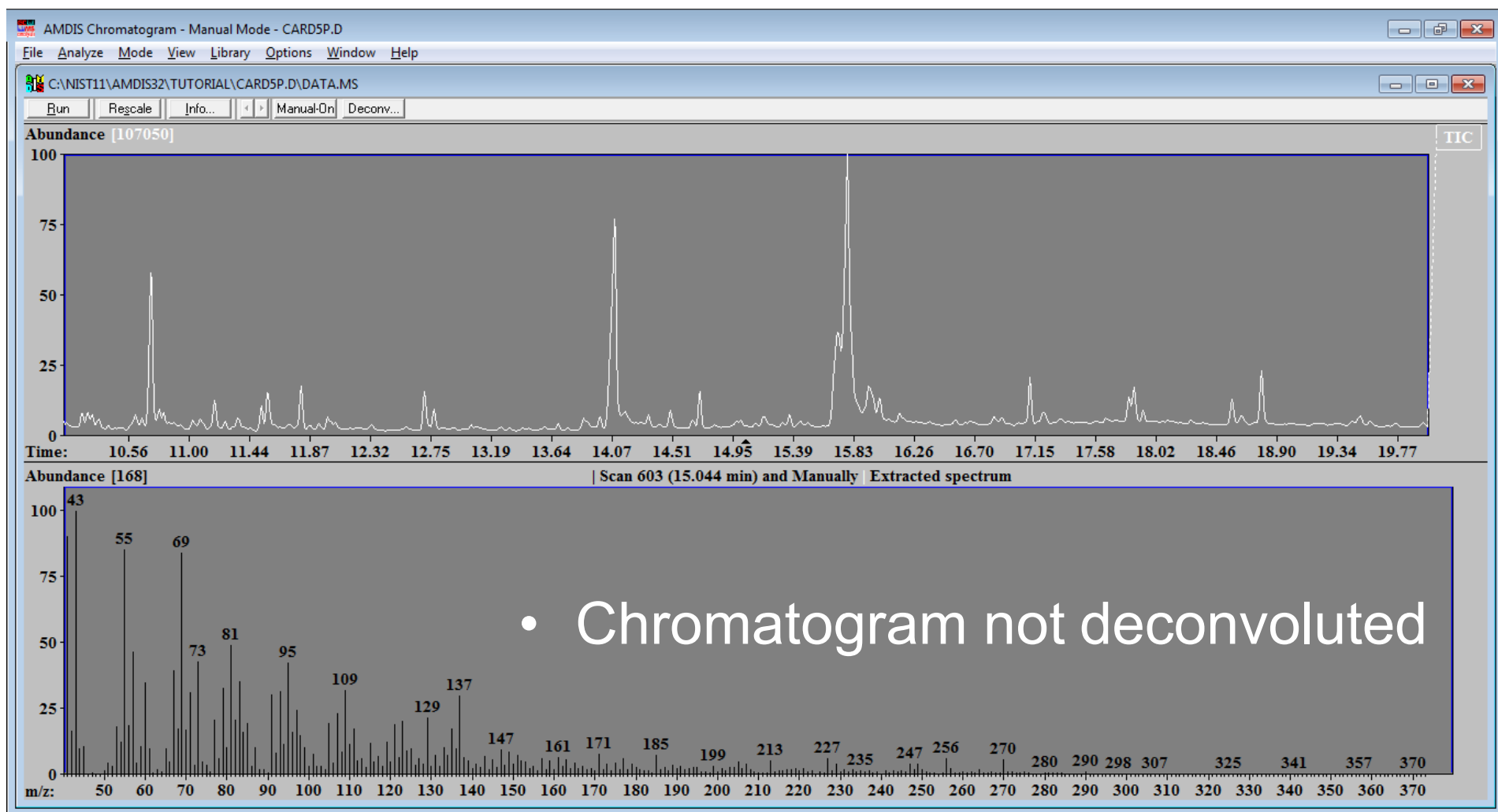
- Always some chromatographic resolution
 - Total co-elution (apex & same shape) can not be deconvoluted
- Always obtain good peak shapes
 - Sharp, Gaussian peaks are easier to deconvolute
- Ensure correct mass range is obtained for deconvolution
- Ensure there are enough data points across peak
 - Improves peak shape, enables accurate identification of apex, enables deconvolution of closely co-eluting peaks
- Get good signal to noise
 - Any data system will handle large, sharp peaks better than working in noise region
 - Reducing noise & improving signal can be applied throughout GC-MS system from carrier gas to MS detector & sample prep



