

Pogonatherumol, a new highly oxygenated norsesquiterpene and flavone C-glycosides from *Pogonatherum crinitum*

Lin Ni,^{1,2} Wei Huang², He-shan Wang³, Hui-you Xu^{1*}

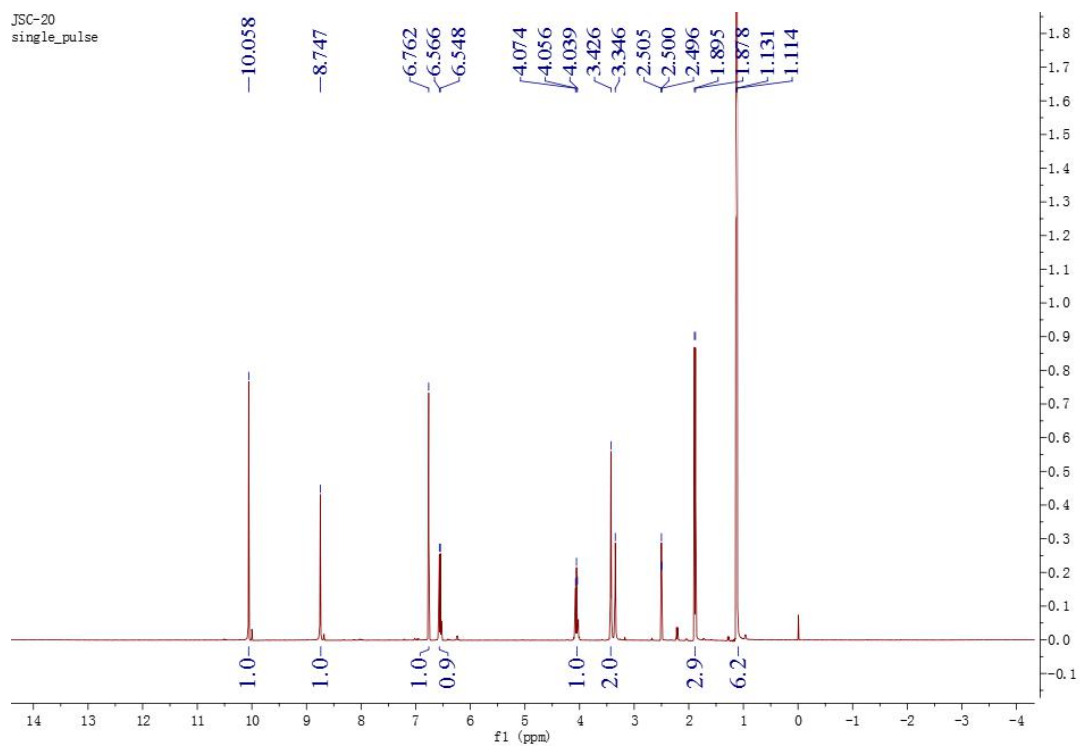
*Corresponding author. E-mail:HuiyouXu@126.com.

