

Phytochemical study of aerial parts of *Leea asiatica*

Hyun Woo Kil^{a1,†}, Taewoong Rho^{1,†} and Kee Dong Yoon^{1,*}

¹ College of Pharmacy and Integrated Research Institute of Pharmaceutical Sciences, The Catholic University of Korea, Bucheon 14662, Republic of Korea; karlwho@naver.com (T.R.); kilhyunwoo@catholic.ac.kr (H.W.K.); kdyoon@catholic.ac.kr (K.D.Y.)

* Correspondence: e-mail kdyoon@catholic.ac.kr; Tel.: +82-2-2164-4091

† These authors contributed equally to this work

Contents

SI 1: ¹H-NMR spectrum of compound **1**.

SI 2: ¹³C-NMR spectrum of compound **1**.

SI 3: ¹H-¹H COSY spectrum of compound **1**.

SI 4: HSQC spectrum of compound **1**.

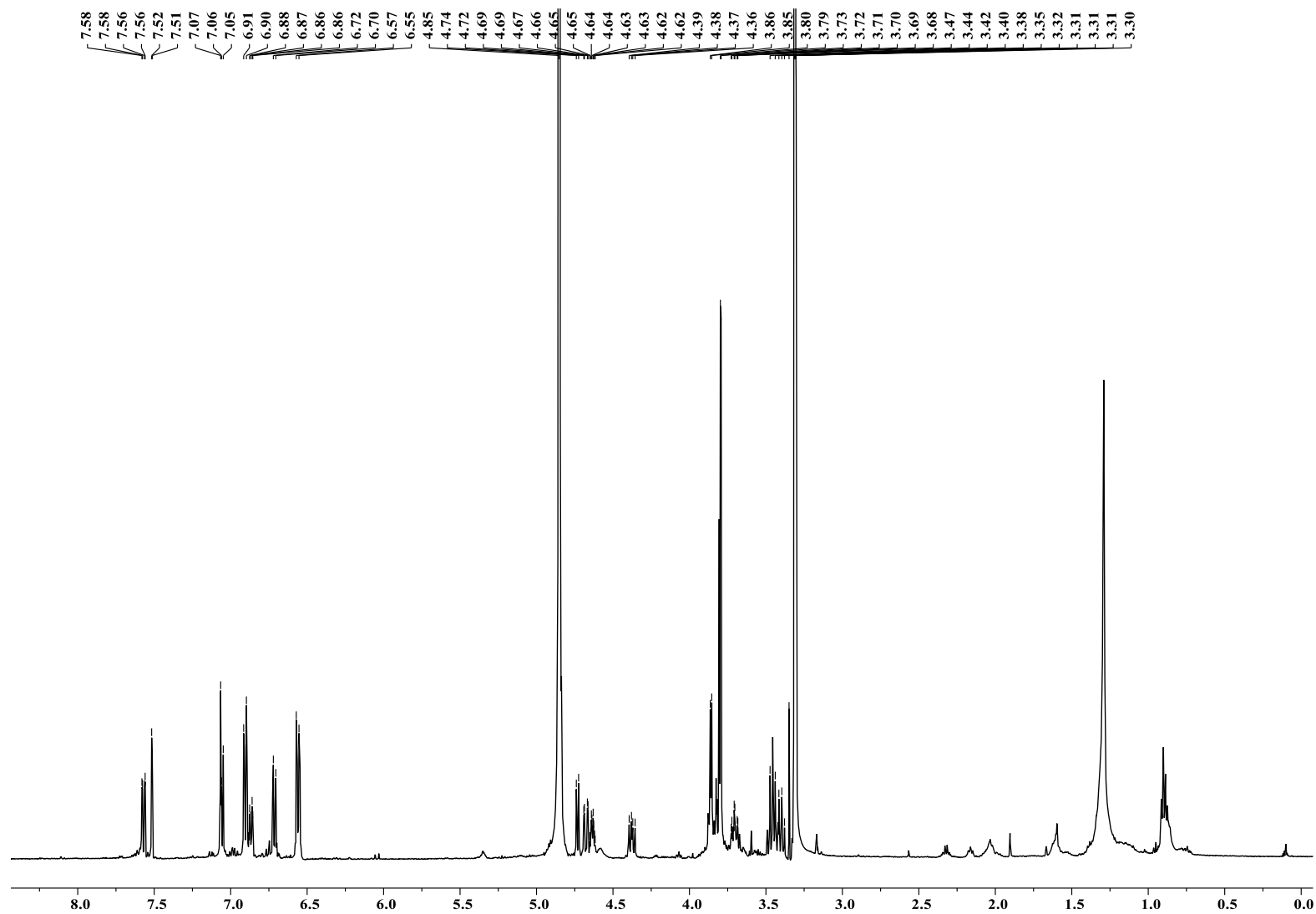
SI 5: HMBC spectrum of compound **1**.

