

# Supplementary materials

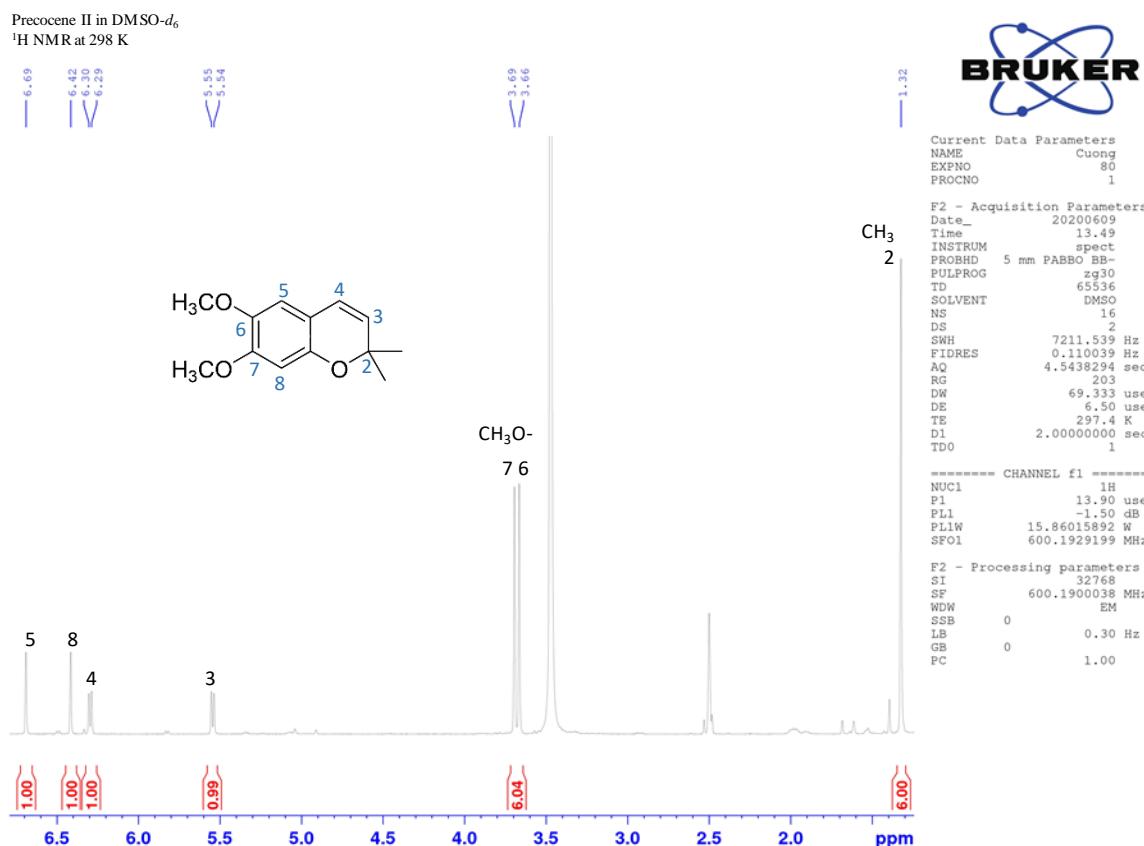
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**Table S1:** NMR data of compound **1** (Precocene II) identified from *A. conyzoides* L. extract in DMSO-*d*<sub>6</sub>

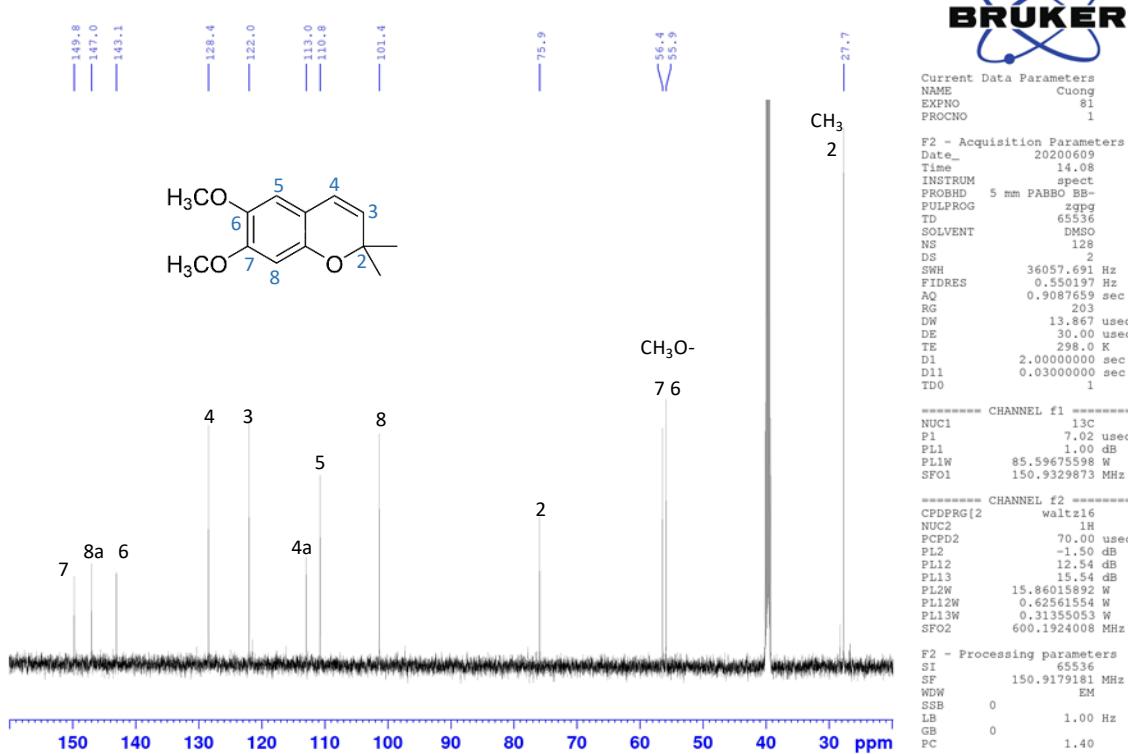
Position	<sup>13</sup> C NMR (150 MHz)	<sup>1</sup> H NMR (600 MHz)
<b>2</b>	75.9	
<b>3</b>	122.0	5.55 (1H, d, <i>J</i> =9.5 Hz)
<b>4</b>	128.4	6.30 (1H, d, <i>J</i> =9.5 Hz)
<b>4a</b>	113.0	
<b>5</b>	110.8	6.69 (1H, s)
<b>6</b>	143.1	
<b>7</b>	149.8	
<b>8</b>	101.4	6.42 (1H, s)
<b>8a</b>	147.0	
-CH <sub>3</sub>	27.7	1.32 (6H, s)
-OCH <sub>3</sub>	55.9	3.69 (3H, s)
	56.4	3.66 (3H, s)

Ref. González *et al.*, *Phytochemistry* **1991**, *30*, 1137–1139.