Supplementary materials

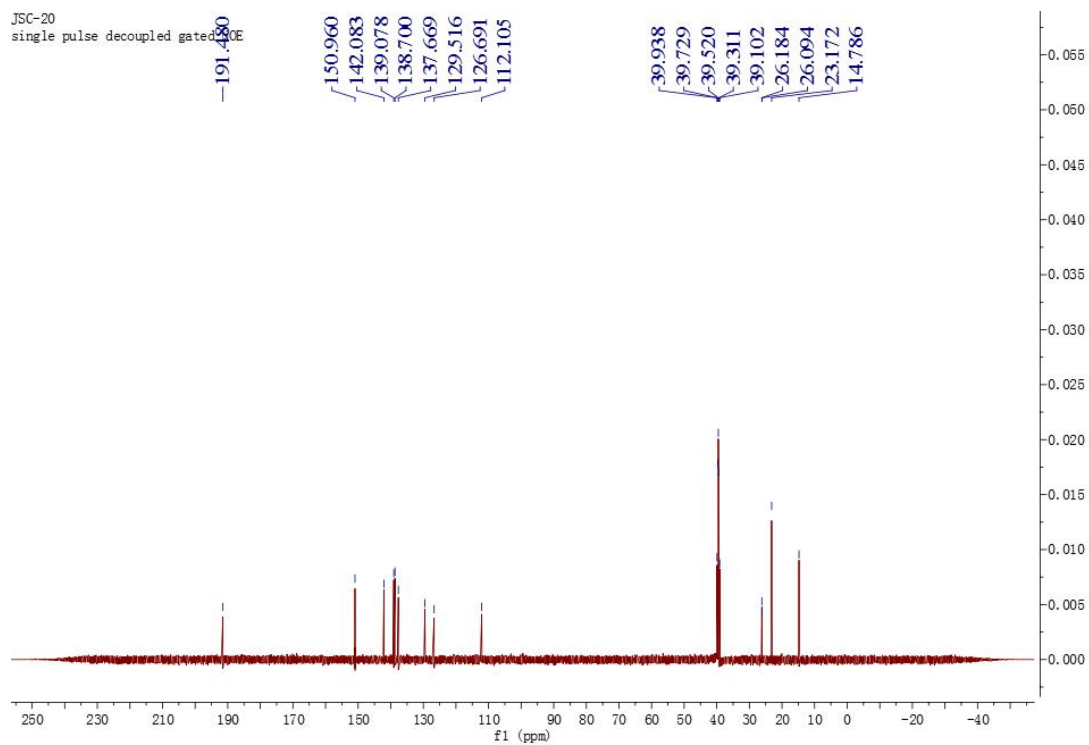
1 College of Plant Protection, Fujian Agriculture and Forestry University, Fuzhou 350002, People's Republic of China;

2 Fujian Colleges and University Engineering Research Institute of Conservation & Utilization of Natural Bioresources, Fujian Agriculture and Forestry University, Fuzhou, 350002, People's Republic of China;

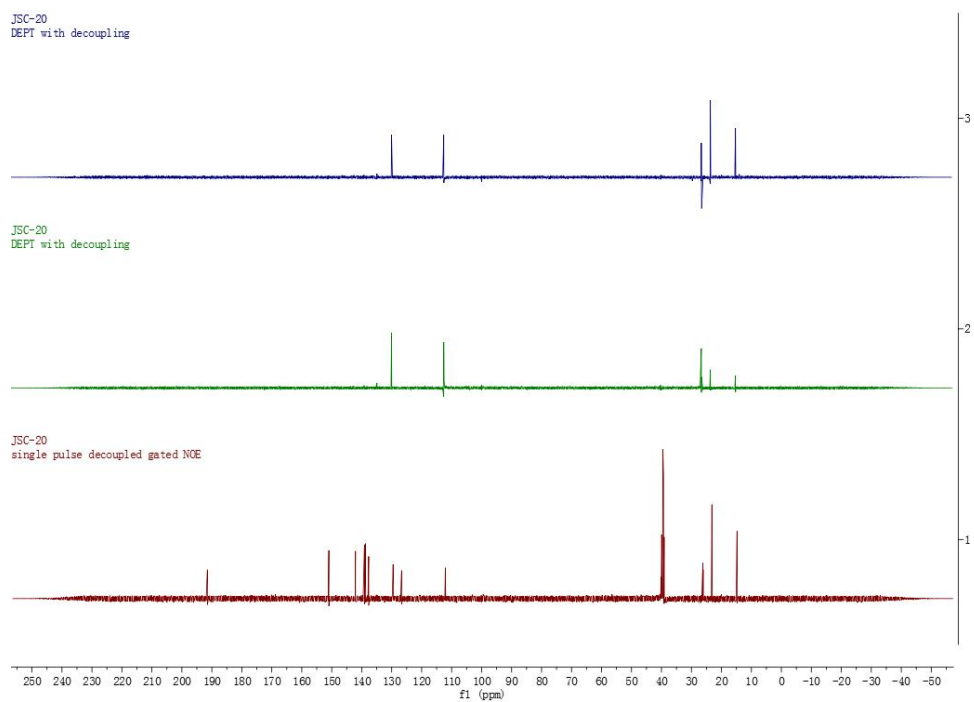
3 College of Pharmacy, Fujian University of Traditional Chinese Medicine, Fuzhou 350108, People's Republic of China.