Applied Deconvolution

Examples

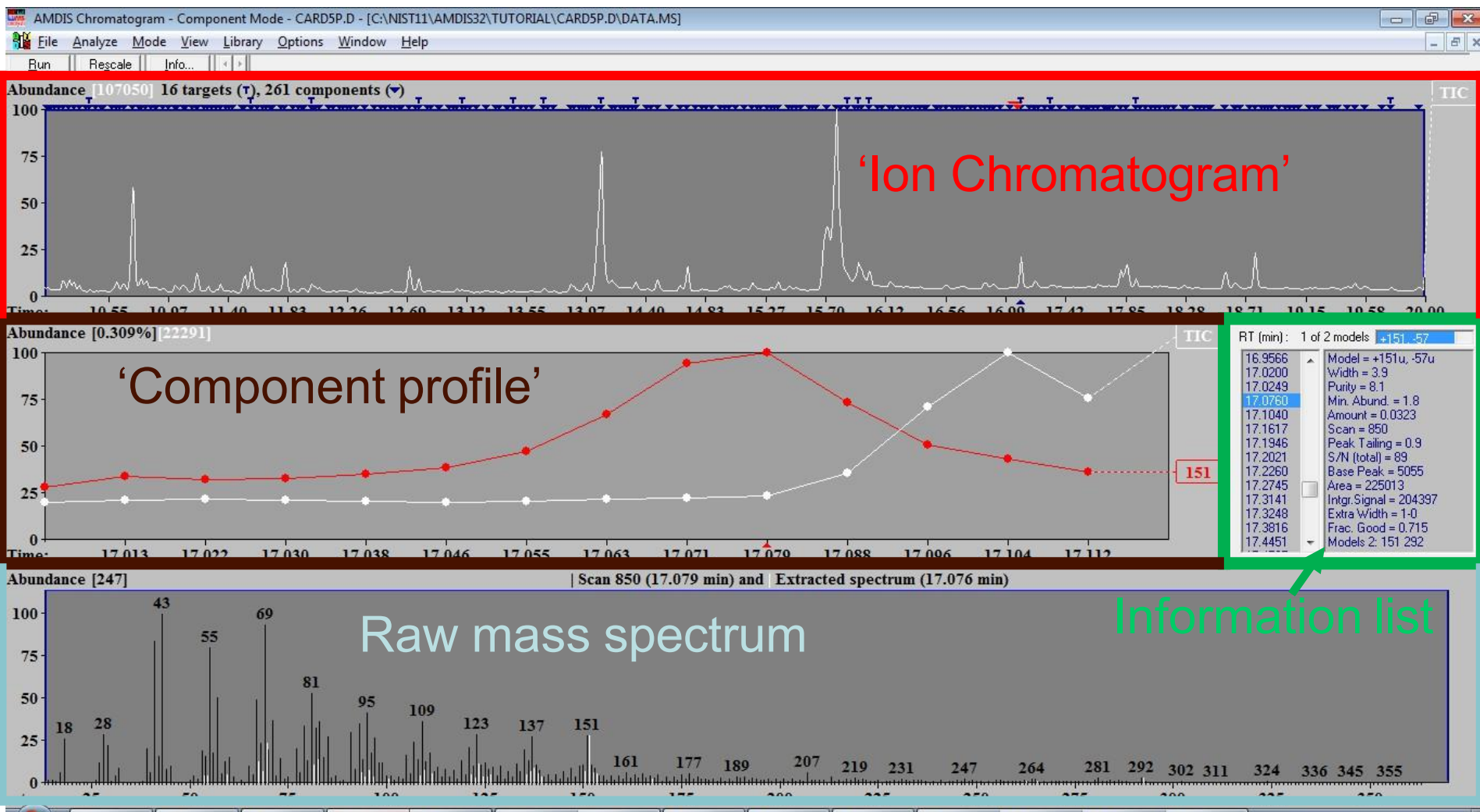
AMDIS Deconvolution



Pesticides in cardamon oil

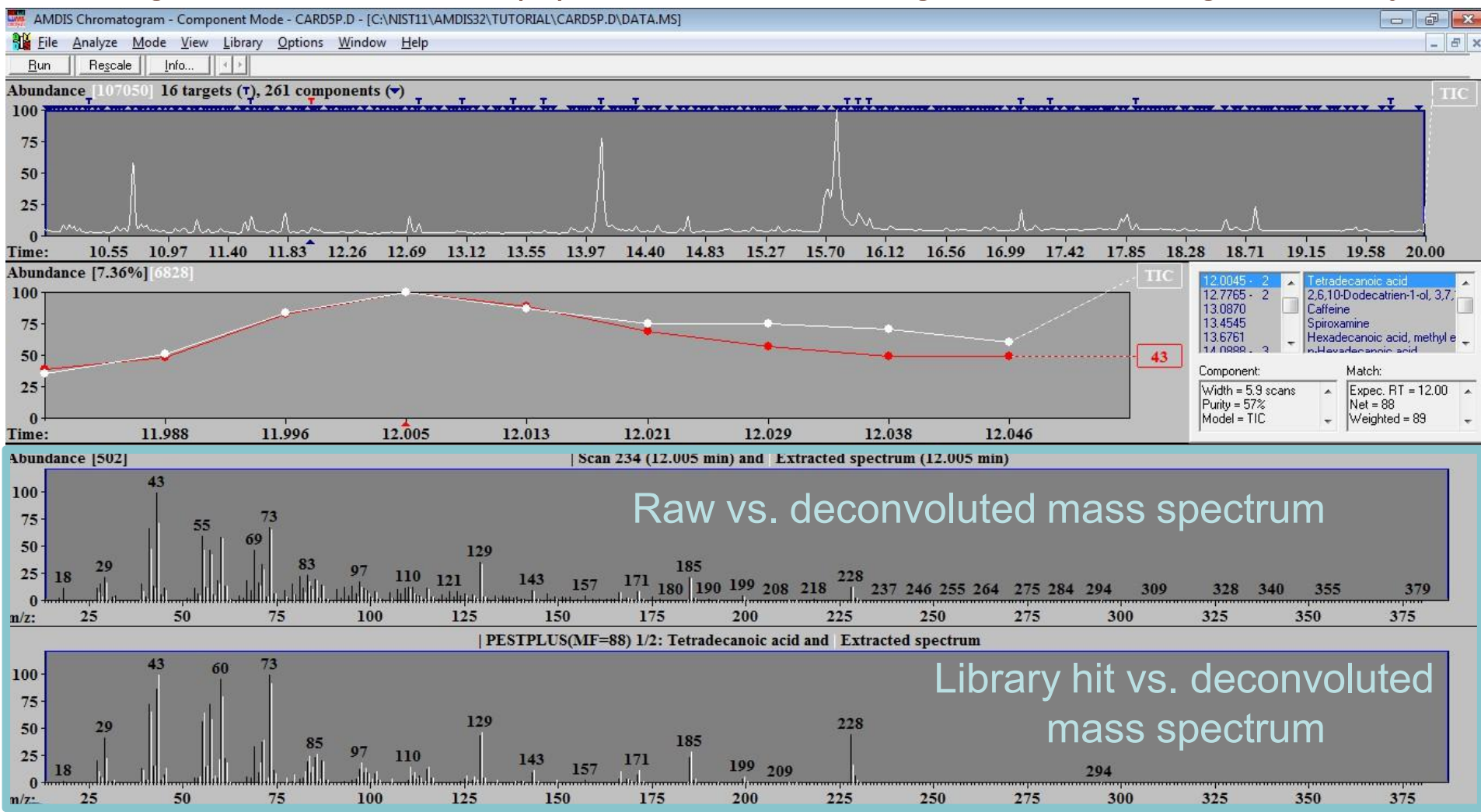
