

Supplementary Materials for

Attenuated Structural Transformation of Aconitine During Sand Frying Process and Anti-arrhythmic Effect of Its Converted Products

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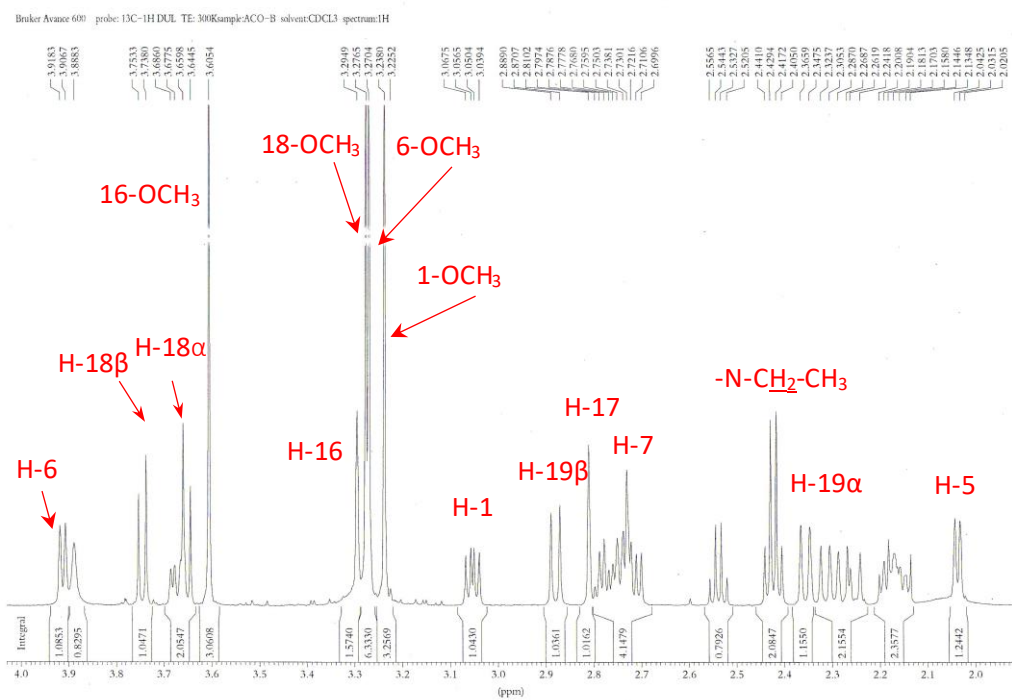


Figure S2. ¹H NMR of pyroaconitine (Detail)

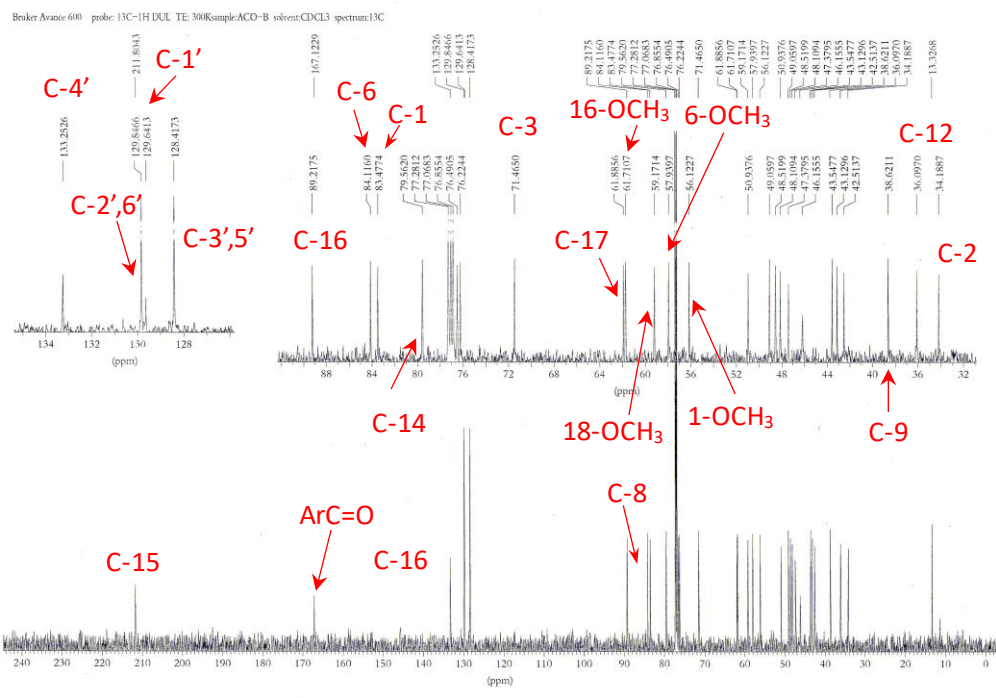


Figure S3. ¹³C NMR of pyroaconitine

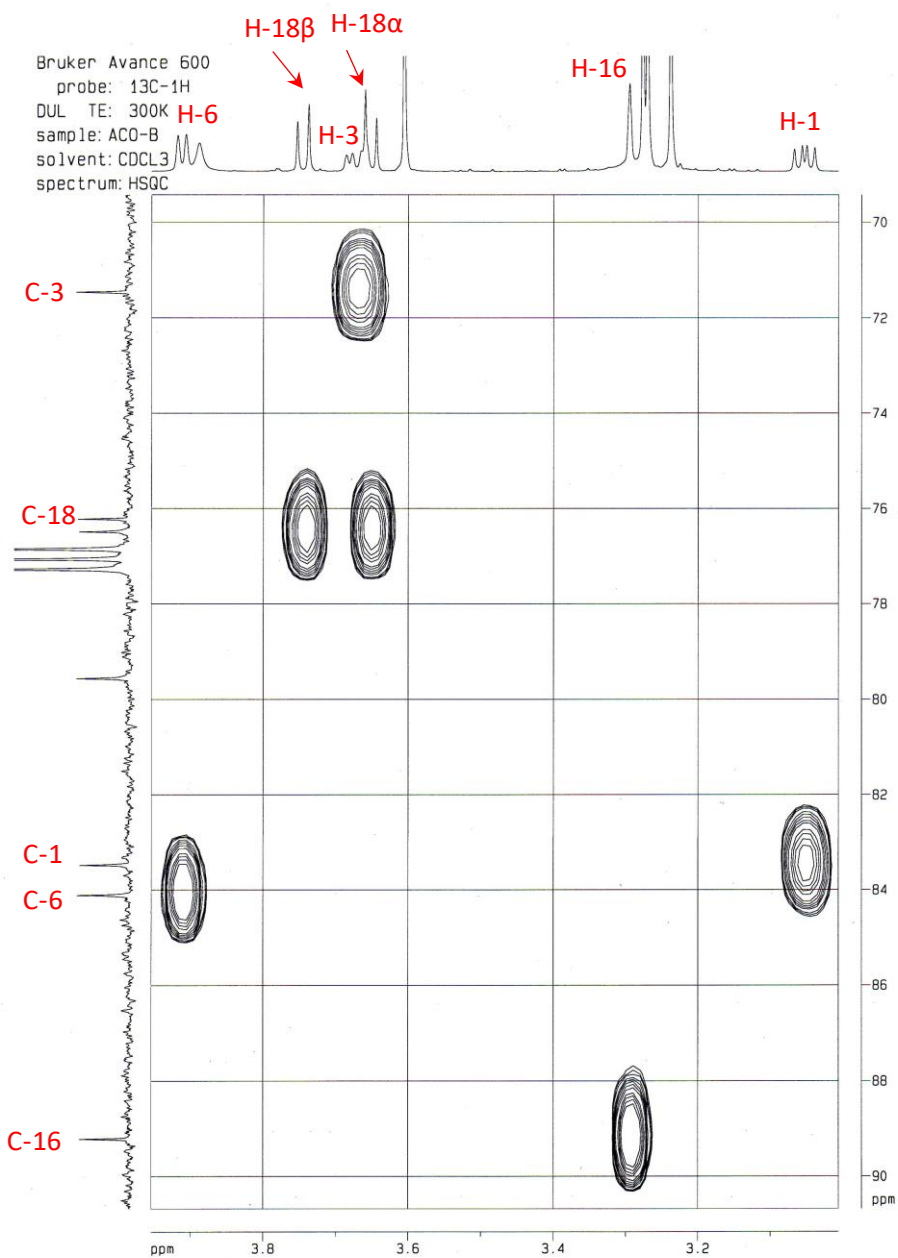


Figure S4. Key HSQC correlations of pyroaconitine (Detail 1)

