

Developing Better Solutions for GC and GC-MS

New Approaches to Data Handling:

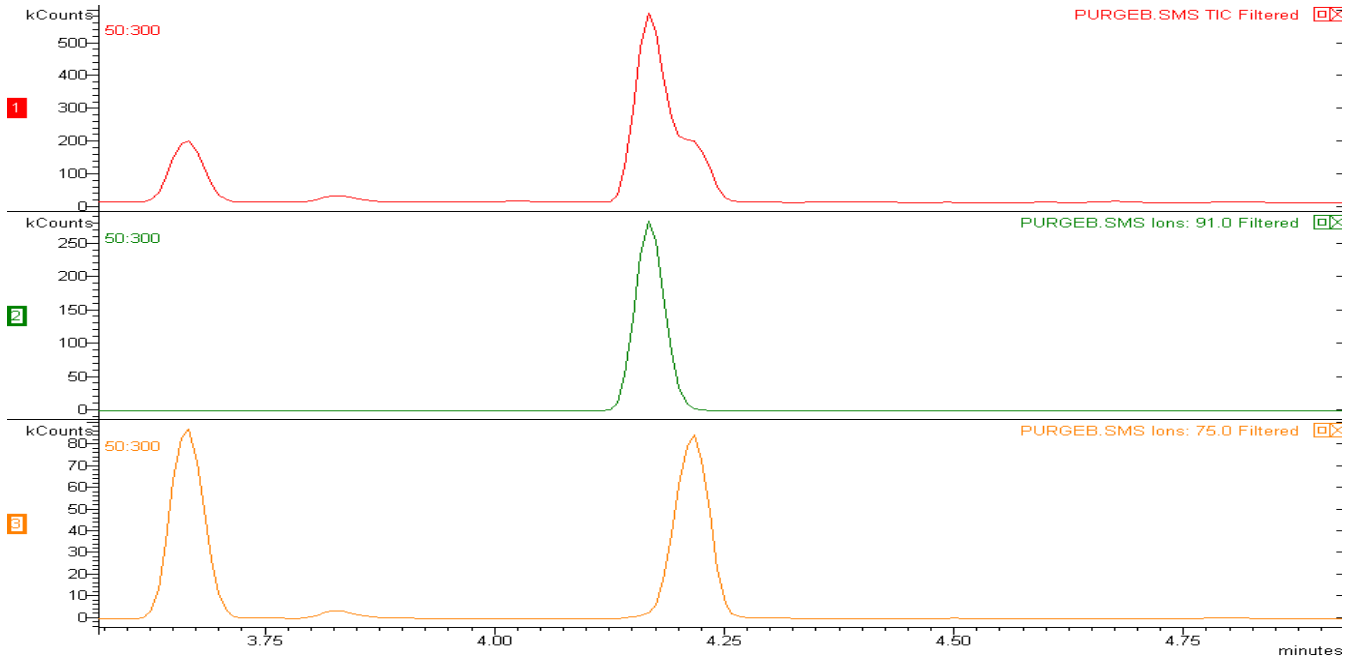
A “game changer” for qual and quant



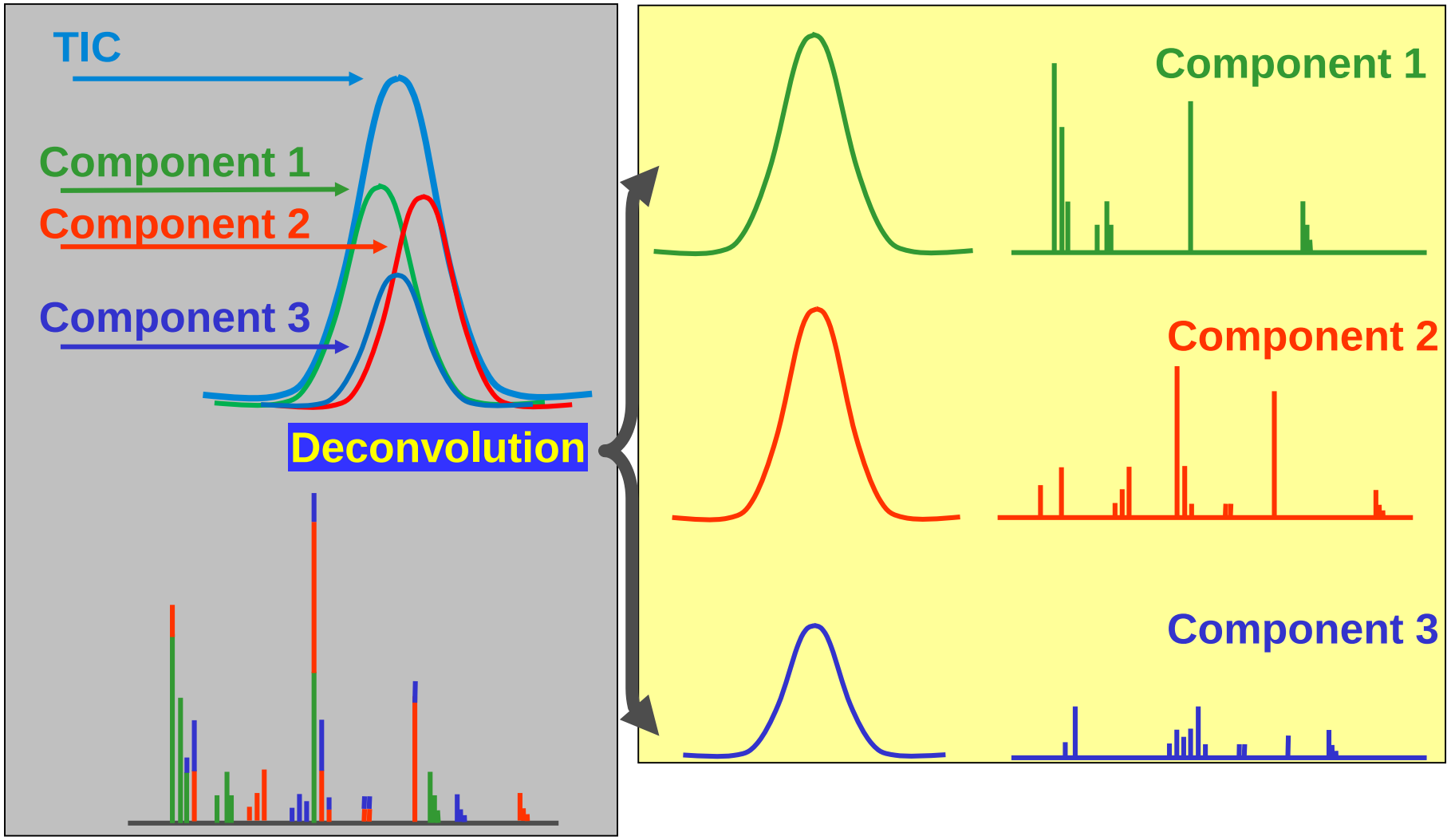
Deconvolution

Where the software “mines” the GC and MS data to separate chemical components or “entities”

Effectively mimicking what the analyst often attempts manually



Deconvolution



Deconvolution

Find a number of chemical components/entities

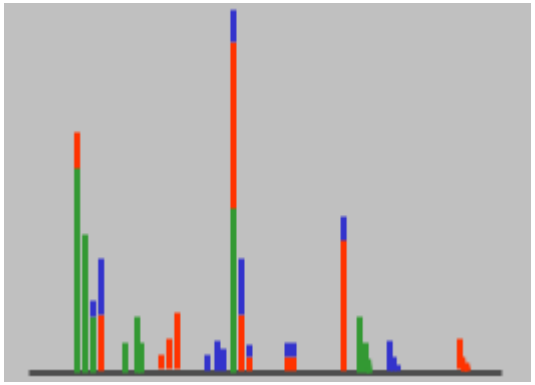
- Have control over the “sensitivity” of such a process
- Retain mass spectrometric information
- Possible ID by Library Search
- Possible Quantification
- Export the information for further interrogation

