**Dendronpholides A-R, cembranoid diterpenes from the Chinese soft coral
Dendronephthya sp.**

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Table 1 ^1H , ^{13}C NMR, HMBC, and NOESY of 2

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.46 m	31.9 CH	C-2, C-14, C-15	H-5, H-20
2	1.08 ddd (3.5,11.0,11.0) 1.71 m	28.1 CH ₂	C-1, C-14, C-3, C-5	
3	1.80 m 1.90 m	32.1 CH ₂		
4		86.4 C		
5	5.25 d (11.5)	71.3 CH	C=O, C-4, C-18, C-C-3, C-6	H-1, H-9
6	1.38 dd (13.5,13.5) 1.50 m	27.9 CH ₂		
7	1.78 m 1.90 m	34.1 CH ₂		
8		133.8 C		
9	5.28 dd (7.5,7.5)	125.2 CH	C-7, C-10, C-11, C-19	H-11, H-5
10	2.60 dd (6.5,8.0)	25.9 CH ₂	C-8, C-9, C-11, C-12	
11	5.53 dd (8.5,8.5)	126.3 CH	C-9, C-10, C-13, C-20	H-13
12		134.7 C		
13	3.94 dd (6.0, 12.0)	75.5 CH	C-12, C-1, C-20	H-11, H-17a (5.55)
14	1.54 m 1.80 m	38.5 CH ₂		
15		145.5 C		
16		169.0 C		
17	5.55 brs 5.97 brs	124.6 CH ₂	C-1, C-15, C-16	
18	1.19 s	24.9 CH ₃	C-3, C-4, C-5	
19	1.67 s	16.8 CH ₃	C-7, C-8, C-9	
20	1.56 s	10.0 CH ₃	C-11, C-12, C-13	H-1, H-10
	2.04 s	21.4 CH ₃ 170.9 C	C=O	

Table 2 ^1H , ^{13}C NMR, HMBC, and NOESY of 3

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.23 ddd (8.0,8.0,10.0)	32.0 CH	C-2, C-14, C-15	H-5, H-20
2	1.10 m 1.80 m	29.4 CH ₂	C-1, C-14, C-3, C-5	
3	1.78 m 2.00 m	32.6 CH ₂		
4		86.4 C		
5	5.34 d (9.0)	71.8 CH	C=O, C-4, C-18, C-C-3, C-6	H-1, H-9
6	1.50 m	27.3 CH ₂		
7	1.75 m 2.00 m	34.7 CH ₂		
8		130.1 C		
9	5.48 m	127.6 CH	C-7, C-10, C-11, C-19	H-11, H-5
10	2.41 brd (14.5) 3.17 ddd (11.0,11.5,14.5)	26.8 CH ₂	C-8, C-9, C-11, C-12	
11	5.07 brd (10.0)	127.8 CH	C-9, C-10, C-13, C-20	H-13
12		135.7 C		
13	4.46 d (11.5)	64.5 CH	C-12, C-1, C-20	H-10 (3.17), H-20
14	1.60 m 1.80 m	39.5 CH ₂		
15		146.2 C		
16		168.6 C		
17	5.47 brs 5.94 brs	123.9 CH ₂	C-1, C-15, C-16	
18	1.20 s	23.9 CH ₃	C-3, C-4, C-5	
19	1.65 s	16.2 CH ₃	C-7, C-8, C-9	
20	1.53 s	17.5 CH ₃	C-11, C-12, C-13	H-13, H-1
	2.05 s	21.2 CH ₃ 170.3 C	C=O	

Table 3 ^1H , ^{13}C NMR, HMBC, and NOESY of 4

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.18 ddd (7.0,7.5,12.5)	38.1 CH	C-2, C-14, C-15	H-20, H-14a
2	1.28 m 1.28 m	26.2 CH ₂	C-1, C-14, C-3, C-5	
3	0.90 ddd (6.0,6.0,12.0) 1.20 m	38.1 CH ₂	C-4, C-5, C-1	
4		74.6 C		
5	3.16 d (10.0)	70.1 CH	C=O, C-4, C-18, C-C-3, C-6	H-7a (2.08), H-9
6	1.22 m 1.50 m	28.9 CH ₂		
7	1.97 brd (12.5) 2.09 dd (12.5,12.5)	34.9 CH ₂	C-5, C-6, C-8, C-9, C-19	
8		135.4 C		
9	5.25 (dd, 7.5,7.5)	124.0 CH ₂	C-7, C-10, C-11, C-19	H-7a, H-5, H-10a (2.40)
10	2.40 ddd (7.0,7.5,12.0) 2.94 ddd (7.5,10.0,12.0)	26.6 CH ₂	C-8, C-9, C-11, C-12	H-9, H-11
11	5.17 brd (10.0)	126.6 CH	C-9, C-10, C-13, C-20	H-10a, H-13
12		133.3 C		
13	3.95 dd (7.0,10.0)	75.4 CH	C-14, C-11, C-20	H-11, H-20, H-14a (1.50)
14	1.45 m 1.50 m	41.4 CH ₂		
15		144.3 C		
16		167.5 C		
17	5.57 brs 6.12 brs	124.9 CH ₂	C-1, C-15, C-16	H-14b (1.40)
18	0.98 s	24.4 CH ₃	C-3, C-4, C-5	
19	1.54 s	16.1 CH ₃	C-7, C-8, C-9	H-10b (2.94)
20	1.60 s	10.0 CH ₃	C-11, C-12, C-13	H-13, H-1, H-10b
MeO	3.67 s	52.1 CH ₃	C=O	

Table 4 ^1H , ^{13}C NMR, HMBC, and NOESY of 5

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.16 m	39.4 CH	C-2, C-14, C-15	H-20, H-14a
2	1.26 m 1.29 m	26.4 CH ₂	C-1, C-14, C-3, C-5	
3	1.40 m 1.70 m	39.2 CH ₂	C-4, C-5, C-1	
4		72.7 C		
5	4.92 d (11.0)	74.8 CH	C=O, C-4, C-18, C-C-3, C-6	H-7a (2.08), H-9
6	1.20 m 1.48 m	29.2 CH ₂		
7	1.92 dd (5.5,13.0) 1.92 dd (5.5,13.0)	33.3 CH ₂	C-5, C-6, C-8, C-9, C-19	
8		134.9 C		
9	5.43 dd (6.0,6.0)	122.6 CH	C-7, C-10, C-11, C-19	H-7a, H-5, H-10a (2.40)
10	2.50 ddd (6.0,7.5,12.0) 2.70 ddd (6.0,8.0,12.0)	26.2 CH ₂	C-8, C-9, C-11, C-12	H-9, H-11
11	5.37 dd (7.5,8.0)	123.9 CH	C-9, C-10, C-13, C-20	H-10a, H-13
12		138.8 C		
13	3.69 dd (6.5,10.0)	73.9 CH	C-14, C-11, C-20	H-11, H-20, H-14a (1.50)
14	1.69 m 1.69 m	38.1 CH ₂		
15		140.5 C		
16		167.7 C		
17	5.30 brs 6.27 brs	124.1 CH ₂	C-1, C-15, C-16	H-14b (1.40)
18	0.95 s	23.7 CH ₃	C-3, C-4, C-5	
19	1.65 s	17.9 CH ₃	C-7, C-8, C-9	H-10b (2.94)
20	1.57 s	10.7 CH ₃	C-11, C-12, C-13	H-13, H-1, H-10b
AcO	2.00 s	21.6 CH ₃ 170.9 C	C=O	
MeO	3.69 s	52.3 CH ₃		

