

**Figure 1.** A contour plot of the 500 MHz ROESY spectrum of anhydroerythromycin A (1) in deuteriated phosphate buffer at apparent pH 7.0, 25 °C.

**Table 1.** 500 MHz ROESY connectivity table of anhydroerythromycin A (1) in deuteriated phosphate buffer at apparent pH 7.0, 25 °C; mixing time is 500 ms

	2	3	4	5	7r	7s	8	10	11	13	14s	14r	15	16	17	18	19	20	21	1'	2'	3'	4'r	4's	5'	6'	7',8'	1"	2"r	2"s	4"	5"	6"	7"	8"
2	•	S	Μ					Μ						Μ																					
3	S	•	V	S												Μ												Μ							
4	Μ	٧	•	V				S							S					Μ															
5		S	V	•											Μ	Μ				Μ												Μ			
7r					•	L	S									S																			
7s					L	•	S										S	S																	
8					S	S	•									S	Μ																		
10	Μ		S					•										Μ																	
11									•								S	Μ	Μ																
13										•		Μ	Μ						Μ																
14s											•	L	V																						
14r										Μ	L	٠	V						S																
15										Μ	V	V	•																						
16	Μ													٠														Μ							
17			S	Μ											•																	Μ			S
18		Μ		Μ	S		S									•																			
19						S	Μ		S								•	S																	
20						S		Μ	Μ								S	•			V														
21									Μ	Μ		S							•																
1'			Μ	Μ																•	S	Μ			L										
2'																		V		S	•				V		Μ								
3'																				Μ		•		V	S		Μ								
4'r																							•	L		S	S								
4's																						۷	L	•	S		S								
5'																				L	V	S		S	•	Μ									
6'																							S		Μ	•									
7',8'																					Μ	Μ	S	S			•								
1"		Μ												Μ														•	Μ	V		V			
2"r																												Μ	•	L	Μ				
2"s																												V	L	•					Μ
4"																													М		٠	S		L	
5"				М											Μ													V			S	٠	L		
6"																																L	•		
7"																															L			•	М
8"															S															Μ				Μ	•
	2	3	4	5	7r	7s	8	10	11	13	14s	14r	15	16	17	18	19	20	21	1'	2'	3'	4'r	4's	5'	6'	7',8'	1"	2"r	2"s	4"	5"	6"	7"	8"

Very small signal: V; Small signal : S; Medium Signal: M; Large signal: L

## Chemical shifts of methylene protons

H-7r:  $\delta$  1.65; H-7s:  $\delta$  2.4; H-14s:  $\delta$  2.0; H-14r:  $\delta$  1.7; H-4'r:  $\delta$  1.62; H-4's:  $\delta$  2.18; H-2"r:  $\delta$  1.7; H-2"s:  $\delta$  2.43. The symbols r and s are used as abbreviations for *proR* and *pros* in this table.

## Full NMR assignments of anhydroerythromycin A 2'-acetate (4) in CDCl<sub>3</sub>

Anhydroerythromycin A 2'-acetate (4) was dissolved in CDCl<sub>3</sub> to a concentration of 30 mg ml<sup>-1</sup>. In the 1D-<sup>1</sup>H spectrum there were three readily recognizable singlets at  $\delta$  3.28, 2.26 and 2.10 integrating respectively to three, six and three protons. These were assigned by inspection to the methyl groups at 8", 7'/8' and 10' respectively. Their corresponding carbon chemical shifts were found from the gHMQC spectrum. The only triplet in the upfield region,  $\delta$  0.83, was assigned to CH<sub>3</sub>-15. C-15 was assigned from the gHMQC spectrum. In the gHMBC spectrum, H<sub>3</sub>-15 coupled to  $\delta$  24.24 (a negative signal in DEPT-135 spectrum) and  $\delta$  81.35. These were consistent with C-14 and C-13, respectively. H<sub>3</sub>-15 showed, in the DQF-COSY spectrum, correlation with H<sub>2</sub>-14 at  $\delta$  1.66 and 2.04. Now the TOCSY spectrum was used to assign  $\delta$  5.17, a double doublet signal in 1D-<sup>1</sup>H spectrum, to H-13. The spin group H-13 to H-14<sub>s</sub>, H-14<sub>r</sub> and H3-15 was very clear in the TOCSY spectrum. In the gHMBC spectrum H-13 demonstrated correlation with C-12 at  $\delta$  82.52 and also it was used to assign  $\delta$  1.29 to H<sub>3</sub>-21, a singlet in the 1D-<sup>1</sup>H spectrum, based on its correlation with C-12 and C-13. C-21 appeared at  $\delta$  25.19 in the gHMQC spectrum.