Deconvolution: ID by Library Search

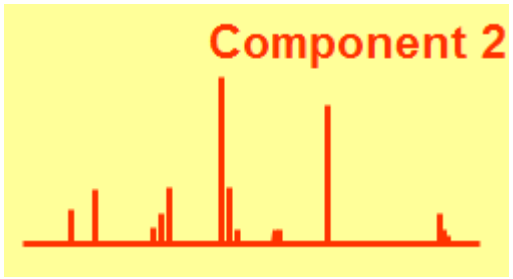
Deconvolution seen as the ultimate “background subtraction”

Clean spectra result in good ID

Not “user” skill dependant



Data



Deconvoluted Data

✓ Library ID

Improved Analysis

Deconvolution: Quantification

As analysts we have always seen the benefit of spectra being “corrected” prior to library searching

We think “How pure is our spectrum” Good data, good match.

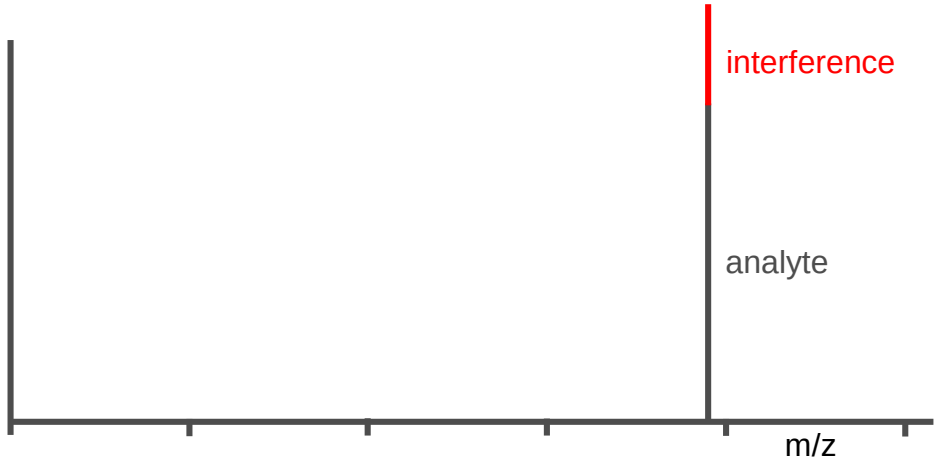
Traditionally, when we quantify on the Quan Ion, do we consider it’s purity?

Generally, no we don’t – we assume the response is solely from our analyte.

Deconvolution: Quantification

EI-SIM (Single Quad)

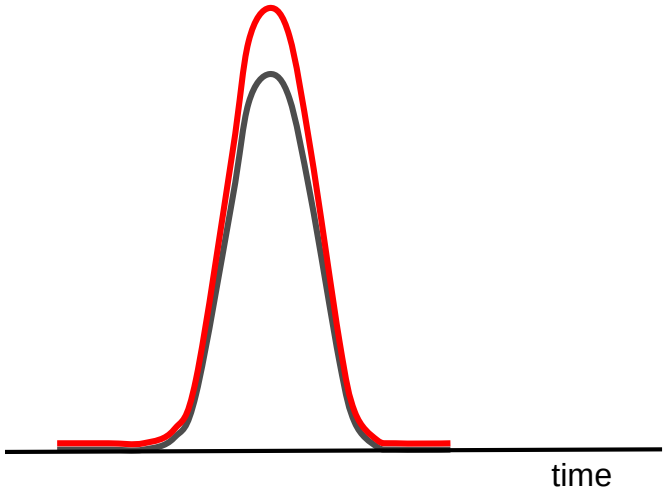
- selectivity proportional to spectral resolution
- no selectivity against ions with same m/z



