

SUPPLEMENTARY MATERIAL

Title: Antitrypanosomal and Antileishmanial Activity of Chalcones and Flavanones from *Polygonum salicifolium*

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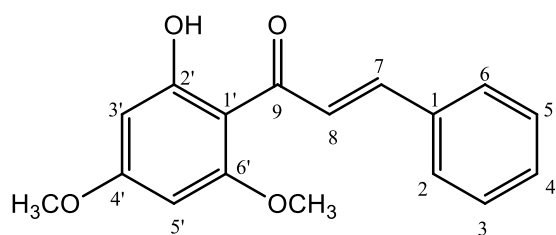
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*, Correspondence:

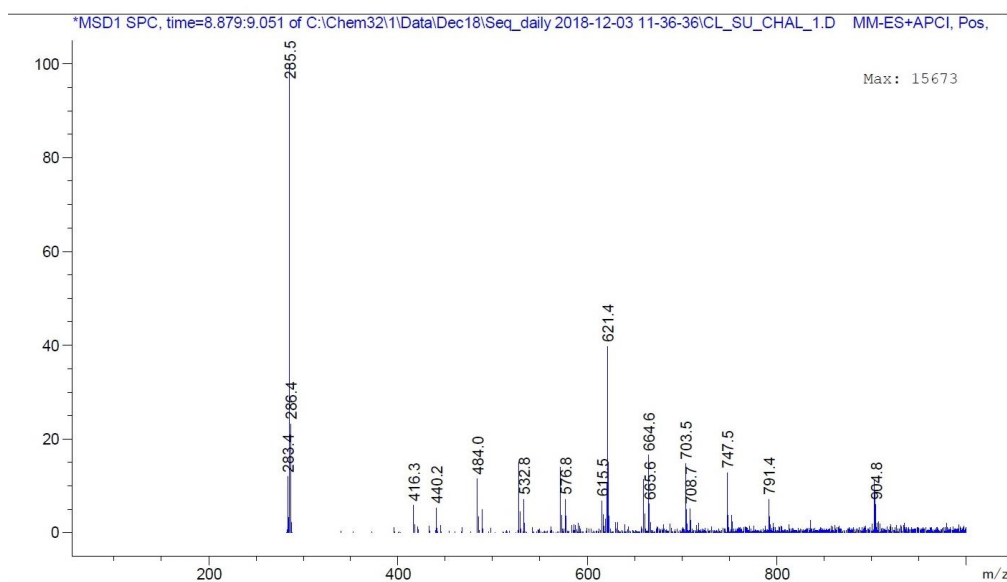
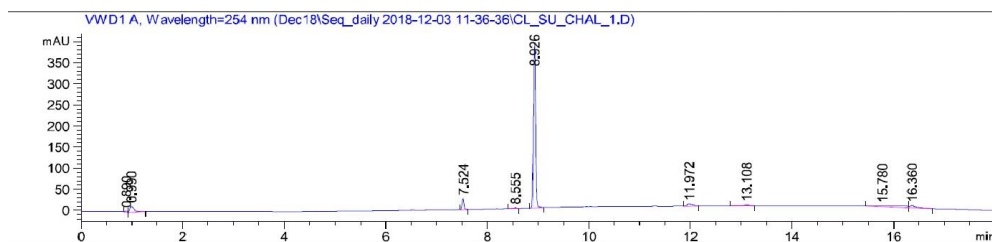
Harry P. de Koning

Email:Harry.De-Koning@glasgow.ac.uk

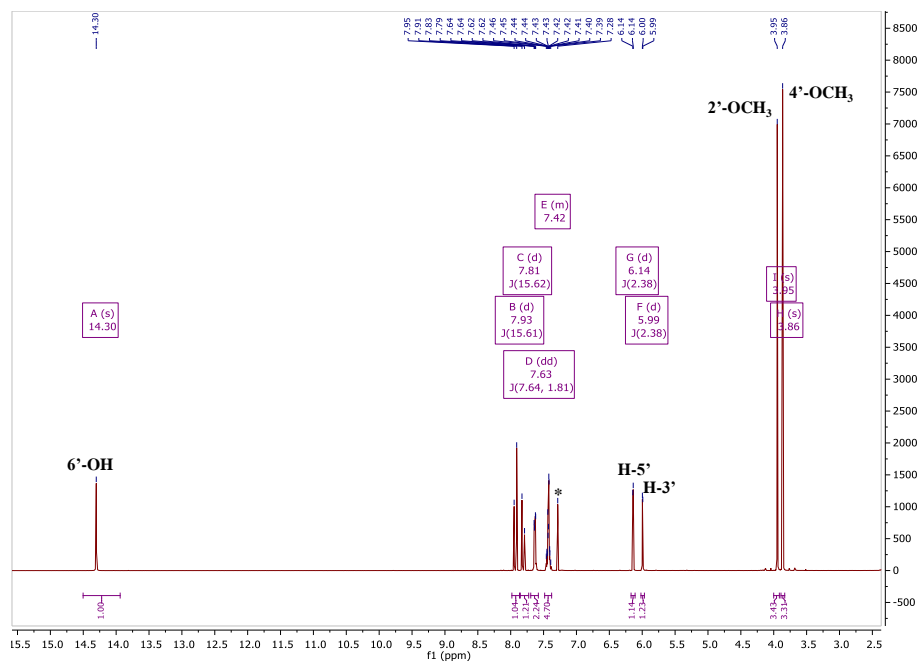
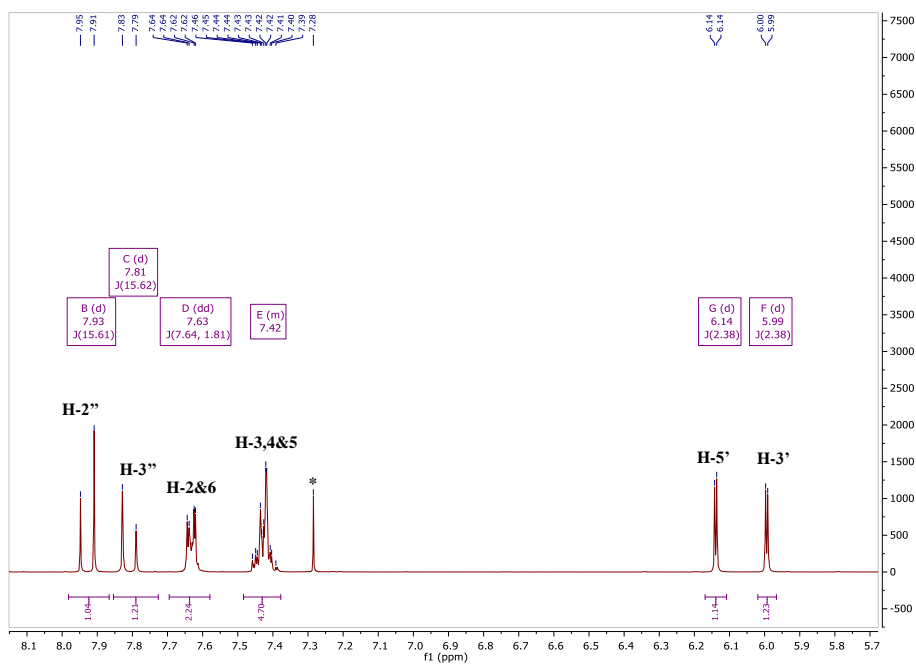
Compound 1



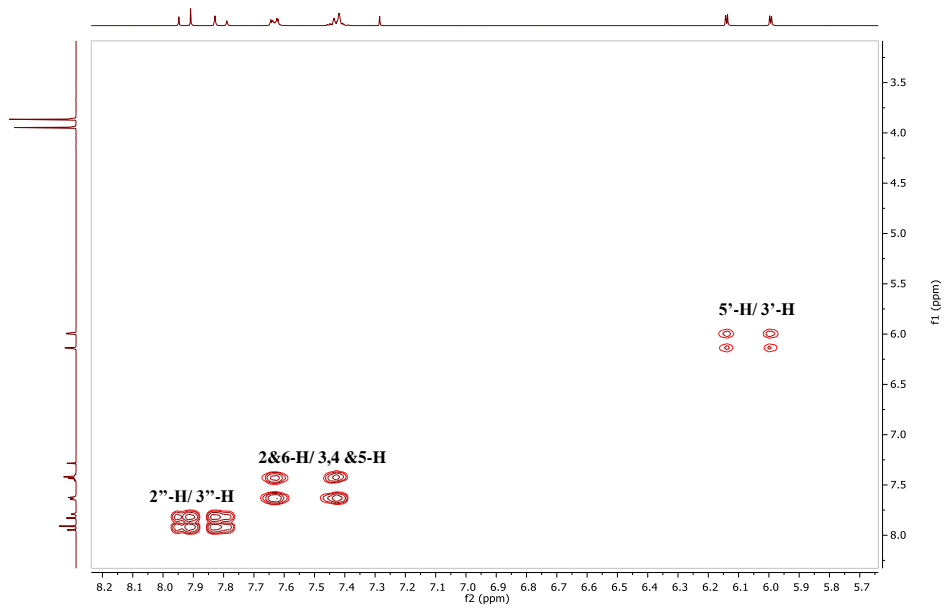
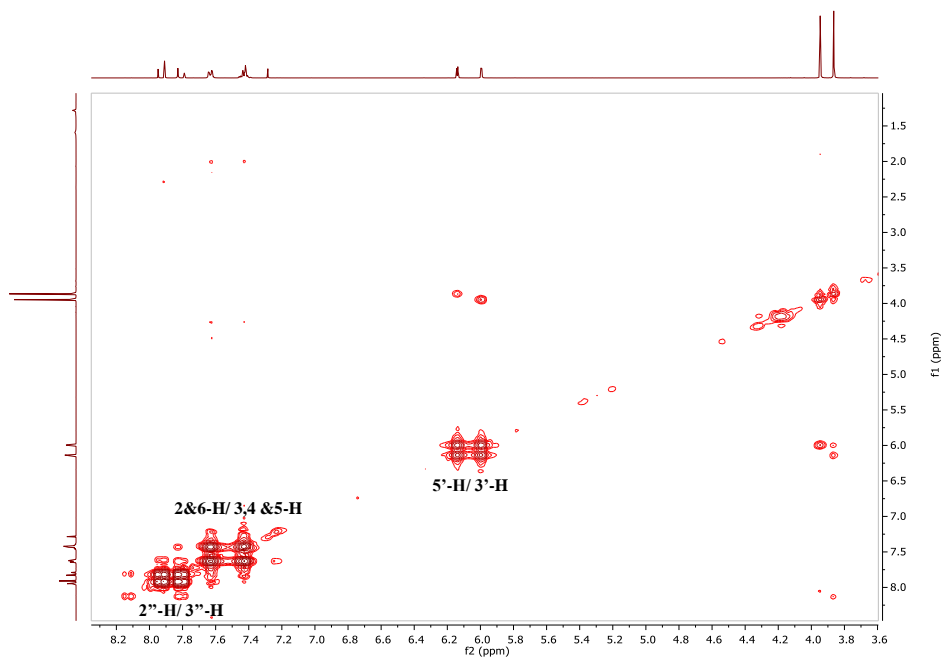
4',6'-dimethoxy-2'-hydroxychalcone



