About OMICS Group

OMICS Group is an amalgamation of Open Access Publications and worldwide international science conferences and events. Established in the year 2007 with the sole aim of making the information on Sciences and technology 'Open Access', OMICS Group publishes 500 online open access scholarly journals in all aspects of Science, Engineering, Management and Technology journals. OMICS Group has been instrumental in taking the knowledge on Science & technology to the doorsteps of ordinary men and women. Research Scholars, Students, Libraries, Educational Institutions, Research centers and the industry are main stakeholders that benefitted greatly from this knowledge dissemination. OMICS Group also organizes 500 International conferences annually across the globe, where knowledge transfer takes place through debates, round table discussions, poster presentations, workshops, symposia and exhibitions.

OMICS International Conferences

OMICS International is a pioneer and leading science event organizer, which publishes around 500 open access journals and conducts over 500 Medical, Clinical, Engineering, Life Sciences, Pharma scientific conferences all over the globe annually with the support of more than 1000 scientific associations and 30,000 editorial board members and 3.5 million followers to its credit.

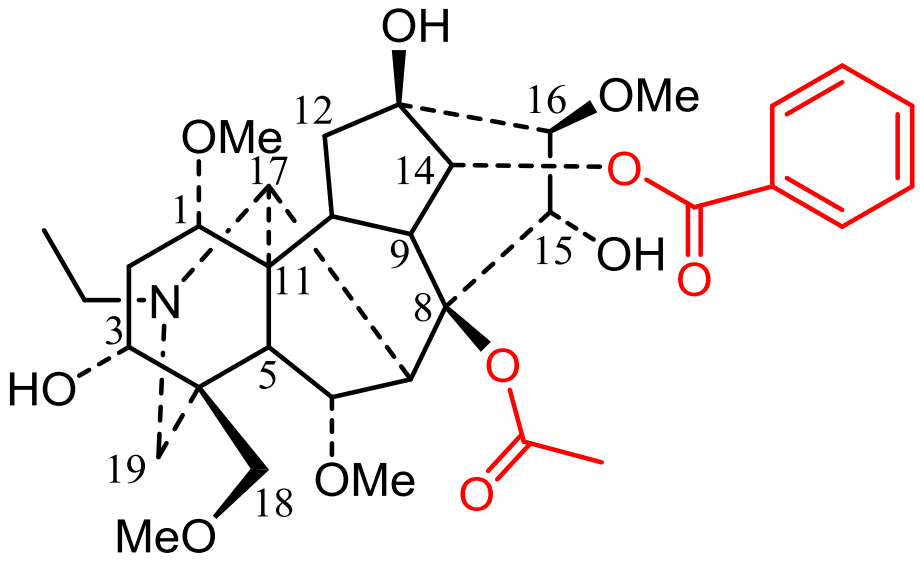
OMICS Group has organized 500 conferences, workshops and national symposiums across the major cities including San Francisco, Las Vegas, San Antonio, Omaha, Orlando, Raleigh, Santa Clara, Chicago, Philadelphia, Baltimore, United Kingdom, Valencia, Dubai, Beijing, Hyderabad, Bengaluru and Mumbai.

