SUPPLEMENTARY MATERIAL

A new bioactive diterpenoid from *Pestalotiopsis adusta*, an endophytic fungus from *Clerodendrum canescens*

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Bioassay-guided fractionation of the culture extract of *Pestalotiopsis adusta*, an endophytic fungus isolated from the medicinal plant *Clerodendrum canescens*, led to the isolation of one new, (10*S*)-12,16-epoxy-17(15→16)-abeo-3,5,8,12,15-abietapentaen-2,7,11,14-tetraone (**1**), and four known diterpenoids, teuvincenone F (**2**), uncinatone (**3**), coleon U (**4**), coleon U-12-methyl ether (**5**). These structures were identified by using spectroscopic methods, including UV, MS, 1D and 2D NMR experiments. This is the first report of these compounds being isolated from a *Pestalotiopsis* species. The cytotoxic activities of the compounds were evaluated, and compounds **1** and **3** demonstrated cytotoxic activities against the HL-60 tumor cell line (IC_{50} < 20 μM).

Keywords: *Pestalotiopsis adusta*; endophytic fungus; abietane diterpenes; cytotoxic activity

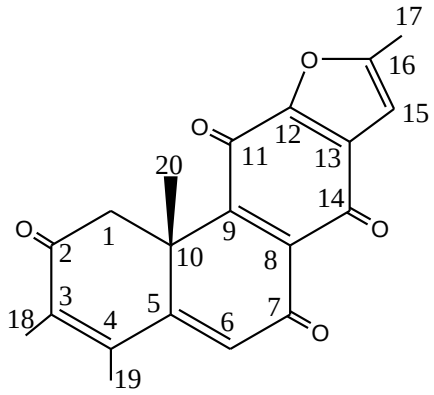


Figure S1 Chemical structure of compound 1