AMDIS Deconvolution

Individual components (peaks): selected component in red

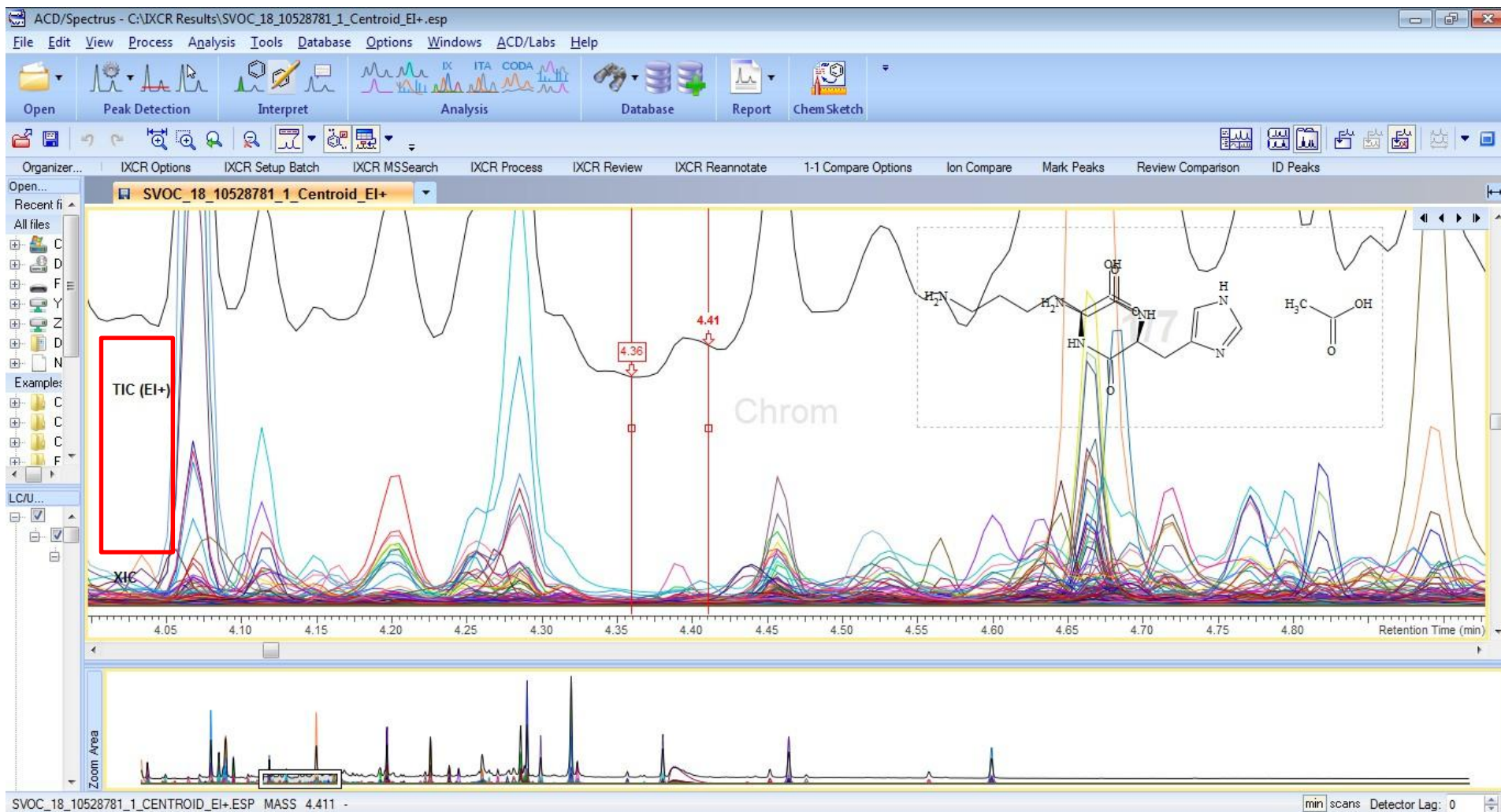


AMDIS Deconvolution

