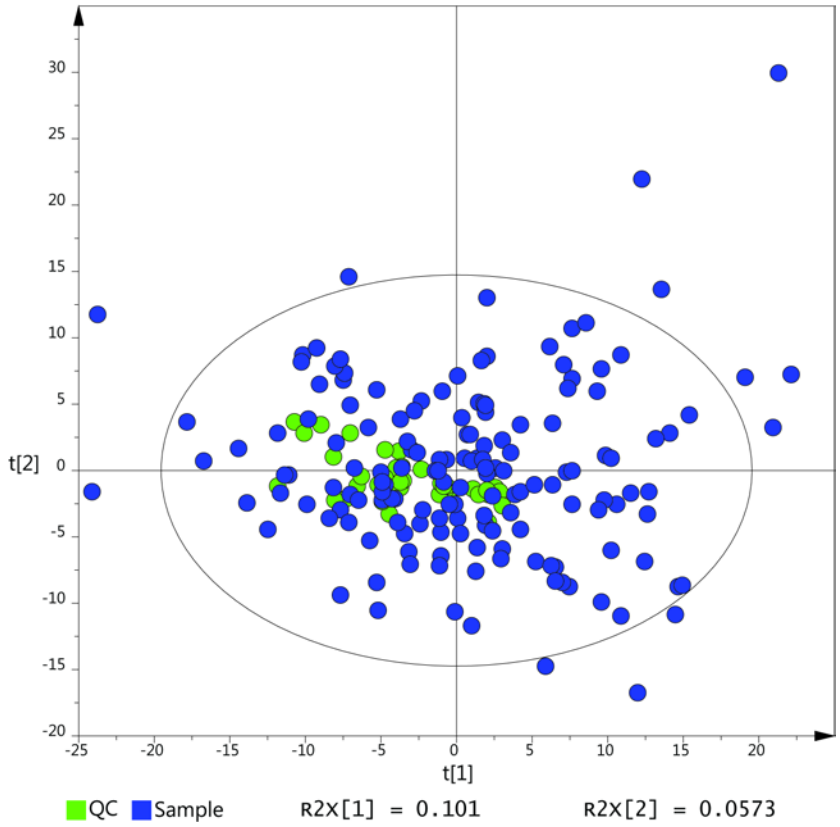
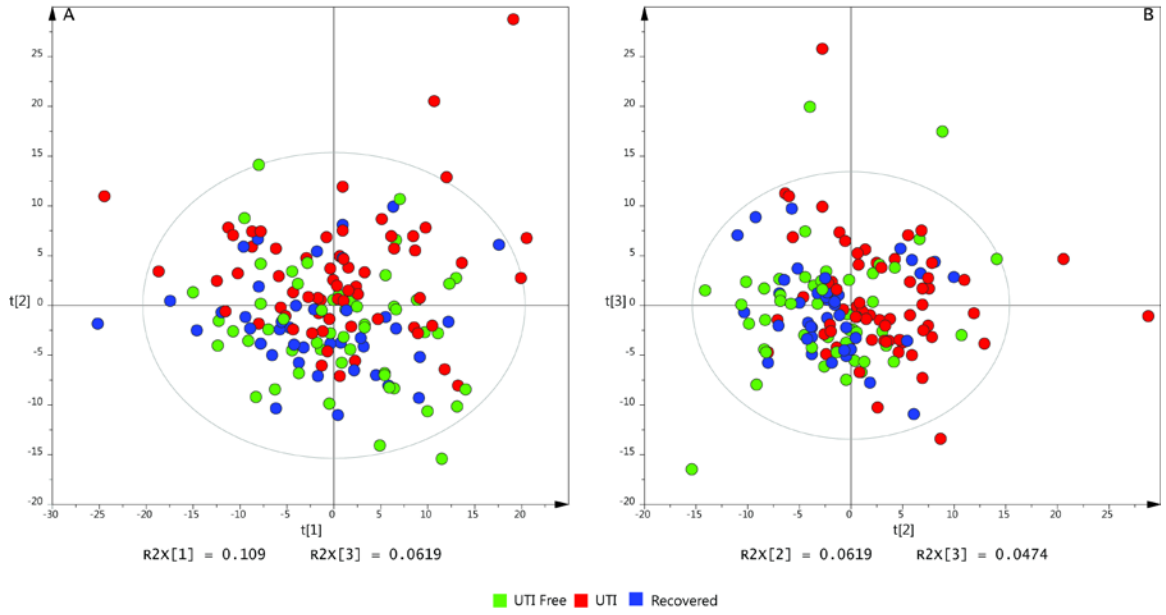
