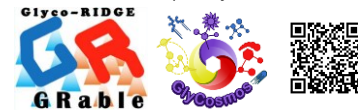


GRable Version 1.0 : 質量分析による グライコプロテオーム解析を加速するソフトウェア

GRable website (in GlyCosmos Portal)



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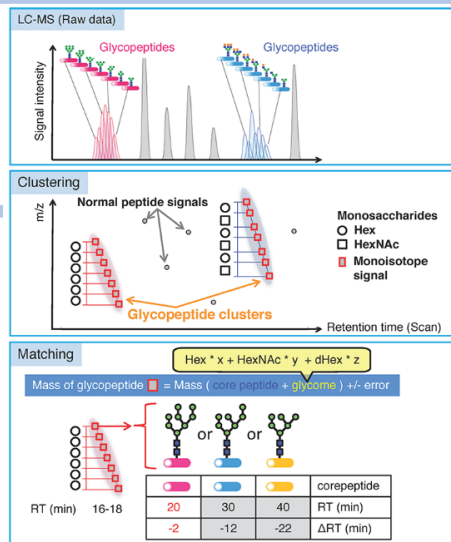
<https://glycosmos.org/grable>

What is GRable?

GRable is a freely available online tool to find **site-specific glycoforms of glycopeptides**. This tool is unique in that it utilizes an **MS1-based** glycoproteomic method named "**Glyco-RIDGE**" (Glycan heterogeneity-based Relational Identification of Glycopeptide signals on Elution profile).

Principle of the Glyco-RIDGE method

First, this method identifies glycopeptide signals based on the chromatographic properties of glycopeptides and mass differences due to the glycan heterogeneity. That is, glycopeptides having the same core peptide but different glycans elute within a narrow range of elution time, so glycopeptide signals with a similar elution time and mass differences corresponding to glycan units can be assigned as a cluster, without MS2 spectrum analyses. In parallel, core peptides present in the glycopeptide sample are identified by IGOT-LC/MS/MS. Then, considering that the mass value of glycopeptide is the sum of those of core peptide and glycan, the combination of peptide and glycan for each glycopeptide is searched from these three lists (the masses and RT lists of glycopeptides, peptides, and glycans).



How to Use

Input data

GRable requires following 4 files:

1. LC/MS data of glycopeptides (.mzML)
2. Core peptide list (.xlsx)
3. Glycan point list (.xlsx)
4. LC/MS/MS data of glycopeptides (.mgf)

Scheme

1. Data Registration

*Deconvoluted data is required

2. Deconvolution

*Unapplicable in this version

3. Range setting

4. Monoisotopic peak picking

5. Clustering

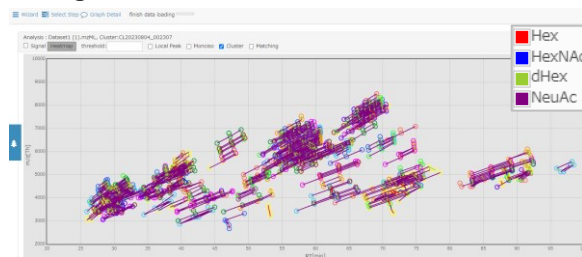
6. Matching

7. Selection

Glycopeptide list

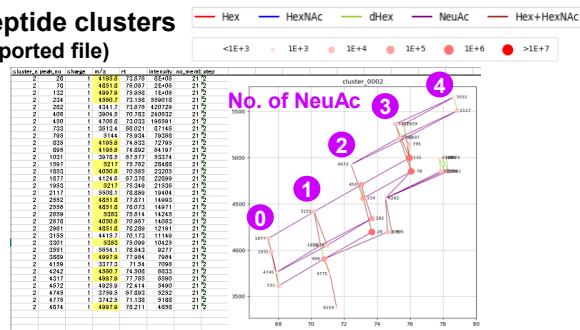
Output data

Clustering view (in the viewer)



All glycopeptide clusters detected from the input data are visualized to overlook the complexity of glycopeptide sample.

Glycopeptide clusters (in the exported file)



Glycopeptides with the same core peptide are depicted as a cluster, facilitating understanding of glycan heterogeneity.

References

Glyco-RIDGE methodology

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 Togayachi *et al. J Am Soc Mass Spectrom* 29:1138-52, 2018.
 Narimatsu *et al. J Proteome Res* 17:4097-112, 2018.

IGOT-LC/MS/MS method

- Kaji *et al. Nat Biotechnol* 21:667-72, 2003.
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Applications of the Glyco-RIDGE method

- Noro *et al. Glycobiology* 31:1268-78, 2021.
 Tasaki *et al. Transp Int* 35:51, 2022.
 Fukuoka *et al. Oncogene* 41:4385-96, 2022.
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 Hiono *et al. J Proteome Res* 23:1408-19, 2024.

GRable development

- Nagai-Okatani *et al. Mol Cell Proteomics* 23:100833, 2024.