Table 5 ^1H , ^{13}C NMR, HMBC, and NOESY of 6

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.23 ddd (4.0,10.5,10.5)	38.5 CH	C-2, C-14, C-15	H-20, H-14a
2	1.18 m 1.20 m	25.3 CH ₂		
3	1.10 ddd (2.0,2.0,12.0) 1.40 ddd (3.5,11.5,12.0)	39.5 CH ₂	C-4, C-5, C-1	
4		78.8 C		
5		214.2 C		
6	2.40 brdd (3.0,14.0) 3.20 ddd (2.0,11.0,14.0)	33.1 CH ₂	C-7, C-8, C-4	
7	2.00 dd (3.0, 15.0) 2.33 ddd (2.0, 11.0,15.0)	31.7 CH ₂	C-5, C-6, C-8, C-9, C-19	
8		133.4 C		
9	5.03 m	122.7 CH	C-7, C-10, C-11, C-19	H-7a, H-5, H-10a (2.46)
10	2.46 m 2.71 ddd (7.5,7.5,13.5)	26.5 CH ₂	C-8, C-9, C-11, C-12	H-9, H-11
11	5.02 m	125.0 CH	C-9, C-10, C-13, C-20	H-10a, H-13
12		135.3 C		
13	3.79 dd (4.5, 10.0)	74.4 CH	C-14, C-11, C-20	H-11, H-20
14	1.50 m 1.60 m	40.0 CH ₂		
15		143.5 C		
16		167.2 C		
17	5.49 brs 6.17 brs	125.2 CH ₂	C-1, C-15, C-16	
18	1.03 s	24.5 CH ₃	C-3, C-4, C-5	
19	1.56 s	16.4 CH ₂	C-7, C-8, C-9	H-10b (2.71)
20	1.52 s	10.7 CH ₃	C-11, C-12, C-13	H-13, H-1, H-10b
EtO	4.15 q (7.0) 1.23 t (7.0)	60.8 CH ₂ 14.5 CH ₃	C=O, Me	

Table 6 ^1H , ^{13}C NMR, HMBC, and NOESY of 7

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.67 m	38.2 CH	C-2, C-14, C-14, C-15	H-14a (1.77)
2	1.55 m 1.71 m	26.8 CH ₂		
3	1.36 dd (12.0,12.0) 1.62 m	36.43 CH ₂	C-4, C-5, C-1	
4		72.8 C		
5	3.87 dd (5.5,10.0)	88.3 CH	C-3, C-4, C-18	H-19
6	1.56 m 1.80 m	27.8 CH ₂		
7	1.56 m 1.76 dd (5.5,12.0,13.5)	35.9 CH ₂	C-5, C-8, C-9, C-19	
8		83.3 C		
9	4.87 d (11.0)	76.1 CH	C=O, C-8, C-7, C-19, C-10	H-11a (0.72)
10	1.60 m 1.90 dd (10.5, 13.0)	24.5 CH ₂		
11	0.72 dd (10.5,13.5) 1.98 dd (8.5, 13.5)	34.9 CH ₂	C-13, C-12, C-9, C-20	
12		61.3 C		
13	2.83 dd (2.5,10.0)	59.0 CH	C-14, C-1, C-12, C-20	
14	1.50 m 1.77 m	32.2 CH ₂		
15		146.0 C		
16		169.0 C		
17	5.60 brs 6.15 brs	124.0 CH ₂	C-1, C-15, C-16	
18	0.95 s	25.4 CH ₃	C-3, C-4, C-5	H-6b (1.80)
19	1.14 s	21.2 CH ₃	C-7, C-8, C-9	H-5
20	1.30 s	17.7 CH ₃	C-11, C-12, C-13	
AcO	2.04 s	21.3 CH ₃ 171.8 C	C=O	

Table 7 ^1H , ^{13}C NMR, HMBC, and NOESY of 8

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.68 m	39.2 CH	C-2, C-14, C-14, C-15	H-14a (1.77)
2	1.67 m 1.74 m	27.4 CH ₂		
3	1.36 dd (11.0,11.0) 1.57 m	37.0 CH ₂	C-4, C-5, C-1	
4		73.6 C		
5	3.88 dd (6.0,10.5)	89.1 CH	C-3, C-4, C-18	H-19
6	1.65 m 1.80 m	28.6 CH ₂		
7	1.60 m 1.75 m	36.7 CH ₂	C-5, C-8, C-9, C-19	
8		84.1 C		
9	4.86 d (11.0)	76.8 CH	C=O, C-8, C-7, C-19, C-10	H-11a (0.72)
10	1.62 m 1.90 dd (9.0,14.0)	25.3 CH ₂		
11	0.73 dd (11.0,13.5) 1.99 dd (9.0,13.5)	35.6 CH ₂	C-13, C-12, C-9, C-20	
12		62.1 C		
13	2.83 dd (3.5,10.0)	59.6 CH	C-14, C-1, C-12, C-20	
14	1.52 m 1.73 m	33.2 CH ₂		
15		144.6 C		
16		168.4 C		
17	5.77 brs 6.25 brs	125.4 CH ₂	C-1, C-15, C-16	
18	0.95 s	26.2 CH ₃	C-3, C-4, C-5	H-6b (1.80)
19	1.15 s	22.1 CH ₃	C-7, C-8, C-9	H-5
20	1.31 s	18.3 CH ₃	C-11, C-12, C-13	
AcO	2.05 s	21.9 CH ₃ 172.7 C	C=O	
MeO	3.70 s	53.2 CH ₃	C=O (C-16)	

Table 8 ^1H , ^{13}C NMR, HMBC, and NOESY of 9

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.85 m	37.8 CH	C-2, C-14, C-14, C-15	H-14a (1.92)
2	1.65 m 1.77 m	26.7 CH ₂		
3	1.63 m 1.65 m	36.0 CH ₂	C-4, C-5, C-1	
4		73.8 C		
5	4.02 dd (6.0,11.0)	87.9 CH	C-3, C-4, C-18	H-19
6	1.68 m 1.77 m	27.4 CH ₂		
7	1.70 m 1.92 m	36.3 CH ₂	C-5, C-8, C-9, C-19	
8		83.8 C		
9	5.04 d (10.5)	75.9 CH	C=O, C-8, C-7, C-19, C-10	H-11a (0.90)
10	1.72 m 1.85 m	24.5 CH ₂		
11	0.90 dd (11.0,14.0) 2.08 m	34.9 CH ₂	C-13, C-12, C-9, C-20	
12		61.3 C		
13	3.03 dd (2.5,10.0)	59.8 CH	C-14, C-1, C-12, C-20	
14	1.62 m 1.92 m	32.4 CH ₂		
15		143.2 C		
16		167.3 C		
17	5.82 brs 6.43 brs	124.2 CH ₂	C-1, C-15, C-16	
18	1.10 s	25.4 CH ₃	C-3, C-4, C-5	H-6b (1.77)
19	1.24 s	21.1 CH ₃	C-7, C-8, C-9	H-5
20	1.38 s	17.3 CH ₃	C-11, C-12, C-13	
AcO	2.08 s	20.9 CH ₃ 171.4 C	C=O	
EtO	1.32 t (7.0) 4.24 q (7.0)	14.2 CH ₃ 60.9 CH ₂	C=O (C-16)	

