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Identification of aconitine artefact in alcoholic extracts

Mai Ahmed
University of Bath, UK

Aconitum napellus is a highly poisonous plant; all of its parts are rich in toxic C₁₉-norditerpenoid alkaloids e.g. aconitine and mesaconitine. General extraction procedures for aconitine and diester diterpenoid alkaloids require maceration in alcohols. Mass spectra of *A. napellus* seed extracts show various alkaloidal contents. HPLC combined with mass spectrometry was used to study the stability of aconitine in methanol, followed by separation and identification of the main artefact whose formation could follow a synchronous fragmentation. The HRMS data from *A. napellus* seed extracts, from methanol and acetone, showed the same alkaloidal profile with an extra peak in the methanolic extract at m/z MH⁺ = 618.3271, MH⁺ of O-methyl-14-O-benzoylaconine requires 618.3278. Its semi-synthesis was carried out by refluxing aconitine in methanol (6 h at 65°C). The suggested mechanism for the formation of this artefact is via a Grob-type fragmentation, cleavage of the C-7-C-17 bond with the nitrogen lone pair and C-7-C-17 orientated anti-parallel to the C-8-acetate bond, and then adding methanol back. The NMR data of the HPLC purified artefact (10 mg) were compared with those of aconitine. Assigning the new O-methyl at C-8 followed from the chemical shift data, δ H 3.14, 3.28, 3.28, 3.31 and 3.74 (each 3H, s) and δ C 49.9, 55.0, 58.5, 59.1 and 62.4 (respectively), while in aconitine, four methoxy singlets appear at δ H 3.16, 3.26, 3.29 and 3.75, with associated carbon signals at δ C 58.1, 56.1, 59.3 and 61.3. Quaternary C-8 resonates at δ C 82.4 in 8-O-methyl-14-O-benzoylaconine and at δ C 92.2 in (8-acetoxy) aconitine.

Biography

Mai Ahmed completed her Master's degree in Pharmaceutical Sciences at the age of 28 years from Assiut University, Egypt and worked there as an assistant lecturer. In 2011, she got a fully funded scholarship (for which we thank the Egyptian Government) and now she is a final year student in the Dept. of Pharmacy and Pharmacology, University of Bath, UK.

ma560@bath.ac.uk

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