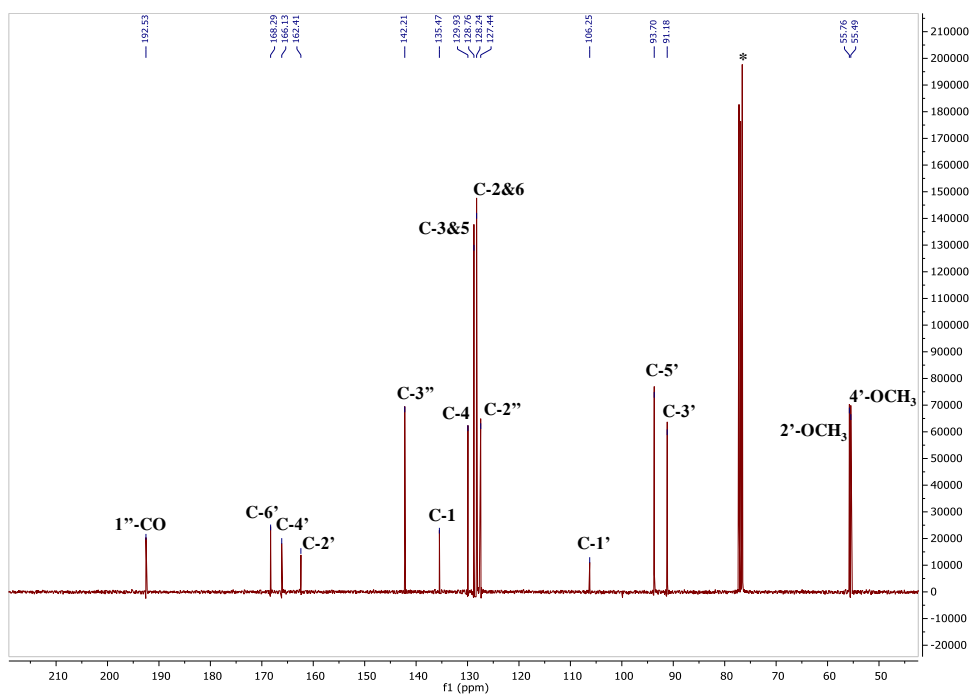
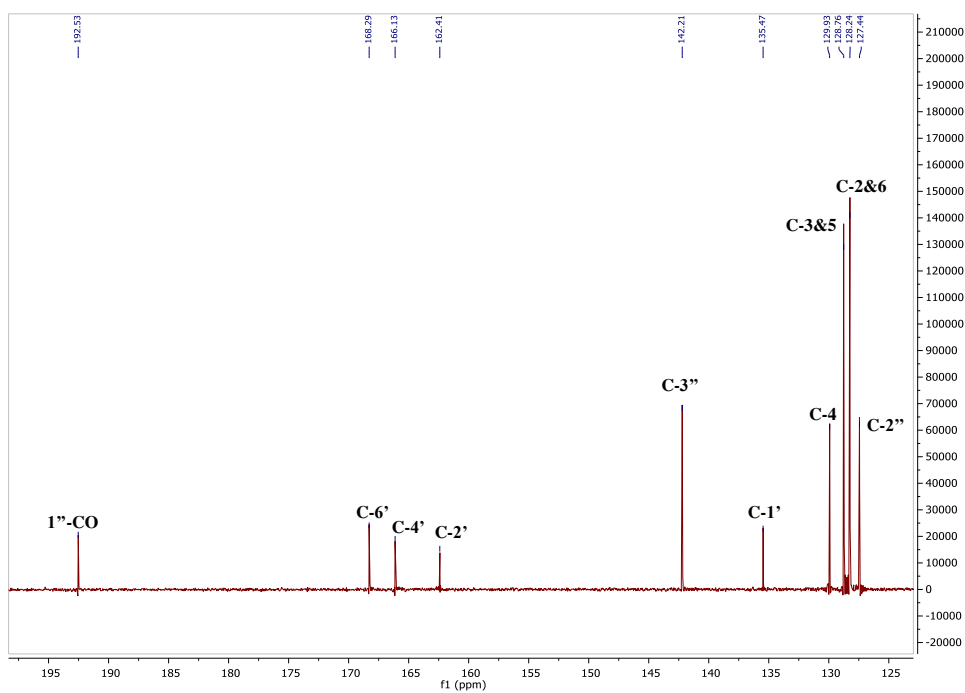
Supplementary material S1: LC-MS spectrum showing $[M+H]^+$ ion for compound 1.

A**B**

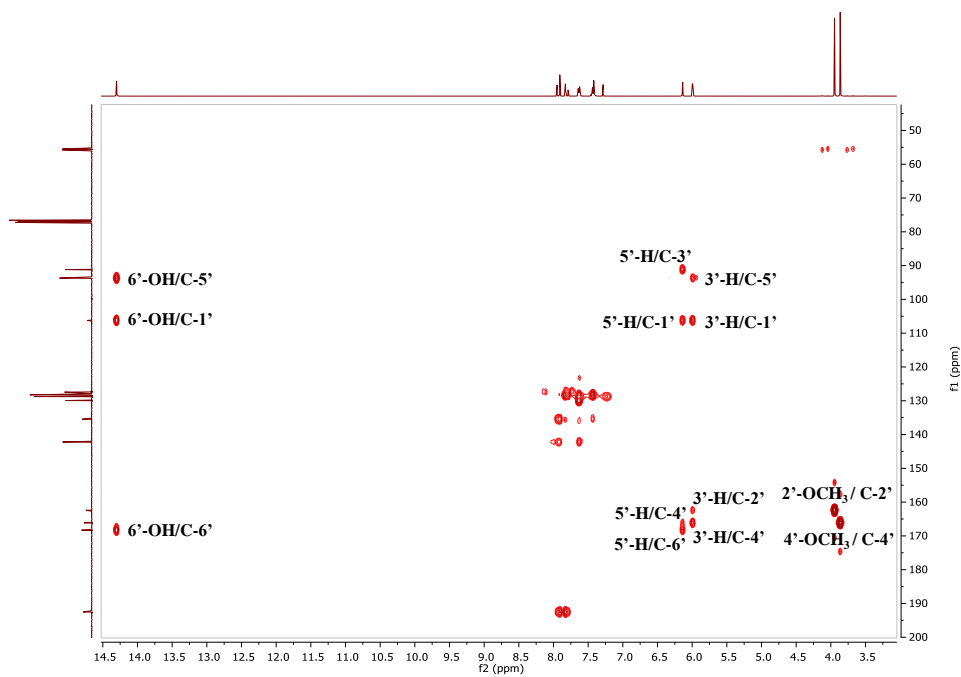
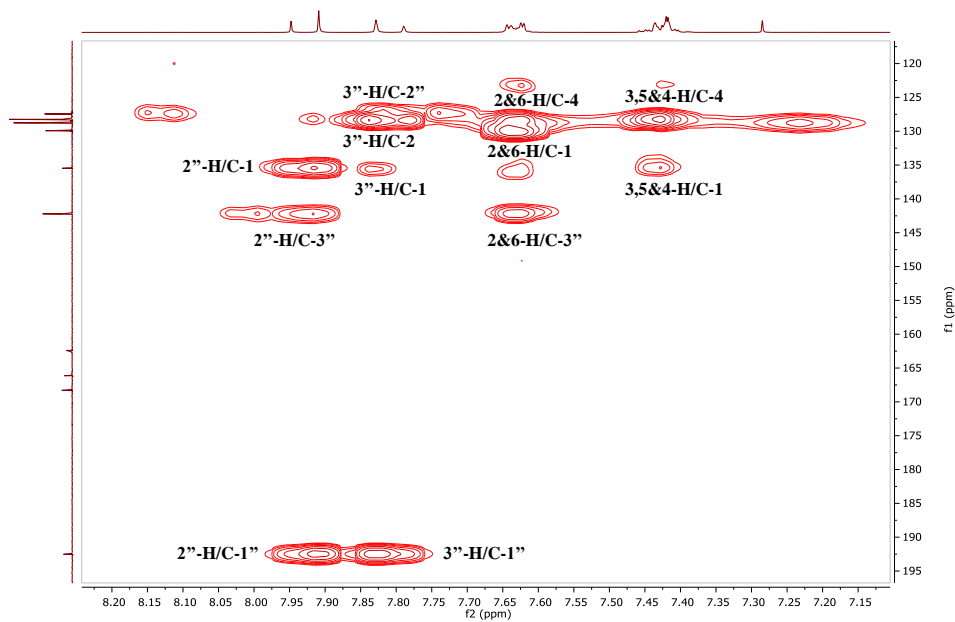
Supplementary material S2: (A) Full and (B) expansion of ^1H NMR spectrum (500 MHz) of compound **1** in CDCl_3 . *Denotes residual solvent peak.

A**B**

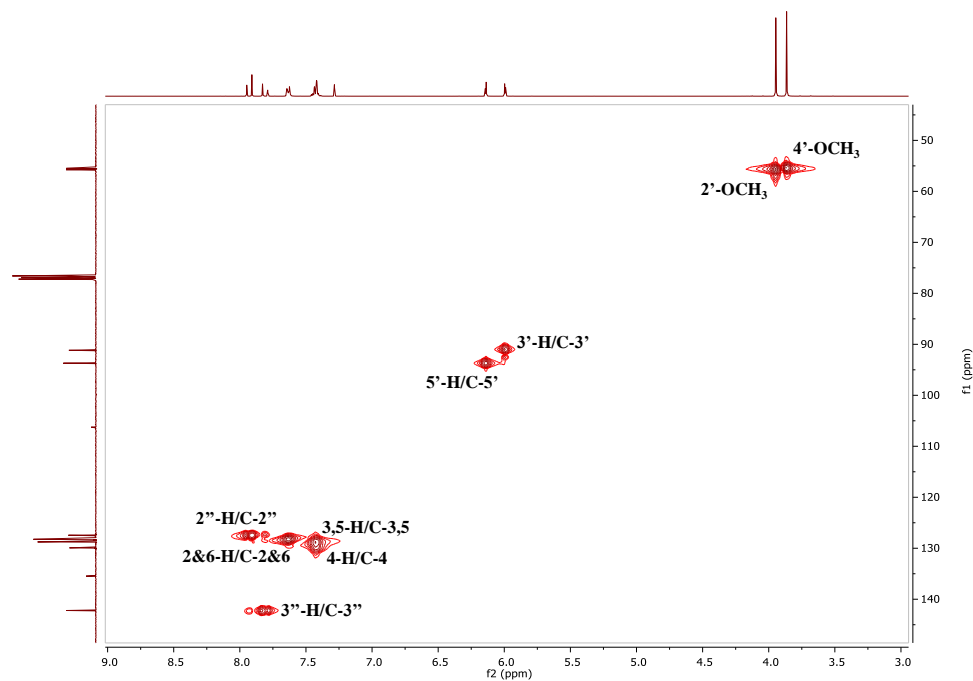
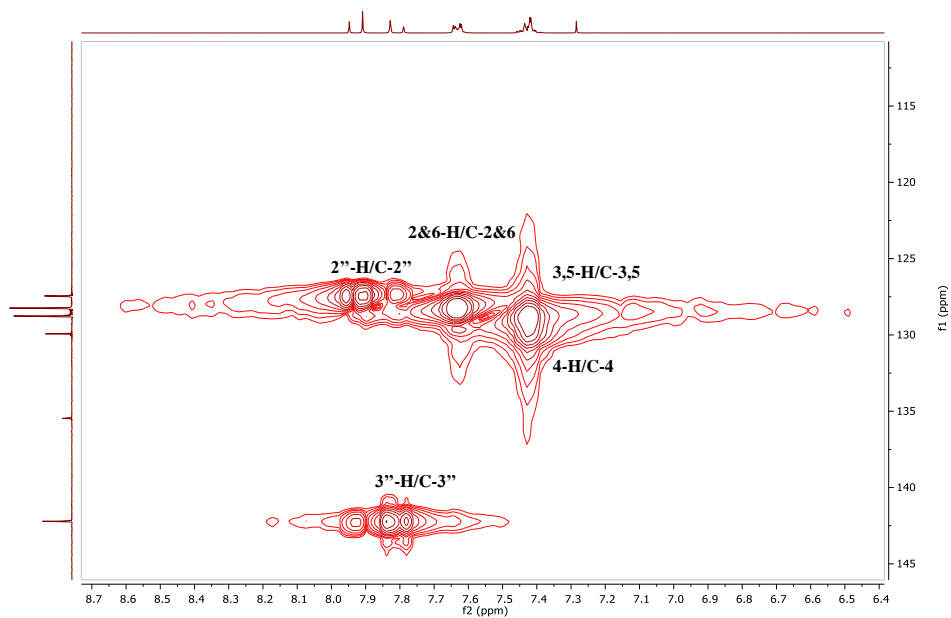
Supplementary material S3: (A) Full and (B) expansion of COSY spectrum of compound **1** in CDCl₃.

A**B**

Supplementary material S4: (A) Full and (B) expansion of ¹³C NMR spectrum of compound 1 in CDCl₃. *Denotes residual solvent peak.

A**B**

Supplementary material S5: (A) Full and (B) expansion of HMBC spectrum of compound 1 in CDCl₃.

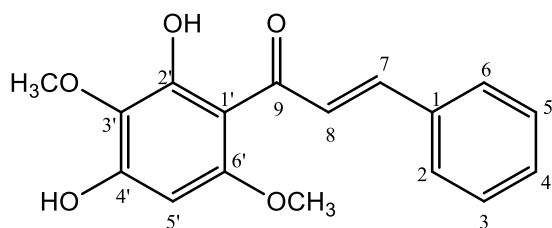
A**B**

Supplementary material S6: (A) Full and (B) expansion of HSQC spectrum of compound 1 in CDCl₃.

