Supporting Information

DNA Methyl Transferase Inhibiting Halogenated Monoterpenes from the Madagascar Red Marine Alga *Portieria hornemannii*

Eric H.Andrianasolo,[†] Dennis France,[‡] Susan Cornell-Kennon,[‡] and William H. Gerwick[†]

Spectral Data for Compound (2) in CDCl₃

- Figure S1. 400 MHz ¹H NMR spectrum of compound (2) in CDCl₃
- Figure S2. 100 MHz ¹³C NMR spectrum of compound (2) in CDCl₃
- **Figure S3**. 400 MHz ¹H-¹H COSY spectrum of compound (2) in CDCl₃
- Figure S4 400 MHz Multi-edited HSQC spectrum of compound (2) in CDCl₃
- Figure S5 400 MHz HMBC spectrum (optimized for J = 8Hz) of compound (2) in CDCl₃
- Figure S6 400 MHz 1D NOE spectrum (irradiation of proton 6.25 ppm) of compound (2) in CDCI₃
- **Figure S7** 400 MHz 1D NOE spectrum (irradiation of proton 2.62 ppm) of compound (**2**) in CDCl₃
- Figure S8 400 MHz 1D NOE spectrum (irradiation of proton 5.68 ppm) of compound (2) in CDCl₃
- **Figure S9** 400 MHz 1D NOE spectrum (irradiation of proton 5.48 ppm) of compound (**2**) in CDCl₃
- Figure \$10 LRCI MS spectrum of compound (2)

[†] College of Pharmacy, Oregon State University, Corvallis, Oregon 97331

[‡] Novartis Institute for Biomedical Research, Summit, New Jersey 07901

Spectral Data for Compound (3) in CDCI₃

- **Figure S11** 400 MHz ¹H NMR spectrum and 100 MHz ¹³C spectrum of compound (**3**) in CDCl₃
- Figure S12 400 MHz ¹H-¹H COSY spectrum of compound (3) in CDCl₃
- Figure S13 400 MHz Multi-edited HSQC spectrum of compound (3) in CDCl₃
- Figure S14 400 MHz HMBC spectrum (optimized for J = 8Hz) of compound (3) in CDCl₃
- **Figure S15** 400 MHz 1D NOE spectrum (irradiation of proton 6.35 ppm) of compound (**3**) in CDCl₃
- **Figure S16** 400 MHz 1D NOE spectrum (irradiation of proton 5.69 ppm) of compound (**3**) in CDCl₃
- Figure S17 400 MHz 1D NOE spectrum (irradiation of proton 5.49 ppm) of compound (3) in CDCl₃
- Figure S18 GC/MS spectrum of compound (3)

Spectral Data for Compound (4) in CDCI₃

- Figure S19 400 MHz ¹H NMR spectrum of compound (4) in CDCl₃
- Figure S20 400 MHz ¹H-¹H COSY spectrum of compound (4) in CDCl₃
- Figure S21 400 MHz HSQC spectrum of compound (4) in CDCl₃ (partial vue of the signal belonging to the two methyl groups)
- **Figure S22** 400 MHz HSQC spectrum of compound (4) in CDCl₃ (partial vue of the signal belonging to the proton doublets at 5.53 and 5.70 ppm)
- Figure S23 400 MHz HSQC spectrum of compound (4) in CDCl₃ (partial vue of the signal belonging to the proton at 6.97 ppm)
- **Figure S24** 400 MHz HMBC spectrum of compound (**4**) in CDCl₃ (observed signal from the two methyl groups)
- **Figure S25** 400 MHz HMBC spectrum of compound (**4**) in CDCl₃ (observed signal from the proton doublets at 5.53 and 5.70 ppm)
- Figure S26 GC/MS spectrum of compound (4)
- Figure S27 LRCI MS spectrum of compound (4)

Data on Algal Sample and Collection Site

- Figure S28 Photo of the voucher sample
- Figure S29 Photo of the collection site