There were two remaining isolated singlets in the 1D-<sup>1</sup>H spectrum at  $\delta$  1.21 and 1.42. These were respectively assigned to H<sub>3</sub>-7" and H<sub>3</sub>-18. Their corresponding carbon chemical shifts were found through the gHMQC spectrum. C-18, in the gHMBC spectrum, showed connections with  $\delta$  3.43, 2.48 and 1.46. These were (non-specifically) H<sub>2</sub>-7 and H-5, but were distinguished by the strong mutual coupling between  $\delta$  1.46 and 2.48 in the DQF-COSY spectrum. Now the gHMQC spectrum was used to assign C-7 and C-5. Both protons attached to C-7 coupled to H-8 at  $\delta$  2.28. C-8 was found from the gHMQC spectrum; in the gHMBC spectrum C-8, in addition to coupling to H<sub>2</sub>-7, coupled to  $\delta$  1.07 which is consistent with H<sub>3</sub>-19.

A new starting point was chosen from the DEPT-135 spectrum. There were two remaining methylene groups at  $\delta$  30.64 and 34.56 were assigned non-specifically to C-2" and C-4'. In the gHMQC spectrum,  $\delta$  34.56 showed proton signals at  $\delta$  1.53 and 2.28 (overlapping H-8). In the TOCSY spectrum these two proton signals coupled to  $\delta$  5.13, a doublet in 1D-<sup>1</sup>H spectrum. This spin group was comfortably consistent with H-2"<sub>s</sub>, H-2"<sub>r</sub> and H-1". Hence the remaining methylene group at  $\delta$  30.56 was assigned to CH<sub>2</sub>-4'. Now the gHMQC spectrum was used to assign C-1" and H-4'. In the TOCSY spectrum, the H-4' at  $\delta$  1.75 coupled to  $\delta$  1.24, 1.33, 2.71, 3.49, 4.34 and 4.83. These interactions demonstrated a clear spin group existing in the desosamine sugar. The most downfield chemical shift was assigned to H-2' that showed correlation, in the DQF-COSY spectrum, with H-1' (at  $\delta$  4.34) and H-3' (at  $\delta$  2.71). The DQF-COSY spectrum was used to assign H-5' (at  $\delta$  3.49) from its correlation with H-4' and subsequently H-6' was determined from its coupling with H-5'. C-1', C-2' and C-3' were assigned using the gHMQC spectrum. C-5' and C-6' were assigned through their connections to H-4' (at  $\delta$  1.75) in the gHMBC spectrum.

In the 1D-<sup>1</sup>H spectrum, there were three overlapping methyl signals at  $\delta$  1.07 – 1.08. One of these had already been assigned to H<sub>3</sub>-19. The TOCSY and DQF-COSY spectra were now used to assign the spin group H-5/H-4/H<sub>3</sub>-17/H-3/H-2/H<sub>3</sub>-16. The remaining 2 methyl groups at  $\delta$  1.07 – 1.08 could now be assigned to H<sub>3</sub>-16 and H<sub>3</sub>-17. The carbon chemical shifts for C-2, C-3, C-4, C-16 and C-17 were found through their corresponding proton chemical shifts in the gHMQC spectrum.

The remaining spin group in the TOCSY spectrum ( $\delta$  3.98,  $\delta$  3.02, 1.87 and 1.21) was assigned to the cladinose sugar, H-5", H-4", OH-4" and H<sub>3</sub>-6" respectively. The OH-4" signal, a broad singlet, was missing in the DQF-COSY and gHMBC spectra. Now the gHMQC spectrum was used to assign C-4", C-5" and C-6". The chemical shift of C-3" was found through its connection to H-1" and H-2" in the gHMBC spectrum.

