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Agilent Technologies

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Varian MS Workstation
Version 6

Quick Start for QuickEP

QUALITY SYSTEM
ISO 9001
CERTIFIED

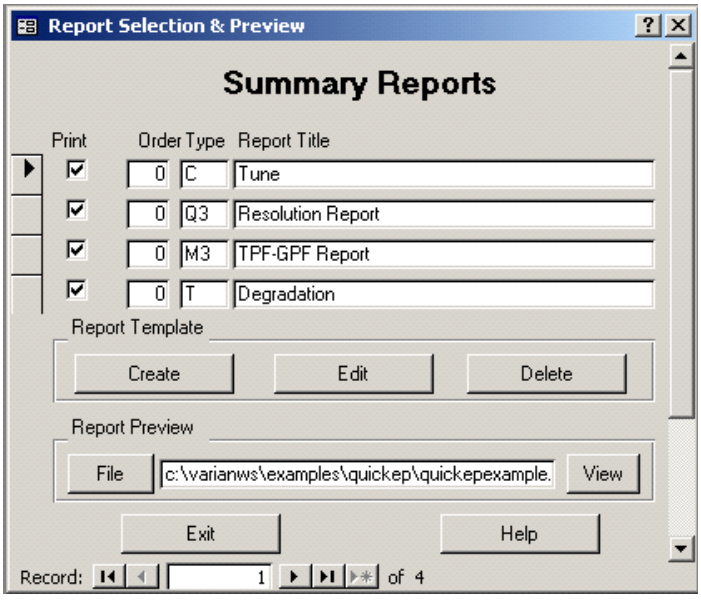
Printed in U.S.A. 03-914987-00:Rev. 1

Quick Start for QuickEP

Purpose

QuickEP is a custom report template used to compute and report system suitability indicators from Varian Workstation data files. The following types of reports may be generated:

1. Resolution between selected target compound peak pairs.
2. Degradation estimates for selected target compounds, where the degradation products are also quantitated as target compounds.
3. Tailing Peak and Gaussian Peak Factors for selected target compounds (TPF-GPF Report).
4. Tune reports for BFB (bromofluorobenzene) or DFTPP (decafluorotriphenylphosphine) based on EPA method 524, 624, CLPVOL, 8240, or 8260 criteria for BFB or method 525,625, CLPSEM, 8250, or 8270 for DFTPP.



Suitability Report Setup Main Page

Usage Notes

1. Acquire and process through data handling the data files to be reported, using a method set up to integrate the target compounds of interest.
2. Create a working QuickEP template using the Custom Reports Star Toolbar button, basing it on QuickEP.mdb.
3. Load the file prepared in Step 1 into the template created in Step 2 by clicking the File button on the template.
4. Select the type of report to be generated by clicking the selector to the left of the report name, and follow the report specific instructions below.

