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¹H and ¹³C NMR spectral assignments of novel chromenylchalcones

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Several types of chalcones containing 2*H*-chromen group were synthesized. Claisen–Schmidt condensation of 2*H*-chromen-3carbaldehydes (I) with methoxy substituted acetophenones afforded (*E*)-3-(2*H*-chromen-3-yl)-1-(methoxyphenyl)prop-2-en-1ones (chromenylchalcones, 1–7). Other types of chromenylchalcone, (*E*)-1-(6-methoxy-2*H*-chromen-3-yl)-3-(methoxyphenyl) prop-2-en-1-ones (8–13) were also obtained between reaction of methoxy substituted benzaldehydes and 1-(6-methoxy-2*H*chromen-3-yl)ethanone (II). Dichromenylchalcones (14–16) were also synthesized through the same reaction between aldehydes (I) and ketone (II). Their complete ¹H-NMR and ¹³C-NMR assignments are reported here and more polysubstituted chromenylchalcones synthesized or isolated from the natural sources in the future can be identified on the basis of the NMR data reported here. Copyright © 2012 John Wiley & Sons, Ltd.

Keywords: NMR; ¹ H NMR; ¹³C NMR; 2D NMR; flavonoid; chalcone

Introduction

Chalcones are one of the secondary metabolites in plants and belong to a flavonoid class with C6-C3-C6 skeletone, which are named A, C, and B-ring [Fig. 1{A)]. Instead of a closed C-ring of flavonoid, however, C3 skeleton of chalcone is α,β -unsaturated carbonyl group [Fig. 1(B)]. Because of their diverse biological activities, various chalcones have been isolated from natural sources and synthesized, and their NMR data have been reported.^[1-3] Benzoflavones are one of the flavonoids, too, and contain one more benzene ring attached to A-ring [Fig. 1(C)]. It has been known that they act as potent inhibitors of breast cancer resistance protein.^[4,5] Because of diverse biological activities of chalcones and benzoflavones, we designed three types of novel chromenylchalcones combined with chalcone and chromenes, which are analogs of benzoflavone, and synthesized them: seven (E)-3-(2H-chromen-3-yl)-1-phenylprop-2-en-1-ones [Fig. 1(D)], six (E)-1-(6-methoxy-2H-chromen-3-yl)-3-phenylprop-2-en-1-ones [Fig. 1 (E)], and three (E)-3-(2H-chromen-3-yl)-1-(6-methoxy-2H-chromen-3-yl) prop-2-en-1-ones [Fig. 1(F)]. Because their NMR data can help us identify newly isolated or synthesized chromenylchalcone derivatives, we report here the complete ¹H and ¹³C NMR data of 16 chromenylchalcones (Fig. 2).

Experimental

Synthesis

All of the chromenylchalcone derivatives (1-16) were synthesized as shown in Scheme 1. Methoxy or bromo substituted salicylaldehydes were treated with acrolein in the presence of K₂CO₃ in dioxane to give corresponding 2*H*-chromen-3-carbaldehydes (I). When the same conditions were applied in reaction between 5-methoxy salicylaldehyde and methylvinylketone, 1-(6-methoxy-2*H*-chromen-3-yl)ethanone (II) was obtained in good yield. Michaels addition of salicylaldehydes to acrolein or

methylvinylketone followed by intramolecular aldol condensation accounts for the formation of chromene aldehydes (I) or chromene methyl ketone (II). Claisen–Schmidt condensation of chromene aldehydes (I) with methoxy substituted acetophenone under basic conditions afforded (*E*)-3-(2*H*-chromen-3-yl)prop-2-en-1ones (chromenylchalcones, **1–7**) as we described in the previous report.^[6] When chromene methyl ketone (II) was treated with methoxy substituted benzaldehydes under the same conditions, other types of chromenylchalcone **8–13** were also obtained. Dichromenylchalcones (**14–16**) were synthesized through the same reaction between chromene aldehydes (I) and chromene methyl ketone (II). To confirm the structures of the synthetic compounds, mass spectrometry was performed on a high-resolution electron impact ionization mass spectrometer (HREIMS, JMS700, Jeol Ltd., Tokyo, Japan).