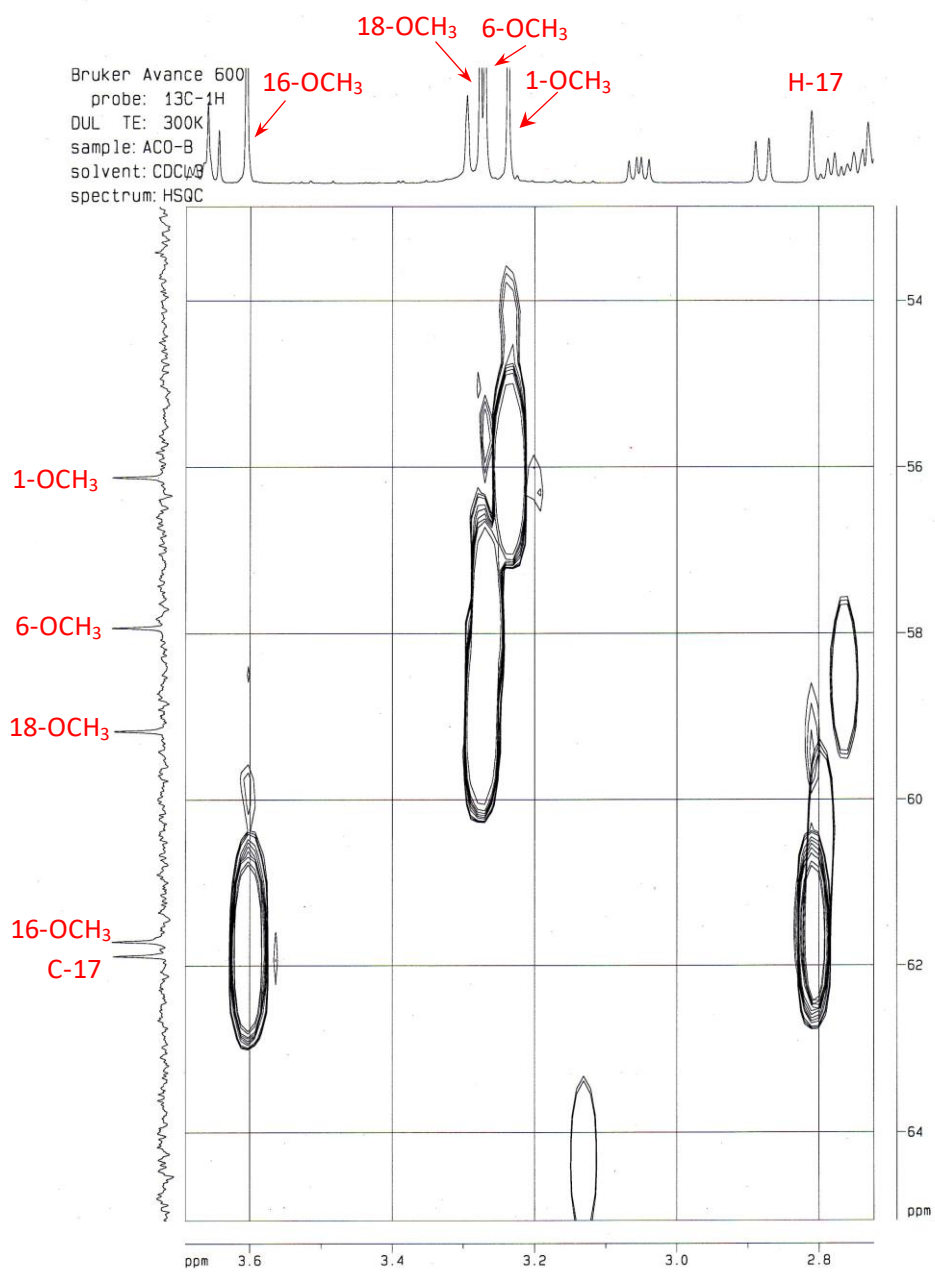


Figure S5. Key HSQC correlations of pyroaconitine (Detail 2)

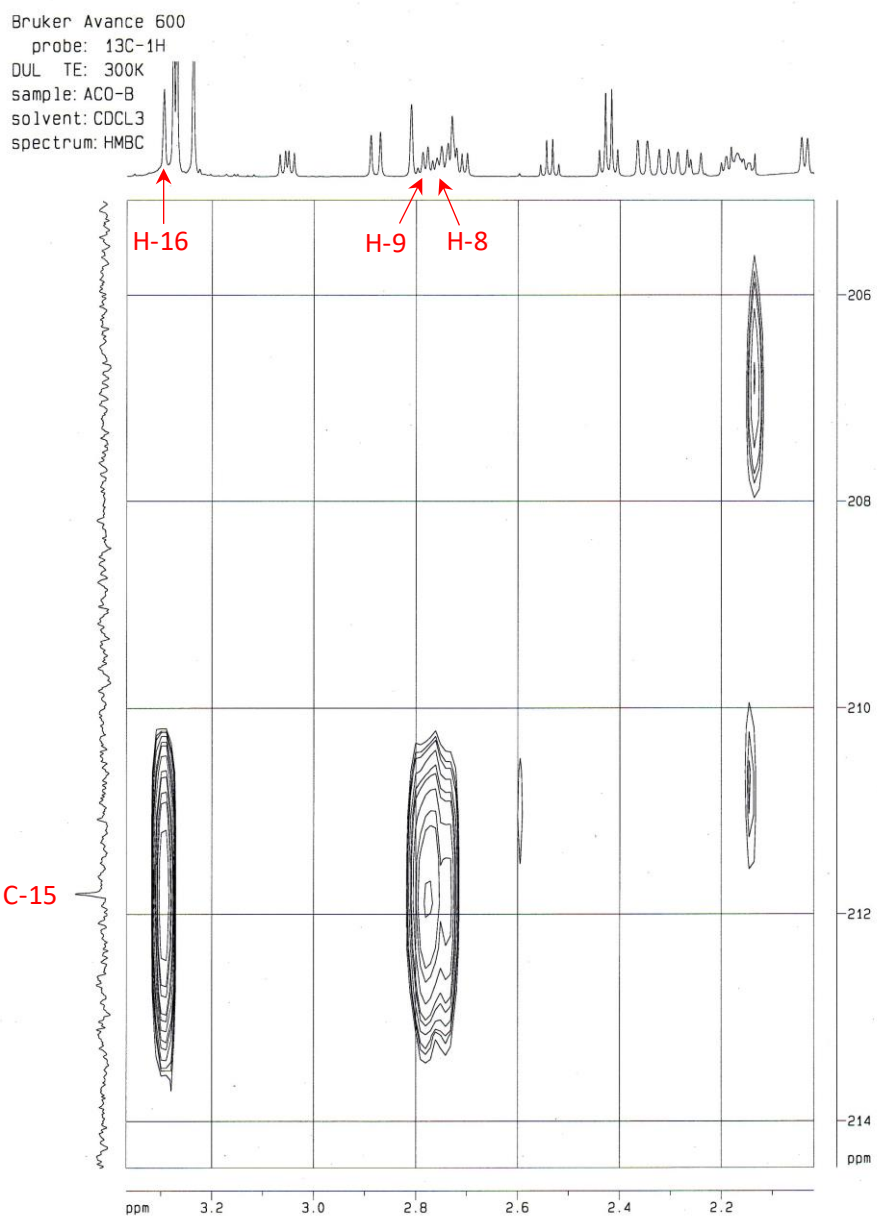


Figure S6. Key HMBC correlations of pyroaconitine (Detail 1)

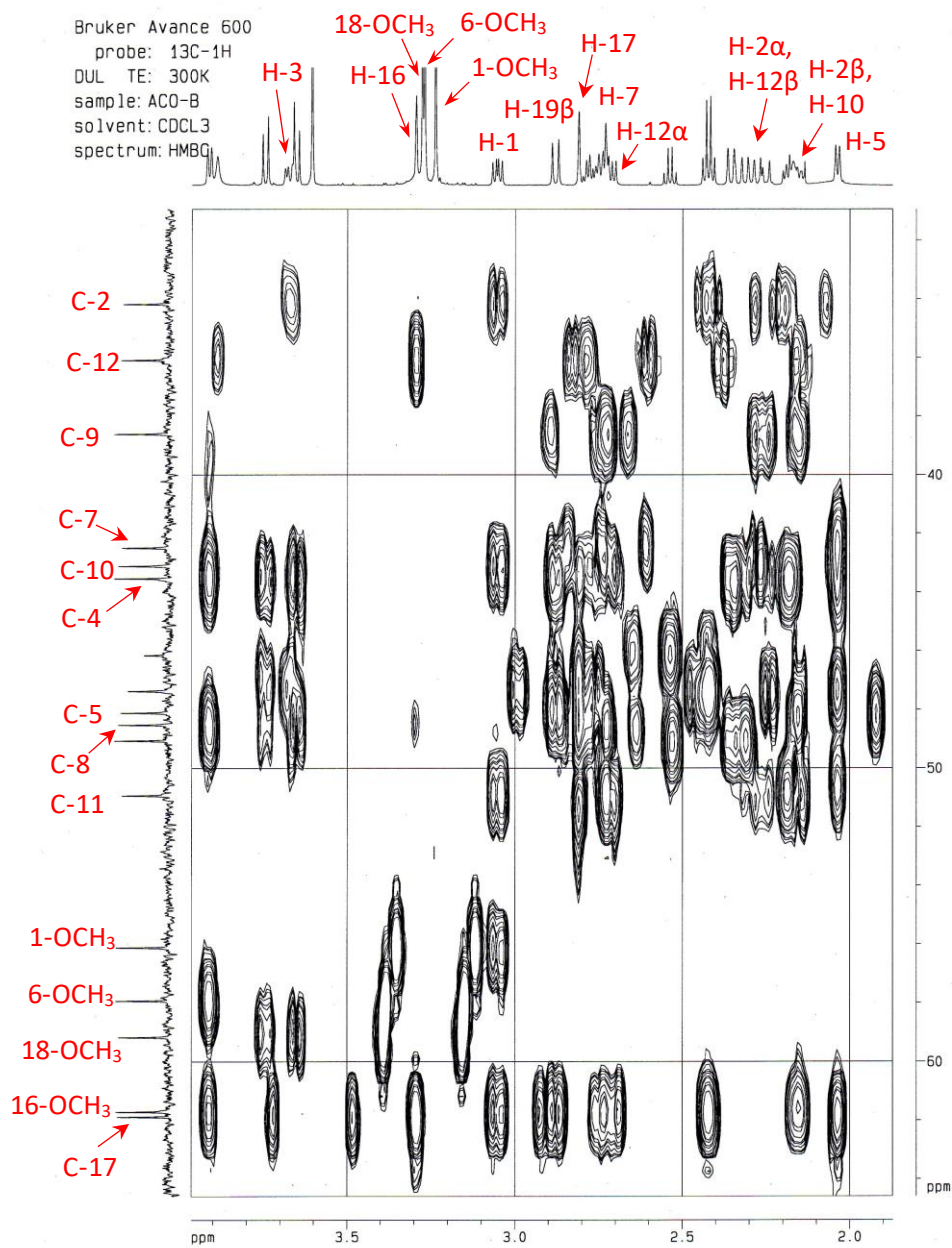


Figure S7. Key HMBC correlations of pyraconitine (Detail 2)

