

Supporting Information

New *ent*-kaurane diterpenoid acids from *Nouelia insignis* Franch and their anti-inflammatory activity

Zhi-li Wu ^{a,b}, Jia-yu Li ^b, Peng-li Huang ^b, Ze-shi Sun ^b, Hui-liang Li ^{a, b, *}, Wei-dong Zhang ^{a, b, *}

Affiliation

^a School of Traditional Chinese Pharmacy, China Pharmaceutical University, Nanjing, Jiangsu 211198, P.R. China

^b School of Pharmacy, Second Military Medical University, Shanghai 200433, P.R. China

Corresponding authors

Tel.: +86 21 81871245

E-mail addresses: faranli@hotmail.com (H.-L. Li), wdzhangy@hotmail.com (W.-D. Zhang).

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Table S1 ¹³C NMR Spectroscopic Data for compounds 1–11 ^a (δ in ppm).

NO	1	2	3	4	5	6	7	8	9	10	11
1	42.6	35.7	41.2	41.4	49.7	49.9	35.0	33.9	42.0	40.3	34.4
2	20.2	27.1	18.8	20.1	64.7	64.8	27.2	25.9	20.3	18.9	27.0
3	39.1	71.5	37.7	39.0	47.7	47.7	72.0	70.3	39.3	37.8	71.5
4	44.5	48.3	43.0	44.7	45.8	45.9	45.0	47.7	44.7	43.3	48.6
5	57.9	50.3	56.7	57.3	56.9	56.9	49.6	48.3	57.7	56.4	49.3
6	22.2	21.9	20.9	21.4	21.4	21.2	21.1	21.0	23.1	21.4	21.2
7	35.1	35.9	34.4	34.5	35.4	34.9	34.9	38.7	36.0	34.3	35.2
8	45.6	46.6	45.3	53.5	53.9	53.7	54.0	45.6	49.3	45.9	54.5
9	52.3	51.6	51.0	52.3	53.1	53.1	53.2	45.4	47.6	46.0	53.1
10	37.8	37.6	36.5	40.8	42.4	42.7	41.4	38.8	40.4	39.0	41.0
11	82.5	77.8	76.3	29.0	19.4	19.6	19.5	17.5	19.7	18.5	19.5
12	79.8	39.7	38.2	71.9	25.6	33.2	33.4	33.1	27.5	26.2	25.8
13	50.7	43.3	38.3	49.4	36.3	39.4	39.5	40.1	45.0	39.5	33.6
14	37.3	38.9	37.5	37.5	38.2	37.7	37.7	36.1	41.6	40.6	38.0
15	82.3	82.9	77.7	226.2	227.0	212.3	212.8	81.8	90.4	79.9	224.0
16	85.4	85.6	86.8	42.9	49.0	151.2	151.4	157.6	84.1	77.1	57.3
17	21.0	20.7	61.8	11.7	10.3	115.4	115.1	103.7	64.6	69.1	59.9
18	181.6	181.3	180.2	181.3	180.7	181.2	183.0	180.2	181.7	180.3	181.0
19	29.6	25.1	28.2	29.4	29.3	29.5	25.3	23.6	29.5	28.1	24.9
20	18.8	18.2	17.0	16.3	17.2	17.3	16.2	14.8	16.3	14.7	15.8

^a NMR Data were measured at 125 MHz in CD₃OD for **1-11**.

Table S2 ¹H NMR Spectroscopic Data for compounds 1–6^a (δ in ppm, *J* in Hz).

NO	1	2	3	4	5	6
1	1.88, 1.19	1.58	1.85, 1.18	1.86, 0.85	2.17, 0.67, t, (12.0)	2.19, 0.70, t, (12.0)
2	1.85, 1.43, m	2.13, 1.57, m	1.86, 1.42, m	1.91, 1.42, m	4.08, m	4.09, m
3	2.16, 1.05, m	3.99, overlap	2.16, 1.04, m	2.13, 1.04, m	2.41, 0.96, t, (12.2)	2.41, 0.97, t, (12.3)
5	1.05, m	1.47, m	1.06, m	1.17, m	1.11, m	1.11, m
6	1.84, 1.70, m	1.76, m	1.85, 1.75, m	1.90, 1.78, m	1.93, 1.81, m	1.95, m
7	1.54, 1.25, m	1.78, 1.21, m	1.56, 1.22, m	1.74, 1.39, m	1.67, 1.36, m	1.82, 1.34, m
9	1.72	1.68	1.70	1.16	1.06	1.19
11	4.09, overlap	4.28, overlap	4.33, overlap	1.93, m	1.71, 1.23, m	1.77, 1.47, m
12	4.14, overlap	2.00, d, (11.4), 1.82,	2.00, d, (11.2), 1.80	4.09, m	1.69, m	1.89, 1.69, m
13	2.14	2.19	2.45	2.41, m	2.44, m	3.07, m
14	1.95, d, (12.7), 1.19	1.95, d, (12.3), 1.14	1.97, d, (12.3), 1.11	2.33, d, (12.5), 1.48	2.45, 1.43	2.43, 1.40
15	2.82, s	2.87, s	3.06, s			
16				2.59	2.30	
17	1.34, s	1.27, s	3.59 dd, (11.5, 5.8)	1.25, d, (7.2)	1.09, d, (7.2)	5.89, 5.32, s
19	1.19, s	1.24, s	1.19, s	1.21, s	1.27, s	1.27, s
20	0.99, s	1.01, s	1.02, s	0.98, s	1.04, s	1.06, s

^a NMR Data were measured at 500 MHz in CD₃OD for **1-6**.

Table S3 ¹H NMR Spectroscopic Data for compounds 7–11 ^a (δ in ppm, *J* in Hz).

NO	7	8	9	10	11
1	1.54, 1.24	1.63, 1.32	1.90, 0.89	1.92, 0.89	1.55, 1.23
2	2.24, 1.53, m	2.19, 1.55, m	1.91, 1.40, m	1.91, 1.40, m	2.18, 1.54, m
3	4.00	3.98	2.12, 1.02, m	2.12, 1.01, m	3.97, overlap
5	1.54, m	1.48, m	1.05, m	1.04, m	1.57, m
6	1.92, 1.80, m	1.86, 1.73, m	1.83, m	1.82, 1.60, m	1.86, 1.76, m
7	1.82, 1.31, m	1.65, 1.29, m	1.91, 1.45, m	1.94, 0.88, m	1.72, 1.34, m
9	1.22	1.44	1.40	1.40	1.14
11	1.72, 1.43, m	1.63, 1.49, m	1.61, 1.53, m	1.69, 1.47, m	1.69, 1.21, m
12	1.89, 1.67, m	1.63, 1.45, m	1.63, 1.47, m	1.76, 1.40, m	1.75, m
13	3.06, m	2.59, m	1.92, m	1.96, m	2.65, m
14	2.46, d, (12.1), 1.38	2.00, d, (11.9), 1.01	1.58, 1.42	1.60, 1.33	2.50, d, (12.2), 1.42
15		3.68	3.42, s	3.06, s	
16					2.50
17	5.88, 5.30, s	5.04, s, 4.91, overlap	3.75 dd, (11.9, 10.2)	3.42, d, (11.2), 3.27 d, (11.3)	3.94, dd, (11.3, 6.6), 3.59, dd, (9.2, 2.1)
19	1.24, s	1.23, s	1.18, s	1.18, s	1.24, s
20	1.08, s	0.99, s	0.99, s	0.97, s	1.05, s

^a NMR Data were measured at 500 MHz in CD₃OD for **7-11**.

Materials and methods

1. General experimental procedures

Column chromatography (CC): silica gel H (10-40 μm) and silica gel (200-300 mesh) (Marine Chemical Factory, Qingdao, P. R. China); MCI gel CHP-20P: (Daiso, Co., Japan) and RP-C₁₈ gel (40–63 μm ; Daiso, Co., Japan) were used for column chromatography; Sephadex LH-20 (Pharmacia Fine Chemicals, Piscataway, NJ, USA). TLC: silica gel plates, visualization by spraying with 10 % H₂SO₄ in EtOH and dragendorff's reagent. Semi-preparative HPLC: Agilent 1260 series (Agilent Technologies, US) with a Zorbax SB-C₁₈ (5 μM , 9.4 mm \times 25 cm) column. NMR Spectra: Bruker Avance III-500 spectrometer (Bruker, Switzerland). MS: Agilent MSD-Trap-XCT (for ESI) and Agilent-6520 Q-TOF mass spectrometer (for HR-ESI). IR: Thermo Scientific Nicolet 6700 (Thermo Scientific, US). UV spectra: Agilent 1260 series DAD detector (Agilent Technologies, US). CD spectrum: Brighttime Chirascan (Applied Photophysics Ltd, UK). Optical rotation: Rudolph Autopo V (Rudolph Research Analytical, Hackettstown, NJ).

2. Plant material

Nouelia insignis Franch were collected from Sichun province of China in August 2020, and identified by Prof. Bao-kang Huang (Department of pharmacognosy, Second Military Medical University, Shanghai, China). A voucher specimen (No. 202008-VS) is deposited in the department of pharmacognosy, Second Military Medical University.

3 Extraction and isolation

The dried and crushed branch of *Nouelia insignis* Franch (20.0 kg) were

ultrasonically extracted with 95% methanol overnight at room temperature (20 L × 3). After remove of solvent, the methanol extract (550.5 g) was extracted with water, petroleum ether (PE) and ethyl acetate (EtOAc) (3 times with 5 L each). The PE extract (124.3 g) was segmented by Silica gel H (10-40 μm) column chromatography eluting with petroleum ether- ethyl acetate (PE / EtOAc, 50:1 to 0:1 v/v) to afford 7 fractions (Fr. 1-7). Fraction 4 (21.6 g) was separated by MCI column chromatography (MeOH/H₂O, 10:90 to 100:0 v/v) to provide 5 subfractions (Fr. 4.1-4.5). Then, fraction 4.3 was separated by ODS (CH₃CN /H₂O, 10:90 to 40:60 v/v) to afford 6 subfractions (Fr. 4.3.1- 4.3.6). Fr. 4.3.2 and Fr. 4.3.4 were purified by semi-preparative RP-C₁₈ HPLC (CH₃OH/H₂O, 63:37 v/v 1.0 mL/min) to give compounds **4** (12.3 mg), **5** (10.2 mg), **13** (9.4 mg), **14** (13.6 mg) and **8** (9.5 mg), **18** (10.6 mg), **19** (9.2 mg), **21** (8.2 mg). Fraction 4.5 was also separated by ODS (CH₃OH /H₂O, 10:90 to 40:60 v/v) to afford compounds **22** (15.2 mg), **23** (9.4 mg). Fraction 5 was initially separated by Sephadex LH-20 CC eluting with CH₃OH/H₂O (55:45) to yield 5 subfractions (Fr. 5.1-5.5). Compounds **1** (14.3 mg) and **2** (10.3 mg) were obtained from Fr. 5.2 by ODS column chromatography (CH₃OH /H₂O, 30:70 to 55:45 v/v). Fr. 5.3-5.4 were purified by ODS column chromatography (CH₃OH /H₂O, 30:70 to 80:20 v/v) and further purified by semi-preparative RP-C₁₈ HPLC (CH₃OH /H₂O, 65:35 v/v 1.0 mL/min) to afford compounds **3** (13.3 mg), **12** (9.8 mg) and **9** (8.3 mg), **10** (11.8 mg), **24** (14.1 mg), **25** (9.7 mg). Fraction 6 was separated on a Sephadex LH-20 CC eluted with MeOH/H₂O (60:40, v/v) to yield 7 sufractions (Fr. 6.1-6.7), Compound **11** (8.3 mg) was obtained from Fr. 6.1 through the ODS column chromatography (CH₃OH /H₂O, 30:70 to 55:45 v/v). Meanwhile,

Purifications of Fr. 6.3 and 6.4 by RP-HPLC (CH₃OH/H₂O, 60:40 v/v 1.0 mL/min) yielded compounds **6** (9.8 mg), **7** (13.1 mg) and **17** (9.1 mg). Fr. 6.5 was separated with ODS column chromatography (CH₃OH /H₂O, 10:90 to 50:50 v/v) and further purified by semi-preparative RP-C₁₈ HPLC (CH₃OH/H₂O, 60:34 v/v 1.0 mL/min) to get compounds **15** (8.8 mg), **16** (12.7 mg) and **26** (13.3 mg). Fraction 7 was separated with ODS column chromatography (CH₃OH /H₂O, 10:90 to 40:60 v/v) and semi-preparative RP-C₁₈ HPLC (CH₃CN/H₂O, 62:38 v/v 1.0 mL/min) to give compounds **20** (9.3 mg) and **27** (8.6 mg). Above all, the whole compounds were obtained (Fig. 1).

Compound characterizations of 1–11

Noeinsiancin A (1)

Colorless needle crystals; $[\alpha]_{25}^D -71.4$ (c 0.06, CH₃OH); IR (KBr) ν_{\max} 3592, 3411, 2974, 2913, 2854, 1677, 1470, 1453, 1197, 1094, 1023, 982, 797, cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S2 and S1; positive HRESIMS m/z 373.1962 ([M+Na]⁺, calcd for C₂₀H₃₀O₅Na, 373.1985). Crystal data for **1**, size 0.20 × 0.14 × 0.09 mm³, orthorhombic, space group P 21 21 21, $a = 7.4300$ (3) Å, $b = 12.6486$ (5) Å, $c = 21.6486$ (13) Å, $V = 1952.27$ (13) Å³, $T = 293.0$ K, $Z = 4$, $D = 1.315$ Mg/m³, λ (CuK α) = 1.54178 Å, $F(000) = 840$, reflections collected/unique 15527/3520 [R (int) = 0.0500], h (−8/8), k (−14/14), l (−26/24), Final R indices $R1 = 0.0389$ and $wR2 = 0.1043$ ($I > 2\sigma(I)$), $R1 = 0.0404$ and $wR2 = 0.1057$ (all data), GOF = 1.093, largest diff. peak/hole, 0.387/−0.236 eÅ⁻³. Absolute structure parameter: 0.04(8). CCDC: 2127069.

Noeinsiancin B (2)

Colorless needle crystals; $[\alpha]_{25}^D -44.8$ (c 0.07, CH₃OH); IR (KBr) ν_{\max} 3593, 3413, 2975, 2911, 1677, 1471, 1445, 1265, 1180, 1394, 1093, 1023, 935, 797 cm⁻¹; ¹H- and

¹³C-NMR data (500 MHz/125 MHz), see Tables S2 and S1; positive HRESIMS *m/z* 373.1963 ([M+Na]⁺, calcd for C₂₀H₃₀O₅Na, 373.1985). Crystal data for **2**, size 0.19 × 0.15 × 0.12 mm³, orthorhombic, space group P21, *a* = 6.6713 (2) Å, *b* = 19.5694 (7) Å, *c* = 7.1999 (2) Å, *V* = 939.04 (5) Å³, *T* = 293.0 K, *Z* = 2, *D* = 1.303 Mg/m³, λ (CuKα) = 1.54178 Å, *F*(000) = 400, reflections collected/unique 11475/3259 [*R* (int) = 0.0428], *h* (−8/8), *k* (−23/23), *l* (−8/8), Final *R* indices *R*1 = 0.0492 and *wR*2 = 0.1288 (*I* > 2σ(*I*)), *R*1 = 0.0503 and *wR*2 = 0.1304 (all data), GOF = 1.040, largest diff. peak/hole, 0.459/−0.227 eÅ^{−3}. Absolute structure parameter 0.02(9), CCDC: 2127070.

Noeinsiancin C (3)

White powder; [α]_D²⁵ −80.3 (*c* 0.065, CH₃OH); IR (KBr) *v*_{max} 3412, 2960, 2916, 2870, 1732, 1690, 1602, 1466, 1447, 1252, 1196, 1088, 1013, 996, 789 cm^{−1}; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S2 and S1; positive HRESIMS *m/z* 373.1960 ([M+Na]⁺, calcd for C₂₀H₃₀O₅Na, 373.1985).

Noeinsiancin D (4)

Colorless needle crystals; [α]_D²⁵ −108.3 (*c* 0.06, CH₃OH); IR (KBr) *v*_{max} 3199, 2945, 2872, 1738, 1708, 1466, 1449, 1245, 1172, 1047, 976, 795, cm^{−1}; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S2 and S1; positive HRESIMS *m/z* 357.2023 ([M+Na]⁺, calcd for C₂₀H₃₀O₄Na, 357.2036). Crystal data for **4**: size 0.200 × 0.150 × 0.130 mm³, orthorhombic, space group P 21, *a* = 11.7128 (3) Å, *b* = 7.9902 (2) Å, *c* = 11.8269 (3) Å, *V* = 1001.54 (4) Å³, *T* = 293 K, *Z* = 2, *D* = 1.215 Mg/m³, λ (CuKα) = 1.541789 Å, *F*(000) = 400, reflections collected/unique 123977/3447 [*R* (int) = 0.0331], *h* (−13/13), *k* (−8/9), *l* (−13/14), Final *R* indices *R*1 = 0.0302 and *wR*2 = 0.0800 (*I* > 2σ(*I*)), *R*1 = 0.0310 and *wR*2 = 0.0911 (all data), GOF = 1.047, largest diff. peak/hole, 0.124/−0.094 eÅ^{−3}. Absolute structure parameter 0.09(6), CCDC: 2090338.

Noeinsiancin E (5)

Colorless needle crystals; $[\alpha]_{25}^D$ -140.2 (c 0.10, CH₃OH); IR (KBr) ν_{\max} 3370, 2964, 2869, 1714, 1448, 1366, 1288, 1169, 1018, 976, 755, cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S2 and S1; positive HRESIMS m/z 357.2023 ([M+Na]⁺, calcd for C₂₀H₃₀O₄Na, 357.2036). Crystal data for **5**: size 0.200 × 0.160 × 0.130 mm³, orthorhombic, space group P 1, $a = 6.4700$ (4) Å, $b = 7.6635$ (5) Å, $c = 9.8461$ (6) Å, $V = 447.19$ (5) Å³, $T = 293$ K, $Z = 1$, $D = 1.242$ Mg/m³, λ (CuK α) = 1.541789 Å, $F(000) = 182$, reflections collected/unique 13755/2977 [R (int) = 0.0359], h (-7/7), k (-9/9), l (-11/11), Final R indices $R1 = 0.0304$ and $wR2 = 0.0799$ ($I > 2\sigma(I)$), $R1 = 0.0305$ and $wR2 = 0.0800$ (all data), GOF = 1.069, largest diff. peak/hole, 0.138/-0.097 eÅ⁻³. Absolute structure parameter 0.07(4), *CCDC*: 2090337.

Noeinsiancin F (6)

Colorless needle crystals; $[\alpha]_{25}^D$ -116.7 (c 0.05, CH₃OH); IR (KBr) ν_{\max} 3426, 2931, 1723, 1467, 1447, 1373, 1270, 1168, 1065, 977, 787 cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S2 and S1; positive HRESIMS m/z 355.1861 ([M+Na]⁺, calcd for C₂₀H₂₈O₄Na, 355.1880). Crystal data for **6**: size 0.15 × 0.07 × 0.05 mm³, orthorhombic, space group P 1.21.1, $a = 6.4502$ (3) Å, $b = 14.2302$ (6) Å, $c = 9.9729$ (4) Å, $V = 905.16$ (7) Å³, $T = 293$ K, $Z = 2$, $D = 1.220$ Mg/m³, λ (CuK α) = 1.34139 Å, $F(000) = 360$, reflections collected/unique 11155/3409 [R (int) = 0.0564], h (-7/7), k (-17/17), l (-12/12), Final R indices $R1 = 0.0407$ and $wR2 = 0.1083$ ($I > 2\sigma(I)$), $R1 = 0.0431$ and $wR2 = 0.1090$ (all data), GOF = 1.080, largest diff. peak/hole, 0.138/-0.097 eÅ⁻³. Absolute structure parameter 0.01(11), *CCDC*: 2156441.

Noeinsiancin G (7)

White powder; $[\alpha]_{25}^D$ -139.3 (c 0.15, CH₃OH); IR (KBr) ν_{\max} 3245, 2934, 2874,

1770, 1470, 1447, 1372, 1271, 1172, 1065, 976, 789 cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S3 and S1; positive HRESIMS 355.1860 ([M+Na]⁺, calcd for C₂₀H₂₈O₄Na, 355.1880)

Noeinsiancin H (8)

Colorless needle crystals; [α]_D²⁵ -85.8 (c 0.06, CH₃OH); IR (KBr) ν_{\max} 3253, 2926, 2857, 1700, 1596, 1447, 1394, 1297, 1167, 1079, 976, 758 cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S3 and S1; positive HRESIMS m/z 357.2023 ([M+Na]⁺, calcd for C₂₀H₃₀O₄Na, 357.2036). Crystal data for **8**: size 0.05 × 0.105 × 0.01 mm³, orthorhombic, space group P2₁2₁2₁, $a = 7.4299$ (10) Å, $b = 10.3592$ (2) Å, $c = 23.4977$ (3) Å, $V = 1808.57$ (5) Å³, $T = 173$ K, $Z = 4$, $D = 1.294$ Mg/m³, λ (CuK α) = 1.34139 Å, $F(000) = 768$, reflections collected/unique 129313420 [R (int) = 0.0399], h (-8/9), k (-12/12), l (-24/28), Final R indices $R1 = 0.0576$ and $wR2 = 0.0799$ ($I > 2\sigma(I)$), $R1 = 0.0305$ and $wR2 = 0.0800$ (all data), GOF = 1.069, largest diff. peak/hole, 0.138/-0.097 eÅ⁻³. Absolute structure parameter 0.07(4), CCDC: 2090340.

Noeinsiancin I (9)

Colorless needle crystals; [α]_D²⁵ -91.3 (c 0.05, CH₃OH); IR (KBr) ν_{\max} 3421, 2941, 1695, 1467, 1444, 1370, 1284, 1160, 1066, 990, 793 cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S3 and S1; positive HRESIMS m/z 375.2123 ([M+Na]⁺, calcd for C₂₀H₃₂O₅Na, 375.2142). Crystal data for **9**: size 0.20 × 0.14 × 0.10 mm³, orthorhombic, space group P 2₁, $a = 8.4122$ (2) Å, $b = 19.7326$ (6) Å, $c = 11.0321$ (3) Å, $V = 1829.87$ (9) Å³, $T = 293$ K, $Z = 4$, $D = 1.279$ Mg/m³, λ (CuK α) = 1.54178 Å, $F(000) = 768$, reflections collected/unique 21478/6401 [R (int) = 0.0438], h (-10/10), k (-23/23), l (-12/13), Final R indices $R1 = 0.0322$ and $wR2 = 0.0841$ ($I > 2\sigma(I)$), $R1 = 0.0327$ and $wR2 = 0.0846$ (all data), GOF = 1.052, largest diff. peak/hole, 0.151/-0.138 eÅ⁻³.

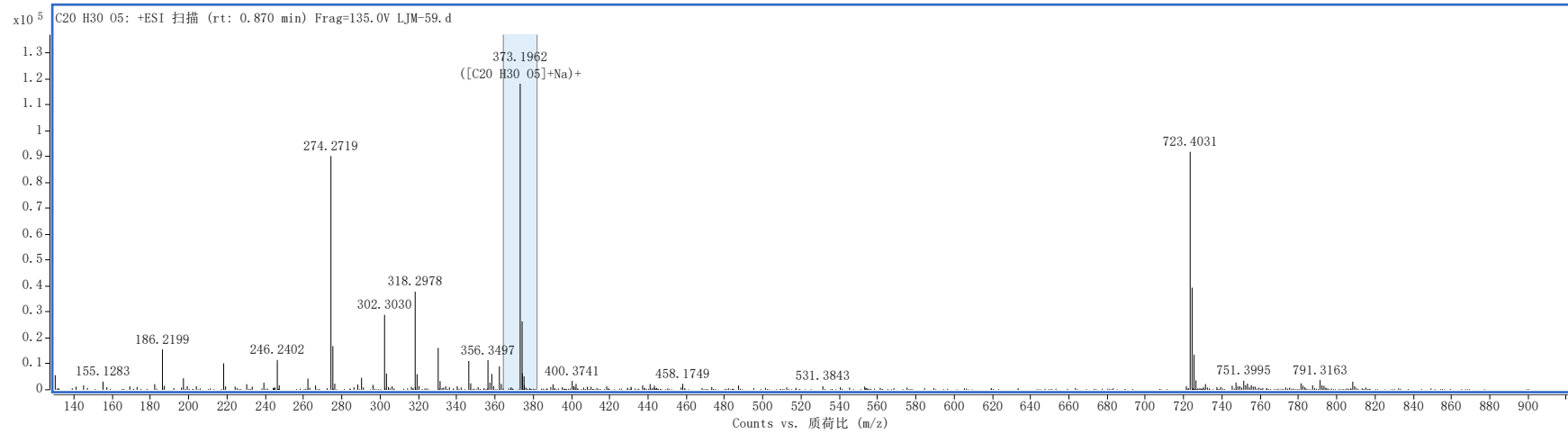
Absolute structure parameter -0.02(5), *CCDC: 2127071*.

Noeinsiancin J (10)

White powder; $[\alpha]_{25}^D$ -87.0 (c 0.10, CH₃OH); IR (KBr) ν_{\max} 3366, 2937, 2898, 1696, 1470, 1408, 1384, 1325, 1264, 1180, 1051, 996, 798 cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S3 and S1; positive HRESIMS m/z 375.2121 ([M+Na]⁺, calcd for C₂₀H₃₂O₅Na, 375.2142).

Noeinsiancin K (11)

White powder; $[\alpha]_{25}^D$ -96.0 (c 0.05, CH₃OH); IR (KBr) ν_{\max} 3483, 2950, 2869, 1721, 1683, 1469, 1402, 1368, 1230, 1160, 1038, 977, 803 cm⁻¹; ¹H- and ¹³C-NMR data (500 MHz/125 MHz), see Tables S3 and S1; positive HRESIMS m/z 373.1966 ([M+Na]⁺, calcd for C₂₀H₃₀O₅Na, 373.1985).



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H30 O5	(M+Na)+	373.1962	80.62	7.45	80.62

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分比(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分比	峰高总百分比	m/z	Diff (ppm)
79.7	119354.7	100	373.1985	2.3	118255.6	100	78.9	373.1962	6.24

Figure S1. HRESIMS spectrum of Noueinsiancin A (1)

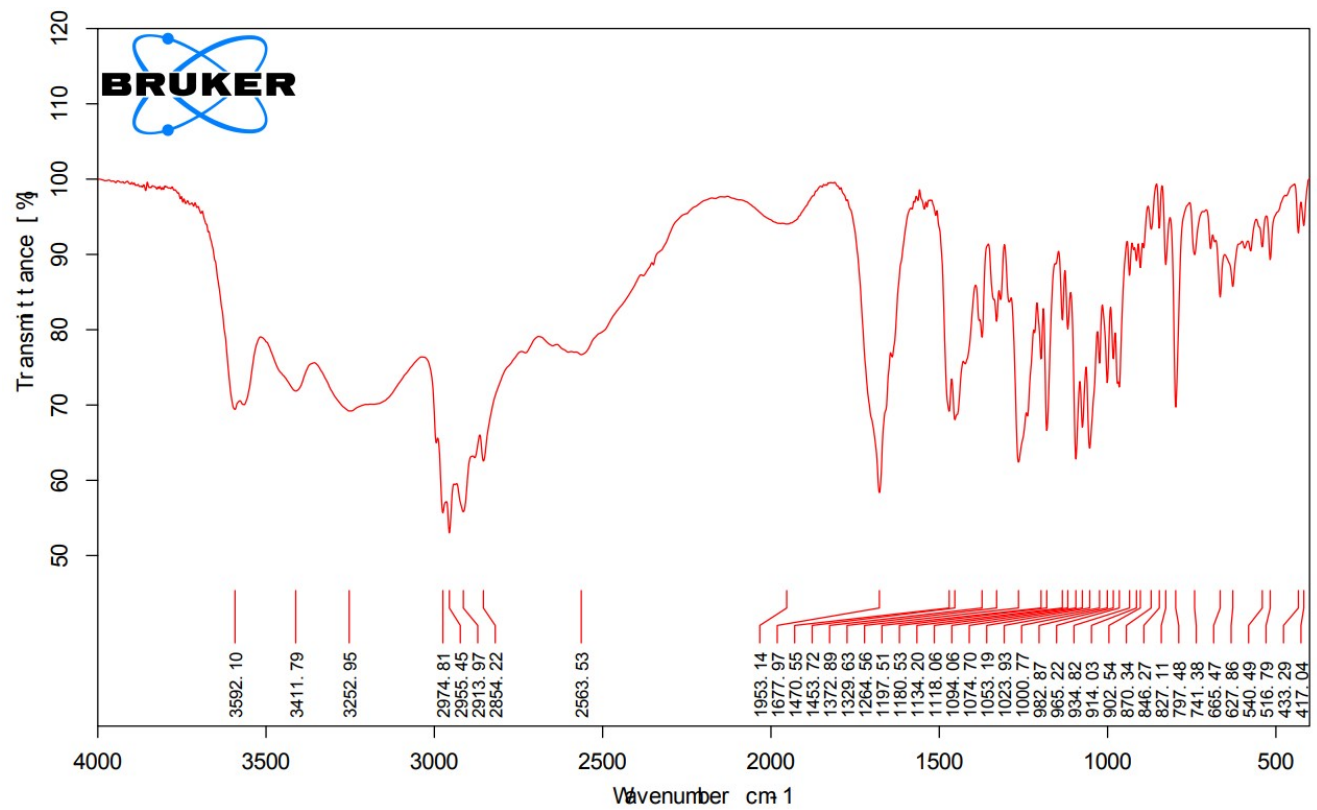


Figure S2. IR spectrum of Noueinsiancin A (1)

Rudolph Research Analytical

Wednesday, 02/09/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-59
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-71.389	0.6213	-70.000	-71.667

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-59	04:28:05 PM	-71.667	SR	-0.043	589	100.00	0.060	19.7	
2	LJM-59	04:28:11 PM	-71.667	SR	-0.043	589	100.00	0.060	19.7	
3	LJM-59	04:28:17 PM	-71.667	SR	-0.043	589	100.00	0.060	19.7	
4	LJM-59	04:28:22 PM	-71.667	SR	-0.043	589	100.00	0.060	19.7	
5	LJM-59	04:28:28 PM	-70.000	SR	-0.042	589	100.00	0.060	19.8	
6	LJM-59	04:28:34 PM	-71.667	SR	-0.043	589	100.00	0.060	19.8	