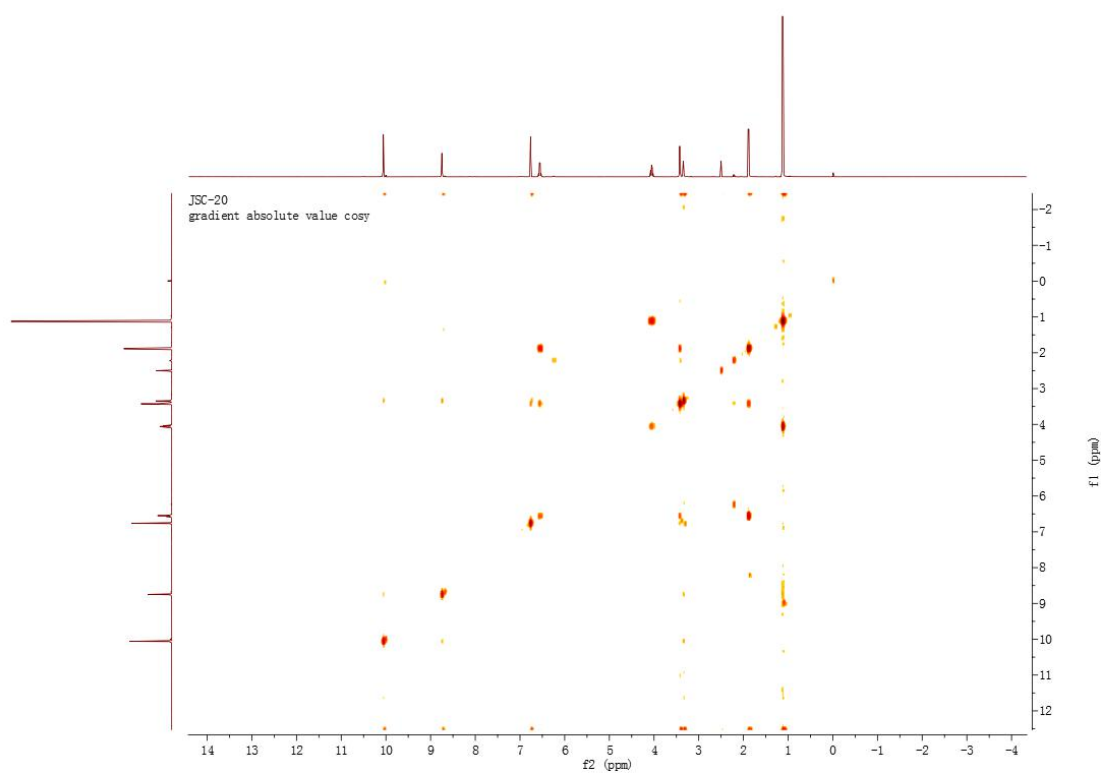
^1H NMR spectrum of Pogonatherumol (400 MHz, $\text{DMSO}-d_6$)



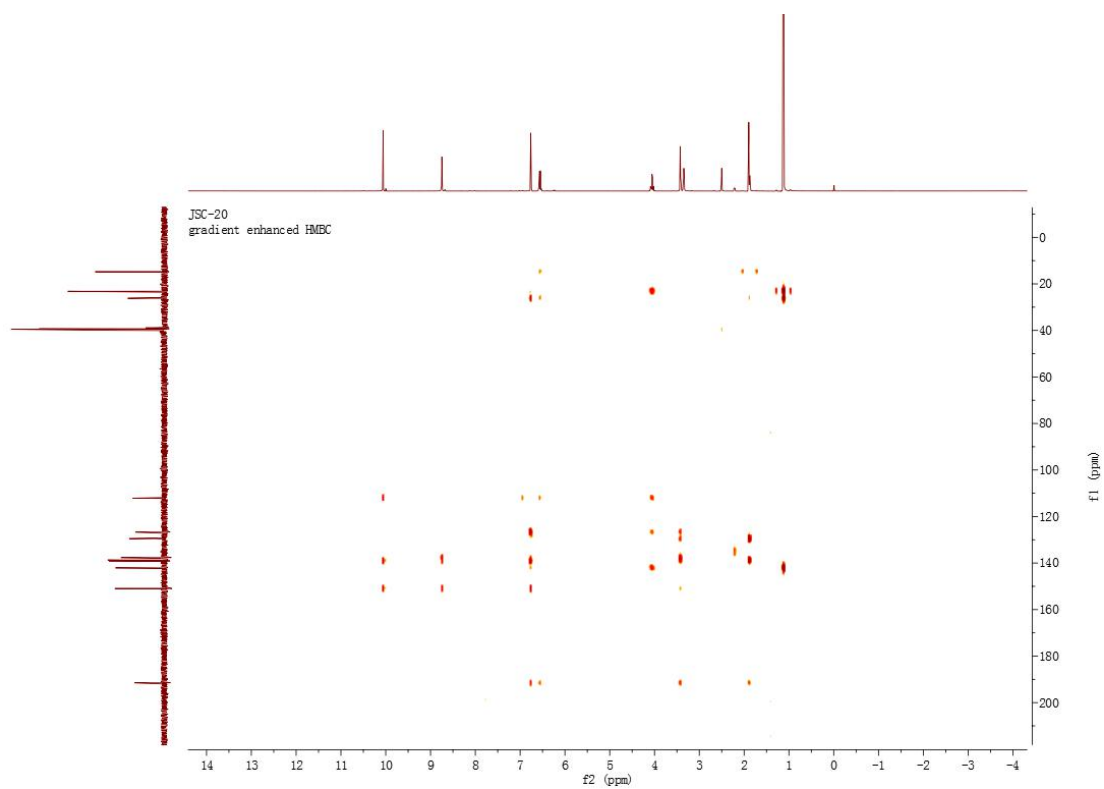
^{13}C NMR spectrum of Pogonatherumol (400 MHz, $\text{DMSO}-d_6$)



