Agilent MSD Productivity ChemStation G1701 & G1710

Performance Report Parameters

Agilent Technologies

Notices

Manual Part Number

G1701-90101

Edition

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1. Introduction

This document describes the calculations used by the Performance Report in the Agilent MSD Productivity ChemStation. These calculations are dependent on the integrator selected for the Data Analysis. The MSD Productivity ChemStation allows use of the Chemstation integrator and the RTE integrator.

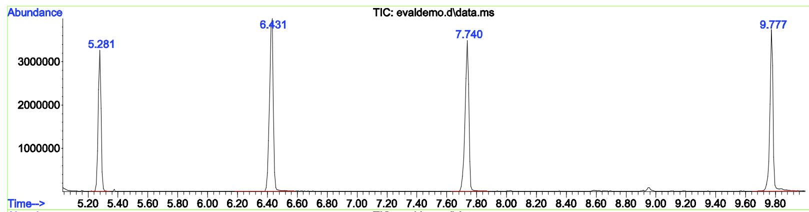
The report is created by selecting Performance Report from the Chromatogram menu. The user is then presented with a dialog and asked to enter a retention time range where the noise will be calculated. A Total Ion Chromatogram (TIC) of this specified noise range is displayed in a new window and the report shown below is printed:

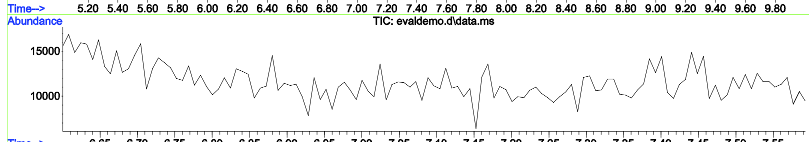
```
Performance Report

Data Path : C:\msdchem\1\data\
Data File : evaldemo.d
Acq On    :  7 Sep 1989  13:59
Operator  : perkins
Sample    : demoscan sample
Misc      : 10 ng per component
ALS Vial  : 1   Sample Multiplier: 1

Integration Parameters: events.e
Integrator: ChemStation

Method    : C:\msdchem\1\METHODS\DEFAULT.M
Title     :
```






```
Noise characteristics:
  Noise start : 6.6  min.
  Noise end   : 7.6 min.
  Number of points: 125
  Maximum noise: 16844 abundances
  Minimum noise: 6382 abundances
  Peak-to-Peak noise: 10462 abundances
  Root-mean-square noise: 1831.09 abundances

The table below is based on an integrated chromatogram.
Tailing calculated at 10% height.
```

#	RetTime	Area	BslPH	PWidth	Resol	Tailing	PtP S/N	RMS S/N	Plates
1	5.28	44191981	3024034	0.023	0.00	1.06	289.05	1651.49	282170
2	6.43	69653044	3920766	0.028	26.63	0.88	374.76	2141.22	301871
3	7.74	59113575	3267388	0.028	27.78	0.80	312.31	1784.40	421345
4	9.78	54668317	3559771	0.024	46.26	0.95	340.26	1944.07	928376

DEFAULT.M Tue Mar 13 14:51:03 2012 Page: 1

2. Report Layout

The report has several sections as described below. Calculations for noise are located in the Noise characteristics section. Calculations relating to individual peaks are shown in the table at the bottom of the report.

Heading

The heading displays the data file and path used by the report, the date the data was acquired, the operator's name, sample name, misc, and vial number. This is followed by the integration parameters file and the name of the integrator used.

RTE Integration Parameters

When the integrator is the RTE integrator, the RTE integration parameter settings are displayed next.

Graphics Area

The top window contains a Total Ion Chromatogram (TIC) of the data file. The lower graphic contains the noise area specified by the user.

Noise characteristics

Noise Start and Noise End

These are the retention time values entered by the user to define the range used for calculating noise.

Number of points

The number of data points found in the specified noise range.

Maximum noise

The abundance value of the data point with the maximum abundance in the noise range.

Minimum noise

The abundance value of the data point with the minimum abundance in the noise range.

Peak-to-Peak noise

$PPNoise$ = Maximum noise - Minimum noise

Root-mean-square noise

$$RMS\ Noise = \sqrt{\left(\frac{(N\sum(x^2) - (\sum x)^2)}{N(N-1)}\right)}$$

Where: N = Number of points
(see definition under Noise characteristics above)

x = abundance of an individual data point

Performance Report Results

#:

Peak number.

RetTime:

Retention time of the peak.

Area:

Area of the peak as determined by the selected integrator.

BslPH:

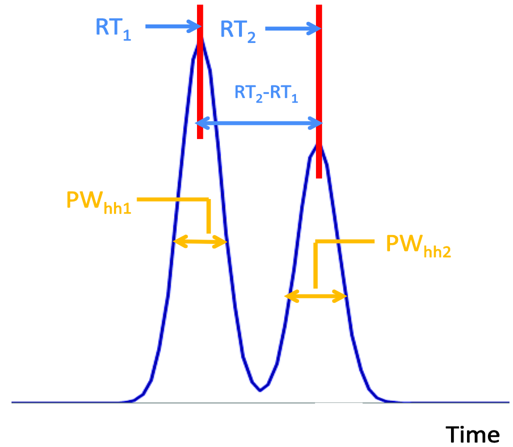
The peak height as measured from the corrected baseline.

