

A Quick-Start Guide to Optimizing Detector Gain for GC/MSD

Authors

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Using detector gain provides a number of important advantages in GC/MS including: better compound response stability over time, better correspondence between instruments, simpler diagnostics, but most importantly, a simple approach to optimize the working concentration range of the MS detector. This application note details this optimizing approach for the concentration range of interest to the analyst.

Introduction

The primary principle of Gain is that the signal for the compound ions is directly proportional to the Gain setting of the acquisition method [1]. This means adjusting the Gain higher, for example, from Gain Factor = 1 to Gain Factor = 5, increases the signal amplification five times higher thereby increasing the response seen in the data analysis for all compounds five-fold also. This reveals the strategy for setting the Gain for the range of analyte concentrations. If the Gain (Factor) is too high, peaks are flat-topped and quantitation is poor at higher concentrations. If the Gain (Factor) is to too low, the low concentration analyte responses are too low.



Procedure

Under optimized GC conditions (for example, injector parameters, GC oven program, and so forth) and MS parameters (for example, scan range, or SIM ions, and so forth) for the analysis, set the GAIN FACTOR = 1 and acquire the highest concentration standard (Figure 1).

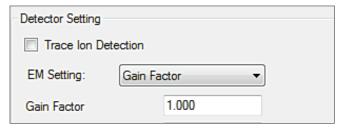


Figure 1. Detector setting.

Identify the most intense extracted ion signal. Find the
most intense ion in any of the compounds and record the
maximum peak height counts. There are at least two
approaches. The Appendix shows a very simple demonstration of the data handling through the MassHunter
GC/MS Qualitative software.

Another approach (ChemStation-based) is to identify all the compounds and build a quantitation database.

- Temporarily set the quantitation method to quantitate the compounds by their peak height.
- 2. Generate a report which will give the peak height counts for each compound's target ion.
- Look through the list and identify the compound, its retention time and the target ion.
- Check that all the peak height counts are under 8 million. If the any exceed 8 million, consider using a larger ion drawout lens [2].
- On the report, find the counts for the largest peak height. Call this LPHt counts.

To calculate a more optimum Gain Factor (GF_{calc}):

$$\frac{\text{[LPHt counts]}}{\text{[1.0]}} = \frac{\text{[3} \times 10^6 \text{ counts]}}{\text{[GF}_{calc}]}$$

٥r

$$\frac{[3 \times 10^6 \text{ counts}]}{[\text{LPHt counts}]} = [\text{GF}_{\text{calc}}]$$

The calculated Gain Factor (GF_{calc}) can be rounded off to the first place behind the decimal point (x.x).

- Set the method Gain Factor to this new value (GF_{calc}) and reacquire the highest concentration standard.
- 7. Recalculate the peak heights and see that the compound with the largest peak height now produces peak height counts ≥ 3 million counts but less than 6 million counts.

If so, acquire the lowest concentration standard and check for good detection of all compounds, both the most and least intense. Some sacrifices may need to be made to accommodate all compounds within the detectors working range. The user should be familiar with the technical note concerning source drawout lenses [2]. Figure 2 shows a flowchart diagraming the logic.

The rules are rather simple for choice of Gain Factor:

- Choose the lowest Gain Factor that allows detection of both the most and least intense ion out of all of the target analytes over the concentration range of interest.
- Do this by identifying these two compounds and their ions and testing the choice of Gain Factor in both the highest and lowest concentration standards.

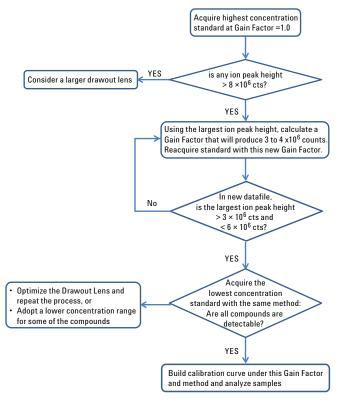
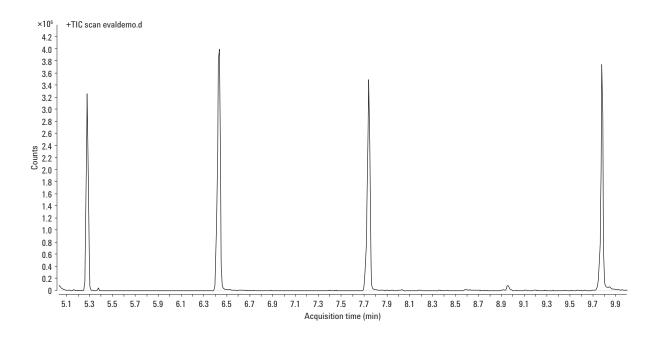


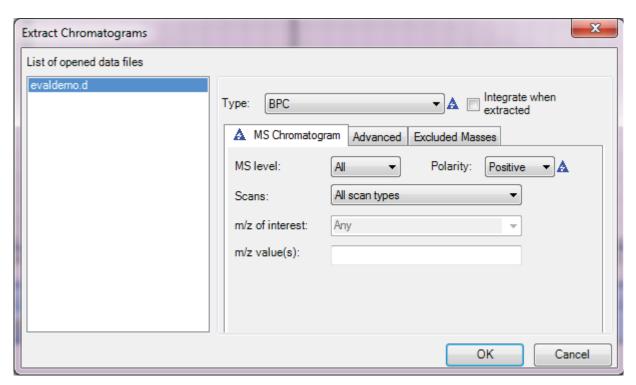
Figure 2. Flowchart of the gain optimization procedure.

