

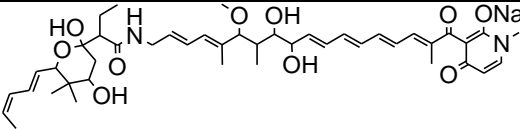
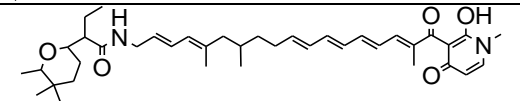
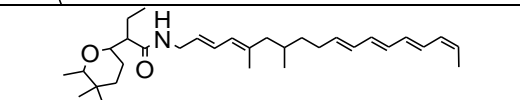
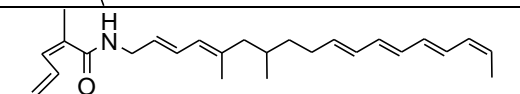
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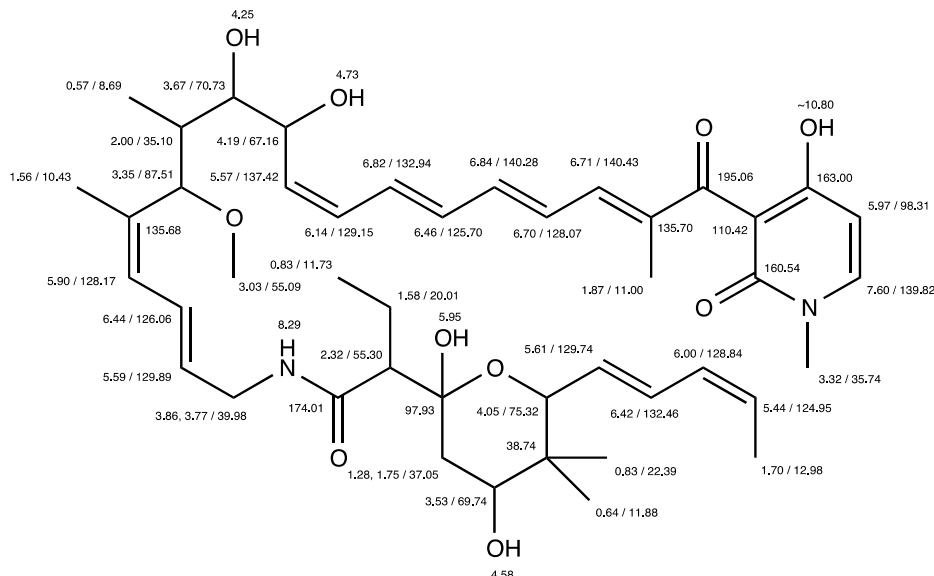
ARTICLE TYPE

SUPPLEMENTARY DATA:

MS-MS analysis of Factumycin.