PWidth:

Peak width for the ChemStation Integrator is the width of the peak at ½ the peak height. For the RTE Integrator, peak width is the width of the peak start minus the peak end.

Resol:

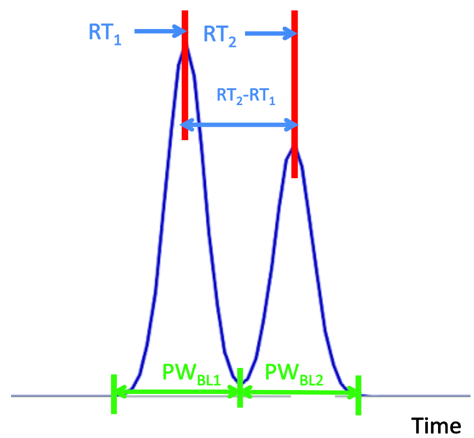
ChemStation Integrator Resolution, as determined using the "ChemStation" Integrator.



$$Resol = 1.18 * \frac{RT_2 - RT_1}{PW_{hh1} + PW_{hh2}}$$

Where: RT_2 = retention time of the second peak;
RT_1 = retention time of the first peak;
PW_{hh1}= peak width at ½ height of the first peak;
PW_{hh2} = peak width at ½ height of the second peak.

RTE Integrator Resolution, as determined using the "RTE" Integrator.



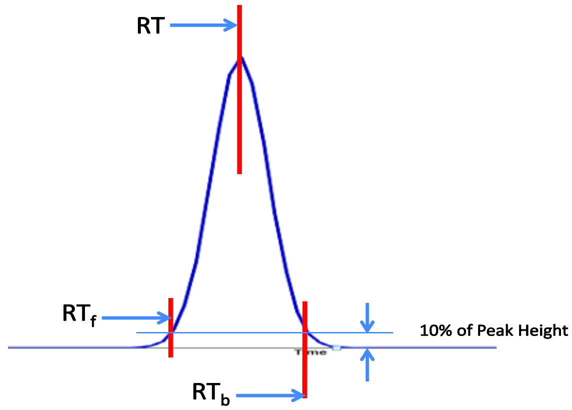
$$Resol = 1.18 * \frac{RT_2 - RT_1}{PW_{BL1} + PW_{BL2}}$$

Where: RT_2 = retention time of the second peak;
RT_1 = retention time of the first peak;
PW_{BL1} = peak width at baseline of the first peak;
PW_{BL2} = peak width at baseline of the second peak.

Please observe that the calculation for *Resolution* when using the RTE integrator does not use the peak width at ½ height. Instead the resolution is calculated using the peak width at the baseline. This is not one of the classical methods for calculating resolution but can be used as a measure to compare resolutions on the Agilent MSD Productivity ChemStation.

Tailing:

Peak Tailing Factor
This is a measure of peak symmetry. For a perfectly symmetric peak, the peak tailing factor = 1.



$$Tailing = \frac{RT_b - RT_f}{2.0 * (RT - RT_f)}$$

Where: RT = retention time of the peak.
RT_b = RT of peak back at 10% of peak height;
RT_f = RT of peak front at 10% of peak height;

PtP S/N:

Peak-to-Peak signal to noise ratio.

$PtP\ S/N\ = (BslPH)/(PPNoise)$

Where: $BslPH$ = baseline corrected peak height;
$PPNoise$ (see definition under Noise characteristics above)

RMS S/N:

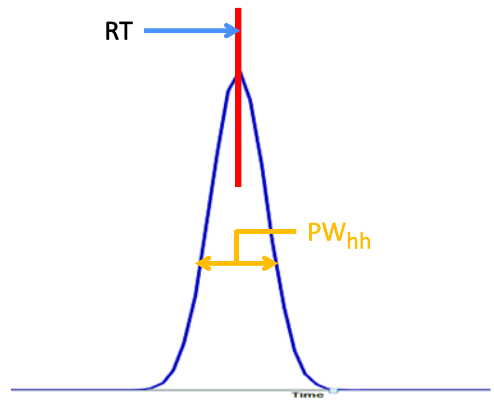
Root Mean Square signal to noise ratio

$RMS\ S/N = (BslPH)/(RMSNoise)$

Where: $BslPH$ = baseline corrected peak height;
$RMSNoise$ (see definition under Noise characteristics above)

Plates:

Number of Theoretical Plates
This is a measure of the column efficiency (the ability to produce narrow peaks). The result is the number of theoretical plates per meter of column length.



$$Plates = 5.54 * \left[\frac{RT}{PW_{hh}}\right]^2$$

Where: RT = retention time of the peak;
PW_{hh} = width of the peak at ½ height.

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