Xanthone and Sesquiterpene Derivatives from the Fruits of *Garcinia scortechinii*

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The fruits of *Garcinia scortechinii* afforded 10 new compounds: four caged-tetraprenylated xanthones (scortechinones Q−T, **1**−**4**), four rearranged xanthones (scortechinones U−X, **5**−**8**), and two sesquiterpene derivatives (scortechterpenes A, B, **9**, **10**), together with 14 known compounds: one sesquiterpene, two biflavonoids, and 11 caged-polyprenylated xanthones. Their structures were elucidated by analysis of spectroscopic data and comparison of the NMR data with those reported previously. All xanthone derivatives were evaluated for antibacterial activity against methicillin-resistant *Staphylococcus aureus*.

Our previous investigation on twigs, latex, and stem bark of *Garcinia scortechinii*, a small slender tree distributed throughout Malaysia and southern Thailand, resulted in the isolation of 15 caged-polyprenylated xanthones (scortechinones A−J[1,2] and L−P[3]) and one degraded caged-tetraprenylated xanthone (scortechinone K[2]). All of them, except scortechinones J and K, have a characteristic structure with a C-7 bridgehead methoxyl group and a 2,3,3-trimethyldihydrofuran unit linked at C-3 and C-4 of the aromatic ring. Among these xanthones, scortechinone B, the major component in all investigated parts of the plant, exhibited significant antibacterial activity against methicillin-resistant *Staphylococcus aureus* (MRSA) strain with an MIC value of 3.38 μM. Some structure−antibacterial activity relationships were established.[3] This paper describes the isolation and identification of four new caged-tetraprenylated xanthones of the same type, four new highly rearranged tetraprenylated xanthones, and two new sesquiterpenes from the fruits of the plant. The effect on the inhibition against MRSA of all new xanthones was also reported.

Results and Discussion

The fruits of *G. scortechinii* were extracted with MeOH, and the MeOH extract was then subjected to chromatographic purifications to obtain 10 new compounds: four caged-tetraprenylated xanthones (scortechinones Q−T, **1**−**4**), four rearranged xanthones (scortechinones U−X, **5**−**8**), and two sesquiterpenes (scortechterpenes A, B, **9**, **10**), along with 14 known compounds: 11 caged-polyprenylated xanthones [scortechinones A (**11**),[1] B (**12**),[1] C,[1] D−F,[2] H,[2] I (**14**),[2] M (**13**),[3] L,[3] and P[3]], two biflavonoids [(+)-volkensiflavone (**15**)[4,5] and (+)-morelloflavone (**16**)[4]], and one sesquiterpene, germacra-4(15),5*E*,10(14)-trien-1β-ol (**17**).[6] All structures were elucidated using 1D and 2D NMR spectroscopic data. The ^{1}H and ^{13}C NMR signals were assigned from DEPT, HMQC, and HMBC spectra.

Caged-polyprenylated xanthones isolated from the latex, stem bark, and twigs of *G. scortechinii* were 7-methoxy caged-polyprenylated xanthones with a 2,3,3-trimethyldihydrofuran unit attached at C-3 and C-4 via an ether linkage at C-3. They are divided into three types: those with and without a C8/C8a double bond and a degraded caged-tetraprenylated xanthone. These compounds were primarily distinguished by UV absorption bands. The caged-polyprenylated xanthones with the C8/C8a double bond and the degraded caged-tetraprenylated xanthones showed a typical UV absorption band in the range 360−368 nm due to a conjugated carbonyl chromophore, while those lacking the C8/C8a double bond gave an absorption band at shorter wavelength (λ_{max} 304 nm). The orientation of H-15 of the dihydrofuran unit in all caged-polyprenylated xanthones, relative to the C-5 prenyl substituent, was assigned by NOEDIFF data.[1−3] When H-15 was *cis* to the C-5 substituent, it was assigned at the α-face. For those with the C8/C8a double bond, the orientation of H-15 at either the α- or β-face was further confirmed by the ^{1}H and ^{13}C chemical shifts of the *gem*-dimethyl groups of the dihydrofuran unit.[1−3] In the case of the dihydrofurans with the β-methine proton, such as scortechinone B (**12**), the *gem*-dimethyl groups appeared at similar δ_H values, but distinctly different δ_C values ($\Delta\delta_C$ ca. 8 ppm). In contrast, the *gem*-dimethyl groups of the dihydrofurans with the α-methine proton, such as scortechinone A (**11**), gave differences in both the ^{1}H and ^{13}C signals of approximately 0.4 and 3 ppm, respectively.

Scortechinone Q (**1**), with a molecular formula of $C_{34}H_{42}O_8$ from HR-MS, showed UV spectral data similar to those of scortechinone A (**11**)[1] with the C8/C8a double bond. Their ^{1}H NMR spectra (Table 1) were also similar except for the fact that one methyl singlet in **11** was replaced by separated methylene signals of a hydroxymethyl group (δ 3.56 and 3.65, both as a doublet, J = 11.5 Hz) in **1**. The location of the hydroxymethyl group was assigned at C-27 due to the HMBC correlations between the oxymethylene protons and C-26, C-27, and C-28. Irradiation of H_a-25, in a NOEDIFF experiment, enhanced signal intensities of H_b-25 and $H_{a,b}$-29, but not H-26, suggesting that the hydroxymethyl substituent was α-oriented. The attachment of other substituents and relative configuration were identical to those of **11**, based on HMBC correlations and NOEDIFF data, respectively (see Supporting Information). The α-orientation of H-15 was further confirmed by the ^{1}H and ^{13}C chemical shifts of Me-17 and Me-18.[2,3] Therefore, scortechinone Q (**1**) was identified as a caged-tetraprenylated xanthone, having an α-hydroxymethyl substituent at C-27.

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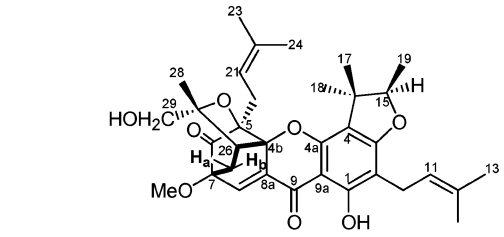
Chart 1



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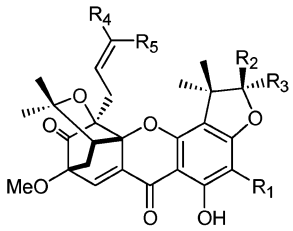
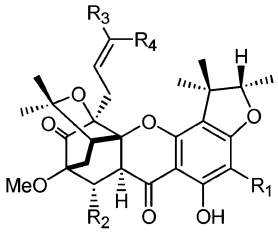


