

# Supporting Information for Aspartocins A (1), B (2), and C (3)

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Figure S1. HPLC chromatogram of the aspartocin complex, which is composed of three analogs, aspartocin A (1), aspartocin B (2), and aspartocin C (3)

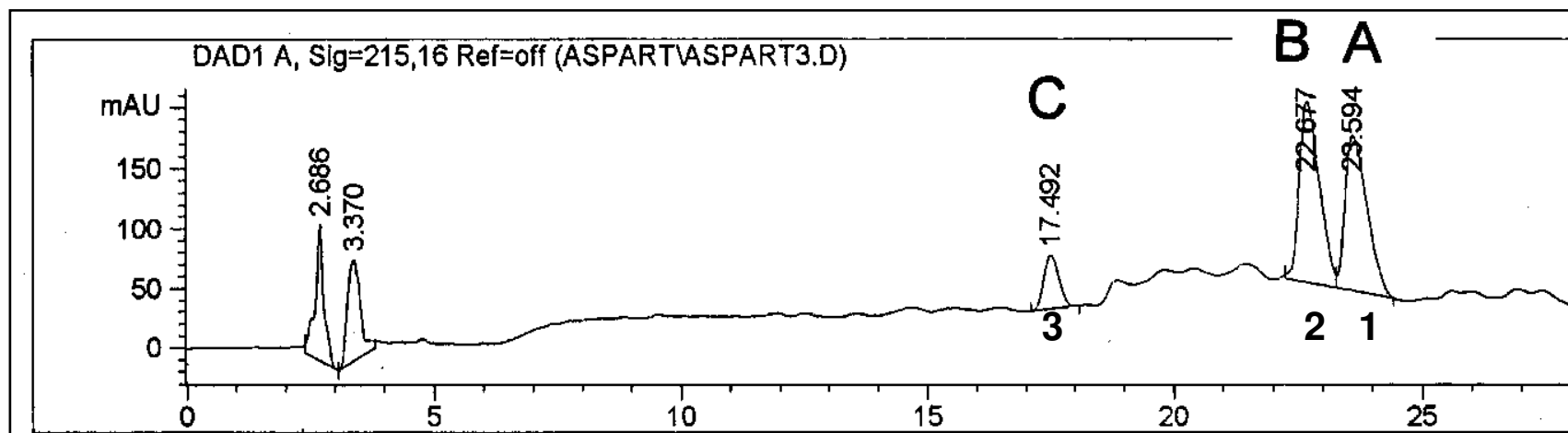


Figure S2. LC-UV-MS data of aspartocin A (1) generated on a Finnigan LCQ LC-MS system

D:\Deca-data\FMK\AspartocinA

12/04/03 04:42:27 PM

antibiotic

AspartocinA  
 Type: Unknown ID: 1 Row: 1  
 Sample Name: antibiotic  
 Flow Rate:: 0.3 mL/min.  
 Notebook #:: L18747  
 Column:: YMC ODS A; 2.0X100mm  
 Solvents:: A = H2O with 0.025% formic acid; B = CH3CN with 0.025% formic acid; C = MeOH with 0.025% formic acid; D =  
 Mobile Phase:: 5 to 50% B in A in 10 min  
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 LC-MSfmk50ACN.meth  
 Processing Method:  
 Vial: 41

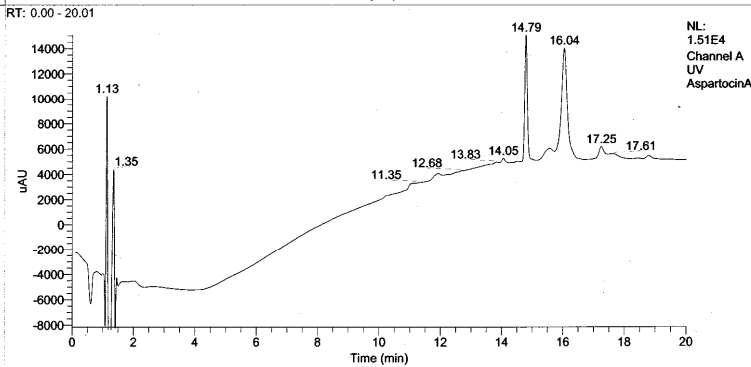
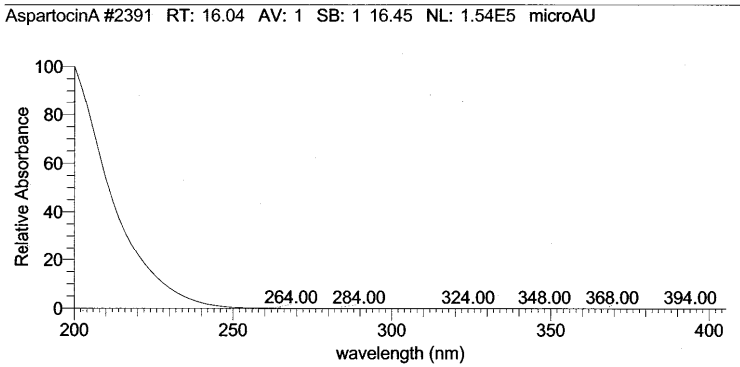
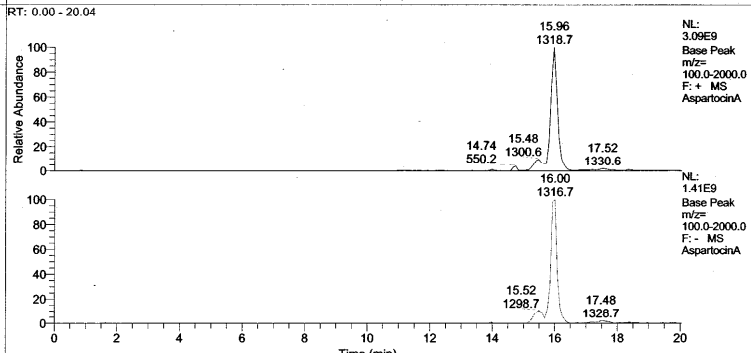
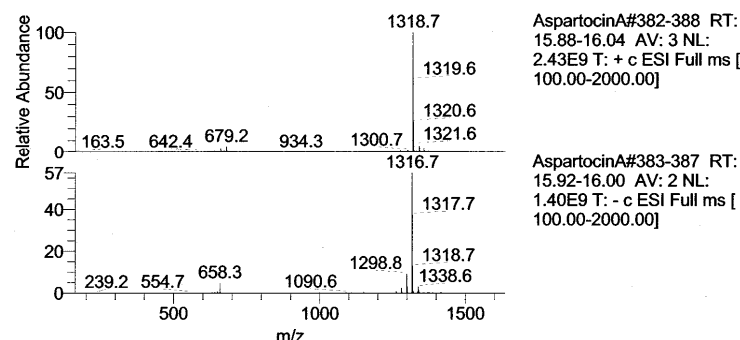
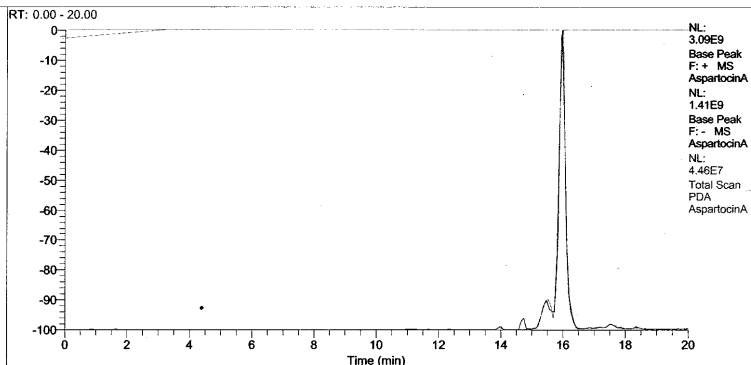


Figure S3.  $^1\text{H}$ -NMR spectrum of aspartocin A (1) in  $\text{DMSO-}d_6$  recorded on Bruker 500 MHz