SI 6: ESI-Q-TOF-MS spectrum of compound **1**.

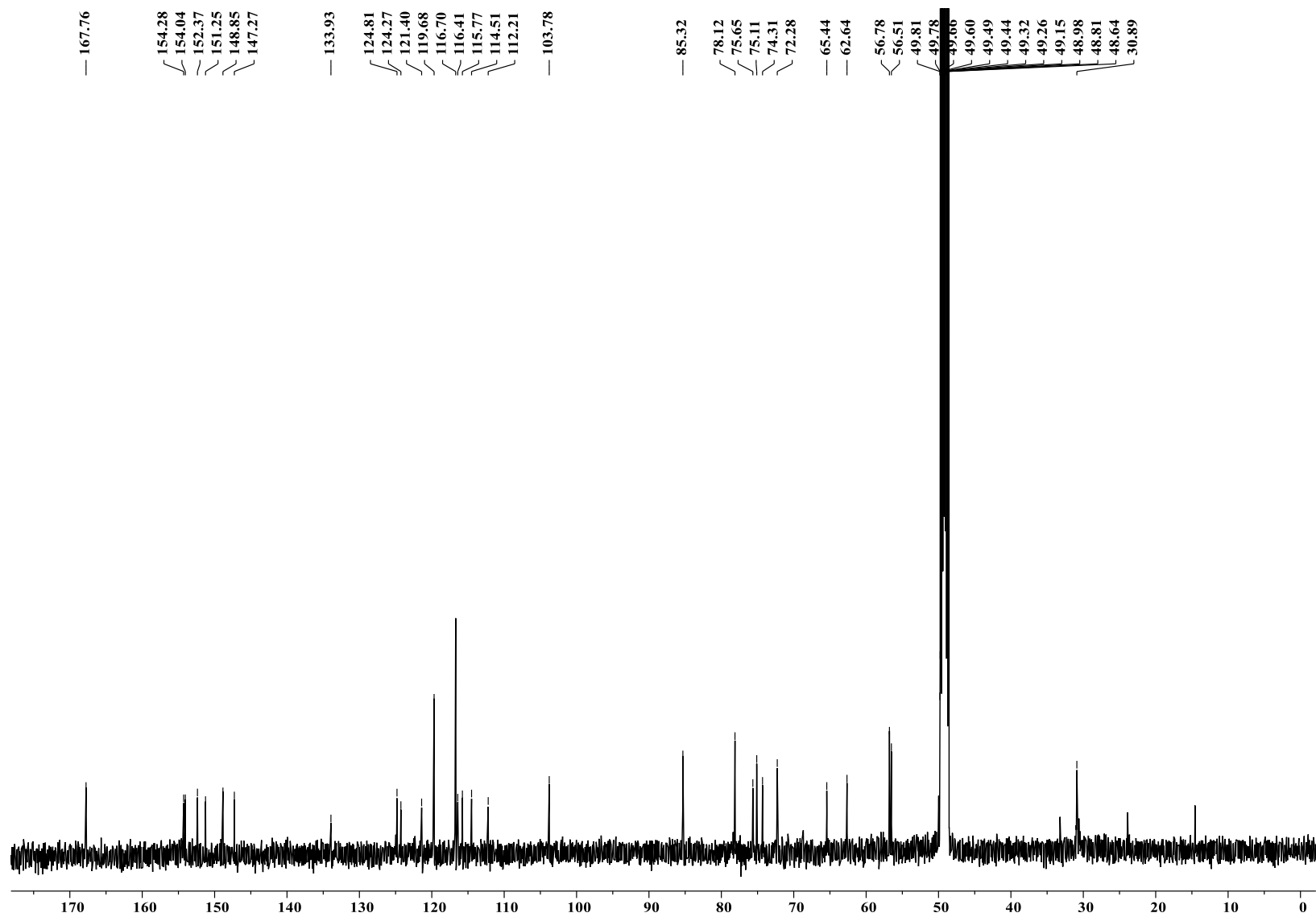
SI 7: UV spectrum of compound **1**.

