Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

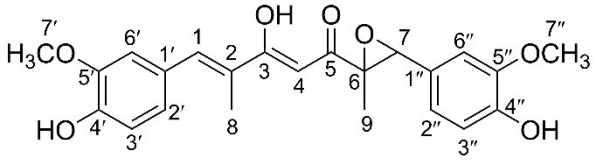
Stability and anti-inflammatory activity of the reduction-resistant curcumin analog, 2,6-dimethyl-curcumin

*Akil I. Joseph[1], Rebecca L. Edwards[1], Paula B. Luis[1], Sai Han Presley[1], Ned A. Porter[2], and Claus Schneider[1]**

[1]Department of Pharmacology, Division of Clinical Pharmacology, and Vanderbilt Institute of Chemical Biology, Vanderbilt University School of Medicine, Nashville, TN 37232, U.S.A.
[2]Department of Chemistry, and Vanderbilt Institute of Chemical Biology, Vanderbilt University, Nashville, TN 37232, U.S.A.

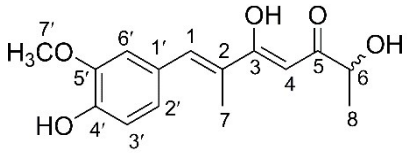
Content:

Table S1. ^{1}H, ^{13}C, COSY, HSQC, and HMBC spectral data for product **3**, 3-hydroxy-5-(4-hydroxy-3-methoxyphenyl)-1-(3-(4-hydroxy-3-methoxyphenyl)-2-methyloxiran-2-yl)-4-methylpenta-2*Z*,4*E*-dien-1-one. The spectra were recorded on a Bruker AV-II 600 MHz spectrometer using D_2O as solvent. ^{13}C chemical shifts were determined from HSQC and HMBC experiments.



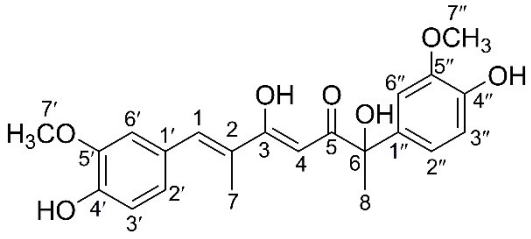
Position	^{1}H (ppm)	Multiplicity	J (Hz)	^{13}C (ppm)	COSY	HMBC
1	7.62	s	-	136.8	7	2',3,6',8
2	-	-	-	124.4	-	-
3	-	-	-	189.7	-	-
4	5.92	s	-	101.2	-	3,6
5	-	-	-	209.0	-	-
6	-	-	-	93.1	-	-
7	4.89	s	-	76.3		2",6"
8	2.22	d	1.01	13.8	1	1,2',3
9	1.33	s	-	18.8	-	5,6,7
1'	-	-	-	128.0	-	-
2'	7.16	dd	8.34,1.87	124.2	3',6'	4',6'
3'	7.02	d	8.16	115.5	2'	1',5'
4'	-	-	-	146.2	-	-
5'	-	-	-	147.0	-	-
6'	7.19	d	2.09	114.5	2'	2',4'
7'	3.87	s	-	55.7	-	5'
1"	-	-	-	131.0	-	-
2"	7.02	dd	8.20,2.00	121.3	3",6"	6",4"
3"	6.95	d	8.10	114.8	2"	1",5"
4"	-	-	-	145.2	-	-
5"	-	-	-	147.3	-	-
6"	7.19	d	2.10	112.2	2"	2",4",5"
7"	3.95	s	-	55.9	7	5"

Table S2. ^{1}H, ^{13}C, COSY, HSQC, and HMBC spectral data for product **4**, 2,5-dihydroxy-7-(4-hydroxy-3-methoxyphenyl)-6-methylhepta-4*Z*,6*E*-dien-3-one. The spectra were recorded on a Bruker AV-II 600 MHz spectrometer using CD_3OD as solvent. ^{13}C chemical shifts were determined from HSQC and HMBC experiments.



