Supporting Information

Cytotoxic and NF-κB Inhibitory Constituents of the Stems of *Cratoxylum cochinchinense* and Their Semi-synthetic Analogues

Yulin Ren,[†] Susan Matthew,[†,‡] Daniel D. Lantvit,[§] Tran Ngoc Ninh,[⊥] Heebyung Chai,[†] James R. Fuchs,[†] Djaja D. Soejarto,[§] Esperanza J. Carcache de Blanco,[†,‡] Steven M. Swanson,[§] and A. Douglas Kinghorn[*,†]

Divisions of Medicinal Chemistry and Pharmacognosy and Pharmacy Practice and Administration, College of Pharmacy, The Ohio State University, Columbus, Ohio 43210, Program for Collaborative Research in the Pharmaceutical Sciences and Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, Chicago, Illinois 60612, and Institute of Ecology and Biological Resources, Vietnamese Academy of Science and Technology, Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

[*] To whom correspondence should be addressed. Tel.: +1 614 247 8094. Fax: +1 614 247 8081.

E-mail: kinghorn.4@osu.edu

[†] Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University.

[‡] Division of Pharmacy Practice and Administration, College of Pharmacy, The Ohio State University.

[§] University of Illinois at Chicago.

[⊥] Institute of Ecology and Biological Resources, Vietnam.

Table of Contents

Figure S1a. Mass spectrum of cochinchinoxanthone (**1**) from *C. cochinchinense*

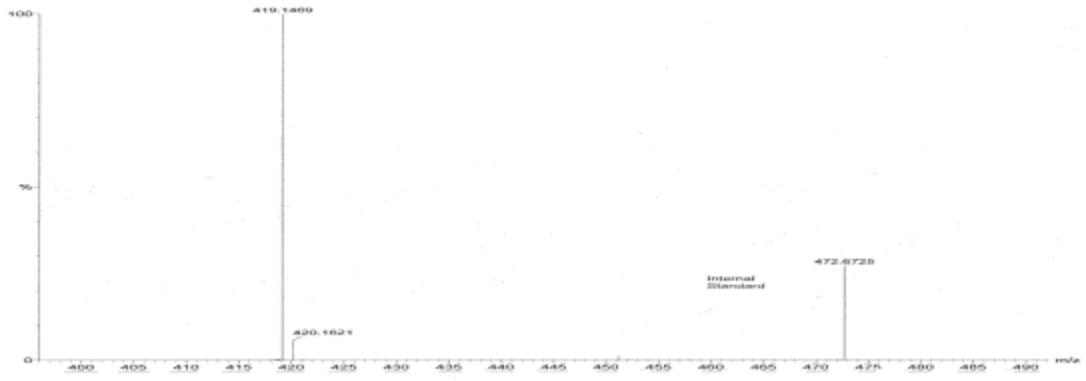


Figure S1b. ^{1}H NMR spectrum of cochinchinoxanthone (**1**) from *C. cochinchinense*

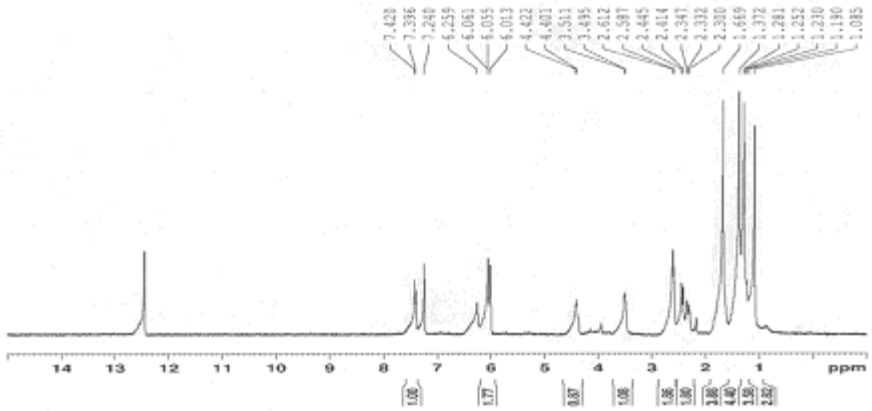


Figure S1c. ^{13}C NMR spectrum of cochinchinoxanthone (**1**) from *C. cochinchinense*

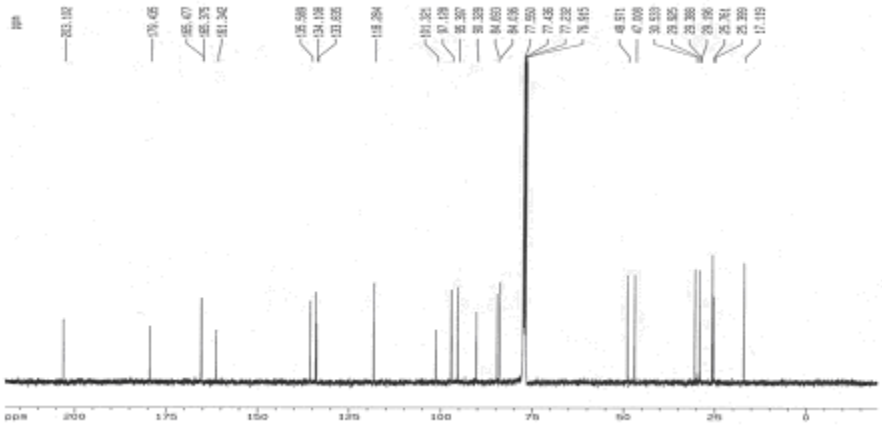


Figure S2a. Mass spectrum of cochinensoxanthone (**2**) from *C. cochinchinense*

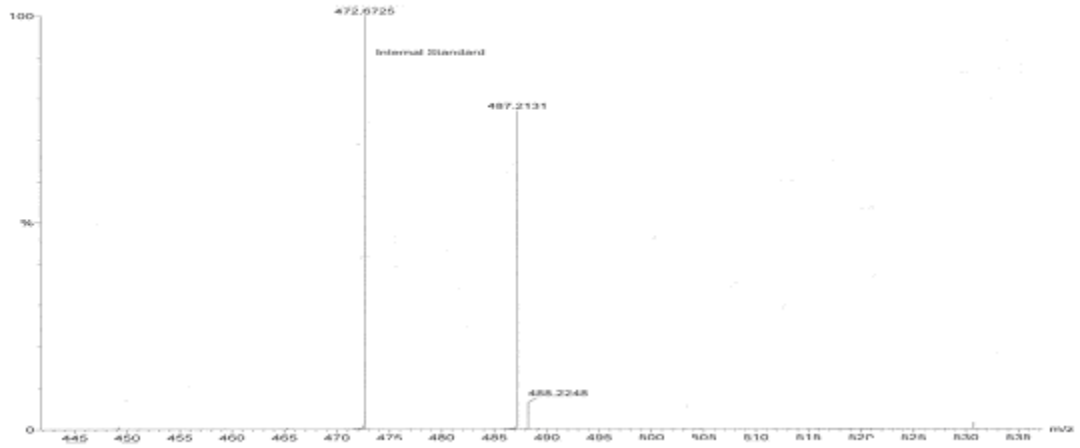


Figure S2b. ^{1}H NMR spectrum of cochinensoxanthone (**2**) from *C. cochinchinense*