2: R_1 =  , $R_2 = R_4 = Me$, $R_3 = H$, $R_5 = CO_2H$

11: R_1 =  , $R_2 = R_4 = R_5 = Me$, $R_3 = H$

12: R_1 =  , $R_2 = H$, $R_3 = R_4 = Me$, $R_5 = CO_2H$

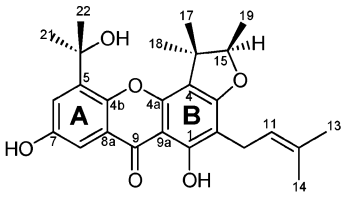
13: R_1 =  , $R_2 = H$, $R_3 = R_4 = Me$, $R_5 = CO_2H$



3: R_1 =  , $R_2 = OMe$, $R_3 = Me$, $R_4 = CO_2H$

4: R_1 =  , $R_2 = OMe$, $R_3 = CHO$, $R_4 = Me$

14: R_1 =  , $R_2 = OMe$, $R_3 = Me$, $R_4 = CO_2H$



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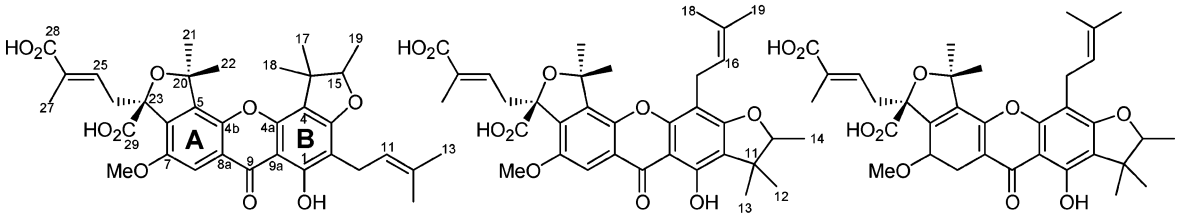
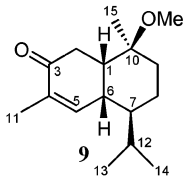


6 **7** **8**



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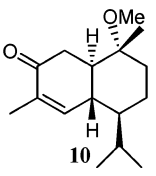

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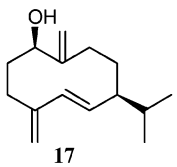

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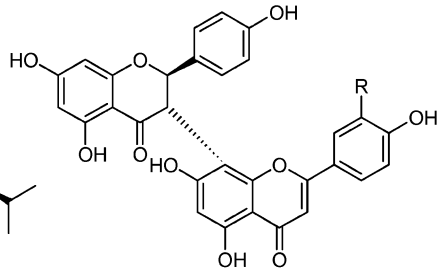

15: R = H

16: R = OH

Scortechinone R (**2**), with a molecular formula of $C_{34}H_{40}O_{10}$ by HR-MS, displayed UV spectroscopic data similar to those of scortechinone M (**13**).[3] The ^1H NMR spectrum (Table 1) indicated that it contained substituents identical to those of **13**. The minor differences were the ^1H and ^{13}C chemical shifts of the *gem*-dimethyl groups of the dihydrofuran unit, which indicated that in **2** H-15 was α-oriented. The NOEDIFF results (see Supporting Information) confirmed this orientation. Therefore, scortechinone R (**2**) was a C-15 epimer of **13**.

Scortechinone S (**3**) ($C_{35}H_{44}O_{11}$, from HR-MS of $[M - MeOH]^+$) showed UV absorption bands similar to those of scortechinone I (**14**),[2] lacking the C8/C8a double bond. The ^1H and ^{13}C NMR data of **3** were similar to those of **14** except for the signals of the 3-methylbut-2-enyl group. These resonances were replaced by a spin system that could be ascribed to a 2-hydroxy-3-methylbut-3-enyl group. This substituent was assigned to be at C-2 by HMBC correlations of the methylene protons ($H_{a,b}$-10) with C-1 and C-3. The attachment of other substituents was identical to **14**, on the basis of HMBC data (see Supporting Information). The NOEDIFF data (see Supporting Information) confirmed the α-orientation of H-8a, the *β*-orientations of H-8 and H-15, and the *Z* configuration of the C21/C22 double bond, which were identical to those of **14**. From these results, scortechinone S (**3**) was identified as the fourth new caged-tetraprenylated xanthone, lacking a C8/C8a double bond, isolated from *G. scortechinii*.

Scortechinone T (**4**), $C_{35}H_{44}O_9$ as determined by HR-MS, exhibited UV absorption bands similar to those of **3** and **14**.[2] The ^1H NMR spectrum (Table 1) was almost identical to that of **14** with an additional singlet of an aldehyde proton at *δ* 9.48. The HMBC correlations between the aldehydic H-23 and C-22 and C-24 suggested that the C-5

Table 1. ^{1}H and ^{13}C NMR Data of Scortechinones Q–T (**1**–**4**)

