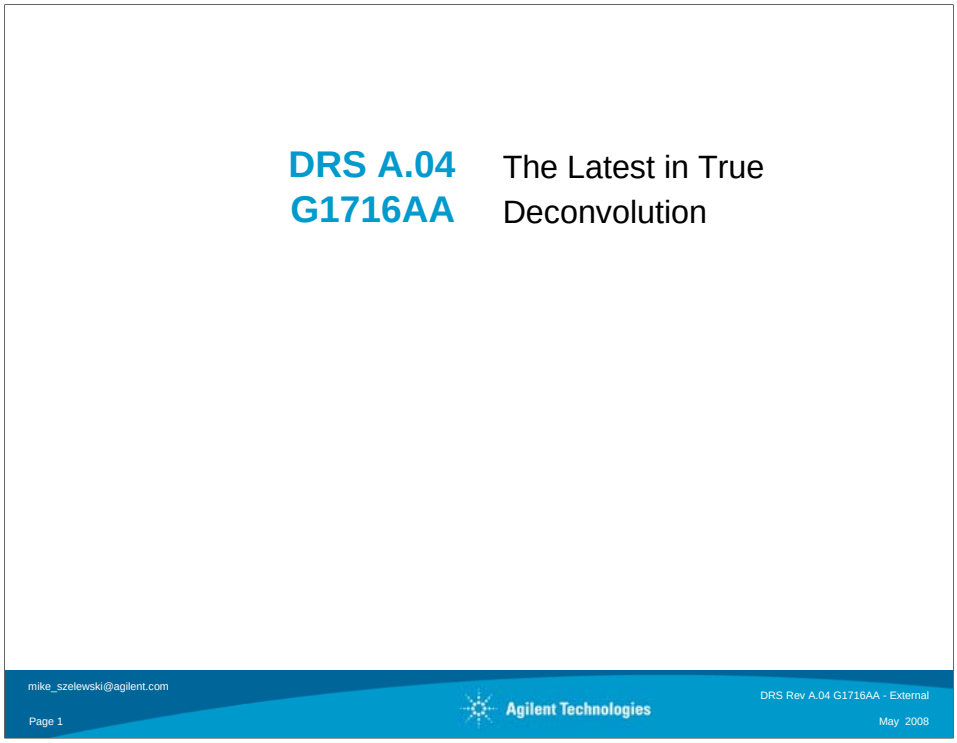


Since the introduction of Deconvolution Reporting Software in 2004, thousands of analysts have taken advantage of its ability to save time in data reduction. This presentation will provide a review of DRS and show the features and benefits of the latest revision, DRS A.04, introduced in 2008.

DRS is Based on Industry Standard AMDIS

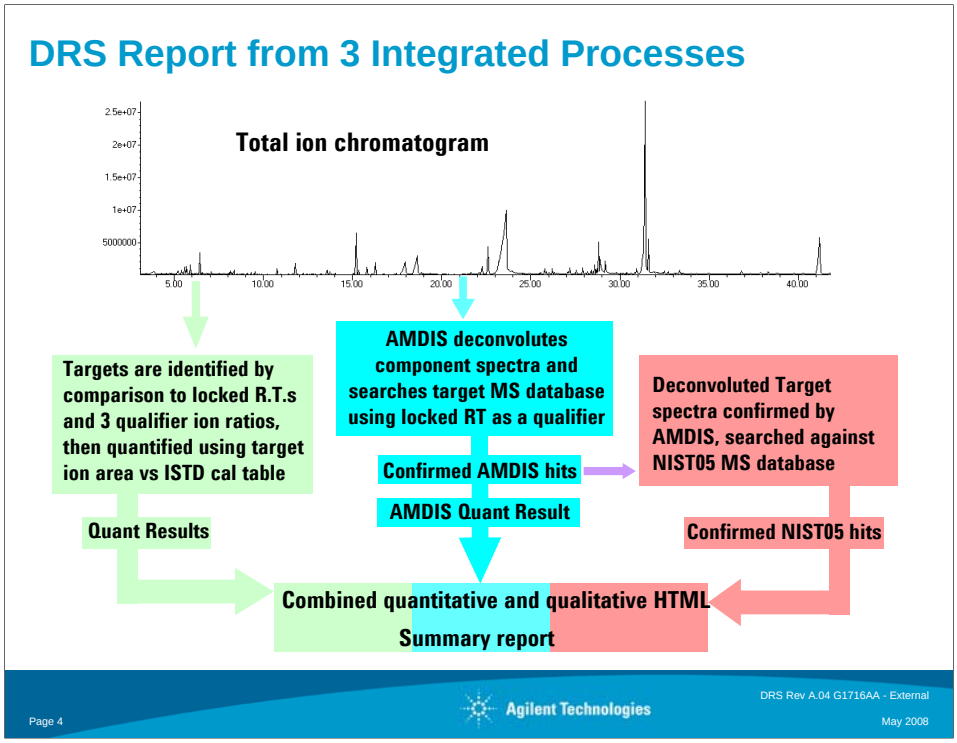
- **Automatic Mass spectral Deconvolution and Identification Software**
  - **Developed to automatically detect chemicals in violation of Chemical Weapons Convention**
  - **Identify compounds at low concentration levels in complex matrices**
  - **Developed by National Institute of Standards and Technology**
  - **Retention Time can be used as a qualifier, so RTL is a big advantage**