NMR spectra

The synthetic chromenylchalcones were dissolved in DMSO- d_6 . The ¹H and ¹³C chemical shifts of the deuterated solvent were 2.50 and 39.5 ppm referenced to TMS, respectively. The NMR samples were prepared at approximately 50 mM, and they were transferred to a 2.5-mm NMR tube. All NMR experiments were carried out on a Bruker Avance 400 spectrometer system

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Figure 1. Structures of (A) flavone, (B) chalcone, (C) benzoflavone, (D) (*E*)-3-(2*H*-chromen-3-yl)-1-phenylprop-2-en-1-one, (E) (*E*)-1-(6-methoxy-2*H*-chromen-3-yl)-3-phenylprop-2-en-1-one, and (F) (*E*)-3-(2*H*-chromen-3-yl)-1- (6-methoxy-2*H*-chromen-3-yl)prop-2-en-1-one.

(9.4 T; Bruker, Karlsruhe, Germany) at 298 K. For the ¹ H NMR analyses, 16 transients were acquired with a 1 s relaxation delay using 32 K data points. The 90° pulse duration was of 11.8 µs, and the spectral width was 4800 Hz. The ¹³C NMR spectra were obtained with a spectral width of 21,000 Hz using 64 K data points. The 90° pulse duration was of 15.0 µs. For the two-dimensional experiments including COSY, TOCSY, NOESY, HMQC, and HMBC, all data were acquired with 2 K × 256 data points ($t_2 \times t_1$). The mixing time for the NOESY experiment was 1 s, and the long-range coupling time for HMBC was 70 ms. Zero-filling of 2 K and the sine-squared bell window function were applied before Fourier transformation using XWin-NMR (Bruker).^[7] All NMR data were analyzed using Sparky.^[8]

Results and Discussion

All chromenylchalcone derivatives (**1–16**) are novel. The procedure to assign the NMR data of chromenylchalcone **16**, (*E*)-1-(6-methoxy-2H-chromen-3-yl)-3-(8-methoxy-2H-chromen-3-yl)prop-2-en-1-one, is explained in detail here. Twenty-three peaks were observed in the ¹³C NMR spectrum. Of them, the most downfield shifted peak at 186.2 ppm was caused by the carbon of ketone group. It showed long-ranged couplings with the ¹H peaks at 7.14 and 7.35 ppm in the HMBC spectrum, which were attached to the ¹³C peaks at 120.0 and 139.4 ppm in the HMQC spectrum, respectively, so that they were assigned C- α and C- β , respectively. In addition, a cross peak between two protons at 7.14 and 7.35 ppm was observed in the COSY spectrum. Because H- β was correlated with two protons at 5.11 and 7.10 ppm attached to two carbons at 65.6 (triplet carbon) and 131.5 (doublet carbon), respectively; they were



de staardere e		mass (m/z)		D	р.	D	D	р.
derivatives	name	(calcd/found)	К1	K ₂	R 3	\mathbf{K}_4	\mathbf{K}_5	к ₆
1	(E)-3-(6-methoxy -2H- chromen -3-yl)-1-(4- methoxyphenyl)prop -2-en-1- one	322.3545/322.1206	Н	н	OMe	н	OMe	Н
2	(E)- 3-(6-methoxy -2H- chromen -3-yl)-1-(3,5- dimethoxyphenyl)prop-2-en- 1-one	352.3805/352.1312	Н	OMe	Н	OMe	OMe	Н
3	(E)-3-(7-methoxy -2H- chromen -3-yl)-1-(4- methoxyphenyl)prop -2-en-1- one	322.3545/322.1205	Н	Н	OMe	Н	Н	OMe
4	(E)-3-(6-methoxy -2H- chromen -3-yl)-1-(2- methoxyphenyl)prop -2-en-1- one	322.3545/322.1205	OMe	н	Н	н	OMe	Н
5	(E)-3-(6-bromo -2H- chromen -3-yl)-1-(3- methoxyphenyl)prop -2-en-1- one	371.2246/370.0201	Н	OMe	Н	Н	Br	Н
6	(E)-3-(6-bromo -2H- chromen -3-yl)-1-(2- methoxyphenyl)prop -2-en-1- one	371.2246/370.0207	OMe	н	Н	Н	Br	Н
7	(E)-3-(6-bromo -2H- chromen -3-yl)-1-(3,5- dimethoxyphenyl)prop -2-en- 1-one	401.2506/400.0312	Н	OMe	Н	OMe	Br	Н



