

Supporting Information

Rec. Nat. Prod. 18:6 (2024) 663-673

Anti-inflammatory Constituents Isolated From *Launaea sarmentosa* Against Infection by LPS-stimulated Macrophages

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Table S1: List of primers and primer sequences

No.	Gene name	Primer probes	Sequence
1	<i>iNOS</i>	Forward	5'- CTTTGCCACGGACGAGAC-3'
		Reverse	5'- TCATTGTACTCTGAGGGCTGAC-3'
2	<i>IL-6</i>	Forward	5'- GCTACCAAACCTGGATATAATCAGGA-3'
		Reverse	5'- CCAGGTAGCTATGGTACTCCAGAA-3'
3	<i>TNF-α</i>	Forward	5'- CTGTAGCCCACGTCGTAGC-3'
		Reverse	5'- TTGAGATCCATGCCGTTG-3'
4	<i>β-actin</i>	Forward	5'- GGAGGGGGTTGAGGTGTT-3'
		Reverse	5'- GTGTGCACTTTTATTGGTCTCAA-3'

iNOS; inducible nitric oxide synthase, *COX-2*; cyclooxygenase-2, *HO-1*; heme oxygenase-1

Table S2: Cytotoxicity of LSm and its fractional extract on LPS-stimulated macrophages

Cytotoxicity (cell viability < 95 %); non-treatad with LPS							
Parameter	Control	non-LPS	50	100	200	400	800
LSm	–	n.a	–	–	–	54.00 \pm 7.32	15.06 \pm 0.87
Hex-ex	–	n.a	–	–	–	89.18 \pm 1.57	23.40 \pm 0.21
Ea-ex	–	n.a	–	–	–	76.54 \pm 5.46	31.06 \pm 1.25
Aq-ex	–	n.a	–	–	–	56.29 \pm 3.43	25.86 \pm 3.27
Cytotoxicity (cell viability < 95 %); treatad with LPS							
	Control	LPS	50	100	200	400	800
LSm	–	94.52 \pm 0.58	–	–	–	79.32 \pm 1.1	19.99 \pm 1.90
Hex-ex	–	93.21 \pm 0.19	–	–	–	27.00 \pm 0.20	2.46 \pm 0.09
Ea-ex	–	94.05 \pm 0.82	–	–	–	90.67 \pm 3.27	31.77 \pm 0.36
Aq-ex	–	91.47 \pm 0.65	–	–	–	85.67 \pm 1.80	62.94 \pm 2.39

“–”: No cytotoxicity; “n.a”: Not applicable; $p < 0.05$.

Table S3: Induction efficiency of NO secretion from isolated compounds in LPS-induced inflammation

No	Compound	IC ₅₀ value of NO inhibition (μ M)
1	Succinic acid	>100
2	Quercetin	27.44 \pm 0.30
3	2(4-Hydroxylphenyl)acetic acid	>100
4	Luteolin-7- <i>O</i> - β -glucopyranoside	30.38 \pm 0.86
5	Quercetin-3- <i>O</i> -rutinoside	>100

1. Supplementary spectroscopic data of compound 1

Table S4: The comparison of NMR data of compound 1 with a similar compound (Succinic acid).

Position	Compound 1 (CD ₃ OD)		Succinic acid (CD ₃ OD) [1]	
	¹³ C-NMR (150 MHz) δ _C ppm	¹ H-NMR (600 MHz) δ _H ppm	¹³ C-NMR (125 MHz) δ _C ppm	¹ H-NMR (500 MHz) δ _H ppm
1, 4	176.1	-	174.8	-
2, 3	29.7	2.59	28.4	2.57

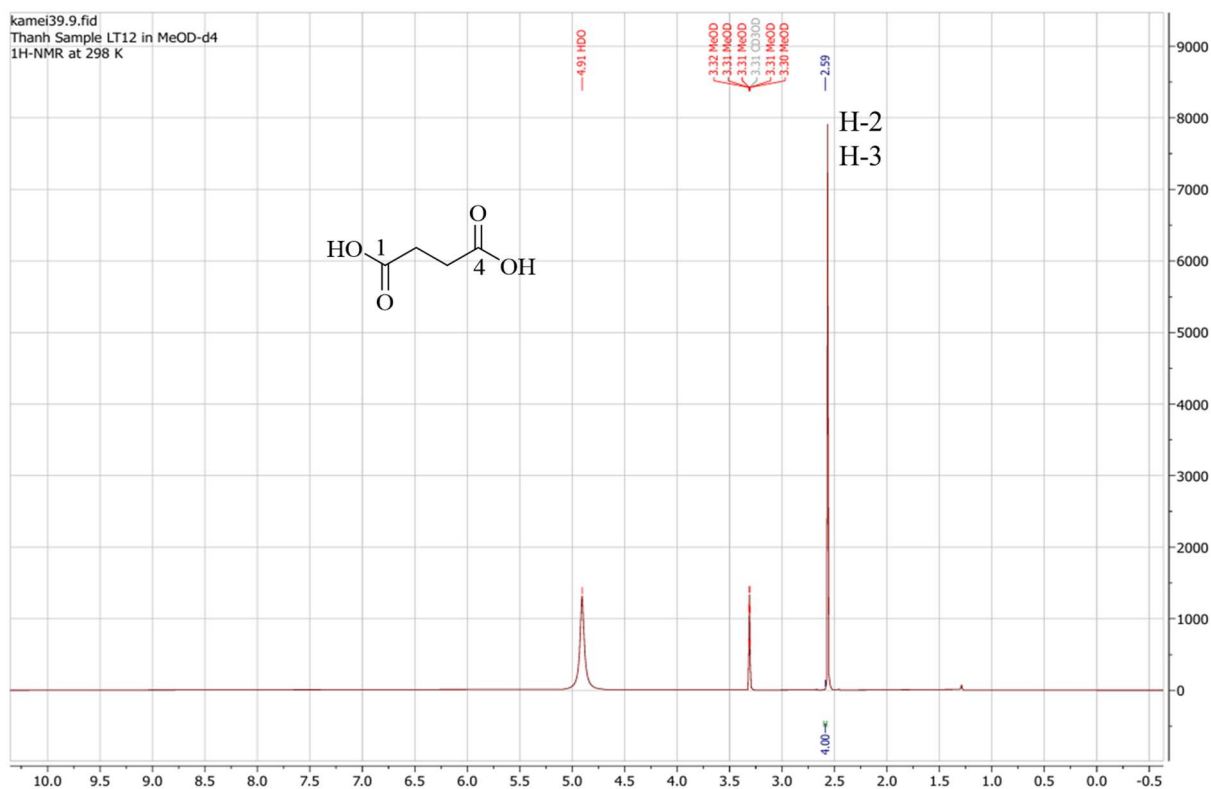


Figure S1: ¹H-NMR (600 MHz, CD₃OD) spectrum of compound 1 (succinic acid)

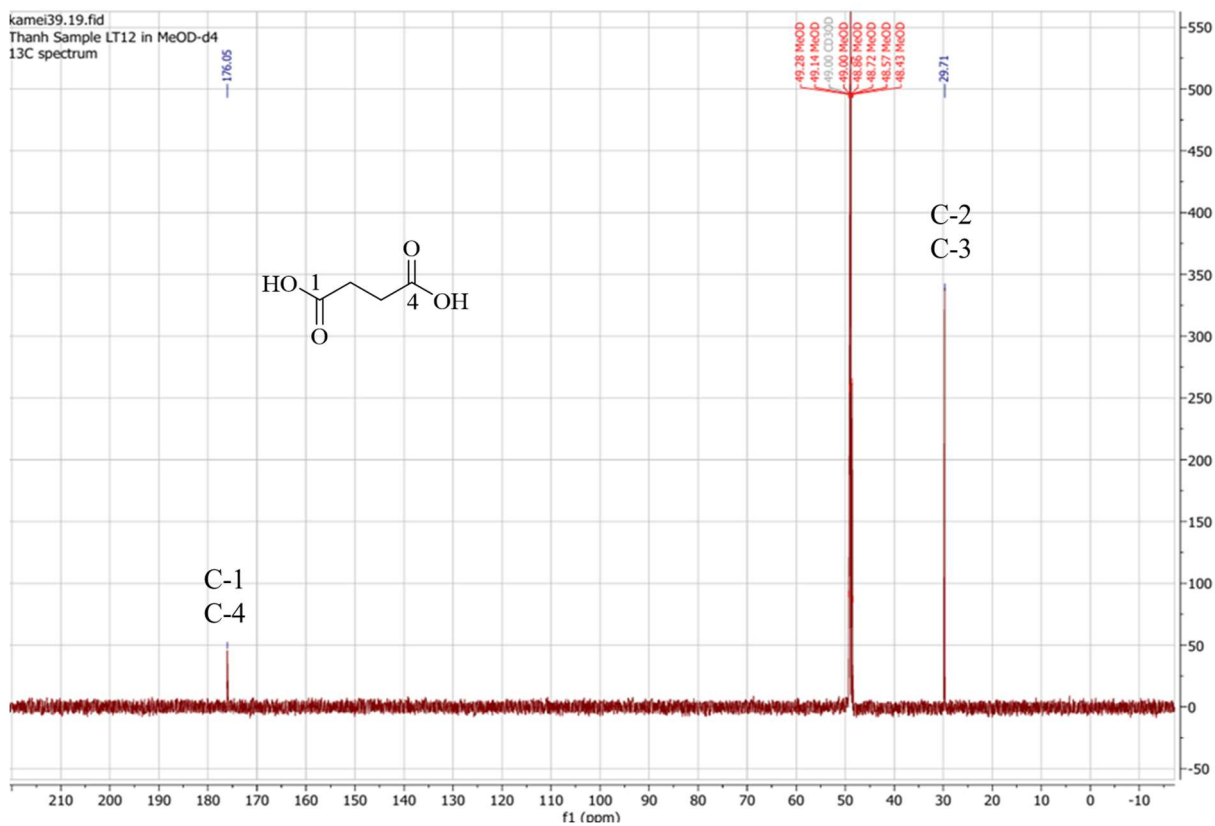


Figure S2: ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound **1** (succinic acid)

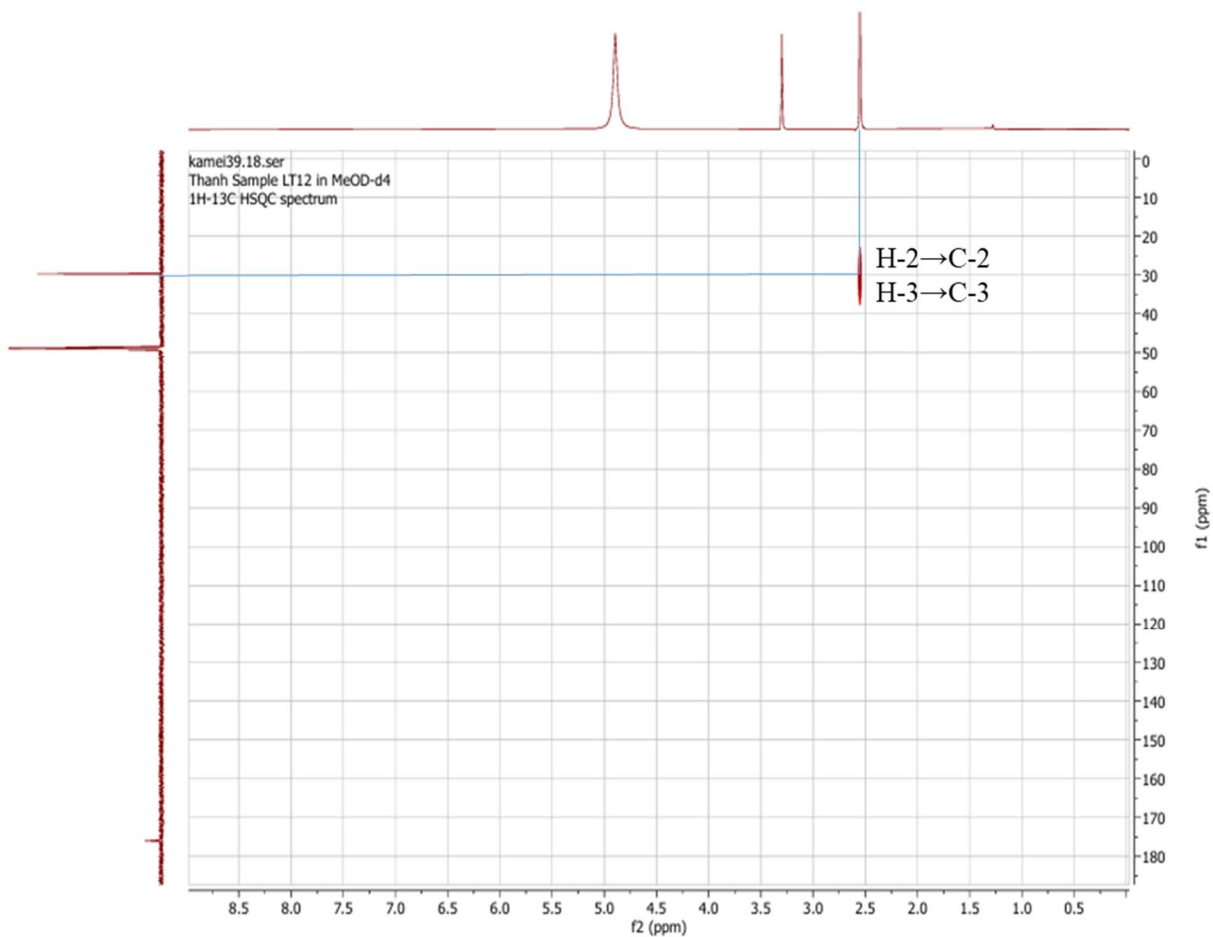
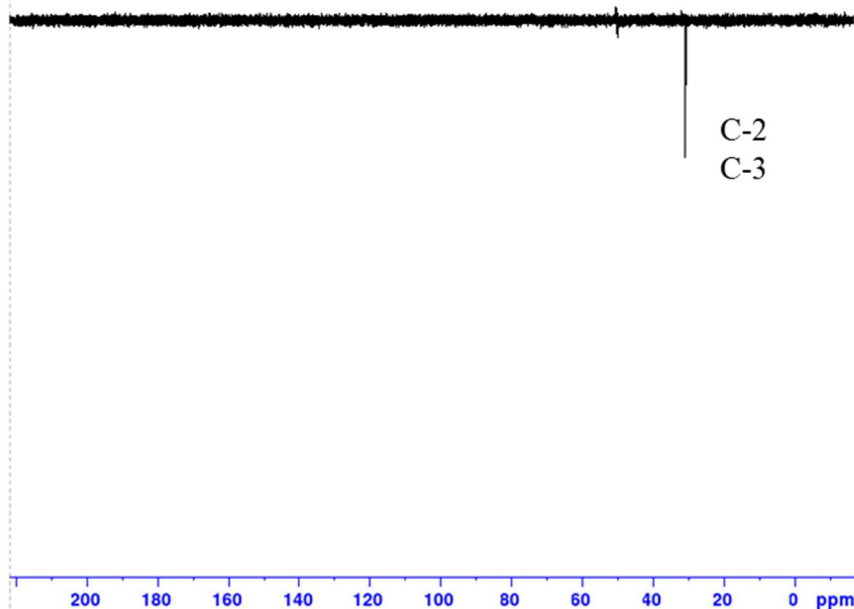