Table 9 ^1H , ^{13}C NMR, HMBC, and NOESY of 10

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.65 m	36.1 CH	C-2, C-14, C-14, C-15	H-14a (1.60)
2	1.55 m 1.55 m	30.9 CH ₂		
3	1.30 dd (5.5,11.0) 2.10 ddd (2.0,11.0,11.0)	34.5 CH ₂	C-4, C-5, C-1	
4		72.8 C		
5	3.78 dd (5.0,11.5)	87.5 CH	C-3, C-4, C-18	H-18, H-19
6	1.55 m 1.70 m	29.4 CH ₂		
7	1.52 m 1.80 m	35.8 CH ₃	C-5, C-8, C-9, C-19	
8		83.5 C		
9	4.81 dd (4.0,9.5)	77.5 CH	C=O, C-8, C-7, C-19, C-10	H-13
10	1.52 m 1.80 m	23.1 CH ₂		
11	1.40 m 1.50 m	35.5 CH ₂	C-13, C-12, C-9, C-20	
12		71.8 C		
13	4.37 d (11.0)	78.0 CH	C-14, C-1, C-12, C-20	H-9, H-2b (1.55)
14	1.60 dd (11.0,14.5) 1.98 brd (14.5)	24.9 CH ₂		
15		141.0 C		
16		166.4 C		
17	5.72 brs 6.22 brs	128.3 CH ₂	C-1, C-15, C-16	H-2b
18	1.05 s	25.2 CH ₃	C-3, C-4, C-5	H-2b
19	1.09 s	23.6 CH ₃	C-7, C-8, C-9	
20	1.12 s	24.1 CH ₃	C-11, C-12, C-13	H-14a
AcO	2.05 s	21.5 CH ₃ 171.2 C	C=O	

Table 10 ^1H , ^{13}C NMR, HMBC, and NOESY of 11

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.60 m	36.0 CH	C-2, C-14, C-14, C-15	H-14a (1.80)
2	1.36 m 1.88 m	29.3 CH ₂		
3	1.19 m 1.46 m	32.2 CH ₂	C-4, C-5, C-1	
4		72.4 C		
5	3.85 dd (4.5,11.0)	88.5 CH	C-3, C-4, C-18	H-18, H-19
6	1.55 m 1.80 m	28.0 CH ₂		
7	1.69 m 2.21 dd (7.5,12.0)	36.2 CH ₂	C-5, C-8, C-9, C-19	
8		82.4 C		
9	4.14 d (11.5)	77.1 CH	C=O, C-8, C-7, C-19, C-10	H-13
10	1.63 m 2.30 brd (14.5)	24.1 CH ₂		
11	1.42 m 1.74 m	36.9 CH ₂	C-13, C-12, C-9, C-20	
12		73.0 C		
13	4.58 brd (10.5)	80.1 CH	C-14, C-1, C-12, C-20	H-9, H-2b (1.36)
14	1.80 m 1.98 brd (14.5)	23.0 CH ₂		
15		140.4 C		
16		166.3 C		
17	5.83 brs 6.37 brs	131.1 CH ₂	C-1, C-15, C-16	H-2b
18	0.92 s	27.9 CH ₃	C-3, C-4, C-5	H-2b
19	1.16 s	21.2 CH ₃	C-7, C-8, C-9	
20	1.04 s	25.6 CH ₃	C-11, C-12, C-13	H-14a
AcO	2.04 s	21.6 CH ₃ 170.9 C	C=O	

Table 11 ^1H , ^{13}C NMR, HMBC, and NOESY of 12

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.68 m	35.9 CH	C-2, C-14, C-14, C-15	H-14a (1.52)
2	1.50 m 1.55 m	30.0 CH ₂		
3	1.25 dd (5.5,12.5) 2.00 dd (11.0,12.5)	34.4 CH ₂	C-4, C-5, C-1	
4		72.4 C		
5	3.77 dd (5.0, 11.5)	87.5 CH	C-3, C-4, C-18	H-18, H-19
6	1.56 m 1.58 m	29.2 CH ₂		
7	1.52 m 1.79 m	35.6 CH ₂	C-5, C-8, C-9, C-19	
8		83.4 C		
9	4.78 brd (10.0)	77.1 CH	C=O, C-8, C-7, C-19, C-10	H-13
10	1.55 m 1.70 m	22.3 CH ₂		
11	1.50 m	30.0 CH ₂	C-13, C-12, C-9, C-20	
12		77.0 C		
13	4.55 d (12.0)	77.2 CH	C-14, C-1, C-12, C-20	H-9, H-2b (1.55)
14	1.52 m 1.99 brd (14.5)	24.5 CH ₂		
15		140.9 C		
16		165.3 C		
17	5.68 brs 6.18 brs	127.3 CH ₂	C-1, C-15, C-16	H-2b
18	1.05 s	25.0 CH ₃	C-3, C-4, C-5	H-2b
19	1.10 s	22.5 CH ₃	C-7, C-8, C-9	
20	1.10 s	17.3 CH ₃	C-11, C-12, C-13	H-14a
AcO	2.04 s	21.3 CH ₃ 170.9 C	C=O	
MeO	3.09 s	49.3 CH ₃		

Table 12 ^1H , ^{13}C NMR, HMBC, and NOESY of 13

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	3.10 m	33.8 CH	C-2, C-14, C-14, C-15	H-14a (1.60)
2	1.62 m 1.98 m	31.8 CH ₂		
3	0.84 m 1.34 m	25.3 CH ₂	C-4, C-5, C-1	
4		71.8 C		
5	3.82 dd (5.0,10.5)	89.1 CH	C-3, C-4, C-18	H-18, H-7b (1.77)
6	1.50 m 1.71 m	26.7 CH ₂		
7	1.60 m 1.76 m	36.4 CH ₂	C-5, C-8, C-9, C-19	
8		82.9 C		
9	4.73 d (10.5)	77.9 CH	C=O, C-8, C-7, C-19, C-10	H-7b (1.77)
10	1.50 m 1.93 m	22.1 CH ₂		
11	1.59 m 1.61 m	38.0 CH ₂	C-13, C-12, C-9, C-20	
12		74.2 C		
13	4.38 d (12.0)	68.3 CH	C-14, C-1, C-12, C-20	H-14a (1.60)
14	1.45 m 1.95 m	21.9 CH ₂		
15		144.5 C		
16		167.7 C		
17	5.43 brs 6.11 brs	123.6 CH ₂	C-1, C-15, C-16	
18	0.81 s	23.9 CH ₃	C-3, C-4, C-5	H-5,
19	1.15 s	21.3 CH ₃	C-7, C-8, C-9	
20	1.23 s	26.7 CH ₃	C-11, C-12, C-13	
AcO	2.05 s	21.3 CH ₃ 171.3 C	C=O	
EtO	1.31 t (7.0) 4.18 q (7.0)	14.6 CH ₃ 60.9 CH ₂		

Table 13 ^1H , ^{13}C NMR, HMBC, and NOESY of 14

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	3.15 m	33.8 CH	C-2, C-14, C-14, C-15	H-14a (1.60)
2	1.33 m 1.70 m	31.8 CH ₂		
3	0.86 m 1.35 m	25.3 CH ₂	C-4, C-5, C-1	
4		71.8 C		
5	3.81 dd (6.5,11.0)	89.0 CH	C-3, C-4, C-18	H-18, H-7b (1.77)
6	1.48 m 1.70 m	26.2 CH ₂		
7	1.60 m 1.77 m	36.4 CH ₂	C-5, C-8, C-9, C-19	
8		82.9 C		
9	4.74 d (10.5)	77.9 CH	C=O (171.3), C-8, C-7, C-19, C-10	H-7b (1.77)
10	1.48 m 1.95 m	22.0 CH ₂		
11	1.48 m 1.72 m	38.0 CH ₂	C-13, C-12, C-9, C-20	
12		74.2 C		
13	4.38 d (11.5)	68.2 CH	C-14, C-1, C-12, C-20	H-14a (1.60)
14	1.60 m 2.05 m	22.2 CH ₂		
15		144.5 C		
16		167.7 C		
17	5.45 brs 6.14 brs	123.6 CH ₂	C-1, C-15, C-16	
18	0.82 s	23.9 CH ₃	C-3, C-4, C-5	H-5,
19	1.16 s	21.3 CH ₃	C-7, C-8, C-9	
20	1.21 s	26.7 CH ₃	C-11, C-12, C-13	
AcO	2.05 s	22.1 CH ₃ 171.3 C	C=O (171.3)	
MeO	3.71 s	52.4 CH ₃	C=O (167.7)	