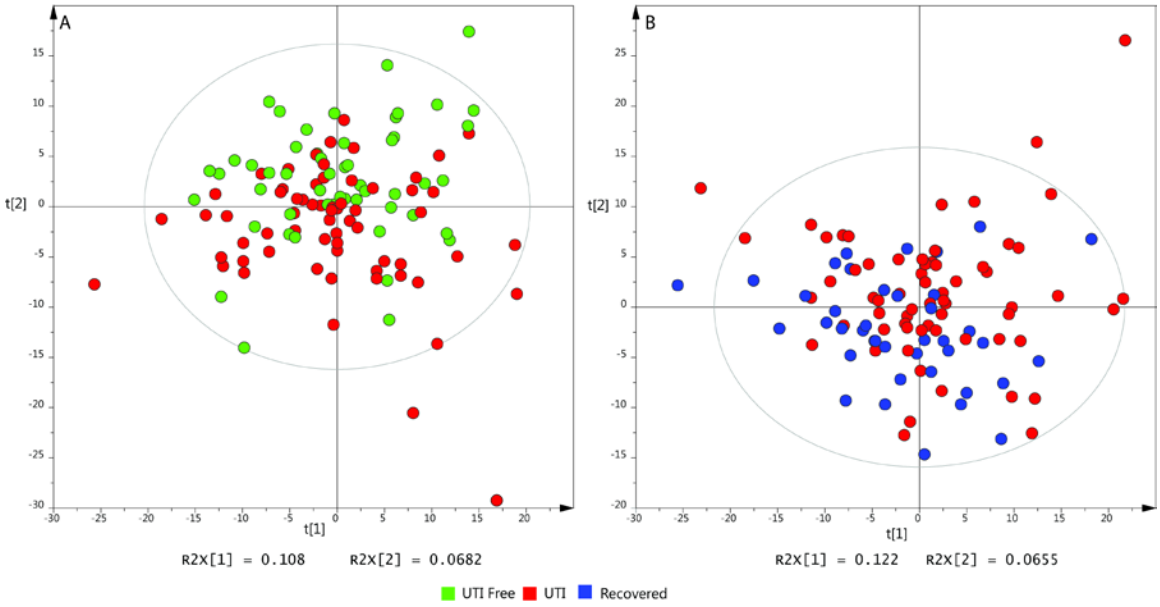
Electronic Supplementary Material (ESI) for Analyst.



