

SUPPLEMENTARY INFORMATION

Table 1. Statistically significant masses depending on the statistical test.

<b>Name of group</b>	<b>Statistics test</b>	<b>N° of features</b>
group I (masses common for all samples)	SUS-plot - condition	79
	SUS-plot - treatment	15
CVCR	T-test	54
	Splot	34
	Jack knife	61
	together	96
DVDR	T-test	21
	Splot	52
	Jack knife	91
	together	104
group II (separation according to treatment CV+DV and CR+DR)	T-test	93
	Splot	14
	Jack knife	46
	together	120

Fig.1

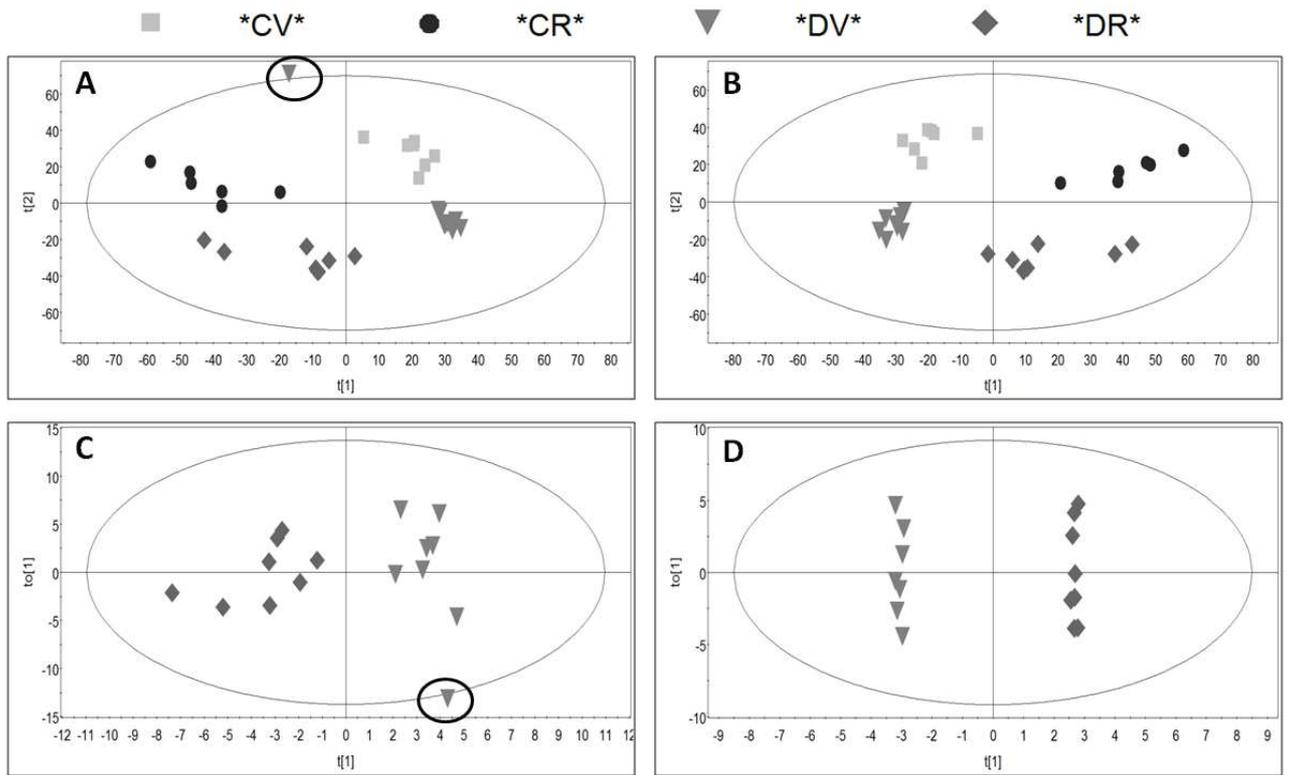


Fig.2

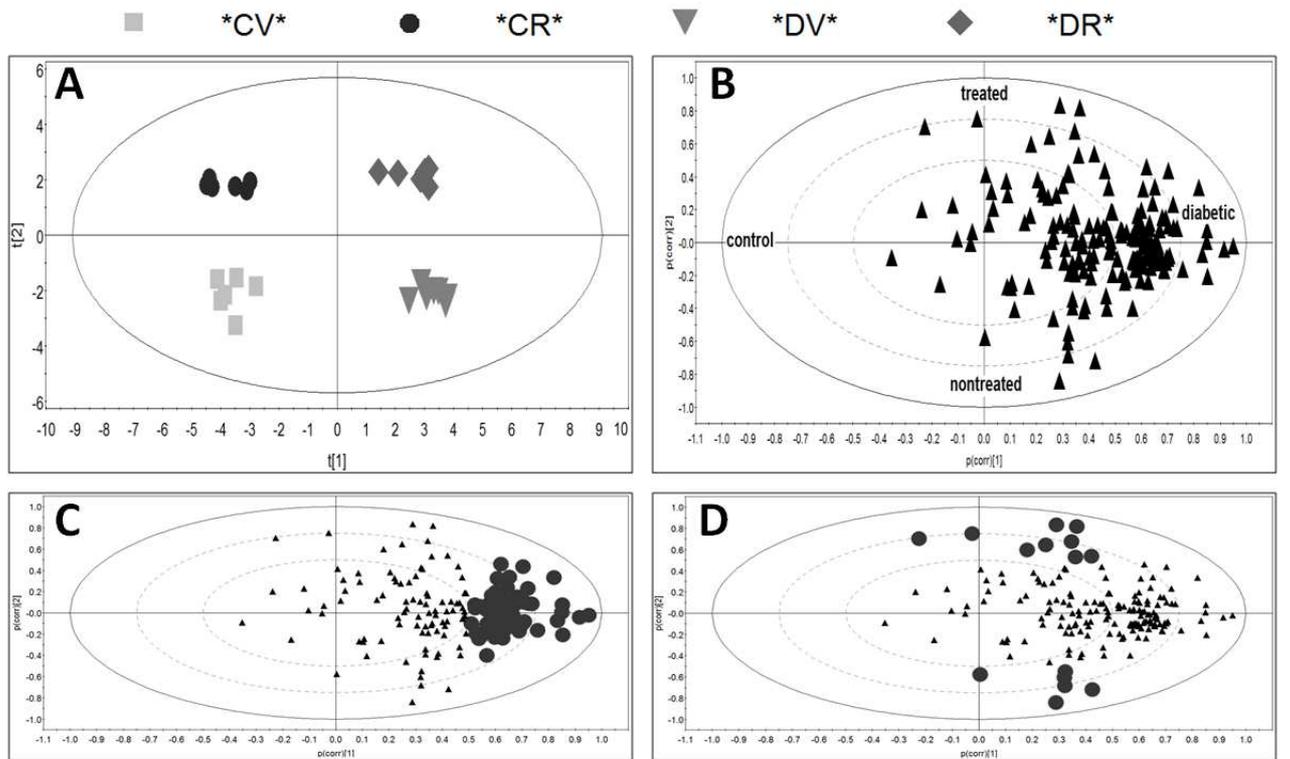
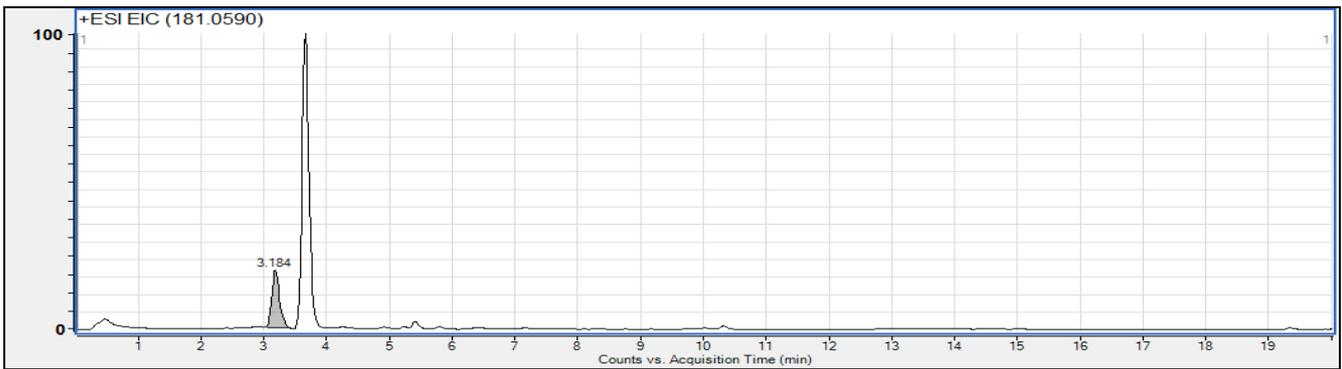