Supplementary Table S1: NMR data for compound 1 in CDCl₃

Position	δ_{H} (mult, <i>J</i> (Hz))	δ_{C}	HMBC correlations
1	-	135.4	-
2, 6	7.62 (2H, <i>dd</i> , 7.6, 1.8)	128.2	C-1, C-4
3, 4, 5	7.42 (3H, <i>m</i>)	128.7 & 129.9	C-1, C-4
7	7.83 (1H, <i>d</i> , 15.6)	142.2	C-1, C-2, C-8, C-9
8	7.91 (1H, <i>d</i> , 15.6)	127.4	C-1, C-7, C-9
9	-	192.5	-
1'	-	106.2	-
2'	-	168.2	-
3'	6.14 (1H, <i>d</i> , 2.6)	93.7	C-1', C-2', C-4', C-5'
4'	-	166.1	-
5'	5.99 (1H, <i>d</i> , 2.6)	91.1	C-1', C-3', C-4', C-6'
6'	-	162.4	-
2'-OH	14.30 (<i>s</i>)	-	C-1', C-2', C-3'
O-CH ₃	3.86 (3H, <i>s</i>)	55.4	C-4'
O-CH ₃	3.95 (3H, <i>s</i>)	55.7	C-6'

Compound 2

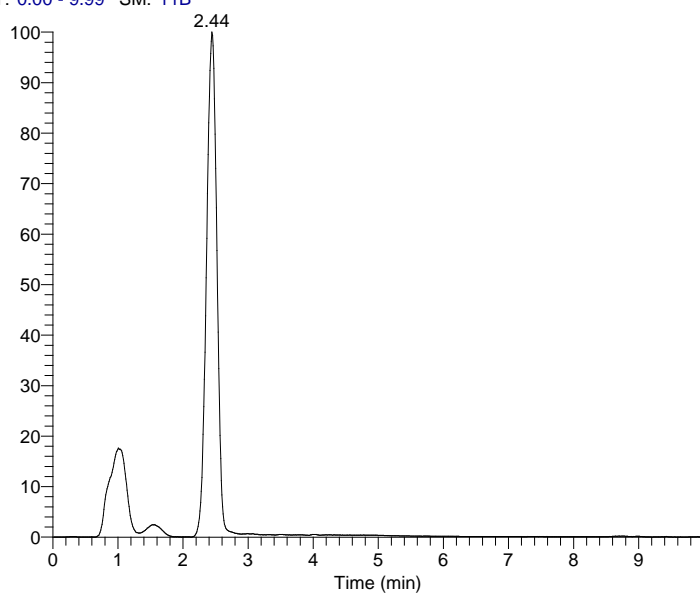


3',6'-dimethoxy-2',4'-dihydroxychalcone.

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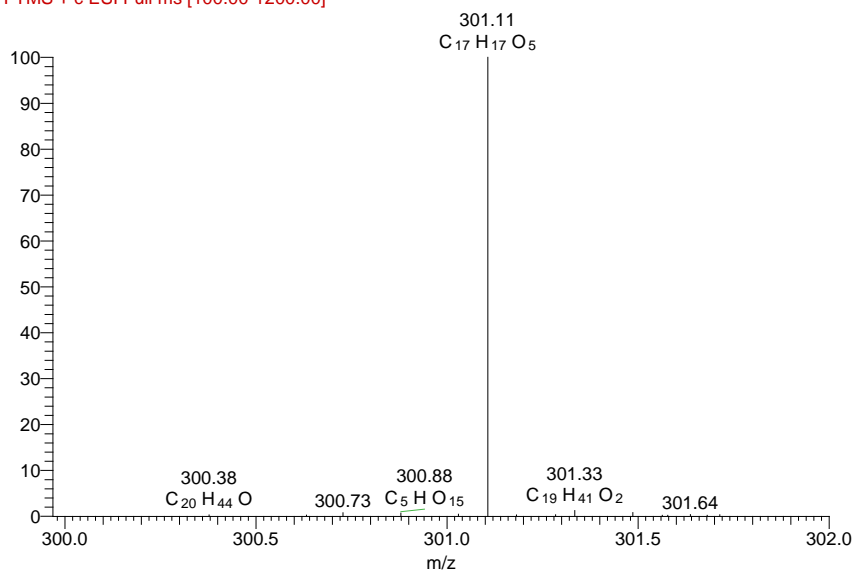
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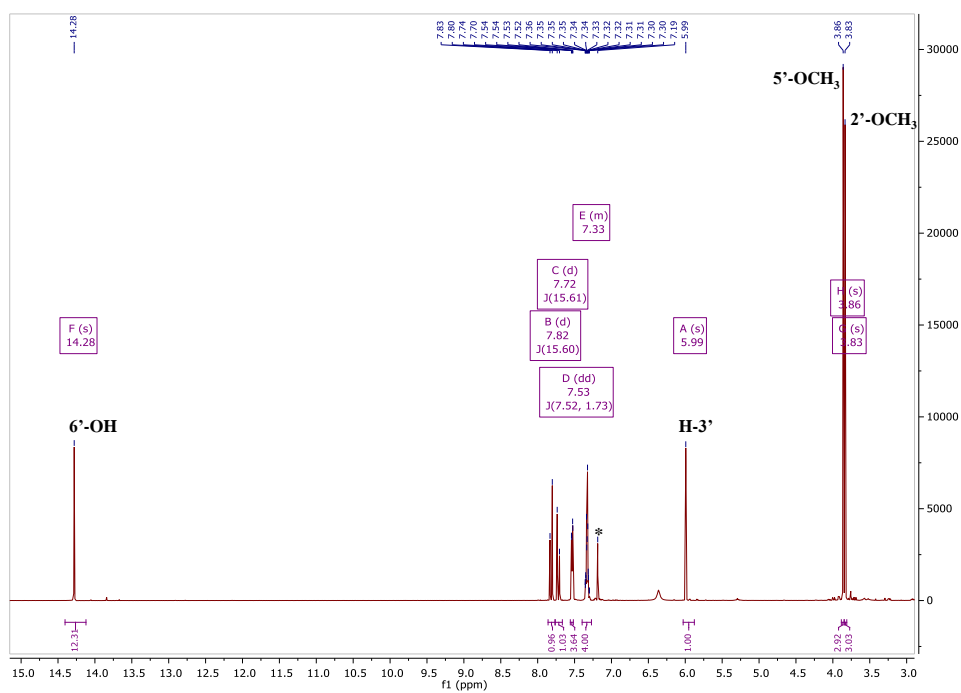
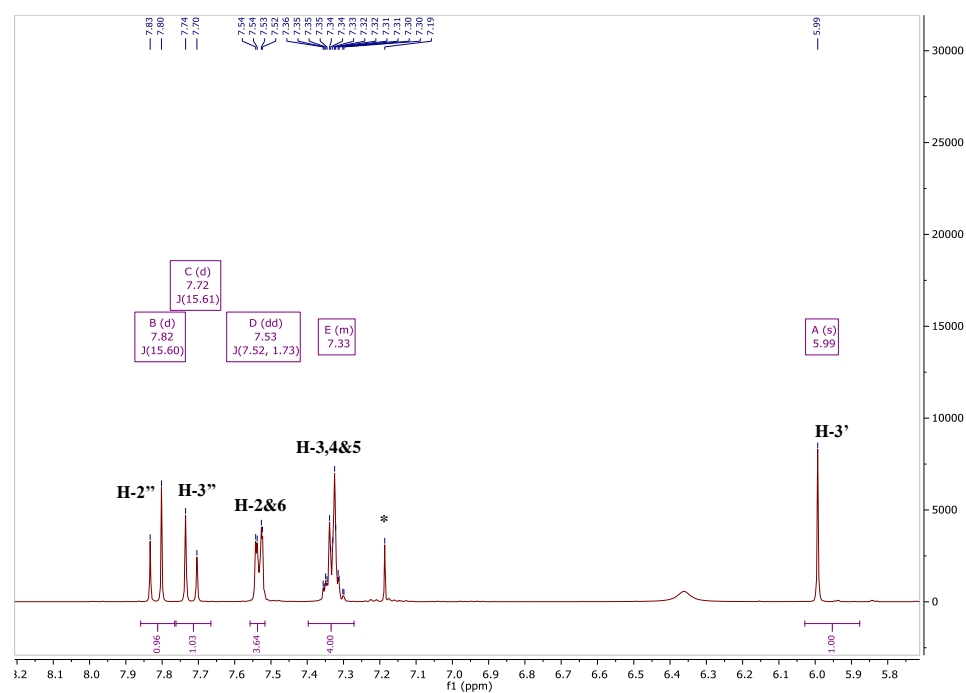


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ms
[100.00-1200.00]
MS P5H-35

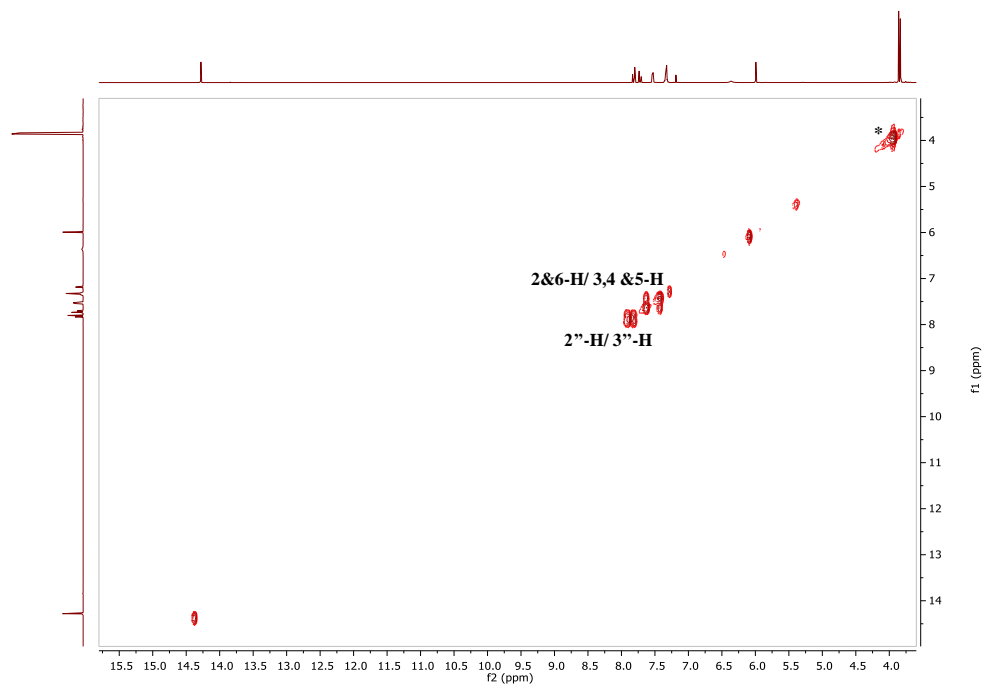
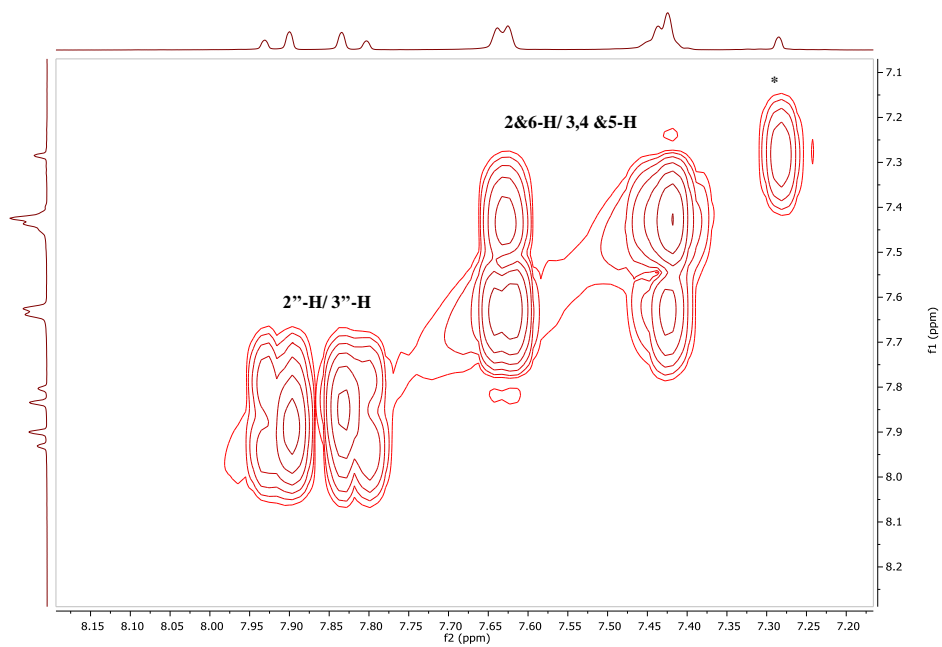
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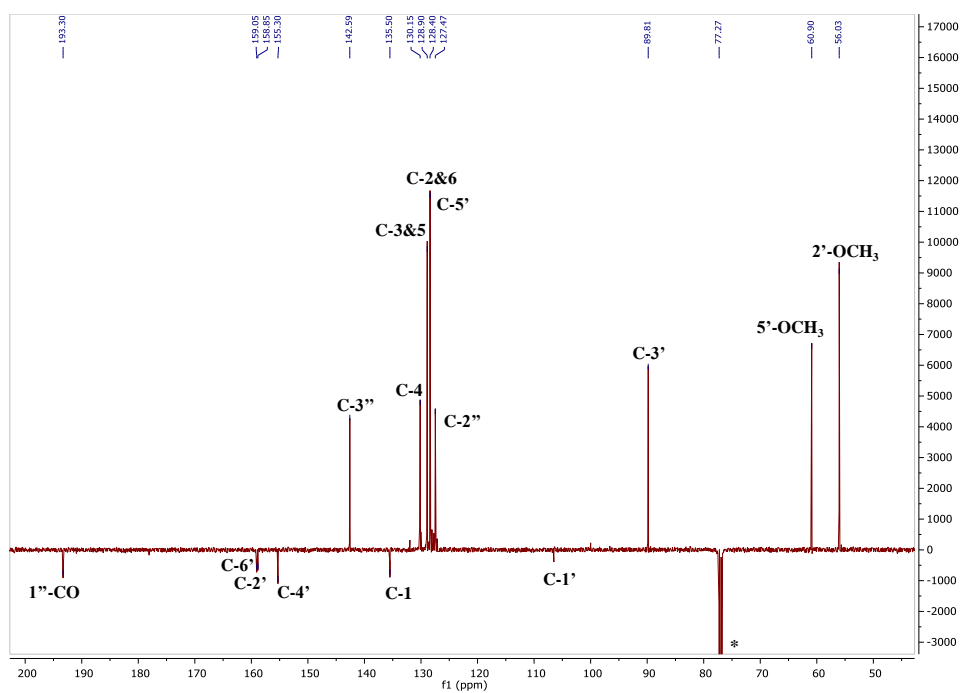
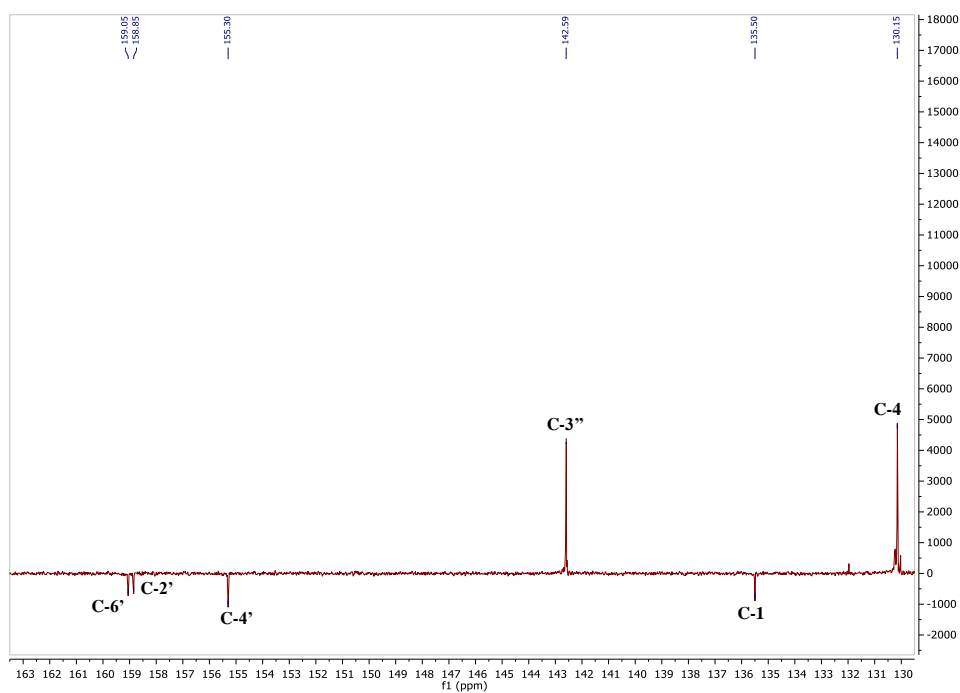
Supplementary material S7: HR-LC-MS spectrum showing [M+H]⁺ ion for compound 2