MS signal visualization

for example EIC 284

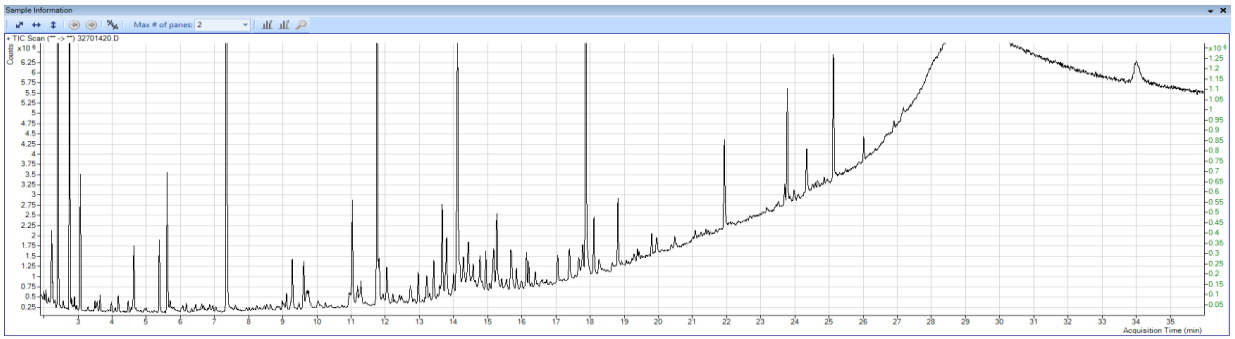
Matrix gives enhanced recovery



Poor accuracy, potential false positives

Deconvolution: MH Target Deconvolution

TIC



Targets are identified by comparison to locked RTs and 1 Quant + 3 Qualifier ion ratios, then quantified using Quant ion area versus calibration table

MH deconvolutes component spectra and performs spectral matching of deconvoluted spectra vs target MS database using RT Window and Library Match Score as qualifiers