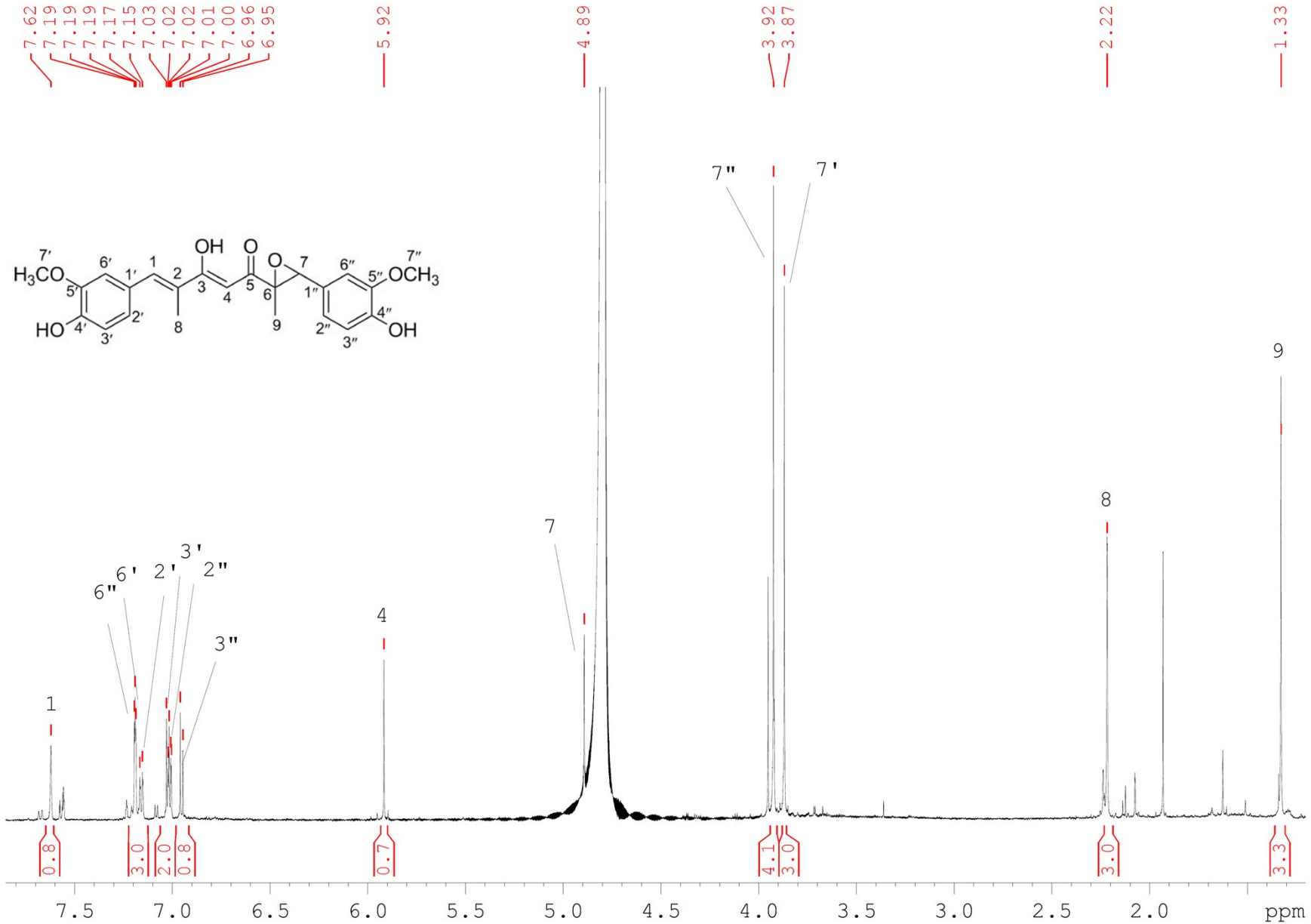
Position	^{1}H (ppm)	Multiplicity	J (Hz)	^{13}C (ppm)	COSY	HMBC
1	7.54	br. s	-	136.8	7	2,2',3,6',7
2	-	-	-	121.7	-	-
3	-	-	-	188.6	-	-
4	5.77	s	-	99.2	-	3,5,6
5	-	-	-	206.6	-	-
6	-	-	-	82.3	-	-
7	2.22	d	1.26	13.6	1	1,1',2,3,6'
8	1.47	s	-	15.4	-	5,6
1'	-	-	-	126	-	-
2'	7.04	dd	8.28,1.98	124.5	3',6'	1,4',6'
3'	6.82	d	8.22	115.6	2'	1',5'
4'	-	-	-	150.3	-	-
5'	-	-	-	148.3	-	-
6'	7.06	d	1.98	113.5	2'	1,2',4',5'
7'	3.87	s	-	55.0	-	5'