Identification of Aconitine Artefact in Alcoholic Extracts

DRUG DISCOVERY, FRANKFURT, GERMANY, AUGUST 2015

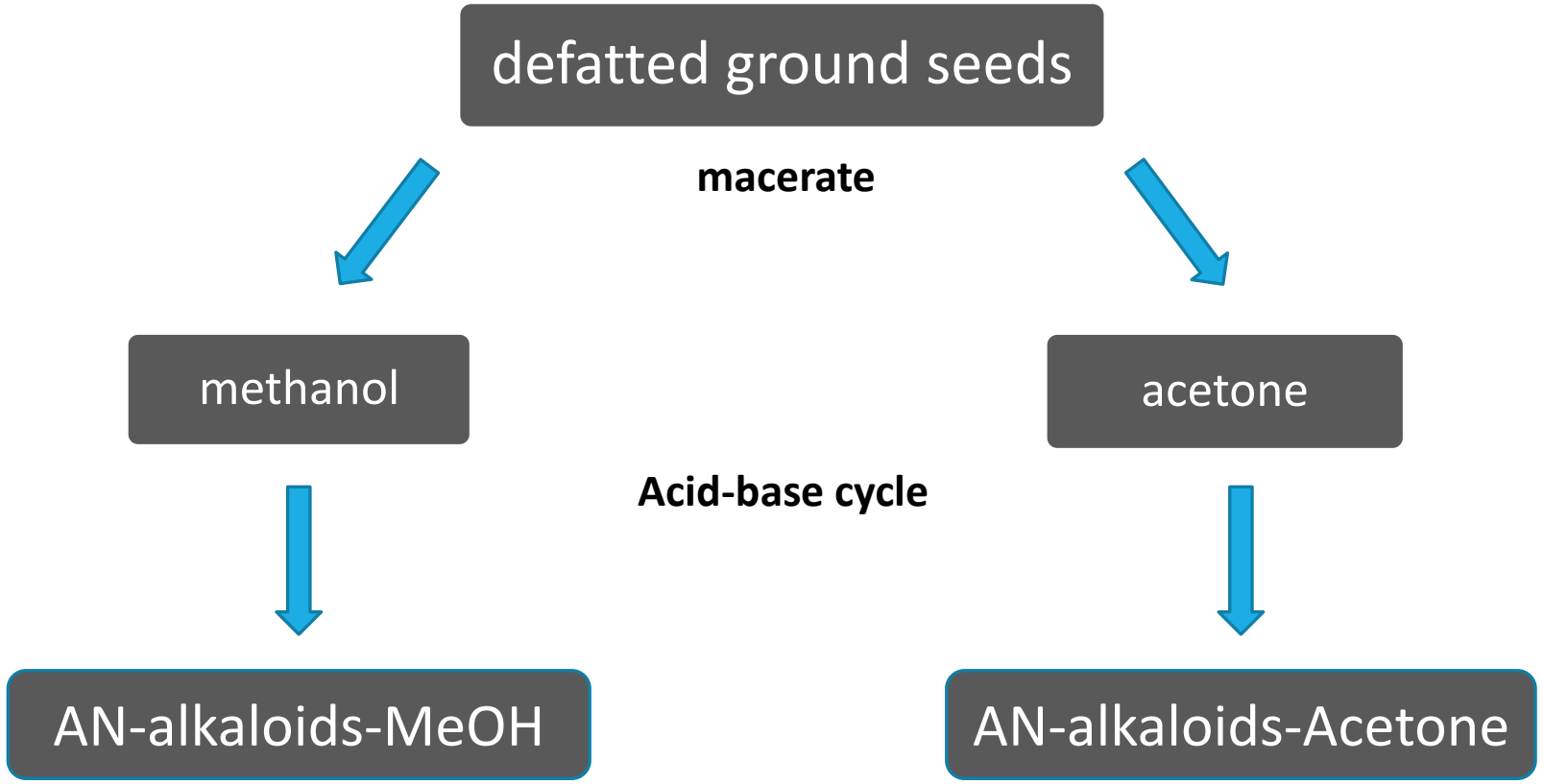
Mai Ahmed

Aconitine



Aconitum napellus

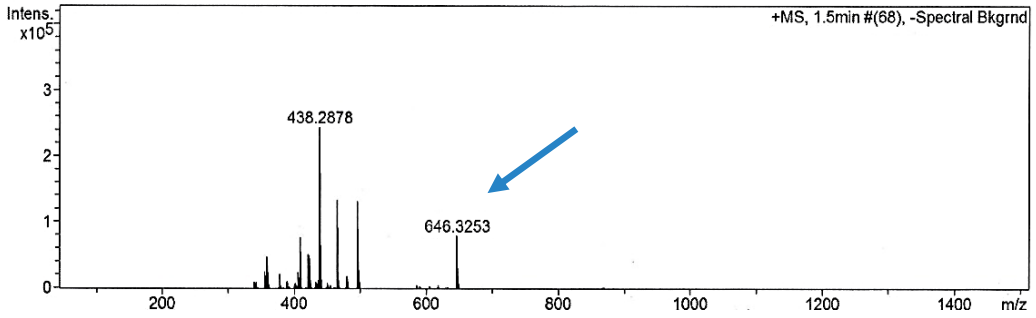
