Alkaloids from *Daphniphyllum longeracemosum*

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Supporting Information

- S3. ^1H NMR (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin A (**1**).
- S4. ^{13}C NMR (Bruker AM-500, 125 MHz, CD_3OD) of daphnilongeranin A (**1**).
- S5. ^1H - ^1H COSY (Varian Mercury-400, 400 MHz, CD_3OD) of daphnilongeranin A (**1**).
- S6. HMQC (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin A (**1**).
- S7. HMBC (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin A (**1**).
- S8. Expanded HMBC (δ_{H} 0.9-4.3 vs δ_{C} 19-68) (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin A (**1**).
- S9. NOESY (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin A (**1**).
- S10. EIMS of daphnilongeranin A (**1**).
- S11. IR of daphnilongeranin A (**1**).
- S12. ^1H NMR (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin B (**2**).
- S13. ^{13}C NMR (Bruker AM-500, 125 MHz, CD_3OD) of daphnilongeranin B (**2**).
- S14. ^1H - ^1H COSY (Varian Mercury-400, 400 MHz, CD_3OD) of daphnilongeranin B (**2**).
- S15. HMQC (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin B (**2**).
- S16. HMBC (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin B (**2**).
- S17. NOESY (Bruker AM-500, 500 MHz, CD_3OD) of daphnilongeranin B (**2**).
- S18. EIMS of daphnilongeranin B (**2**).
- S19. IR of daphnilongeranin B (**2**).
- S20. ^1H NMR (Bruker AM-500, 500 MHz, CDCl_3) of daphnilongeranin C (**3**).
- S21. ^{13}C NMR (Bruker AM-500, 500 MHz, CDCl_3) of daphnilongeranin C (**3**).
- S22. ^1H - ^1H COSY (Varian Mercury-400, 400 MHz, CDCl_3) of daphnilongeranin C (**3**).

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- S23. HMQC (Bruker AM-500, 500 MHz, CDCl₃) of daphnilongeranin C (**3**).
- S24. HMBC (Varian Mercury-400, 400 MHz, CDCl₃) of daphnilongeranin C (**3**).
- S25. Expanded HMBC (δ_{H} 0.96-3.88 vs δ_{C} 19-68) (Varian Mercury-400, 400 MHz, CDCl₃) of daphnilongeranin C (**3**).
- S26. ROESY (Varian Inova-600, 600 MHz, CDCl₃) of daphnilongeranin C (**3**).
- S27. EIMS of daphnilongeranin C (**3**).
- S28. IR of daphnilongeranin C (**3**).
- S29. ¹H NMR (Bruker AM-500, 500 MHz, CD₃OD) of daphnilongeranin D (**4**).
- S30. ¹³C NMR (Bruker AM-500, 125 MHz, CD₃OD) of daphnilongeranin D (**4**).
- S31. ¹H-¹H COSY (Varian Mercury-400, 400 MHz, CD₃OD) of daphnilongeranin D (**4**).
- S32. HMQC (Bruker AM-500, 500 MHz, CD₃OD) of daphnilongeranin D (**4**).
- S33. Expanded HMQC (δ_{H} 0.85-3.35 vs δ_{C} 19-50) (Bruker AM-500, 500 MHz, CD₃OD) of daphnilongeranin D (**4**).
- S34. HMBC (Bruker AM-500, 500 MHz, CD₃OD) of daphnilongeranin D (**4**).
- S35. Expanded HMBC (δ_{H} 0.75-2.25 vs δ_{C} 19-45) (Bruker AM-500, 500 MHz, CD₃OD) of daphnilongeranin D (**4**).
- S36. EIMS of daphnilongeranin D (**4**).
- S37. IR of daphnilongeranin D (**4**).
- S38. Figures of the ¹H-¹H COSY (—), the selected HMBC (H→C) and key NOESY correlations (↔) of **1** and **2**.
- S39. Figures of the ¹H-¹H COSY (—), the selected HMBC (H→C) and key ROESY correlations (↔) of **3** and the ¹H-¹H COSY (—), the selected HMBC (H→C) of **4**.

¹H NMR of daphnilongeranin A (1) run in CD₃OD

^{13}C NMR of daphnilongeranin A (1) run in CD_3OD

^1H - ^1H COSY of daphnilongeranin A (1)

HMQC of daphnilongeranin A (1)

HMBC of daphnilongeranin A (1)

NOESY of daphnilongeranin A (1)

EIMS of daphnilongeranin A (1)

SPEC: 152009
 Samp: DL-19
 Comm: Finnigan/MAT95/70eV/Tsou:200c/R:1000
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
 Oper: WANG_JESIMM.CAS Client: S/N:SW01-0001
 Base: 110.0 Inten : 30849280
 Norm: 110.0 RIC : 78725693
 Peak: 1000.00 mmu

31-May-05 Elapse: 02:56.5 27
 Start : 15:22:06 32

Inlet :
 Masses: 50 > 750
 #peaks: 467

IR of daphnilongeranin A (1)

¹H NMR of daphnilongeranin B (**2**) run in CD₃OD

^{13}C NMR of daphnilongeranin B (2) run in CD_3OD

Chemical structure of compound **1** is shown in the top right corner. The structure is a complex polycyclic molecule with a quaternary carbon atom bonded to a methyl group, a hydrogen atom, and two other groups. The molecule contains several stereocenters and a carbonyl group.