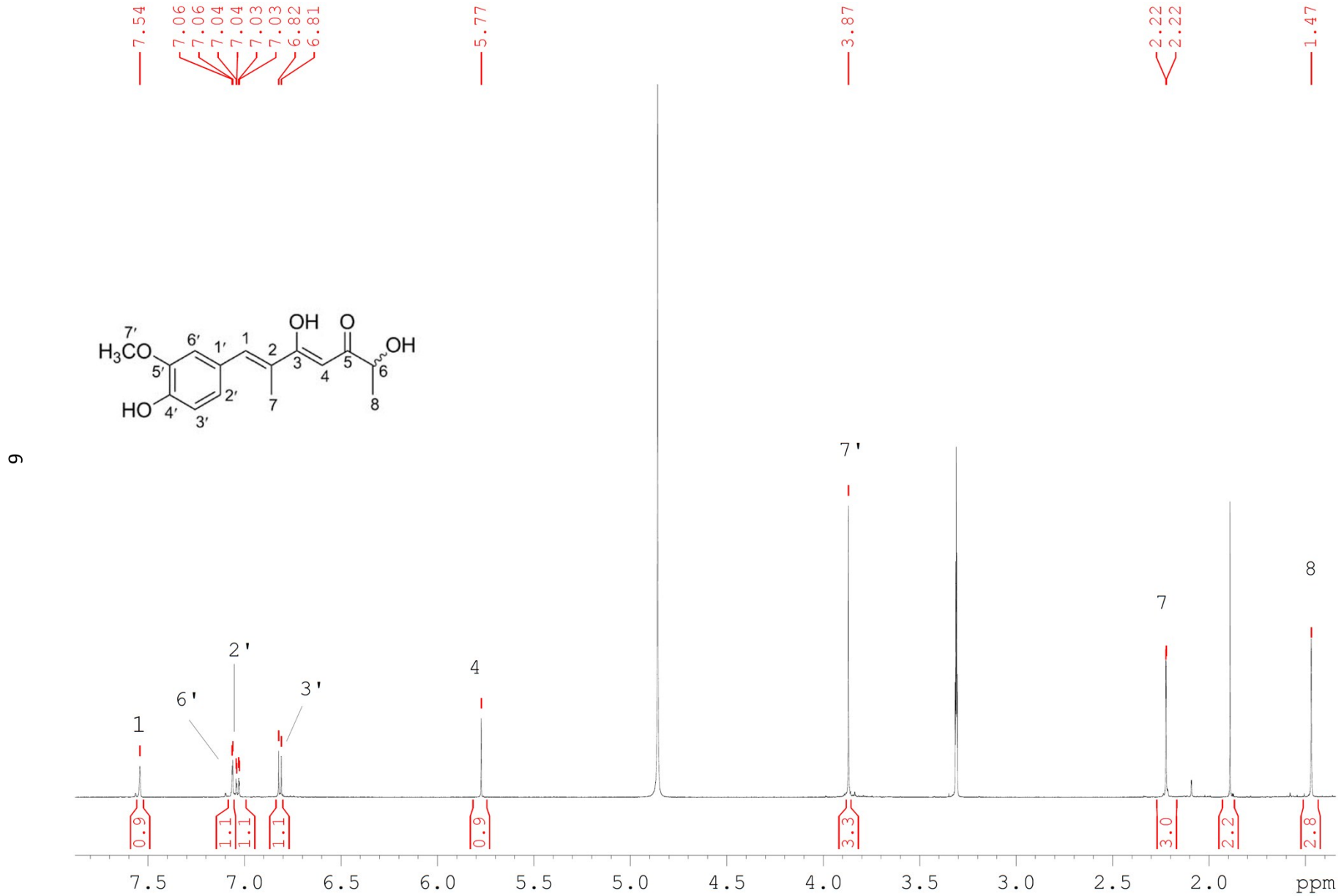
Table S3. ^{1}H, ^{13}C, COSY, HSQC, and HMBC spectral data for product **5**, 2,5-dihydroxy-2,7-bis(4-hydroxy-3-methoxyphenyl)-6-methylhepta-4*Z*,6*E*-dien-3-one. The spectra were recorded on a Bruker AV-II 600 MHz spectrometer using CD_3OD as solvent. Carbon chemical shifts were determined in a ^{13}C-NMR experiment.

