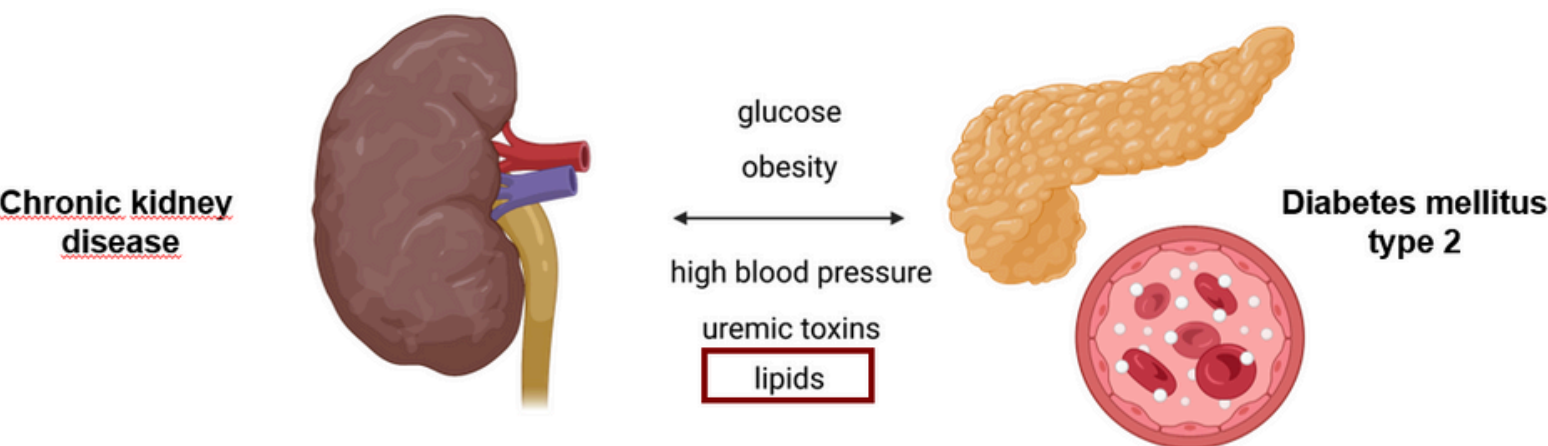


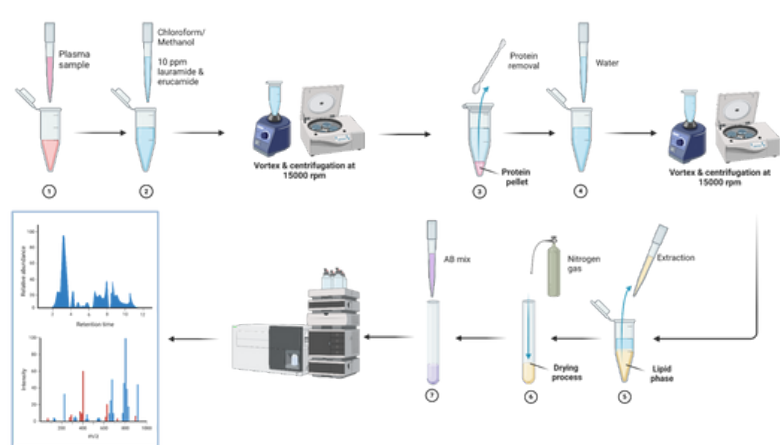
STSM: Extracting MS signals features relevant to chronic disease classification