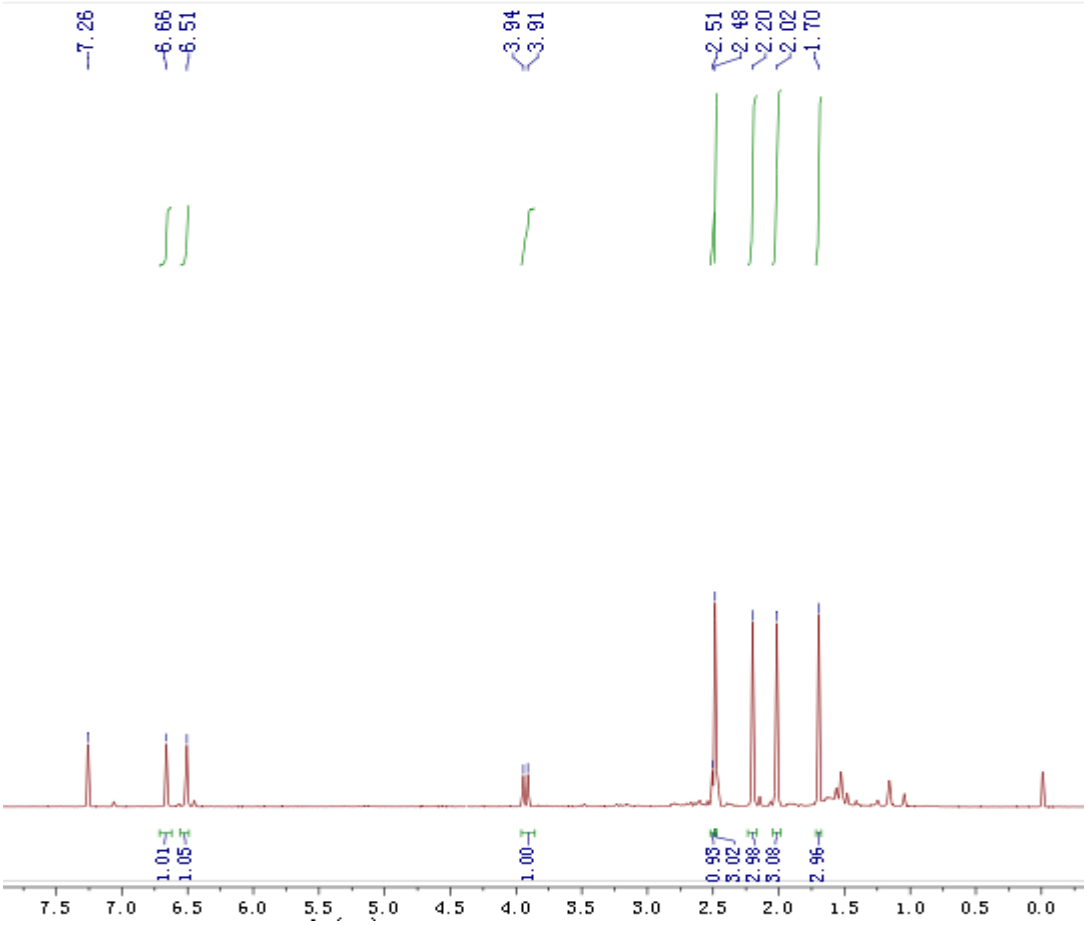


Figure S2. ^{1}H NMR of compound **1**

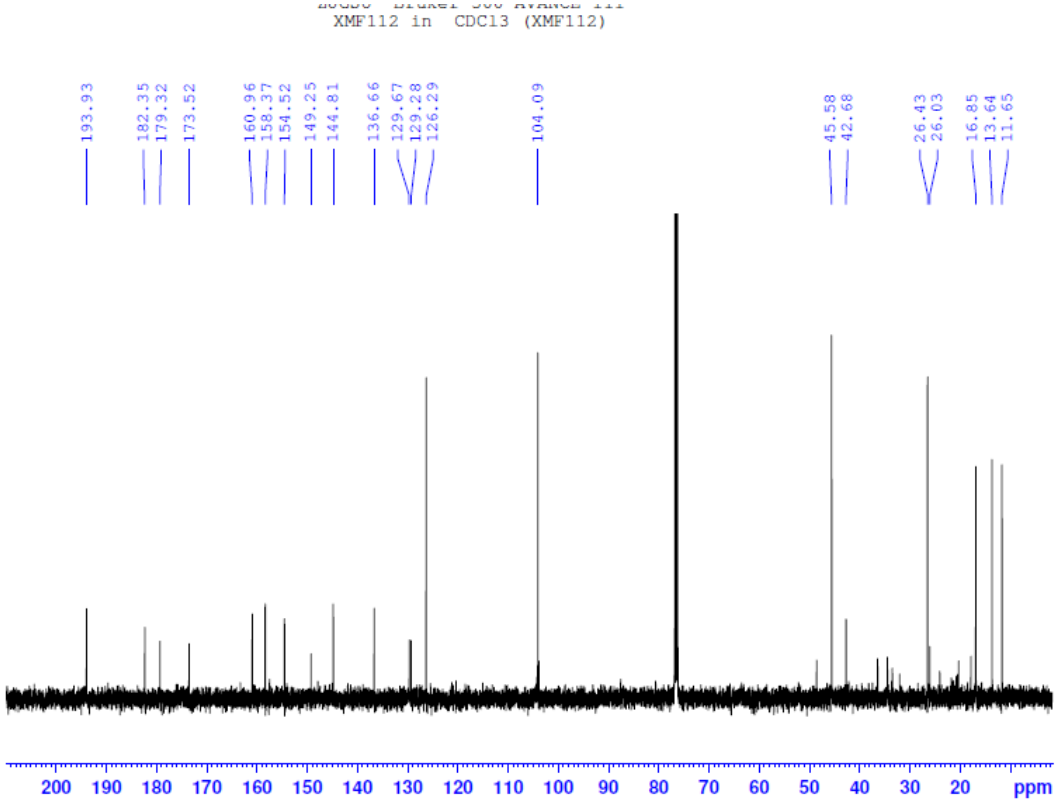


Figure S3. ^{13}C NMR of compound **1**

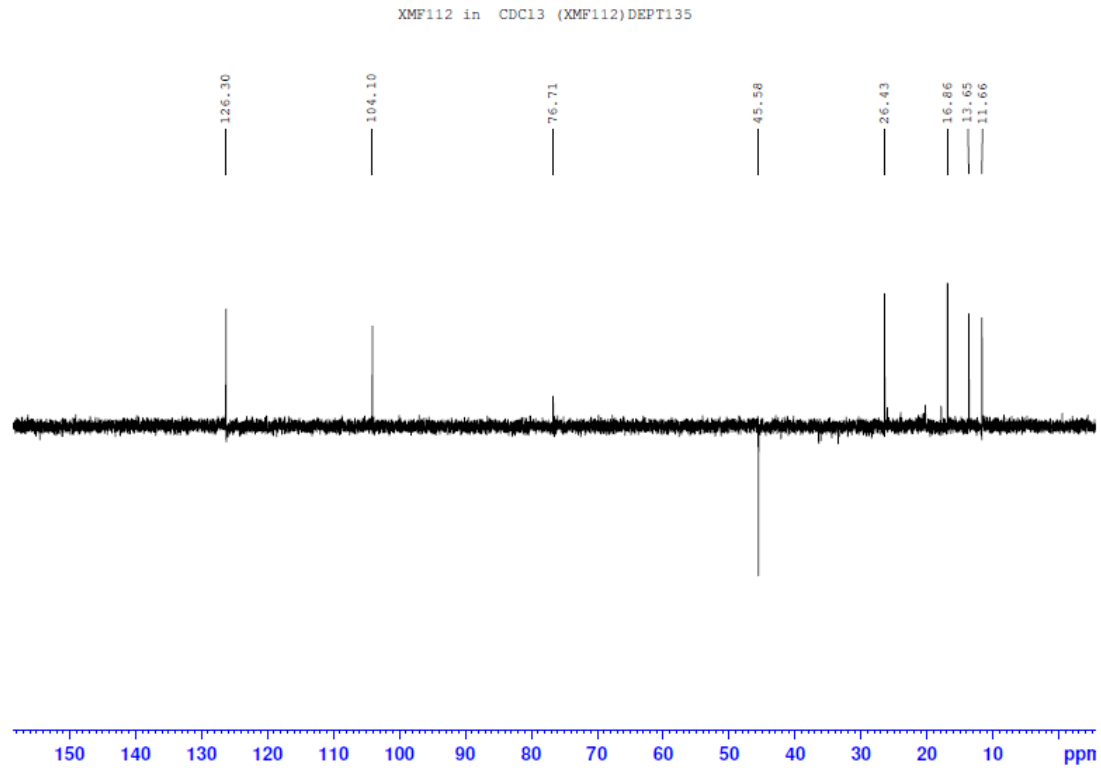


Figure S4. DEPT 135 NMR of compound **1**

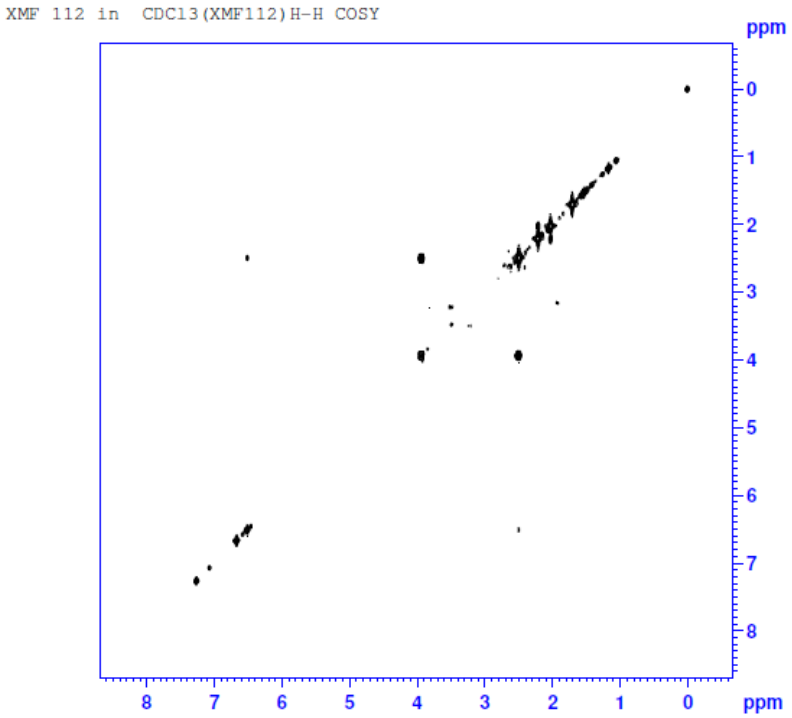


Figure S5. H-H COSY of compound **1**

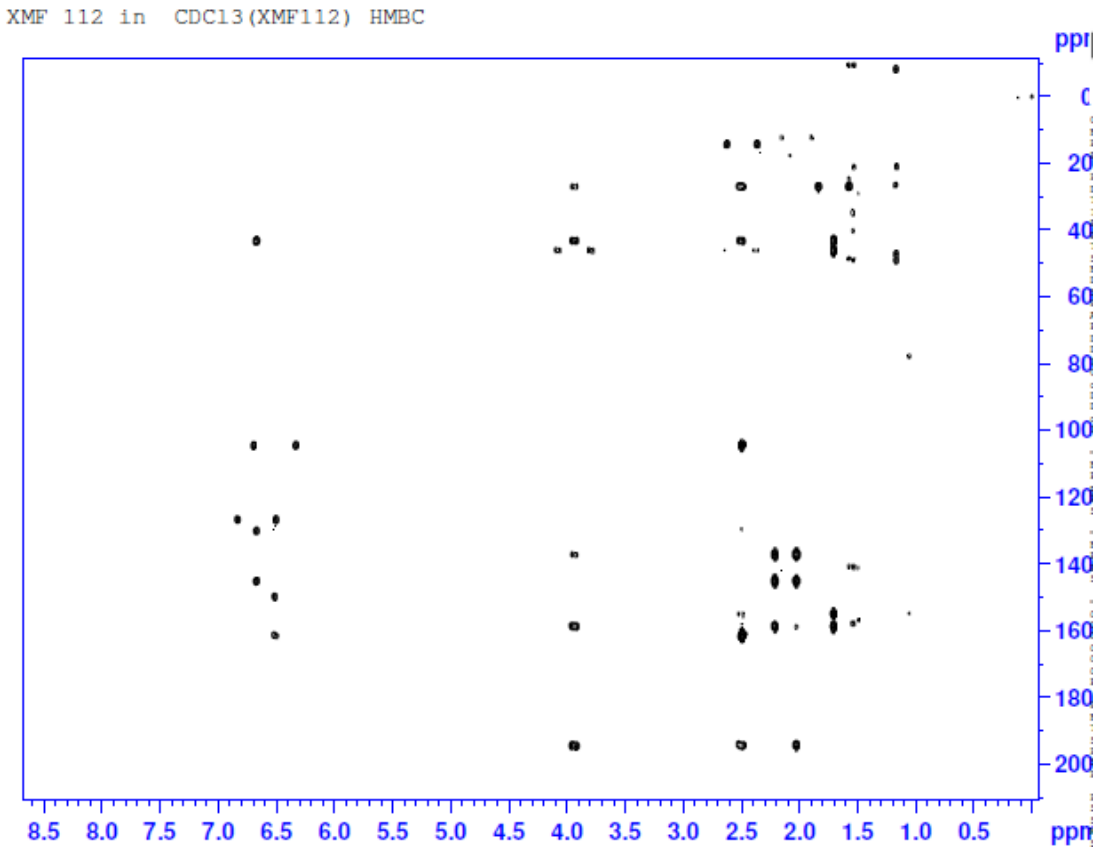


Figure S6. HMBC of compound **1**

