

Antiproliferative Bistramides from *Trididemnum cyclops* from Madagascar

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Supporting Information

¹H NMR Data for Bistramides A and D

¹H NMR Spectrum of 39-Oxobistramide K (**1**) in CD₃OD

ROESY Spectrum of 39-Oxobistramide K (**1**) in CD₃OD

COSY Spectrum of 39-Oxobistramide K (**1**) in CD₃OD

HSQC Spectrum of 39-Oxobistramide K (**1**) in CD₃OD

HMBC Spectrum of 39-Oxobistramide K (**1**) in CD₃OD

¹H NMR Spectrum of Bistramide A (**2**) in CD₃OD

¹³C NMR Spectrum of Bistramide A (**2**) in CDCl₃

COSY Spectrum of Bistramide A (**2**) in CDCl₃

HMBC Spectrum of Bistramide A (**2**) in CDCl₃

¹H NMR Spectrum of Bistramide D (**3**) in CD₃OD

CD Spectrum of 39-Oxobistramide K (**1**) in CH₃OH

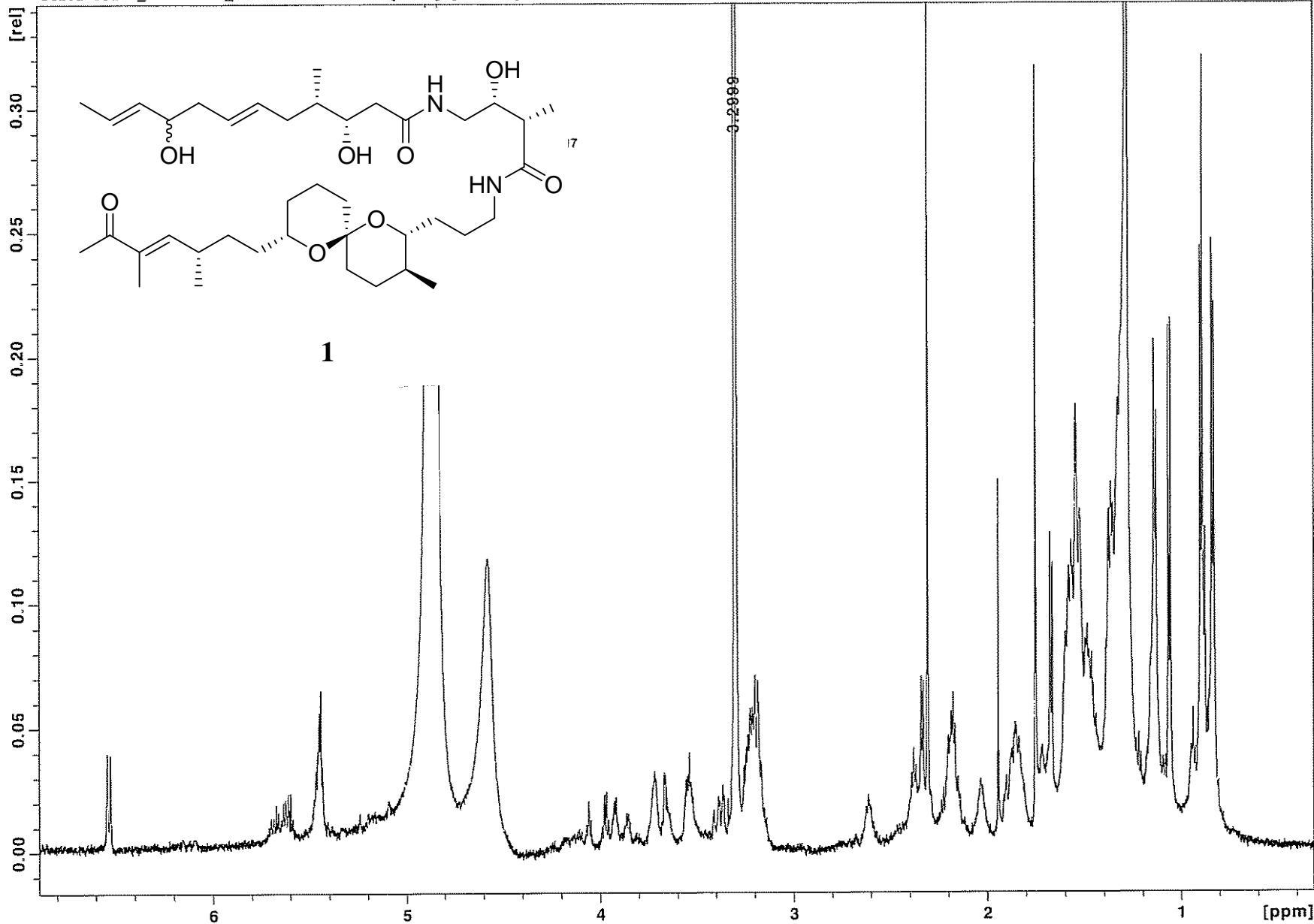
CD Spectrum of Bistramide A (**2**) in CH₃OH

Photograph of NB 04-05-31 (*Trididemnum cyclops*)