SI 8: Comparison of ¹H and ¹³C NMR data between compound **1** and (-)-4-hydroxy-3-methoxyphenol β-D-{6-O-[4-O-(7S,8R)-(4-hydroxy-3-methoxyphenylglycerol-8-yl)-3-methoxybenzoyl]}-glucopyranoside [Ref. 17].

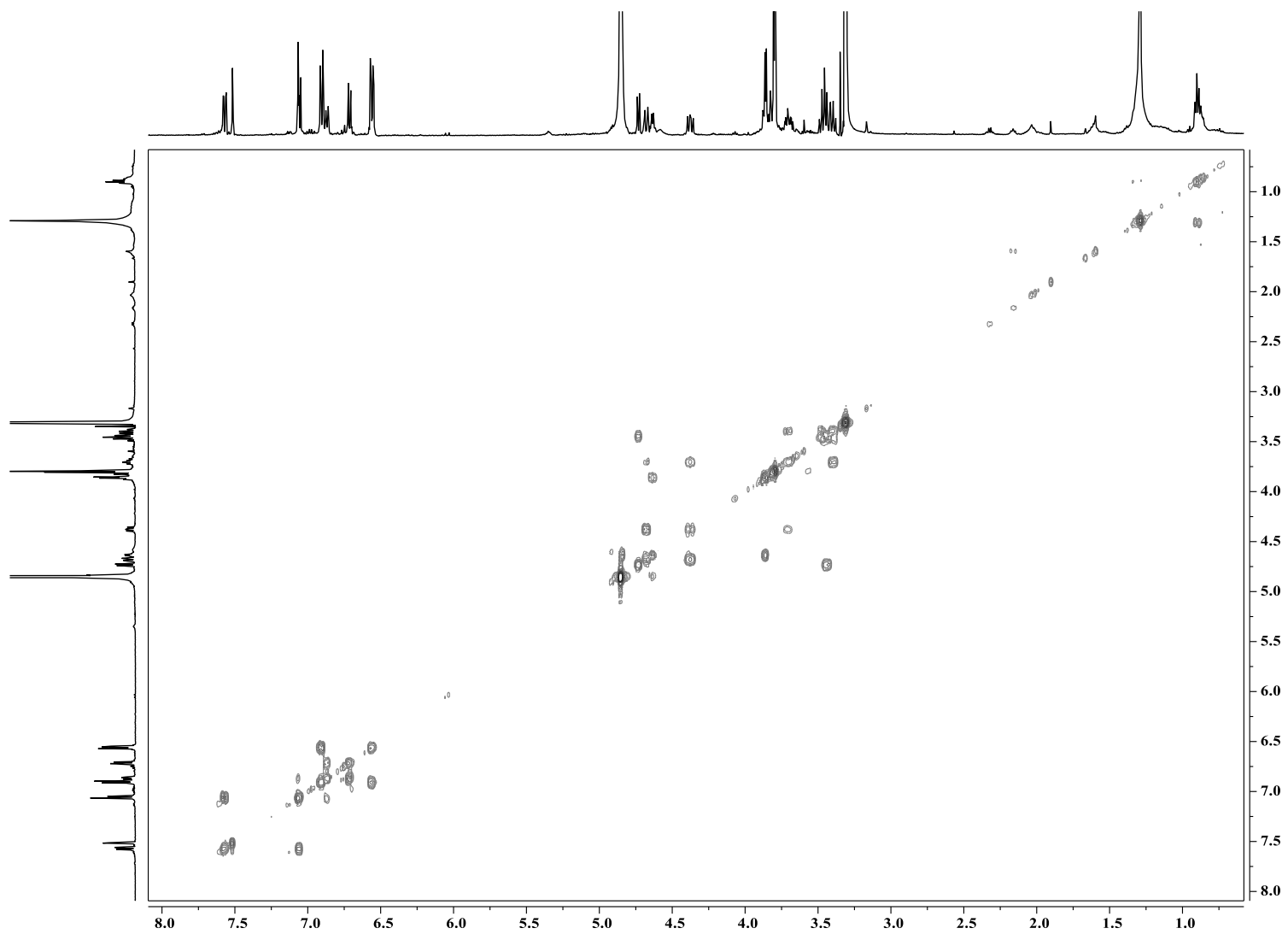
SI 9: Isolation scheme of compounds **1–24** from the aerial parts of *Leea asiatica*.



