# DERIVATIZATION-TARGETED ANALYSIS OF AMINO COMPOUNDS IN NEUTRAL LOSS ACQUISITION MODE BY LIQUID CHROMATOGRAPHY COUPLED TO TRIPLE QUADRUPOLE MASS SPECTROMETRY

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Amino compounds form a significant part of metabolites, which are small molecules generated by the many cellular metabolism pathways. It is estimated that the human metabolome consists of over 100,000 compounds [1]. One of the widely used techniques for metabolites identification is liquid chromatography-tandem mass spectrometry (LC-MS/MS), due to its sensitivity and the fact that it provides information about the molecular mass and functional group of compounds. Ions (from the first mass analyser) collide with an inert gas in a cell (collision cell), where fragments are generated and thereafter, go through the second mass analyser and detector. There are several operational modes available with this set up, for instance, multiple reaction monitoring (MRM) and neutral loss scan (NLS), with the latter allowing the detection of all the compounds that lose a specific neutral fragment upon fragmentation.

Identification of all metabolites is difficult, given the amount and different chemical properties of each. There is no available technique with enough selectivity and sensitivity that would englobe this wide range of diversity. A way to overcome this issue is through derivatization, where a moiety is introduced in the compound of interest (in this work, amines) by a chemical reaction. Derivatives have better LC separation and higher sensitivity than the starting material. In this work, diethyl ethoxymethylenemalonate (DEEMM) was chosen as the derivatization reagent for amines, because of the simplicity of the reaction and the derivatives' constant fragmentation pattern: the loss of neutral fragment 46 (ethanol) from the parent ion. This follows to employ NLS and, therefore, it is possible to identify all the compounds (mostly compounds with primary and secondary amino groups) that react with DEEMM.

References

1. Wishart, D.S. Advances in metabolite identification. *Bioanalysis* 3(15), 1769–1782 (2011).

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