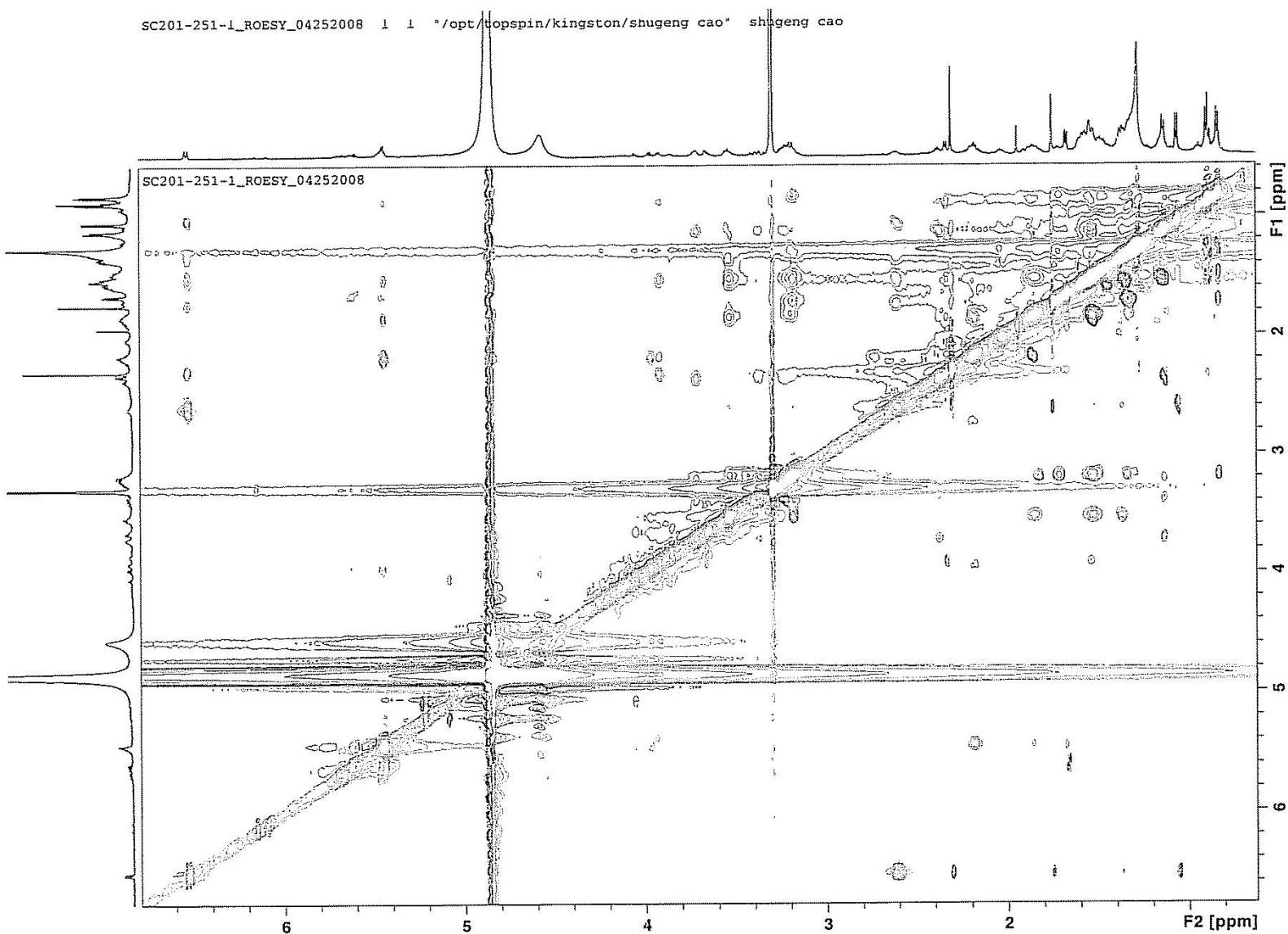
¹H NMR Data for Bistramide A (2): ¹H NMR (CDCl₃) δ_H 0.80 (3H, d, *J* = 6.5 Hz, H-24), 0.86 (3H, d, *J* = 7.0 Hz, H-10), 0.94 (3H, d, *J* = 6.5 Hz, H-35), 1.24 (3H, d, *J* = 6.5 Hz, H-17), 1.25 (3H, d, *J* = 7.5 Hz, H-40), 1.10 – 1.90 (24H, m, H-7, 8, 9, 20, 21, 23, 25, 26, 28, 29, 30, 32, 33), 1.91 (3H, dd, *J* = 1.5, 6.5 Hz, H-1), 2.19 (1H, m, Ha-12), 2.33 (1H, m, H-24), 2.37 (1H, m, H-16), 2.52 (1H, dd, *J* = 3.0, 16.5 Hz, Ha-5), 2.76 (1H, dd, *J* = 11.5, 15.0 Hz, Hb-12), 2.90 (1H, dd, *J* = 9.0, 17.0 Hz, Hb-5), 3.14 (1H, t, *J* = 9.5 Hz, H-22), 3.25 (1H, m, Ha-14), 3.30 (2H, m, H-19), 3.46 (1H, m, H-31), 3.51 (1H, m, Hb-14), 3.71 (1H, m, H-15), 4.06 (1H, dd, *J* = 4.5, 11.0 Hz, H-11), 4.19 (1H, m, H-6), 5.18 (1H, d, *J* = 9.0 Hz, H-36), 6.12 (1H, dd, *J* = 1.5, 16.0 Hz, H-3), (1H, dd, *J* = 6.5, 16.0 Hz, H-2), 6.96 (1H, t, *J* = 5.5 Hz, NH-19), 7.32 (1H, t, *J* = 5.5 Hz, NH-14).

¹H NMR Data for Bistramide D (3): ¹H NMR (CD3OD) δ_H 0.83 (3H, d, *J* = 6.5 Hz, H-24), 0.85 (3H, d, *J* = 7.0 Hz, H-10), 0.95 (3H, d, *J* = 6.5 Hz, H-35), 1.14 (3H, d, *J* = 7.0 Hz, H-17), 1.20 (3H, d, *J* = 6.5 Hz, H-40), 1.25 – 1.95 (22H, m, H-7, 9, 20, 21, 23, 25, 26, 28, 29, 30, 32, 33), 1.35 (2H, m, H-8), 1.38 (2H, m, H-33), 1.43 and 1.65 (2H, m, H-5), 1.61 (3H, s, H-38), 1.67 (d, *J* = 6.5 Hz, H-1), 2.23 (1H, dd, *J* = 4.0, 15.0 Hz, Ha-12), 2.38 (2H, m, H-16, 34), 2.70 (1H, dd, *J* = 11.0, 15.0 Hz, Hb-12), 3.15-3.20 (2H, m, Ha-14, 22), 3.23 (2H, m, H-19), 3.44 (1H, dd, *J* = 4.0, 14.0 Hz, Hb-14), 3.52 (1H, m, H-31), 3.73 (1H, m, H-15), 3.81(1H, m, H-6), 4.11 (1H, m, H-4), 4.14 (1H, m, H-39), 4.27 (1H, ddd, *J* = 4.0, 6.5, 8.5 Hz, H-11), 5.13 (1H, d, *J* = 9.0 Hz, H-36), 5.45 (1H, ddd, *J* = 1.5, 7.0, 15.5 Hz, H-3), 5.64 (1H, dd, *J* = 7.0, 15.5 Hz, H-2).

