Supporting Information

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A new 8′,9′-dinor 8,4′-oxyneolignan Glucoside from *Dendrobium Aurantiacum* var. *Denneanum*

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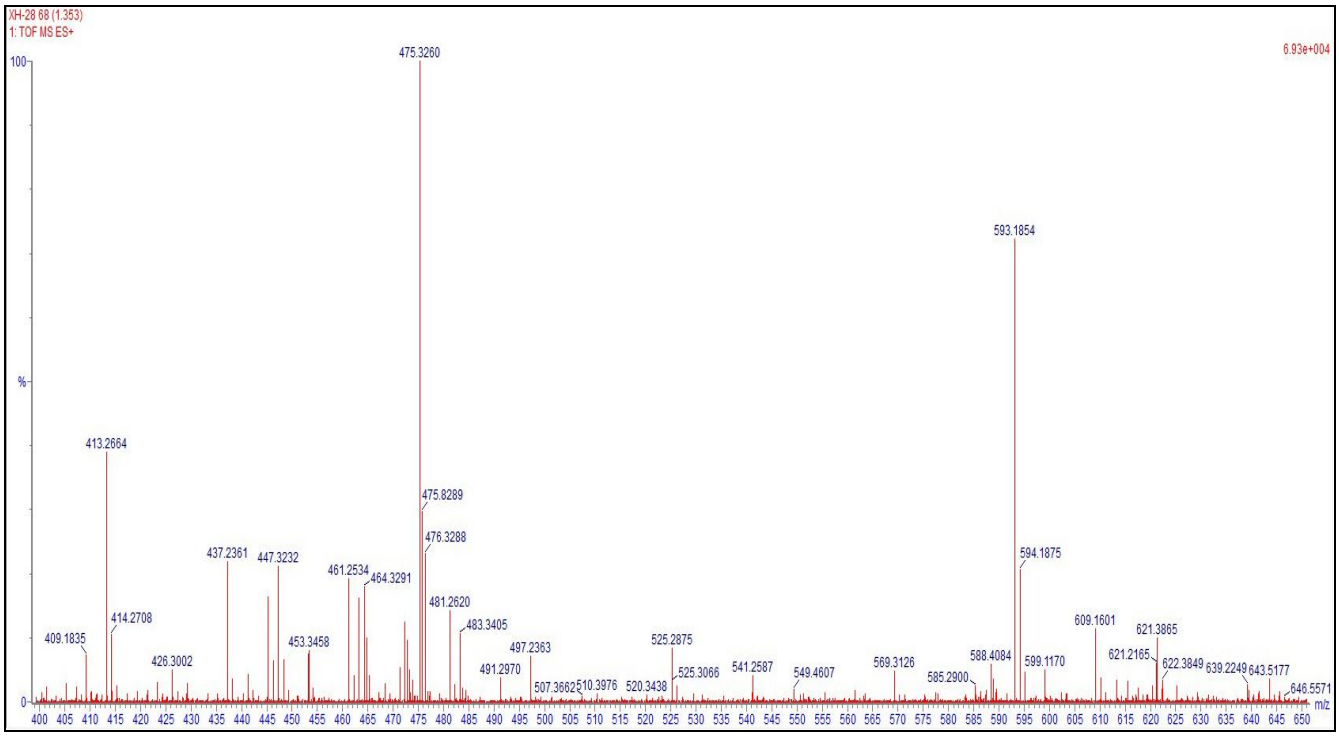
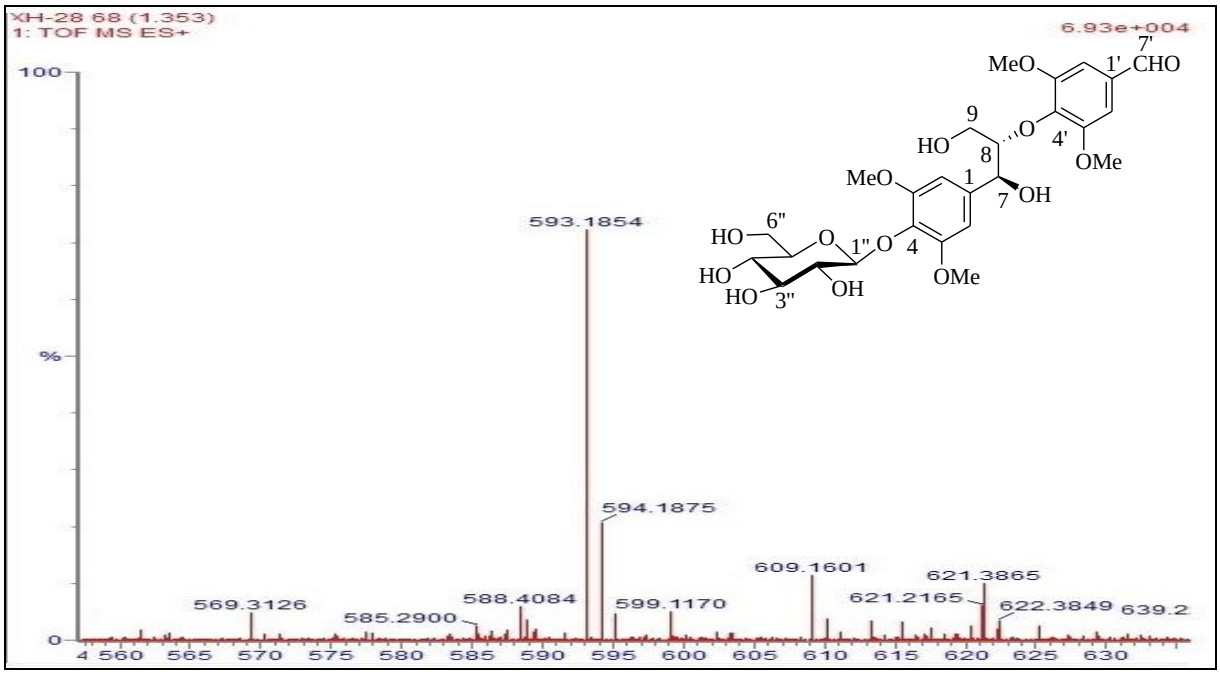
Table of Contents **Page**