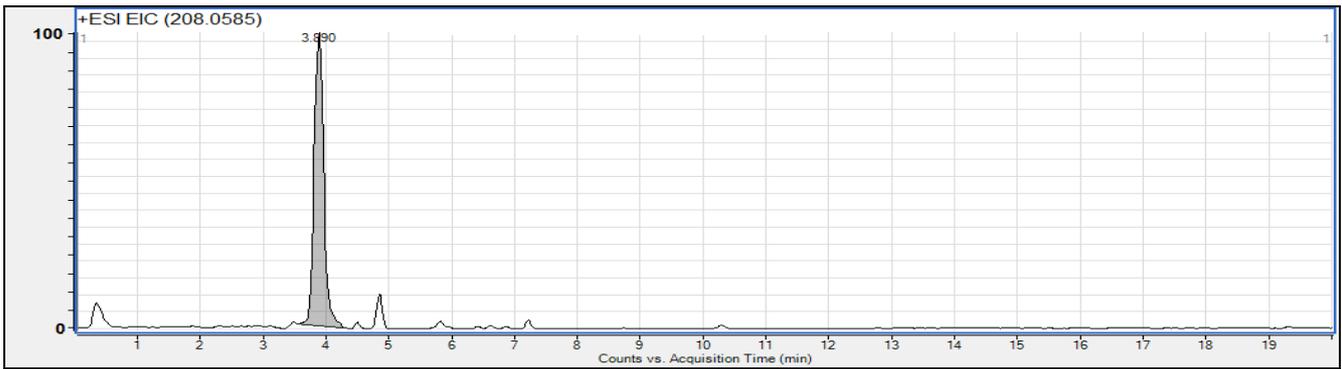
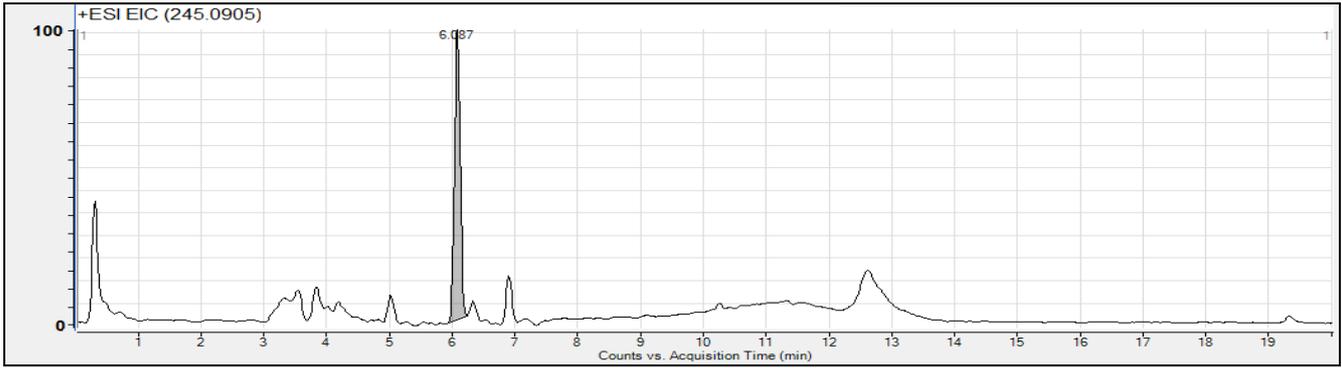
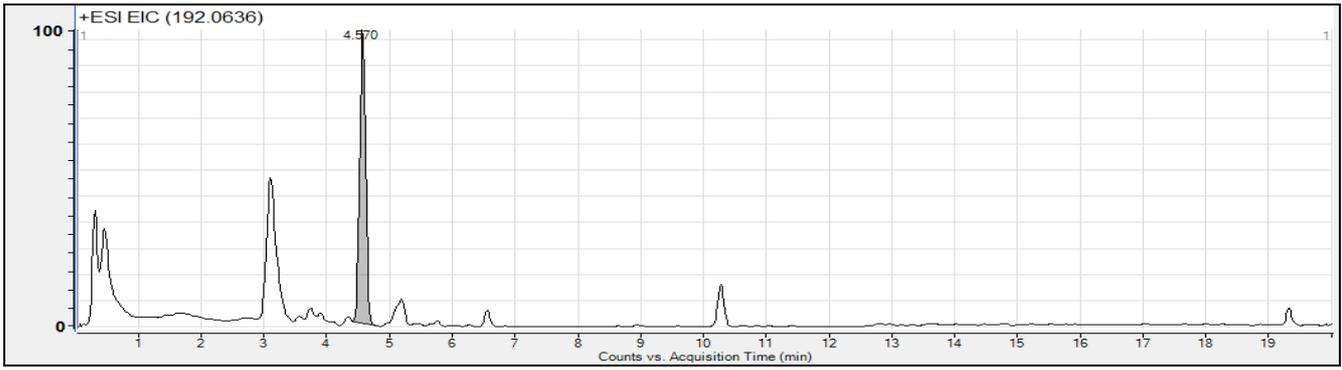
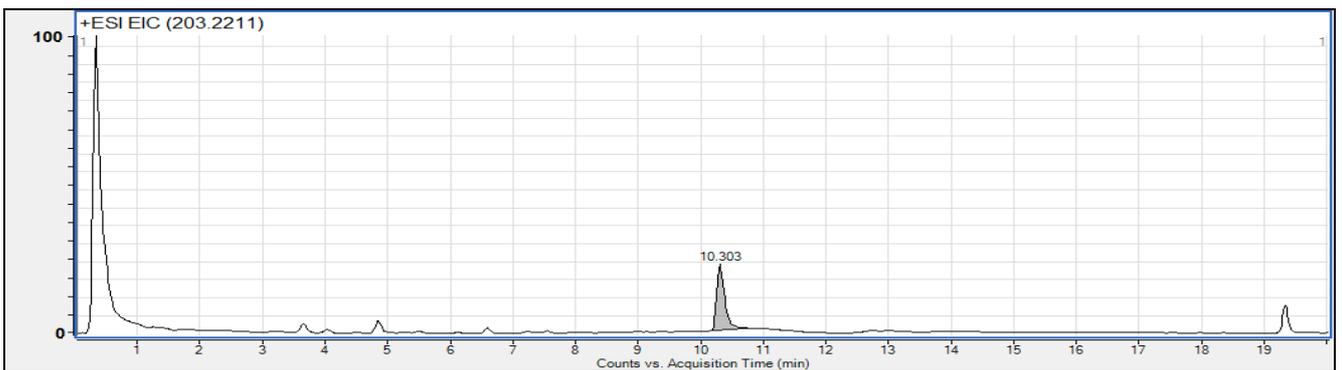
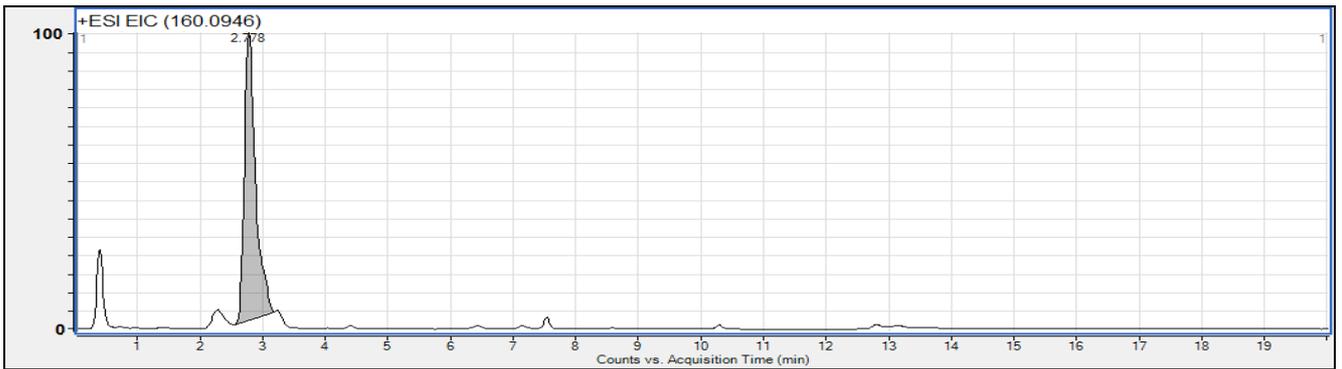