Bruker Avance 600
probe: ^{13}C -1H
DUL TE: 300K
sample: ACO-B
solvent: CDCl_3
spectrum: HMBC

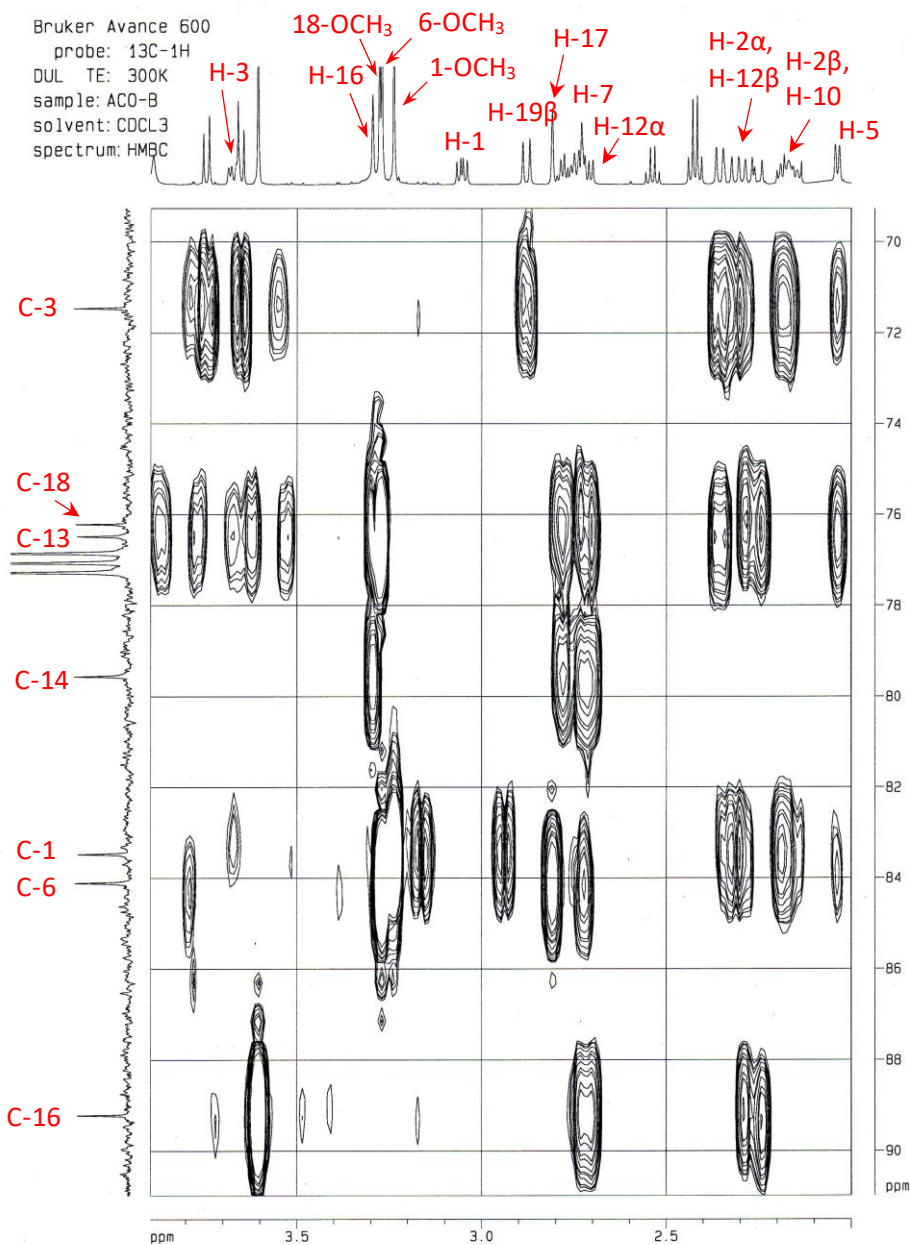


Figure S8. Key HMBC correlations of pyraconitine (Detail 3)

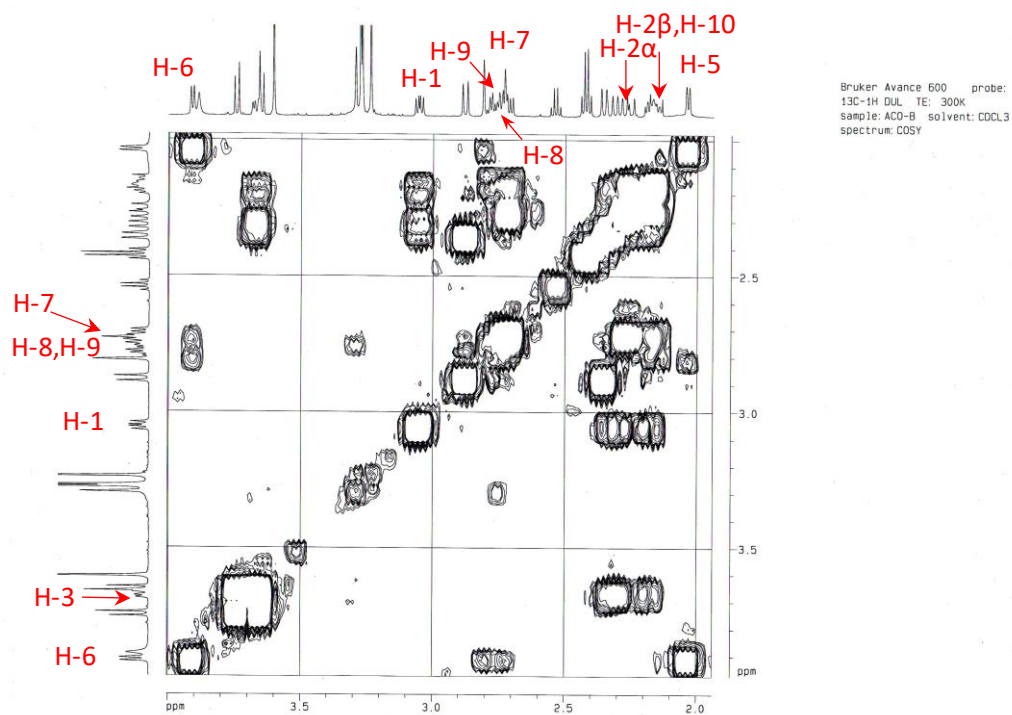


Figure S9. Key ^1H - ^1H COSY correlations of pyroaconitine (Detail 1)

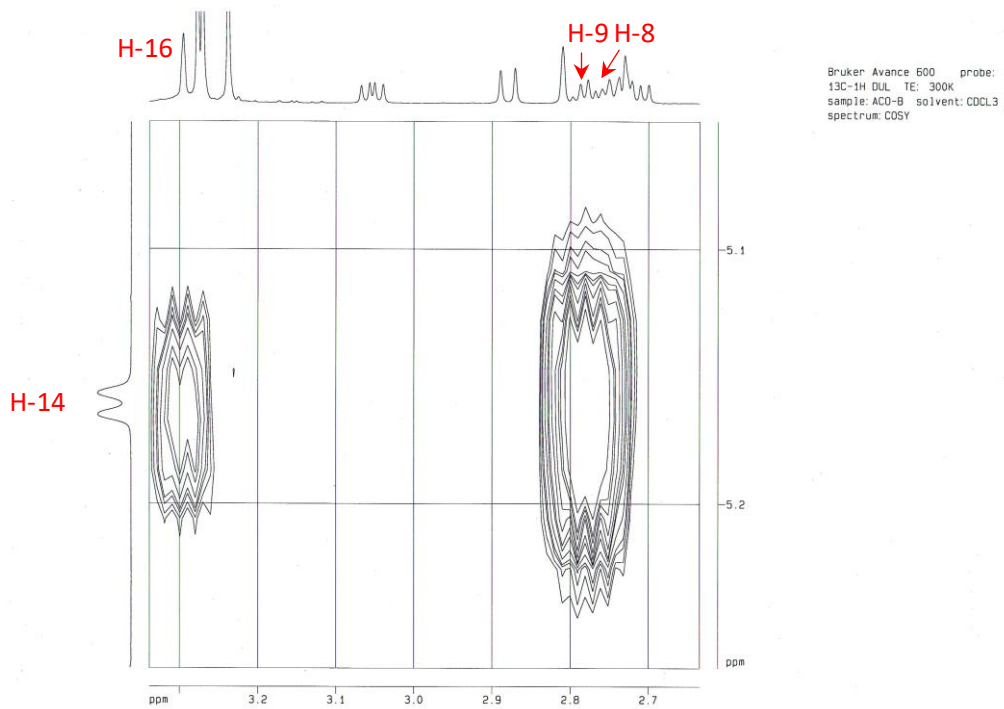


Figure S10. Key ^1H - ^1H COSY correlations of pyroaconitine (Detail 2)