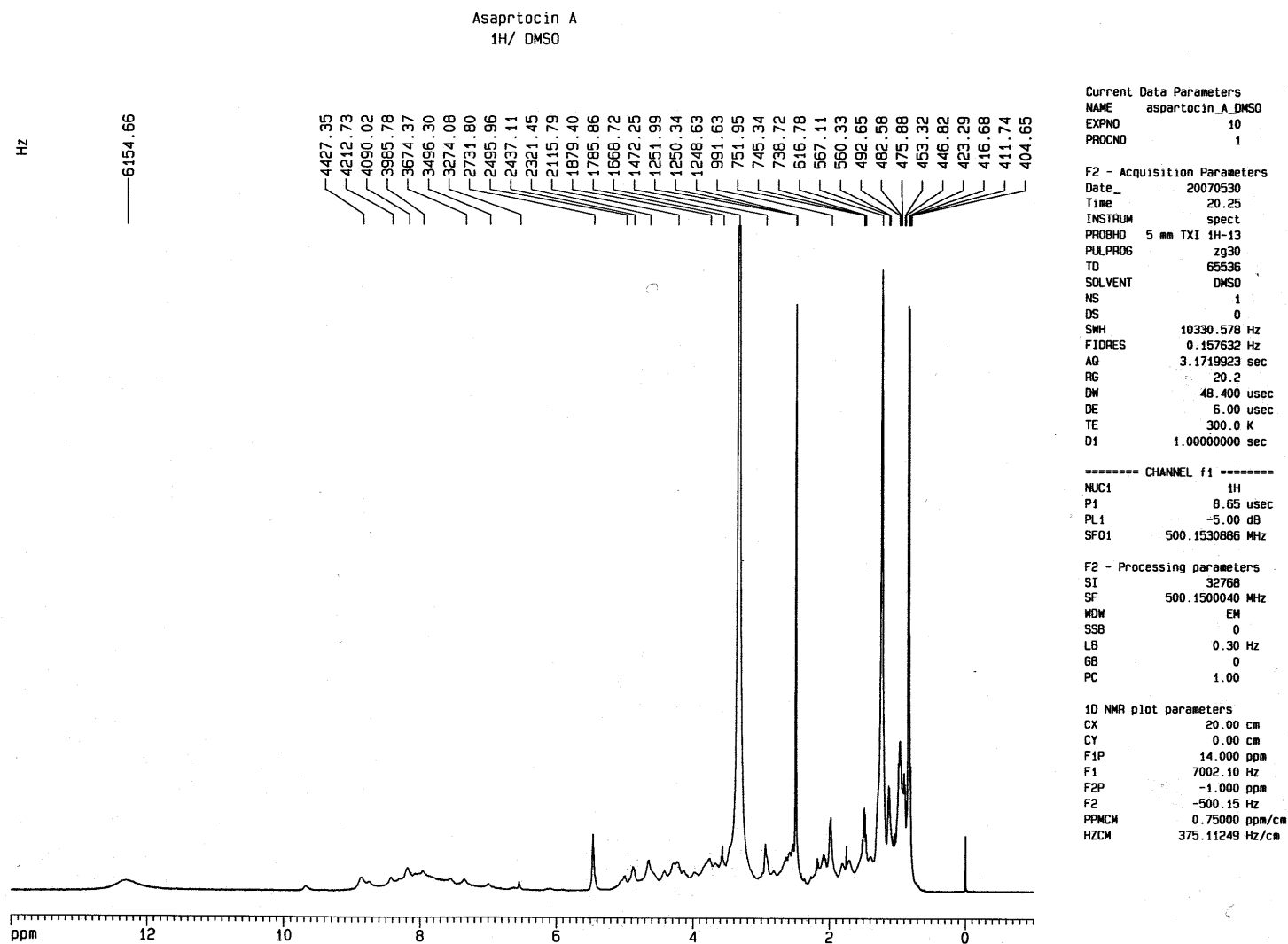


Figure S4. COSY-DQF spectrum of aspartocin A (1) in DMSO- $d_6$  recorded on Bruker 500 MHz

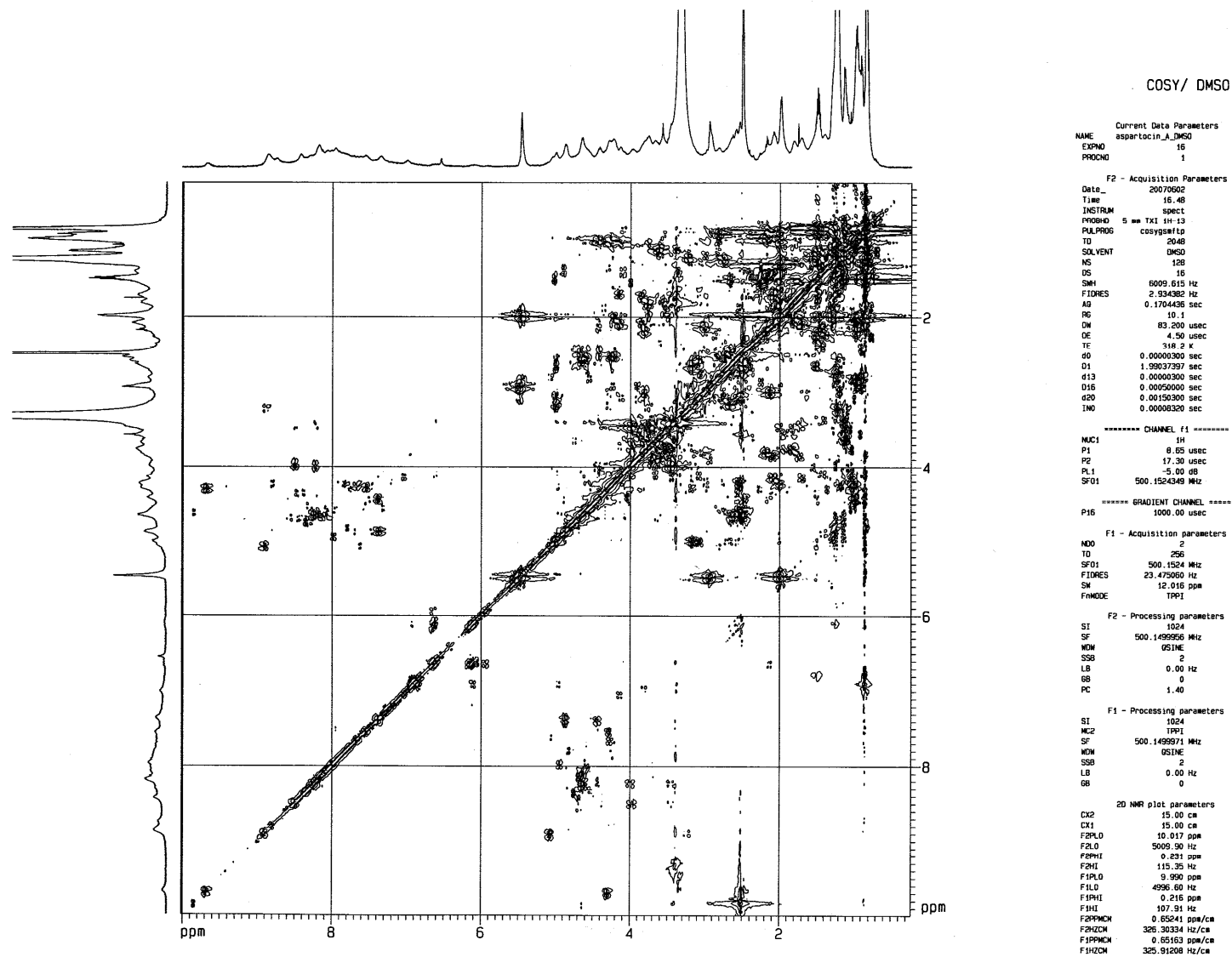


Figure S5. HSQC spectrum of aspartocin A (1) in DMSO-*d*<sub>6</sub> recorded on Bruker DRX 500 MHz

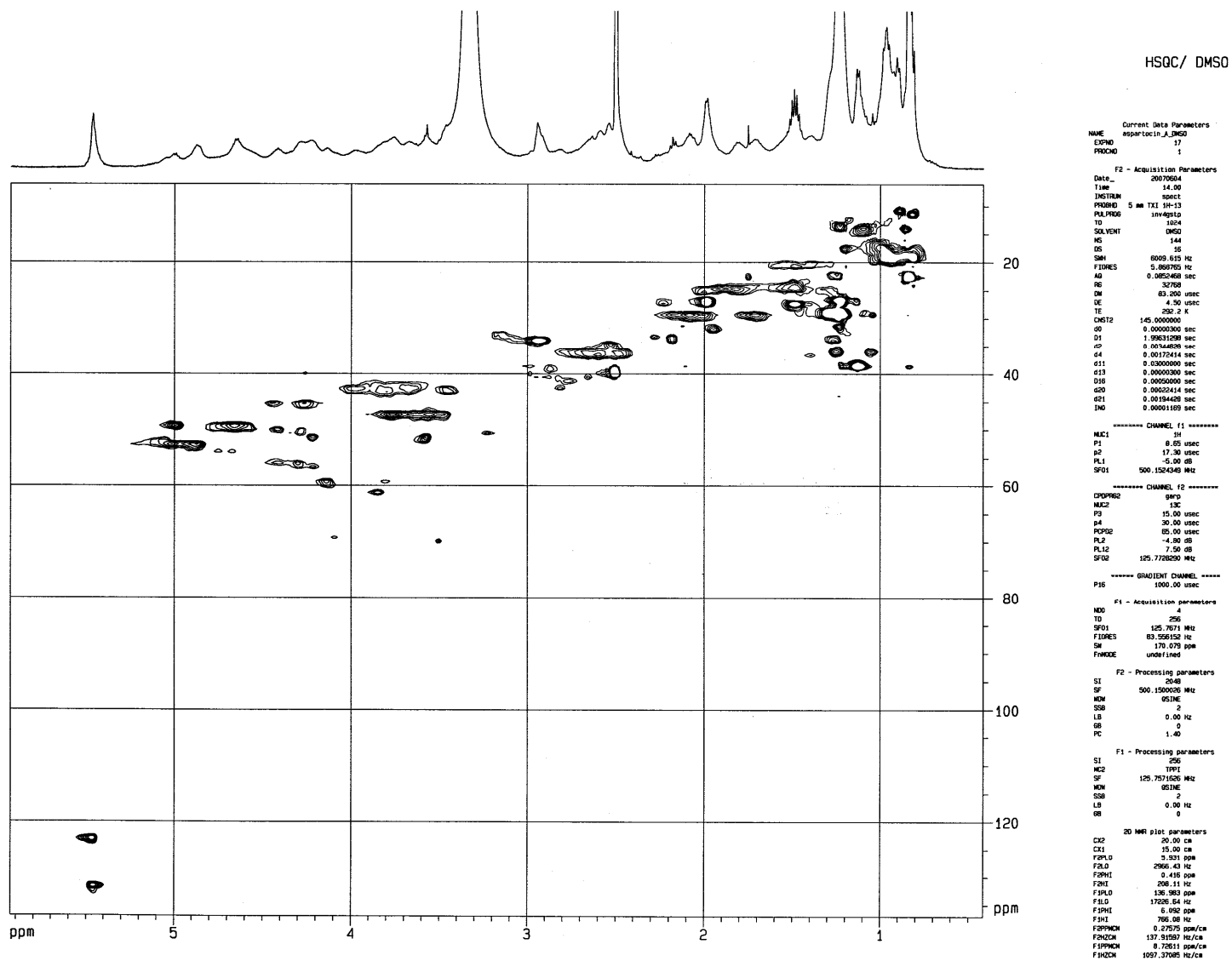




Figure S6. TOCSY spectrum of aspartocin A (1) in DMSO-*d*<sub>6</sub> recorded on Bruker DRX 500 MHz