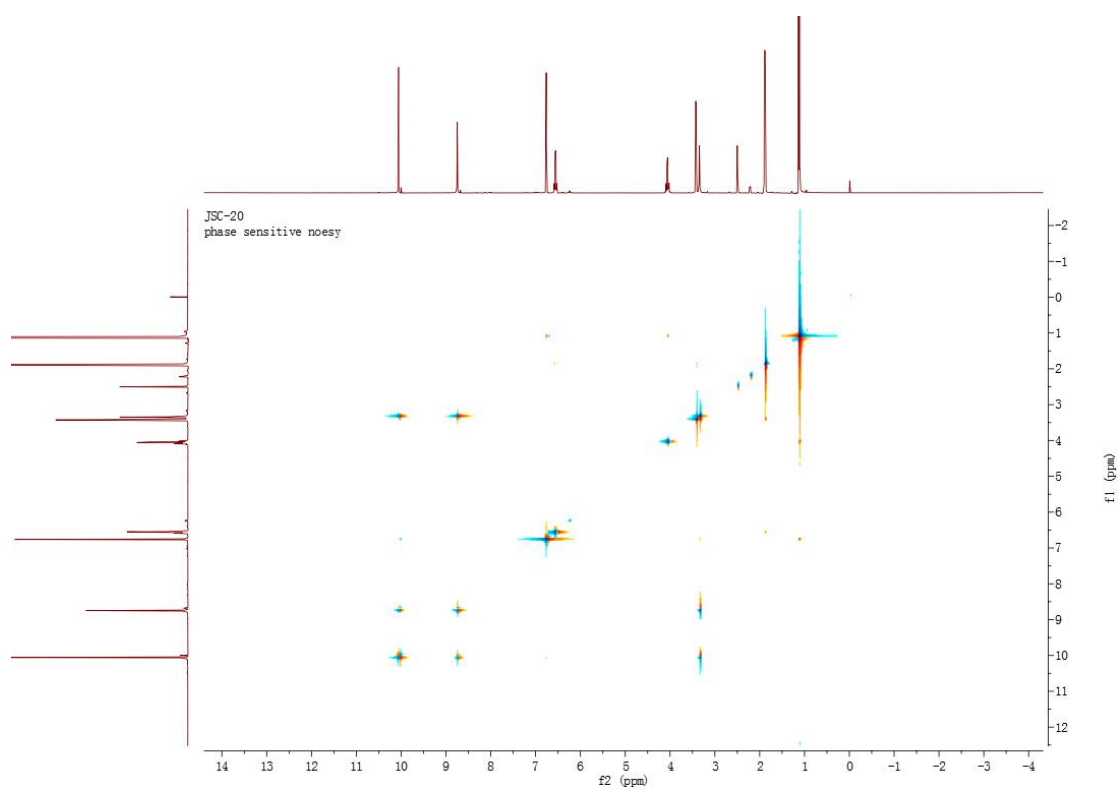
DEPT spectrum of Pogonatherumol (400 MHz, DMSO- d_6)