Figure S3: HSQC spectrum of compound **1** (succinic acid)

Thanh Sample LT12 in MeOD-d4
13C DEPT135 spectrum



Current Data Parameters
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EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231219
Time 14.24
INSTRUM spect
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PULPROG dept135
TD 65536
SOLVENT MeOD
NS 22
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 30.00 usec
TE 297.4 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1

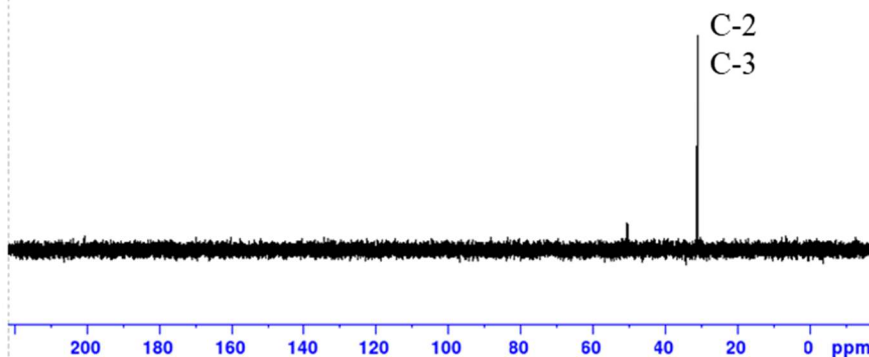
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P2 23.40 usec
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PL1W 85.59675598 W
SFO1 150.9329873 MHz

===== CHANNEL f2 =====
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NUC2 1H
P3 13.90 usec
P4 27.80 usec
PCPD2 70.00 usec
PL2 -1.50 dB
PL12 12.54 dB
PL2W 15.86015892 W
PL12W 0.52561554 W
SFO2 600.1924008 MHz

F2 - Processing parameters
SI 65536
SF 150.9175544 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S4: DEPT-135 spectrum of compound 1 (succinic acid)

Thanh Sample LT12 in MeOD-d4
13C DEPT90 spectrum



Current Data Parameters
NAME kame139
EXPNO 21
PROCNO 1

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Time 14.28
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PULPROG dept90
TD 65536
SOLVENT MeOD
NS 58
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 30.00 usec
TE 297.2 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.70 usec
P2 23.40 usec
PL1 1.00 dB
PL1W 85.59675598 W
SFO1 150.9329873 MHz

===== CHANNEL f2 =====
CPDPRG12 waitz16
NUC2 1H
P3 13.90 usec
P4 27.80 usec
PCPD2 70.00 usec
PL2 -1.50 dB
PL12 12.54 dB
PL2W 15.86015892 W
PL12W 0.52561554 W
SFO2 600.1924008 MHz

F2 - Processing parameters
SI 65536
SF 150.9175544 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S5: DEPT-90 spectrum of compound 1 (succinic acid)

2. Supplementary spectroscopic data of compound 2.

Table S5: The comparison of NMR data of compound 2 with a similar compound (Quercetin).

Position	Compound 2 (CD ₃ OD)		Quercetin (CD ₃ OD) [2]	
	¹³ C-NMR (150 MHz) δ _C ppm	¹ H-NMR (600 MHz) δ _H ppm	¹³ C-NMR (125 MHz) δ _C ppm	¹ H-NMR (500 MHz) δ _H ppm
2	-	148.8	-	148.6
3	-	137.2	-	137.2
4	-	177.3	-	177.3
5	-	162.5	-	162.6
6	6.20 (1H, <i>d</i> , <i>J</i> = 1.8 Hz)	99.3	6.20 (1H, <i>d</i> , <i>J</i> = 2.0 Hz)	99.1
7	-	165.6	-	165.6
8	6.41 (1H, <i>d</i> , <i>J</i> = 1.8 Hz)	94.4	6.41 (1H, <i>d</i> , <i>J</i> = 2.0 Hz)	94.4
9	-	158.3	-	158.2
10	-	104.5	-	104.5
1'	-	124.2	-	124.1
2'	7.75 (1H, <i>d</i> , <i>J</i> = 2.4 Hz)	116.0	7.75 (1H, <i>d</i> , <i>J</i> = 2.2 Hz)	116.0
3'	-	146.2	-	146.2
4'	-	148.0	-	148.0
5'	6.91 (1H, <i>d</i> , <i>J</i> = 9 Hz)	116.2	6.99 (1H, <i>d</i> , <i>J</i> = 8.5 Hz)	116.2
6'	7.66 (1H, <i>dd</i> , <i>J</i> = 9.0, 2.4 Hz)	121,7	7.65 (1H, <i>dd</i> , <i>J</i> = 8.5; 2 Hz)	121,7

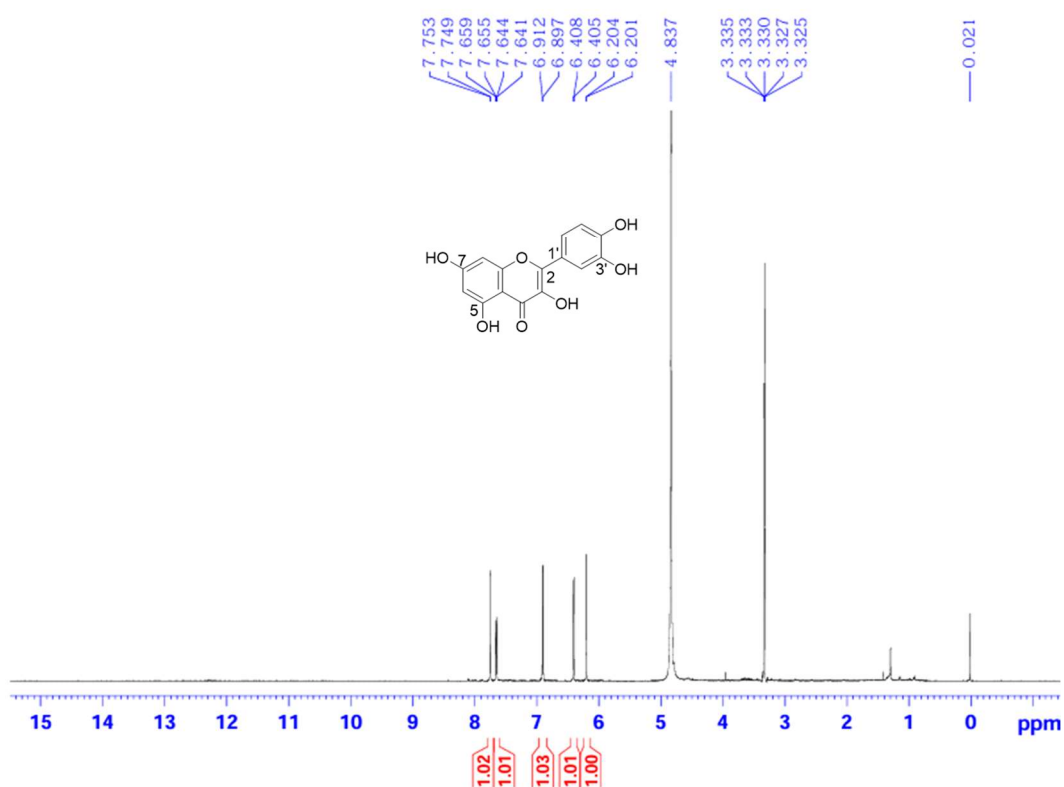


Figure S6: ¹H-NMR (600 MHz, CD₃OD) spectrum of compound 2 (quercetin)

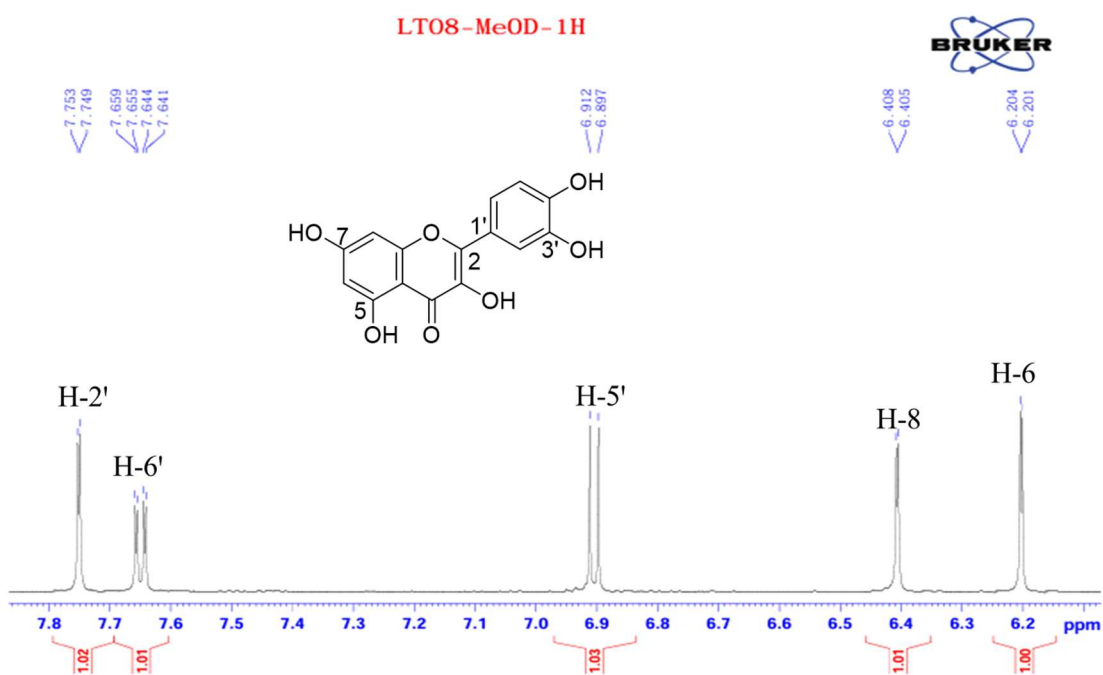


Figure S7: ¹H-NMR (600 MHz, CD₃OD) spectrum of compound 2 (quercetin) (from δ_H 6 ppm to δ_H 8 ppm)