Supplementary Figure 1. The score plot of a PCA model built on the entire data set, 24 components cover 56% of variance, dots are colored according to their ID: QC and samples.

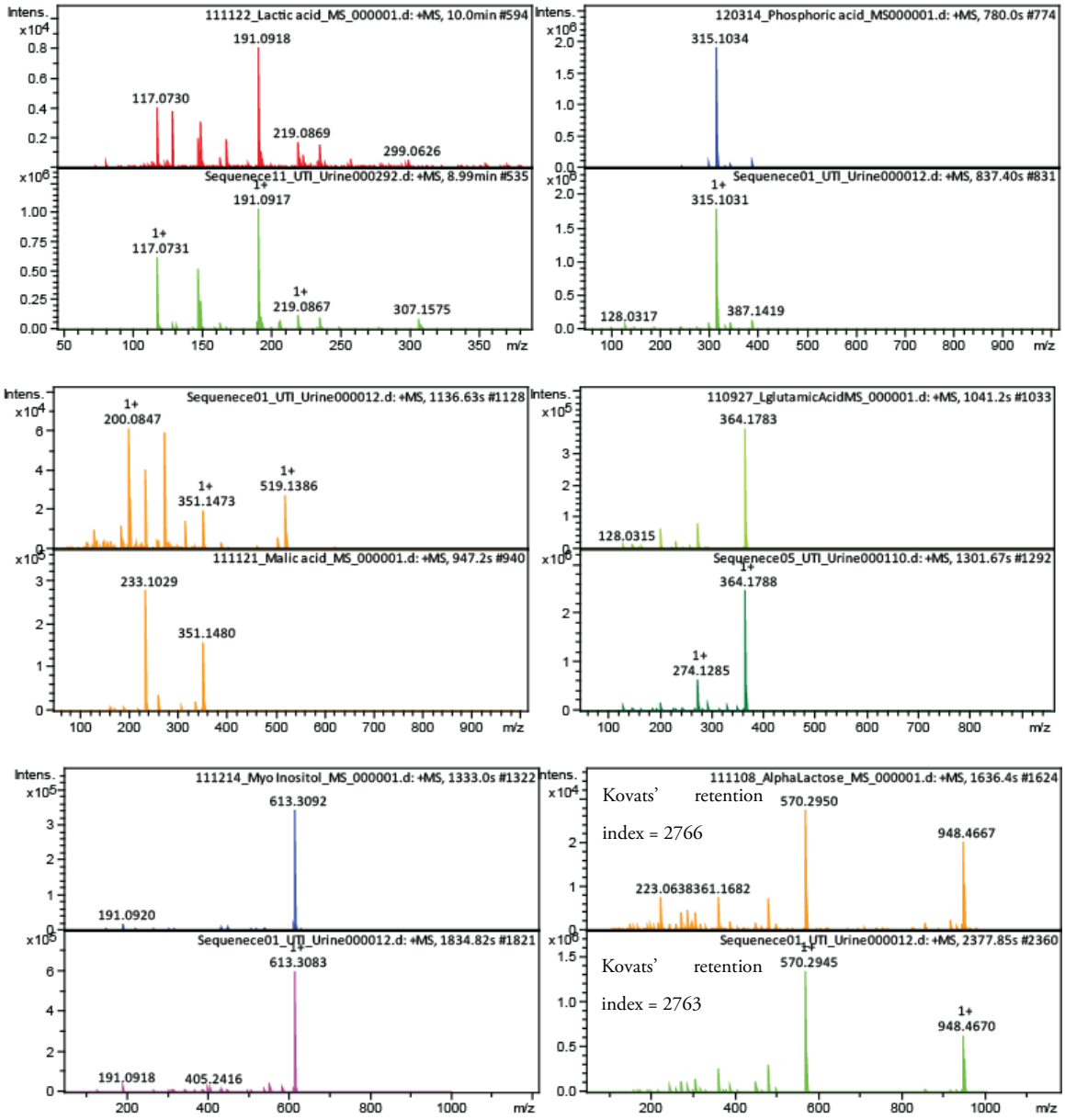


Supplementary Figure 2. A score plots showing the first and second (A) and the second and third (B) components of the PCA model (24 components cover 59% of the variance) built of 155 clinical samples. The samples are coloured according to the infectious status. The first and the second components display a major trend which cover more than 16% of the total variability (A). However, the second and the third component show a tendency in the cluster of the controls and UTI patients t=30 days against UTI patients t=0 day (B).



