Supporting Information

Sulfated Meroterpenoids from the Brazilian Sponge *Callyspongia* sp. are Inhibitors of the Antileishmaniasis Target Adenosine Phosphoribosyl Transferase

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Table 1. ^1H (600 MHz) and ^{13}C (150 MHz) NMR data obtained for isoakaterpin (**3**) in 4:1 $\text{CD}_3\text{OD}/\text{C}_6\text{D}_6$.

Carbon	δ_{C} ppm (mult.)	δ_{H} ppm (int., mult., J/Hz)
1	37.1 (t)	2.50 (1H, d, 13.9); 3.44 (1H, d, 13.9)
2	43.2 (s)	
3	38.4 (d)	1.72 (1H, m)
4	26.2 (t)	1.18 (1H, m); 1.95 (1H, m)
5	28.5 (t)	1.37 (1H, m); 2.01 (1H, m)
6	43.6 (s)	
7	46.5 (d)	1.62 (1H, m)
8	22.2 (t)	1.95 (1H, m); 2.29 (1H, br d, 13.2)
9	25.6 (t)	1.67 (1H, m); 1.94 (1H, m)
10	34.2 (t)	2.18 (1H, br dd, 13.5, 4.0); 2.38 (1H, td 13.5, 6.4)
11	153.7 (s)	
12	37.8 (t)	0.78 (1H, td 13.0, 3.1); 1.92 (1H, m)
13	25.0 (t)	0.94 (1H, td, 13.2, 3.3); 1.35 (1H, m)
14	43.0 (s)	
15	46.1 (d)	1.24 (1H, m)
16	32.4 (t)	1.26 (1H, m); 1.45 (1H, m)
17	31.2 (t)	1.05 (1H, m); 1.76 (1H, m)
18	45.0 (d)	1.63 (1H, m)
19	147.4 (s)	
20	118.0 (d)	5.38 (1H, br dd, 4.6, 2.6)
21	24.3 (t)	2.00 (1H, m); 2.10 (1H, m)
22	32.5 (t)	1.10 (1H, m); 1.39 (1H, m)
23	32.8 (s)	
24	16.7 (q)	1.16 (3H, d, 7.0)
25	25.1 (q)	1.10 (3H, s)
26	108.7 (t)	4.73 (1H, br s); 4.83 (1H, br s)
27	17.1 (q)	0.84 (3H, d, 6.6)
28	24.3 (q)	1.03 (3H, s)
29	28.5 (q)	1.00 (3H, s)
30	28.5 (q)	0.85 (3H, s)
1'	150.3 (s)	
2'	135.3 (s)	
3'	125.2 (d)	7.47 (1H, d, 2.8)
4'	150.0 (s)	
5'	120.5 (d)	7.26 (1H, dd, 8.9, 2.8)
6'	123.4 (d)	7.56 (1H, d, 8.9)

Figure 1. ^1H (CD_3OD , 600 MHz) and ^{13}C (CD_3OD , 150 MHz) spectra of ilhabelanol (**1**).

Figure 2. ^1H (CD_3OD , 600 MHz) and ^{13}C (CD_3OD , 150 MHz) spectra of ilhabrene (**2**).

Figure 3. ^1H (CD_3OD , 600 MHz) and ^{13}C (CD_3OD , 150 MHz) spectra of isoakaterpin (**3**).

Figure 4. ^1H ($\text{CD}_3\text{OD}/\text{C}_6\text{D}_6$ 4:1, 600 MHz) and ^{13}C ($\text{CD}_3\text{OD}/\text{C}_6\text{D}_6$ 4:1, 150 MHz) spectra of isoakaterpin (**3**).

Figure 5. Comparison of the ^{13}C NMR data reported for model compounds **4** (CDCl₃, 75 MHz), **5** (CDCl₃, 100 MHz), **7** (CD₃OD, 125 MHz) and **8** (CDCl₃, 125 MHz) with that obtained for the A and B rings of ilhabelanol (**1**) and isoakaterpin (**3**).