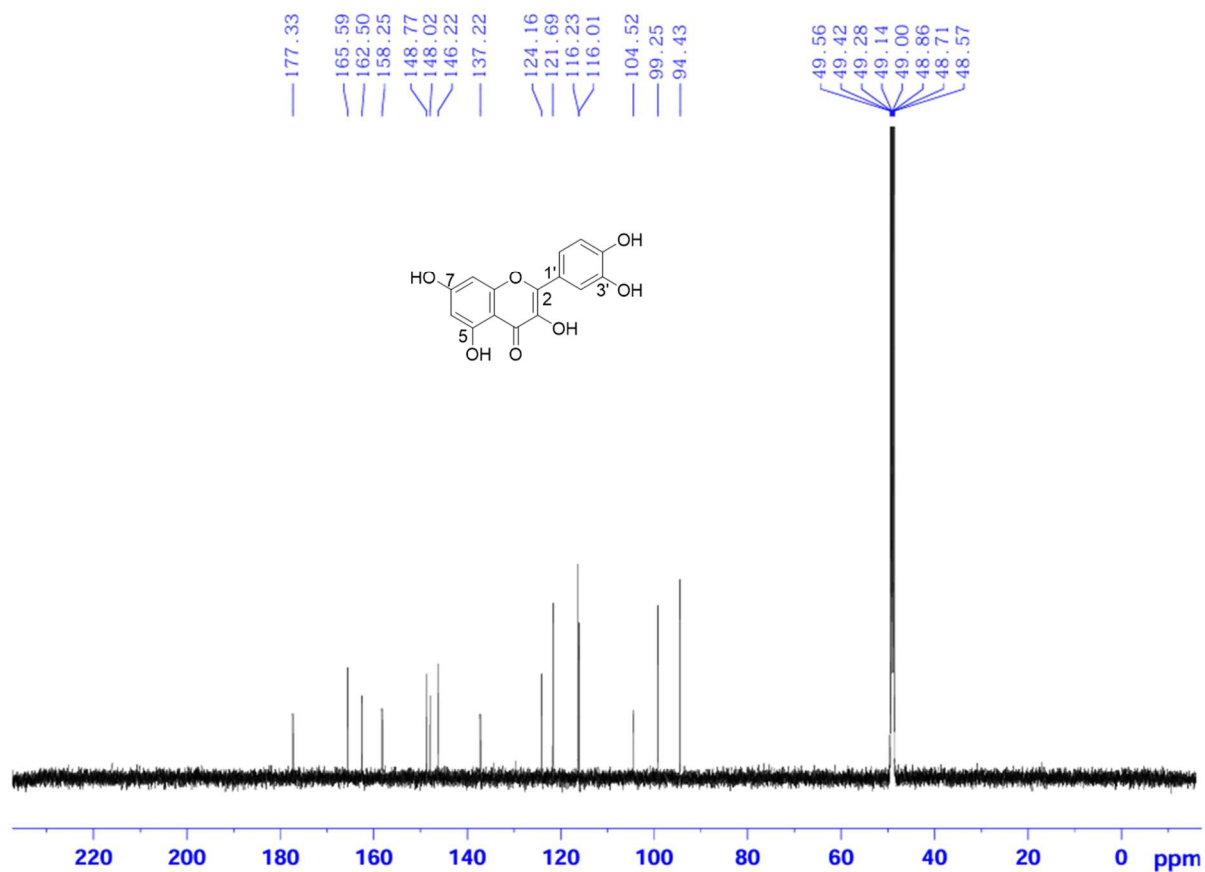


Figure S8: ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound 2 (quercetin)

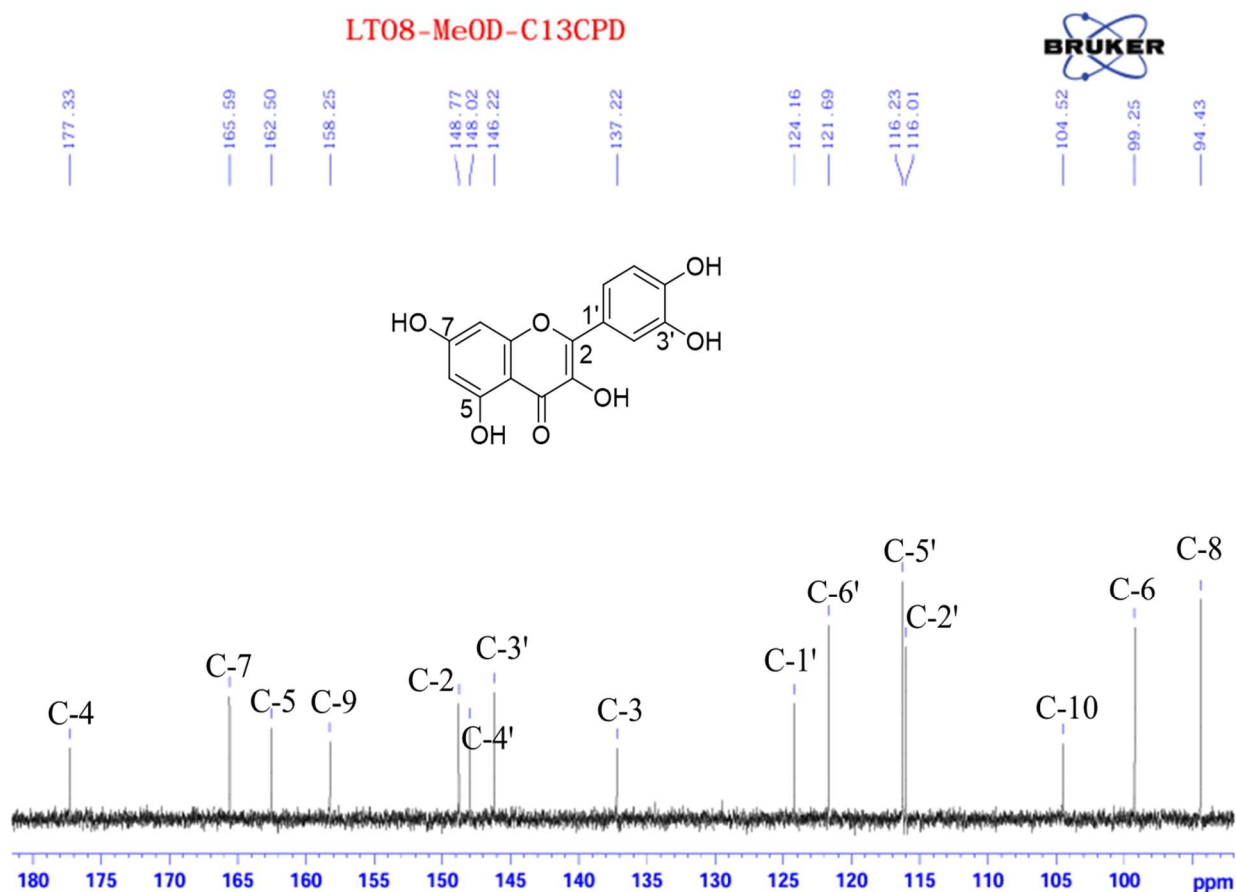


Figure S9: ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound **2** (quercetin) (from δ_{C} 95 ppm to δ_{C} 180 ppm)

4. Supplementary spectroscopic data of compound **3**.

Table S6: The comparison of NMR data of compound **3** with a similar compound (Quercetin-3-*O*-rutinoside).

Position	Compound 3 ($\text{DMSO-}d_6$)		Quercetin-3- <i>O</i> -rutinoside ($\text{DMSO-}d_6$)[5]	
	^{13}C -NMR (150 MHz) δ_{C} ppm	^1H -NMR (600 MHz) δ_{H} ppm	^{13}C -NMR (125 MHz) δ_{C} ppm	^1H -NMR (500 MHz) δ_{H} ppm
2	-	156.5	-	156.5
3	-	133.3	-	133.3
4	-	177.3	-	177.3
5	-	161.2	-	161.2
6	6.19 (1H, <i>d</i> , <i>J</i> = 1.8 Hz)	98.6	6.19 (1H, <i>d</i> , <i>J</i> = 2.0 Hz)	98.7
7	-	164.0	-	164.2

8	6.38 (1H, <i>d</i> , <i>J</i> = 1.8 Hz)	93.5	6.38 (1H, <i>d</i> , <i>J</i> = 2.0 Hz)	93.6
9	-	156.4	-	156.4
10	-	103.9	-	103.9
1'	-	121.1	-	121.1
2'	7.55 (1H, <i>m</i> , <i>J</i> = 8.4; 2.4 Hz)	115.2	7.53 (1H, <i>m</i> , <i>J</i> = 8.5; 2.0 Hz)	115.2
3'	-	144.7	-	144.7
4'	-	148.4	-	148.4
5'	6.84 (1H, <i>d</i> , <i>J</i> = 8.4 Hz)	116.2	6.84 (1H, <i>d</i> , <i>J</i> = 8.2 Hz)	116.2
6'	7.55 (1H, <i>m</i> , <i>J</i> = 8.4; 2.4 Hz)	121.5	7.53 (1H, <i>m</i> , <i>J</i> = 8.5; 2.0 Hz)	121.7
1''	5.35 (1H, <i>d</i> , <i>J</i> = 7.2 Hz)	101.1	5.34 (1H, <i>d</i> , <i>J</i> = 7.3 Hz)	101.2
2''	3.21 – 3.39 (1H, <i>m</i>)	74.0	3.15 – 3.41 (<i>m</i>)	74.1
3''	3.21 – 3.39 (1H, <i>m</i>)	76.4	3.15 – 3.41 (<i>m</i>)	76.4
4''	3.21 – 3.39 (1H, <i>m</i>)	70.0	3.15 – 3.41 (<i>m</i>)	70.0
5''	3.21 – 3.39 (1H, <i>m</i>)	75.9	3.15 – 3.41 (<i>m</i>)	75.9
6''	3.21 – 3.39 (1H, <i>m</i>) 3.72 (1H, <i>d</i> , <i>J</i> = 10.2 Hz)	66.9	3.15 – 3.41 (<i>m</i>)	66.8
1'''	4.39 (1H, <i>brd</i> , <i>J</i> = 0.6 Hz)	100.7	4.38 (1H, <i>s</i>)	100.7
2'''	3.04 – 3.09 (1H, <i>m</i>)	70.3	3.05 – 3.10 (<i>m</i>)	70.4
3'''	3.04 – 3.09 (1H, <i>m</i>)	70.5	3.05 – 3.10 (<i>m</i>)	70.5
4'''	3.04 – 3.09 (1H, <i>m</i>)	71.8	3.05 – 3.10 (<i>m</i>)	71.8
5'''	3.04 – 3.09 (1H, <i>m</i>)	68.2	3.05 – 3.10 (<i>m</i>)	68.2

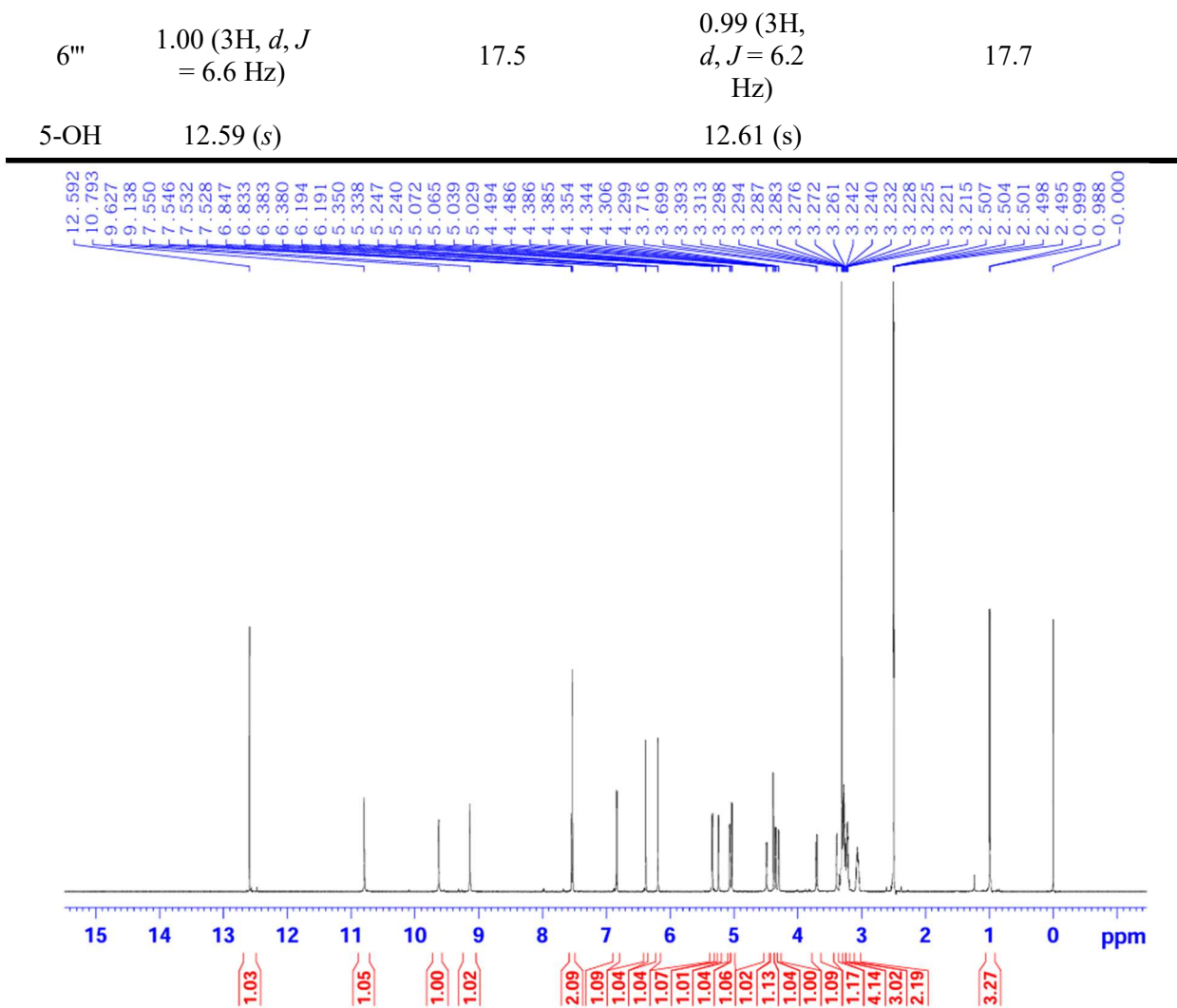


Figure S10: ¹H-NMR (600 MHz, DMSO-*d*₆) spectrum of compound **3** (quercetin-3-*O*-rutinoside)