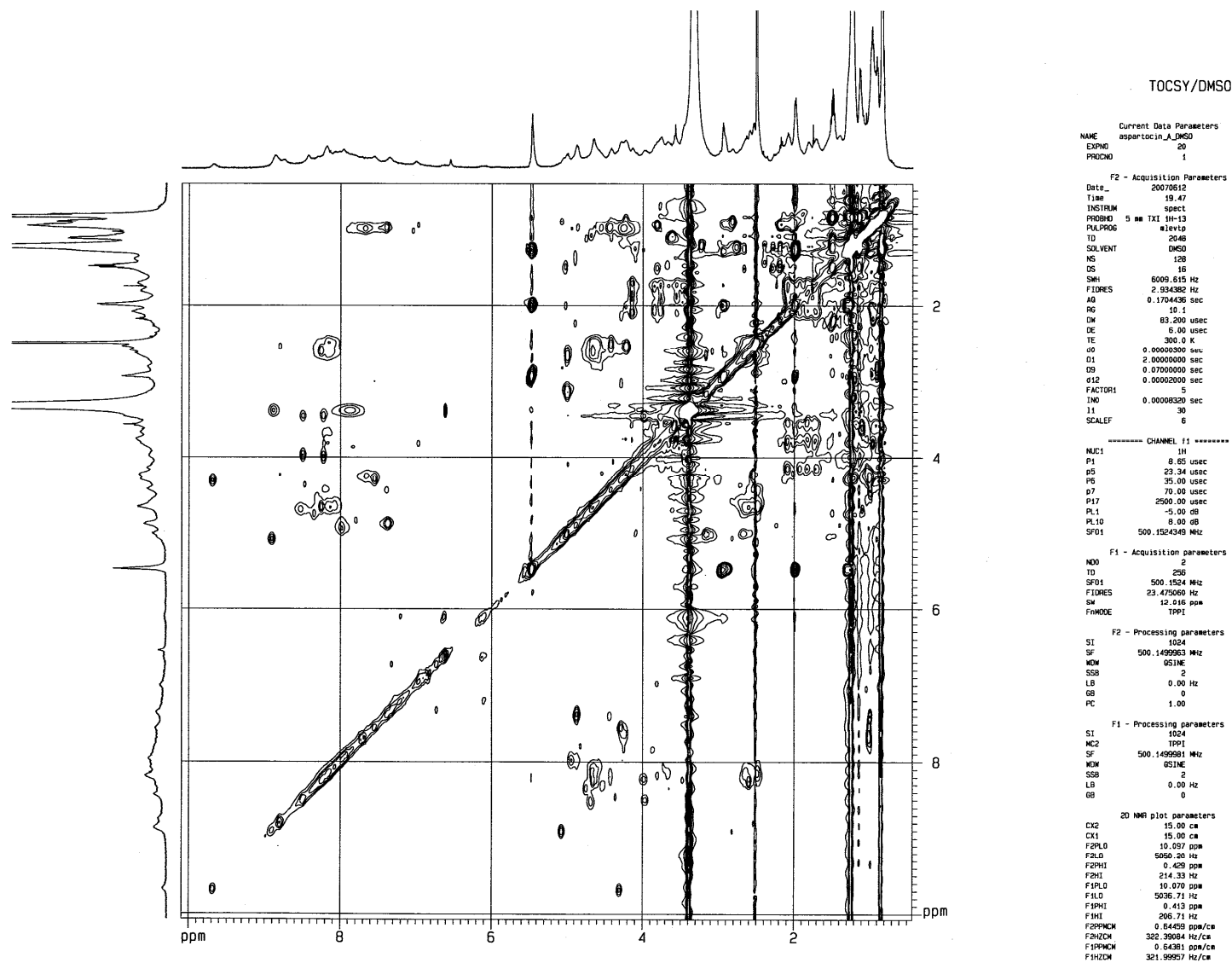


Figure S7. HSQC-TOCSY spectrum of aspartocin A (1) in DMSO- $d_6$  recorded on Bruker DRX 500 MHz

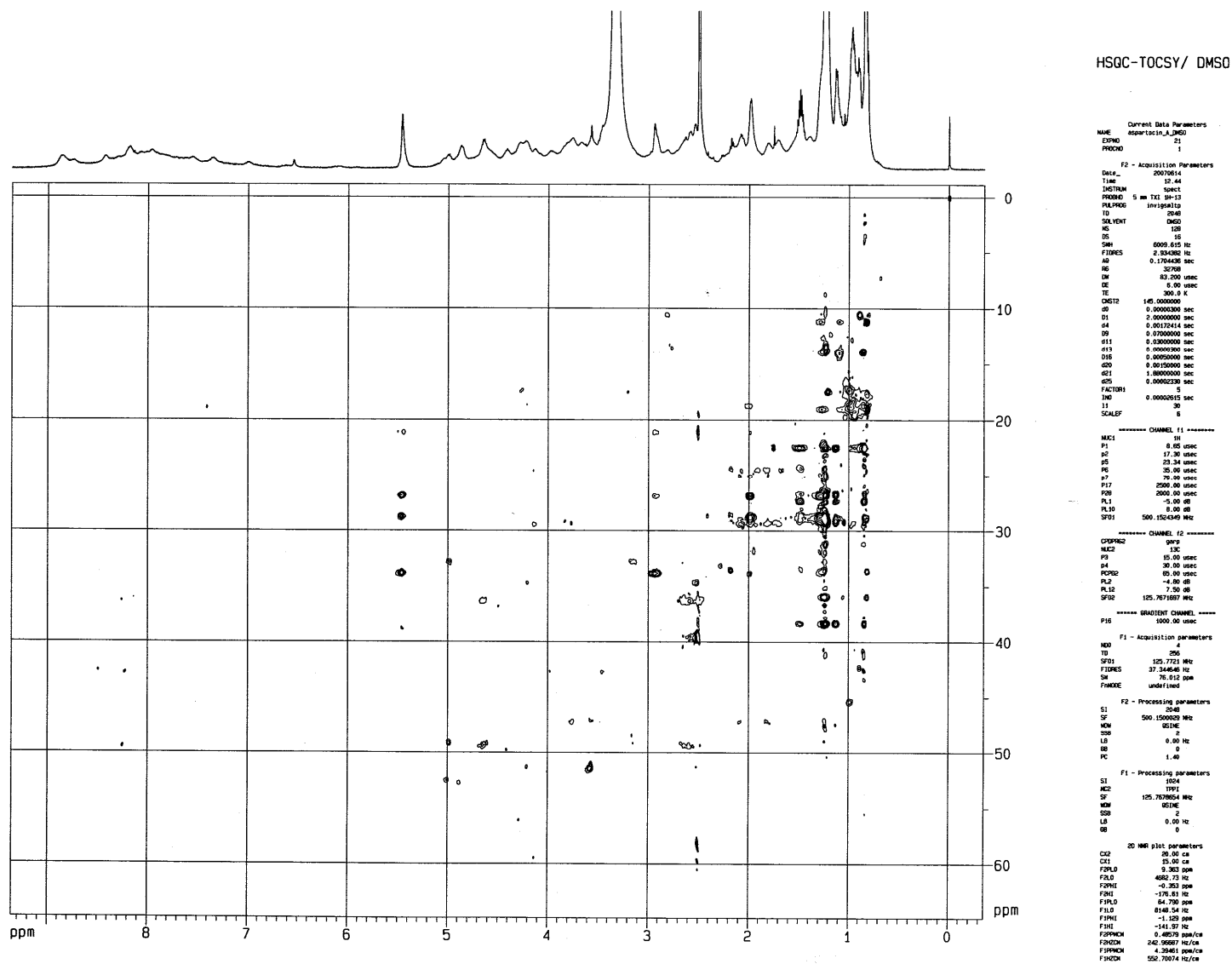


Figure S8. NOESY spectrum of aspartocin A (1) in DMSO- $d_6$  recorded on Bruker DRX 500 MHz