SC201-251-1_1HinCD3OD_04222008 1 1 /opt/topspin/kingston shugeng cao

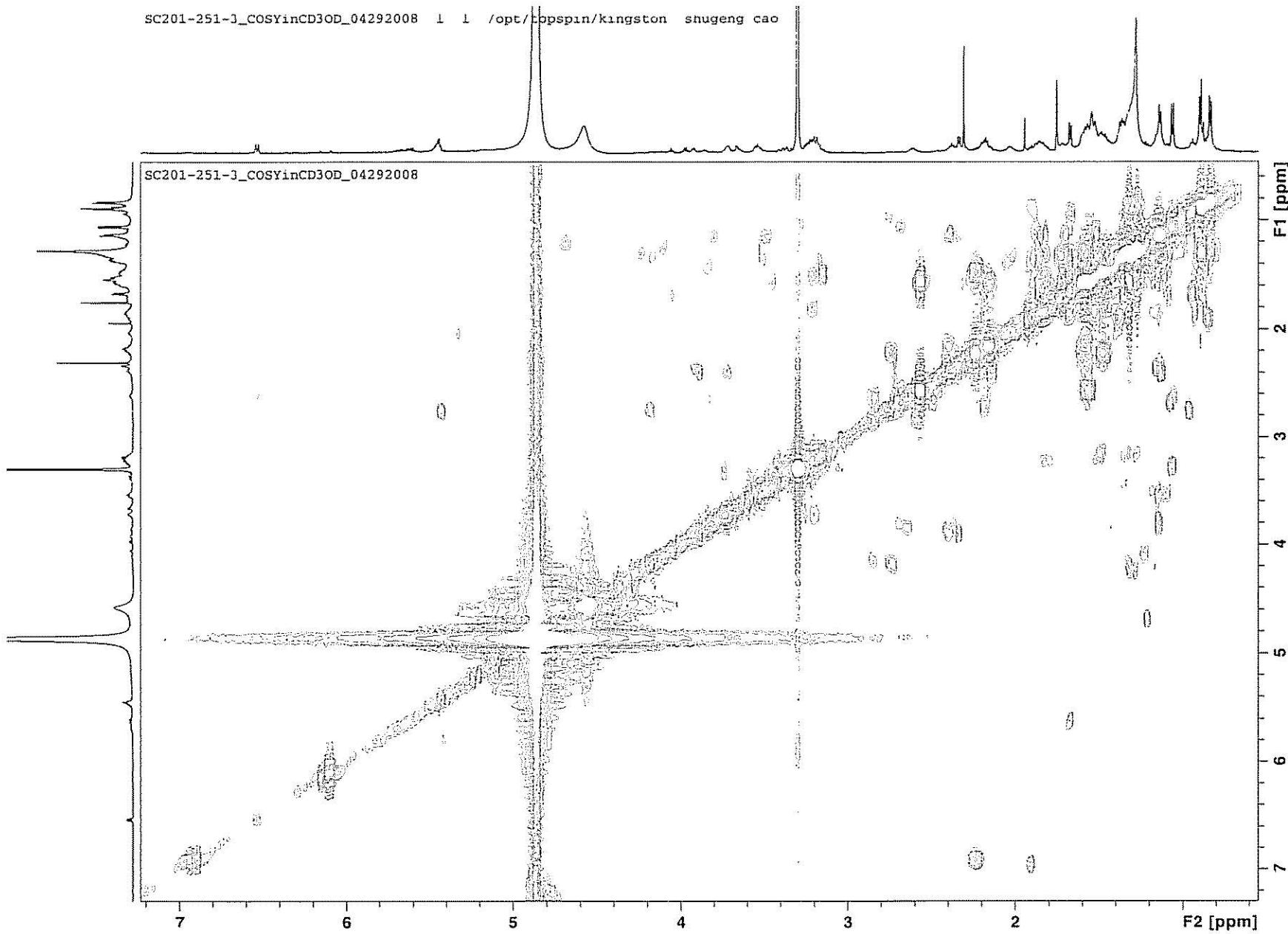


^1H NMR Spectrum of 39-Oxobistramide K (**1**) in CD_3OD



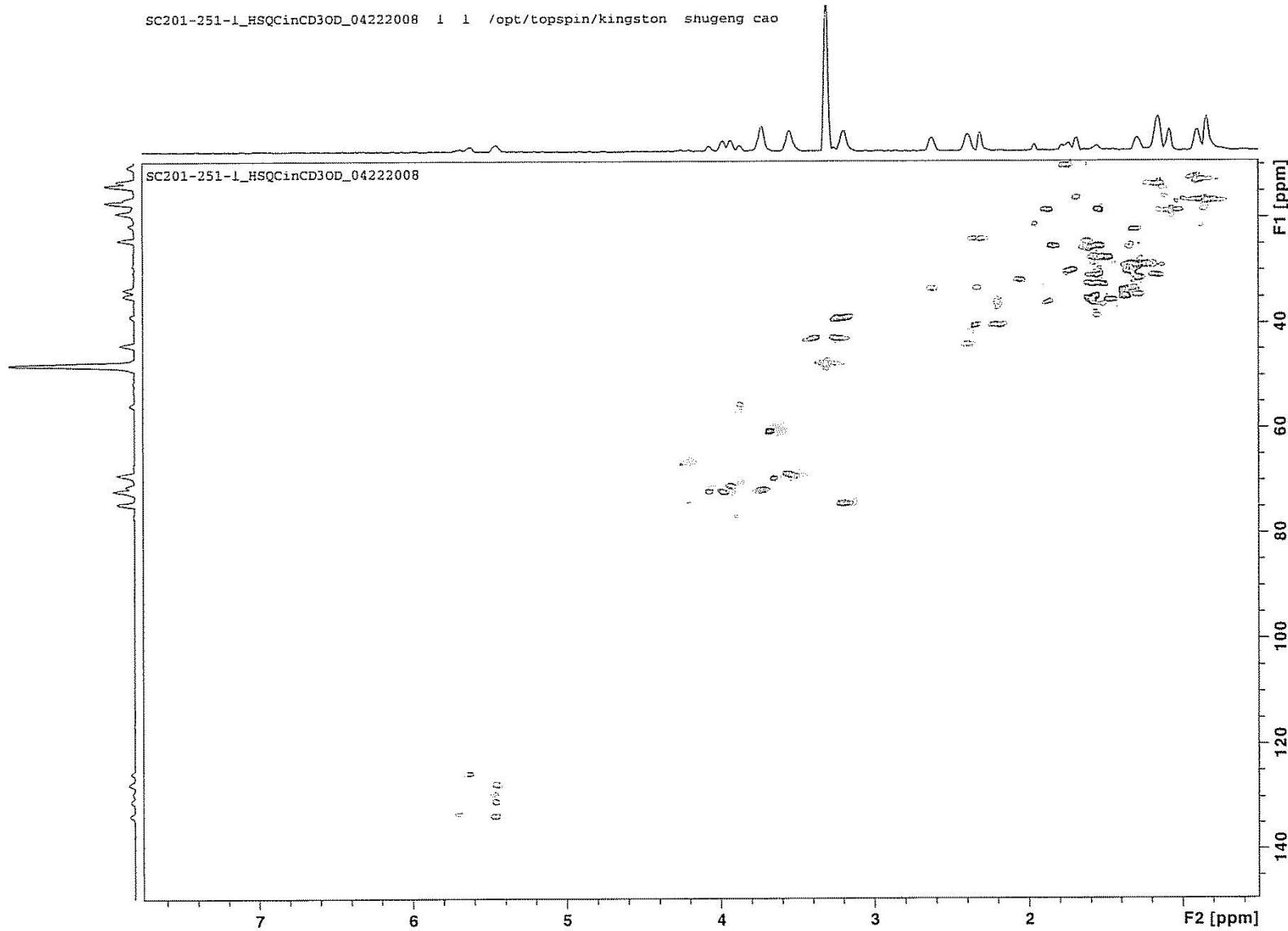
ROESY Spectrum of 39-Oxobistramide K (1) in CD_3OD

