



Hands-on Automated MS Data Analysis using Lipid Data Analyzer (LDA)

Part V – Summary and outlook

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- LC-MS¹ data: Identification and quantitation of intact lipid species
- MSⁿ data: Verification of lipid class and structural information about the lipid molecular species
- Isomeric/isobaric and co-eluting species are common in lipidomics
- Both, positive and negative ion mode are required to cover all classes in lipidomics
- Decision rules are a versatile and reliable tool for high-quality lipid annotations
- FPs cannot be entirely avoided – how to identify them:
 - ECN model
 - fragmentation patterns

Summary

- Free of charge: http://genome.tugraz.at/lda2/lda_download.shtml
- And open-source: <https://github.com/ThallingerLab/LDA2>
- Plenty of published (test) data:
http://genome.tugraz.at/lda2/lda_data.shtml
<http://www.ebi.ac.uk/metabolights/MTBLS391>
<http://www.ebi.ac.uk/metabolights/MTBLS394>
<http://www.ebi.ac.uk/metabolights/MTBLS396>
<http://www.ebi.ac.uk/metabolights/MTBLS398>
<http://www.ebi.ac.uk/metabolights/MTBLS462>
- Comprehensive user manual: http://genome.tugraz.at/lda2/lda_documentation.shtml
- Video tutorial: <https://www.youtube.com/watch?v=GiKM-urfNIg>

Hartler J, *et al.*, Bioinformatics, 2011

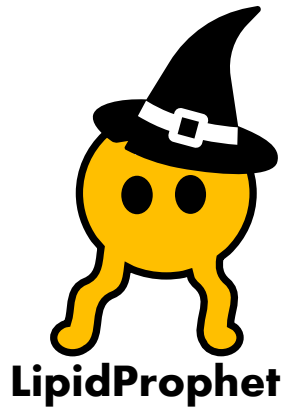
Hartler J, *et al.*, Nature Methods, 2017

Recent LDA extensions

- **Sphingolipids**
Hartler J, *et al.*, Analytical Chemistry, 2020
- **Glycolipidomics: Glycosyl inositol phospho ceramides (GIPCs)**
Panzenboeck L, *et al.*, Metabolites, 2020
- **Oxidized lipids**
Krettler CA, *et al.*, Studies in Health Technology and Informatics, 2020
- **Glycolipidomics: Gangliosides**
Hohenwallner K, *et al.*, JACS Au, 2022
- **Accurate triglyceride quantitation**
Vigor C, *et al.*, Food Chemistry, 2022
- **LDA for shotgun and FAIMS shotgun workflows**
Hohenwallner K, *et al.*, Analytical Chemistry, 2024



LDA module for accurate and automated C=C identification based on retention time



A universal confidence classifier that supports FDR-controlled lipid identification in lipidomics.

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