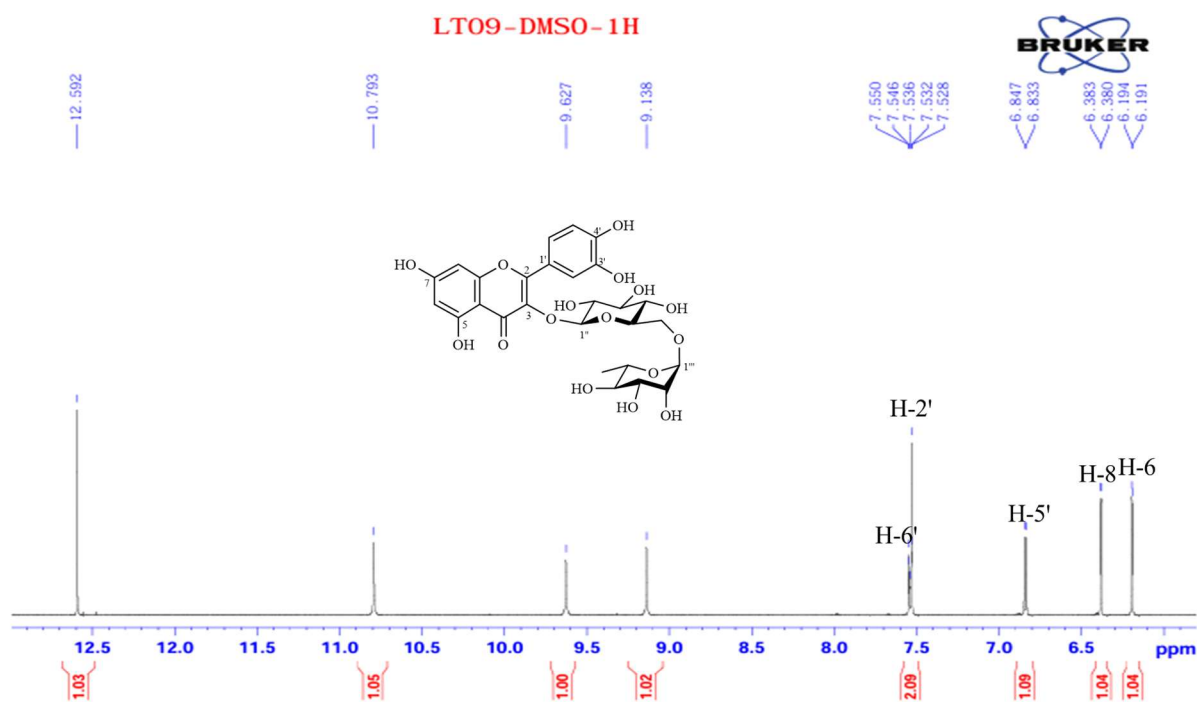


Figure S11: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **3** (quercetin-3-*O*-rutinoside) (from δ_H 6 ppm to δ_H 13 ppm)

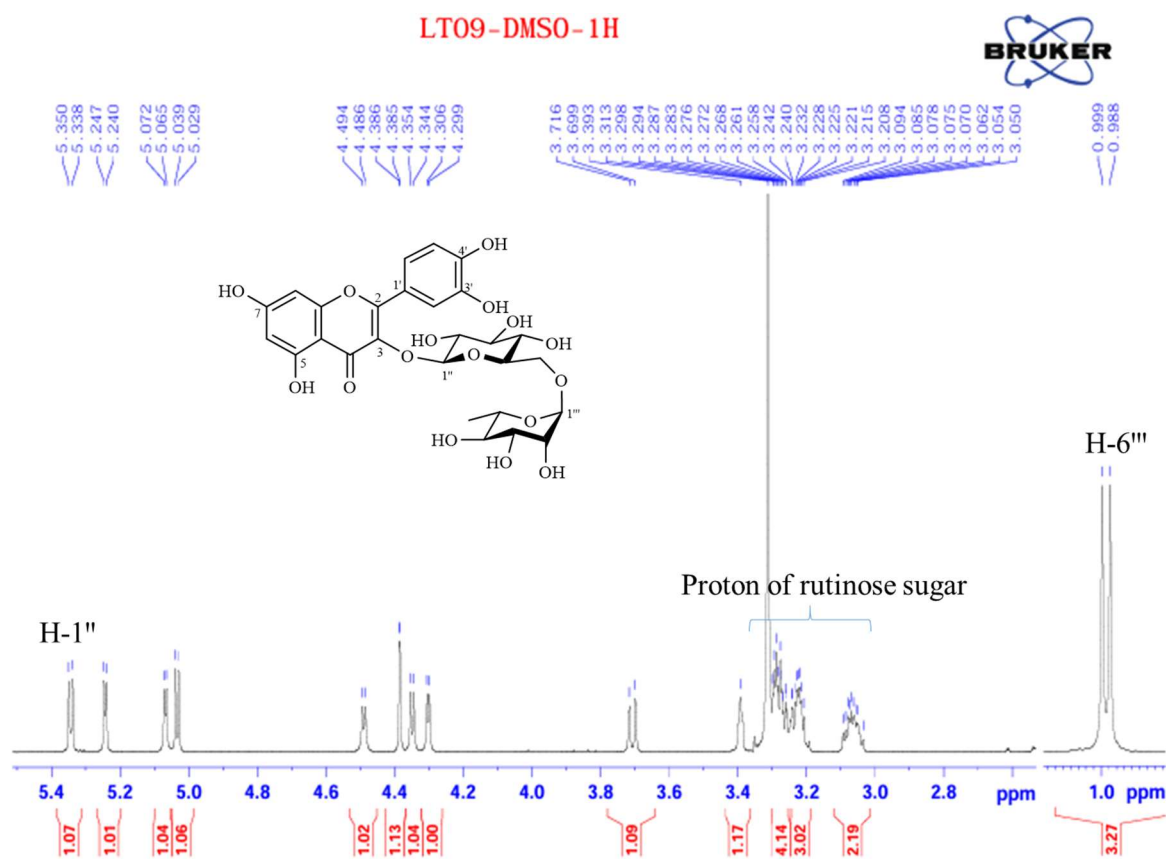


Figure S12: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **3** (quercetin-3-*O*-rutinoside) (from δ_H 1.0 ppm to δ_H 5.5 ppm)

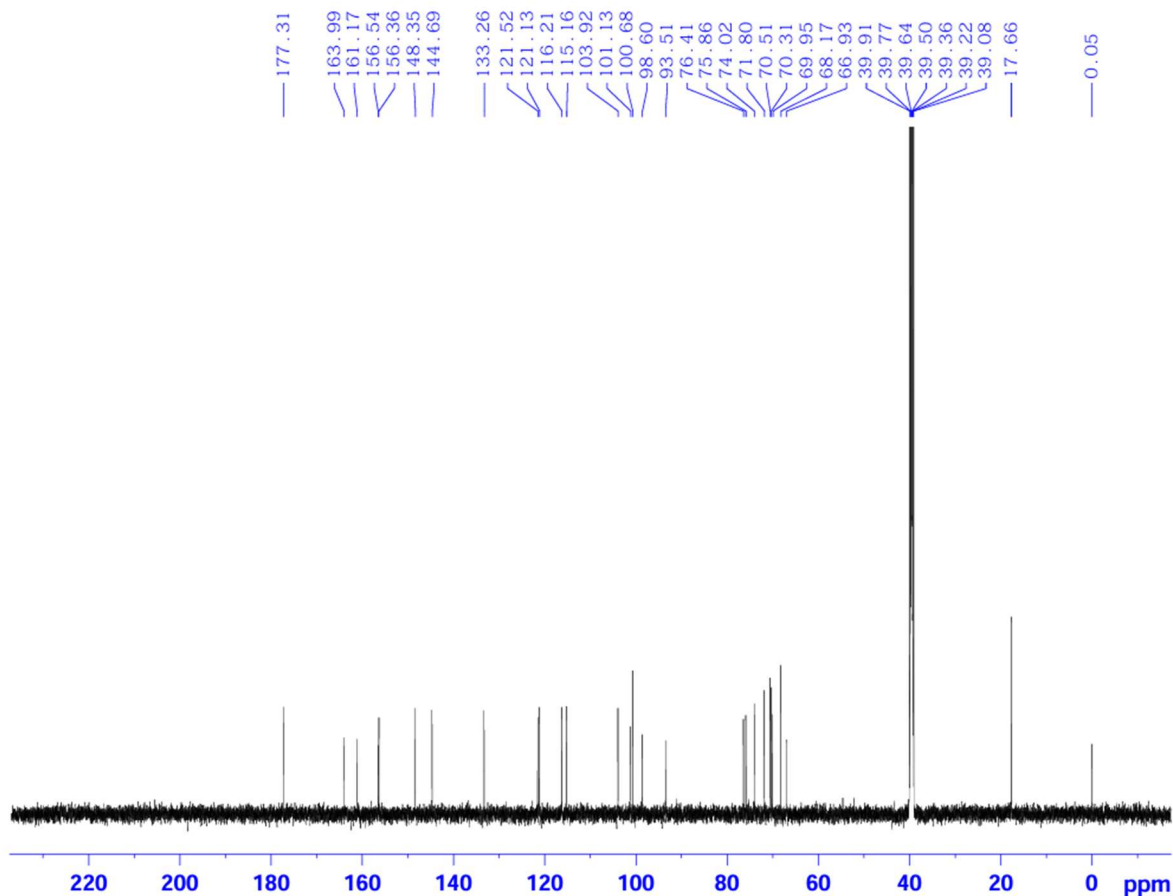


Figure S13: ^{13}C -NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compound **3** (quercetin-3-*O*-rutinoside)

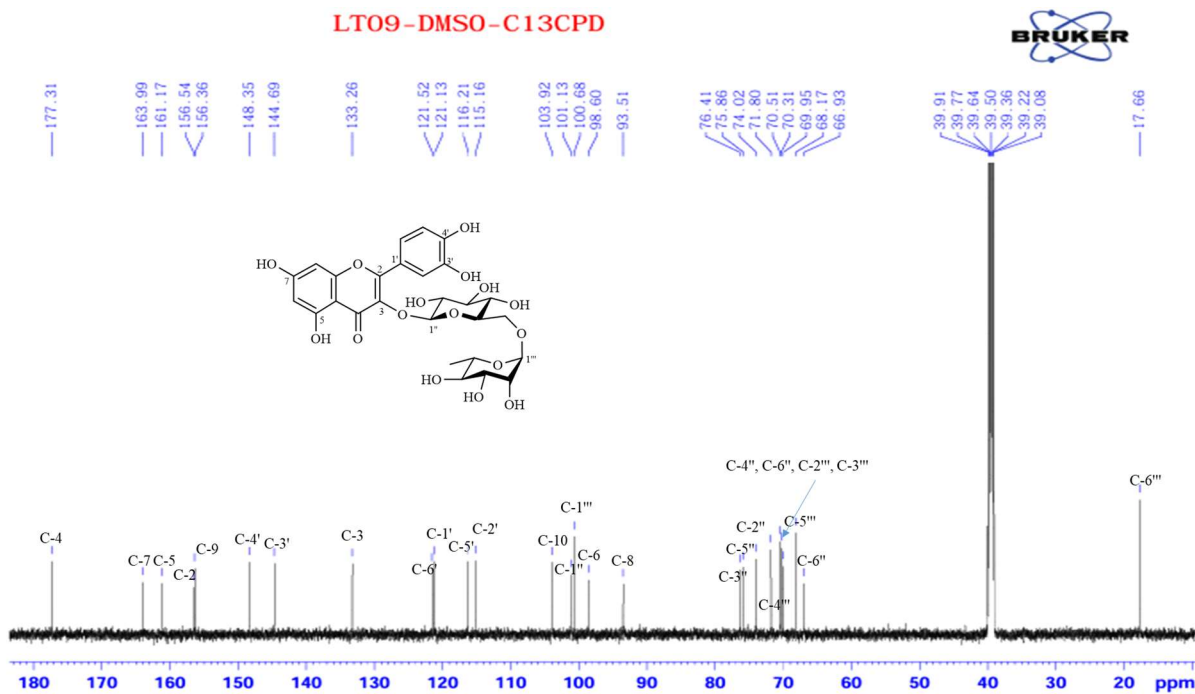


Figure S14: ^{13}C -NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compound **3** (quercetin-3-*O*-rutinoside) (from δ_{C} 20 ppm to δ_{C} 185 ppm)

4. Supplementary spectroscopic data of compound 4.

Table S7: The comparison of NMR data of compound 4 with a similar compound (Luteolin-7-*O*- β -glucopyranoside).