Table 14 ^1H , ^{13}C NMR, HMBC, and NOESY of 15

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.98 m	33.6 CH	C-2, C-14, C-14, C-15	H-13
2	1.25 m 1.65 m	31.0 CH ₂		
3	0.90 m 1.40 m	26.4 CH ₂	C-4, C-5, C-1	
4		71.8 C		
5	3.83 dd (6.0,11.0)	89.0 CH	C-3, C-4, C-18	H-18, H-7b (1.74)
6	1.45 m 1.71 m	26.8 CH ₂		
7	1.55 m 1.74 m	36.4 CH ₂	C-5, C-8, C-9, C-19	
8		83.0 C		
9	4.70 d (10.0)	78.4 CH	C=O (171.2), C-8, C-7, C-19, C-10	H-7b (1.74)
10	1.50 m 1.92 m	23.4 CH ₂		
11	1.45 m 1.75 m	38.2 CH ₂	C-13, C-12, C-9, C-20	
12		75.1 C		
13	3.34 d (10.5)	81.2 CH	C-14, C-1, C-12, C-20	H-17a (5.42), H-1, H-20
14	1.40 m 1.45 m	30.1 CH ₂		
15		145.8 C		
16		167.5 C		
17	5.42 brs 6.08 brs	122.8 CH ₂	C-1, C-15, C-16	
18	0.84 s	24.2 CH ₃	C-3, C-4, C-5	H-5
19	1.13 s	21.2 CH ₃	C-7, C-8, C-9	
20	1.16 s	24.7 CH ₃	C-11, C-12, C-13	H-13
AcO	2.04 s	21.3 CH ₃ 171.2 C	C=O (171.2)	
MeO	3.43 s	60.2 CH ₃	C-13	
EtO	1.23 t (7.0) 4.16 q (7.0)	14.6 CH ₃ 60.8 CH ₂	CH ₂ (60.8) C=O (167.5)	

Table 15 ^1H , ^{13}C NMR, HMBC, and NOESY of 16

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.63 ddd (3.0,10.5,10.5)	37.7 CH	C-2, C-14, C-14, C-15	H-20
2	1.30 m 1.73 m	25.6 CH ₂		
3	1.16 m 1.46 m	42.5 CH ₂		
4		72.6 C		
5	3.59 dd (7.0,7.0)	86.4 CH	C-3, C-4, C-18	H-19
6	1.72 m	26.1 CH ₂		
7	1.41 m 1.58 m	36.7 CH ₂		
8		84.4 C		
9	4.65 d (11.0)	78.3 CH	C=O, C-8, C-7, C-19, C-10	
10	2.15 brd (13.5) 2.48 ddd (11.0,10.5,13.5)	30.1 CH ₂	C-8, , C-11, C-12	
11	5.26 d (10.5)	122.5 CH	C-13, C-12, C-9, C-20	H-5
12		135.7 C		
13	3.99 brd (10.0)	75.0 CH	C-14, C-1, C-12, C-20	H-11
14	1.40 m 1.54 m	42.4 CH ₂		
15		145.8 C		
16		167.5 C		
17	5.46 brs 6.09 brs	124.9 CH ₂	C-1, C-15, C-16	
18	0.93 s	19.8 CH ₃	C-3, C-4, C-5	
19	1.10 s	19.6 CH ₃	C-7, C-8, C-9	H-5
20	1.54 s	10.7 CH ₃	C-11, C-12, C-13	H-1
AcO	2.04 s	21.7 CH ₃ 170.5 C	C=O (170.5)	
EtO	1.20 t (7.0) 4.13 q (7.0)	14.8 CH ₃ 60.9 CH ₂	CH ₂ (60.9) C=O (167.5)	

Table 16 ^1H , ^{13}C NMR, HMBC, and NOESY of 17

position	δ_{H} (ppm, Hz)	δ_{C} (DEPT, HMQC)	HMBC (H $\rightarrow$ C)	NOESY
1	2.65 m	37.4 CH	C-2, C-14, C-14, C-15	H-20
2	1.29 m 1.73 m	25.5 CH ₂		
3	1.17 m 1.47 m	42.2 CH ₂	C-4, C-5, C-1	
4		72.4 C		
5	3.58 dd (7.0,7.0)	85.9 CH	C-3, C-4, C-18	H-19
6	1.72 m 1.75 m	25.8 CH ₂		
7	1.42 m 1.56 m	36.5 CH ₂		
8		84.2 C		
9	4.64 d (11.5)	78.1 CH	C=O (170.2), C-8, C-7, C-19, C-10	
10	2.15 brd (13.5) 2.45 m	29.9 CH ₂		
11	5.25 d (10.0)	122.2 CH	C-13, C-9, C-20	H-5
12		135.5 C		
13	3.98 dd (3.5,10.5)	74.7 CH	C-14, C-1, C-12, C-11, C-20	H-11
14	1.42 m 1.57 m	42.2 CH ₂		
15		145.3 C		
16		167.8 C		
17	5.49 brs 6.11 brs	124.8 CH ₂	C-1, C-15, C-16	
18	0.92 s	19.6 CH ₃	C-3, C-4, C-5	
19	1.11 s	19.3 CH ₃	C-7, C-8, C-9	H-5
20	1.54 s	10.4 CH ₃	C-11, C-12, C-13	H-1
AcO	2.01 s	21.4 CH ₃ 170.2 C	C=O (170.2)	
MeO	3.66 s	52.1 CH ₃	C=O (167.8)	

The list of original spectroscopic copies

1. ^1H NMR spectrum of **2**
2. ^{13}C NMR and DEPT spectra of **2**
3. COSY spectrum of **2**
4. HMQC spectrum of **2**
5. HMBC spectrum of **2**
6. NOESY spectrum of **2**
7. IR spectrum of **2**
8. MS spectrum of **2**
9. ^1H NMR spectrum of **3**
10. ^{13}C NMR and DEPT spectra of **3**
11. COSY spectrum of **3**
12. HMQC spectrum of **3**
13. HMBC spectrum of **3**
14. NOESY spectrum of **3**
15. IR spectrum of **3**
16. MS spectrum of **3**
17. ^1H NMR spectrum of **4**
18. ^{13}C NMR and DEPT spectra of **4**
19. COSY spectrum of **4**
20. HMQC spectrum of **4**
21. HMBC spectrum of **4**
22. NOESY spectrum of **4**
23. IR spectrum of **4**
24. MS spectrum of **4**
25. ^1H NMR spectrum of **5**
26. ^{13}C NMR and DEPT spectra of **5**
27. COSY spectrum of **5**
28. HMQC spectrum of **5**
29. HMBC spectrum of **5**
30. NOESY spectrum of **5**
31. IR spectrum of **5**
32. MS spectrum of **5**
33. ^1H NMR spectrum of **6**
34. ^{13}C NMR spectrum of **6**
35. COSY spectrum of **6**
36. EDHSQC spectrum of **6**
37. HMBC spectrum of **6**
38. NOESY spectrum of **6**
39. IR spectrum of **6**
40. MS spectrum of **6**
41. ^1H NMR spectrum of **7**
42. ^{13}C NMR spectrum of **7**

