

SUPPLEMENTARY MATERIAL

A new secoiridoid glycoside from the fruits of *Cornus officinalis* (Cornaceae)

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A new secoiridoid glycoside, 7 β -*O*-dimethyl butanedioate morroniside (**1**) was isolated from the fruits of *Cornus officinalis* (Cornaceae) along with the known compound, caffeoyltartaric acid dimethyl ester (**2**) which was isolated from the family Cornaceae for the first time. Their structures were elucidated by physical and spectroscopic data analysis, including 1D and 2D NMR, ESI-MS, and CD experiments.

Keywords: *Cornus officinalis*; Cornaceae; secoiridoid glycoside

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We provided the original NMR spectra for 7 β -*O*-dimethyl butanedioate morroniside (**1**) and experimental data for caffeoyltartaric acid dimethyl ester (**2**).

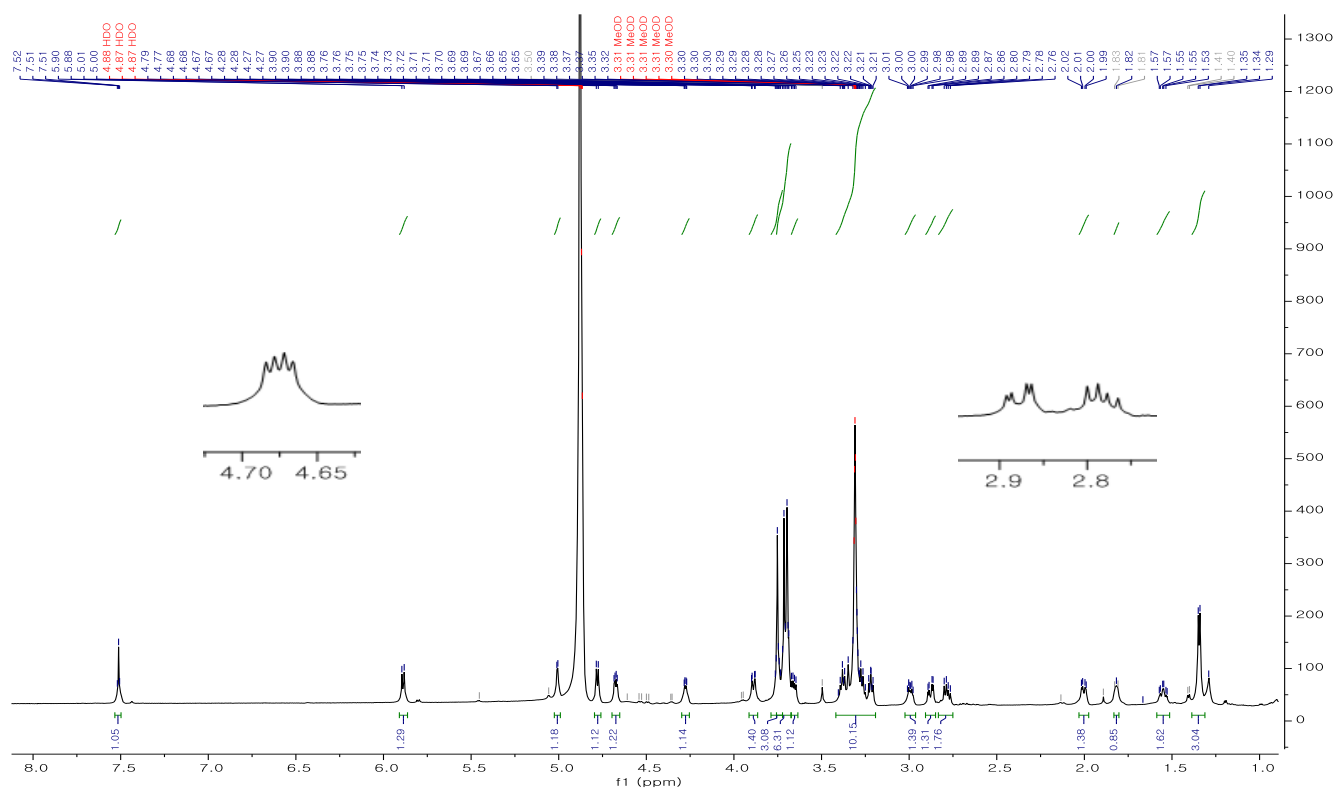


Figure S1. ^1H -NMR (700 MHz, CD_3OD) spectrum of compound **1**.