		1		**2**		**3**		**4**	
position	C-type	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	C	12.87 (s, OH)	163.0	13.26 (s, OH)	164.1	12.27 (s, OH)	162.0	12.08 (s, OH)	161.7
2	C		105.3		102.3		102.4		105.6
3	C		166.9		168.3		167.4		166.9
4	C		113.7		113.8		113.9		113.6
4a	C		154.3		154.4		152.7		152.0
4b	C		83.7		89.1		87.1		86.1
5	C		84.9		84.0		86.5		87.1
6	C=O		198.9		203.1		205.4		205.4
7	C		88.0		85.1		81.4		81.7
7-OCH_3	CH_3	3.50 (s)	51.8	3.64 (s)	53.9	3.49 (s)	52.4	3.52 (s)	52.3
8	CH	7.08 (d, 1.0)	134.9	7.52 (d, 1.0)	134.8	4.46 (s)	75.1	4.48 (s)	75.3
8-OCH_3	CH_3					3.39 (s)	57.5	3.40 (s)	57.7
8a	C		131.5		132.4	3.20 (s)	48.9	3.09 (s)	49.3
9	C=O		176.5		177.9		192.2		191.7
9a	C		101.9		101.3		102.6		102.4
10	CH_2	3.20 (d, 7.0)	21.4	a: 2.93 (dd, 14.5, 10.5) b: 2.71 (dd, 14.5, 3.5)	28.3	a: 2.90 (dd, 14.0, 4.0) b: 2.77 (dd, 14.0, 9.0)	29.1	3.21 (m)	21.4
11	CH	5.25 (tm, 7.0)	121.7	4.51 (dd, 10.5, 3.5)	74.8	4.27 (dd, 9.0, 4.0)	75.5	5.24 (tm, 7.0)	121.4
12	C		132.0		147.1		147.4		133.0
13	CH_3	1.69 (s)	25.8					1.69 (s)	25.8
	CH_2			a: 5.06 (brs) b: 4.89 (brs)	110.6	a: 4.99 (s) b: 4.84 (s)	110.4		
14	CH_3	1.75 (s)	17.7	1.85 (s)	18.3	1.84 (s)	18.1	1.76 (s)	17.7
15	CH	4.50 (q, 6.5)	90.9	4.53 (q, 6.5)	91.1	4.41 (q, 6.3)	90.6	4.42 (q, 6.5)	90.1
16	C		43.7		43.1		44.0		43.9
17	CH_3	1.19 (s)	21.1	1.15 (s)	21.1	1.44 (s)	26.1	1.45 (s)	26.2
18	CH_3	1.55 (s)	25.2	1.57 (s)	23.6	1.12 (s)	22.1	1.09 (s)	22.3
19	CH_3	1.38 (d, 6.5)	14.5	1.39 (d, 6.5)	13.7	1.34 (d, 6.3)	13.9	1.35 (d, 6.5)	13.8
20	CH_2	a: 2.66 (dd, 13.5, 10.0) b: 2.62 (dm, 13.5)	28.1	a: 3.57 (dd, 15.5, 11.0) b: 2.78 (dm, 15.5)	28.9	a: 3.24 (ddm, 16.0, 7.0) b: 3.12 (ddm, 16.0, 7.0)	28.4	a: 3.04 (dd, 16.5, 6.5) b: 2.96 (dd, 16.5, 6.5)	27.9
21	CH	4.48 (m)	117.8	5.40 (dm, 11.0)	135.7	6.59 (tm, 7.0)	137.3	7.01 (t, 6.5)	148.6
22	C		136.4		129.4		128.4		139.8
23	CH_3	1.59 (s)	25.8	1.67 (t, 1.5)	21.2	1.97 (d, 1.5)	20.9		
	CH							9.48 (s)	195.0
24	CH_3	1.61 (s)	17.9					1.76 (s)	9.4
	C=O				167.8		170.4		
25	CH_2	a: 2.84 (d, 12.5) b: 1.76 (dd, 12.5, 10.0)	33.8	a: 2.32 (d, 13.5) b: 1.72 (dd, 13.5, 9.5)	30.6	a: 2.04 (d, 14.0) b: 1.64 (dd, 14.0, 8.5)	23.9	a: 2.07 (d, 14.5) b: 1.64 (dd, 14.5, 8.5)	23.8
26	CH	2.57 (d, 10.0)	41.4	2.62 (d, 9.5)	49.6	2.72 (d, 8.5)	45.3	2.73 (d, 8.5)	45.3
27	C		85.2		83.6		82.8		82.2
28	CH_3	1.41 (s)	25.1	1.71 (s)	30.7	1.43 (s)	30.5	1.42 (s)	30.5
29	CH_2	a: 3.65 (d, 11.5) b: 3.56 (d, 11.5)	67.9						
	CH_3			1.29 (s)	28.7	1.22 (s)	27.2	1.22 (s)	27.3

3-carboxybut-2-enyl substituent in **14** was replaced by a 2-butenyl-3-carboxaldehyde unit in **4**. An NOE enhancement of H-23 after irradiation of the olefinic H-21 established an *E* configuration for the C21/22 double bond. This was in agreement with the observed signal of H-21, which was shifted to much lower field than that found in **14**. The HMBC correlations between the methylene protons ($H_{a,b}$-20) of the 2-butenyl-3-carboxaldehyde group and C-4b and C-6 confirmed the attachment of the 2-butenyl-3-carboxaldehyde substituent at C-5. The orientations of H-8, H-8a, and H-15 were proved to be identical to those of **14** by the NOEDIFF data (see Supporting Information). Thus, scortechinone T (**4**) is a new naturally occurring caged-tetraprenylated xanthone, having a C-5 2-butenyl-3-carboxaldehyde unit.

Scortechinone U (**5**) was analyzed as $C_{26}H_{30}O_6$ by HR-MS. The xanthone chromophore was evident by its UV absorption bands,[7] while hydroxyl and conjugated carbonyl absorption bands were evident in the IR spectrum. Its ^{1}H NMR spectrum (Table 2) contained signals of one hydrogen-bonded hydroxyl group (δ 13.90, s), two *meta*-coupled aromatic protons [δ 7.75 (1H, d, J = 3.5 Hz) and 7.56 (1H, d, J = 3.5 Hz)], one prenyl unit [δ 5.28 (1H, tm, J = 7.0 Hz), 3.30 (2H, d, J = 7.0 Hz), 1.78 (3H, s), and 1.66 (3H, s)], one 2,3,3-trimethyldihydrofuran ring [δ 4.55 (1H, q, J = 6.5 Hz), 1.66 (3H, s), 1.44 (3H, d, J = 6.5 Hz), and 1.33 (3H, s)], one 2-hydroxyisopropyl group [δ 1.87 (3H, s) and 1.79 (3H, s)], and two hydroxyl groups [δ 9.12 (brs) and 4.63 (brs)]. The location of all subunits was established by HMBC data (see Supporting Information). The hydrogen-bonded hydroxyl group at C-1 gave ^3J cross-peaks with C-2 and C-9a. HMBC correlations between the methylene protons (H-10) of the prenyl group and C-1, C-2, and C-3 established the attachment of the prenyl group at C-2, *ortho* to the hydrogen-bonded hydroxyl group. Two *meta* aromatic protons were attributed to H-6 and H-8, respectively, on the basis of the chemical shifts and the HMBC correlations of H-6/C-4b, C-7, and C-8 and those of H-8/C-4b and C-6. According to the chemical shift of C-7, C-7 carried a hydroxyl substituent. The hydroxyisopropyl group was assigned at C-5, *ortho* to H-6, by ^3J correlations of H-6/C-20 and those of the *gem*-dimethyl protons (Me-21 and Me-22)/C-5. NOE enhancement of Me-21 and Me-22, upon irradiation of H-6, supported the above assignment. From

Table 2. ^{1}H and ^{13}C NMR Data of Scortechinones U–X (**5**–**8**)