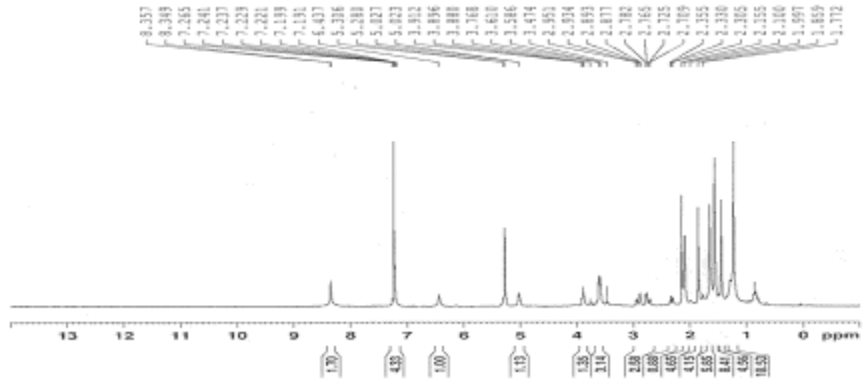


Figure S2c. ^{13}C NMR spectrum of cochinensoxanthone (**2**) from *C. cochinchinense*

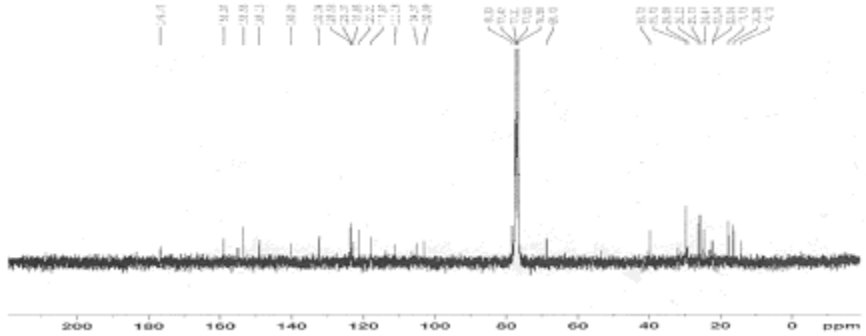


Figure S3a. Mass spectrum of 4-methyl-3,6-di-*O*-methyl-α-mangostin (**10**) from α-mangostin

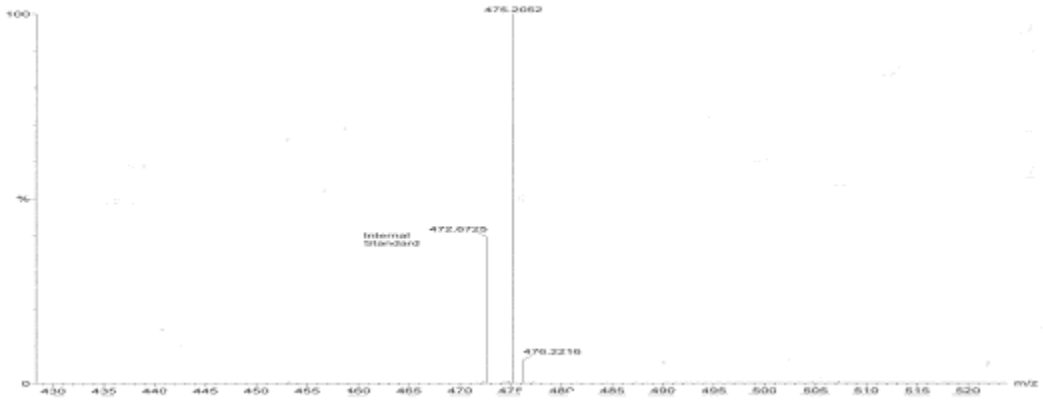


Figure S3b. ^{1}H NMR spectrum of 4-methyl-3,6-di-*O*-methyl-α-mangostin (**10**) from α-mangostin

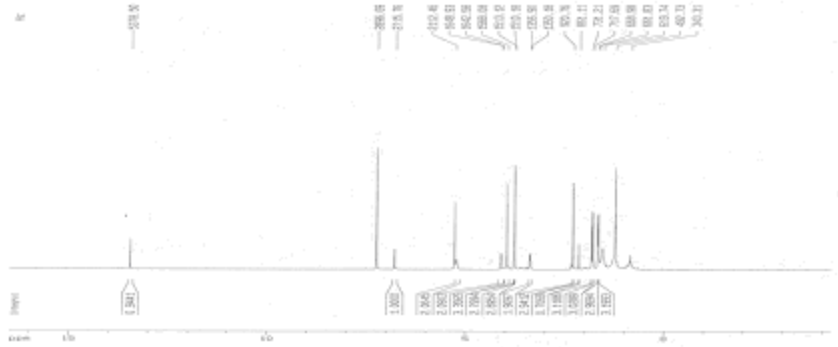


Figure S3c. ^{13}C NMR spectrum of 4-methyl-3,6-di-*O*-methyl-α-mangostin (**10**) from α-mangostin

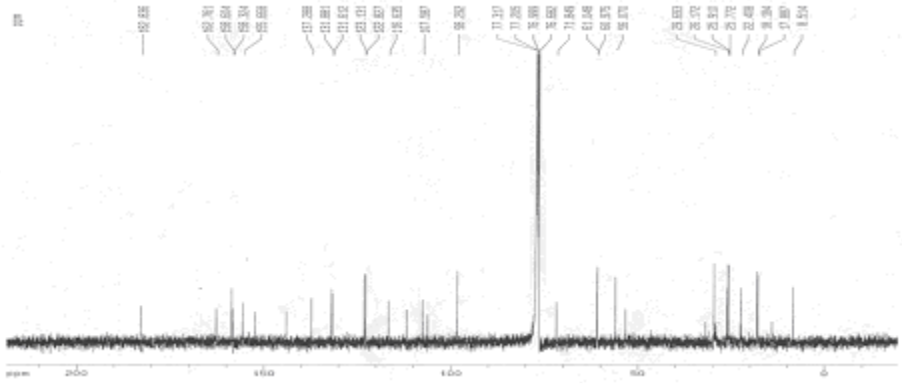


Figure S4a. Mass spectrum of 18-*O*-formyl-3-isomangostin hydrate (**13**) from α-mangostin

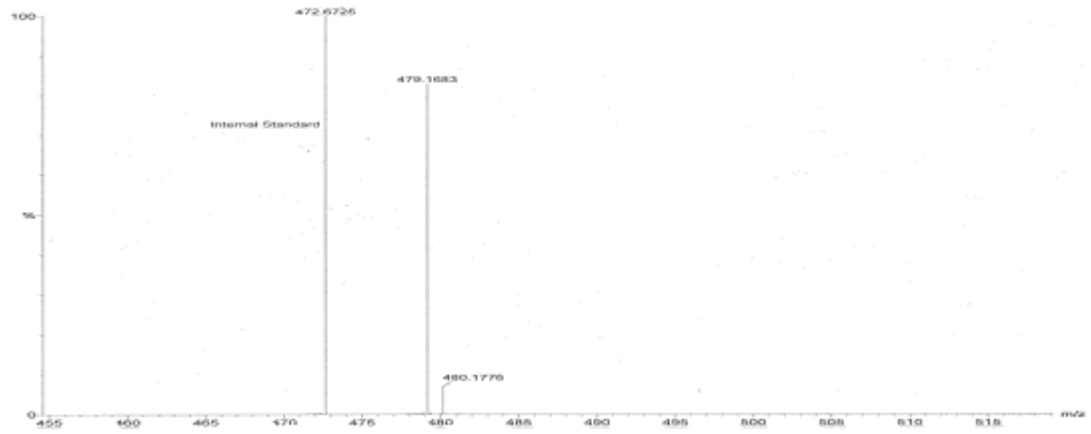


Figure S4b. ^{1}H NMR spectrum of 18-*O*-formyl-3-isomangostin hydrate (**13**) from α-mangostin

