METABOLOMICS INFRASTRUCTURE LINZ

Bernd Reichl
Feb 11th 2020

JOHANNES KEPLER
UNIVERSITÄT LINZ

Interreg
EUROPÄISCHE UNION
Österreich-Tschechische Republik
Europäischer Fonds für regionale Entwicklung

Institute of
Analytical Chemistry

Metabolomics laboratory

Dedicated metabolomics sample preparation lab

- Tissue homogenizer
- Thermal shaker
- Mixing devices
- Solvent evaporator

Agilent 6560 IM-QToF

Installation: March 2018

1st training: April 2018

2nd training: January 2019

IM user meeting (Agilent): March 2019

Next IM user meeting (Agilent): Feb 2020

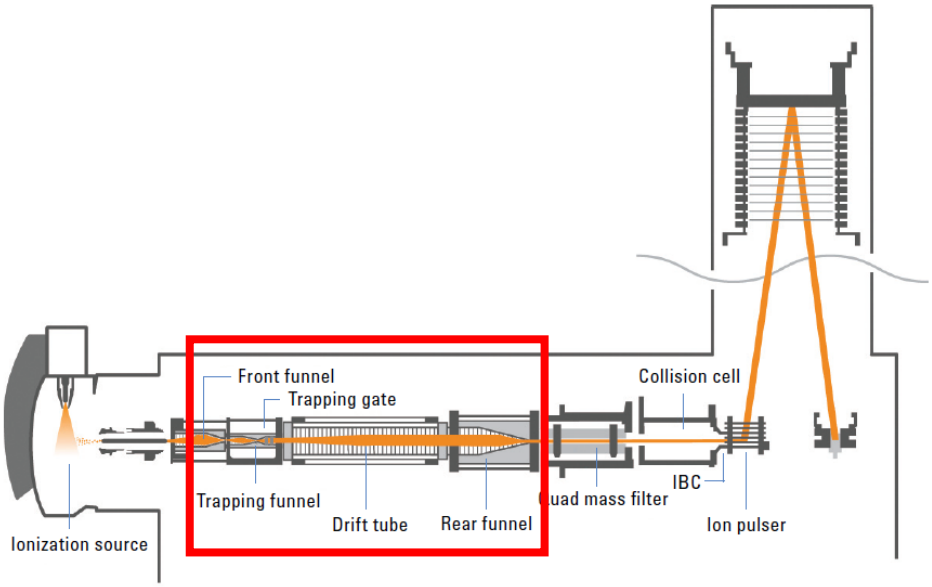
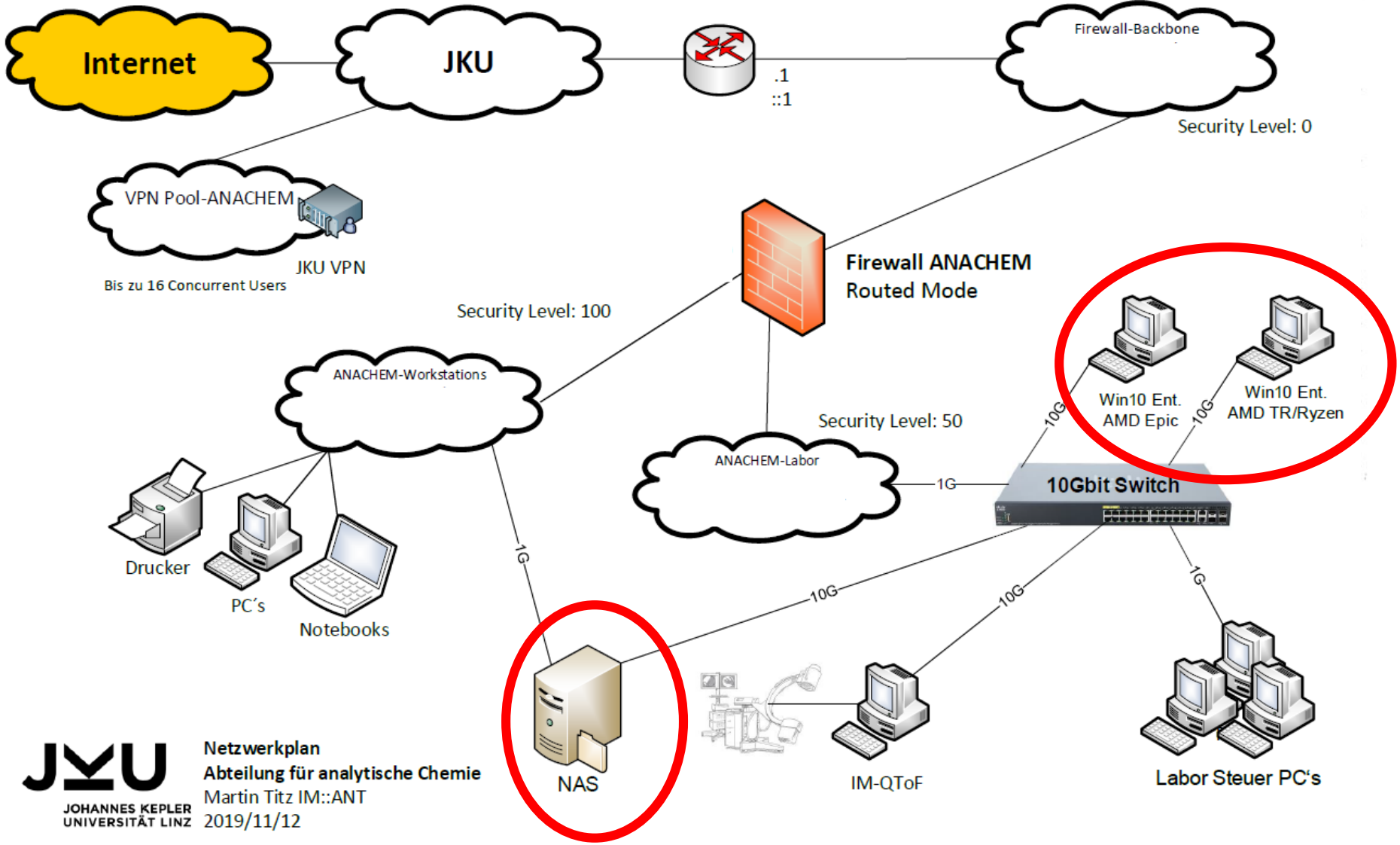