derivatives	name	mass (m/z) (calcd/found)	R_1	R_2	R_3	R_4	R_5
8	(E)-1-(6-methoxy-2H- chromen-3-yl)-3-(3,5- dimethoxyphenyl)prop-2-en- 1-one	352.3805/352.1313	н	OMe	н	OMe	н
9	(E)-1-(6-methoxy-2H- chromen-3-yl)-3-(2,4- dimethoxyphenyl)prop-2-en- 1-one	352.3805/353.1375	OMe	Н	OMe	Н	Н
10	(E)-1-(6-methoxy-2H- chromen-3-yl)-3-(2,4,5- trimethoxyphenyl)prop-2-en- 1-one	382.4065/383.1458	OMe	н	OMe	OMe	н
11	(E)-1-(6-methoxy-2H- chromen-3-yl)-3-(2,4,6- trimethoxyphenyl)prop-2-en- 1-one	382.4065/383.1468	OMe	Н	OMe	Н	OMe
12	(E)-1-(6-methoxy-2H- chromen-3-yl)-3-(2- methoxyphenyl) prop-2-en-1- one	322.3545/323.1266	OMe	Н	Н	Н	Н
13	(E)-1-(6-methoxy-2H- chromen-3-yl)-3-(4- methoxyphenyl) prop-2-en-1- one	322.3545/323.1273	Н	н	OMe	Н	Н



Figure 2. Structures, nomenclature, and HREIMS data of chromenylchalcones 1–16.



Scheme 1. Synthetic methods used to prepare chromenylchalcones 1–16.

determined to be H-2' and H-4', respectively. In the HMBC spectrum, C-4' was long-range coupled to the proton at 6.81 ppm, and it was assigned H-5'. C-5' (120.0 ppm), determined on the basis of the HMQC spectrum, showed a long-ranged coupling with the proton at 6.98 ppm, so that it was determined H-7'. From the interpretation of the COSY spectrum, the ¹H peak at 6.90 ppm was assigned H-6'. Because of the long-ranged coupling between the carbon peak at 147.4 ppm and H-6' was observed in the HMBC spectrum, it was C-8'. The methoxy proton at 3.79 ppm showed a long-ranged coupling with C-8', so that it was assigned 8'-OMe. The carbon (143.1 ppm) showing long-range couplings with H-5' and H-7' was determined C-9'. Because the ¹³C at 122.7 ppm was longrange coupled to H-6', it was C-10'. Of the two methoxy carbons at 55.7 and 55.5 ppm, because the former was assigned 8'-OMe, the later should be 6-OMe. The carbon showing the long-range coupling with the proton of 6-OMe at 3.75 ppm was observed at 154.0 ppm, which was assigned C-6. The proton at 6.85 ppm showing the long-ranged coupling with C-6 was H-8. Likewise, the carbon observed at 121.6 ppm was C-10. A triplet carbon at 63.8 ppm was C-2. From the interpretation of HMBC,