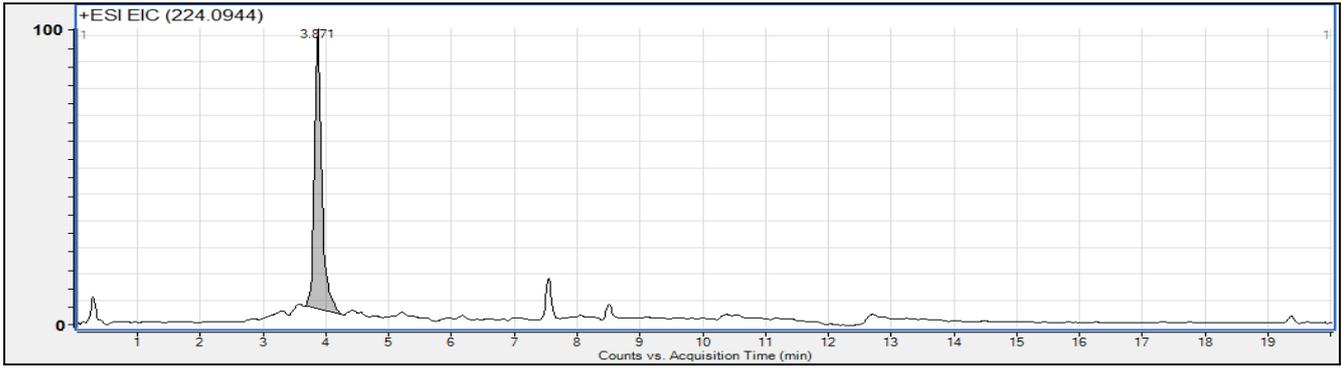
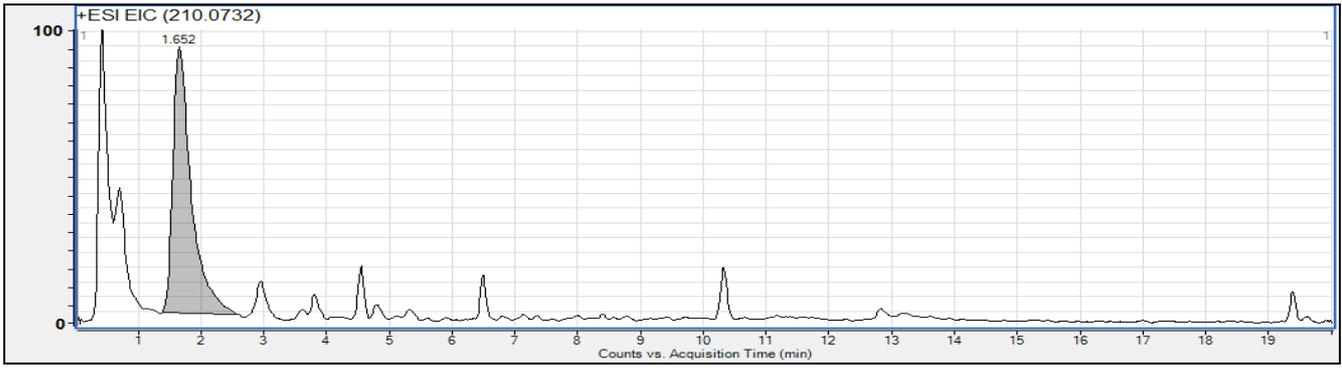
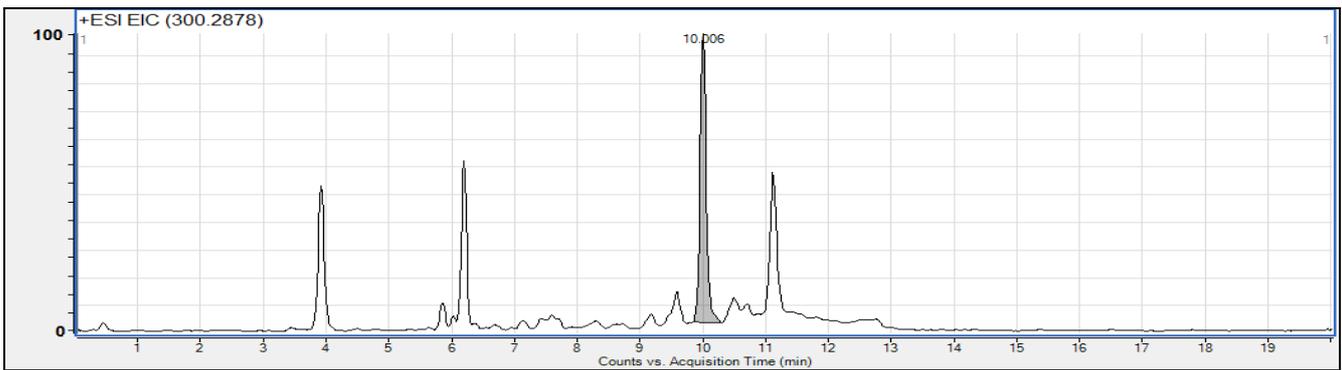
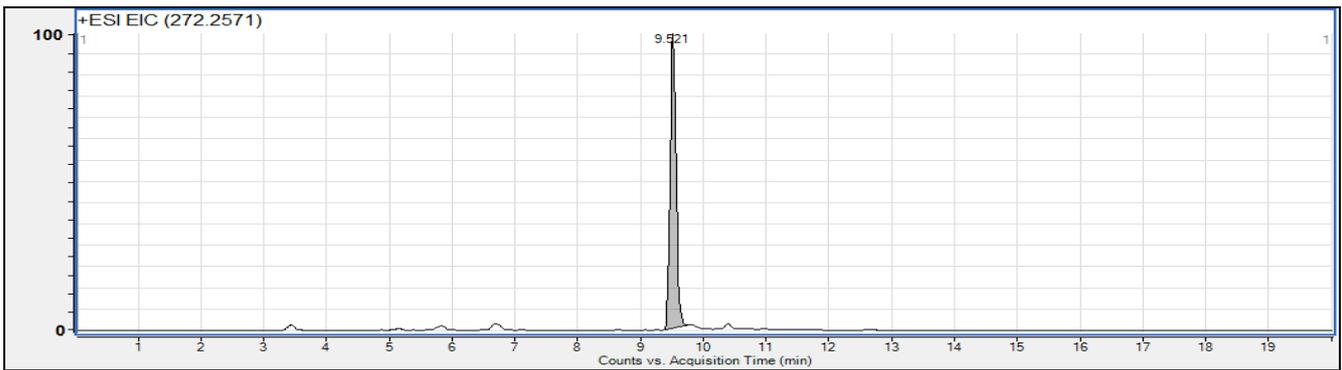
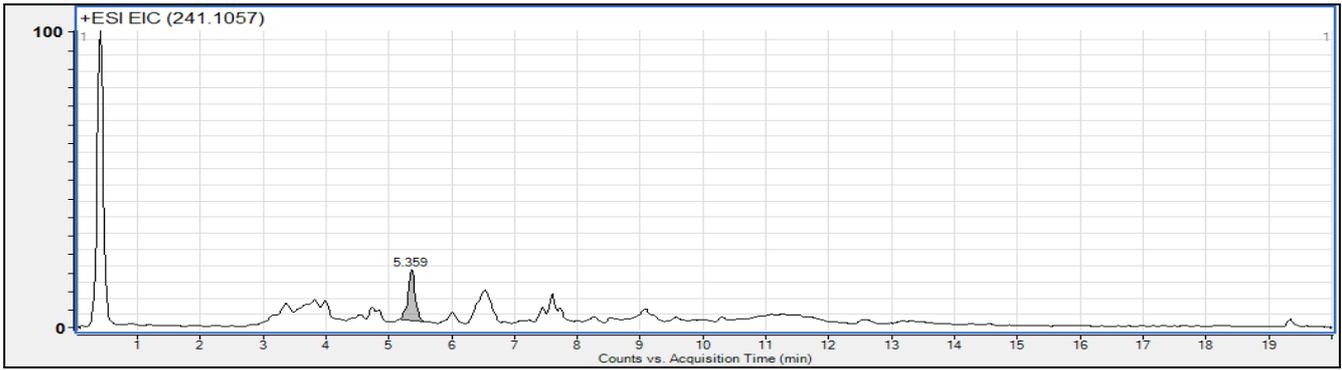