Tutorial

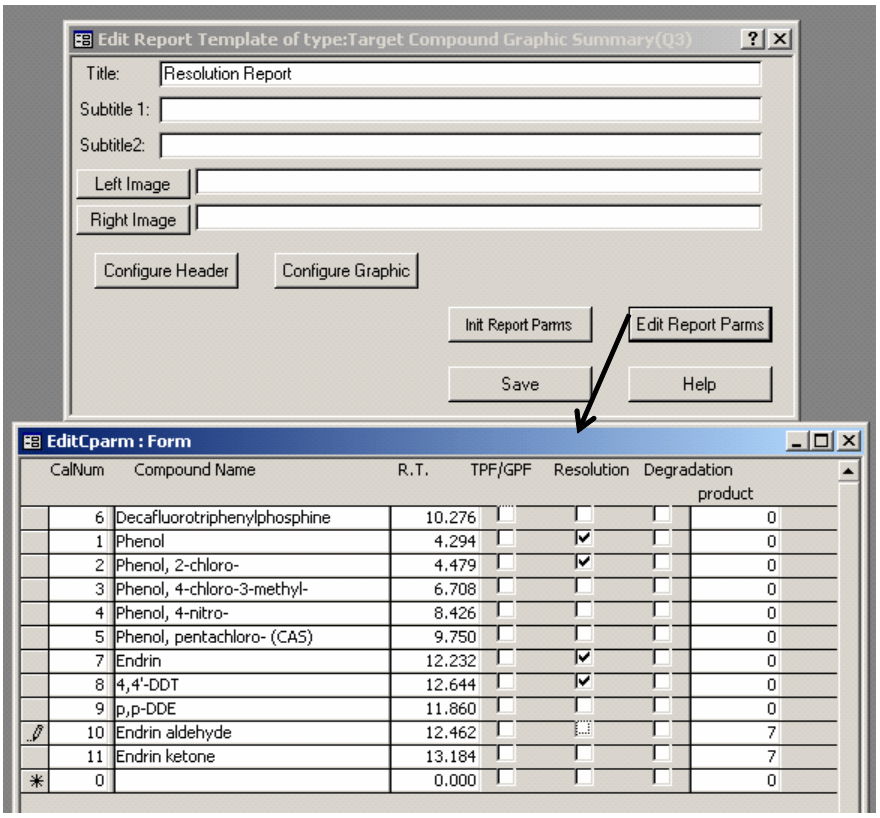
An example data file, QuickEPexample.sms is included in the Varian WS\Examples\QuickEP directory. This file will allow creating the different reports of the software. For the tune report, select the DFTTP as the tune compound, and Method 525 as the tune criteria. (You may also choose from the same directory the BFBTune.sms file to evaluate the VOC tune criteria.)

The different reports allow the configuration of Header, Footer, graphic and or text reports. These specifications will allow creating the report in the format desired. Follow on line help on the set up of these formats.