S1: HRESI-MS Spectrum of Compound **1** ((–)-(7*S*,8*S*)-4-Hydroxy-3,3′,5,5′-tetramethoxy-8′,9′-dinor-8,4′-oxyneoligna-7,9-diol-7′-al 4-O-*β*-D-glucopyranoside)



Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

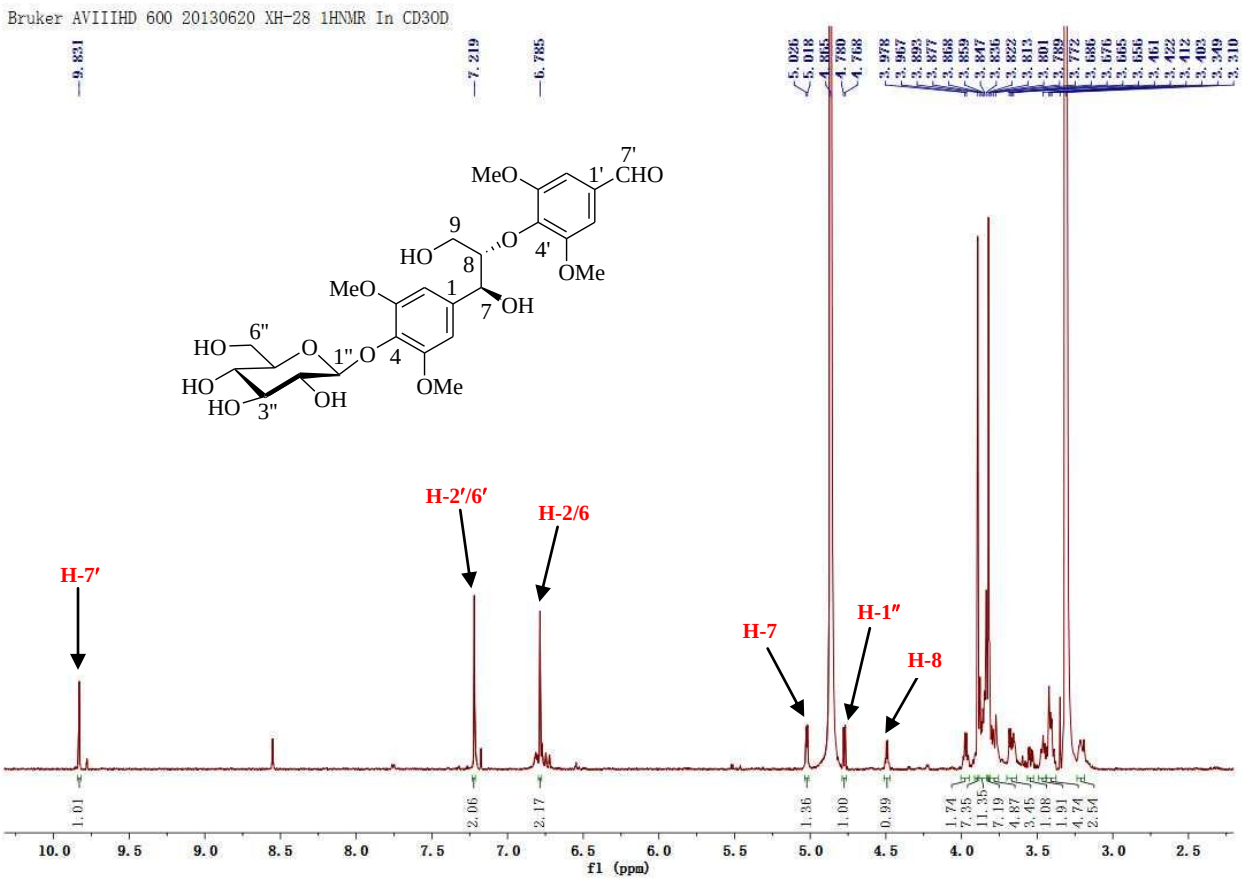
Monoisotopic Mass, Even Electron Ions

247 formula(e) evaluated with 1 results within limits (up to 100 closest results for each mass)