DRS uses industry standard AMDIS as its deconvolution engine. Developed by NIST, AMDIS is specifically designed to find compounds at low levels in dirty matrices. AMDIS is retention time independent so compounds can be found anywhere in the chromatogram. Compounds identified by AMDIS can be further filtered by retention time or retention index, therefore Retention Time Locking is an advantage.

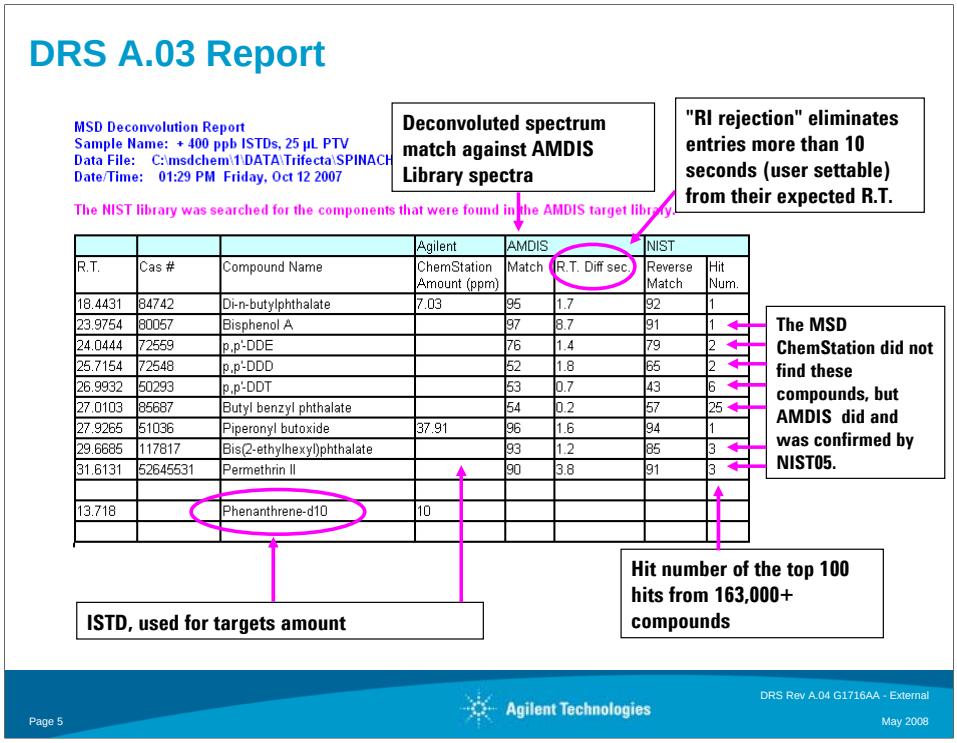
True Deconvolution using AMDIS

- **Automatic Mass spectral Deconvolution and Identification Software**
  - **All spectra are deconvoluted, not just those selected by the user**
  - **Identification is based on full spectral matching**
    - **User does not have to "pick" ions**
    - **More confidence in result using all ions**
  - **Published algorithims, not proprietary**
  - **Accepted for world-wide use**