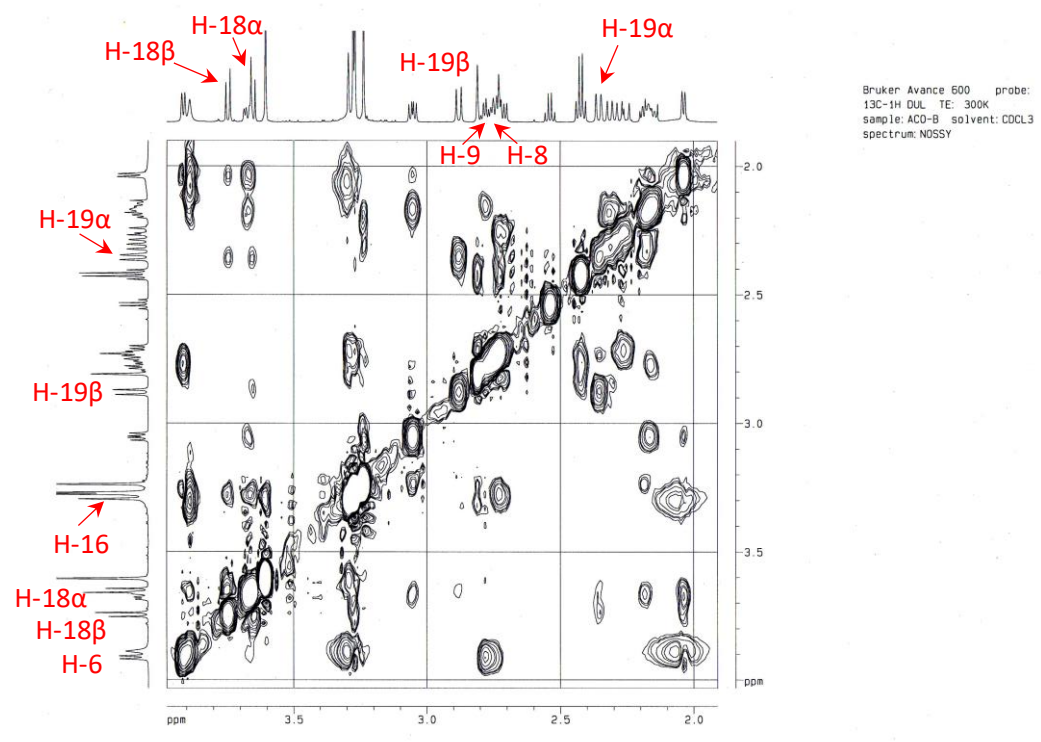


Figure S11. Key NOESY correlations of pyroaconitine (Detail 1)

Mass Spectrum SmartFormula Report

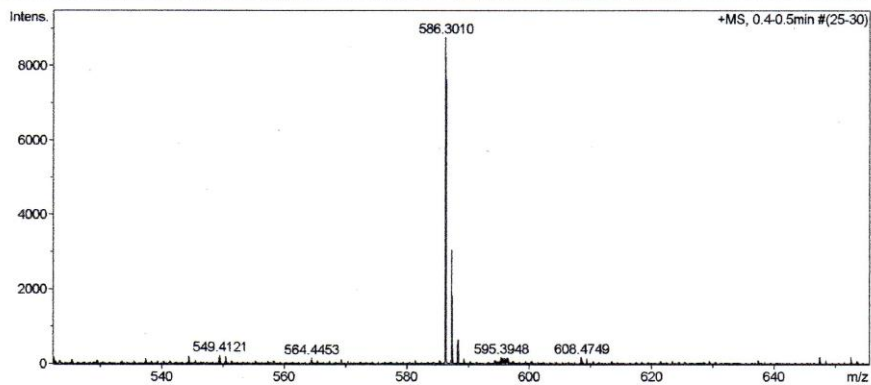
Analysis Info

Method tune_low_NEW.m
Sample Name ACO-B
Comment

Operator Ma
Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	Formula	m/z	err [ppm]	mSigma	N-Rule	e ⁻ Conf
586.3010	C ₃₂ H ₄₄ N ₂ O ₉	586.3011	0.2	4.92	ok	even

Figure S12. High-resolution ESI-MS of pyroaconitine

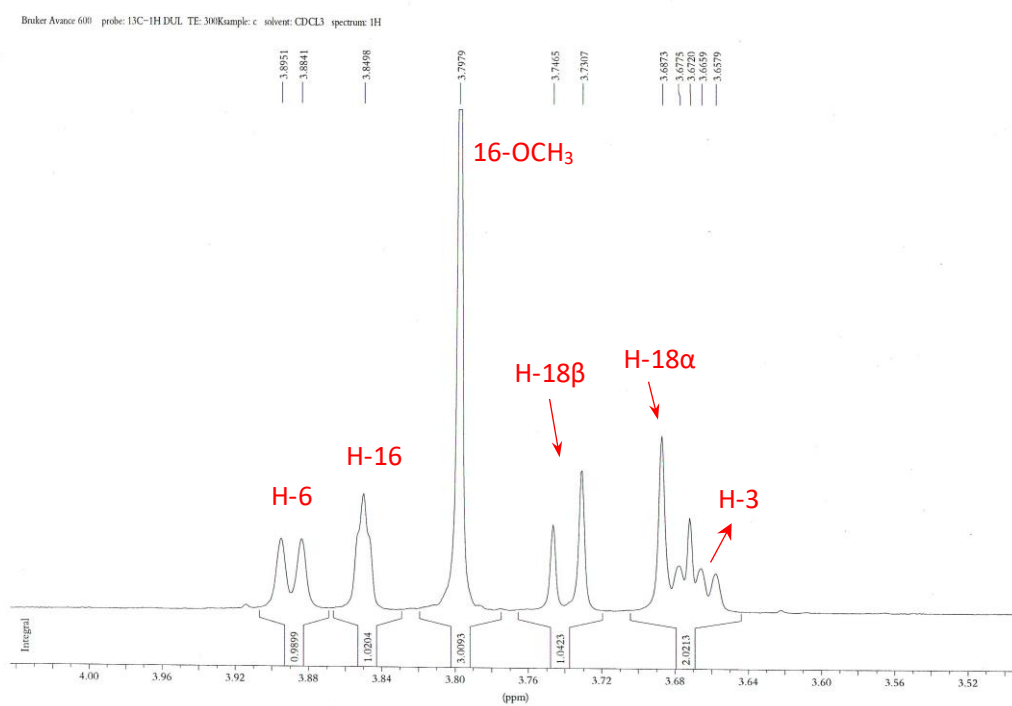


Figure S14. ¹H NMR of 16-epi-pyroaconitine (Detail 1)

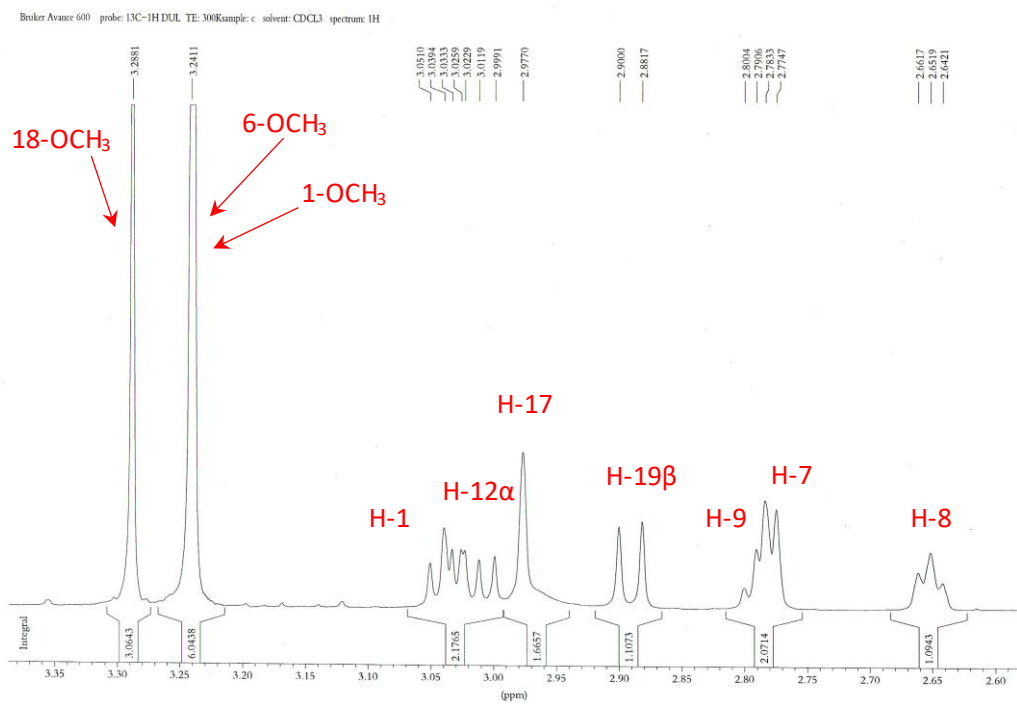


Figure S15. ¹H NMR of 16-epi-pyraconitine (Detail 2)