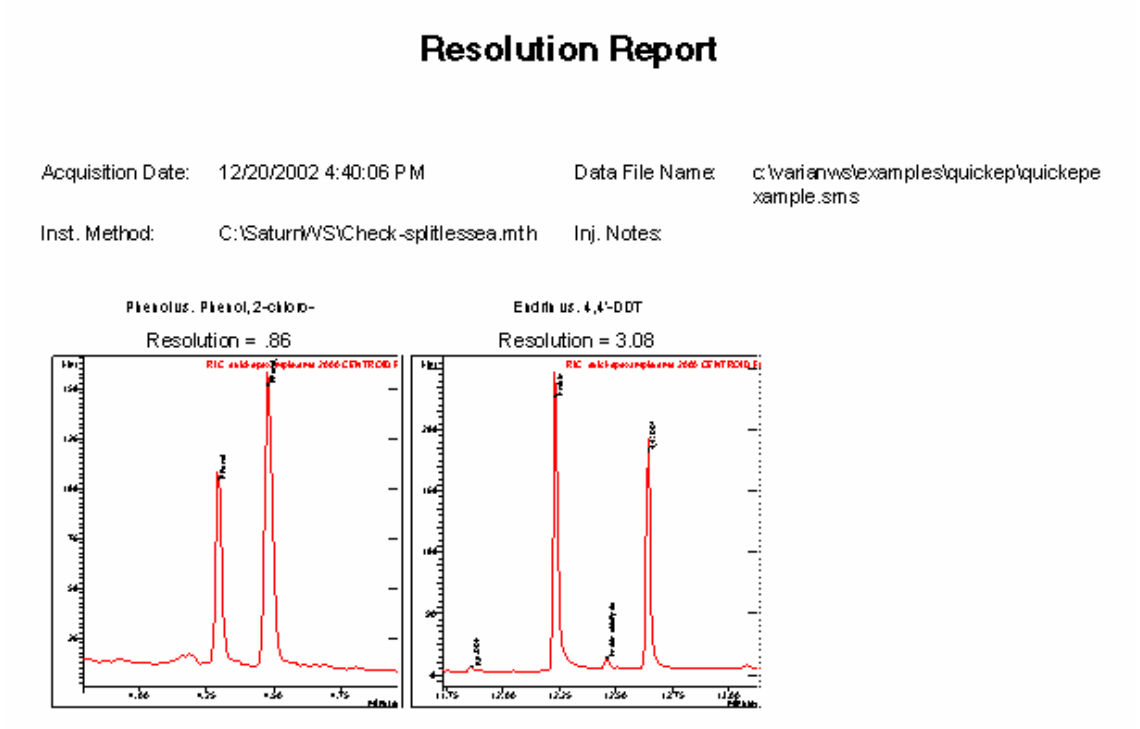
Resolution Report

1. Click the edit button to open the Edit Report Template form.
2. Click the Init Report Parms button. This will copy the target compound list from the current data file into the report configuration list and clears all report settings.
3. Click the Edit Report Parms button to open the report setup screen.
4. Click checkboxes in the Resolution column to select the resolution peak pairs. Resolution will be reported for adjacent pairs of checked peaks on this form.
5. Click Close on the Edit Cparm form and save on the Edit Report Template form.
6. Click the View button to display a page select form. Select the page to be viewed then click the Preview button to view the report page. Up to six resolution compound pairs will be displayed per page.

To display subsequent resolution reports from files quantitated using the same method, execute Step 6, skipping Steps 1 through 5).



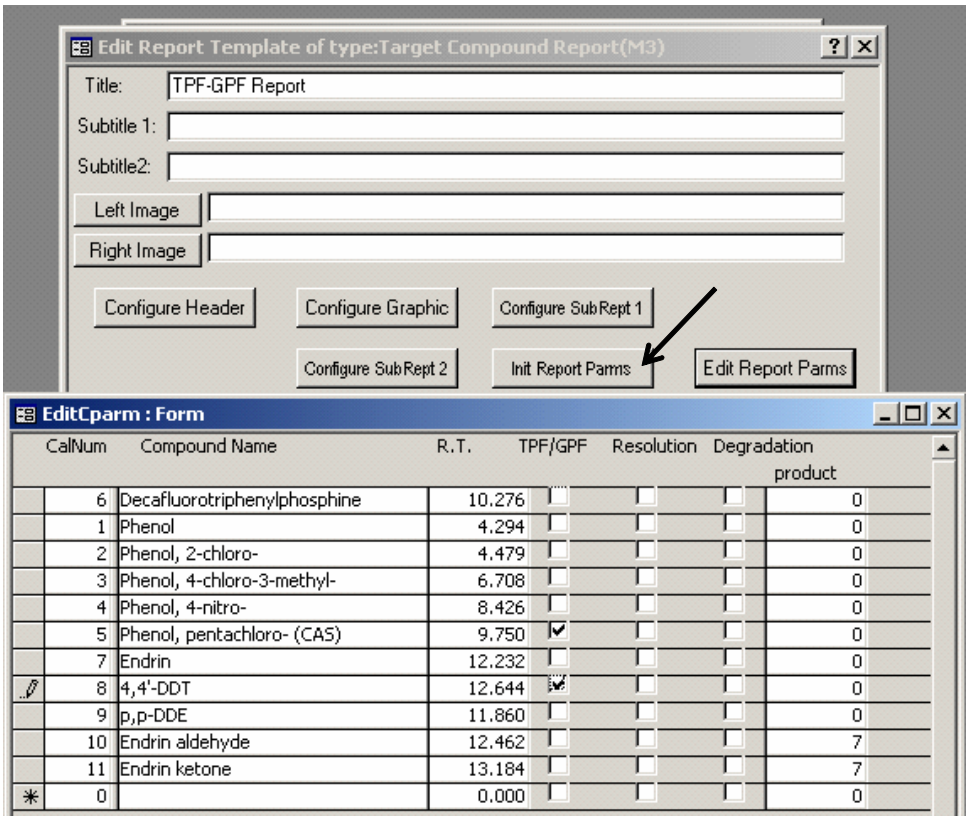
Set Up for Resolution Report



Tailing Peak and Gaussian Peak Factor Report

1. Click the edit button to open the Edit Report Template form.
2. Click the Init Report Parms button. This will copy the target compound list from the current data file into the report configuration list and clears all report settings.
3. Click the Edit Report Parms button to open the report setup screen.
4. Click checkboxes in the TPF/GPF column to select the reportable peaks. The report will include the checked peaks on this form.
5. Click Close on the Edit Cparm form and save on the Edit Report Template form.
6. Click the View button to display a page select form. Select the page to be viewed then click the Preview button to view the report page. Up to six compounds will be displayed per report page.