**Figure S1:** <sup>1</sup>H NMR spectrum of compound **1** recorded in DMSO-*d*<sub>6</sub>

Precocene II in DMSO-*d*<sub>6</sub>  
<sup>13</sup>C NMR at 298 K

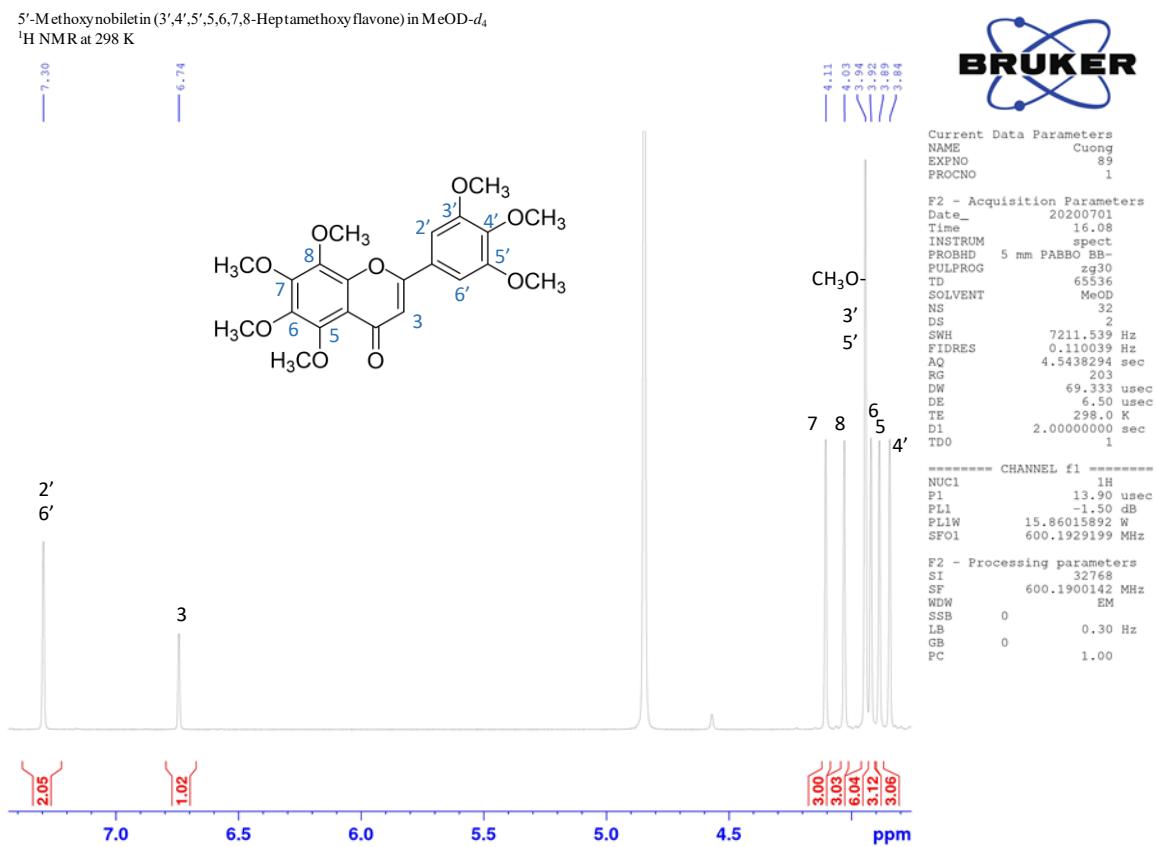


**Figure S2:** <sup>13</sup>C NMR spectrum of compound 1 recorded in DMSO-*d*<sub>6</sub>

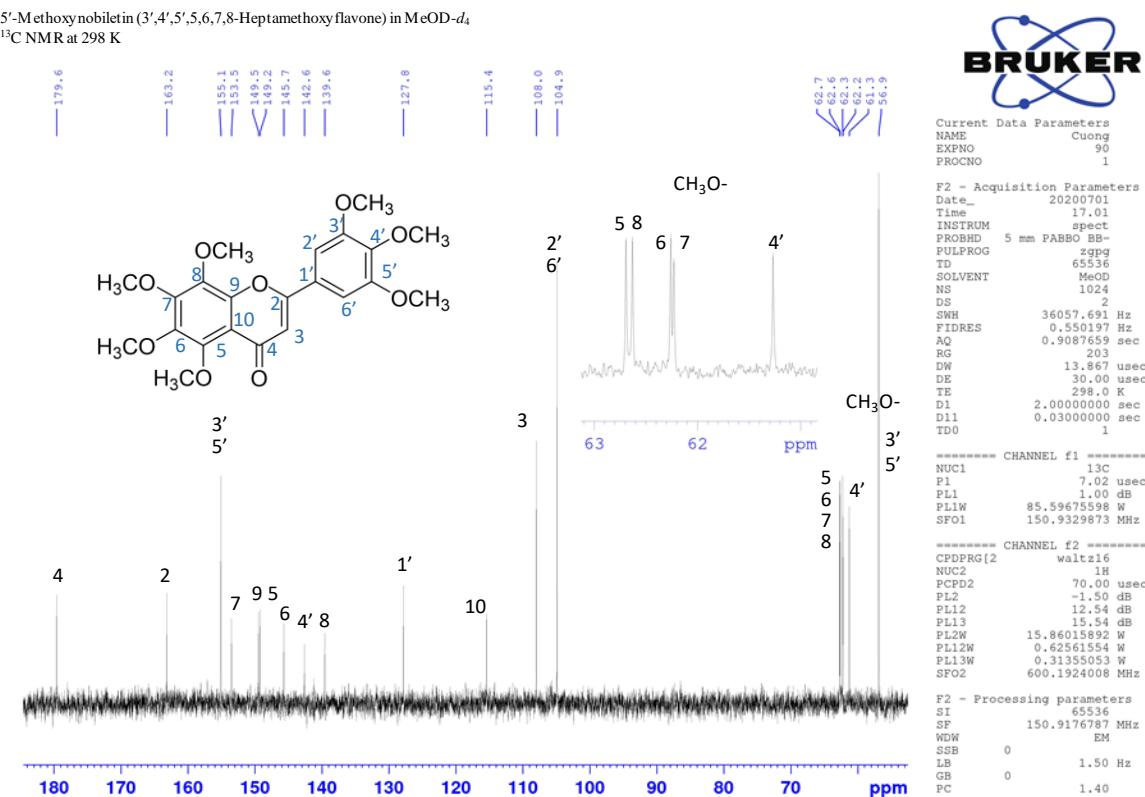
**Table S2:** NMR data of compound **2** (5'-Methoxynobeleitin) identified from *A. conyzoides* L. extract in MeOD-*d*<sub>4</sub>