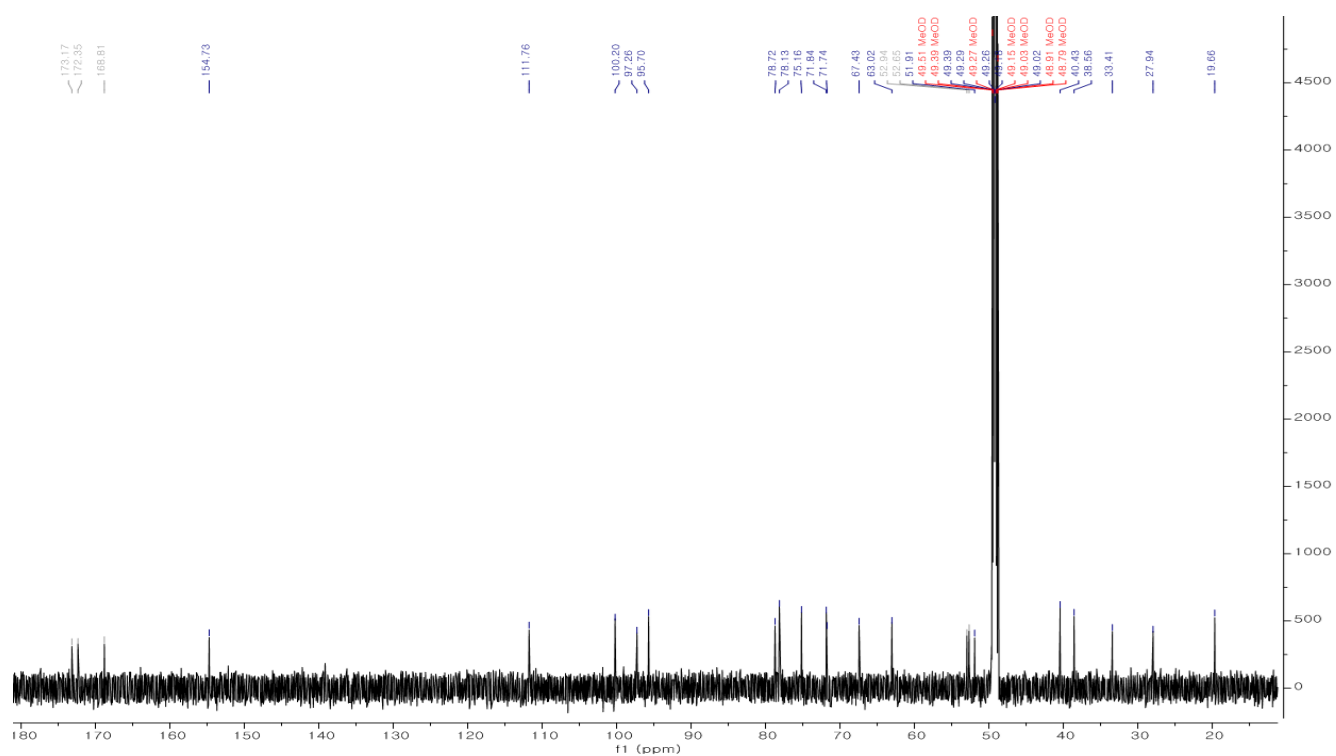


Figure S2. ^{13}C -NMR (175 MHz, CD_3OD) spectrum of compound **1**.