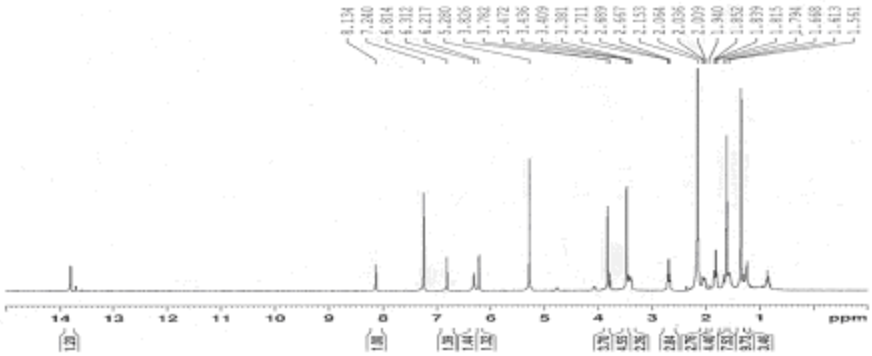


Figure S4c. ^{13}C NMR spectrum of 18-*O*-formyl-3-isomangostin hydrate (**13**) from α-mangostin

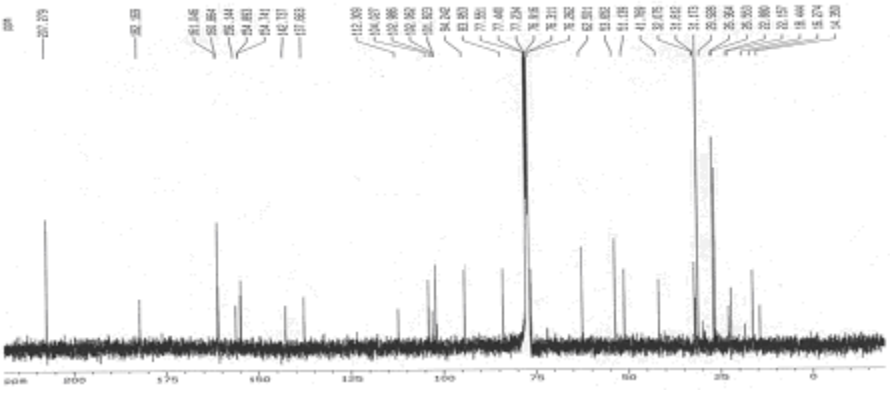


Figure S5a. Mass spectrum of 3,7-di-*O*-acetylcochinchinone A (**16**) from cochinchinone A

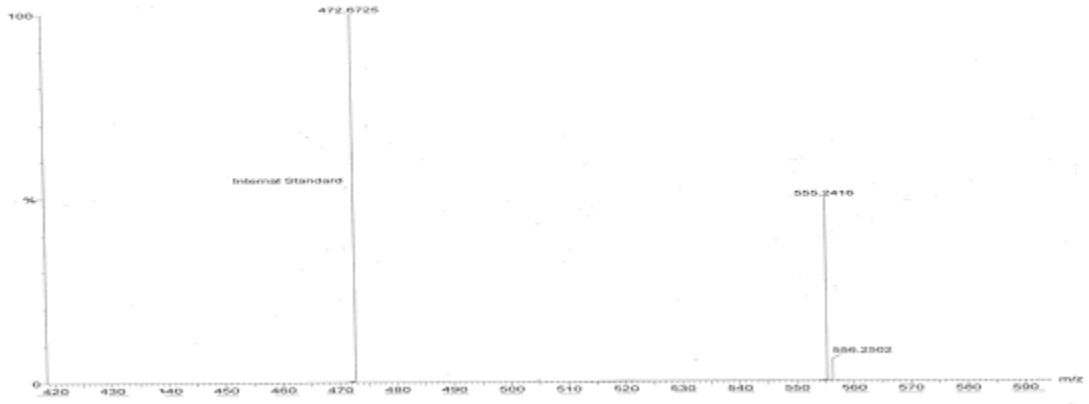


Figure S5b. ^{1}H NMR spectrum of 3,7-di-*O*-acetylcochinchinone A (**16**) from cochinchinone A

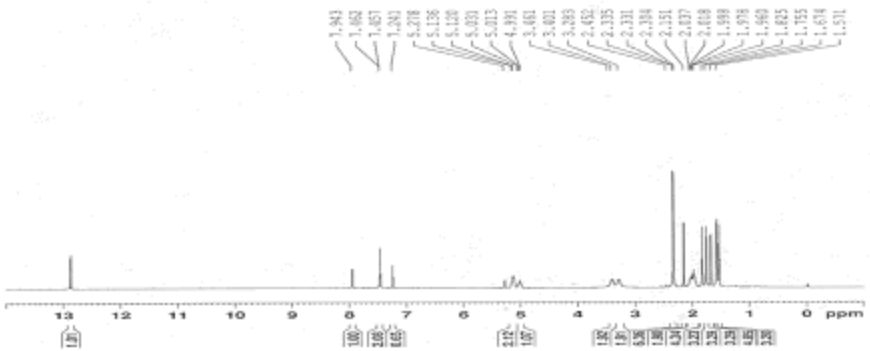


Figure S5c. ^{13}C NMR spectrum of 3,7-di-*O*-acetylcochinchinone A (**16**) from cochinchinone A

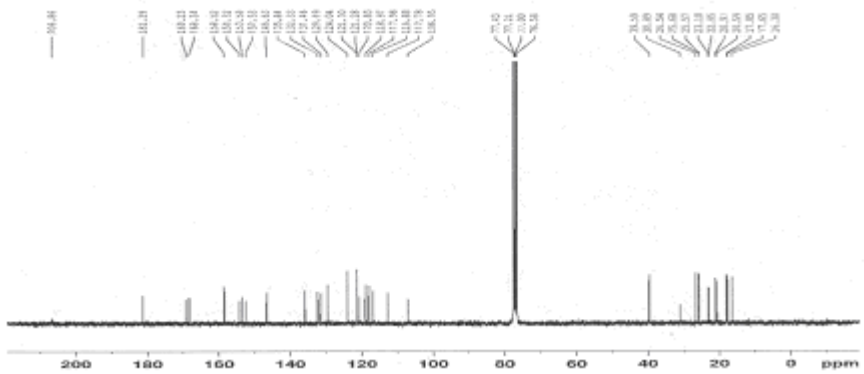


Figure S6a. Mass spectrum of 7-*O*-methylcochinchinone A (**17**) from cochinchinone A

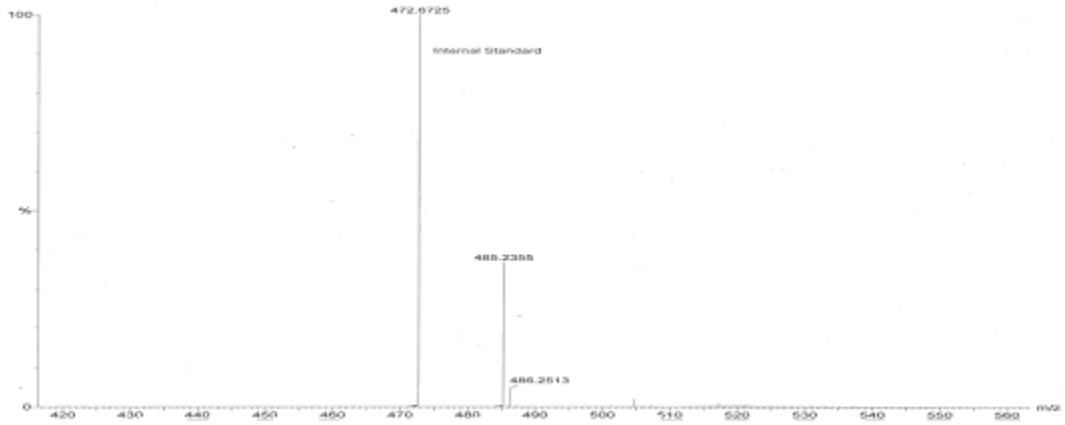


Figure S6b. ^{1}H NMR spectrum of 7-*O*-methylcochinchinone A (**17**) from cochinchinone A