To display subsequent TPF/GPF reports from files quantitated using the same method, load the next data file and execute Step 6, skipping Steps 1 through 5.



CalNum	Compound Name	R.T.	TPF/GPF	Resolution	Degradation product
6	Decafluorotriphenylphosphine	10.276	☐	☐	0
1	Phenol	4.294	☐	☐	0
2	Phenol, 2-chloro-	4.479	☐	☐	0
3	Phenol, 4-chloro-3-methyl-	6.708	☐	☐	0
4	Phenol, 4-nitro-	8.426	☐	☐	0
5	Phenol, pentachloro- (CAS)	9.750	☑	☐	0
7	Endrin	12.232	☐	☐	0
8	4,4'-DDT	12.644	☑	☐	0
9	p,p-DDE	11.860	☐	☐	0
10	Endrin aldehyde	12.462	☐	☐	7
11	Endrin ketone	13.184	☐	☐	7
0		0.000	☐	☐	0

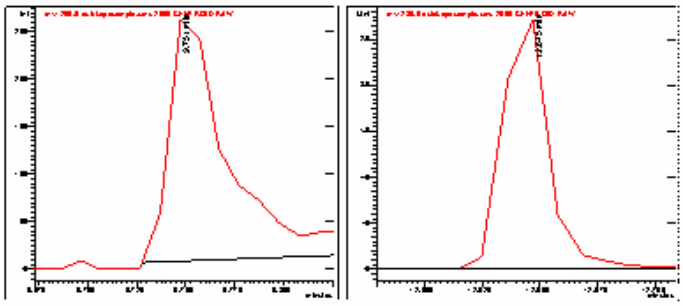
Set up for Tailing/Gaussian Factor Reports

TPF-GPF Report

Acquisition Date:	12/20/2002 4:40:06 PM	Data File Name:	c:\varianws\examples\quickep\quickepexample.sms
Inst. Method:	C:\Saturn\VS\Check-splitlessea.mth	Inj. Notes:	

Phenol, pentachloro- (
RT = 9.751 Area = 579

4,4'-DDT
RT = 12.645 Area = 38213



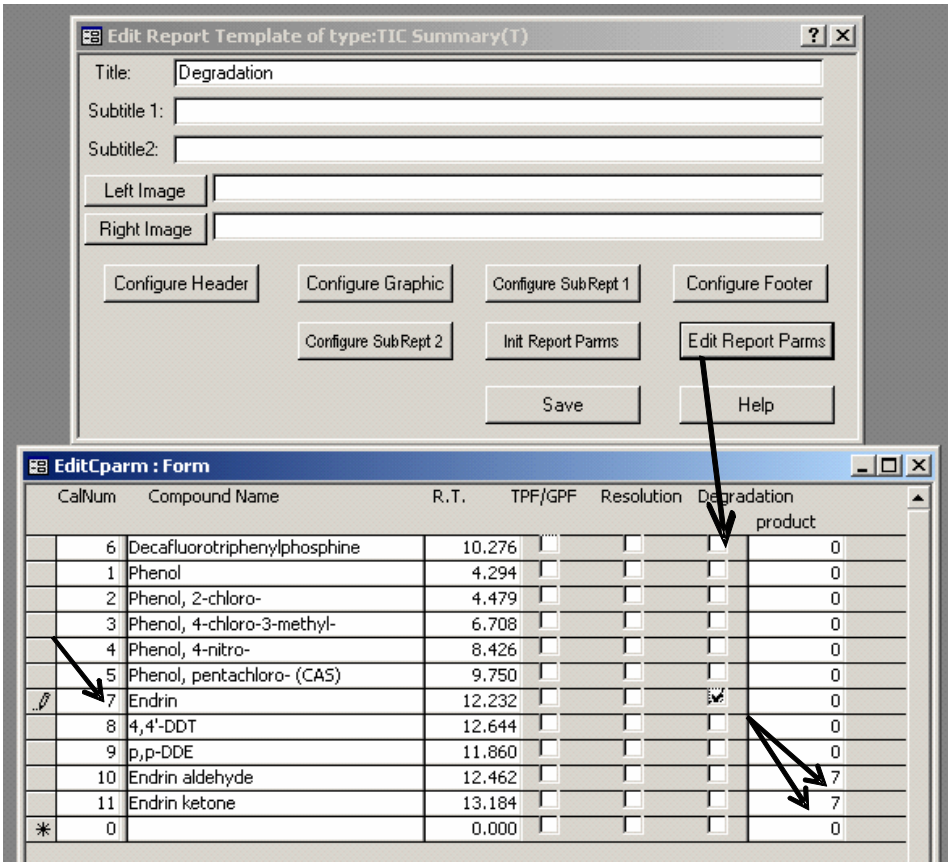
Compound Name	RT	TPF	GPF
Phenol, pentachloro- (CA	9.751	7.726	0.335
4,4'-DDT	12.645	0.874	0.995