C-1 and C-9' were the most downfield signals in the 1D-<sup>13</sup>C spectrum. The assignment of C-1 to  $\delta$  178.57 was confirmed by the presence in the gHMBC spectrum of a crosspeak to a high frequency double doublet at  $\delta$  5.17, characteristic of H-13. The C-1 signal in the gHMBC spectrum was in fact folded back at about  $\delta$  35.8. This C-9' quaternary signal was assigned at  $\delta$  170.10 and showed couplings to H-2' and H<sub>3</sub>-10' in the gHMBC spectrum.

There was a quaternary signal in the 1D-<sup>13</sup>C spectrum that demonstrated couplings to  $\delta$  2.47 (H-7), 1.94 (H-4) and 1.42 (H<sub>3</sub>-18). This signal must be C-6. Therefore the remaining quaternary signal in the 1D-<sup>13</sup>C spectrum at  $\delta$  116.03 was assigned to C-9 showing connections to H<sub>3</sub>-19, H-8 and H-7 (at  $\delta$  1.46) in the gHMBC spectrum. In addition to these correlations, C-9 in the gHMBC spectrum also coupled to  $\delta$  2.97 and 1.31. The signal at  $\delta$  1.31 was an isolated doublet in the 1D-<sup>1</sup>H spectrum integrated to three protons. This was consistent with H<sub>3</sub>-20, the only remaining methyl group. The signal at  $\delta$  2.97, overlapping with H-2, was then assigned to H-10; this signal showed a correlation with H<sub>3</sub>-20 in the DQF-COSY spectrum. H-10 also coupled to  $\delta$  3.50, assigned to H-11. A signal that appeared only in the TOCSY spectrum at  $\delta$  2.02, overlapping with H-14 in the 1D-<sup>1</sup>H spectrum, coupled to H-10 and H-11, and was assigned to 11-OH. The completion of the assignments was carried out by assigning C-10 and C-11 through their appearance in the gHMQC spectrum. The full assignments are summarized in table 1.