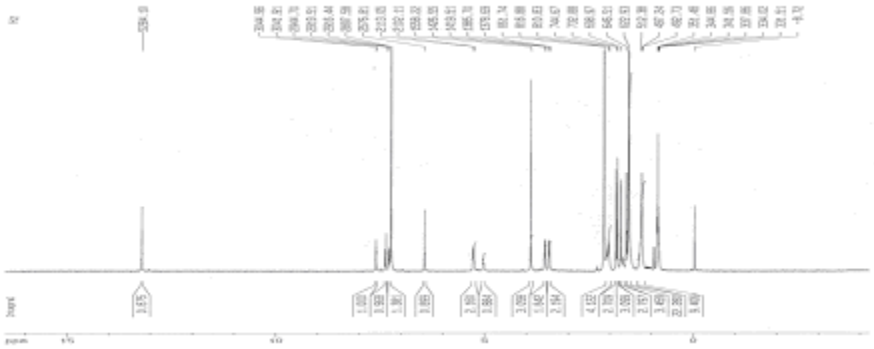


Figure S6c. ^{13}C NMR spectrum of 7-*O*-methylcochinchinone A (**17**) from cochinchinone A

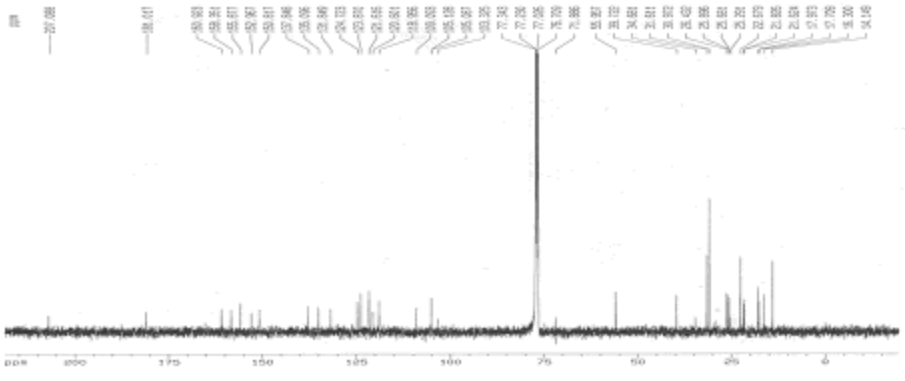


Figure S7a. Mass spectrum of 3,7-di-*O*-methylcochinchinone A (**18**) from cochinchinone A

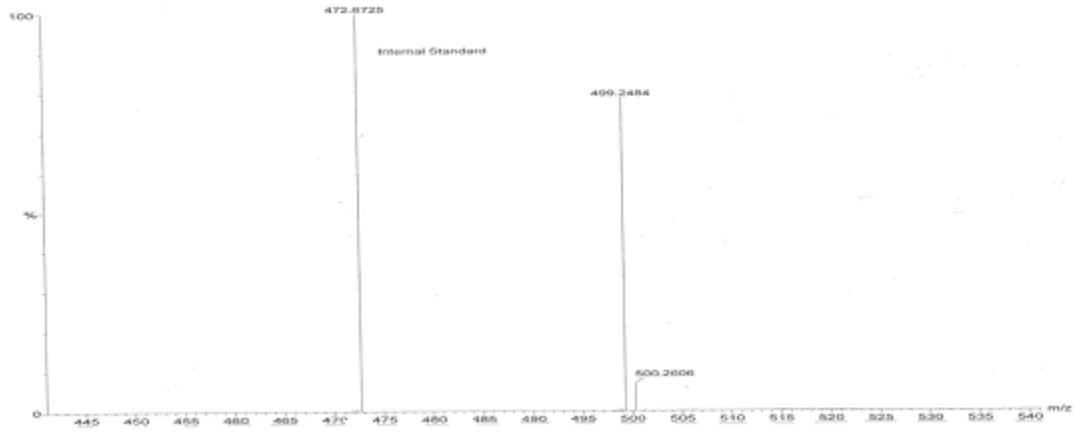


Figure S7b. ^{1}H NMR spectrum of 3,7-di-*O*-methylcochinchinone A (**18**) from cochinchinone A

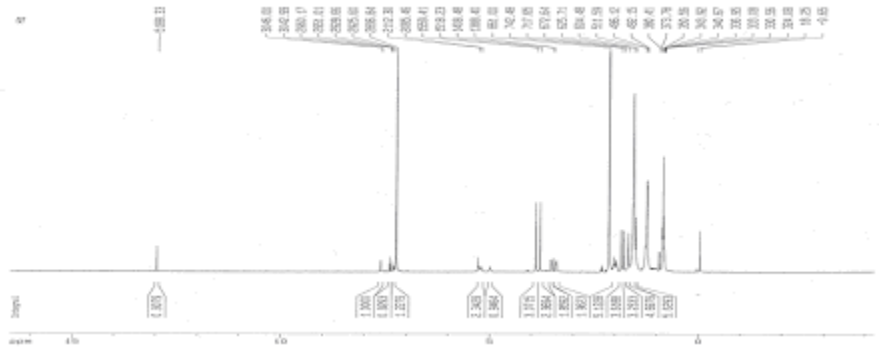


Figure S7c. ^{13}C NMR spectrum of 3,7-di-*O*-methylcochinchinone A (**18**) from cochinchinone A

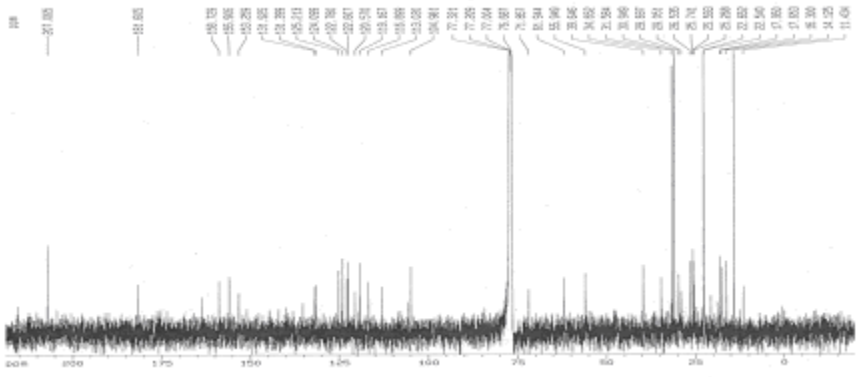


Figure S8a. Mass spectrum of 7-*O*-benzoylcochinchinone A (**19**) from cochinchinone A

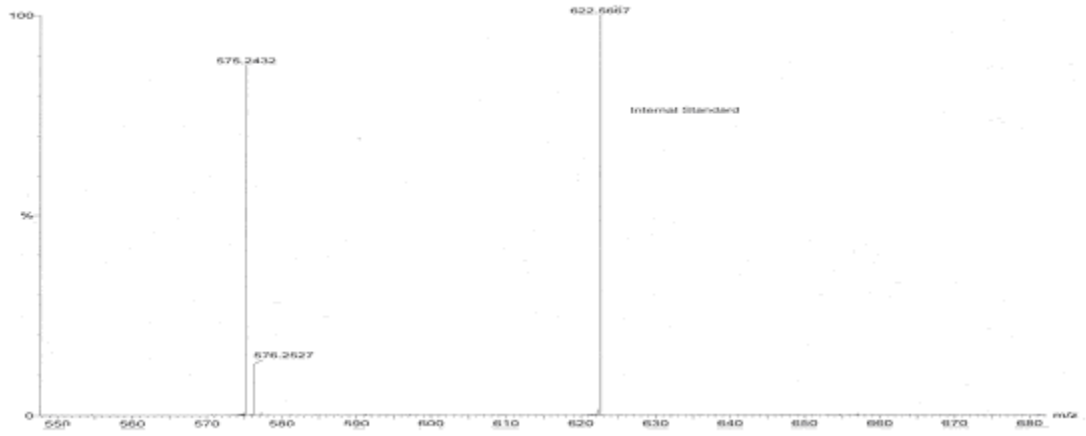


Figure S8b. ^{1}H NMR spectrum of 7-*O*-benzoylcochinchinone A (**19**) from cochinchinone A