Signature

Figure S3. OR Value of Noueinsiancin A (1) in CH₃OH

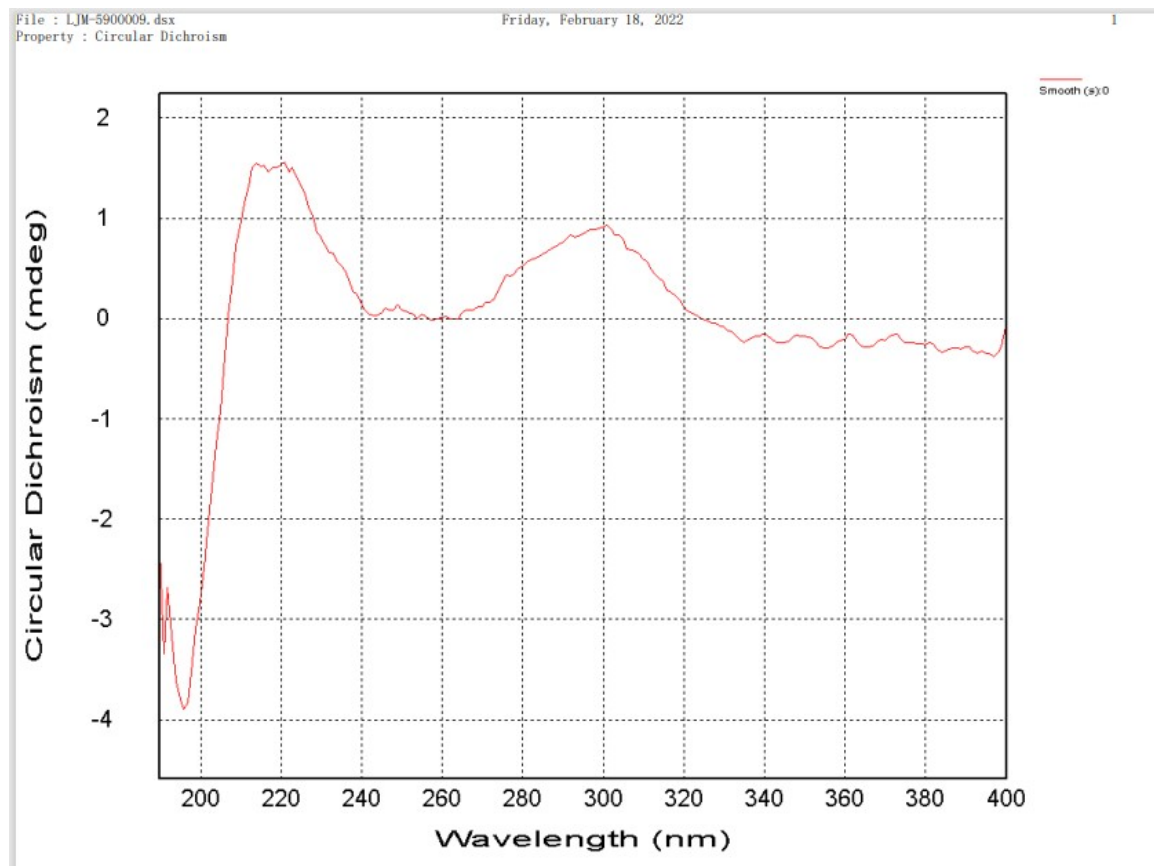


Figure S4. CD Value of Noueinsiancin A (1) in CH₃OH

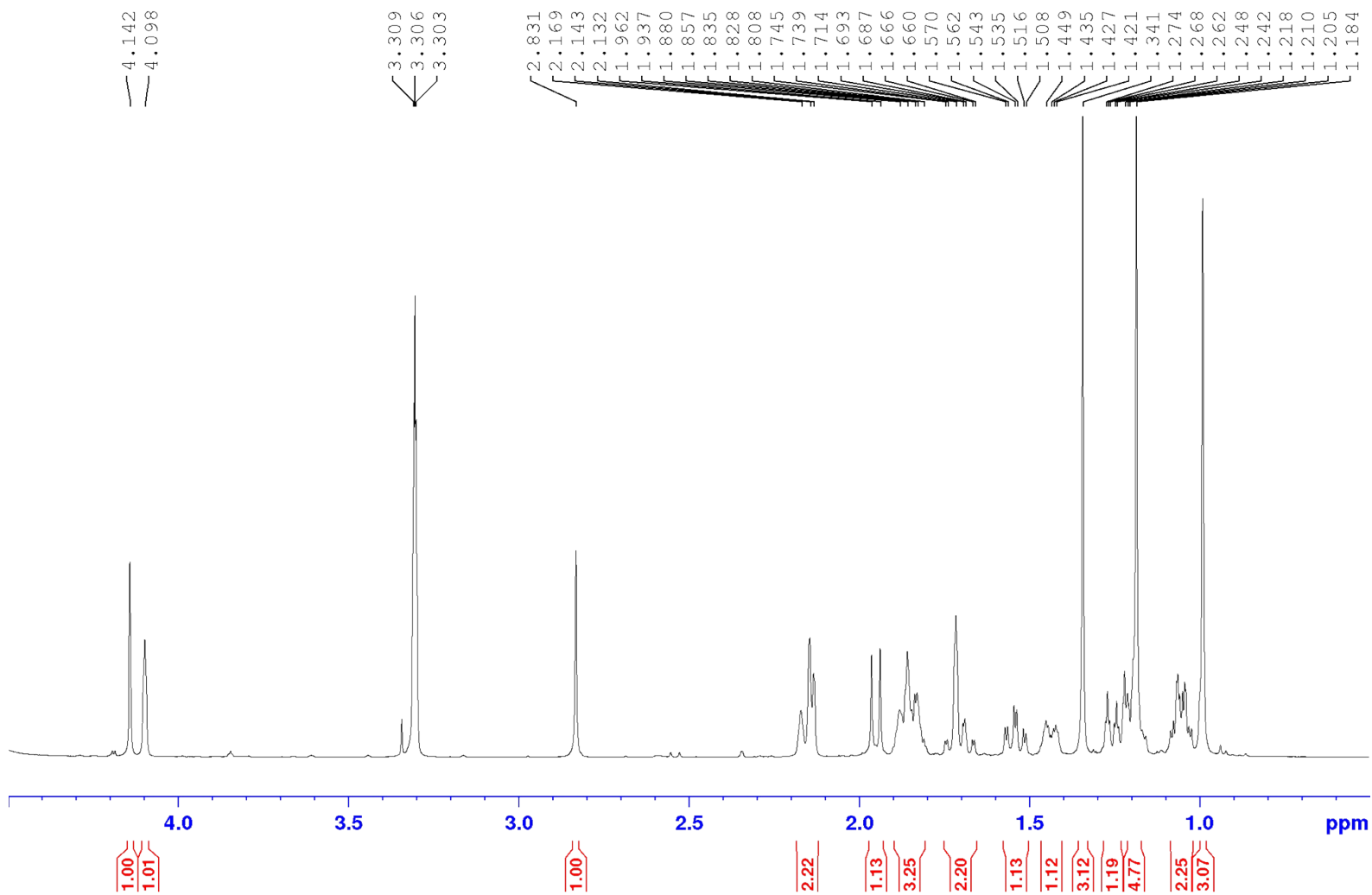


Figure S5. ¹H NMR spectrum of Noueinsiancins A (1) in CD₃OD

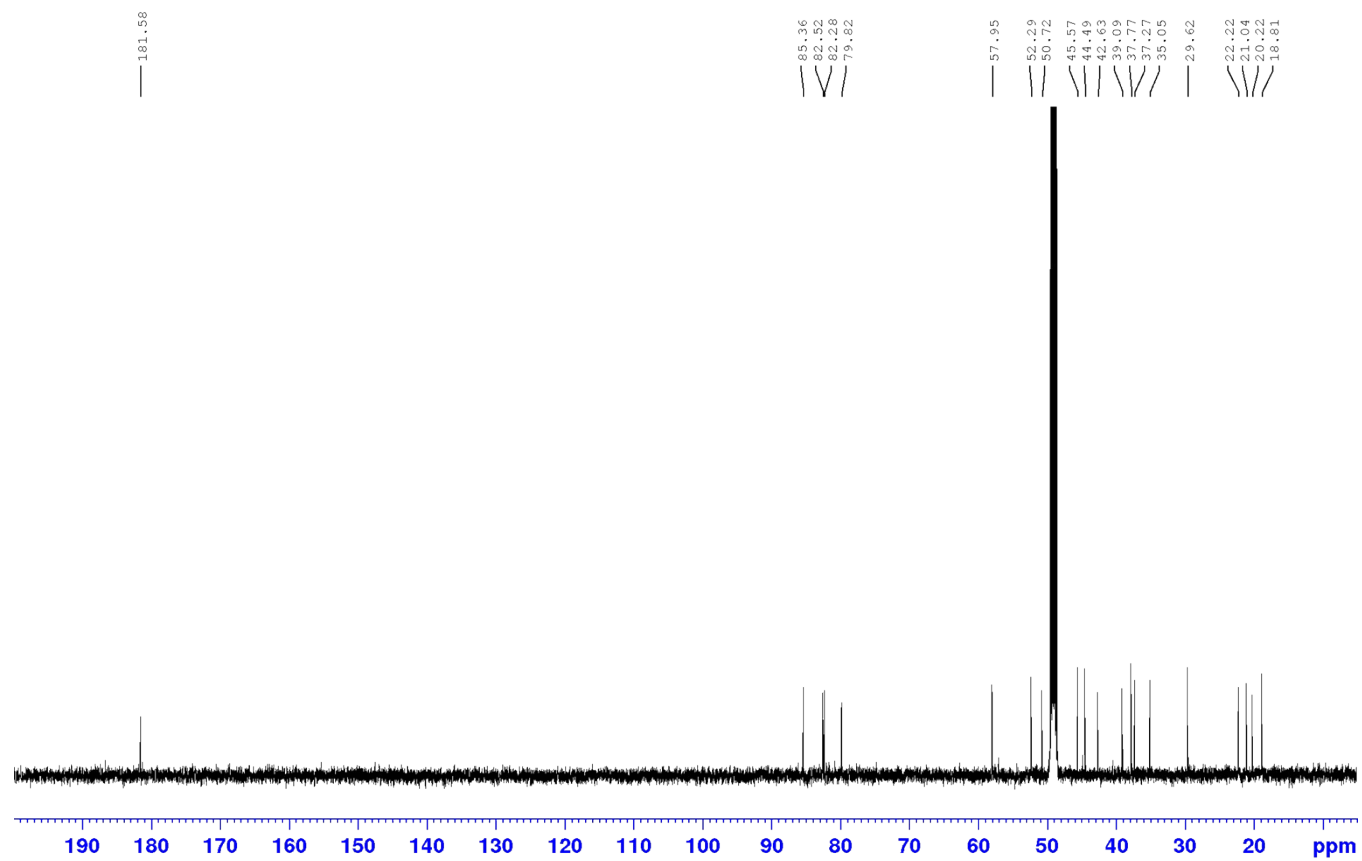


Figure S6. ^{13}C NMR spectrum of Noueinsiancin A (1) in CD_3OD

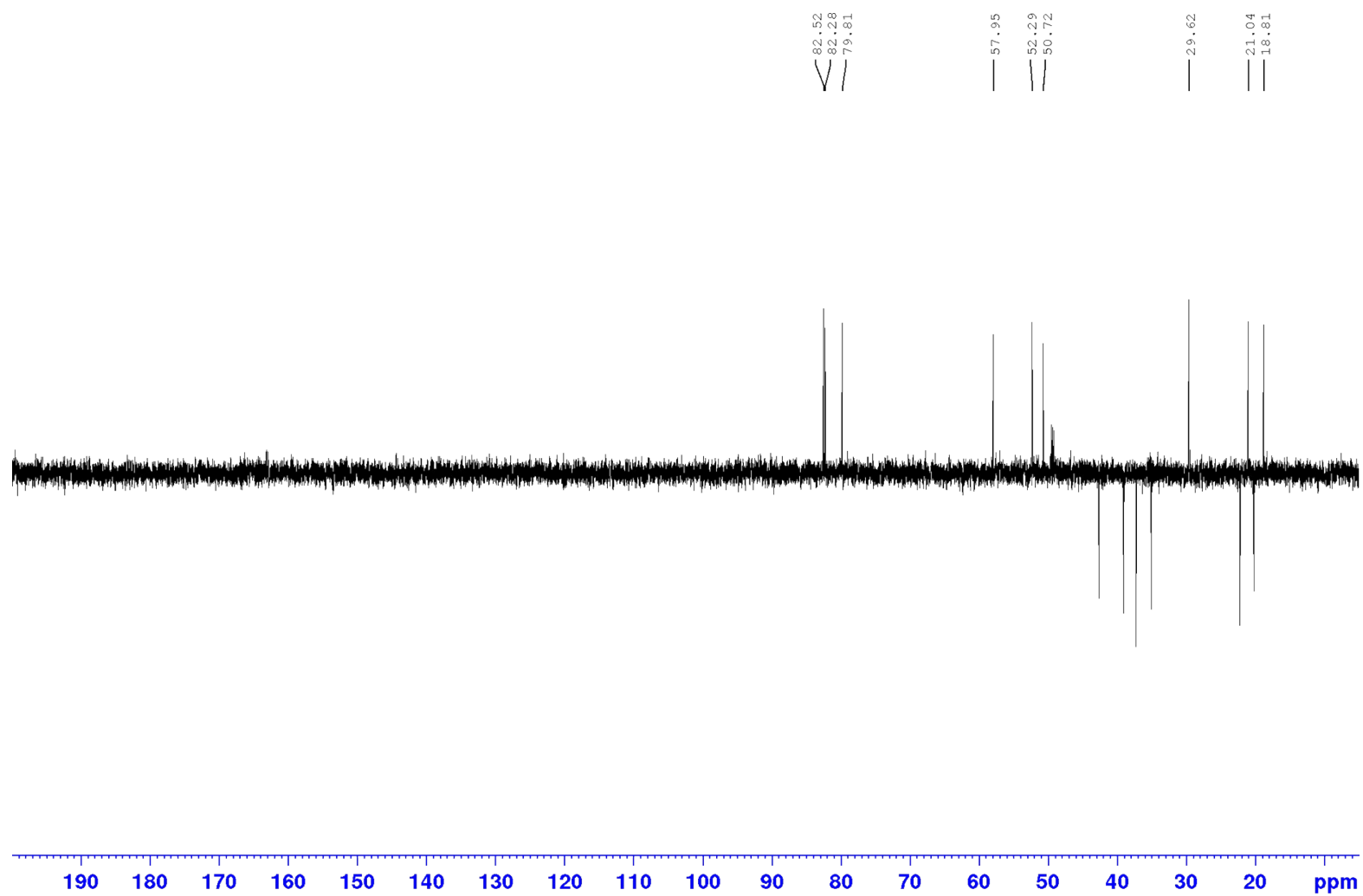


Figure S7. DEPT-135 NMR spectrum of Nouveinsiancin A (1) in CD₃OD

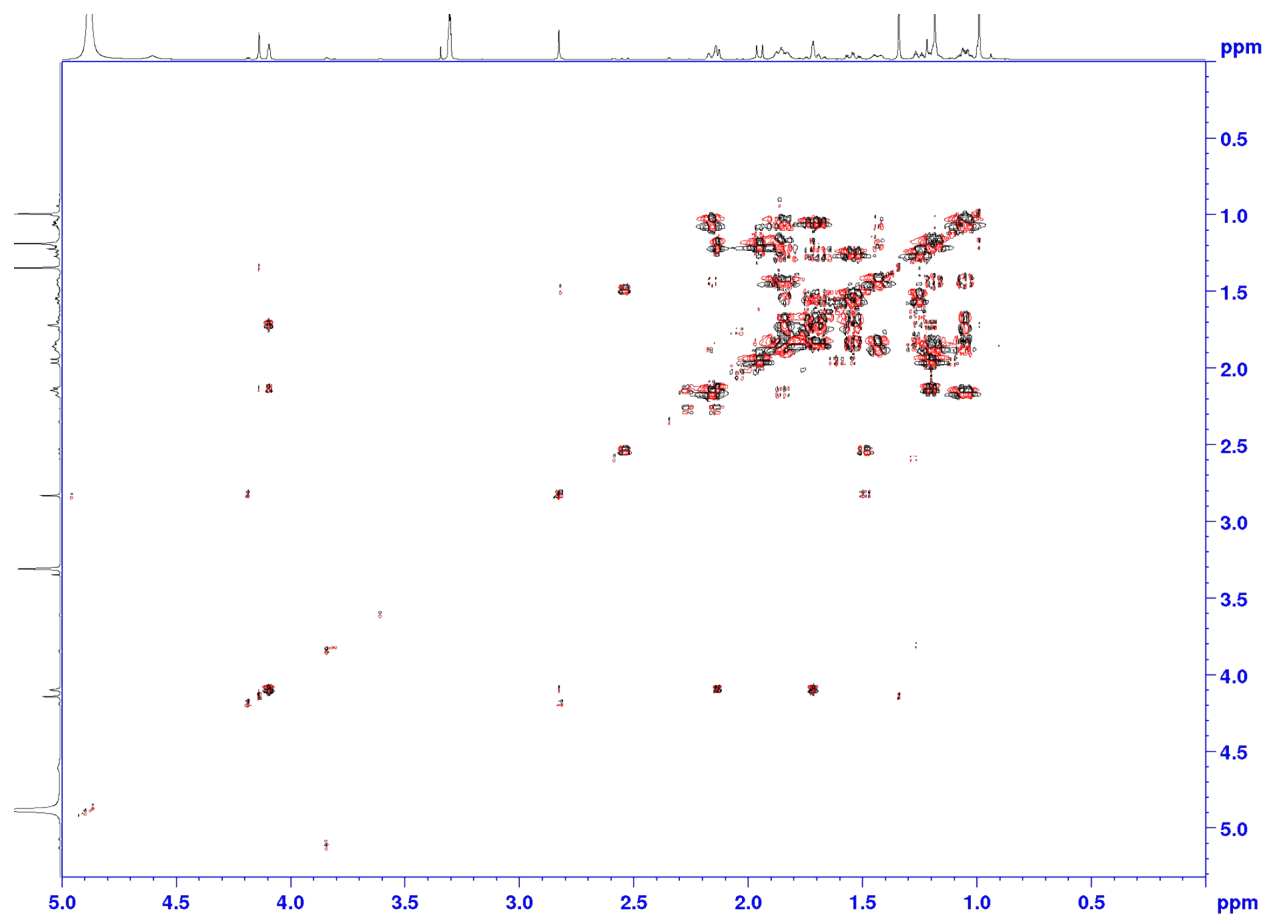


Figure S8. ^1H - ^1H COSY spectrum of Noueinsiancin A (1) in CD_3OD

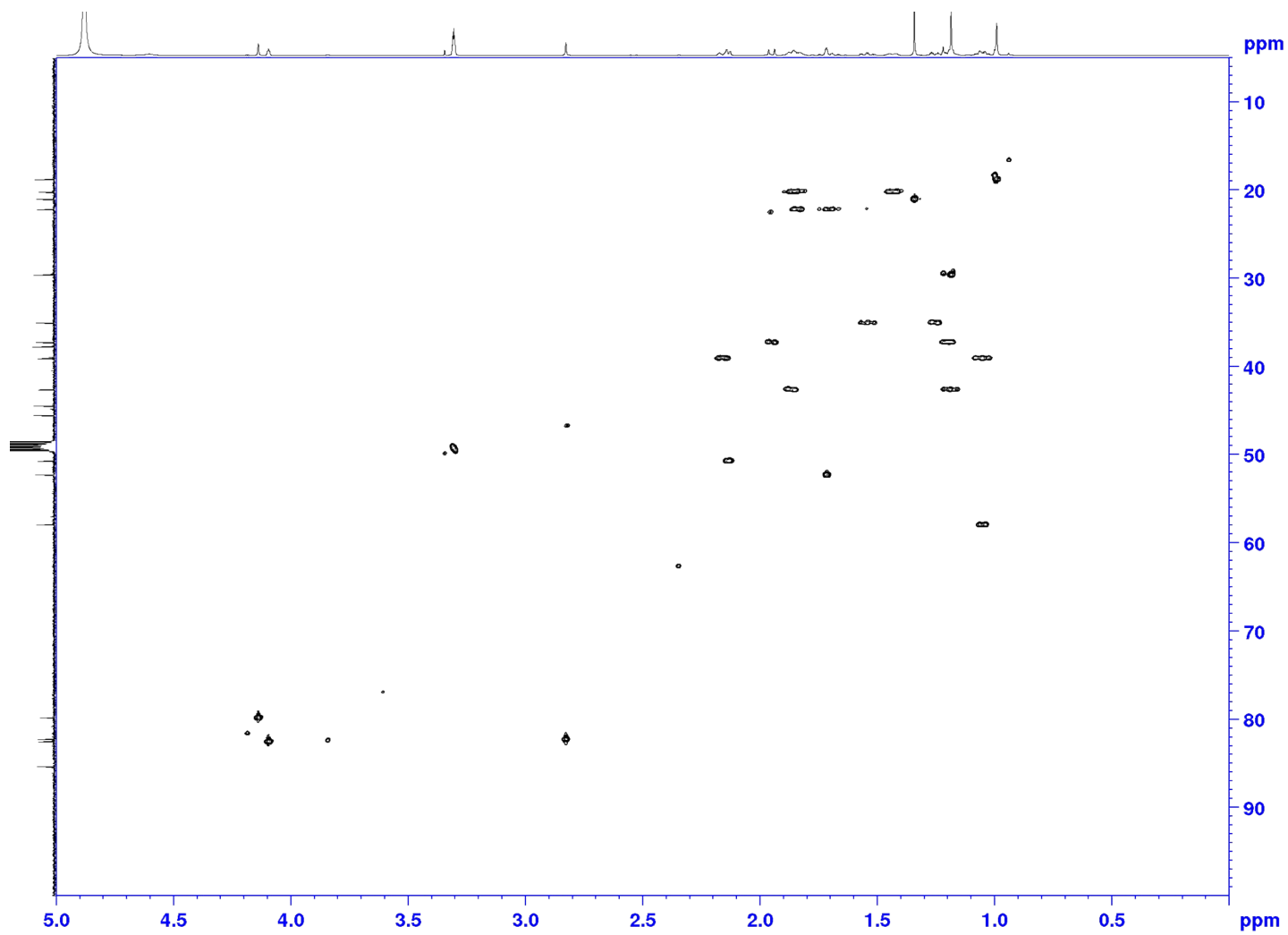


Figure S9. HSQC spectrum of Noueinsiancin A (1) in CD₃OD

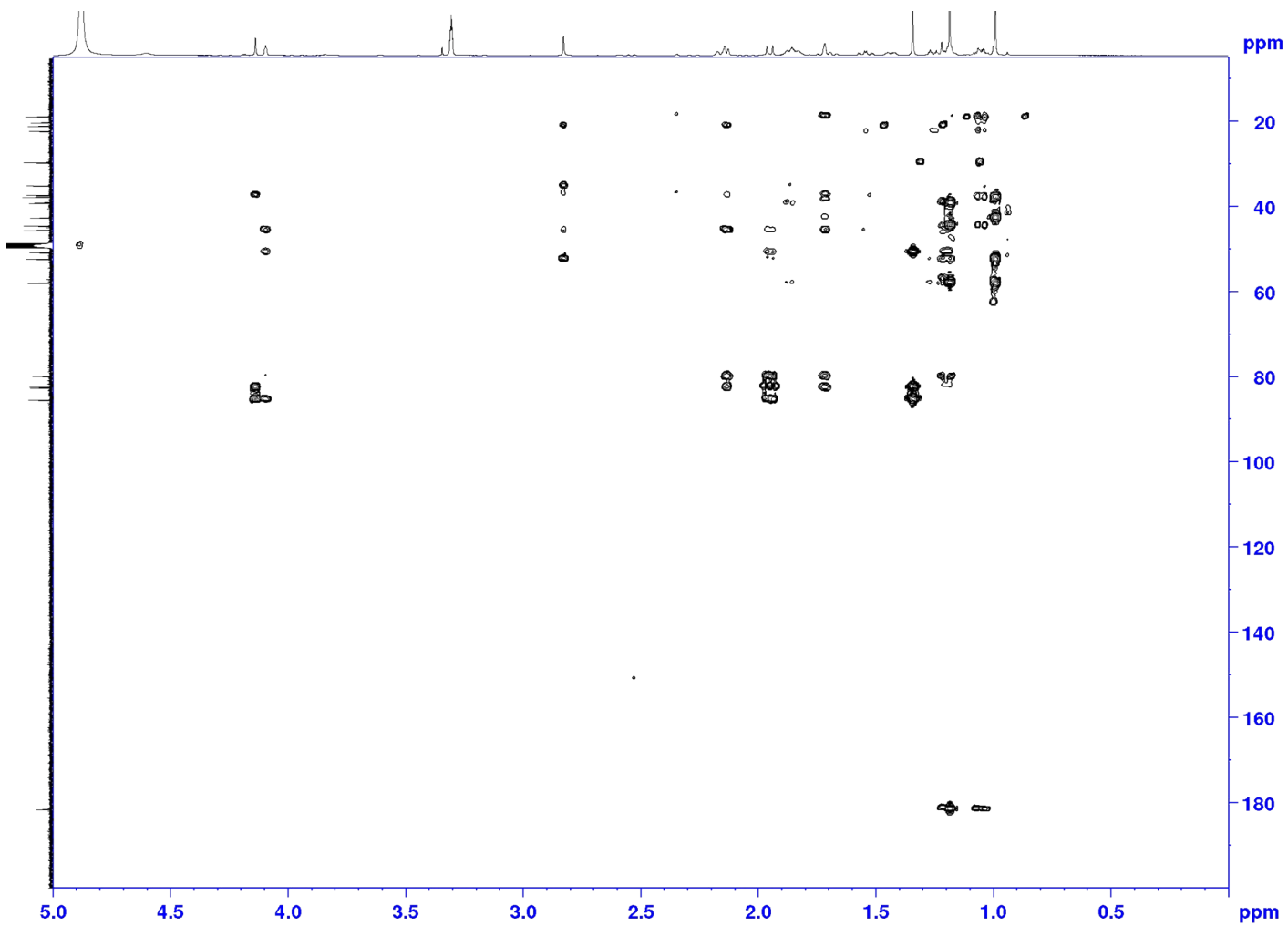


Figure S10. HMBC spectrum of Noueinsiancin A (1) in CD₃OD

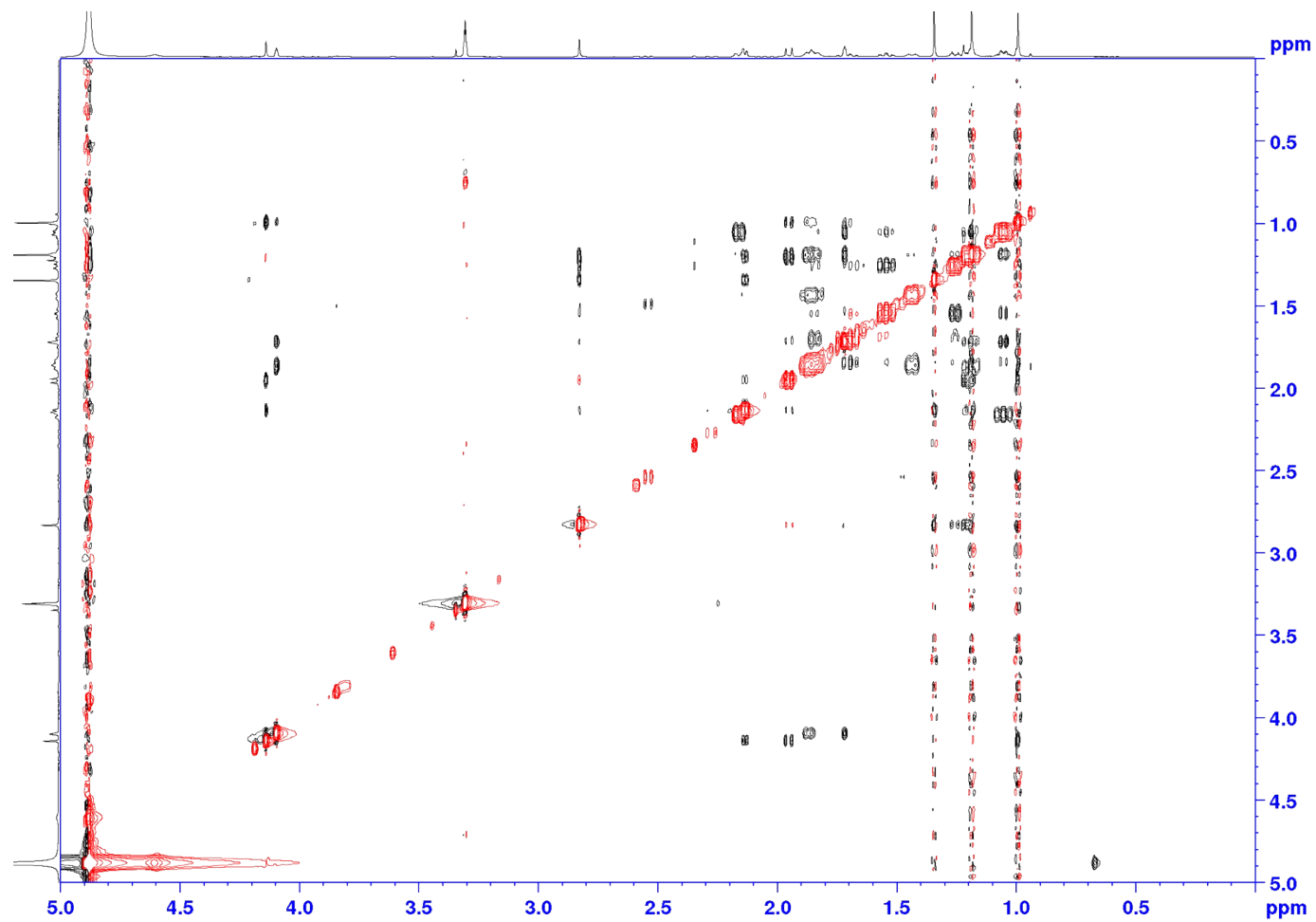


Figure S11. NOESY spectrum of Noueinsiancin A (1) in CD₃OD

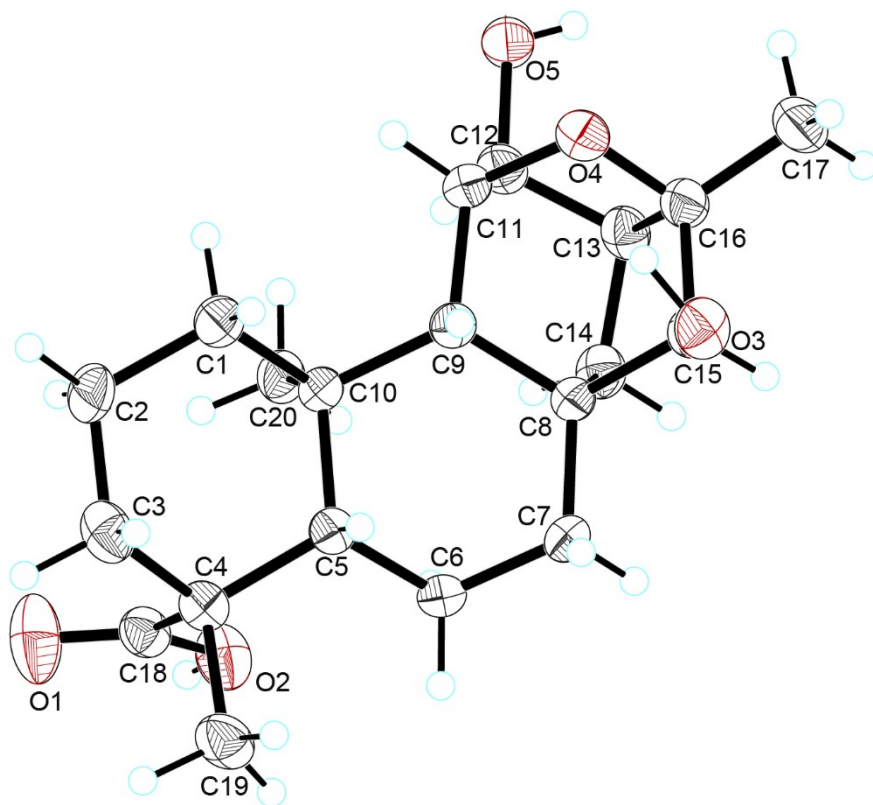
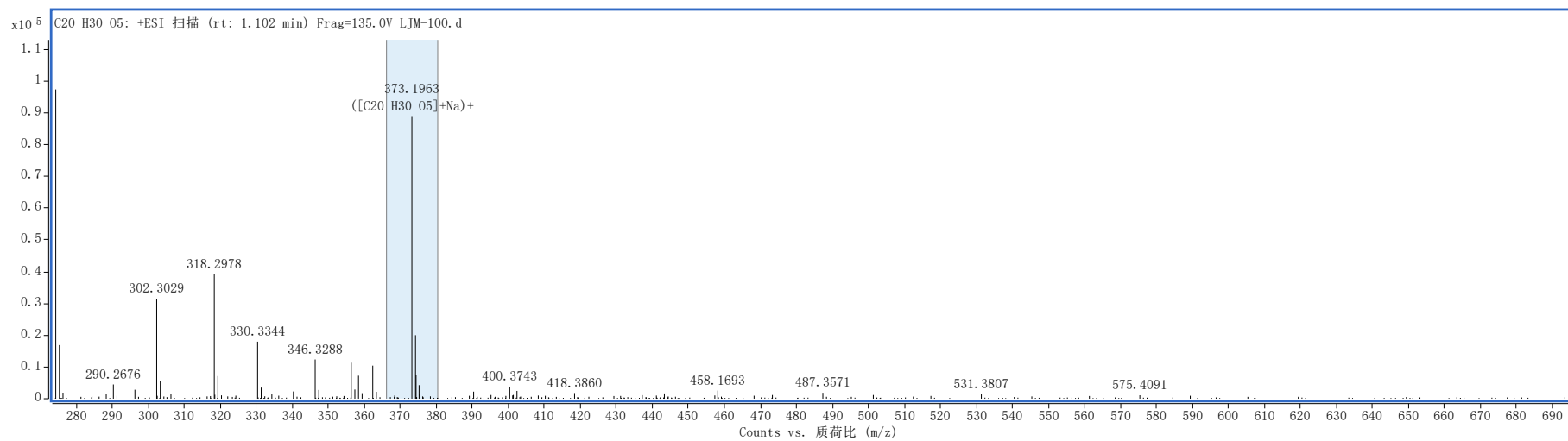


Figure S12. X-ray structure of Nouveinsiancin A (1)



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H30 O5	(M+Na)+	373.1963	81.76	7.22	81.76

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.7	90242.2	100	373.1985	2.2	89005.8	100	78.6	373.1963	6

Figure S13. HRESIMS spectrum of Noueinsiancin B (2)

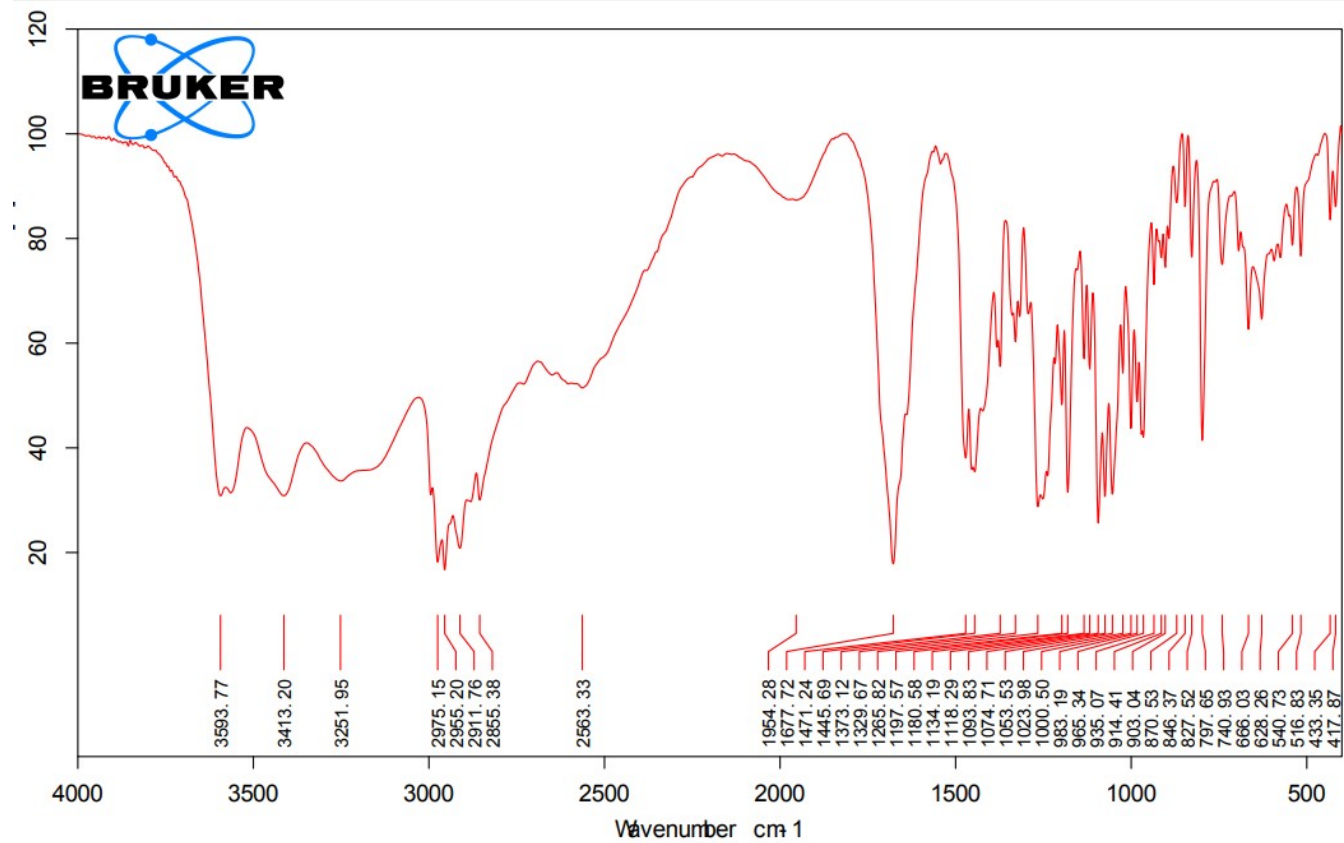


Figure S14. IR spectrum of Nouveinsiancin B (2)

Rudolph Research Analytical

Thursday, 02/10/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-100
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum						
6	-44.762	0.6732	-44.286	-45.714						
S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-100	07:18:04 PM	-45.714	SR	-0.032	589	100.00	0.070	19.7	
2	LJM-100	07:18:11 PM	-44.286	SR	-0.031	589	100.00	0.070	19.7	
3	LJM-100	07:18:17 PM	-44.286	SR	-0.031	589	100.00	0.070	19.7	
4	LJM-100	07:18:22 PM	-45.714	SR	-0.032	589	100.00	0.070	19.7	
5	LJM-100	07:18:27 PM	-44.286	SR	-0.031	589	100.00	0.070	19.8	
6	LJM-100	07:18:33 PM	-44.286	SR	-0.031	589	100.00	0.070	19.8	

Signature

Figure S15. OR Value of Noueinsiancin B (2) in CH₃OH

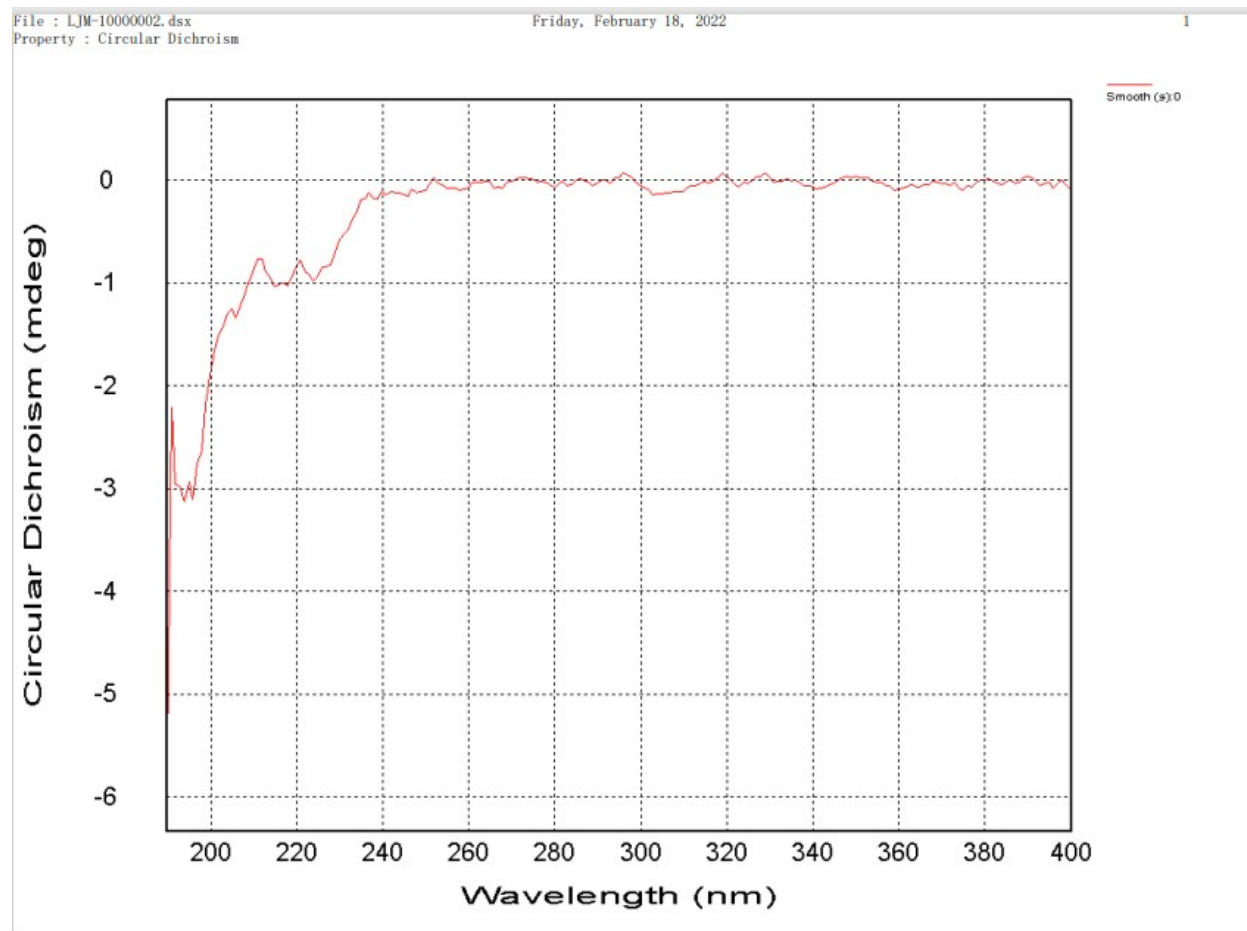


Figure S16. CD Value of Noueinsiancin B (2) in CH₃OH

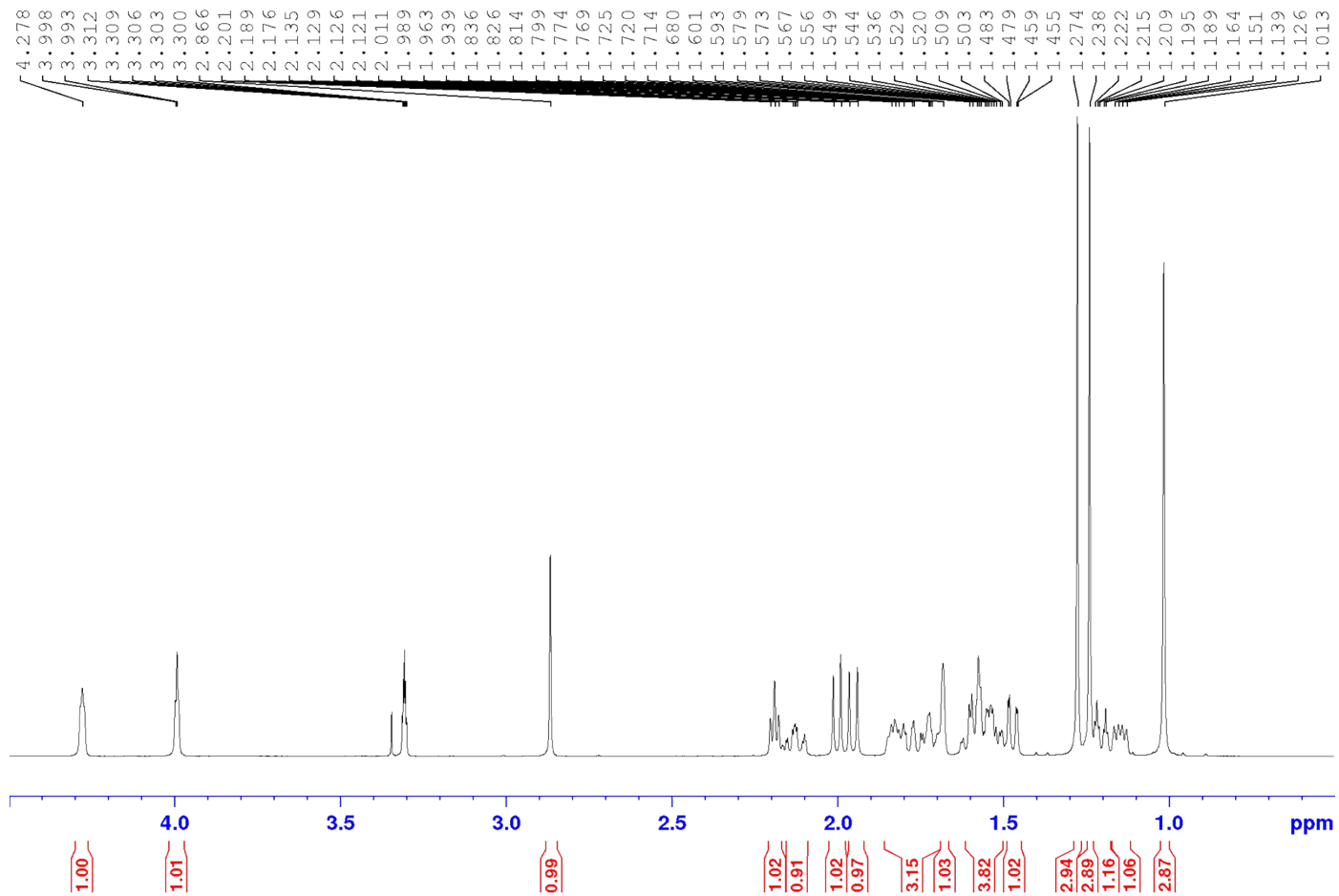


Figure S17. ¹H NMR spectrum of Noueinsiancin B (2) in CD₃OD

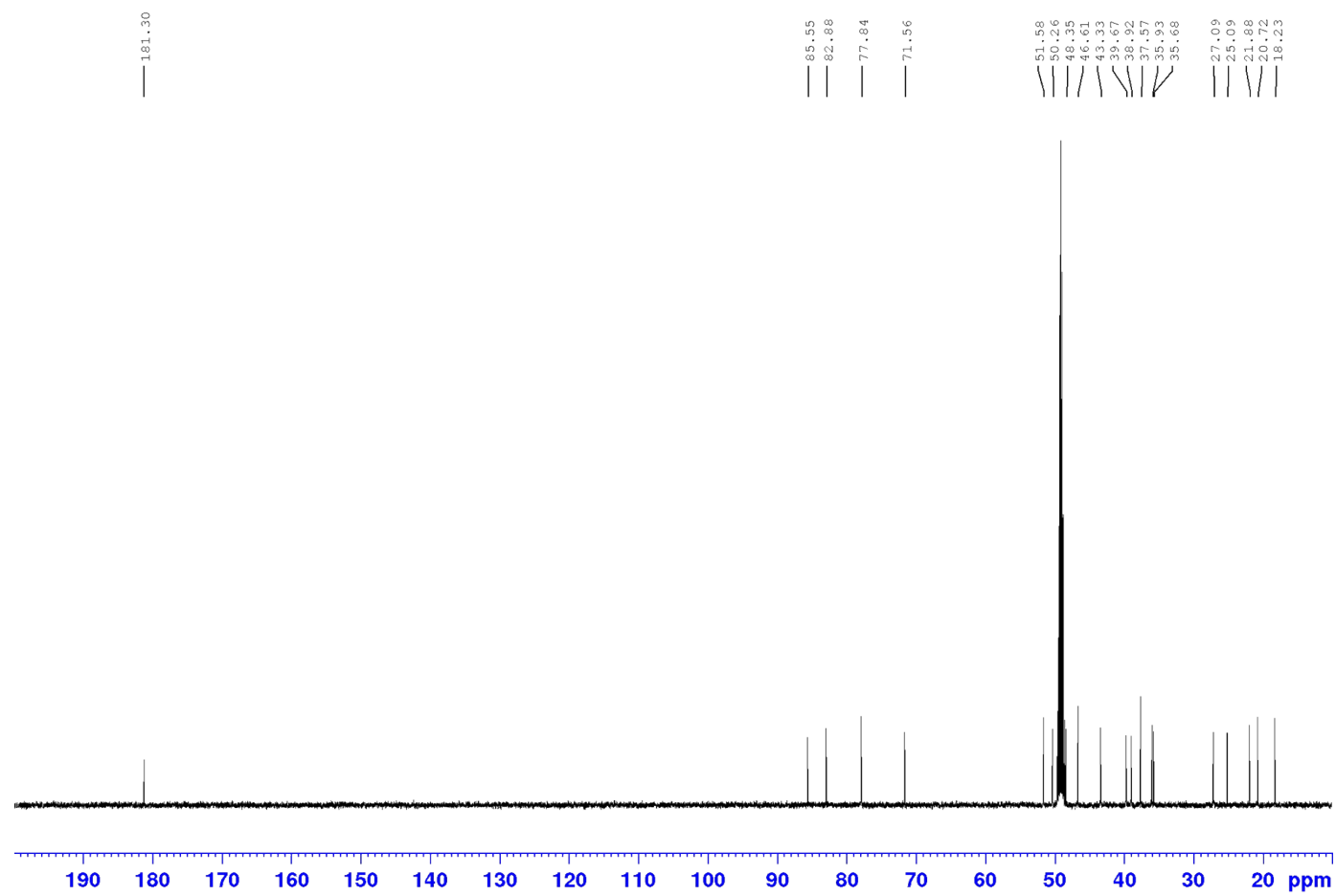


Figure S18. ¹³C NMR spectrum of Noueinsiancin B (2) in CD₃OD

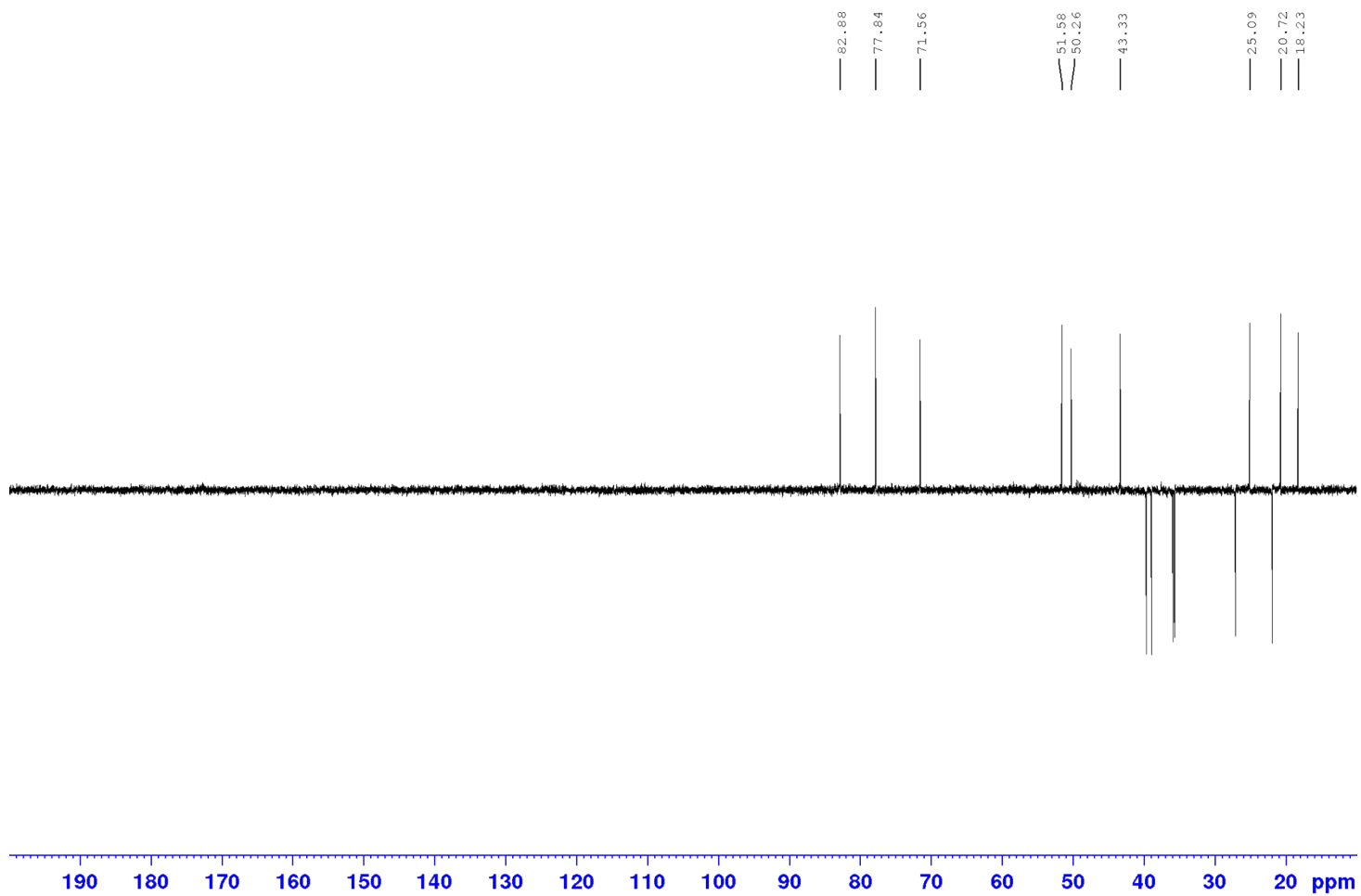


Figure S19. DEPT-135 NMR spectrum of Noueinsiancin B (2) in CD₃OD

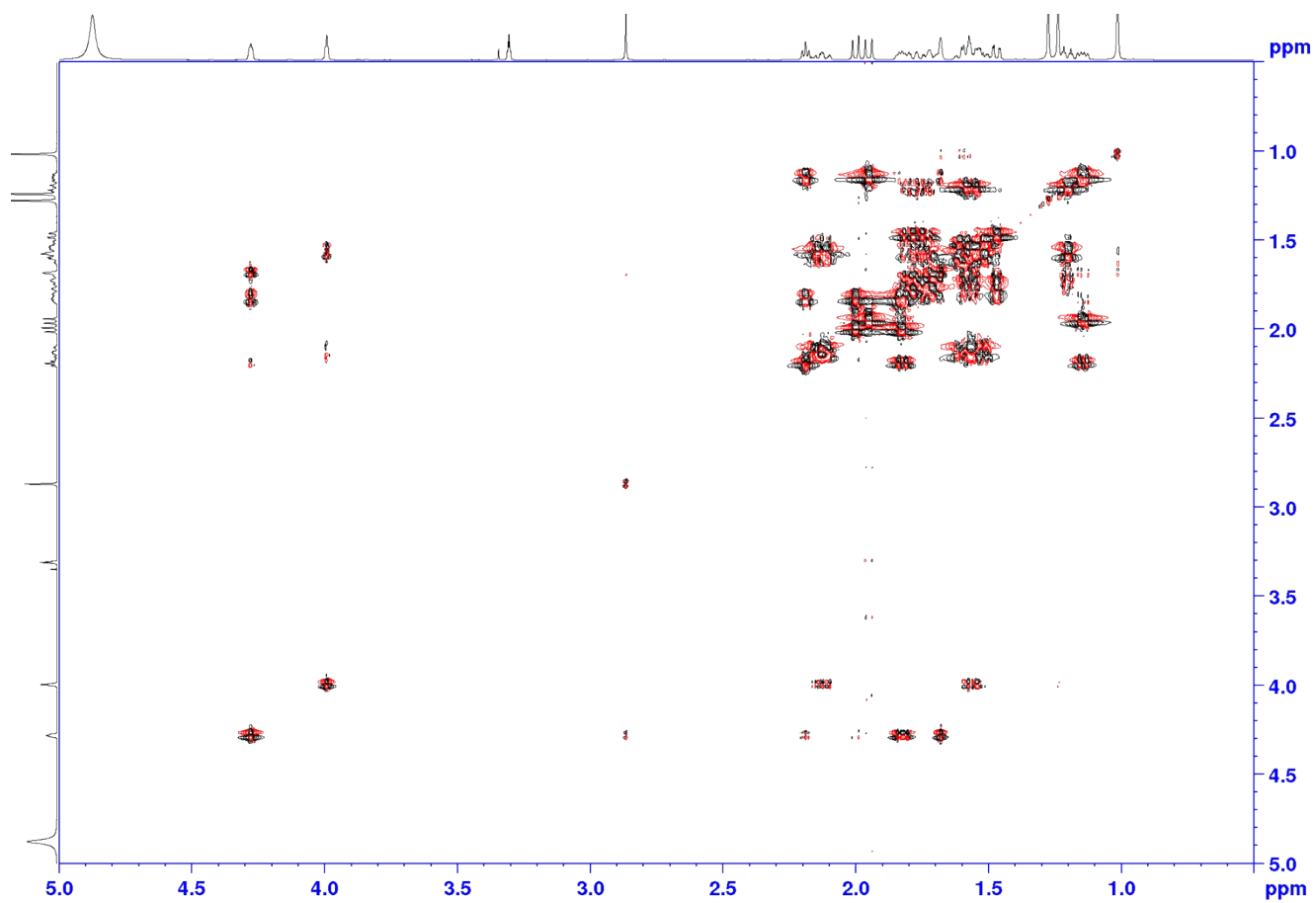


Figure S20. ^1H - ^1H COSY spectrum of Nouveinsiancin B (2) in CD_3OD

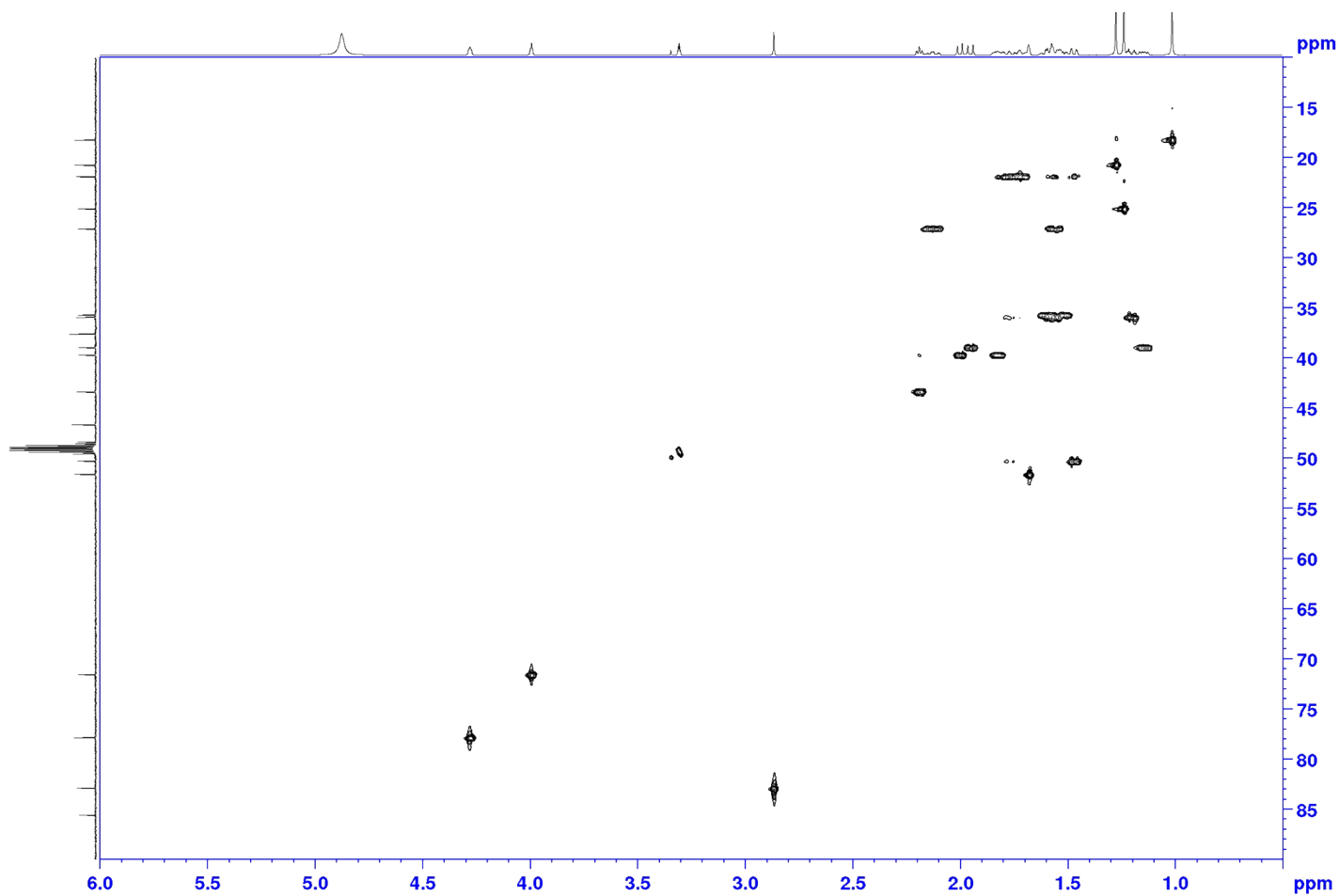


Figure S21. HSQC spectrum of Noueinsiancin B (2) in CD_3OD

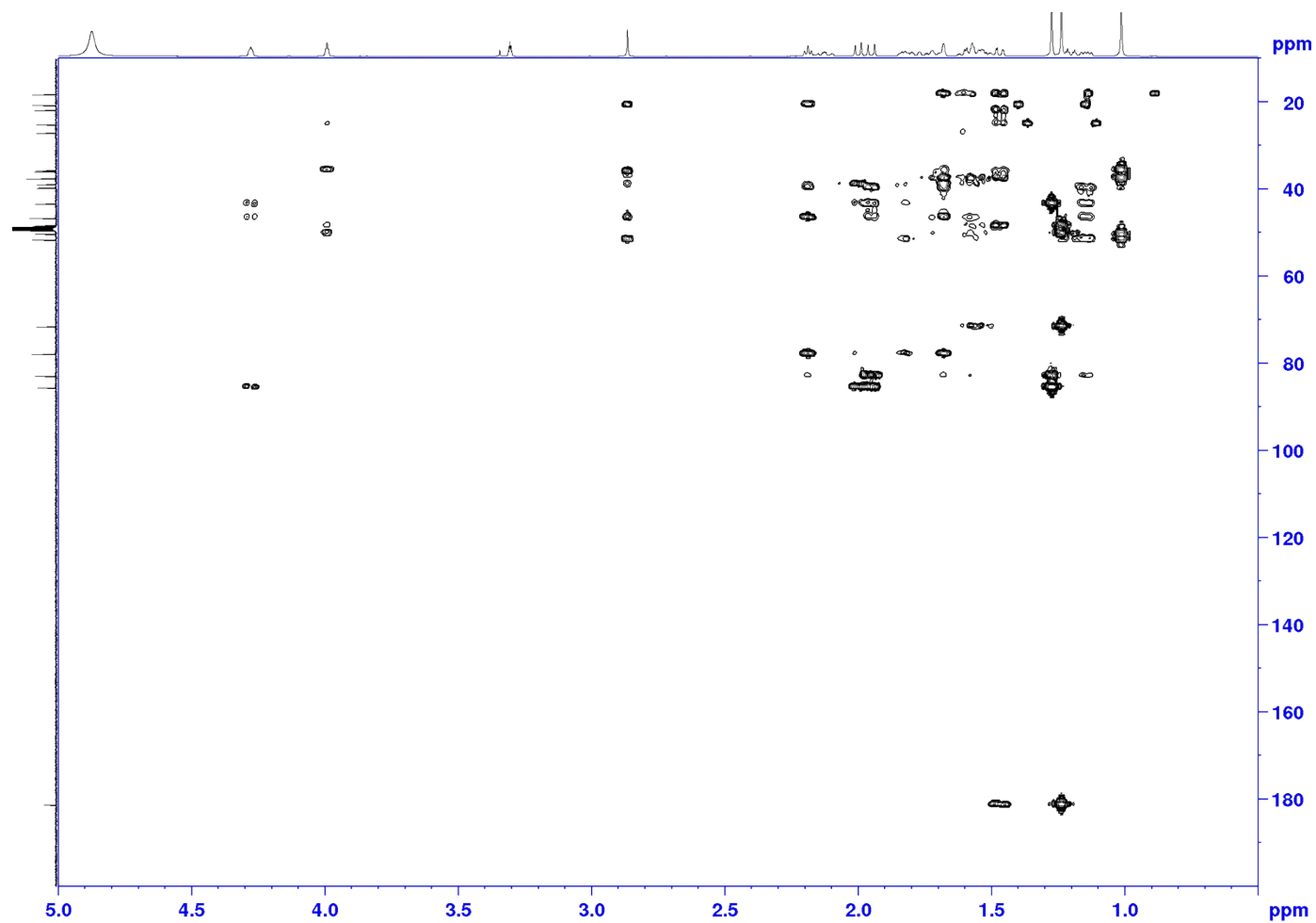


Figure S22. HMBC spectrum of Noueinsiancin B (2) in CD₃OD

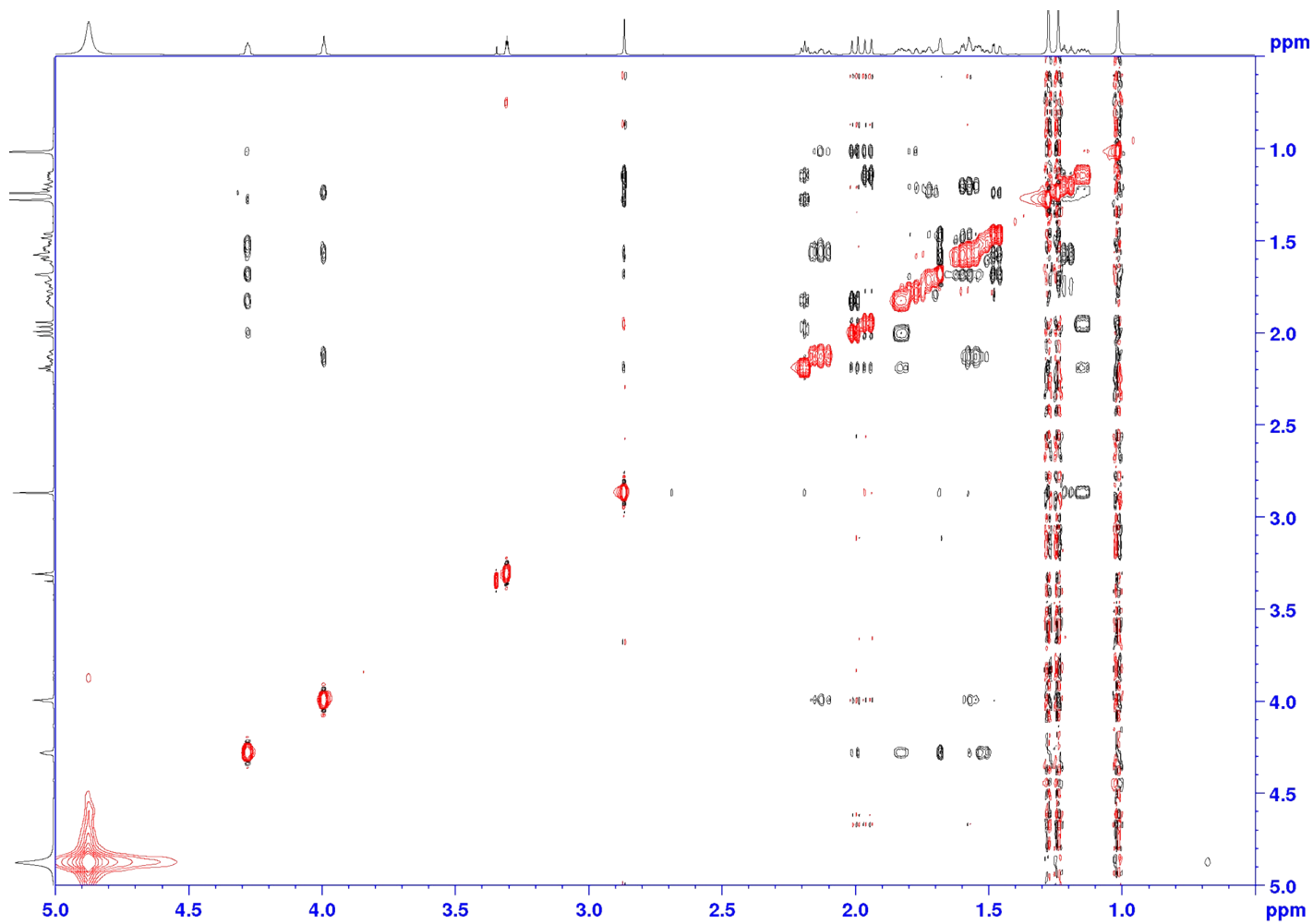


Figure S23. NOESY spectrum of Noueinsiancin B (2) in CD₃OD

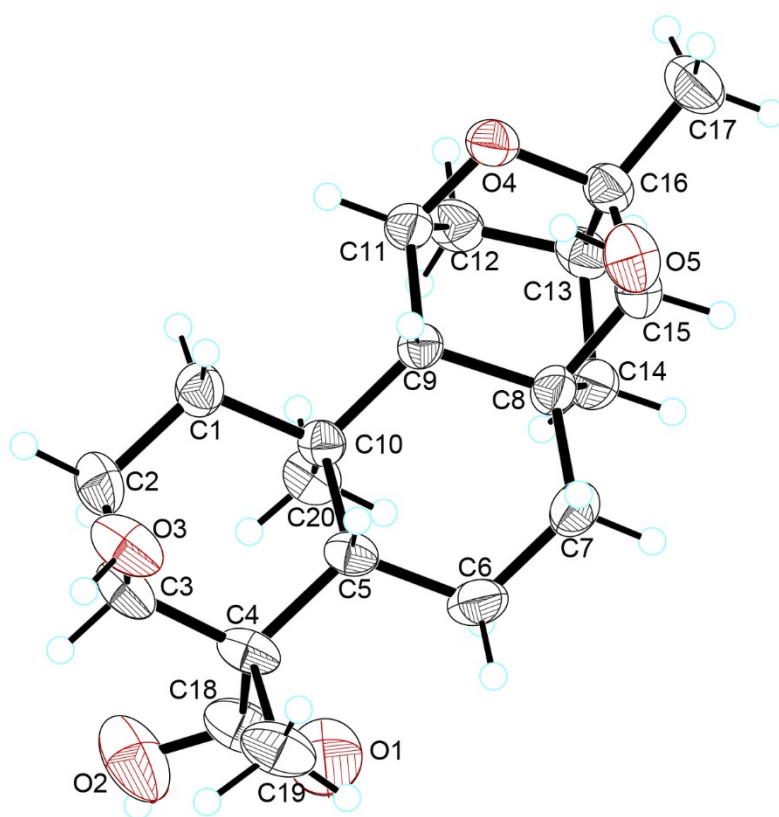
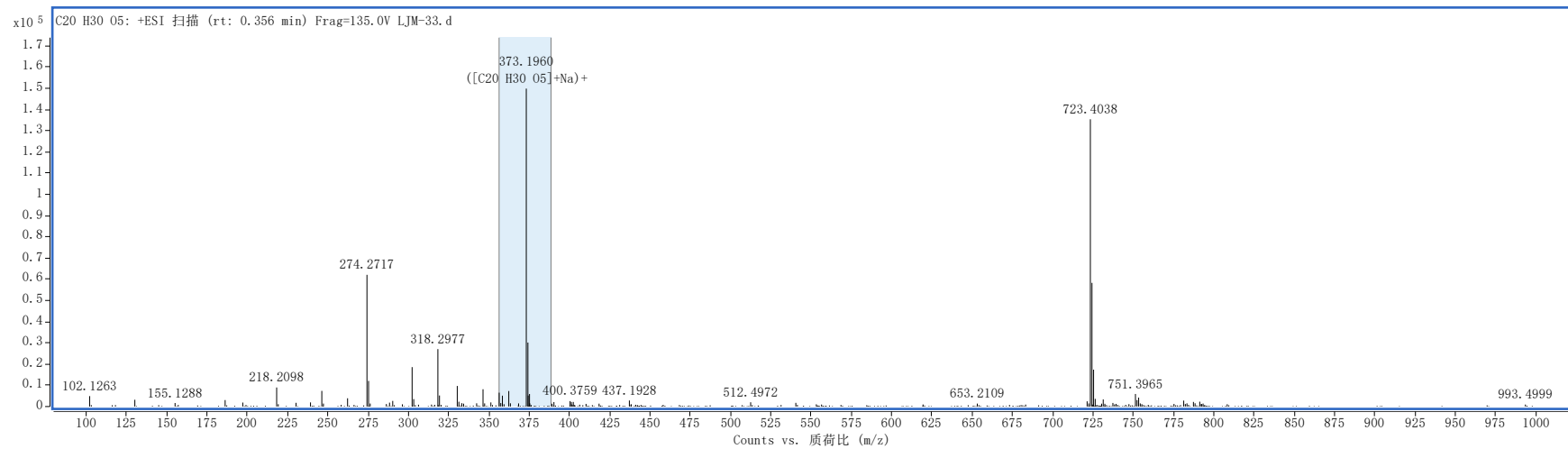