All data processing performed within Mass Hunter Quant SW

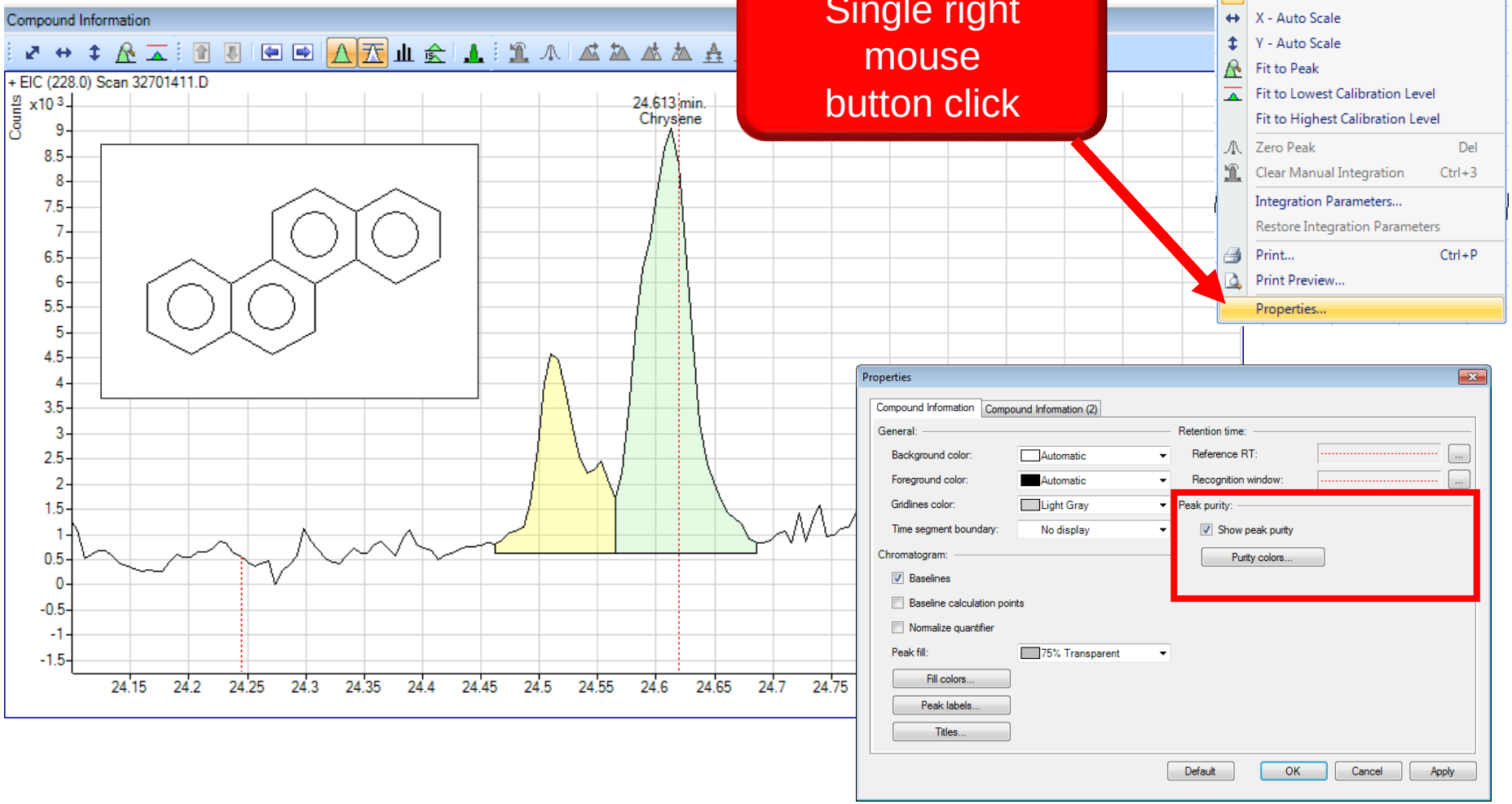
Quant Results

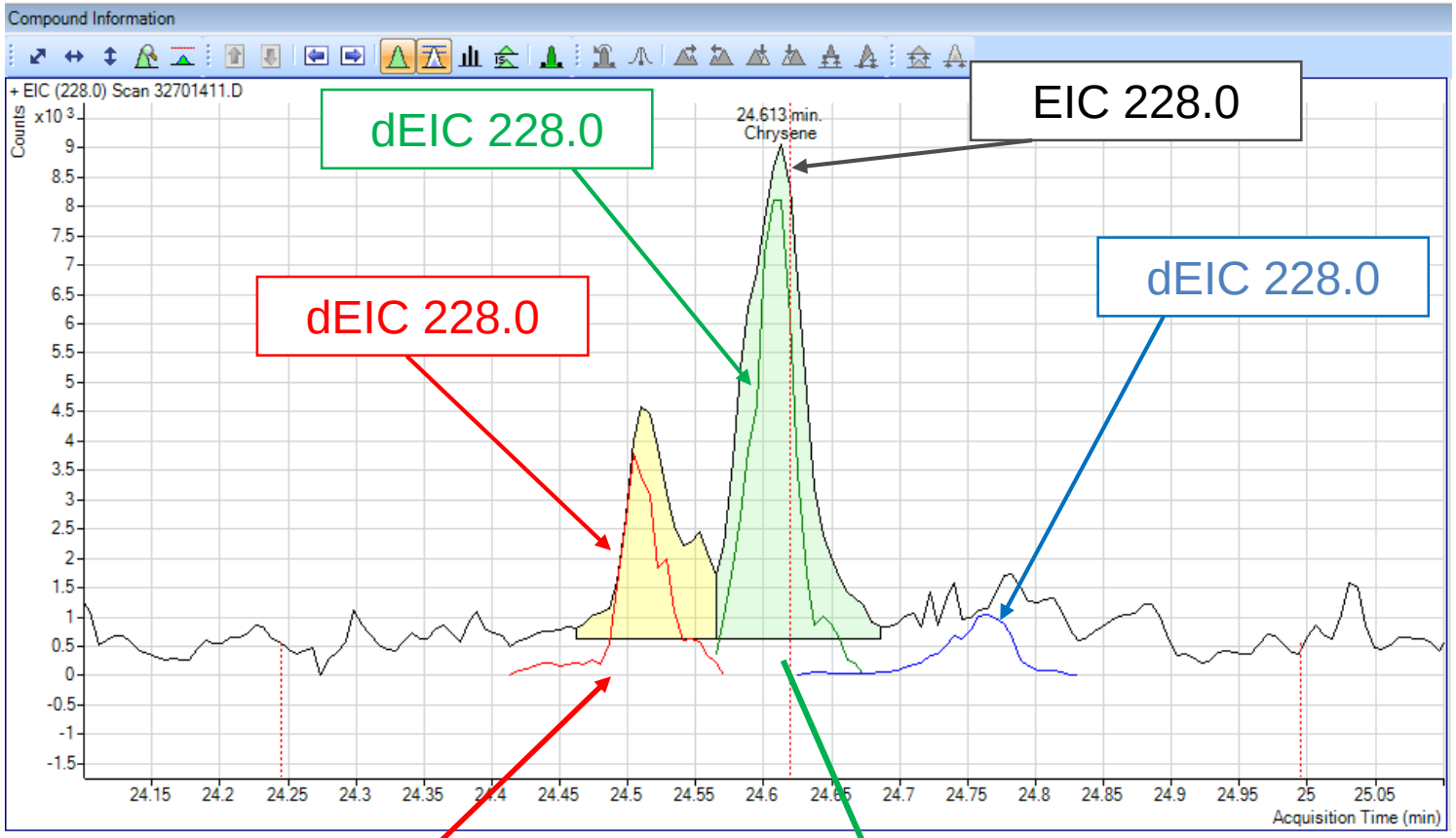
Qualitative Results

Review results in Mass Hunter Batch-at-a-Glance and Compounds-at-a-Glance

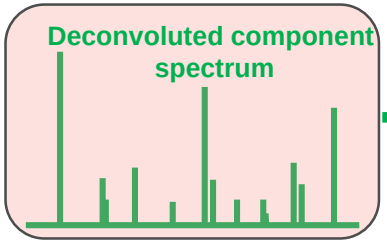
Combined quantitative and qualitative Target Deconvolution .pdf Summary report

TD : Chrysene in Water Extract example (Quant Ion EIC m/z 228.0)