AMDIS does true deconvolution. All spectra are deskewed then separated from each other and from background. This is different from other software packages that only separate compounds specified by the user. The full deconvoluted "clean" spectrum is used for library matching, resulting in high confidence in the results. This identification is not based on the user having to preselect a few ions. Deconvoluted spectra can also be used to build new libraries or they can be added to existing user libraries. Government labs throughout the world use AMDIS to detect trace chemical weapons.



DRS integrates 3 processes. The first level of identification and quantitation is based on target and qualifier ion ratios, combined with locked retention times. The next identification is based on comparing the "clean" full AMDIS spectrum to a user library. Deconvoluted ions are also available for quantitation. The third confirmation of a compound's identity is based on searching the 163,000+ NIST library, using the AMDIS deconvoluted spectrum. Results from each of these three processes are combined in an easy to read report.



The easy to read DRS report shows retention time, CAS# and name. A quantitative amount based on user calibration comes from the standard MSD Chemstation calculations. DRS A.04 provides additional quantitation capabilities that will be seen later. Match factors based on "clean" spectra and retention time differences from expected are provided by AMDIS. The NIST search results include match factors and position of the found compound in the top 100 NIST hits.

DRS A.04 based on these Customer Requests

- Bring AMDIS information into MSD QEdit
- Provide optional quantitation on AMDIS data
- Keep look, feel and functionality of QEdit
- Display full raw, deconvoluted, and library spectra without accessing AMDIS
- Provide graphics output of AMDIS and MSD data
- Provide MSD and AMDIS amounts in both quant and DRS reports
- Make AMDIS Library building easier
- Provide an easy way to update RTs in AMDIS

DRS has been enhanced based on inputs from chemists worldwide that have experience using earlier DRS revisions, the MSD Chemstation and AMDIS. QEdit is the data review process in the MSD Chemstation. Users requested that all information from AMDIS deconvolution be presented and used in the familiar QEdit environment.

DRS A.04 Features 1 of 2

Import AMDIS information – manually in QEdit or automatically upon entering QEdit

Display AMDIS deconvoluted and library spectra along with the associated MSD raw spectrum

Display AMDIS extracted ion profile overlayed with MSD target ion & qualifiers

Display AMDIS extracted ion profile for integration in a separate window, while the MSD target ion is displayed in its own window

Manually integrate, independently, either the MSD Target ion or the AMDIS ion

As a result of the user recommendations, DRS A.04 incorporates a long list of enhanced features. These are used for rapid data review and a second level of quantitation based on deconvoluted Extracted Ion Currents from AMDIS.

DRS A.04 Features 2 of 2

Distinct indicators in the QQEdit list for each type of data: “x” if found by the MSD and “A” if found by AMDIS

Calibration can be updated using AMDIS results from a standard after updating with MSD results

Uses the current Method quant Integrator

Works using height or area data

Response and Amount for MSD and AMDIS displayed side-by-side, and independently updated with man-int

This is a continued list of DRS A.04 features that increase productivity in data review. Users do not have to learn a new quantitation package and can work in the familiar QEdit view.

DRS A.04 Features – Reporting Results

Simple Text Report: displayed in QEdit to show MSD and AMDIS matching results

Graphics Report: one page/compound showing MSD Target ion and Qualifiers, AMDIS ion Profile, all 3 spectra, and both sets of quant results

Summary Quant report: from Data Analysis View reports AMDIS compounds and amounts after MSD results

DRS A.04 Report: Both sets of Quantitative Results are displayed along with AMDIS settings in the header

In addition to the extensive list of new and enhanced features, DRS A.04 allows reporting of results in four different formats.