Figure S24. X-ray structure of Nouveinsiancin B (2)



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H30 O5	(M+Na)+	373.1960	81.47	7.7	81.47

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.7	148045.5	100	373.1985	2.6	149803.4	100	80.6	373.196	6.91

Figure S25. HRESIMS spectrum of Nouveinsiancin C (3)

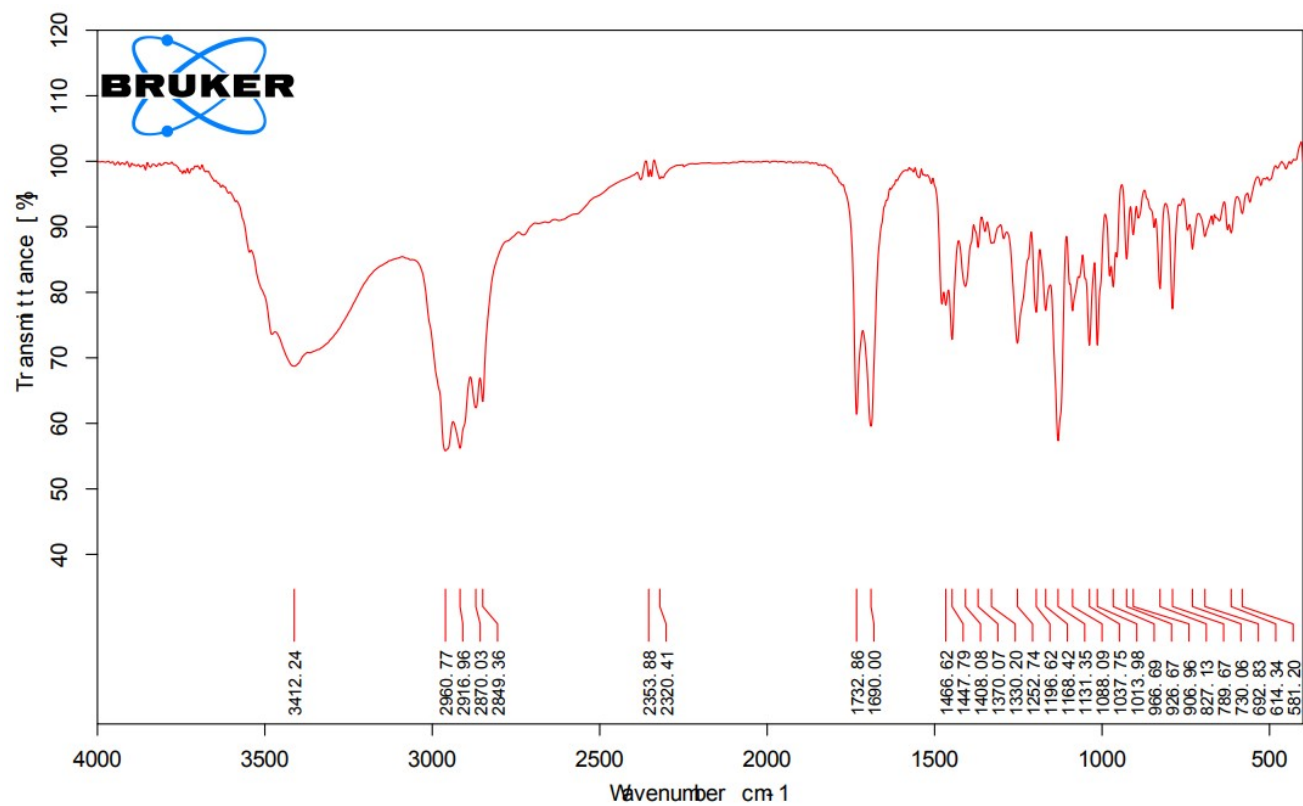


Figure S26. IR spectrum of Noueinsiancin C (3)

Rudolph Research Analytical

Wednesday, 02/09/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-33
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-80.256	0.5732	-80.000	-81.538

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-33	03:53:04 PM	-81.538	SR	-0.053	589	100.00	0.065	20.2	
2	LJM-33	03:53:10 PM	-80.000	SR	-0.052	589	100.00	0.065	20.2	
3	LJM-33	03:53:16 PM	-80.000	SR	-0.052	589	100.00	0.065	20.1	
4	LJM-33	03:53:22 PM	-80.000	SR	-0.052	589	100.00	0.065	20.1	
5	LJM-33	03:53:27 PM	-80.000	SR	-0.052	589	100.00	0.065	20.1	
6	LJM-33	03:53:33 PM	-80.000	SR	-0.052	589	100.00	0.065	20.1	

Signature

Figur

e S27. OR Value of Noueinsiancin C (3) in CH₃OH

Property : Circular Dichroism

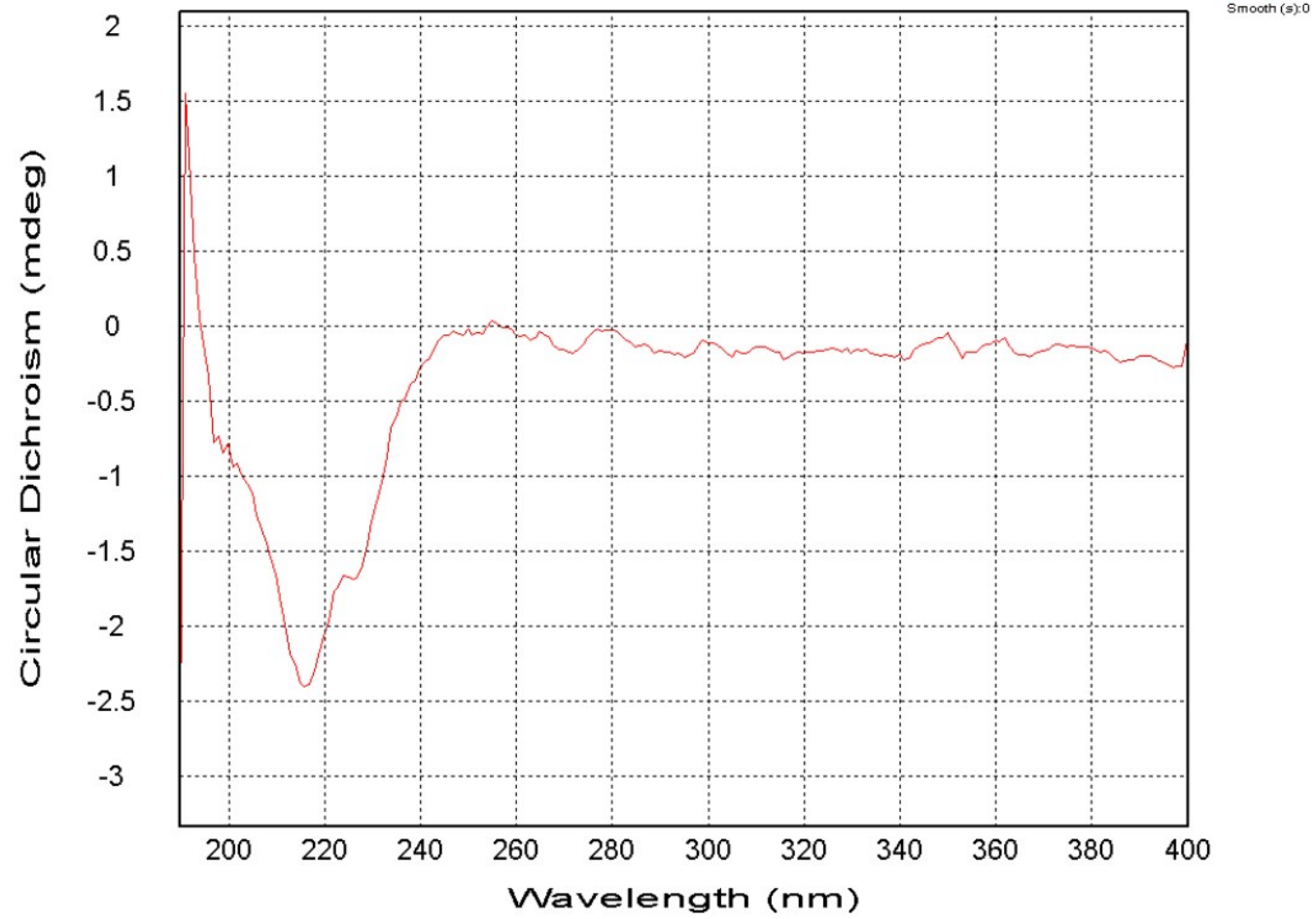


Figure S28. CD Value of Noueinsiancin C (3) in CH₃OH

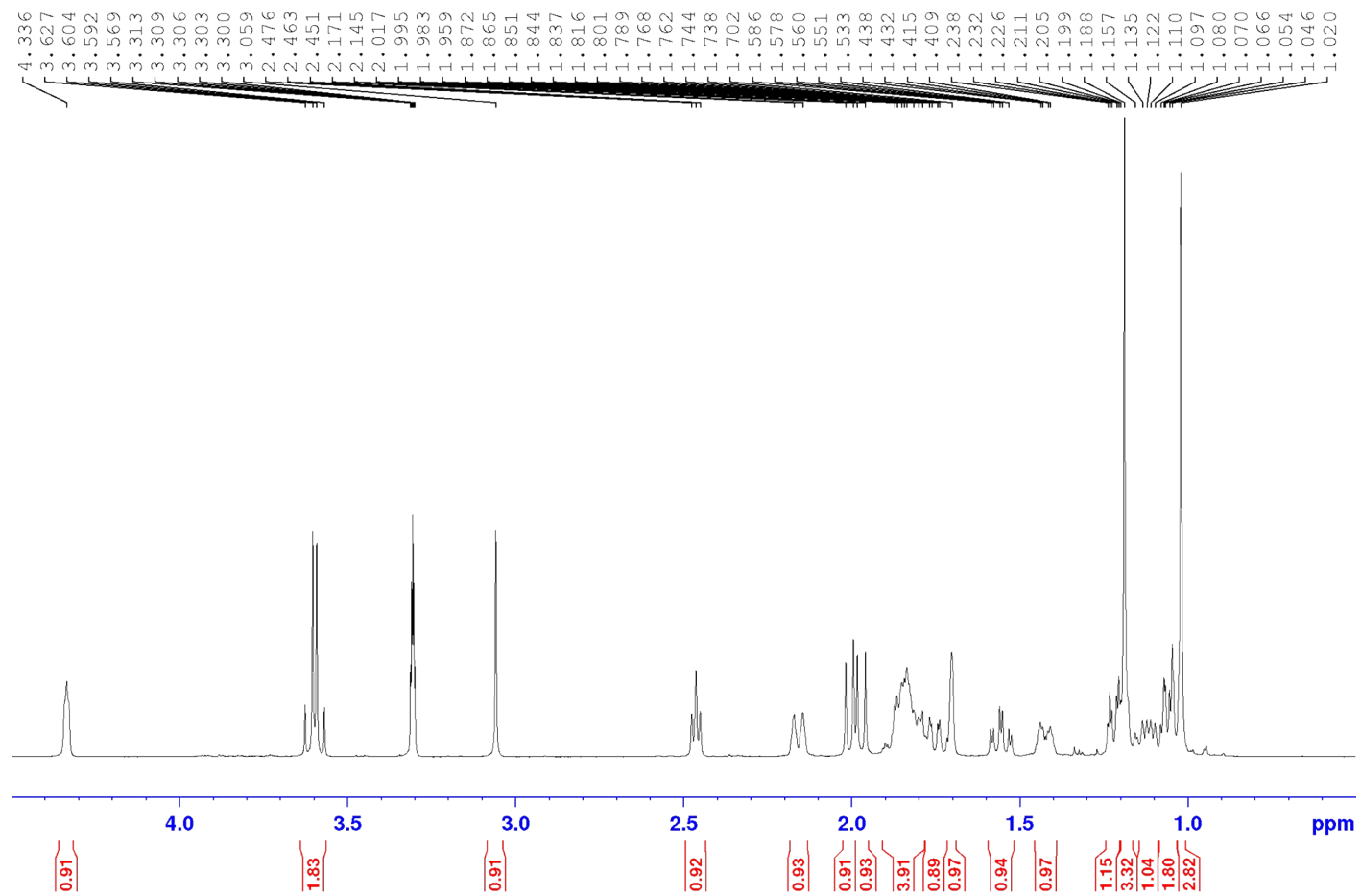


Figure S29. ¹H NMR spectrum of Noueinsiancin C (3) in CD₃OD

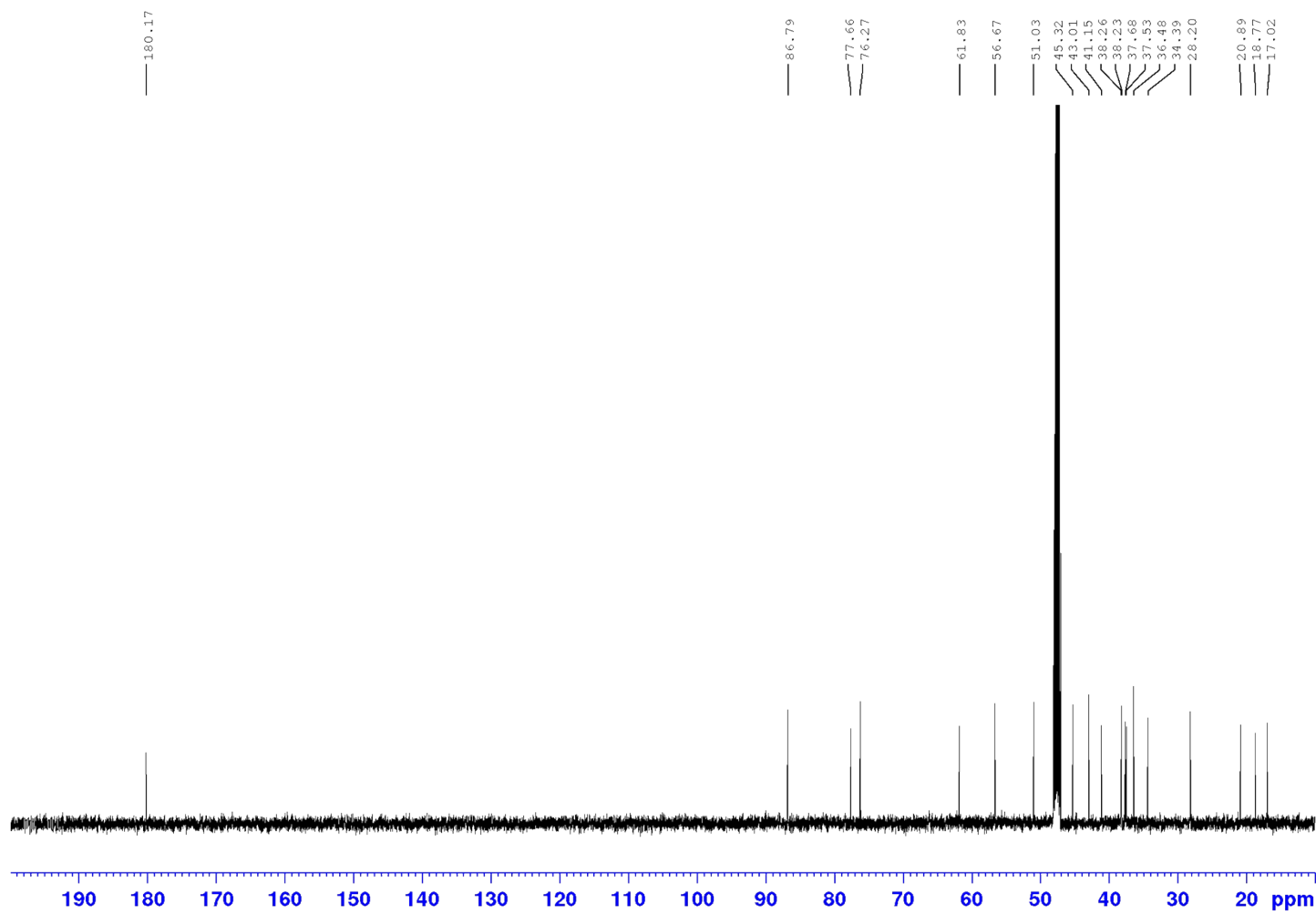


Figure S30. ¹³C NMR spectrum of Noueinsiancin C (3) in CD₃OD

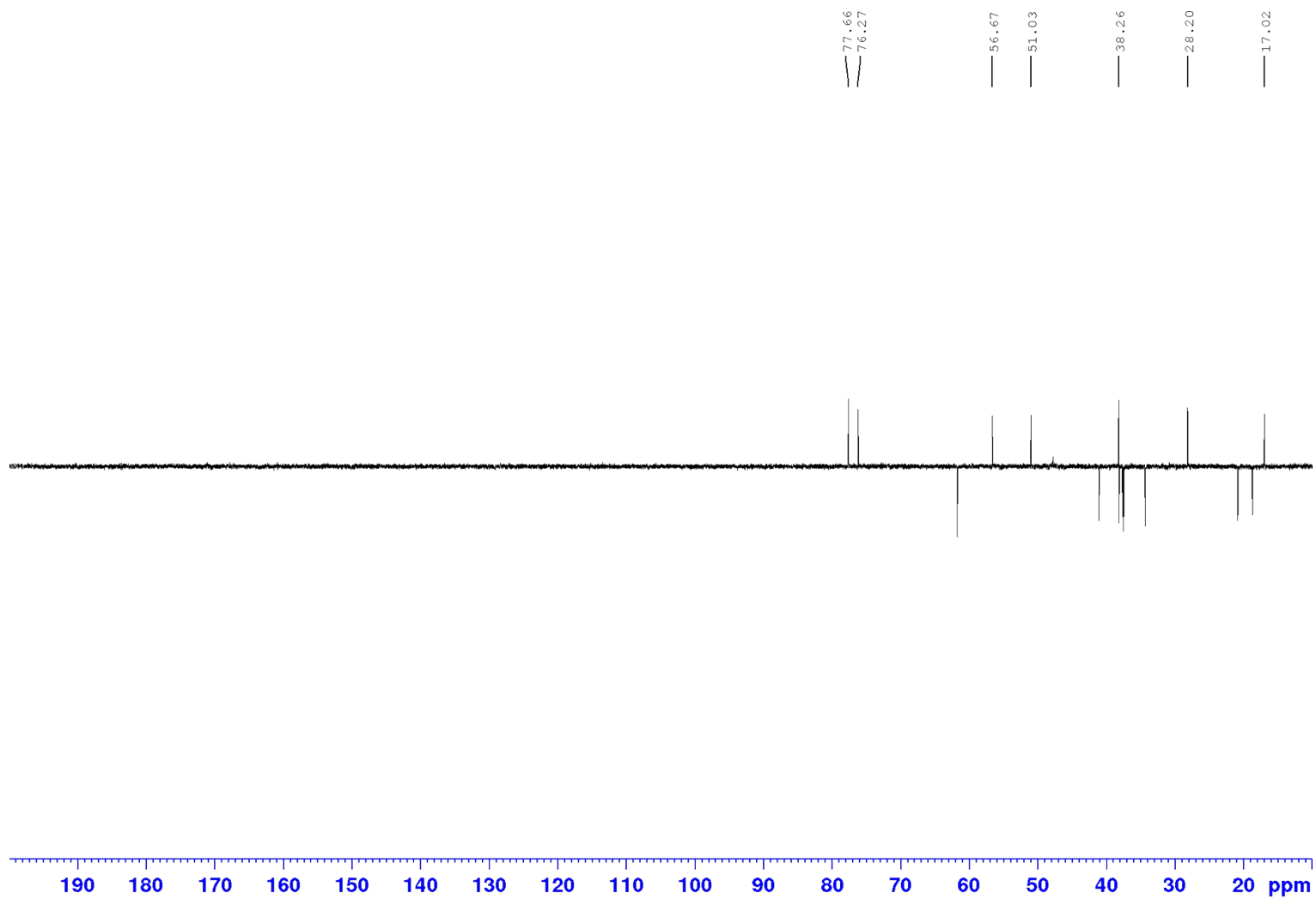


Figure S31. DEPT-135 NMR spectrum of Noueinsiancin C (3) in CD₃OD

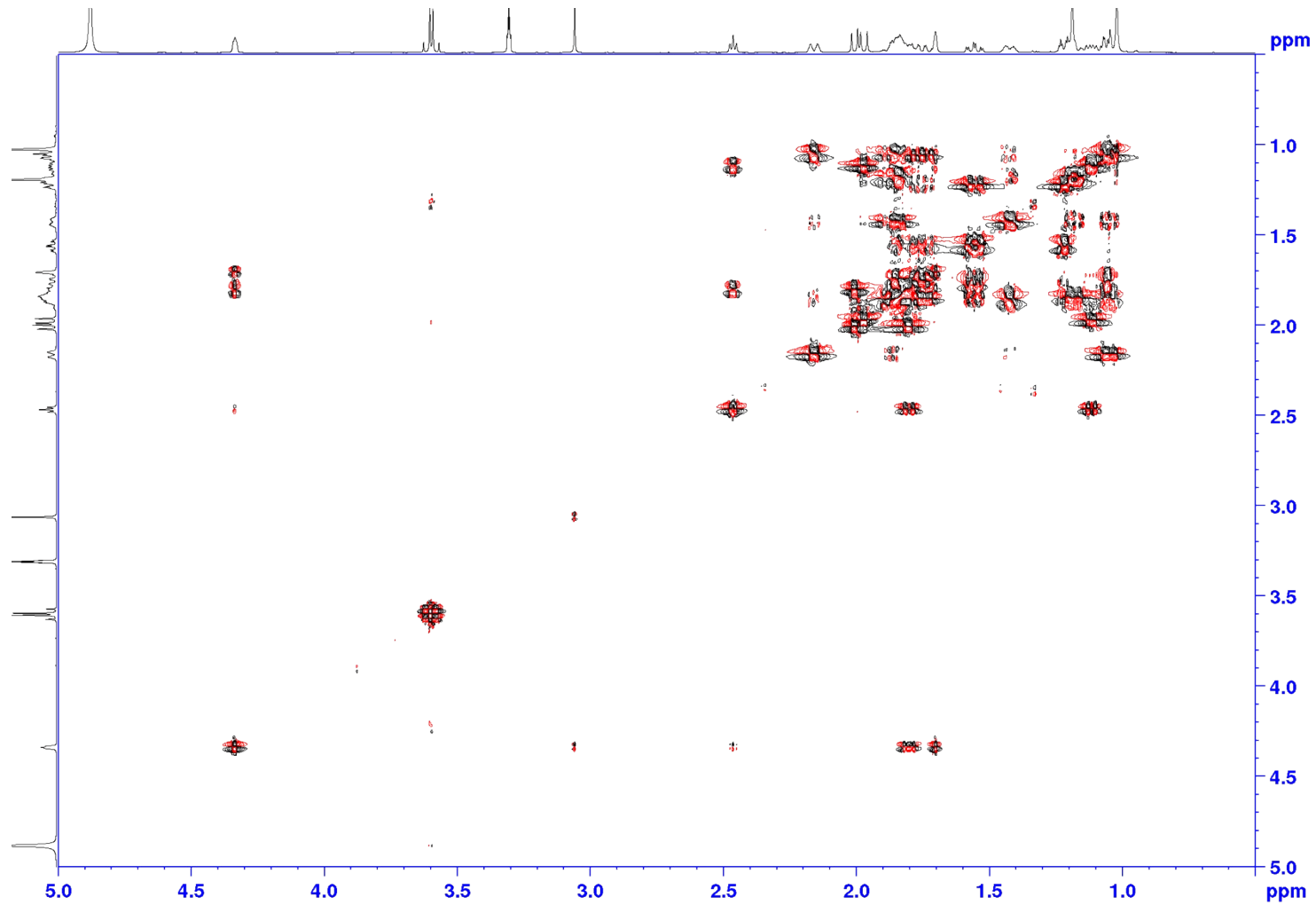


Figure S32. ^1H - ^1H COSY spectrum of Noueinsiancin C (3) in CD_3OD

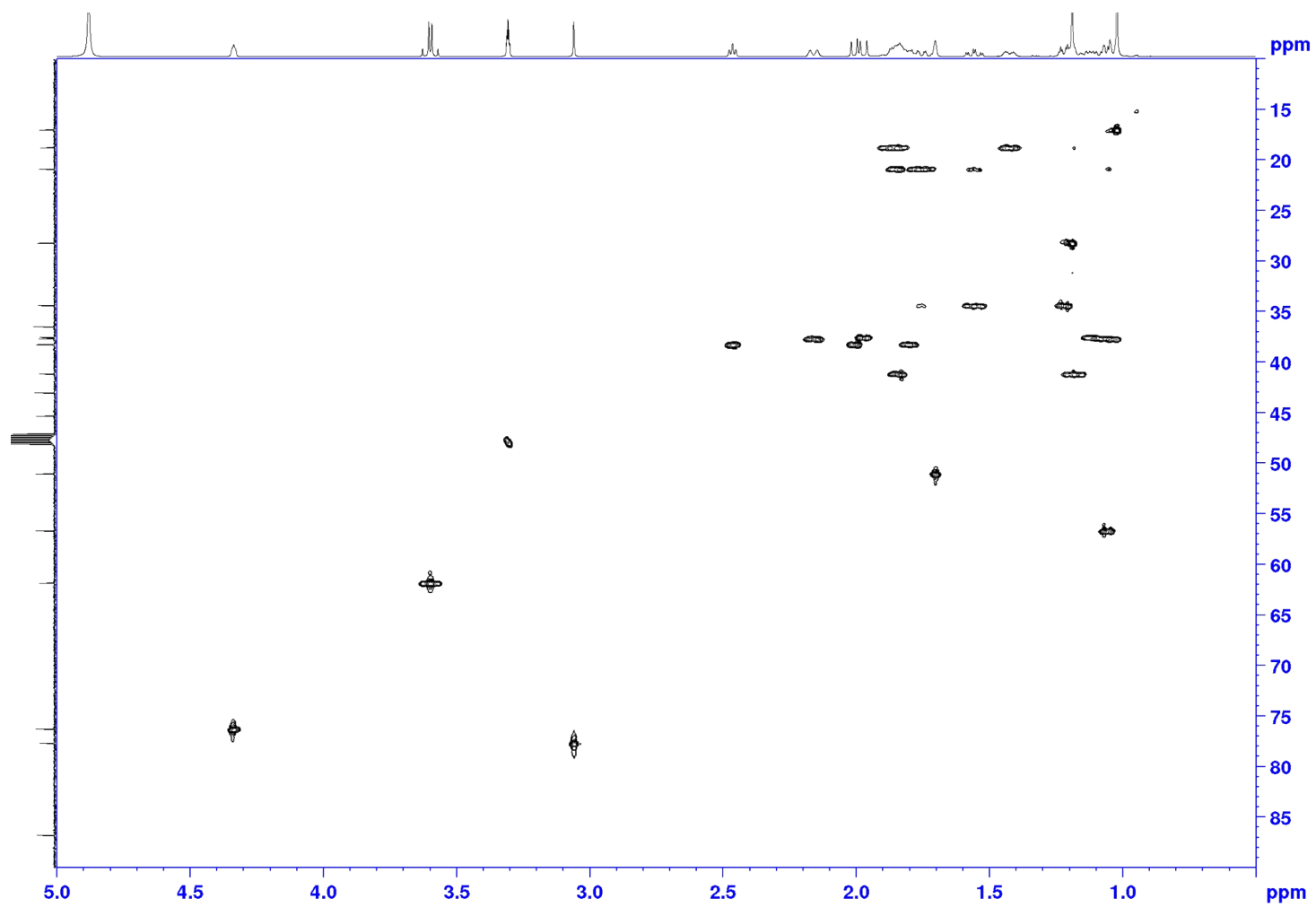


Figure S33. HSQC spectrum of Noueinsiancin C (3) in CD₃OD

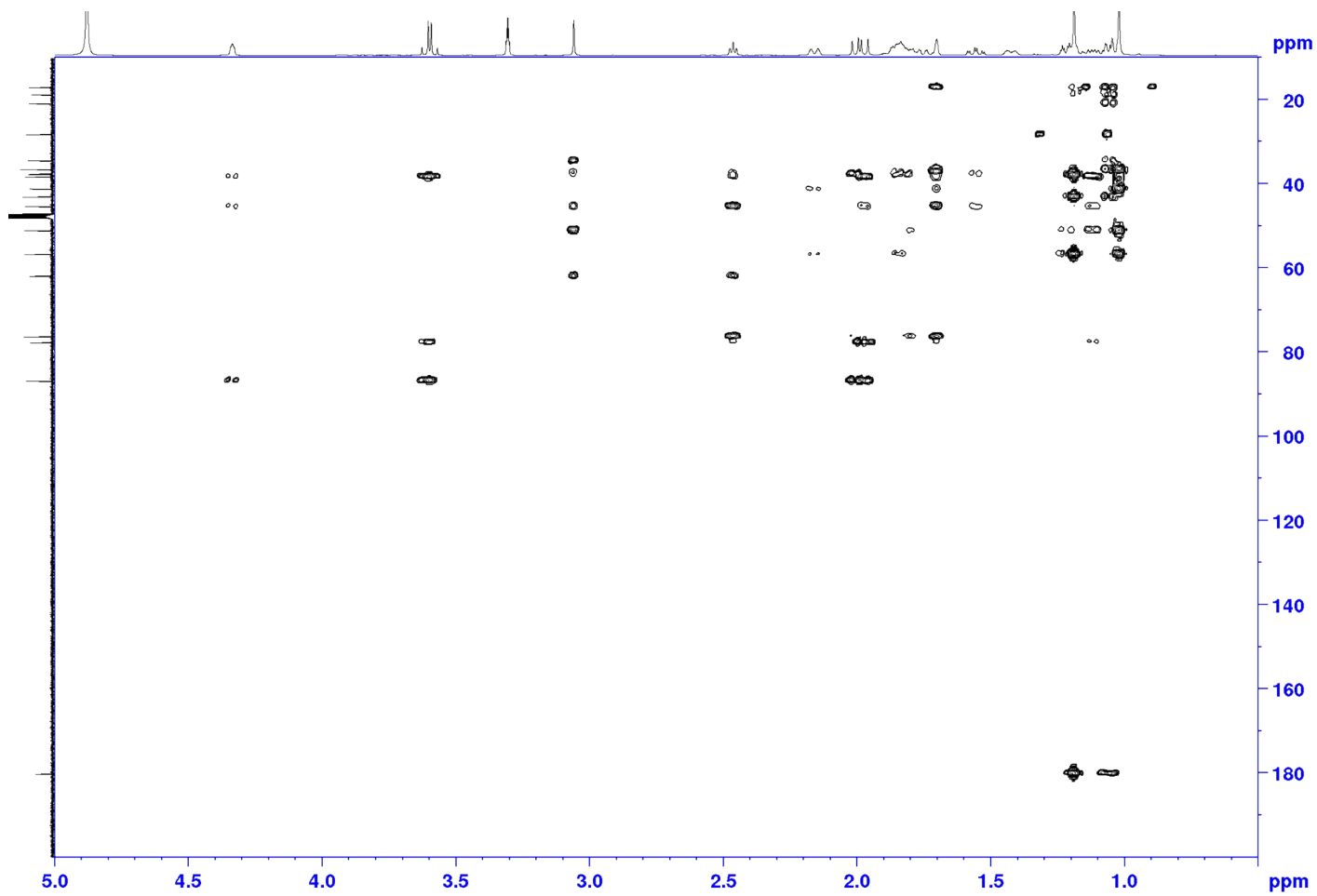


Figure S34. HMBC spectrum of Noueinsiancin C (3) in CD₃OD

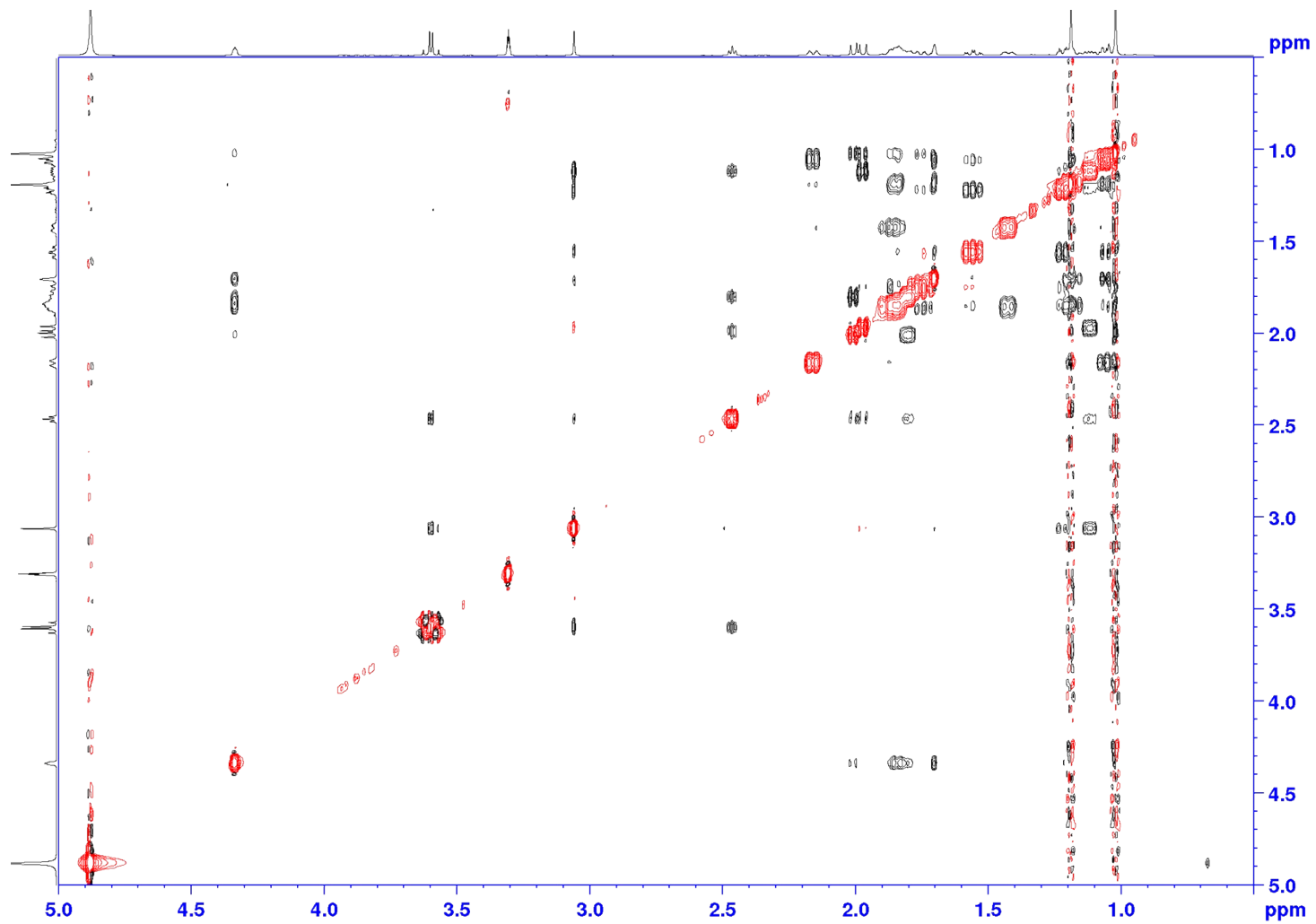
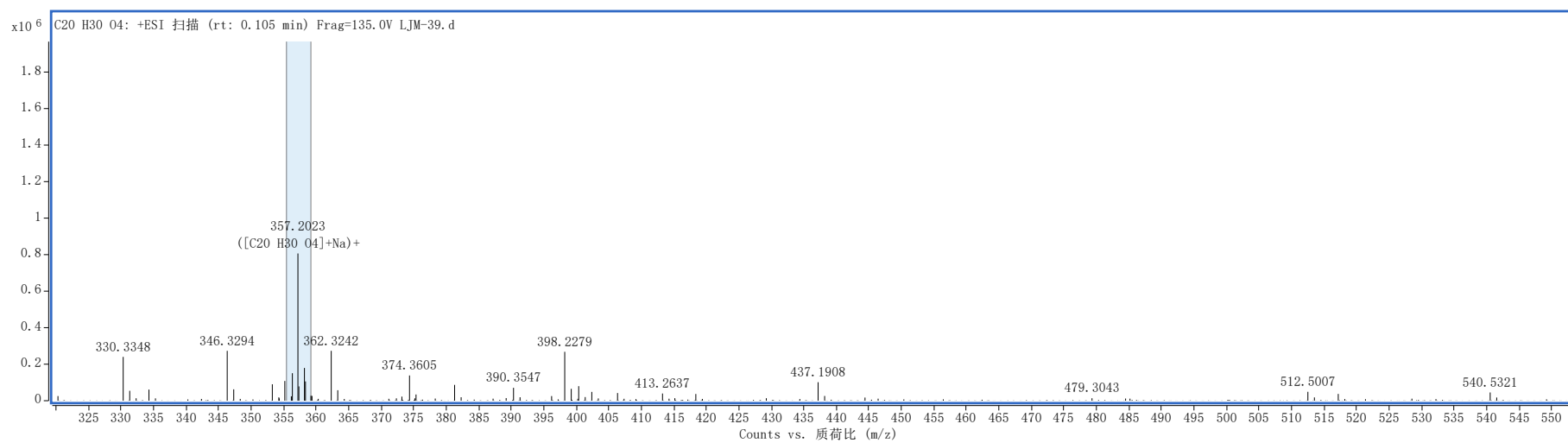


Figure S35. NOESY spectrum of Noueinsiancin C (3) in CD₃OD



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (谱库)	分数 (DB)	分数 (MFG)
TRUE	MFG	C20 H30 O4	(M+Na)+	357.2023	92.42	4.59			92.42

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.8	809437.4	100	357.2036	1.3	807306.1	100	79.6	357.2023	3.75
17.7	179119.3	22.1	358.207	2.1	179631.9	22.3	17.7	358.2049	5.92

Figure S36. HRESIMS spectrum of Noueinsiancin D (4)

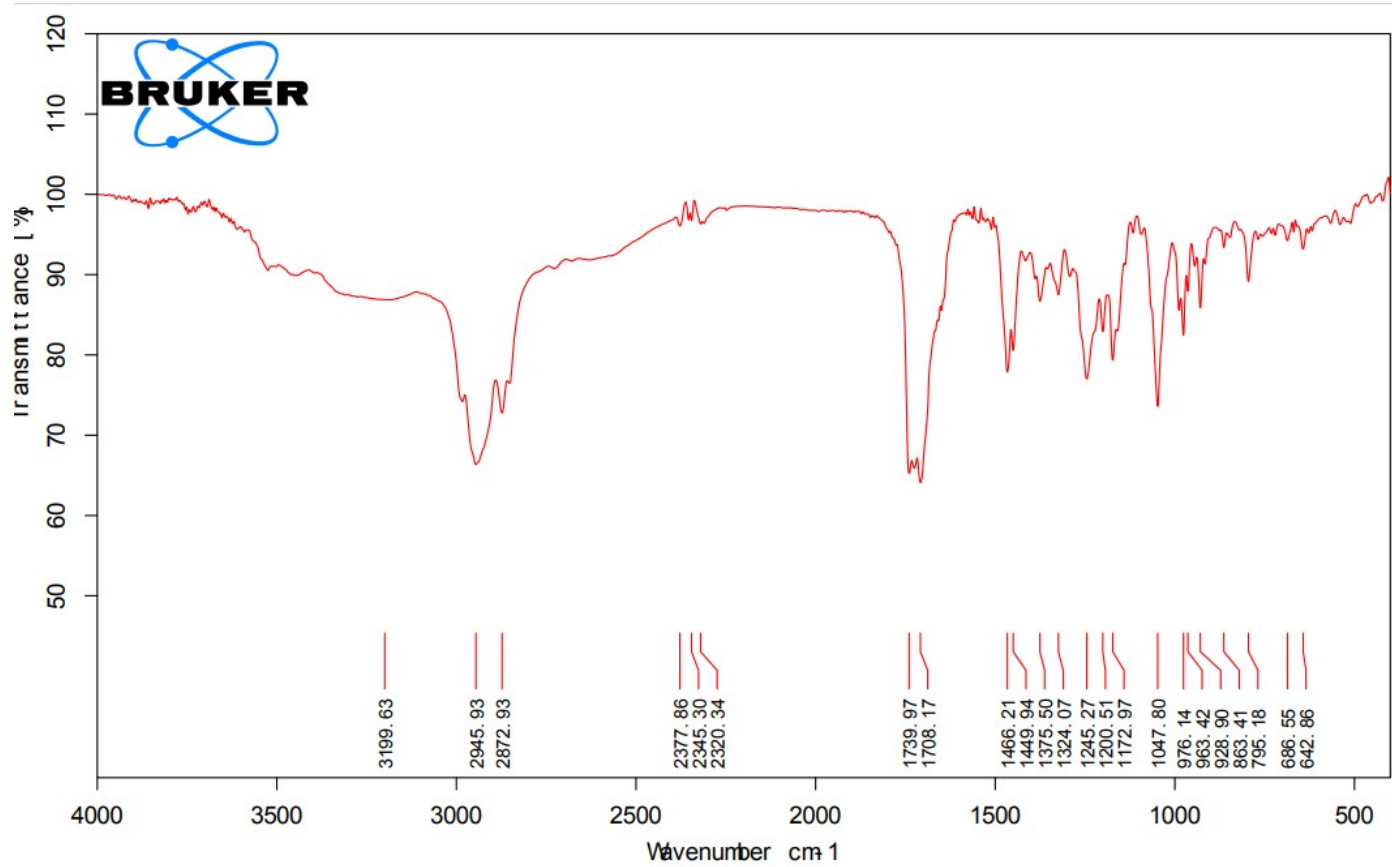


Figure S37. IR spectrum of Nouveinsiancin D (4)