Compound Name	RT	Area	Amount	BC
Phenol, pentachloro- (CA	9.751	579	1.071	BB
4,4'-DDT	12.645	38213	1.003	BB

Degradation Report

1. Click the edit button to open the Edit Report Template form.
2. Click the Init Report Parms button. This will copy the target compound list from the current data file into the report configuration list and clears all report settings.
3. Click the Edit Report Parms button to open the report setup screen.
4. Click checkboxes in the Degradation column to select the degradation parent peak(s). In the listboxes under Product, enter in each degradation product peak line the CalNum of the parent peak(s).
5. Click Close on the Edit Cparm form and save on the Edit Report Template form.
6. Click the View button to preview the report.

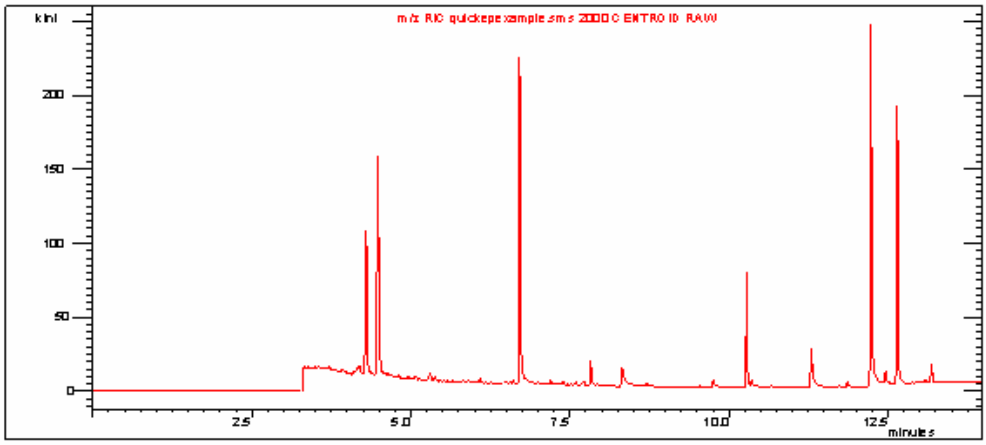
To display subsequent degradation reports from files quantitated using the same method, load the next data file and click the View button.



Set up for degradation Report

Degradation

Acquisition Date:	12/20/2002 4:40:06 PM	Data File Name:	c:\varianws\examples\quickep\quickepexample.sms
Inst. Method:	C:\SaturnWS\Check-splitlessea.mth	Operator Name:	
Inj. Notes:		Instrument ID:	Saturn GC/MS #1



Test

Compound Name	RT	Area	Amount	Calib. RT	BC	Units	IntegWin
Endrin	12.232	6294	1.000	12.232	BB		0.20