A**B**

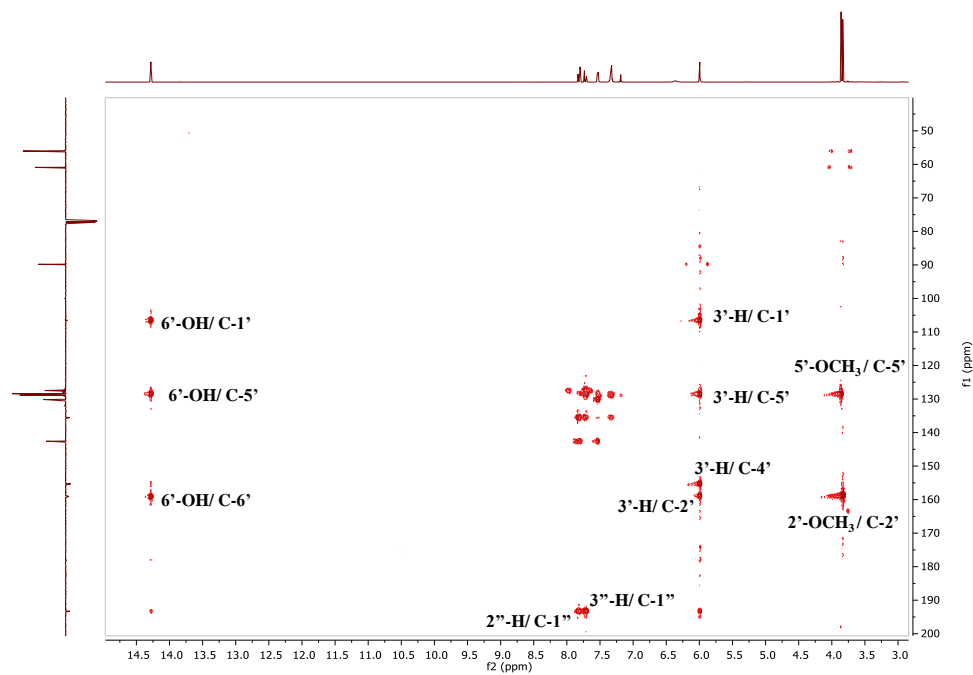
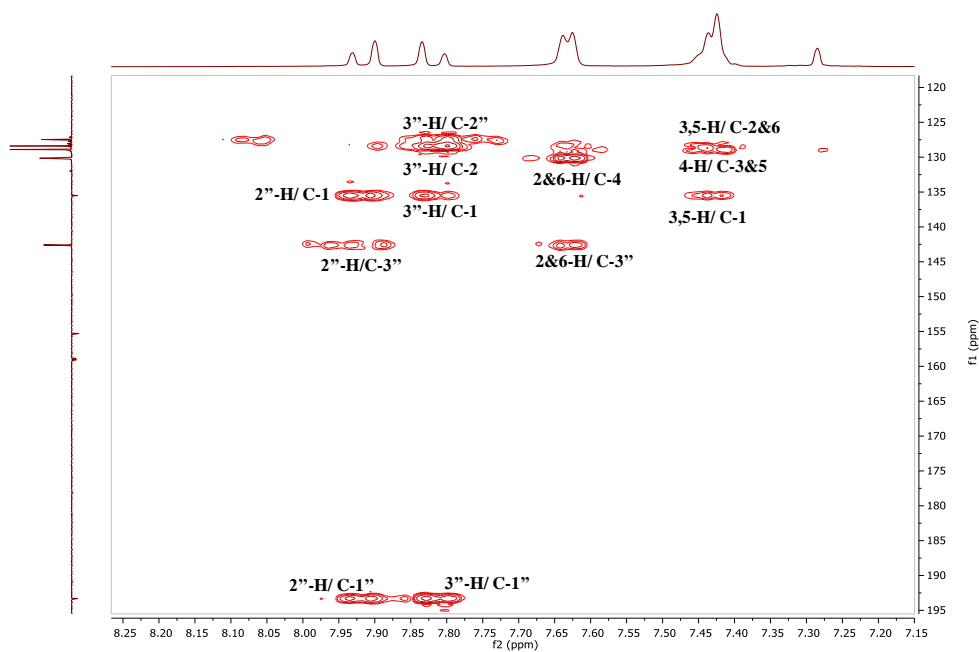
Supplementary material 8: (A) Full ^1H NMR spectrum (500 MHz) of compound **2** in CDCl_3 and (B) expansion of the aromatic region. *Denotes residual solvent peak.

A**B**

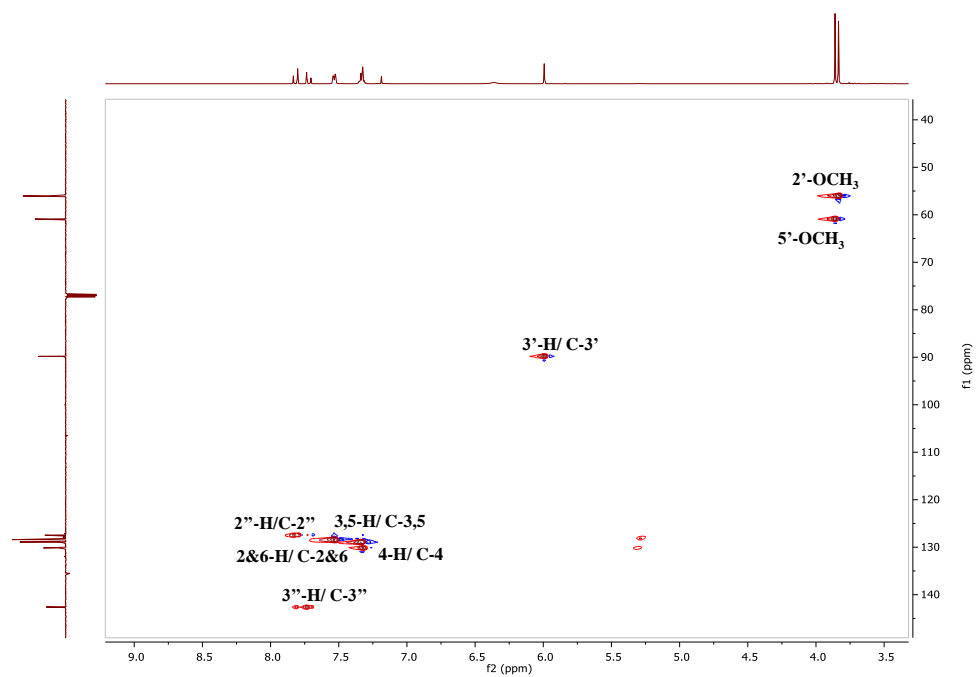
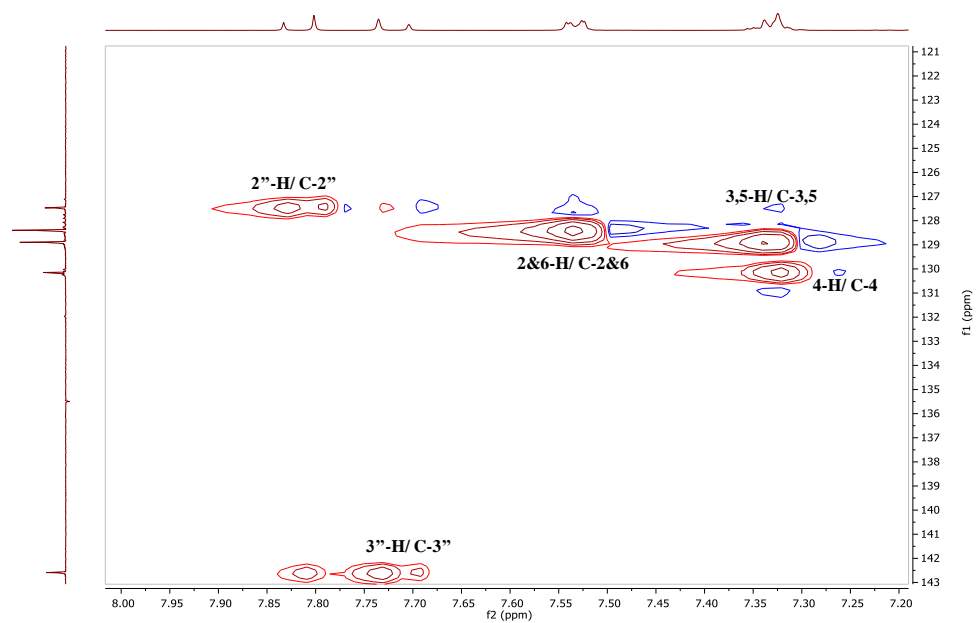
Supplementary material S9: (A) Full and (B) expansion of COSY spectrum of compound 2 in CDCl₃.