		5		**6**		**7**		**8**	
position	C-type	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	C	13.90 (s, OH)	161.8	13.15 (s, OH)	161.4	12.87 (s, OH)	157.0	12.36 (s, OH)	155.4
2	C		107.2		107.6		117.4		118.0
3	C		165.6		165.5		165.3		163.3[a]
4	C		112.8		113.2		103.5		102.8
4a	C		151.6		151.3		155.0		154.2
4b	C		147.5		147.2		147.5		163.2[a]
5	C		140.6		145.1		145.1		140.4
6	CH	7.75 (d, 3.5)	122.3		128.2		128.0		122.8
7	C		154.1		150.8		150.8		
	CH							4.50 (t, 8.0)	74.8
7-OH		9.12 (brs)							
7-OCH_3	CH_3			4.10 (s)	57.3	4.09 (s)	57.0	3.54 (s)	58.0
8	CH	7.56 (d, 3.5)	108.0	7.44 (s)	109.4	7.44 (s)	109.3		
	CH_2							a: 2.70 (dd, 18.0, 8.0)	27.1
								b: 2.59 (dd, 18.0, 8.0)	
8a	C		122.5		117.0		116.8		111.6
9	C=O		181.4		181.4		182.0		178.7
9a	C		103.7		104.5		105.1		105.9
10	CH_2	3.30 (d, 7.0)	22.2	3.28 (d, 7.5)	22.2				
	CH					4.58 (q, 6.5)	91.6	4.47 (q, 6.5)	90.6
11	CH	5.28 (tm, 7.0)	122.6	5.26 (tm, 7.5)	122.4				
	C						44.4		43.8
12	C		132.0		132.2				
	CH_3					1.49 (s)	25.4	1.46 (s)	25.1
13	CH_3	1.66 (s)	25.8	1.64 (s)	25.8	1.24 (s)	20.8	1.21 (s)	20.5
14	CH_3	1.78 (s)	17.8	1.75 (s)	17.8	1.41 (d, 6.5)	14.6	1.37 (d, 6.5)	14.4
15	CH	4.55 (q, 6.5)	90.9	4.64 (q, 6.5)	91.7				
	CH_2					3.47 (d, 7.5)	22.5	3.37 (m)	21.9
16	C		44.7		44.7				
	CH					5.34 (tm, 7.5)	122.4	5.22 (tm, 7.0)	121.6
17	CH_3	1.33 (s)	22.0	1.33 (s)	21.4				
	C						132.5		132.3
18	CH_3	1.66 (s)	26.0	1.61 (s)	26.0	1.84 (s)	17.7	1.77 (s)	17.8
19	CH_3	1.44 (d, 6.5)	14.2	1.43 (d, 6.5)	14.8	1.64 (s)	25.9	1.67 (s)	25.7
20	C		71.5		87.2		87.2		88.0
20-OH		4.63 (brs)							
21	CH_3	1.79 (s)	30.5	1.61 (s)	28.8	1.61 (s)	28.8	1.38 (s)	26.7
22	CH_3	1.87 (s)	30.2	1.53 (s)	30.2	1.53 (s)	30.2	1.38 (s)	26.6
23	C				91.6		91.7		91.0
24	CH_2			a: 3.54 (dd, 15.0, 7.5)	36.0	a: 3.54 (ddm, 15.0, 7.5)	36.0	a: 3.31 (dd, 16.0, 8.0)	35.6
				b: 3.28 (dd, 15.0, 7.5)		b: 3.26 (ddm, 15.0, 7.5)		b: 3.10 (dd, 16.0, 8.0)	
25	CH			6.59 (tm, 7.5)	139.3	6.58 (tm, 7.5)	139.3	6.78 (tm, 7.5)	140.6
26	C				129.9		129.9		129.0
27	CH_3			1.70 (d, 1.5)	12.8	1.69 (d, 1.0)	12.8	1.77 (s)	12.4
28	C=O				168.9		168.9		173.0
29	C=O				172.0		172.0		175.0

[a] Interchangeable.

these results, the dihydrofuran unit was placed at C-3 and C-4 of ring B. *gem*-Dimethyl protons (Me-17 and Me-18) of the 2,3,3-trimethyldihydrofuran ring showing HMBC correlations with C-4, not with C-3, supported the attachment of the hydrofuran ring at C-3 and C-4 of the xanthone nucleus with an ether linkage at C-3. Signal enhancement of Me-22, upon irradiation of Me-17, confirmed that the hydroxyisopropyl moiety was adjacent to the dihydrofuran unit. Me-17 was *trans* to H-15 since irradiation of H-15 enhanced the signals of Me-18 and Me-19, but not Me-17. Thus, scortechinone U (**5**) was determined as 1,7-dihydroxy-5-(2′-hydroxyisopropyl)-2-(3-methylbutyl-2-enyl)-4″,4″,5″-trimethylfurano(2″,3″:3,4)xanthone.

Scortechinone V (**6**), with a molecular formula of $C_{34}H_{38}O_{10}$ by HR-MS of $[M - CO_2]^+$, exhibited UV and IR data similar to those of **5**. Additional IR absorption bands at 3600–2500 (a hydroxyl group of carboxylic group) and 1694 (a carbonyl group of carboxylic group) cm^{-1} indicated the presence of a carboxylic acid functional group. The ^{1}H NMR spectrum (Table 2) showed a hydrogen-bonded hydroxy proton at δ 13.15 (s), characteristic signals of a prenyl group [δ 5.26 (1H, tm, J = 7.5 Hz), 3.28 (2H, d, J = 7.5 Hz), 1.75 (3H, s), and 1.64 (3H, s)], and a 2,3,3-trimethyldihydrofuran ring [δ 4.64 (1H, q, J = 6.5 Hz), 1.61 (3H, s), 1.43 (3H, d, J = 6.5 Hz), and 1.33 (3H, s)]. These data together with HMBC data (see Supporting Information) identical to those of **5** indicated that **5** and **6** had the same structure of ring B. In addition, the ^{1}H NMR spectrum exhibited an aromatic proton singlet at δ 7.44, an *O*-methyl resonance at δ 4.10, characteristic signals of a 3-carboxybut-2-enyl group [δ 6.59 (1H, tm, J = 7.5 Hz), 3.54 (1H, dd, J = 15.0 and 7.5 Hz), 3.28 (1H, dd, J = 15.0 and 7.5 Hz), and 1.70 (3H, d, J = 1.5 Hz)], and two *gem*-dimethyl signals of an oxyisopropyl group at δ 1.61 (3H, s) and 1.53 (3H, s). The location of these substituents on ring A of the xanthone nucleus was established by the following HMBC data (see Supporting Information). The aromatic proton singlet, which was attributed to H-8 according to the chemical shift, showed ^2J cross-peaks with C-7 and C-8a and ^3J cross-peaks with C-4b and C-6. An HMBC correlation between the methoxy protons and C-7 confirmed the *O*-methyl group at C-7. In addition, the HMBC spectrum showed correlations between one of the methylene protons, H_b-24, of the 3-carboxybut-2-enyl group with C-6, C-23, and C-29 of the carboxyl group, and between the olefinic H-25 with C-23. These data established the attachment of the carboxyl group and the

3-carboxybut-2-enyl group at C-23, the latter linked with C-6 of the xanthone moiety. The *gem*-dimethyl protons (Me-21 and Me-22) of the oxyisopropyl group gave cross-peaks with the remaining aromatic carbon at C-5 and an oxyquaternary carbon at C-20, indicating the presence of the oxyisopropyl group at C-5. On the basis of the established molecular formula, a dihydrofuran unit was constructed by forming an ether linkage between two oxyquaternary carbons, C-20 and C-23. Irradiation of H-25 of the 3-carboxybut-2-enyl unit enhanced the signal intensity of Me-21, not Me-27, indicating that the carboxyprenyl unit had an *E* configuration and *cis*-relationship to Me-21. Signal enhancement of Me-18, upon irradiation of H-15, suggested their *cis*-relationship. The relative configuration of the hydrofuran rings could not be determined because Me-18 and Me-21 resonated at the same chemical shift. Therefore, scortechinone V (**6**) was identified as 1-hydroxy-7-methoxy-2′,2′-dimethyl-5′-carboxy-5′-(3-carboxybut-2-enyl)-furano(3′,4′:5,6)-2-(3-methylbutyl-2-enyl)-4″,4″,5″-trimethylfurano(2″,3″:3,4)xanthone.