Figure S1. 400 MHz ¹H NMR spectrum of compound (2) in CDCl₃

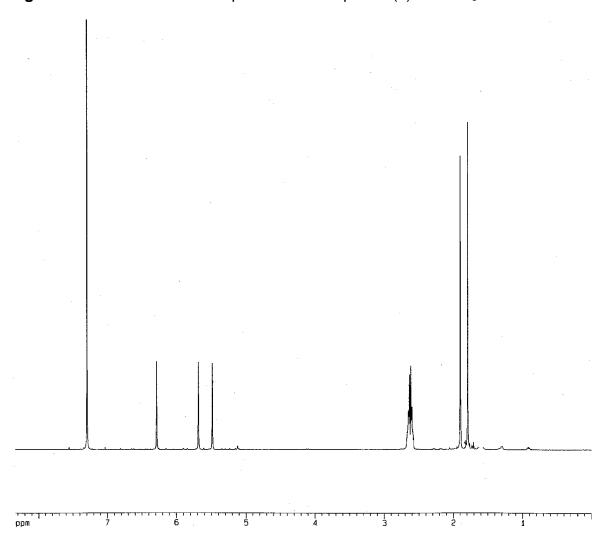


Figure S2. 100 MHz 13 C NMR spectrum of compound (2) in CDCl $_3$

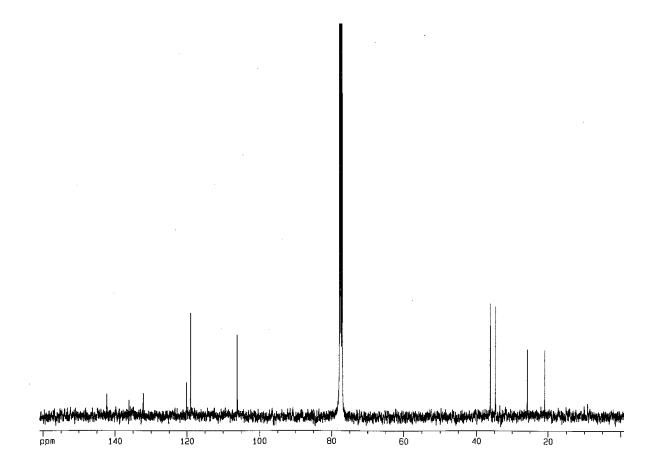


Figure S3. 400 MHz ¹H-¹H COSY spectrum of compound (2) in CDCl₃

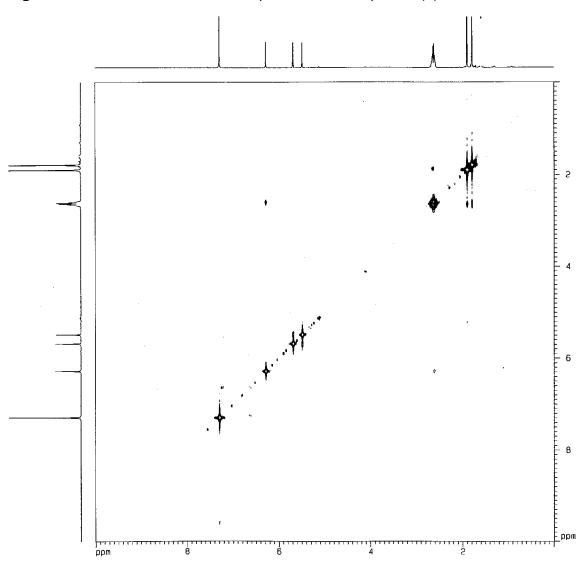


Figure S4 400 MHz Multi-edited HSQC spectrum of compound (2) in CDCl₃ 50

Figure S5 400 MHz HMBC spectrum (optimized for J = 8Hz) of compound (2) in CDCl₃

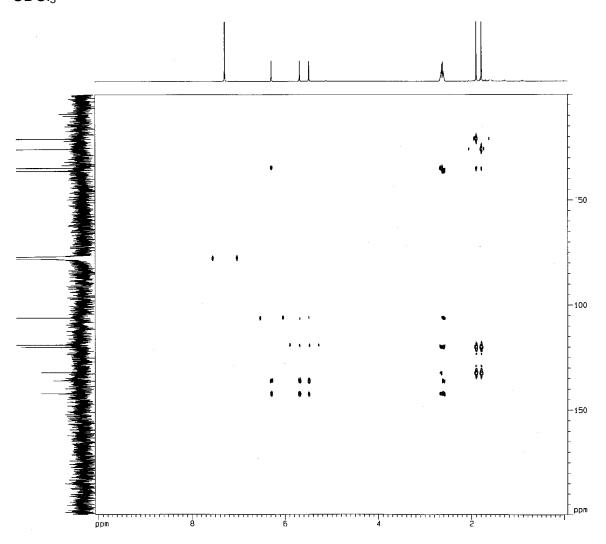


Figure S6 400 MHz 1D NOE spectrum (irradiation of proton 6.25 ppm) of compound (2) in \mbox{CDCI}_3