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Positin	Multiplicity	<sup>1</sup> H (ppm)	J <sub>HH</sub> (Hz)	<sup>13</sup> C (ppm)	HMBC Connectivities $(^{13}C \rightarrow ^{1}H)$					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1	_	_	_	178.57	H(2), H(3), H <sub>3</sub> (16), H(13)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2	m	2.96 <sup>b</sup>	_	46.37	H <sub>3</sub> (16)					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	dd	4.31	6.6, 3.9	76.34	H(4), H(5), H <sub>3</sub> (16), H(1")					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	4	dq	1.94	13.2, 6.7	44.08	H(3), H(5), H <sub>3</sub> (17)					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	d	3.43	5.5	85.58	H(4), H(7), H <sub>3</sub> (17), H <sub>3</sub> (18), H(1')					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6	_	_	_	81.29	H(4), H(7), H <sub>3</sub> (18)					
brt 2.48 13.6 H3 (4) 8 obscured 2.28 - 41.28 H3(19), H2(7) 9 116.03 H(7), H(8), H(10), H3(19), H3(20) 10 m 2.97 <sup>b</sup> - 51.58 H3(20) 11 obscured 3.50 - 87.23 H(10), H3(20), H3(21) 11-OH obscured 2.04 12 82.58 H(13), H3(21) 13 dd 5.17 11.7, 2.9 81.36 H(14), H3(15), H3(21) 14 dddd 1.66 14.1, 7.3, 2.9 24.24 H3(15), H3(21) 15 t 0.83 7.4 10.95 H2(14) 16 d 1.07 6.6 14.75 H(2) 17 d 1.08 7.0 15.97 H(4), H(5) 18 s 1.42 - 28.56 H(5), H2(7) 19 d 1.07 6.6 12.24 H7(7), H3(8) 20 d 1.31 7.3 14.03 H(10), H1(1) 21 s 1.29 - 25.19 - 11 d 4.34 7.7 100.80 H(15), H2(7) 19 d 1.07 6.6 12.24 H7(7), H8) 20 d 1.31 7.3 14.03 H(10), H(11) 21 s 1.29 - 25.19 - 11 d 4.34 7.7 100.80 H3(5), H2(7) 2' dd 4.83 10.6, 7.6 71.14 H(3'), H(4') 3' ddd 2.71 4.3 63.46 H(2') H3(4'), H3(7')8') 4' obscured 1.33 - 30.64 H3(6') 5' m 3.49 <sup>a</sup> - 69.02 H(4'), H3(7')8') 4' obscured 1.33 - 30.64 H3(6') 5' m 3.49 <sup>a</sup> - 69.02 H(4'), H3(7')8') 4' obscured 1.33 - 30.64 H3(6') 5' m 3.49 <sup>a</sup> - 69.02 H(4'), H3(7')8') 4' obscured 1.53 15.2, 4.9 34.56 H3(7), H3(7')8') 4' obscured 1.53 4.4 95.42 H(3), H3(7')8') 9' 7 72.83 H(1"), H2(7')8') 9' 7 72.83 H(1"), H2(7'), H3(8") 4'' d 3.02 9.9 78.23 H(1"), H2(7'), H3(8") 4'' d 3.02 9.9 78.23 H(1"), H2(7'), H3(8") 4'' dd 3.02 9.9 78.23 H2(7'), H3(8") 4'' dd 3.02 9.9 78.	7	dd	1.46	12.6. 6.6	41.26	H₃(18)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		brt	2.48	13.6							
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	obscured	2.28	_	41.28	H <sub>3</sub> (19), H <sub>2</sub> (7)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	9	-	_	_	116.03	H(7), H(8), H(10), H <sub>3</sub> (19), H <sub>3</sub> (20)					
11         obscured         3.50         -         87.23         H(10), H_3(20), H_3(21)           11-OH         obscured         2.04         -         -         -           12         -         -         -         82.58         H(13), H_3(21)           13         dd         5.17         11.7, 2.9         81.36         H(14), H_3(15), H_3(21)           14         dddd         1.66         14.1, 7.3, 2.9         24.24         H_3(15), H(13)           m         2.04         -         -         -         -           15         t         0.83         7.4         10.95         H_2(14)           16         d         1.07         6.6         14.75         H(2)           17         d         1.08         7.0         15.97         H(4), H(5)           18         s         1.42         -         28.56         H(5), H_2(7)           19         d         1.07         6.6         12.24         H(7), H(8)           20         d         1.31         7.3         14.03         H(10), H(11)           21         s         1.29         -         25.19         -           14         obscured </td <td>10</td> <td>m</td> <td>2.97<sup>b</sup></td> <td>_</td> <td>51.58</td> <td>H<sub>3</sub>(20)</td>	10	m	2.97 <sup>b</sup>	_	51.58	H <sub>3</sub> (20)					