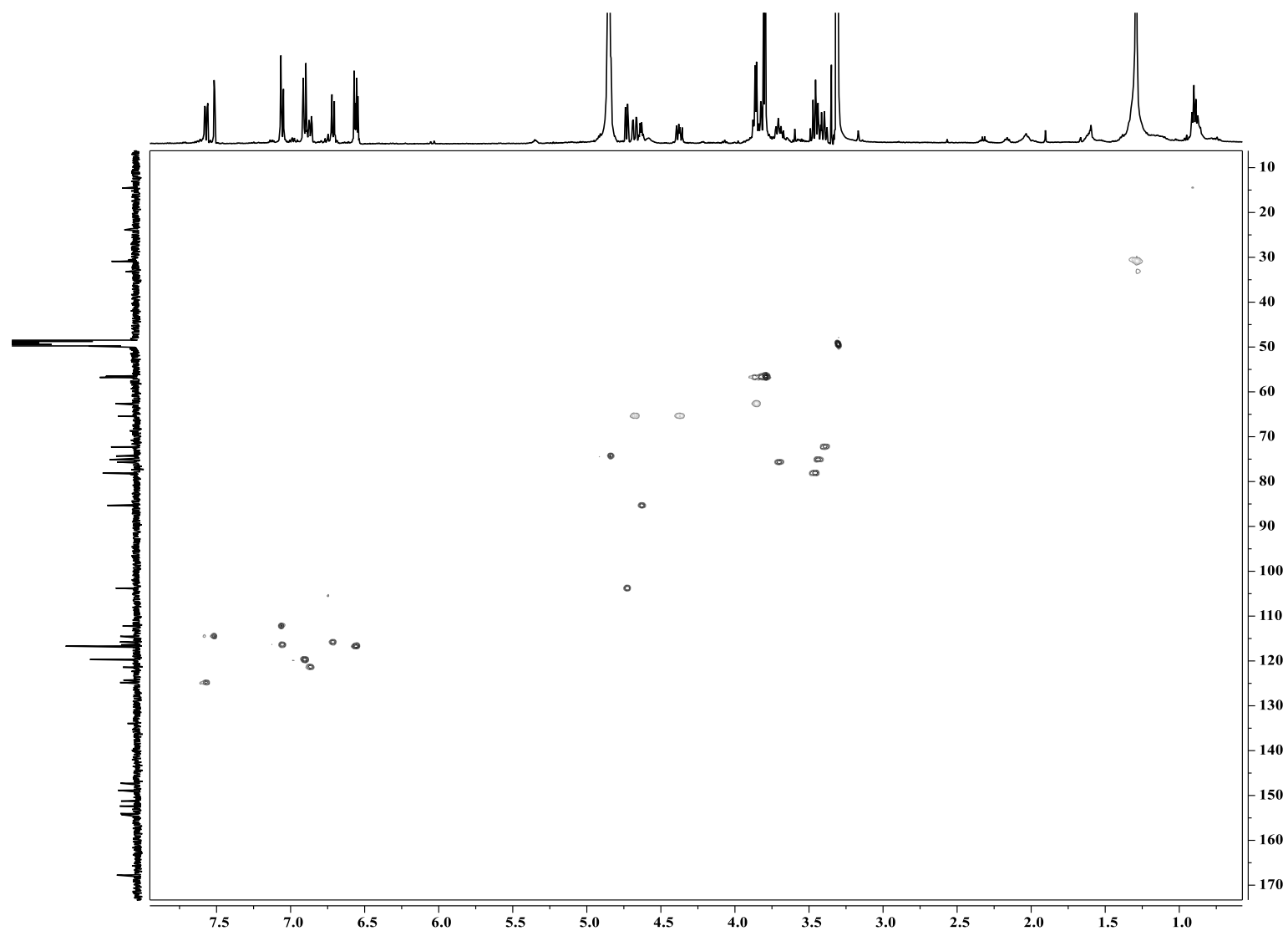
SI 1. ^1H -NMR spectrum of compound 1.