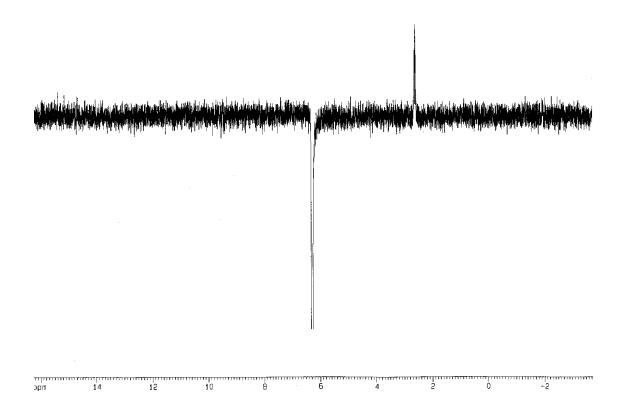


Figure S7 400 MHz 1D NOE spectrum (irradiation of proton 2.62 ppm) of compound (2) in $CDCl_3$

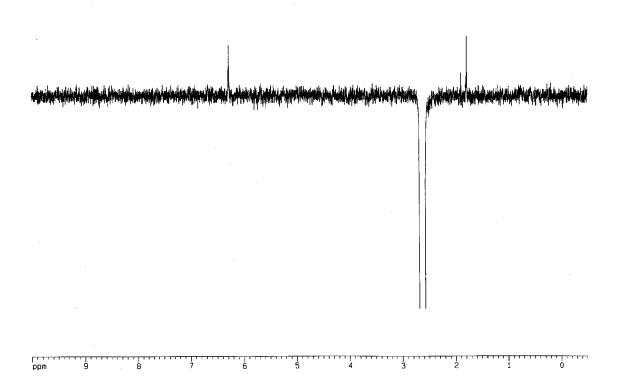


Figure S8 400 MHz 1D NOE spectrum (irradiation of proton 5.68 ppm) of compound (2) in $CDCl_3$

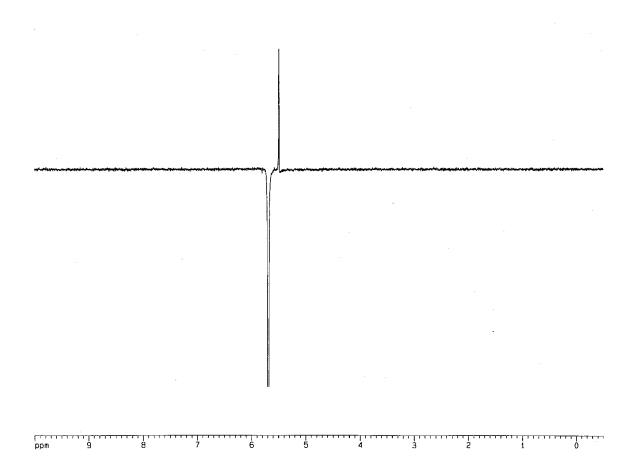


Figure S9 400 MHz 1D NOE spectrum (irradiation of proton 5.48 ppm) of compound (2) in $CDCl_3$

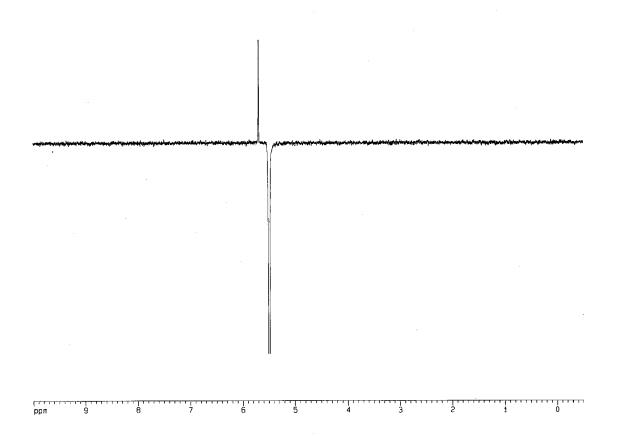


Figure S10 LRCI MS spectrum of compound (2)

