Supplementary Material (ESI) for Organic and Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2010

Supporting Information for:

Dermacozines, a New Phenazine Family from Deep-sea Dermacocci Isolated from a Mariana Trench Sediment

Wael M. Abdel-Mageed^{a,b}, Bruce F. Milne^c, Marcell Wagner^d, Marc Schumacher^e, Peter

Sandor^f, Wasu Pathom-aree^g, Michael Goodfellow^g, Alan T. Bull^h, Koki Horikoshiⁱ, Rainer Ebel^a, Marc Diederich^e, Hans-Peter Fiedler^d and Marcel Jaspars^{a*}

a.) Marine Biodiscovery Centre, Department of Chemistry' University of Aberdeen' Old

Aberdeen, AB24 3UE, Scotland, UK.

Tel: +44 1224 272895; Fax: +44 1224 272921; Email: m.jaspars@abdn.ac.uk

b.) Department of Pharmacognosy Faculty of Pharmacy Assiut University Assiut, Egypt.

c.) Center for Computational Physics, Physics Department, University of Coimbra, Rua Larga,3004-516, Coimbra, Portugal.

d.) Mikrobiologisches Institut, Universität Tübingen Auf der Morgenstelle 28, D-72076
Tübingen, Germany.

e.) Laboratoire de Biologie Moléulaire et Cellulaire du Cancer, Hôpital Kirchberg, 9 rue Edward Steichen, L-2540 Luxembourg, Grand-Duchy of Luxembourg.

f.) Varian Deutschland GmbH, Alsfelder Strasse 6, 64289 Darmstadt, Germany.

g.) School of Biology, University of Newcastle, Ridley Building, Newcastle upon Tyne NE17RU, UK.

h.) Department of Biosciences, University of Kent, Canterbury, Kent CT2 7NJ, UK.

i.) Extremobiosphere Research Center, Japan Agency for Marine-Earth Science and Technology, 2-15 Natsushima-cho, Yokosuka 237-0061, Japan.

CONTENTS

	Page
S1. UV spectrum of dermacozine A (1) (in Ethanol)	5
S2. ¹ H NMR spectrum of dermacozine A (1) (400 MHz, DMSO)	5
S3. ¹³ C NMR spectrum of dermacozine A (1) (100 MHz, DMSO)	6
S4. HSQC spectrum of dermacozine A (1) (400 MHz, DMSO)	6
S5. ¹ H- ¹ H COSY spectrum of dermacozine A (1) (400 MHz, DMSO)	7
S6. HMBC spectrum of dermacozine A (1) (400 MHz, DMSO)	7
S7. LRESIMS spectrum of dermacozine A (1) (in Methanol)	8
S8. HRESIMS spectrum of dermacozine A (1) (in Methanol)	8
S9. UV spectrum of dermacozine B (2) (in Ethanol)	9
S10. ¹ H NMR spectrum of dermacozine B (2) (400 MHz, DMSO)	9
S11. ¹³ C NMR spectrum of dermacozine B (2) (100 MHz, DMSO)	10
S12. HSQC spectrum of dermacozine B (2) (400 MHz, DMSO)	10
S13. ¹ H- ¹ H COSY spectrum of dermacozine B (2) (400 MHz, DMSO)	11
S14. HMBC spectrum of dermacozine B (2) (400 MHz, DMSO)	11
S15. ¹ H NMR spectrum of dermacozine B (2) (400 MHz, DMSO- d_6 /CD ₃ OD)	12
S16. ¹ H- ¹ H COSY spectrum of dermacozine B (2) (400 MHz, DMSO- d_6 /CD ₃ OD)	12
S17. LRESIMS spectrum of dermacozine B (2) (in Methanol)	13
S18. HRESIMS spectrum of dermacozine B (2) (in Methanol)	13
S19. UV spectrum of dermacozine C (3) (in Ethanol)	14
S20. ¹ H NMR spectrum of dermacozine C (3) (400 MHz, DMSO)	14
S21. ¹³ C NMR spectrum of dermacozine C (3) (100 MHz, DMSO)	15
S22. HSQC spectrum of dermacozine C (3) (400 MHz, DMSO)	15
S23. HMBC spectrum of dermacozine C (3) (400 MHz, DMSO)	16
S24. ¹ H NMR spectrum of dermacozine C (3) (400 MHz, DMSO- d_6 /CD ₃ OD)	16