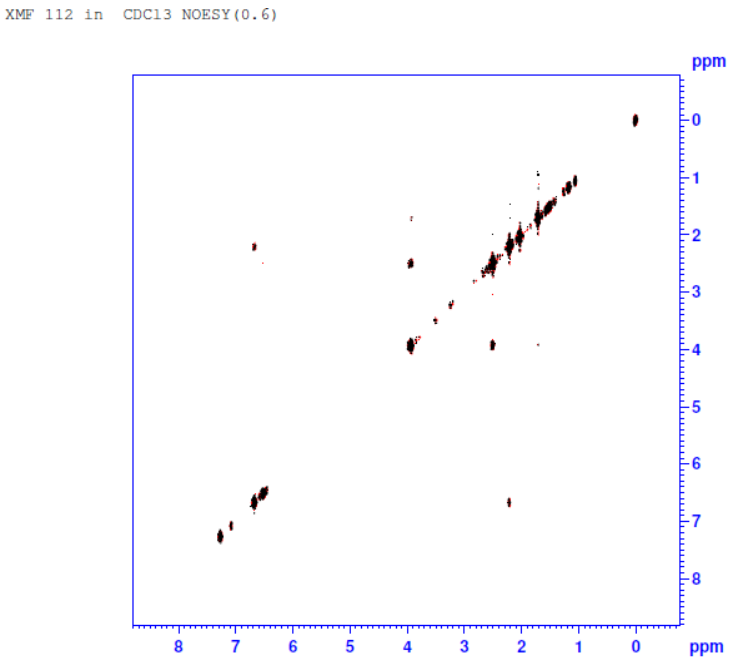
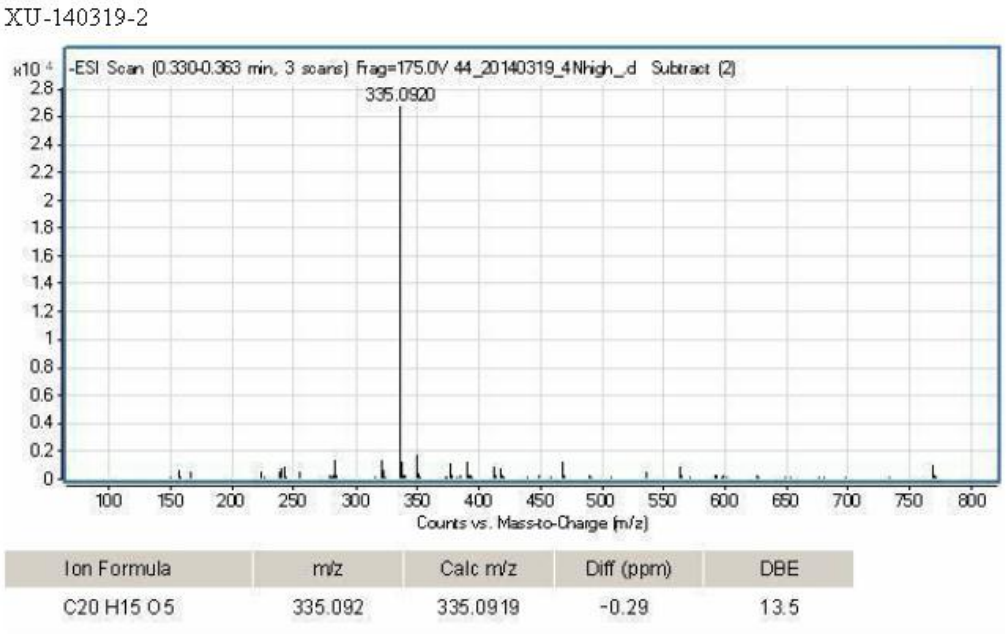


Figure S6. NOESY of compound **1**



Ion Formula	m/z	Calc m/z	Diff (ppm)	DBE
C20 H15 O5	335.092	335.0919	-0.29	13.5

Figure S7. MS of compound **1**

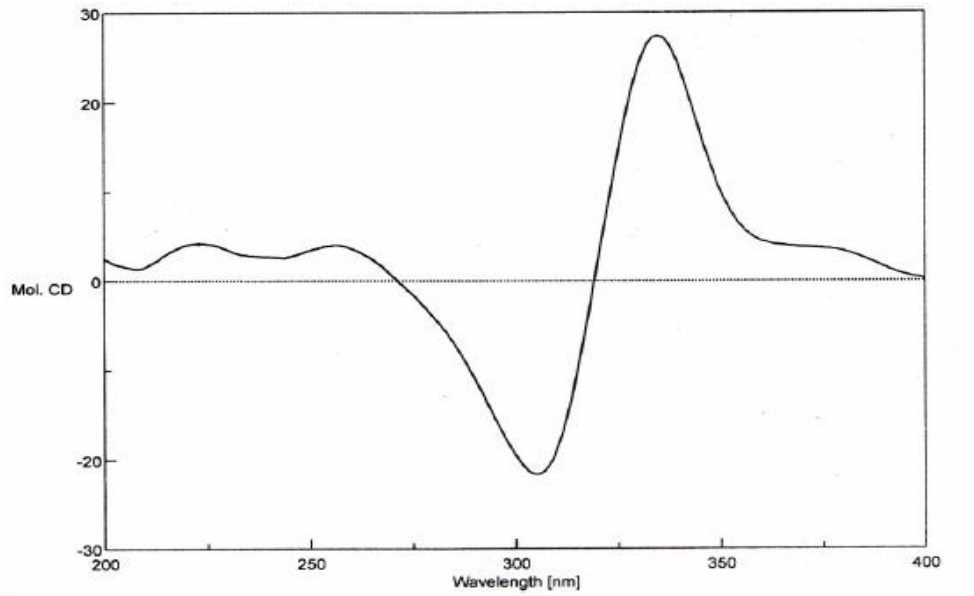


Figure S8. ECD spectrum of compound **1**

Table S1 NMR spectroscopic data in $CDCl_3$.for compound **1**.