Position	<sup>13</sup> C NMR (150 MHz)	<sup>1</sup> H NMR (600 MHz)
<b>2</b>	163.2	
<b>3</b>	108.0	6.74 (1H, s)
<b>4</b>	179.6	
<b>5</b>	149.2	
<b>6</b>	145.7	
<b>7</b>	153.5	
<b>8</b>	139.6	
<b>9</b>	149.5	
<b>10</b>	115.4	
<b>1'</b>	127.8	
<b>2'</b>	104.9	7.30 (2H, s)
<b>3'</b>	155.1	
<b>4'</b>	142.6	
<b>5'</b>	155.1	
<b>6'</b>	104.9	7.30 (2H, s)
<b>5-OCH<sub>3</sub></b>	62.7	3.89 (3H, s)
<b>6-OCH<sub>3</sub></b>	62.3	3.92 (3H, s)
<b>7-OCH<sub>3</sub></b>	62.2	4.11 (3H, s)
<b>8-OCH<sub>3</sub></b>	62.6	4.03 (3H, s)
<b>3'-OCH<sub>3</sub></b>	56.9	3.94 (3H, s)
<b>4'-OCH<sub>3</sub></b>	61.3	3.84 (3H, s)
<b>5'-OCH<sub>3</sub></b>	56.9	3.94 (3H, s)

Ref. Le-Van *et al.*, *Phytochemistry* **1979**, *18*, 1859–1861; Nour *et al.*, *J. Ethnopharmacol.* **2010**, *129*, 127–130.



**Figure S3:**  $^1\text{H}$  NMR spectrum of compound **2** recorded in MeOD- $d_4$



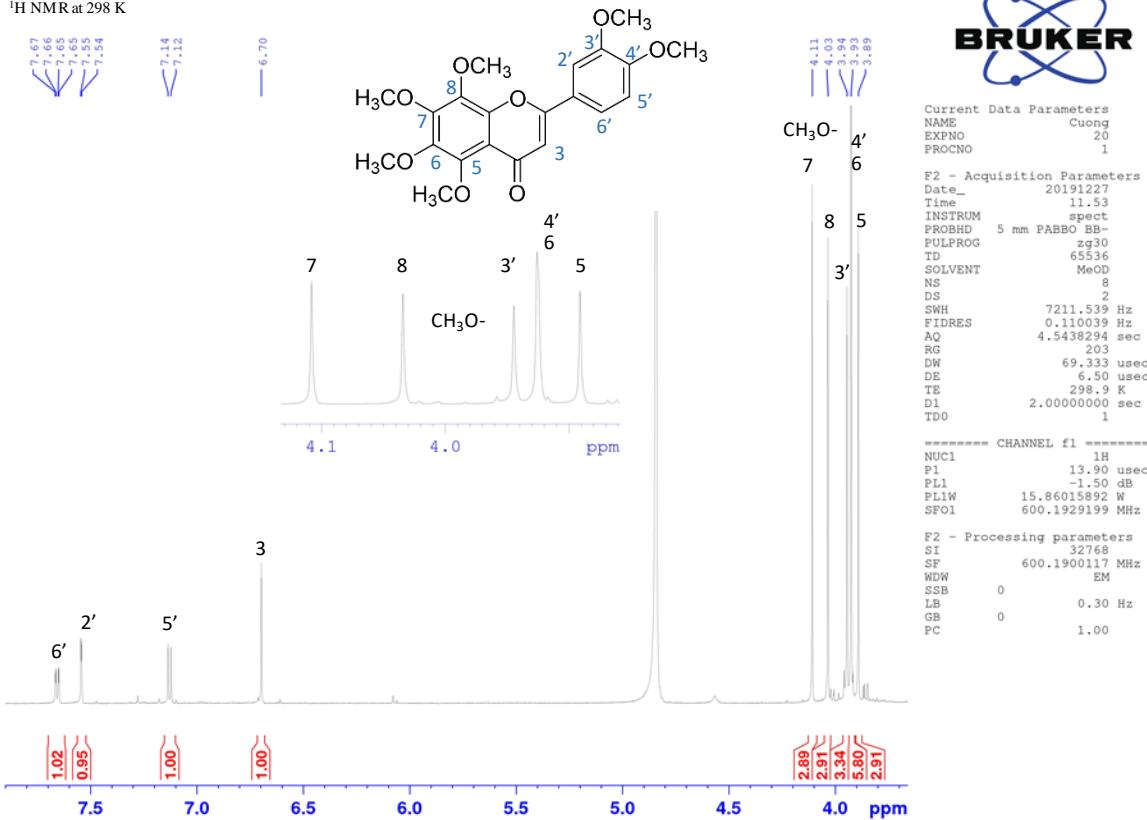
**Figure S4:**  $^{13}\text{C}$  NMR spectrum of compound **2** recorded in  $\text{MeOD-}d_4$

**Table S3:** NMR data of compound **3** (Nobiletin) identified from *A. conyzoides* L. extract in MeOD-*d*<sub>4</sub>

Position	<sup>13</sup> C NMR (150 MHz)	<sup>1</sup> H NMR (600 MHz)	HMBC ( <sup>1</sup> H → <sup>13</sup> C)
<b>2</b>	163.7		
<b>3</b>	107.1	6.70 (1H, s)	C-2, 4, 10, 1'
<b>4</b>	179.7		
<b>5</b>	149.3		
<b>6</b>	145.7		
<b>7</b>	153.5		
<b>8</b>	139.7		
<b>9</b>	149.5		
<b>10</b>	115.5		
<b>1'</b>	124.9		
<b>2'</b>	110.4	7.54 (1H, d, <i>J</i> = 2.0 Hz)	C-2, 3', 4', 6'
<b>3'</b>	151.0		
<b>4'</b>	154.1		
<b>5'</b>	113.0	7.13 (1H, d, <i>J</i> = 8.4 Hz)	C-1', 3', 4'
<b>6'</b>	121.4	7.66 (1H, dd, <i>J</i> = 8.4, 2.0 Hz)	C-2, 2', 4'
<b>5'-OCH<sub>3</sub></b>	62.8	3.89 (3H, s)	C-5
<b>6'-OCH<sub>3</sub></b>	62.4	3.93 (3H, s)	C-6
<b>7'-OCH<sub>3</sub></b>	62.3	4.11 (3H, s)	C-7
<b>8'-OCH<sub>3</sub></b>	62.8	4.03 (3H, s)	C-8
<b>3'-OCH<sub>3</sub></b>	56.7	3.94 (3H, s)	C-3'
<b>4'-OCH<sub>3</sub></b>	56.7	3.93 (3H, s)	C-4'