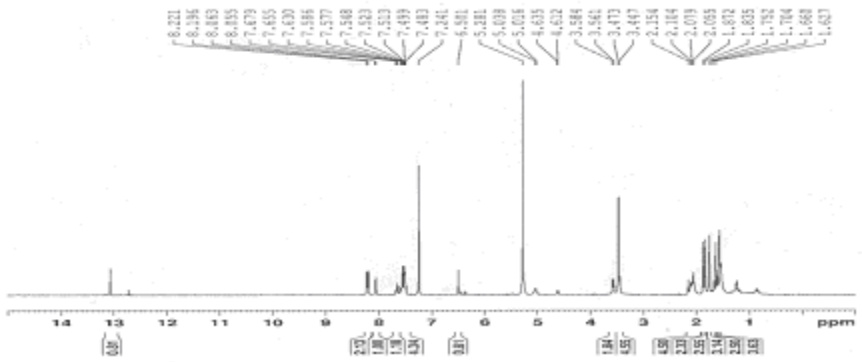
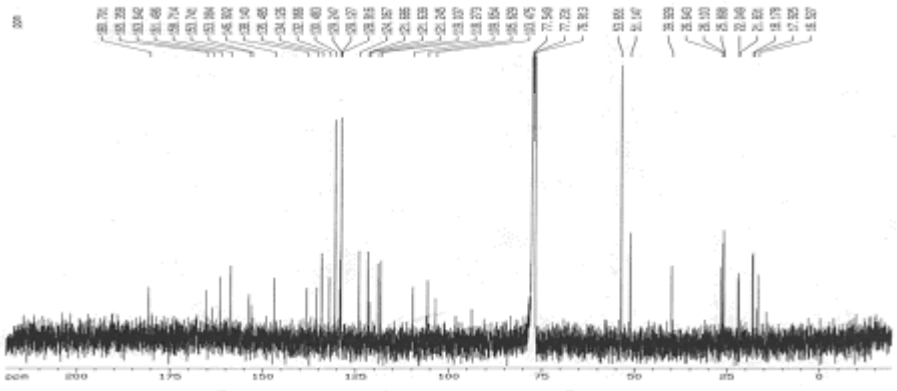
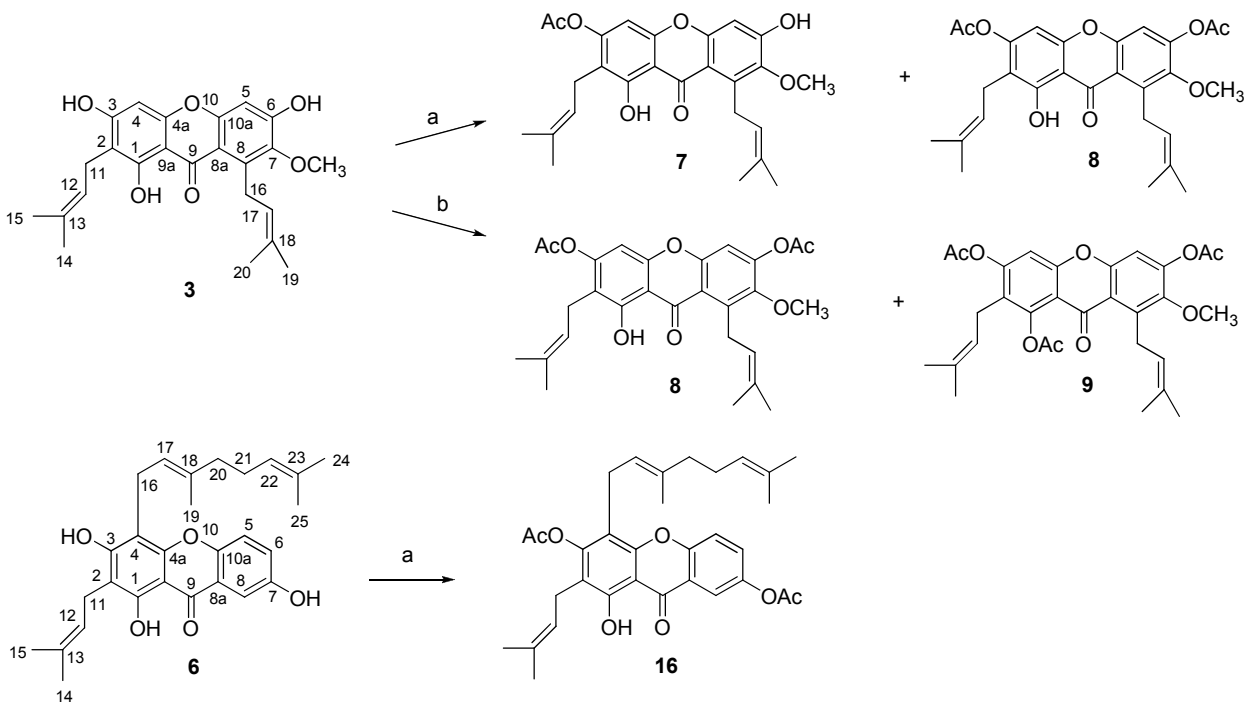


Figure S8c. ^{13}C NMR spectrum of 7-*O*-benzoylcochinchinone A (**19**) from cochinchinone A

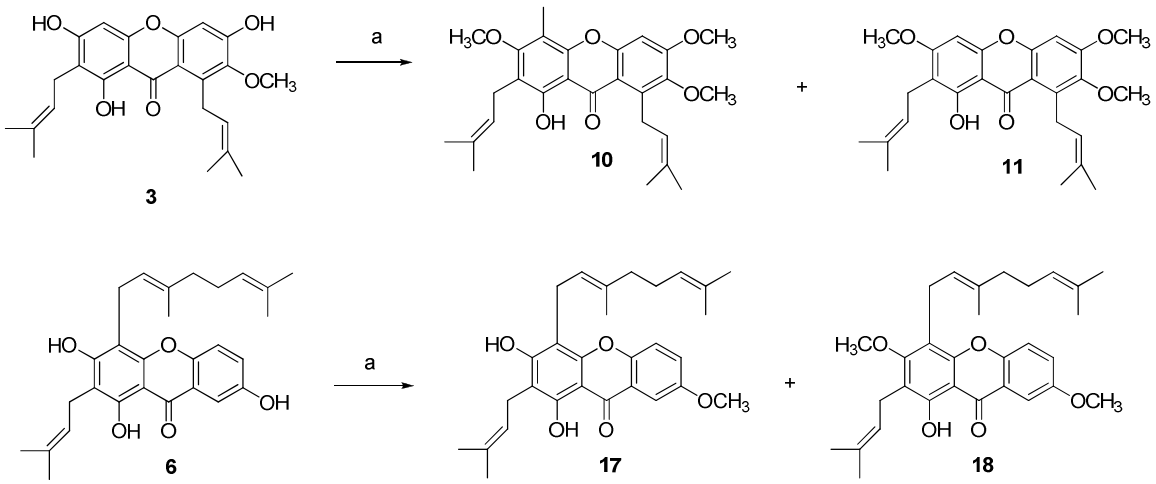


Scheme S1. Acetylation of α-mangostin (**3**) and cochinchinone A (**6**).