Elements Used:

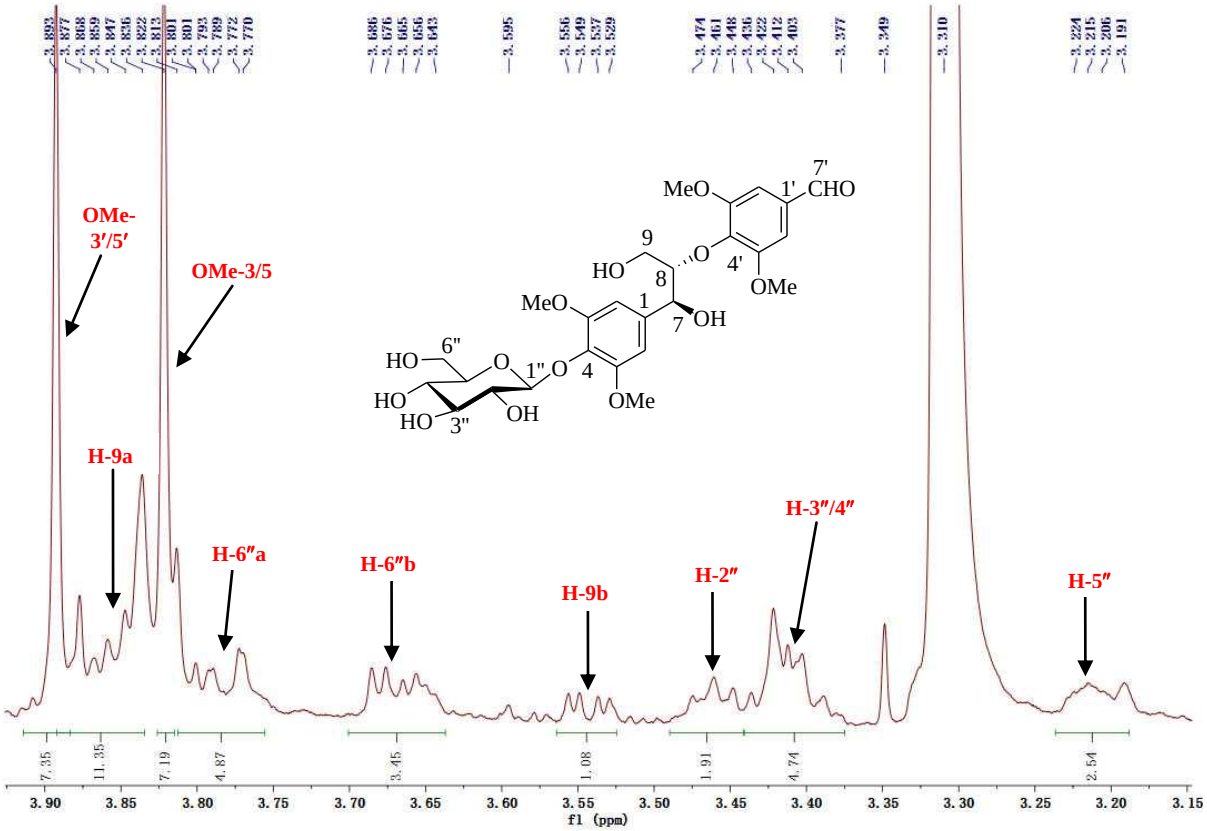
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
593.1854	593.1846	0.8	1.3	9.5	C26 H34 O14 Na	308.1	n/a	n/a	26	34	14	1