Scortechinone W (**7**), with a molecular formula of $C_{34}H_{38}O_{10}$ from HR-MS of $[M - CO_2]^+$, displayed UV and IR absorption bands similar to those of **6**. The ^1H and ^{13}C NMR (Table 2) and HMBC data (see Supporting Information) of ring A revealed that **6** and **7** had identical rings A. In addition, the ^1H NMR spectrum showed characteristic signals of a hydrogen-bonded hydroxy proton (δ 12.87, s), a 2,3,3-trimethyldihydrofuran ring [δ 4.58 (1H, q, J = 6.5 Hz), 1.49 (3H, s), 1.41 (3H, d, J = 6.5 Hz), and 1.24 (3H, s)], and a 3-methylbutyl-2-enyl unit [δ 5.34 (1H, tm, J = 7.5 Hz), 3.47 (2H, d, J = 7.5 Hz), 1.84 (3H, s), and 1.64 (3H, s)]. The location of these substituents on ring B was established by the following HMBC data (see Supporting Information). The hydrogen-bonded hydroxy proton, at C-1, showed ^3J cross-peaks with C-2 and C-9a. The 2,3,3-trimethyldihydrofuran ring was fused in a linear fashion at C-2 with an ether linkage at C-3, according to ^3J HMBC correlations between Me-12 and Me-13 with C-2. The remaining 3-methylbutyl-2-enyl unit was attached at C-4 by the ^3J correlations of H-15/C-3 and C-4a. The chemical shifts of the *gem*-dimethyl groups of both dihydrofuran rings were established by the NOEDIFF data (see Supporting Information). However, the NOEDIFF results could not determine the relative configuration of the dihydrofuran units. Attempts to recrystallize **7** in various solvent systems were unsuccessful. Thus, scortechinone W (**7**) was assigned as 1-hydroxy-7-methoxy-2′,2′-dimethyl-5′-carboxy-5′-(3-carboxylbut-2-enyl)furano(3′,4′:5,6)-4-(3-methylbutyl-2-enyl)-4″,4″,5″-trimethylfurano(2″,3″:3,2)-xanthone.

Scortechinone X (**8**), with a molecular formula $C_{34}H_{40}O_{10}$ (HR-MS), showed IR absorption bands for the hydroxyl group of a carboxylic group, acid carbonyl, and conjugated carbonyl groups. The UV spectrum displayed an absorption band at 278 nm, a shorter wavelength than those found in **5**−**7**. The ^1H NMR spectrum (Table 2) was similar to that of **7** except for the fact that a singlet aromatic proton (δ 7.44, H-8) was replaced by the signals of an oxymethine proton at δ 4.50 (t, J = 8.0 Hz) and methylene protons at δ 2.70 (dd, J = 18.0 and 8.0 Hz) and 2.59 (dd, J = 18.0 and 8.0 Hz). These indicated that **8** had the same structure of ring B as that of **7**. The HMBC and NOEDIFF data (see Supporting Information) confirmed these assignments. The oxymethine proton and methylene protons were attributed to H-7 and H-8, respectively, since H-7 showed ^3J correlations in the HMBC spectrum with C-5 and C-8a, while both methylene protons, H-8, gave ^3J correlations with C-4b and C-6. A methoxyl group was assigned to be at C-7 due to a HMBC correlation between the methoxy protons and C-7. Furthermore, the location of other substituents on ring A was identical to that of **7**, on the basis of HMBC data (see Supporting Information). Again, the relative configuration of both dihydrofuran units could not be assigned by NOEDIFF data. In addition, the orientation of 7-OMe was not determined because of equivalence of the ^1H resonances of Me-21 and Me-22 and those of Me-18 and Me-27. Therefore, scortechinone X (**8**) was determined as the first naturally occurring xanthone derivative, lacking a C7/C8 double bond, which was isolated from *G. scortechinii*. The stability of compound **8** with its cyclohexadiene moiety is notable.

Scortechterpene A (**9**) had a molecular formula of $C_{16}H_{26}O_2$ from HR-MS. The IR spectrum suggested the presence of an α,β-unsaturated carbonyl system.[8] The UV absorption band supported the presence of an α,β-unsaturated ketone.[9] The ^1H and ^{13}C NMR and DEPT data revealed that **9** had the skeleton of a cadinane type sesquiterpene.[8,9] Comparison of these data with those of 10α-hydroxyamorphane-4-en-3-one[8,10] indicated that the hydroxyl group of 10α-hydroxyamorphane-4-en-3-one was replaced by an *O*-methyl group in **9**. This demonstrated that the methoxyl group was located at C-10, which was proved by an HMBC correlation between the methoxy protons and C-10. The COSY, HMQC, and HMBC data of **9** led to unambiguous assignments of NMR data. The location of the isopropyl group and the position of the α,β-unsaturated ketone moiety were supported by HMBC data (see Supporting Information). The relative configuration was deduced from analyses of splitting patterns together with the coupling constant of H-5 and NOEDIFF data between H-1 and H-6. In the ^1H NMR spectrum, H-5 appeared as a double quartet with coupling constants of 6.3 and 1.5 Hz, which was coupled to H-6 and Me-11, respectively. The coupling constant of 6.3 Hz between H-5 and H-6 provided evidence for the *cis*-fusion: in *trans*-fusion, H-5 appeared as a broad singlet, while for *cis*-fusion, H-5 resonated as a doublet with a coupling constant of 6.5 Hz.[8] Since H-6 appeared as a doublet of doublets of doublets with the large coupling (J = 10.2 Hz) and the smallest coupling (J = 5.1 Hz) constants with H-7 and H-1, respectively, H-6 and the 7-isopropyl substituent were located at the β-axial and β-equatorial positions, respectively. Irradiation of H_{ax}-6 produced signal enhancement of H_{eq}-1 and 10-OMe, supporting the assignment of *cis*-fusion and also indicating the location of 10-OMe at the β-axial position, *cis* to both H_{eq}-1 and H_{ax}-6. Thus, scortechterpene A (**9**) was identified as 10-methoxyamorphan-4-en-3-one.