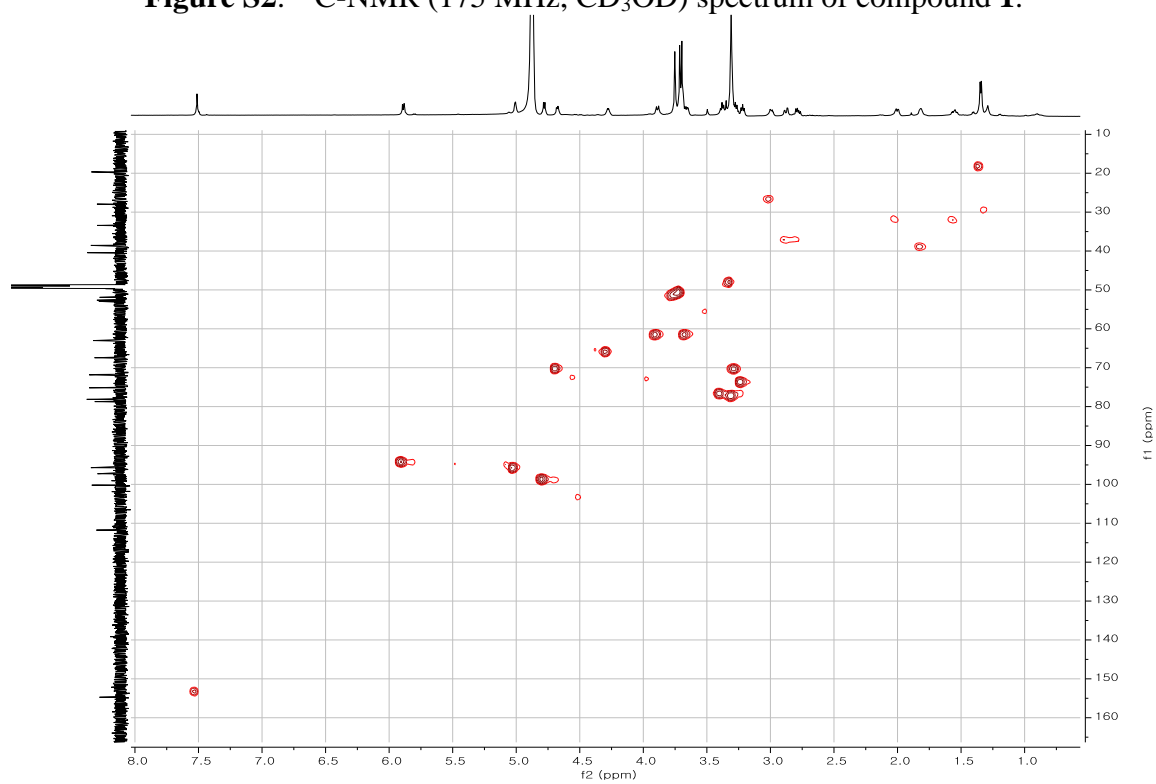


Figure S3. HSQC NMR spectrum of compound **1**.

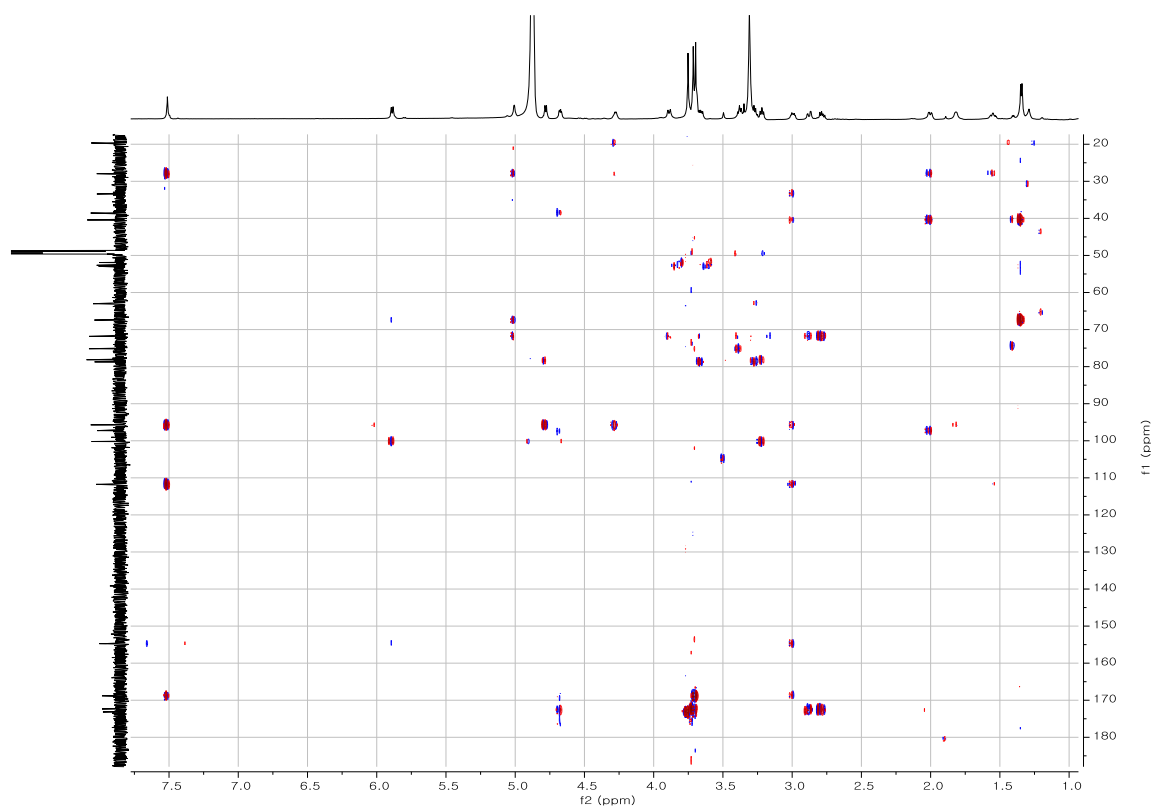


Figure S4. HMBC NMR spectrum of compound **1**.