A**B**

Supplementary Spectrum S10: (A) Full and (B) expansion of DEPTq ^{13}C NMR spectrum of compound 2 in CDCl_3 . *Denotes residual solvent peak.

A**B**

Supplementary material S11: (A) Full and (B) expansion of HMBC spectrum of compound 2 in CDCl₃.

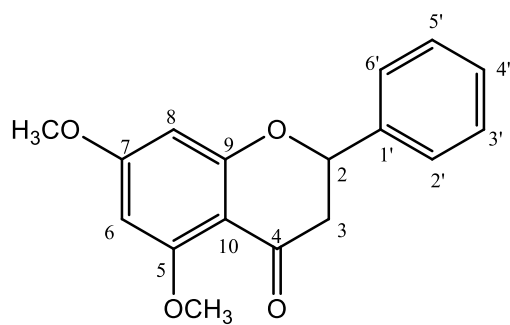
A**B**

Supplementary material S12: (A) Full and (B) expansion of HSQC spectrum of compound 2 in CDCl₃.

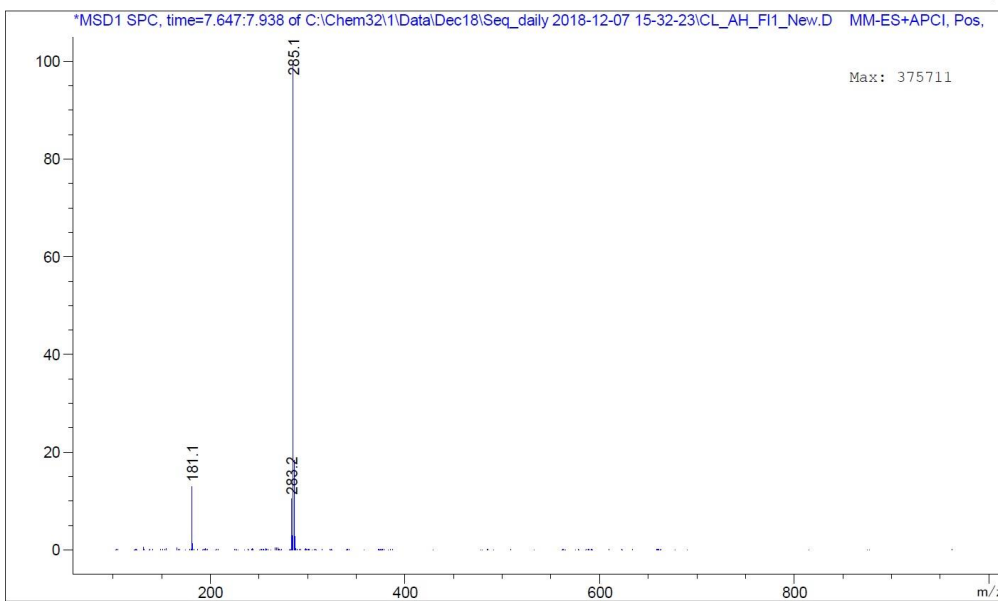
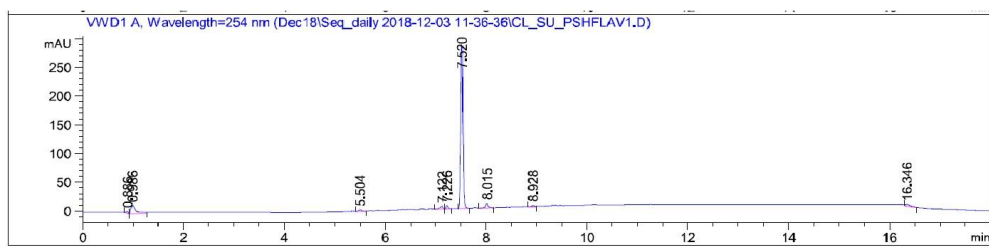
Supplementary Table S2: NMR data for compound 2 in CDCl₃

Position	δ_{H} (mult, <i>J</i> (Hz))	δ_{C}	HMBC
1	-	135.5	-
2, 6	7.53 (2H, dd, 7.5, 1.7)	128.4	C-1, C-7
3, 4, 5	7.33 (3H, m)	128.9, 130.1	C-1, C4
7	7.72 (1H, d, 15.6)	142.5	C-1, C-9, C-8
8	7.82 (1H, d, 15.6)	127.4	C-1, C-9, C-7
9	-	193.3	-
1'	-	106.5	-
2'	-	159.0	C-1', C-2', C-3'
3'	-	128.4	-
4'	-	155.3	-
5'	5.99 (1H, s)	89.8	C-1', C-3', C-4', C-6'
6'	-	158.8	-
2'-OH	14.2 (s)	-	-
O-CH ₃	3.83 (3H, s)	60.1	C-4'
O-CH ₃	3.86 (3H, s)	56.0	C-6'

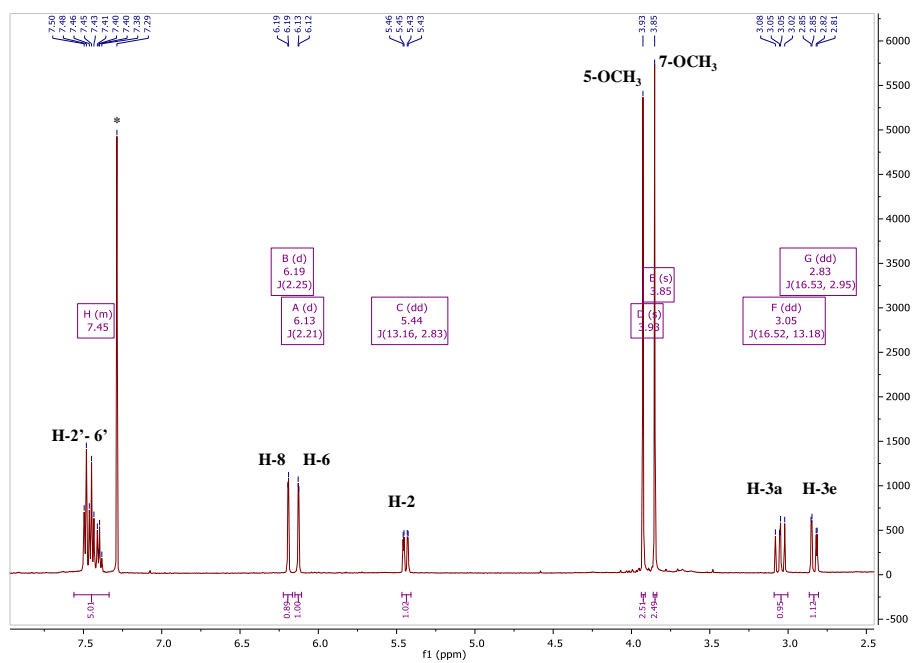
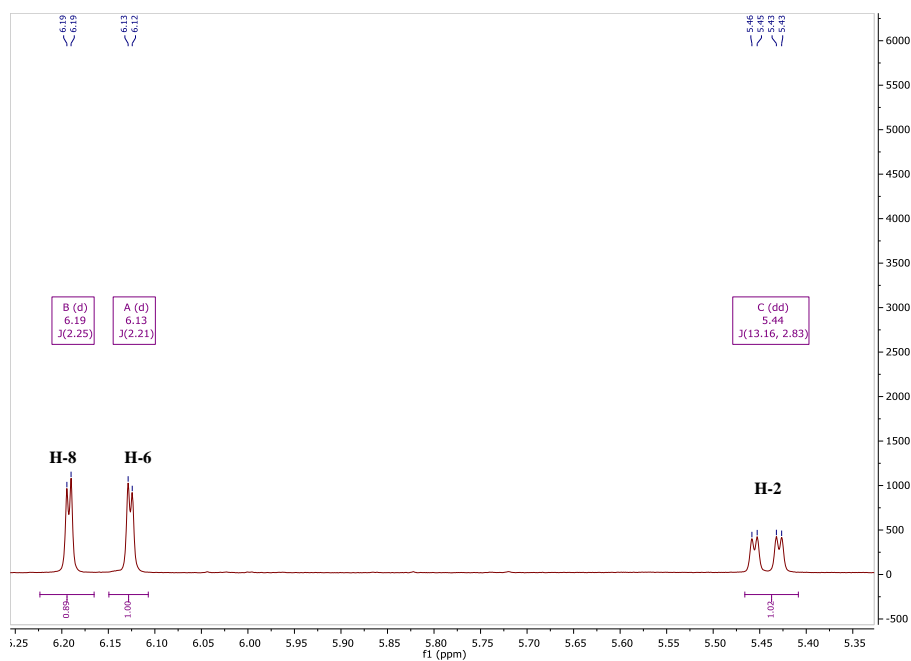
Compound 3



5,7-dimethoxyflavanone

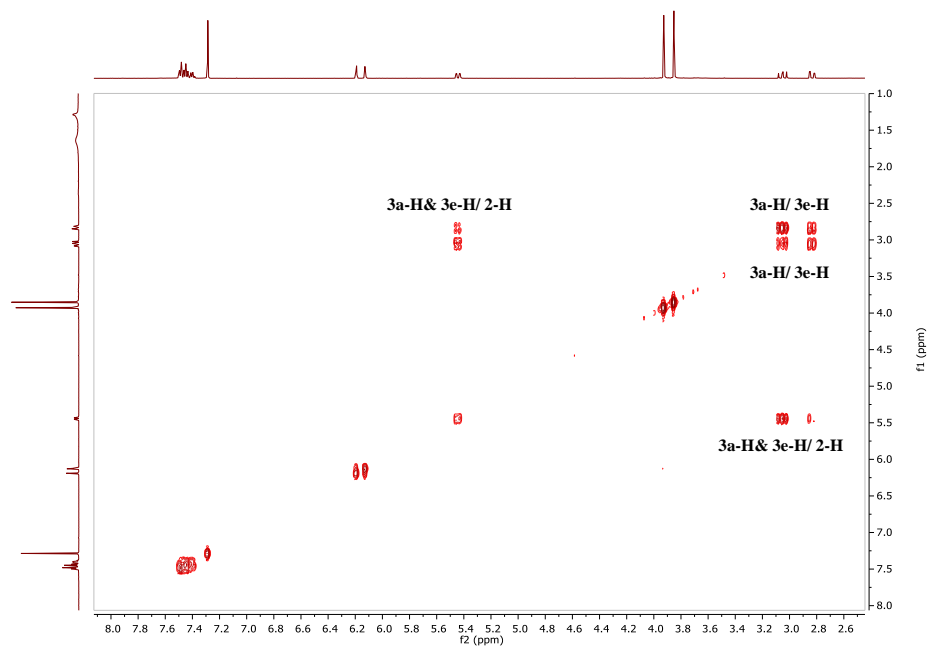


Supplementary material S13: LC-MS spectrum showing $[M+H]^+$ ion for compound 3.