Table 1. The ¹ H NMR chemical shifts of chromenylchalcones 1–16										
δ of ¹ H (J, Hz)										
Position	1	2	3	4	5	6	7	8		
2	8.12(d, 8.8)	7.22(d, 2.3)	8.10(d, 8.7)	_	7.49(d, 2.7)	_	7.22(d, 2.2)	4.96(s)		
3	7.08(d, 8.8)		7.07(d, 8.7)	7.18(d, 8.4)	—	7.19(d, 8.4)	—			
4	—	6.79(d, 2.3)	_	7.54 (ddd, 1.8,	7.23(dd,	7.54 (ddd, 2.0,	6.80(d, 2.2)	8.06(s)		
5	7.08(d, 8.8)	_	7.07(d, 8.7)	7.06(d, 7.4)	7.49(d, 7.9)	7.06(d, 7.5)	_	6.98(d, 3.0)		
6	8.12(d, 8.8)	7.22(d, 2.3)	8.10(d, 8.7)	7.48(dd,	7.62(d, 7.9)	7.43(dd,	7.22(d, 2.2)	_		
				1.8, 7.4)		2.0, 7.5)				
7	_	_	_	_	_	_	_	6.93(dd,		
8	_	_	_	_	_	_	_	6.86(d, 8.8)		
2′	5.10(s)	5.10(s)	5.14(s)	4.98(s)	4.26(s)	4.16(s)	5.20(s)	7.04(d, 2.2)		
4'	7.08(s)	7.12(s)	7.08(s)	7.04(s)	7.28(s)	7.17(s)	7.12(s)	6.60(d, 2.2)		
5'	6.82(m)	6.82(m)	7.14(d, 8.4)	6.80(m)	7.57(d, 2.5)	7.56(d, 2.5)	7.41(d, 2.5)	_		
6′	—	_	6.55(dd, 2.2, 8.4)	—	_	_	_	7.04(d, 2.2)		
7′	6.82(m)	6.82(m)	_	6.80(m)	7.36(dd, 2.5, 8.7)	7.36(dd, 2.5, 8.7)	7.36(dd, 2.5, 8.6)	—		
8′	6.82(m)	6.82(m)	6.49(d, 2.2)	6.80(m)	6.85(d, 8.7)	6.85(d, 8.7)	6.84(d, 8.6)	_		
α	7.28(d, 15.5)	7.22(d, 15.5)	7.18(d, 15.5)	6.79(d, 15.5)	7.33(d, 15.5)	7.02(d, 15.7)	7.24(d, 15.4)	7.79(d, 15.6)		
β	7.43(d, 15.5)	7.45(d, 15.5)	7.42(d, 15.5)	7.21(d, 15.5)	7.49(d, 15.5)	7.26(d, 15.7)	7.42(d, 15.4)	7.55(d, 15.6)		
2-OMe	—	_	—	3.86(s)	—	3.87(s)	—			
3-OMe	—	3.84(s)	—	—	3.84(s)	—	3.84(s)	—		
4-OMe	3.88(s)	_	3.87(s)	—	_	_	—	_		
5-OMe	—	3.84(s)	_	—	—	—	3.84(s)	—		
6-OMe			—	—	—	—	—	3.75(s)		
3'-OMe			—	—	—	—	—	3.82(s)		
5'-OMe	—		—	—	—	—	—	3.82(s)		
6'-OMe	3.73(s)	3.72(s)	—	3.71(s)	—	_	—	—		
7'-OMe	—	—	3.77(s)	δ of ¹ H (J, Hz)	_	_	_	—		
Position	9	10	11	12	13	14	15	16		
2	4.94(d, 0.7)	4.95(d, 0.7)	4.93(d, 0.9)	4.95(d, 0.9)	4.95(s)	4.93(s)	4.93(s)	4.94(s)		
4	7.92(s)	7.91(s)	7.72(s)	7.99(s)	8.00(s)	7.96(s)	7.93(s)	7.96(s)		

(Continues)

Table 1. (Continued)											
δ of ¹ H (J, Hz)											
Position	9	10	11	12	13	14	15	16			
5	6.97(d, 3.0)	6.97(d, 3.0)	7.10(d, 3.0)	6.97(d, 3.0)	6.95(d, 2.6)	6.93(s)	6.93(s)	6.95(s)			
7	7.90(dd,	6.90(dd, 3.0,	6.88(dd,	6.91(dd,	6.91(dd,	6.92(m)	6.90(m)	6.93(d, 8.6)			
	3.0, 8.8)	8.8)	3.0, 8.8)	3.0, 8.8)	2.6, 8.8)						
8	6.83(d, 8.8)	6.83(d, 8.8)	6.82(d, 8.8)	6.84(d, 8.8)	6.83(d, 8.8)	6.84(m)	6.83(m)	6.85(d, 8.6)			
2′	—	—		—	7.80(d, 8.5)	5.06(s)	5.11(s)	5.11(s)			
3′	6.64(s)	6.74(s)	6.32(s)	7.11(d, 8.4)	7.02(d, 8.5)	—	—	—			
4′	—	—	_	7.45 (ddd, 1.6,	—	7.07(s)	7.07(s)	7.10(s)			
				7.5, 8.4)							
5′	6.63(m)	—	6.32(s)	7.04(d, 7.5)	7.02(d, 8.5)	6.80(m)	7.13(d, 8.4)	6.81(dd,			
								1.4, 7.9)			
6′	7.87(d, 8.9)	7.47(s)	—	7.93(dd, 1.6, 7.5)	7.80(d, 8.5)	_	6.55(d, 8.4)	6.90(m)			
7′	—	—	—	—	—	6.81(m)	—	6.98(dd, 1.4,			
								7.9)			
8′				_		6.81(m)	6.49(s)				
α	7.62(d, 15.6)	7.60(d, 15.7)	7.72(d, 15.7)	7.75(d, 15.8)	7.67(d, 15.5)	7.15(d, 15.5)	7.05(d, 15.4)	7.14(d, 15.5)			
β	7.88(d, 15.6)	7.93(d, 15.7)	7.98(d, 15.7)	7.94(d, 15.8)	7.58(d, 15.5)	7.33(d, 15.5)	7.33(d, 15.4)	7.35(d, 15.5)			
6-OMe	3.74(s)	3.74(s)	3.74(s)	3.74(s)	3.74(s)	3.74(s)	3.75(s)	3.75(s)			
2'-OMe	3.90(s)	3.89(s)	3.93(s)	3.89(s)	—	—	—	—			
3'-OMe	—	—	—	_	—	_	_	—			
4'-OMe	3.84(s)	3.87(s)	3.86(s)	_	3.82(s)	_	_	—			
5'-OMe	—	3.82(s)	_	_	—	—	—	—			
6'-OMe	—	—	3.93(s)	_	—	3.71(s)	—	—			
7'-OMe	—	—	—	_	—	—	3.77(s)	—			
8'-OMe			—	—				3.79(s)			

