

Construction of novel lipidomics platform combined of targeted and non-targeted analysis

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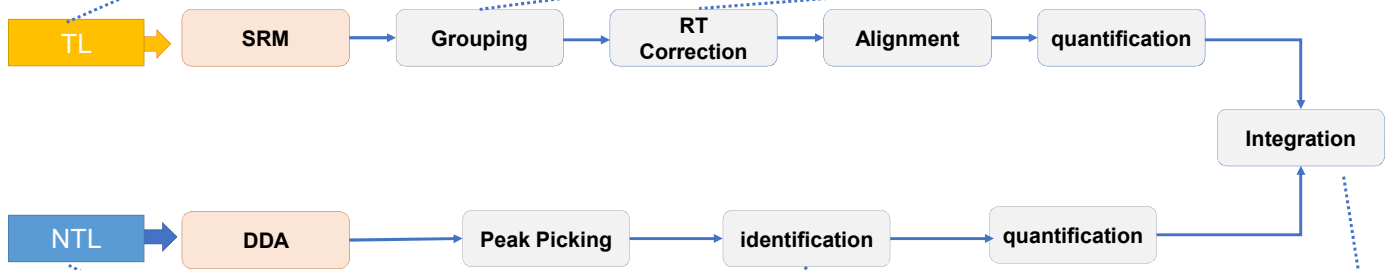
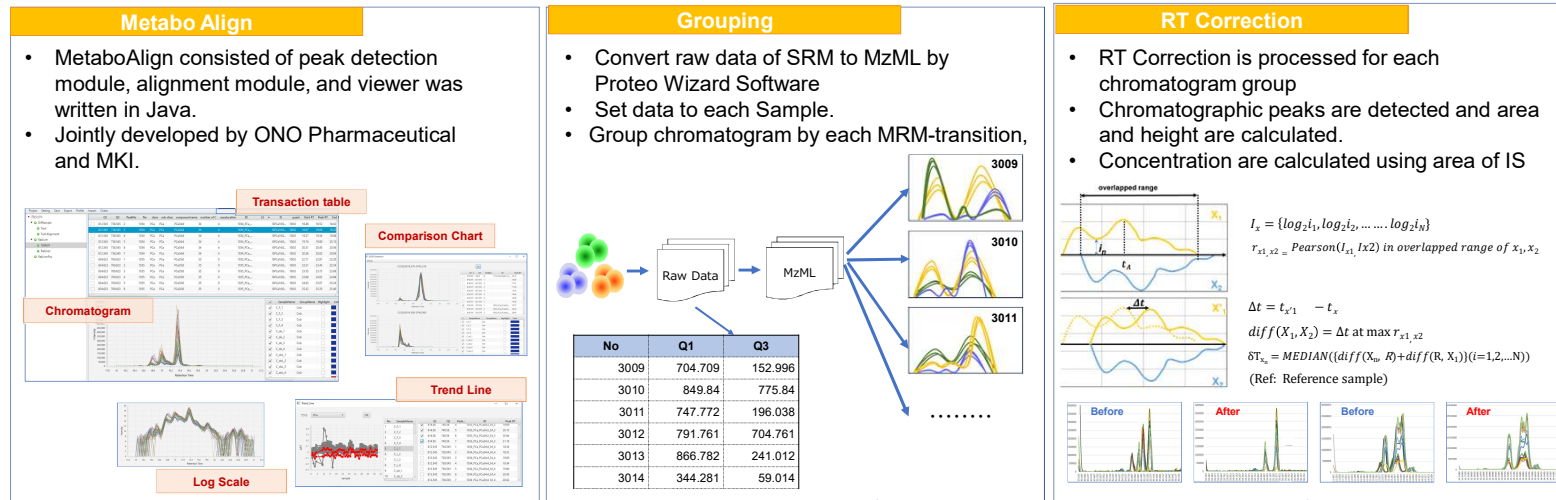
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Introduction:

Targeted lipidomics (TL) using selected ion monitoring (SRM) enable high sensitive quantitative analysis for certain lipids in biological sample. However overlapped chromatographic peaks from isomer and fluctuations in retention time of chromatograms cause miss alignment among samples. Here we developed novel lipidomics platform named **MetaboAlign** which solve these issues combining TL with Non-targeted lipidomics(NTL) on data dependent acquisition (DDA).

Architecture of MetaboAlign:



About Lipid Search

- A powerful tool for lipidomics.
- Jointly developed by Professor Ryo Taguchi (Univ. of Tokyo) and MKI
- Sold for global market by Thermo Fisher Scientific
- Latest version is 4.2

LipidSearch

Lipid Molec table, Alignment Detail, Lipid Profile

Identification (NTL)

- Creating the database with combination of partial structures
- Containing >1.5 million lipid species (v4.0) and their predicted fragment ions
- High speed analysis
- High accuracy peak detection algorithms
- Unique ID algorithms for various kinds of scan
- Alignment of identified lipids between different samples

1. Basic structures, 2. Fatty acids, 3. Adduct ions, 4. Combinations and fragmentation

Class	ver.2.0	ver.4.1
GPL_GL_SL	59,228	632,583
OXG_L	--	321,376
SP_Cer_SPD	--	36,580
ONE	--	544
Co	--	5
CL	--	649,528
GGL	--	99,273
Labeled IS	--	3,808
SUM	59,228	1,743,497

Integration

- Lipid species identified by Lipid Search are assigned to each chromatographic peak of SRM
- Q1 to m/z of precursor ion
- Q3 to m/z product ion
- RT is same within tolerance

NTL: $PC(X_1:Y_1)$, $PC(X_2:Y_2)$, $PC(X_3:Y_3)$

Q3: Class specific ion

Results and Discussion:

Demonstration

- We applied this software to rat liver sample (n10).
- SRM data were measured by 4000 Qtrap (Sciex)
- DDA data were measured by QExactive HF (Thermo Fisher Scientific)
- As a result, 861 kinds of lipid species were identified by NTL, 496 of which were acquired as lipid profiles by TL.

PC(38:4)+CH3COO
Q1: 868.607 Q3: 794.607 (M-CH3)

PS(38:2)-H
Q1: 814.56 Q3: 727.56 (M-Serine+H2O-H)

PE(38:5)-H
Q1: 764.524 Q3: 196.0

Conclusion

- Novel lipidomics platform combined TL with NTL was developed.
- Rapid and accurate quantitative analysis of large sample sets was achieved using the software

Acknowledgement

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