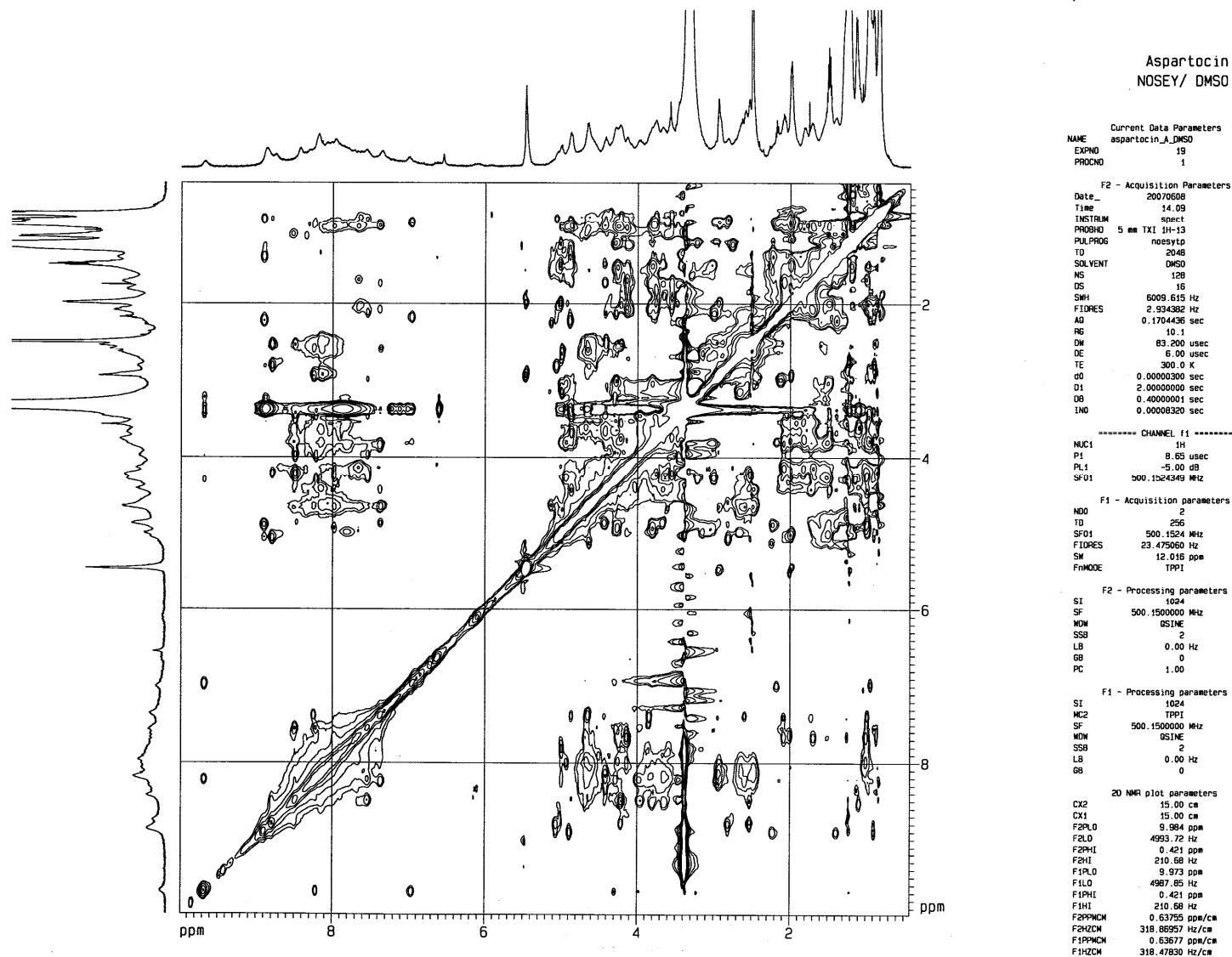


Figure S9. ROESY spectrum of aspartocin A (1) in DMSO- $d_6$  recorded on Bruker DRX 500 MHz

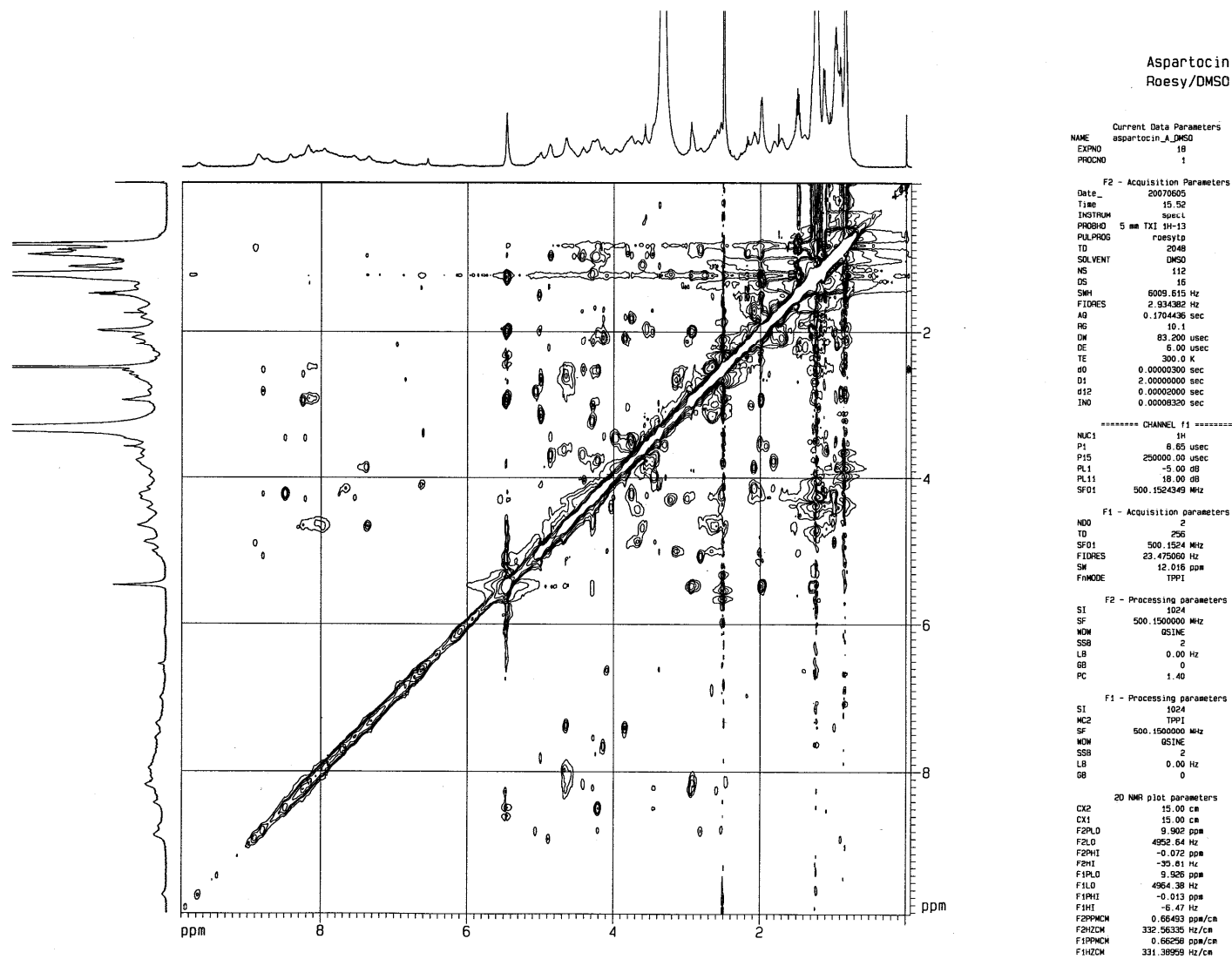


Figure S10. <sup>1</sup>H-NMR spectrum of aspartocin A (1) in MeOH-d<sub>4</sub> recorded on Bruker DPX 400 MHz