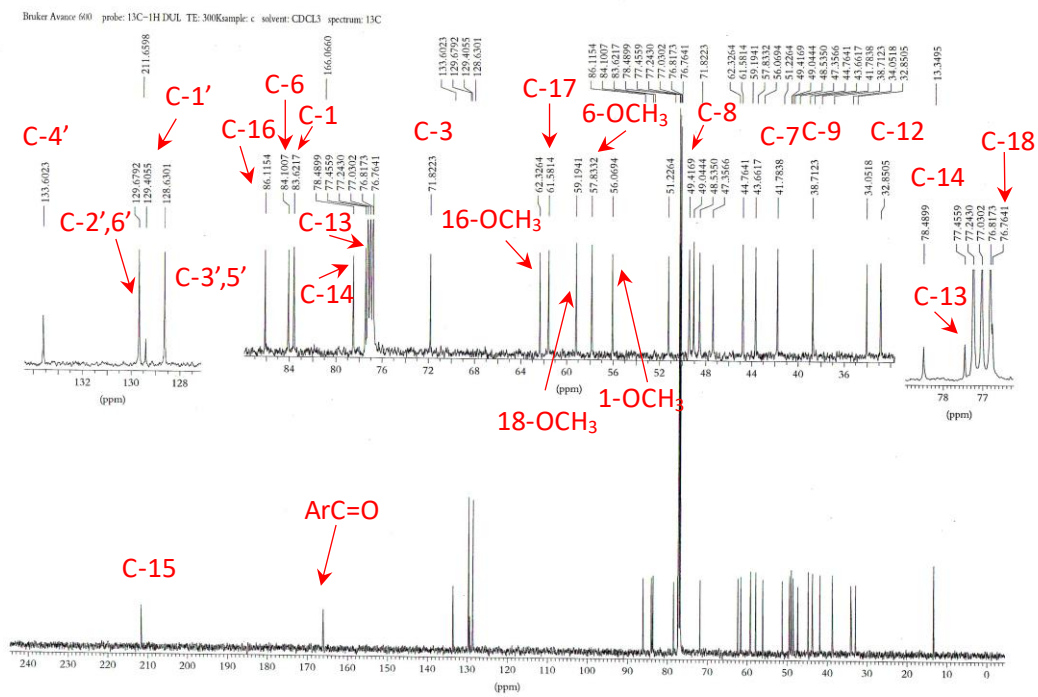


Figure S16. ¹³C NMR of 16-epi-pyroaconitine

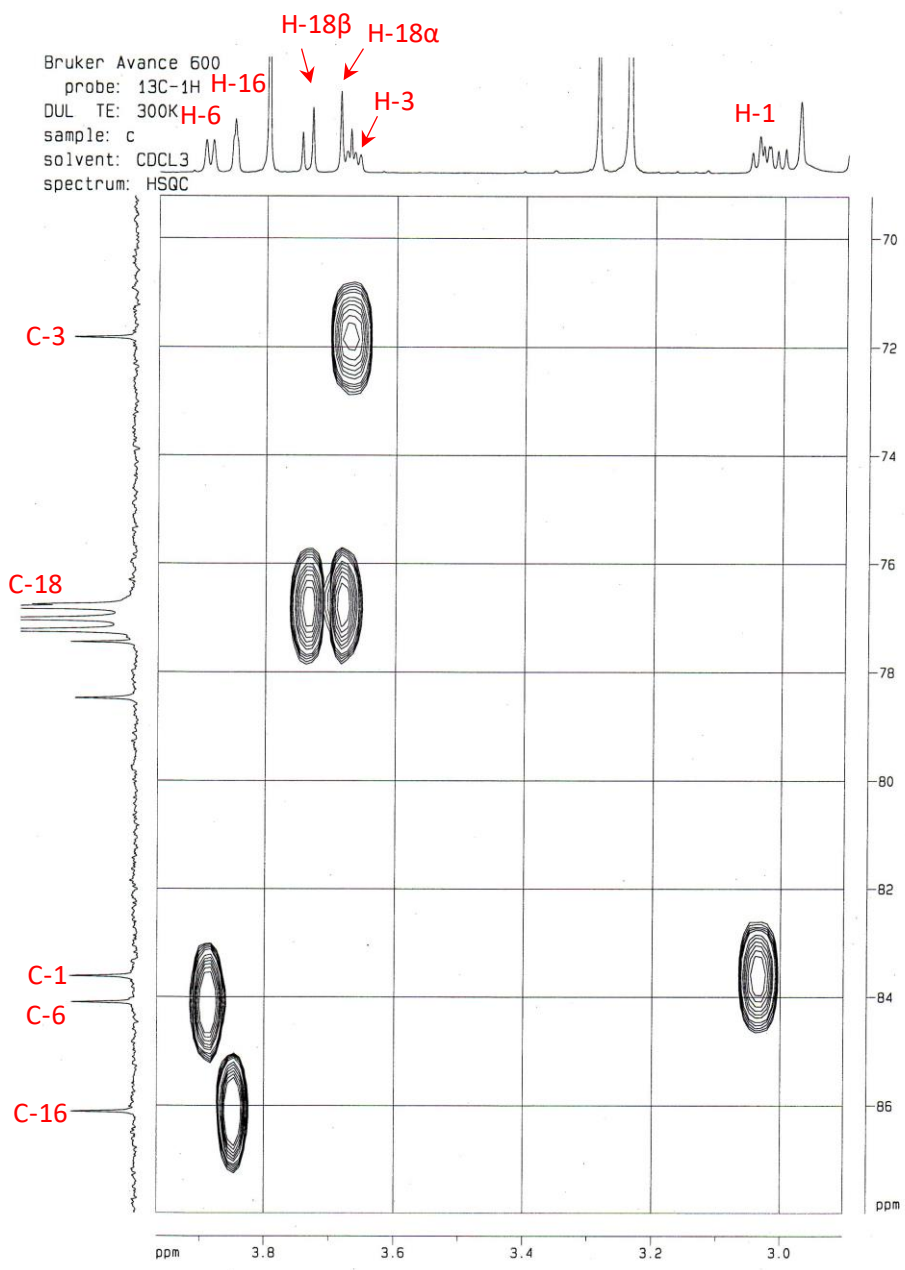


Figure S17. Key HSQC correlations of 16-epi-pyroaconitine (Detail 1)

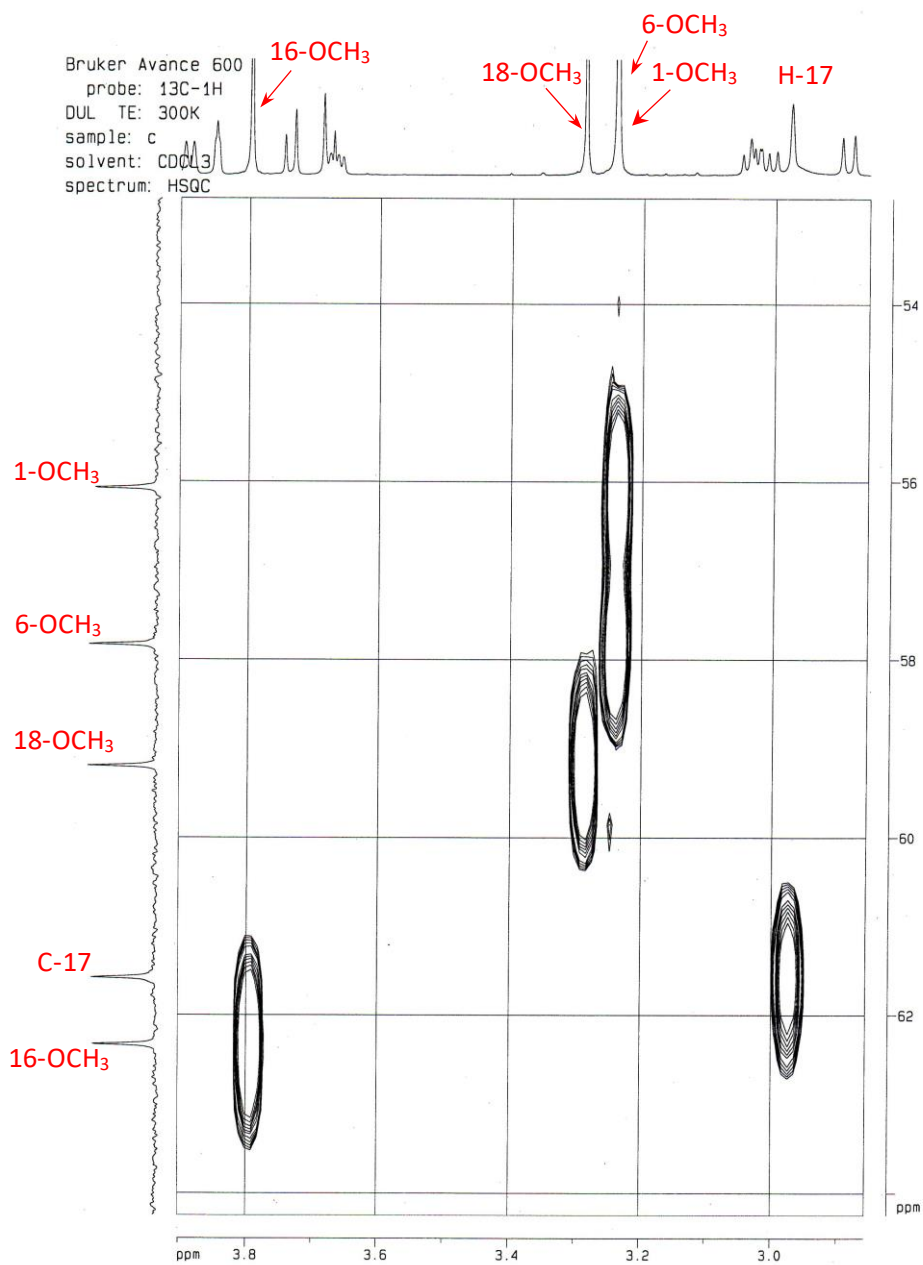


Figure S18. Key HSQC correlations of 16-epi-pyroaconitine (Detail 2)