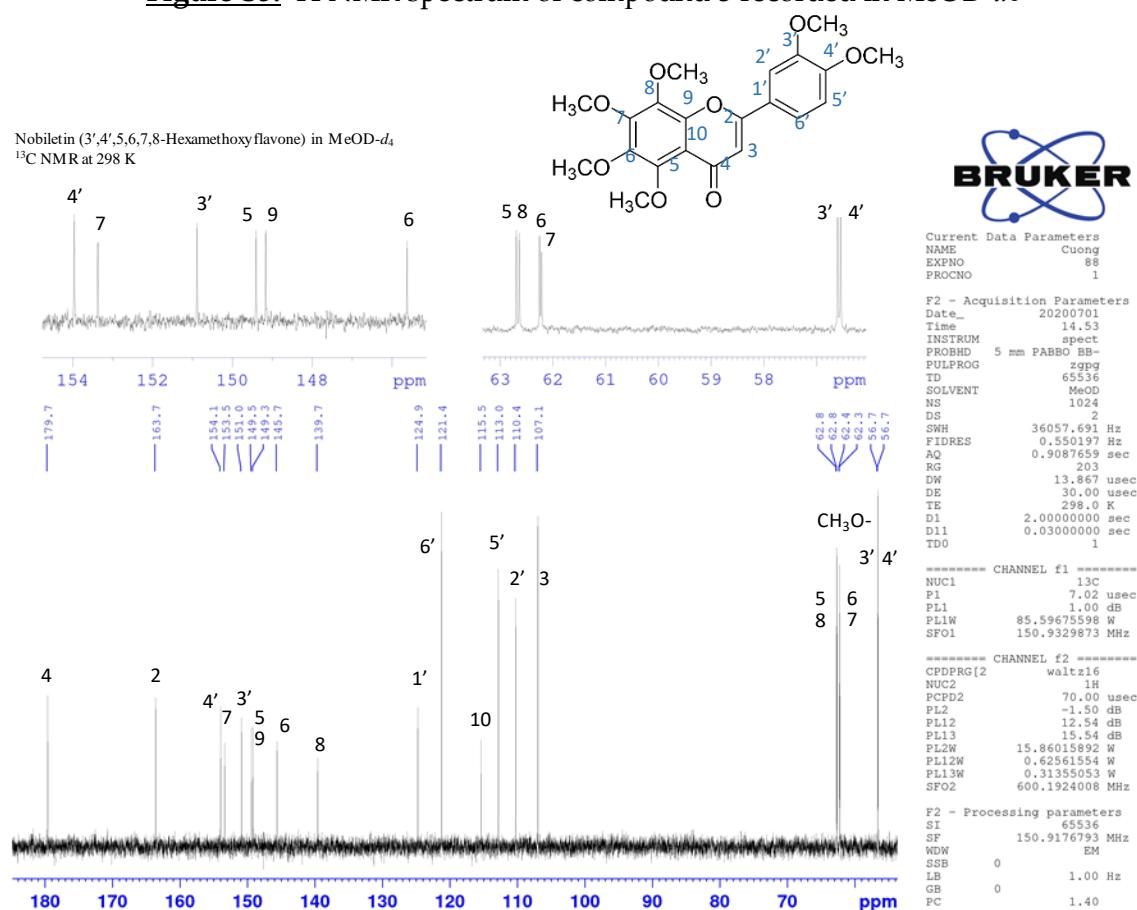
Ref. Chen *et al.*, *J. Agric. Food Chem.* **1997**, *45*, 364–368.

Nobiletin (3',4',5,6,7,8-Hexamethoxyflavone) in MeOD-*d*<sub>4</sub>  
<sup>1</sup>H NMR at 298 K