43. COSY spectrum of **7**
44. HMQC spectrum of **7**
45. HMBC spectrum of **7**
46. NOESY spectrum of **7**
47. IR spectrum of **7**
48. MS spectrum of **7**
49. ^1H NMR spectrum of **8**
50. ^{13}C NMR and DEPT spectra of **8**
51. COSY spectrum of **8**
52. HMQC spectrum of **8**
53. HMBC spectrum of **8**
54. NOESY spectrum of **8**
55. IR spectrum of **8**
56. MS spectrum of **8**
57. ^1H NMR spectrum of **9**
58. ^{13}C NMR and DEPT spectra of **9**
59. COSY spectrum of **9**
60. HMQC spectrum of **9**
61. HMBC spectrum of **9**
62. NOESY spectrum of **9**
63. IR spectrum of **9**
64. MS spectrum of **9**
65. ^1H NMR spectrum of **10**
66. ^{13}C NMR spectrum of **10**
67. COSY spectrum of **10**
68. HMQC spectrum of **10**
69. HMBC spectrum of **10**
70. NOESY spectrum of **10**
71. IR spectrum of **10**
72. MS spectrum of **10**
73. ^1H NMR spectrum of **11**
74. ^{13}C NMR and DEPT spectra of **11**
75. COSY spectrum of **11**
76. HMQC spectrum of **11**
77. HMBC spectrum of **11**
78. NOESY spectrum of **11**
79. IR spectrum of **11**
80. MS spectrum of **11**
81. ^1H NMR spectrum of **12**
82. ^{13}C NMR and DEPT spectra of **12**
83. COSY spectrum of **12**
84. HMQC spectrum of **12**
85. HMBC spectrum of **12**
86. NOESY spectrum of **12**

87. IR spectrum of **12**
88. MS spectrum of **12**
89. ^1H NMR spectrum of **13**
90. ^{13}C NMR spectrum of **13**
91. COSY spectrum of **13**
92. HMQC spectrum of **13**
93. HMBC spectrum of **13**
94. NOESY spectrum of **13**
95. IR spectrum of **13**
96. MS spectrum of **13**
97. ^1H NMR spectrum of **14**
98. ^{13}C NMR spectrum of **14**
99. COSY spectrum of **14**
100. HMQC spectrum of **14**
101. HMBC spectrum of **14**
102. NOESY spectrum of **14**
103. IR spectrum of **14**
104. MS spectrum of **14**
105. ^1H NMR spectrum of **15**
106. ^{13}C NMR spectrum of **15**
107. COSY spectrum of **15**
108. HMQC spectrum of **15**
109. HMBC spectrum of **15**
110. NOESY spectrum of **15**
111. IR spectrum of **15**
112. MS spectrum of **15**
113. ^1H NMR spectrum of **16**
114. ^{13}C NMR and DEPT spectra of **16**
115. COSY spectrum of **16**
116. HMQC spectrum of **16**
117. HMBC spectrum of **16**
118. NOESY spectrum of **16**
119. IR spectrum of **16**
120. MS spectrum of **16**
121. ^1H NMR spectrum of **17**
122. ^{13}C NMR spectrum of **17**
123. COSY spectrum of **17**
124. HMQC spectrum of **17**
125. HMBC spectrum of **17**
126. NOESY spectrum of **17**
127. IR spectrum of **17**
128. MS spectrum of **17**
129. ^1H NMR spectrum of **18**
130. ^{13}C NMR and DEPT spectra of **18**

- 131. COSY spectrum of **18**
- 132. HMQC spectrum of **18**
- 133. HMBC spectrum of **18**
- 134. NOESY spectrum of **18**
- 135. IR spectrum of **18**
- 136. MS spectrum of **18**
- 137. ^1H NMR spectrum of **19**
- 138. ^{13}C NMR spectrum of **19**
- 139. COSY spectrum of **19**
- 140. HMQC spectrum of **19**
- 141. HMBC spectrum of **19**
- 142. NOESY spectrum of **19**
- 143. IR spectrum of **19**
- 144. MS spectrum of **4**

The list of original spectroscopic copies

1. ^1H NMR spectrum of **2**

Avance 500 Bruker, A&T Center BN
Sample: May-f11-7, Solvent: DMSO
Spectrum: May-7 28

2. ^{13}C NMR and DEPT spectra of **2**

Avance 500 Bruker, A&T Center BNU
Sample: May-f11-7, Solvent: DMSO
Spectrum: May-7 35 ^{13}C

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-7, Solvent:DMSO
Spectrum:May-7 34 dept90

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-7, Solvent:DMSO
Spectrum:May-7 33 dept135

3. DQFCOSY spectrum of **2**

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-7, Solvent:DMSO
Spectrum:May-7 29 cosy

4. HMQC spectrum of **2**

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-7, Solvent:DMSO
Spectrum:May-7 30 HMQC

5. HMBC spectrum of 2

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-7, Solvent:DMSO
Spectrum:May-7 31 HMBCGP

6. NOESY spectrum of 2

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-7, Solvent:DMSO
Spectrum:May-7 32 noesy

7. IR spectrum of 2

8 MS spectrum of 2

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/106/pdata/1/massan
XMASS Mass Analysis Constraints

Ion mass = 399.2139670
Charge = +1
Tolerance = 0.0100000
DBE min = -2
DBE max = 200
Max Candidates = 100

Atom	#(min, max)	Wt*(min, max)
C	15 30	0.00 100.00
H	15 50	0.00 100.00
O	0 10	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
***	Mass Analysis for mass				399.2139670	
1	22	32	5	1	399.2141791	5.313e-07
2	24	31	5	0	399.2165845	6.557e-06

9. ^1H NMR spectrum of **3**

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-5, Solvent:DMSO
Spectrum:may-9 39 1H

10. ^{13}C NMR and DEPT spectra of **3**

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-5, Solvent:DMSO
Spectrum:may-9 46 13C

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-5, Solvent:DMSO
Spectrum:may-9 45 DEPT90

11. COSY spectrum of **3**

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-5, Solvent:DMSO
Spectrum:may-9 40 COSY

12. HMQC spectrum of **3**

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-5, Solvent:DMSO
Spectrum:may-9 41 HMQC

13. HMBC spectrum of **3**

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-5, Solvent:DMSO
Spectrum:may-9 42 HMBC

14. NOESY spectrum of **3**

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-5, Solvent:DMSO
Spectrum:may-11 9 noesy

15. IR spectrum of **3**

16. MS spectrum of 3

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/43/pdata/1/massana
XMASS Mass Analysis Constraints

Ion mass = 377.2321570

Charge = +1

Tolerance = 0.0030000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	20 40	0.00 100.00
H	20 55	0.00 100.00
O	4 20	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
***	Mass Analysis for mass 377.2321570					
1	22	33	5	0	377.2322337	2.034e-07

17. ¹H NMR spectrum of 4

Avance 500 Bruker, A&T Center BNU

Sample:May-fil-2, Solvent:DMSO

Spectrum:May-7 5 HNMR

18. ^{13}C NMR and DEPT spectra of **4**

Avance 500 Bruker, A&T Center BNU
 Sample:May-f11-2, Solvent:DMSO
 Spectrum:May-7 11 ^{13}C

Avance 500 Bruker, A&T Center BNU
 Sample:May-f11-2, Solvent:DMSO
 Spectrum:May-7 10 DEPT90

Avance 500 Bruker, A&T Center BNU
 Sample:May-f11-2, Solvent:DMSO
 Spectrum:May-7 9 DEPT135