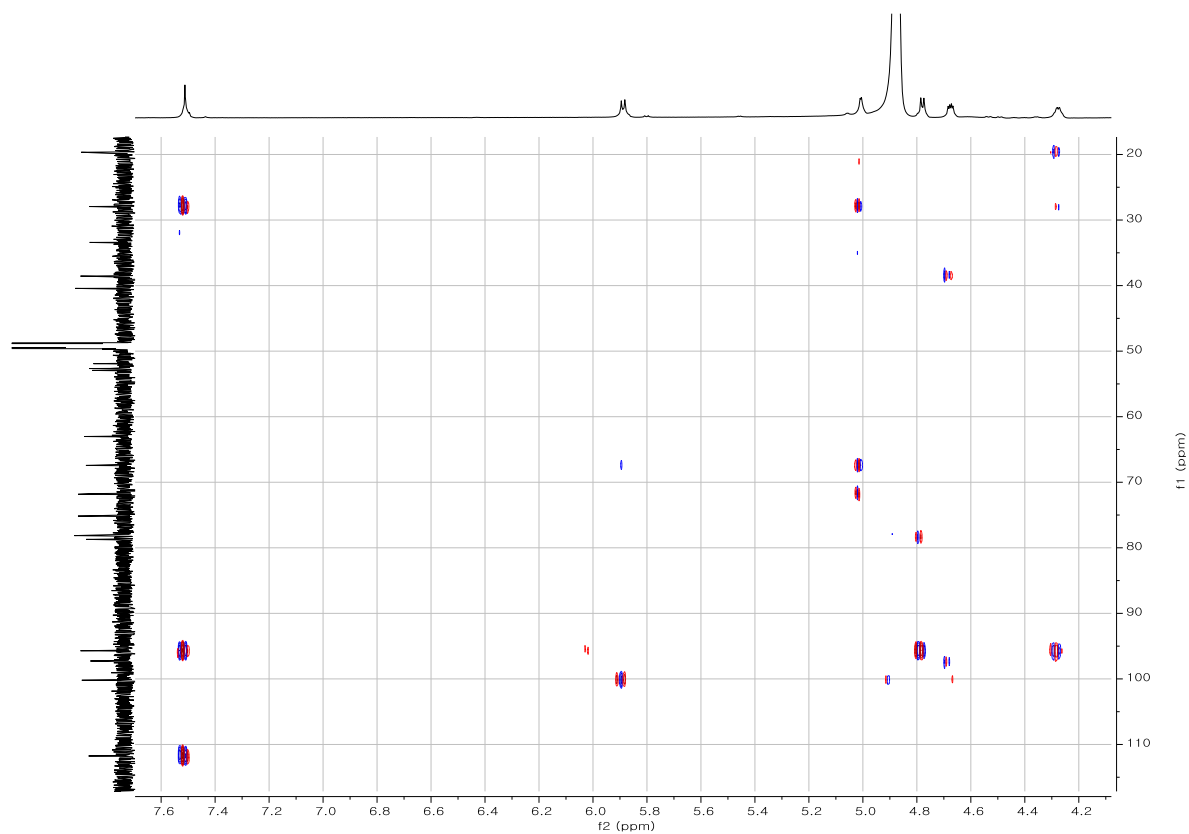


Figure S5. Expansion of the HMBC NMR spectrum of compound **1**.