Rudolph Research Analytical

Wednesday, 02/09/2022

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-39
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum						
6	-108.333	0.0000	-108.333	-108.333						
S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-39	04:04:41 PM	-108.333	SR	-0.065	589	100.00	0.060	19.7	
2	LJM-39	04:04:47 PM	-108.333	SR	-0.065	589	100.00	0.060	19.7	
3	LJM-39	04:04:53 PM	-108.333	SR	-0.065	589	100.00	0.060	19.7	
4	LJM-39	04:04:58 PM	-108.333	SR	-0.065	589	100.00	0.060	19.7	
5	LJM-39	04:05:04 PM	-108.333	SR	-0.065	589	100.00	0.060	19.8	
6	LJM-39	04:05:10 PM	-108.333	SR	-0.065	589	100.00	0.060	19.8	

Signature

Figure S38. OR Value of Noueinsiancin D (4) in CH₃OH

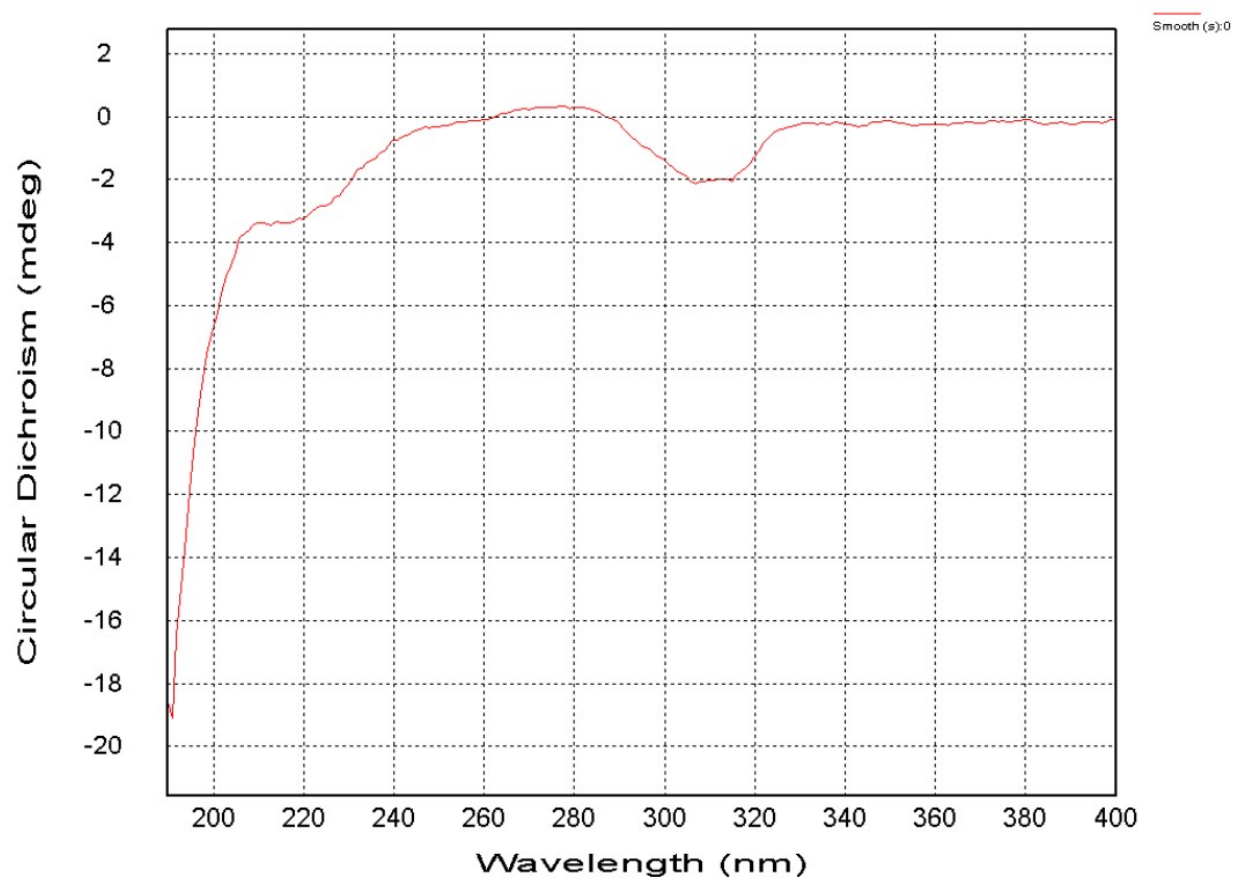


Figure S39. CD Value of Noueinsiancin D (4) in CH₃OH

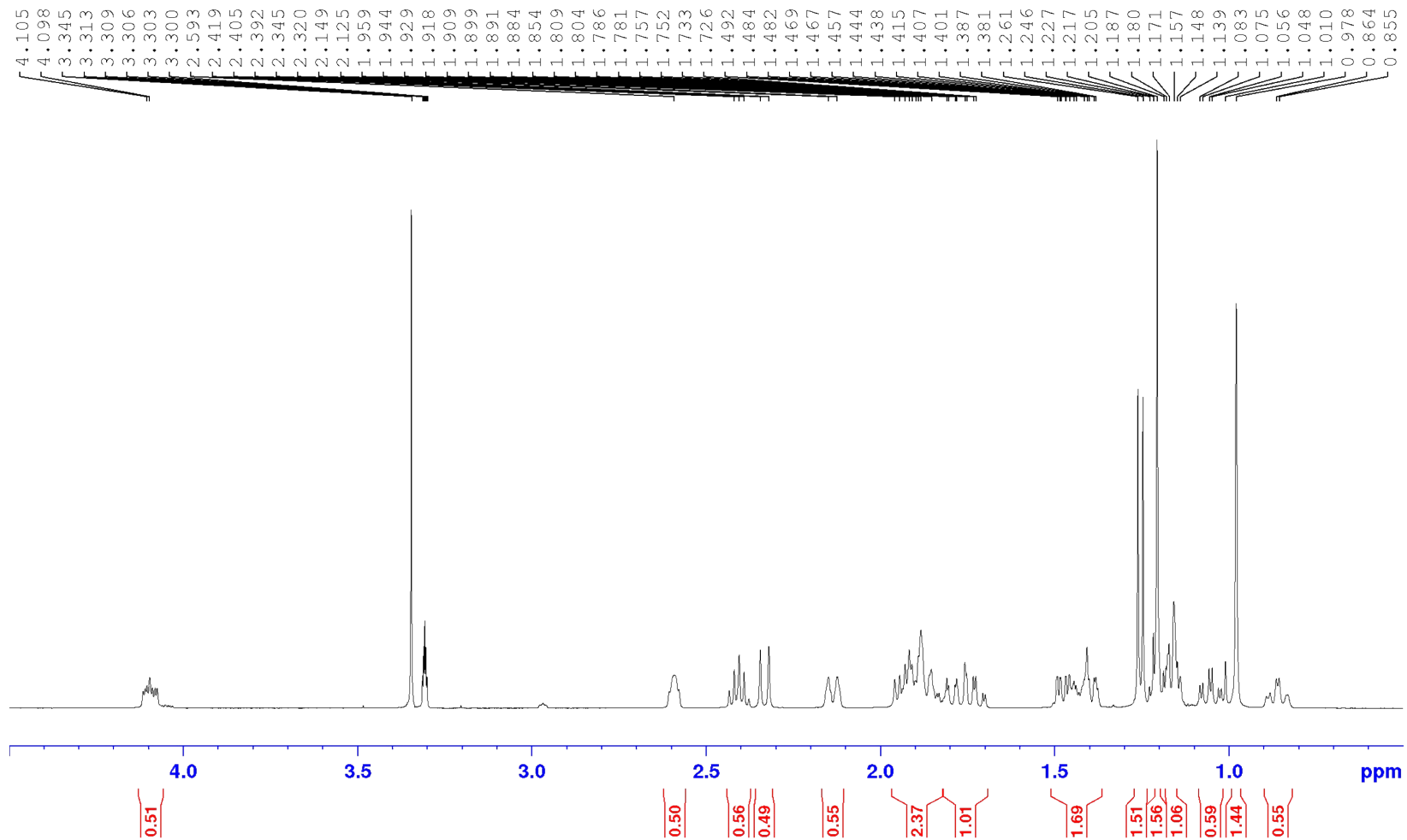


Figure S40. ¹H NMR spectrum of Noueinsiancin D (4) in CD₃OD

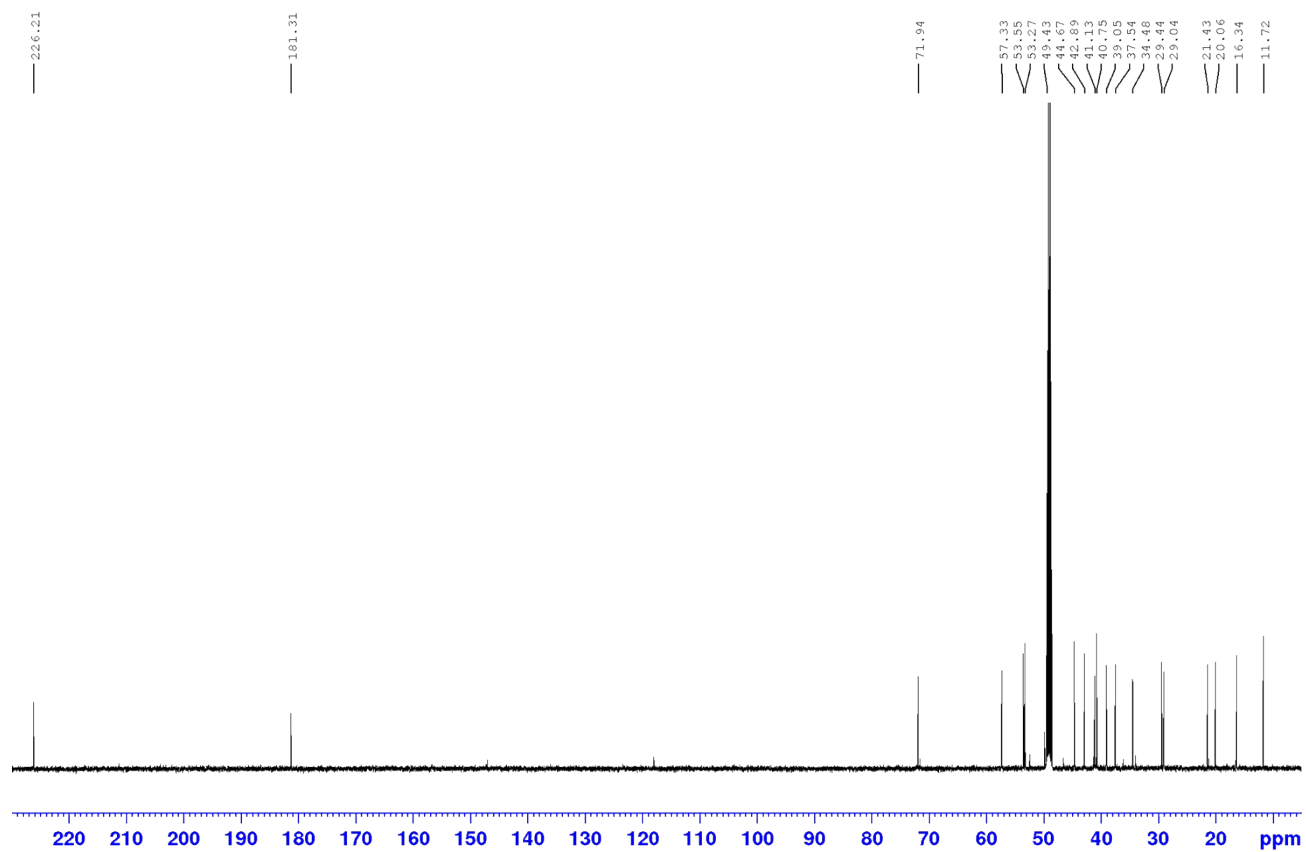


Figure S41. ^{13}C NMR spectrum of Noueinsiancin D (4) in CD_3OD

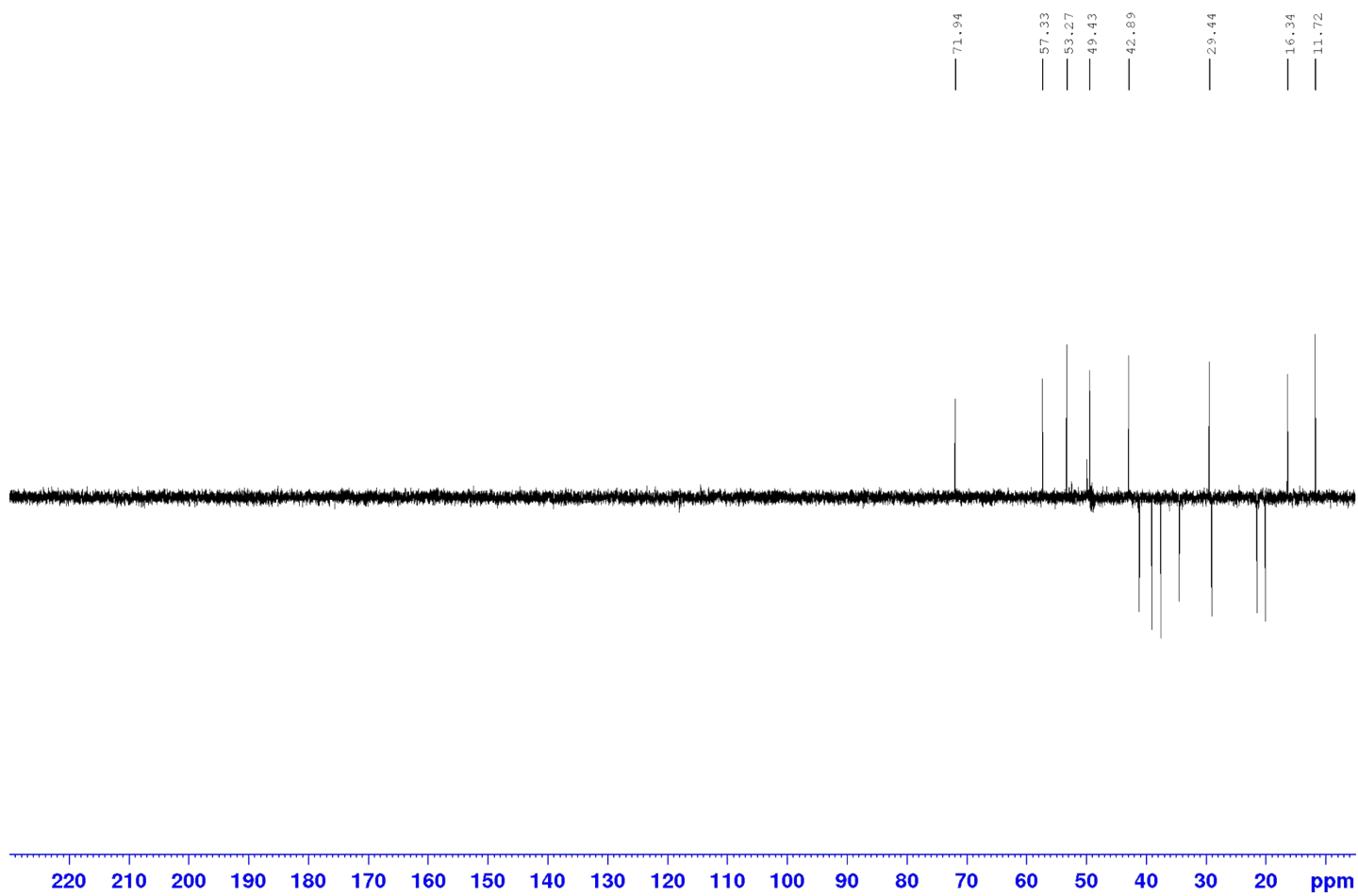


Figure S42. DEPT-135 NMR spectrum of Noueinsiancin D (4) in CD₃OD

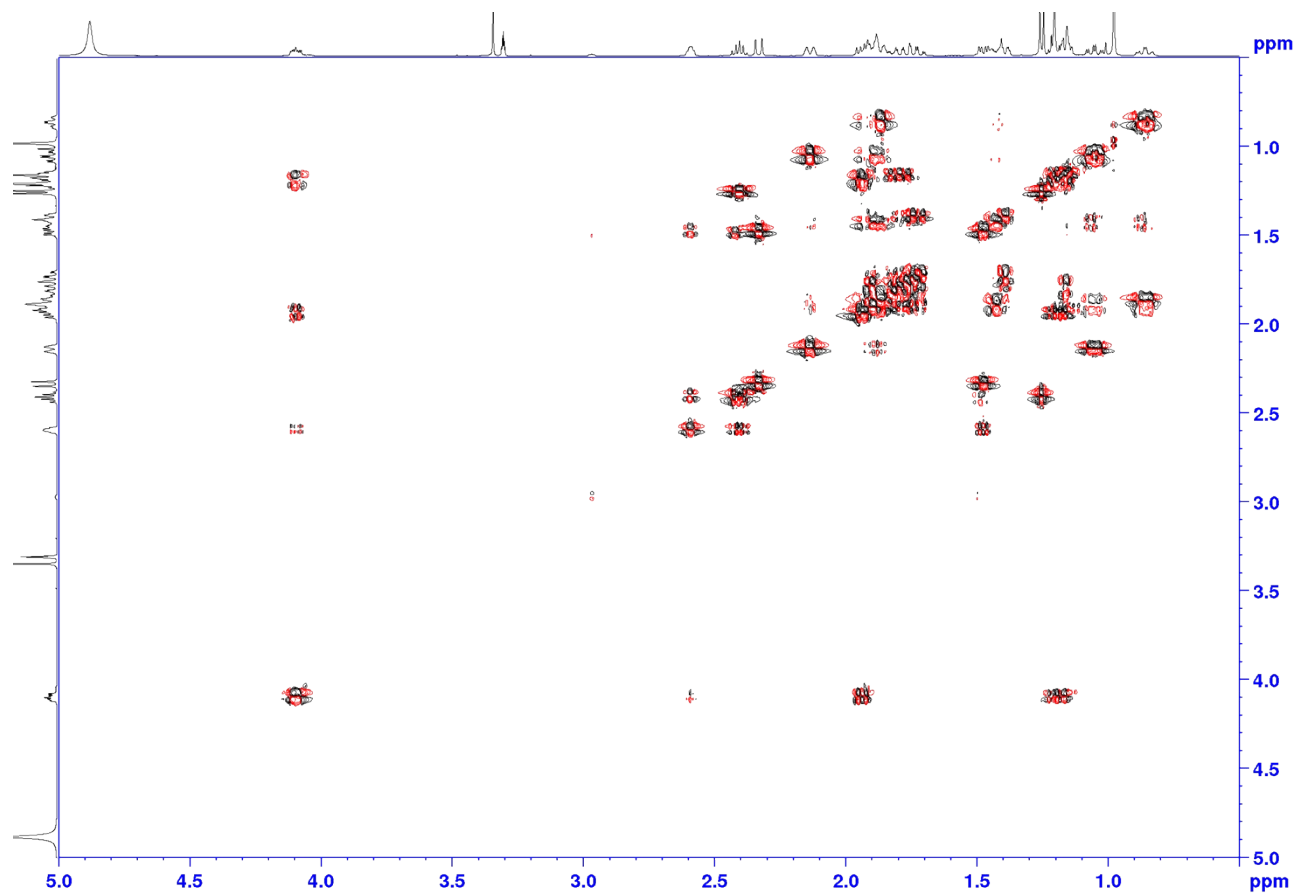


Figure S43. ^1H - ^1H COSY spectrum of Nouveinsiancin D (4) in CD_3OD

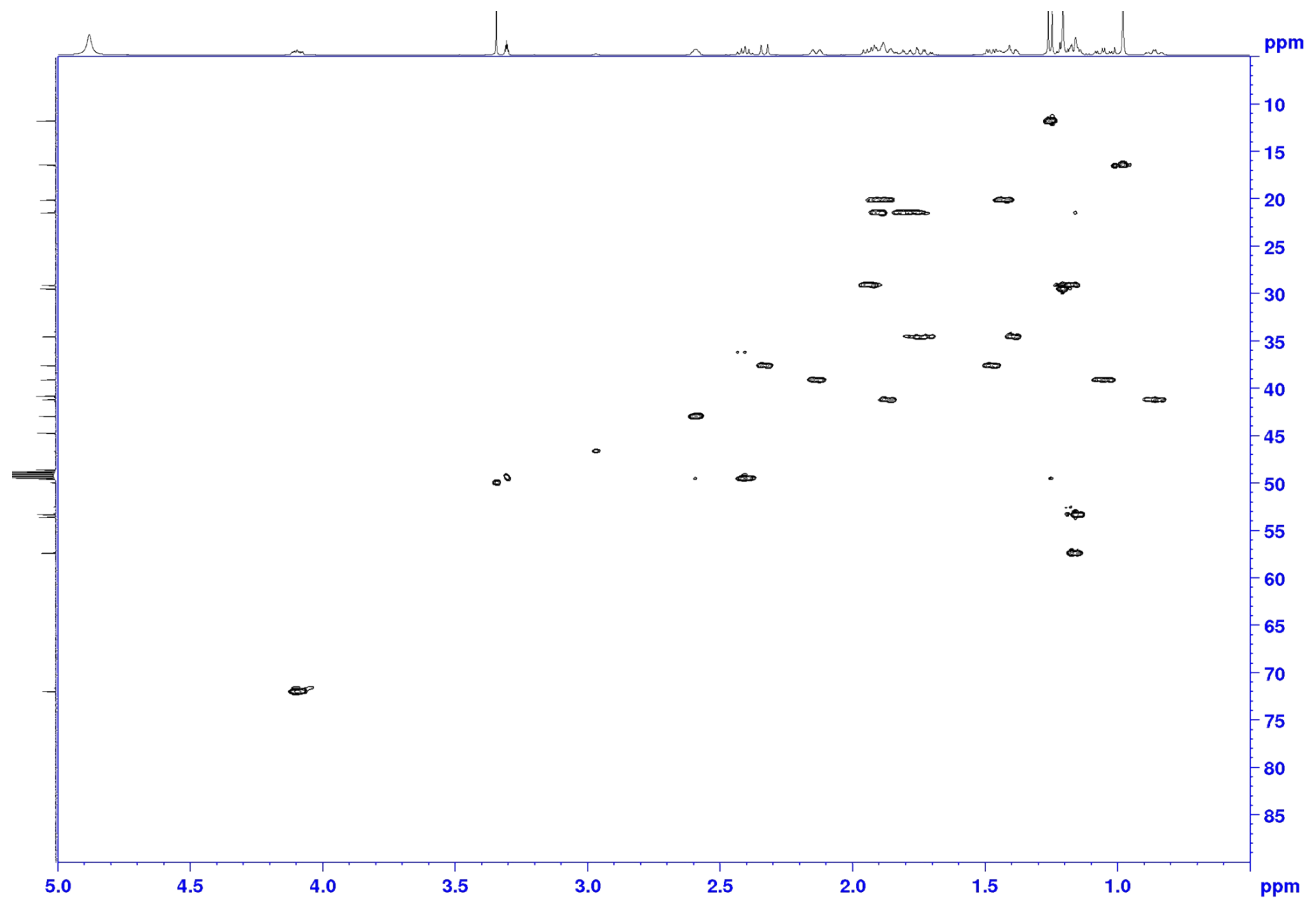


Figure S44. HSQC spectrum of Noueinsiancin D (4) in CD₃OD

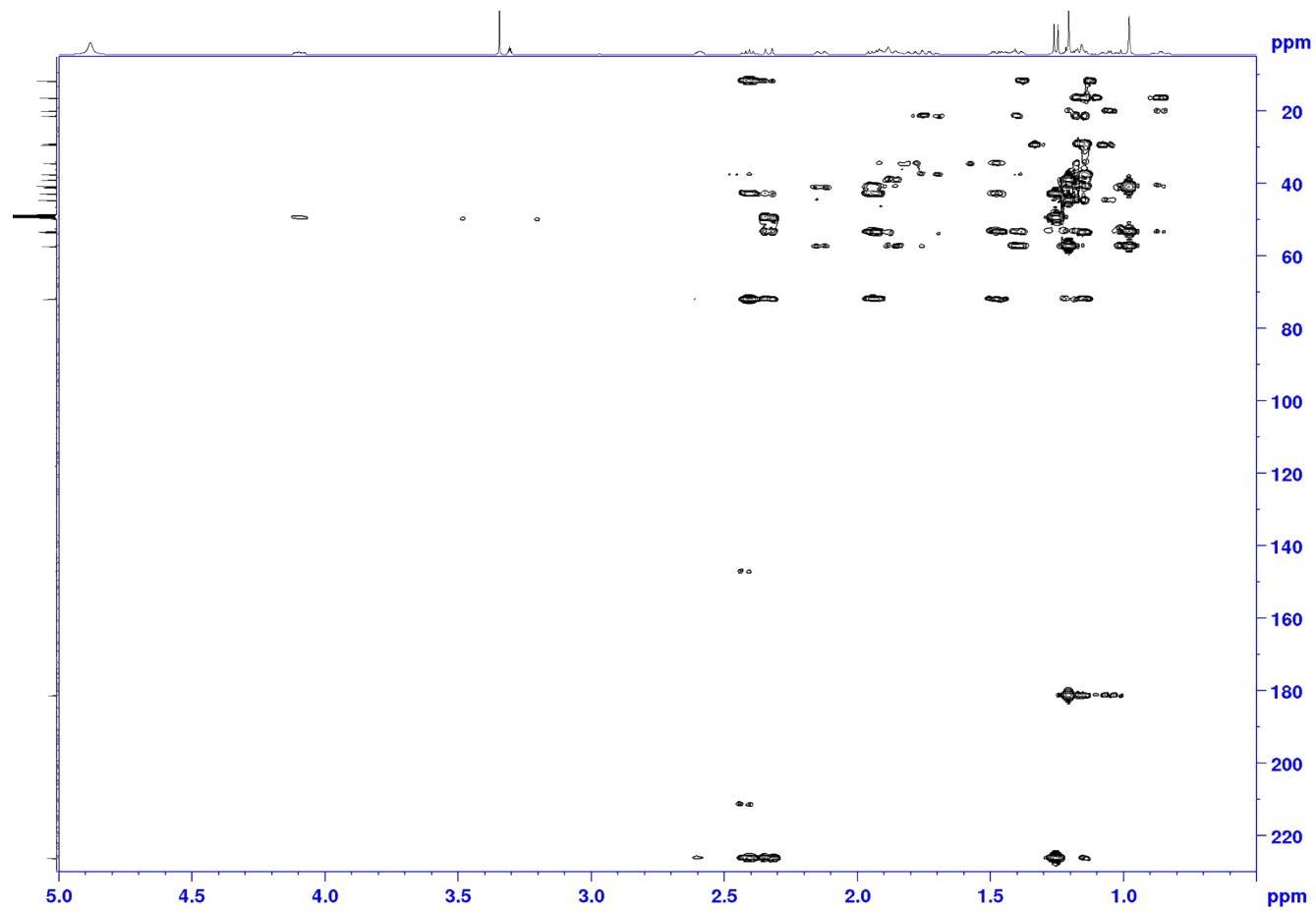


Figure S45. HMBC spectrum of Noueinsiancin D (4) in CD₃OD

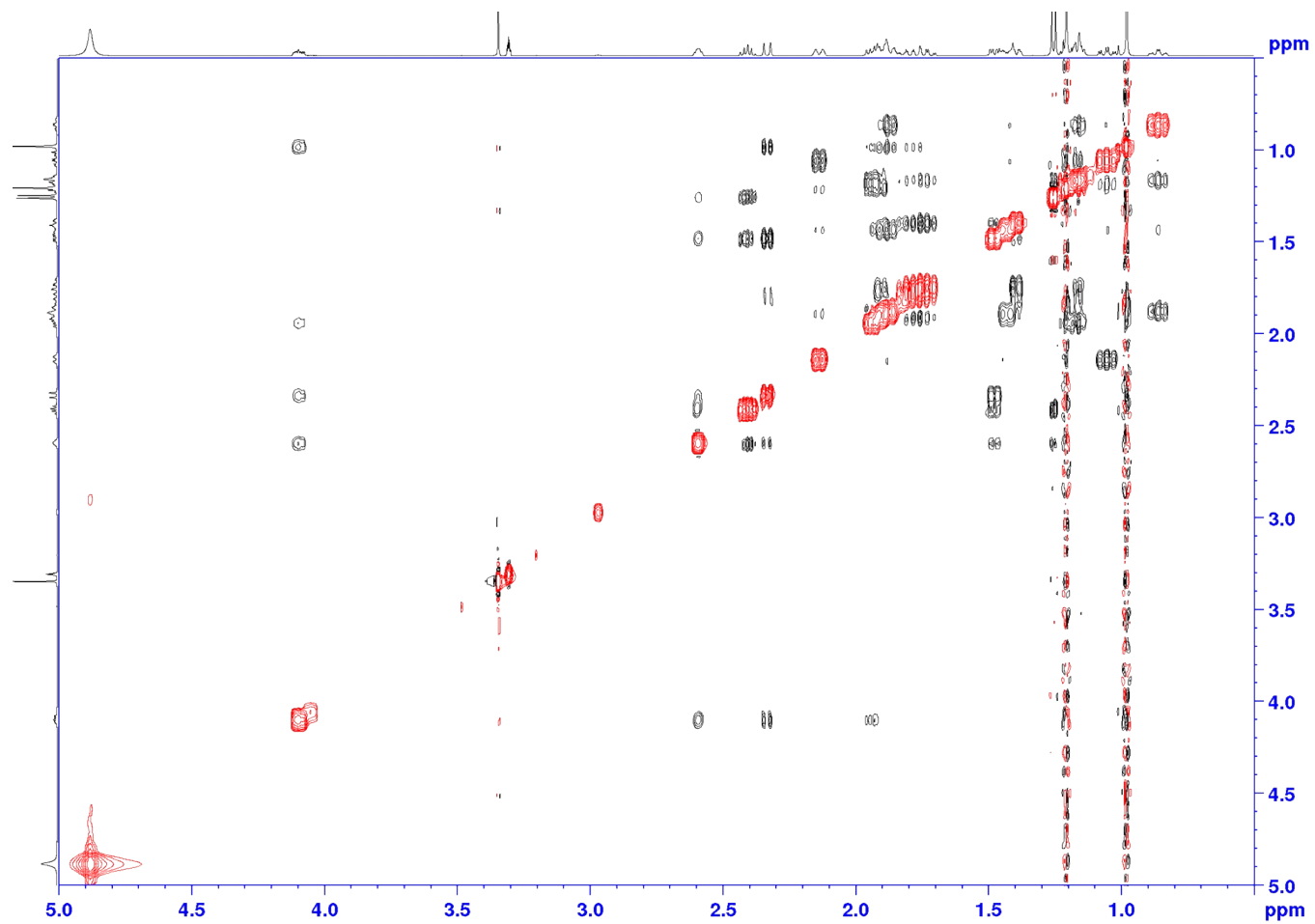


Figure S46. NOESY spectrum of Noueinsiancin D (4) in CD₃OD

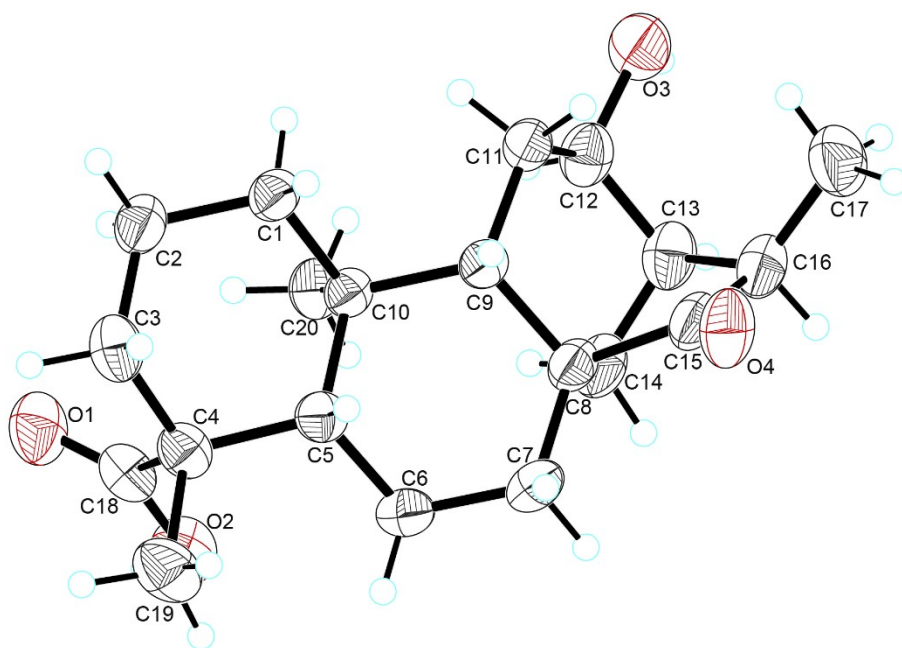
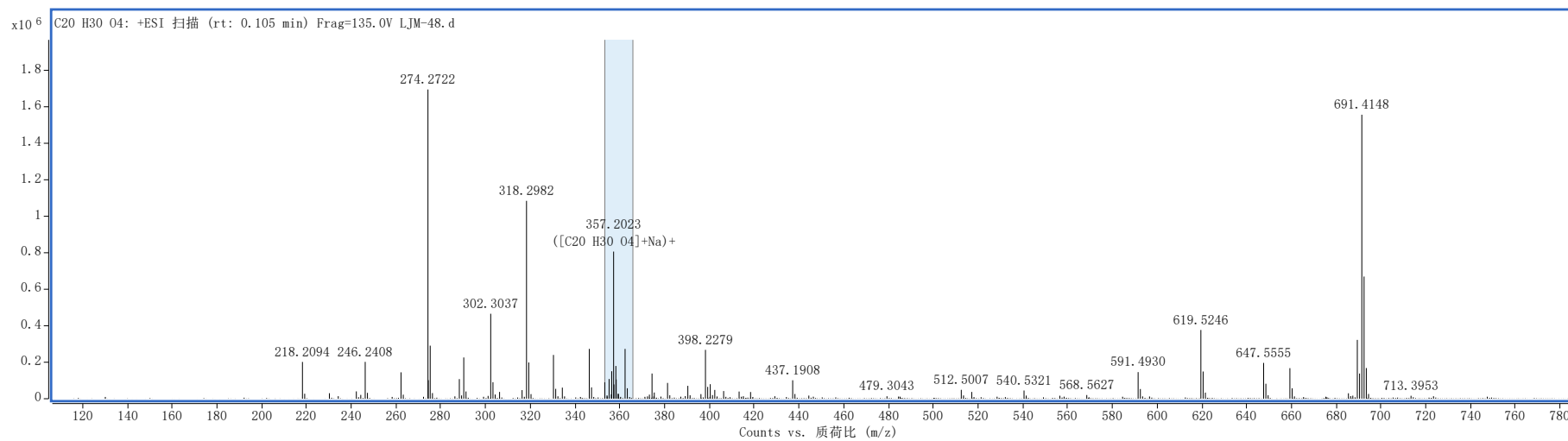


Figure S47. X-ray structure of Noueinsiancin D (4)



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H30 O4	(M+Na)+	357.2023	92.42	4.59	92.42

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.8	809437.4	100	357.2036	1.3	807306.1	100	79.6	357.2023	3.75

Figure S48. HRESIMS spectrum of Noueinsiancin E (5)

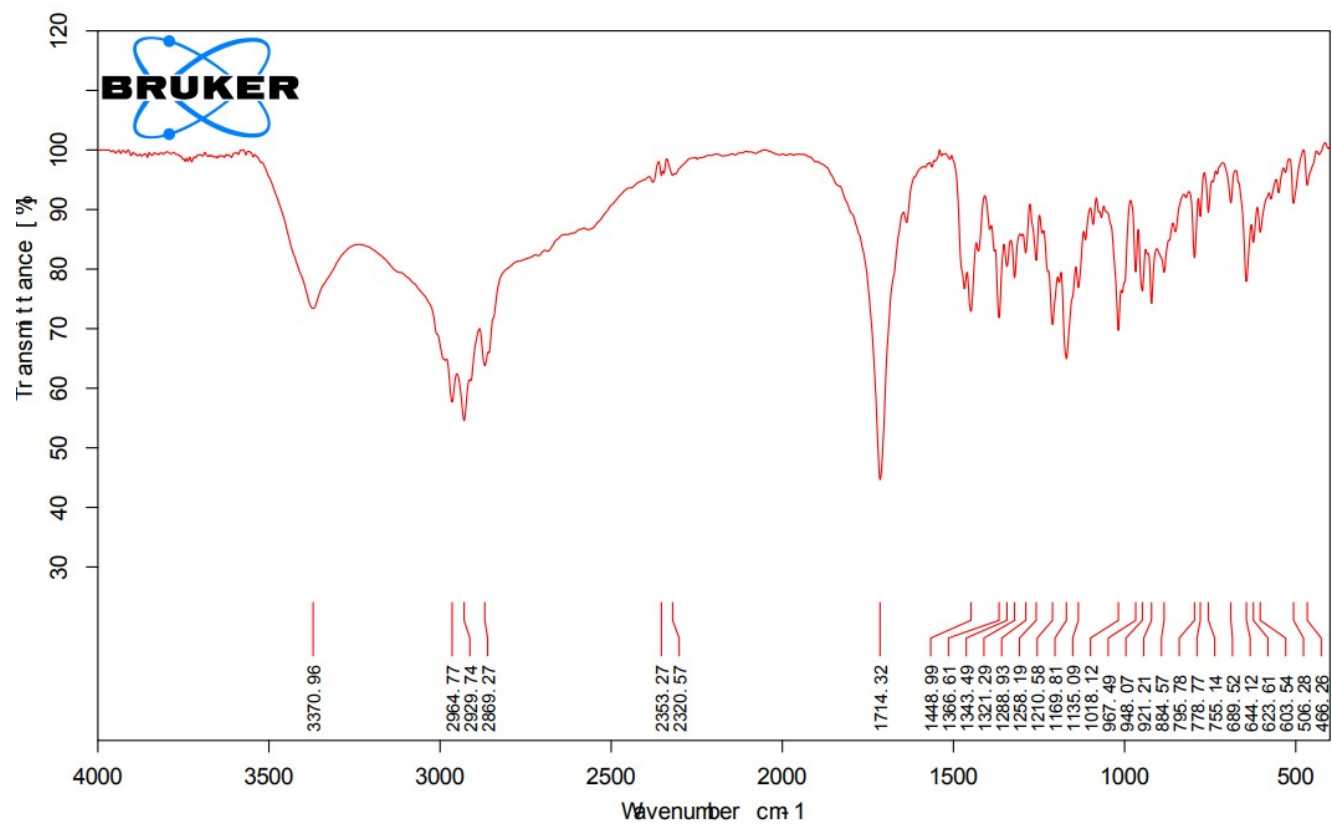


Figure S49. IR spectrum of Noueinsiancin E (5)

Rudolph Research Analytical

Wednesday, 02/09/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-48
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-140.167	0.6872	-139.000	-141.000

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-48	04:15:44 PM	-141.000	SR	-0.141	589	100.00	0.100	20.1	
2	LJM-48	04:15:49 PM	-141.000	SR	-0.141	589	100.00	0.100	20.1	
3	LJM-48	04:15:55 PM	-140.000	SR	-0.140	589	100.00	0.100	20.1	
4	LJM-48	04:16:01 PM	-140.000	SR	-0.140	589	100.00	0.100	20.1	
5	LJM-48	04:16:07 PM	-140.000	SR	-0.140	589	100.00	0.100	20.0	
6	LJM-48	04:16:13 PM	-139.000	SR	-0.139	589	100.00	0.100	20.0	