Extraction of diterpenoid alkaloids from *A. napellus* seeds



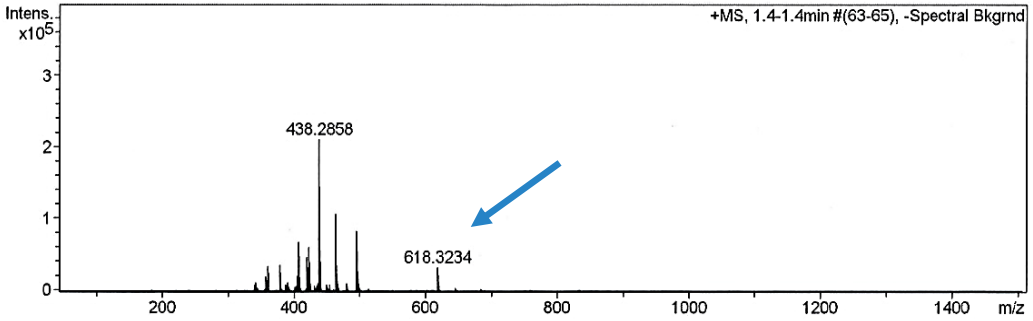
HRMS data of *A. napellus* extracts

Both extracts showed the same alkaloidal profile except for an extra peak at MH^+ 618 in the methanolic extract.