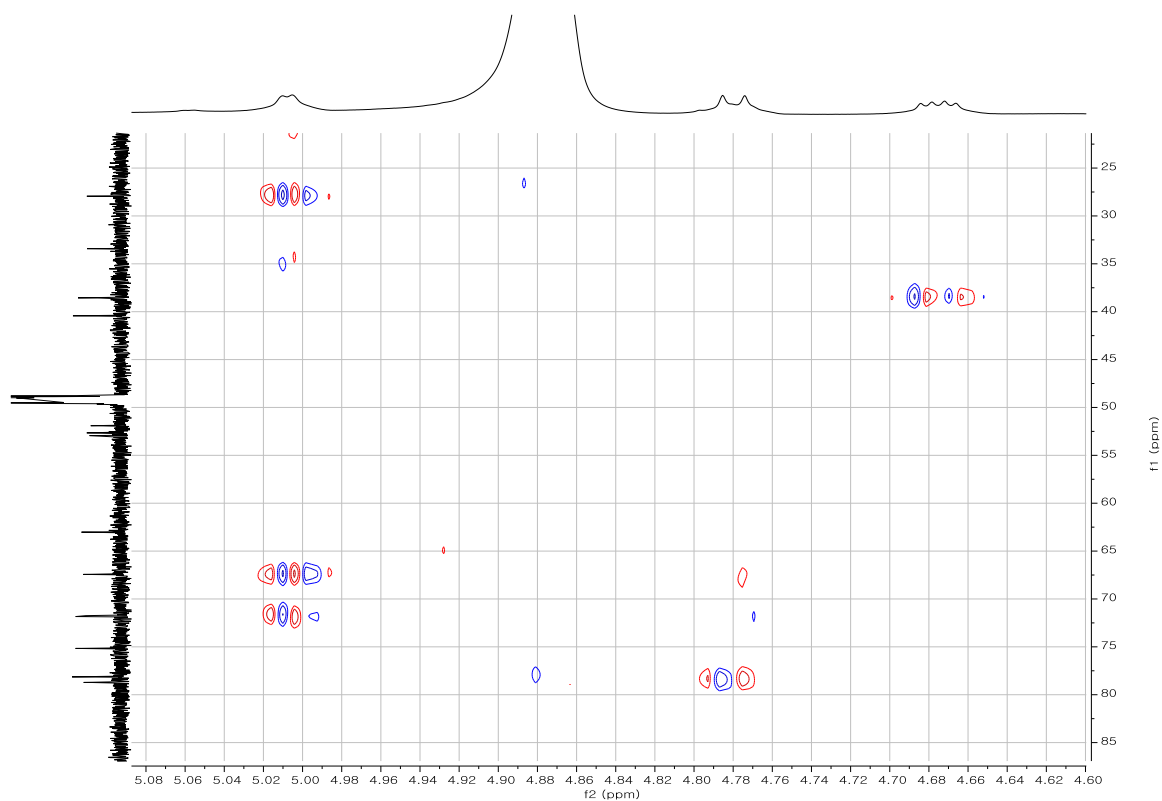


Figure S5. Expansion of the HMBC NMR spectrum of compound **1** (continued).

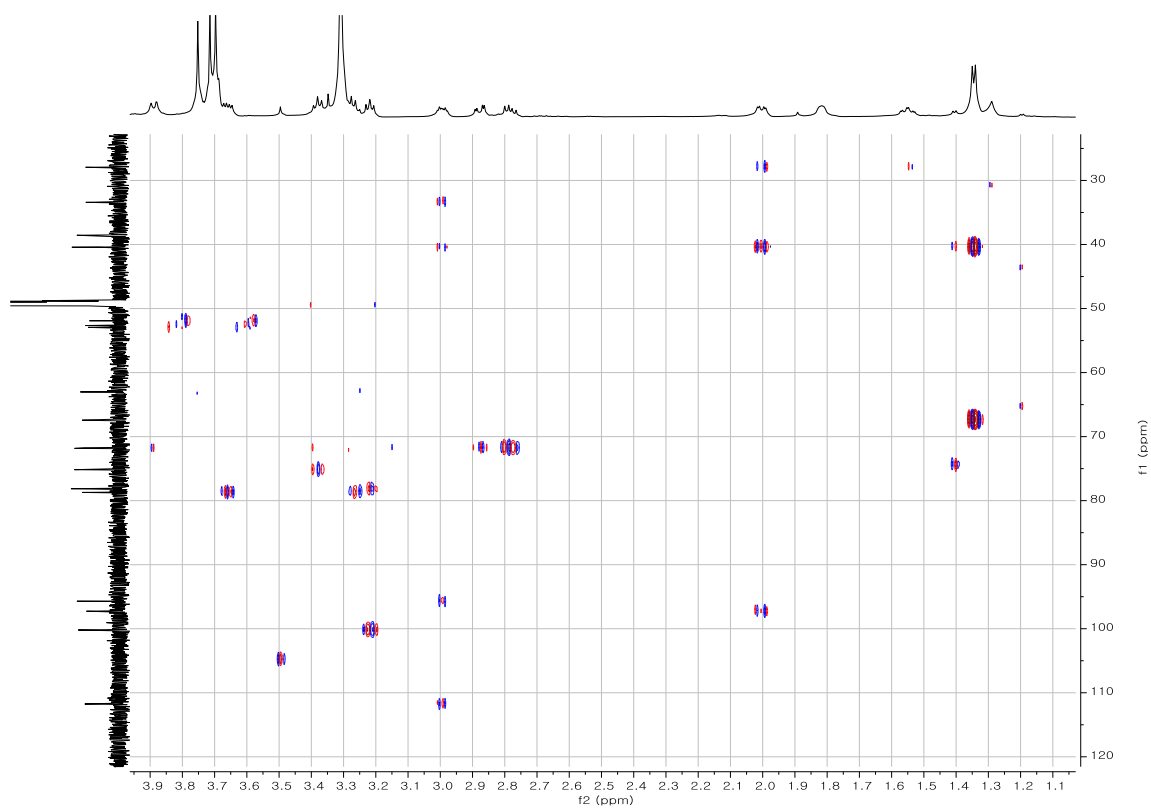


Figure S5. Expansion of the HMBC NMR spectrum of compound **1** (continued).