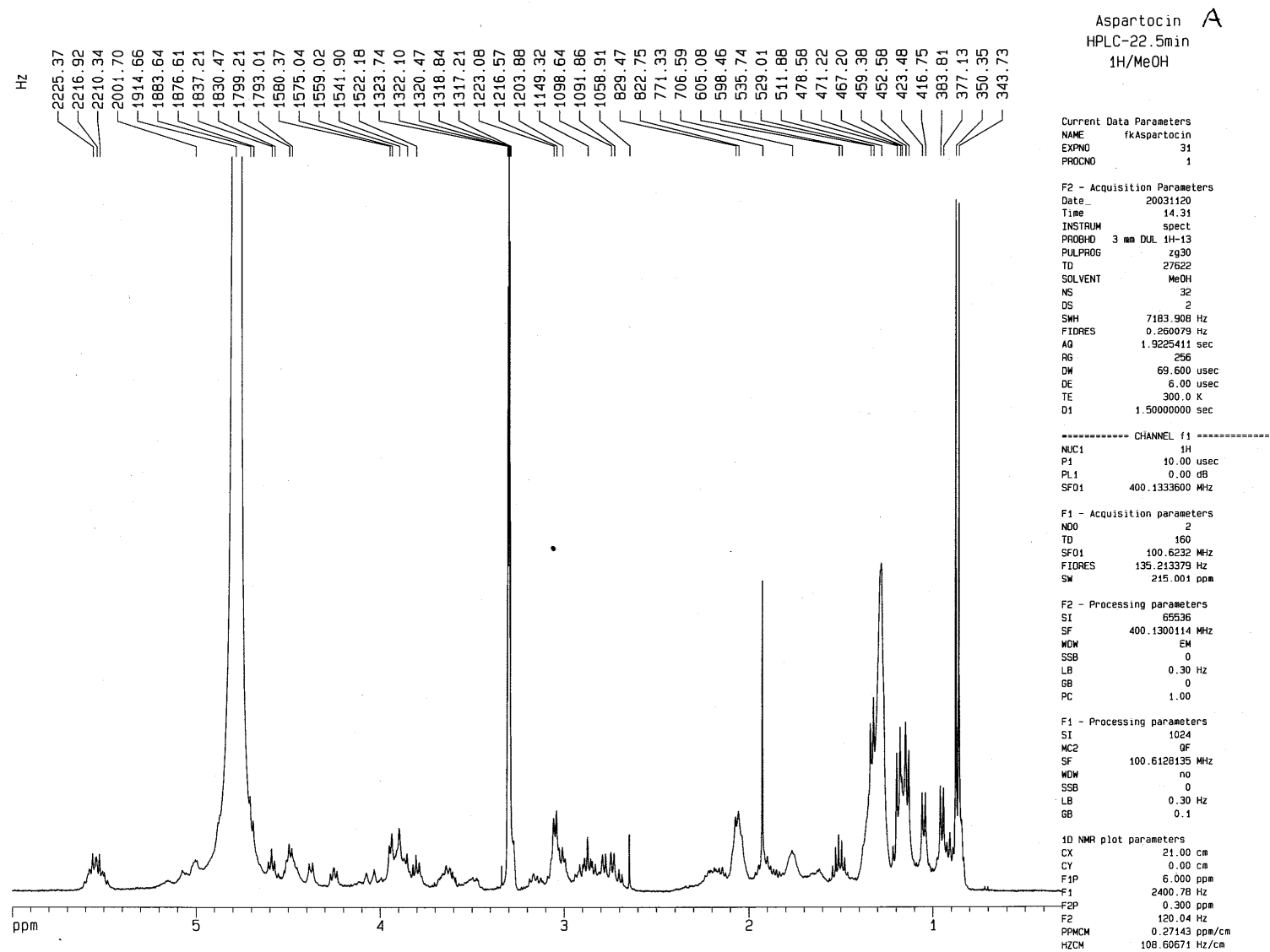


Figure S11. LC-UV-MS data of aspartocin B (2) generated on a Finnigan LCQ LC-MS system

D:\Deca-data\FMK\AspartocinB

12/04/03 05:03:41 PM

antibiotic

AspartocinB  
 Type: Unknown ID: 1 Row: 1  
 Sample Name: antibiotic  
 Flow Rate: 0.3 mL/min.  
 Notebook #: L18747  
 Column: YMC ODS A; 2.0X100mm  
 Solvents: A = H2O with 0.025% formic acid; B = CH3CN with 0.025% formic acid; C = MeOH with 0.025% formic acid; D =  
 Mobile Phase: 5 to 50% B in A in 10 min  
 Instrument Method: D:\New Xcalibur\Xcalibur\methods\fmkMeCN LC-MSfmk50ACN.meth  
 Processing Method:  
 Vial: 42

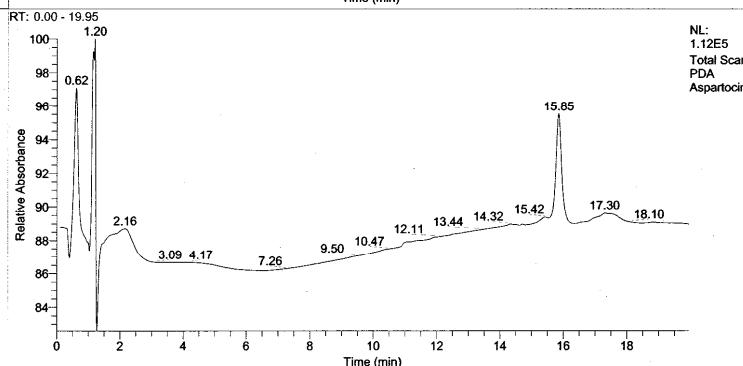
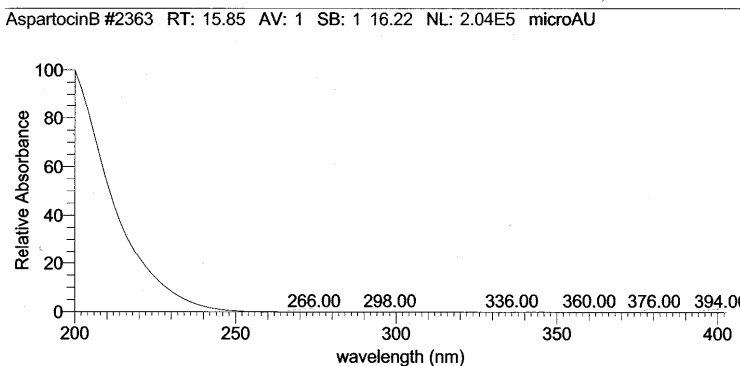
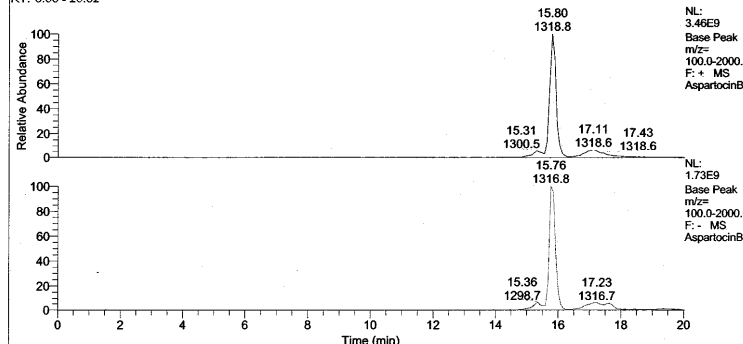
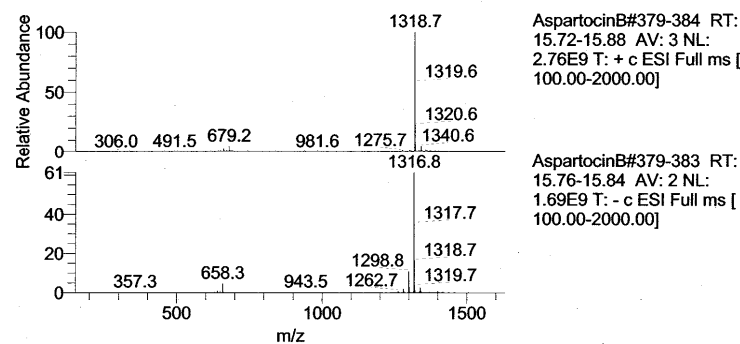
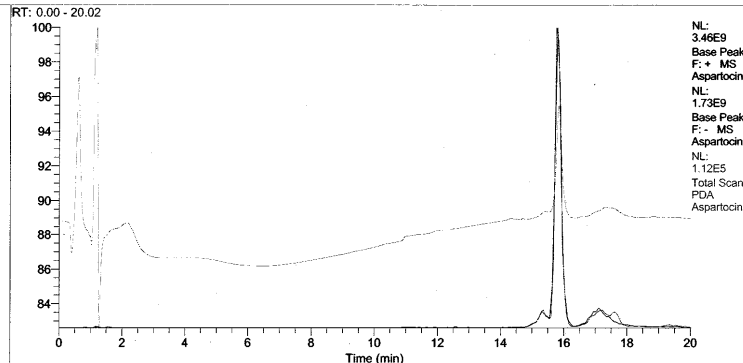


Figure S12. <sup>1</sup>H-NMR spectrum of aspartocin B (2) in MeOH-d<sub>4</sub> recorded on Bruker DPX 400 MHz