19. COSY spectrum of 4

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-2, Solvent:DMSO
Spectrum:May-7 6 COSY

20. HMQC spectrum of 4

Avance 500 Bruker, A&T Center BNU
Sample:May-f11-2, Solvent:DMSO
Spectrum:May-7 7 HMQC

21. HMBC spectrum of 4

22. NOESY spectrum of 4

Avance 500 Bruker, A&T Center BNU
 sample:may-f11-2, Solvent:DMSO
 spectrum:may-7 45 noesy

23. IR spectrum of 4

24. MS spectrum of 4

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/113/pdata/1/massar
XMASS Mass Analysis Constraints

Ion mass [1] = 389.2292970
Ion mass [2] = 433.2190530

Charge = +1
Tolerance = 0.0100000

DBE min = -2
DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	15 30	0.00 100.00
H	15 50	0.00 100.00
O	0 10	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 389.2292970						
1	21	34	5	1	389.2298283	1.365e-06
2	30	29	0	0	389.2263648	7.533e-06
3	23	33	5	0	389.2322337	7.545e-06

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 433.2190530						
1	22	34	7	1	433.2196565	1.393e-06
2	24	33	7	0	433.2220619	6.945e-06

25. ^1H NMR spectrum of 5

Avance 500 Bruker, A&T Center BNU
sample:may-f9-10, Solvent:DMSO
spectrum:may-05 36 1H

26. ^{13}C NMR and DEPT spectra of **5**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-10, Solvent:DMSO
 spectrum:may-05 42 ^{13}C

27. COSY spectrum of 5

Avance 500 Bruker, A&T Center BNU
sample:may-f9-10, Solvent:DMSO
spectrum:may-05 37 COSY

28. HMQC spectrum of 5

Avance 500 Bruker, A&T Center BNU
sample:may-f9-10, Solvent:DMSO
spectrum:may-05 38 HMQC

29. HMBC spectrum of 5

Avance 500 Bruker, A&T Center BNU
sample:may-f9-10, Solvent:DMSO
spectrum:may-05 39 HMBC

30. NOESY spectrum of 5

Avance 500 Bruker, A&T Center BNU
sample:may-f9-10, Solvent:DMSO
spectrum:may-05 40 NOESY

31. IR spectrum of 5

32. MS spectrum of 5

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/155/pdata/1/massar
XMASS Mass Analysis Constraints

Ion mass [1] = 373.2363830
Ion mass [2] = 431.2398170

Charge = +1
Tolerance = 0.0100000

DBE min = -2
DBE max = 200

Max Candidates = 100

*** Mass Analysis for mass 431.2398170

V1	23	36	6	1	431.2403916	1.332e-06
2	25	35	6	0	431.2427970	6.910e-06

33. ¹H NMR spectrum of 6

Avance 500 Bruker, A&T Center BNU
sample:may-f9-7-1, Solvent:DMSO
spectrum:may-05 12 1H

34. ^{13}C NMR spectrum of **6**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-7-1, Solvent:DMSO
 spectrum:may-05 17 ^{13}C

35. COSY spectrum of 6

Avance 500 Bruker, A&T Center BNU
sample:may-f9-7-1, Solvent:DMSO
spectrum:may-05 13 COSY

36. EDHSQC spectrum of 6

Avance 500 Bruker, A&T Center BNU
sample:may-f9-7-1, Solvent:DMSO
spectrum:may-06 25

37. HMBC spectrum of 6

Avance 500 Bruker, A&T Center BNU
sample:may-f9-7-1, Solvent:DMSO
spectrum:may-05 14 HMBC

38. NOESY spectrum of 6

Avance 500 Bruker, A&T Center BNU
sample:may-f9-7-1, Solvent:DMSO
spectrum:may-05 16 NOESY

39. IR spectrum of 6

40. MS spectrum of 6

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/158/pdata/1/massar
XMASS Mass Analysis Constraints

Ion mass = 401.2292690

Charge = +1

Tolerance = 0.0100000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	20 30	0.00 100.00
H	30 50	0.00 100.00
O	3 10	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
***	Mass Analysis for mass	401.2292690				
✓	22	34	5	1	401.2298283	1.394e-06
2	24	33	5	0	401.2322337	7.389e-06

41. ¹H NMR spectrum of 7

Avance 500 Bruker, A&T Center BNU
sample:may-ba-7, Solvent:DMSO
spectrum:may-1 10 1H

42. ^{13}C NMR spectrum of **7**

Avance 500 Bruker, A&T Center BNU
sample:may-ba-7, Solvent:DMSO
spectrum:may-1 17 ^{13}C

43. COSY spectrum of **7**

Avance 500 Bruker, A&T Center BNU
sample:may-ba-7, Solvent:DMSO
spectrum:may-1 11 COSY

44. HMQC spectrum of **7**

Avance 500 Bruker, A&T Center BNU
sample:may-ba-7, Solvent:DMSO
spectrum:may-1 12 HMQC

45. HMBC spectrum of **7**

Avance 500 Bruker, A&T Center BNU
sample:may-ba-7, Solvent:DMSO
spectrum:may-1 13 HMBC

46. NOESY spectrum of 7

Avance 500 Bruker, A&T Center BNU
sample:may-Ba-7 Solvent:DMSO
spectrum:1 noesy

47. IR spectrum of 7

48. MS spectrum of 7

/disk2b/SPECS_SIMS/N-SIMS-LinWenHan/16/pdata/1 xspec Fri Jun 9 07:04:06 2006

XMASS Mass Analysis for /disk2b/SPECS_SIMS/N-SIMS-LinWenHan/16/pdata/1/massana
XMASS Mass Analysis Constraints

Ion mass = 409.2230010

Charge = -1

Tolerance = 0.0030000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	15 25	0.00 100.00
H	15 45	0.00 100.00
O	0 12	0.00 100.00

#	C	H	O	mass	error
*** Mass Analysis for mass 409.2230010					
1	22	33	7	409.2231591	3.863e-07

49. ^1H NMR spectrum of **8**

50. ^{13}C NMR and DEPT spectra of **8**

MAY-f7-7

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: auto_01Jul2004

Pulse Sequence: DEPT

51. COSY spectrum of 8

MAY-f7-7

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: auto_11Nov2004-22:24:46

Pulse Sequence: gCDSY

Solvent: DMSO
Ambient temperature
Files: yun_0725 -
INOVA-500 "unknown"

Relax. delay 1.000 sec
Acq. time 0.212 sec
Width 4821.6 Hz
2D Width 4821.6 Hz
18 repetitions
256 increments
OBSERVE H1 499.5555361 MHz
DATA PROCESSING
Sg. sine bell 0.106 sec
F1 DATA PROCESSING
Sg. sine bell 0.029 sec
F1 size 4096 X 4096
Total time 1 hr, 25 min, 47 sec

52. HMQC spectrum of 8

MAY-f7-7
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: auto_11Nov2004-22:24:46
 Pulse Sequence: gHSQC

53. HMBC spectrum of 8

MAY-f7-7
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: auto_11Nov2004-22:24:46
 Pulse Sequence: gHMBC

54. 1D NOESY spectrum of 8

Avance 500 Bruker, A&T Center BNU

sample:may-f7-7 Solvent:DMSO

spectrum: 1

55. IR spectrum of 8

56. MS spectrum of 8

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/108/pdata/1/massan
XMASS Mass Analysis Constraints

Ion mass = 447.2351040

Charge = +1

Tolerance = 0.0100000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	15 30	0.00 100.00
H	15 50	0.00 100.00
O	0 10	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 447.2351040						
1	23	36	7	1	447.2353057	4.510e-07
2	25	35	7	0	447.2377111	5.829e-06