The 2D COSY NMR spectrum displays the following features:

- Diagonal Peaks:** These represent the 1D ¹H NMR spectrum, showing peaks at approximately 3.3, 3.2, 3.1, 3.0, 2.9, 2.8, 2.7, 2.6, 2.5, 2.4, 2.3, 2.2, 2.1, 2.0, 1.9, 1.8, 1.7, 1.6, 1.5, 1.4, 1.3, 1.2, and 1.1 ppm.
- Cross-peaks:** These indicate scalar coupling between protons. Key cross-peaks are observed at (3.3, 3.3), (3.2, 3.2), (3.1, 3.1), (3.0, 3.0), (2.9, 2.9), (2.8, 2.8), (2.7, 2.7), (2.6, 2.6), (2.5, 2.5), (2.4, 2.4), (2.3, 2.3), (2.2, 2.2), (2.1, 2.1), (2.0, 2.0), (1.9, 1.9), (1.8, 1.8), (1.7, 1.7), (1.6, 1.6), (1.5, 1.5), (1.4, 1.4), (1.3, 1.3), (1.2, 1.2), and (1.1, 1.1).

HMOC of daphnilongeranin B (2)

HMBC of daphnilongeranin B (2)

NOESY of daphnilongeranin B (2)

EIMS of daphnilongeranin B (2)

SPEC: 152811
Samp: DL-21
Comm: Finnigan/MAT95/70eV/Tsou:200c/R:1000
Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
Oper: WANG_J@SIMM.CAS Client: S/N:SW01-0001
Base: 325.2 Inten: 4664474
Norm: 325.2 RIC: 60095271
Peak: 1000.00 mmu

25-Aug-05 Elapse: 02:24.8 22
Start: 11:31:04 74
Inlet: 50 > 750
Masses: 533
#peaks: 533

¹H NMR of daphnilongeranin C (**3**) run in CDCl₃

^{13}C NMR of daphnilongeranin C (**3**) run in CDCl_3

^1H - ^1H COSY of daphnilongeranin C (3)

HMQC of daphnilongeranin C (3)

HMBC of daphnilongeranin C (3)

CDCL3 HMBC

Expanded HMBC (δ_{H} 0.96-3.88 vs δ_{C} 19-68) of daphnilongeranin C (3)

ROESY of daphnilongeranin C (**3**)

EIMS of daphnilongeranin C (3)

SPEC: 152891
Samp: DL-23
Comm: Finnigan/MAT95/70eV/Tsou:200c/R:1000
Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
Oper: WANG_J@SIMM.CAS Client: S/N:SW01-0001
Base: 310.2 Inten: 1336299
Norm: 310.2 RIC: 11033219
Peak: 1000.00 mmu

02-Sep-05 Elapse: 02:09.9 20
Start: 15:33:06 20

Inlet: 50 > 750
Masses: 403
#peaks: 403

^1H NMR of daphnilongeranin D (4) run in CD_3OD

^{13}C NMR of daphnilongeranin D (4) run in CD_3OD

^1H - ^1H COSY of daphnilongeranin D (4)

HMQC of daphnilongeranin D (4)

Expanded HMQC (δ_{H} 0.85-3.35 vs δ_{C} 19-50) of daphnilongeranin D (4)

HMBC of daphnilongeranin D (4)

Expanded HMBC (δ_{H} 0.75-2.25 vs δ_{C} 19-45) of daphnilongeranin D (4)

EIMS of daphnilongeranin D (4)

SPEC: 152892
Samp: DL-9
Comm: Finnigan/MAT95/70eV/Tsou:200c/R:1000
Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
Oper: WANG_J@SIMM.CAS Client: S/N:SW01-0001
Base: 286.2 Inten: 9844437
Norm: 286.2 RIC: 57203400
Peak: 1000.00 mmu

02-Sep-05 Elapse: 02:20.7 22
Start: 15:36:16 23
Inlet: 50 > 750
Masses: 570
#peaks: 570

Figure 1. A: ^1H - ^1H COSY (—) and the selected HMBC (H $\rightarrow$ C) of **1**.
 B: Key NOESY correlations ($\leftrightarrow$) of **1**.

Figure 2. A: ^1H - ^1H COSY (—) and the selected HMBC (H $\rightarrow$ C) of **2**.
 B: Key NOESY correlations ($\leftrightarrow$) of **2**.

Figure 3. A: ^1H - ^1H COSY (—) and the selected HMBC (H $\rightarrow$ C) of **3**.
 B: Key ROESY correlations ($\leftrightarrow$) of **3**.

Figure 4. ^1H - ^1H COSY (—) and selected HMBC (H $\rightarrow$ C) correlations of **4**.