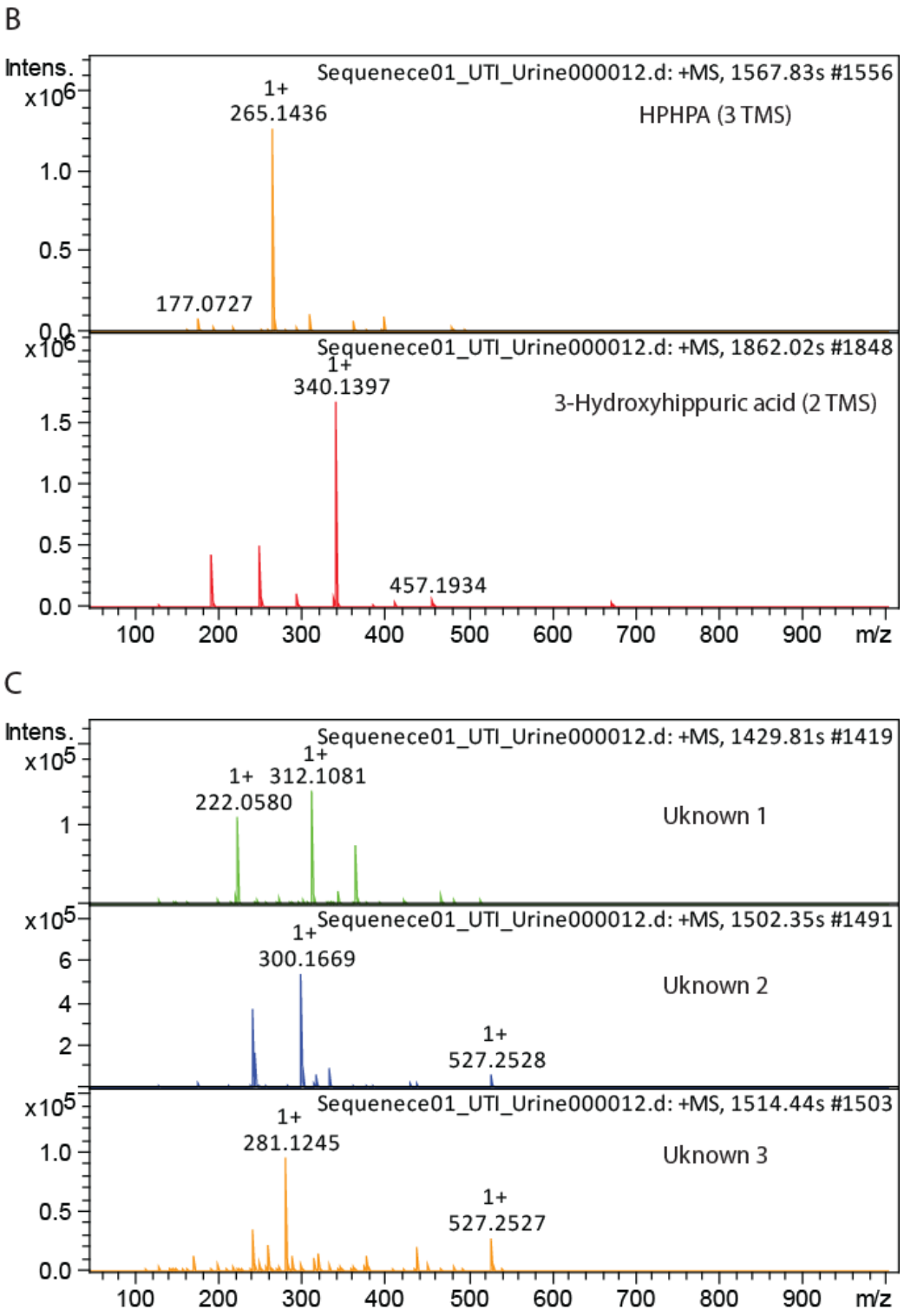
Supplementary Figure 3. PCA score plots for the models built for cross-sectional (A) and longitudinal data (B) parts separately. A) UTI Free + UTI t=0; 9 components cover 57% of the variance. B) UTI t=0 + UTI t=30; 16 components cover 55% of the variance .