DRS A.04 Report before importing AMDIS results

MSD Deconvolution Report
Sample Name: + 400 ppb ISTDs, 25 µL PTV
Data File: C:\msdchem\1\DATA\Trifecta\SPINACH.D
Date/Time: 07:33 AM Thursday, Apr 10 2008

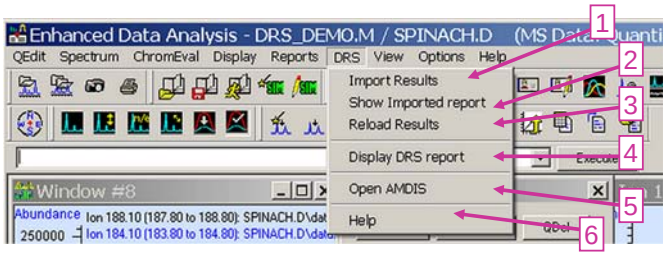
Adjacent Peak Subtraction = 1
Resolution = High
Sensitivity = High
Shape Requirements = Medium

The NIST library was searched for the components that were found in the AMDIS target library.

			Amount (ppm)		AMDIS		NIST	
R.T.	Cas #	Compound Name	Chem station	AMDIS	Match	R.T. Diff sec.	Reverse Match	Hit Num.
18.4431	84742	Di-n-butylphthalate	7.18		95	1.7	92	1
23.9754	80057	Bisphenol A			97	8.7	91	1
24.0647	72559	p,p'-DDE			66	2.6	60	2
25.7154	72548	p,p'-DDD			52	1.8	65	2
26.9932	50293	p,p'-DDT			53	0.7	43	6
27.0103	85687	Butyl benzyl phthalate			54	0.2	57	25
27.9265	51036	Piperonyl butoxide	37.8		96	1.6	94	1
29.6648	117817	Bis(2-ethylhexyl)phthalate			94	1.0	86	3
31.6131	52645531	Permethrin II			90	3.8	91	3
13.718		Phenanthrene-d10	10					

This is the new DRS A.04 report, before importing AMDIS results. It is similar to the A.03 report and includes a separate column for reporting quantitative results based on AMDIS. The key AMDIS deconvolution settings are now shown on the right side of the header.

DRS A.04 QEdit Menu Items



1- Import spectra and extracted ion from AMDIS

2- Displays Text Report with MSD and AMDIS Results

3- Reloads existing results from AMDIS results file

4- Displays DRS report with updated amounts

5- Opens AMDIS standalone

6- Link to DRS Help

The QEdit view now has a separate menu item for DRS. All commonly used operations involving AMDIS results are available in this pull-down.

DRS A.04 Report after importing AMDIS results,
before review and manual integration

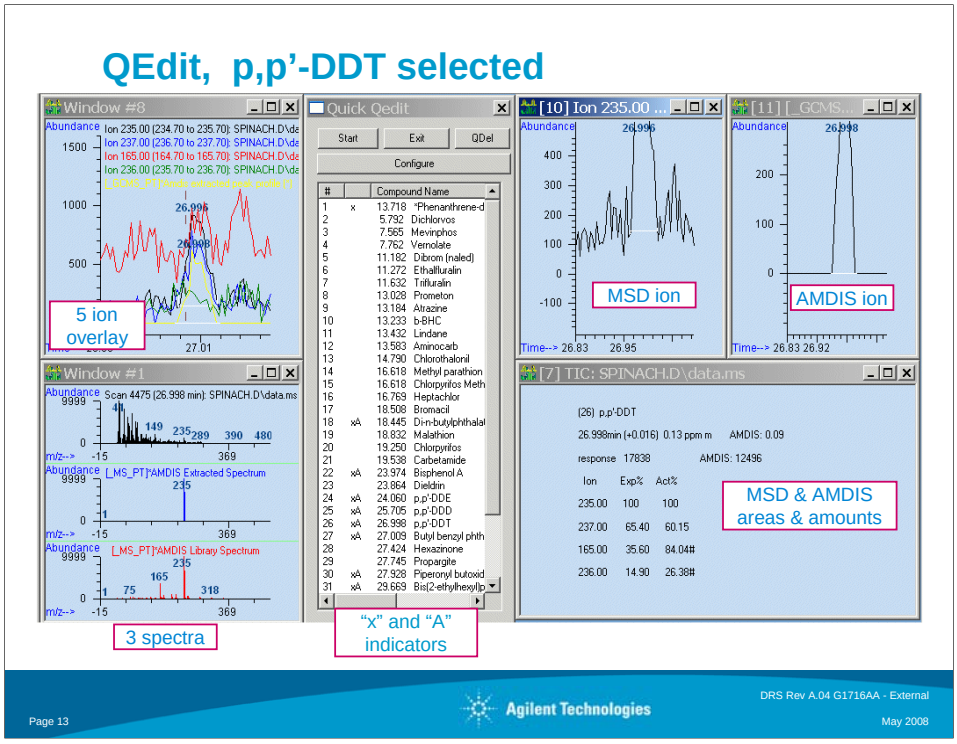
MSD Deconvolution Report
Sample Name: + 400 ppb ISTDs, 25 pL PTV
Data File: C:\msdchem\1\DATA\Trifecta\SPINACH.D
Date/Time: 07:37 AM Thursday, Apr 10 2008

