

Supporting Information

Bioactive diterpenes from Brazilian native plant (*Moquiniastrum pulchrum*) and their application in weed control.

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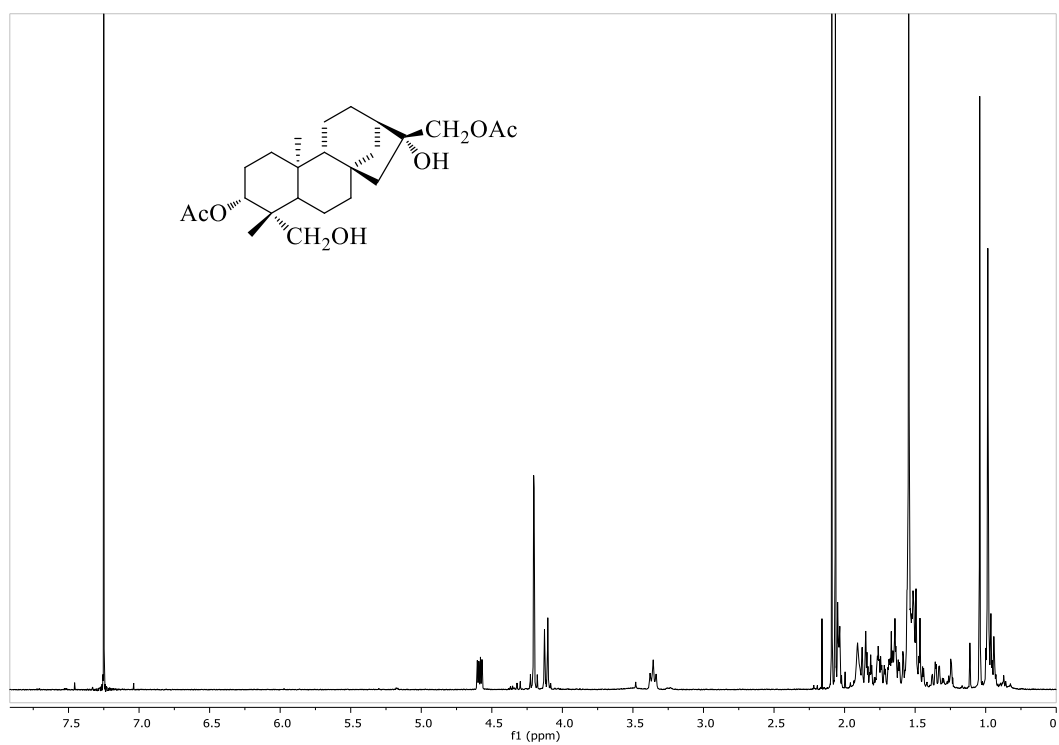
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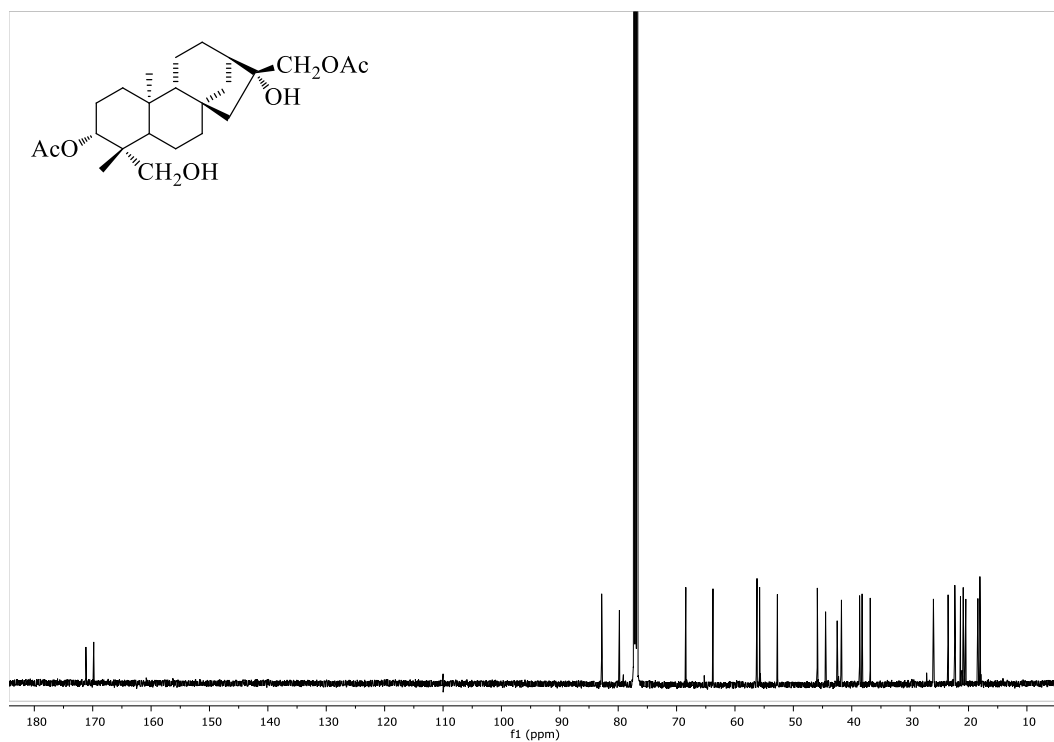
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Phone: +34 956 01 27 90; Fax: +34 956 01 62 88.