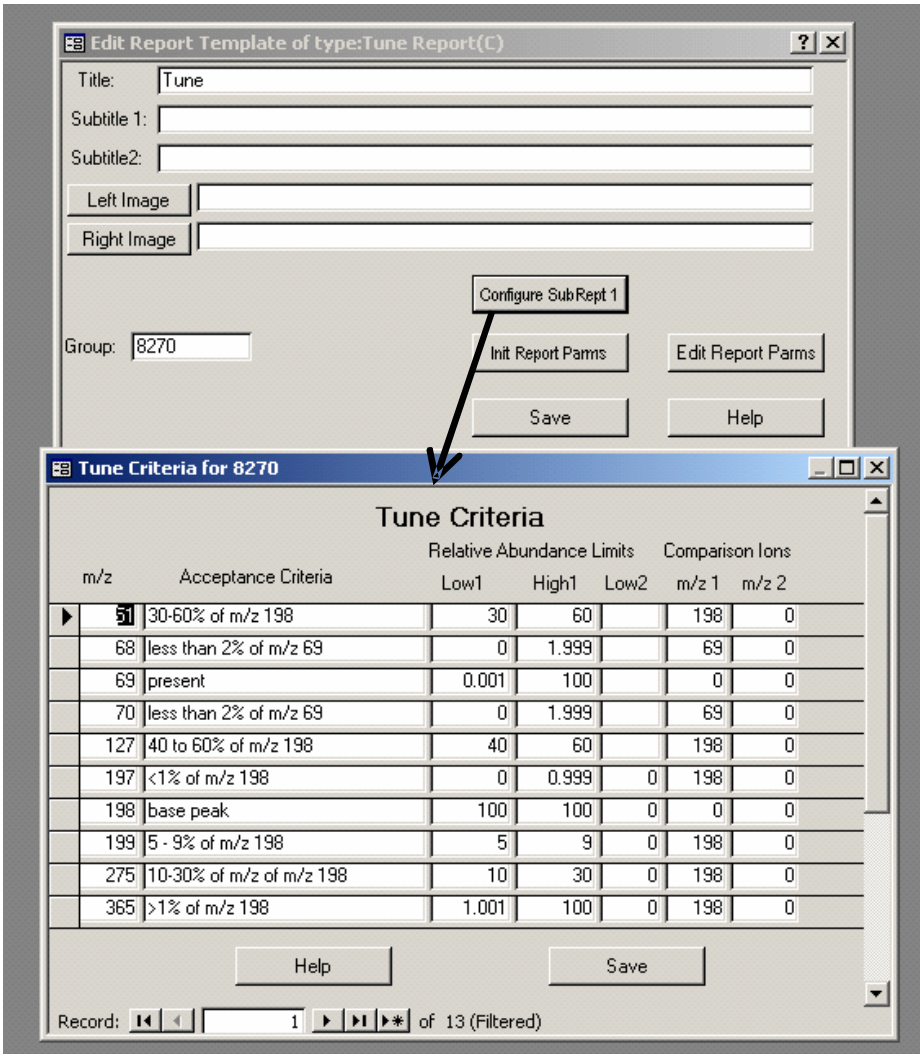
Degradation Product

Compound Name	RT	Area	Amount	Calib. RT	BC	Units	IntegWin
Endrin aldehyde	12.463	557	1.000	12.462	BB		0.20
Endrin ketone	13.184	788	1.000	13.184	BB		0.20

% Degradation of Endrin : = 17.6

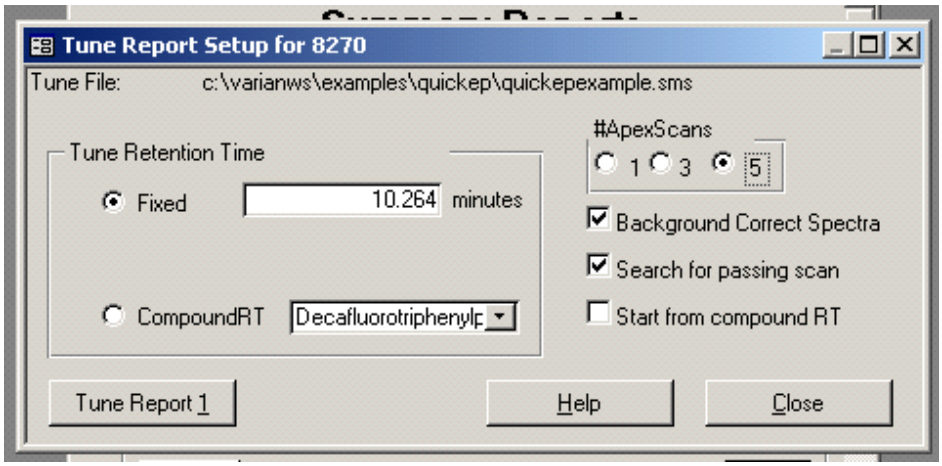
Tune Report

1. Click the edit button to open the Edit Report Template form.
2. Edit the Group text box to contain EPA method designator for the Tune Criteria to be used. (524,624,CLPVOL, 8240 or 8260 for BFB; 525, 625, CLPSEM, 8250, or 8270 for DFTPP).
3. (optional) Click the ConfigSubRept1 button to review or edit the Tune criteria to be used. Close the ConfigSubRept1 dialog
4. Close the Edit Report Template dialog.