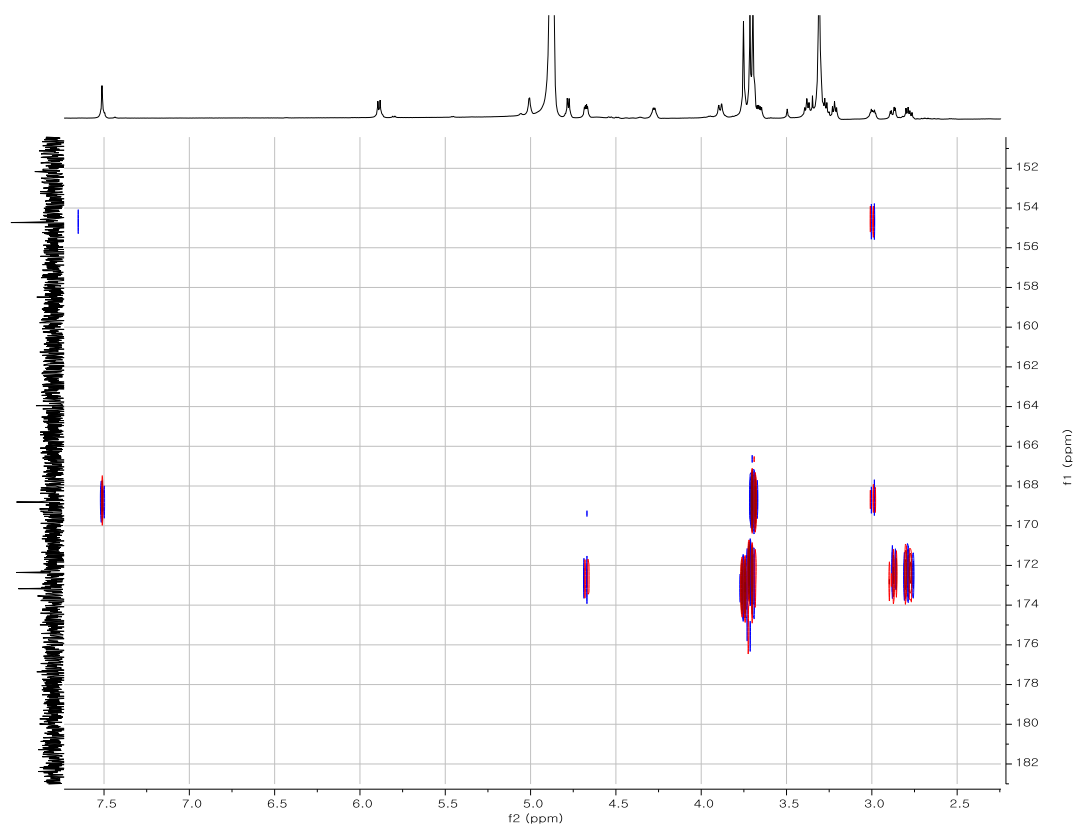


Figure S5. Expansion of the HMBC NMR spectrum of compound **1** (continued).