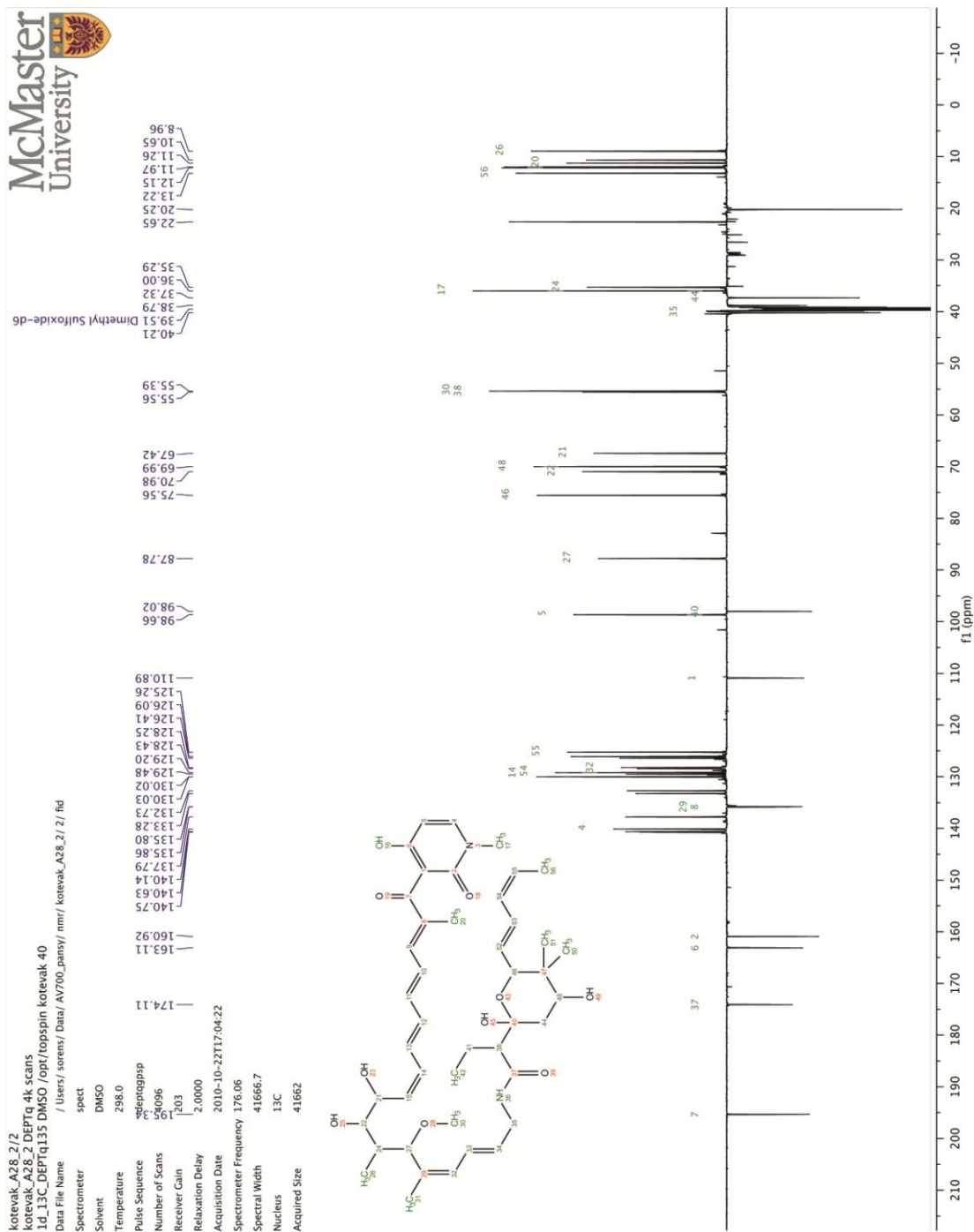
Fragment	Molecular formula	[M+H] ⁺ calc.	[M+H] ⁺ obs.
	C ₄₄ H ₆₁ N ₂ NaO ₁₀	801.4304	801.4233
	C ₃₉ H ₅₆ N ₂ O ₅	633.4269	633.3235
	C ₃₂ H ₅₁ NO ₂	482.4000	482.2824
	C ₂₆ H ₃₇ NO	380.2955	380.2167

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Supplementary Figure 1. Structural assignment of Factumycin. Chemical shift values are as observed in the HSQC / HMBC spectra.

Factumycin: yellow powder; HR negative MS m/z 777.4444 for $[M-H]^-$ (calculated for $C_{44}H_{61}N_2O_{10}$, 777.4326); ¹H NMR (700 MHz, DMSO-*d*₆) δ 10.77 (s, 1H), 8.29 (t, J = 5.7 Hz, 1H), 7.60 (d, J = 7.5 Hz, 1H), 6.84 (m, 1H), 6.81 (m, 1H), 6.71 (m, 1H), 6.70 (m, 1H), 6.46 (m, 1H), 6.43 (m, 1H), 6.42 (m, 1H), 6.14 (t, J = 11.2 Hz, 1H), 6.00 (td, J = 11.2, 1.9 Hz, 1H), 5.97 (d, J = 7.5 Hz, 1H), 5.90 (d, J = 10.7 Hz, 1H), 5.62 (m, 1H), 5.59 (m, 1H), 5.56 (d, J = 9.7 Hz, 1H), 5.44 (dq, J = 10.8, 7.1 Hz, 1H), 4.19 (t, J = 8.7 Hz, 1H), 4.06 (d, J = 5.4 Hz, 1H), 3.86 (m, 1H), 3.77 (m, 1H), 3.67 (dd, J = 8.6, 1.7 Hz, 1H), 3.54 (dd, J = 11.6, 4.8 Hz, 1H), 3.35 (d, J = 10.0 Hz, 1H), 3.32 (s, 3H), 3.03 (s, 3H), 2.32 (dd, J = 9.1, 6.0 Hz, 1H), 2.00 (m, 1H), 1.87 (s, 3H), 1.75 (dd, J = 12.6, 4.7 Hz, 1H), 1.70 (dd, J = 7.1, 1.7 Hz, 3H), 1.58 (m, 2H), 1.56 (s, 3H), 1.28 (t, J = 12.1 Hz, 1H), 0.84 (m, 3H), 0.84 (s, 3H), 0.65 (s, 3H), 0.57 (d, J = 7.0 Hz, 3H). ¹³C NMR (176 MHz, DMSO-*d*₆) δ 195.34, 174.11, 163.11, 160.92, 140.75, 140.63, 140.14, 137.79, 135.86, 135.80, 133.28, 132.73, 130.03, 130.02, 129.48, 129.20, 128.43, 128.25, 126.41, 126.09, 125.26, 110.89, 98.66, 98.02, 87.78, 75.56, 70.98, 69.99, 67.42, 55.56, 55.39, 40.21, 38.79, 37.32, 36.00, 35.29, 22.65, 20.25, 13.22, 12.15, 11.97, 11.26, 10.65, 8.96.