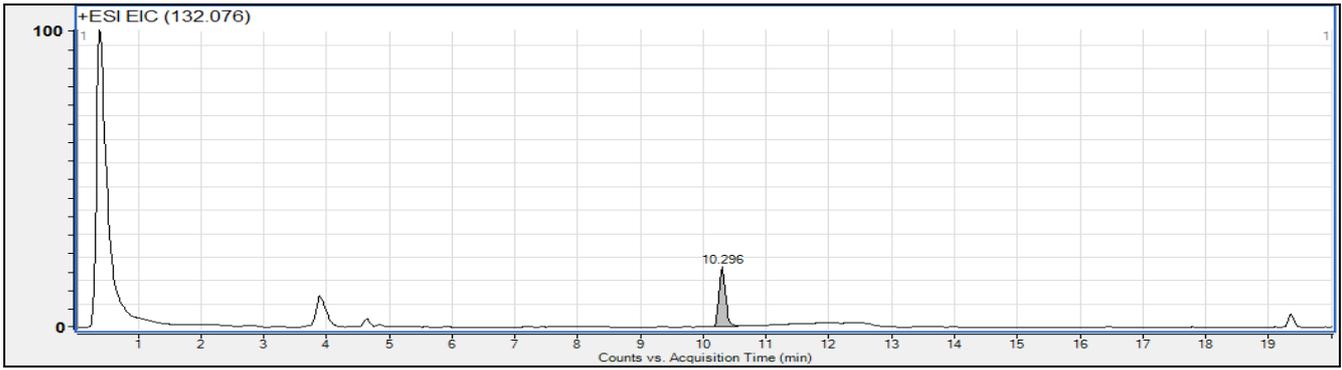
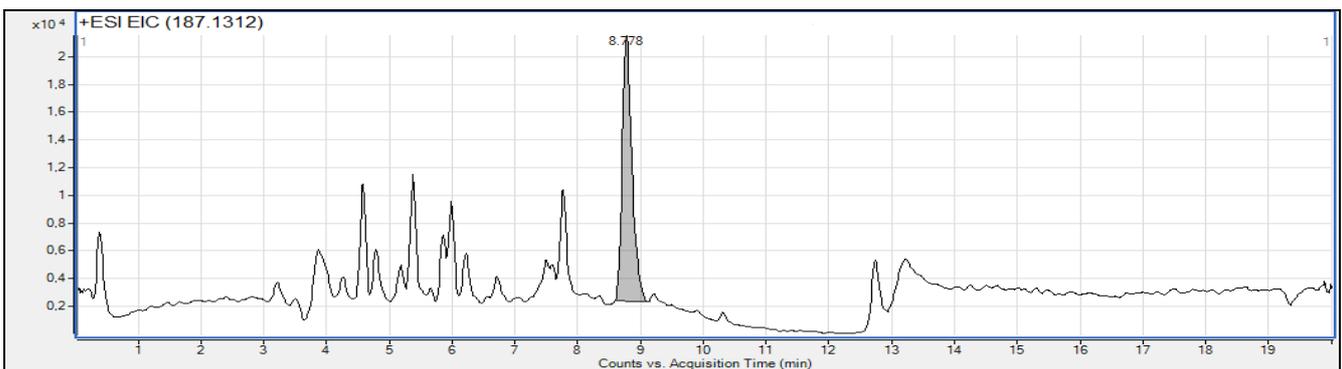
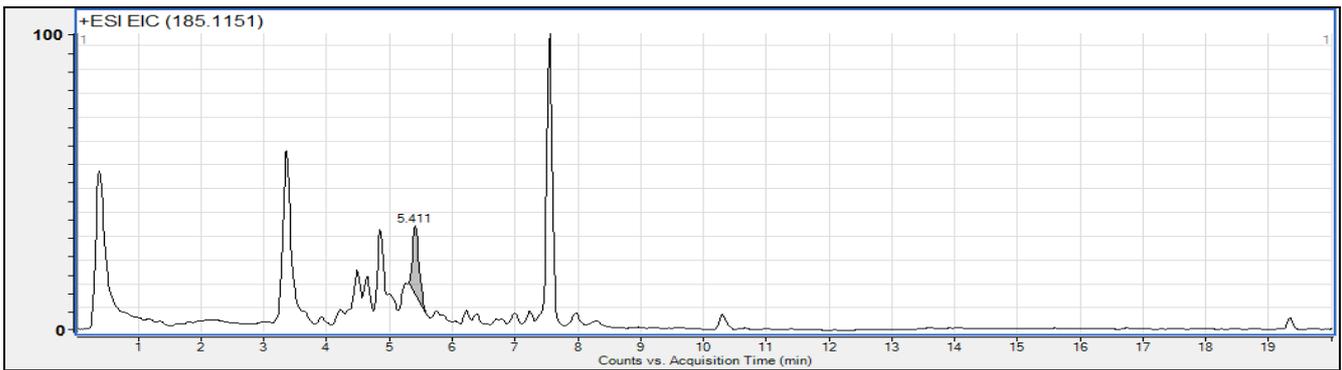
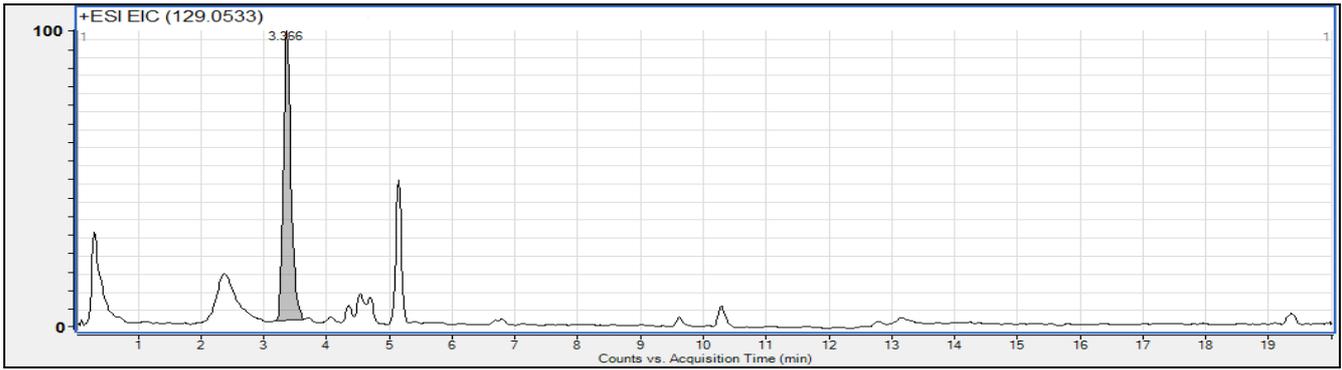
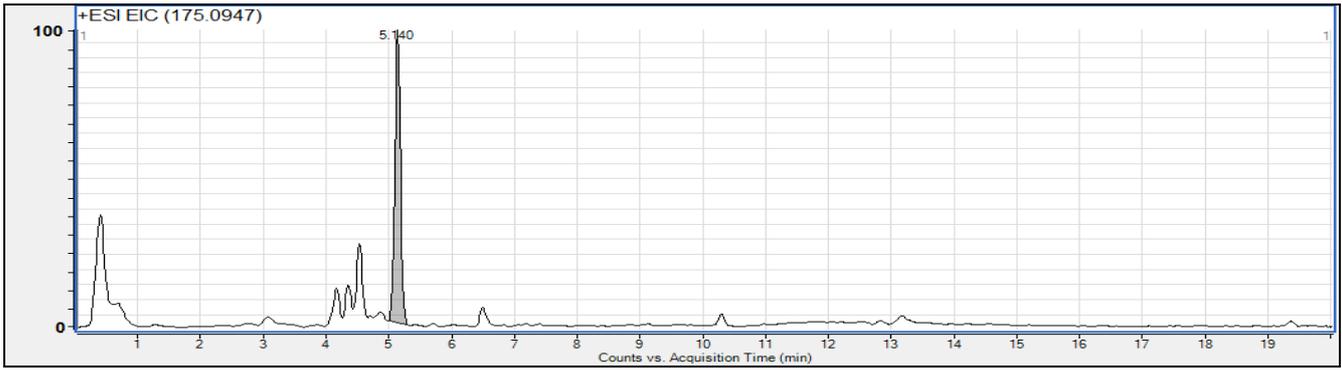