A

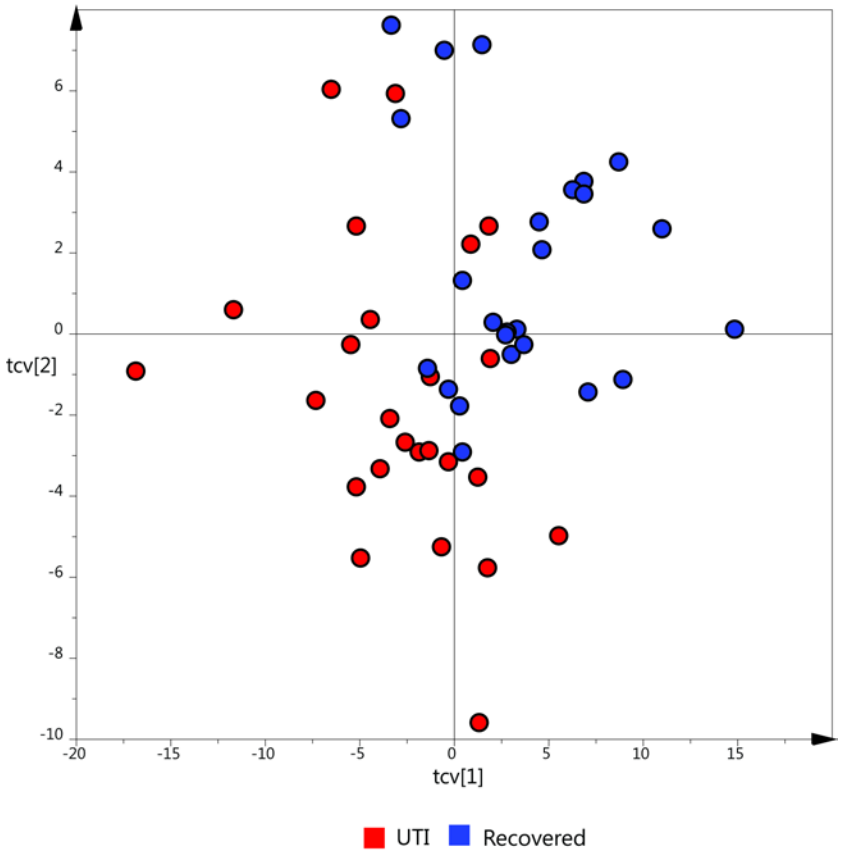


Kovats' retention index = 2766

Kovats' retention index = 2763

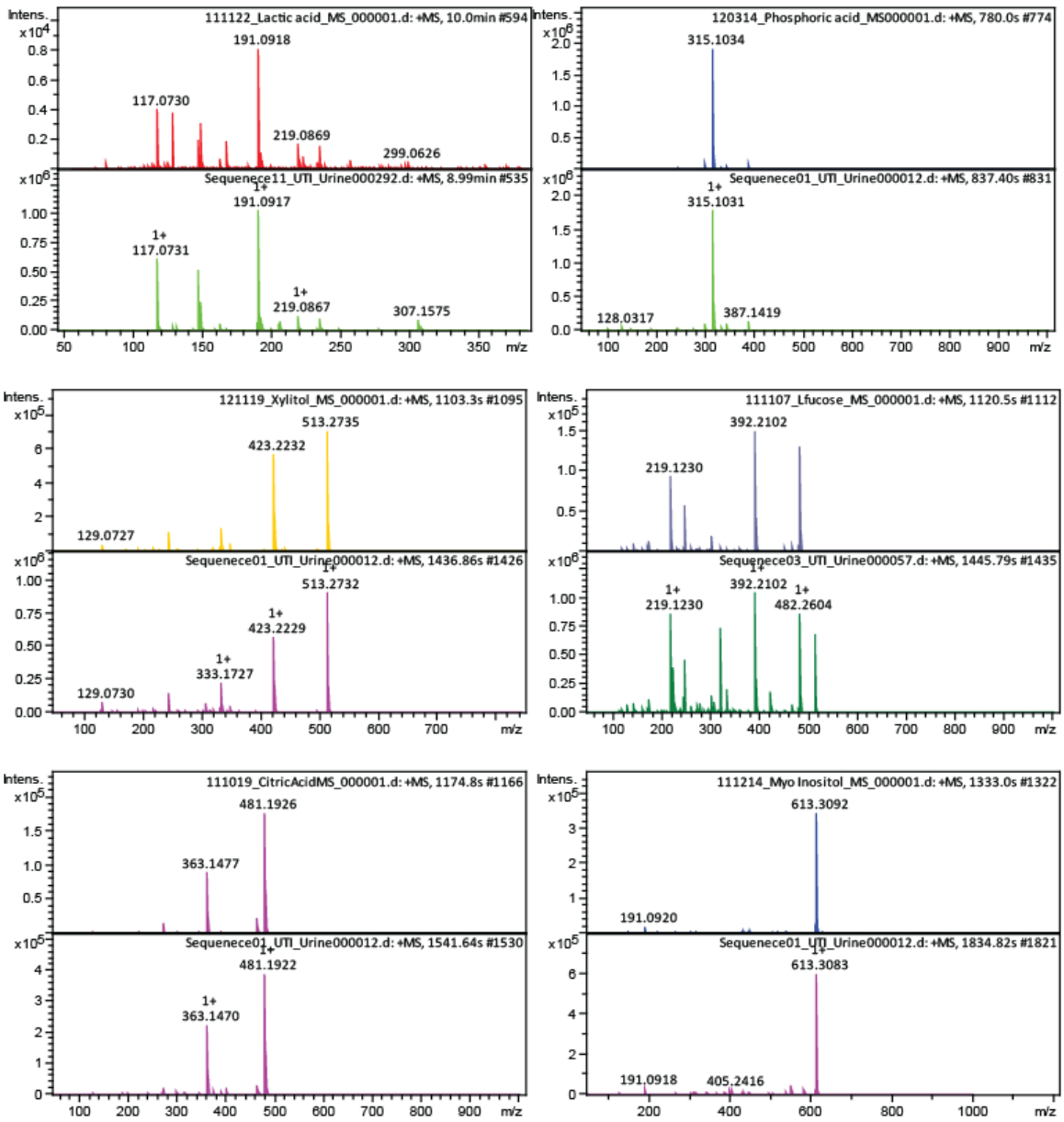


Supplementary Figure 4. MS spectra of classifiers reported in Table 2. A) Compounds identified with library matching B) compounds identified with *de novo* identification protocol and C) Unknown compounds.



Supplementary Figure 5. Cross-validates score plot of a PLS-DA built on UTI subjects (*E.coli*) who presented samples at both time point t=0 and t=30 days (50 samples in total). R2X=0.186, R2Y=0.816 Q2=0.46.