Table 2. The ¹³ C NMR chemical shifts of chromenylchalcones 1–16										
δ of ¹³ C										
Position	1	2	3	4	5	6	7	8		
1	131.2	139.6	130.5	128.7	139.2	128.8	139.4	_		
2	131.4	106.3	130.7	157.7	112.7	157.7	106.3	63.9		
3	114.5	160.7	113.9	112.3	159.5	112.4	160.7	131.8		
4	163.7	104.8	163.1	133.0	119.0	133.0	105.0	134.1		
5	114.5	160.7	113.9	120.5	130.0	120.6	160.7	113.3		
6	131.4	106.3	130.7	129.4	120.7	129.5	106.3	154.0		
7	—	—	—	—	—	—	—	118.5		
8	—	—	—	—		—	—	116.7		
9	—	—	—	—	—	—	—	148.9		
10	—	—	—	—	—	—	—	121.6		
1′	—	—	—	—	—	—	—	136.6		
2′	65.2	64.61	64.9	64.5	64.7	65.4	64.9	106.7		
3′	130.9	130.6	126.8	130.2	134.8	134.7	130.9	160.7		
4′	131.9	132.0	131.5	131.4	137.8	137.3	130.2	102.5		
5′	112.7	112.2	129.2	112.2	132.0	132.0	130.0	160.7		
6′	154.4	153.9	108.0	153.9	109.8	109.8	112.8	106.7		
7′	117.0	116.7	161.7	116.5	132.6	132.6	133.0	—		
8′	116.7	116.3	101.3	116.2	117.5	117.6	117.7	—		
9′	148.6	148.2	155.7	148.0	155.5	155.6	153.4	—		
10′	123.3	122.7	115.3	122.6	124.9	125.0	124.2	—		
α	121.9	121.4	119.8	126.3	122.0	127.2	122.2	121.2		
β	140.5	141.0	140.5	139.4	147.1	145.6	140.5	142.5		
C=0	187.6	188.4	187.0	191.8	189.2	192.2	188.4	186.5		
2-OMe	—	—	—	55.7	—	55.7	—	—		

(Continues)

Table 2. (Continued)

				δ of ¹³ C				
Position	1	2	3	4	5	6	7	8
3-OMe	_	55.5	_		55.3	_	55.5	_
4-OMe	56.1	_	55.5		_	—	_	—
5-OMe	_	55.5	—	—	—	—	55.5	—
6-OMe	—	_	—		_	—	_	55.4
3'-OMe	_	—	—	—	—	—	_	55.5
5'-OMe	—	—	—	—	—	—	—	55.5
6'-OMe	56.0	55.4	—	55.4	—	—	_	—
7'-OMe	—	—	55.4	—	—	—	—	—
				δ of ¹³ C				
Position	9	10	11	12	13	14	15	16
2	64.0	64.1	64.2	63.9	63.9	63.8	63.9	63.8
3	132.1	132.2	132.4	131.9	131.9	131.8	131.9	131.8
4	132.9	132.7	131.7	133.7	133.4	133.8	133.4	133.8
5	113.3	113.2	113.7	113.4	113.3	113.2	113.1	113.2
6	153.9	153.9	153.9	153.9	153.9	154.0	153.9	154.0
7	118.0	118.1	117.9	118.3	118.2	118.5	118.3	118.5
8	116.5	116.6	116.4	116.6	116.6	116.6	116.6	116.7
9	148.7	148.8	148.7	148.8	148.8	148.8	148.8	148.8
10	121.7	121.7	121.7	121.6	121.7	121.6	121.6	121.6
1′	115.9	114.2	105.0	122.9	127.3	—	_	—
2′	159.8	154.2	161.3	158.1	130.5	64.7	64.9	65.6
3′	98.2	97.5	91.0	111.8	114.4	130.4	126.5	129.7
4'	163.0	152.9	163.2	132.2	161.2	131.5	131.7	131.5
5′	106.3	143.0	91.0	120.4	114.4	112.2	129.2	120.0
6′	129.5	111.1	161.3	128.0	130.5	153.9	108.1	121.5
7′	_	_	_	—	—	116.5	161.8	114.2
8′	—	—	_	—	—	116.2	101.2	147.4
9′	_	_	_	—	_	148.1	155.7	143.1
10′	—	—	_	—	—	122.7	115.3	122.7
α	117.7	117.4	119.0	120.6	118.3	120.2	118.5	120.0
β	137.0	136.9	133.8	136.7	142.3	139.2	139.7	139.4
C = 0	186.5	186.5	187.4	186.6	186.4	186.2	186.1	186.2
6-OMe	55.4	55.5	55.5	55.4	55.4	55.4	55.4	55.5
2'-OMe	55.8	56.4	56.1	55.7	—	—	—	—
4'-OMe	55.5	55.8	55.5		55.3	_	_	—
5'-OMe	—	56.5	—		—	_	—	—
6'-OMe	—	—	56.1	_	_	55.4	_	—
7'-OMe	_	—	—	—	—	—	55.4	—
8'-OMe	_	—	—	_	—		—	55.7