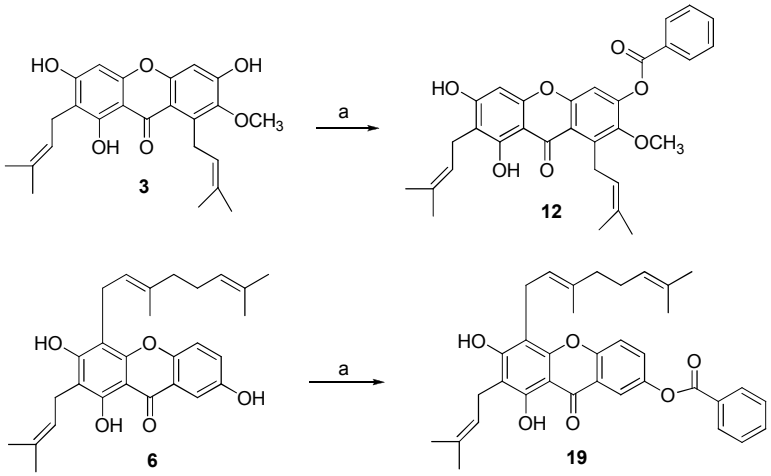
a: acetic anhydride and pyridine, 60 ºC, 1 h. b: acetic anhydride and pyridine, 70 ºC, 2 h.

Scheme S2. Methylation of α-mangostin (**3**) and cochinchinone A (**6**).



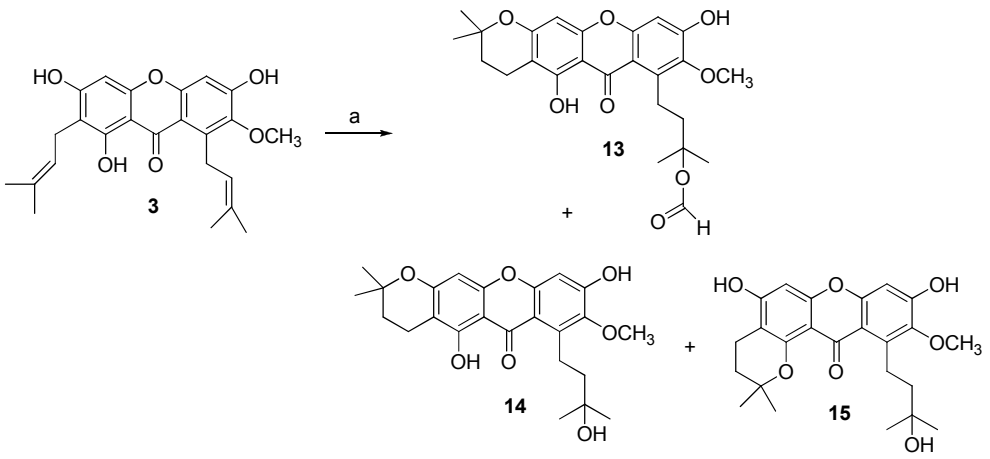
a: methyl iodide and silver oxide (1:1) in dichloromethane, reflux, 2 h.

Scheme S3. Benzoylation of α-mangostin (**3**) and cochinchinone A (**6**).



a: benzoic acid and DCC in dichloromethane, reflux, 2 h.

Scheme S4. Cyclization of α-mangostin (**3**).



a: formic acid and DCC in dichloromethane, reflux, 2 h.

Table S1. ^{1}H NMR Spectroscopic Data of Compounds **3-7**

position	**3**[a]	**4**[b]	**5**[c]	**6**[c]	**7**[c]
4	6.28 d (1.2)	6.37 s			6.59 s
5	6.82 d (1.2)	6.81 s	7.37 d (9.0)	7.27 d (9.0)	6.82 s
6			7.24 dd (3.0, 9.0)	7.22 dd (2.4, 9.0)	
8			7.59 d (3.0)	7.61 d (2.4)	
11	3.45 d (7.2)	3.36 d (7.1)	3.47 d (7.2)	3.46 d (6.5)	3.03 d (7.0)
12	5.29 t (7.2)	5.33 m	5.26 t (7.2)	5.31 t (6.5)	5.23 m
13					
14	1.76 s	1.64 s	1.76 s	1.76 s	1.67 s
15	1.83 s	[i]1.78 s	1.84 s	1.84 s	1.76 s
16	4.09 d (6.3)	4.20 d (6.7)	3.54 d (6.9)	3.55 d (6.5)	4.07 d (6.3)
17	5.25 t (6.3)	5.33 m	5.28 t (6.9)	5.26 t (6.5)	5.23 m
19	1.68 s	1.64 s	1.72 s	1.87 s	1.67 s
20	1.81 s	[i]1.84 s	1.87 s	2.09 m	1.81 s
21				2.09 m	
22				5.04 t (6.5)	
24				1.63 s	
25				1.57 s	
OMe-7	3.79 s				3.79 s
OAc-3					2.36 s
OH-1	13.78 s	13.97 s	13.15 s	12.98 s	13.60 s
OH-3	6.13 s				
OH-6	6.29 s				6.34 s
OH-7			6.44 s		

[a]Data (δ) measured in acetone-d_6 at 300 MHz. [b]Data (δ) measured in acetone-d_6 at 400 MHz. [c]Data (δ) measured in $CDCl_3$ at 300 MHz. s = singlet, d = doublet, t = triplet, m = multiplet, dd = double doublet. *J* values presented in Hz and omitted if the signals overlapped as multiplets. [i]interchangeable.

Table S2. ^{13}C NMR Spectroscopic Data of Compounds **3**-**7**

position	**3**[a]	**4**[b]	**5**[c]	**6**[c]	**7**[d]
1	160.7 C	162.8 C	158.3 C	158.3 C	160.9 C
2	108.4 C	99.4 C	108.8 C	109.2 C	115.9 C
3	161.6 C	161.8 C	160.9 C	161.1 C	156.0 C
4	93.3 CH	93.0 CH	105.3 C	105.1 C	100.2 CH
4a	155.1 C	155.8 C	153.1 C	153.0 C	154.4 C
5	101.6 CH	101.2 CH	119.1 CH	119.0 CH	101.6 CH
6	154.5 C	149.6 C	123.7 CH	124.0 CH	153.6 C
7	142.6 C	141.8 C	151.8 C	152.3 C	142.7 C
8	137.1 C	131.4 C	109.3 CH	109.0 CH	137.2 C
8a	112.3 C	110.8 C	120.9 C	120.6 C	112.2 C
9	182.1 C	183.3 C	180.8 C	180.9 C	182.6 C
9a	103.7 C	103.8 C	103.3 C	103.2 C	106.8 C
10a	155.8 C	153.6 C	150.7 C	150.4 C	155.0 C
11	21.5 CH_2	22.1 CH_2	21.7 CH_2	21.6 CH_2	22.3 CH_2
12	121.4 CH	123.6 CH	122.8 CH	121.6 CH	121.4CH
13	135.8 C	131.4 C	135.5 C	135.0 C	132.4 C
14	25.8 CH_3	[i]26.1 CH_3	25.8 CH_3	25.8 CH_3	25.7 CH_3
15	18.0 CH_3	[ii]18.4 CH_3	17.9 CH_3	17.9 CH_3	18.2 CH_3
16	26.6 CH_2	26.5 CH_2	21.9 CH_2	21.8 CH_2	26.6 CH_2
17	123.2 CH	124.6 CH	122.5 CH	121.6 CH	122.8 CH
18	132.1 C	129.1 C	133.8 C	137.9 C	132.2 C
19	25.8 CH_3	[i]26.0 CH_3	25.8 CH_3	16.3 CH_3	25.8 CH_3
20	18.2 CH_3	[ii]18.0 CH_3	17.9 CH_3	39.7 CH_2	17.8 CH_3
21				26.4 CH_2	
22				123.9 CH	
23				131.8 C	
24				25.6 CH_3	
25				17.7 CH_3	
OMe-7	62.1 CH_3				62.1 CH_3
Me-4					
OAc-3					168.6 C
					21.0 CH_3

[a]Data (δ) measured in acetone-d_6 at 75.5 MHz. [b]Data (δ) measured in acetone-d_6 at 100.6 MHz. [c]Data (δ) measured in $CDCl_3$ at 75.5 MHz. [d]Data (δ) measured in $CDCl_3$ at 100.6 MHz. [i,ii]interchangeable.