Position	Compound 4 (DMSO- <i>d</i> ₆)		Luteolin-7- <i>O</i> - β -D-glucopyranoside (DMSO- <i>d</i> ₆) [4]	
	¹³ C-NMR (150 MHz) δ_C ppm	¹ H-NMR (600 MHz) δ_H ppm	¹³ C-NMR (125 MHz) δ_C ppm	¹ H-NMR (500 MHz) δ_H ppm
2	-	164.5	-	164.9
3	6.75 (1H, <i>s</i>)	103.2	6.76 (1H, <i>s</i>)	103.5
4	-	181.9	-	182.3
5	-	161.1	-	161.6
6	6.45 (1H, <i>d</i> , <i>J</i> = 2.4 Hz)	99.5	6.45 (1H, <i>d</i> , <i>J</i> = 1.7 Hz)	99.9
7	-	162.9	-	163.4
8	6.79 (1H, <i>d</i> , <i>J</i> = 1.8 Hz)	94.7	6.79 (1H, <i>d</i> , <i>J</i> = 1.7 Hz)	95.1
9	-	156.9	-	157.4
10	-	105.3	-	105.8
1'	-	121.4	-	121.6
2'	7.43 (1H, <i>d</i> , <i>J</i> = 2.4 Hz)	113.6	7.43 (1H, <i>d</i> , <i>J</i> = 8.4 Hz)	113.9
3'	-	145.8	-	146.4
4'	-	149.9	-	150.7
5'	6.92 (1H, <i>d</i> , <i>J</i> = 8.4 Hz)	116.0	6.90 (1H, <i>d</i> , <i>J</i> = 8.4 Hz)	116.4
6'	7.46 (1H, <i>dd</i> , <i>J</i> = 8.4; 2.4 Hz)	119.1	7.45 (1H, <i>dd</i> , <i>J</i> = 8.3; 2.3 Hz)	119.6
1''	5.09 (1H, <i>d</i> , <i>J</i> = 7.2 Hz)	99.9	5.08 (1H, <i>d</i> , <i>J</i> = 7.3 Hz)	100.3
2''	3.28 (1H, <i>m</i>)	73.1	3.26 (1H, <i>m</i>)	73.6
3''	3.45 (1H, <i>m</i>)	77.1	3.45 (1H, <i>m</i>)	77.6

4''	3.21 (1H, <i>t</i> , $J = 9.0; 9.6$ Hz)	69.6	3.17 (1H, <i>m</i>)	70.0
5''	3.34 (1H, <i>m</i>)	76.4	3.30 (1H, <i>m</i>)	76.9
6''	3.50 (1H, <i>m</i>)	60.6	3.48 (1H, <i>m</i>)	61.1
	3.73 (1H, <i>d</i> , $J = 11.4$ Hz)		3.72 (1H, <i>d</i> , $J = 9.9$ Hz)	

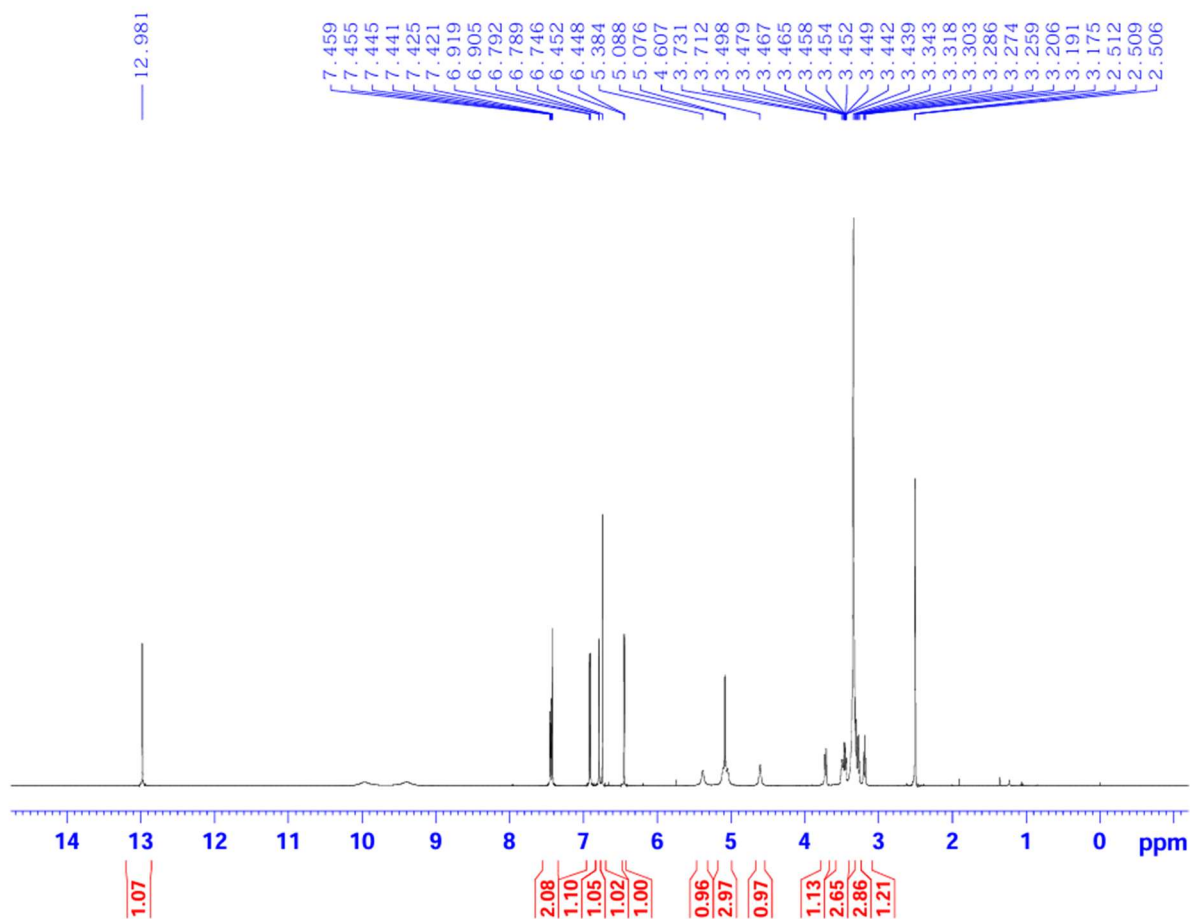


Figure S15: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **4** (luteolin-7-*O*- β -D-glucopyranoside)

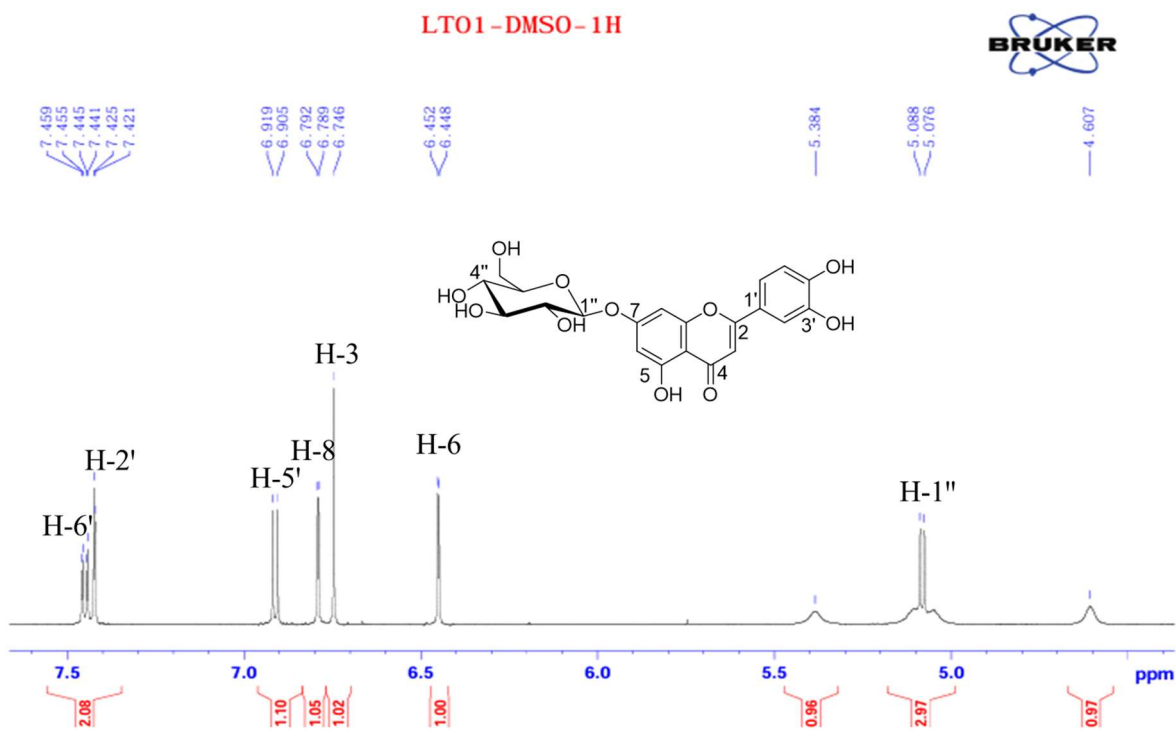


Figure S16: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **4** (luteolin-7-*O*- β -D-glucopyranoside) (from δ_{H} 4 ppm to δ_{H} 7.5 ppm)

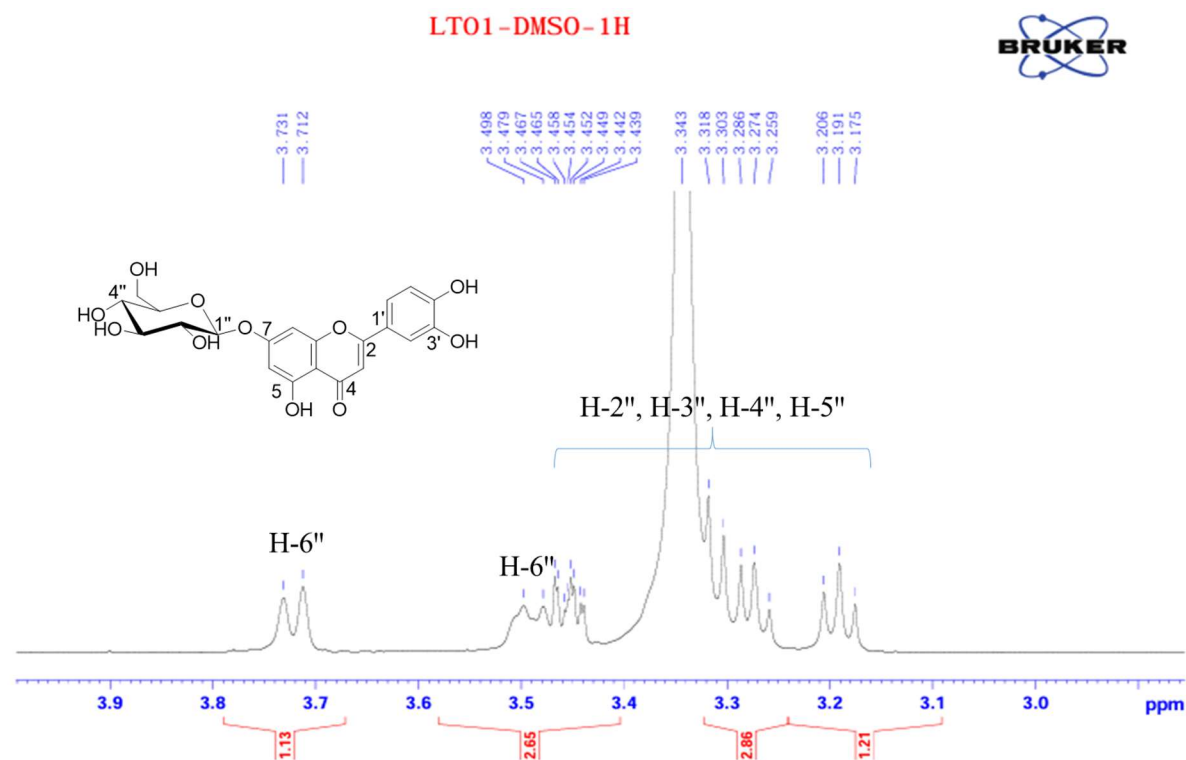


Figure S17: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **4** (luteolin-7-*O*- β -D-glucopyranoside) (from δ_{H} 3 ppm to δ_{H} 4 ppm)

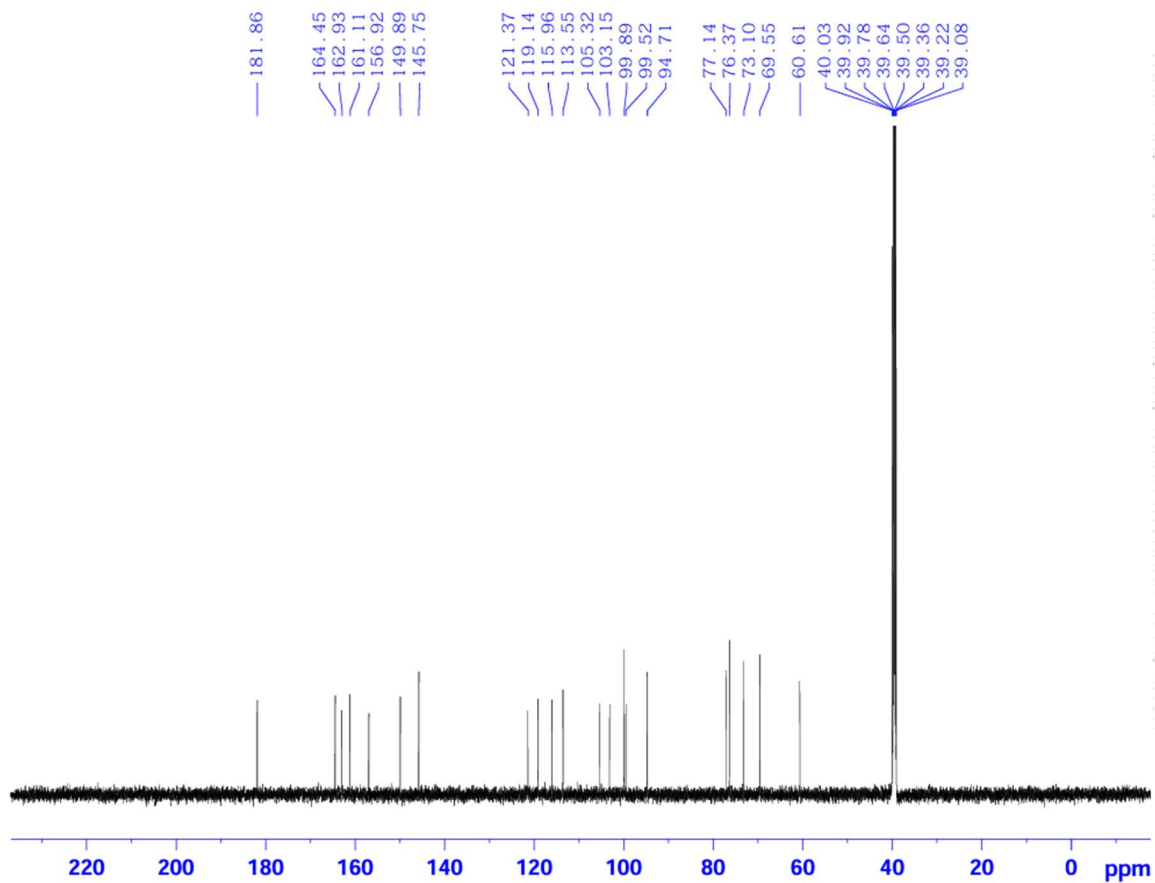


Figure S18: ^{13}C -NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compound **4** (luteolin-7-*O*- β -D-glucopyranoside)