S25. ¹ H- ¹ H COSY spectrum of dermacozine C (3) (400 MHz, DMSO- d_6 /CD ₃ OD)	17
S26. LRESIMS spectrum of dermacozine C (3) (in Methanol)	17
S27. UV spectrum of dermacozine D (4) (in Ethanol)	18
S28. ¹ H NMR spectrum of dermacozine D (4) (400 MHz, CDCl ₃)	18
S29. ¹³ C NMR spectrum of dermacozine D (4) (100 MHz, CDCl ₃)	19
S30. HSQC spectrum of dermacozine D (4) (400 MHz, CDCl ₃)	19
S31. ¹ H- ¹ H COSY spectrum of dermacozine D (4) (400 MHz, CDCl ₃)	20
S32. HMBC spectrum of dermacozine D (4) (400 MHz, CDCl ₃)	20
S33. ¹ H NMR spectrum of dermacozine D (4) (400 MHz, DMSO- d_6)	21
S34. HSQC spectrum of dermacozine D (4) (400 MHz, DMSO- d_6)	21
S35. ¹ H- ¹ H COSY spectrum of dermacozine D (4) (400 MHz, DMSO- d_6)	22
S36. HMBC spectrum of dermacozine D (4) (400 MHz, DMSO- d_6)	
S37. LRESIMS spectrum of dermacozine D (4) (in Methanol)	23
S38. HRESIMS spectrum of dermacozine D (4) (in Methanol)	23
S39. A) UV spectrum of dermacozine E (5) (in Ethanol)	24
B) Acidic and basic vs. neutral UV spectra of dermacozine E	24
S40. ¹ H NMR spectrum of dermacozine E (5) (600 MHz, CDCl ₃)	25
S41. ¹³ C NMR spectrum of dermacozine E (5) (150 MHz, CDCl ₃)	25
S42. HSQC spectrum of dermacozine E (5) (600 MHz, CDCl ₃)	26
S43. ¹ H- ¹ H COSY spectrum of dermacozine E (5) (600 MHz, CDCl ₃)	26
S44. HMBC spectrum of dermacozine E (5) (600 MHz, CDCl ₃)	27
S45.Expanded HMBC spectrum of dermacozine E (5) (600 MHz, DMSO)	27
S46. ¹⁵ N HSQC spectrum of dermacozine E (5) (600 MHz, DMSO)	
S47. ¹⁵ N HMBC spectrum of dermacozine E (5) (600 MHz, DMSO)	
S48. LRESIMS spectrum of dermacozine E (5) (in Methanol)	29
S49. HRESIMS spectrum of dermacozine E (5) (in Methanol)	29

S50. UV spectrum of dermacozine F (6) (in Ethanol)	30
S51. ¹ H NMR spectrum of dermacozine F (6) (400 MHz, DMSO- <i>d</i> ₆)	30
S52. ¹³ C NMR spectrum of dermacozine F (6) (100 MHz, DMSO- d_6)	31
S53. HSQC spectrum of dermacozine F (6) (400 MHz, DMSO- <i>d</i> ₆)	31
S54. ¹ H- ¹ H COSY spectrum of dermacozine F (6) (400 MHz, DMSO- d_6)	32
S55. HMBC spectrum of dermacozine F (6) (400 MHz, DMSO- <i>d</i> ₆)	32
S56. LRESIMS spectrum of dermacozine F (6) (in Methanol)	33
S57. HRESIMS spectrum of dermacozine F (6) (in Methanol)	33
S58. UV spectrum of dermacozine G (7) (in Ethanol)	34
S59. ¹ H NMR spectrum of dermacozine G (7) (400 MHz, DMSO- d_6)	34
S60. HSQC spectrum of dermacozine G (7) (400 MHz, DMSO- <i>d</i> ₆)	35
S61. ¹ H- ¹ H COSY spectrum of dermacozine G (7) (400 MHz, DMSO- d_6)	35
S62. HMBC spectrum of dermacozine G (7) (400 MHz, DMSO- <i>d</i> ₆)	36
S63. LRESIMS spectrum of dermacozine G (7) (in Methanol)	37
S64. HRESIMS spectrum of dermacozine G (7) (in Methanol)	37
Table S1: Observed HMBC correlations of dermacozines A-G (1-7)	38



S1. UV spectrum of dermacozine A (1) (in Ethanol)