11-OH       obscured       2.04       -       -       -         12       -       -       82.58       H(13), H_3(21)         13       dd       5.17       11.7, 2.9       81.36       H(14), H_3(15), H_3(21)         14       dddd       1.66       14.1, 7.3, 2.9       24.24       H_3(15), H(13)         m       2.04       -       -       -         15       t       0.83       7.4       10.95       H_2(14)         16       d       1.07       6.6       14.75       H(2)         17       d       1.08       7.0       15.97       H(4), H(5)         18       s       1.42       -       28.56       H(7), H(8)         20       d       1.31       7.3       14.03       H(10), H(11)         21       s       1.29       -       25.19       -         1'       d       4.34       7.7       100.80       H(2), H_3(7)/8)         2'       dd       2.71       4.3       63.46       H(2) H_2(4), H_3(7)/8)         4'       obscured       1.33       -       30.64       H(3), H_3(6')         6'       d       1.24       6.0	11	obscured	3.50	_	87.23	H(10), H <sub>3</sub> (20), H <sub>3</sub> (21)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	11-OH	obscured	2.04	-	-	-					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12	_	_	_	82.58	H(13), H <sub>3</sub> (21)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	13	dd	5.17	11.7, 2.9	81.36	H(14), H <sub>3</sub> (15), H <sub>3</sub> (21)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14	dddd	1.66	14.1, 7.3, 2.9	24.24	H <sub>3</sub> (15), H(13)					
15       t       0.83       7.4       10.95       H2(14)         16       d       1.07       6.6       14.75       H(2)         17       d       1.08       7.0       15.97       H(4), H(5)         18       s       1.42       -       28.56       H(5), H2(7)         19       d       1.07       6.6       12.24       H(7), H(8)         20       d       1.31       7.3       14.03       H(10), H(11)         21       s       1.29       -       25.19       -         1'       d       4.34       7.7       100.80       H(5), H2(2)         2'       dd       4.83       10.6, 7.6       71.14       H(3'), H(4')         23.7, 12.4,       3'       ddd       2.71       4.3       63.46       H(2') H2(4'), H3(7'/8')         4'       obscured       1.33       -       30.64       H3(6')       14.4')         7'/8'       s       2.26       -       40.65       H(3'), H3(6')         6'       d       1.24       6.0       21.04       H(4')         7'/8'       s       2.26       -       40.65       H(3'), H3(10'),		m	2.04	_							
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	15	t	0.83	7.4	10.95	H <sub>2</sub> (14)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	16	d	1.07	6.6	14.75	H(2)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	17	d	1.08	7.0	15.97	H(4), H(5)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	18	S	1.42	_	28.56	H(5), H <sub>2</sub> (7)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	19	d	1.07	6.6	12.24	H(7), H(8)					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	d	1.31	7.3	14.03	H(10), H(11)					
