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SUPPORTING INFORMATION

The Structures of Five Components of the Actinomycin Z Complex from *Streptomyces fradiae*, Two of which Contain 4-Chlorothreonine

Helmut Lackner, Isabel Bahner, Nobuharu Shigematsu, Lewis K. Pannell and Anthony B. Mauger

Table 1. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₁

Table 2. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₂

Table 3. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₃

Table 4. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₄

Figure: 2D NMR Connectivities for Actinomycin Z₁

Figure: 2D NMR Connectivities for Actinomycin Z₅

**Table 1. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₁
(Parent Ion m/z 1301.6)**

<u>m/z</u>	<u>Fragment lost (except those in parentheses)</u>
1002	H-4-O-5-MePro-Sar-MeAla-OH
972	H-3-OH-5-MePro-Sar-MeVal-OH
903	H-D-Val-4-O-5-MePro-Sar-MeAla-OH
875	H-D-Val-3-OH-5-MePro-Sar-MeVal-OH
673	H-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH
574	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH <i>or</i> H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + H-4-O-5-MePro-Sar-MeAla-OH
475	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-D-Val-3-OH-5-MePro-Sar-MeVal-OH
429	(H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + H) ⁺
330	(H-3-OH-5-MePro-Sar-MeVal-OH + H) ⁺

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**Table 2. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₂
(Parent Ion m/z 1285.6)**

<u>m/z</u>	<u>Fragment lost (except those in parentheses)</u>
986	H-4-O-5-MePro-Sar-MeAla-OH
956	H-3-OH-5-MePro-Sar-MeVal-OH
887	H-D-Val-4-O-5-MePro-Sar-MeAla-OH
857	H-D-Val-3-OH-5-MePro-Sar-MeVal-OH
657	H-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH
558	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH <i>or</i> H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + H-4-O-5-MePro-Sar-MeAla-OH
459	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-D-Val-3-OH-5-MePro-Sar-MeVal-OH
429	(H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + H) ⁺
330	(H-3-OH-5-MePro-Sar-MeVal-OH + H) ⁺

**Table 3. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₃
(Parent Ion m/z 1319.5)**

<u>m/z</u>	<u>Fragment lost (except those in parentheses)</u>
1020	H-4-O-5-MePro-Sar-MeAla-OH
990	H-3-OH-5-MePro-Sar-MeVal-OH
984	H-4-O-5-MePro-Sar-MeAla-OH and HCl
921	H-D-Val-4-O-5-MePro-Sar-MeAla-OH
891	H-D-Val-3-OH-5-MePro-Sar-MeVal-OH
691	H-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH
655	H-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH + HCl
592	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH <i>or</i> H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + H-4-O-5-MePro-Sar-MeAla-OH
556	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-3-OH-5-MePro-Sar-MeVal-OH + HCl <i>or</i> H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + H-4-O-5-MePro-Sar-MeAla-OH + HCl
493	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-D-Val-3-OH-5-MePro-Sar-MeVal-OH
458	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + HCl
429	(H-D-Val-3-OH-5-MePro-Sar-MeVal-OH + H) ⁺
330	(H-3-OH-5-MePro-Sar-MeVal-OH + H) ⁺

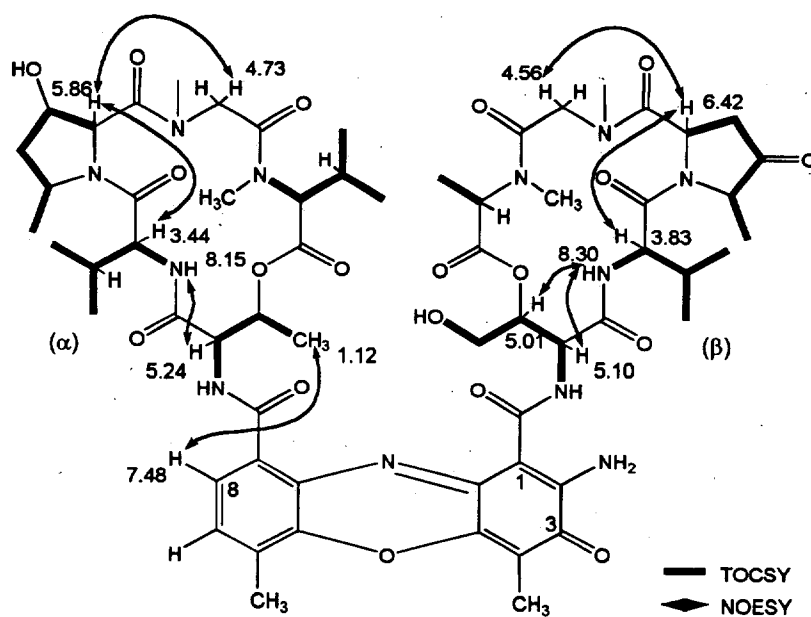
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**Table 4. Daughter Ion Spectra in Linked Scan FABMS of Actinomycin Z₄
(Parent Ion m/z 1269.6)**

<u>m/z</u>	<u>Fragment lost (except those in parentheses)</u>
970	H-4-O-5-MePro-Sar-MeAla-OH
956	H-5-MePro-Sar-MeVal-OH
871	H-D-Val-4-O-5-MePro-Sar-MeAla-OH
858	H-D-Val-5-MePro-Sar-MeVal-OH
657	H-4-O-5-MePro-Sar-MeAla-OH + H-5-MePro-Sar-MeVal-OH
558	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-5-MePro-Sar-MeVal-OH <i>or</i> H-D-Val-5-MePro-Sar-MeVal-OH + H-4-O-5-MePro-Sar-MeAla-OH
459	H-D-Val-4-O-5-MePro-Sar-MeAla-OH + H-D-Val-5-MePro-Sar-MeVal-OH
413	(H-D-Val-5-MePro-Sar-MeVal-OH + H) ⁺
314	(H-5-MePro-Sar-MeVal-OH + H) ⁺

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2D NMR Connectivities in Actinomycin Z₁



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2D NMR Connectivities in Actinomycin Z₅