S2. ¹H NMR spectrum of dermacozine A (1) (400 MHz, DMSO-*d*₆)







S4. HSQC spectrum of dermacozine A (1) (400 MHz, DMSO-*d*₆)



S5. ¹H-¹H COSY NMR spectrum of dermacozine A (1) (400 MHz, DMSO-*d*₆)



S6. HMBC spectrum of dermacozine A (1) (400 MHz, DMSO-d₆)



S7. LRESIMS spectrum of dermacozine A (1) (in Methanol)



18/03/2008 08:05:25

CMEP755MAT95

MAT 95 XP

S8. HRESIMS spectrum of dermacozine A (1) (in Methanol)



S9. UV spectrum of dermacozine B (2) (in Ethanol)



S10. ¹H NMR spectrum of dermacozine B (2) (400 MHz, DMSO-*d*₆)



S11. ¹³C NMR spectrum of dermacozine B (2) (100 MHz, DMSO-*d*₆)



S12. HSQC NMR spectrum of dermacozine B (2) (400 MHz, DMSO-d₆)



S13. ¹H-¹H COSY spectrum of dermacozine B (2) (400 MHz, DMSO-*d*₆)



S14. HMBC spectrum of dermacozine B (2) (400 MHz, DMSO-*d*₆)



S15. ¹H NMR spectrum of dermacozine B (2) (400 MHz, DMSO-*d*₆/CD₃OD)



S16. ¹H-¹H COSY spectrum of dermacozine B (2) (400 MHz, DMSO-*d*₆/CD₃OD)



S17. LRESIMS spectrum of dermacozine B (2) (in Methanol)



S18. HRESIMS spectrum of dermacozine B (2) (in Methanol)



S19. UV spectrum of dermacozine C (3) (in Ethanol)



S20. ¹H NMR spectrum of dermacozine C (**3**) (400 MHz, DMSO-*d*₆)



S21. ¹³C NMR spectrum of dermacozine C (3) (100 MHz, DMSO-*d*₆)



S22. HSQC spectrum of dermacozine C (3) (400 MHz, DMSO-d₆)



S23. HMBC spectrum of dermacozine C (3) (400 MHz, DMSO-d₆)



S24. ¹H NMR spectrum of dermacozine C (**3**) (400 MHz, DMSO-*d*₆/CD₃OD)



S25. ¹H-¹H COSY spectrum of dermacozine C (**3**) (400 MHz, DMSO-*d*₆/CD₃OD)



S26. LRESIMS spectrum of dermacozine C (3) (in Methanol)



S27. UV spectrum of dermacozine D (4) (in Ethanol)



S28. ¹H NMR spectrum of dermacozine D (**5.04**) (400 MHz, CDCl₃)



S29. ¹³C NMR spectrum of dermacozine D (4) (100 MHz, CDCl₃)



S30. HSQC spectrum of dermacozine D (4) (400 MHz, CDCl₃)



S31. ¹H-¹H COSY spectrum of dermacozine D (4) (400 MHz, CDCl₃)



S32. HMBC spectrum of dermacozine D (4) (400 MHz, CDCl₃)

Supplementary Material (ESI) for Organic and Biomolecular Chemistry This journal is The Royal Society of Chemistry 2010







S34. HSQC spectrum of dermacozine D (4) (400 MHz, DMSO-d₆)



S35. ¹H-¹H COSY spectrum of dermacozine D (4) (400 MHz, DMSO-*d*₆)



S36. ¹H-¹³C HMBC spectrum of dermacozine D (4) (400 MHz, DMSO-*d*₆)



S37. LRESIMS spectrum of dermacozine D (4) (in Methanol)



S38. HRESIMS spectrum of dermacozine D (4) (in Methanol)



S39. A) UV spectrum of dermacozine E (5) in (Ethanol).B) Acidic and basic vs. neutral UV spectra of dermacozine E.