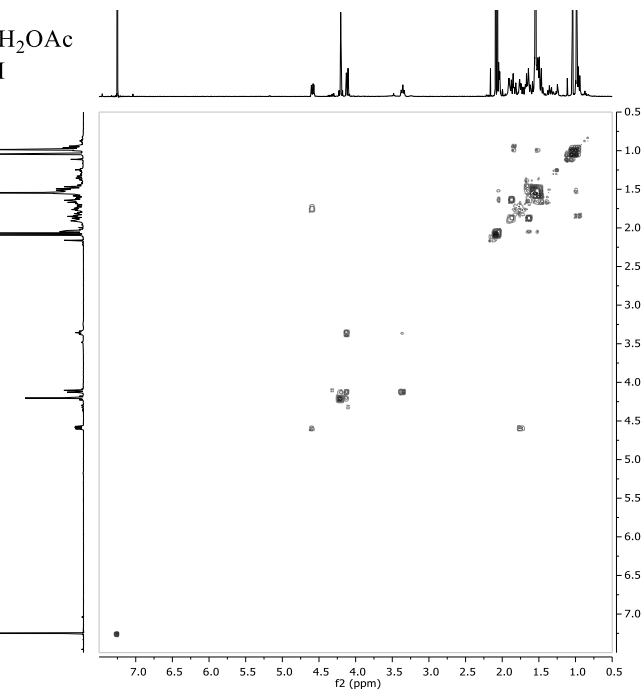
- S3 ^1H NMR spectrum of moquinian A (4) (500 MHz, Cl_3CD)
- S3 ^{13}C NMR spectrum of moquinian A (4) (125 MHz, Cl_3CD)
- S5 ^1H - ^1H COSY spectrum of moquinian A (4) (125 MHz, Cl_3CD)
- S5 HSQC spectrum of moquinian A (4) (125 MHz, Cl_3CD)
- S7 HMBC spectrum of moquinian A (4) (125 MHz, Cl_3CD)
- S7 TOF MS spectra of moquinian A (4)
- S9 ^1H NMR spectrum of moquinian B (5) (500 MHz, MeOH)
- S9 ^{13}C NMR spectrum of moquinian B (5) (125 MHz, MeOH)
- S10 ^1H - ^1H COSY spectrum of moquinian B (5) (125 MHz, MeOH)
- S10 HSQC spectrum of moquinian B (5) (125 MHz, MeOH)
- S11 HMBC spectrum of moquinian B (5) (125 MHz, MeOH)
- S11 TOF MS spectra of moquinian B (5)