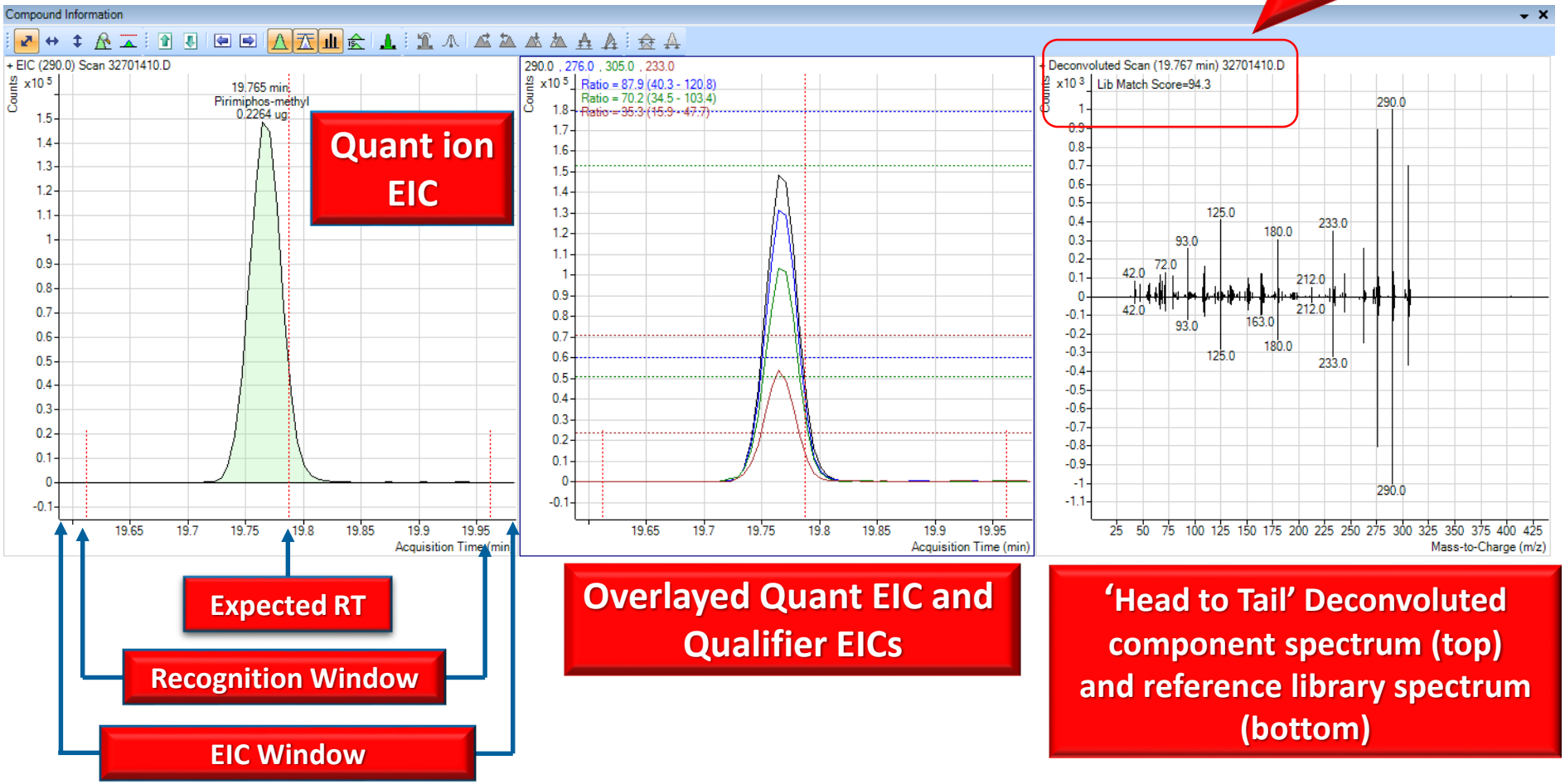


In the event of a component dEIC overlap, TD Quant result is corrected for interference (Purity)



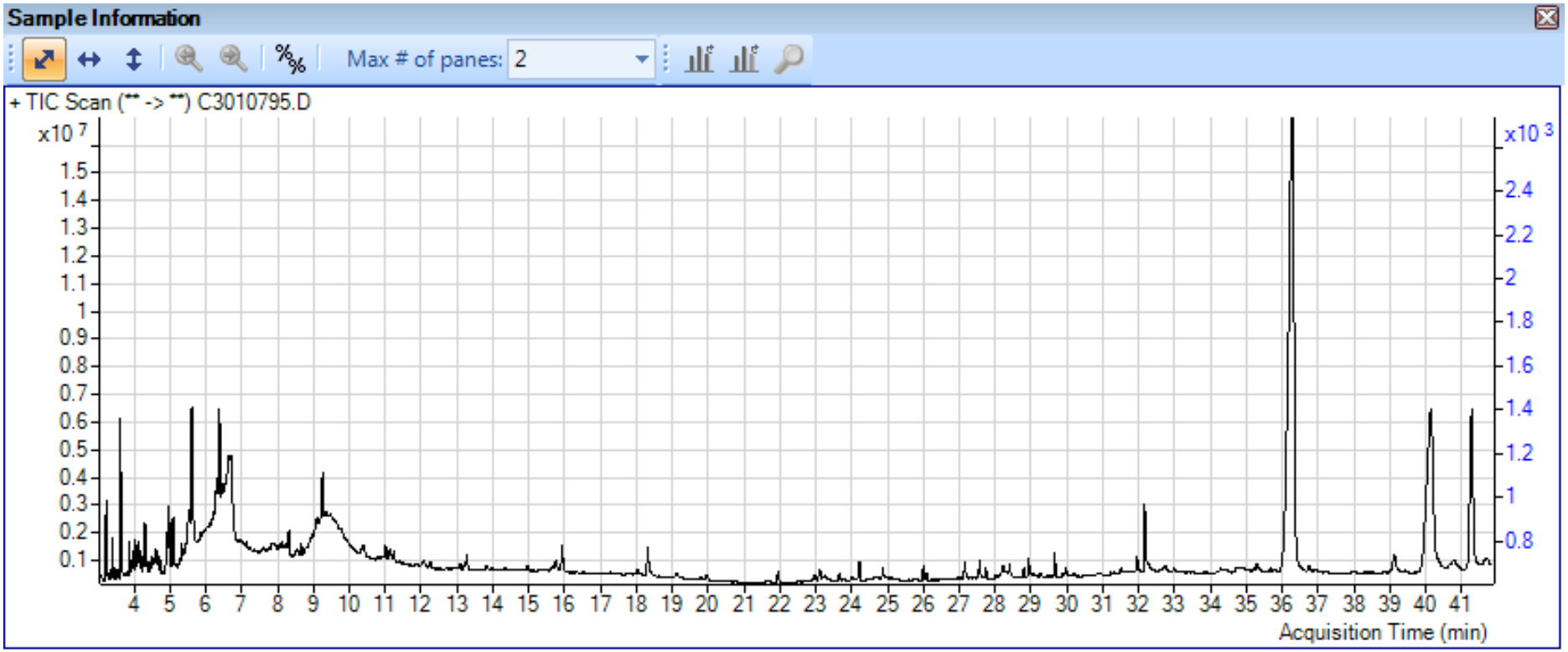
- Compared to entry in reference MS Library
- RT Difference calculated
- LMS calculated
- Purity calculated