Figure 3. Schematic of the Agilent IM-QTOF instrument. The ion mobility spectrometer is coupled to a quadrupole time-of-flight mass spectrometer using a hexapole ion guide.

Data storage and processing



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Netzwerkplan
Abteilung für analytische Chemie
Martin Titz IM::ANT
2019/11/12

IM-QToF applications

Lipidomics (Bernd Reichl)

- Establishing lipidomics workflow
- ESI optimization (DoE)
- Repeatability of CCS determination

Metabolomics (Thomas Bögl)

- Establishing metabolomics workflow

Pharmaceutical drugs (Armin Guntner)

- CCS values as predictors for blood brain barrier permeation

Plant metabolomics (Franz Mlynek)

- CCS values as measure to assign drug metabolites to parent drugs

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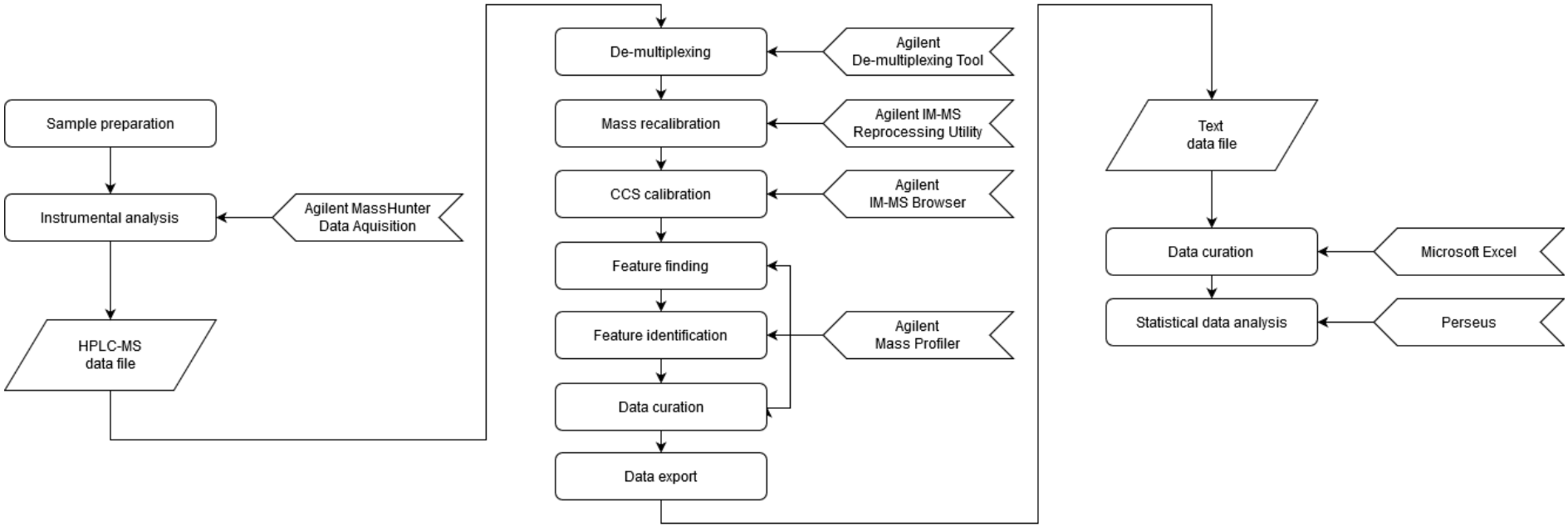
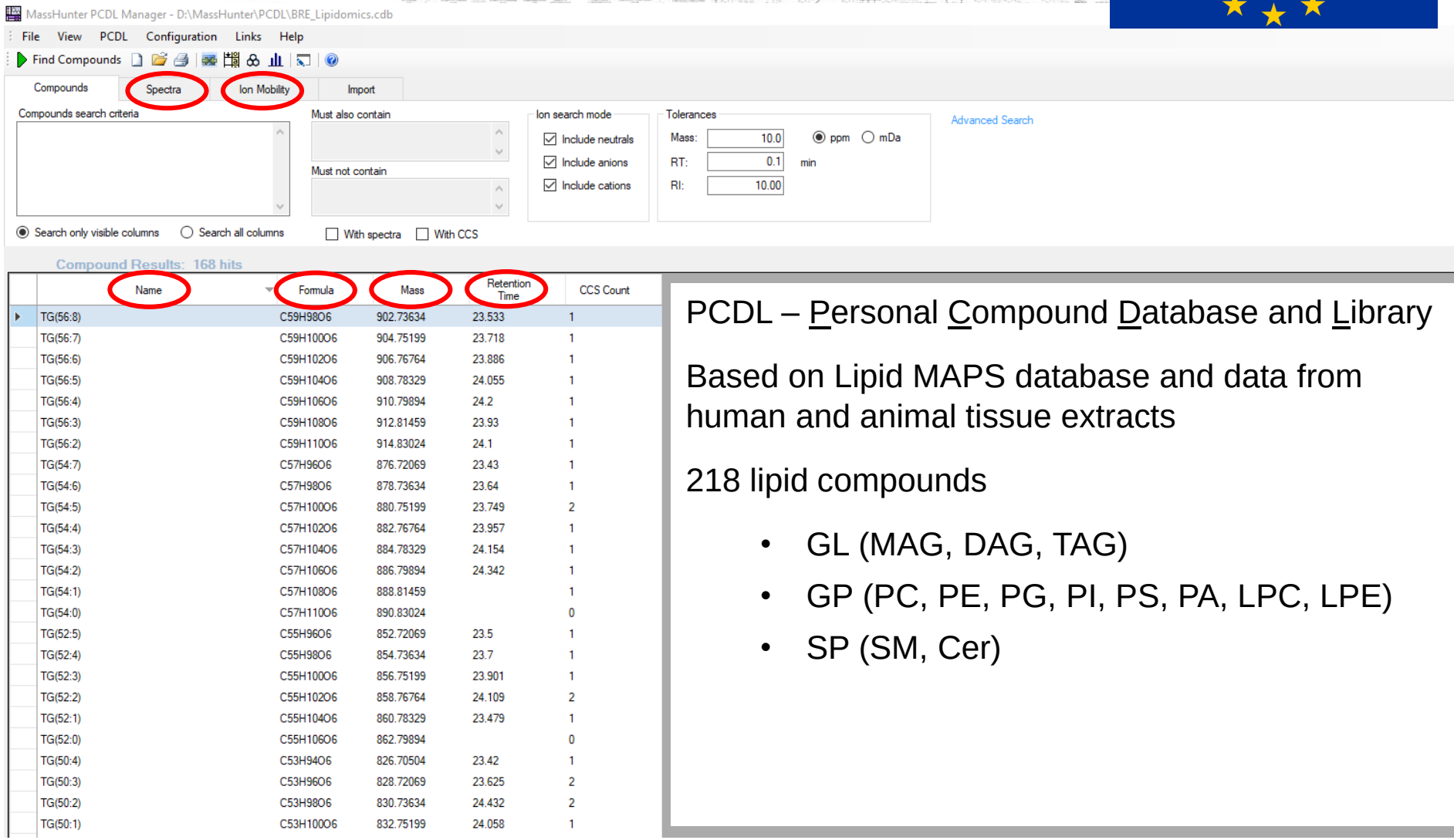
Lipidomics workflow