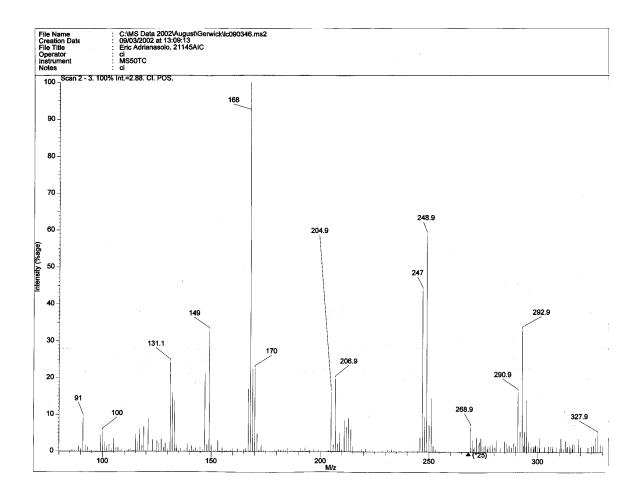
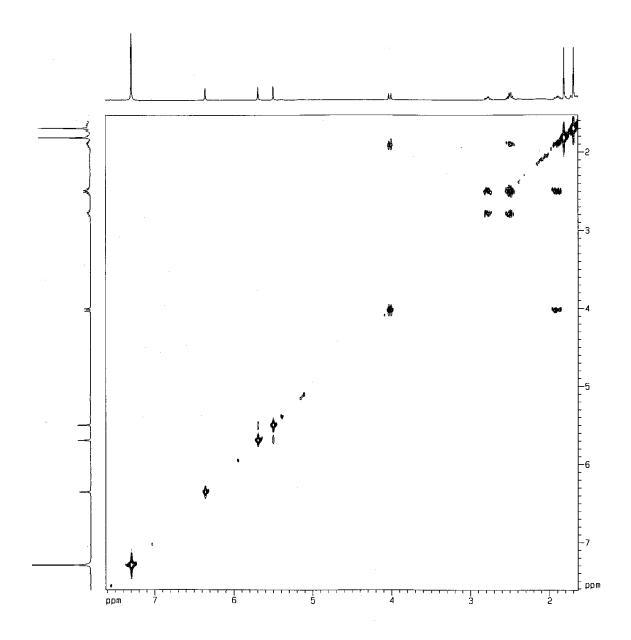


Figure S11 400 MHz ¹H NMR spectrum and 100 MHz ¹³C spectrum of compound (3) in CDCl₃

Figure S12 400 MHz ¹H-¹H COSY spectrum of compound (3) in CDCl₃



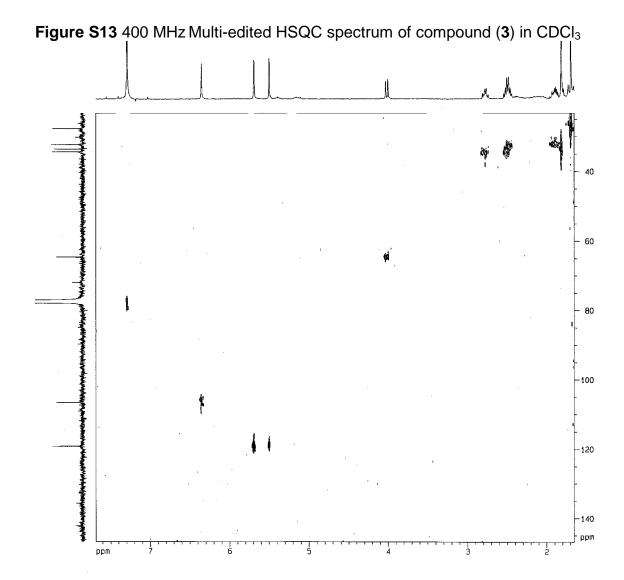


Figure S14 400 MHz HMBC spectrum (optimized for J = 8Hz) of compound (3) in CDCI₃ 100 e a

Figure S15 400 MHz 1D NOE spectrum (irradiation of proton 6.35 ppm) of compound (3) in \mbox{CDCI}_3