Compound Information: Mass Hunter Quant Batch at a Glance with TD



Full scan TIC of Grape Extract

Analyzed using the Agilent RTL (1x) Pesticide Method and the RTLPEST3.L Pesticide library (converted to Mass Hunter .reflibrary.xml format)



Mass Hunter TD Report : Grape Extract

R.T.	Cas #	Compound Name	Amount/Conc	LMS	R.T. Diff(sec)	Purity

Targeted Deconvolution Report

Sample Name: 1ul Splitless injection
Data File: C3010795.D
Quant Batch Name: C:\Users\csandy\Desktop\LGC Grapes RTL 1x ESTD\GRAPES\QuantResults\TD_Grapes_II.batch.bin
Last Calib Update: 5/30/2013 9:51:58 AM

R.T.	Cas #	Compound Name	Amount/Conc	LMS	R.T. Diff(sec)	Purity
3.5255	108-95-2	Phenol	2.0961	82	-1.4	100.0
3.8376	541-73-1	1,3-Dichlorbenzene	0.0612	70	4.8	100.0
4.1955	95-48-7	2-Methylphenol	0.5341	82	-3.0	91.4
4.3698	106-44-5	4-Methylphenol	0.5170	78	-2.7	95.8
4.3698	108-39-4	m-Cresol	0.4263	76	-3.2	95.4
7.0678	92-52-4	Biphenyl	0.0640	68	-2.2	100.0
7.9672	85-41-6	Phthalimide	0.3002	76	-0.8	68.0
8.5637	33704-61-9	Cashmeran	0.9683	57	-3.4	100.0
8.7472	90-43-7	o-Phenylphenol	0.6008	84	-2.1	100.0
8.8757	100-02-7	4-Nitrophenol	0.4561	59	1.4	100.0
9.9586	84-66-2	Diethyl phthalate	0.5515	86	0.0	93.4
15.9327	84-69-5	Diisobutyl phthalate	25.7540	96	2.3	100.0
18.4105	84-74-2	Di-n-butylphthalate	4.0803	89	-0.3	100.0
19.1722	90-98-2	4,4'-Dichlorobenzophenone	0.5411	78	-1.7	96.8
20.1541	81-84-5	Naphthalic anhydride	0.0712	80	-1.8	100.0
21.6867	55219-65-3	Triadimenol	0.5555	69	1.1	100.0
21.9436	32809-16-8	Procymidone	4.4251	95	-1.1	99.7
24.6416	85509-19-9	Flusilazole	0.7549	76	2.9	100.0
25.9998	563-12-2	Ethion	3.5314	90	-0.1	100.0
28.4042	36734-19-7	Iprodione	1.8311	82	0.8	100.0
28.6244	18181-80-1	Bromopropylate	0.0595	63	0.5	100.0
28.7988	115-32-2	p,p'-Dicofol	2.1221	87	0.1	100.0
29.3310	84-61-7	Dicyclohexyl phthalate	0.3242	57	2.5	100.0
29.6614	117-81-7	Bis(2-ethylhexyl)phthalate	9.9592	96	0.8	100.0
30.6892	13457-18-6	Pyrazophos	0.4960	72	-1.8	100.0