S40. ¹H NMR spectrum of dermacozine E (5) (600 MHz, DMSO- d_6)

S41. ¹³C NMR spectrum of dermacozine E (5) (150 MHz, DMSO-*d*₆)

S42. ¹H-¹³C HSQC spectrum of dermacozine E (**5**) (600 MHz, DMSO-*d*₆)

S43. ¹H-¹H COSY spectrum of dermacozine E (**5**) (600 MHz, DMSO-*d*₆)

S44. ¹H-¹³C HMBC spectrum of dermacozine E (**5**) (600 MHz, DMSO-*d*₆)

S45. Expanded HMBC spectrum of dermacozine E (5) (600 MHz, DMSO-d₆)

S46. ¹H-¹⁵N HSQC spectrum of dermacozine E (**5**) (600 MHz, DMSO-*d*₆)

S47. 1 H- 15 N HMBC spectrum of dermacozine E (5) (600 MHz, DMSO- d_{6})

S48. LRESIMS spectrum of dermacozine E (5) (in Methanol)

S49. HRESIMS spectrum of dermacozine E (5) (in Methanol)

S50. UV spectrum of dermacozine F (6) (in Ethanol)

S51. ¹H NMR spectrum of dermacozine F (6) (400 MHz, DMSO-*d*₆)

S52. ¹³C NMR spectrum of dermacozine F (6) (100 MHz, DMSO-*d*₆)

S53. ¹H-¹³C HSQC spectrum of dermacozine F (6) (400 MHz, DMSO-*d*₆)

S54. ¹H-¹H COSY spectrum of dermacozine F (6) (400 MHz, DMSO-*d*₆)

S55. HMBC spectrum of dermacozine F (6) (400 MHz, DMSO-d₆)

S56. LRESIMS spectrum of dermacozine F (6) (in Methanol)

S57. HRESIMS spectrum of dermacozine F (6) (in Methanol)

S58. UV spectrum of dermacozine G (7) (in Methanol)

S59. ¹H NMR spectrum of dermacozine G (7) (400 MHz, DMSO-*d*₆)

S60. HSQC spectrum of dermacozine G (7) (400 MHz, DMSO-d₆)

S61. ¹H-¹H COSY spectrum of dermacozine G (7) (400 MHz, DMSO-*d*₆)

S62. HMBC spectrum of dermacozine G (7) (400 MHz, DMSO-d₆)

Abdel- Mageed et al.

S63. LRESIMS spectrum of dermacozine G (7) (in Methanol)

S64. HRESIMS spectrum of dermacozine G (7) (in Methanol)

No.	1	2	3	4	5*	6	7
1 2 3 4 5	C-4, 10a, 11 C-1, 4a C-2, 10a	C-4, 10a, 11, 13 C-2, 4a, 10a, 13	C-4, 10a, 11, 13 C-2, 3, 4a, 10a, 13	C-4, 10a, 11 C-1, 4a C-2, 10a	C-4, 10a, 11 C-1, 4, 4a C-2, 10a	C-4, 10a, 11 C-1, 4a C-2, 10a	C-4, 10a, 11 C-1, 4a C-2, 10a
6 7 8 9 10 11 12	C-5a, 9, 13 C-6, 9a C-5a, 7 C-4a, 5a	C-5a, 9, 20 C-6, 9a C-5a, 7 C-4a, 5a	C-5a, 9, 20 C-6, 9a C-5a, 7 C-1, 4a, 5a, 9, 9a	C-6, 9a, 15 C-5a, 7 C-1, 4a, 5a, 9	C-6, 7, 9a, 16 C-5a, 7 C-1	C-6, 7, 9a, 16 C-5a, 7	C-6, 9a, 16 C-5a, 7
13 14	C-6				C-6, 16		
15 16 17 18 19 20 21 22 23 24	C-4a, 5a	C-13, 17, 19 C-14, 18 C-15, 19 C-14, 16 C-13, 15, 17 C-20 C-4a, 5a	C-13, 17, 19 C-14, 18 C-15, 19 C-14, 16 C-13, 15, 17 C-20 C-4a, 5a	C-15, 19 C-16 C-17, 21 C-16, 17, 21 C-15, 19 C-22 C-4a, 5a	C-16, 20 C-17 C-18, 22 C-17 C-16, 20 C-4a, 5a	C-16, 20, 22 C-17, 21 C-18, 22 C-17, 19 C-16, 18, 20 C-4a, 5a	C-16, 20, 22 C-17 C-17 C-16, 18, 20 C-4a, 5a

^a All spectra were recorded at 400 MHz in DMSO-*d*₆ solution, except where noted.

* Recorded at 600 MHz in DMSO- d_6 solution.

TABLE S1. Observed HMBC correlations (H→ C) of dermacozines A-G (1-7)