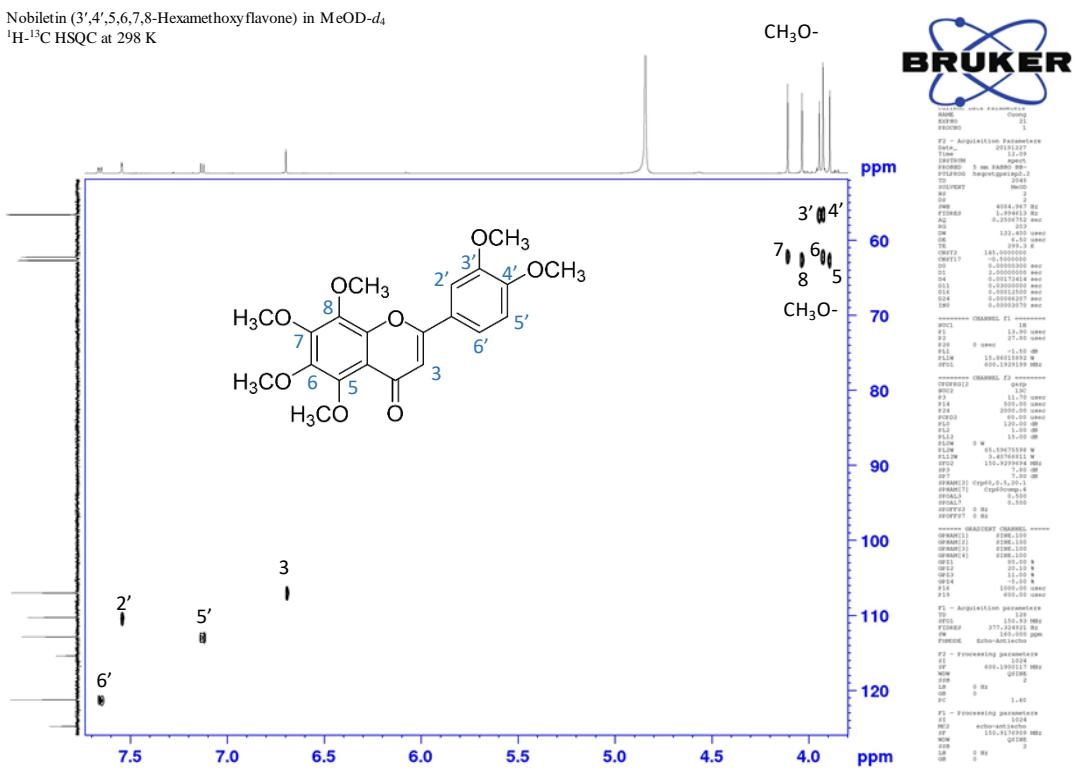


**Figure S5:** <sup>1</sup>H NMR spectrum of compound 3 recorded in MeOD-*d*<sub>4</sub>

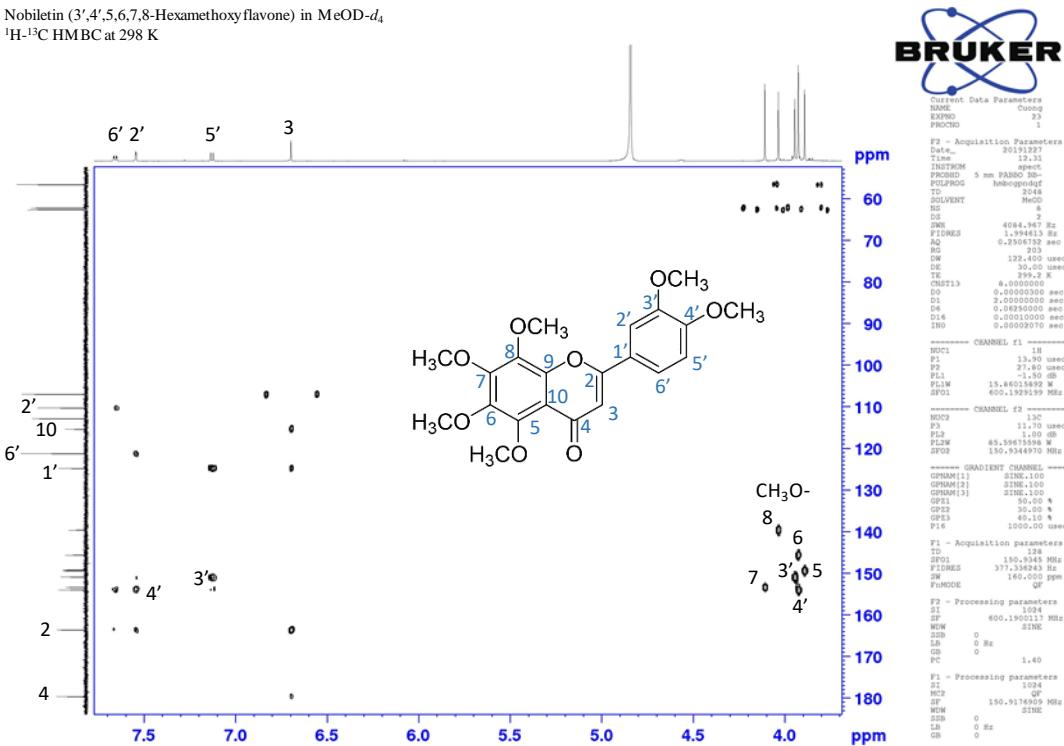
Nobiletin (3',4',5,6,7,8-Hexamethoxyflavone) in MeOD-*d*<sub>4</sub>  
<sup>13</sup>C NMR at 298 K



