

## Identification of Lipo-Alkaloids and Fatty Acids in *Aconitum carmichaelii* Using Liquid Chromatography-Mass Spectrometry and Gas Chromatography-Mass Spectrometry

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**Abstract :** Lipo-alkaloid is a kind of C19-norditerpenoid alkaloids existed in *Aconitum* species, which usually contains an aconitane skeleton and one or two fatty acid residues. The structures are very similar to that of diester-type alkaloids, which are considered as the main bioactive components in *Aconitum carmichaelii*. They have anti-inflammatory, anti-nociceptive, and anti-proliferative activities. So far, more than 200 lipo-alkaloids were reported from plants, semisynthesis, and biotransformations. In our research, by the combination of ultra-high performance liquid chromatography-quadrupole-time of flight mass spectrometry (UHPLC-Q-TOF-MS) and an in-house database, 148 lipo-alkaloids were identified from *A. carmichaelii*, including 93 potential new compounds and 38 compounds with oxygenated fatty acid moieties. To our knowledge, this is the first time of the reporting of the oxygenated fatty acids as the side chains in naturally-occurring lipo-alkaloids. Considering the fatty acid residues in lipo-alkaloids should come from the free acids in the plant, the fatty acids and their relationship with lipo-alkaloids were further investigated by GC-MS and LC-MS. Among 17 fatty acids identified by GC-MS, 12 were detected as the side chains of lipo-alkaloids, which accounted for about 1/3 of total lipo-alkaloids, while these fatty acid residues were less than 1/4 of total fatty acid residues. And, total of 37 fatty acids were determined by UHPCL-Q-TOF-MS, including 18 oxidized fatty acids firstly identified from *A. carmichaelii*. These fatty acids were observed as the side chains of lipo-alkaloids. In addition, although over 140 lipo-alkaloids were identified, six lipo-alkaloids, 8-O-linoleoyl-14-benzoylmesaconine (1), 8-O-linoleoyl-14-benzoylaconine (2), 8-O-palmitoyl-14-benzoylmesaconine (3), 8-O-oleoyl-14-benzoylmesaconine (4), 8-O-pal-benzoylaconine (5), and 8-O-ole-Benzoylaconine (6), were found to be the main components, which accounted for over 90% content of total lipo-alkaloids. Therefore, using these six components as standards, a UHPLC-Triple Quadrupole-MS (UHPLC-QQQ-MS) approach was established to investigate the influence of processing on the contents of lipo-alkaloids. Although it was commonly supposed that the contents of lipo-alkaloids increased after processing, our research showed that no significant change was observed before and after processing. Using the same methods, the lipo-alkaloids in the lateral roots of *A. carmichaelii* and the roots of *A. kusnezoffii* were determined and quantified. The contents of lipo-alkaloids in *A. kusnezoffii* were close to that of the parent roots of *A. carmichaelii*, while the lateral roots had less lipo-alkaloids than the parent roots. This work was supported by Macao Science and Technology Development Fund (086/2013/A3 and 003/2016/A1).

**Keywords :** *Aconitum carmichaelii*, fatty acids, GC-MS, LC-MS, lipo-alkaloids

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