57. ^1H NMR spectrum of **9**

Avance 500 Bruker, A&T Center BNU
sample:MAY-P-26-2, Solvent:CDCl₃
spectrum:may-4 1

58. ^{13}C NMR and DEPT spectra of **9**

Avance 500 Bruker, A&T Center BNU
sample:MAY-P-26-2, Solvent:CDCl₃
spectrum:may-4 8 ^{13}C

Avance 500 Bruker, A&T Center BNU
sample:MAY-P-26-2, Solvent:CDCl3
spectrum:may-4 7 DEPT90

Avance 500 Bruker, A&T Center BNU
sample:MAY-P-26-2, Solvent:CDCl3
spectrum:may-4 6 DEPT135

59. COSY spectrum of 9

Avance 500 Bruker, A&T Center BNU
 sample:MAY-P-26-2, Solvent:CDCl₃
 spectrum:may-4 2 COSY

60. HMQC spectrum of 9

Avance 500 Bruker, A&T Center BNU
 sample:MAY-P-26-2, Solvent:CDCl₃
 spectrum:may-4 3 HMQC

61. HMBC spectrum of 9

Avance 500 Bruker, A&T Center BNU
sample:MAY-P-26-2, Solvent:CDCl₃
spectrum:may-4 4 HMBC

62. NOESY spectrum of 9

Avance 500 Bruker, A&T Center BNU
sample:may-p-26-2, Solvent:cdcl₃
spectrum:may-4 14

63. IR spectrum of **9**

64. MS spectrum of **9**

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/63/pdata/1/massana
 XMASS Mass Analysis Constraints

Ion mass [1] = 461.2513420
 Ion mass [2] = 421.2560720
 Ion mass [3] = 439.2686660

Charge = +1
 Tolerance = 0.0060000

DBE min = -2
 DBE max = 200

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 461.2513420						
1	24	38	7	1	461.2509549	8.392e-07
2	26	37	7	0	461.2533603	4.376e-06

65. ^1H NMR spectrum of **10**

Avance 500 Bruker, A&T Center BNU
 sample:may-ba-5, Solvent:DMSO
 spectrum:may-01 1

66. ^{13}C NMR spectrum of **10**

Avance 500 Bruker, A&T Center BNU
 sample:may-ba-5, Solvent:DMSO
 spectrum:may-01 6

67. COSY spectrum of **10**

Avance 500 Bruker, A&T Center BNU
 sample:may-ba-5, Solvent:DMSO
 spectrum:may-01 1

68. HMQC spectrum of **10**

Avance 500 Bruker, A&T Center BNU
sample:may-ba-5, Solvent:DMSO
spectrum:may-01 1

69. HMBC spectrum of **10**

Avance 500 Bruker, A&T Center BNU
sample:may-ba-5, Solvent:DMSO
spectrum:may-01 4 HMBGCP

70. NOESY spectrum of **10**

Avance 500 Bruker, A&T Center BNU
sample:MAY-ba-5 Solvent:DMSO
spectrum:20 noesy

71. IR spectrum of **10**

72. MS spectrum of **10**

73. ^1H NMR spectrum of **11**

74. ^{13}C NMR and spectra of **11**

75. COSY spectrum of **11**

76. HMQC spectrum of 11

MAY-Ba-6
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: gHSQC

77. HMBC spectrum of 11

may-ba-6
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: gHMBC

78. NOESY spectrum of **11**

Avance 500 Bruker, A&T Center BNU
sample:may-ba-6 Solvent:DMSO
spectrum: 1

79. IR spectrum of **11**

80. MS spectrum of **11**

81. ^1H NMR spectrum of **12**

Avance 500 Bruker, A&T Center BNU
Sample:may-f7-10, Solvent:DMSO
Spectrum:may-9 34

82. ^{13}C NMR and DEPT spectra of **12**

Avance 500 Bruker, A&T Center BNU
Sample: may-f7-10, Solvent: DMSO
Spectrum: may-9 30

Avance 500 Bruker, A&T Center BNU
Sample: may-f7-10, Solvent: DMSO
Spectrum: may-9 28

Avance 500 Bruker, A&T Center BNU
Sample: may-f7-10, Solvent: DMSO
Spectrum: may-9 29 dept135

83. COSY spectrum of **12**

Avance 500 Bruker, A&T Center BNU
Sample:may-f7-10, Solvent:DMSO
Spectrum:may-9 35 COSY

84. HMQC spectrum of **12**

Avance 500 Bruker, A&T Center BNU
Sample:may-f7-10, Solvent:DMSO
Spectrum:may-9 36 HMQC

85. HMBC spectrum of **12**

Avance 500 Bruker, A&T Center BNU
Sample:may-f7-10, Solvent:DMSO
Spectrum:may-9 37 HMBC

86. NOESY spectrum of **12**

Avance 500 Bruker, A&T Center BNU
Sample:may-f7-10, Solvent:DMSO
Spectrum:may-9 38 NOESY

87. IR spectrum of **12**

25

12

88. MS spectrum of **12**

Acq. File: MT20080401170005.wiff

Printing Date: Tuesday, April 01, 2008 Workstation: QSTAR

89. ^1H NMR spectrum of **13**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-9, Solvent:DMSO
 spectrum:may-05 22 1H

90. ^{13}C NMR spectrum of **13**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-9, Solvent:DMSO
 spectrum:may-05 28 13C

91. COSY spectrum of **13**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-9, Solvent:DMSO
 spectrum:may-05 23 COSY

92. EDHSQC spectrum of **13**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-9, Solvent:DMSO
 spectrum:may-07 hmqc 10

93. HMBC spectrum of **13**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-9, Solvent:DMSO
 spectrum:may-05 24 HMBC

94. NOESY spectrum of **13**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-9, Solvent:DMSO
 spectrum:may-05 26 NOESY

95. IR spectrum of **13**

96. MS spectrum of **13**

97. ^1H NMR spectrum of **14**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-3, Solvent:DMSO
spectrum:may-06 23

98. ^{13}C NMR spectrum of **14**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-3, Solvent:DMSO
spectrum:may-05 6 ^{13}C

99. COSY spectrum of **14**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-3, Solvent:DMSO
spectrum:may-05 2 COSY

100. EDHSQC spectrum of **14**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-3, Solvent:DMSO
spectrum:may-06 23

101. HMBC spectrum of **14**

102. NOESY spectrum of **14**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-6-3, Solvent:DMSO
 spectrum:may-05 4 NOESY

103. IR spectrum of **14**

104. HRESIMS spectrum of **14**

105. ^1H NMR spectrum of **15**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-1, Solvent:DMSO
spectrum:may-05 7

106. ^{13}C NMR spectrum of **15**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-1, Solvent:DMSO
spectrum:may-05 11 13C

107. COSY spectrum of **15**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-1, Solvent:DMSO
spectrum:may-05 8 COSY

108. HMQC spectrum of **15**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-1, Solvent:DMSO
spectrum:may-05 9 HMQC

109. HMBC spectrum of **15**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-6-1, Solvent:DMSO
spectrum:may-05 10 HMBCGP

110. NOESY spectrum of **15**

Avance 500 Bruker, A&T Center BNU
 sample:may-f9-6-1 Solvent:DMSO
 spectrum:1 noe

111. IR spectrum of **15**

112. MS spectrum of 15

XMASS Mass Analysis for /disk2b/SPECS SIMS/P-SIMS-LinWenHan/160/pdata/1/massan
 XMASS Mass Analysis Constraints