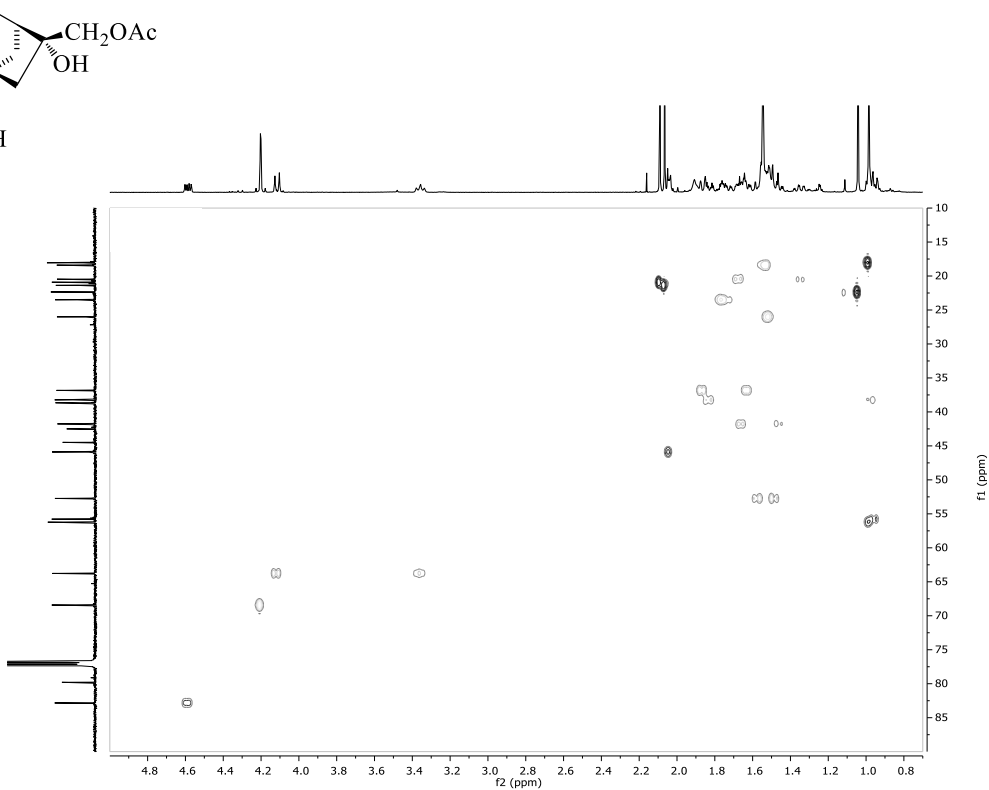
^1H NMR spectrum of moquinian A (4) (500 MHz, CDCl_3)



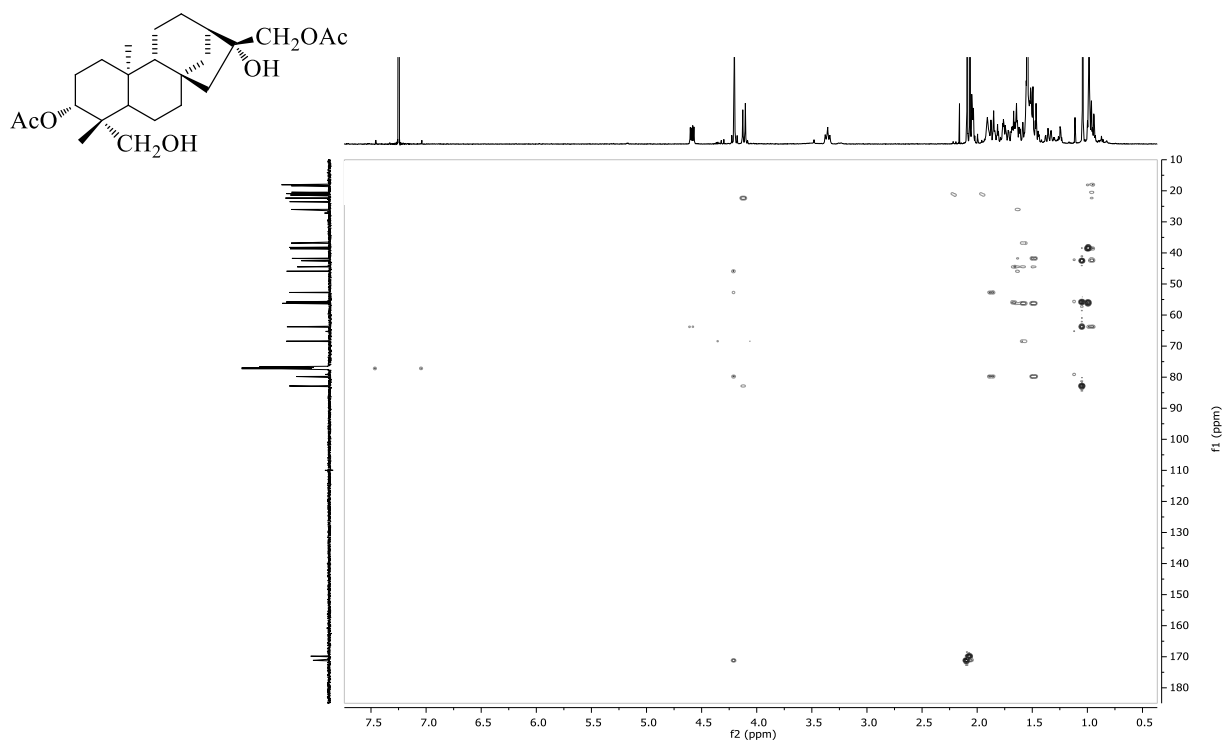
^{13}C NMR spectrum of moquinian A (4) (125 MHz, CDCl_3)