SC201-251-3_COSYinCD3OD_04292008 1 1 /opt/tbppspin/kingston shugeng cao



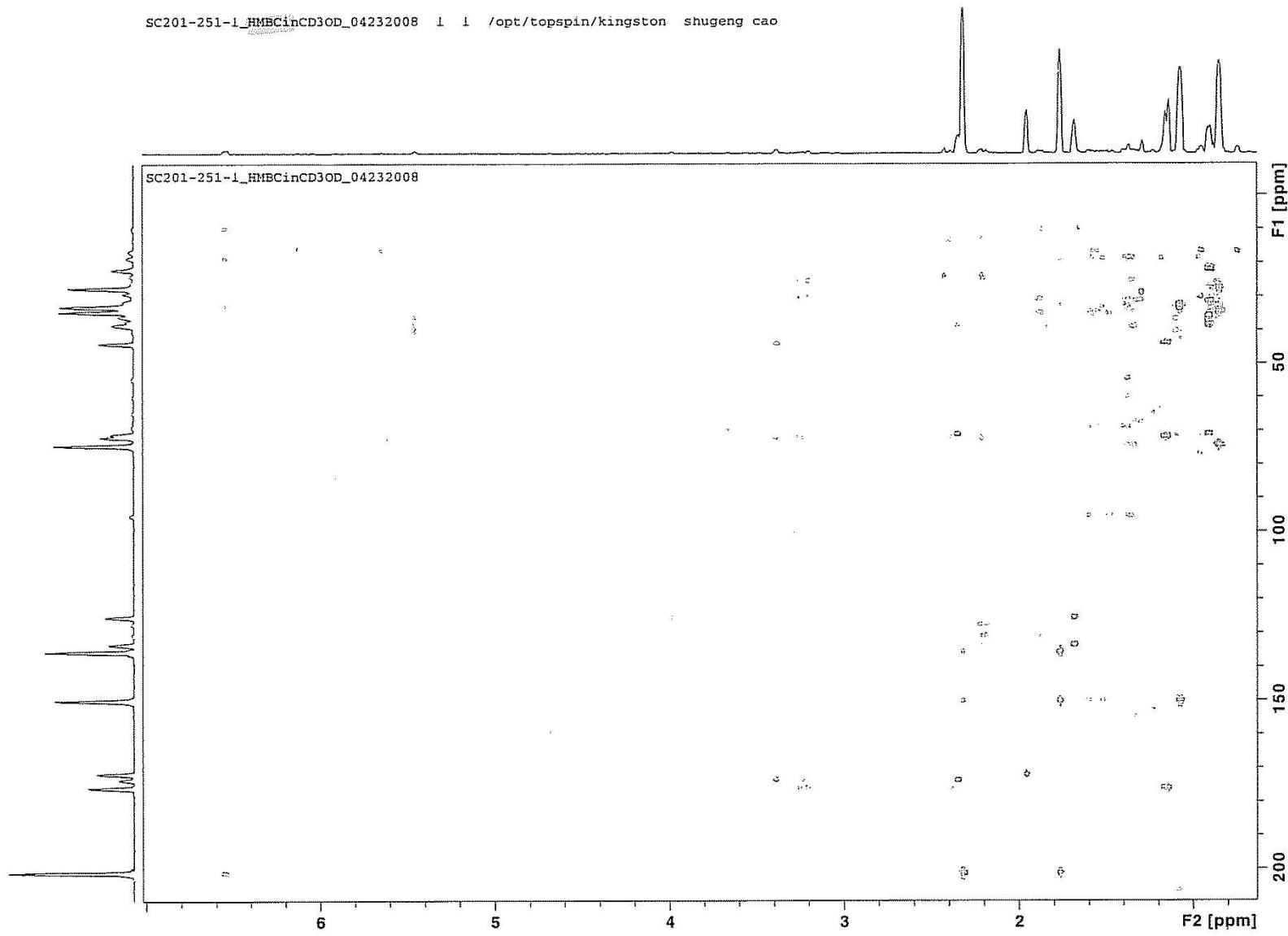
COSY Spectrum of 39-Oxobistramide K (1) in CD_3OD

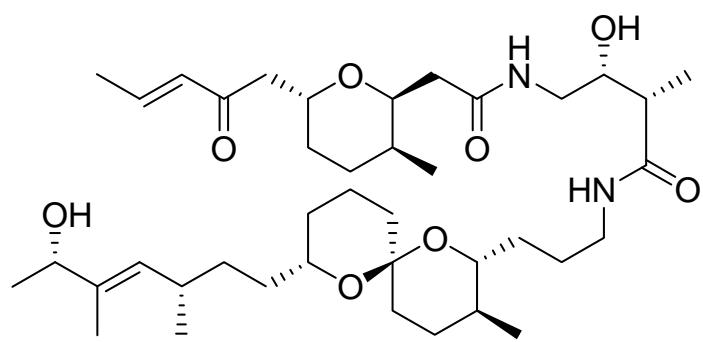
SC201-251-1_HSQCinCD3OD_04222008 1 1 /opt/topspin/kingston shugeng cao



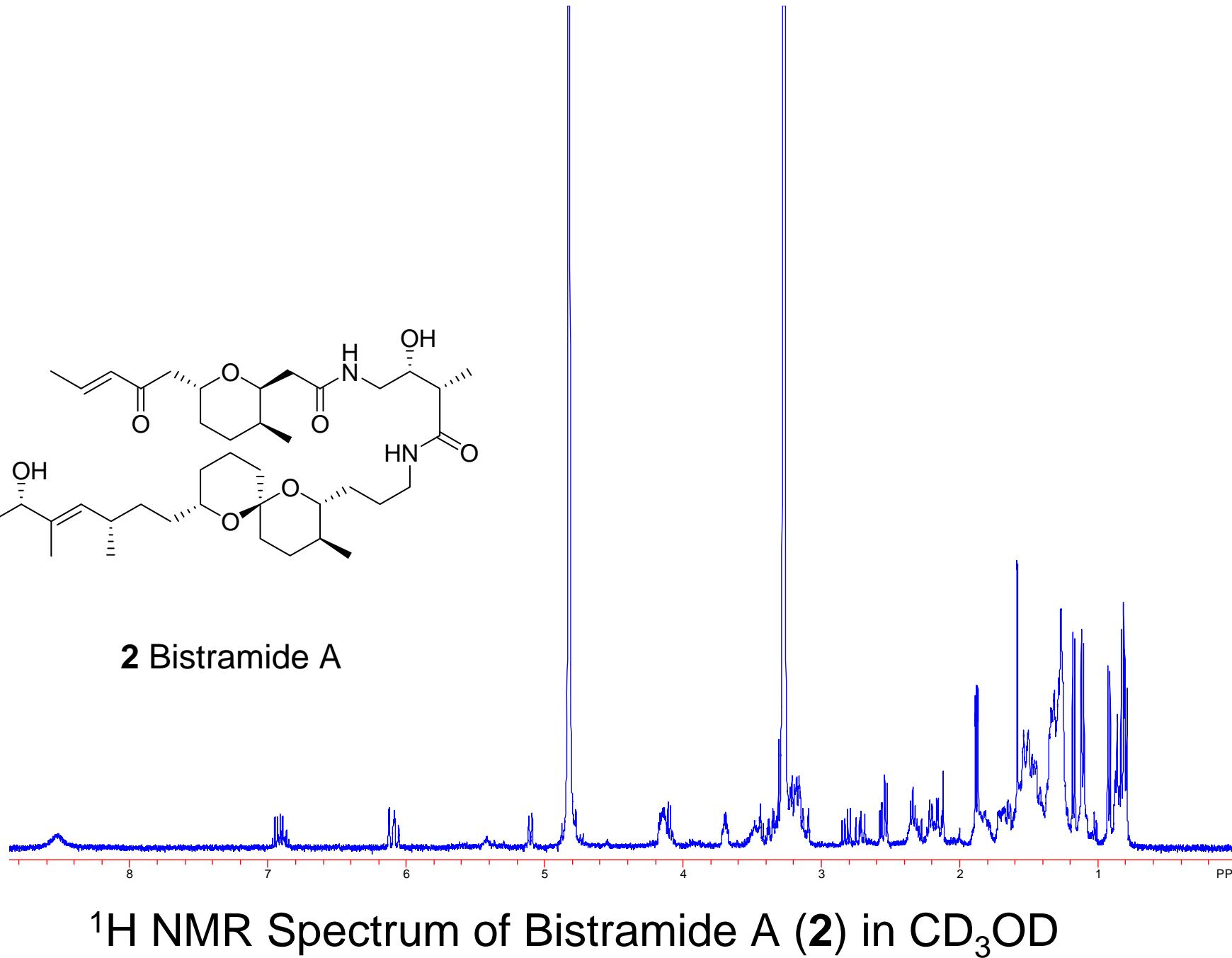
HSQC Spectrum of 39-Oxobistramide K (1) in CD_3OD