Adjacent Peak Subtraction = 1
Resolution = High
Sensitivity = High
Shape Requirements = Medium

The NIST library was searched for the components that were found in the AMDIS target library.

			Amount (ppm)		AMDIS		NIST	
R.T.	Cas #	Compound Name	Chem station	AMDIS	Match	R.T. Diff sec.	Reverse Match	Hit Num.
18.4431	84742	Di-n-butylphthalate	7.18	6.25	95	1.7	92	1
23.975	80057	Bisphenol A		12.74	97	8.7	91	1
24.0647	72559	p,p'-DDE		0.19	66	2.6	60	2
25.715	72548	p,p'-DDD		0.13	52	1.8	65	2
26.993	50293	p,p'-DDT		0.09	53	0.7	43	6
27.010	85687	Butyl benzyl phthalate		0.16	54	0.2	57	25
27.9265	51036	Piperonyl butoxide	37.8	33.12	96	1.6	94	1
29.6648	117817	Bis(2-ethylhexyl)phthalate		2.74	94	1.0	86	3
31.613	52645531	Permethrin II		201.65	90	3.8	91	3
13.718		Phenanthrene-d10	10					

After importing AMDIS results the DRS report can be re-displayed. The nine compounds found by AMDIS have quantitative amounts, based on the deconvoluted target ion. Automatic integration of the clean target ion is easily accomplished without the typical chemical noise of a dirty matrix.



This is the QEdit view, with p,p'-DDT selected. Data review time is significantly reduced with AMDIS information integrated into QEdit.

5 ion overlay - MSD target ion, 3 qualifier ions and target ion from AMDIS (yellow). Verify RTs

3 spectra – raw "dirty" spectrum, AMDIS "clean" deconvoluted spectrum, and AMDIS library spectrum displayed. Visually verify library match.

MSD target ion used for quantitation - can be manually integrated.

AMDIS deconvolved target ion - can be manually integrated.

MSD & AMDIS areas & amounts – displays integrated area (or height) and calculated amounts for MSD and AMDIS target ions. Individually updated with manual integrations.

"x" and "A" – target compound list or QQEdit list. "x" indicates MSD target found (or manually integrated) and "A" indicates compound found by DRS-AMDIS.

DRS A.04 Report after importing AMDIS results,

QEdit reviewed with manual integrations

MSD Deconvolution Report
Sample Name: + 400 ppb ISTDs, 25 µL PTV
Data File: C:\msdchem\1\DATA\Trifecta\SPINACH.D
Date/Time: 07:41 AM Thursday, Apr 10 2008

Adjacent Peak Subtraction = 1
Resolution = High
Sensitivity = High
Shape Requirements = Medium

The NIST library was searched for the components that were found in the AMDIS target library.