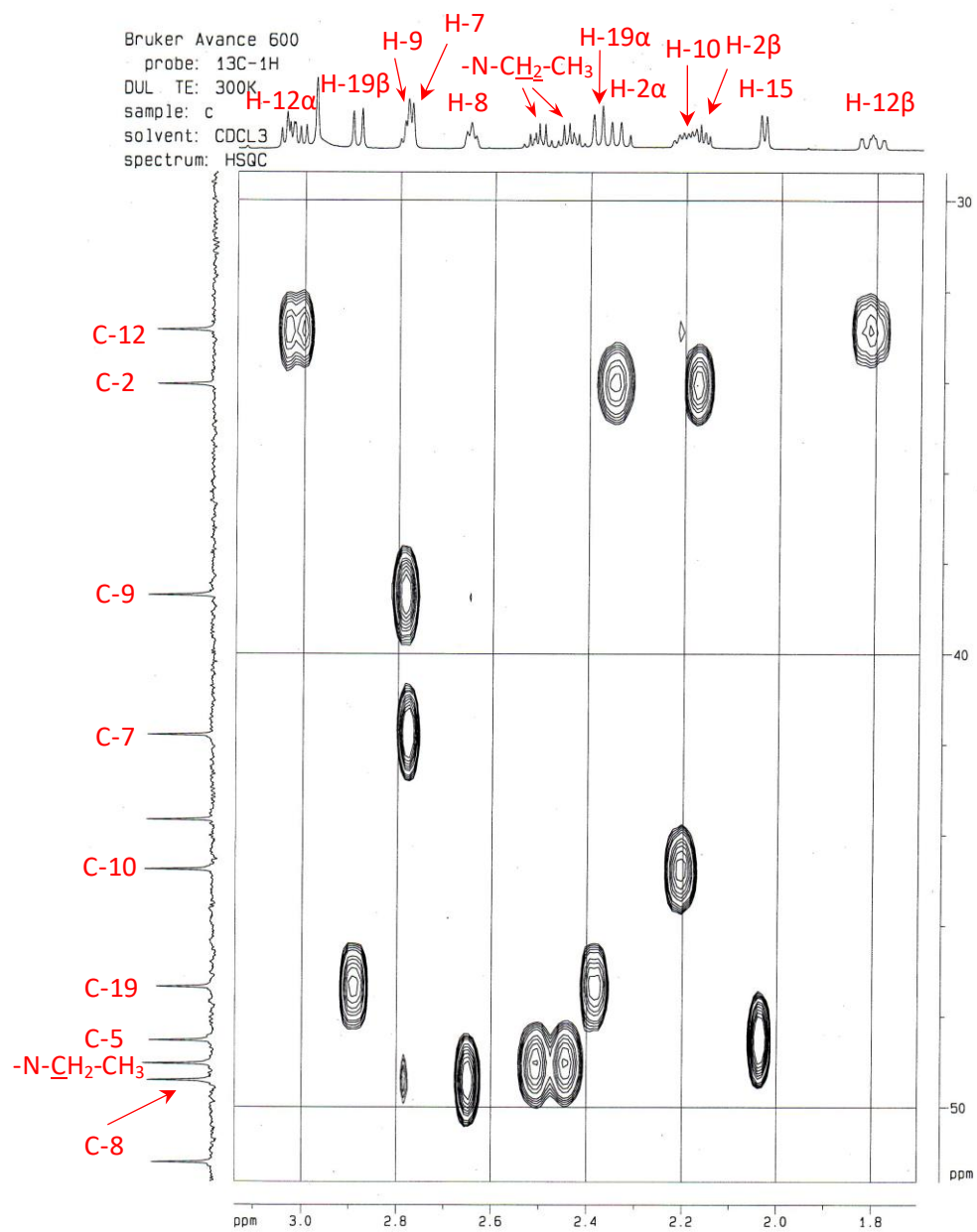


Figure S19. Key HSQC correlations of 16-epi-pyroaconitine (Detail 3)

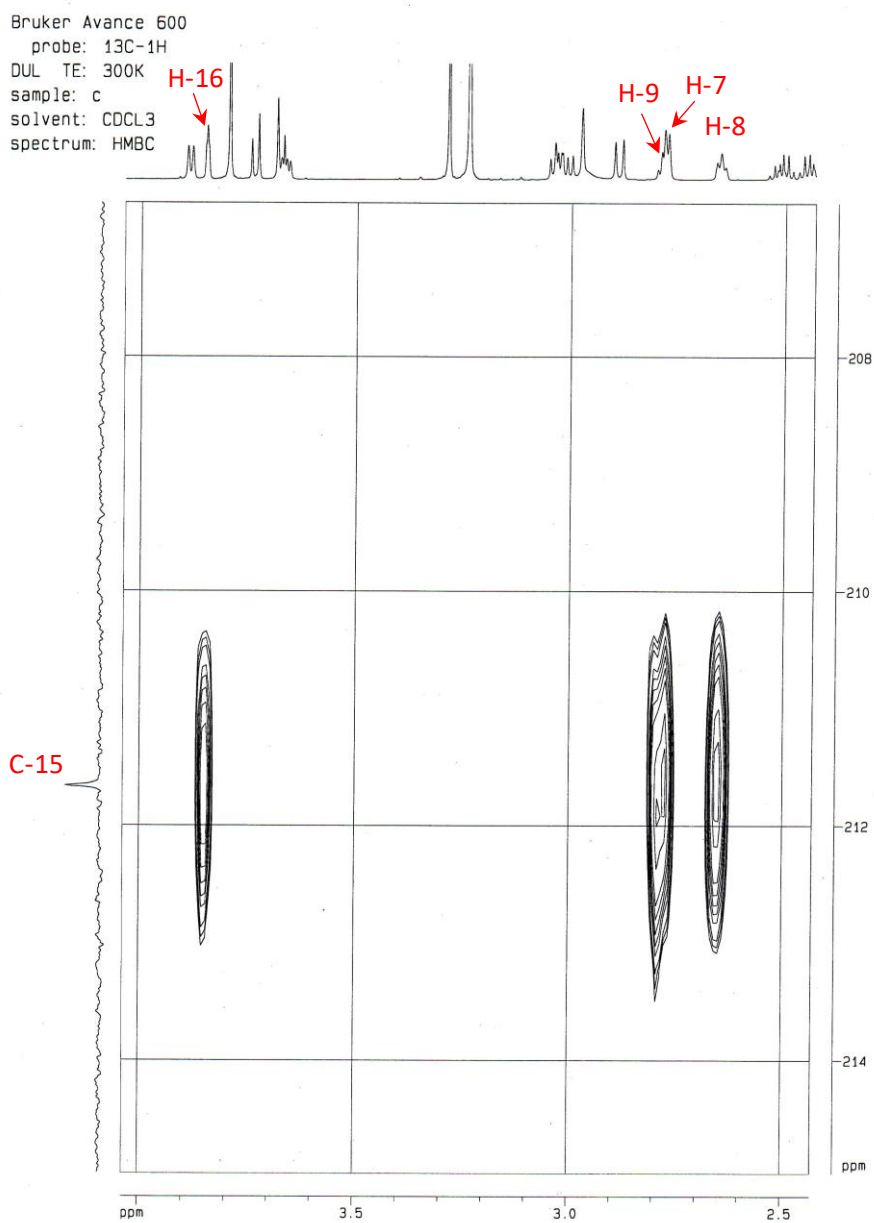


Figure S20. Key HMBC correlations of 16-epi-pyraconitine (Detail 1)

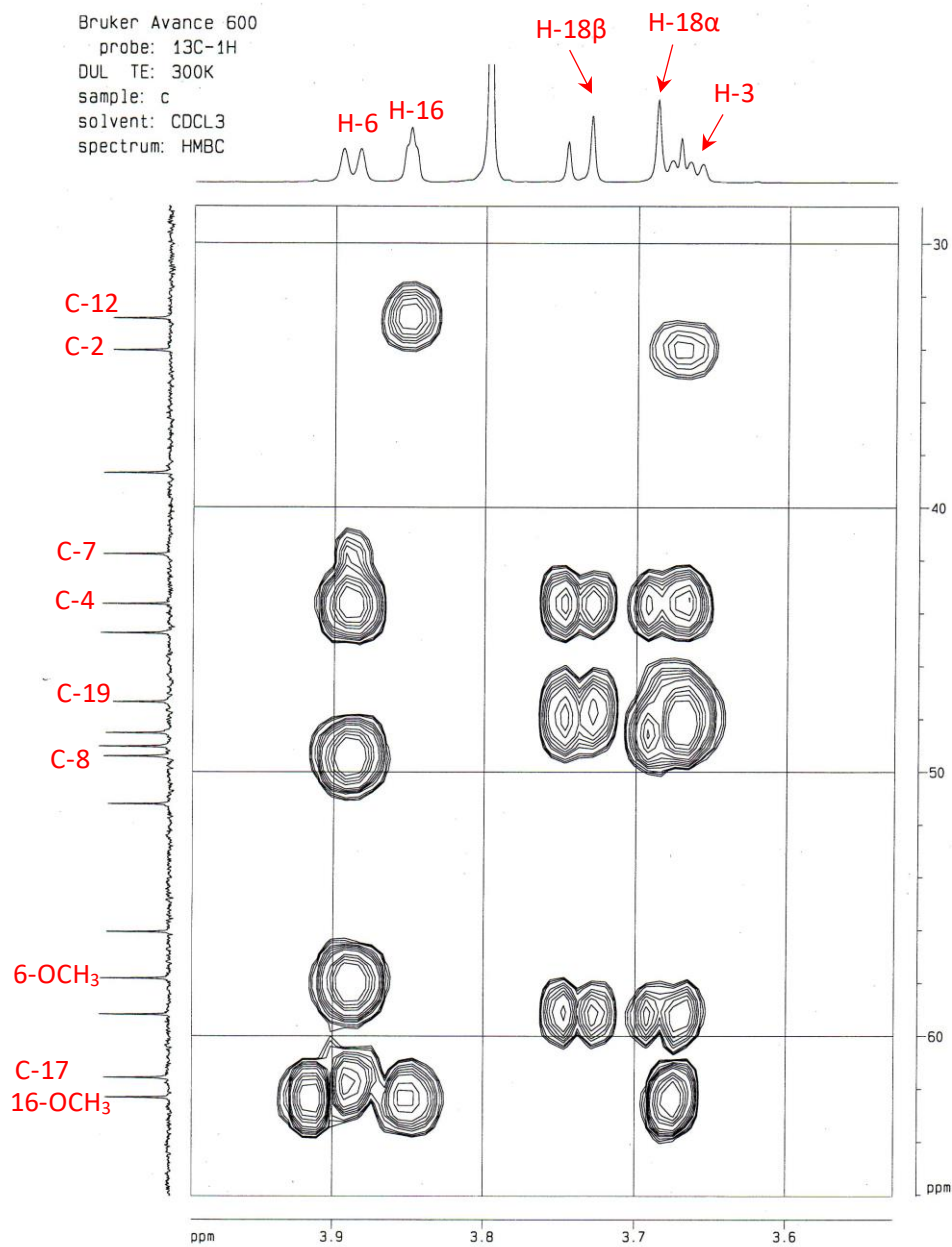


Figure S21. Key HMBC correlations of 16-epi-pyroaconitine (Detail 2)