LT01-DMSO-C13CPD

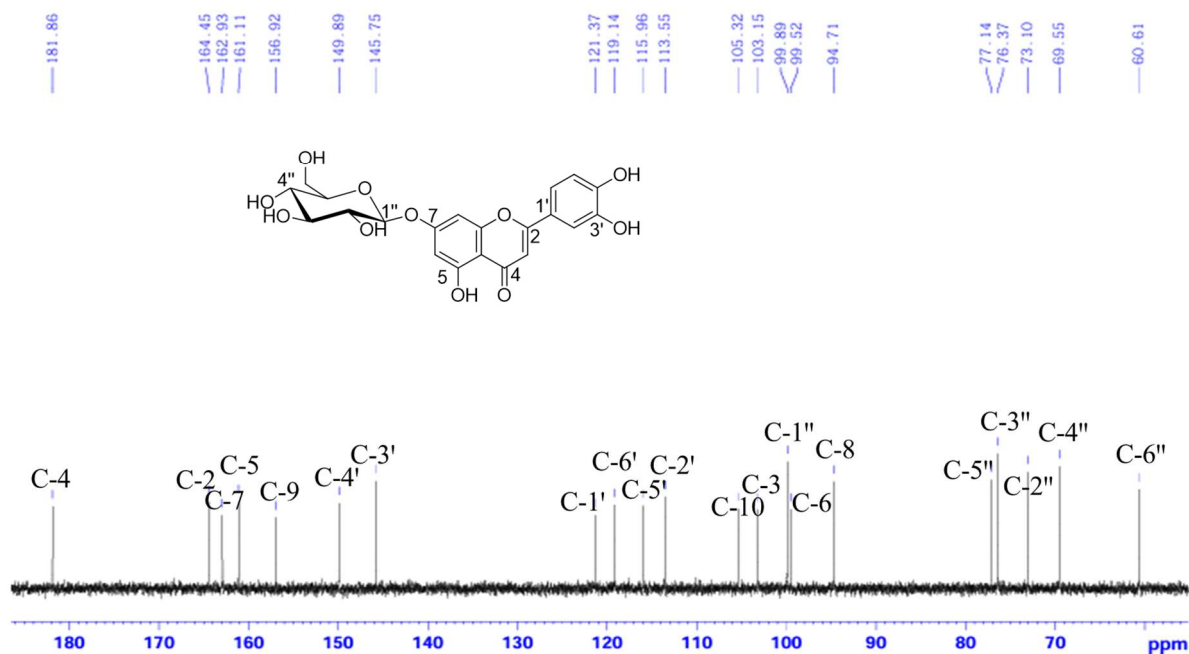


Figure S19: ^{13}C -NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of compound 4 (luteolin-7-*O*-β-D-glucopyranoside) (from δ_{C} 60 ppm to δ_{C} 185 ppm)

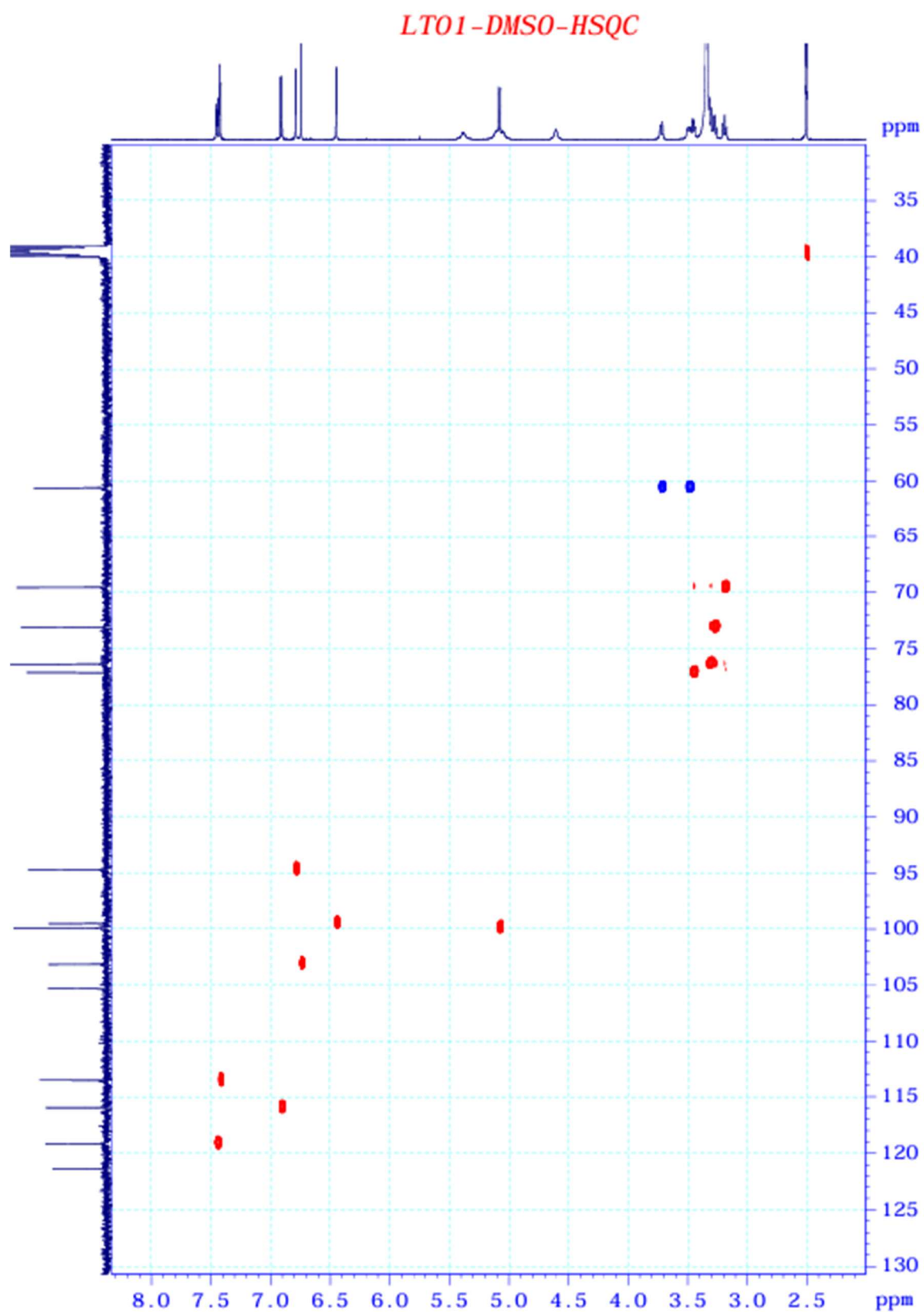


Figure S20: HSQC spectrum of compound 4 (luteolin-7-*O*- β -D-glucopyranoside)

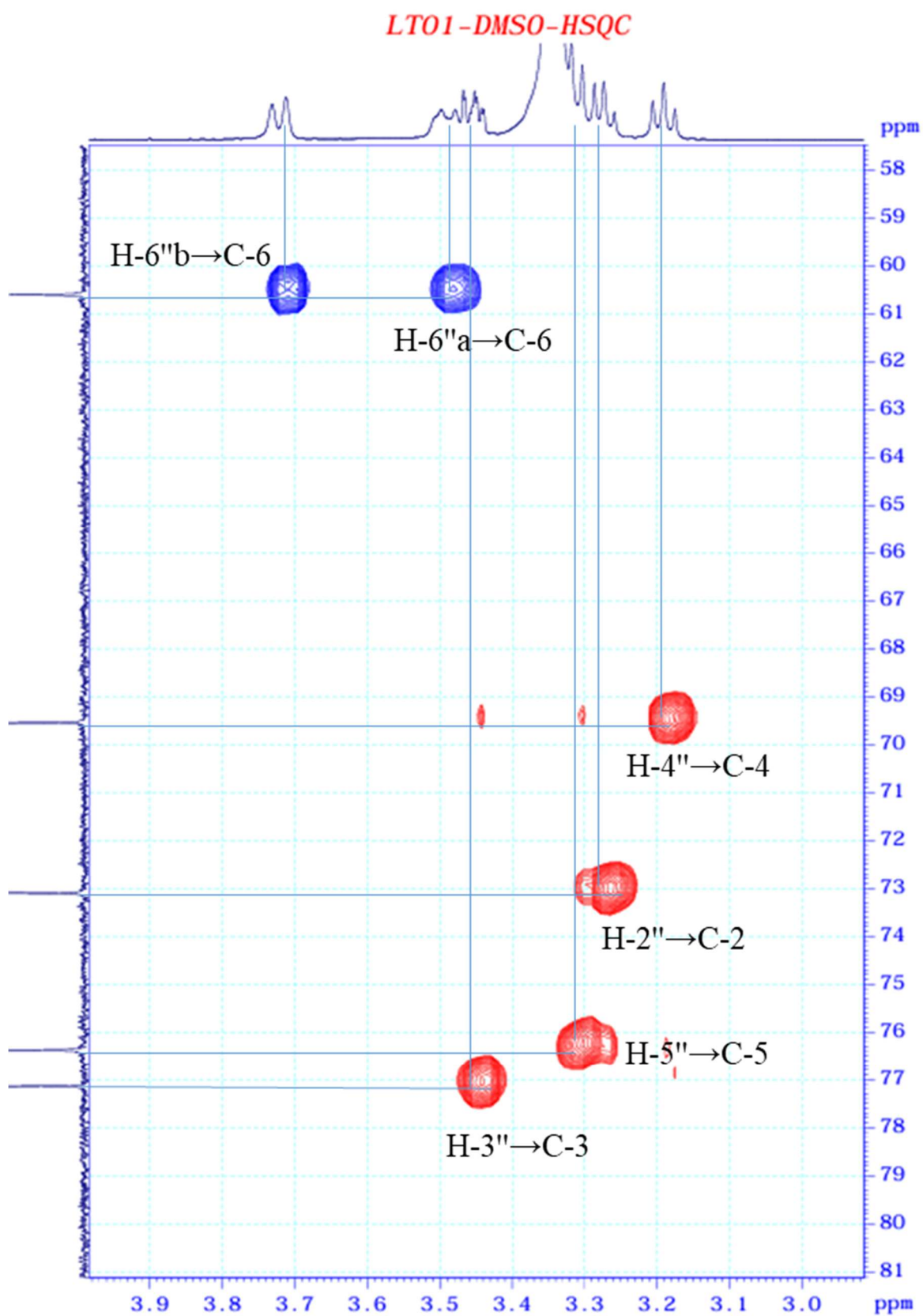


Figure S21: HSQC spectrum of compound **4** (luteolin-7-*O*- β -D-glucopyranoside) (from δ_C 57 ppm to δ_C 8 ppm)