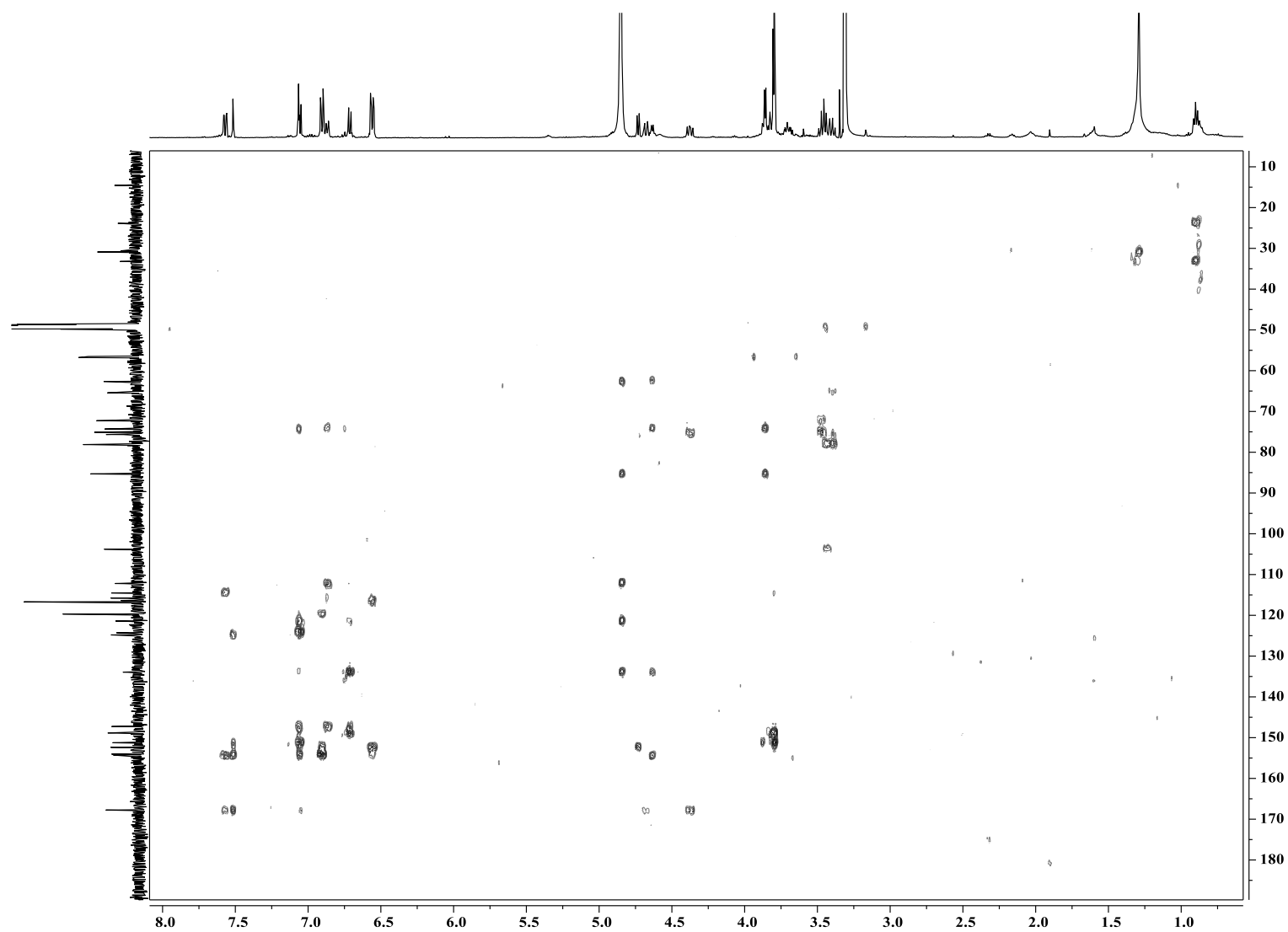
SI 2. ^{13}C -NMR spectrum of compound 1.