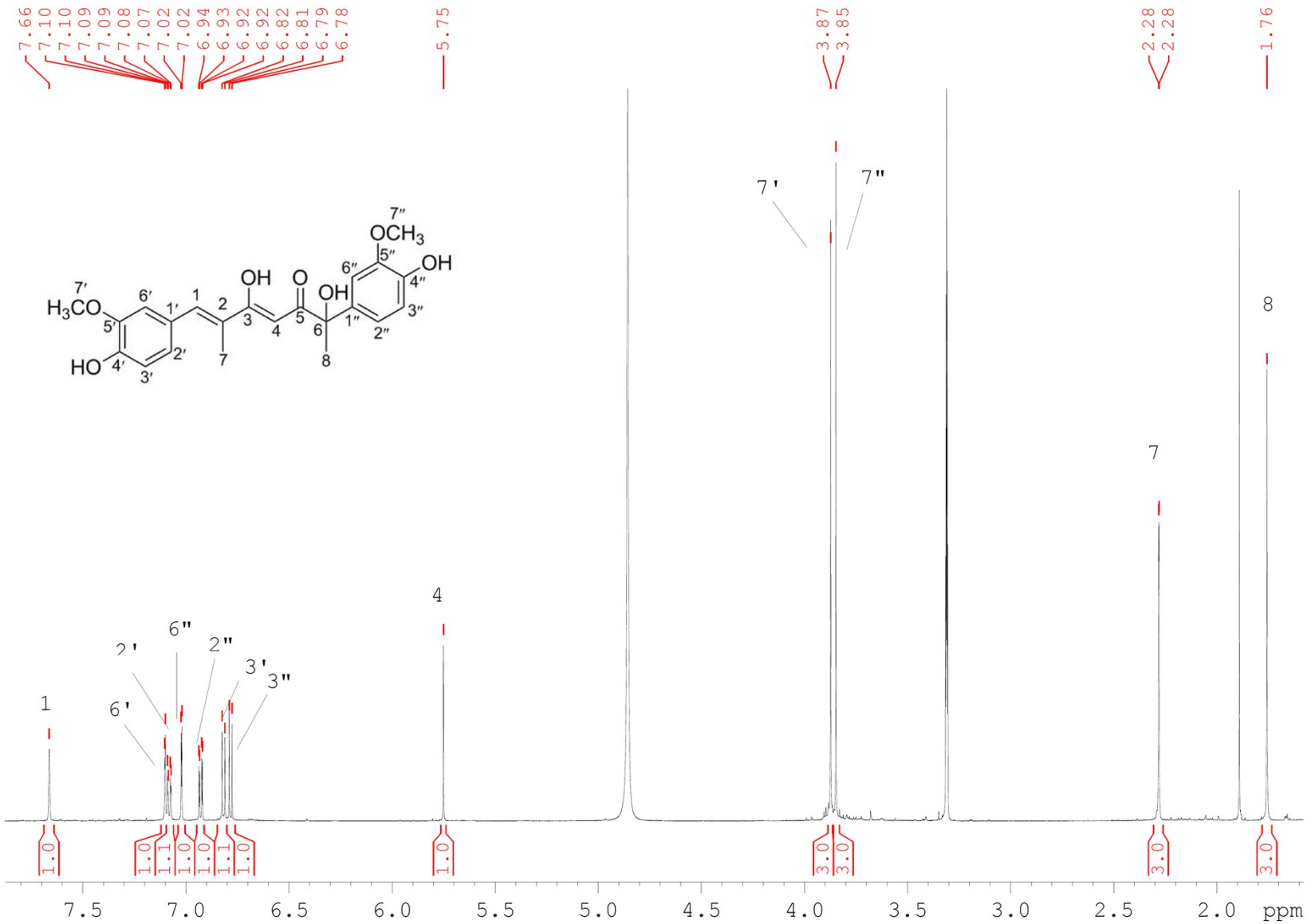


Position	^{1}H (ppm)	Multiplicity	J (Hz)	^{13}C (ppm)	COSY	HMBC
1	7.66	s	-	138.8	7	2',3,6',7
2	-	-	-	122.2	-	-
3	-	-	-	188.9	-	-
4	5.75	s	-	99.1	-	3,5,6
5	-	-	-	207.5	-	-
6	-	-	-	91.7	-	-
7	2.28	d	1.08	15.2	1	1,2,2',3,6'
8	1.76	s	-	24.3	-	1",5,6
1'	-	-	-	127.1*	-	-
2'	7.08	dd	8.22,2.09	126.6	3',6'	1,4',6'
3'	6.81	d	8.16	117.7	2'	2',4',5'
4'	-	-	-	152.8*	-	-
5'	-	-	-	150.3	-	-
6'	7.10	d	1.92	115.0	2'	1,2',4',5'
7'	3.87	s	-	56.3	-	5'
1"	-	-	-	131.0	-	-
2"	6.93	dd	8.31,2.13	118.8	3",6"	3",4",6,6"
3"	6.78	d	8.34	116.3	2"	1",5",2",4"
4"	-	-	-	148.2	-	-
5"	-	-	-	149.1	-	-
6"	7.02	d	2.10	109.8	2"	1",2",4",6
7"	3.85	s	-	56.4	-	5"

*no seen in the ^{13}C NMR spectra but seen in the HMBC spectra.


7.62
7.19
7.19
7.19
7.17
7.15
7.03
7.02
7.02
7.01
7.00
6.96
6.95
5.92
4.89
3.92
3.87
2.22
1.33
7"
7'
9
8
7
6"
6'
2'
3'
2"
4
3"
1
0.8
3.0
2.0
0.8
0.7
4.1
3.0
3.0
3.3
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm


7.54
7.06
7.06
7.04
7.04
7.03
7.03
6.82
6.81
5.77
3.87
2.22
2.22
1.47
OH
O
OH
HO
1
2
3
4
5
6
7
8
1′
2′
3′
4′
5′
6′
7′
H3CO
1
6'
2'
3'
4
7'
7
8
0.9
1.1
1.1
1.1
0.9
3.3
3.0
2.2
2.8
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm


7.66
7.10
7.10
7.09
7.09
7.08
7.07
7.02
7.02
6.94
6.93
6.92
6.92
6.82
6.81
6.79
6.78
5.75
3.87
3.85
2.28
2.28
1.76
7'
7"
8
7
4
1
6'
2'
6"
2"
3'
3"
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1.0
1.1
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1.0
1.1
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3.0
3.0
3.0
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm

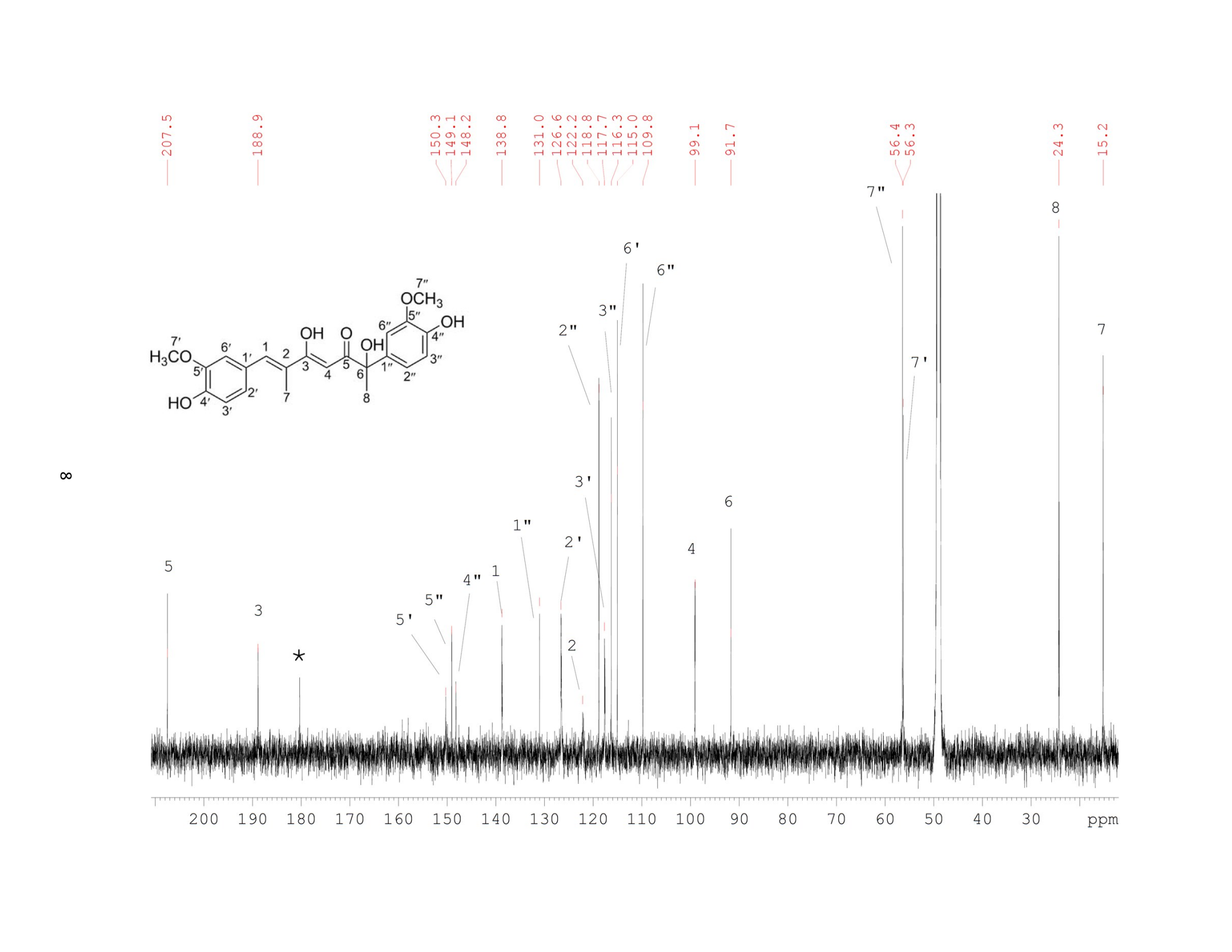
207.5
188.9
150.3
149.1
148.2
138.8
131.0
126.6
122.2
118.8
117.7
116.3
115.0
109.8
99.1
91.7
56.4
56.3
24.3
15.2
7"
8
6'
6"
3"
2"
7
7'
3'
6
1"
2'
4
1
4"
5"
5'
3
2
5
*
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

Table S4. HR-MS data ($[M - H]^-$) of products **2**-**5**.

Product	Found	Calculated	Error (ppm)
2	411.1446	411.1449	0.49
3	411.1448	411.1449	0.20
4	259.0978	259.0976	0.77
5	381.1346	381.1344	0.52