Scortechterpene B (**10**) was analyzed for $C_{16}H_{26}O_2$ by HR-MS. The IR and UV spectra were almost identical to those of **9**. The ^1H NMR spectrum was similar to that of **9** except for a signal of an olefinic H-5 which appeared as a broad singlet. This result suggested that **10** had a *trans*-fused ring system.[8] The location of the methyl, methoxyl, and isopropyl groups and conjugated ketone functionality was identical to that of **9**, according to HMBC correlations (see Supporting Information). Irradiation of H_{ax}-6 enhanced the signal of Me-15, but not H_{ax}-1. These supported the *trans*-fused ring system and also indicated the β-axial orientation of Me-15. Signal enhancement of H_{ax}-7 and equatorial 10-OMe, upon irradiation of H_{ax}-1, established the β-equatorial and α-equatorial orientations of the isopropyl and methoxyl groups at C-7 and C-10, respectively. Therefore, scortechterpene B (**10**) was a diastereomer of **9**, differing in the stereochemistry at C-1 and C-10.

Table 3. Antibacterial Activity of Scortechinones A (11), B (12), I (14), and Q–X (**1**–**8**)

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**11**	**12**	**14**	vancomycin
MIC (μM)	>221	>210	100	>105	>292	106	52.8	>210	228	3.38	12.8	1.38

Among all new xanthones isolated from the fruits of *G. scortechinii*, scortechinone W (**7**) exhibited the best activity against methicillin-resistant *Staphylococcus aureus* (MRSA) with a minimum inhibitory concentration (MIC) of 52.8 μM. Others exhibited less activity (Table 3). The standard vancomycin had an MIC value of 1.38 μM. Scortechinones S (**3**) and T (**4**) were much less active than scortechinone I (**14**). These results supported previous conclusions on the important role of the C-2 prenyl group and the carboxyl group of the C-5 substituent.[3] In addition, scortechinone Q (**1**) showed activity similar to scortechinone A (**11**), indicating that a modified polar methyl substituent at C-27 did not play an important role in the activity.

Up to now, our investigation on *G. scortechinii* led to the isolation of 19 caged-polyprenylated xanthones, one degraded caged-tetraprenylated xanthone, and four highly rearranged tetraprenylated ones. Caged-polyprenylated xanthones are considered to have a mixed shikimate-triacetate and isoprenoid biosynthesis origin.[11] Quillinan and Scheinmann suggested that the caged scaffold of these molecules arises in nature from a tandem Claisen/Diels–Alder rearrangement.[12] In 2001, Wu et al. proposed a plausible biosynthesis of the gaudispirolactone, the first degraded xanthone isolated from *G. gaudichaudii*.[13] Isolation of the highly rearranged xanthones (**5**–**8**) might provide insight in the biosynthesis of these molecules.

Experimental Section

General Experimental Procedures. Melting points were determined on an electrothermal melting point apparatus (Electrothermal 9100) and were reported without correction. Infrared spectra (IR) were obtained on a FTS165 FT-IR spectrometer. Ultraviolet (UV) absorption spectra were measured with a Specord S100 spectrophotometer (Analytik Jena Ag) or a UV-1601 spectrophotometer (Shimadzu). ^{1}H and ^{13}C NMR spectra were recorded on either a 300 MHz Bruker AVANCE spectrometer or a 500 MHz Varian UNITY INOVA spectrometer using $CDCl_3$ solution or as otherwise stated with TMS as internal standard. Optical rotations were measured with sodium D line (589 nm) on a JASCO P-1020 polarimeter. EIMS and HREIMS data were determined on VG ZAB 2SEQ or MAT 95 XL mass spectrometers. Column chromatography was performed on silica gel (Merck) type 100 (70–230 mesh ASTM) using a gradient system of increasing polarity (MeOH–$CHCl_3$) or as otherwise stated, or silica gel 60 RP-18 (40–63 μm) (Merck) with a gradient system of decreasing polarity (MeOH–H_2O) or Sephadex LH-20 with pure MeOH. Flash column chromatography was carried out on silica gel (Merck) type 60 (230–400 mesh ASTM). Thin-layer chromatography (TLC) was performed on silica gel 60 F_{254} or RP-18 F_{254s} (Merck).

Plant Material. The fruits of *G. scortechinii* were collected at the Ton Nga Chang Wildlife Sanctuary, Hat Yai, Songkhla, Thailand, in June 2000. The plant was identified by Dr. Prakart Sawangchote, Department of Biology, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla, where a voucher specimen has been deposited.

Isolation. The fruits (1120 g) of *G. scortechinii*, cut into small segments, were extracted with MeOH (3 × 2.5 L) at room temperature over a period of 7 days. Evaporation of the combined MeOH extracts to dryness in vacuo afforded a brown-yellow gum in 94.4 g. The crude MeOH extract was divided in two parts by dissolving in $CHCl_3$. The $CHCl_3$-soluble part was evaporated to dryness under reduced pressure to give a yellow solid (24.8 g), which was further fractionated by column chromatography to yield 10 fractions. Fraction 2 (0.6 g, eluted with $CHCl_3$) was subjected to column chromatography using solvent mixtures of increasing polarity (5% EtOAc–light petroleum to pure MeOH) to yield three subfractions. The third subfraction (24 mg, eluted with 10% EtOAc–light petroleum) was separated on precoated TLC using 10% EtOAc–light petroleum (5 runs) to afford **9** (2.3 mg) and **10** (3.9 mg). Fraction 3 (2.2 g, eluted with $CHCl_3$) was purified by column chromatography with solvent mixtures of increasing polarity ($CHCl_3$ to 20% MeOH–$CHCl_3$) to afford four subfractions. Scortechinone A (**11**) (38.0 mg) was obtained from the second subfraction. The third subfraction (0.5 g, eluted with 0.5% MeOH–$CHCl_3$), upon repeated flash column chromatography using $CHCl_3$, gave three subfractions. Scortechinones D (4.7 mg), E (2.3 mg), and L (5.1 mg) were obtained from the second subfraction (60 mg of 0.44 g, eluted with $CHCl_3$) after purification on precoated TLC using 8% EtOAc–light petroleum (13 runs). Fraction 4 (0.8 g, eluted with 1% MeOH–$CHCl_3$) was further separated by column chromatography to yield eight subfractions. The second subfraction (60 mg, eluted with $CHCl_3$) was subjected to column chromatography, using 10% EtOAc–light petroleum, to afford three subfractions. Compound **17** (2.0 mg) was obtained from the second subfraction (27 mg) after purification on precoated TLC using a mixture of EtOAc, CH_2Cl_2, and light petroleum (0.1:8:2) (3 runs). Further separation of the fourth subfraction (129.0 mg, eluted with 0.2% MeOH–$CHCl_3$) by column chromatography eluted with a gradient system of EtOAc–hexane (from 8% to 40% EtOAc–hexane), followed by precoated TLC with 1% MeOH–$CHCl_3$ (2 runs), gave **1** (11.8 mg). Fraction 5 (1.4 g, eluted with 1–2% MeOH–$CHCl_3$) was fractionated by column chromatography to give two subfractions. The first subfraction (0.8 g, eluted with 0.1–7% MeOH–$CHCl_3$), upon repeated flash column chromatography using 1% EtOAc–light petroleum, gave three subfractions. Compound **4** (8.2 mg) and scortechinone H (2.4 mg) were obtained from the second (16 mg) and third (12 mg) subfractions, respectively, after purification on precoated TLC using 20% EtOAc–light petroleum (5 runs) and 15% EtOAc–light petroleum (21 runs). Fraction 6 (12.5 g, 2% MeOH–$CHCl_3$) was subjected to column chromatography to yield six subfractions. Scortechinone B (**12**) (100 mg) was obtained from the second subfraction. The fourth subfraction (3.8 g, eluted with 4% MeOH–$CHCl_3$) was further purified by column chromatography to afford three subfractions. The second and third subfractions (56.0 and 62.0 mg) were further separated by precoated TLC with 30% EtOAc–light petroleum to afford scortechinones C (3.5 mg), F (1.6 mg), I (**14**) (10.4 mg), and M (**13**) (3.4 mg). The fifth subfraction (0.6 g, eluted with 4–8% MeOH–$CHCl_3$) was further purified by column chromatography on reversed-phase silica gel with solvent mixtures of decreasing polarity (70% MeOH–H_2O to pure MeOH) to give four subfractions. The second (108.0 mg) and third (35.0 mg) subfractions were subjected to column chromatography, followed by precoated TLC with 25% EtOAc–light petroleum to yield **2** (2.3 mg) and scortechinone P (9.8 mg). Fraction 7 (1.38 g, eluted with 3% MeOH–$CHCl_3$) was separated by column chromatography on Sephadex LH-20 to afford four subfractions. The second subfraction (0.90 g), upon repeated column chromatography on Sephadex LH-20, gave three subfractions. The second subfraction (0.48 g) gave **3** (2.5 mg) after purification on column chromatography followed by precoated TLC with 10% acetone–$CHCl_3$ (6 runs). The third subfraction (26 mg) was separated by column chromatography with solvent mixtures of increasing polarity (1–10% MeOH–$CHCl_3$) and subsequent precoated TLC with 30% EtOAc–light petroleum (5 runs) to yield **5** (4.2 mg). Fraction 9 (2.6 g, eluted with 7% MeOH–$CHCl_3$) was separated by column chromatography on Sephadex LH-20 to afford three subfractions. The second subfraction (1.7 g) was

