

(1) Supporting information, NOEs of (2)

NOEs of (2). Data from ^1H - ^1H -ROESY. Sample amount ca 10mg to 0.6ml MEOD. NOEs from 21-CH₂ are taken from ^1H - ^1H -ROESY of ganefromycin α . NOE intensities are denoted as S (strong), M (medium), or W (weak). Distances are obtained from molecular mechanics calculation and are shown in Ångstrom (Å). ? after a distance indicates unknown conformation. When evaluating the NOE's obtained from the ^1H - ^1H -ROESY data, no correction was made for the spin-locking offset. Mostly the data were treated qualitatively, and when NOE intensities were compared, they were close in chemical shift so only very small difference in intensities were expected.

H2		H5 - H7 = S 2.4	H9 - H10a = S 2.4	H8 - H11 = VW 3.7
H2 - H4 = S 2.5 Å		H7 - H8 = M 2.6?	H9 - H10e = S,W 2.7	H10a - H11 = M? 3.1
H3		H7 - H9 = W 3.0?	H10a	H10e - H11 = S? 2.4
H3 - H5 = S 2.4	H8		H8 - H10a = S 2.7	H11 - H12 = S 2.5
H4	H6 - H8 = S 3.5?		H9 - H10a = S 2.4	H11 - H13 = M 2.8
H2 - H4 = S 2.5	H7 - H8 = M 2.6?		H10a - CH ₃ ¹² = S 2.2	H12
H4 - H6 = X 2.4	H8 - H9 = X 2.4		H10a - H12 = M 3.0	H10a - H12 = M 3.0
H5	H8 - CH ₃ ¹² = M 3.4		H10a - H11 = M? 3.1	H10e - H12 = M 2.8
H3 - H5 = S 2.4	H8 - H11 = VW 3.7		H10e	H11 - H12 = S 2.5
H5 - H7 = S 2.4	H8 - H10a = S 2.7		H8 - H10e = M,W 3.8	H12 - CH ₃ ¹² = S 2.5
H6	H8 - H10e = M,W 3.8		H9 - H10a = S,W 2.7	H12 - H13 = M 3.0
H4 - H6 = X 2.4	H9		H10e - CH ₃ ¹² = M 3.4	H13
H6 - H8 = S 3.5?	H6 - H9 = M 4.8?		H10e - H12 = M 2.8	H11 - H13 = M 2.8
H6 - H9 = M 4.8?	H7 - H9 = W 3.0?		H10e - H11 = S? 2.4	H12 - H13 = M 3.0
H6 - H11 = VW 3.5?	H8 - H9 = X 2.4		H11	H13 - CH ₃ ¹² = M 2.5
H7	H9 - CH ₃ ¹² = W 4.5		H6 - H11 = VW 3.5?	H13 - H15 = S 2.2

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H13 - CH ₃ ¹³ = S 3.6 Å	H16 - H18 = W 3.5	CH ₂ ^{21a} - H23 = S 2.6?	H27 - H28 = W 3.0
CH₃¹²	H16 - CH ₃ ¹⁴ = S 2.4	H23 - H24 = S 2.4	H27 - H29 = S 2.4
H8 - CH ₃ ¹² = M 3.4	H17	H24	H28
H9 - CH ₃ ¹² = W 4.5	H15 - H17 = S 2.4	H23 - H24 = S 2.4	H26 - H28 = M 2.4
H10a - CH ₃ ¹² = S 2.2	H17 - H18 = M 2.5	H24 - CH ₃ ^{25eq} = S 2.7	H27 - H28 = W 3.0
H10e - CH ₃ ¹² = M 3.4	H18	H24 - H26 = S 2.5	H28 - H29 = W 3.1
H12 - CH ₃ ¹² = S 2.5	H16 - H18 = W 3.5	CH₃^{25eq}	H28 - CH ₃ ³⁰ = S 2.8
H13 - CH ₃ ¹² = M 2.5	H17 - H18 = M 2.5	CH ₃ ^{25eq} - H24 = S 2.7	H29
CH₃¹³	H21	H26 - CH ₃ ^{25eq} = S 2.7	H27 - H29 = S 2.4
H13 - CH ₃ ¹³ = S 3.6	H21 - CH ₂ ^{21a} = S 2.7?	H27 - CH ₃ ^{25eq} = S 3.7?	H28 - H29 = W 3.1
CH ₃ ¹³ - CH ₃ ¹⁴ = M,W	H21 - CH ₂ ^{21b} = M 3.0?	CH₃^{25ax}	H29 - H30 = M 2.3
CH₃¹⁴	H21 - H23 = M 3.4	CH ₃ ^{25ax} - H21 = W 3.8	H30
CH ₃ ¹³ - CH ₃ ¹⁴ = M,W	H21 - CH ₃ ^{25ax} = W 3.8	CH ₃ ^{25ax} - H26 = W 3.5	H29 - H30 = M 2.3
H16 - CH ₃ ¹⁴ = S 2.4	CH₂^{21a}	CH ₃ ^{25ax} - H27 = S 2.9	H30 - CH ₃ ³⁰ = M 2.7
H15	H21 - CH ₂ ^{21a} = S 2.7?	H26	CH₃³⁰
H13 - H15 = S 2.2	CH ₂ ^{21a} - H23 = S 2.6?	H24 - H26 = S 2.5	H28 - CH ₃ ³⁰ = S 2.8
H15 - H17 = S 2.4	CH₂^{21b}	H26 - CH ₃ ^{25e} = M 3.5	H30 - CH ₃ ³⁰ = M 2.7
H16	H21 - CH ₂ ^{21b} = W 3.0?	H26 - H27 = S 3.0?	
	H23	H26 - H28 = M 2.4?	
	H21 - H23 = W 3.4	H27	
		H26 - H27 = S 3.0?	