Target components (T) found: match against the target library

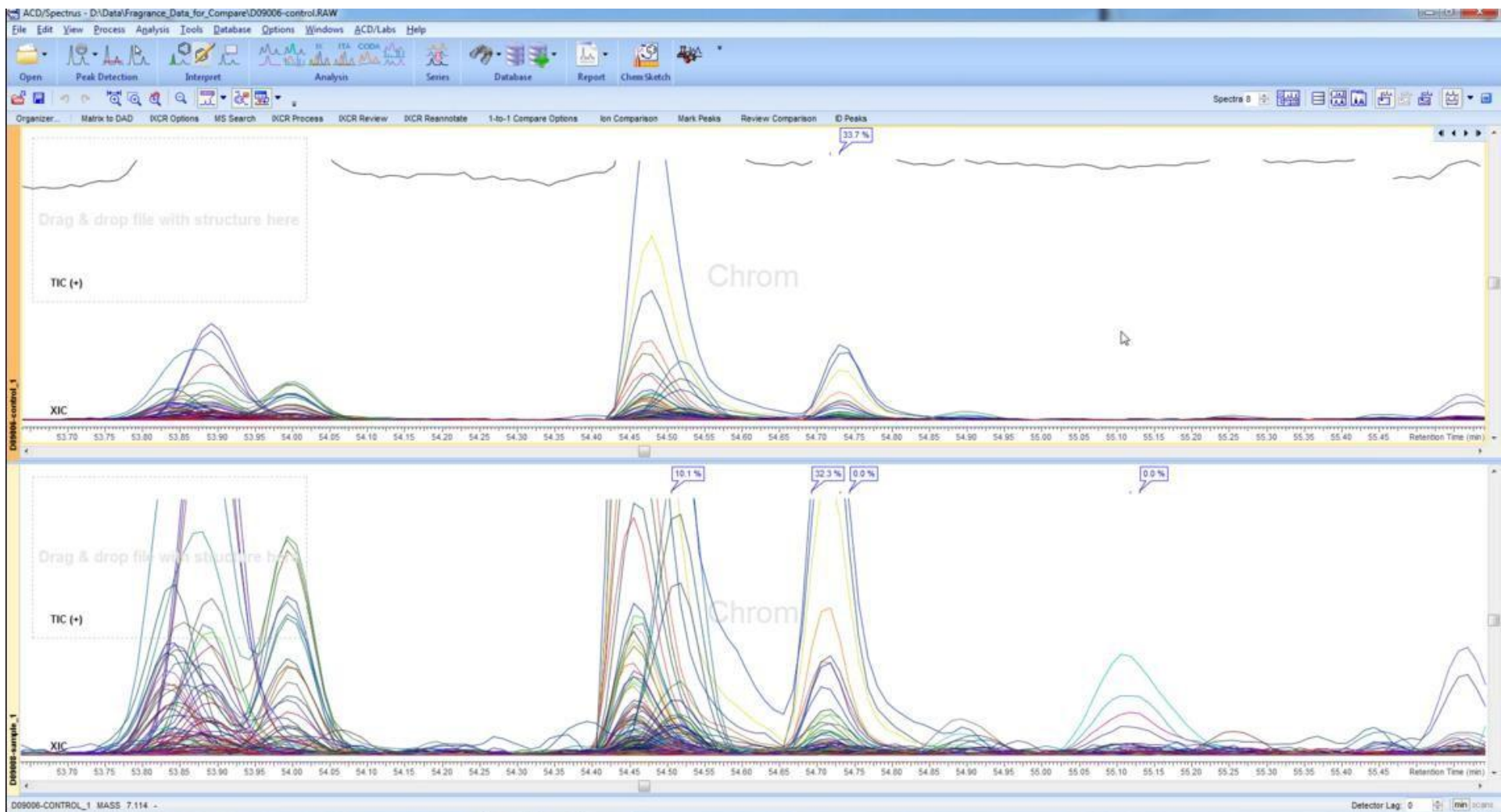


SVOCs in an Environmental sample



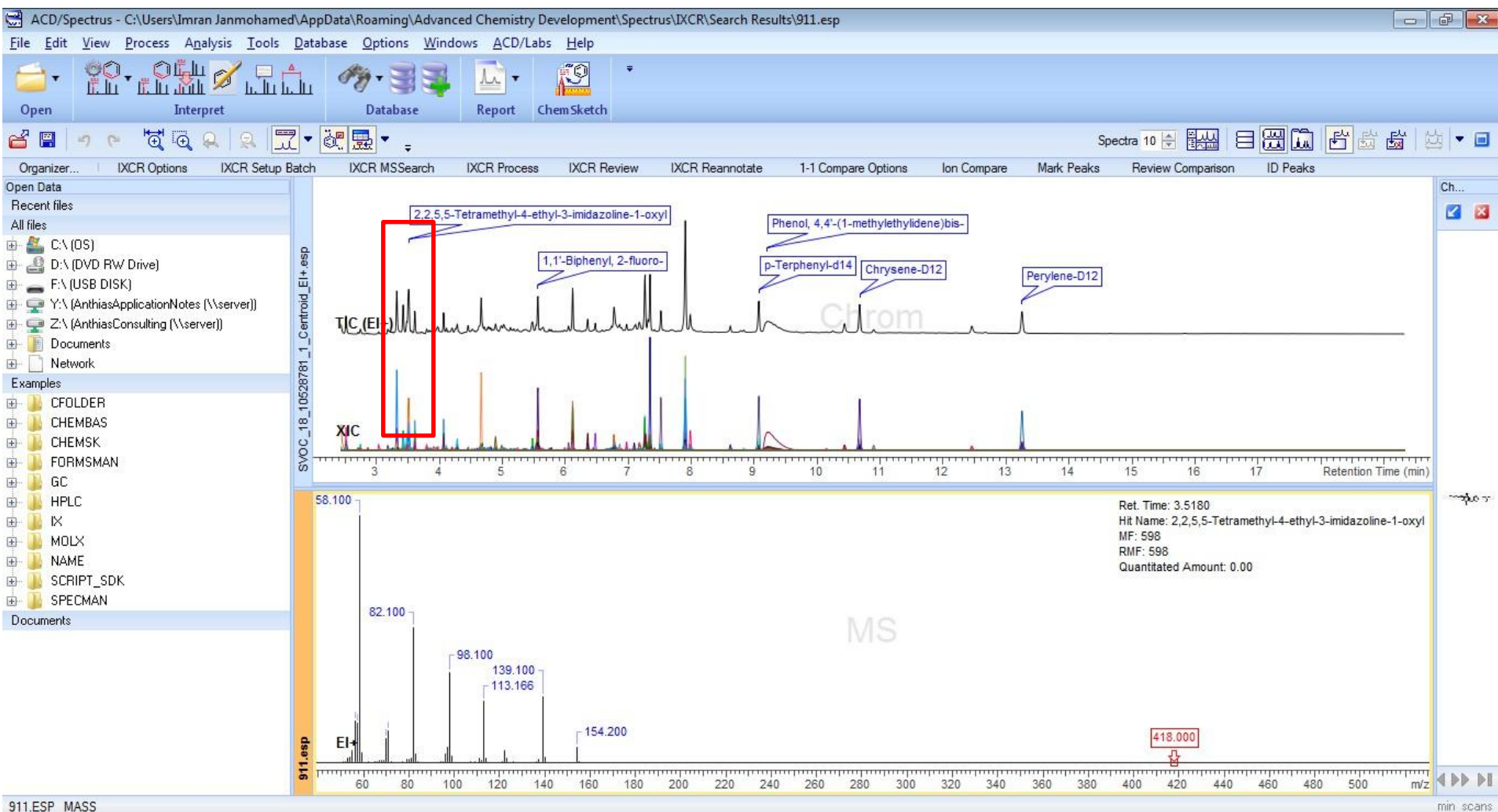