**Figure S6:** <sup>13</sup>C NMR spectrum of compound 3 recorded in MeOD-*d*<sub>4</sub>



**Figure S7:**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **3** recorded in MeOD- $d_4$

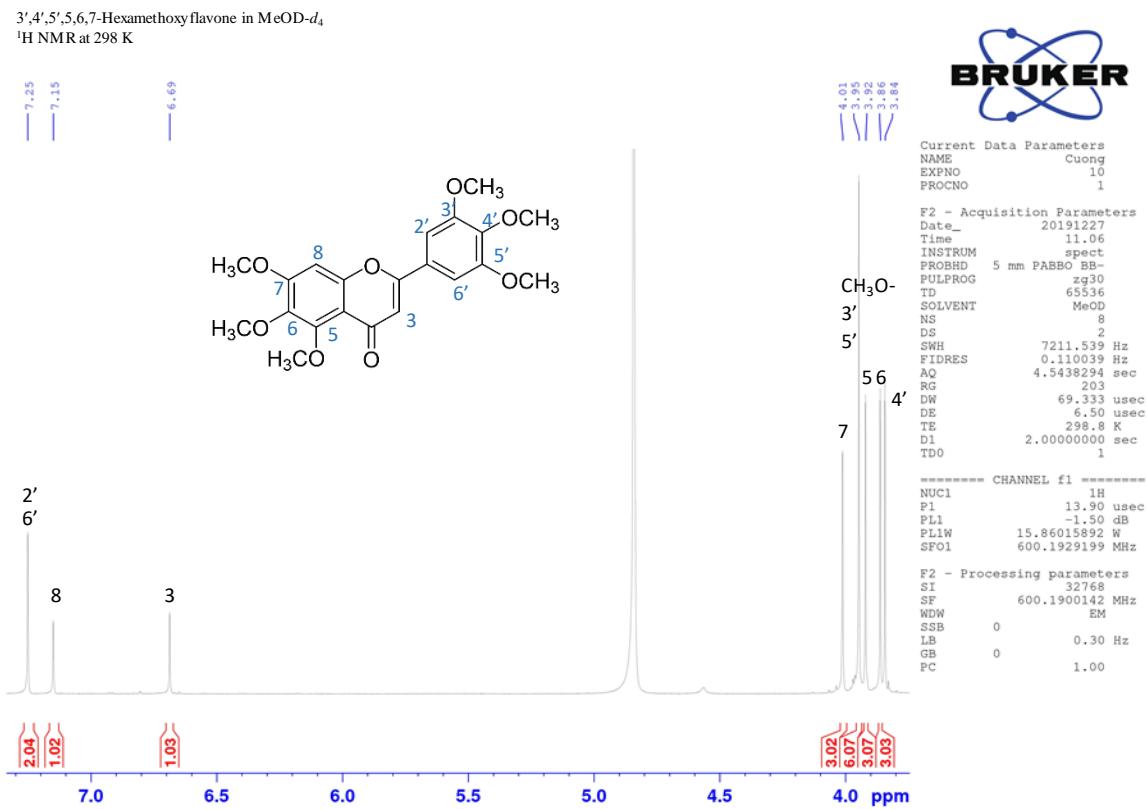


**Figure S8:**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **3** recorded in MeOD- $d_4$

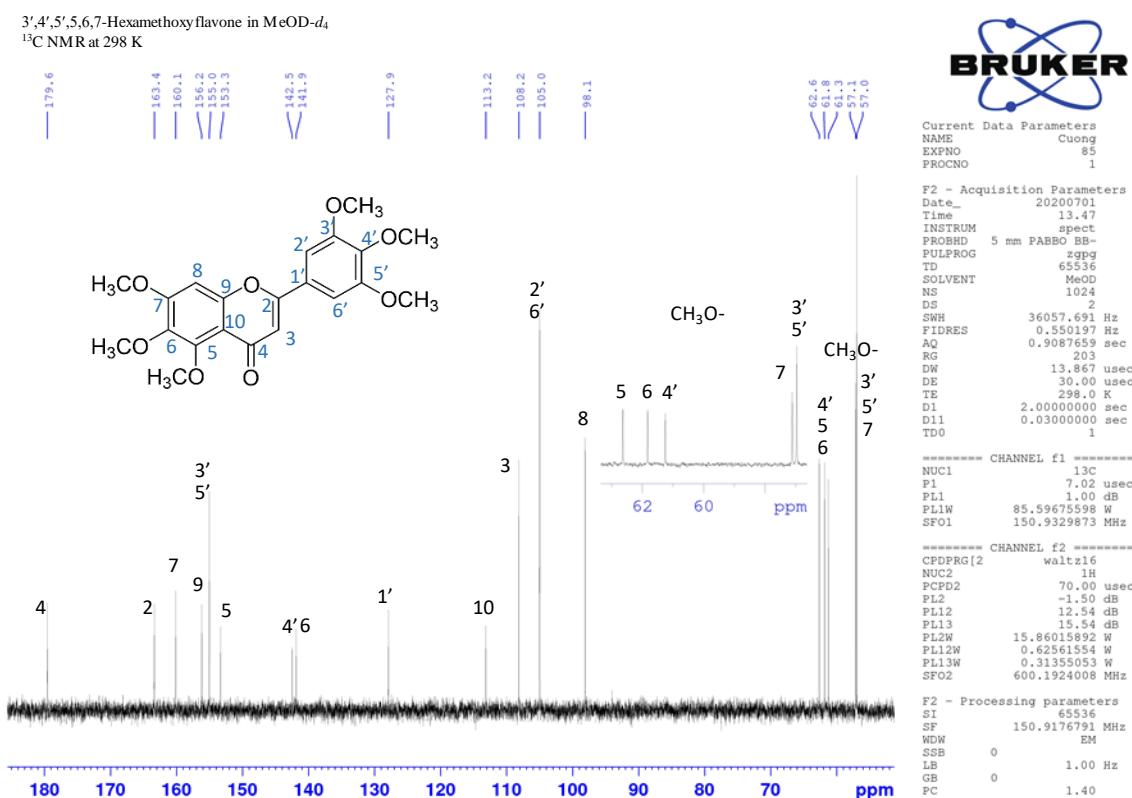
**Table S4:** NMR data of compound **4** (*3',4',5',5,6,7*-Hexamethoxyflavone) identified from *A. conyzoides* L. extract in MeOD-*d*<sub>4</sub>

Position	<sup>13</sup> C NMR (150 MHz)	<sup>1</sup> H NMR (600 MHz)	HMBC ( <sup>1</sup> H → <sup>13</sup> C)
<b>2</b>	163.4		
<b>3</b>	108.2	6.69 (1H, s)	C-1', 2, 4, 10
<b>4</b>	179.6		
<b>5</b>	153.3		
<b>6</b>	141.9		
<b>7</b>	160.1		
<b>8</b>	98.1	7.15 (1H, s)	C-4,6,7,9,10
<b>9</b>	156.2		
<b>10</b>	113.2		
<b>1'</b>	127.9		
<b>2'</b>	105.0	7.25 (2H, s)	C-2, 1', 3', 4', 6'
<b>3'</b>	155.0		
<b>4'</b>	142.5		
<b>5'</b>	155.0		
<b>6'</b>	105.0	7.25 (2H, s)	C-2, 1', 2', 4', 5'
<b>5'-OCH<sub>3</sub></b>	62.6	3.92 (3H, s)	C-5
<b>6'-OCH<sub>3</sub></b>	61.8	3.86 (3H, s)	C-6
<b>7'-OCH<sub>3</sub></b>	57.1	4.01 (3H, s)	C-7
<b>3'-OCH<sub>3</sub></b>	57.0	3.95 (3H, s)	C-3'
<b>4'-OCH<sub>3</sub></b>	61.3	3.84 (3H, s)	C-4'
<b>5'-OCH<sub>3</sub></b>	57.0	3.95 (3H, s)	C-5'

Ref. Chen *et al.*, *Chem. Pharm. Bull.* **1984**, 32, 166-169.