Establishment of in house lipid database



Name	Formula	Mass	Retention Time	CCS Count
TG(56:8)	C59H98O6	902.73634	23.533	1
TG(56:7)	C59H100O6	904.75199	23.718	1
TG(56:6)	C59H102O6	906.76764	23.886	1
TG(56:5)	C59H104O6	908.78329	24.055	1
TG(56:4)	C59H106O6	910.79894	24.2	1
TG(56:3)	C59H108O6	912.81459	23.93	1
TG(56:2)	C59H110O6	914.83024	24.1	1
TG(54:7)	C57H96O6	876.72069	23.43	1
TG(54:6)	C57H98O6	878.73634	23.64	1
TG(54:5)	C57H100O6	880.75199	23.749	2
TG(54:4)	C57H102O6	882.76764	23.957	1
TG(54:3)	C57H104O6	884.78329	24.154	1
TG(54:2)	C57H106O6	886.79894	24.342	1
TG(54:1)	C57H108O6	888.81459		1
TG(54:0)	C57H110O6	890.83024		0
TG(52:5)	C55H96O6	852.72069	23.5	1
TG(52:4)	C55H98O6	854.73634	23.7	1
TG(52:3)	C55H100O6	856.75199	23.901	1
TG(52:2)	C55H102O6	858.76764	24.109	2
TG(52:1)	C55H104O6	860.78329	23.479	1
TG(52:0)	C55H106O6	862.79894		0
TG(50:4)	C53H94O6	826.70504	23.42	1
TG(50:3)	C53H96O6	828.72069	23.625	2
TG(50:2)	C53H98O6	830.73634	24.432	2
TG(50:1)	C53H100O6	832.75199	24.058	1

PCDL – Personal Compound Database and Library

Based on Lipid MAPS database and data from human and animal tissue extracts

218 lipid compounds

- GL (MAG, DAG, TAG)
- GP (PC, PE, PG, PI, PS, PA, LPC, LPE)
- SP (SM, Cer)