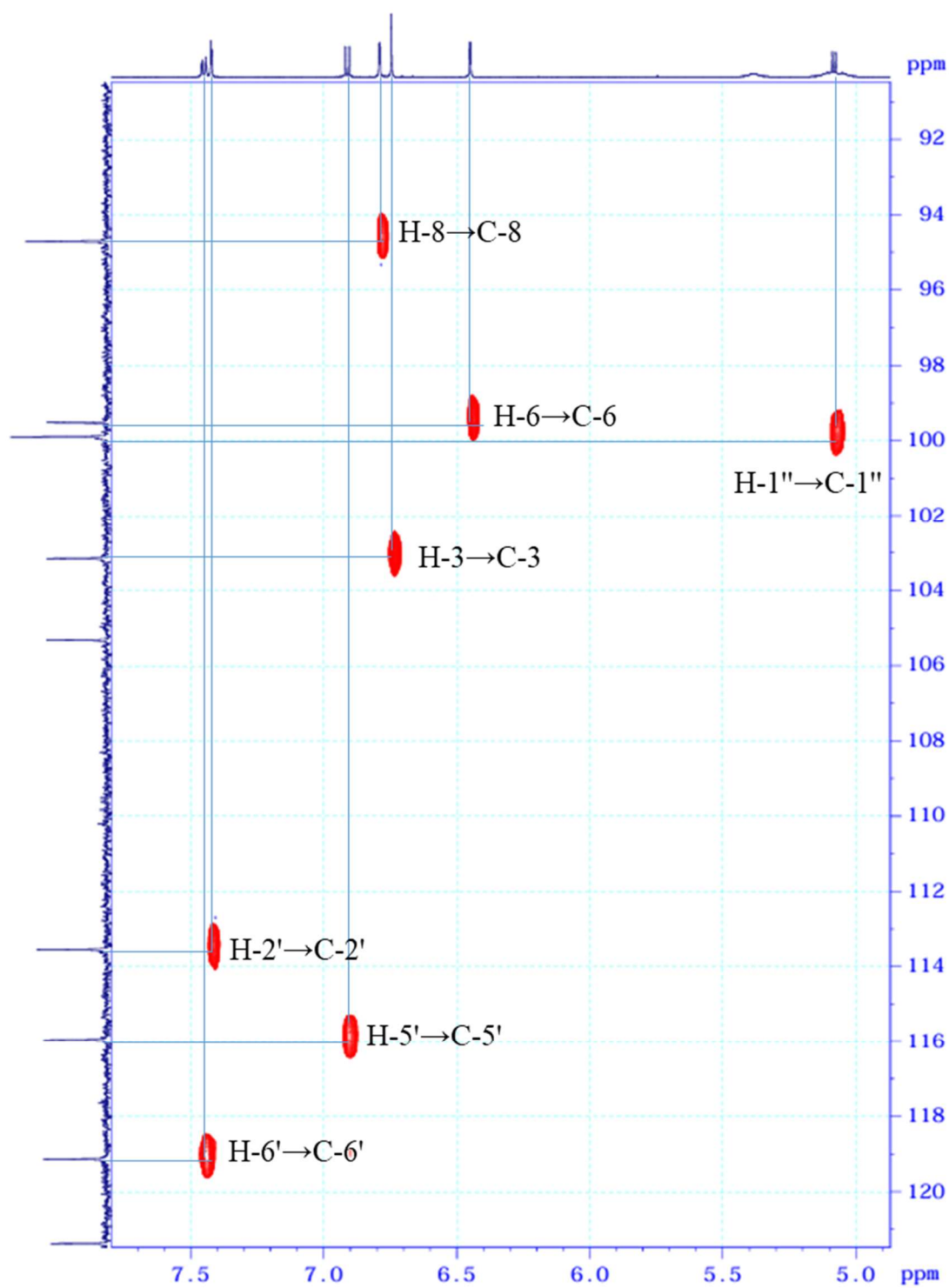


Figure S22: HSQC spectrum of compound **4** (luteolin-7-*O*- β -D-glucopyranoside) (from δ_C 90 ppm to δ_C 120 ppm)

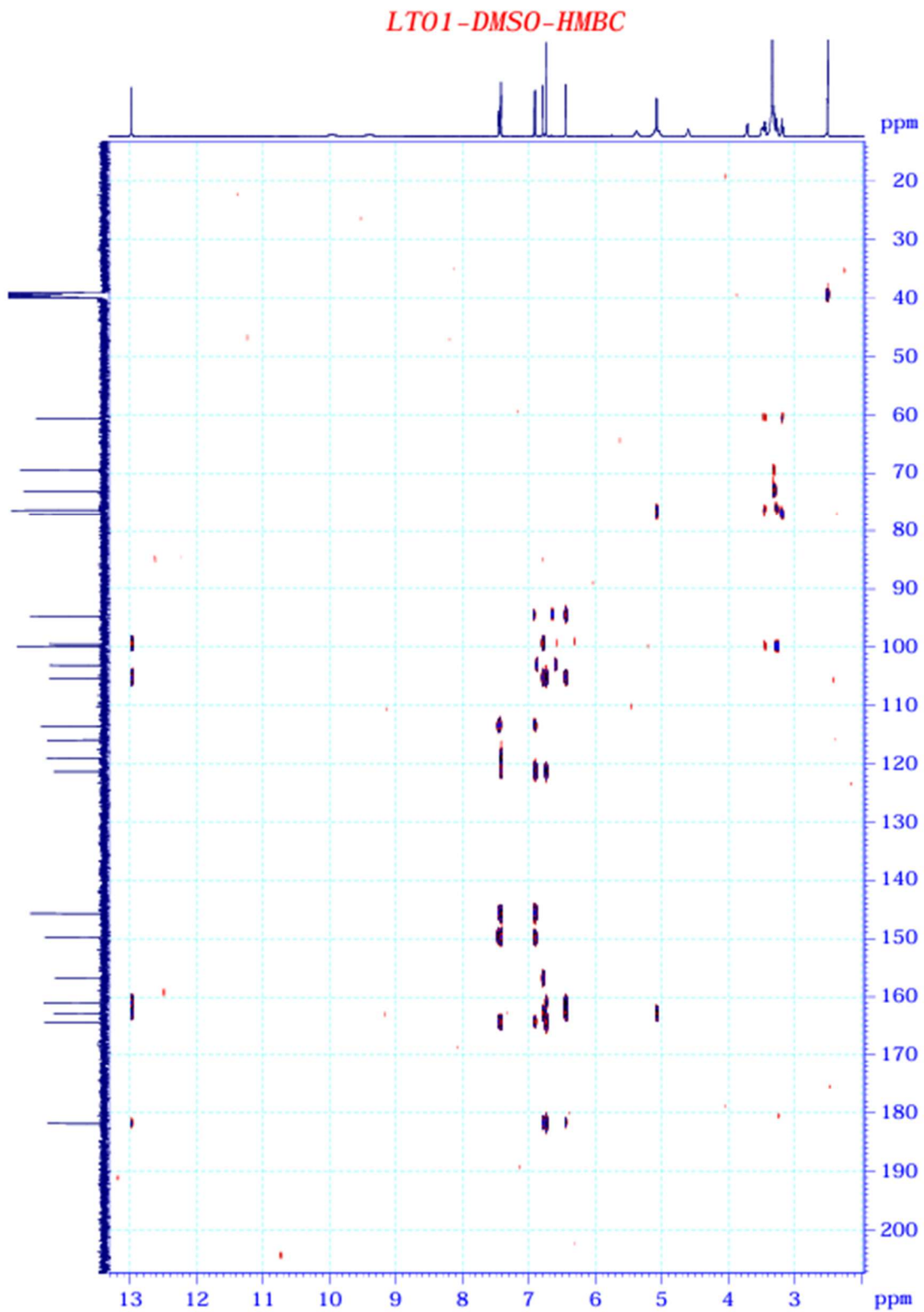


Figure S23: HMBC spectrum of compound 4 (luteolin-7-*O*-β-D-glucopyranoside)

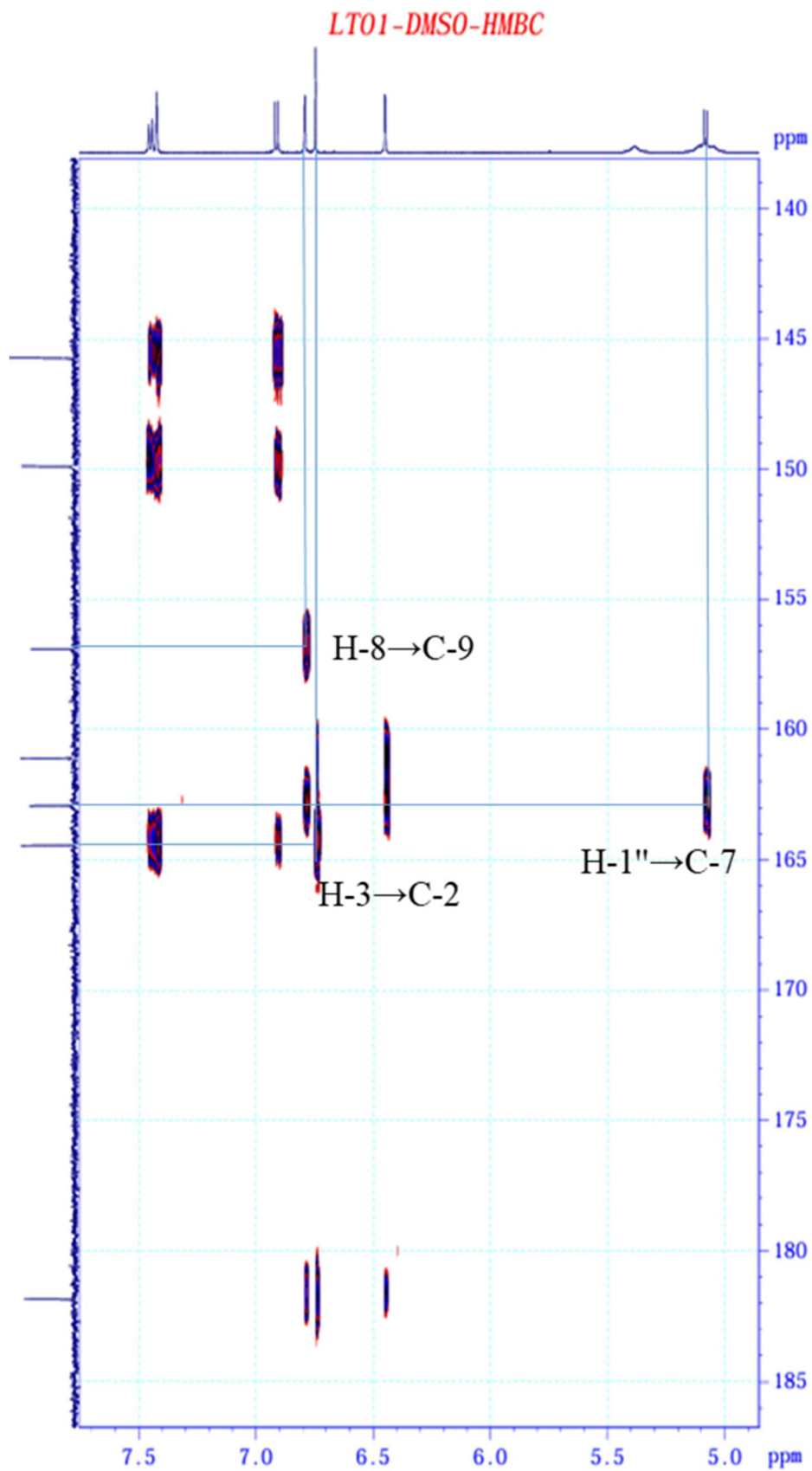


Figure S24: HMBC spectrum of compound 4 (luteolin-7-*O*- β -D-glucopyranoside) (from δ_C 140 ppm to δ_C 185 ppm)

LTO1-DMSO-HMBC

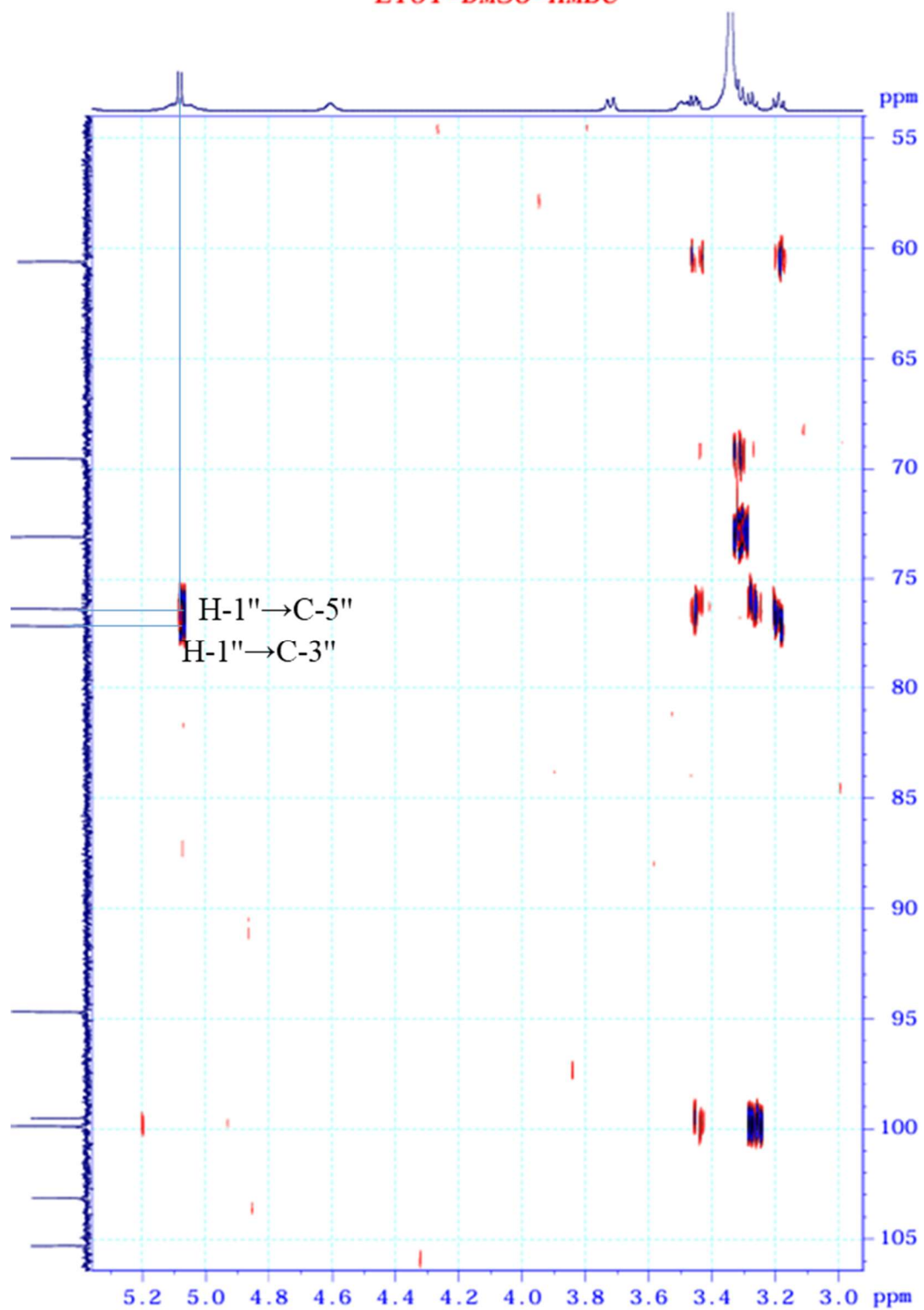


Figure S25: HMBC spectrum of compound 4 (luteolin-7-*O*-β-D-glucopyranoside) (from δ_C 55 ppm to δ_C 105 ppm)