			Amount (ppm)		AMDIS		NIST	
R.T.	Cas #	Compound Name	Chem station	AMDIS	Match	R.T. Diff sec.	Reverse Match	Hit Num.
18.4431	84742	Di-n-butylphthalate	7.18	6.25	95	1.7	92	1
23.974	80057	Bisphenol A	15.39	12.74	97	8.7	91	1
24.060	72559	p,p'-DDE	0.58	0.19	66	2.6	60	2
25.705	72548	p,p'-DDD	0.16	0.13	52	1.8	65	2
26.9932	50293	p,p'-DDT	0.13	0.09	53	0.7	43	6
27.009	85687	Butyl benzyl phthalate	0.26	0.16	54	0.2	57	25
27.9265	51036	Piperonyl butoxide	37.8	33.12	96	1.6	94	1
29.6648	117817	Bis(2-ethylhexyl)phthalate	3.12	2.74	94	1.0	86	3
31.6131	52645531	Permethrin II	213.63	201.65	90	3.8	91	3
13.718		Phenanthrene-d10	10					

The DRS report after QEdit review and manual integrations. In addition to the identified targets, AMDIS has deconvoluted all spectra. These unknown spectra can be library searched against NIST from AMDIS.

Text report comparing MSD and AMDIS RTs and amounts available in QEdit

Compound	R.T.	AMDIS R.T.	Delta	Conc.	AMDIS Conc.	Units
18) Di-n-butylphthalate	18.445	18.443	0.002	7.18	6.25	ppm
22) Bisphenol A	23.974	23.975	-0.001	15.39	12.74	ppm
24) p,p'-DDE	24.060	24.065	-0.005	0.58	0.19	ppm
25) p,p'-DDD	25.705	25.715	-0.010	0.16	0.13	ppm
26) p,p'-DDT	26.998	26.993	0.005	0.13	0.09	ppm
27) Butyl benzyl phthalate	27.009	27.010	-0.002	0.26	0.16	ppm
30) Piperonyl butoxide	27.928	27.927	0.001	37.80	33.12	ppm
31) Bis(2-ethylhexyl)phthalate	29.669	29.665	0.004	3.12	2.74	ppm
34) Permethrin II	31.614	31.613	0.001	213.63	201.65	ppm

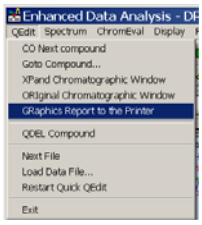
This is a simple text report that is available. Retention time of compounds are shown for both the MSD Chemstation and for AMDIS, along with the difference. Quantitative amounts are also displayed for both.

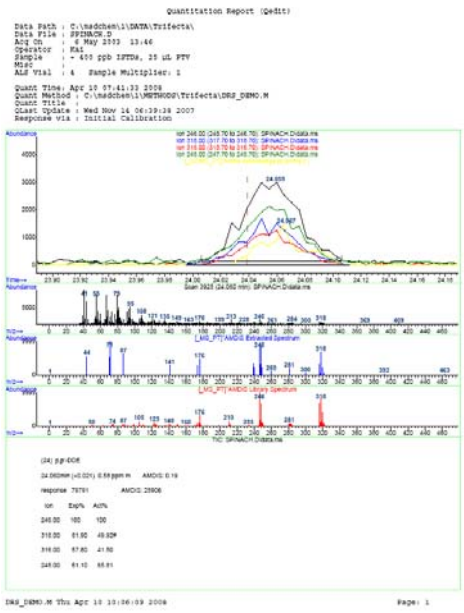
Graphics Report

MSD and AMDIS 5-ion overlay

Raw, deconvoluted and library spectra

MSD and AMDIS areas and amounts





This is a full graphics report from QEdit, one page for each compound. The MSD Chemstation target and 3 qualifier ions are overlaid with the AMDIS deconvoluted target ion. The raw Chemstation spectrum is reported together with the full deconvoluted "clean" spectrum and AMDIS library spectrum. At the bottom of the page are listed the responses and quantitative amounts.