1d4.341.7100.80 $H(3), H(2)$ 2'dd4.8310.6, 7.671.14 $H(3'), H(4')$ 23.7, 12.4,23.7, 12.4,1.33-30.64 $H(2') H_2(4'), H_3(7'/8')$ 4'obscured1.33-30.64 $H_3(6')$ brdd1.7513.2, 2.65'm3.49°-69.02 $H(4'), H_3(6')$ 6'd1.246.021.04 $H(4')$ 7'/8's2.26-40.65 $H(3'), H_3(7'/8')$ 9'170.10 $H(2'), H_3(10'),$ 10's2.10-21.64 $H(4')$ 1"d5.134.495.42 $H(3), H_2(2")$ 2"dd1.5315.2, 4.934.56 $H_3(7")$ obscured2.283"3"4"d3.029.978.23 $H(2"), H_3(7"), H_3(8")$ 4"-OHbrs1.875"dq3.989.3, 6.265.15 $H(1"), H(4"), H_3(6")$ 6"d1.21°-21.63 $H_3(17), H(2")$ 9"10'9.978.23 $H(1"), H(4"), H_3(6")$ 4"5"dq3.989.3, 6.265.15 $H(1"), H(4"), H_3(6")$ 6"d1.21°- </td <td>21 1'</td> <td>S</td> <td>1.29</td> <td>_ 7 7</td> <td>25.19</td> <td></td>	21 1'	S	1.29	_ 7 7	25.19						
2       dd       1.30       23.7, 12.4,       1.11       1.(0), 1(1')         3'       ddd       2.71       4.3       63.46       H(2') H <sub>2</sub> (4'), H <sub>3</sub> (7'/8')         4'       obscured       1.33       -       30.64       H(2') H <sub>2</sub> (4'), H <sub>3</sub> (6')         5'       m       3.49 <sup>a</sup> -       69.02       H(4'), H <sub>3</sub> (6')         6'       d       1.24       6.0       21.04       H(4')         7'/8'       s       2.26       -       40.65       H(3'), H <sub>3</sub> (7'/8')         9'       -       -       -       170.10       H(2'), H <sub>3</sub> (10'),         10'       s       2.10       -       21.64       H(4')         1"       d       5.13       4.4       95.42       H(3), H <sub>2</sub> (2")         2"       dd       1.53       15.2, 4.9       34.56       H <sub>3</sub> (7")         obscured       2.28       -       -       -       -         3"       -       -       72.83       H(1"), H(2"), H <sub>3</sub> (6")         4"       d       3.02       9.9       78.23       H(2"), H(5"), H <sub>3</sub> (6")         4"-OH       brs       1.87       -       -       -         5"	2'	u dd	4.34	10676	71 14	п(5), п(2) Н(3') Н(4')					
3'       ddd       2.71       4.3       63.46       H(2') H_2(4'), H_3(7'/8')         4'       obscured       1.33       -       30.64       H_3(6')         5'       m       3.49 <sup>a</sup> -       69.02       H(4'), H_3(6')         6'       d       1.24       6.0       21.04       H(4')         7'/8'       s       2.26       -       40.65       H(3'), H_3(7'/8')         9'       -       -       170.10       H(2'), H_3(10'),         10'       s       2.10       -       21.64       H(4')         1''       d       5.13       4.4       95.42       H(3), H_2(2'')         2''       dd       1.53       15.2, 4.9       34.56       H_3(7'')         obscured       2.28       -       -       -       -         3''       -       -       72.83       H(1''), H(2''), H_3(7''), H_3(8'')         4''       d       3.02       9.9       78.23       H(2''), H(4''), H_3(6'')         4''-OH       brs       1.87       -       -       -         5''       dq       3.98       9.3, 6.2       65.15       H(1''), H(4''), H_3(6'')         6''       <	-	44	1.00	23.7, 12.4,							
4'       obscured $1.33$ - $30.64$ $H_3(6')$ 5'       m $3.49^a$ - $69.02$ $H(4'), H_3(6')$ 6'       d $1.24$ $6.0$ $21.04$ $H(4')$ 7'/8'       s $2.26$ - $40.65$ $H(3'), H_3(7'/8')$ 9'       -       -       - $170.10$ $H(2'), H_3(10'),$ 10'       s $2.10$ - $21.64$ $H(4')$ 1"       d $5.13$ $4.4$ $95.42$ $H(3), H_2(2")$ 2"       dd $1.53$ $15.2, 4.9$ $34.56$ $H_3(7")$ obscured $2.28$ -       -       - $72.83$ $H(1"), H(2"), H_3(7"), H_3(8")$ 4"       d $3.02$ $9.9$ $78.23$ $H(2"), H_5", H_3(6")$ 4"-OH       brs $1.87$ -       -       -         5"       dq $3.98$ $9.3, 6.2$ $65.15$ $H(1"), H(4"), H_3(6")$ 6"       d $1.21^a$ $7.7$ $17.75$ $H(4")$ 7"       s $1.21^a$	3'	ddd	2.71	4.3	63.46	H(2') H <sub>2</sub> (4'), H <sub>3</sub> (7'/8')					