S2: Expansion of HRESI-MS Spectrum of Compound **1**

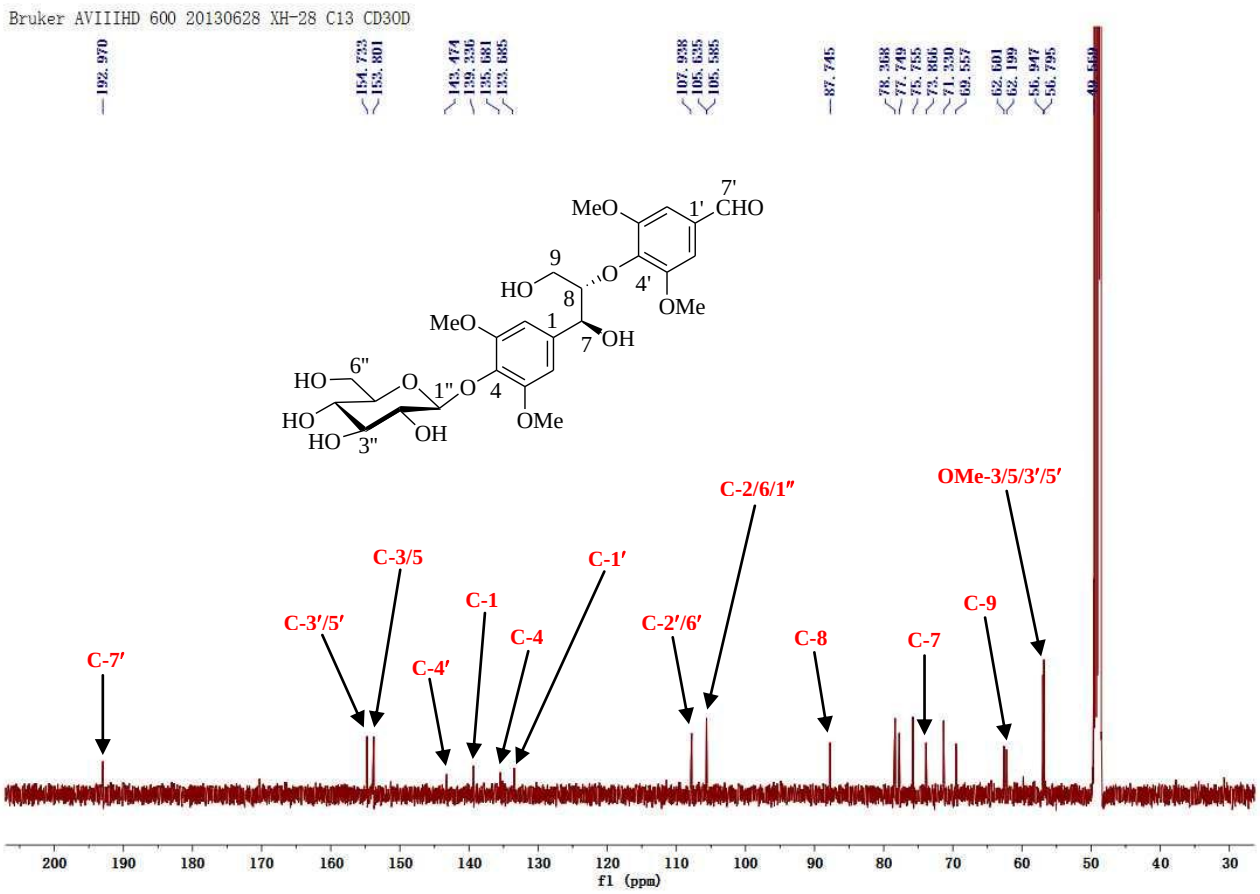


S3: ^{1}H-NMR (600 MHz, CD_3OD) Spectrum of Compound **1**

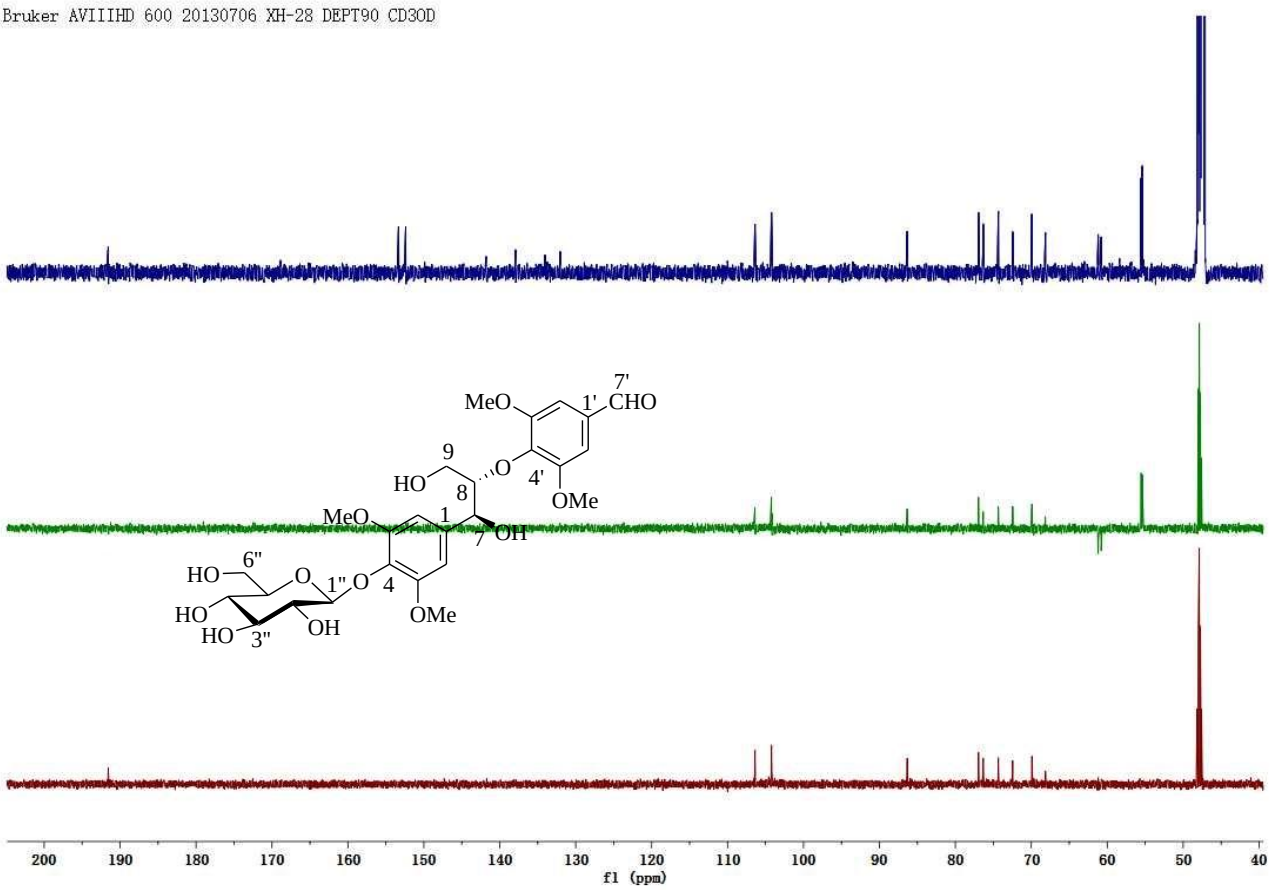
(–)-(7S,8S)-4-Hydroxy-3,3′,5,5′-tetramethoxy-8′,9′-dinor-8,4′-oxyneoligna-7,9-diol-7′-al 4-O-β-D-glucopyranoside ***(1)****:* Colorless gum. $[\alpha]_D^{20}$ = –31.2 (*c* = 0.04, MeOH). IR ν_{max} (KBr): 3359, 2923, 2853, 1596, 1503, 1461, 1422, 1332, 1123, 1057, 875, 799, 713 cm^{-1}. ^{1}H-NMR (CD_3OD, 600 MHz), *δ*: 9.83 (1H, s, H-7′), 7.22 (2H, s, H-2′/6′), 6.69 (2H, s, H-2/6), 5.02 (1H, d, H-7), 4.77 (1H, d, H-1″), 4.49 (1H, m, H-8), 3.89 (6H, s, OMe-3′/5′), 3.84 (1H, m, H-9a), 3.82 (6H, s, OMe-3/5), 3.78 (1H, dd, H-6″a), 3.67 (1H, dd, H-6″b), 3.54 (1H, dd, H-9b), 3.46 (1H, m, H-2″), 3.41 (2H, m, H-3″/4″), 3.20 (1H, m, H-5″). ^{13}C-NMR (CD_3OD, 150 MHz), *δ*: 193.0 (C-7′), 154.7 (C-3′/5′), 153.8 (C-3/5), 143.5 (C-4′), 139.3 (C-1), 135.7 (C-4), 133.7 (C-1′), 107.9 (C-2′/6′), 105.6 (C-2/6/1″), 87.7 (C-8), 78.4 (C-5″), 77.7 (C-3″), 75.8 (C-2″), 73.9 (C-7), 71.3 (C-4″), 62.6 (C-6″), 62.2 (C-9), 56.9 (OMe-3/5), 56.8 (OMe-3′/5′). HRESIMS: *m/z* 593.1854 $[M+Na]^+$ (calcd. for $C_{26}H_{34}O_{14}Na$, 593.1846).



