Analysis of GC-IMS Peak Table Stability

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1. Load Peak Table

```
df <- read.csv("../../data/peak_table_pool.csv")
df <- df %>% rename(SampleID = 1)
```

1.1. Visualisation

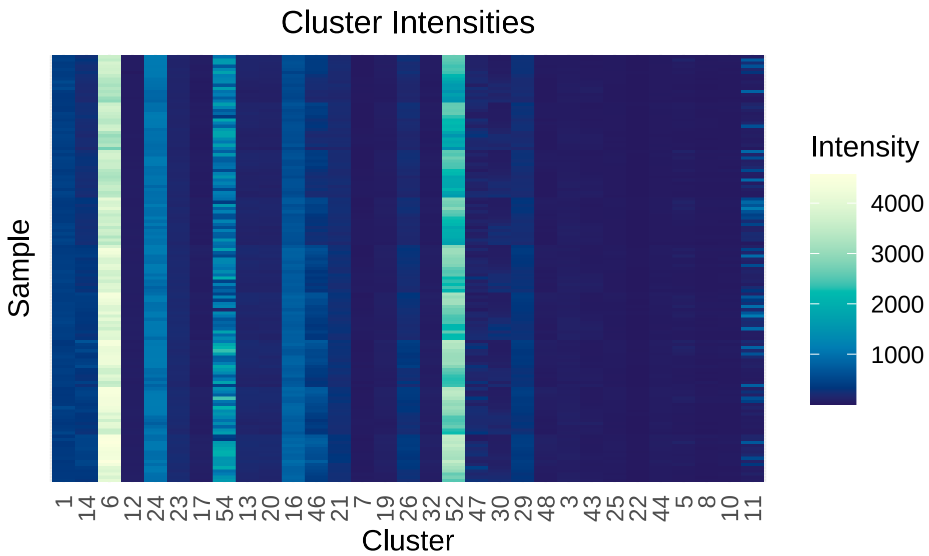


Figure 1: Cluster intensity values across samples

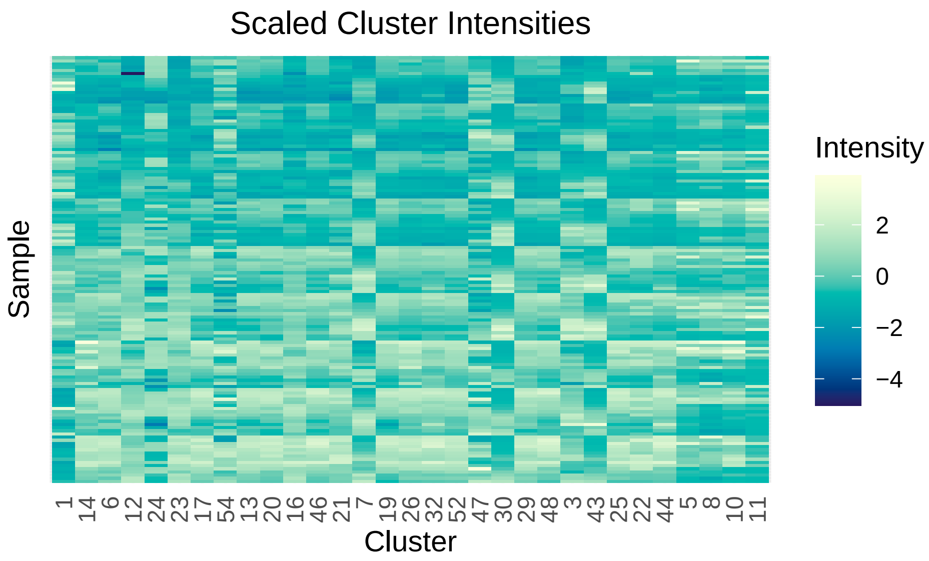


Figure 2: Scaled Cluster intensity values across samples

Scaling: (`scale(x, center = TRUE, scale = TRUE)`) is done by: - **Centering** by subtracting the column means - **Scaling** by dividing the (centered) columns of x by their standard deviations.

2. Stability of the Peaks

This analysis builds upon two previous reports: the linearity analysis, which demonstrated strong temporal trends in signal intensity and motivated the use of `batch` as an ordinal numeric variable; and the baseline correction report, which addressed signal overestimation due to background effects in GC-IMS data. These preprocessing steps form the foundation for the current evaluation of signal stability across sessions.

2.1. Relative Standard Deviation (RSD)

In this section, we assess the technical variability of each cluster by computing the Relative Standard Deviation (RSD) of its intensity values across repeated measurements:

$$RSD = \frac{\text{Standard Deviation}}{\text{Mean}} \times 100$$

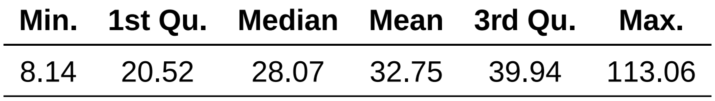
Relative Standard Deviation (RSD), or Coefficient of Variation (CV), which are typically considered equivalent in this context, are commonly used to quantify the variability of a given feature—such as the intensity of a detected compound—across replicate measurements (e.g., repeated injections or pooled QC samples in metabolomics studies) (Zhang et al., 2020; Schiffman et al., 2019; Sarmad et al., 2022).

2.1.1. Computing the RSD per cluster

In GC-IMS data analysis, peaks detected across different samples can be grouped into clusters when they are assumed to originate from the same compound (see the previous preprocessing workflow with GCIMS package) . Their intensity values in each sample reflect the abundance or concentration of the corresponding compound. Therefore, the **intensity of each cluster across samples** becomes the **feature we evaluate when assessing technical stability across replicate measurements.**

To do so, we compute the Relative Standard Deviation (RSD) for each cluster across all 135 samples. The RSD expresses the variation of a signal relative to its average intensity, allowing us to identify clusters that show stable responses across the dataset versus those affected by technical variability.

