Class exercise

LC-MS/MS analysis urine samples from human patients gave rise to the following selected negative ion chromatogram at m/z 448.307.

Graphical user interface, application, table, Excel

Description automatically generated

This ion was searched for in the MS/MS data

Graphical user interface, chart, application, table, Excel

Description automatically generated

The dots were doubled clicked on to produce these MSMS spectra

Graphical user interface, application, table

Description automatically generated

Table, Excel

Description automatically generated

What is this compound? Hint: a search in Google may help. If so, then explain the MSMS spectra. Is the peak eluting at 5.5 min the same as the one at 6.0-6.1?

Another ion was found to be interesting, and it had an ion mass of m/z 528.267 – here’s its ion MSMS spectrum. What is it? The small unmarked peak on the left is m/z 74.026

Graphical user interface, application, table, Excel

Description automatically generated

Hint: you have probably noticed the similar ions from the previous MSMS spectra.

Another ion of interest was at m/z 624.335

Graphical user interface, application, table, Excel

Description automatically generated

Here’s the search MSMS plot

Graphical user interface, application, table, Excel

Description automatically generated

And here’s the MSMS spectrum at ~5.50 min

Graphical user interface, application

Description automatically generated

What do you think this compound is? Note the common ion again