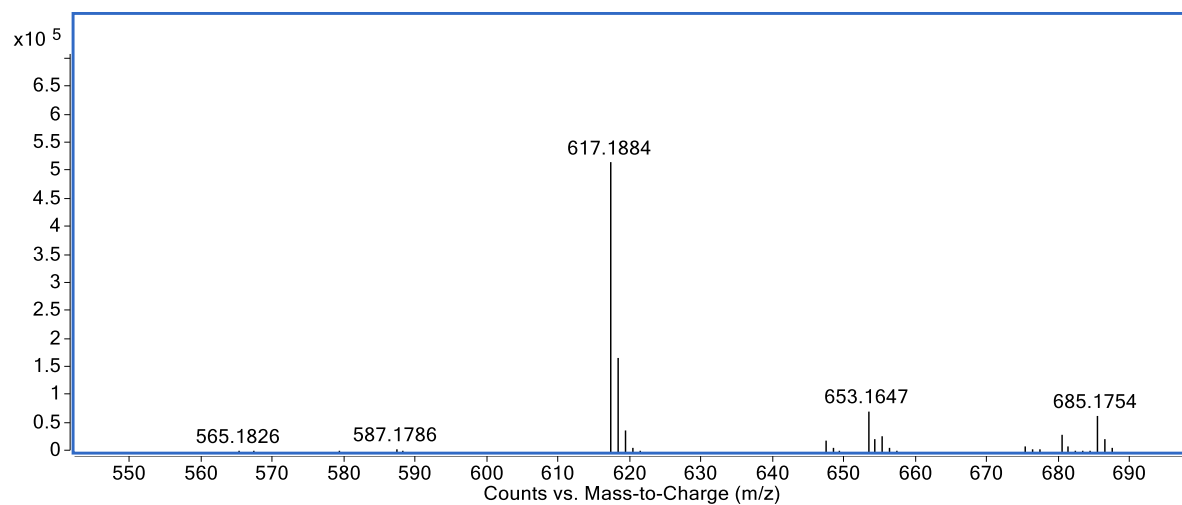
SI 3. ^1H - ^1H COSY spectrum of compound **1**.



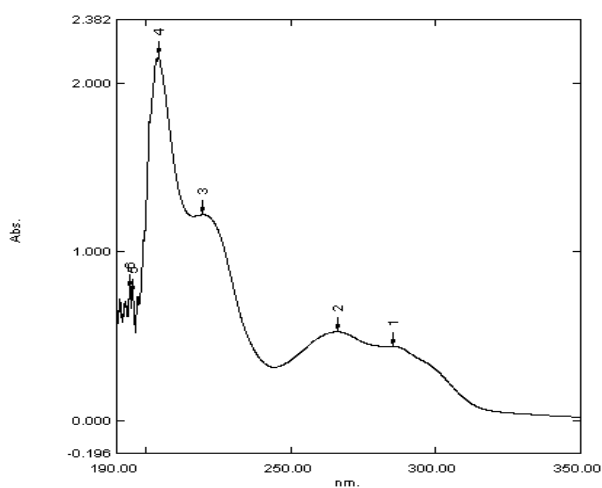
SI 4. HSQC spectrum of compound 1.



SI 5. HMBC spectrum of compound 1.



SI 6. ESI-Q-TOF-MS spectrum of compound 1.



1: 285.10 / 0.437
 2: 266.10 / 0.526
 3: 219.80 / 1.222
 4: 204.50 / 2.167

SI 7. UV spectrum of compound 1.