SC201-251-1_HMBCinCD3OD_04232008 1 1 /opt/topspin/kingston shugeng cao

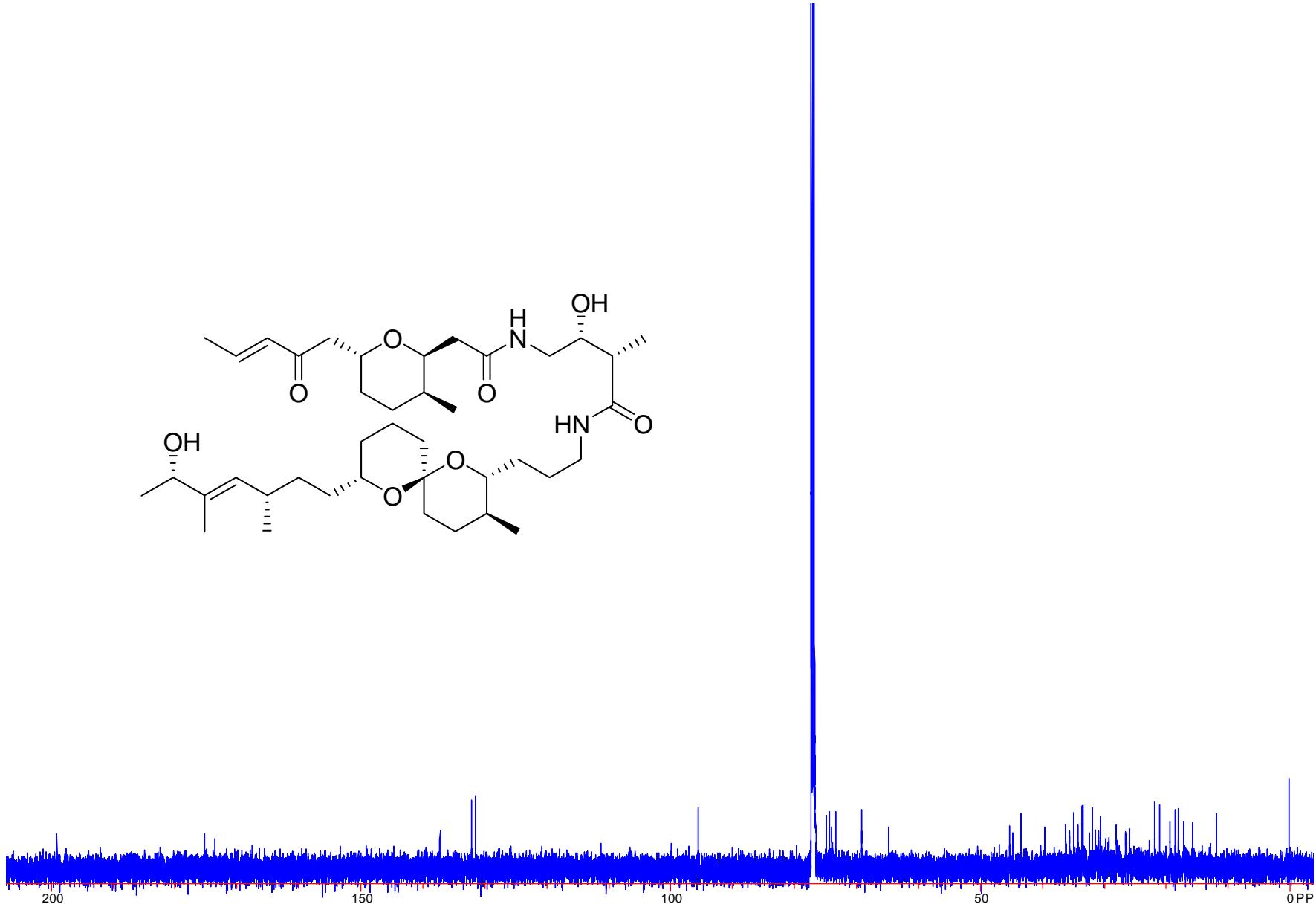
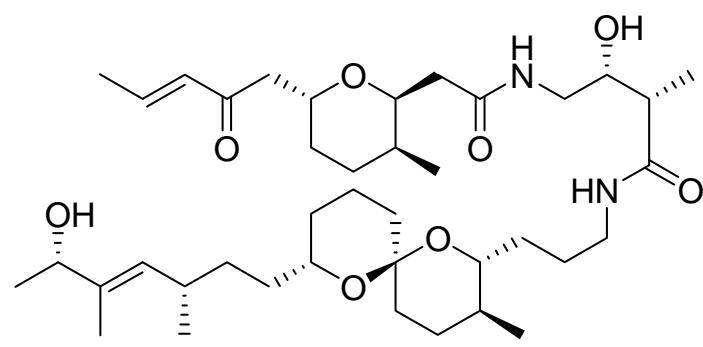