^1H - ^1H COSY spectrum of moquinian A (4) (125 MHz, Cl_3CD)



HSQC spectrum of moquinian A (4) (125 MHz, Cl_3CD)



HMBC spectrum of moquinian A (4) (125 MHz, Cl₃CD)

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

173 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

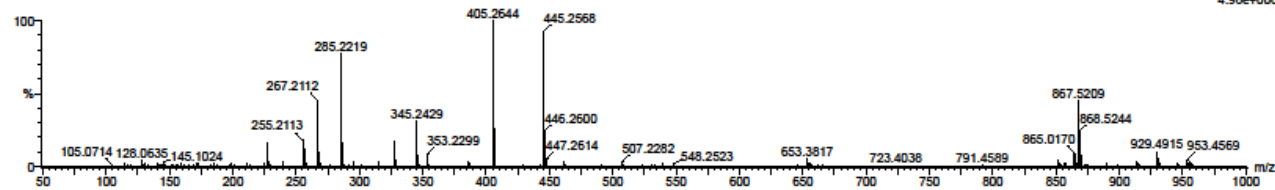
Elements Used:

C: 0-100 H: 0-100 O: 0-20 Na: 0-1

chcn

d4-d11 496 (4.590)

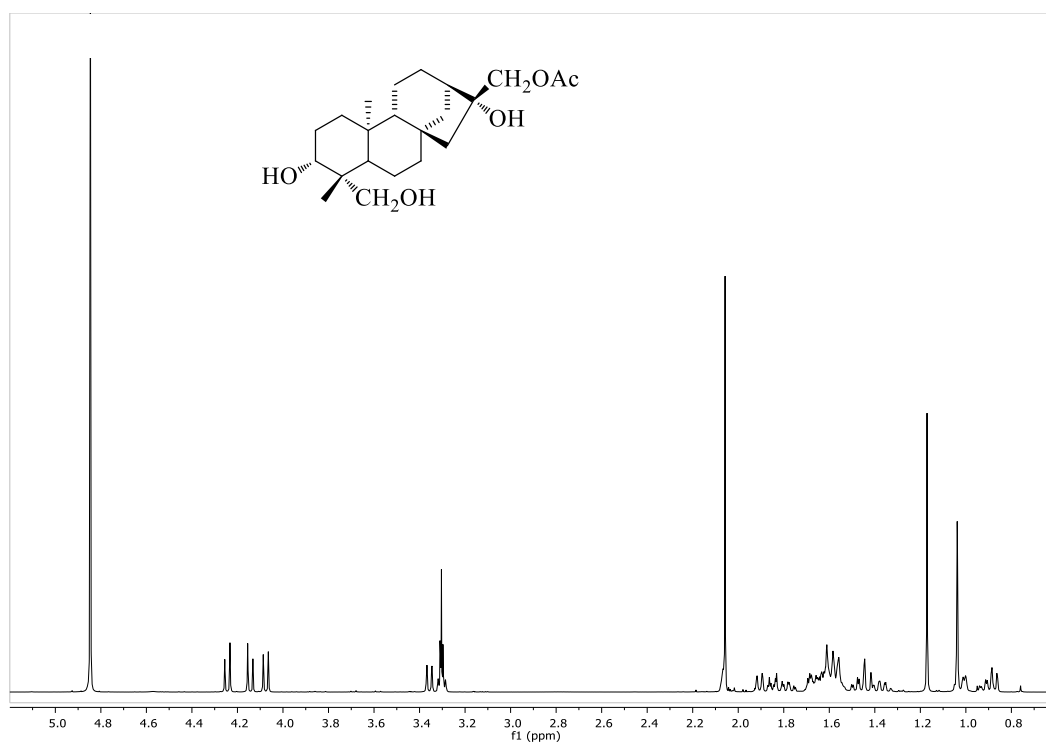
1: TOF MS ES+
4.98e+006



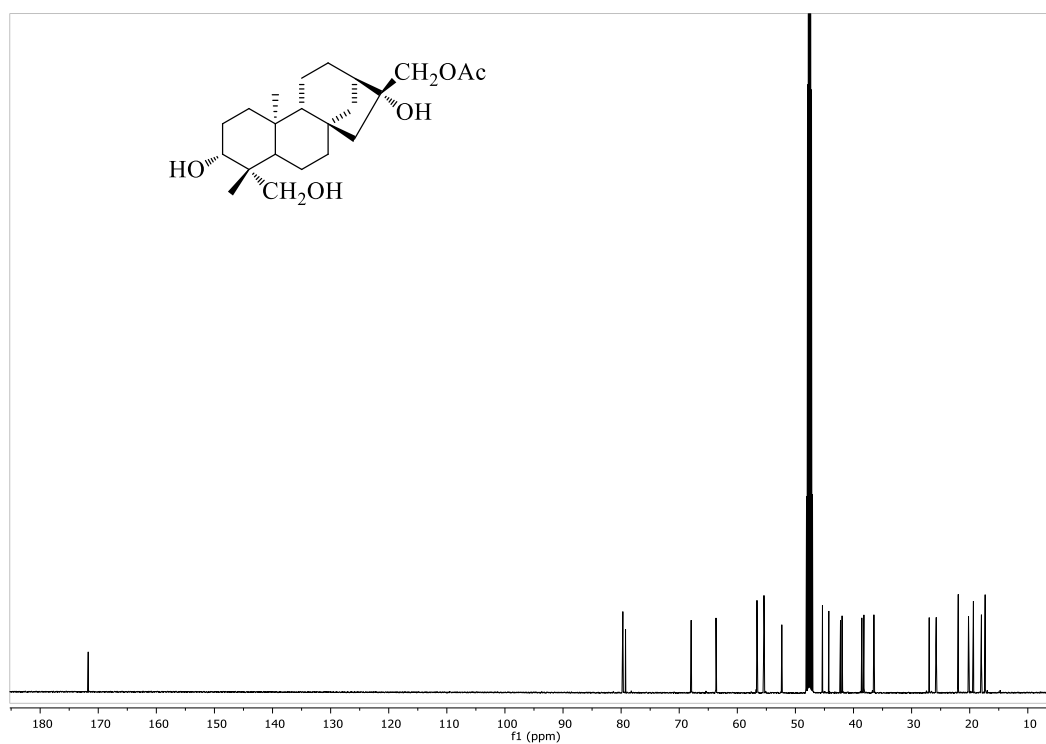
Minimum: -1.5
Maximum: 1.0 10.0 80.0

Mass	Calc. Mass	mDa	PFM	DBE	i-FIT	Norm	Conf(%)	Formula
445.2568	445.2566	0.2	0.4	5.5	1233.5	n/a	n/a	C ₂₄ H ₃₈ O ₆ Na