^1H , ^1H COSY spectrum of Pogonatherumol (400 MHz, DMSO- d_6)



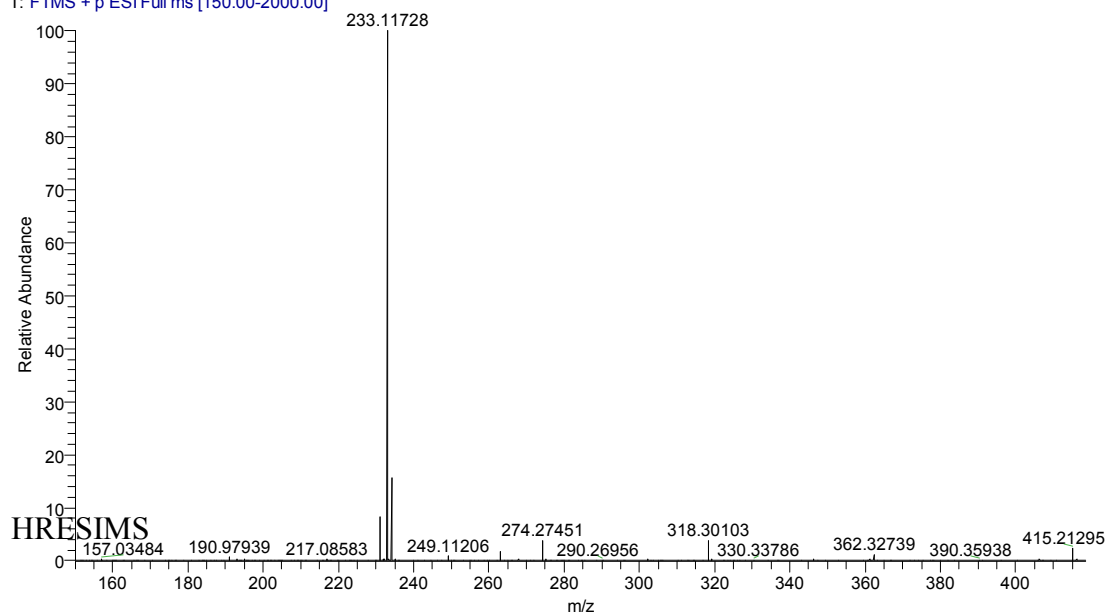
HMBC spectrum of Pogonatherumol (400 MHz, DMSO-*d*₆)



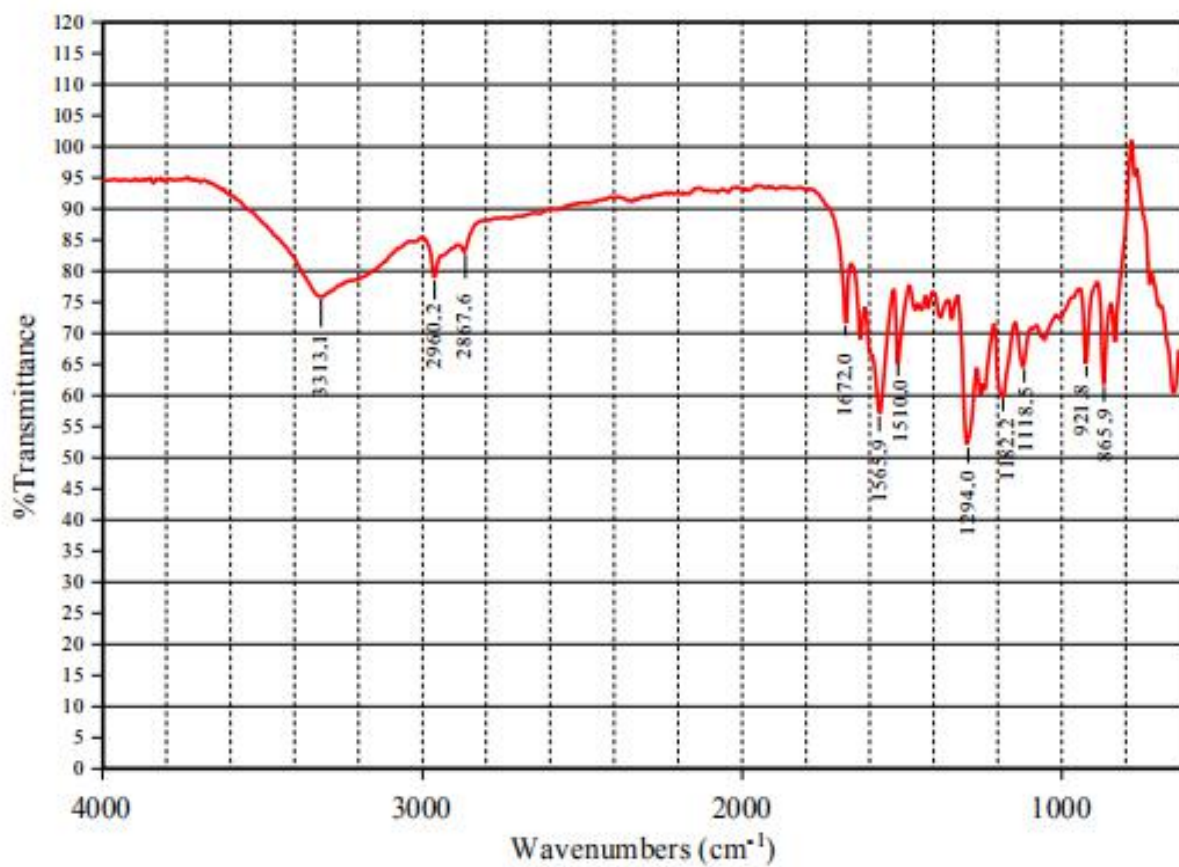
NOESY spectrum of Pogonatherumol (400 MHz, DMSO-*d*₆)