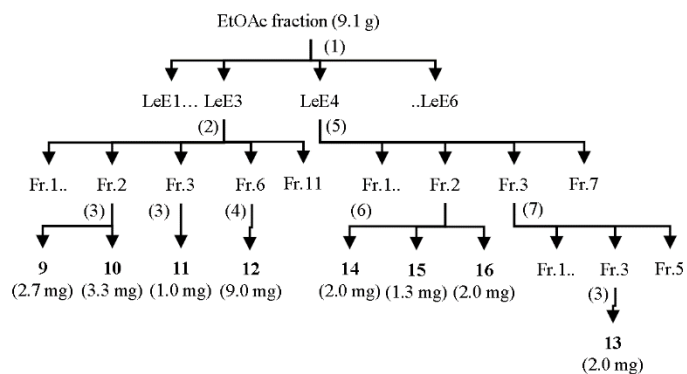
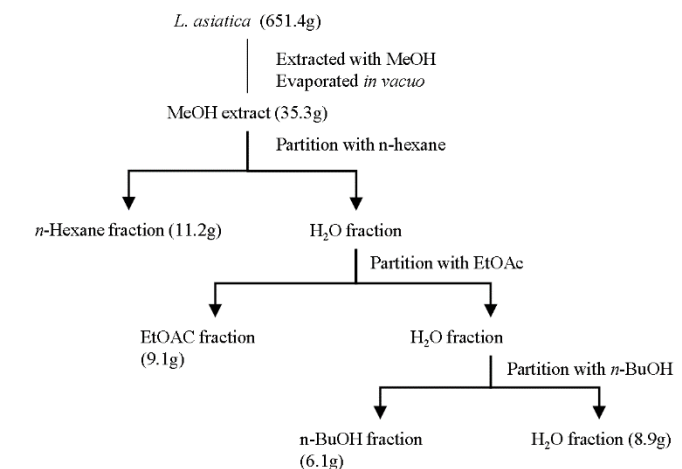
SI 8. Comparison of ¹H- and ¹³C-NMR data between compound **1** and (-)-4-hydroxy-3-methoxyphenol β-D-[6-O-[4-O-(7S,8R)-(4-hydroxy-3-methoxyphenylglycerol-8-yl)-3-methoxybenzoyl]]-glucopyranoside [Ref. 17]

Compound 1*			Reference compound (Ref. 16)*	
Position	¹ H-NMR	¹³ C-NMR	¹ H-NMR	¹³ C-NMR
1		152.3		152.5
2	6.91 d (9.0)	119.6	6.63 s	104.1
3	6.56 d (9.0)	116.7		149.2
4		154		143.1
5	6.56 d (9.0)	116.7	6.47 d (8.0)	115.9
6	6.91 d (9.0)	119.6	6.48 d (8.0)	110.2
1'	4.73 d (7.4)	103.7	4.70 d (7.5)	103.7
2'	3.44 o***	75.1	3.38 dd (8.5, 7.5)	75.0
3'	3.45 o***	78.1	3.42 t (8.5)	78.0
4'	3.39 brt (9.1)	72.2	3.34 t (8.5)	72.1
5'	3.71 m**	75.6	3.66 m**	75.6
6'	4.68 dd (11.7, 2.1), 4.37 dd (11.7, 7.6)	65.4	4.64 d (11.0), 4.34 dd (11.0, 6.0)	65.3
1''		124.2		124.2
2''	7.51 d (2.0)	114.5	7.49 s	114.2
3''		151.2		151.0
4''		154.2		154.4
5''	7.06 d (8.5)	116.4	7.04 d (8.5)	116.1
6''	7.57 dd (8.5, 2.0)	124.8	7.50 d (8.5)	124.8
7''		167.7		167.6
1'''		133.9		133.7
2'''	7.07 o***	112.2	7.00 s	111.7
3'''		148.8		148.9
4'''		147.2		147.2
5'''	6.71 d (8.1)	115.7	6.70 d (8.0)	115.9
6'''	6.87 dd (8.1, 2.2)	121.4	6.82 brd (8.0)	120.7
7'''	4.84 o***	74.3	4.85 d (5.0)	74.0
8'''	4.64 m**	85.3	4.52 m**	85.8
9'''	3.86 brd (4.9)	62.6	3.73 dd (12.0, 4.0), 3.50 dd (12.0, 6.0)	62.6
3-OMe			3.61 s	56.3
3''-OMe	3.79 s	56.7	3.81 s	56.6
3'''-OMe	3.80 s	56.5	3.77 s	56.4