Appendix: an example of estimating a more optimum Gain Factor using EVALDEMO.D

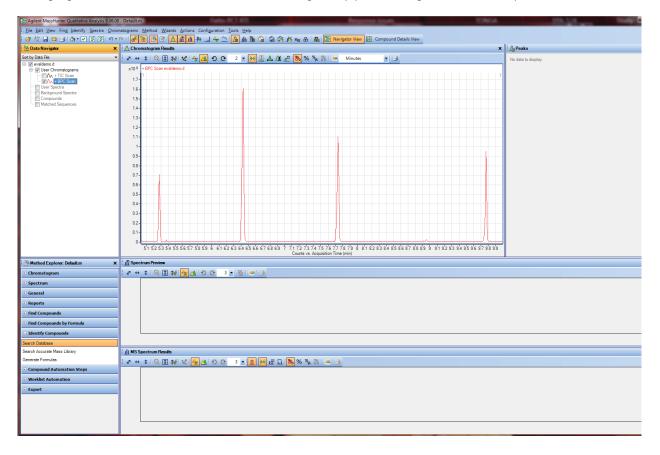
1. Using MassHunter Qualitative Analysis load the file EVALDEMO.D found in the C:\MassHunter\GCMS\1\data directory.



2. Use Extract Chromatograms (found under the menu item Chromatograms) with the type Base Peak Chromatogram (BPC).



3. Highlight ONLY BPC Scan under the *User Chromatograms* (by unchecking the TIC Scan box).



Then execute Integrate Chromatogram (under the Chromatograms menu item). Turn on the Peak Table () so the results can be viewed.

| Peaks: +BPC Scan | | | | | | | | | | | | |
|------------------|----------|-------|------------|------------|--------|---------|---------|-------|--|--|--|--|
| F | Peak ⊽+⊐ | RT ₽ | Area +¤ | Height +¤ | Type + | Width 中 | FWHM +□ | SNR ₽ | | | | |
| F | 5 | 9.772 | 1295596.16 | 946705.31 | | 0.137 | 0.021 | | | | | |
| | 4 | 8.955 | 34610.13 | 21537.31 | | 0.1 | 0.049 | | | | | |
| | 3 | 7.737 | 1851998.76 | 1102033.31 | | 0.13 | 0.025 | | | | | |
| | 2 | 6.431 | 2737375.79 | 1607889.31 | | 0.137 | 0.026 | | | | | |
| | 1 | 5.278 | 950077.57 | 705681.31 | | 0.066 | 0.022 | | | | | |

 Click twice in the table on the header for peak height to sort the table in order of high-to-low for peak height of the BPC. This will bring the most intense ion peak heights to the top of the list.

| 1 | Peaks: + BPC Scan | | | | | | | | | | | | |
|---|-------------------|---|-------|------------|------------|---------------|---------|---------|-------|--|--|--|--|
| | Peak | þ | RT 中 | Area +¤ | Height ∇+ | Type + | Width 中 | FWHM +□ | SNR ₽ | | | | |
| ▶ | | 2 | 6.431 | 2737375.79 | 1607889.31 | | 0.137 | 0.026 | | | | | |
| | | 3 | 7.737 | 1851998.76 | 1102033.31 | | 0.13 | 0.025 | | | | | |
| | | 5 | 9.772 | 1295596.16 | 946705.31 | | 0.137 | 0.021 | | | | | |
| | | 1 | 5.278 | 950077.57 | 705681.31 | | 0.066 | 0.022 | | | | | |
| | | 4 | 8.955 | 34610.13 | 21537.31 | | 0.1 | 0.049 | | | | | |

6. Record this highest height value, which is in this case 1607889 and belongs to the second peak in the chromatogram (at 6.431 minutes). Note that the least intense target ion belongs to the compound at 8.955 minutes.

Assuming this was collected under a Gain Factor of 1.0, we can calculate a better Gain Factor by the equation:

Better Gain Factor =
$$\frac{3,000,000}{1,607,889} = 1.87 \approx 1.9$$

This suggests the sample should be reacquired at a new Gain Factor of 1.9 and then examined in BPC for Peak 2 to see that the peak height is within the proper range (> 3 million counts in height but less than 6 million counts). If this is true, then the lowest concentration standard should be acquired at this Gain Factor and the least intense peak(s) examined for their intensity. In this example that is the peak at 8.955 minutes (peak 4).

References

- 1. Enhancements to Gain Normalized Instrument Tuning: Understanding the Benefits and Features (5989-7654EN).
- 2. 5977 El Source Selection Guide (5991-2106EN).

For More Information

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