further purified by column chromatography to yield 10 subfractions. The fourth (103.0 mg, eluted with 2% MeOH−$CHCl_3$) and seventh (216.0 mg, eluted with 4−7% MeOH−$CHCl_3$) subfractions were purified by column chromatography on reversed-phase silica gel with solvent mixtures of decreasing polarity (70% MeOH−H_2O to pure MeOH) and subsequent purification on precoated TLC with 30% EtOAc−light petroleum to afford **6** (3.1 mg), **7** (3.3 mg), and **8** (4.7 mg). The $CHCl_3$-insoluble part was evaporated to dryness under reduced pressure to give a brown solid (20.0 g). This was further fractionated by column chromatography on Sephadex LH-20 to afford three subfractions. The second subfraction (1.51 g) was further separated by column chromatography on reversed-phase silica gel with solvent mixtures of decreasing polarity (50% MeOH−H_2O to pure MeOH) to yield four subfractions. The second (75.0 mg) and third (349.0 mg) subfractions, upon repeated column chromatography on Sephadex LH-20, afforded **15** (28.0 mg) and **16** (33.0 mg), respectively.

Scortechinone Q (1): yellow gum, $[\alpha]^{28}_D$ −36° (*c* 0.10, MeOH); UV (MeOH) λ_{max} (log ϵ) 350 (4.02); IR (neat) ν_{max} 3432, 1749, 1614 cm^{-1}; ^1H NMR (500 MHz), Table 1; ^{13}C NMR (125 MHz), Table 1; EIMS *m/z* 578 $[M]^+$ (4), 518 (74), 480 (100), 424 (28), 366 (27), 308 (19), 149 (44); HREIMS *m/z* 578.2883 (calcd for $C_{34}H_{42}O_8$, 578.2880).

Scortechinone R (2): yellow gum; $[\alpha]^{28}_D$ −58° (*c* 0.04, MeOH); UV (MeOH) λ_{max} (log ϵ) 365 (4.01); IR (neat) ν_{max} 3700−3200, 1745, 1690, 1631 cm^{-1}; ^1H NMR (500 MHz), Table 1; ^{13}C NMR (125 MHz), Table 1; EIMS *m/z* 608 $[M]^+$ (4), 580 (30), 536 (27), 509 (100), 473 (32), 436 (33), 383 (43), 243 (38), 233 (52); HREIMS *m/z* 608.2619 (calcd for $C_{34}H_{40}O_{10}$, 608.2621).

Scortechinone S (3): yellow gum; $[\alpha]^{28}_D$ −39° (*c* 0.08, MeOH); UV (MeOH) λ_{max} (log ϵ) 304 (3.97); IR (neat) ν_{max} 3600−2500, 1749, 1693, 1633 cm^{-1}; ^1H NMR (500 MHz), Table 1; ^{13}C NMR (125 MHz), Table 1; EIMS *m/z* 608 $[M\text{-MeOH}]^+$ (4), 579 (29), 536 (29), 508 (100), 382 (14), 276 (14), 233 (22); HREIMS *m/z* 608.2627 $[M - MeOH]^+$ (calcd for $C_{34}H_{40}O_{10}$, 608.2627).

Scortechinone T (4): yellow gum; $[\alpha]^{28}_D$ −28° (*c* 0.10, MeOH); UV (MeOH) λ_{max} (log ϵ) 303 (4.16); IR (neat) ν_{max} 3480, 1749, 1682, 1633 cm^{-1}; ^1H NMR (500 MHz), Table 1; ^{13}C NMR (125 MHz), Table 1; EIMS *m/z* 608 $[M]^+$ (30), 553 (20), 438 (29), 381 (34), 291 (67), 289 (80), 259 (73), 233 (100); HREIMS *m/z* 608.2982 (calcd for $C_{35}H_{44}O_9$, 608.2985).

Scortechinone U (5): yellow solid, mp 148.8−150.0 °C; $[\alpha]^{28}_D$ −273° (*c* 0.06, MeOH); UV (MeOH) λ_{max} (log ϵ) 322 (4.14), 267 (4.48), 241 (4.46); IR (neat) ν_{max} 3427, 1640 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6), Table 2; ^{13}C NMR (125 MHz, acetone-d_6), Table 2; EIMS *m/z* 438 $[M]^+$ (21), 423 (15), 405 (16), 383 (100), 365 (23), 349 (30), 309 (23); HREIMS *m/z* 438.2037 (calcd for $C_{26}H_{30}O_6$, 438.2042).