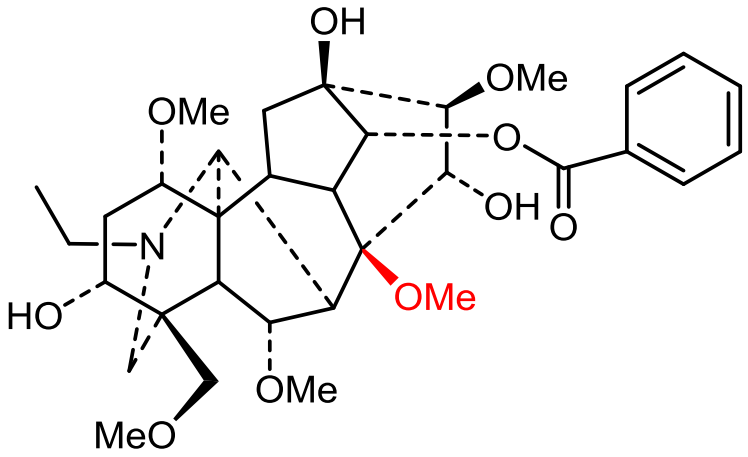
AN-alkaloids-MeOH



AN-alkaloids-Acetone



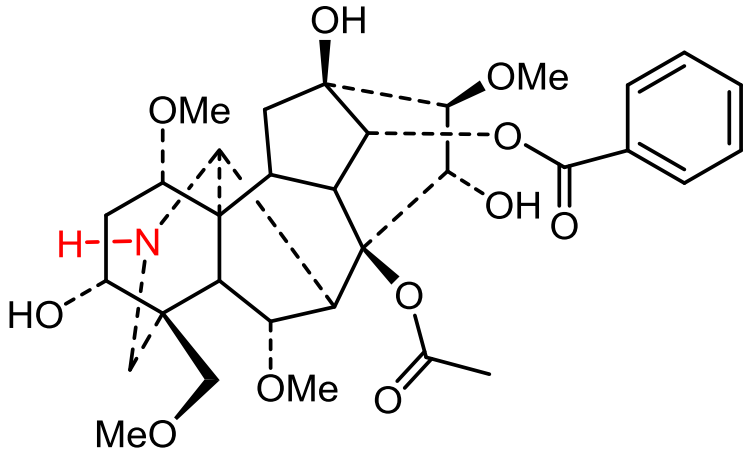
HRMS data of the aconitine artefact



14-*O*-benzoyl-8-*O*-methylaconine MH^+ 618.3278

$C_{33}H_{48}NO_{10}$

-(CO)



***N*-deethylaconitine MH^+ 618.68**

$C_{32}H_{43}NO_{11}$

-(C_2H_4)

Semi-synthesis of aconitine artefact

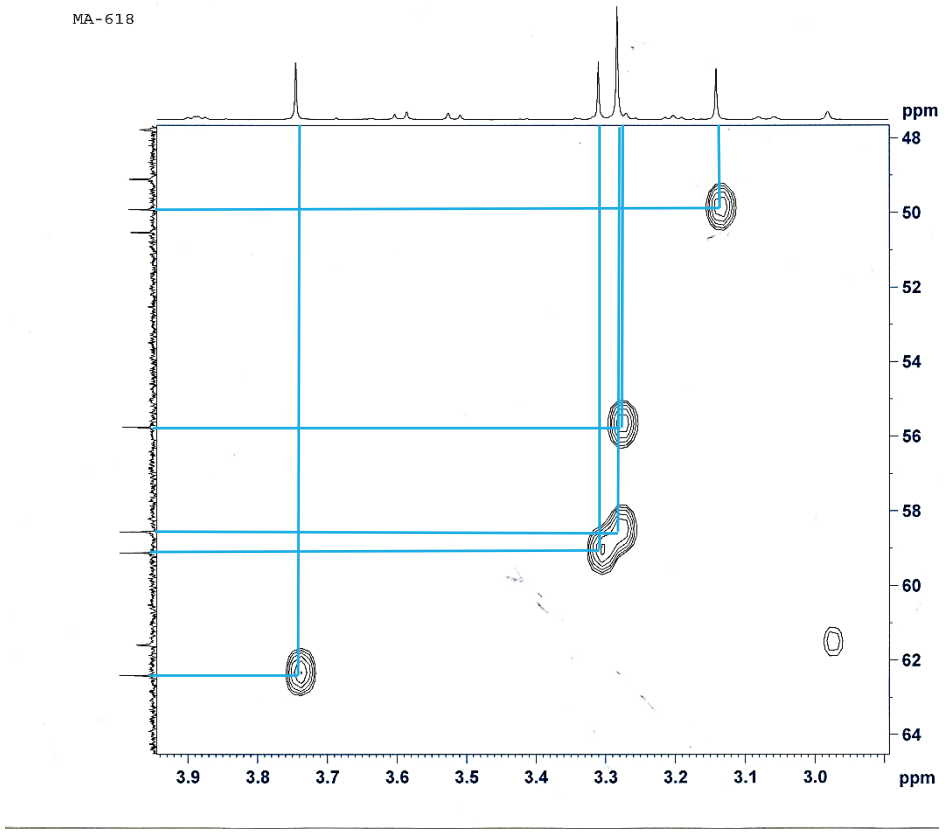
Aconitine was refluxed in methanol (at 65 ^{o}C for 6 hrs), purified by HPLC using C18 Gemini column 5µ 250 x 10 mm (mobile phase: acetonitrile : water with 0.3% conc. NH_3 [9:1 v/v], 3 mL/min; sample 100 µL, UV detection at λ = 232 nm), R_t 8 min. 10 mg were purified and NMR data were recorded in $CDCl_3$ using a Bruker 500 MHz NMR machine.