Courtesy of ACD/Labs

ACD/Spectrus Deconvolution



Courtesy of ACD/Labs

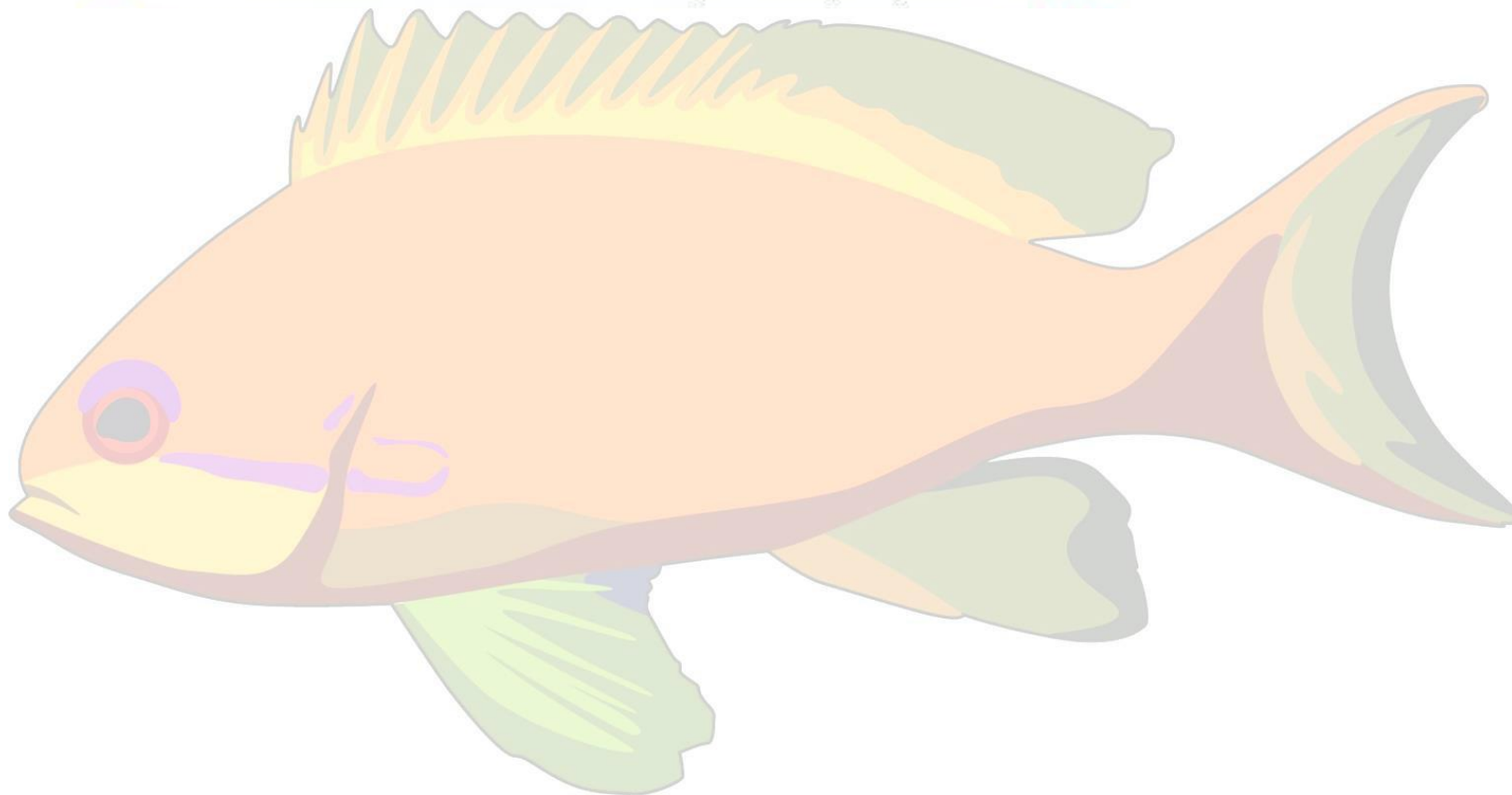
ACD/Spectrus Deconvolution