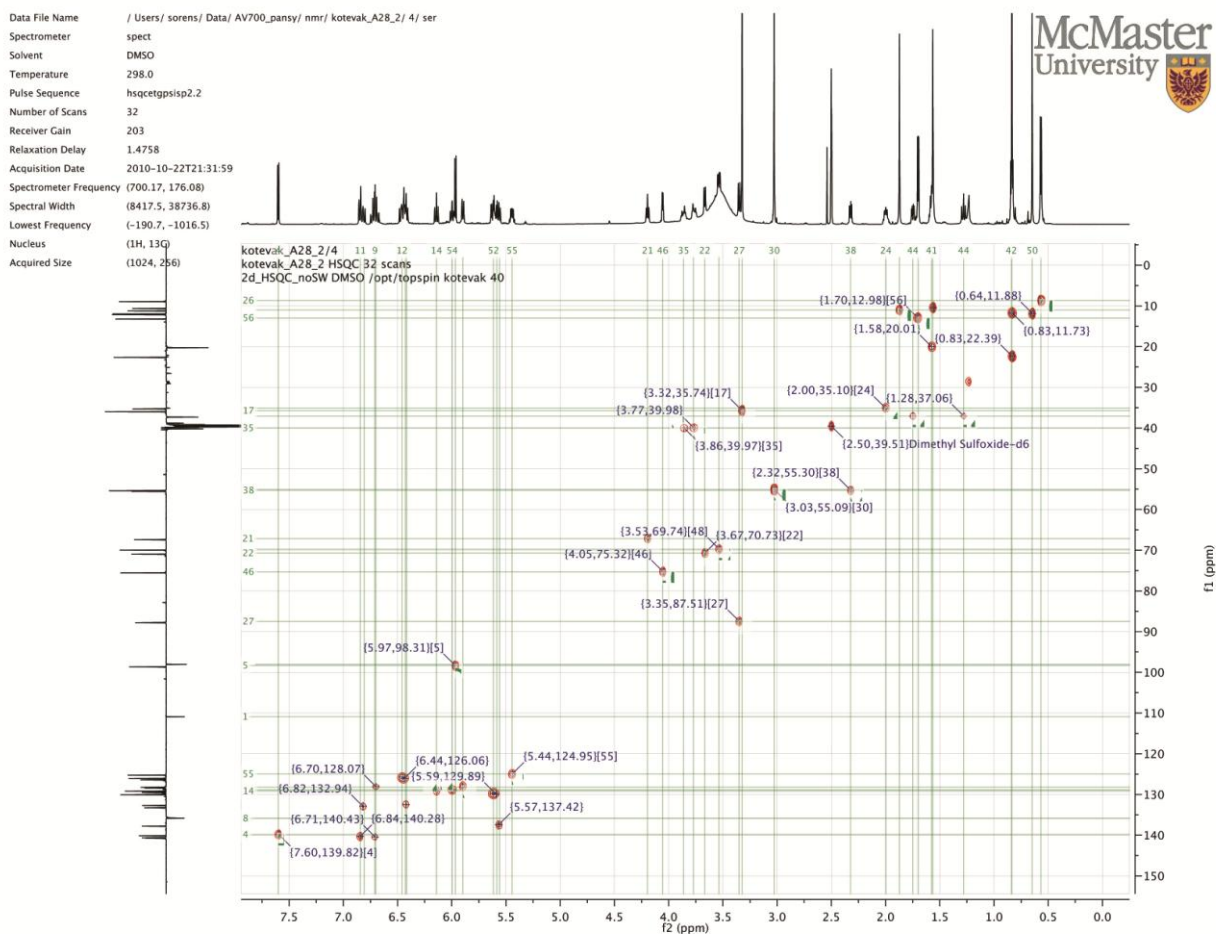


Supplementary Figure 3: DEPT q spectra of Factumycin

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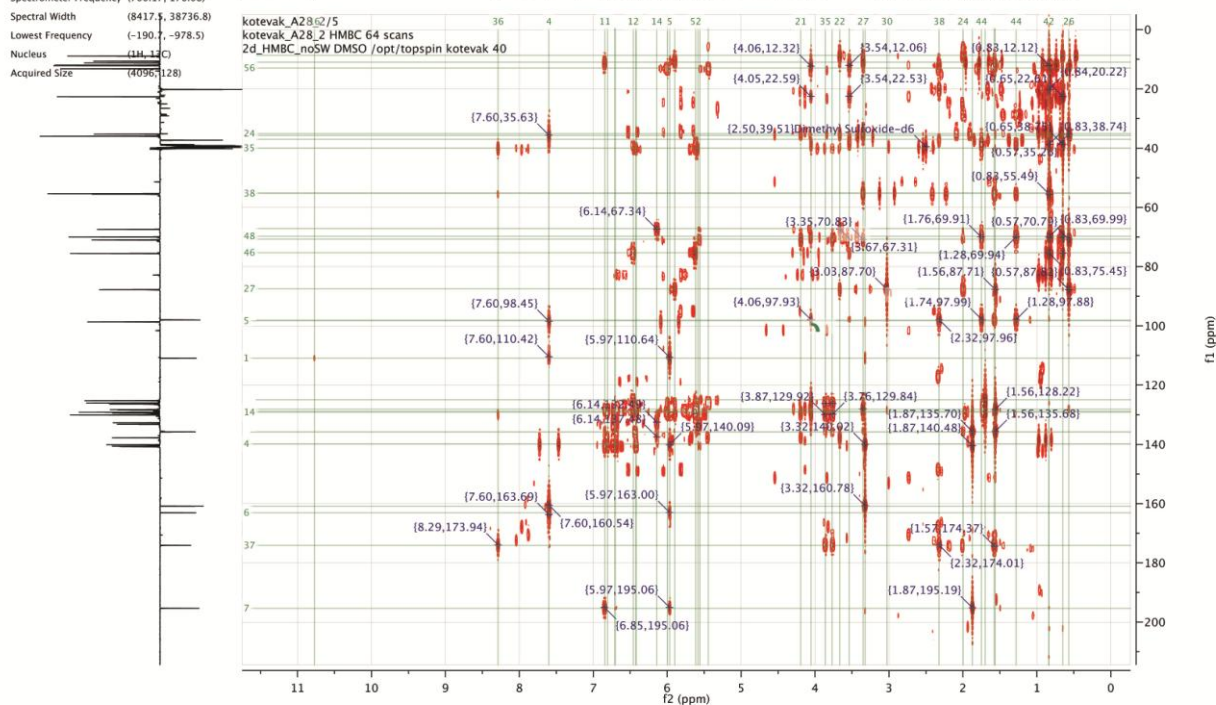
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Supplementary Figure 4: HSQC spectra of Factumycin.

Data File Name / Users/soresns/Data/AV700_pansy/nmr/kotevak_A28_2/5/ser
Spectrometer spect
Solvent DMSO
Temperature 298.0
Pulse Sequence hmbcgp12ndqf
Number of Scans 64
Receiver Gain 203
Relaxation Delay 1.4959
One-bond JHX 145
Long-range JHX 8
Acquisition Date 2010-10-23T01:07:19
Spectrometer Frequency (700.17, 176.08)
Spectral Width (8417.5, 38736.8)
Lowest Frequency (-190.7, -978.5)
Nucleus (1H, 13C)
Acquired Size (4095, 128)



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Supplementary figure 5: HMBC spectra of Factumycin.

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