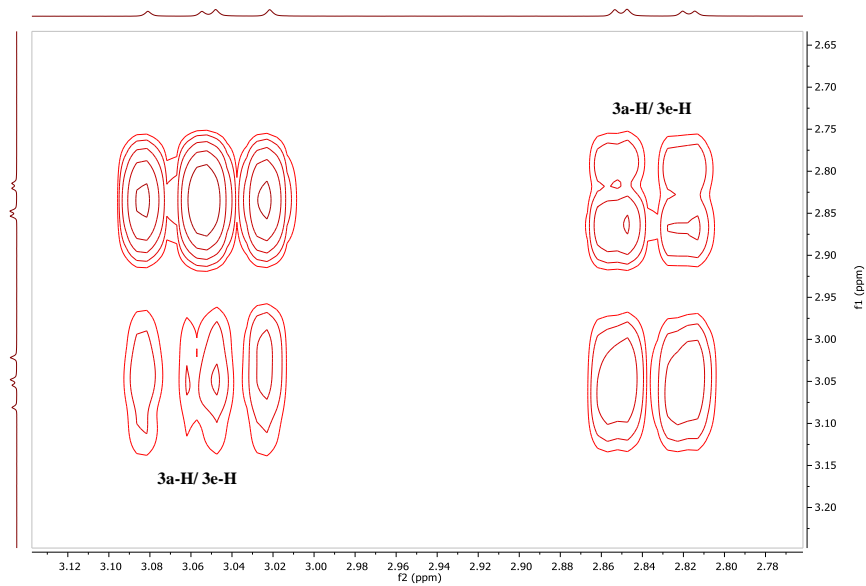
A**B**

Supplementary material S14: (A) Full and (B) expansion of ^1H NMR spectrum (500 MHz) in CDCl_3 of compound 3. *Denotes residual solvent peak

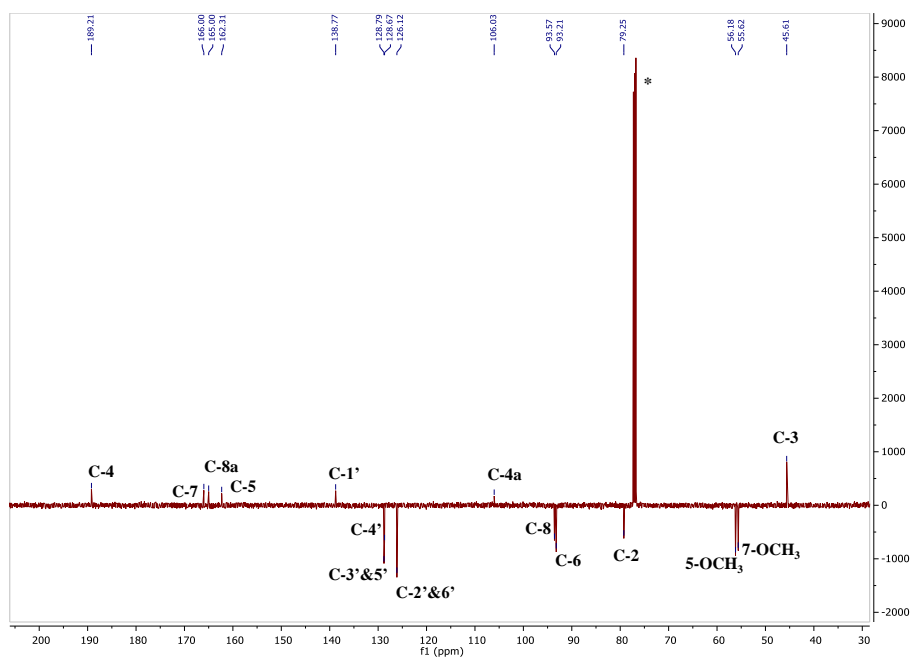
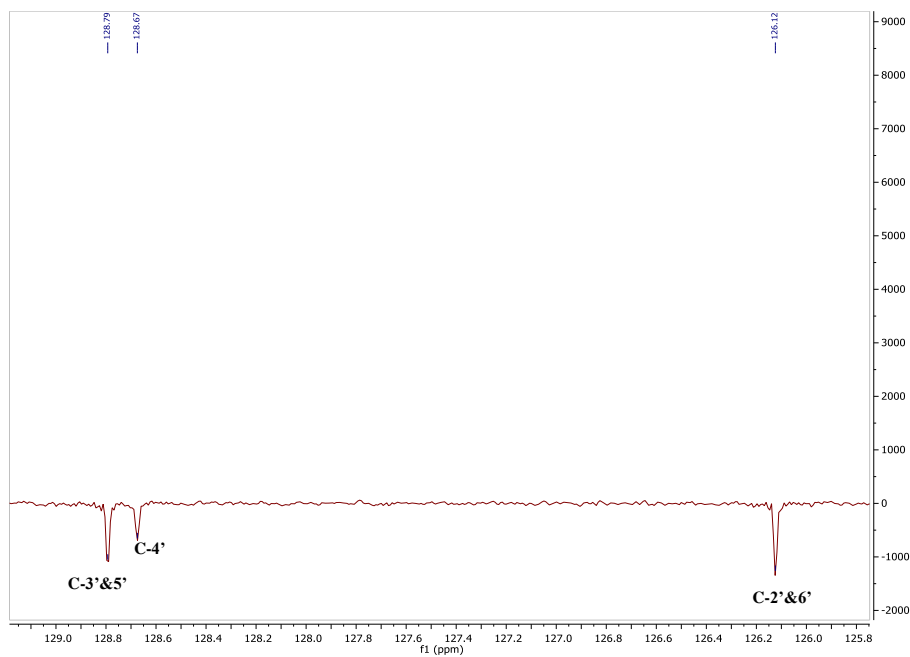
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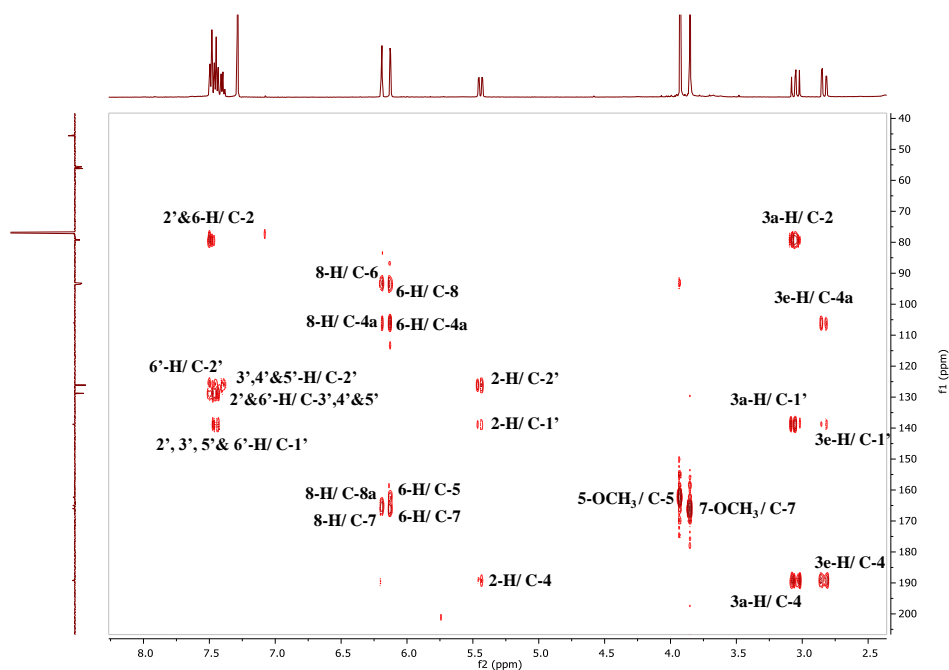
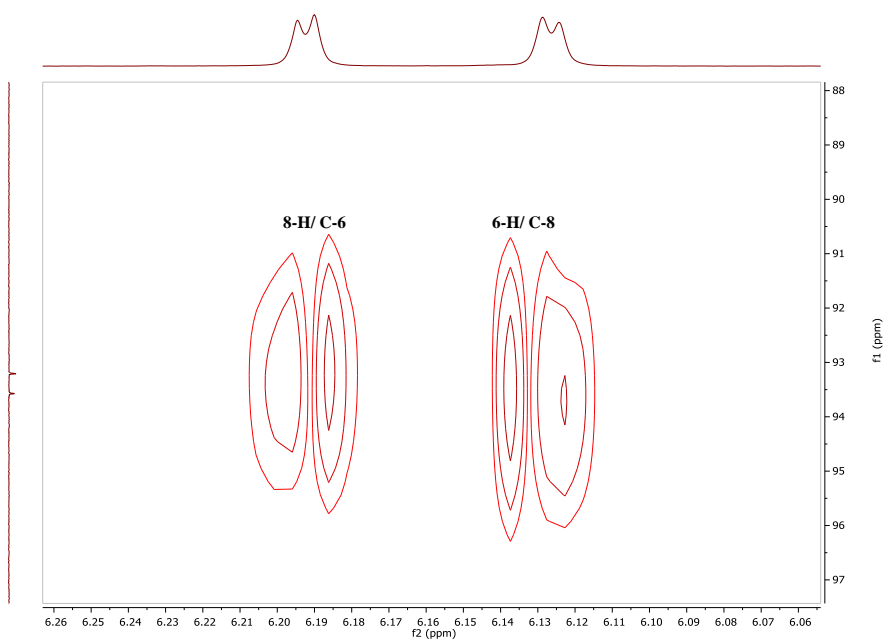
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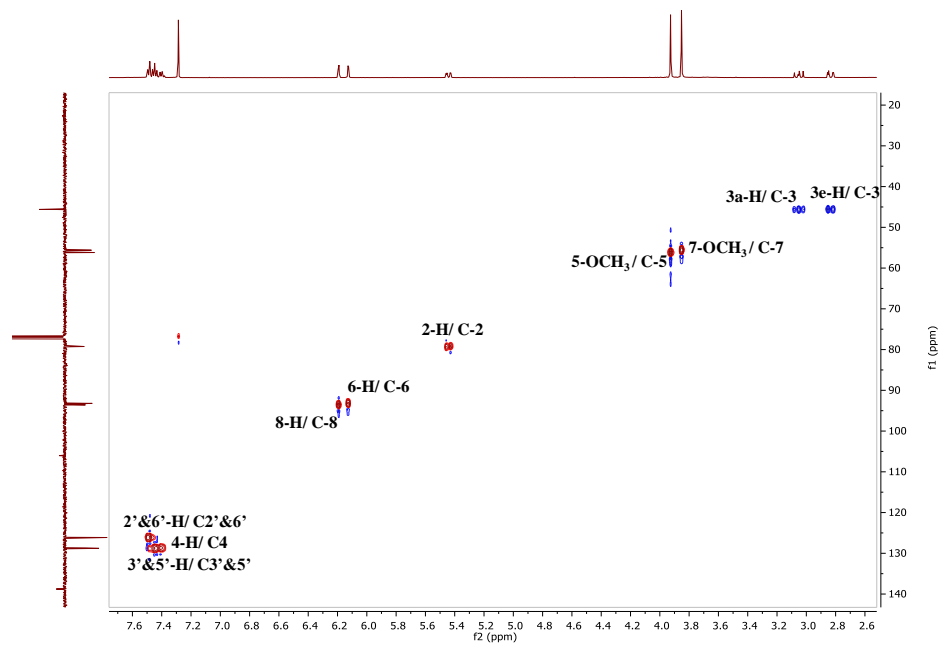
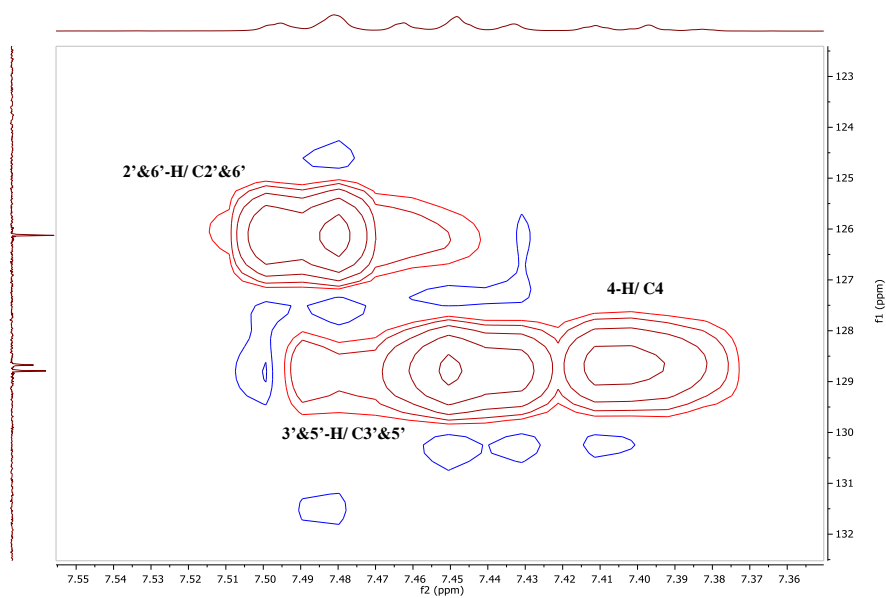
Supplementary Spectrum S15: (A) Full and (B) expansion of COSY spectrum of compound **3** in CDCl₃.

A**B**

Supplementary material S16: (A) Full and (B) expansion of DEPTq 135 ¹³C NMR spectrum of compound **3** in CDCl₃. *Denotes residual solvent peak

A**B**

Supplementary material S17: (A) Full and (B) expansion of HMBC spectrum of compound **3** in CDCl₃.

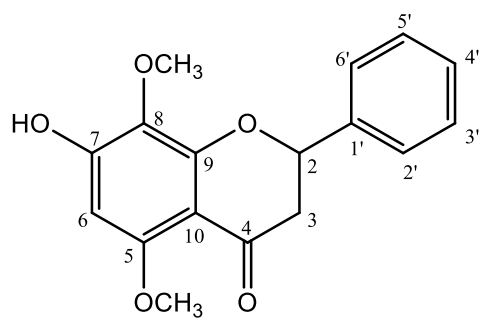
A**B**

Supplementary material S18: (A) Full and (B) expansion of HSQC spectrum of compound 3 in CDCl₃.