brdd $1.75$ $13.2, 2.6$ 5'm $3.49^a$ - $69.02$ $H(4'), H_3(6')$ 6'd $1.24$ $6.0$ $21.04$ $H(4')$ 7'/8's $2.26$ - $40.65$ $H(3'), H_3(7'/8')$ 9' $170.10$ $H(2'), H_3(10'),$ 10's $2.10$ - $21.64$ $H(4')$ 1"d $5.13$ $4.4$ $95.42$ $H(3), H_2(2")$ 2"dd $1.53$ $15.2, 4.9$ $34.56$ $H_3(7")$ obscured $2.28$ 3"72.83 $H(1"), H(2"), H_3(7"), H_3(8")$ 4"d $3.02$ $9.9$ $78.23$ $H(2"), H(5"), H_3(6")$ 4"-OHbrs $1.87$ 5"dq $3.98$ $9.3, 6.2$ $65.15$ $H(1"), H(4"), H_3(6")$ 6"d $1.21^a$ $7.7$ $17.75$ $H(4")$ 7"s $1.21$ - $21.63$ $H_3(17), H(2")$	4'	obscured	1.33	_	30.64	H <sub>3</sub> (6')					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		brdd	1.75	13.2, 2.6							
6       d       1.24       6.0       21.04       H(4)         7'/8'       s       2.26       -       40.65       H(3'), H_3(7'/8')         9'       -       -       -       170.10       H(2'), H_3(10'),         10'       s       2.10       -       21.64       H(4')         1"       d       5.13       4.4       95.42       H(3), H_2(2")         2"       dd       1.53       15.2, 4.9       34.56       H_3(7")         obscured       2.28       -       -       -       72.83       H(1"), H(2"), H_3(7"), H_3(8")         4"       d       3.02       9.9       78.23       H(2"), H(5"), H_3(6")         4"-OH       brs       1.87       -       -       -         5"       dq       3.98       9.3, 6.2       65.15       H(1"), H(4"), H_3(6")         6"       d       1.21 <sup>a</sup> 7.7       17.75       H(4")         7"       s       1.21       -       21.63       H_3(17), H(2")	5'	m	3.49°	_	69.02	$H(4'), H_3(6')$					
$7/8'$ s $2.26$ $ 40.65$ $H(3'), H_3(7/8')$ 9' $  170.10$ $H(2'), H_3(10'),$ 10'       s $2.10$ $ 21.64$ $H(4')$ 1"       d $5.13$ $4.4$ $95.42$ $H(3), H_2(2")$ 2"       dd $1.53$ $15.2, 4.9$ $34.56$ $H_3(7")$ $obscured$ $2.28$ $   72.83$ $H(1"), H(2"), H_3(7"), H_3(8")$ 4"       d $3.02$ $9.9$ $78.23$ $H(2"), H(5"), H_3(6")$ 4"-OH       brs $1.87$ $  -$ 5"       dq $3.98$ $9.3, 6.2$ $65.15$ $H(1"), H(4"), H_3(6")$ 6"       d $1.21^a$ $7.7$ $17.75$ $H(4")$ 7"       s $1.21$ $ 21.63$ $H_3(17), H(2")$	5	a	1.24	6.0	21.04	H(4)					
9'       -       -       -       170.10 $H(2'), H_3(10'),$ 10'       s       2.10       -       21.64 $H(4')$ 1"       d       5.13       4.4       95.42 $H(3), H_2(2")$ 2"       dd       1.53       15.2, 4.9       34.56 $H_3(7")$ obscured       2.28       -       -       -         3"       -       -       72.83 $H(1"), H(2"), H_3(7"), H_3(8")$ 4"       d       3.02       9.9       78.23 $H(2"), H(5"), H_3(6")$ 4"-OH       brs       1.87       -       -       -         5"       dq       3.98       9.3, 6.2       65.15 $H(1"), H(4"), H_3(6")$ 6"       d       1.21 <sup>a</sup> 7.7       17.75 $H(4")$ 7"       s       1.21       -       21.63 $H_3(17), H(2")$	778	S	2.26	_	40.65	$H(3^{\circ}), H_{3}(7^{\circ})$					
10'       s       2.10       -       21.64       H(4')         1"       d       5.13       4.4       95.42       H(3), H_2(2")         2"       dd       1.53       15.2, 4.9       34.56       H_3(7")         obscured       2.28       -       -       -         3"       -       -       72.83       H(1"), H(2"), H_3(7"), H_3(8")         4"       d       3.02       9.9       78.23       H(2"), H(5"), H_3(6")         4"-OH       brs       1.87       -       -       -         5"       dq       3.98       9.3, 6.2       65.15       H(1"), H(4"), H_3(6")         6"       d       1.21 <sup>a</sup> 7.7       17.75       H(4")         7"       s       1.21       -       21.63       H_3(17), H(2")	9'	-	-	—	170.10	$H(2'), H_3(10'),$					