NMR data of aconitine artefact

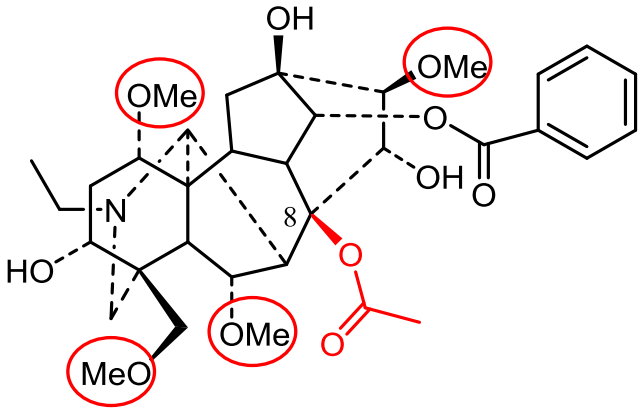
The ^{13}C-NMR data revealed the presence of 33 carbon atoms while the DEPT experiment showed the presence of 5 methylenes, and 6 quaternary carbons.

The NMR data revealed the presence of *N*-ethyl fragment, 5 methoxyl groups and absence of acetoxyl group.

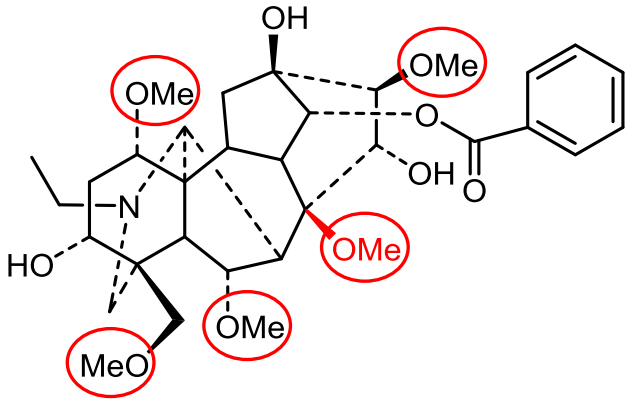
Quaternary C-8 resonates at δC 82.4 in 14-*O*-benzoyl-8-*O*-methylaconine and at δC 92.2 in (8-acetoxy) aconitine.



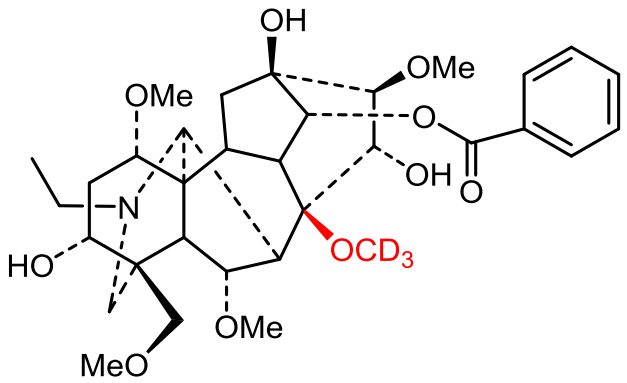
Aconitine and its artefacts



aconitine



artefact



deuterated artefact

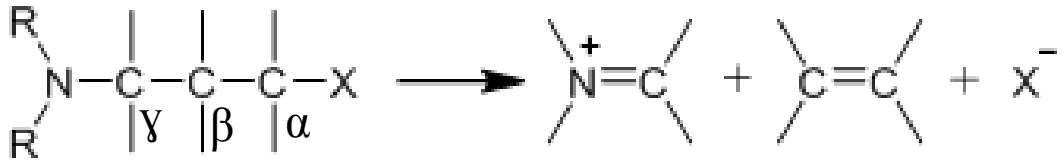
Aconitine reacted with different alcohols