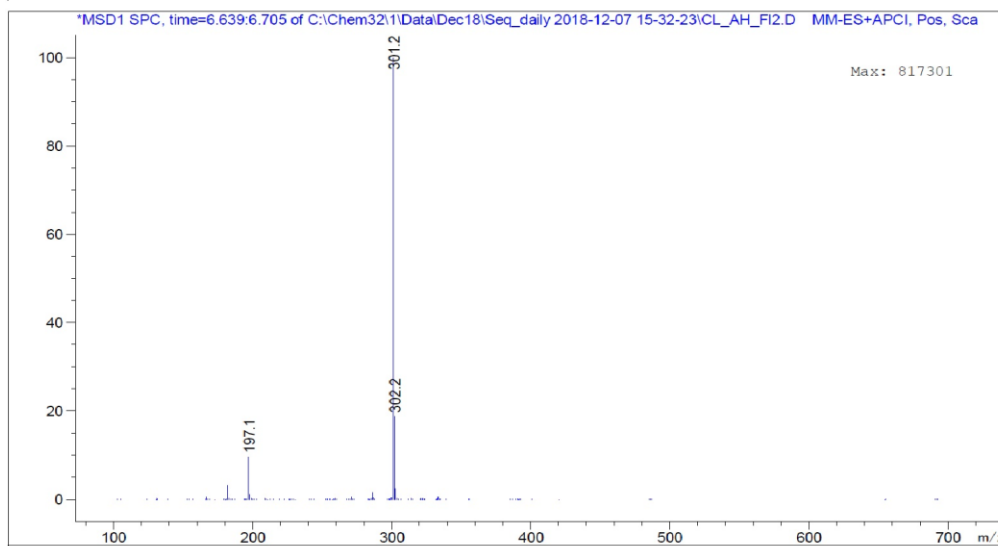
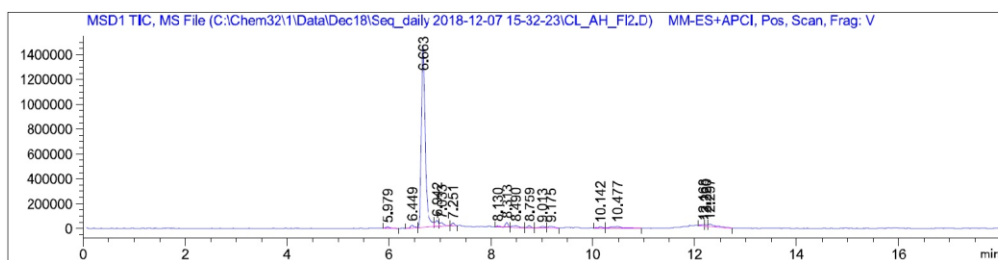
Supplementary Table S3: NMR data for compound 3 in CDCl₃.

Position	δ_{H} (mult, <i>J</i> (Hz))	δ_{C}	HMBC
2	5.44 (1H, dd, 13.1, 2.8)	79.2	C-2', C-1', C-4
3	2.83 (1H, dd, 16.5, 2.8), 3.05 (1H, dd, 16.5, 13.1)	45.6	C-1', C-4, C-10
4	-	189.2	-
5	-	162.3	-
6	6.13 (1H, d, 2.2)	93.2	C-8, C-5, C-7, C-10
7	-	166.0	-
8	6.19 (1H, d, 2.2)	93.6	C-6, C-9, C-10
9	-	165.0	-
10	-	106.0	-
1'	-	138.7	-
2', 6'	7.5 (2H, m)	126.1	C-1', C-2, C-3', C-4', C-5'
3', 4', 5'	7.38 (3H, m)	128.7, 128.8	C-2', C-1'
5-OCH ₃	3.98 (3H, s)	56.1	C-5
7-OCH ₃	3.85 (3H, s)	55.6	C-7

Compound 4

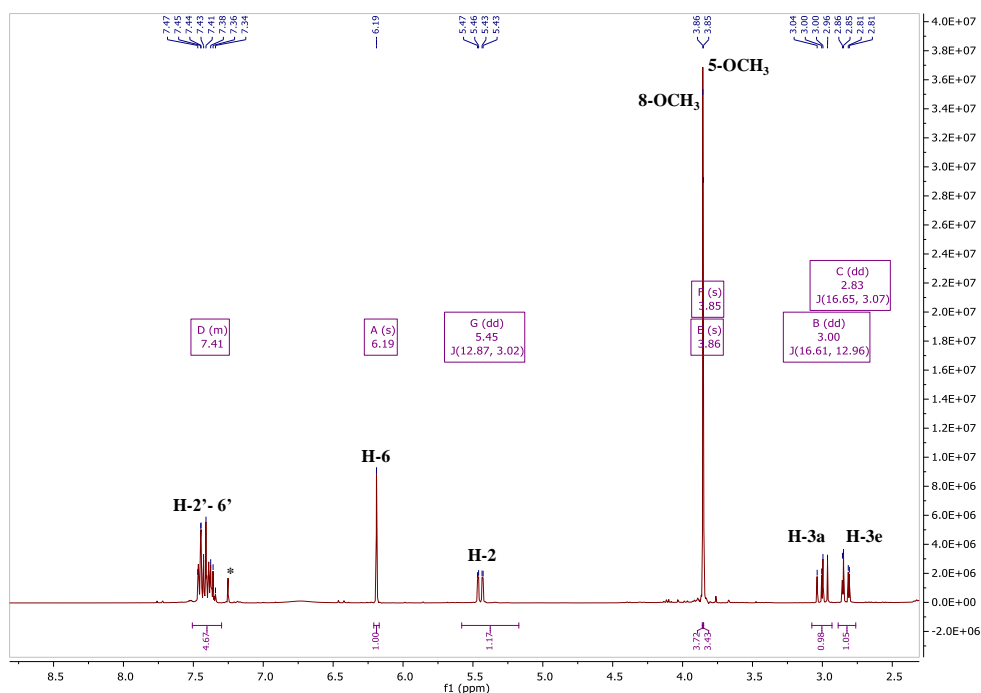


7-hydroxy-5,8-dimethoxy flavanone.

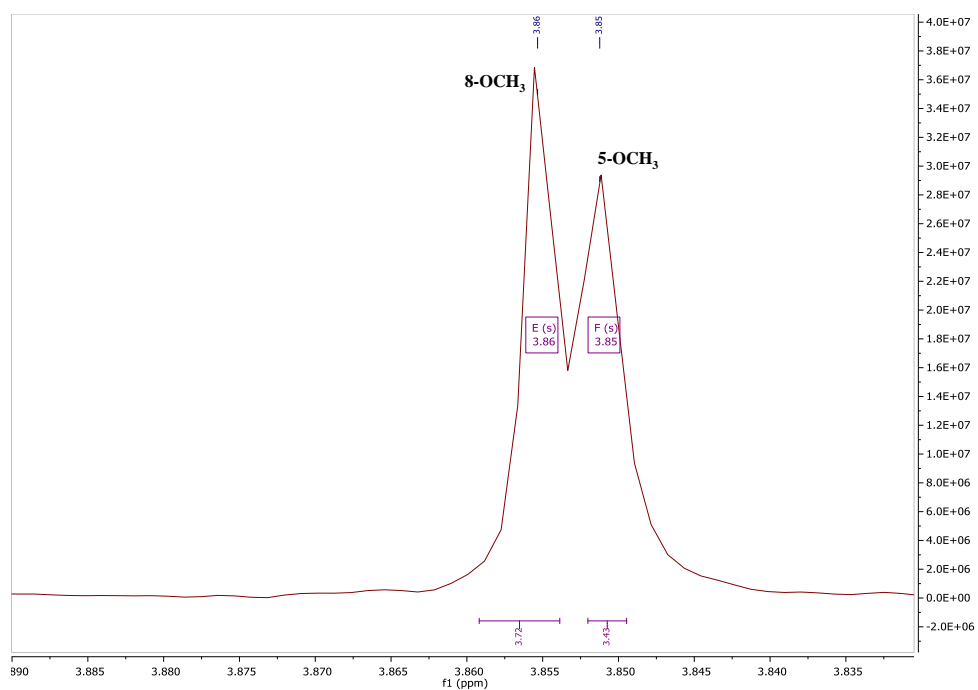


Supplementary material S19: LC-MS spectrum showing $[M+H]^+$ ion for compound 4

A

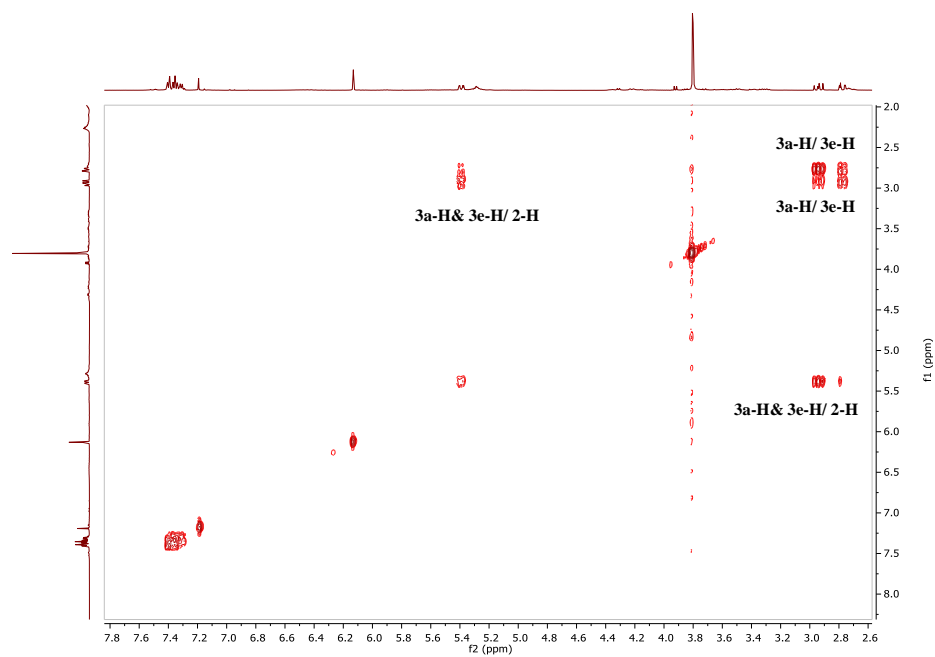


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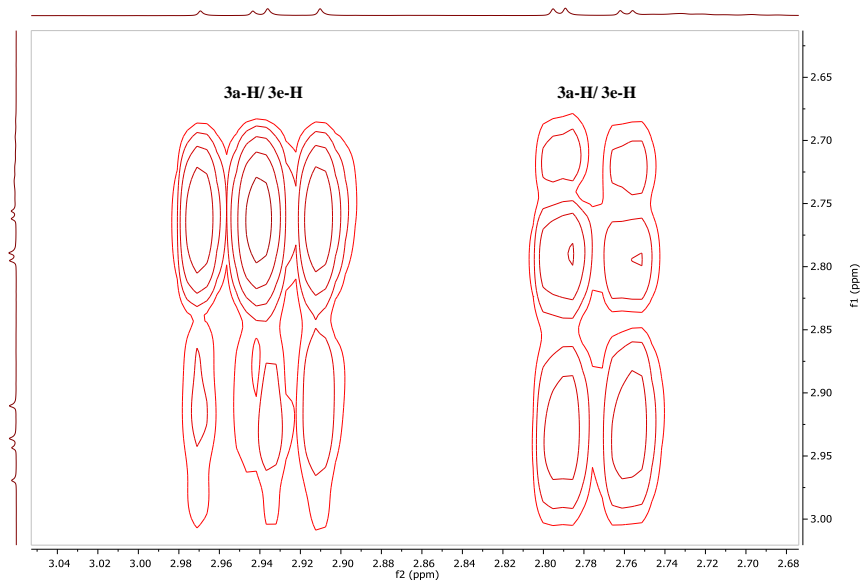


Supplementary material S20: (A) Full ^1H NMR spectrum (500 MHz) of compound **4** in CDCl_3 and (B) expansion of the methoxy region. *Denotes residual solvent peak.