HRMS (ESI) m/z calcd for $C_{14}H_{17}O_3^+$ (M+H) $^+$ 233.11722, found 233.11728.

81 #7 RT: 0.12 AV: 1 NL: 9.64E6
T: FTMS + p ESI Full ms [150.00-2000.00]



HRMS spectrum of Pogonatherumol



IR spectrum of Pogonatherumol

Compound 2

^1H -NMR (400 MHz, $\text{DMSO-}d_6$) δ : 13.65 (1H, s, 5-OH), 8.32 (1H, s, 4'-OH), 8.00 (2H, d, $J = 9.5$ Hz, H-2', 6'), 6.92 (2H, d, $J = 9.5$ Hz, H-3', 5'), 6.72 (1H, s, H-3), 4.80 (1H, d, $J = 10.5$ Hz, H-1'''), 4.56 (1H, d, $J = 11.5$ Hz, H-1''); ^{13}C -NMR (100 MHz, $\text{DMSO-}d_6$) δ : 163.7 (C-2), 102.4 (C-3), 182.0 (C-4), 161.2 (C-5), 109.0 (C-6), 161.2 (C-7), 103.9 (C-8), 154.0 (C-9), 102.9 (C-10), 121.3 (C-1'), 128.8 (C-2', 6'), 116.0 (3', 5'), 159.7 (C-4'), 74.0 (C-''1), 70.5 (C-2''), 79.2 (C-3'', 5''), 70.6 (C-4''), 68.6 (C-6''), 75.3 (C-1'''), 69.9 (C-2'''), 74.0 (C-3'''), 70.2 (C-4'''), 70.6 (C-5''').

Compound 3

^1H -NMR (400 MHz, $\text{DMSO-}d_6$) δ : 13.60 (1H, s, 5-OH), 10.29 (1H, s, 7-OH), 9.19 (1H, s, 4'-OH), 8.32 (2H, d, $J = 8.2$ Hz, H-2', 6'), 6.92 (2H, d, $J = 8.2$ Hz, H-3', 5'), 6.85 (1H, s, H-3); ^{13}C -NMR (100 MHz, $\text{DMSO-}d_6$) δ : 165.3 (C-2), 102.2 (C-3), 182.4 (C-4), 156.5 (C-5), 109.0 (C-6), 162.2 (C-7), 106.0 (C-8), 156.1 (C-9), 104.7 (C-10), 121.9 (C-1'), 130.7 (C-2', 6'), 116.7 (C-3', 5'), 159.1 (C-4'), 75.1 (C-1''), 69.3 (C-2''), 74.7 (C-3''), 70.1 (C-4''), 71.0 (C-5''), 74.7 (C-1'''), 69.1 (C-2'''), 79.7 (C-3'''), 70.5 (C-4'''), 81.5 (C-5'''), 62.2 (C-6''').