Courtesy of ACD/Labs

Deconvolution of co-eluting compounds

- Identification of 2-Chloroacetophenone (CAP)

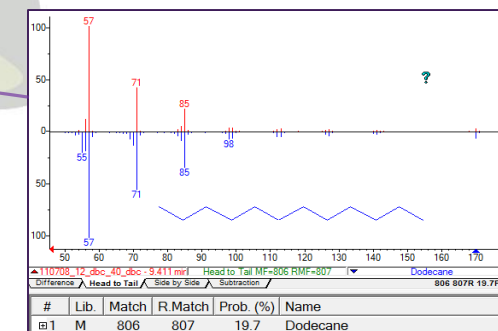
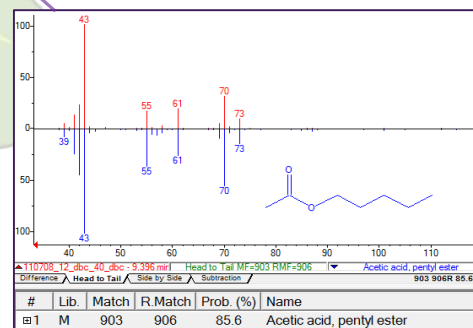
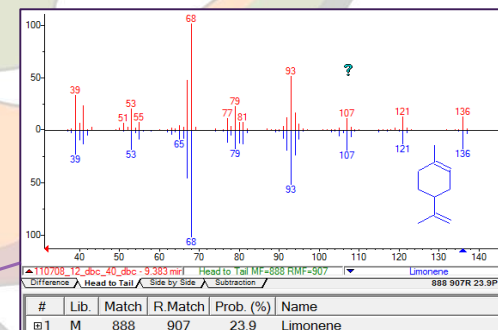
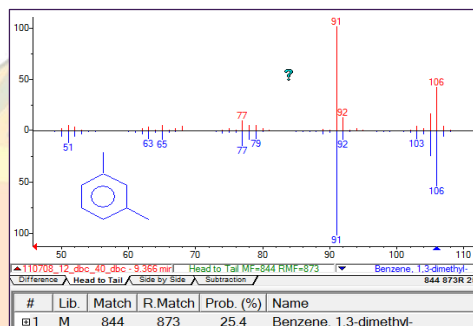
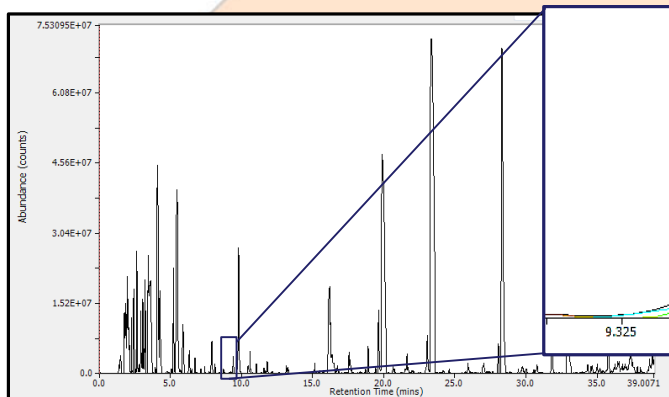