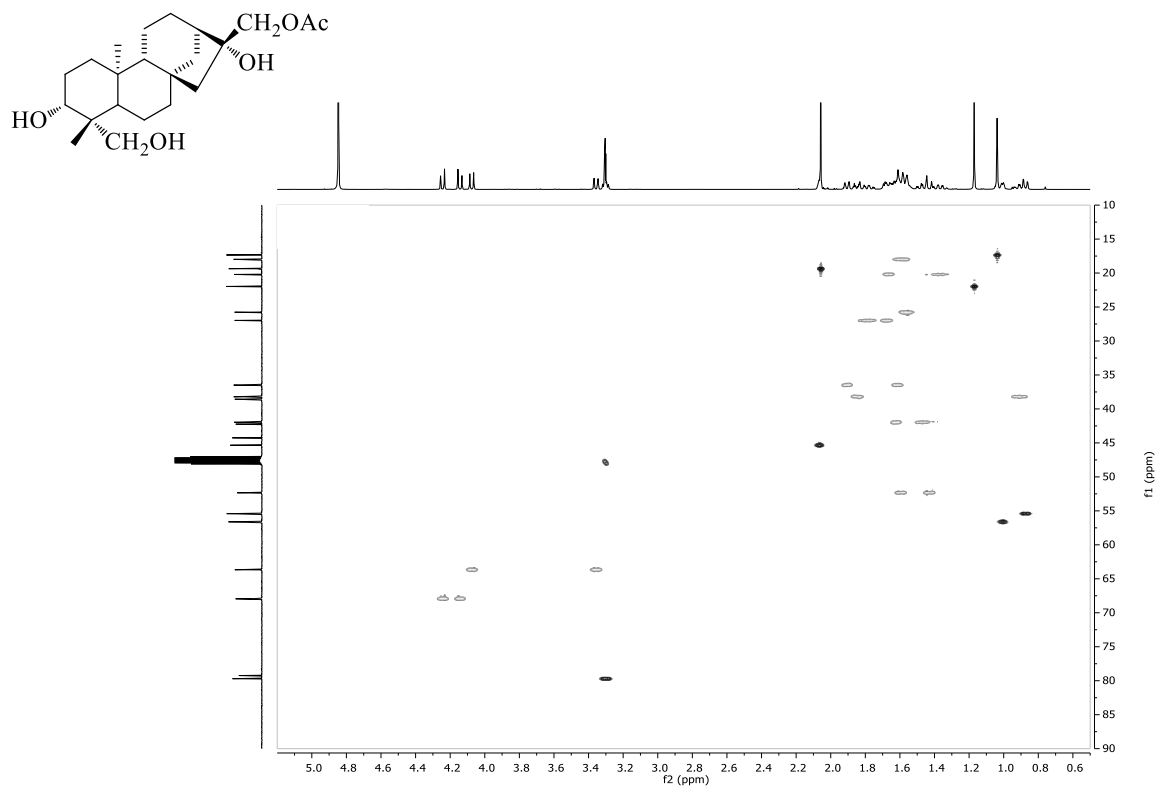
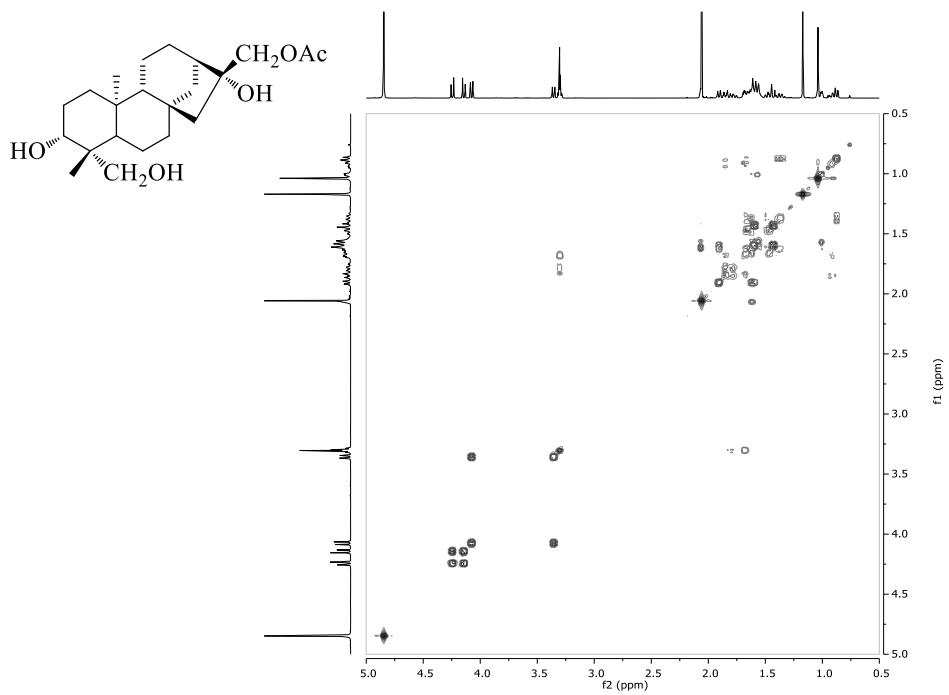
TOF MS spectrum of moquinian A (4)