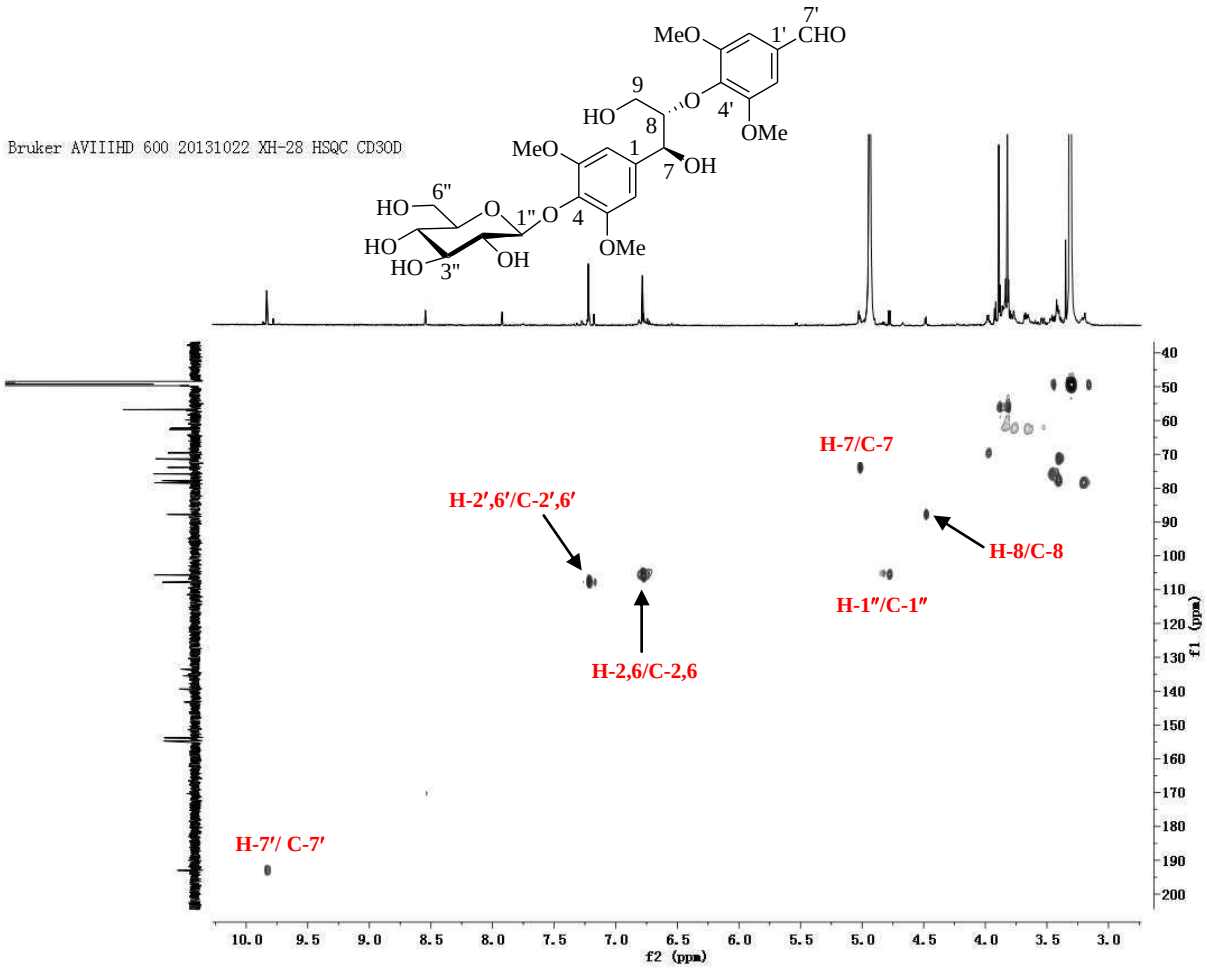
S4: Expansion of the ^{1}H-NMR Spectrum of Compound **1** (From 3.15 to 3.95 ppm)



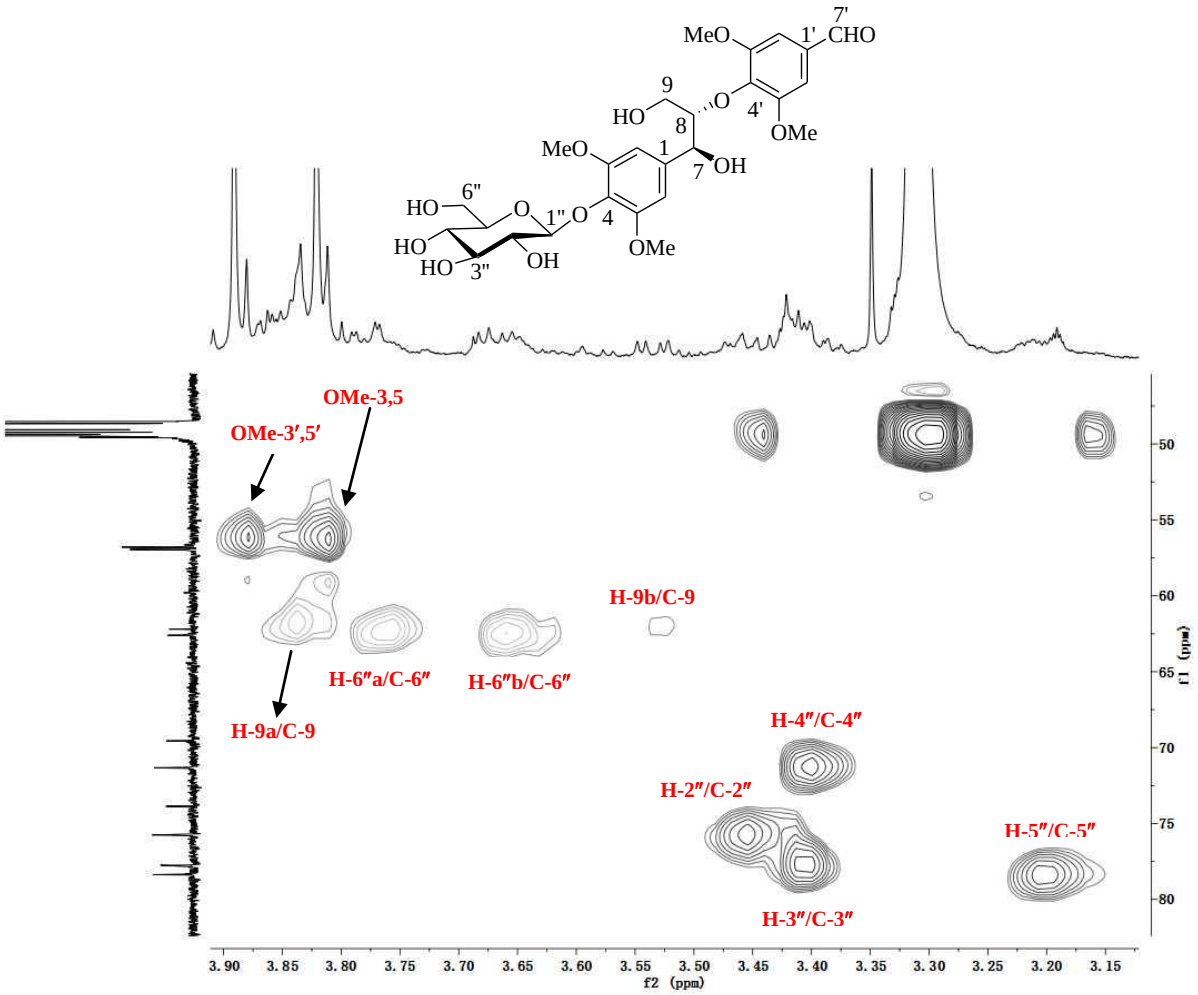
S5: ^{13}C-NMR (150 MHz, CD_3OD) Spectrum of Compound **1**