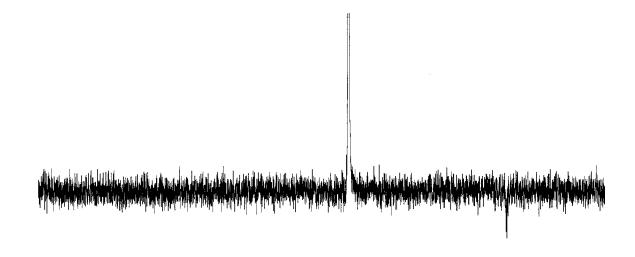




Figure S16 400 MHz 1D NOE spectrum (irradiation of proton 5.69 ppm) of compound (3) in \mbox{CDCI}_3

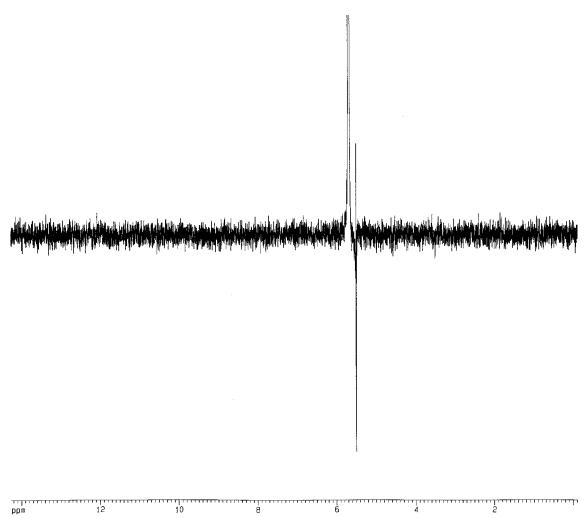


Figure S17 400 MHz 1D NOE spectrum (irradiation of proton 5.49 ppm) of compound (3) in \mbox{CDCI}_3

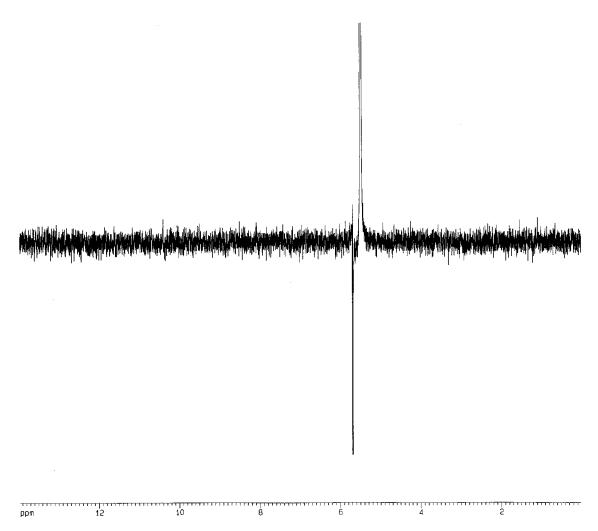


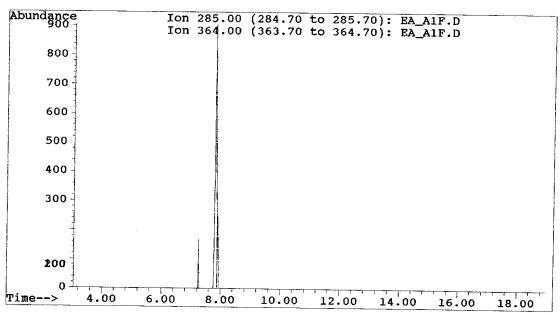
Figure S18 GC/MS spectrum of compound (3)