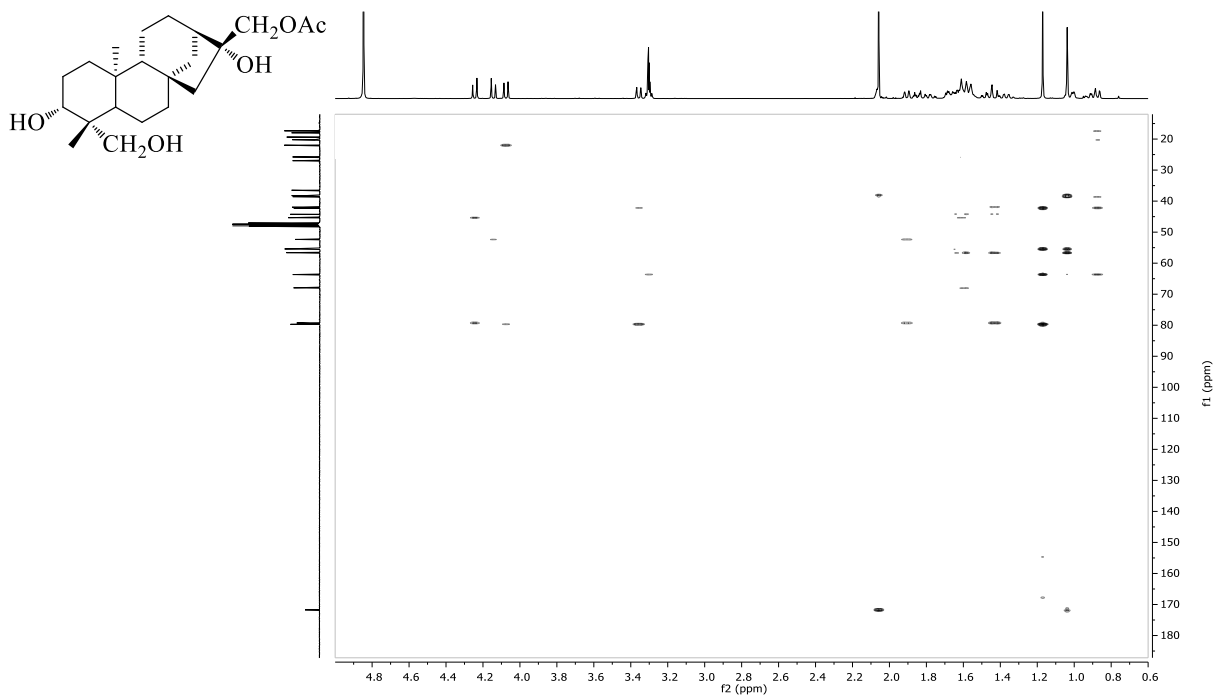
¹H NMR spectrum of moquinian B (5) (500 MHz, MeOH)



¹³C NMR spectrum of moquinian B (5) (125 MHz, MeOH)



HSQC spectrum of moquinian B (5) (125 MHz, MeOH)



HMBC spectrum of moquinian B (5) (125 MHz, MeOH)

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

159 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

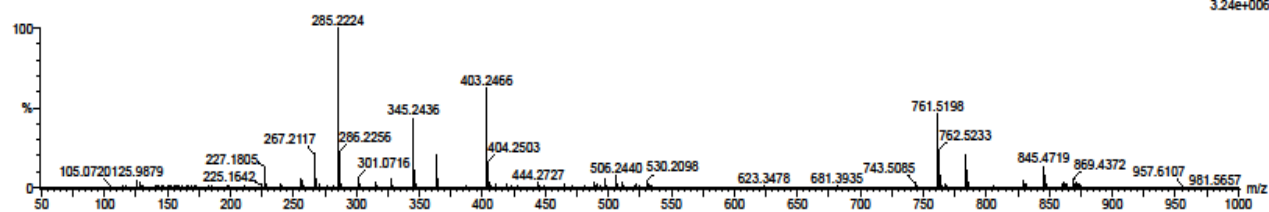
Elements Used:

C: 0-100 H: 0-100 O: 0-20 Na: 0-1

chon

d5-dl1 433 (4.016)

1: TOF MS ES+
3.24e+006



Minimum: -1.5
Maximum: 1.0 10.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
403.2466	403.2460	0.6	1.5	4.5	1266.1	n/a	n/a	C22 H36 O5 Na

TOF MS spectra of moquinian B (5)