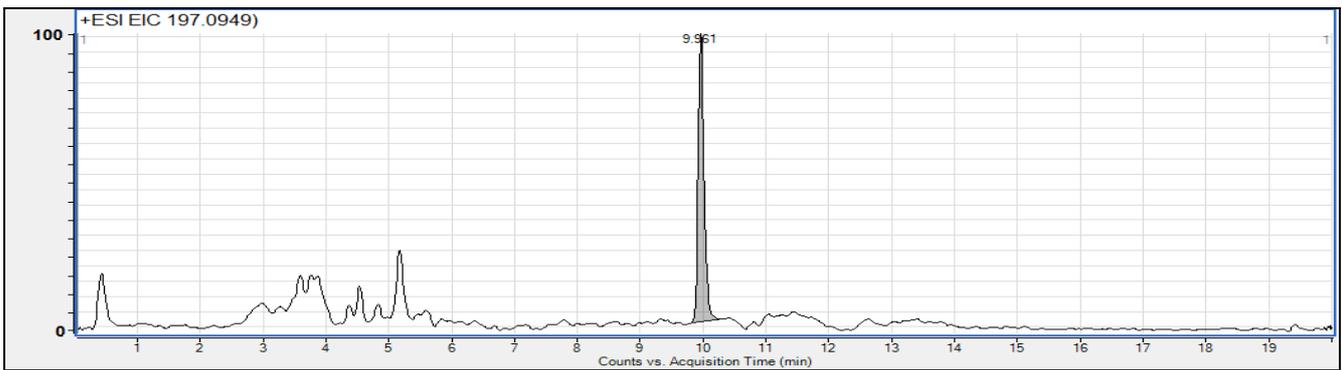
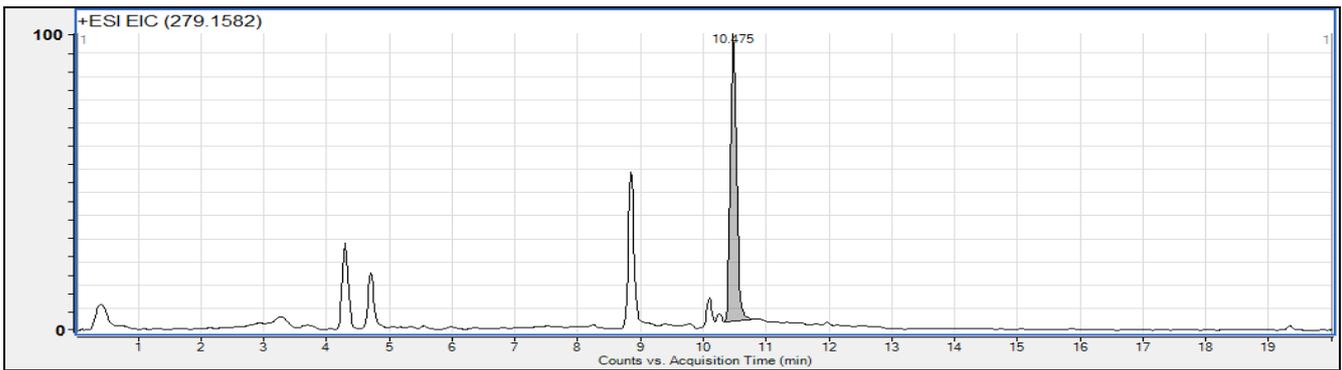
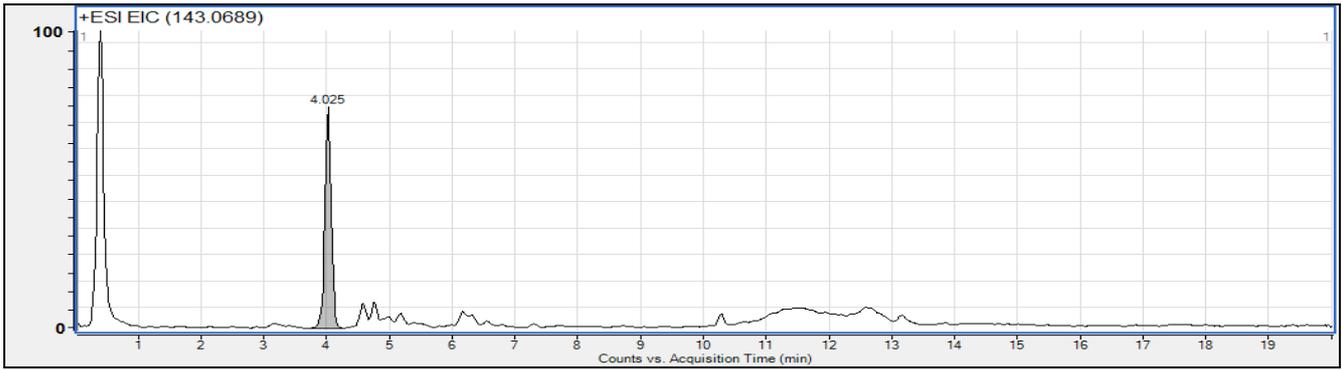
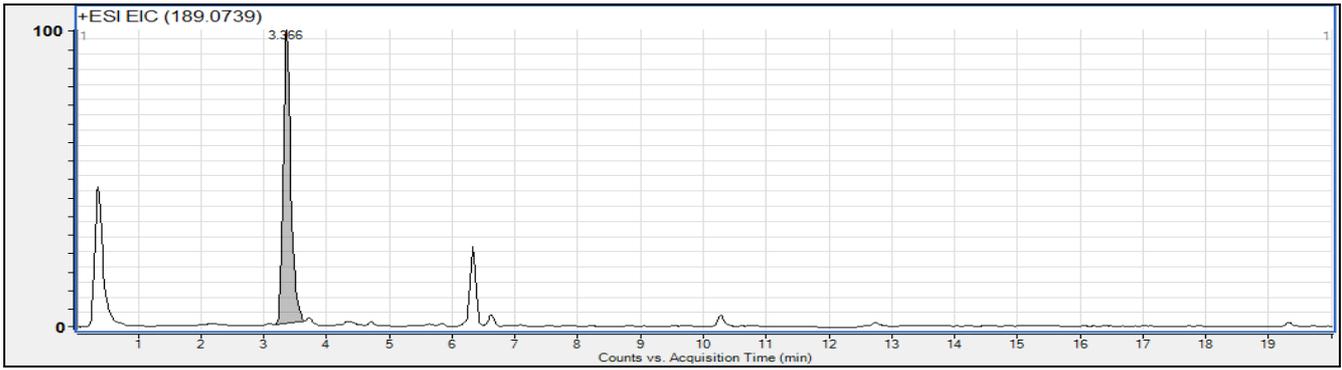
Fig.3