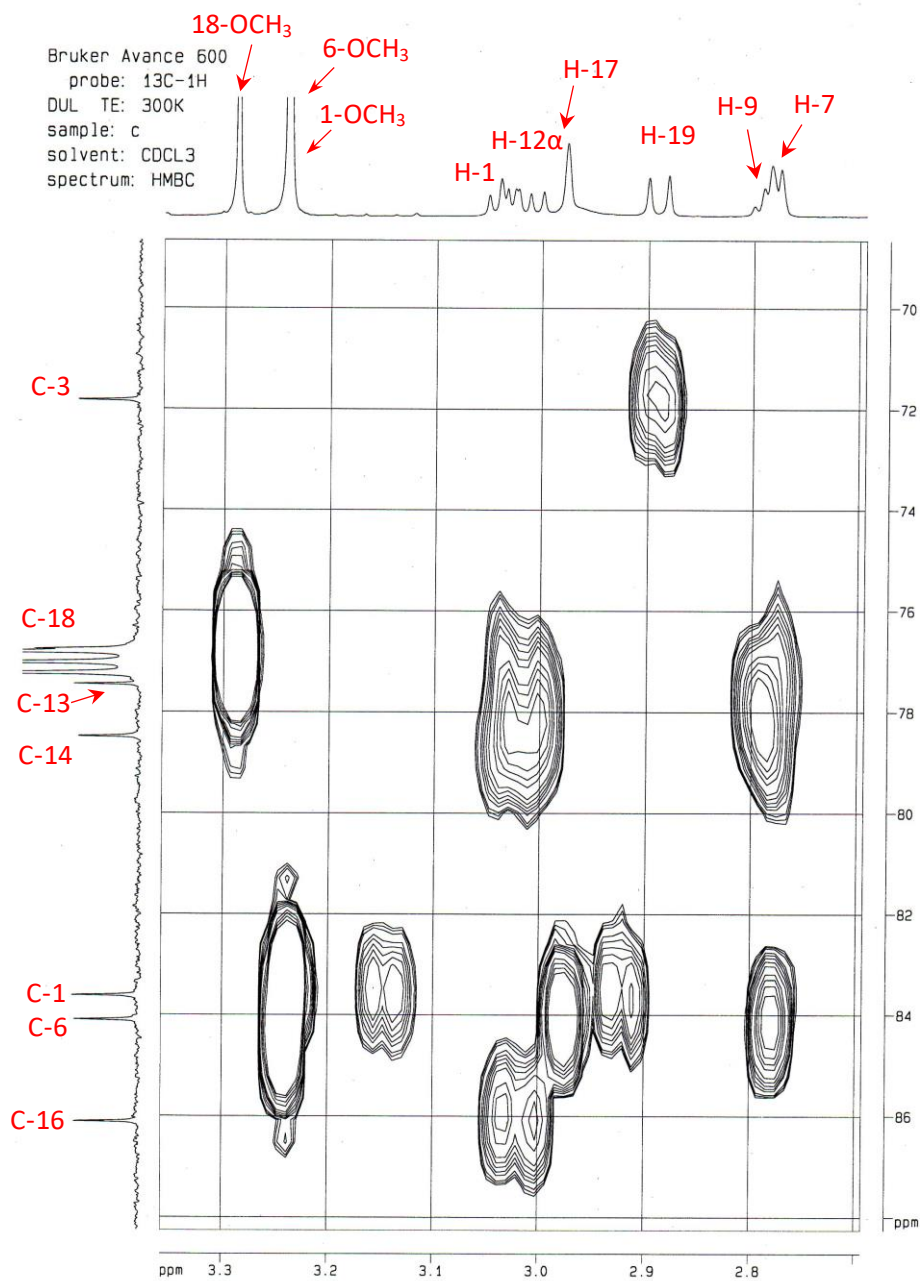


Figure S22. Key HMBC correlations of 16-epi-pyraconitine (Detail 3)

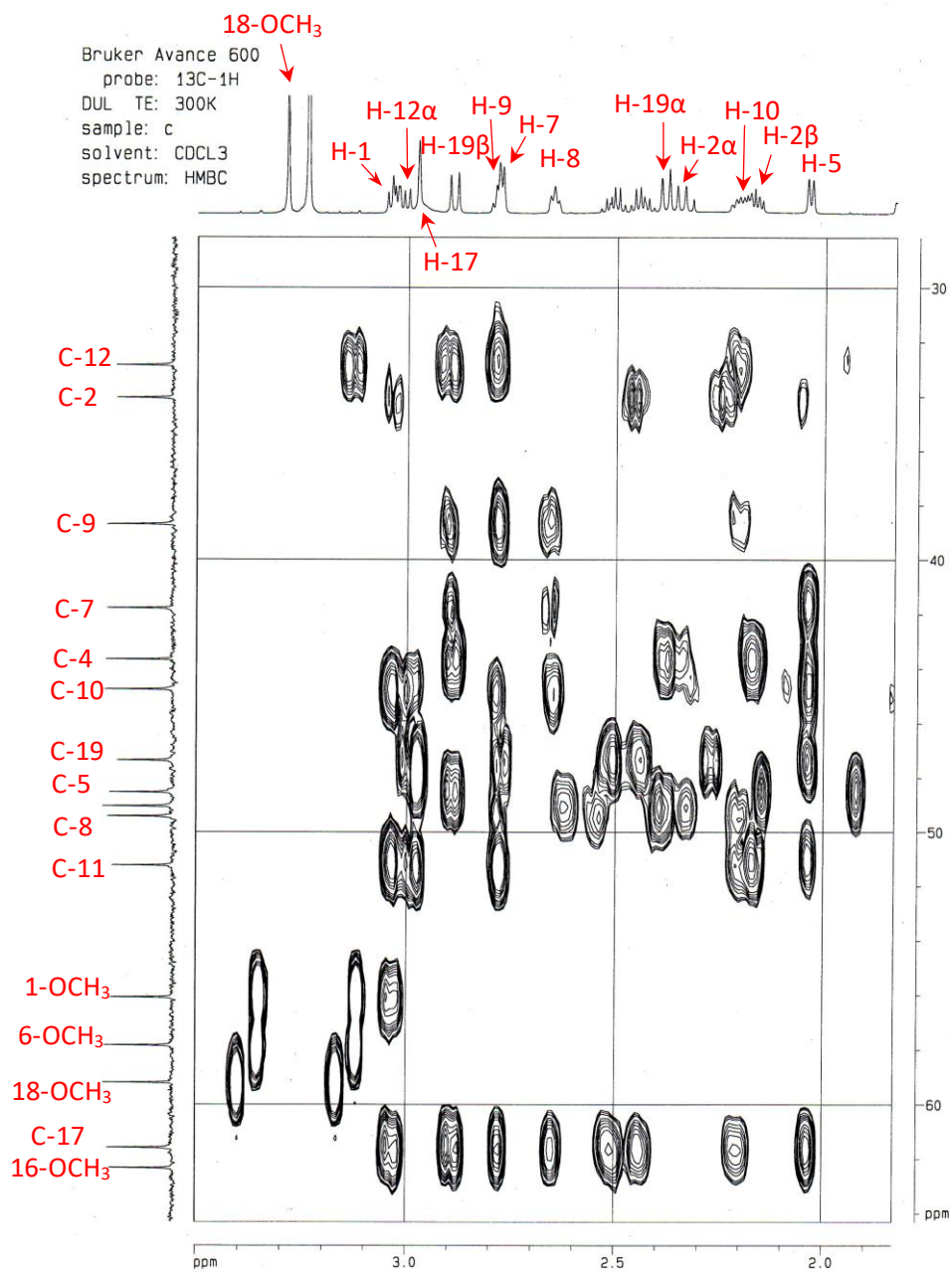


Figure S23. Key HMBC correlations of 16-epi-pyroaconitine (Detail 4)