Summary Statistics of RSD Values



Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
8.14	20.52	28.07	32.75	39.94	113.06

Figure 3: Summary statistics of RSD values

RSD Values Distribution .

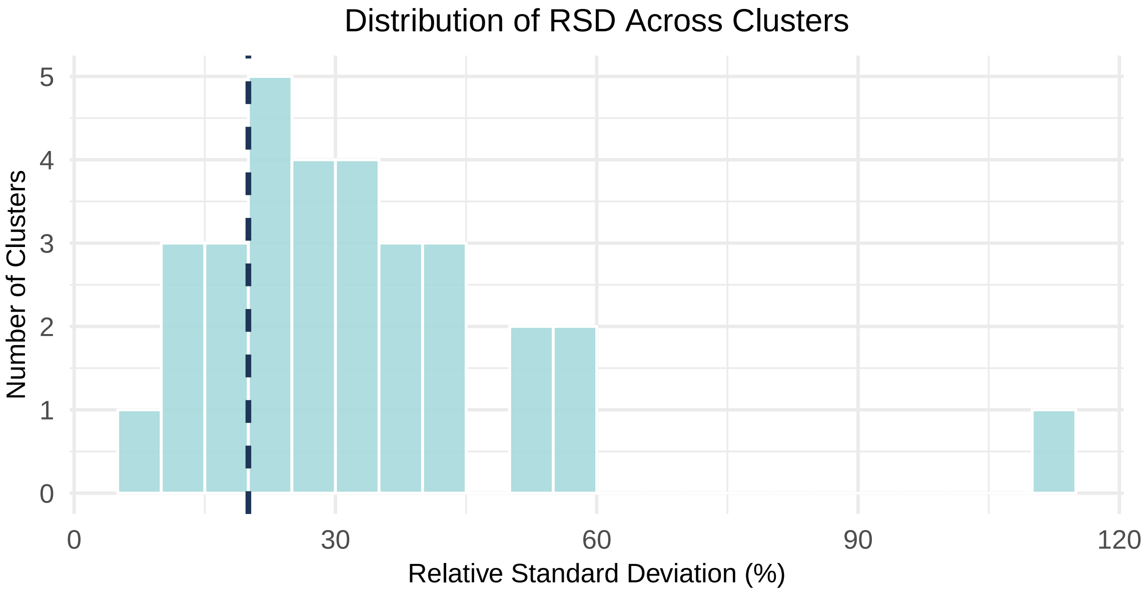


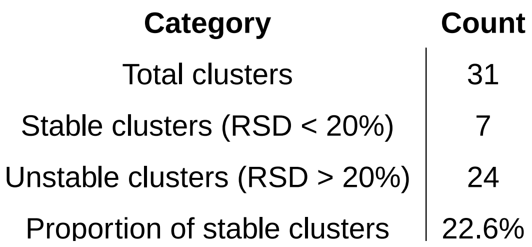
Figure 4: Distribution of RSD values across all clusters

The histogram shows the distribution of RSD values across all clusters in the corrected peak table. Most clusters exhibit RSD values between 15% and 50%, although some extend beyond this range, with one exceeding 100%. A dashed vertical line marks the 20% threshold, which we use as a reference point based on common practices in metabolomics (as further discussed below).

2.2. Assessment of Stable Clusters Based on RSD

In the context of metabolomics data analysis, it is common practice to filter out features that exhibit excessive variability from the dataset: features with a CV above **20–30%** are typically filtered out to retain only reproducible signals (Zhang et al., 2020; Schiffman et al., 2019; Sarmad et al., 2022).

Although our experimental context differs, we adopt a **20% RSD threshold** as an **orientative reference** to evaluate **how many clusters exhibit variability levels in line with those considered acceptable in similar contexts**. This threshold is not applied as a strict filter, but rather as a descriptive benchmark for technical stability.



Category	Count
Total clusters	31
Stable clusters (RSD < 20%)	7
Unstable clusters (RSD > 20%)	24
Proportion of stable clusters	22.6%

Figure 5: Summary of cluster stability

Only 22.6% of the clusters exhibit a relative standard deviation below 20%, suggesting that a small subset of the clusters, which likely correspond to specific metabolites, are stable across the dataset and may be considered for further analysis. This highlights the presence of substantial variability among many features.

3. References

- Zhang, X., Dong, J., & Raftery, D. (2020). *Five Easy Metrics of Data Quality for LC–MS-Based Global Metabolomics.* Analytical Chemistry, 92(17), 12925–12933. https://doi.org/10.1021/acs.analchem.0c01493

- Schiffman, C. et al. (2019). *Filtering procedures for untargeted LC-MS metabolomics data.* BMC Bioinformatics, 20, 334. https://doi.org/10.1186/s12859-019-2871-9

- Sarmad, S., Viant, M. R., Dunn, W. B., Goodacre, R., Wilson, I. D., Chappell, K. E., Griffin, J. L., O'Donnell, V. B., Naicker, B., Lewis, M. R., Suzuki, T., & UK Consortium on Metabolic Phenotyping (MAP/UK). (2022). *A proposed framework to evaluate the quality and reliability of targeted metabolomics assays from the UK Consortium on Metabolic Phenotyping (MAP/UK).* Nature Protocols, 17(7), 1808–1820. https://doi.org/10.1038/s41596-022-00801-8