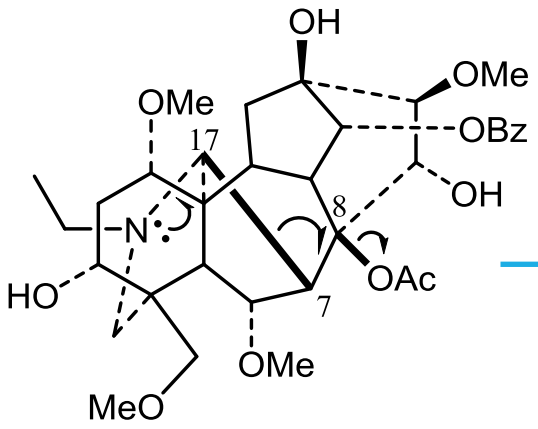
High Resolution Time-of-Flight mass spectra were obtained on a Bruker Daltonics micrOTOF spectrometer using electrospray ionisation (ESI).

Alcohol	Artefact	m/z (found)	Molecular formula
methanol	14-*O*-benzoyl-8-*O*-methylaconine	618.3291 Da	$C_{33}H_{48}NO_{10}$ requires 618.3278
d_4-methanol	14-*O*-benzoyl-8-*O*-trideuteriated methylaconine	621.3490 Da	$C_{33}H_{45}D_3NO_{10}$ requires 621.3461
ethanol	14-*O*-benzoyl-8-*O*-ethylaconine	632.3459 Da	$C_{34}H_{50}NO_{10}$ requires 632.3429
d_6-ethanol	14-*O*-benzoyl-8-*O*-pentadeuteriated ethylaconine	637.3759 Da	$C_{34}H_{45}D_5NO_{10}$ requires 637.3743

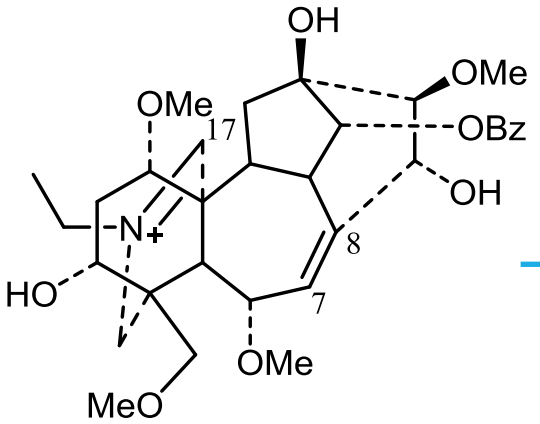
Grob-type fragmentation

It takes place when the free electron pair of the nitrogen atom and C_α-X bond are oriented anti-parallel to the C_β-C_γ bond which undergoes cleavage.

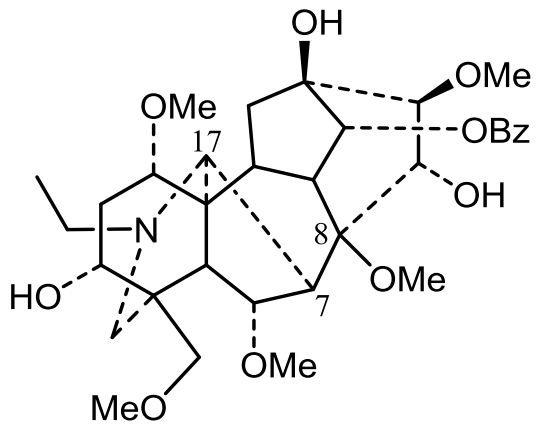




aconitine



MeOH



14-*O*-benzoyl-8-*O*-methylaconine

Conclusions

Alcoholic solvents should be avoided in any extraction procedure for aconitine and diester-diterpenoid alkaloids. Isolation of 8-*O*-alkylated diterpenoid alkaloids is most probably due to artefact formation. Medicinal formulations such as tinctures that involve extracts in ethanol are likely to suffer extensive degradation of diester alkaloids during preparation and/or storage and, on this occasion, be less toxic than the parent alkaloids.

Let us meet again..

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