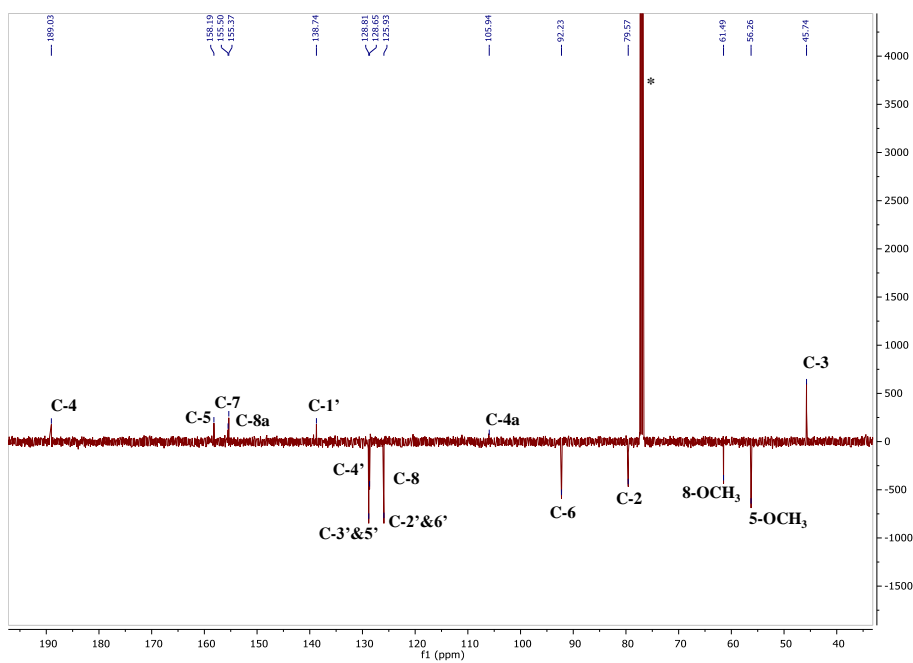
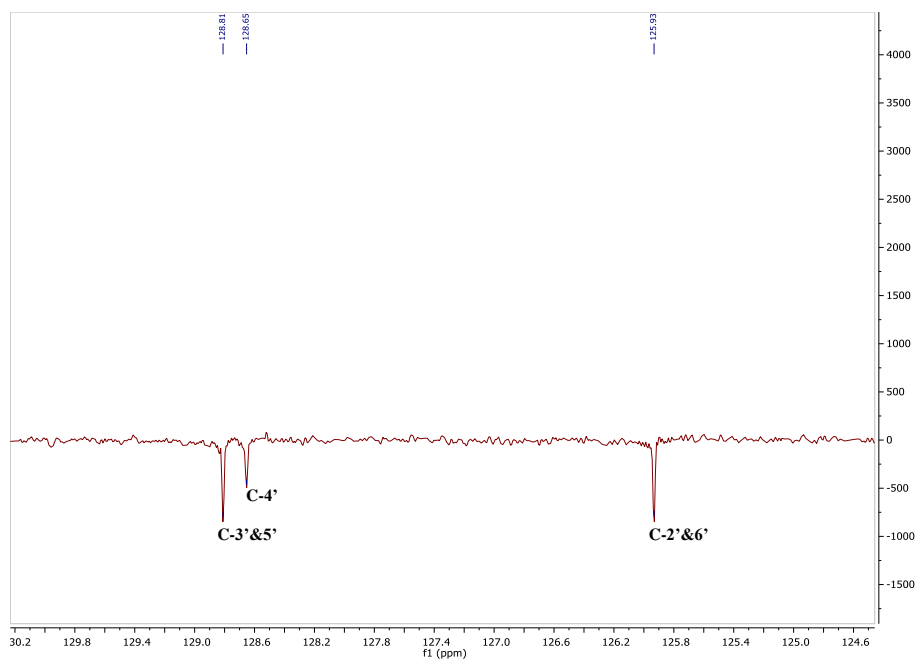
A



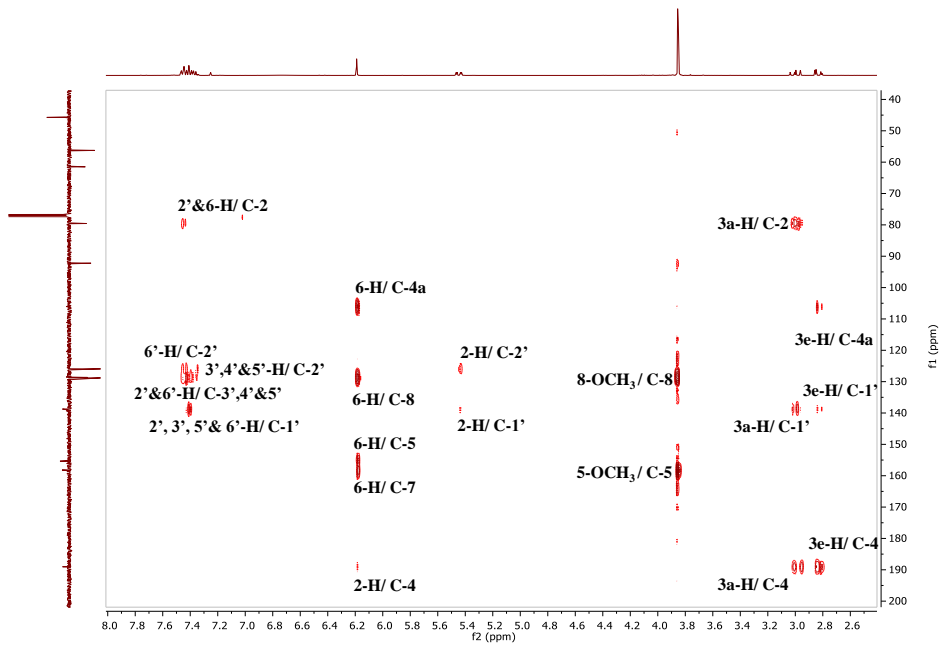
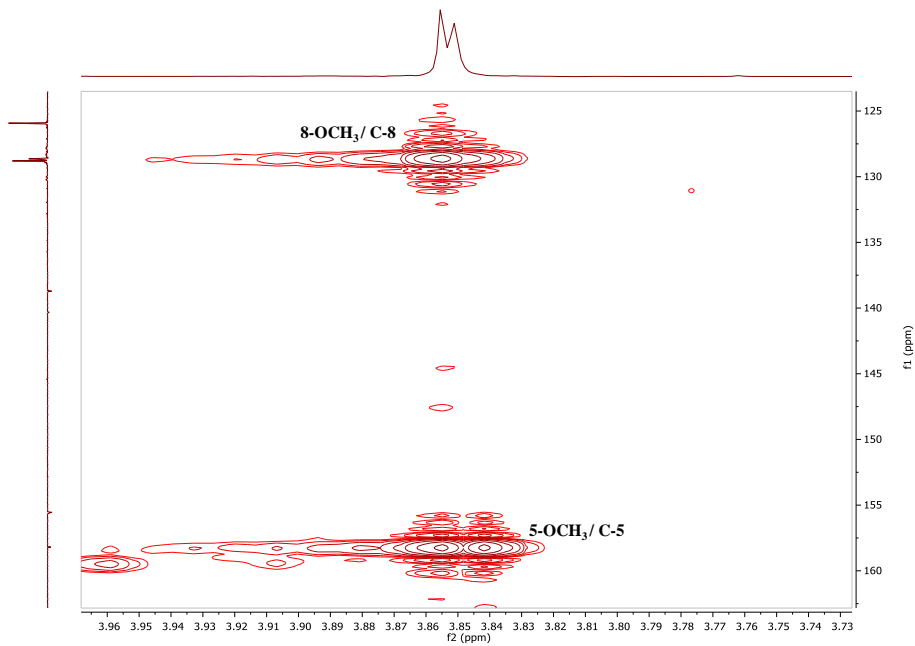
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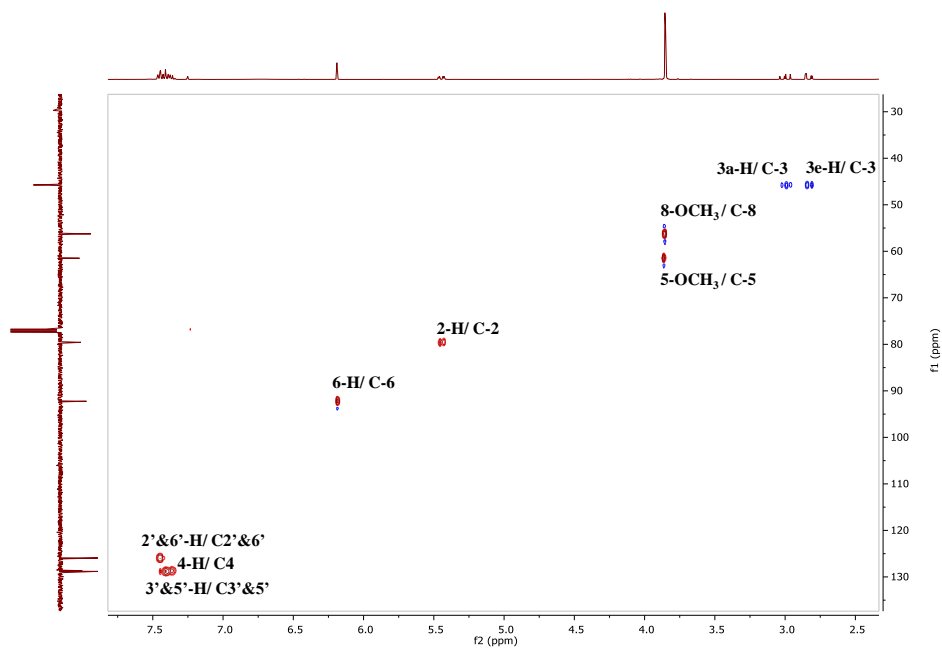
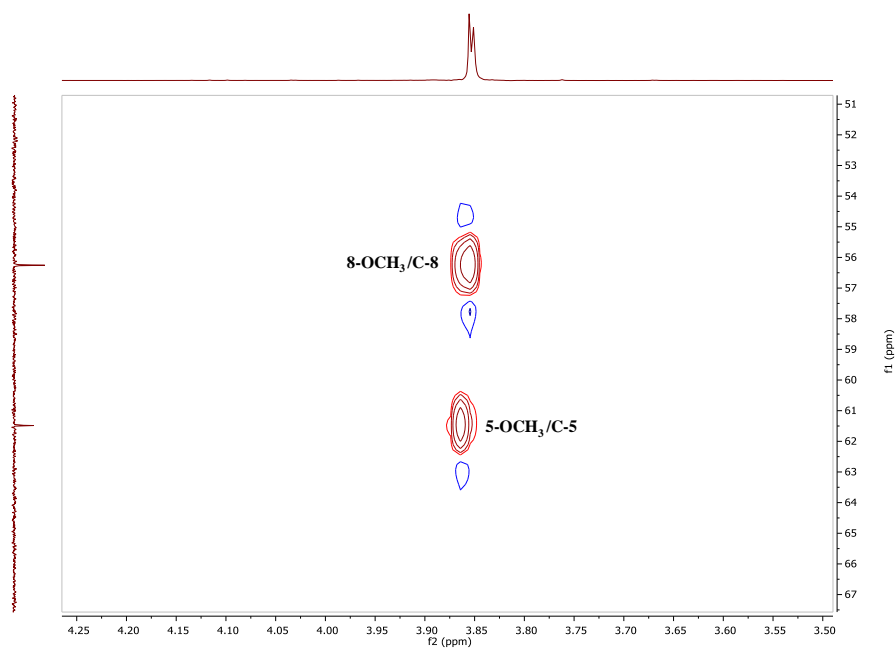
Supplementary Spectrum S21: (A) Full and (B) expansion of COSY spectrum of compound 4 in CDCl₃.

A**B**

Supplementary material S22: (A) Full DEPTq 135 ^{13}C -NMR spectrum in CDCl_3 of compound **4** and (B) expansion of B ring signals.

A**B**

Supplementary material 23: (A) Full HMBC spectrum in CDCl₃ and (B) expansion of the methoxy region of compound 4.

A**B**

Supplementary material S24: (A) Full and (B) expansion of HSQC spectrum of compound 4 in CDCl₃.

Supplementary Table S4: NMR data for compound 4 in CDCl₃.

Position	δ_{H} (mult, J (Hz))	δ_{C}	HMBC
2	5.45 (1H, dd, 12.9, 3.0)	79.6	C-1', C-2', C-4
3	2.83 (1H, dd, 16.6, 3.1), 3.0 (1H, dd, 16.6, 13.0)	45.7	C-1', C-4, C-10
4	-	189.0	-
5	-	158.1	-
6	6.20 (1H, s)	92.1	C-5, C-7, C-8, C-10
7	-	156.0	-
8	-	128.6	-
9	-	155.5	-
10	-	105.9	-
1'	-	138.7	-
2', 6'	7.47 (2H, m)	125.9	C-2, C-3', C-4', C-5'
3', 4', 5'	7.34 (3H, m)	128.8	C-2', C-1'
5-OCH ₃	3.85 (3H, s)	56.1	C-5
8-OCH ₃	3.86 (3H, s)	61.4	C-8