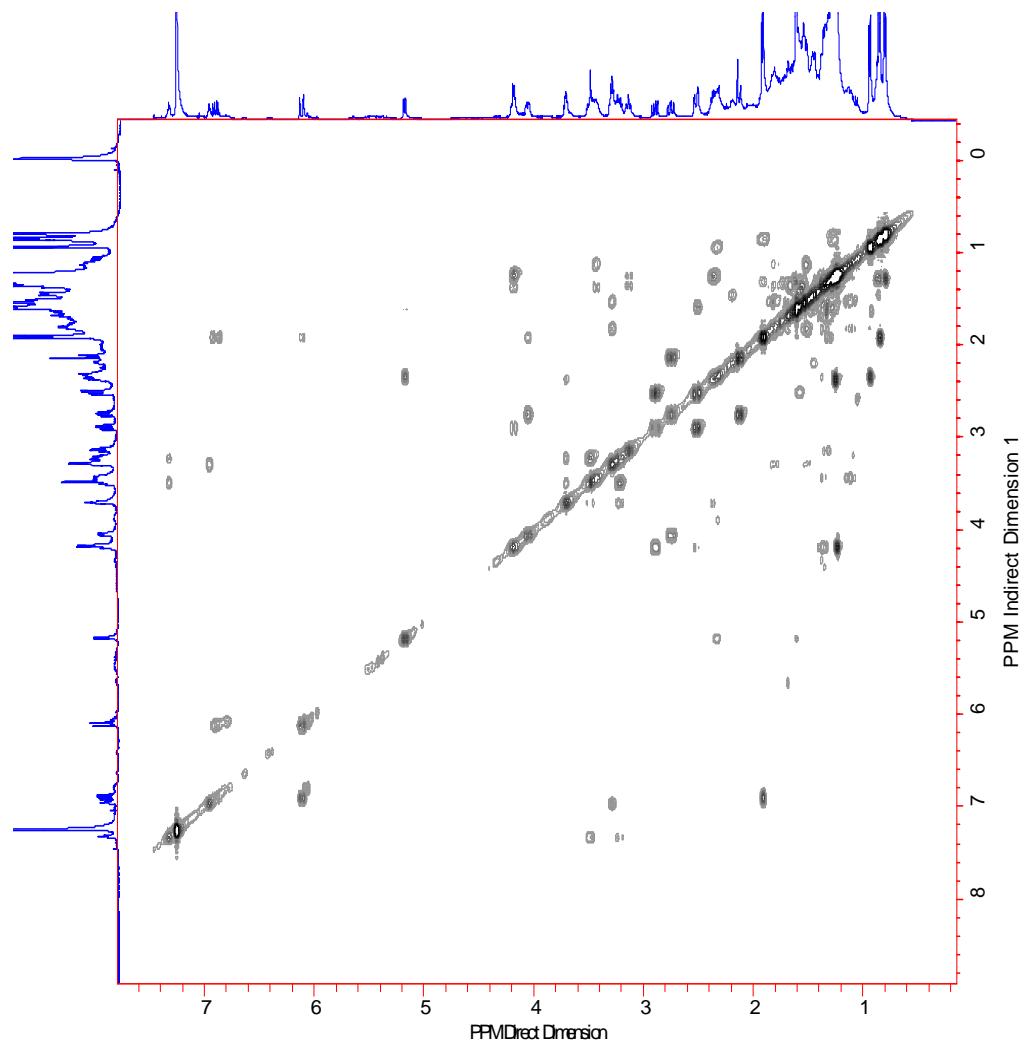
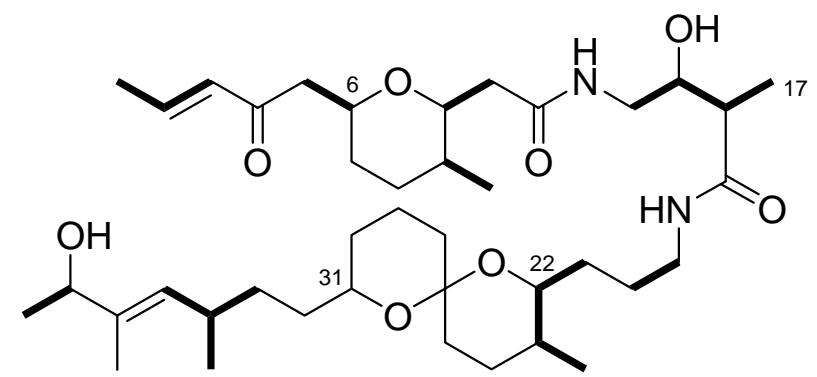
2 Bistramide A



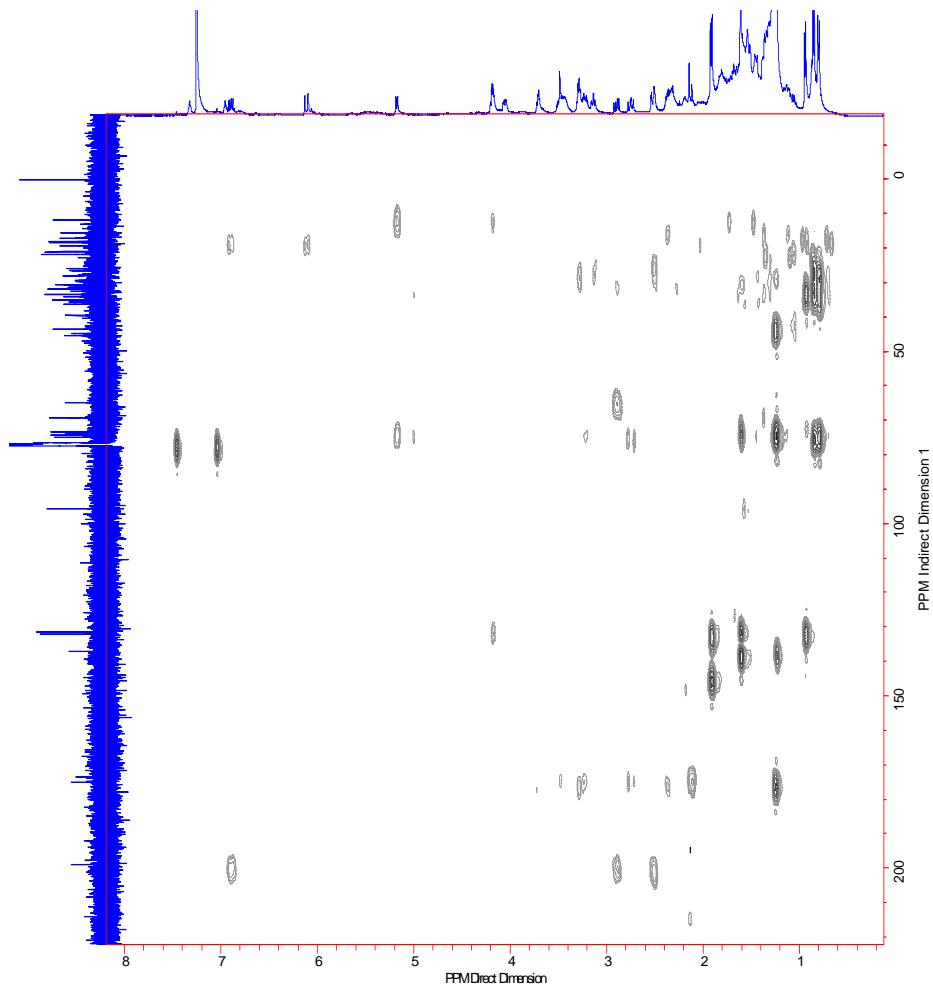
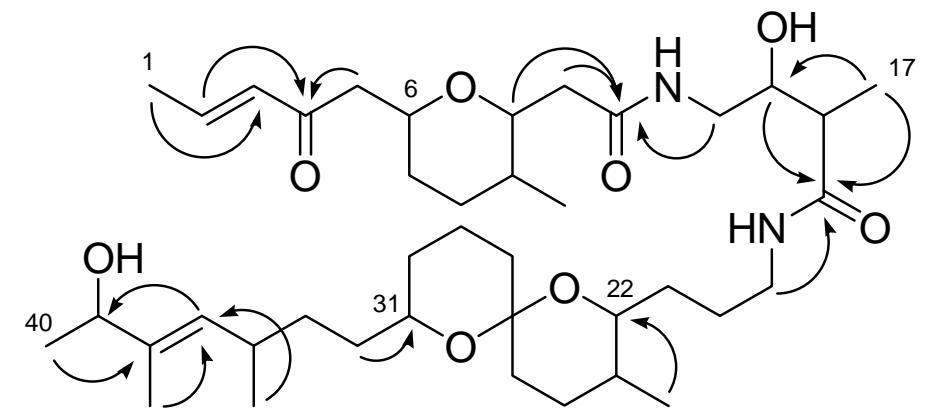
^1H NMR Spectrum of Bistramide A (**2**) in CD_3OD