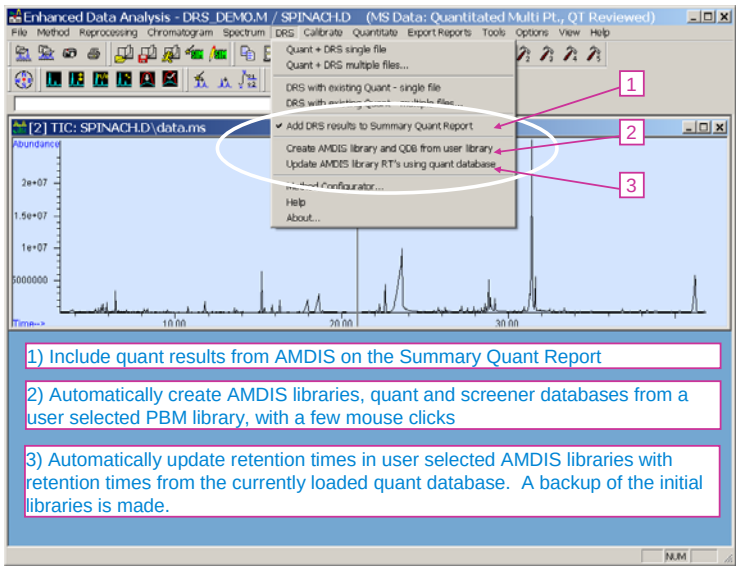
Summary Quant Report optionally includes both MSD Chemstation and AMDIS amounts

Compound	R.T.	QIon	Response	Conc	Units
Internal Standards					
1) Phenanthrene-d10	13.718	188	4953294	10.00	ppm
Target Compounds					
18) Di-n-butylphthalate	18.445	149	989364m	7.18	ppm
22) Bisphenol A	23.974	213	2119577m	15.39	ppm
24) p,p'-DDE	24.060	246	79791m	0.58	ppm
25) p,p'-DDD	25.705	235	21489m	0.16	ppm
26) p,p'-DDT	26.998	235	17838m	0.13	ppm
27) Butyl benzyl phthalate	27.009	149	35766m	0.26	ppm
30) Piperonyl butoxide	27.928	176	5208006m	37.80	ppm
31) Bis(2-ethylhexyl)phtha...	29.669	149	429941m	3.12	ppm
34) Permethrin II	31.614	183	29430854m	213.63	ppm
AMDIS Imported Quantitation Results					
18) Di-n-butylphthalate	18.443	149	861673	6.25	ppm
22) Bisphenol A	23.975	213	1754970	12.74	ppm
24) p,p'-DDE	24.065	246	25906	0.19	ppm
25) p,p'-DDD	25.715	235	17508	0.13	ppm
26) p,p'-DDT	26.993	235	12496	0.09	ppm
27) Butyl benzyl phthalate	27.010	149	21499	0.16	ppm
30) Piperonyl butoxide	27.927	176	4563220	33.12	ppm
31) Bis(2-ethylhexyl)phtha...	29.665	149	377661	2.74	ppm
34) Permethrin II	31.613	183	27779700	201.65	ppm

partial report

This is the fourth report type that is available, a Summary Quant Report. The DRS results are optionally added based on the checkbox shown on the next slide, choice (1).

Enhanced Data Analysis DRS Menu: New A.04 Items



In addition to the features and productivity enhancements already discussed two more important tools are new to DRS A.04. Choice 2 provides rapid AMDIS database creation from an existing user library. Choice 3 updates AMDIS RTs with those found in the current MSD Chemstation quant database.

DRS A.04 – Summary

AMDIS used for deconvolution – the industry standard

Build an AMDIS library from a user library with a few mouse clicks and save time

Use QEdit for data reduction – no need to learn new software

Quantitate on both MSD and AMDIS data – compare results for large differences

Display raw, deconvoluted, and library full spectra without accessing AMDIS – easy to review

Identify compounds on full spectra – more confidence in correct identification than using a few ions

Choose from 4 different reports – no customizing needed

DRS A.04 is an evolution, built on the recommendations of worldwide users. DRS A.04 provides a second level of quantitation, that based on AMDIS deconvoluted data. Productivity gains can be realized using this fully integrated software package.