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Lipidomics PCDL

218 lipids in total

150 with RTs

94 with CCS values

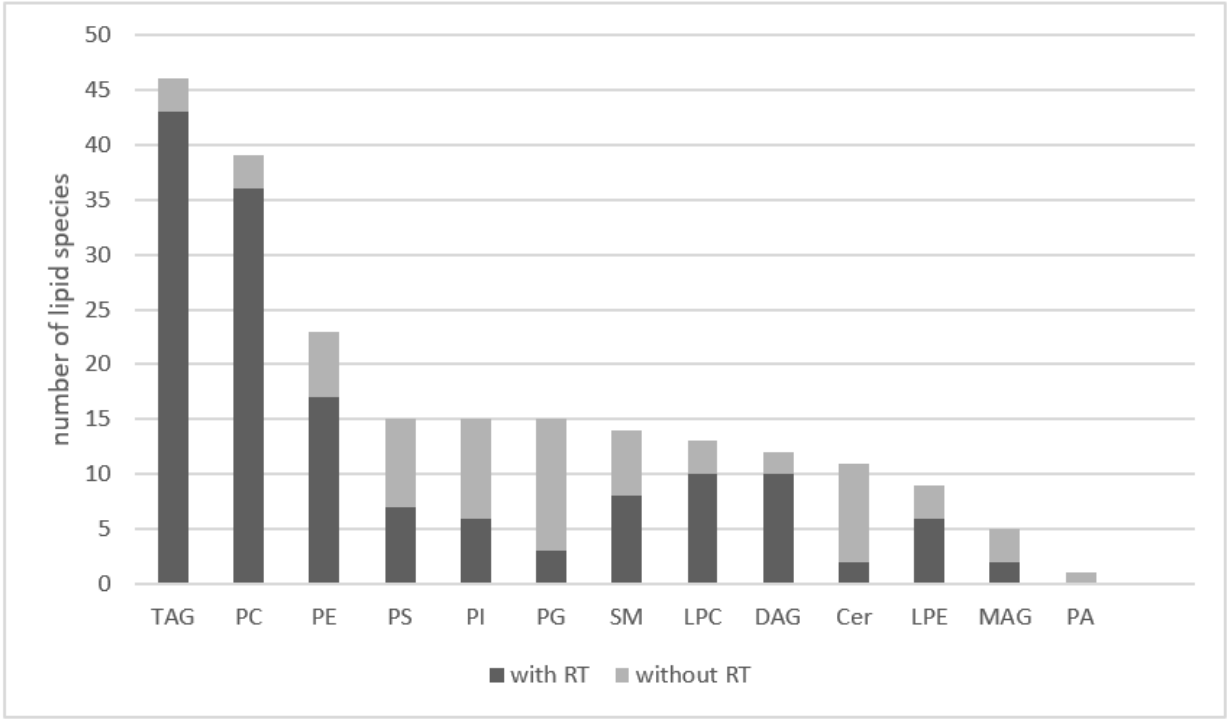

Figure 15: Overview on lipid classes and numbers of individual lipid species included in the final PCDL. The bars show numbers of lipid species per lipid class and the ratio of compounds attributed with RTs (dark grey) and compounds without RTs (bright grey). The lipid classes with highest total numbers of individual compounds are TG (46 species), PC (39 species) and PE (23 species). The total number of lipid species covered in the final PCDL was 218.

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Repeatability of CCS determination

Table 19: Mean CCS values and relative standard deviations (RSDs) of eight investigated deuterated lipid standards in a mixed standard (methanol matrix) and in a pooled animal tissue matrix. CCS values and RSDs were calculated for all analysed samples (methanol matrix and pooled animal tissue matrix, n=24), for methanol matrix (n=12), and for pooled animal tissue matrix (n=12). CCS values from the CCS compendium are added, showing good reproducibility (n.a. = not available).*

	All samples		methanol matrix		animal tissue matrix		CCS compendium
	mean CCS (Å²)	RSD (%)	mean CCS (Å²)	RSD (%)	mean CCS (Å²)	RSD (%)	CCS (Å²)
dPC	285.90	0.13	285.70	0.11	286.09	0.11	285.4
dLPC	234.61	0.12	234.68	0.12	234.54	0.12	235.0
dPE	273.20	0.12	273.38	0.10	273.02	0.11	273.5
dLPE	218.44	0.13	218.45	0.13	218.44	0.13	217.8
dSM	288.02	0.12	287.88	0.11	288.17	0.12	287.8
dCer	253.66	0.15	253.89	0.11	253.42	0.11	n.a.
dTG	311.86	0.11	312.02	0.10	311.70	0.11	n.a.
dDG	257.31	0.11	257.33	0.12	257.28	0.11	258.0

Differences ≤ 0.19%

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Thank you for your attention

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