Table of Contents

Figure S1. HPLC chromatogram of the aspartocin complex

Figure S2. LC-UV-MS data of aspartocin A (I)

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

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

Figure S5. HSQC spectrum of aspartocin A (I) in DMSO-$d_6$ recorded on Bruker DRX 500 MHz

Figure S6. TOCSY spectrum of aspartocin A (I) in DMSO-$d_6$ recorded on Bruker DRX 500 MHz

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

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

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

Figure S10. $^1$H-NMR spectrum of aspartocin A (I) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz

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

Figure S12. $^1$H-NMR spectrum of aspartocin B (2) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz

Figure S13. $^{13}$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-$d_4$ recorded on Bruker DPX 400 MHz

Figure S15. HSQC spectrum of aspartocin B (2) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz

Figure S16. HMBC spectrum of aspartocin B (2) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz
Figure S17. TOCSY spectrum of aspartocin B (2) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz

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

Figure S19. $^1$H-NMR spectrum of aspartocin C (3) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz
Figure S1. HPLC chromatogram of the aspartocin complex, which is composed of three analogs, aspatocin 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

Aspartocin A
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: 41

Aspartocin A #382-388 RT: 15.98-16.04 AV: 3 NL 2.43E9 T: + c ESI Full ms [100.00-2000.00]
Aspartocin A #383-387 RT: 15.92-16.00 AV: 2 NL 1.40E9 T: - c ESI Full ms [100.00-2000.00]

Aspartocin A #2391 RT: 16.04 AV: 1 SB: 1 16.45 NL: 1.54E5 microAU
Figure S3. $^1$H-NMR spectrum of aspartocin A (1) in 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-$d_6$ recorded on Bruker DRX 500 MHz
Figure S6. TOCSY spectrum of aspartocin A (1) in DMSO-$d_6$ 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. $^1$H-NMR spectrum of aspartocin A (1) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz
Figure S11. LC-UV-MS data of aspartocin B (2) generated on a Finnigan LCQ LC-MS system
Figure S12. $^1$H-NMR spectrum of aspartocin B (2) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz
Figure S13. $^{13}$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-$d_4$ recorded on Bruker DPX 400 MHz
Figure S15. HSQC spectrum of aspartocin B (2) in MeOH-\textit{d}_4 recorded on Bruker DPX 400 MHz
Figure S16. HMBC spectrum of aspartocin B (2) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz
Figure S17. TOCSY spectrum of aspartocin B (2) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz
Figure S18. LC-UV-MS data of aspartocin C (3) generated on a Finnigan LCQ LC-MS system
Figure S19. $^1$H-NMR spectrum of aspartocin C (3) in MeOH-$d_4$ recorded on Bruker DPX 400 MHz