Table S3. ^{1}H NMR Spectroscopic Data of Compounds **8, 9**, **11**-**13**

position	**8**	**9**	**11**	**12**	**13**
4	6.62 s	7.09 s	6.31 s	6.30 s	6.22 s
5	7.11 s	7.11 s	6.72 s	7.24 s	6.81 s
11	3.31 d (6.9)	3.25 d (6.9)	3.35 d (6.9)	3.47 d (6.9)	2.71 t (6.6) m
12	5.16 m	5.01 t (6.9)	5.23 m	5.23 m	1.85 t (6.6)
14	1.67 s	1.65 s	1.67 s	1.76 s	1.35 s
15	1.76 s	1.73 s	1.78 s	1.83 s	1.35 s
16	4.13 d (6.3)	4.06 d (5.4)	4.13 d (6.3)	4.17 d (6.3)	3.41 m
17	5.16 m	5.16 t (5.4)	5.23 m	5.23 m	2.06 m
19	1.67 s	1.65 s	1.67 s	1.67 s	1.61 s
20	1.82 s	1.80 s	1.83 s	1.81 s	1.61 s
OMe-3			3.89 s		
OMe-6			3.94 s		
OMe-7	3.79 s	3.74 s	3.78 s	3.75 s	3.83 s
OAc	2.37 s	2.44 s			
OAc	2.32 s	2.36 s			
OAc		2.32 s			
3'				8.24 d (7.5)	
4'				7.56 t (7.5)	
5'				7.68 t (7.5)	
6'				7.56 t (7.5)	
7'				8.24 d (7.5)	
OH-1	13.30 s		13.42 s	13.60 s	13.89 s
OH-3				6.19 s	
OH-6					6.31 s
OH-7					
OCOH-13					8.13 s

Data (δ) measured in $CDCl_3$ at 300 MHz. s = singlet, d = doublet, t = triplet, m = multiplet. *J* values presented in Hz and omitted if the signals overlapped as multiplets.

Table S4. ^{13}C NMR Spectroscopic Data of Compounds **8, 9, 11-13**

position	**8**[a]	**9**[a]	**11**[a]	**12**[b]	**13**[b]
1	161.0 C	154.5 C	159.9 C	160.9 C	161.1 C
2	[i]116.2 C	120.9 C	111.6 C	108.8 C	104.0 C
3	154.9 C	148.8 C	163.4 C	162.4 C	160.9 C
4	100.3 CH	108.9 CH	88.6 CH	93.7 CH	94.2 CH
4a	153.7 C	153.2 C	155.4 C	154.1 C	154.9 C
5	110.6 CH	110.2 CH	98.2 CH	110.9 CH	103.0 CH
6	149.4 C	148.5 C	158.0 C	149.4 C	156.1 C
7	146.8 C	146.8 C	144.0 C	146.9 C	142.7 C
8	139.2 C	139.0 C	137.3 C	139.2 C	137.7 C
8a	[i]116.9 C	118.9 C	112.2 C	117.2 C	112.3 C
9	182.9 C	176.1 C	182.0 C	182.5 C	182.2 C
9a	107.1 C	113.6 C	104.0 C	104.2 C	102.1 C
10a	154.1 C	153.1 C	155.2 C	155.4 C	154.7 C
11	22.3 CH_2	23.5 CH_2	21.4 CH_2	21.7 CH_2	16.3 CH_2
12	121.3 CH	123.0 CH	122.3 CH	121.5 CH	32.1 CH_2
13	132.3 C	132.4 C	131.8 C	136.3 C	76.3 C
14	[ii]25.7 CH_3	[iii]25.6 CH_3	25.8 CH_3	26.1 CH_3	27.0 CH_3
15	18.2 CH_3	18.2 CH_3	17.8 CH_3	18.2 CH_3	27.0 CH_3
16	26.5 CH_2	26.2 CH_2	26.2 CH_2	26.7 CH_2	22.2 CH_2
17	122.6 CH	123.6 CH	123.3 CH	123.1 CH	41.8 CH_2
18	132.3 C	131.7 C	131.7 C	132.4 C	84.0 C
19	[ii]25.8 CH_3	[iii]25.8 CH_3	25.9 CH_3	26.1 CH_3	26.6 CH_3
20	17.8 CH_3	17.9 CH_3	18.2 CH_3	18.4 CH_3	26.6 CH_3
OMe-3			55.8 CH_3		
OMe-6			56.0 CH_3		
OMe-7	61.7 CH_3	61.6 CH_3	60.9 CH_3	62.1 CH_3	62.5 CH_3
OAc	167.9 C	169.2 C			
	20.9 CH_3	21.2 CH_3			
OAc	168.4 C	168.1 C			
	21.0 CH_3	21.0 CH_3			
OAc		168.0 C			
		21.0 CH_3			
1'				164.3 C	
2'				128.9 C	
3'				130.6 CH	
4'				129.0 CH	
5'				134.4 CH	
6'				129.0 CH	
7'				130.6 CH	
OCOH-13					161.1 CH

[a]Data (δ) were measured in $CDCl_3$ at 75.5 MHz. [b]Data (δ) were measured in $CDCl_3$ at 100.6 MHz. [i, ii,or iii]interchangeable.

Table S5. ^{1}H NMR Spectroscopic Data of Compounds **14**, **15**, 3-Geranyloxy-1,7-dihydroxyxanthone, 1,7-Dihydroxy-4-methoxyxanthone, and Euxanthone

position	**14**[a]	**15**[a]	3-geranyloxy-1,7-dihydroxyxanthone[a]	1,7-dihydroxy-4-methoxyxanthone[b]	euxanthone[c]
2			6.32 d (2.2)	6.73 d (9.0)	6.78 d (8.2)
3				7.25 d (9.0)	7.72 t (8.2)
4	6.20 s	6.37 s	6.52 d (2.2)		7.02 d (8.2)
5	6.81 s	6.71 s	7.47 d (9.3)	7.54 d (9.0)	7.54 d (9.0)
6			7.37 dd (3.3, 9.3)	7.33 dd (3.0, 9.0)	7.45 dd (3.0, 9.0)
8			7.57 d (3.3)	7.61 d (3.0)	7.61 d (3.0)
11	2.66 m	2.67 m	4.73 d (7.0)		
12	1.88 m	1.84 m	5.49 t (7.0)		
14	1.35 s	1.37 s	1.79 s		
15	1.35 s	1.37 s	2.14 m		
16	3.48 m	3.38 m	2.14 m		
17	1.81 m	1.80 m	5.06 t (6.6)		
19	1.30 s	1.28 s	1.63 s		
20	1.30 s	1.28 s	1.59 s		
OMe-3				3.96 s	
OMe-7	3.84 s	3.80 s			
OH-1	13.98 s		12.90 s	12.01 s	12.72 s
OH-3		9.56 s			
OH-6		9.21 s			

[a]Data (δ) measured in acetone-d_6 at 300 MHz. [b]Data (δ) measured in $CDCl_3$ at 300 MHz. [c]Data (δ) measured in acetone-d_6 at 400 MHz. s = singlet, d = doublet, t = triplet, m = multiplet, dd = double doublet. *J* values presented in Hz and omitted if the signals overlapped as multiplets.