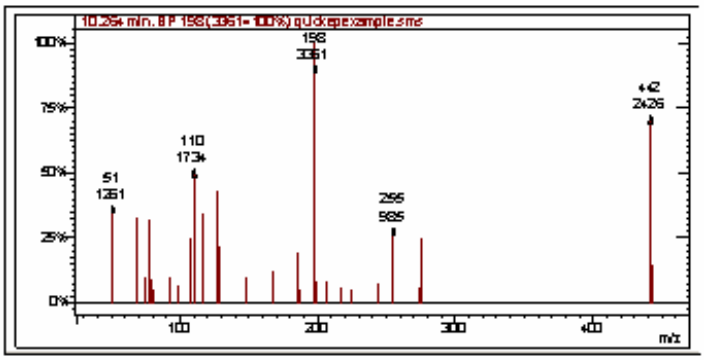


5. Click the View button to open the Tune Report Setup form.
6. Select the appropriate target compound in the compound selection box. Set the other settings appropriately, then click the Tune Report 1 button to view (after a calculation delay) the report.

To display subsequent Tune reports from files quantitated using the same method, execute Steps 5 and 6, skipping Steps 1 through 4.



DFTPP 8270A Report



Lab File ID quickepexample.sms

Injection Date: 12/20/2002

Injection Time: 16:40

m/z	Acceptance Criterion	Value	Pass/Fail
51	30-60 % of m/z 198	37.52	PASS
68	less than 2 % of m/z 69	0.00	PASS
69	present	33.14	PASS
70	less than 2 % of m/z 69	0.00	PASS
127	40 to 60 % of m/z 198	43.26	PASS
197	<1 % of m/z 198	0.00	PASS
198	base peak	100.00	PASS
199	5 - 9 % of m/z 198	8.39	PASS
275	10-30 % of m/z of m/z 198	25.47	PASS
365	>1 % of m/z 198	4.55	PASS
441	present and <m/z 443	47.29	PASS
442	>40 % of m/z 198	72.18	PASS
443	17-23 % of m/z 442	21.27	PASS

Other Information

New report templates can be generated for all report types by clicking the Create button and selecting the type of report to be created.

The fields and field order displayed in Degradation and TPF/GPF reports may be altered. To do this, select the report to be edited, click the Edit button, and use the forms invoked by ConfigSubRept1 and ConfigSubRept2 buttons to configure the reporting fields, and or use the Configure Graphic button to modify the report graphic(s).

To print reports automatically as part of the processing of a recalc list:

1. Configure the reports to be printed in the template.
2. Select (check) the print boxes of the report types to be generated, and edit if desired the print order sequence numbers on the template.
3. Close the template.
4. In the recalc list, enter the full pathname of the report template to be used in the autolink field of each file to be reported.

When the recalc sequence is executed the designated template for each file will be opened and will print the selected reports.

Calculation Definitions

- Resolution = (RT2 – RT1)/(average width of peaks at baseline)
- Gaussian peak factor = 1.83* (width at half height)/(width at 10% of height), using quantitation ion chromatogram profile.
- Tailing peak factor = (Trailing peak half width at 10% of height)/(Leading peak half width at 10% of height), computed using quantitation ion chromatogram profile.
- Degradation % = 100* (Sum of areas of degradation product areas)/(Parent area + Sum of degradation product areas).

NOTE: Areas should be TIC based.

Problem Solving Note

If quantitation baselines start or end above 10% of peak apex height, the TPF and GPF calculations will fail (return 0/report as N/A). TPF and GPF should only be done on baseline resolved peaks. Incorrect values may be computed if the peak being measured is fused to a second peak with a valley point > 10% of peak apex height (the algorithm could search over the top of the fused peak to find incorrect baseline point).