

CHEMBIOCHEM

Supporting Information

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Supporting Information

for

Elucidation of Oxygenation Steps during Oviedomycin Biosynthesis and
Generation of Derivatives with Increased Antitumor Activity

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NMR data of new Oviedomycin derivatives

Table S1. ^1H (400 MHz) and ^{13}C NMR (100 MHz) spectral data of prejadomycin-2-carboxylate (**2**), 4a, 12b-dehydro-UWM6 (**5**), in $[\text{D}_6]\text{DMSO}$ (chemical shifts in ppm; multiplicity in parentheses and coupling constants in Hz).

Position	2			5		
	d_{H} (ppm)	d_{C} (ppm)	HMBC	d_{H} (ppm)	d_{C} (ppm)	HMBC
1	-	156.8		-	207.8	
1-OH	14.75 ^[a] , 1H, s (br)	-		-	-	
2	-	131.3		2.42, 1.88, 2H, d, 13.8	52.9	4a, 12b
2-COOH	9.85 ^[a] , 1H, s (br)	175.2		-	-	
3	-	164.4		-	75.8	
4	2.62, 2.59, 2H, dd, 14.8	40.6	2, 12b	2.66, 1.98, 2H, dd, 14.7	42.3	3, 13
4a	-	71.6		-	142.8	
4-OH	3.96 ^[a] , 1H, s	-		-	-	
5	2.94, 2.35, 2H, dd, 17.4	43.8	4a, 6a, 12b	3.08, 2.83, 2H, dd, 16.7	51.3	6a, 12b
6	-	202.7		-	202.5	
6a	-	111.1		-	111.9	
7	-	166.9		-	165.9	
7a	-	118.2		-	116.6	
7-OH	15.54 ^[a] , 1H, s (br)	-		15.62, 1H, s (br)	-	
8	-	157.2		-	157.3	
8-OH	9.42 ^[a] , 1H, s	-		9.88, 1H, s	-	
9	6.88, 1H, d, 8.2	108.9	7a, 8 11	6.87, 1H, d, 8.9	109.0	7a, 11
10	7.56, 1H, t, 8.2	132.7	8, 9, 11a	7.52, 1H, t, 8.9	133.8	8, 11a
11	7.25, 1H, d, 8.2	112.6	7a, 9, 10	7.25, 1H, d, 8.9	113.4	7a, 9, 12
11a	-	138.7		-	139.9	
12	6.85, 1H, s	119.5	6a, 11a	6.76, 1H, s	118.2	6a, 7a
12a	-	135.25		-	135.2	
12b	-	101.2		-	137.6	
13-CH ₃	1.96, 3H, s	21.6	2, 3	1.11, 3H, s	29.8	2, 3, 4

[a] Exchangeable with D_2O .

Table S2: ^1H (400 MHz) and ^{13}C NMR (100 MHz) of 5-hydroxy-dehydrorabelomycin (**8**) and 9-hydroxy-rabelomycin (**9**) in $[\text{D}_6]\text{DMSO}$ (chemical shifts in ppm; multiplicity in parentheses and coupling constants in Hz).

Position	8		9	
	d_{H} (ppm)	d_{C} (ppm)	d_{H} (ppm)	d_{C} (ppm)
1	-	158.5	-	196.0
2	6.82, d, 1.9, 1H	117.5	2.94, d, 13.1, 1H; 2.67, d, 13.1, 1H	53.3
3	-	139.3	-	71.1
4	7.54, 1H, d, 1.9	113.1	3.11, d, 15.3, 1H; 2.98, d, 15.3, 1H	43.6
4 ^a	-	129.9	-	150.0
5	-	151.2	7.07, s, 1H	121.2
6	-	154.9	-	162.2
6-OH	11.60, brs, 1H	-	11.99, brs, 1H	-
6 ^a	-	110.5	-	116.8
7	-	192.9	-	191.8
7 ^a	-	115.2	-	115.7
8	-	160.5	-	151.9
8-OH	12.56, brs, 1H	-	11.95, brs, 1H	-
9	7.30, d, 7.5, 1H	122.7	-	152.21
10	7.78, t, 7.5, 1H	137.7	7.20, d, 8.0, 1H	120.7
11	7.69, d, 7.5, 1H	119.5	7.40, d, 8.0, 1H	120.0
11 ^a	-	136.5	-	125.5
12	-	187.6	-	181.6
12 ^a	-	137.3	-	137.9
12b	-	118.0	-	128.9
3-CH ₃	2.39, s, 3H	21.2	1.28, s, 3H	29.6