File : C:\HPCHEM\1\DATA\EA_A1F.D

Operator

8 Mar 104 5971 - De Acquired Instrument:

Sample Name: Misc Info : Vial Number: 1



2:08 pm using AcqMethod DEFAULT

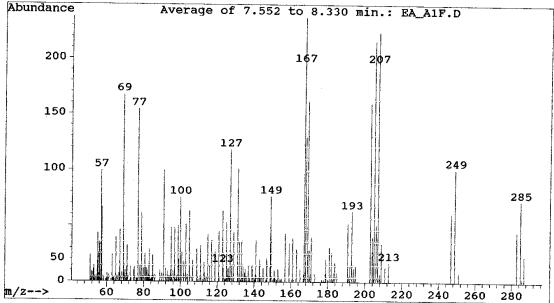


Figure S19. 400 MHz ¹H NMR spectrum of compound (4) in CDCl₃

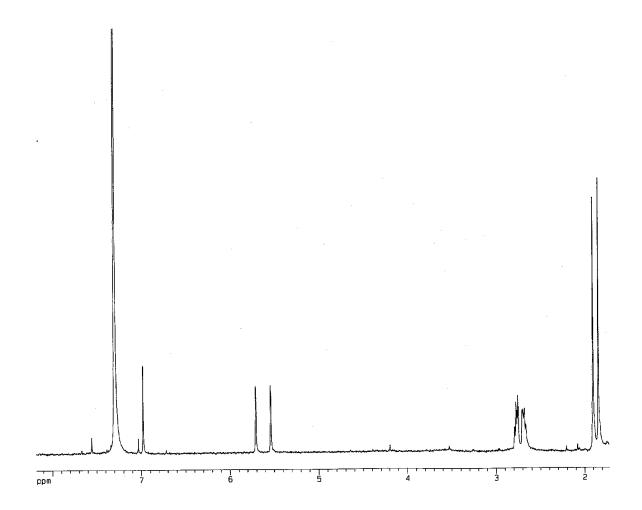


Figure S20 400 MHz ¹H-¹H COSY spectrum of compound (4) in CDCl₃

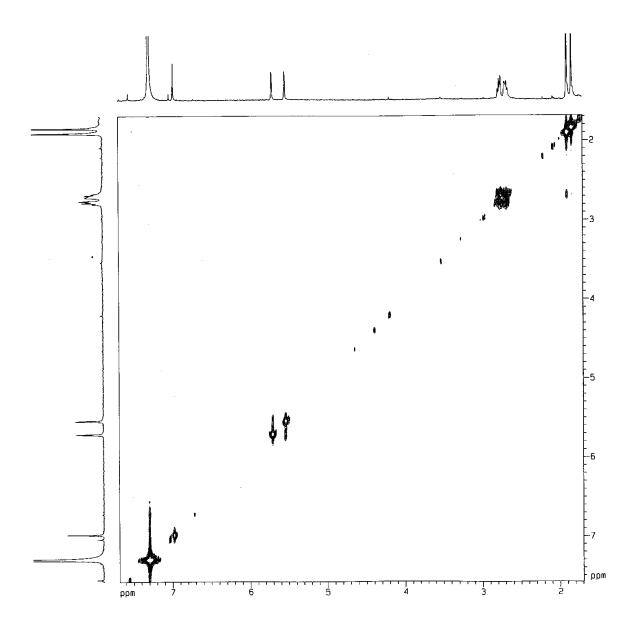


Figure S21 400 MHz HSQC spectrum of compound (4) in CDCl $_3$ (partial vue of the signal belonging to the two methyl groups)

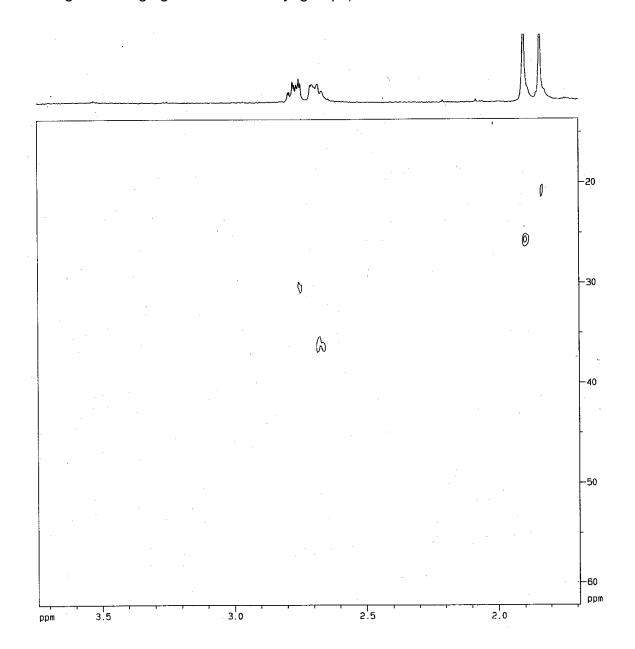


Figure S22 400 MHz HSQC spectrum of compound (4) in CDCl $_3$ (partial vue of the signal belonging to the proton doublets at 5.53 and 5.70 ppm)