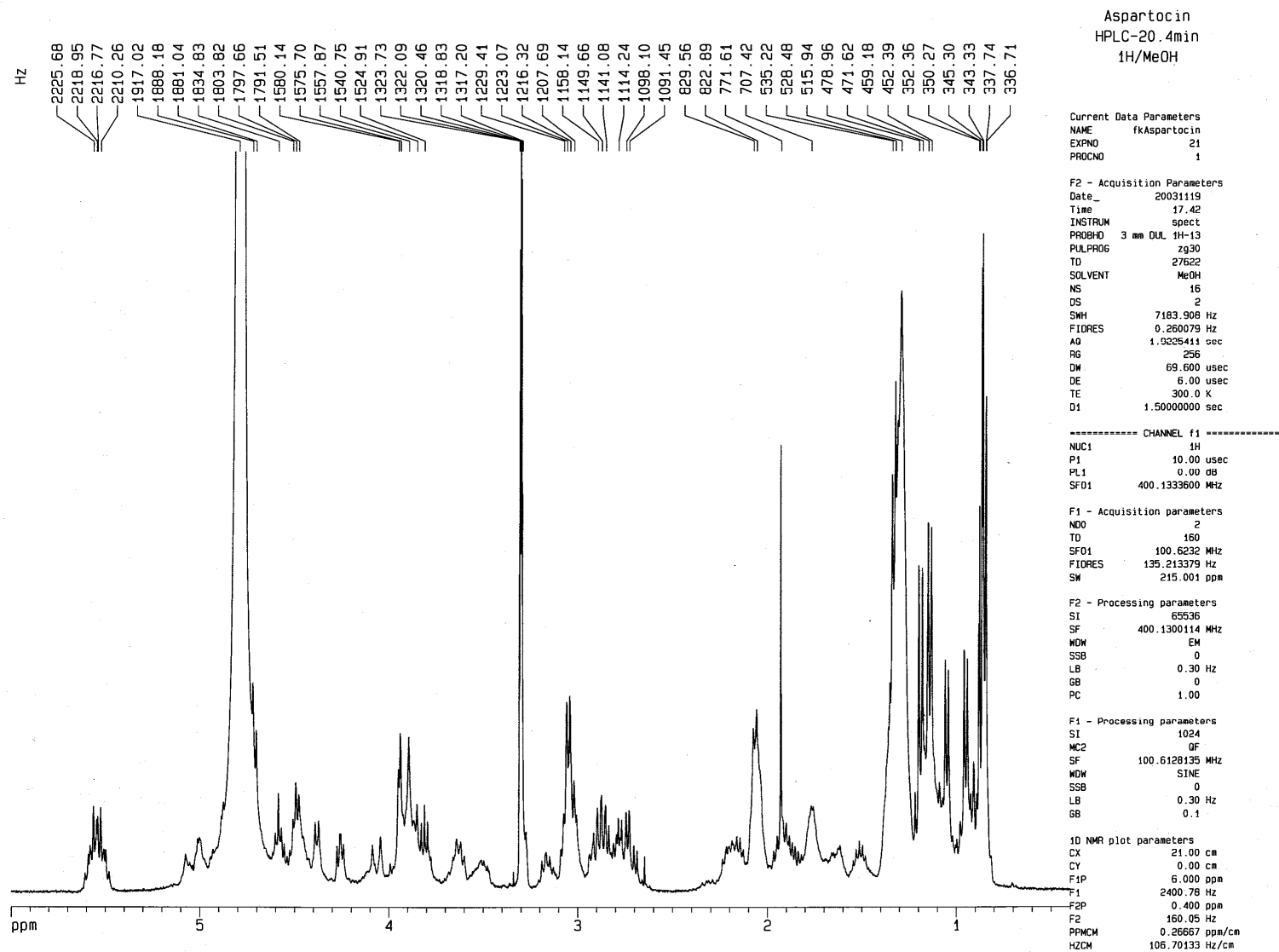


Figure S13.  $^{13}\text{C}$ -NMR spectrum of aspartocin B (2) in MeOH- $d_4$  recorded on Bruker DPX 100 MHz

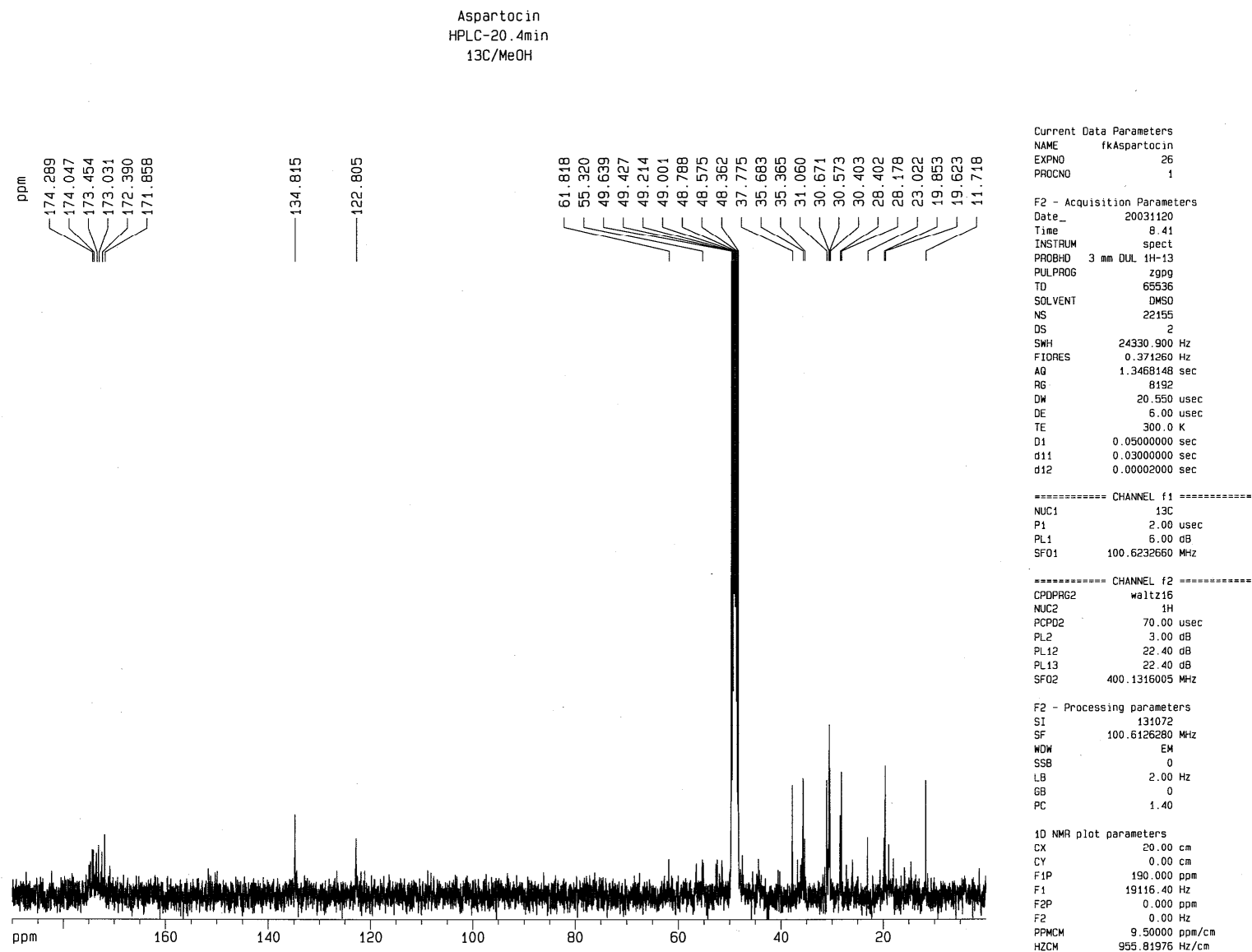




Figure S14. COSY spectrum of aspartocin B (2) in MeOH-*d*<sub>4</sub> recorded on Bruker DPX 400 MHz

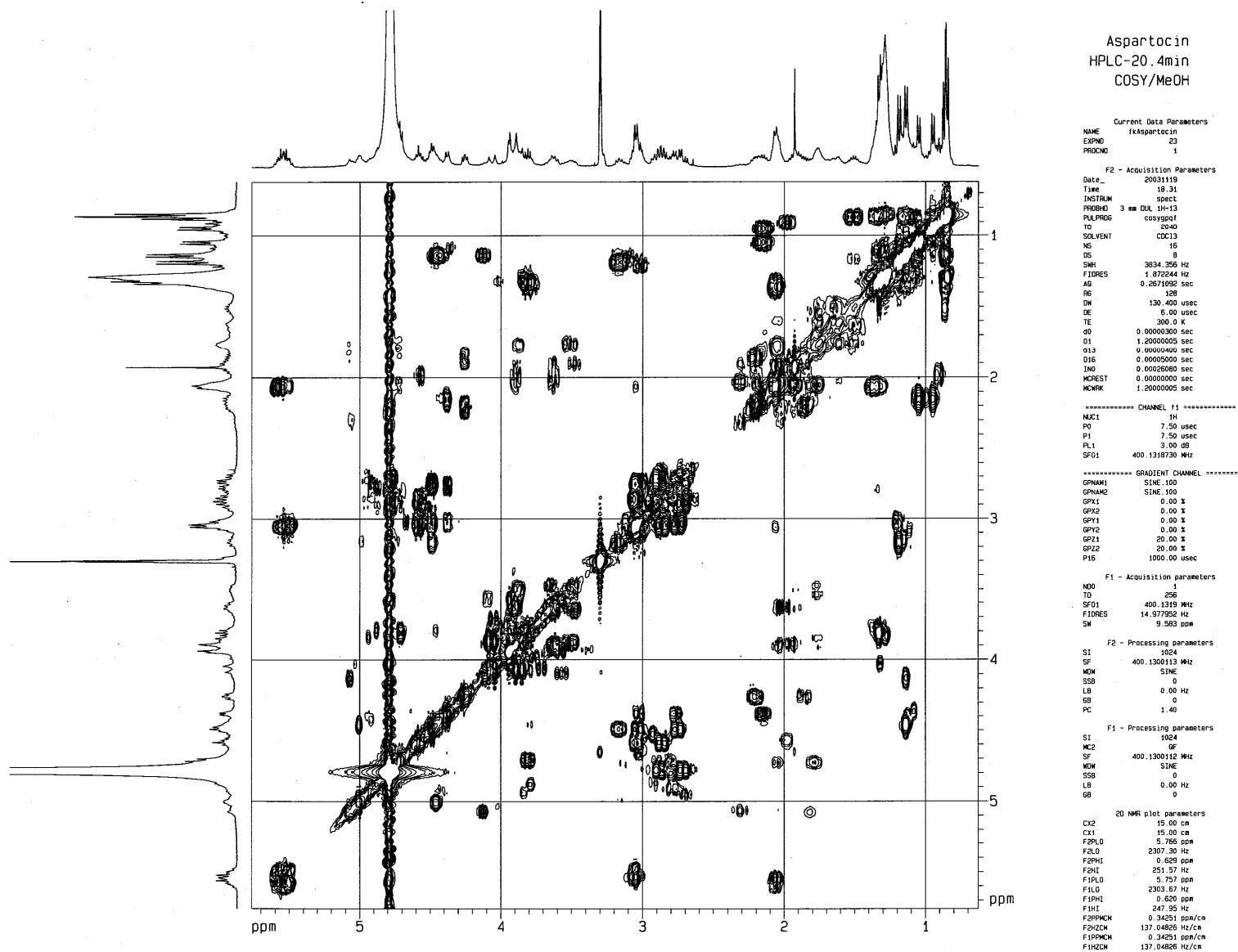


Figure S15. HSQC spectrum of aspartocin B (2) in MeOH-*d*<sub>4</sub> recorded on Bruker DPX 400 MHz