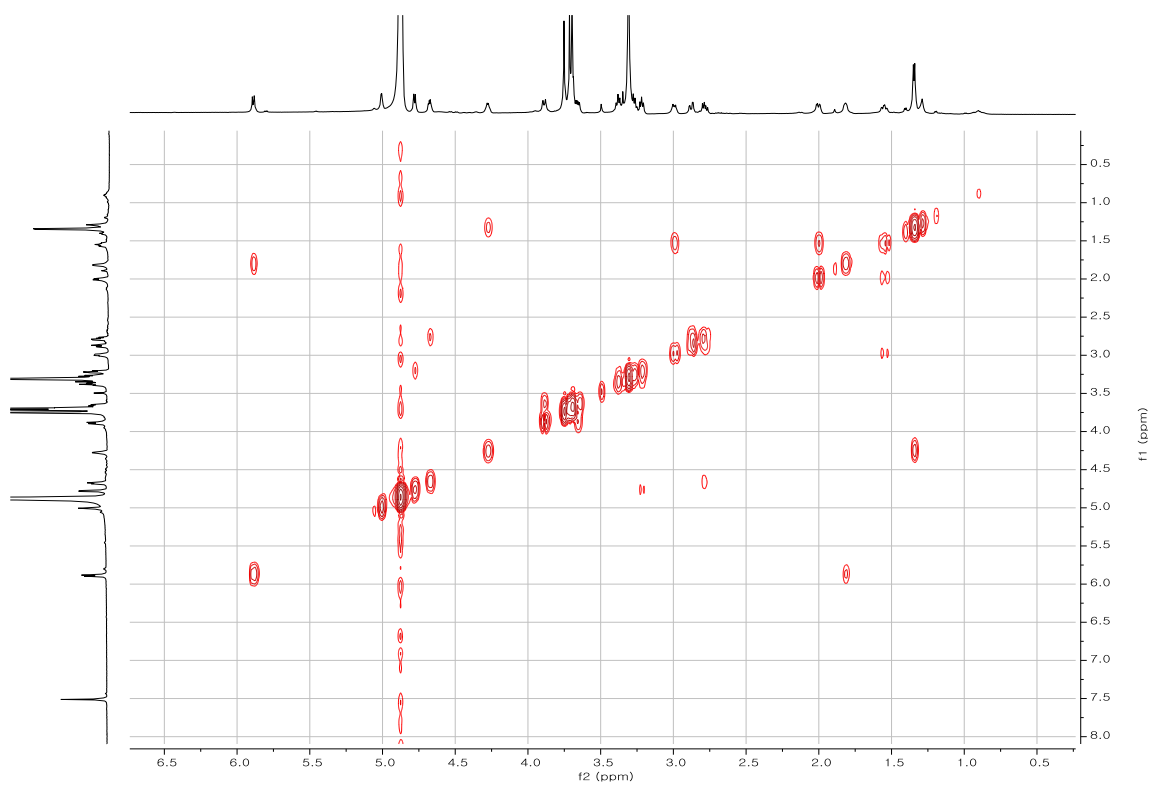


Figure S6. COSY NMR spectrum of compound **1**.

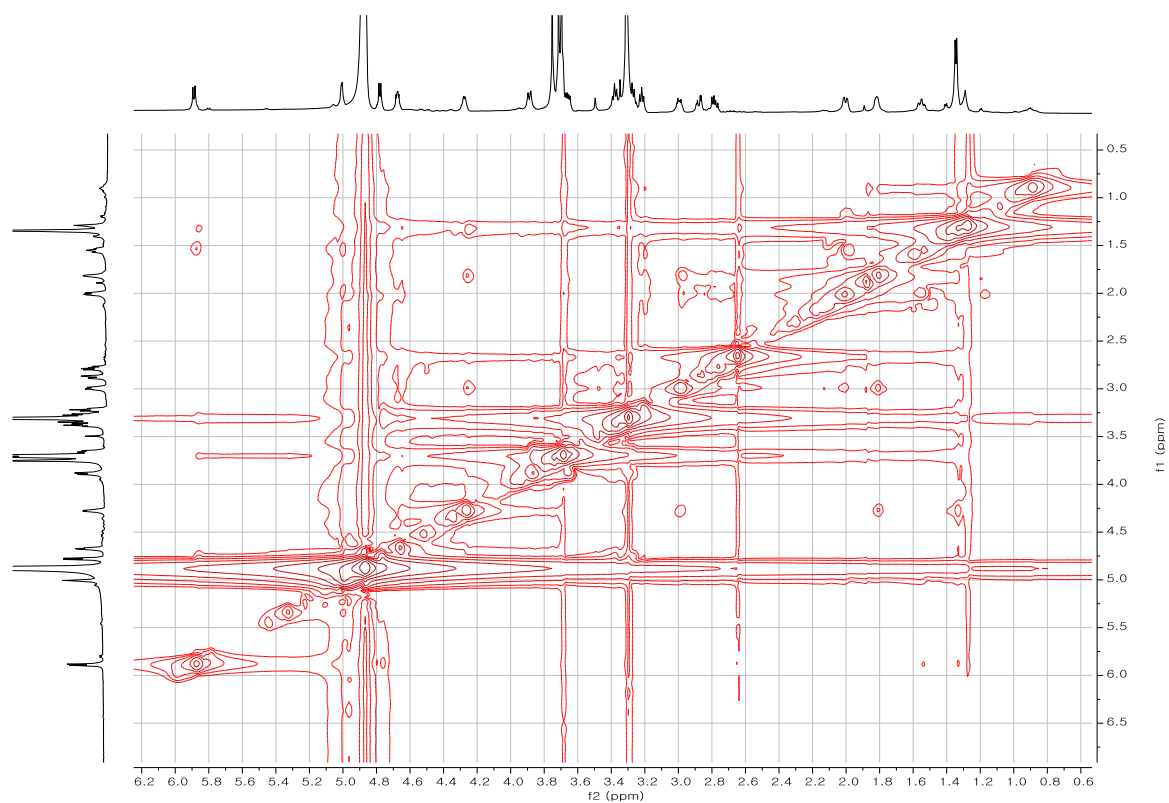


Figure S7. NOESY NMR spectrum of compound **1**.