Scortechinone V (6): yellow solid, decomposed at 213 °C; $[\alpha]^{28}_D$ +28° (*c* 0.22, MeOH); UV (MeOH) λ_{max} (log ϵ) 328 (4.10), 277 (4.25), 267 (4.28), 243 (4.32); IR (neat) ν_{max} 3600−2500, 1694, 1642 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6), Table 2; ^{13}C NMR (125 MHz, acetone-d_6), Table 2; EIMS *m/z* 562 $[M - CO_2]^+$ (80), 506 (46), 490 (77), 463 (100), 447 (34), 433 (54), 419 (50), 407 (76), 379 (80), 349 (36), 323 (43); HREIMS *m/z* 562.2563 $[M - CO_2]^+$ (calcd for $C_{33}H_{38}O_8$, 562.2567).

Scortechinone W (7): yellow solid, decomposed at 210 °C; $[\alpha]^{28}_D$ +61° (*c* 0.22, MeOH); UV (MeOH) λ_{max} (log ϵ) 325 (4.07), 277 (4.20), 266 (4.24), 247 (4.25); IR (neat) ν_{max} 3600−2500, 1704, 1656 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6), Table 2; ^{13}C NMR (125 MHz, acetone-d_6), Table 2; EIMS *m/z* 562 $[M - CO_2]^+$ (20), 489 (22), 463 (100), 435 (22), 375 (21), 349 (20), 323 (25); HREIMS *m/z* 562.2576 $[M - CO_2]^+$ (calcd for $C_{33}H_{38}O_8$, 562.2567).

Scortechinone X (8): yellow gum; $[\alpha]^{28}_D$ +96° (*c* 0.61, MeOH); UV (MeOH) λ_{max} (log ϵ) 278 (3.94); IR (neat) ν_{max} 3600−2500, 1697, 1651 cm^{-1}; ^1H NMR (500 MHz), Table 2; ^{13}C NMR (125 MHz), Table 2; EIMS *m/z* 608 $[M]^+$ (8), 576 (19), 520 (42), 488 (73), 463 (70), 432 (100), 406 (48), 393 (71), 391 (36); HREIMS *m/z* 608.2620 (calcd for $C_{34}H_{40}O_{10}$, 608.2621).

Scortechterpene A (9): colorless gum; $[\alpha]^{28}_D$ +266° (*c* 0.08, $CHCl_3$); UV (MeOH) λ_{max} (log ϵ) 240 (3.88); IR (neat) ν_{max} 1732, 1673 cm^{-1}; ^1H NMR (300 MHz) δ 6.95 (1H, dq, J = 6.3 and 1.5 Hz, H-5), 3.17 (3H, s, 10-OMe), 2.60 (1H, ddd, J = 10.2, 6.3, and 5.1 Hz, H-6), 2.37 (2H, m, H-2), 2.25 (1H, m, H-1), 1.85 (1H, d sep, J = 7.0 and 2.5 Hz, H-12), 1.79 (3H, t, J = 1.5 Hz, Me-11), 1.78 (1H, m, H-9a), 1.47 (1H, m, H-7), 1.36 (2H, m, H-8), 1.29 (1H, m, H-9b), 1.12 (3H, s, Me-15), 0.92, 0.89 (each 3H, d, J = 7.0 Hz, Me-13, Me-14); ^{13}C NMR (75 MHz) δ 199.6 (C, C-3), 151.0 (CH, C-5), 134.7 (C, C-4), 75.0 (C, C-10), 48.9 (CH_3, 10-OMe), 43.0 (CH, C-7), 42.6 (CH, C-1), 36.9 (CH_2, C-2), 35.4 (CH, C-6), 30.3 (CH_2, C-9), 27.8 (CH, C-12), 21.5 (CH_3, C-15), 21.4 (CH_3, C-13), 19.2 (CH_2, C-8), 16.0 (CH_3, C-11), 15.7 (CH_3, C-14); EIMS *m/z* 250 $[M]^+$ (19), 218 (16), 207 (24), 175 (51), 162 (17), 135 (19), 85 (100), 72 (23), 69 (13); HREIMS *m/z* 250.1934 (calcd for $C_{16}H_{26}O_2$, 250.1933).

Scortechterpene B (10): colorless gum; $[\alpha]^{28}_D$ +72° (*c* 0.17, $CHCl_3$); UV (MeOH) λ_{max} (log ϵ) 238 (3.85); IR (neat) ν_{max} 1738, 1681 cm^{-1}; ^1H NMR (300 MHz) δ 6.80 (1H, brs, H-5), 3.20 (3H, s, 10-OMe), 2.71 (1H, dd, J = 15.0 and 1.8 Hz, H-2a), 2.24 (1H, d sep, J = 6.9 and 2.1 Hz, H-12), 2.14 (1H, m, H-6), 2.07 (1H, dd, J = 15.0 and 13.5 Hz, H-2b), 1.98 (1H, m, H-1), 1.87 (1H, m, H-9a), 1.78 (3H, dd, J = 2.1 and 1.5 Hz, Me-11), 1.69 (1H, m, H-8a), 1.48 (1H, m, H-9b), 1.24 (1H, m, H-8b), 1.18 (1H, m, H-7), 1.12 (3H, s, Me-15), 0.98, 0.83 (each 3H, d, J = 6.9 Hz, Me-13, Me-14); ^{13}C NMR (75 MHz) δ 200.4 (C, C-3), 146.2 (CH, C-5), 135.3 (C, C-4), 74.8 (C, C-10), 48.2 (CH_3, 10-OMe), 47.8 (CH, C-1), 45.0 (CH, C-7), 40.5 (CH, C-6), 38.3 (CH_2, C-2), 34.9 (CH_2, C-9), 26.2 (CH, C-12), 21.5 (CH_3, C-13), 21.0 (CH_2, C-8), 17.9 (CH_3, C-15), 15.9 (CH_3, C-11), 15.2 (CH_3, C-14); EIMS *m/z* 250 $[M]^+$ (13), 218 (16), 207 (20), 175 (65), 165 (21), 147 (10), 135 (19), 91 (16), 85 (100), 72 (29), 69 (12); HREIMS *m/z* 250.1944 (calcd for $C_{16}H_{26}O_2$, 250.1933).

Antibacterial Activity Testing. MICs were determined by the agar microdilution method.[14] The test substances were dissolved in DMSO (Merck, Germany). Serial 2-fold dilutions of the test substances were mixed with melted Mueller-Hinton agar (Difco) in the ratio of 1:100 in microtiter plates with flat-bottomed wells (Nunc, Germany). Final concentration of the test substances in agar ranged from 128 to 0.03 μg/mL. MRSA isolated from a clinical specimen, Songklanakarin Hospital, was used as test strain. Inoculum suspensions (10 μL) were spotted on agar-filled wells. The inoculated plates were incubated at 35 °C for 18 h. MICs were recorded by reading the lowest substance concentration that inhibited visible growth. Vancomycin was used as a positive control drug. Growth controls were performed on agar containing DMSO.

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Supporting Information Available: Tables of selected HMBC correlations and NOEDIFF data of **1**−**10**. This material is available free of charge via the Internet at http://pubs.acs.org.

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