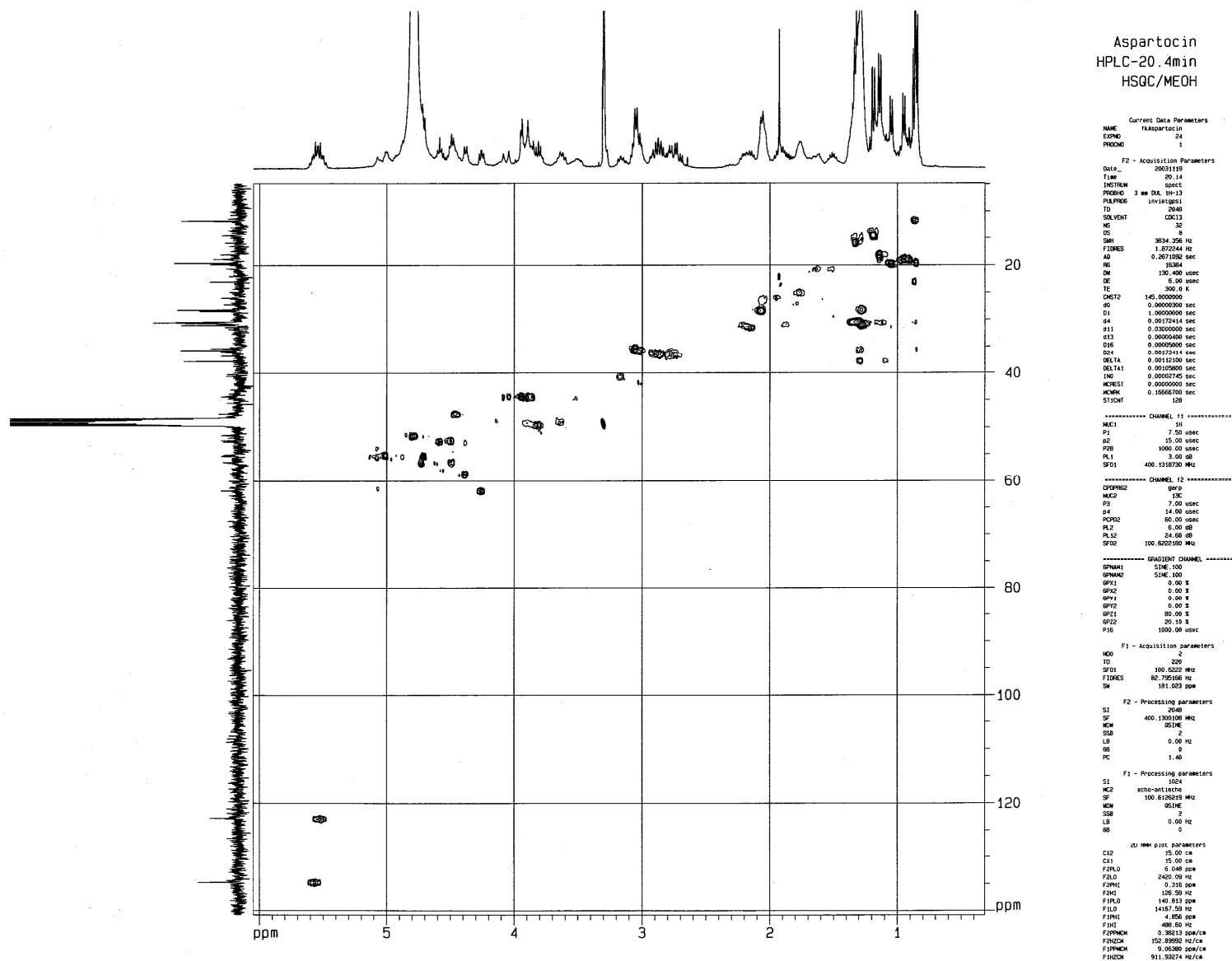


Figure S16. HMBC spectrum of aspartocin B (2) in MeOH-*d*<sub>4</sub> recorded on Bruker DPX 400 MHz

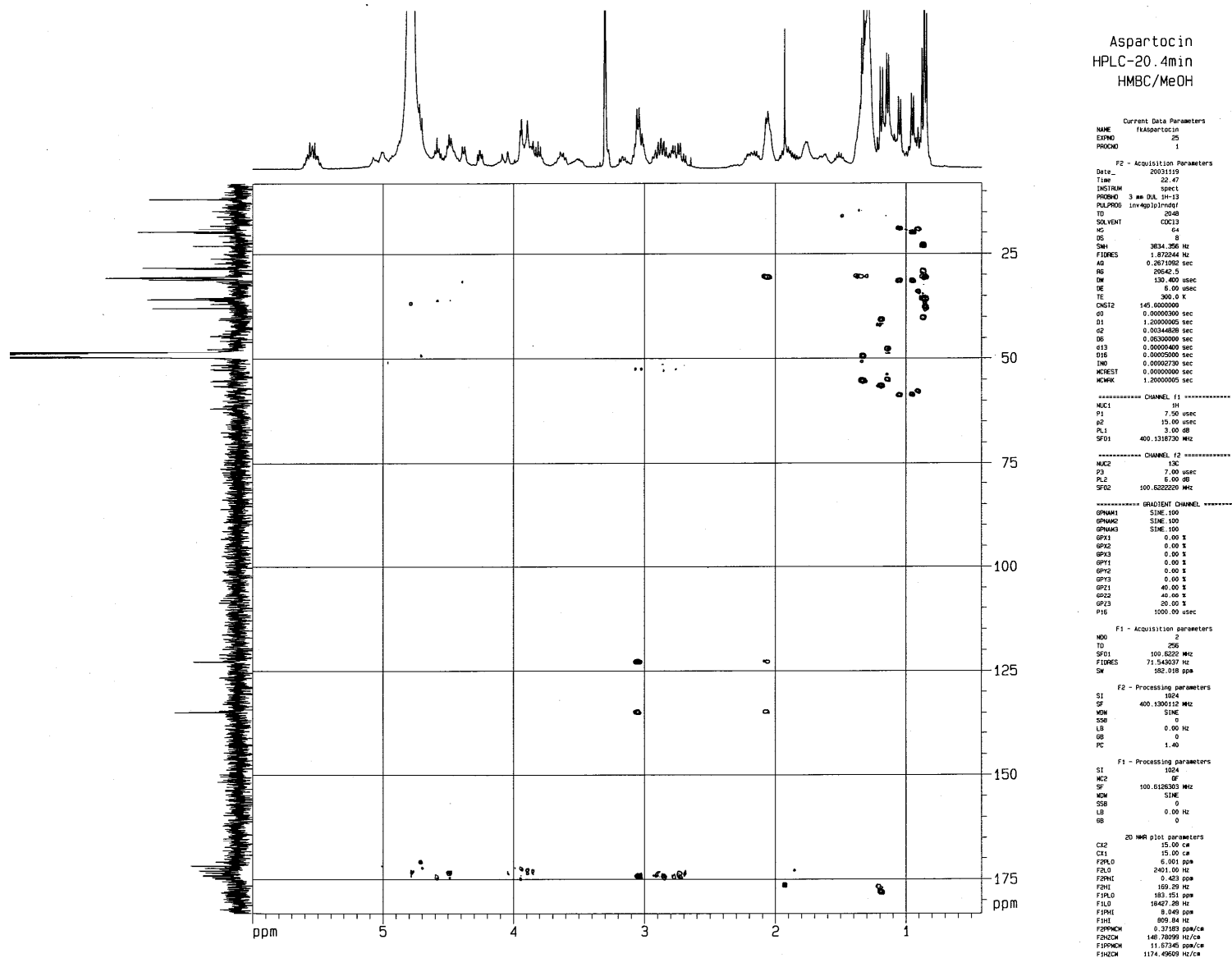


Figure S17. TOCSY spectrum of aspartocin B (2) in MeOH-*d*<sub>4</sub> recorded on Bruker DPX 400 MHz