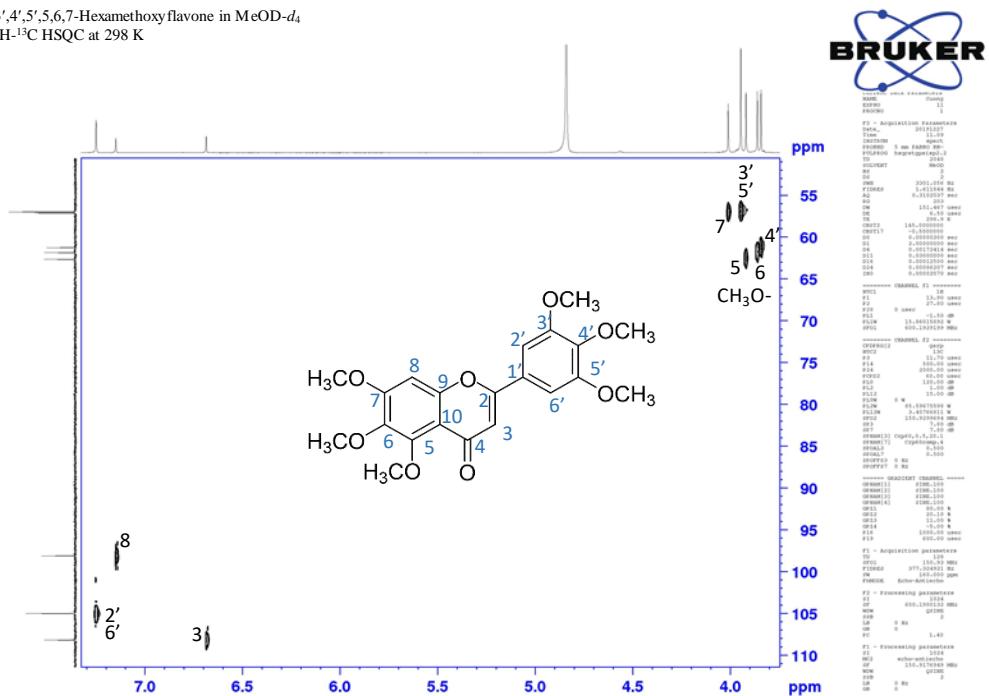


**Figure S9:**  $^1\text{H}$  NMR spectrum of compound 4 recorded in MeOD- $d_4$



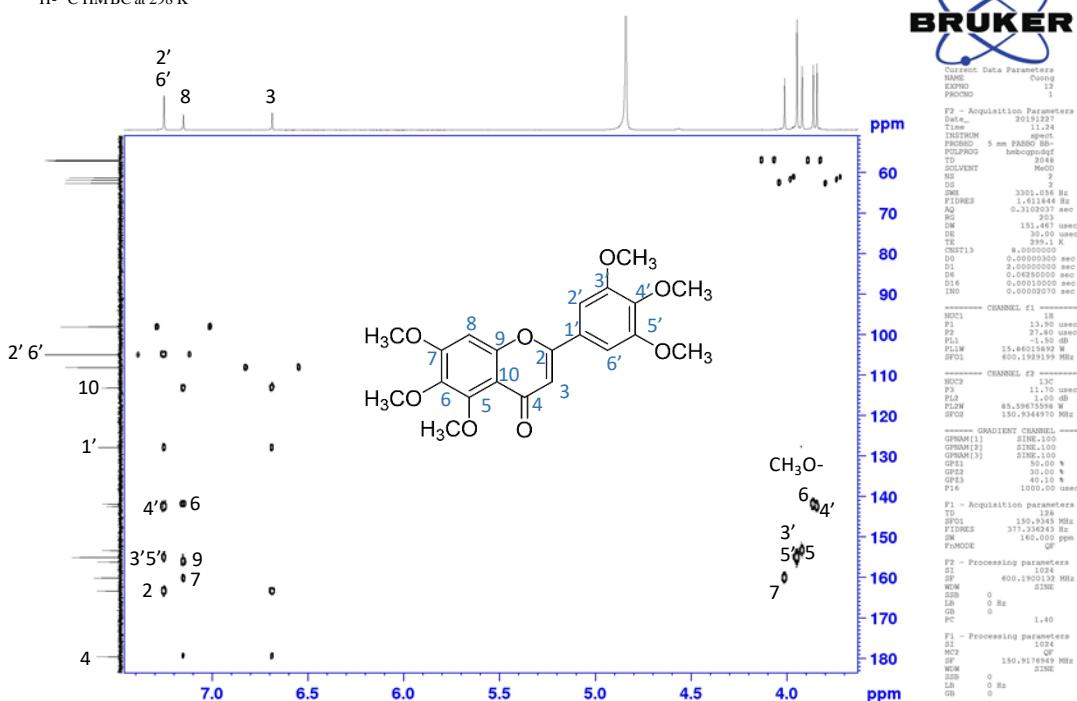
**Figure S10:**  $^{13}\text{C}$  NMR spectrum of compound 4 recorded in  $\text{MeOD-}d_4$

3',4',5',5,6,7-Hexamethoxyflavone in MeOD-*d*<sub>4</sub>  
<sup>1</sup>H-<sup>13</sup>C HSQC at 298 K



**Figure S11:** <sup>1</sup>H-<sup>13</sup>C HSQC spectrum of compound 4 recorded in MeOD-*d*<sub>4</sub>

3',4',5',5,6,7-Hexamethoxyflavone in MeOD-*d*<sub>4</sub>  
<sup>1</sup>H-<sup>13</sup>C HMBC at 298 K



**Figure S12:** <sup>1</sup>H-<sup>13</sup>C HMBC spectrum of compound 4 recorded in MeOD-*d*<sub>4</sub>

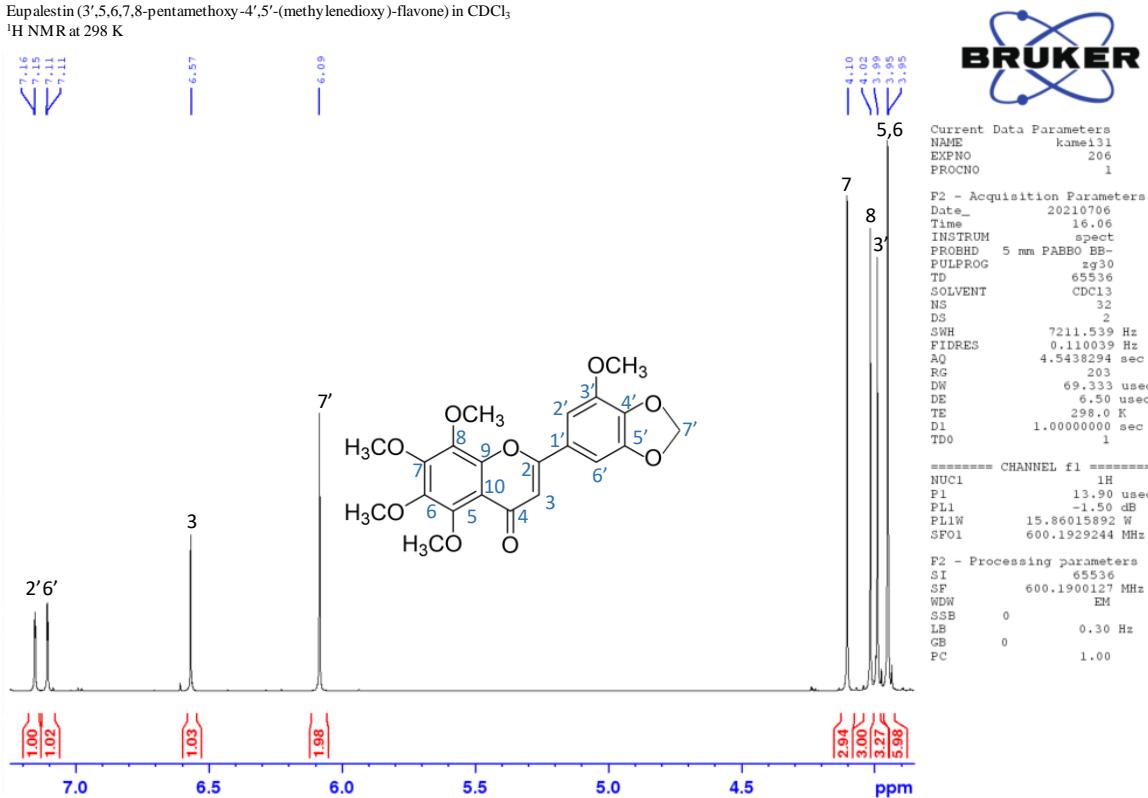
**Table S5:** NMR data of compound 5 (Eupalestin) identified from *A. conyzoides* L. extract in CDCl<sub>3</sub>

Position	<sup>13</sup> C NMR* (150 MHz)	<sup>1</sup> H NMR (600 MHz)	HMBC ( <sup>1</sup> H → <sup>13</sup> C)
2	160.6		
3	107.2	6.57 (1H, s)	C-2, 4, 10, 1'
4	177.2		
5	148.8		
6	143.3		
7	151.4		
8	138.1		
10	114.7		
1'	125.6		
2'	106.4	7.16 (1H, d, <i>J</i> = 1.5 Hz)	C-2, 3', 4', 6'
3'	143.8		
4'	138.1		
5'	149.6		
6'	100.3	7.11 (1H, dd, <i>J</i> = 1.5 Hz)	C-1', 3', 4'
7'	102.2	6.09 (2H, s)	C-2, 2', 4'
5 -OCH <sub>3</sub>	61.9	3.95 (3H, s)	C-5
6 -OCH <sub>3</sub>	61.9	3.95 (3H, s)	C-6
7 -OCH <sub>3</sub>	61.5	4.10 (3H, s)	C-7
8 -OCH <sub>3</sub>	61.8	4.02 (3H, s)	C-8
3'-OCH <sub>3</sub>	56.6	3.99 (3H, s)	C-3'

\*<sup>13</sup>C NMR chemical shift values were determined by the HSQC and HMBC spectra.