1"       d $5.13$ $4.4$ $95.42$ $H(3), H_2(2")$ 2"       dd $1.53$ $15.2, 4.9$ $34.56$ $H_3(7")$ obscured $2.28$ $  31"$ $ -$ 3" $  72.83$ $H(1"), H(2"), H_3(7"), H_3(8")$ $4"$ $d$ $3.02$ $9.9$ $78.23$ $H(2"), H(5"), H_3(6")$ 4"-OH       brs $1.87$ $  -$ 5"       dq $3.98$ $9.3, 6.2$ $65.15$ $H(1"), H(4"), H_3(6")$ 6"       d $1.21^a$ $7.7$ $17.75$ $H(4")$ 7"       s $1.21$ $ 21.63$ $H_3(17), H(2")$	10'	S	2.10	_	21.64	H(4')					
2"       dd       1.53       15.2, 4.9       34.56 $H_3(7")$ obscured       2.28       -       -       -       -         3"       -       -       72.83       H(1"), H(2"), H_3(7"), H_3(8")         4"       d       3.02       9.9       78.23       H(2"), H(5"), H_3(6")         4"-OH       brs       1.87       -       -       -         5"       dq       3.98       9.3, 6.2       65.15       H(1"), H(4"), H_3(6")         6"       d       1.21 <sup>a</sup> 7.7       17.75       H(4")         7"       s       1.21       -       21.63       H_3(17), H(2")	1"	d	5.13	4.4	95.42	H(3), H <sub>2</sub> (2")					
3"       -       -       72.83       H(1"), H(2"), H_3(7"), H_3(8")         4"       d       3.02       9.9       78.23       H(2"), H(5"), H_3(6")         4"-OH       brs       1.87       -       -       -         5"       dq       3.98       9.3, 6.2       65.15       H(1"), H(4"), H_3(6")         6"       d       1.21 <sup>a</sup> 7.7       17.75       H(4")         7"       s       1.21       -       21.63       H_3(17), H(2")	2"	dd	1.53	15.2, 4.9	34.56	H <sub>3</sub> (7")					
$3"$ -       -       -       72.83       H(1"), H(2"), H_3(7"), H_3(8")         4"       d       3.02       9.9       78.23       H(2"), H(5"), H_3(6")         4"-OH       brs       1.87       -       -       -         5"       dq       3.98       9.3, 6.2       65.15       H(1"), H(4"), H_3(6")         6"       d       1.21 <sup>a</sup> 7.7       17.75       H(4")         7"       s       1.21       -       21.63       H_3(17), H(2")	0.1	obscured	2.28	_	70.00						
4"       d $3.02$ $9.9$ $78.23$ $H(2"), H(5"), H_3(6")$ 4"-OH       brs $1.87$ -       -       -         5"       dq $3.98$ $9.3, 6.2$ $65.15$ $H(1"), H(4"), H_3(6")$ 6"       d $1.21^a$ $7.7$ $17.75$ $H(4")$ 7"       s $1.21$ - $21.63$ $H_3(17), H(2")$	3"	-	-	-	72.83	$H(1^{\circ}), H(2^{\circ}), H_3(7^{\circ}), H_3(8^{\circ})$					
4"-OH       brs $1.87$ -       -       -       -         5"       dq $3.98$ $9.3, 6.2$ $65.15$ $H(1"), H(4"), H_3(6")$ 6"       d $1.21^a$ $7.7$ $17.75$ $H(4")$ 7"       s $1.21$ $ 21.63$ $H_3(17), H(2")$ 8"       c $3.28$ $40.22$ $40.22$	4"	d	3.02	9.9	78.23	H(2"), H(5"), H <sub>3</sub> (6")					
5"dq $3.98$ $9.3, 6.2$ $65.15$ $H(1"), H(4"), H_3(6")$ 6"d $1.21^a$ $7.7$ $17.75$ $H(4")$ 7"s $1.21$ - $21.63$ $H_3(17), H(2")$ 8"c $3.28$ 40.22	4"-OH	brs	1.87	-	-	-					
6"d $1.21^{a}$ $7.7$ $17.75$ $H(4")$ 7"s $1.21$ - $21.63$ $H_3(17), H(2")$ 8"c $2.28$ 40.22	5"	dq	3.98	9.3, 6.2	65.15	H(1"), H(4"), H <sub>3</sub> (6")					
$I''' = S = 1.21 - 21.63 H_3(17), H(2'')$	6"	d	1.21 <sup>ª</sup>	7.7	17.75	H(4")					
	/" 8"	S	1.21 3.28	-	21.63 40.33	H <sub>3</sub> (17), H(2")					

Table 2. The full <sup>1</sup>H and <sup>13</sup>C NMR assignments of anhydroerythromycin A 2'-acetate in CDCl<sub>3</sub>.

a: partially obscured



**Figure 2.** A contour plot of the 500 MHz DQF-COSY spectrum of anhydroerythromycin A 2'-acetate (4) in CDCl<sub>3</sub>.



Figure 3. A contour plot of the 500 MHz TOCSY spectrum of anhydroerythromycin A 2'-acetate (4) in CDCl<sub>3</sub>.



Figure 4. A contour plot of the 500 MHz gHMQC spectrum of anhydroerythromycin A 2'-acetate (4) in CDCl<sub>3</sub>.



Figure 5. A contour plot of the 500 MHz GHMBC spectrum of anhydroerythromycin A 2'-acetate (4) in CDCl<sub>3</sub>.