Signature

Figure S50. OR Value of Noueinsiancin E (5) in CH₃OH

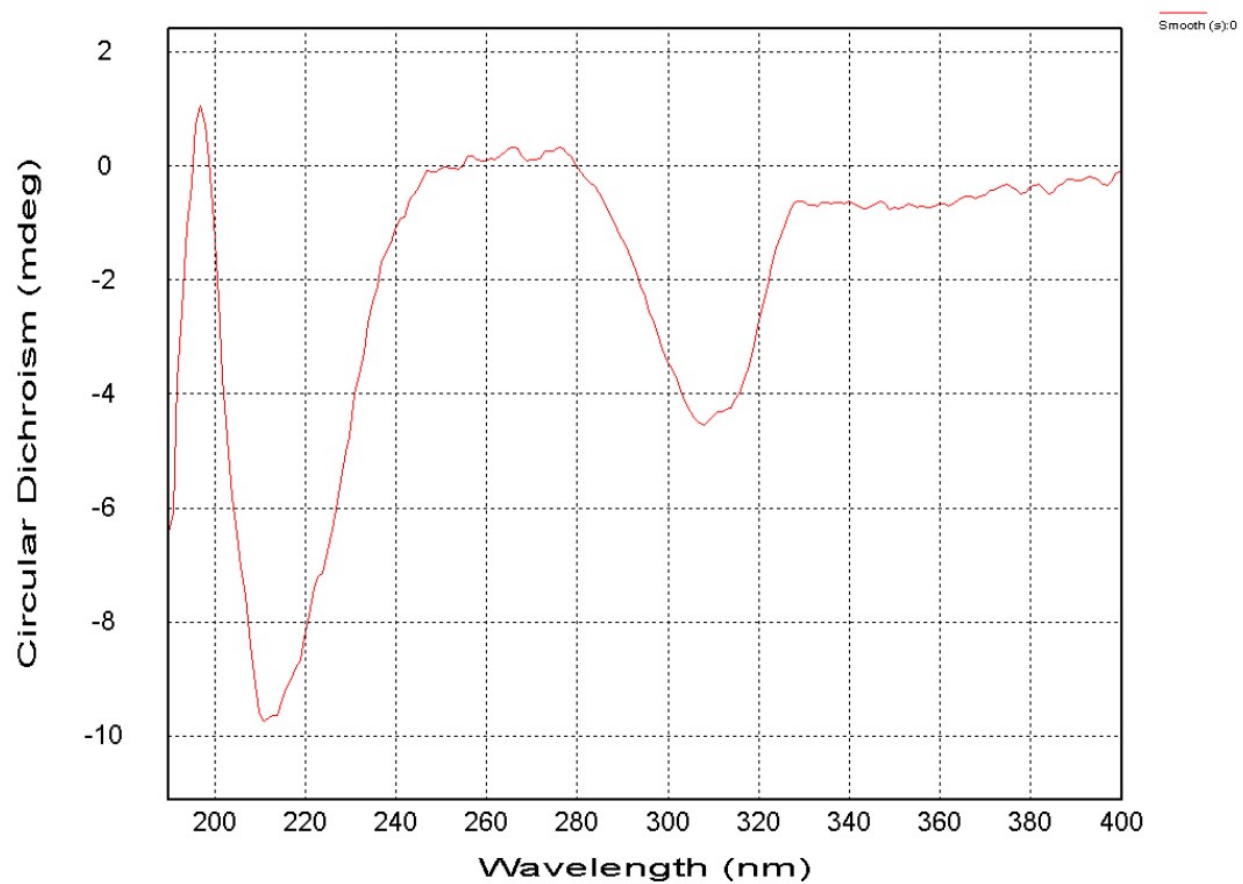


Figure S51. CD Value of Noueinsiancin E (5) in CH₃OH

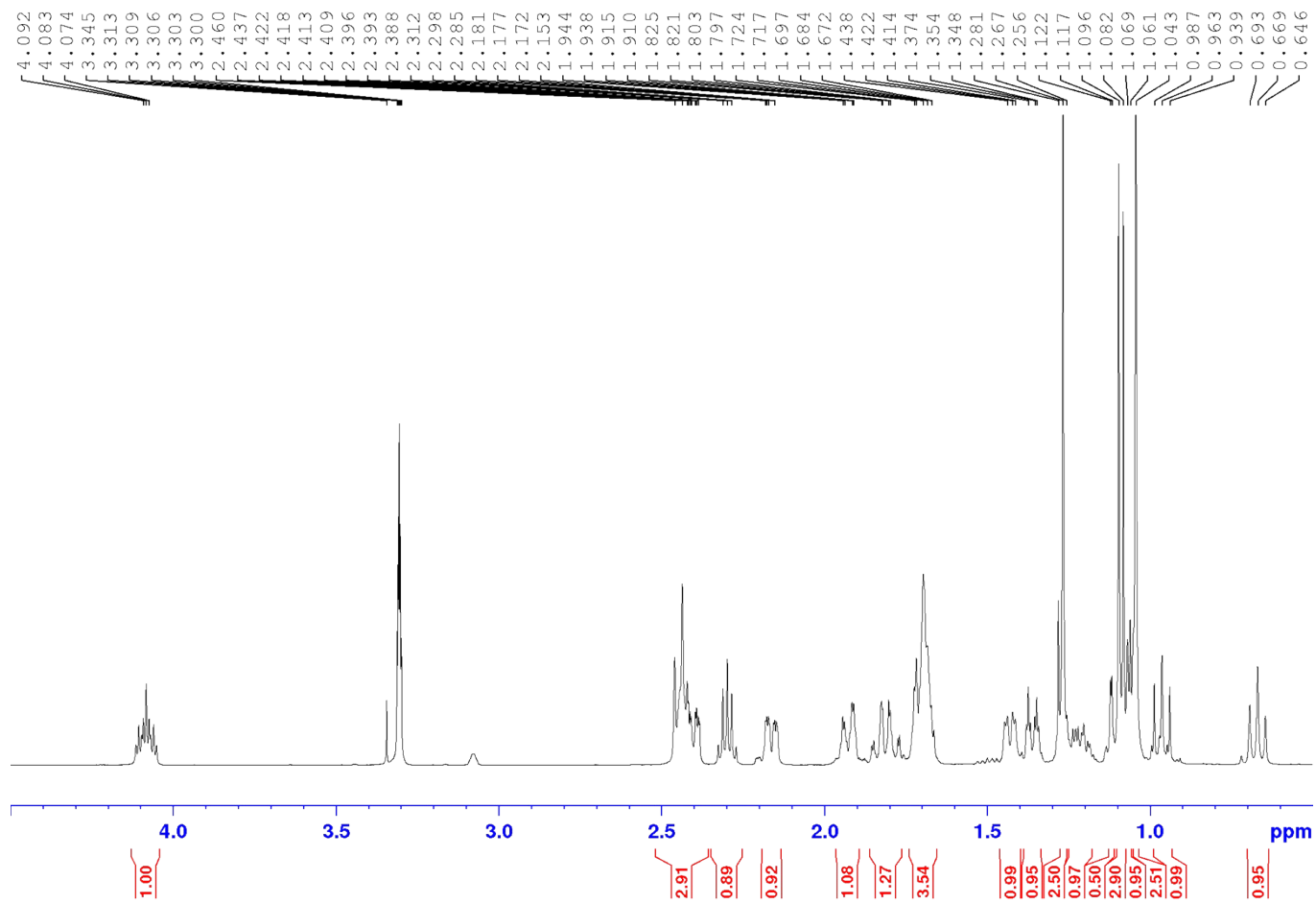


Figure S52. ¹H NMR spectrum of Noueinsiancin E (5) in CD₃OD

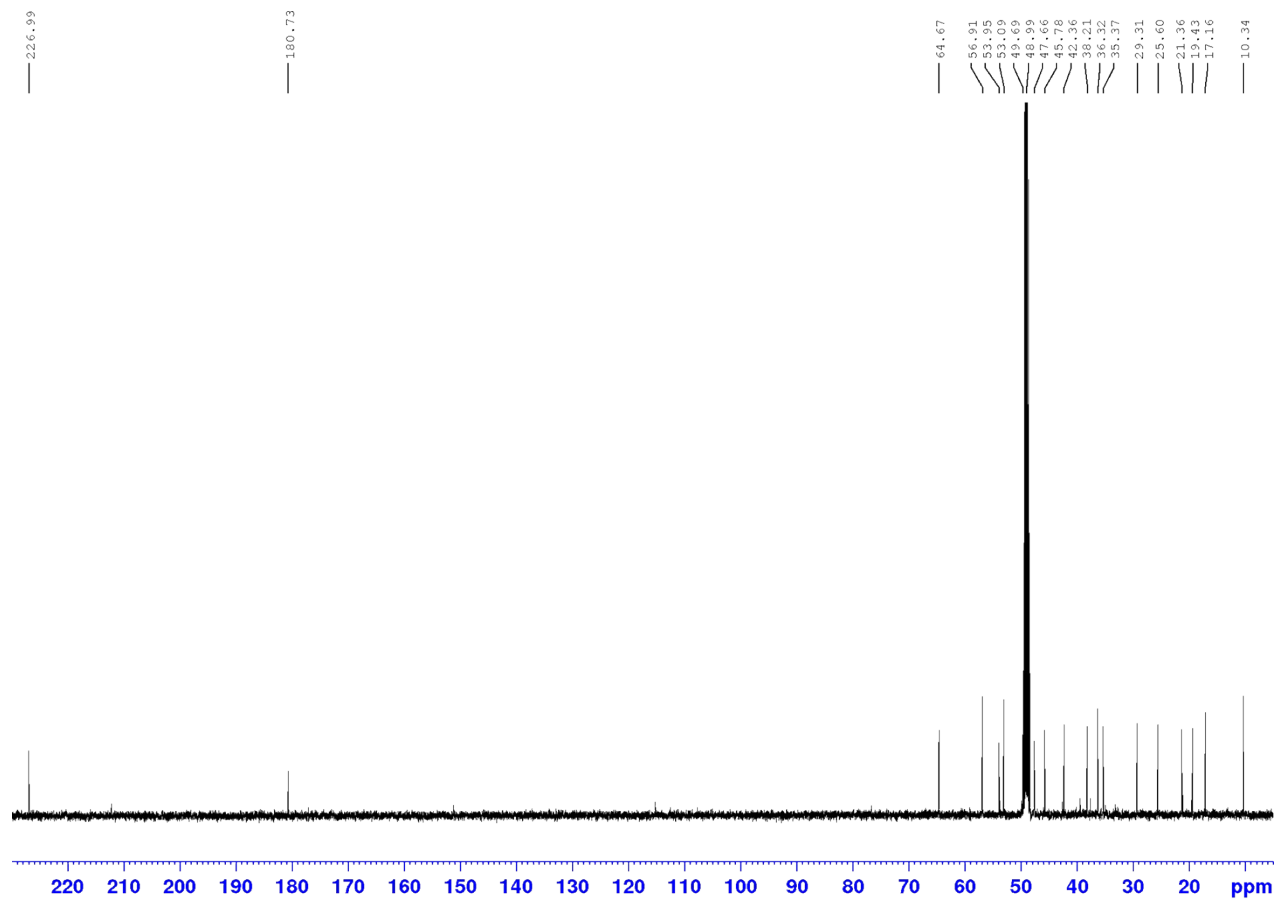


Figure S53. ¹³C NMR spectrum of Noueinsiancin E (5) in CD₃OD

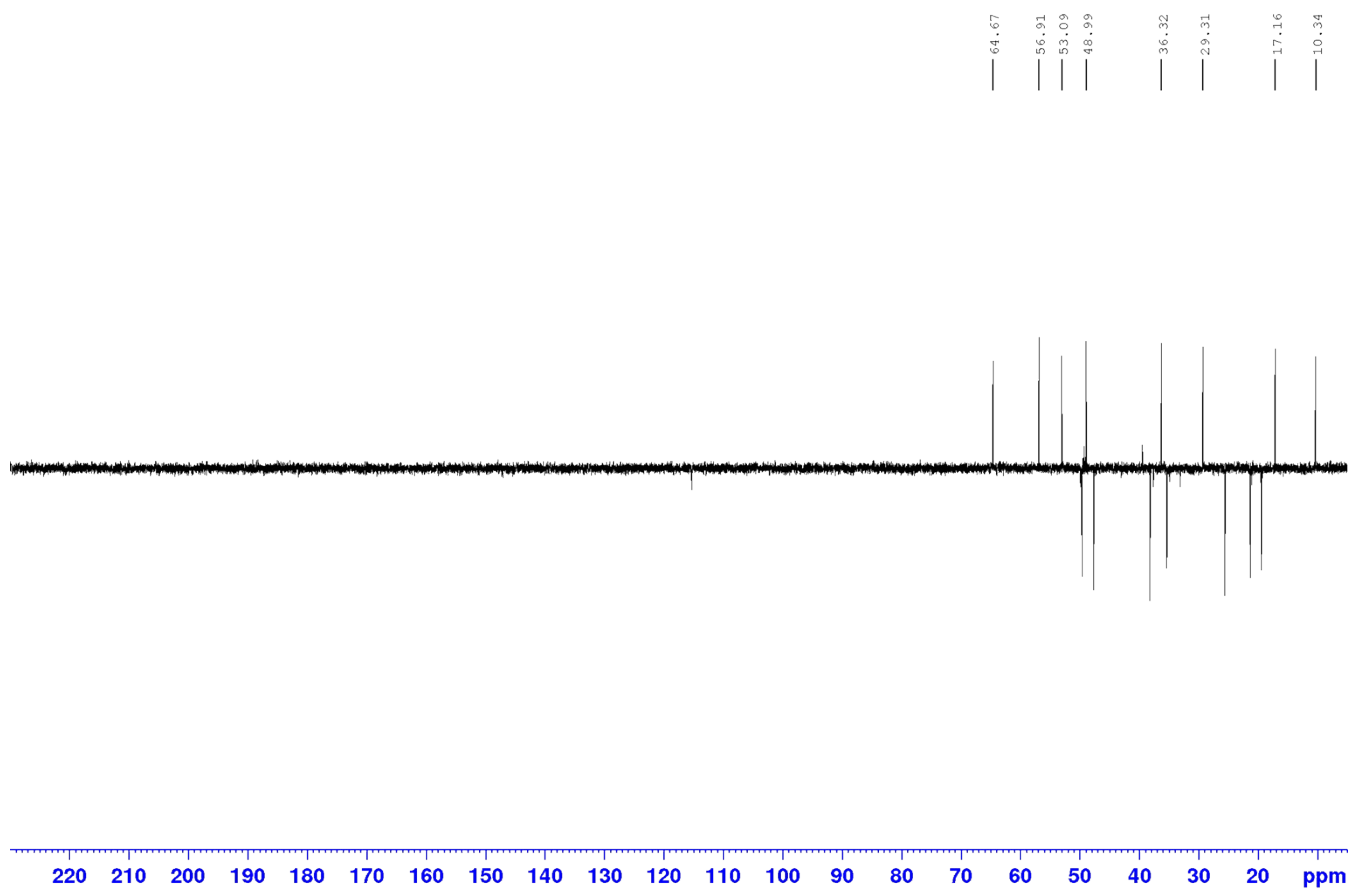


Figure S54. DEPT-135 NMR spectrum of Noueinsiancin E (5) in CD₃OD



Figure S55. ^1H - ^1H COSY spectrum of Noueinsiancin E (5) in CD_3OD

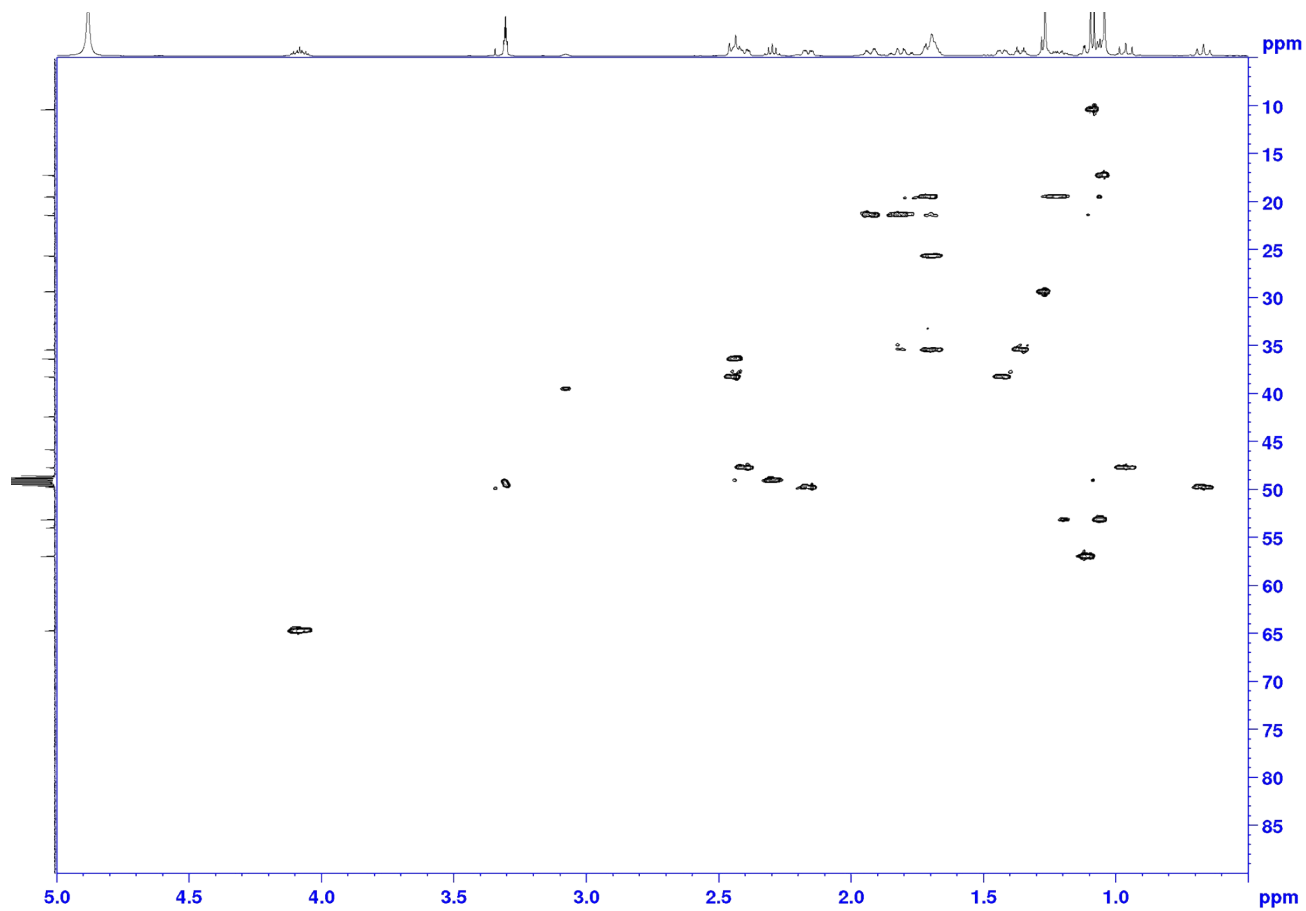


Figure S56. HSQC spectrum of Noueinsiancin E (5) in CD₃OD

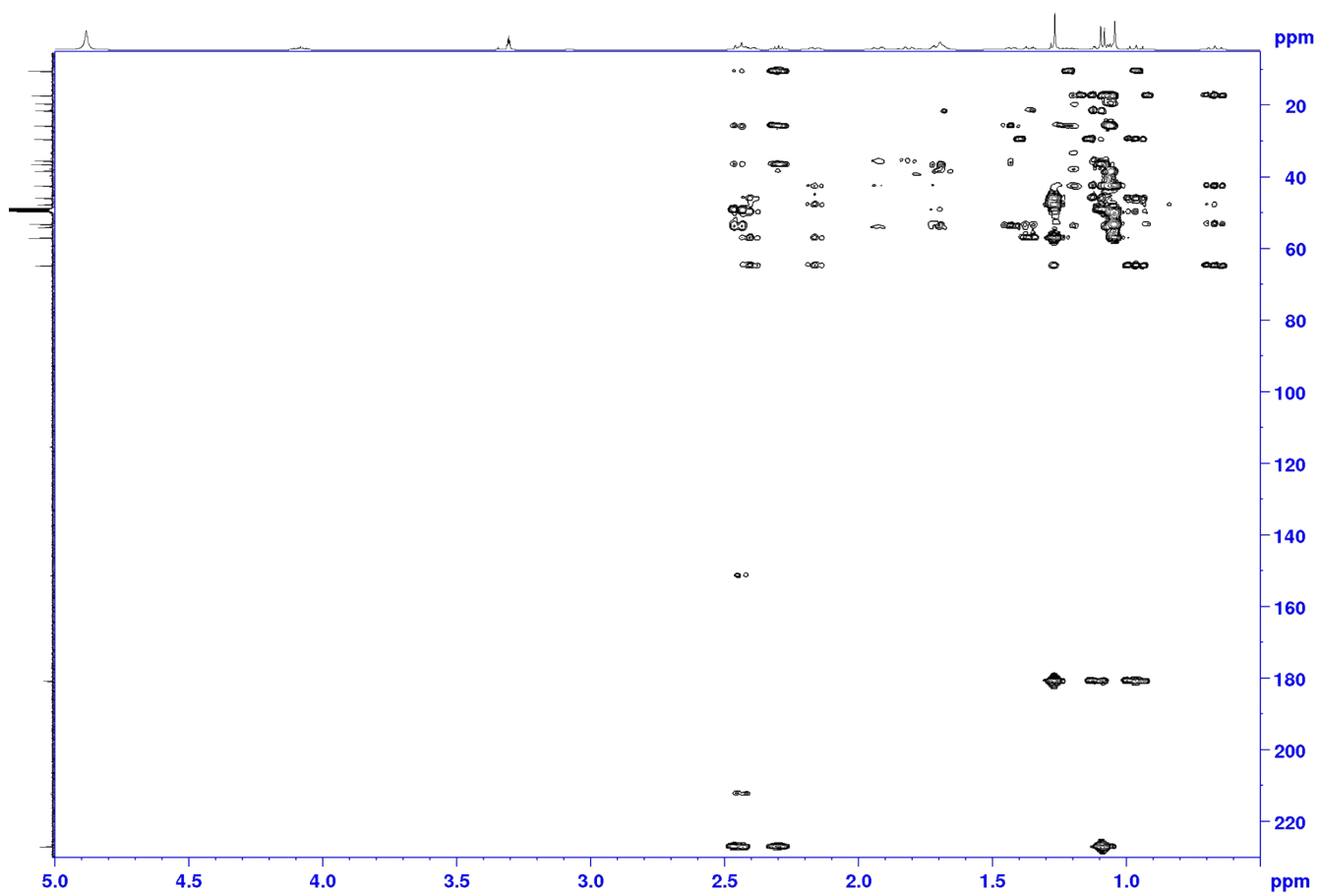


Figure S57. HMBC spectrum of Noueinsiancin E (5) in CD₃OD

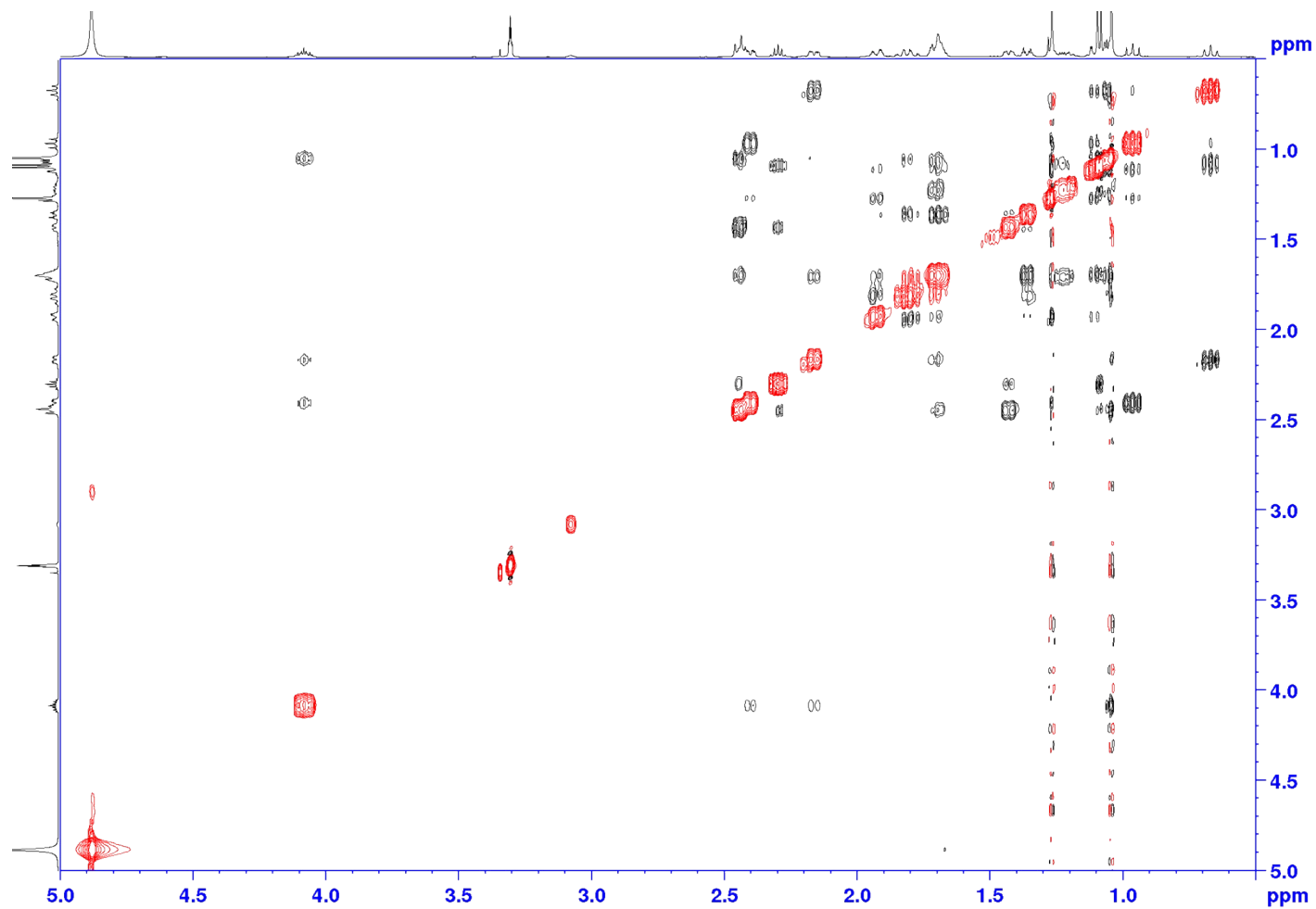


Figure S58. NOESY spectrum of Noueinsiancin E (5) in CD₃OD

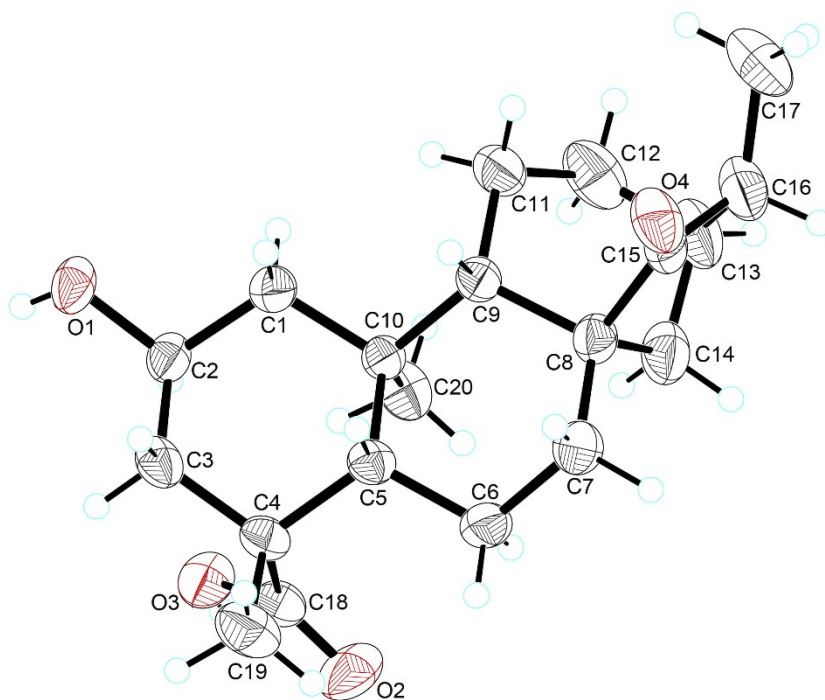
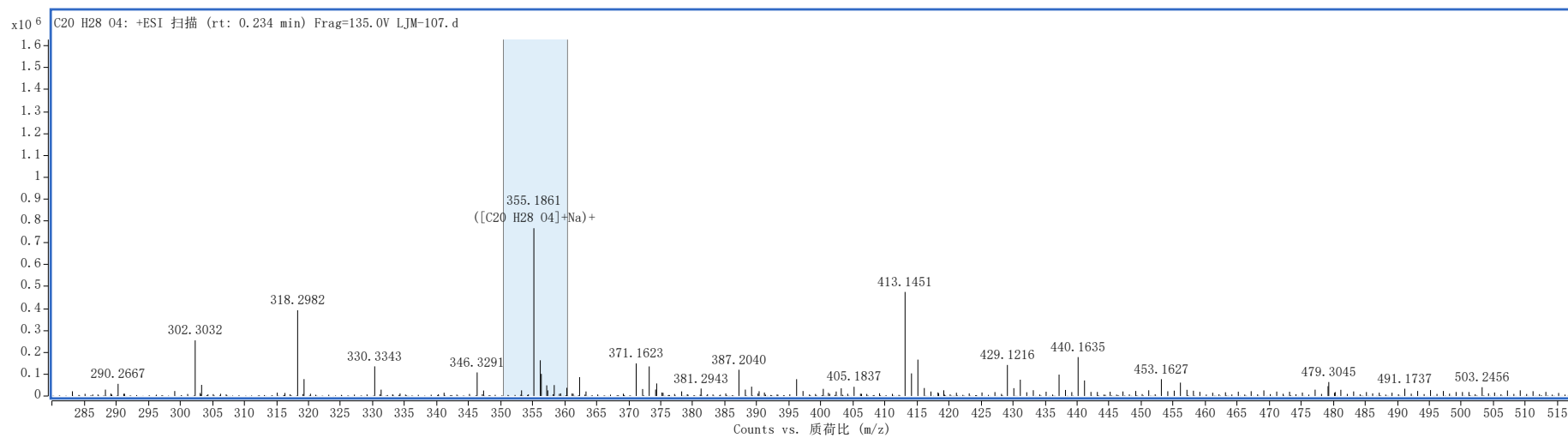


Figure S59. X-ray structure of Nouveinsiancin E (5)



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H28 O4	(M+Na)+	355.1861	86.1	5.69	86.1

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.8	781568.1	100	355.188	1.8	766863.7	100	78.3	355.1861	5.17

Figure S60. HRESIMS spectrum of Noueinsiancin F (6)

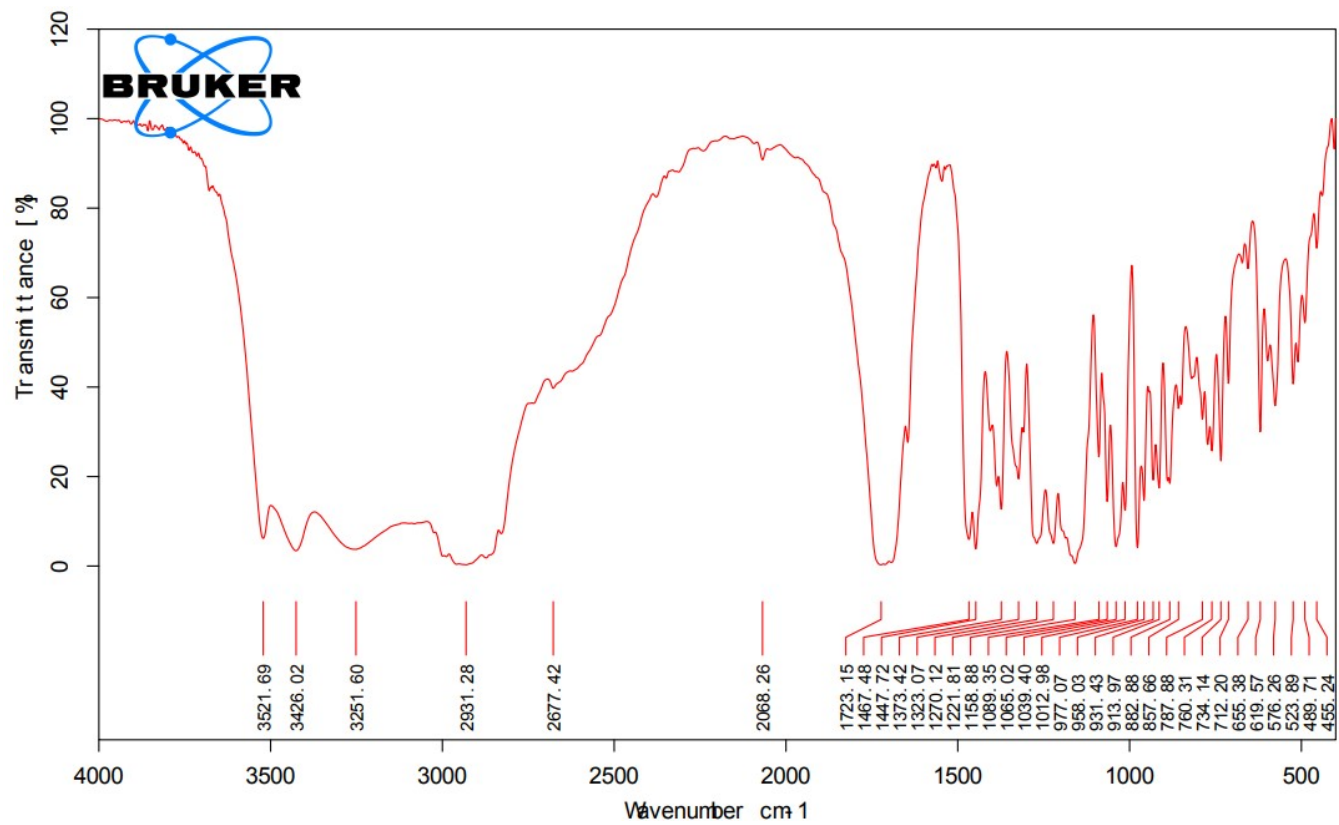


Figure S61. IR spectrum of Nouveinsiancin F (6)

Rudolph Research Analytical

Thursday, 02/10/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-109
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum						
6	-116.667	0.9428	-116.000	-118.000						
S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-109	08:01:05 PM	-116.000	SR	-0.058	589	100.00	0.050	19.7	
2	LJM-109	08:01:10 PM	-118.000	SR	-0.059	589	100.00	0.050	19.7	
3	LJM-109	08:01:16 PM	-116.000	SR	-0.058	589	100.00	0.050	19.7	
4	LJM-109	08:01:21 PM	-118.000	SR	-0.059	589	100.00	0.050	19.7	
5	LJM-109	08:01:27 PM	-116.000	SR	-0.058	589	100.00	0.050	19.7	
6	LJM-109	08:01:32 PM	-116.000	SR	-0.058	589	100.00	0.050	19.8	