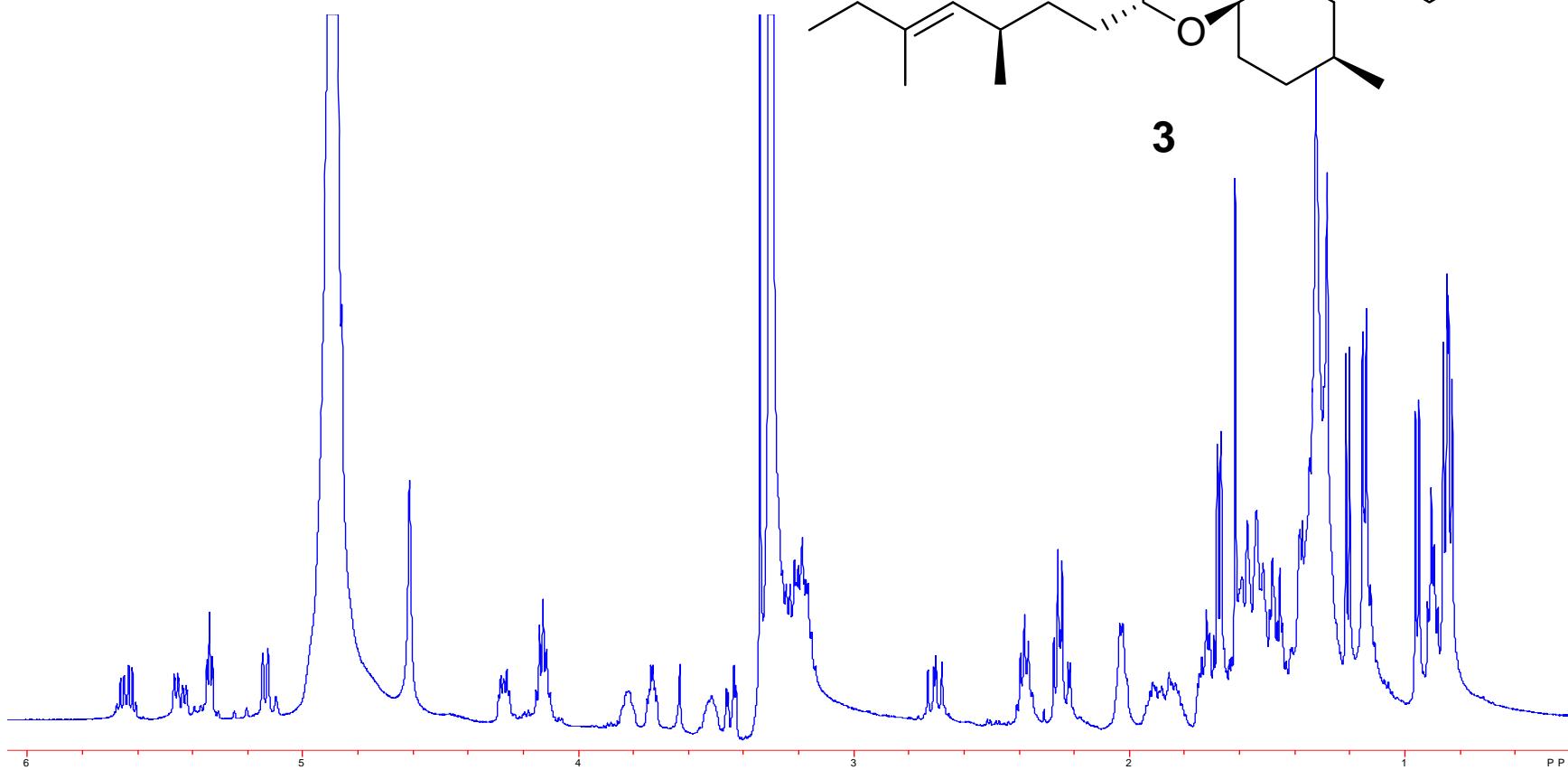
¹³C NMR Spectrum of Bistramide A (**2**) in CDCl₃



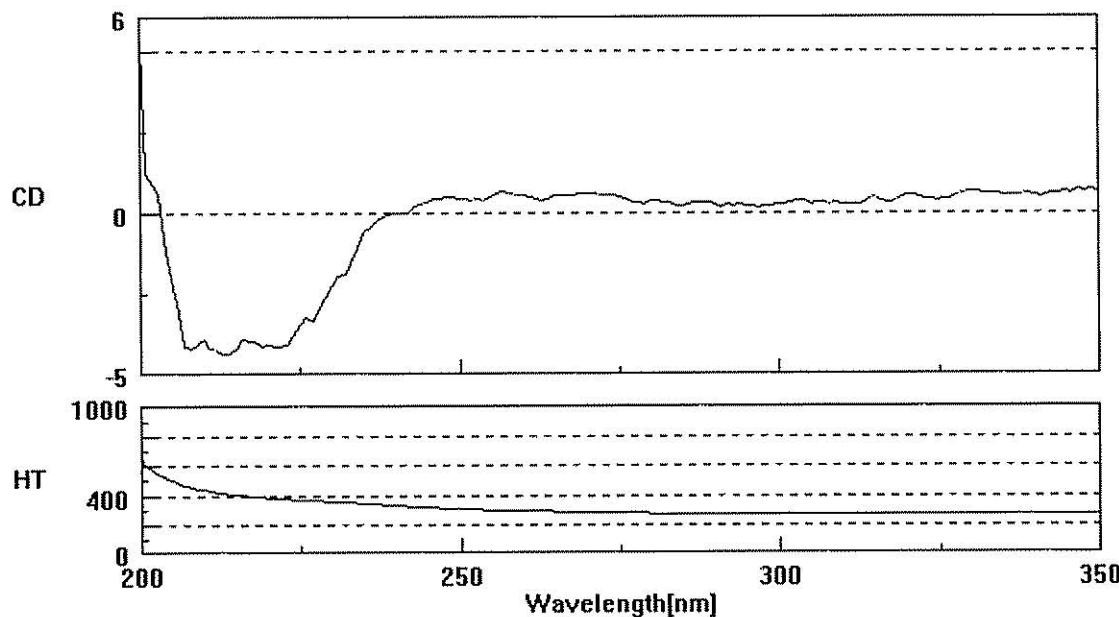
COSY Spectrum of Bistramide A (**2**) in CDCl_3



HMBC Spectrum of Bistramide A (**2**) in CDCl_3



^1H NMR Spectrum of Bistramide D (**3**) in CD_3OD



File Name : noname01.jws

Date : 12/12/108 1:49PM

Sample : SC-201-251-1

Cell Length : 0.2 cm

Concentration : 0 M

Solvent : CH₃OH

Temperature : Room Temp.