Diesel Oil containing trace CWA agent compounds

Courtesy of Markes International

Aroma profiling of Cheddar Cheese

Deconvolution of masked or co-eluting peaks

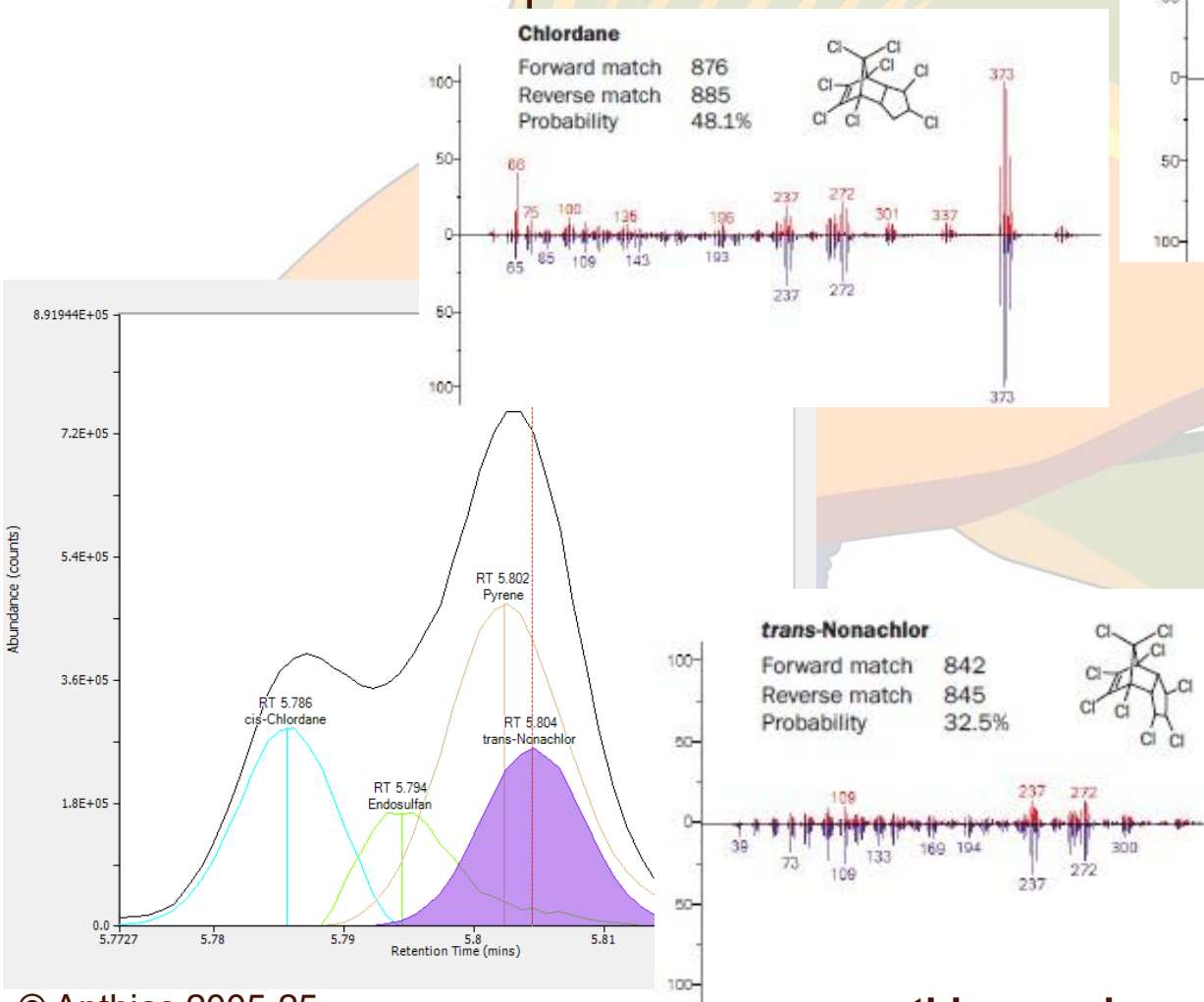


Courtesy of Markes International

TargetView deconvolution


Fast GCMS analysis of an EPA Pesticide
and PAH mixture

Deconvolution of four pollutants



Courtesy of Markes International

- Help to identify peaks you don't know are there!
- Can provide cleaned-up mass spectra that is difficult to get manually
- Can be used on full scan + SIM/MRM data
- After peak finding & deconvolution, can search libraries automatically & use retention time/index as qualifier
- Software dependent, need to optimise settings to pull out all useful peaks
 - Too many 'noise' peaks vs. missing peaks of interest
- Cannot be used identify isomers
 - Can use retention indices automatically
- Cannot deconvolute peaks of identical retention time & shape



Questions?
&
Thank you