STSM Goal



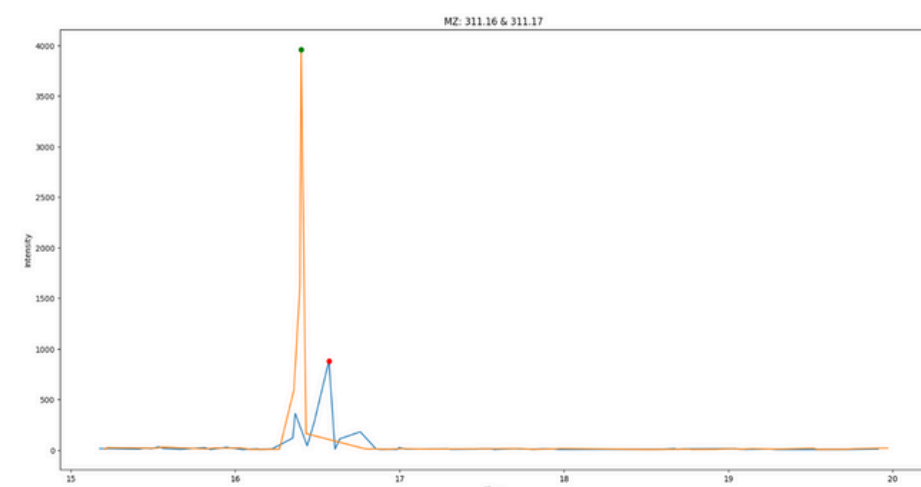
The aim of this STSM was to integrate advanced Data Science and Machine Learning algorithms and methodologies to extract common patterns within MSA signals of blood plasma, across patients with and without a specific chronic disease. More precisely, the aim was to identify novel regulators or key molecules associated with diabetes-related CKD.

Methodology



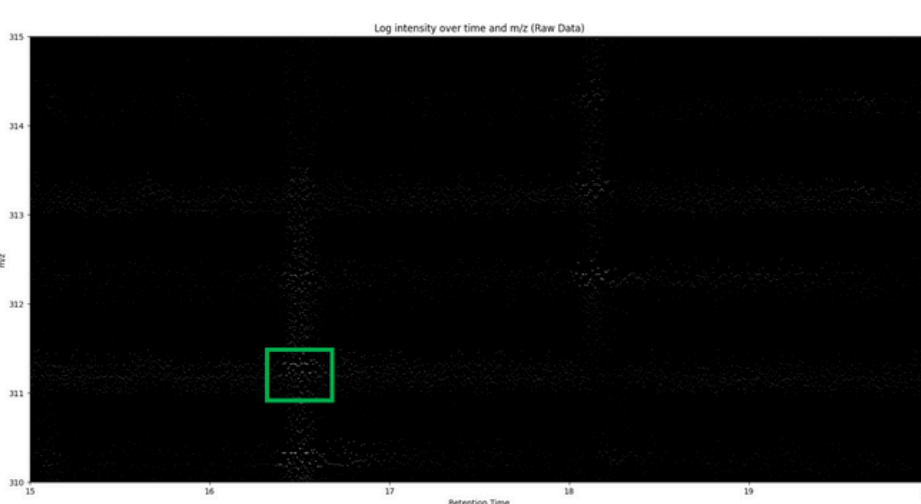
Lipid isolation and mass spectrometry analysis of samples of approx. 600 patients