5. Supplementary spectroscopic data of compound 5.

Table S8: The comparison of NMR data of compound 5 with a similar compound (2-(4-hydroxyphenyl)acetic acid)

Position	Compound 3 (CD ₃ OD)		2-(4-Hydroxyphenyl)acetic acid (CD ₃ OD) [3]	
	¹³ C-NMR (150 MHz) δ _C ppm	¹ H-NMR (600 MHz) δ _H ppm	¹³ C-NMR (125 MHz) δ _C ppm	¹ H-NMR (500 MHz) δ _H ppm
1	-	126.8	-	127.1
2, 6	7.09 (2H, <i>d</i> , <i>J</i> = 8.4 Hz)	131.3	7.08 (2H, <i>d</i> , <i>J</i> = 8.3 Hz)	131.5
3, 5	6.74 (2H, <i>d</i> , <i>J</i> = 8.4 Hz)	116.2	6.72 (2H, <i>d</i> , <i>J</i> = 8.5 Hz)	116.3
4	-	157.4	-	157.6
7	3.50 (2H, <i>s</i>)	41.1	3.5 (2H, <i>s</i>)	41.7
8	-	176.3	-	176.2

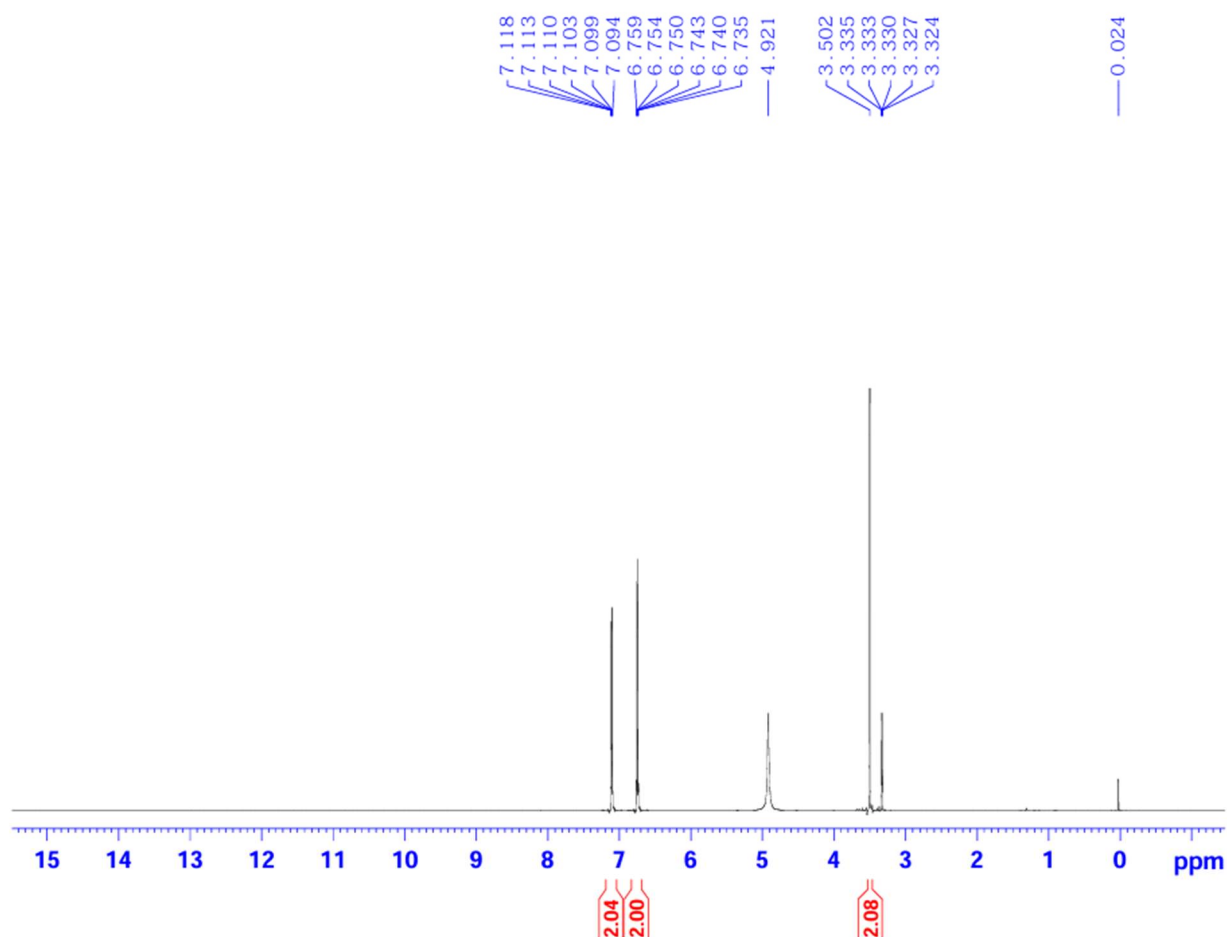


Figure S26: ¹H-NMR (600 MHz, CD₃OD) spectrum of compound 5 (2-(4-Hydroxyphenyl)acetic acid)

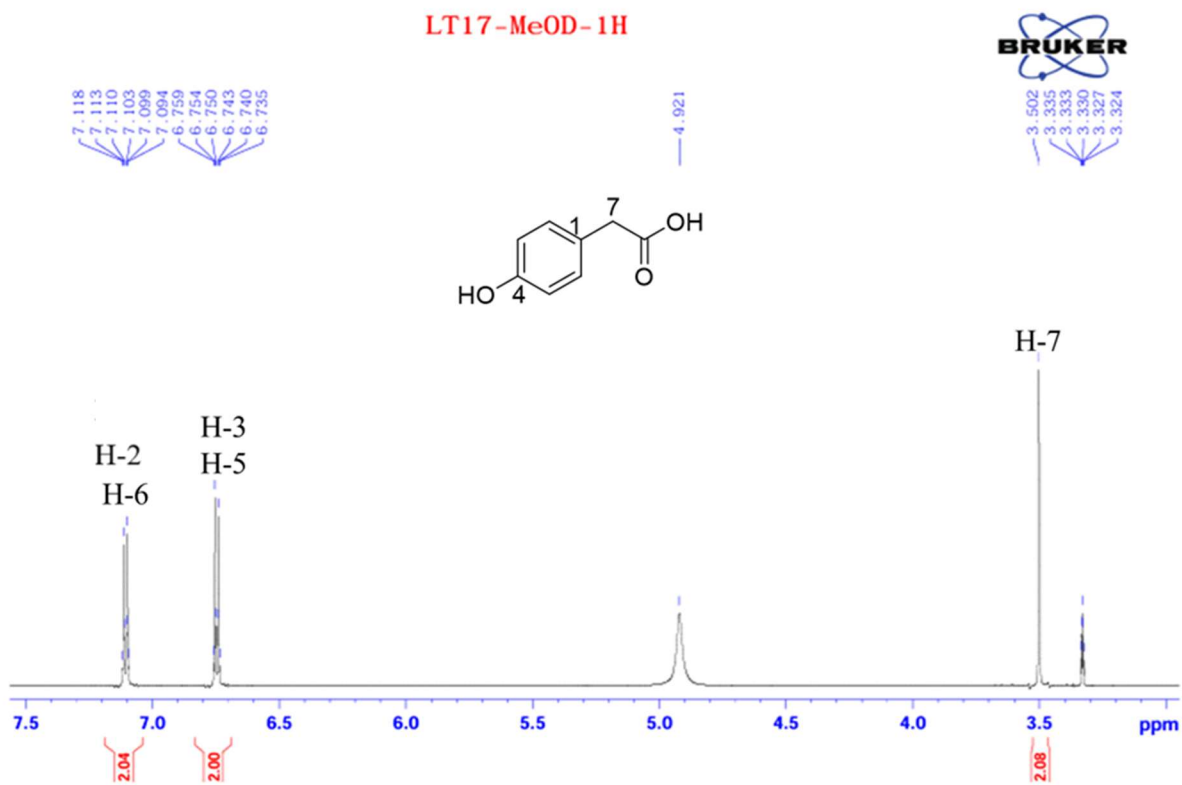


Figure S27: ¹H-NMR (600 MHz, CD₃OD) spectrum of compound **5** (2-(4-Hydroxyphenyl)acetic acid) (from δ_{H} 3 ppm to δ_{H} 7.5 ppm)

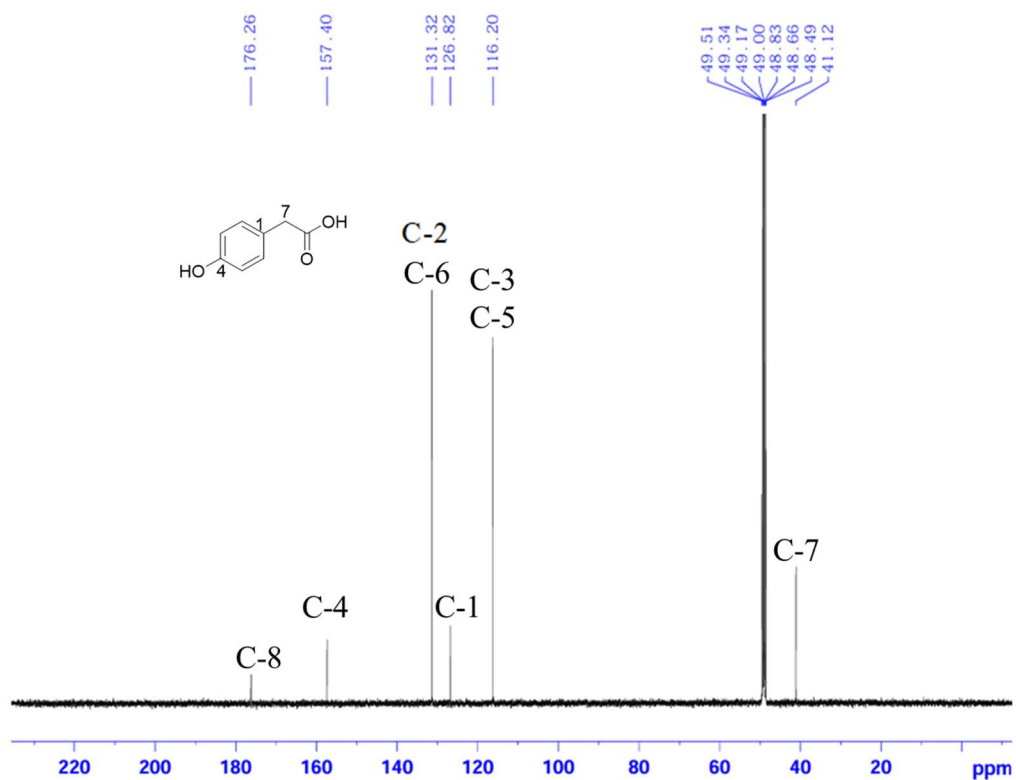


Figure S28: ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound **5** (2-(4-Hydroxyphenyl)acetic acid)

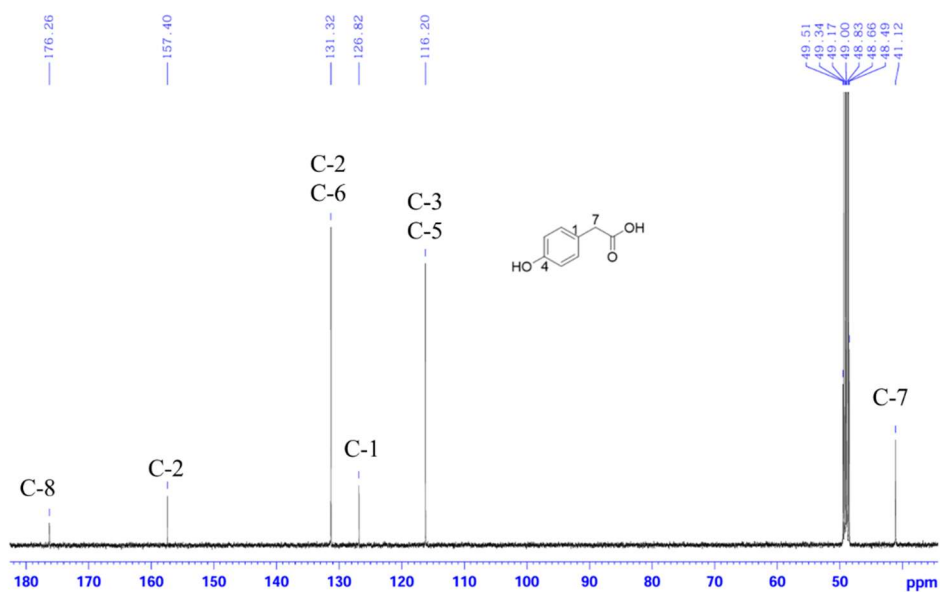


Figure S29: ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound **5** (2-(4-Hydroxyphenyl)acetic acid)
(from δ_{C} 40 ppm to δ_{C} 180 ppm)