Signature

Figure S62. OR Value of Noueinsiancin F (6) in CH₃OH

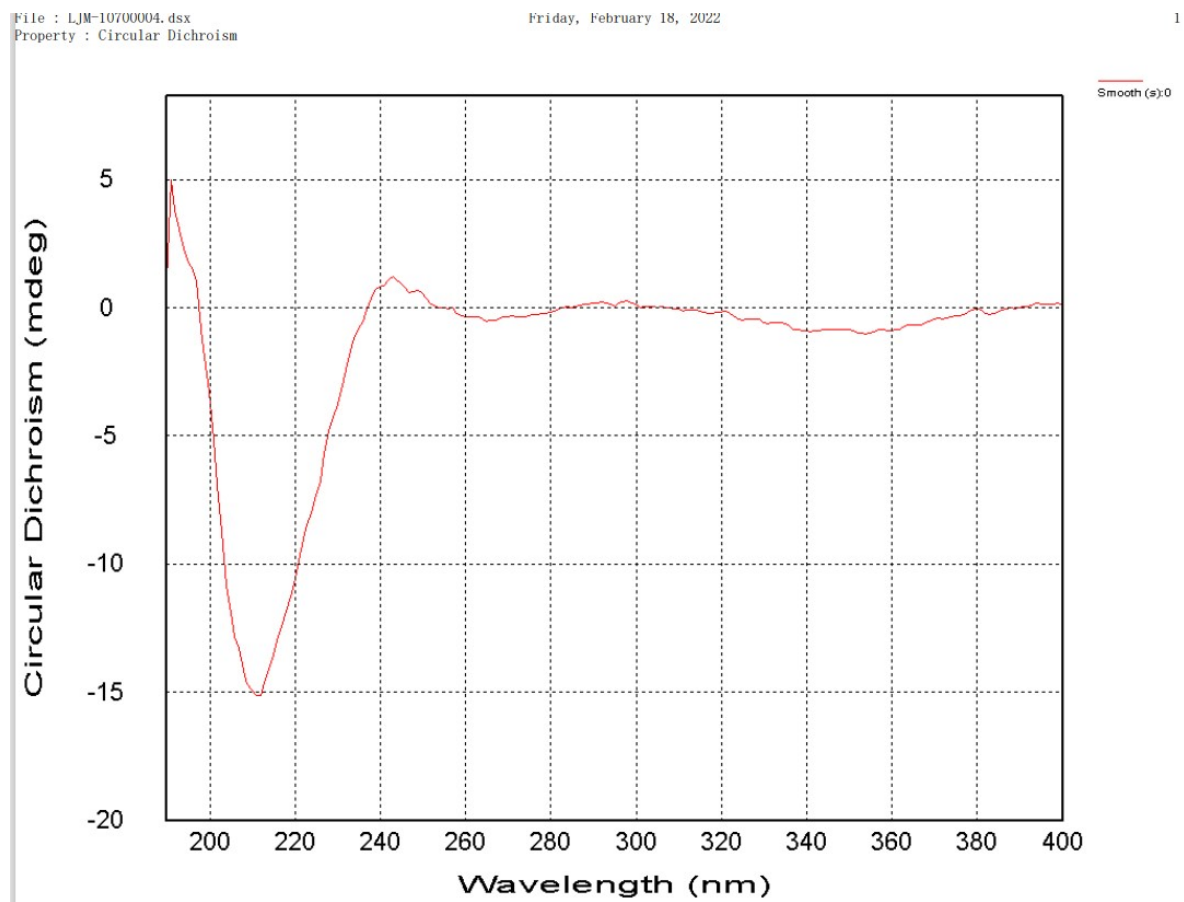


Figure S63. CD Value of Nouveinsancin F (6) in CH₃OH

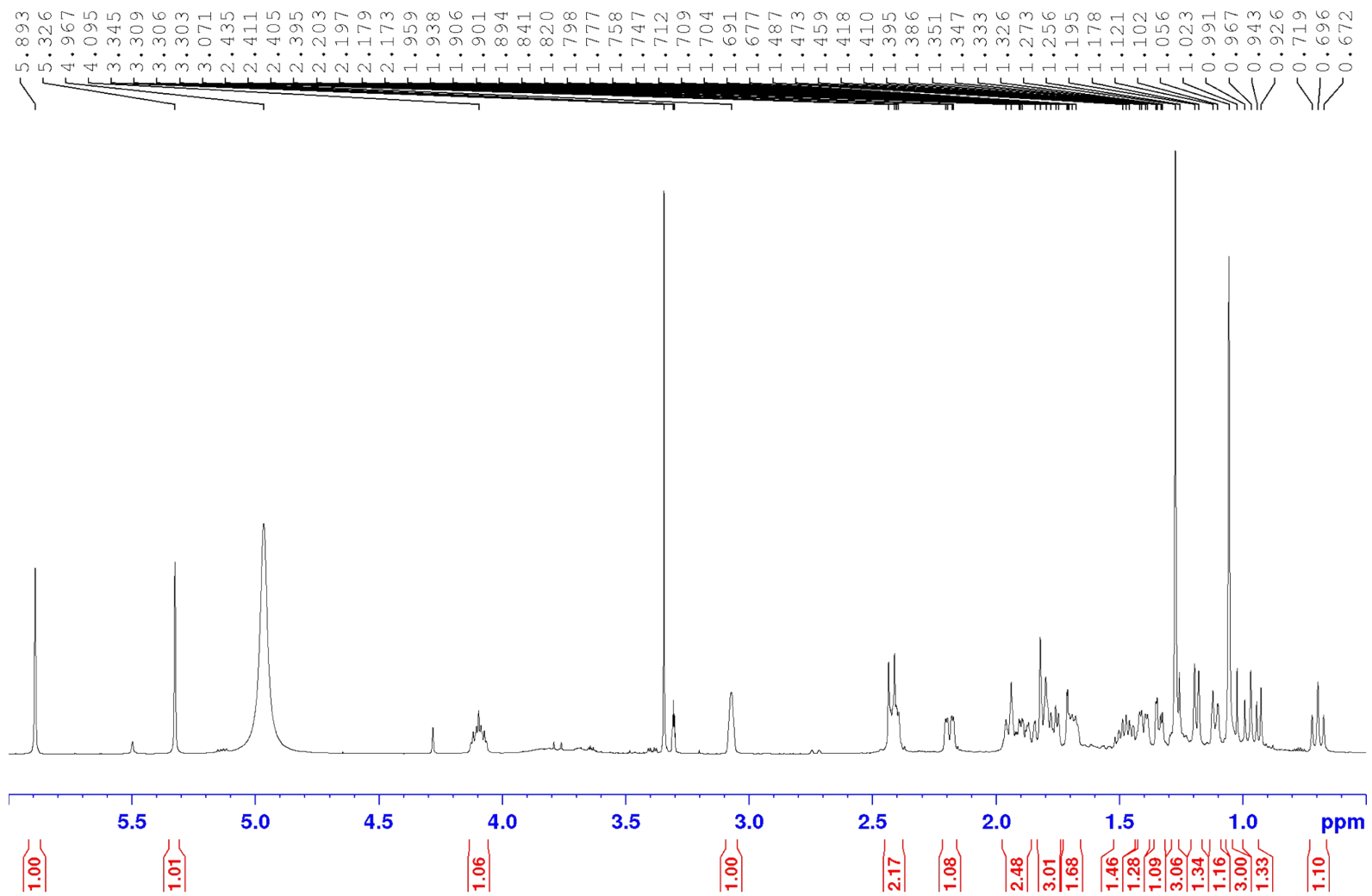


Figure S64. ¹H NMR spectrum of Noueinsiancin F (6) in CD₃OD

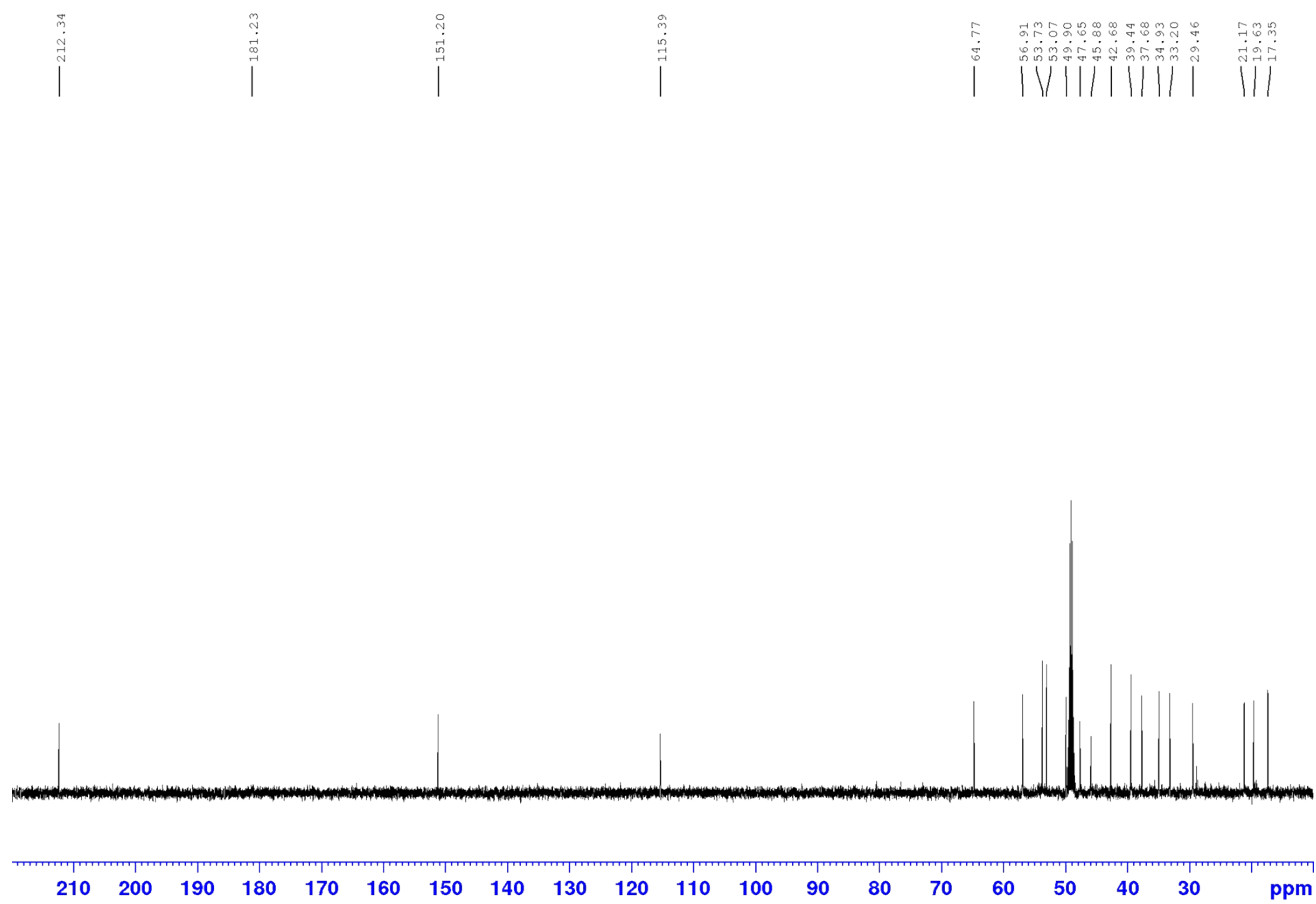


Figure S65. ^{13}C NMR spectrum of Nouveinsiancin F (6) in CD_3OD

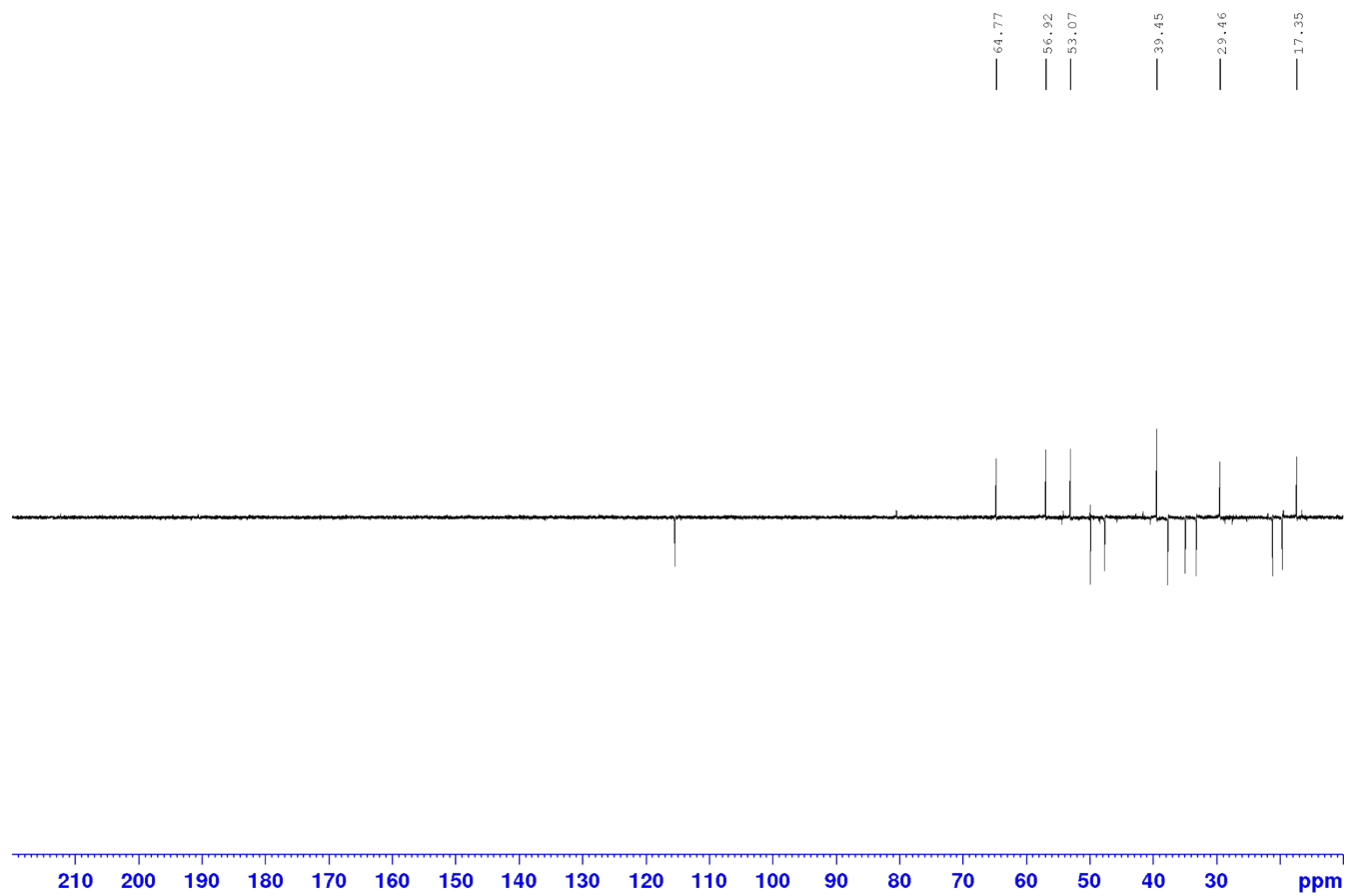


Figure S66. DEPT-135 NMR spectrum of Noueinsiancin F (6) in CD₃OD

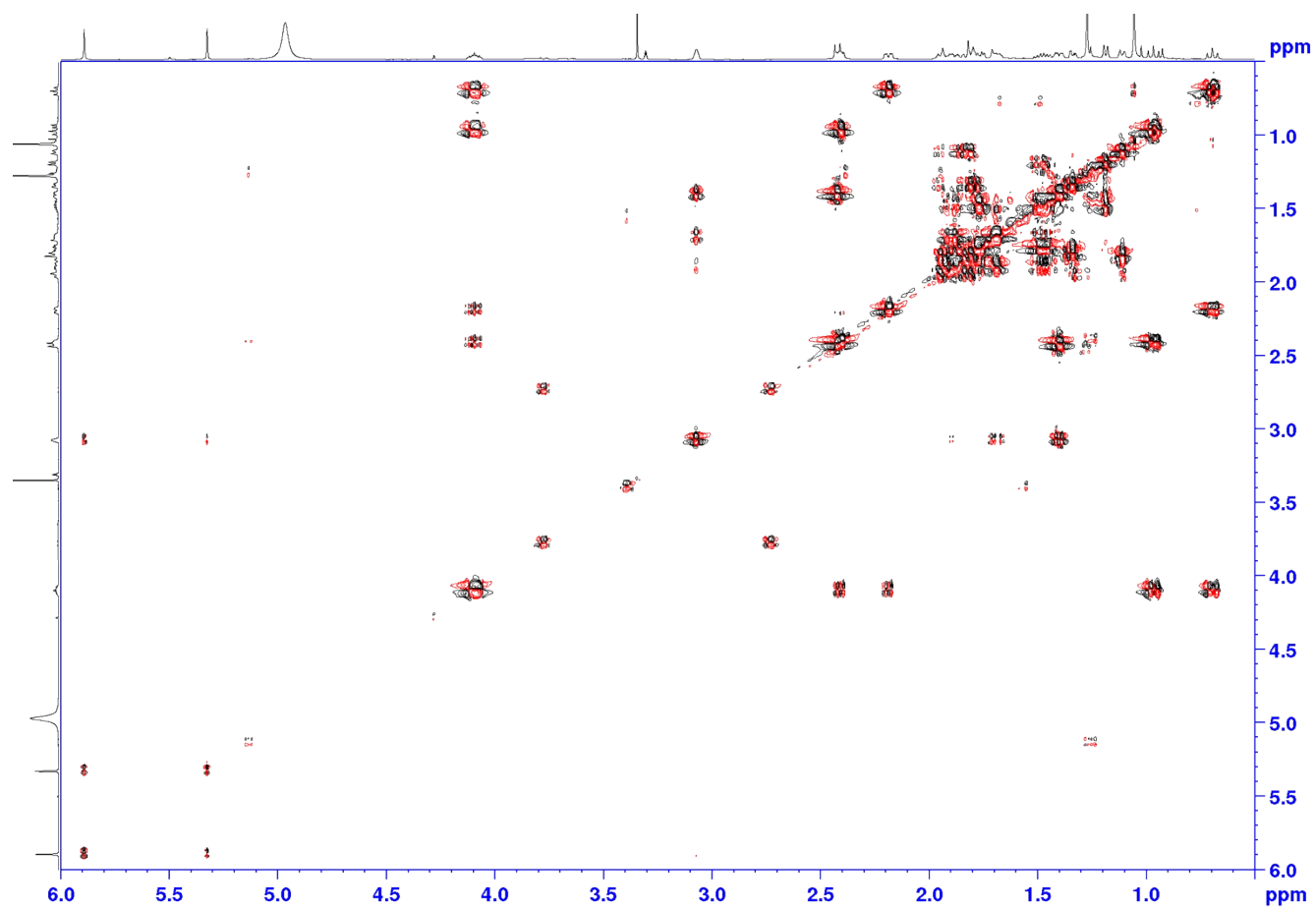


Figure S67. ^1H - ^1H COSY spectrum of Nouveinsancin F (6) in CD_3OD

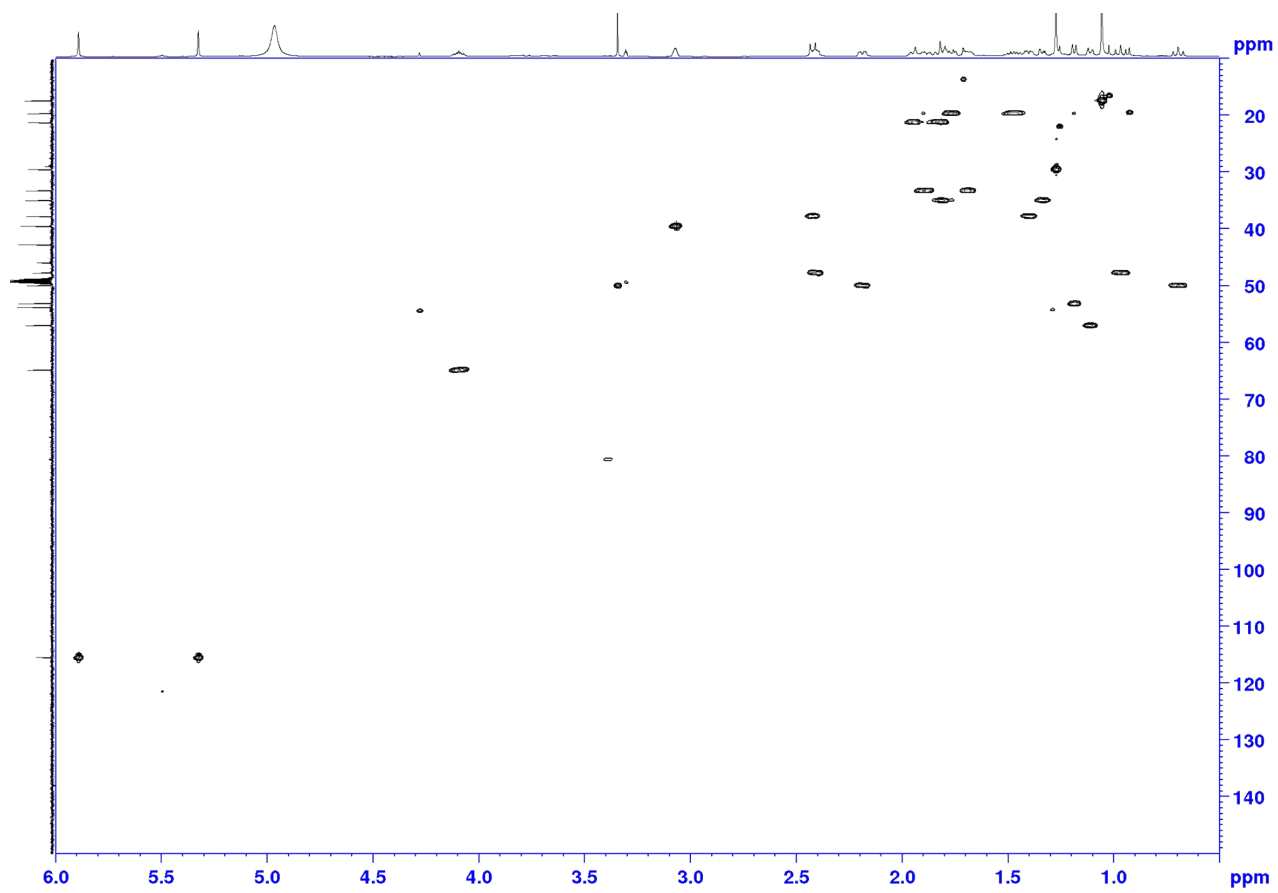


Figure S68. HSQC spectrum of Nouveinsiancin F (6) in CD₃OD

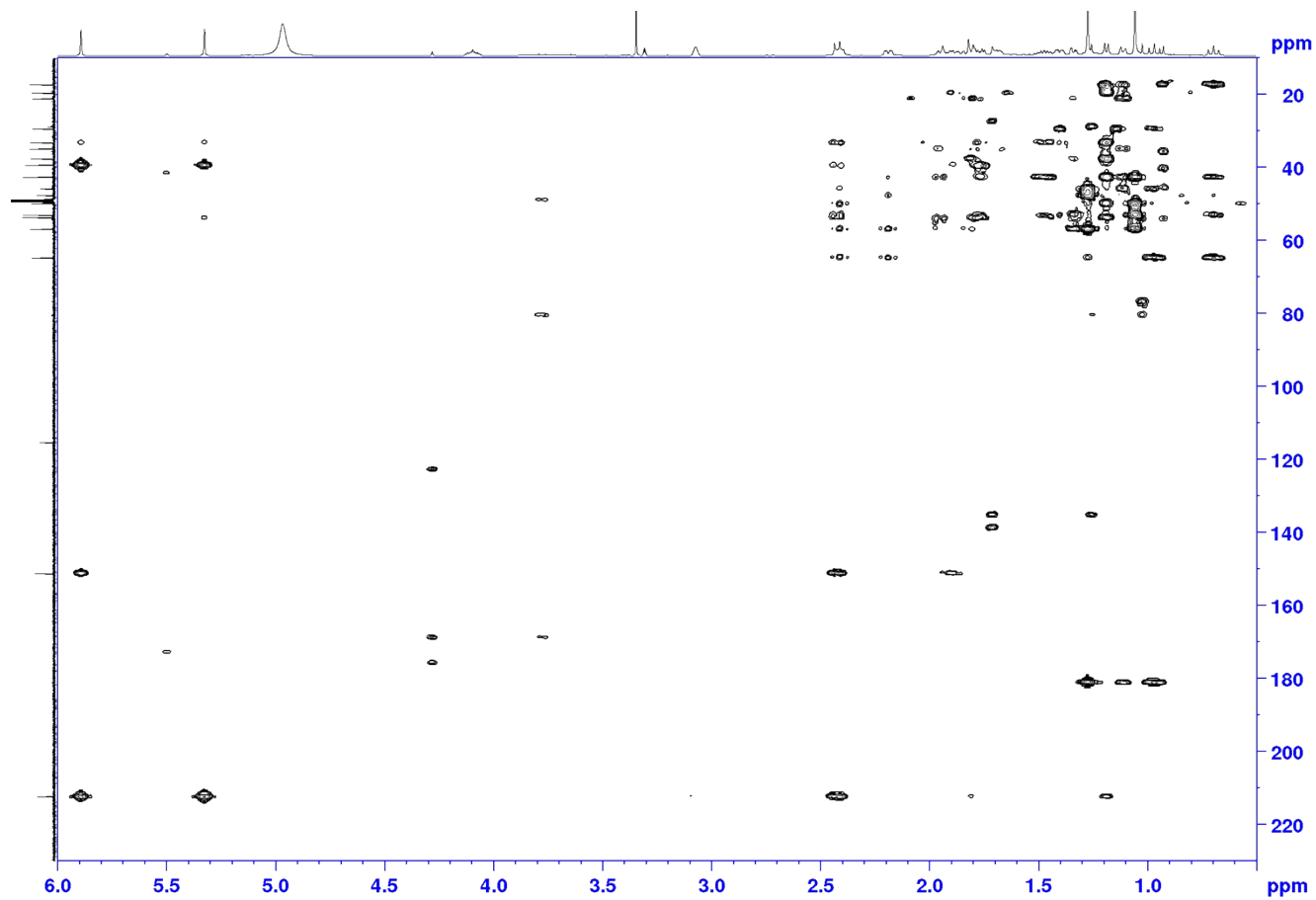


Figure S69. HMBC spectrum of Noueinsiancin F (6) in CD_3OD

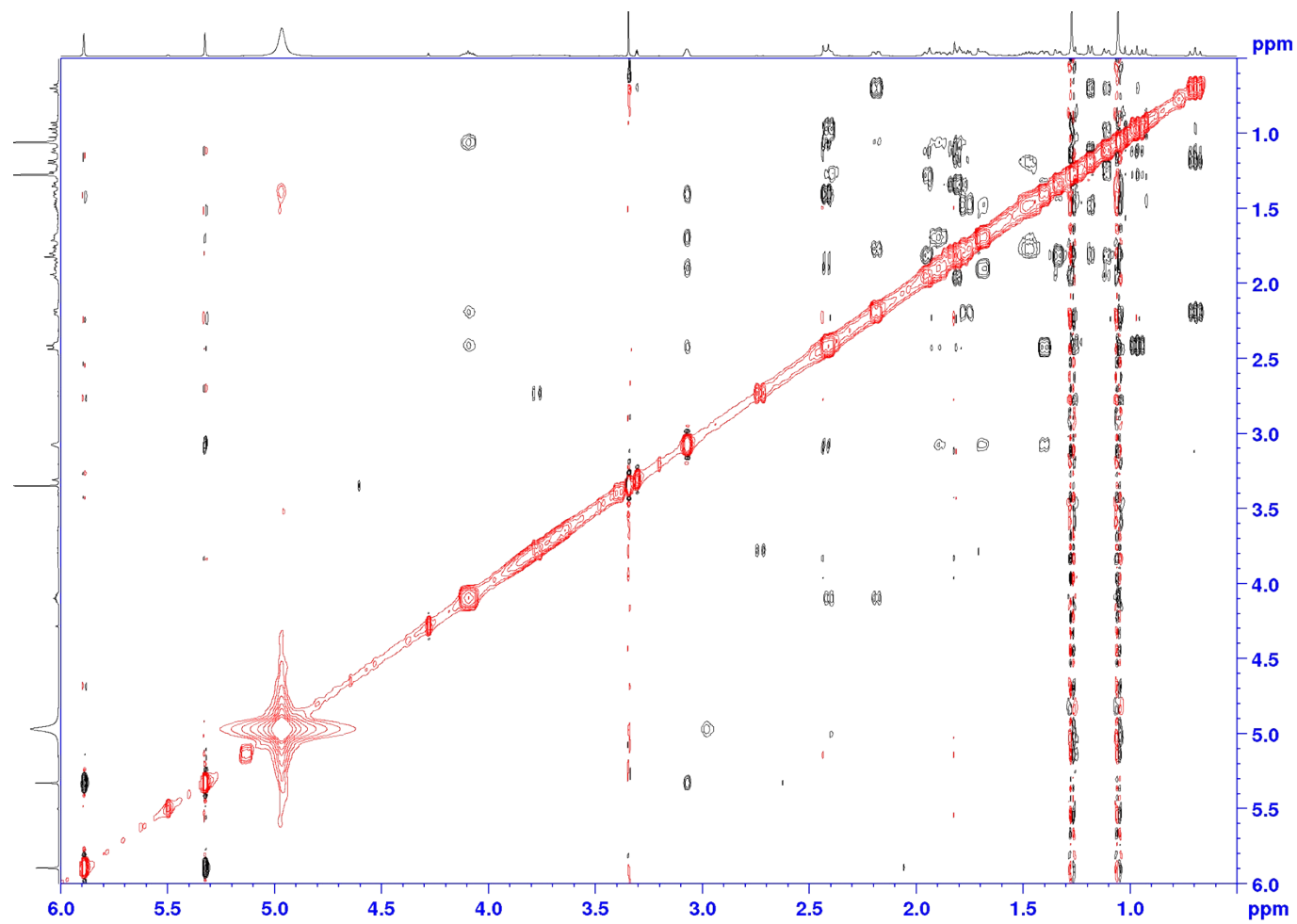


Figure S70. NOESY spectrum of Noueinsiancin F (6) in CD₃OD

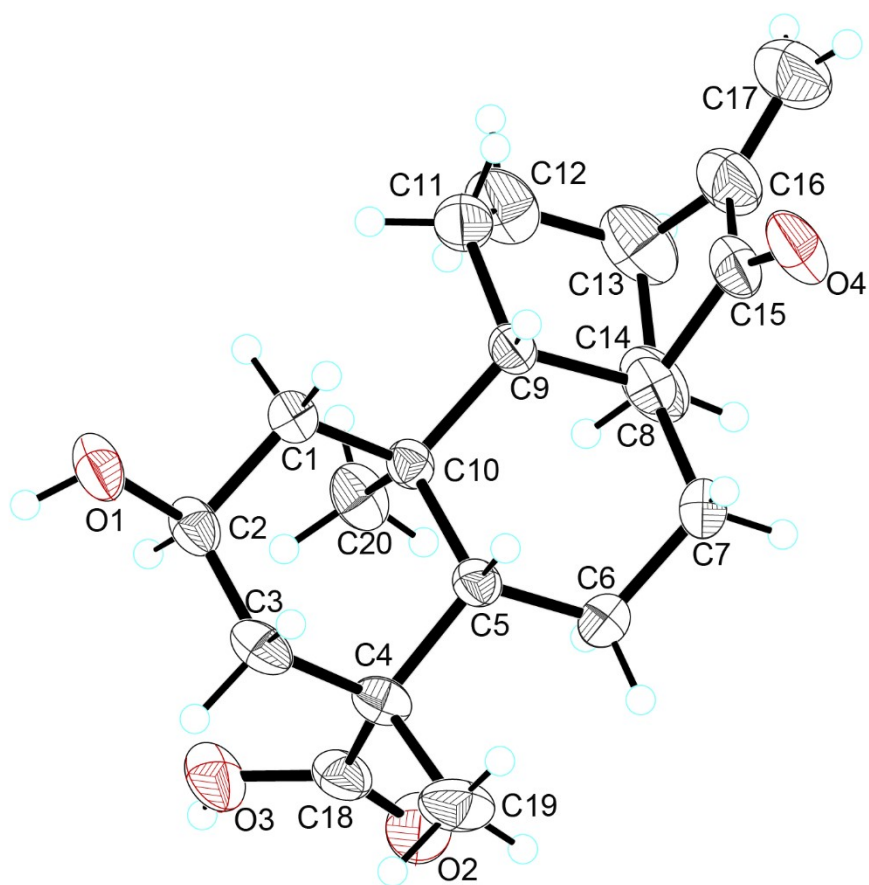
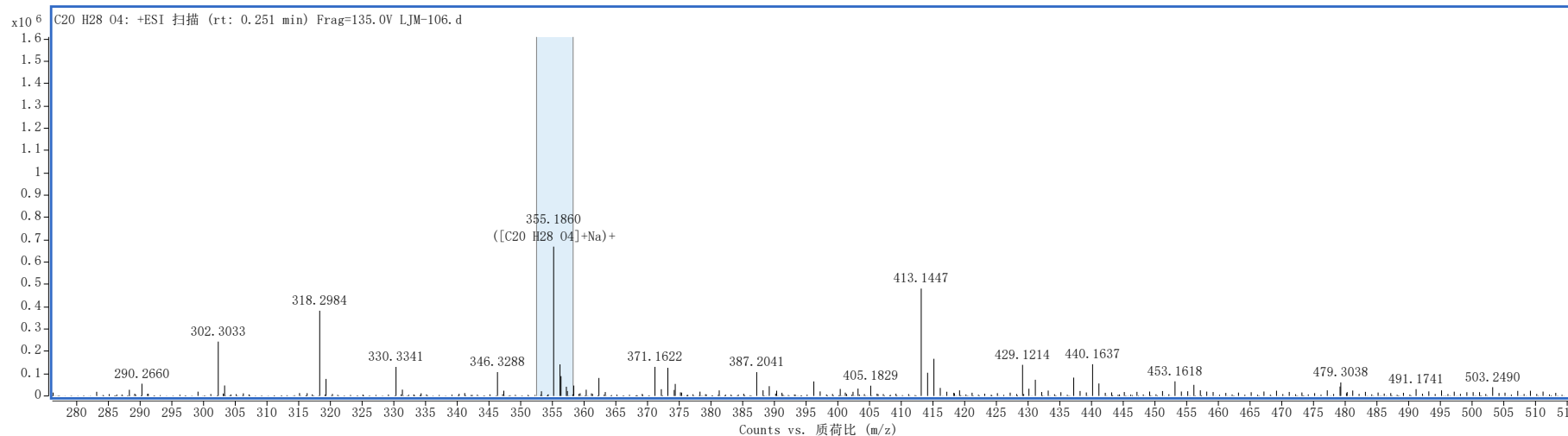


Figure S71. X-ray structure of Noueinsiancin F (6)



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H28 O4	(M+Na)+	355.1860	85.21	6.04	85.21

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.8	680361.9	100	355.188	2	669184.3	100	78.5	355.186	5.63

Figure S72. HRESIMS spectrum of Noueinsiancin G (7)

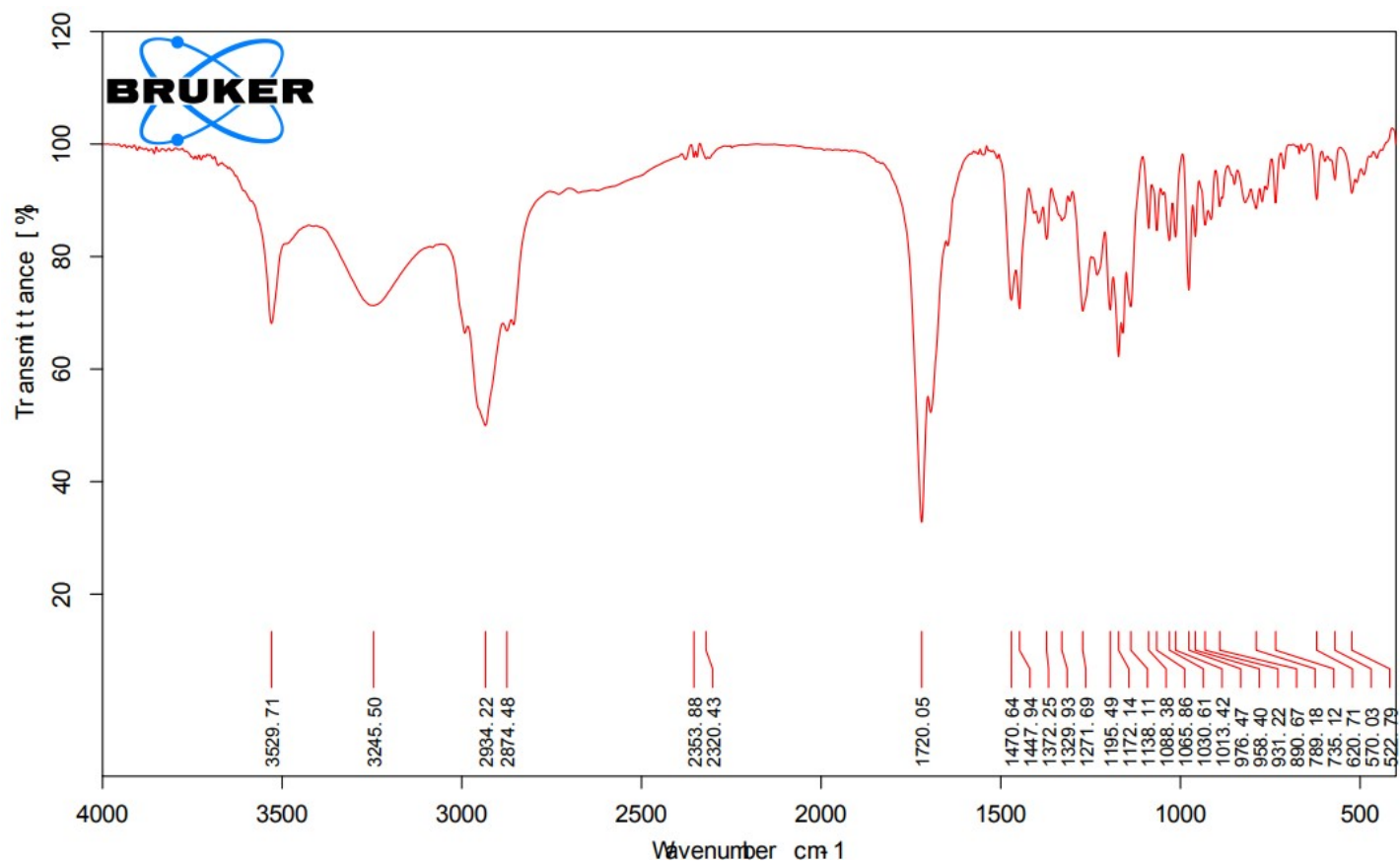


Figure S73. IR spectrum of Nouveinsiancin G (7)

Rudolph Research Analytical

Thursday, 02/10/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-106
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum						
6	-139.333	0.0000	-139.333	-139.333						
S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-106	07:46:08 PM	-139.333	SR	-0.209	589	100.00	0.150	20.1	
2	LJM-106	07:46:13 PM	-139.333	SR	-0.209	589	100.00	0.150	20.1	
3	LJM-106	07:46:19 PM	-139.333	SR	-0.209	589	100.00	0.150	20.1	
4	LJM-106	07:46:25 PM	-139.333	SR	-0.209	589	100.00	0.150	20.1	
5	LJM-106	07:46:30 PM	-139.333	SR	-0.209	589	100.00	0.150	20.0	
6	LJM-106	07:46:36 PM	-139.333	SR	-0.209	589	100.00	0.150	20.0	

Signature

Figure S74. OR Value of Noueinsiancin G (7) in CH₃OH

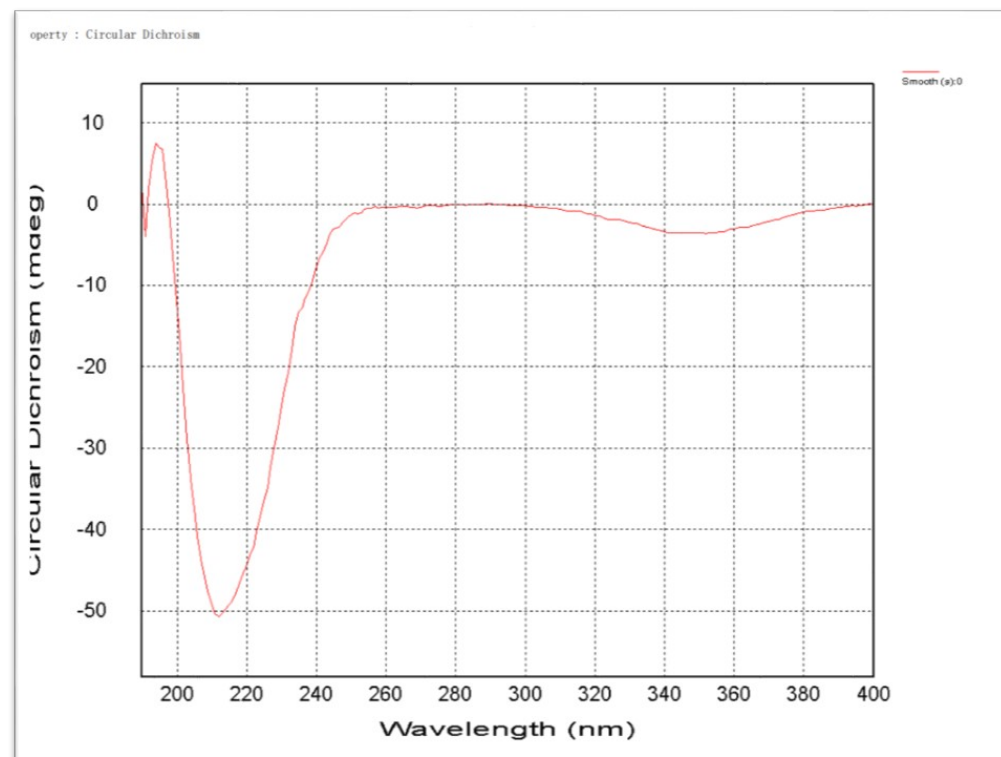


Figure S75. CD Value of Noueinsiancin G (7) in CH₃OH

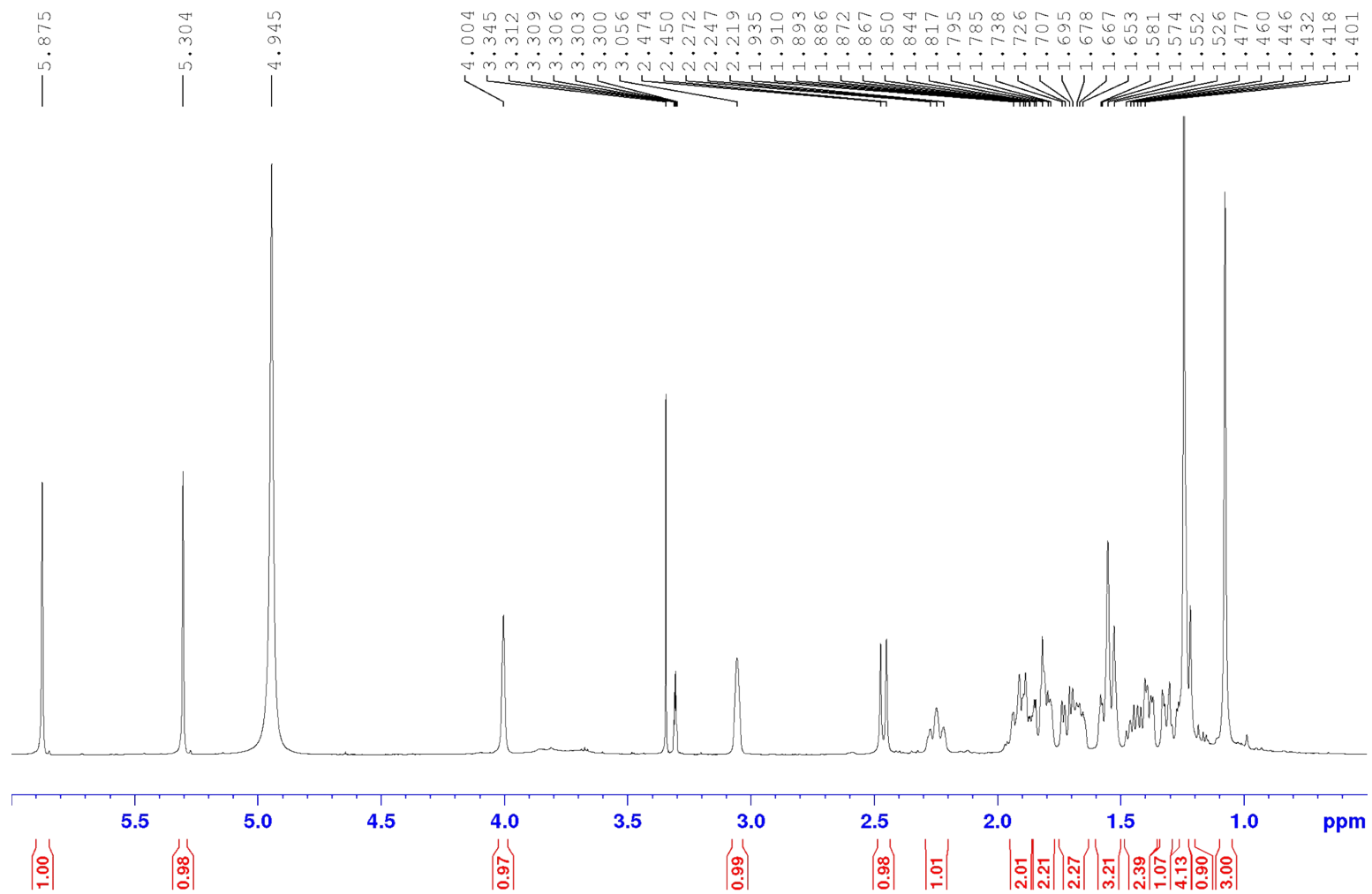


Figure S76. ¹H NMR spectrum of Noueinsiancin G (7) in CD₃OD

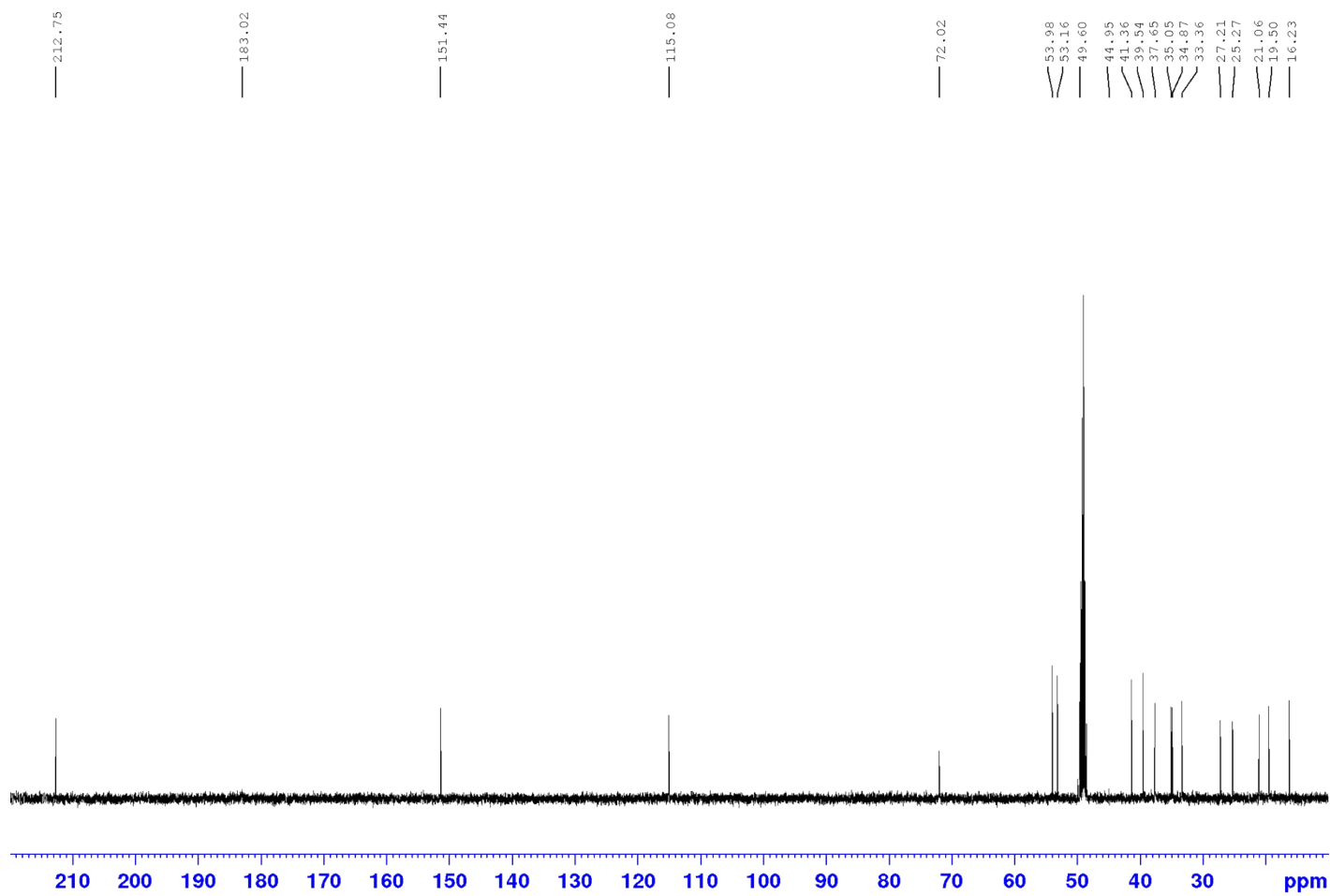


Figure S77 ^{13}C NMR spectrum of Noueinsiancin G (7) in CD_3OD

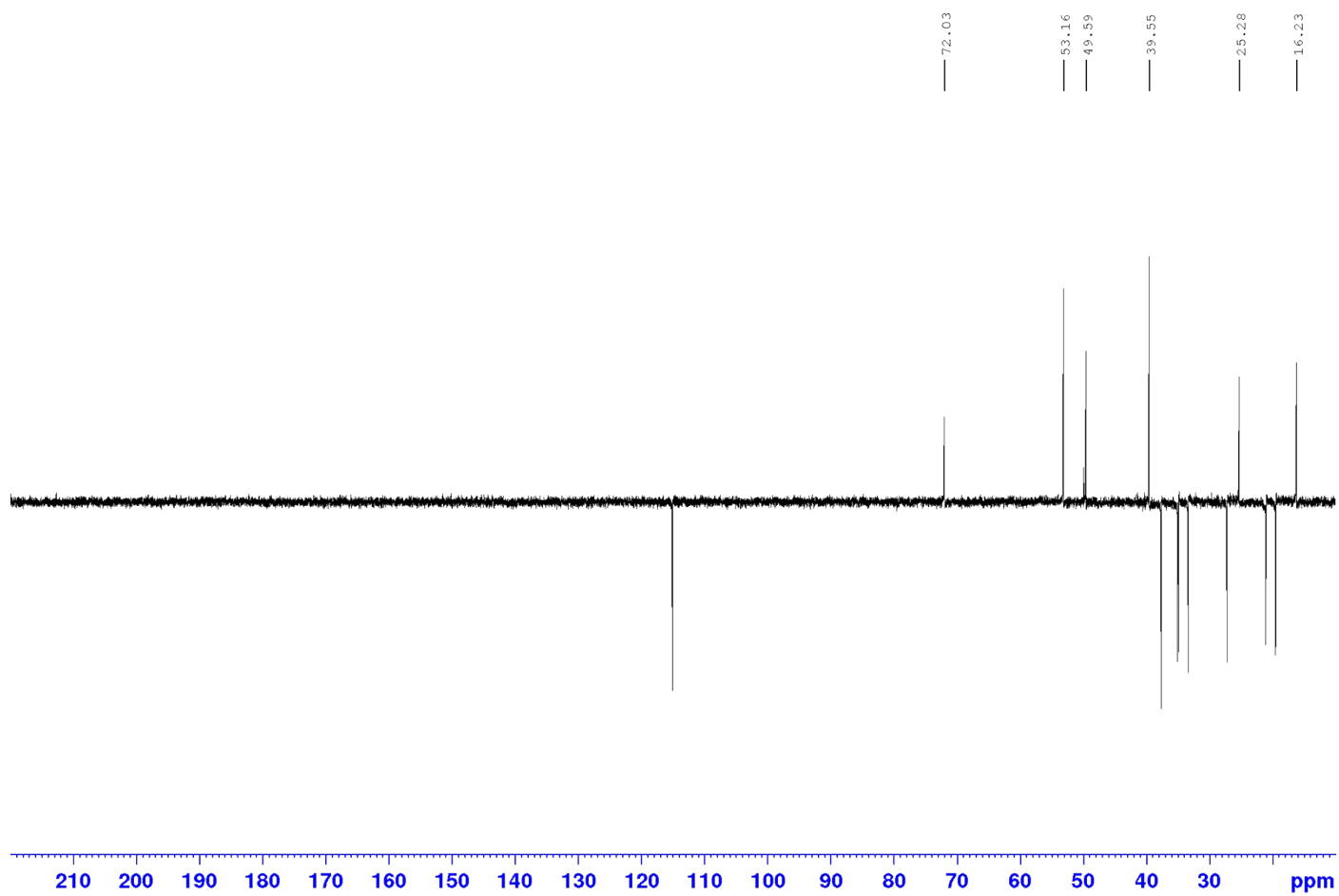


Figure S78. DEPT-135 NMR spectrum of Noueinsiancin G (7) in CD₃OD

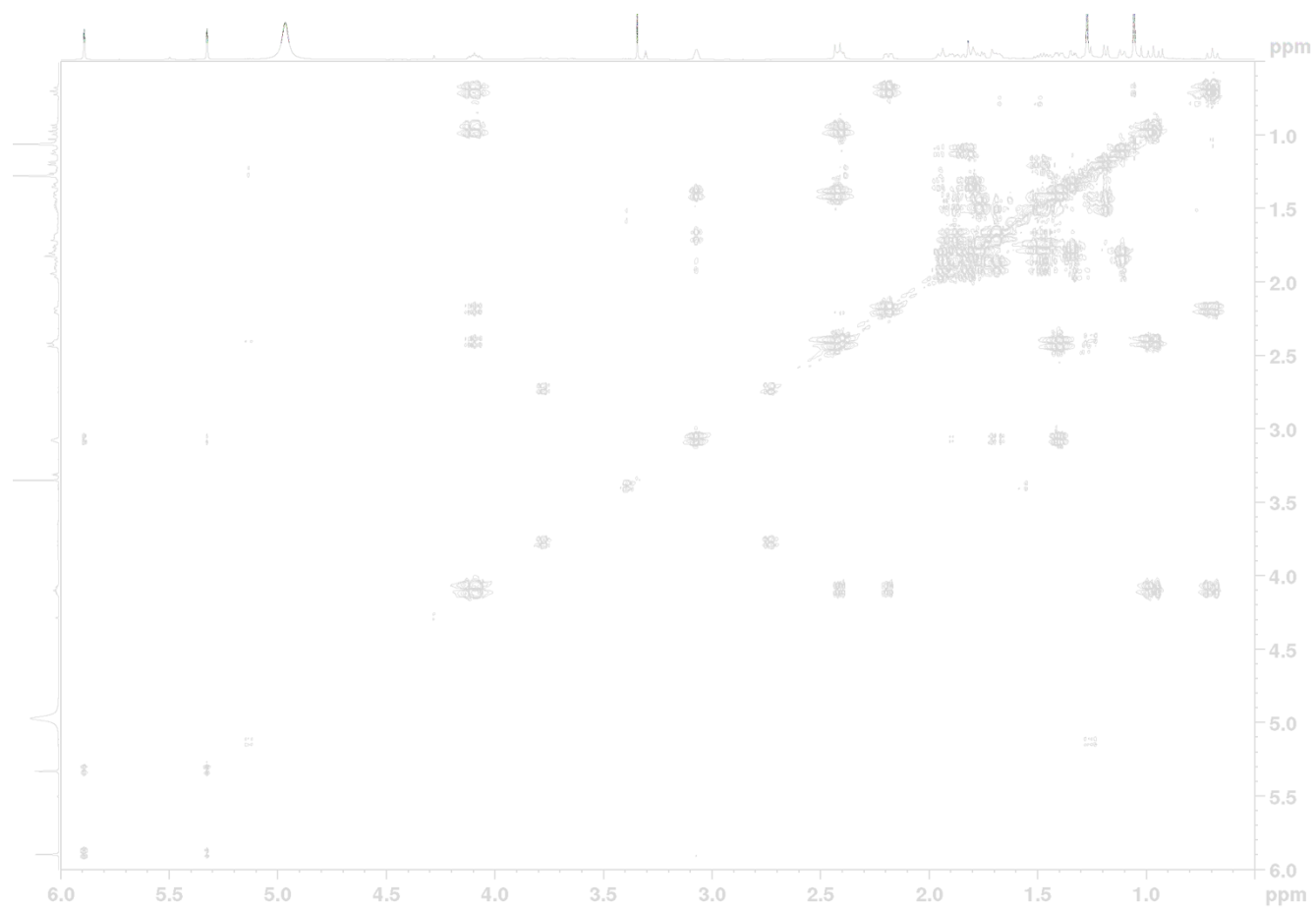


Figure S79. ^1H - ^1H COSY spectrum of Nouveinsiancin G (7) in CD_3OD

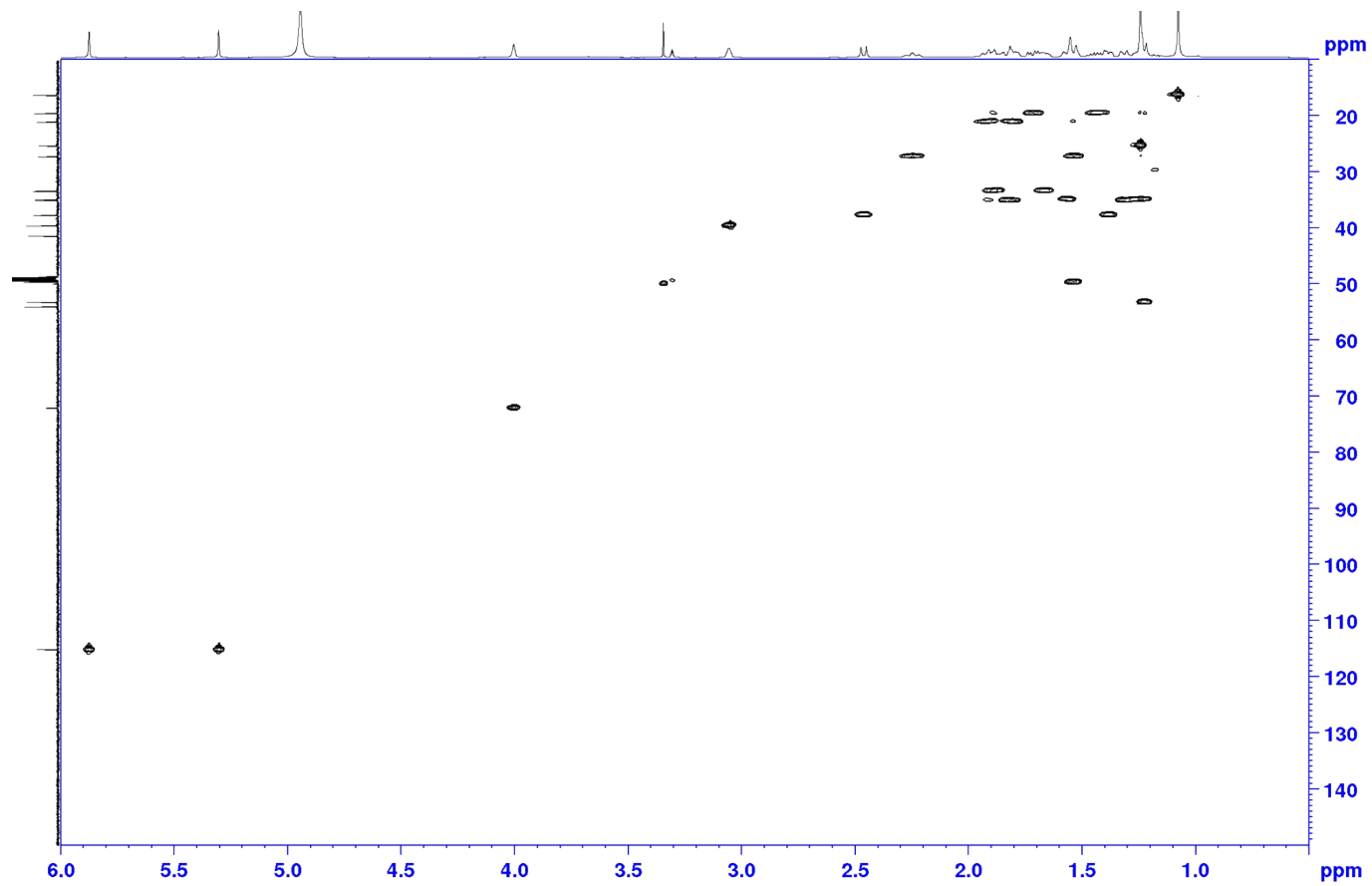


Figure S80. HSQC spectrum of Noueinsiancin G (7) in CD₃OD

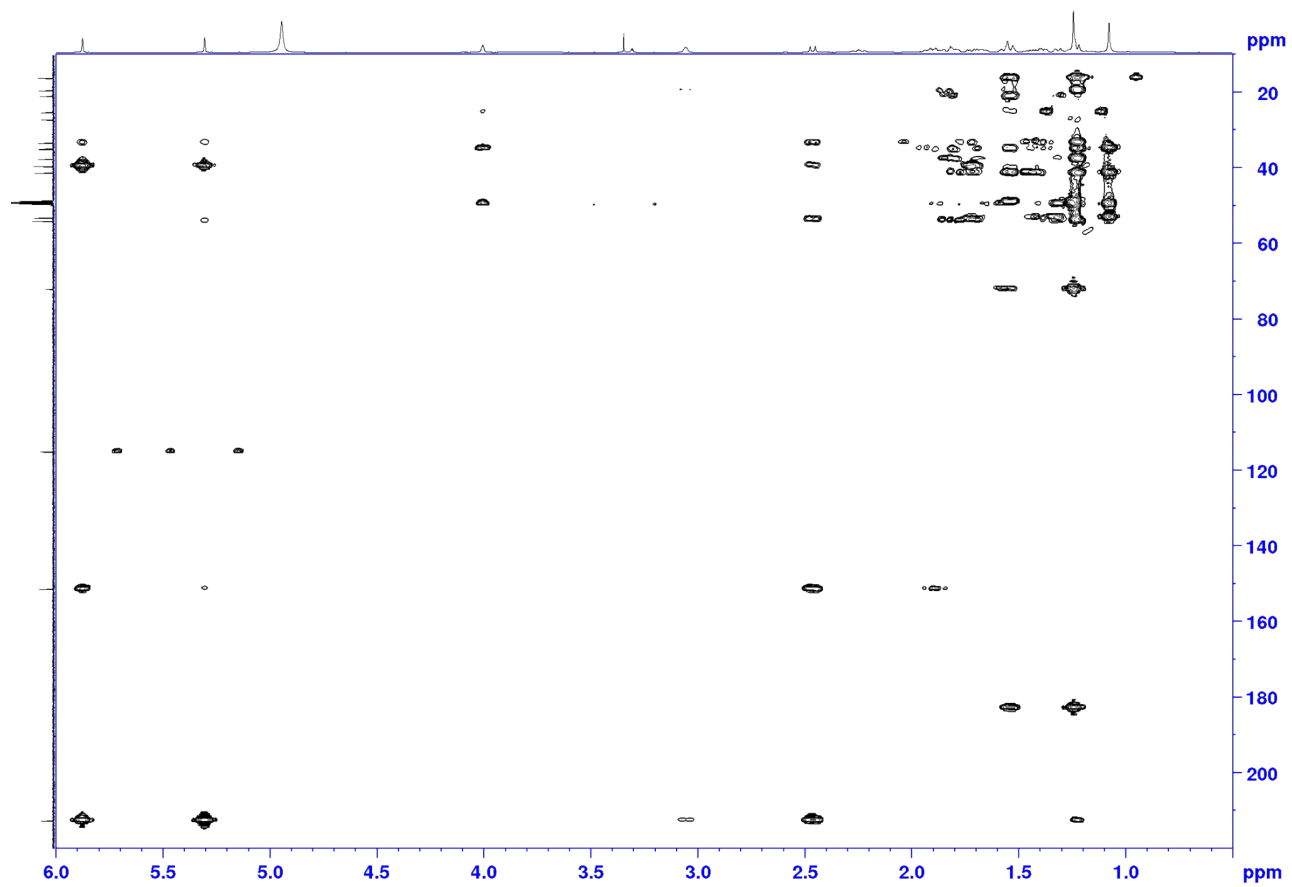


Figure S81. HMBC spectrum of Noueinsiancin G (7) in CD₃OD

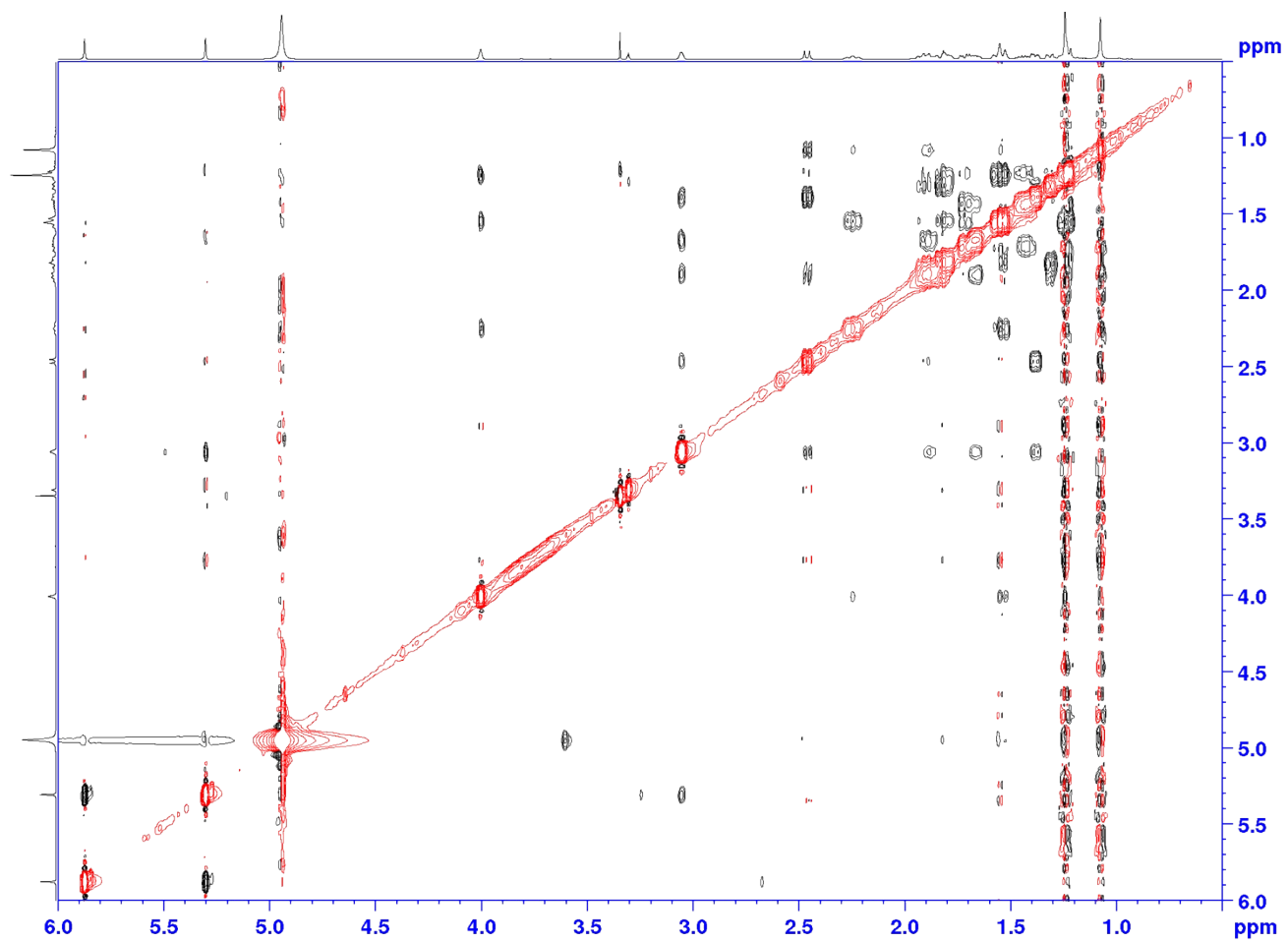
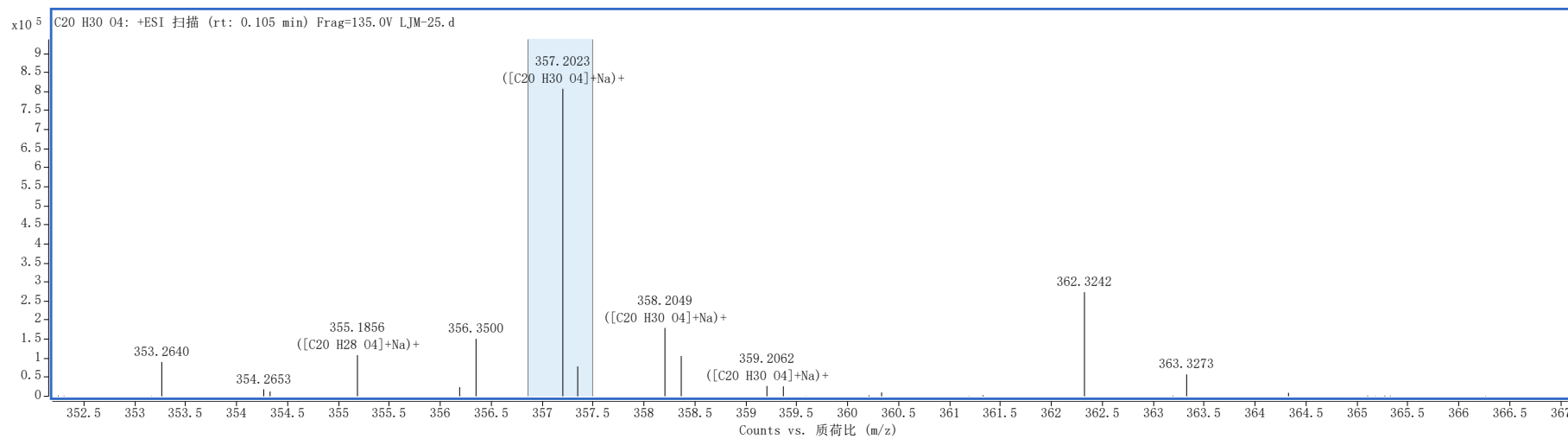


Figure S82. NOESY spectrum of Noueinsiancin G (7) in CD₃OD



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H30 O4	(M+Na)+	357.2023	92.42	4.59	92.42