## Figure captions

### Figure 1

Influence of outliers in model quality and separation. Upper part presents the plot with (A) and without (B) a rat which was not diabetic. Lower part shows plot with (C) and without (D) a rat with urine from only 18 hours. Outliers are marked by the circles. (A) Scores plot for a PCA model built with the whole data set normalized to urine volume for all samples including outliers. Quality parameters for the model: explained variance:  $R^2=0.27$ , predicted variance:  $Q^2=0.05$ . (B) Scores plot for a PCA model built with the whole data set normalized to urine volume for samples without outlier. Quality parameters for the model: explained variance:  $R^2=0.21$ , predicted variance:  $Q^2=0.08$ . (C) Scores plot for OPLS-DA model built with the masses common for diabetics samples (DV+DR) with outlier. Quality parameters for the model: explained variance:  $R^2=0.56$ , predicted variance:  $Q^2=0.19$ . (D) Scores plot for OPLS-DA model built with the masses common for diabetics samples (DV+DR) without outlier. Quality parameters for the model: explained variance:  $R^2=0.99$ , predicted variance:  $Q^2=0.85$ .

### Figure 2

(A) Scores plot for O2PLS model built with the masses common for samples, with two Y variables: condition and treatment. Quality parameters for the model: Explained variance  $R^2=0.97$ , predicted variance:  $Q^2=0.81$ . (B) SUS-plot built for O2PLS with the masses common for all samples. Each triangle presents a single mass. (C) SUS-plot with marked by dots statistically significant variables for the condition (control – diabetic). (D) SUS-plot with marked by dots statistically significant variables for the treatment (treated – nontreated).

### Figure 3

Extracted Ion Chromatograms (EICs) for all identified compounds that are presented in the table 1. The chromatograms are ordered in the same way as in the table.