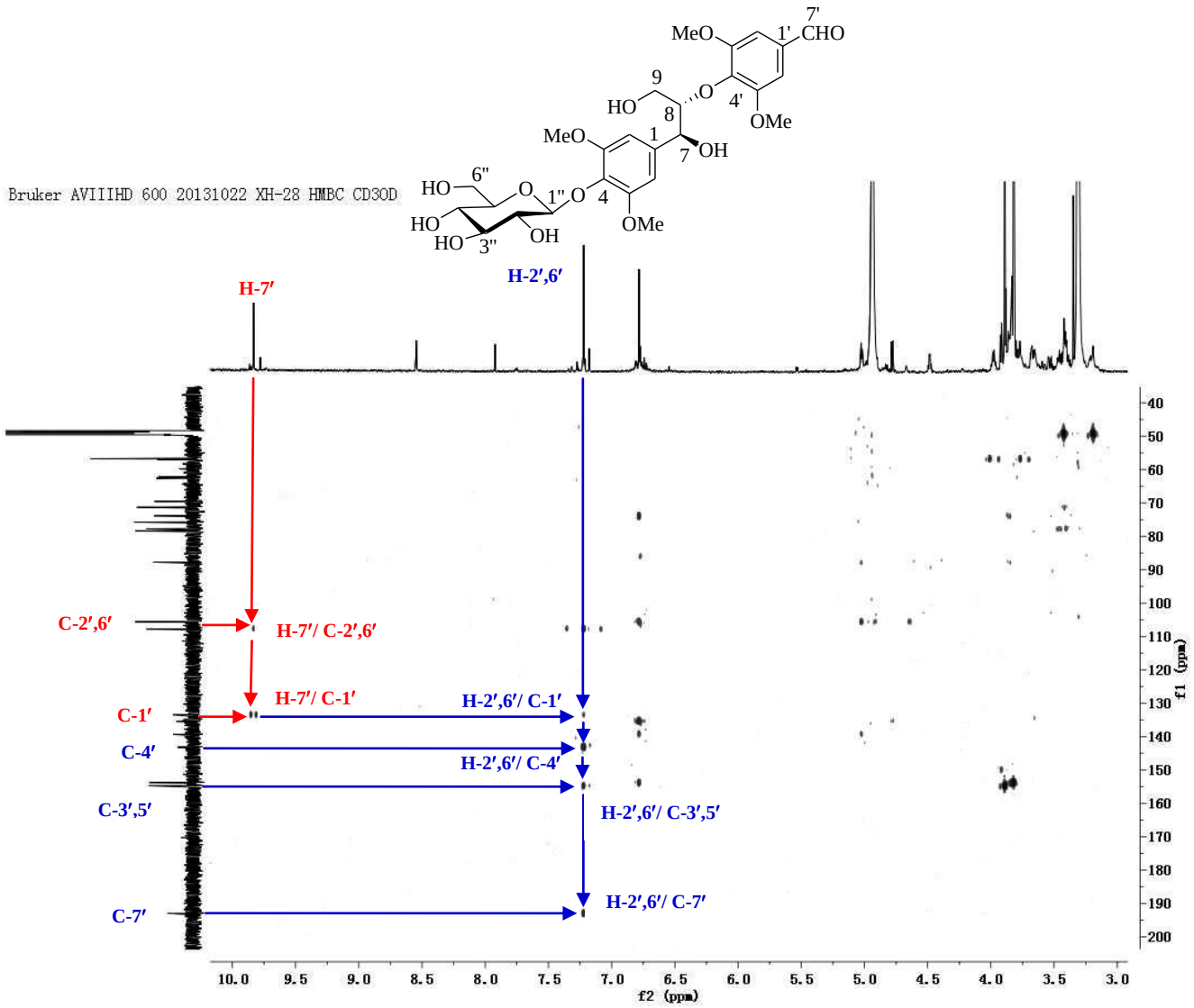
S6: DEPT Spectrum of Compound **1**



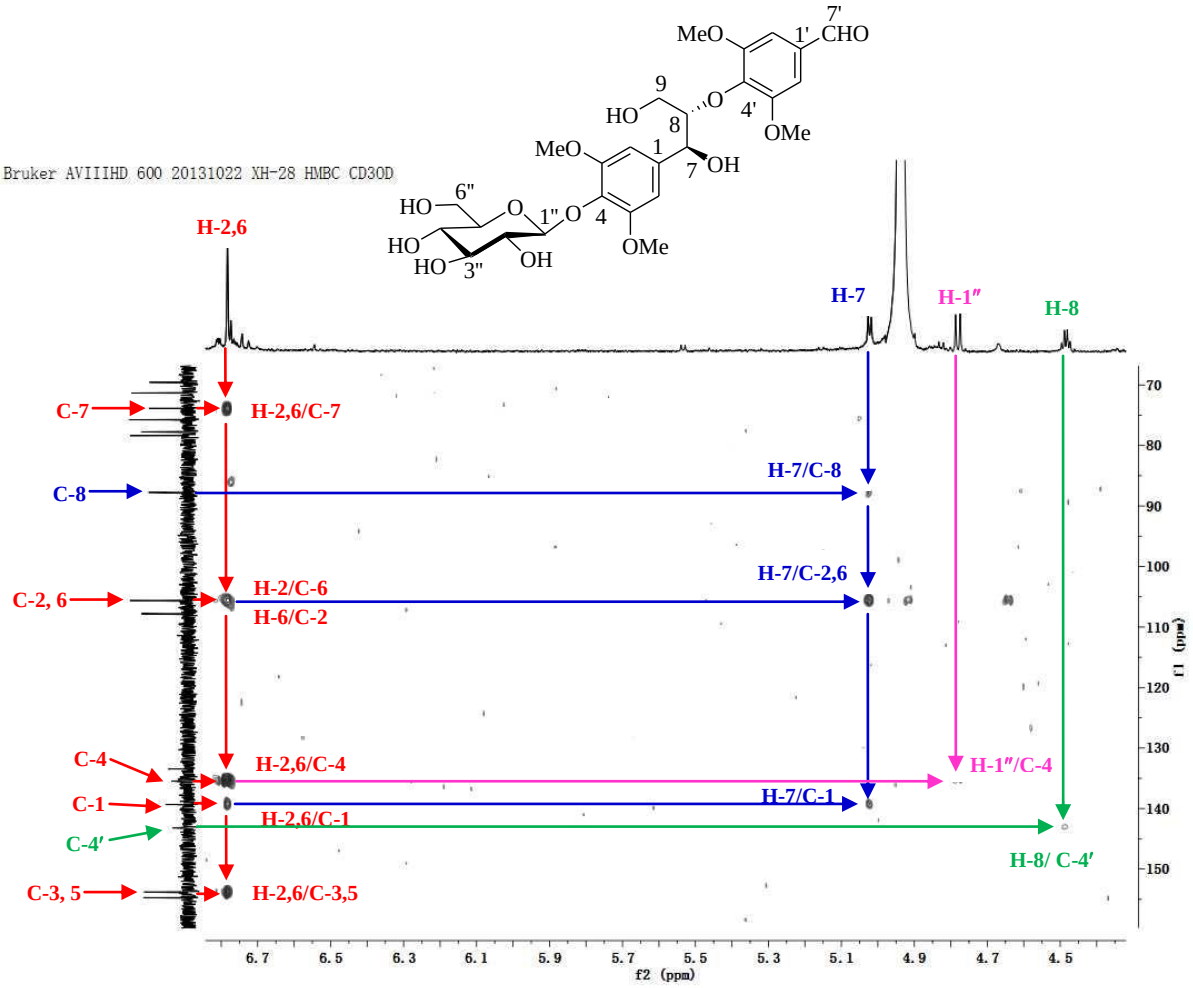
S7: HSQC (600 MHz) Spectrum of Compound **1**



S8: Expansion of HSQC Spectrum of Compound **1** (From 3.08 to 3.93 ppm)



S9: HMBC (600 MHz) Spectrum of Compound **1**



S10: Expansion of HMBC Spectrum of Compound **1** (From 4.30 to 6.90 ppm)