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数 (计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.8	809437.4	100	357.2036	1.3	807306.1	100	79.6	357.2023	3.75

Figure S83. HRESIMS spectrum of Noueinsiancin H (8)

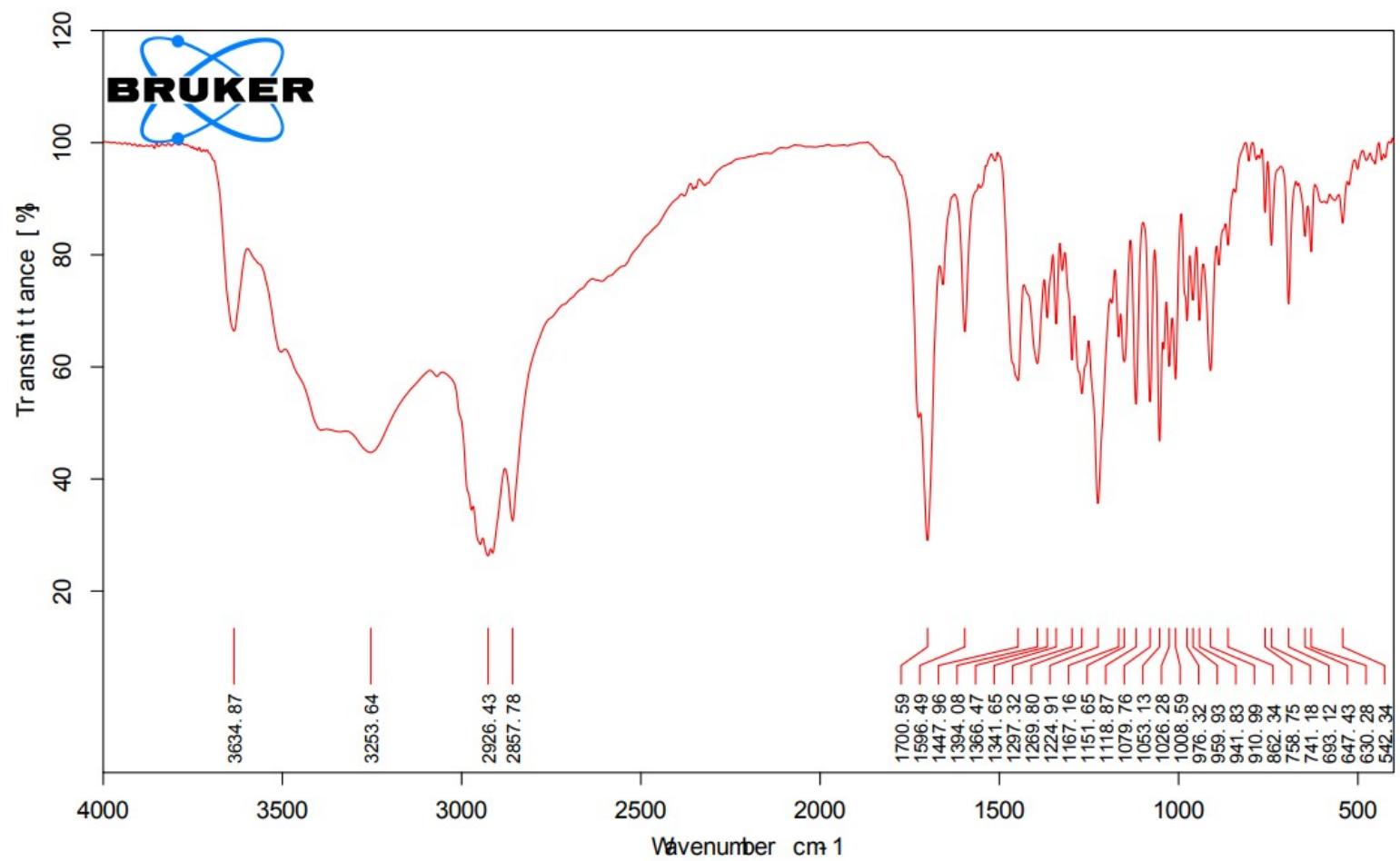


Figure S84. IR spectrum of Nouveinsiancin H (8)

Rudolph Research Analytical

Wednesday, 02/09/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-25
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-85.834	0.8335	-85.000	-86.667

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-25	03:30:51 PM	-85.000	SR	-0.051	589	100.00	0.060	20.2	
2	LJM-25	03:30:57 PM	-86.667	SR	-0.052	589	100.00	0.060	20.2	
3	LJM-25	03:31:03 PM	-86.667	SR	-0.052	589	100.00	0.060	20.2	
4	LJM-25	03:31:11 PM	-86.667	SR	-0.052	589	100.00	0.060	20.1	
5	LJM-25	03:31:17 PM	-85.000	SR	-0.051	589	100.00	0.060	20.1	
6	LJM-25	03:31:23 PM	-85.000	SR	-0.051	589	100.00	0.060	20.1	

Signature

Figure S85. OR Value of Noueinsiancin H (8) in CH3OH

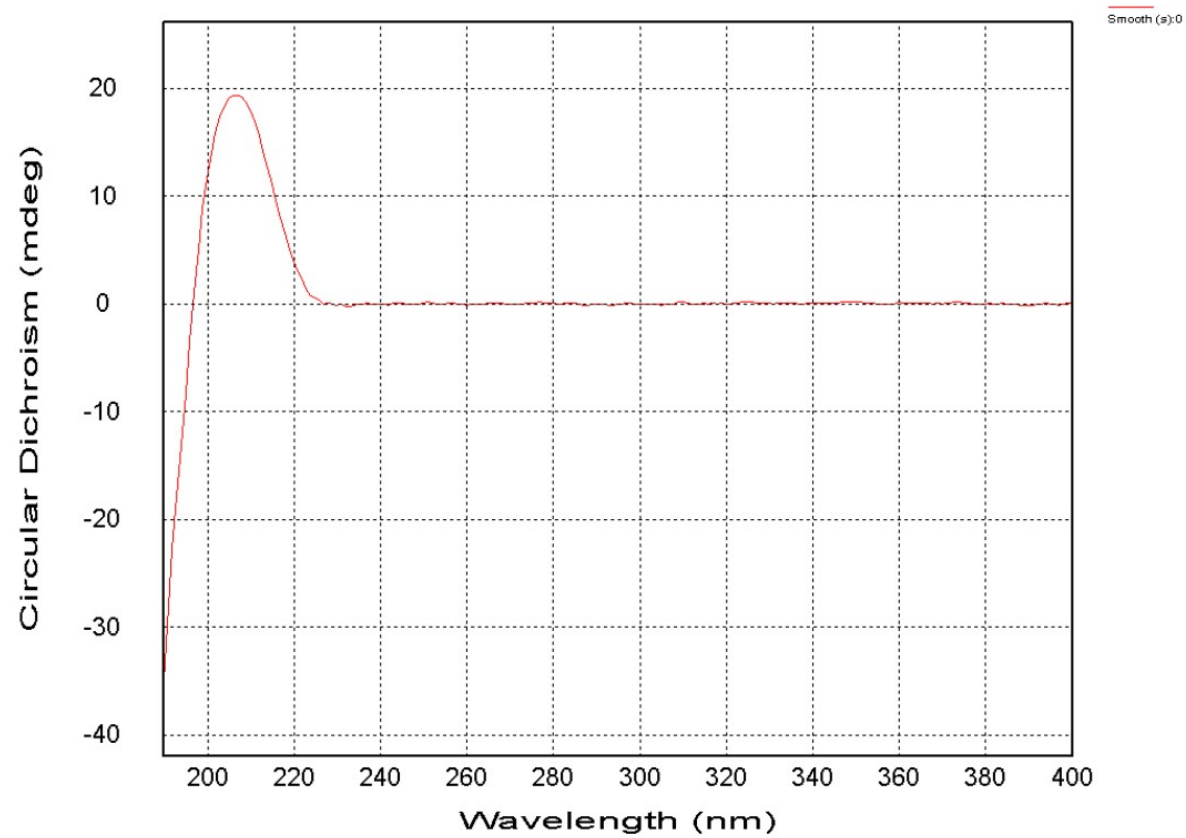


Figure S86. CD Value of Noueinsiancin H (8) in CH₃OH

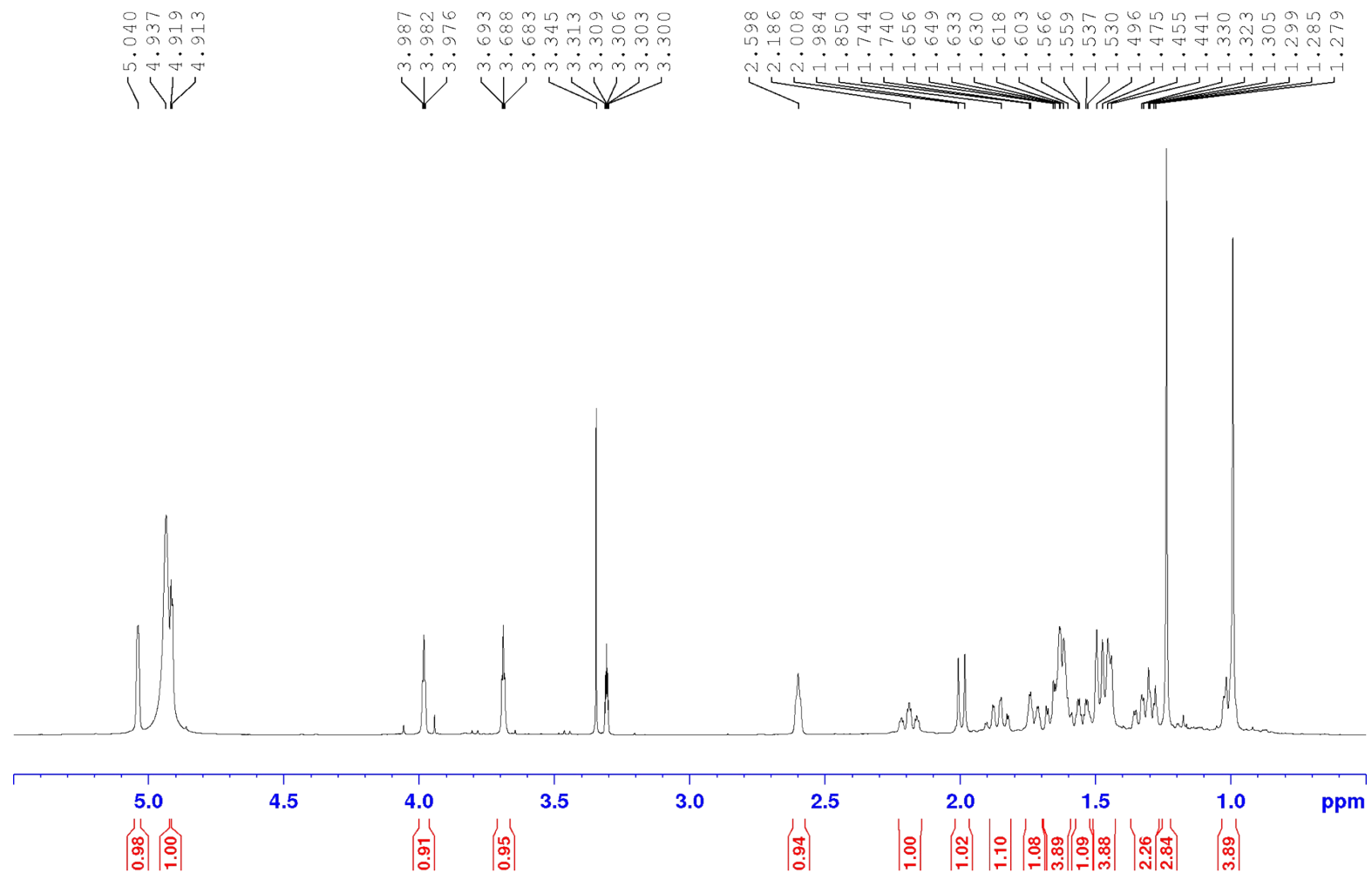


Figure S87. ¹H NMR spectrum of Nouveinsiancin H (8) in CD₃OD.

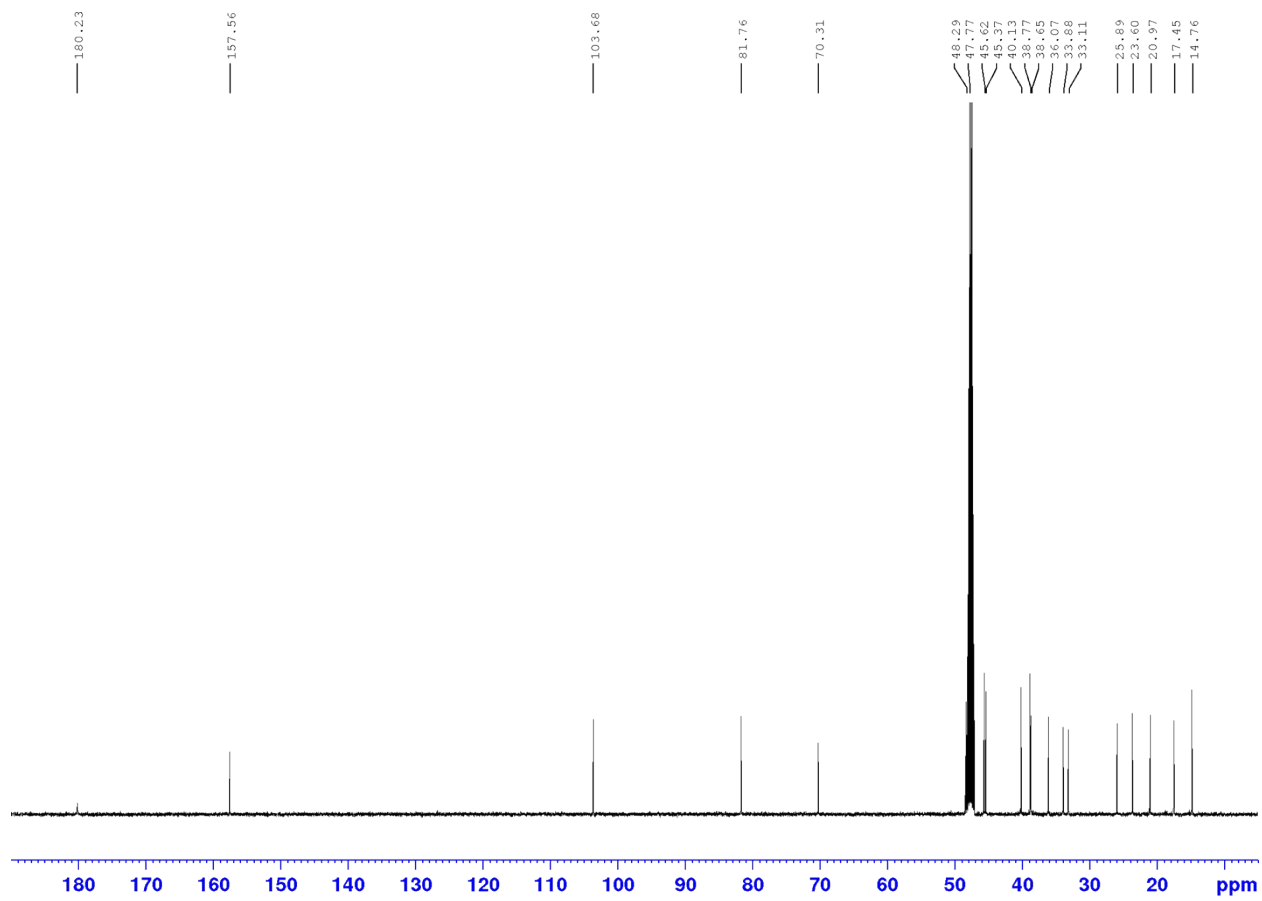


Figure S88. ^{13}C NMR spectrum of Noueinsiancin H (8) in CD_3OD

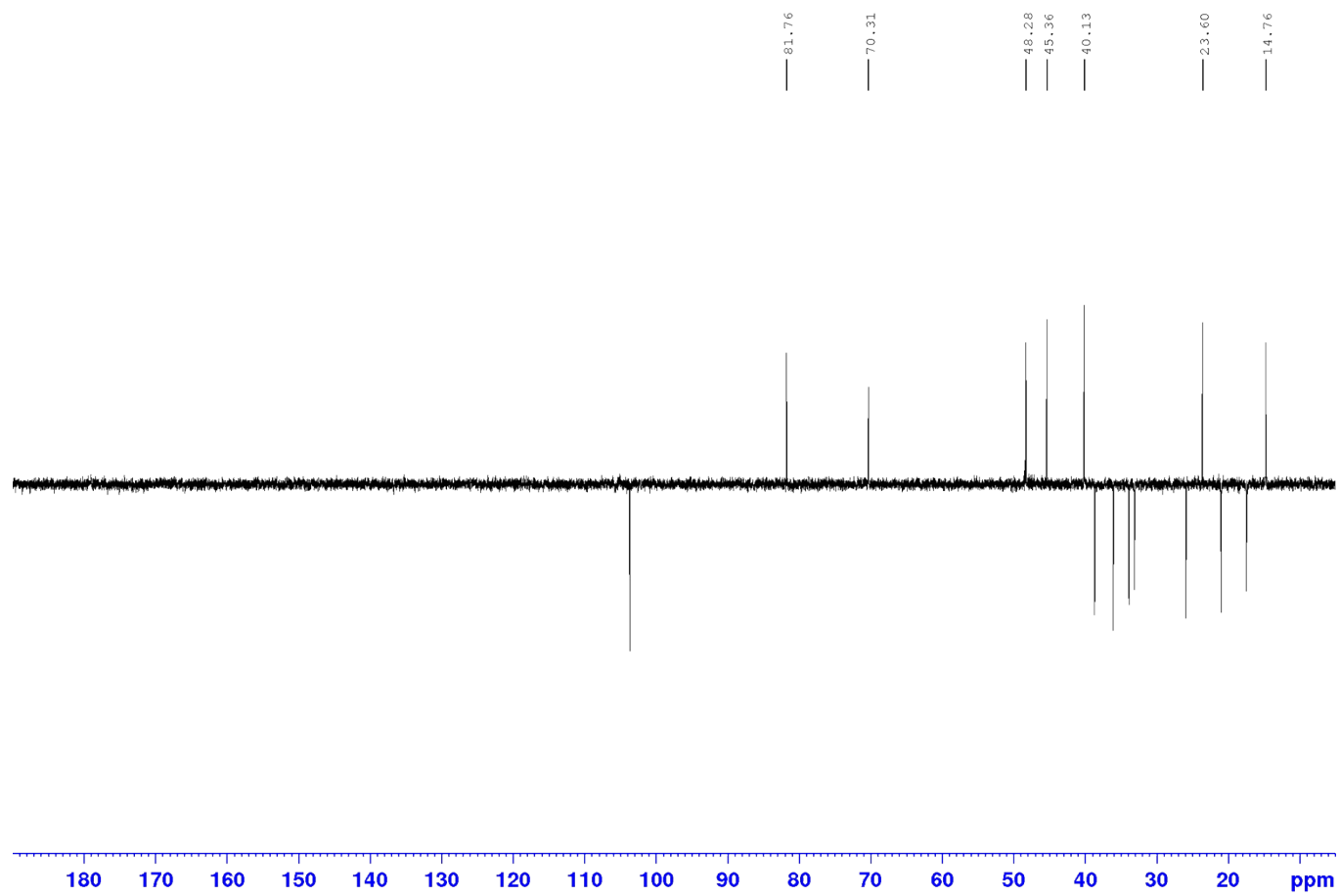


Figure S89. DEPT-135 NMR spectrum of Noueinsiancin H (8) in CD₃OD

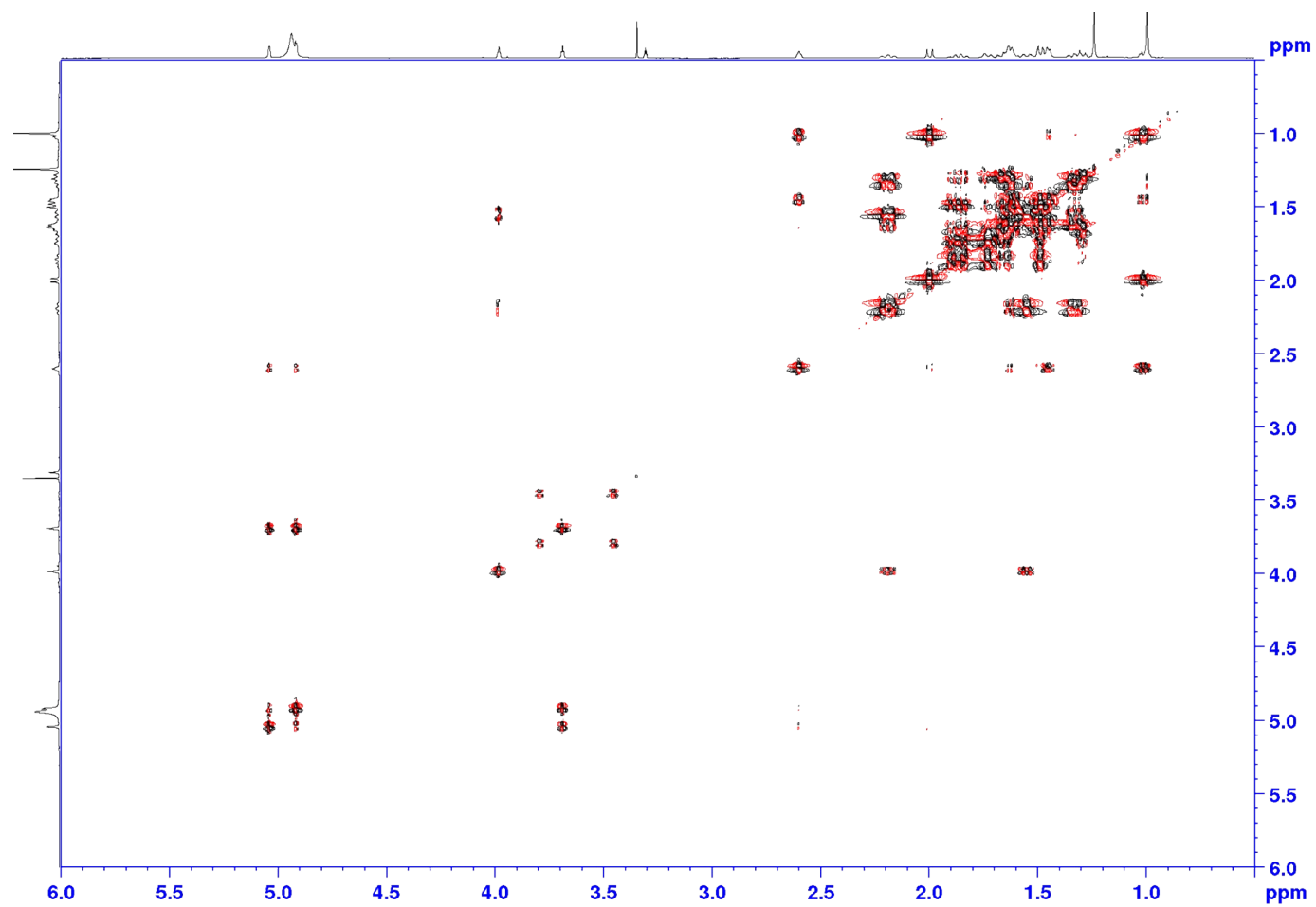


Figure S90. ^1H - ^1H COSY spectrum of Noueinsiancin H (8) in CD_3OD

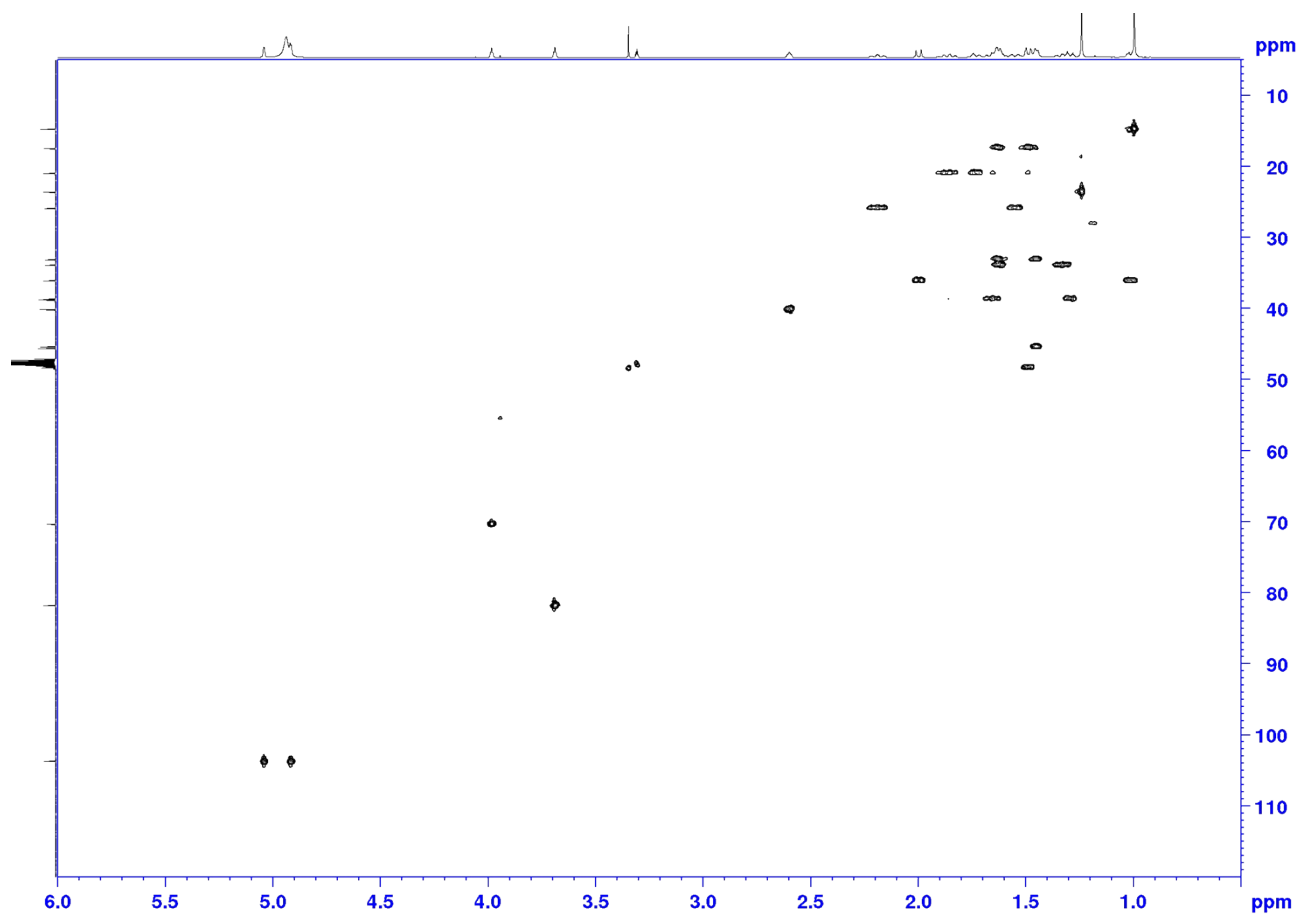


Figure S91. HSQC spectrum of Noueinsiancin H (8) in CD₃OD

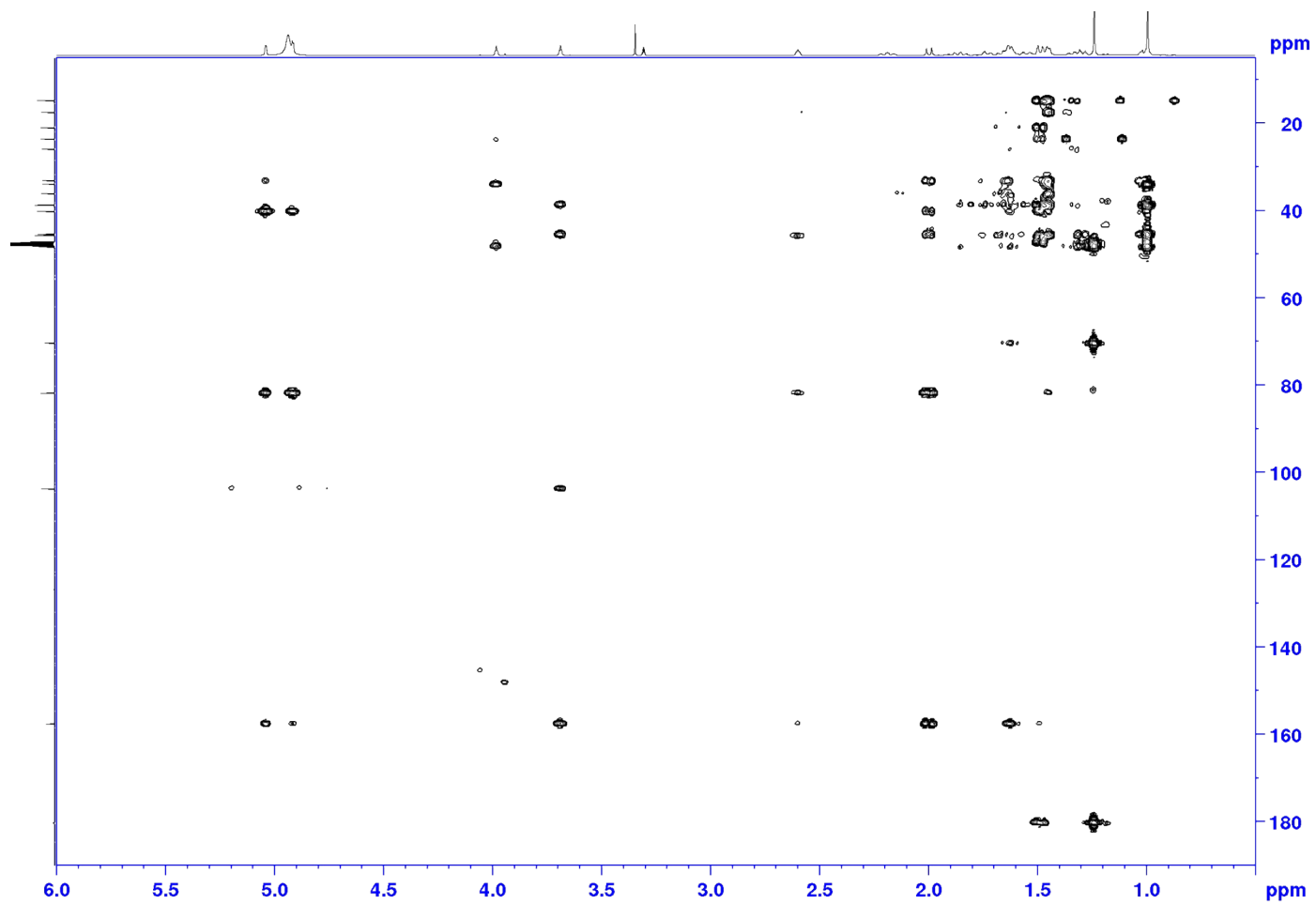


Figure S92. HMBC spectrum of Noueinsiancin H (8) in CD₃OD

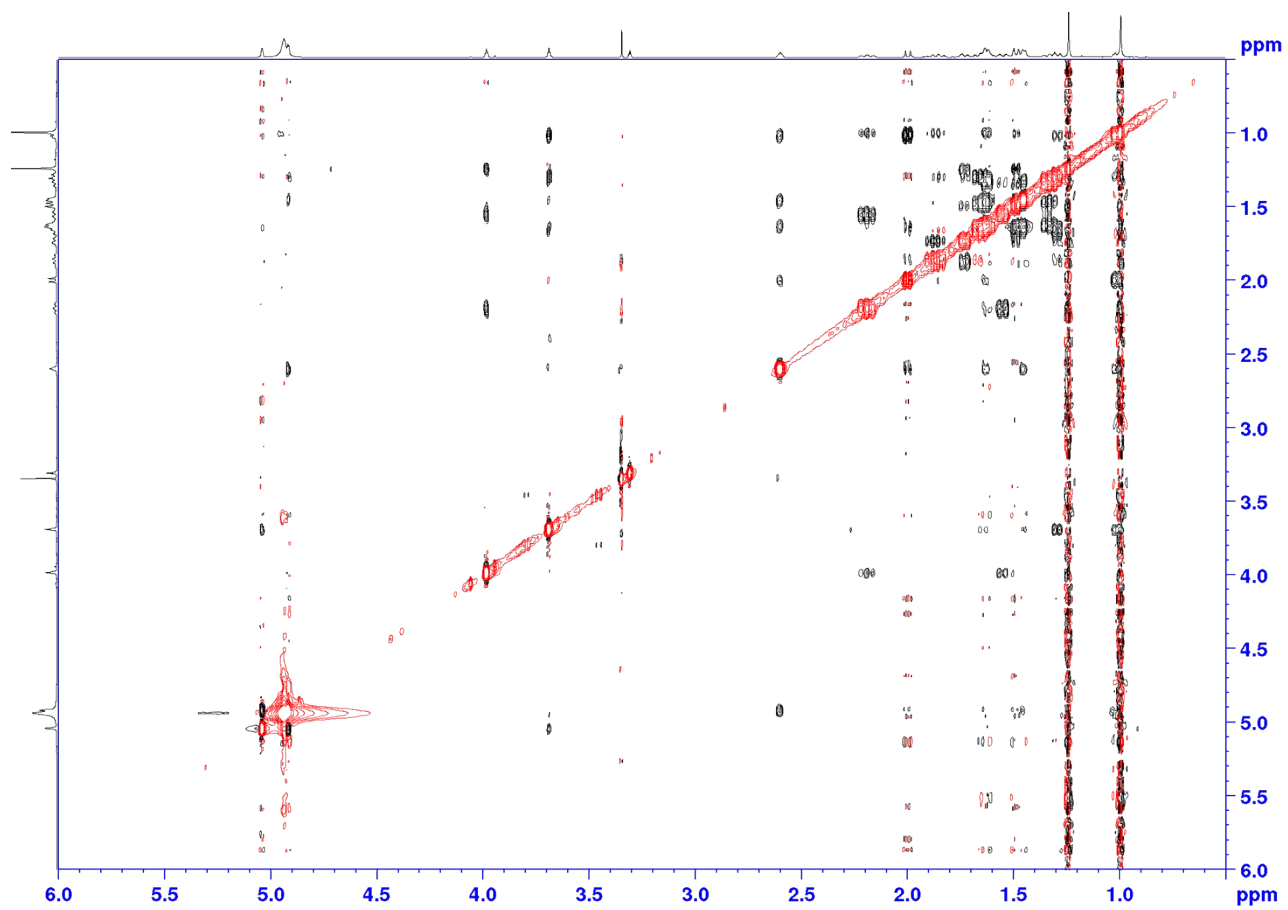


Figure S93. NOESY spectrum of Noueinsiancin H (8) in CD₃OD

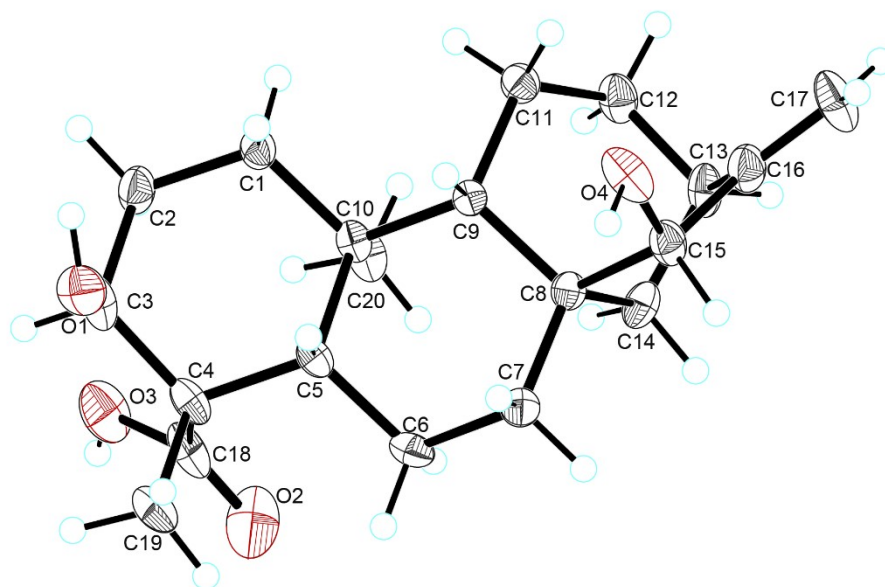
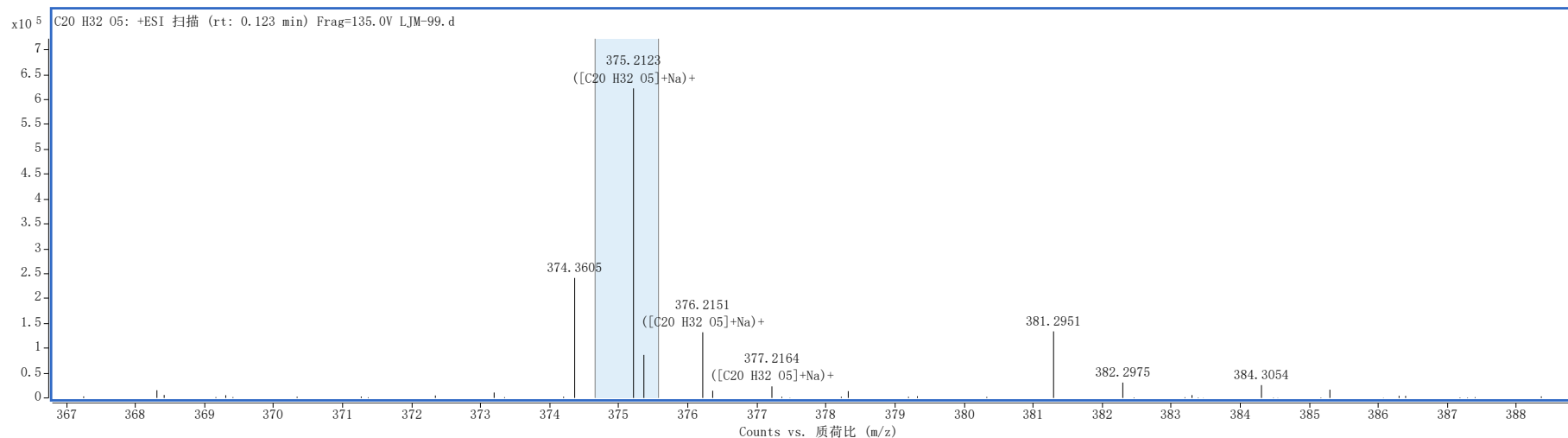


Figure S94. X-ray structure of Nouveinsiancin H (8)



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H32 O5	(M+Na)+	375.2123	88.51	5.77	88.51

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数 (计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.6	619689.8	100	375.2142	1.9	622758.6	100	80	375.2123	4.95

Figure S95. HRESIMS spectrum of Noueinsiancin I (9)

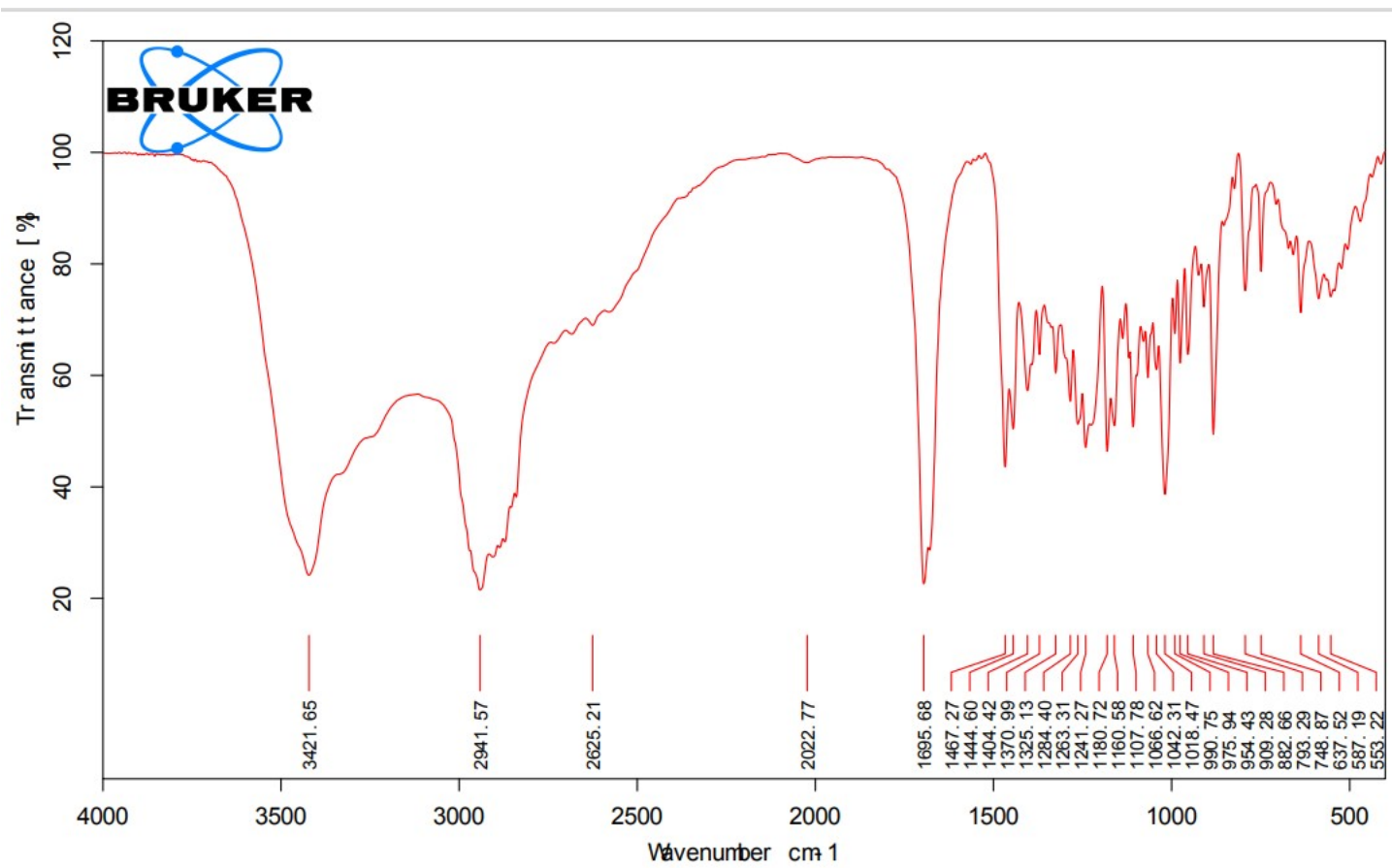


Figure S96. IR spectrum of Nouveinsiancin I (9)

Rudolph Research Analytical

Thursday, 02/10/2022

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-99
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-91.333	0.9428	-90.000	-92.000

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-99	07:04:13 PM	-90.000	SR	-0.045	589	100.00	0.050	20.3	
2	LJM-99	07:04:19 PM	-92.000	SR	-0.046	589	100.00	0.050	20.2	
3	LJM-99	07:04:25 PM	-90.000	SR	-0.045	589	100.00	0.050	20.2	
4	LJM-99	07:04:31 PM	-92.000	SR	-0.046	589	100.00	0.050	20.2	
5	LJM-99	07:04:36 PM	-92.000	SR	-0.046	589	100.00	0.050	20.2	
6	LJM-99	07:04:42 PM	-92.000	SR	-0.046	589	100.00	0.050	20.1	