Table S6. ^{13}C NMR Spectroscopic Data of Compounds **14**, **15**, 3-Geranyloxy-1,7-dihydroxyxanthone, 1,7-Dihydroxy-4-methoxyxanthone, and Euxanthone

position	**14**[a]	**15**[a]	3-geranyloxy-1,7-dihydroxyxanthone[a]	1,7-dihydroxy-4-methoxyxanthone[b]	Euxanthone[a]
1	161.8 C	157.6 C	164.3 C	154.7 C	162.8 C
2	104.6 C	107.9 C	98.3 CH	108.5 CH	110.6 CH
3	161.7 C	160.9 C	167.2 C	120.3 CH	137.9 CH
4	94.5 CH	93.7 CH	93.8 CH	140.1 C	107.9 CH
4a	155.7 C	155.6 C	157.9 C	150.9 C	151.2 C
5	102.7 CH	101.9 CH	119.9 CH	119.9 CH	120.4 CH
6	157.6 C	157.0 C	125.4 CH	124.8 CH	126.2 CH
7	144.5 C	144.1 C	150.9 C	146.0 C	154.9 C
8	140.3 C	139.7 C	109.4 CH	109.1 CH	109.2 CH
8a	112.0 C	115.2 C	122.0 C	121.2 C	121.9 C
9	183.0 C	176.6 C	181.5 C	181.9 C	183.1 C
9a	103.4 C	105.4 C	104.1 C	109.2 C	108.0 C
10a	156.6 C	155.1 C	155.1 C	152.1 C	157.4 C
11	16.9 CH_2	17.8 CH_2	66.5 CH_2		
12	32.4 CH_2	32.1 CH_2	120.0 CH		
13	77.0 C	79.3 C	142.4 C		
14	27.0 CH_3	27.0 CH_3	16.8 CH_3		
15	27.0 CH_3	27.0 CH_3	40.2 CH_2		
16	23.3 CH_2	22.7 CH_2	27.0 CH_2		
17	45.8 CH_2	45.6 CH_2	124.7 CH		
18	70.6 C	70.3 C	132.3 C		
19	29.1 CH_3	29.4 CH_3	25.9 CH_3		
20	29.1 CH_3	29.4 CH_3	17.8 CH_3		
OMe-3				57.4 CH_3	
OMe-7	61.7 CH_3	61.7 CH_3			

[a]Data (δ) measured in acetone-d_6 at 100.6 MHz. [b]Data (δ) measured in $CDCl_3$ at 75.5 MHz.

Physical data of known xanthones isolated or derivatized from *C. cochinchinense*

α-Mangostin (3): Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 243 (4.80), 256 (4.72), 316 (4.66) nm; IR (dried film) ν_{max} 3400, 2966, 2916, 1645, 1608, 1572, 1464, 1209, 1187, 1157, 1080, 841 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S1 and S2; positive ESIMS *m*/*z* 433.2 for $C_{24}H_{26}O_6Na$.

γ-Mangostin (4): Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 243 (4.34), 259 (4.33), 317 (4.17) nm; IR (dried film) ν_{max} 3387, 2924, 1644, 1615, 1460, 1284, 1196, 785 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S1 and S2; positive ESIMS *m*/*z* 419.1 for $C_{23}H_{24}O_6Na$.

1,3,7-Trihydroxy-2,4-di-isoprenylxanthone (5): Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 237 (4.49), 265 (4.49), 317 (4.16) nm; IR (dried film) ν_{max} 3380, 2975, 2926, 1645, 1616, 1585, 1485, 1344, 1221, 1134, 1095, 804 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S1 and S2; positive ESIMS *m*/*z* 403.2 for $C_{23}H_{24}O_5Na$.

Cochinchinone A (6): Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 235 (4.65), 268 (4.65), 317 (4.31) nm; IR (dried film) ν_{max} 3363, 2914, 1641, 1614, 1570, 1485, 1377, 1232, 1172, 1027, 820 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S1 and S2; positive ESIMS *m*/*z* 471.2 for $C_{28}H_{32}O_5Na$.

3-*O*-Acetyl-α-mangostin (7): Amorphous light yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 236 (4.41), 252 (4.37), 308 (4.19) nm; IR (dried film) ν_{max} 3393, 2917, 2849, 1750, 1632, 1606, 1575, 1464, 1432, 1375, 1278, 1159, 1073 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S1 and S2; positive ESIMS *m*/*z* 475.2 for $C_{26}H_{28}O_7Na$.

3,6-Di-*O*-acetyl-α-mangostin (8): Amorphous light yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 237 (4.61), 262 (4.66), 294 (4.25) nm; IR (dried film) ν_{max} 3444, 2917, 1773, 1646, 1603, 1459, 1426, 1373, 1274, 1180, 1142, 1024, 887 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S3 and S4; positive ESIMS *m*/*z* 517.1 for $C_{28}H_{30}O_8Na$.

3,6,7-Tri-*O*-acetyl-α-mangostin (9): Amorphous white powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 242 (4.82), 262 (4.48), 294 (4.20) nm; IR (dried film) ν_{max} 2919, 2852, 1775, 1658, 1618, 1456, 1425, 1369, 1263, 1191, 1139, 1067, 896 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S3 and S4; positive ESIMS *m*/*z* 559.2 for $C_{30}H_{32}O_9Na$.

3,6-Di-*O*-methyl-α-mangostin (11): Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 244 (4.72), 261 (4.73), 312 (4.56) nm; IR (dried film) ν_{max} 2927, 1647, 1599, 1458, 1427, 1375, 1278, 1214, 1173, 825 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S3 and S4; positive ESIMS *m*/*z* 461.3 for $C_{26}H_{30}O_6Na$.

6-*O*-Benzoyl-α-mangostin (12): Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 241 (4.66), 311 (4.31) nm; IR (dried film) ν_{max} 3404, 2924, 1748, 1646, 1458, 1424, 1259, 1178, 1061, 1024, 770 cm^{-1}; ^{1}H and ^{13}C NMR data, see Table S3 and S4; positive ESIMS *m*/*z* 537.3 for $C_{31}H_{30}O_7Na$.

18-*O*-Formyl-3-isomangostin hydrate (13): Amorphous white powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 242 (4.30), 318 (4.21) nm; IR (dried film) ν_{max} 3382, 2978, 1648, 1601, 1463, 1371, 1285, 885 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S3 and S4; positive ESIMS *m*/*z* 479.1 for $C_{25}H_{28}O_8Na$.

3-Isomangostin hydrate (14): Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 243 (4.41), 317 (4.24) nm; IR (dried film) ν_{max} 2931, 1646, 1601, 1463, 1285, 1158, 811 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S5 and S6; positive ESIMS *m*/*z* 451.2 for $C_{24}H_{28}O_7Na$.

1-Isomangostin hydrate (15): Amorphous white powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 244 (4.46), 305 (4.26) nm; IR (dried film) ν_{max} 2929, 2854, 1651, 1625, 1597, 1459, 1368, 1275, 1157, 1088 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S5 and S6; positive ESIMS *m*/*z* 451.3 for $C_{24}H_{28}O_7Na$

3-Geranyloxy-1,7-dihydroxyxanthone: Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 237 (4.38), 259 (4.52), 309 (4.12) nm; IR (dried film) ν_{max} 3383, 2922, 1653, 1610, 1575, 1488, 1301, 1165, 1080, 791 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S5 and S6; positive ESIMS *m*/*z* 403.2 for $C_{23}H_{24}O_5Na$.

1,7-Dihydroxy-4-methoxyxanthone: Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 236 (4.18), 267 (4.20) nm; IR (dried film) ν_{max} 3362, 1651, 1608, 1582, 1489, 1363, 1284, 1237, 1176, 1086, 1046, 810 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S5 and S6; positive ESIMS *m*/*z* 281.1 for $C_{14}H_{10}O_5Na$.

Euxanthone: Amorphous yellow powder (*n*-hexane) showing a purple color under UV light at 365 nm; UV (MeOH) λ_{max} (log ε) 235 (4.95), 259 (5.05) nm; IR (dried film) ν_{max} 3351, 1645, 1609, 1476, 1361, 1234, 1048, 829 cm^{-1}; ^{1}H and ^{13}C NMR data, see Tables S5 and S6; positive ESIMS *m*/*z* 251.1 for $C_{13}H_8O_4Na$.

Evaluation of 3,6-di-*O*-acetyl-α-mangostin (**8**) in an in vivo hollow fiber assay