C-4 (133.8 ppm), C-9 (148.8 ppm), H-7 (6.93 ppm), and H-5 (6.95 ppm) were determined. Two undetermined carbons at 129.7 and 131.8 ppm were decided to be C-3' and C-3, respectively, based on the long-ranged couplings with H- α and H- β , respectively. The complete assignments of the ¹H and ¹³C NMR data of chromenylchalcone **16** are listed in Tables 1 and 2, respectively. Similarly, the ¹H and ¹³C NMR data of 15 chromenylchalcones were acquired and are listed in Tables 1 and 2, respectively.

Chromenylchalcones synthesized here consist of three types: (*E*)-3-(2*H*-chromen-3-yl)-1-methoxyphenylprop-2-en-1-ones (**1–7**), (*E*)-1-(6-methoxy-2*H*-chromen-3-yl)-3-methoxyphenylprop-2-en-1-ones (**8–13**), and (*E*)-3-(2*H*-chromen-3-yl)-1-(6-methoxy-2*H*chromen-3-yl)prop-2-en-1-ones (**14–16**). Chromenylchalcones **2** and **8** contain the same number and position of the substituents. Although the ¹³C chemical shifts of C-2 and C-6 of chromenylchalcone **2** are upfield shifted than those of C-2' and C-6' of chromenylchalcone **8**, the chemical shift of C-4 of chromenylchalcone **2** is downfield shifted than C-4' of chromenylchalcone **8**. Likewise, chromenylchalcones **1** and **13** contain the same number and position of the substituents. The ¹³C chemical shifts of C-1–C-6 of chromenylchalcone **1** where benzene ring is attached to ketone group are downfield shifted than those of C-1'–C-6' of chromenylchalcone **13** where benzene ring is attached to C- β . This trend is observed in chromenylchalcones **8–13** where 2*H*-chromene group is attached to ketone group and in chromenylchalcones **1**, **2**, and **4** where 2*H*-chromene group is attached to C- β . The ¹³C chemical shifts contained in 2*H*-chromene group except C-2 and C-10 of chromenylchalcones **8–13** are downfield shifted than those of chromenylchalcones **1**, **2**, and **4**. In

dichromenylchalcones **14–16**, even the position of methoxy group is different with each other, the ¹³C chemical shift of C-2 is upfield shifted than that of C-2'. The ¹³C chemical shifts of C- α , C- β , and carbonyl carbon of (*E*)-3-(2*H*-chromen-3-yl)-1-phenylprop-2-en-1-ones (**1–7**) are downfield shifted than those of (*E*)-1-(6-methoxy-2*H*-chromen-3-yl)-3-phenylprop-2-en-1-ones (**8–13**). The reversed trends are observed in the ¹H chemical shifts: The ¹H chemical shifts of H- α and H- β of chromenylchalcones **1–7** are upfield shifted than those of chromenylchalcones **8–13**. More polysubstituted chromenylchalcones synthesized or isolated from the natural sources in the future can be identified on the basis of the NMR data reported here.

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