H/C	δ_H (*J* in Hz)	δ_C	HMBC
1	2.51, *m*, α; 3.91, *dd* (16.5, 9.3) β	45.5, t	C-2, C-3, C-10, C-20
2	–	193.9, s	–
3	–	136.6, s	–
4	–	144.8, s	–
5	–	158.3, s	–
6	6.66,*s*	126.2, d	C-4, C-8, C-10
7	–	182.3, s	–
8	–	129.6, s	–
9	–	154.5, s	–
10	–	42.6, s	–
11	–	179.3, s	–
12	–	160.9, s	–
13	–	129.2, s	–
14	–	173.5, s	–
15	6.51, *s*	104.0, d	C-12, C-16
16	–	149.2, s	–
17	2.48, *s*	13.6, q	C-15
18	2.02, *s*	11.6, q	C-3, C-4, C-5, C-19
19	2.20, *s*	16.8, q	C-3, C-4, C-5, C-18
20	1.70, *s*	26.4, q	C-1, C-5, C-10

^1H and ^{13}C NMR data were measured at 500 and 125 MHz, respectively. Chemical shifts are given in δ values.

Abbreviations: s, singlet; m, multiplet; dd, doublet of doublets.

teuvincenone F (**2**) ^{13}C-NMR (125 MHz, $CDCl_3$) δ: 46.0 (C-1), 197.4 (C-2), 136.4 (C-3), 146.2 (C-4), 161.3 (C-5), 123.8 (C-6), 190.3 (C-7), 108.9 (C-8), 131.4 (C-9), 42.6 (C-10), 131.4 (C-11), 152.2 (C-12), 117.7 (C-13), 155.4 (C-14), 101.5 (C-15), 148.8 (C-16), 14.9 (C-17), 12.0 (C-18), 17.5 (C-19), 25.4 (C-20).

uncinatone (**3**) ^{13}C-NMR (125 MHz, $CDCl_3$) δ: 29.2 (C-1), 30.2 (C-2), 140.4 (C-3), 125.3 (C-4), 165.2 (C-5), 118.5 (C-6), 190.1 (C-7), 109.3 (C-8), 136.1 (C-9), 39.5 (C-10), 130.8 (C-11), 153.7 (C-12), 110.9 (C-13), 154.2 (C-14), 34.5 (C-15), 83.0 (C-16), 22.1 (C-17), 20.6 (C-18), 14.9 (C-19), 22.0 (C-20).

coleon U (**4**) ^{13}C-NMR (125 MHz, $CDCl_3$) δ: 28.9 (C-1), 18.4 (C-2), 36.0 (C-3), 36.5 (C-4), 141.3 (C-5), 143.2 (C-6), 182.3 (C-7), 104.8 (C-8), 137.4 (C-9), 40.8 (C-10), 132.4 (C-11), 150.3 (C-12), 117.8 (C-13), 156.0 (C-14), 26.2 (C-15), 20.2 (C-16), 20.2 (C-17), 26.6 (C-18), 31.5 (C-19), 27.4 (C-20).

coleon U-12-methyl ether (**5**) ^{13}C-NMR (125 MHz, $CDCl_3$) δ: 29.8 (C-l), 17.5 (C-2), 36.3 (C-3), 36.5 (C-4), 138.4 (C-5), 141.9 (C-6), 183.6 (C-7), 109.1 (C-8), 145.5 (C-9), 41.5 (C-10), 135.7 (C-11), 156.1 (C-12), 125.6 (C-13), 151.2 (C-14), 26.0 (C-15), 20.30 (C-16), 20.30 (C-17), 27.0 (C-18), 27.3 (C-19), 27.9 (C-20), 62.1 (C-21).