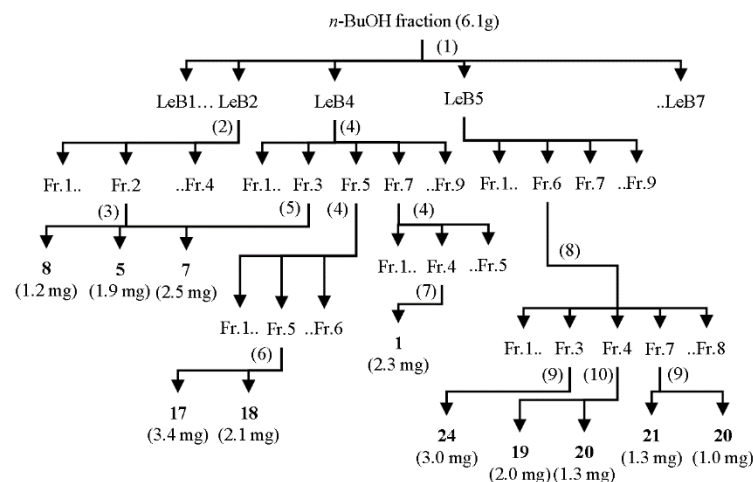
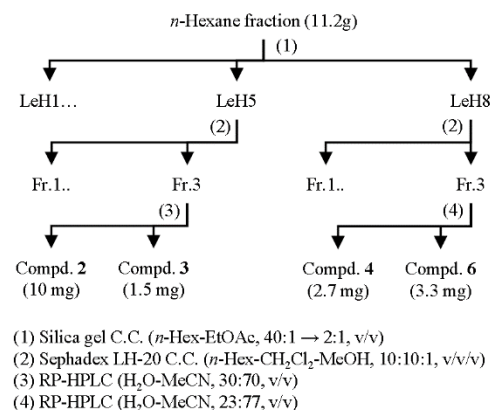
*Compounds were dissolved in CD₃OD.

**m: multiplet

***o: resonance was overlapped.



- (1) Silica gel C.C. (CHCl₃-MeOH, 20:1 → 1:1, v/v)
 (2) RP-MPLC (H₂O-MeOH, 70:30 → 50:50, v/v)
 (3) RP-HPLC (H₂O-MeCN, 30:70, v/v)
 (4) RP-HPLC (H₂O-MeCN, 35:65, v/v)
 (5) RP-MPLC (H₂O-MeOH, 80:20 → 10:90, v/v)
 (6) RP-HPLC (H₂O-MeCN, 30:70 → 70:30, v/v)
 (7) Silica gel C.C. (CHCl₃-MeOH, 9:1 → 2:1, v/v)



- (1) Diaion HP20 C.C. (H₂O-MeOH, 10:90 → 0:100, v/v) / (2) RP-MPLC (H₂O-MeOH, 95:5 → 40:60, v/v)
 (3) RP-HPLC (H₂O-MeCN, 80:20, v/v) / (4) Sephadex LH-20 C.C. (MeOH)
 (5) RP-HPLC (H₂O-MeCN, 80:20 → 30:70, v/v) / (6) RP-HPLC (H₂O-MeCN, 85:15 → 50:50, v/v)
 (7) RP-HPLC (H₂O-MeCN, 80:20, v/v) / (8) RP-MPLC (H₂O-MeOH, 90:10 → 30:70, v/v)
 (9) RP-HPLC (H₂O-MeCN, 80:20 → 55:45, v/v) / (10) RP-HPLC (H₂O-MeCN, 80:20 → 50:50, v/v)

SI 9. Isolation scheme of compounds 1–24 from the aerial parts of *Leea asiatica*.