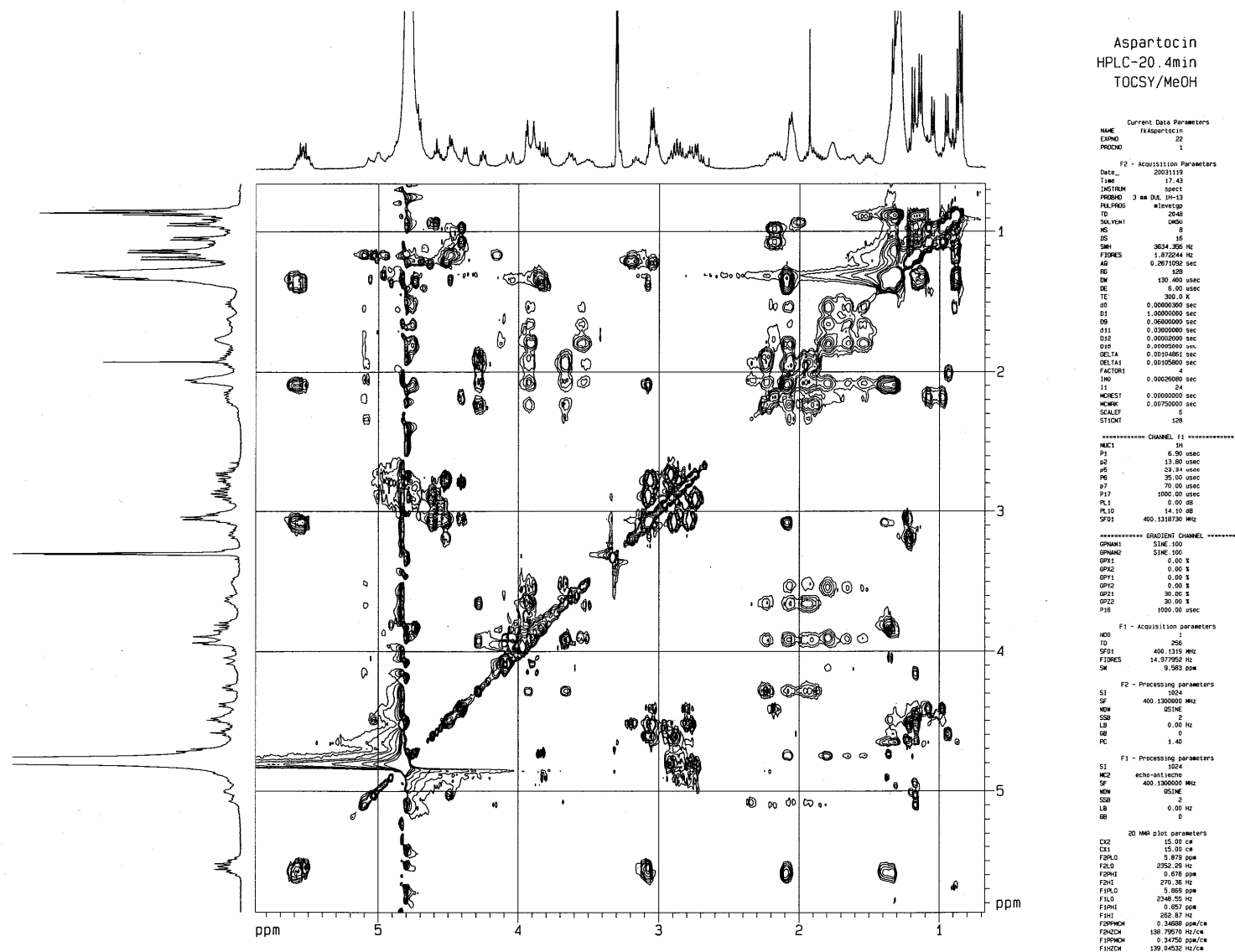


Figure S18. LC-UV-MS data of aspartocin C (**3**) generated on a Finnigan LCQ LC-MS system

D:\Deca-data\FMK\AspartocinC

12/04/03 05:24:59 PM

antibiotic

AspartocinC  
 Type: Unknown ID: 1 Row: 1  
 Sample Name: antibiotic  
 Flow Rate:: 0.3 mL/min.  
 Notebook #:: L18747  
 Column:: YMC ODS A; 2.0X100mm  
 Solvents:: A = H2O with 0.025% formic acid; B = CH3CN with 0.025% formic acid; C = MeOH with 0.025% formic acid; D =  
 Mobile Phase:: 5 to 50% B in A in 10 min  
 Instrument Method: D:\New Xcalibur\Xcalibur\methods\fmkMeCN LC-MSfmk50ACN.meth  
 Processing Method:  
 Vial: 43

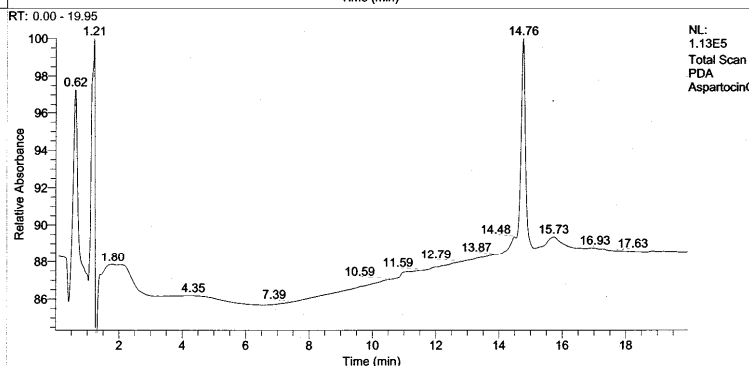
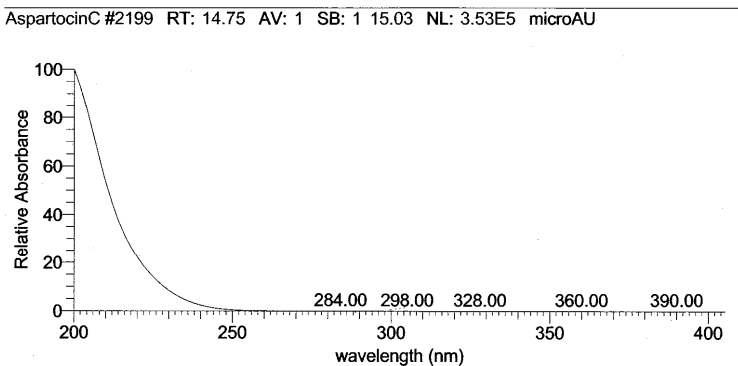
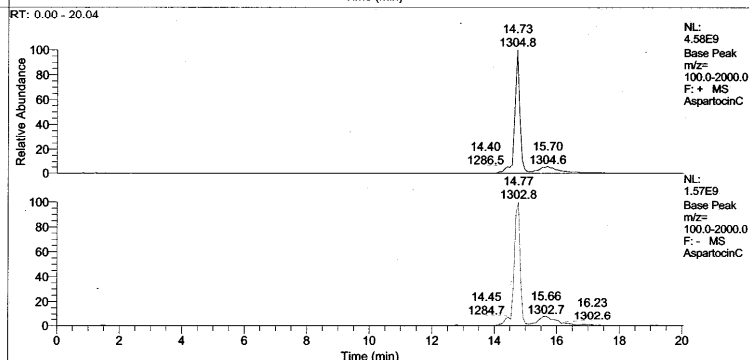
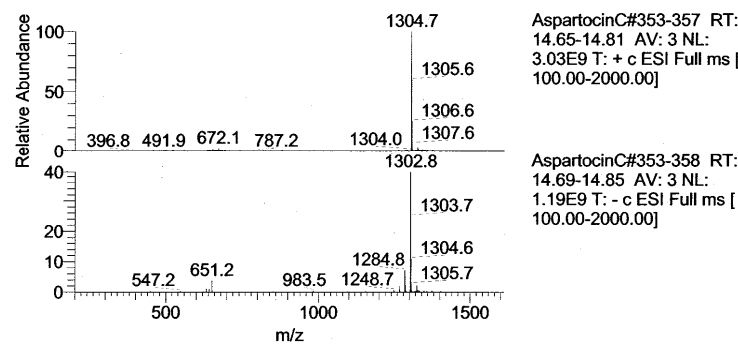
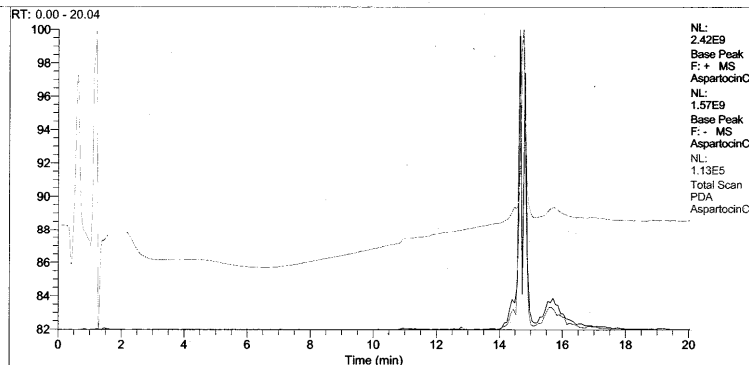


Figure S19. <sup>1</sup>H-NMR spectrum of aspartocin C (**3**) in MeOH-*d*<sub>4</sub> recorded on Bruker DPX 400 MHz