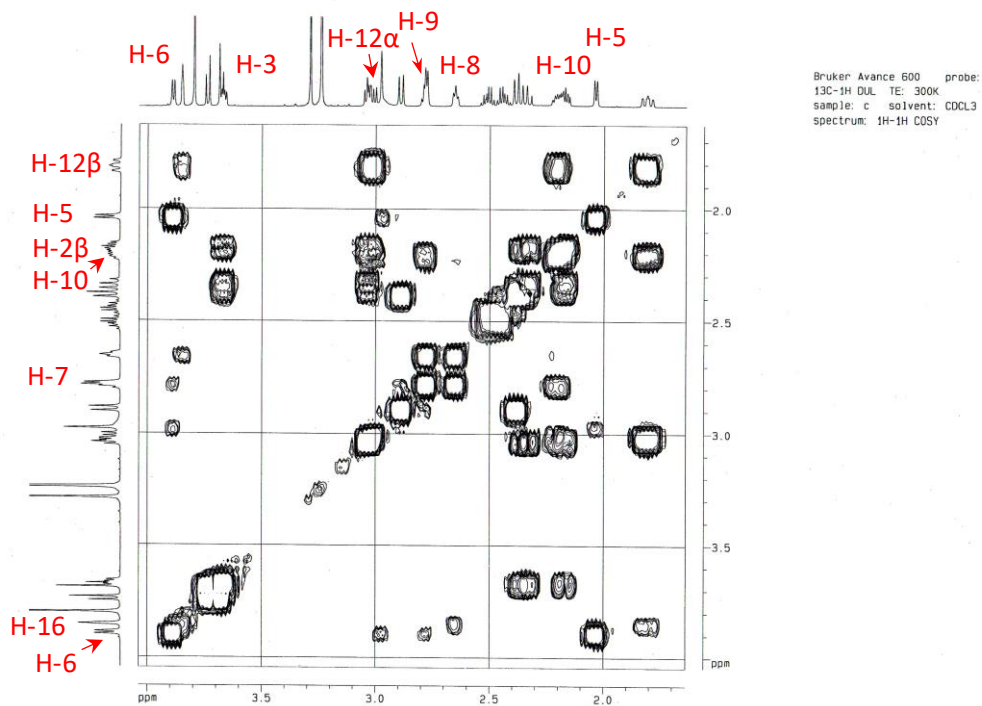


Figure S24. Key ^1H - ^1H COSY correlations of 16-epi-pyroaconitine (Detail 1)

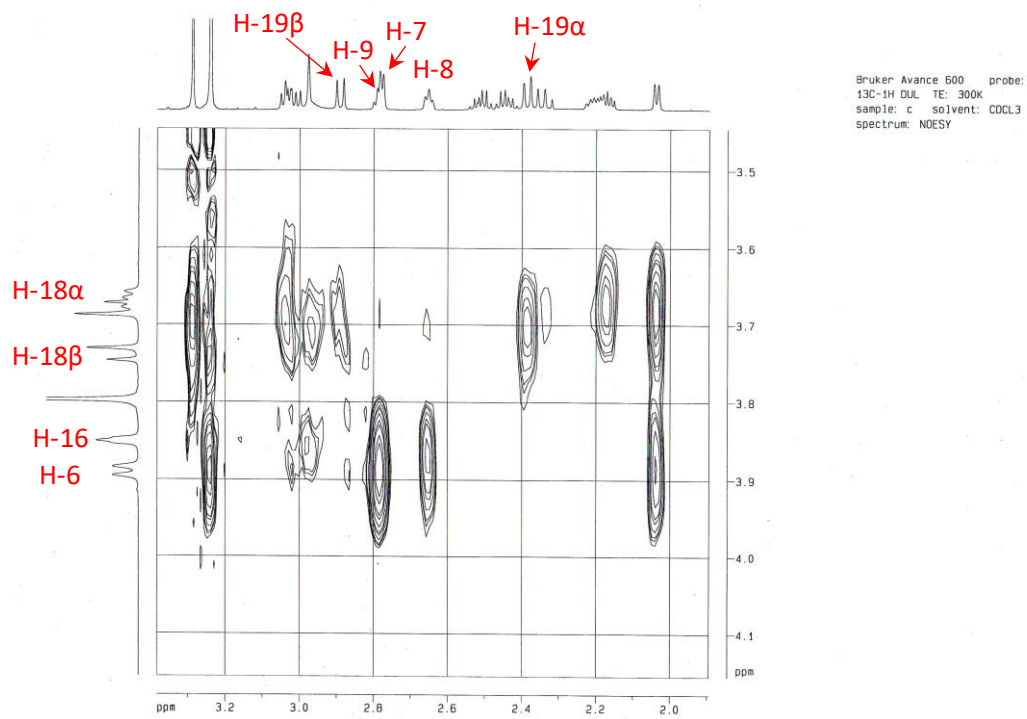


Figure S25. Key NOESY correlations of 16-epi-pyroaconitine (Detail 1)

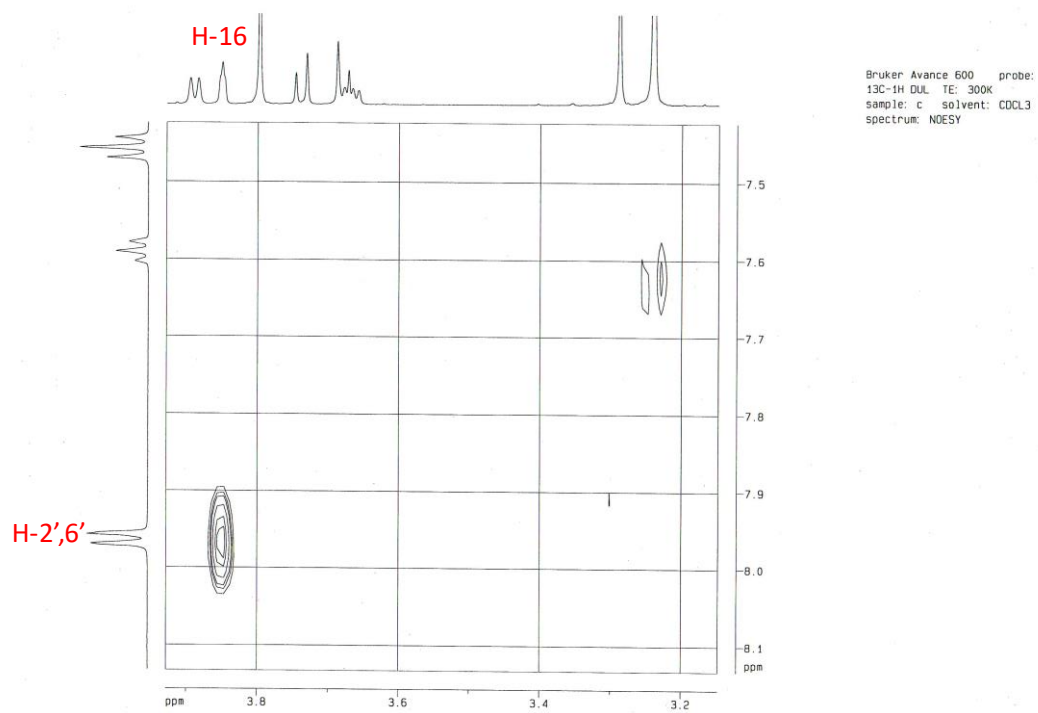


Figure S26. Key NOESY correlations of 16-epi-pyroaconitine (Detail 2)

Mass Spectrum SmartFormula Report

Analysis Info

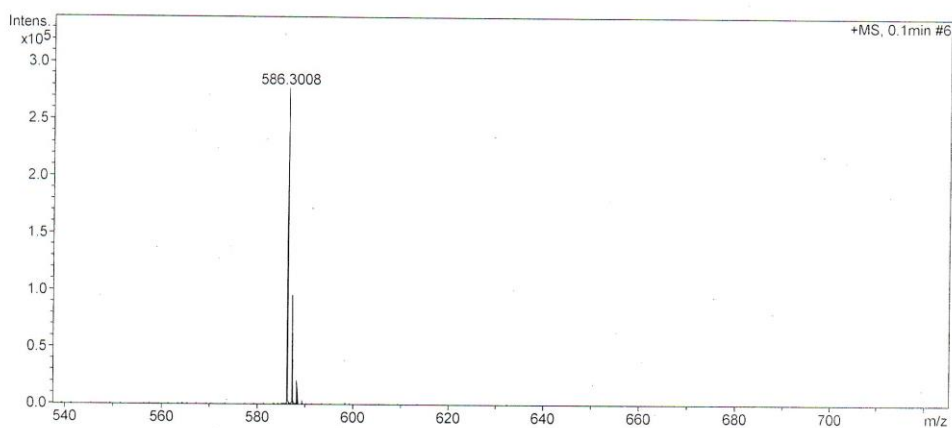
Analysis Name D:\Data\USER-2016\WYJ-C.d
Method tune_low_NEW.m
Sample Name WYJ-C
Comment

Acquisition Date 5/31/2016 4:23:53 PM

Operator Ma
Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	Formula	m/z	err [ppm]	mSigma	N-Rule	e ⁻ Conf
586.3008						
	C 32 H 44 N O 9	586.3011	0.5	4.62	ok	even
	C 29 H 36 N 11 O 3	586.2997	-1.8	7.69	ok	even
	C 28 H 40 N 7 O 7	586.2984	-4.1	7.83	ok	even
	C 33 H 40 N 5 O 5	586.3024	2.8	17.00	ok	even

Figure S27. High-resolution ESI-MS of 16-epi-pyroaconitine.

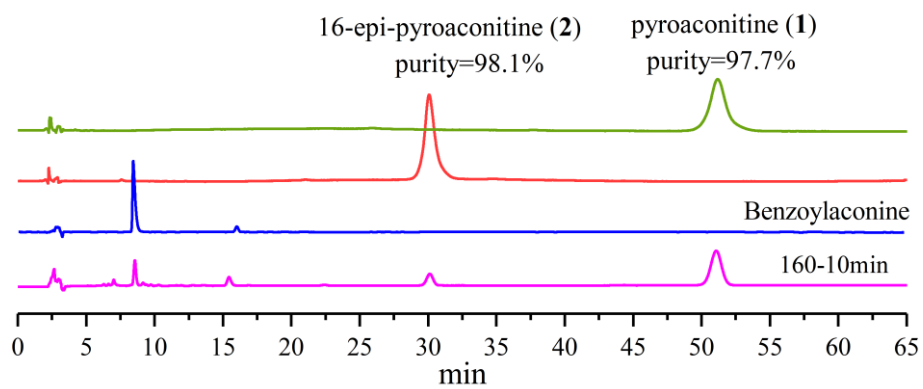


Figure S28. Purity test results of compounds 1 and 2.