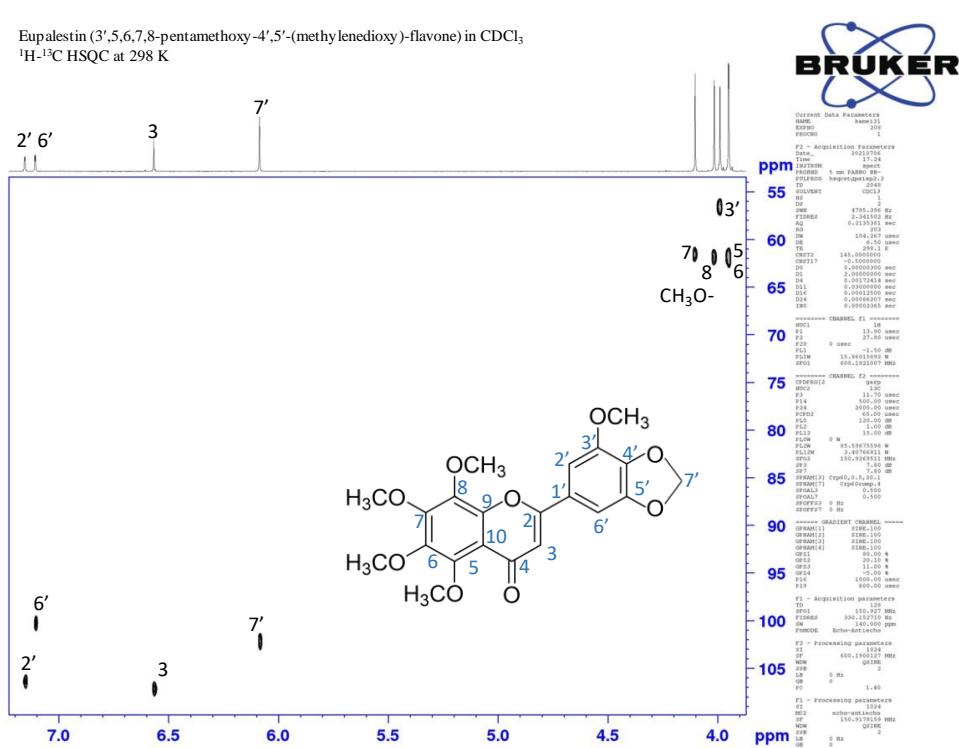
Ref. Le-Van *et al.*, *Phytochemistry* **1979**, *18*, 1859–1861.

Eupalestin (*3',5,6,7,8-pentamethoxy-4',5'-(methylenedioxy)-flavone*) in CDCl<sub>3</sub>.  
<sup>1</sup>H NMR at 298 K



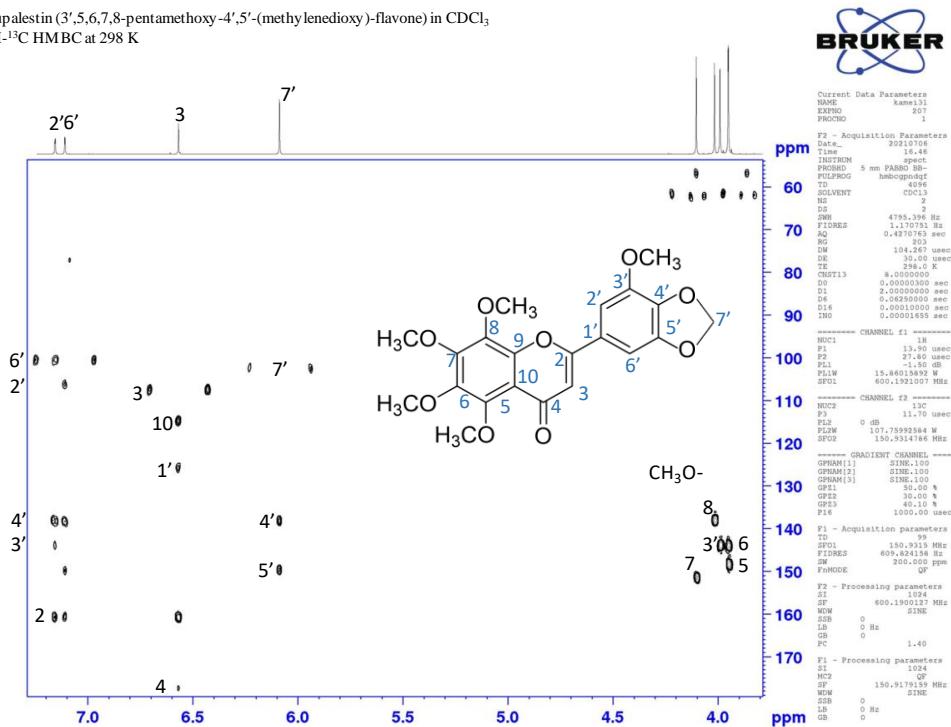
**Figure S13:**  $^1\text{H}$  NMR spectrum of compound **5** recorded in  $\text{CDCl}_3$

Eupalestin (*3'*,*5*',*6*,*7*,*8*-pentamethoxy-*4*',*5*'-(methylenedioxy)-flavone) in CDCl<sub>3</sub>  
<sup>1</sup>H-<sup>13</sup>C HSQC at 298 K



**Figure S14:**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **5** recorded in  $\text{CDCl}_3$

Eupalestin (*3'*,*5*,*6*,*7*,*8*-pentamethoxy-*4'*,*5'*-(methylenedioxy)-flavone) in CDCl<sub>3</sub>  
<sup>1</sup>H-<sup>13</sup>C HMBC at 298 K



**Figure S15:** <sup>1</sup>H-<sup>13</sup>C HMBC spectrum of compound 5 recorded in CDCl<sub>3</sub>