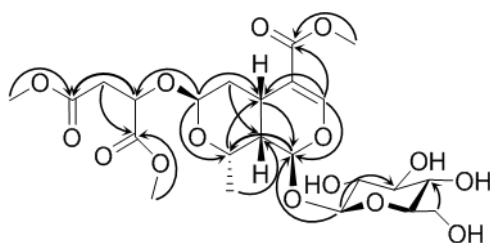


Figure S8. Key HMBC correlations ($^1\text{H} \rightarrow ^{13}\text{C}$) of compound **1**.

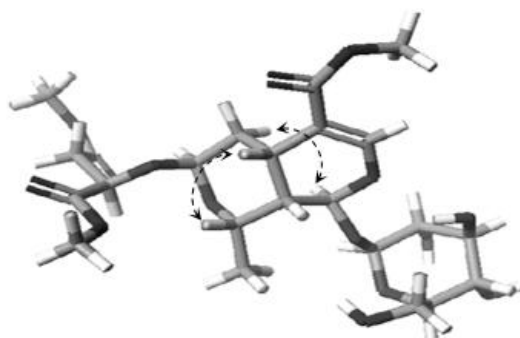


Figure S9. Key NOESY correlations of compound **1**.

Table S1. ^1H - (400 MHz) and ^{13}C -NMR (100 MHz) data of compound **2** in CD_3OD (δ in ppm).

Positions	δ_{H}	δ_{C}	HMBC ($^1\text{H} \rightarrow ^{13}\text{C}$)
1	-	127.5	
2	7.22 (1H, d, $J = 1.9$ Hz)	111.8	1, 3, 4, 6, 7
3	-	149.6	
4	-	151.3	
5	6.82 (1H, d, $J = 8.3$ Hz)	116.6	1, 3, 4
6	7.10 (1H, dd, $J = 8.3, 1.9$ Hz)	124.6	2, 4, 7
7	7.71 (1H, d, $J = 16$ Hz)	148.4	2, 6, 8, 9
8	6.43 (1H, d, $J = 16$ Hz)	114.1	1, 9
9	-	167.9	
1'	-	172.2	
2'	5.56 (1H, d, $J = 3.0$ Hz)	75.3	9, 1', 3', 4'
3'	4.71 (1H, d, $J = 3.0$ Hz)	72.1	1', 2', 4'
4'	-	169.1	
1'-OCH ₃	3.80 (3H, s)	53.0	1'
4'-OCH ₃	3.76 (3H, s)	53.0	4'

Spectral data of compound 2.

Caffeoyltartaric acid dimethyl ester (2): yellowish white powder; $[\alpha]_{\text{D}}^{25} +6.0$ ($c = 0.1$, MeOH); CD ($c = 0.16$ mM, MeOH) $\Delta\epsilon_{185} +9.20$, $\Delta\epsilon_{216} - 21.2$; UV (MeOH) λ_{max} nm (log ϵ): 328.5 (4.58), 235 (4.37); IR (KBr) ν_{max} cm^{-1} : 3457, 2919, 1742, 1593, 1515, 1151; ^1H -NMR (CD_3OD , 400 MHz) and ^{13}C -NMR (CD_3OD , 100 MHz), see Table 1; Key COSY correlations: H-7/H-8, H-2'/H-3'; Key NOESY correlations: H-2/H-7; H-6/H-8; Key HMBC correlations: H-2/C-1, C-3, C-4, C-6, C-7; H-5/C-1, C-3, C-4; H-6/C-2, C-4, C-7; H-7/C-2, C-6, C-8, C-9; H-8/C-1, C-9; H-2'/C-9, C-1', C-3', C-4'; H-3'/C-1', C-2', C-4'; OCH₃-1'/C-1'; OCH₃-4'/C-4'; HRESIMS m/z 340.0795 $[\text{M}]^+$ (calcd for $\text{C}_{15}\text{H}_{16}\text{O}_9$, 340.0794).