Operator : KH

Organization : VT

Comment :

Data mode : CD

Ch2-mode : HT

Range : 400 - 200 nm

Band width : 1.0 nm

Sensitivity : 10 mdeg

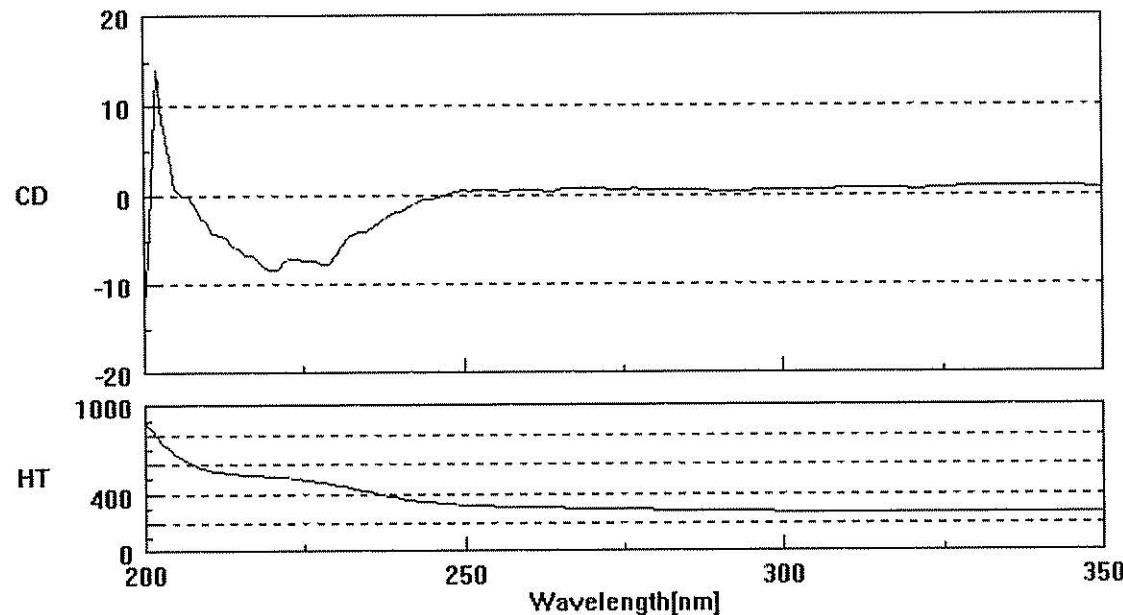
Resolution : 1 nm

Response : 1 sec

Speed : 200 nm/min

Accumulation : 2

CD Spectrum of 39-Oxobistramide K (1) in CH₃OH



File Name : noname02.jws

Date : 12/12/108 1:51PM

Sample : BTM-193-143-146-27

Cell Length : 0.1 cm

Concentration : 0 M

Solvent : CH₃OH

Temperature : Room Temp.

Operator : KH

Organization : VT

Comment :

Data mode : CD

Ch2-mode : HT

Range : 400 - 200 nm

Band width : 1.0 nm

Sensitivity : 10 mdeg

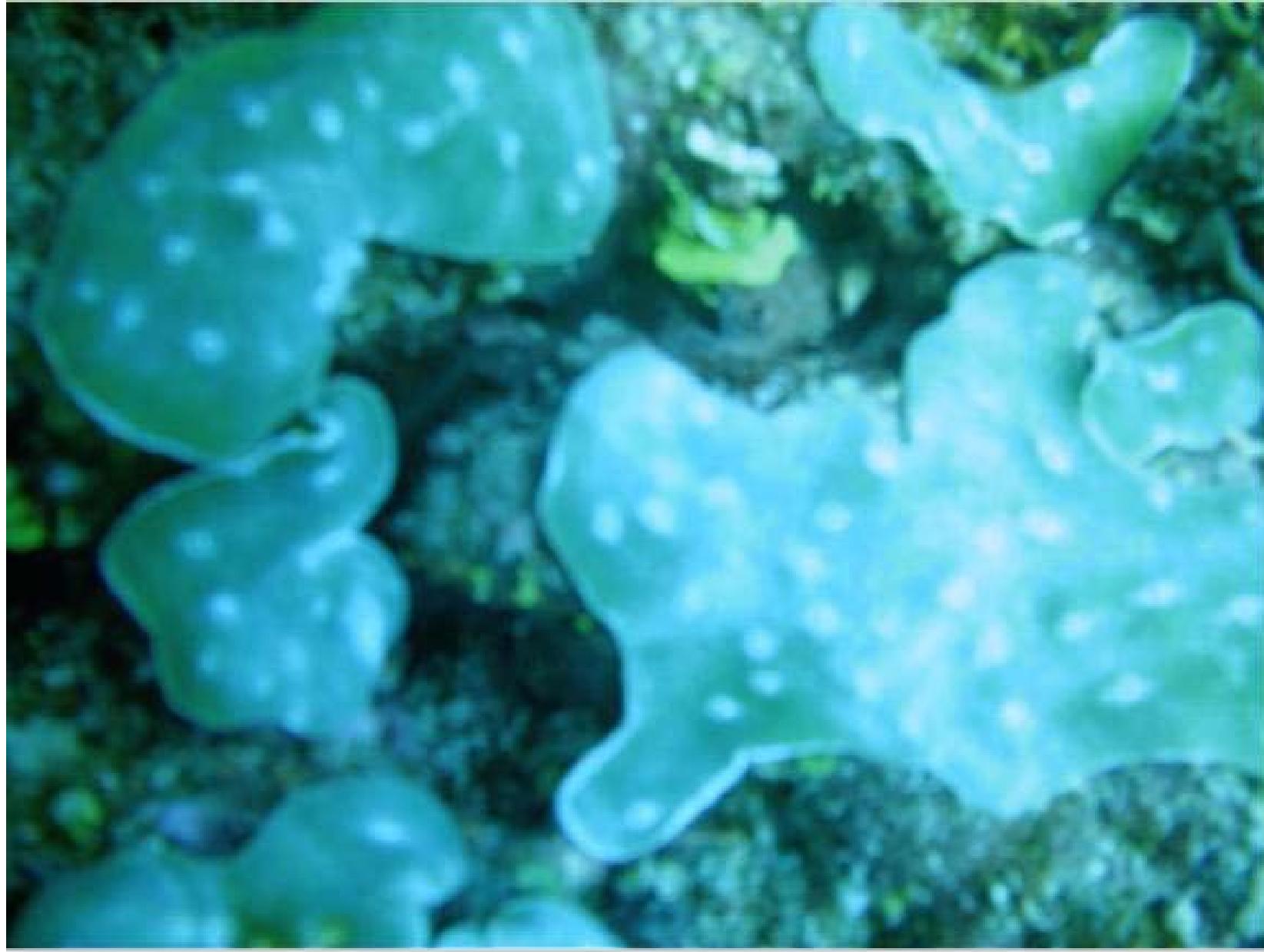
Resolution : 1 nm

Response : 1 sec

Speed : 200 nm/min

Accumulation : 2

CD Spectrum of Bistramide A (2) in CH₃OH



NB 04-05-31 (*Trididemnum cyclops*)