Data preparation and mass signal detection

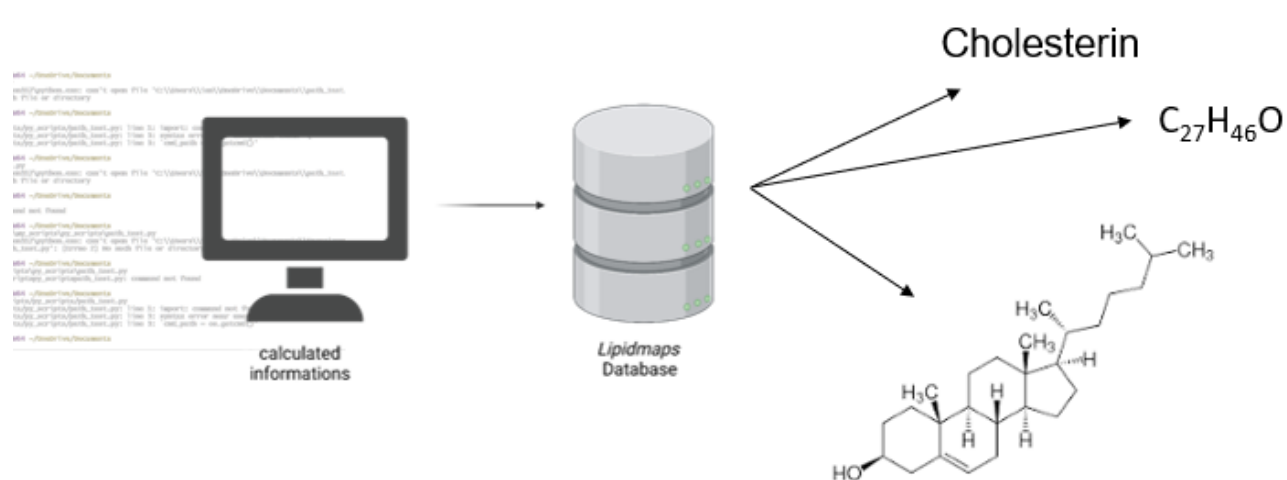


Finding common mass signal across patient groups

Comparison of groups and statistical analysis



Mass signal refinement and lipid mapping



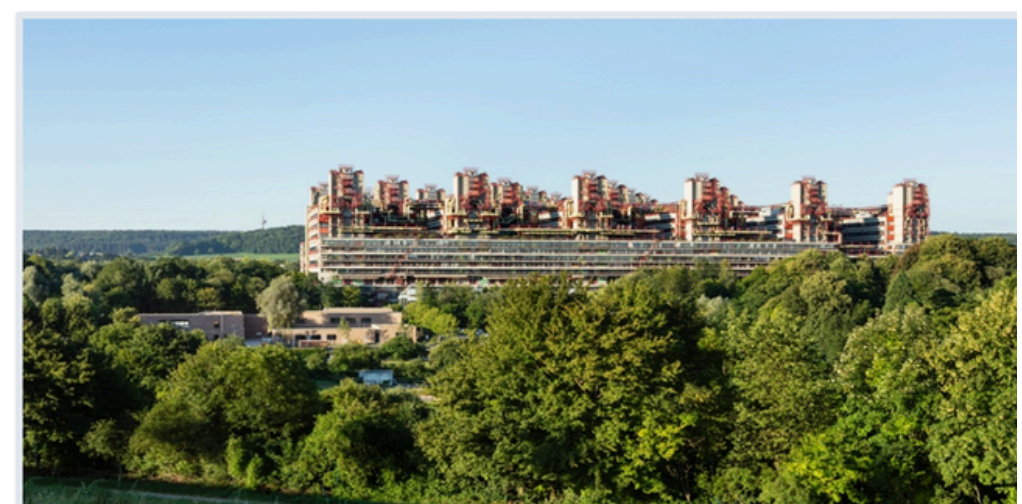
Results and Next Steps

Input Mass	Matched Mass	Delta	Name	Formula	Ion
663.5	663.4983	0.0017	DG 40:9	C43H66O5	[M+H] ⁺
444.5	444.3683	0.1317	CAR 18:0;O	C25H49NO5	[M+H] ⁺
194	194.0659	0.0659	FA 6:2;O4	C6H8O6	[M+NH4] ⁺
685.5	685.5279	0.0279	CerPE 36:3;O2	C38H73N2O6P	[M+H] ⁺
549.5	549.4643	0.0357	FA 33:0;O	C33H66O3K	[M+K] ⁺

Identification of the top ten most important lipids

Selection of samples with the highest intensity for these lipids and perform a new mass spectrometry analysis (MS2) for identification

Mass spectrometric lipid database and reference substance will be used to compare the fragment spectra



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In collaboration with: Juliane Hermann, PhD



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Grantee: Ana Todorovska, PhD candidate