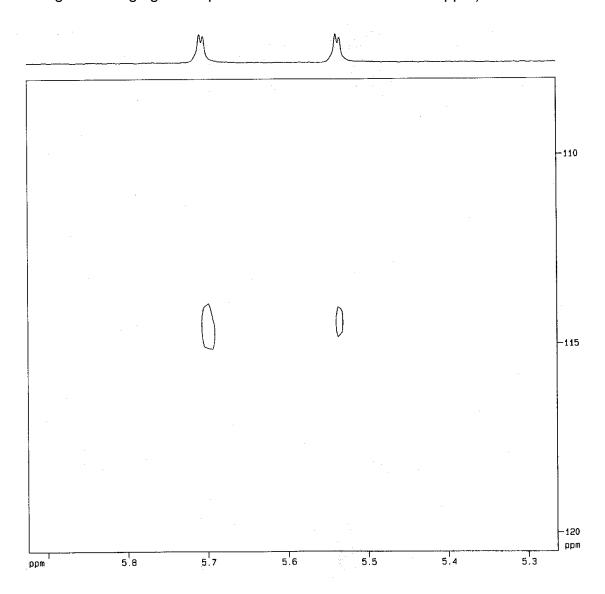


Figure S23 400 MHz HSQC spectrum of compound (4) in CDCl $_3$ (partial vue of the signal belonging to the proton at 6.97 ppm)

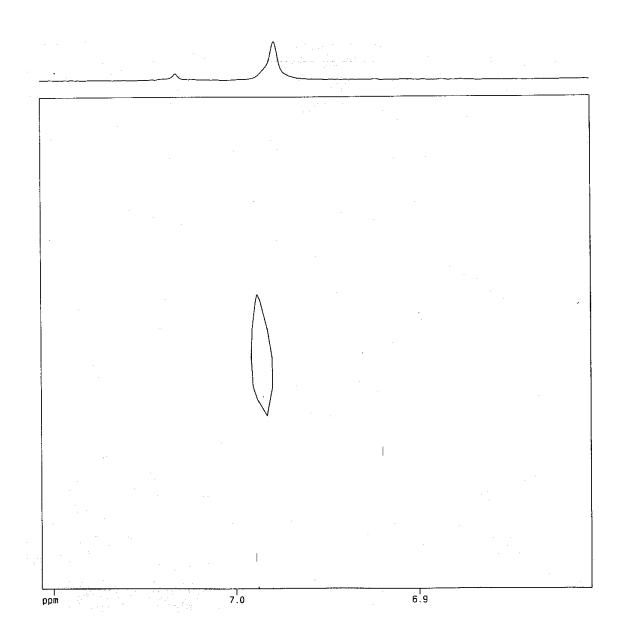


Figure S24 400 MHz HMBC spectrum of compound (4) in $CDCl_3$ (observed signal from the two methyl groups)

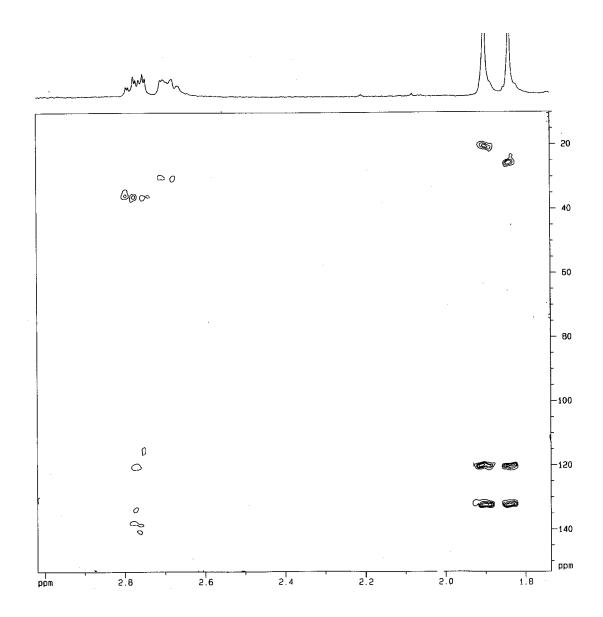


Figure S25 400 MHz HMBC spectrum of compound (4) in CDCl $_3$ (observed signal from the proton doublets at 5.53 and 5.70 ppm)