Ion mass = 493.2769300

Charge = +1

Tolerance = 0.0100000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	20 30	0.00 100.00
H	30 50	0.00 100.00
O	3 10	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 493.2769300						
1	25	42	8	1	493.2771674	4.813e-07
2	27	41	8	0	493.2795728	5.358e-06

113. ¹H NMR spectrum of 16

114. ¹³C NMR and DEPT spectra of 16

may-f8-2
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: auto_01Jul2004
 Pulse Sequence: s2pul
 Solvent: DMSO
 Ambient Temperature
 User: i-1457
 File: vnmr0841
 INOVA-500 "unknown"
 Relax. delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 0.500 sec
 Width 3129.3 Hz
 2552 repetitions
 OBSERVE C13, 125.6110800 MHz
 DECOUPLE H1, 499.5813930 MHz
 POWER 41 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 131072
 Total time 2 hr, 5 min, 31 sec

may-f8-2
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: auto_01Jul2004
 Pulse Sequence: DEPT

may-f9-2

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: auto_11Nov2004-22:24:46

Pulse Sequence: gCOSY

Solvent: DMSO
Ambient temperature
File: yun.0543
INOVA-500 "unknown"

Relax. delay 1.000 sec
Acq. time 0.179 sec
Width 5711.0 Hz
2D width 5711.0 Hz
16 repetitions
256 increments
OBSERVE Hz: 499.5490557 MHz
DATA PROCESSING
3d, sine bell 0.090 sec
F1 DATA PROCESSING
Sq. sine bell 0.022 sec
FT size 4096 x 4096
Total time 1 hr, 23 min, 14 sec

116. HMQC spectrum of 16

may-f9-2

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: auto_11Nov2004-22:24:46

Pulse Sequence: gHMQC

117. HMBC spectrum of 16

may-f9-2
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: auto_11Nov2004-22:24:46
 Pulse Sequence: gHMBC

118. NOESY spectrum of 16

Avance 500 Bruker, A&T Center BNU
 Sample:may-f9-2, Solvent:DMSO
 Spectrum:may-11 13nosy

119. IR spectrum of 16

120. MS spectrum of **16**

/disk2b/SPECS_SIMS/P-SIMS-LinWenHan/47/pdata/1 xspec Mon Mar 20 13:19:40 2006

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/47/pdata/1/massana
XMASS Mass Analysis Constraints

Ion mass = 461.2505910

Charge = +1

Tolerance = 0.0030000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)		Wt%(min, max)	
C	20	40	0.00	100.00
H	20	55	0.00	100.00
O	4	20	0.00	100.00
Na	0	1	0.00	100.00

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 461.2505910						
1	24	38	7	1	461.2509549	7.890e-07

121. ^1H NMR spectrum of **17**

Avance 500 Bruker, A&T Center BNU
 sample:may-r-1, Solvent:DMSO
 spectrum:may-06 11

122. ^{13}C NMR spectrum of **17**

Avance 500 Bruker, A&T Center BNU
 sample:may-r-1, Solvent:DMSO
 spectrum:may-06 33

123. COSY spectrum of 17

Avance 500 Bruker, A&T Center BNU
 sample:may-r-1, Solvent:DMSO
 spectrum:may-06 12 cosygpsw

124. HMQC spectrum of 17

Avance 500 Bruker, A&T Center BNU
sample:may-r-1, Solvent:DMSO
spectrum:may-06 13 hmqc

125. HMBC spectrum of 17

Avance 500 Bruker, A&T Center BNU
sample:may-r-1, Solvent:DMSO
spectrum:may-06 14 HMBGCP

126. NOESY spectrum of **17**

Avance 500 Bruker, A&T Center BNU
sample:may-fr-1 NOE Solvent:dmsd
spectrum: 1

127. IR spectrum of **17**

128. MS spectrum of 17

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/167/pdata/1/massar
XMASS Mass Analysis Constraints

Ion mass = 447.2344110

Charge = +1

Tolerance = 0.0100000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	3 30	0.00 100.00
H	5 50	0.00 100.00
O	0 10	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 447.2344110						
✓ 1	23	36	7	1	447.2353057	2.001e-06
2	25	35	7	0	447.2377111	7.379e-06
3	30	32	2	1	447.2294368	1.112e-05

129. ^1H NMR spectrum of **18**

Avance 500 Bruker, A&T Center BNU
 Sample:may-f11-4, Solvent:DMSO
 Spectrum:may-10 1

130. ^{13}C NMR spectrum of **18**

Avance 500 Bruker, A&T Center BNU
 Sample:may-f11-4, Solvent:DMSO
 Spectrum:may-10 8

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-4, Solvent:DMSO
Spectrum:may-10 6 dept90

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-4, Solvent:DMSO
Spectrum:may-10 7 dept135

131. COSY spectrum of **18**

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-4, Solvent:DMSO
Spectrum:may-10 1

132. HMQC spectrum of 18

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-4, Solvent:DMSO
Spectrum:may-10 3

133. HMBC spectrum of 18

Avance 500 Bruker, A&T Center BNU
Sample:may-f11-4, Solvent:DMSO
Spectrum:may-10 4 HMBGCP

134. NOESY spectrum of **18**

Avance 500 Bruker, A&T Center BNU
sample:MAY-f11-4 Solvent:DMSO
spectrum:1 noesy

135. IR spectrum of **18**

136. MS spectrum of 18

/disk2b/SPECS_SIMS/P-SIMS-LinWenHan/41/pdata/1 xspec Mon Mar 20 12:35:32 2006

XMASS Mass Analysis for /disk2b/SPECS_SIMS/P-SIMS-LinWenHan/41/pdata/1/massana
XMASS Mass Analysis Constraints

Ion mass = 453.2483620

Charge = +1

Tolerance = 0.0030000

DBE min = -2

DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
C	20 40	0.00 100.00
H	20 55	0.00 100.00
O	4 20	0.00 100.00
Na	0 1	0.00 100.00

#	C	H	O	Na	mass	error
*** Mass Analysis for mass 453.2483620.						
1	24	37	8	0	453.2482744	1.932e-07

137. ^1H NMR spectrum of **19**

Avance 500 Bruker, A&T Center BNU
sample: may-f9-5-1; Solvent: DMSO
spectrum: may-f9-5-1 1

138. ^{13}C NMR spectrum of **19**

Avance 500 Bruker, A&T Center BNU
sample: may-f9-5-1, Solvent: DMSO
spectrum: may-04 B ZGDC

139. COSY spectrum of 19

Avance 500 Bruker, A&T Center BNU
sample:may-f9-5-1, Solvent:DMSO
spectrum:may-04 2 cosy

140. HMQC spectrum of 19

Avance 500 Bruker, A&T Center BNU
sample:may-f9-5-1, Solvent:DMSO
spectrum:may-04 3 hmqc

141. HMBC spectrum of **19**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-5-1, Solvent:DMSO
spectrum:may-04 4 HMBCGP

142. NOESY spectrum of **19**

Avance 500 Bruker, A&T Center BNU
sample:may-f9-5-1;NOE Solvent:DMSO
spectrum:may-f9-5-1 1

143. IR spectrum of 19

144. MS spectrum of 19

XMASS Mass Analysis for /disk2b/SPECS_SIMS/N-SIMS-LinWenHan/13/pdata/1/mas
XMASS Mass Analysis Constraints

Charge = -1
Tolerance = 0.0030000

DBE min = -2
DBE max = 200

Max Candidates = 100

Atom	#(min, max)		Wt%(min, max)	
C	15	25	0.00	100.00
H	15	45	0.00	100.00
O	0	12	0.00	100.00

#	C	H	O	mass	error
*** Mass Analysis for mass 409.2228970					
1	22	33	7	409.2231591	6.404e-07