A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117.0730
219.0869
299.0626
Sequenece11_UTI_Urine000292.d: +MS, 8.99min #535
191.0917
117.0731
219.0867
307.1575
120314_Phosphoric acid_MS000001.d: +MS, 780.0s #774
315.1034
Sequenece01_UTI_Urine000012.d: +MS, 837.40s #831
315.1031
128.0317
387.1419
121119_Xylitol_MS_000001.d: +MS, 1103.3s #1095
513.2735
423.2232
129.0727
Sequenece01_UTI_Urine000012.d: +MS, 1436.86s #1426
513.2732
423.2229
333.1727
129.0730
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219.1230
Sequenece03_UTI_Urine000057.d: +MS, 1445.79s #1435
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219.1230
482.2604
111019_CitricAcidMS_000001.d: +MS, 1174.8s #1166
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363.1470
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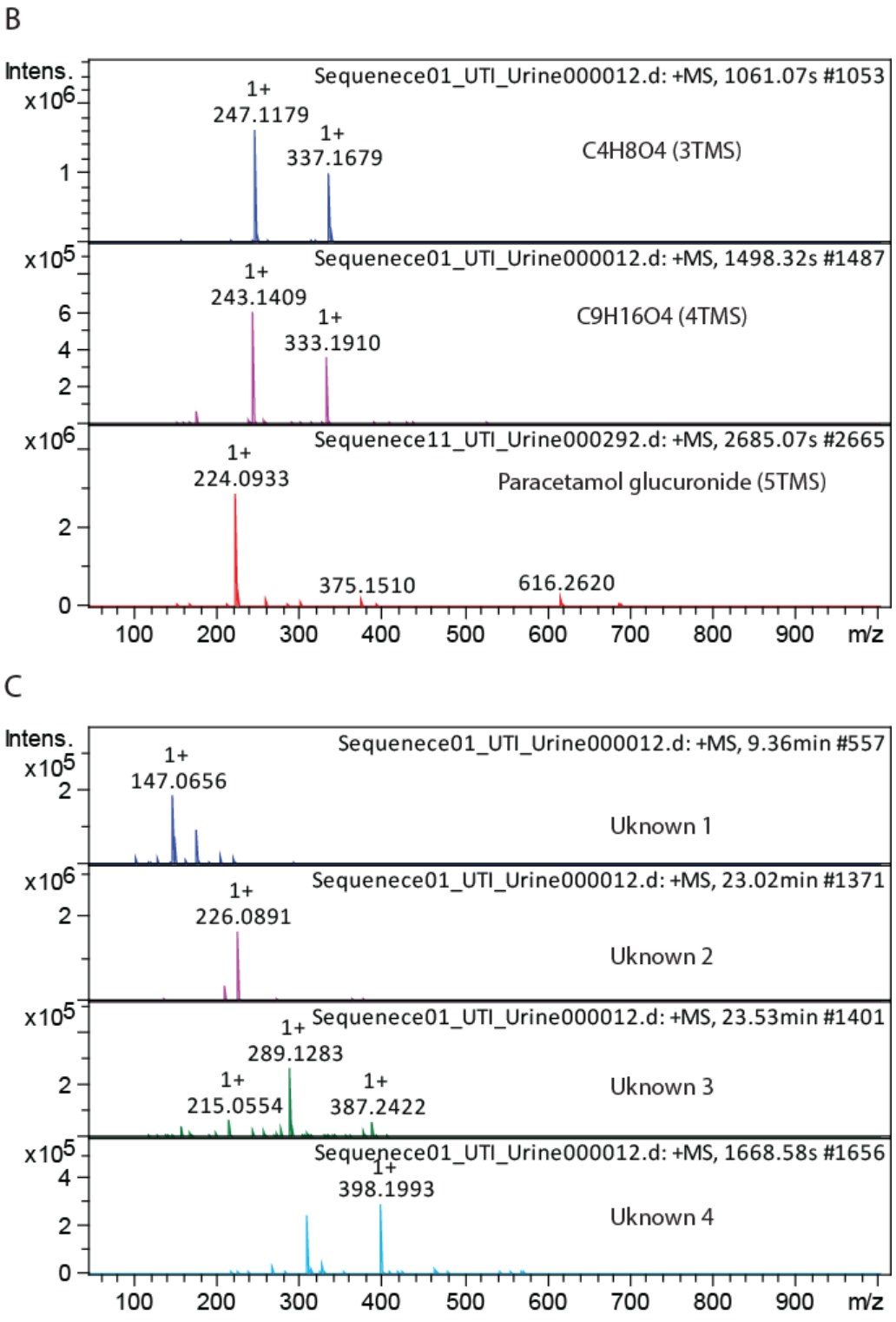
191.0918
405.2416



Supplementary Figure 6. MS spectra of classifiers reported in Table 4. A) compounds identified with library matching B) Compounds identified with *de novo* identification protocol and C) Unknown compounds.