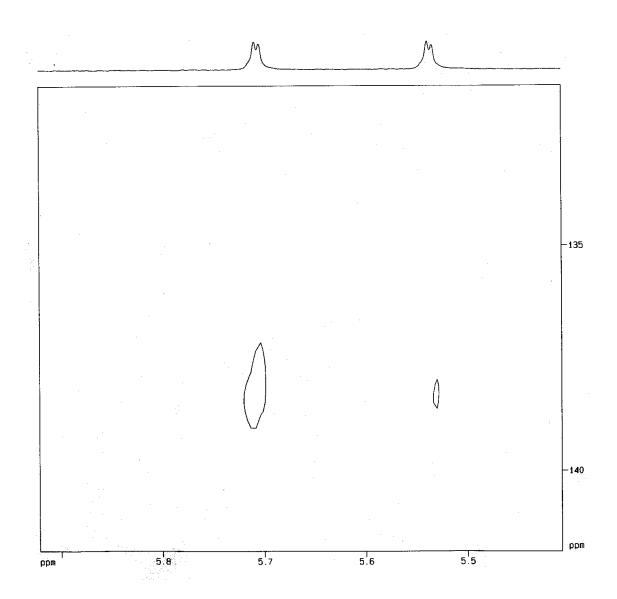


Figure S26 GC/MS spectrum of compound (4)

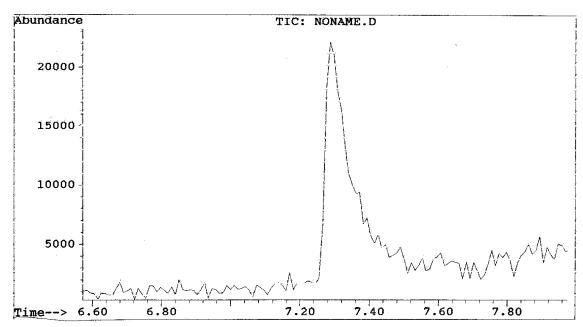
: C:\HPCHEM\I\DATA\NONAME.D File

Operator : eric

8 Mar 104 10:00 am using AcqMethod DEFAULT 5971 - De Acquired

Instrument : Sample Name: 21141a1a4

Misc Info Vial Number: 1



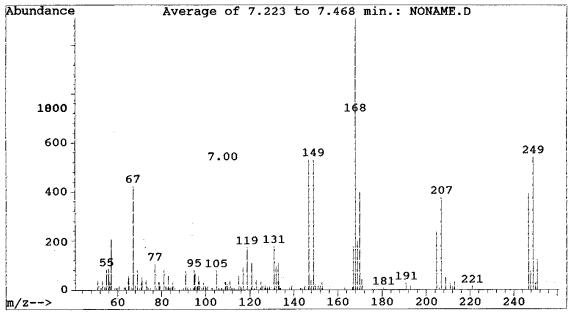


Figure S27 LRCI MS spectrum of compound (4)

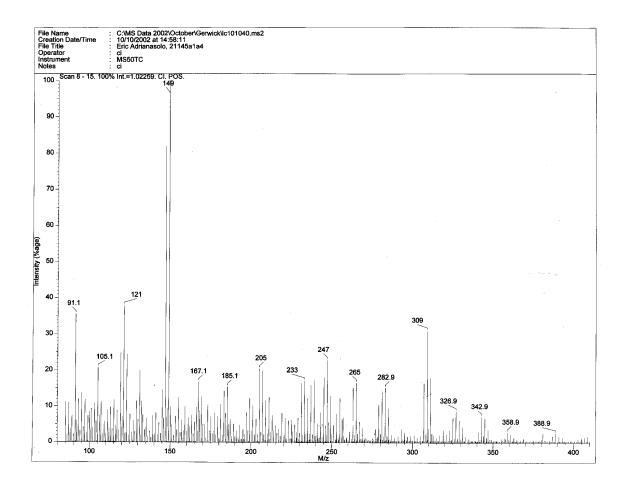


Figure S28 Photo of the voucher sample



Figure \$29 Photo of the collection site