Signature

Figure S97. OR Value of Noueinsiancin I (9) in CH₃OH

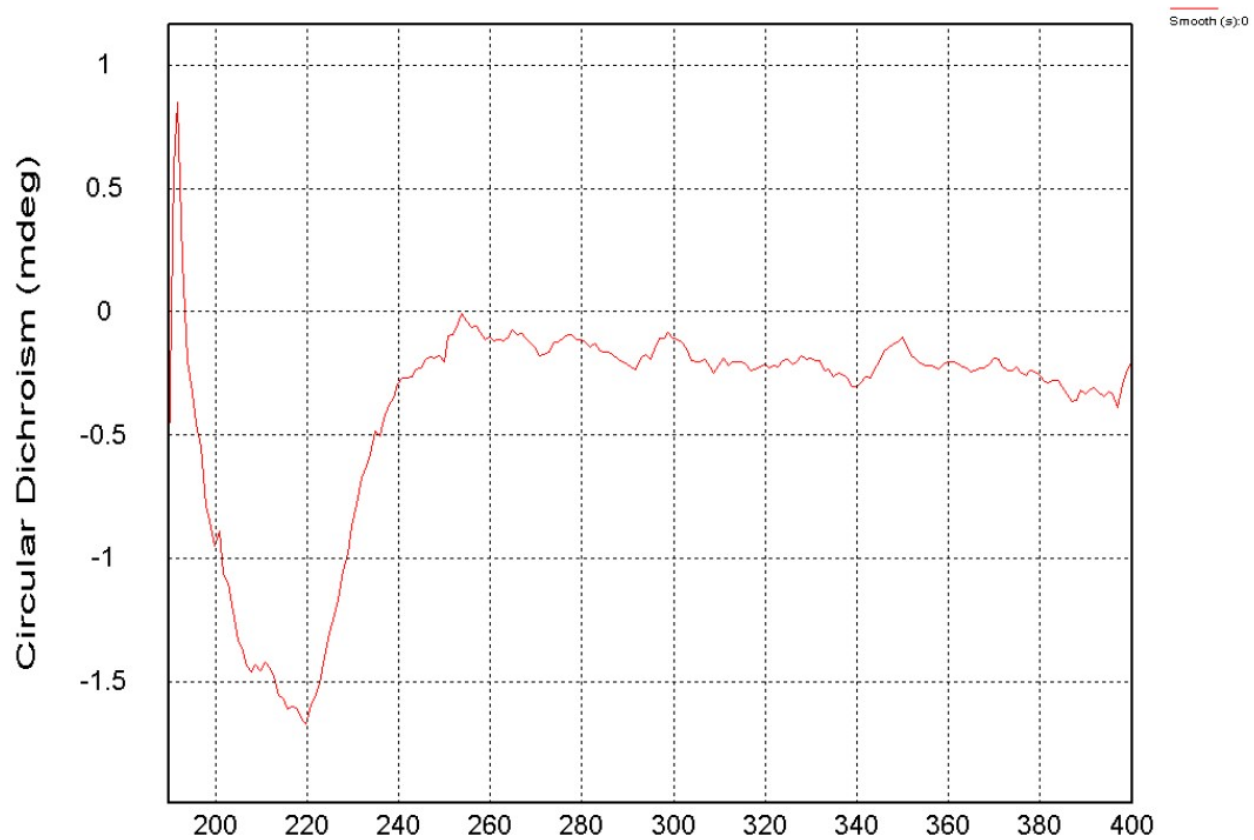


Figure S98. CD Value of Noueinsiancin I (9) in CH₃OH

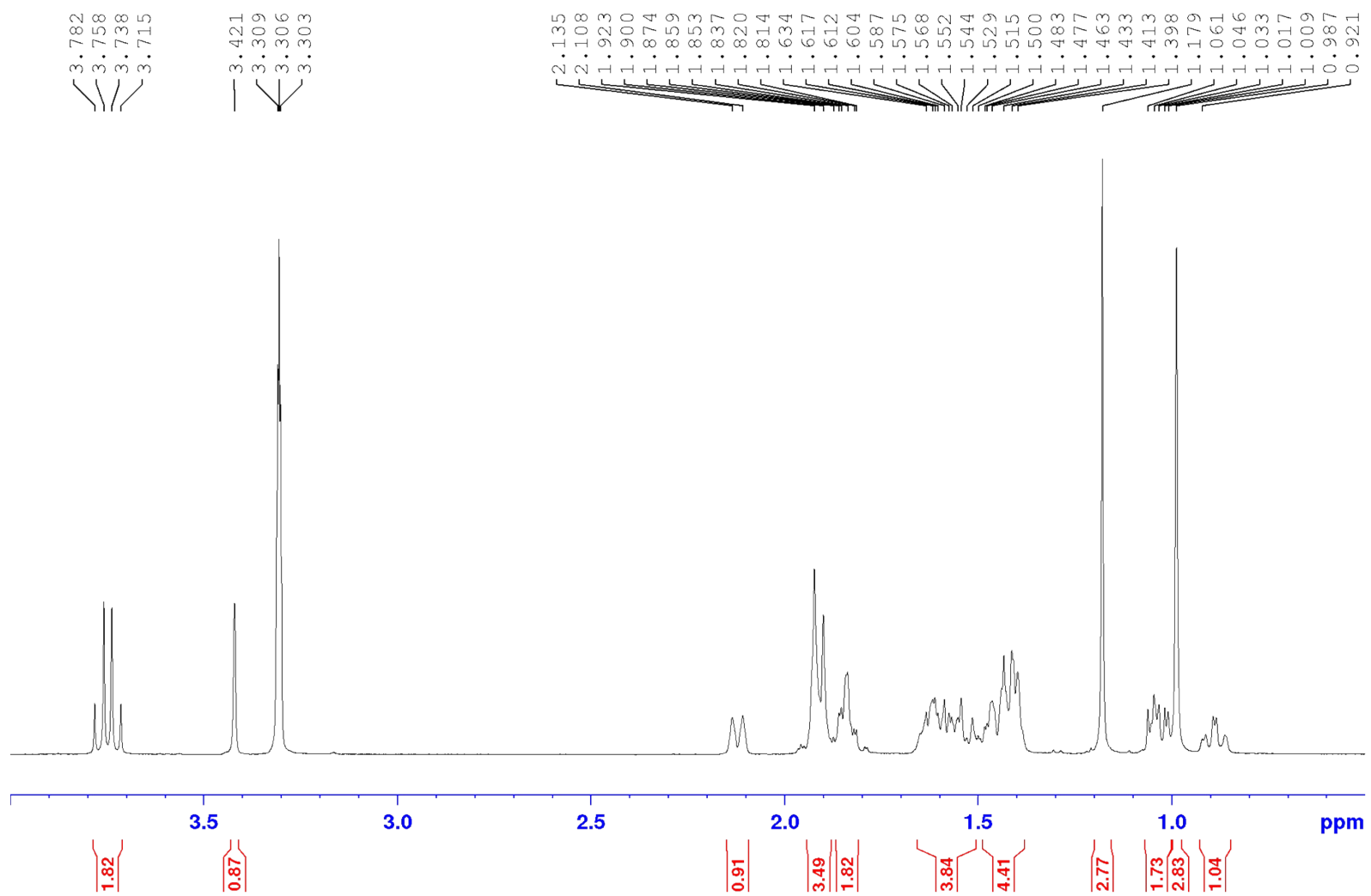


Figure S99. ^1H NMR spectrum of Noueinsiancin I (9) in CD_3OD

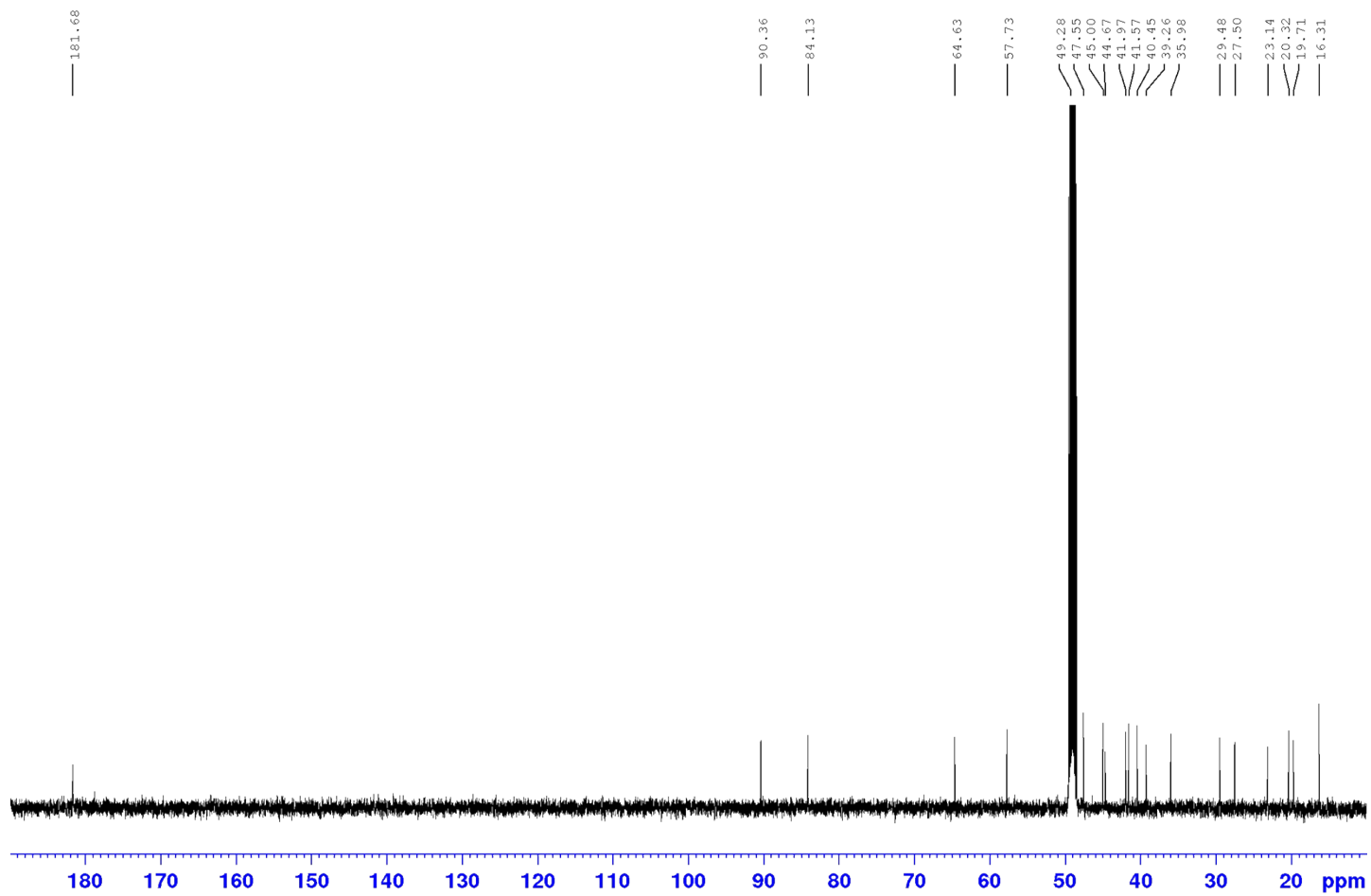


Figure S100. ^{13}C NMR spectrum of Noueinsiancin I (9) in CD_3OD

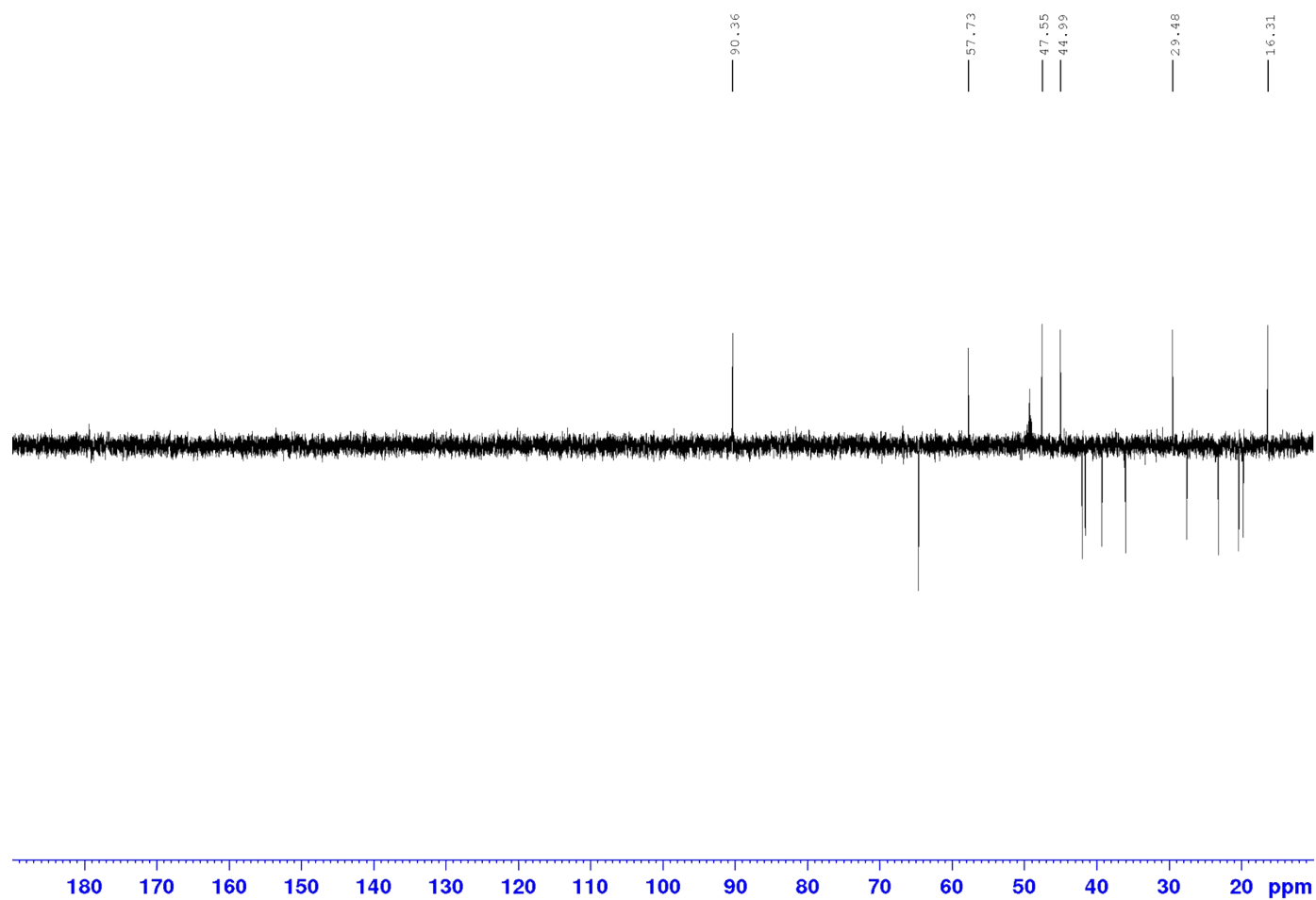


Figure S101. DEPT-135 NMR spectrum of Noueinsiancin I (9) in CD₃OD

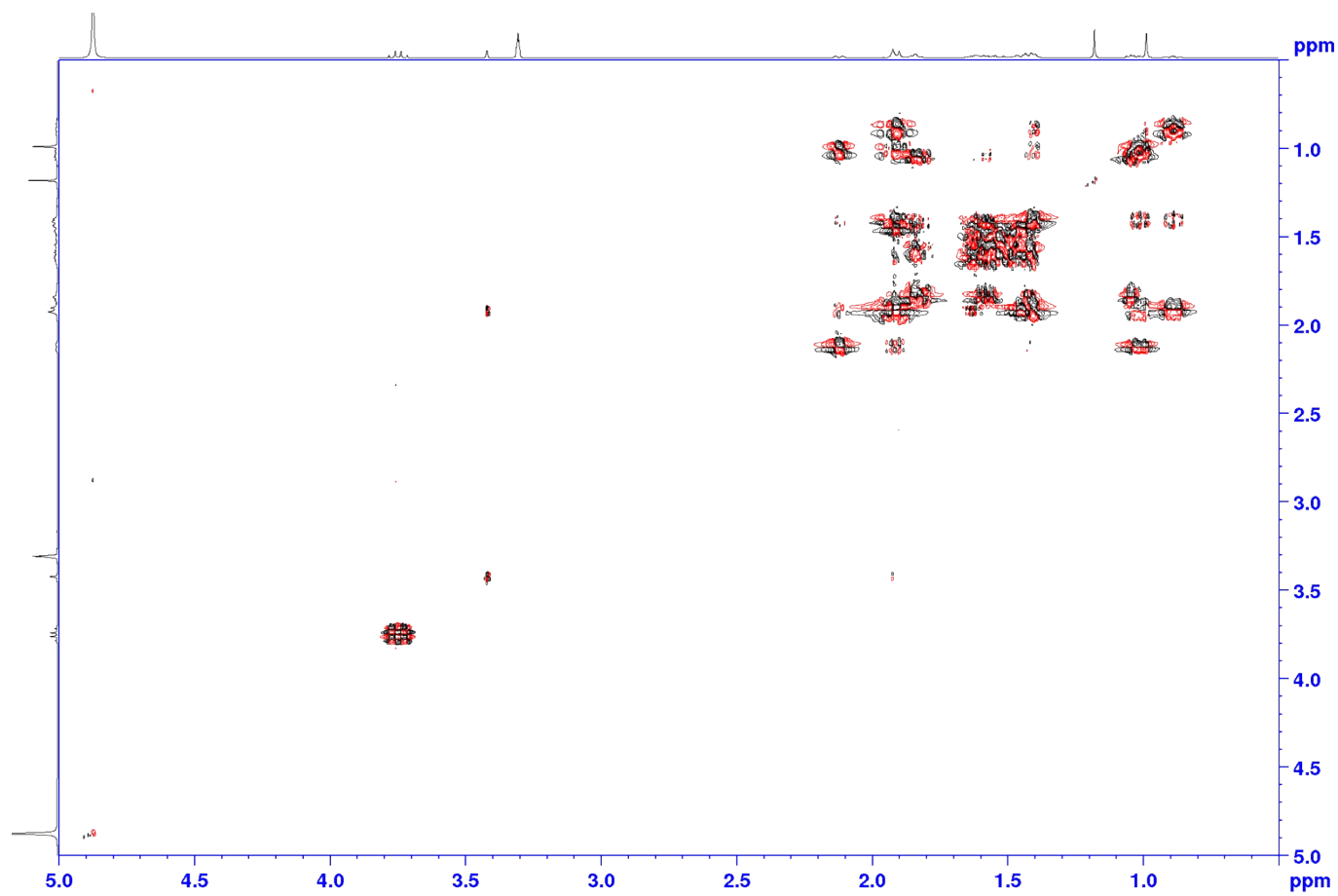


Figure S102. ^1H - ^1H COSY spectrum of Nouveinsiancin I (9) in CD_3OD

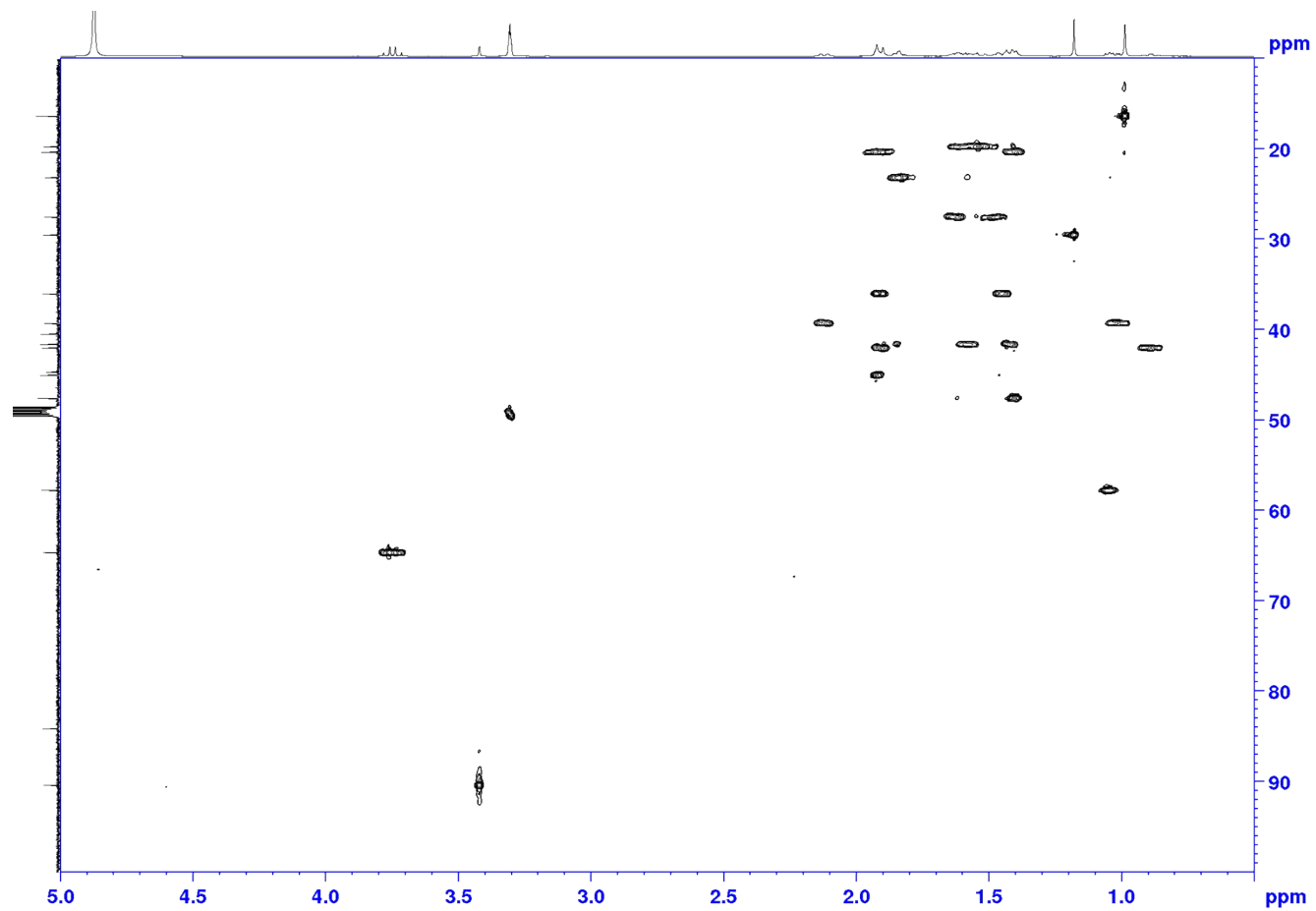


Figure S103. HSQC spectrum of Noueinsiancin I (9) in CD₃OD

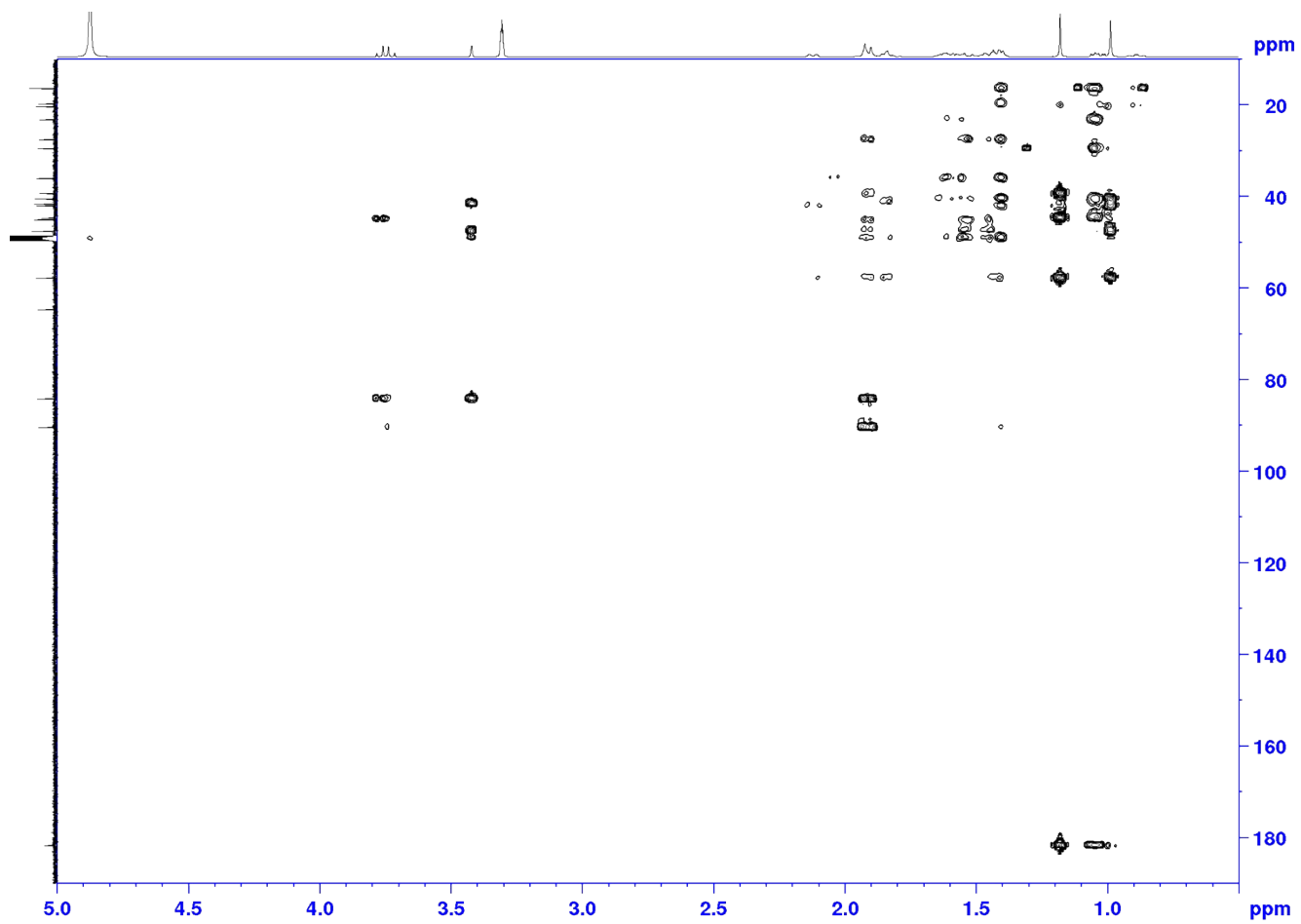


Figure S104. HMBC spectrum of Noueinsiaincin I (9) in CD₃OD

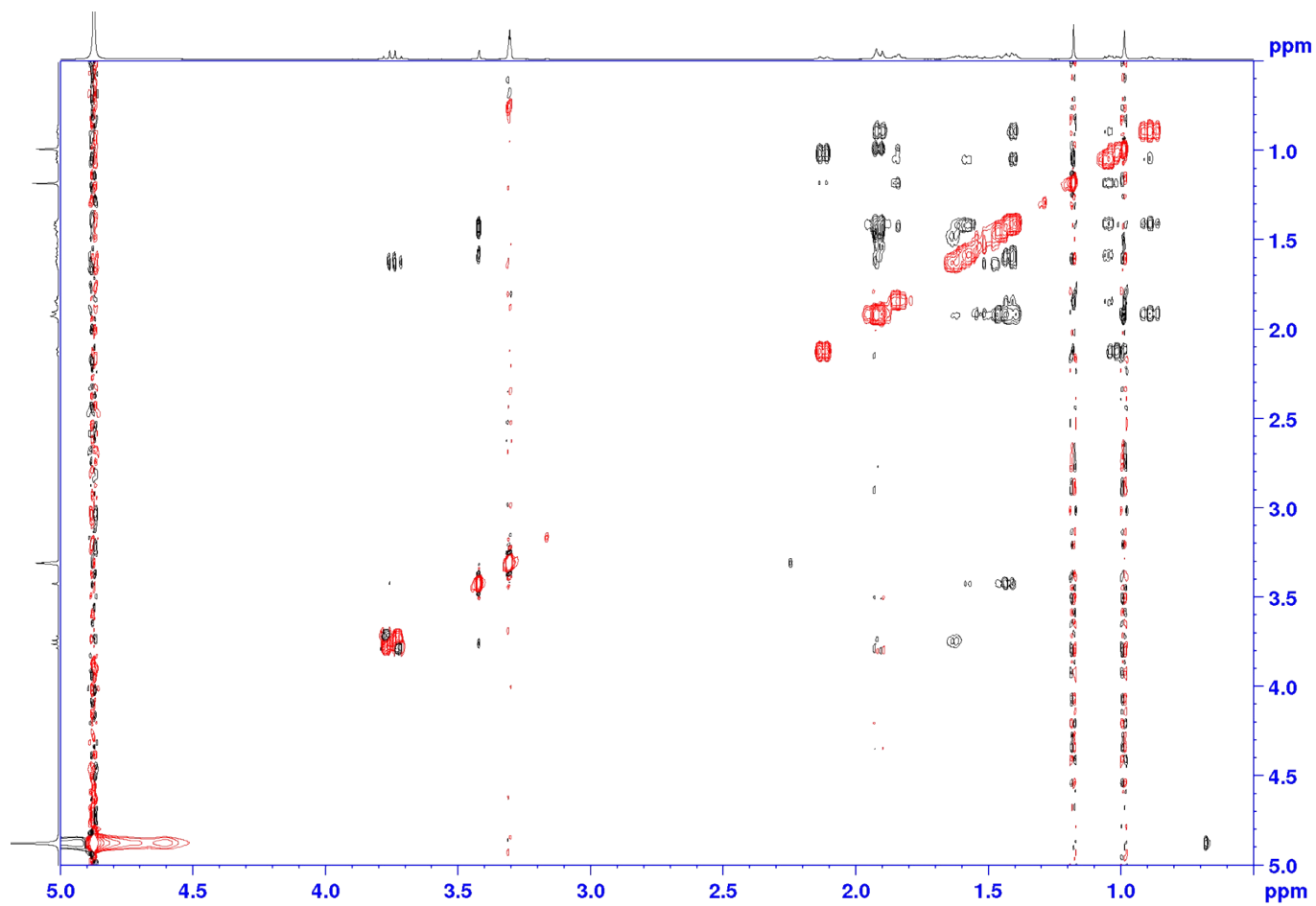


Figure S105. NOESY spectrum of Noueinsiancin I (9) in CD₃OD

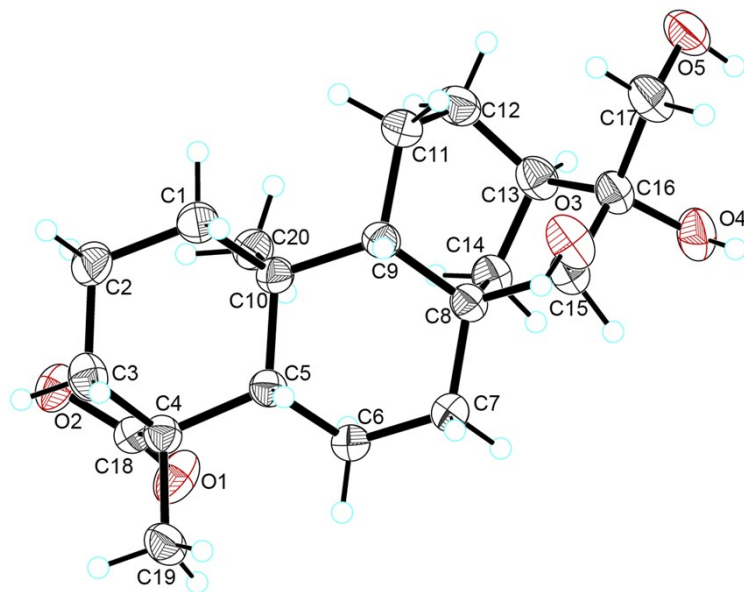
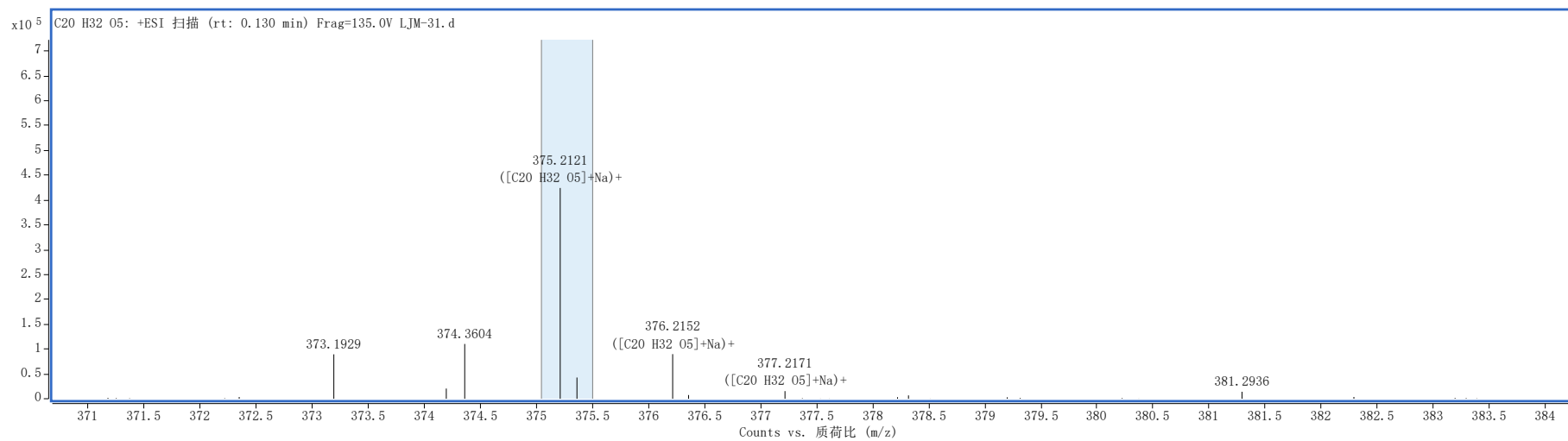


Figure S106. X-ray structure of Noueinsiancin I (9)



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H32 O5	(M+Na)+	375.2121	87.64	6.25	87.64

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.6	421699.4	100	375.2142	2.1	424357.5	100	80.1	375.2121	5.67

Figure S107. HRESIMS spectrum of Nouveinsiancin J (10)

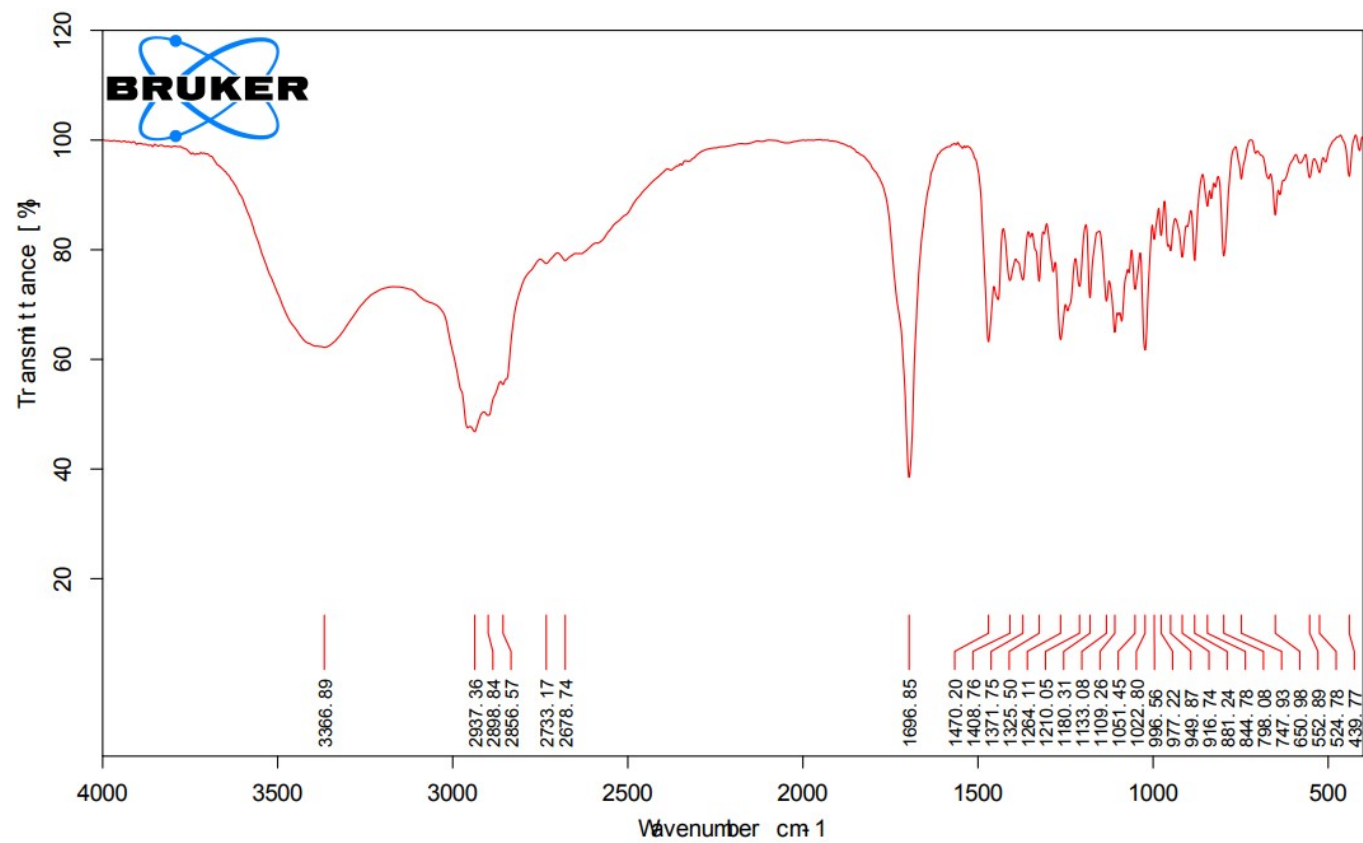


Figure S108. IR spectrum of Noueinsiancin J (10)

Rudolph Research Analytical

Wednesday, 02/09/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-31
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum						
6	-87.000	0.0000	-87.000	-87.000						
S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-31	03:42:49 PM	-87.000	SR	-0.087	589	100.00	0.100	19.7	
2	LJM-31	03:42:54 PM	-87.000	SR	-0.087	589	100.00	0.100	19.7	
3	LJM-31	03:43:00 PM	-87.000	SR	-0.087	589	100.00	0.100	19.7	
4	LJM-31	03:43:06 PM	-87.000	SR	-0.087	589	100.00	0.100	19.7	
5	LJM-31	03:43:12 PM	-87.000	SR	-0.087	589	100.00	0.100	19.8	
6	LJM-31	03:43:18 PM	-87.000	SR	-0.087	589	100.00	0.100	19.8	

Signature

Figure S109. OR Value of Noueinsiancin J (10) in CH₃OH

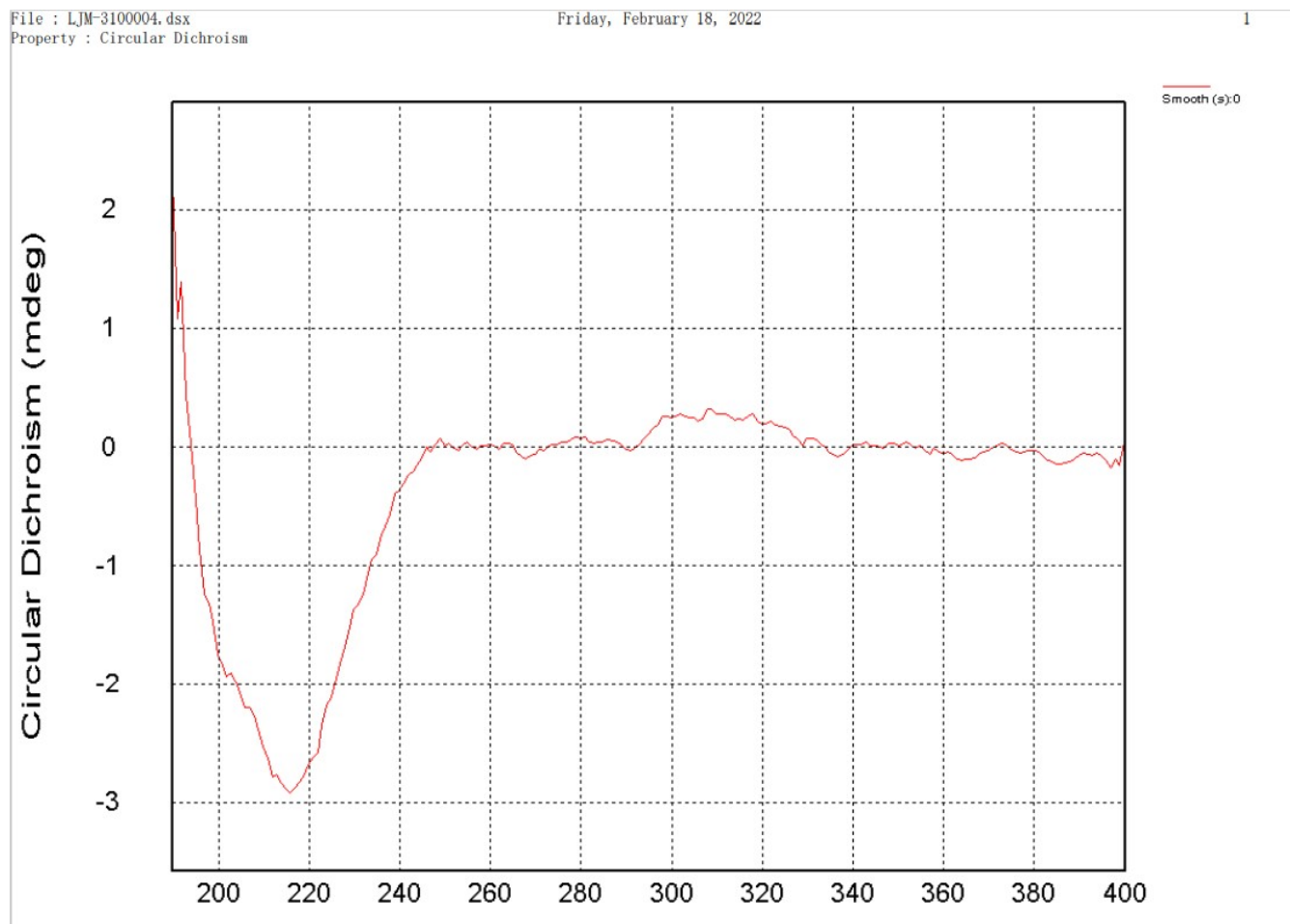


Figure S110. CD Value of Noueinsiancin J (10) in CH₃OH

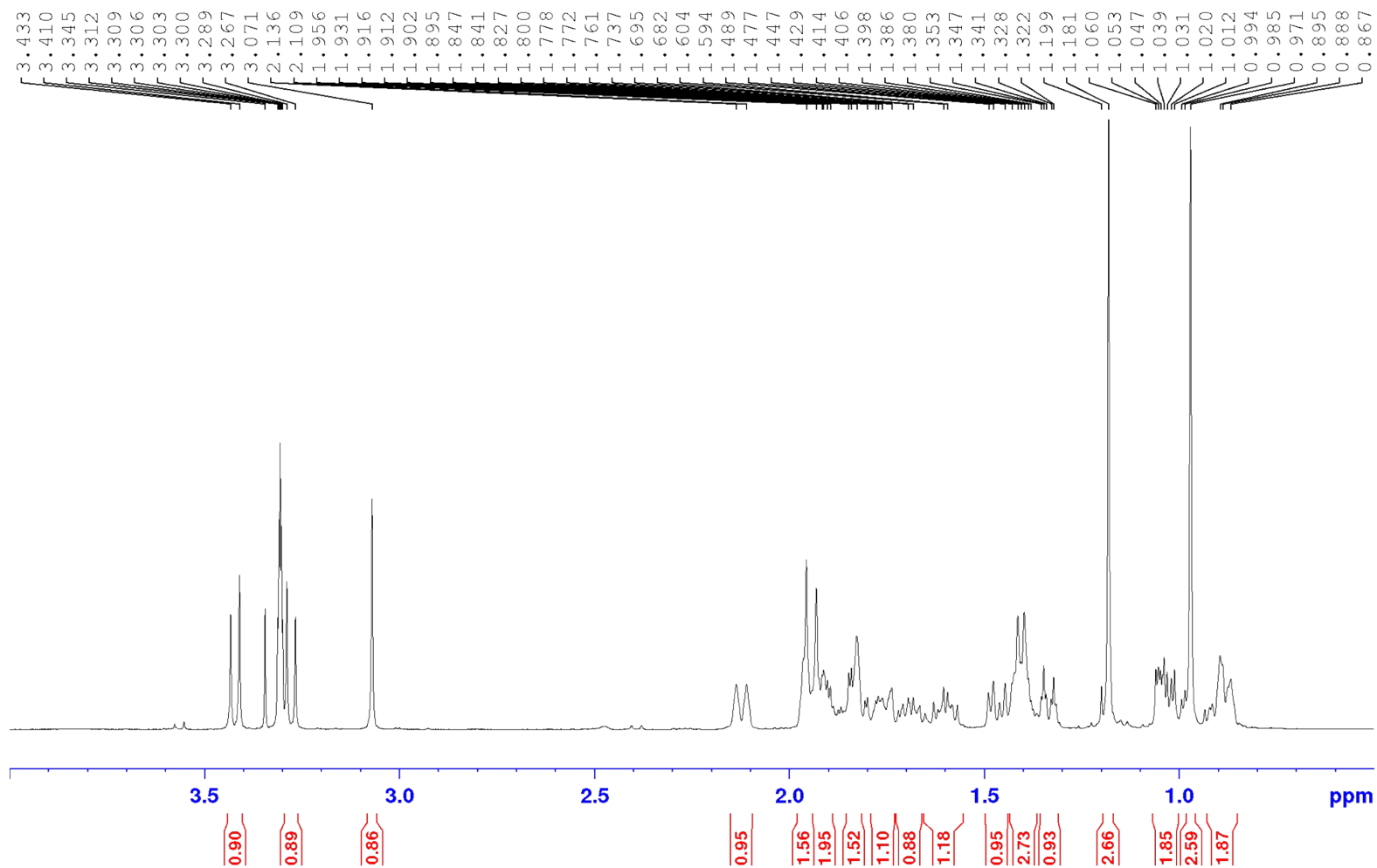


Figure S111. ¹H NMR spectrum of Noueinsiancin J (10) in CD₃OD

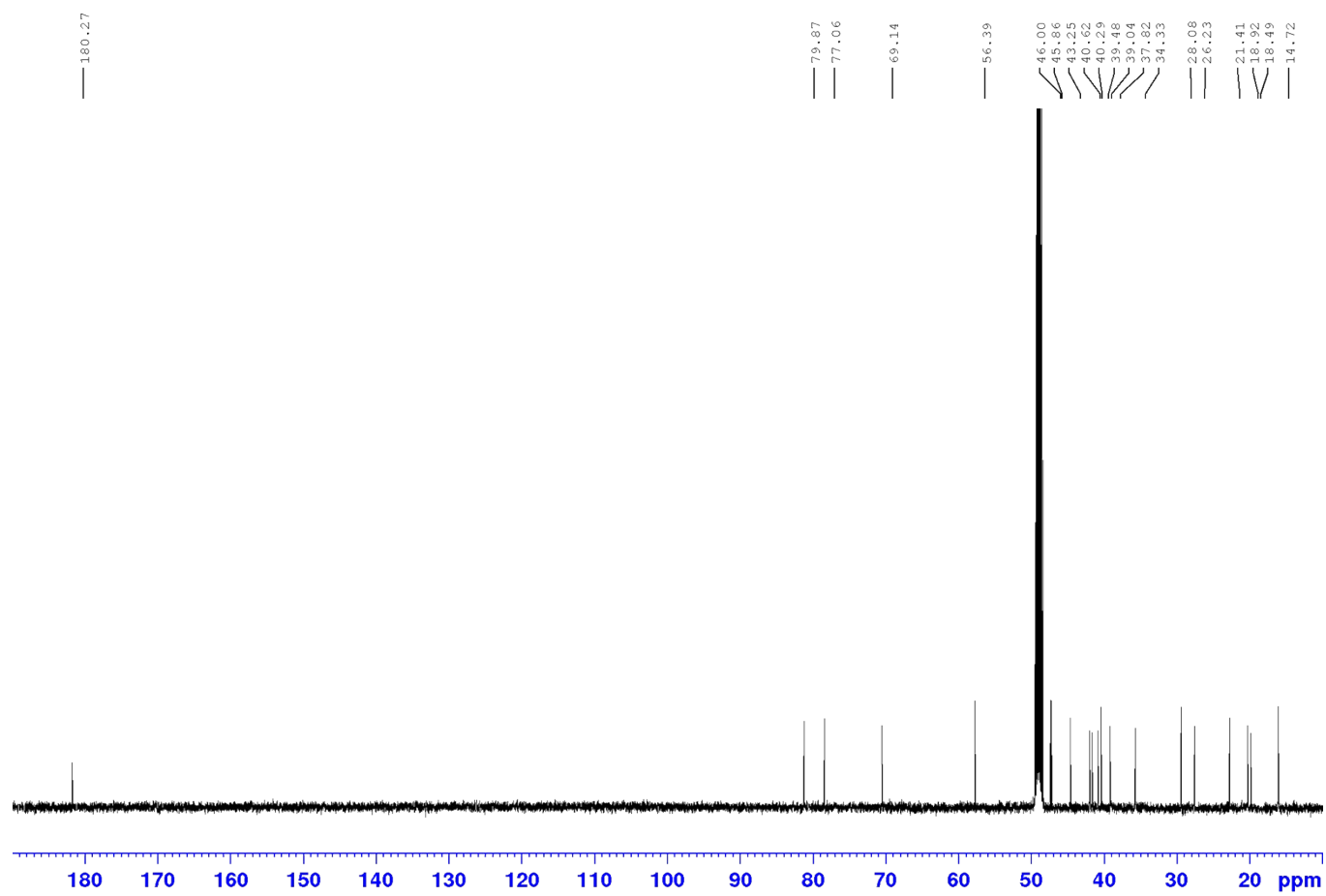


Figure S112. ¹³C NMR spectrum of Noueinsiancin J (10) in CD₃OD

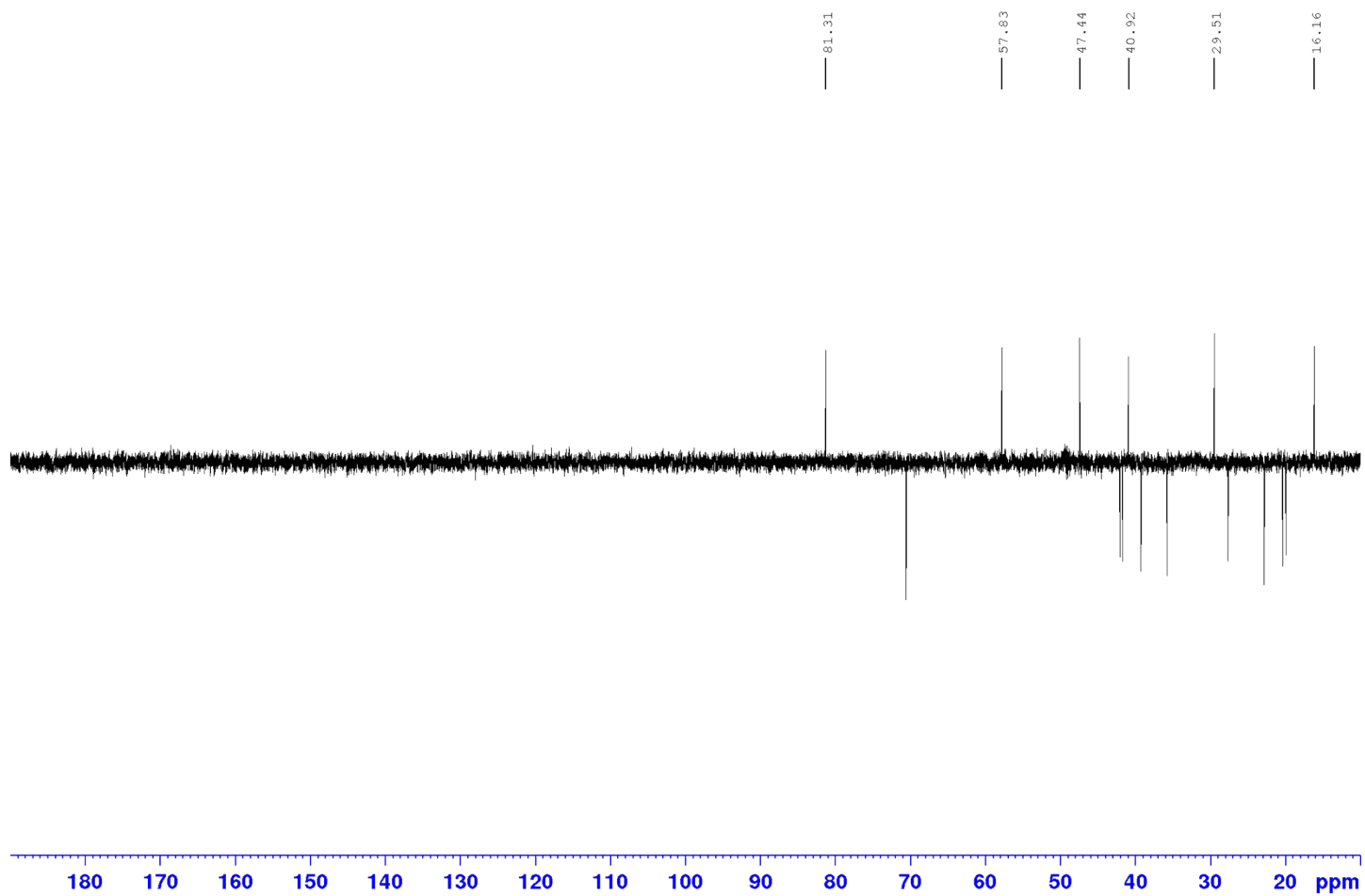


Figure S113. DEPT-135 NMR spectrum of Noueinsiancin J (10) in CD₃OD

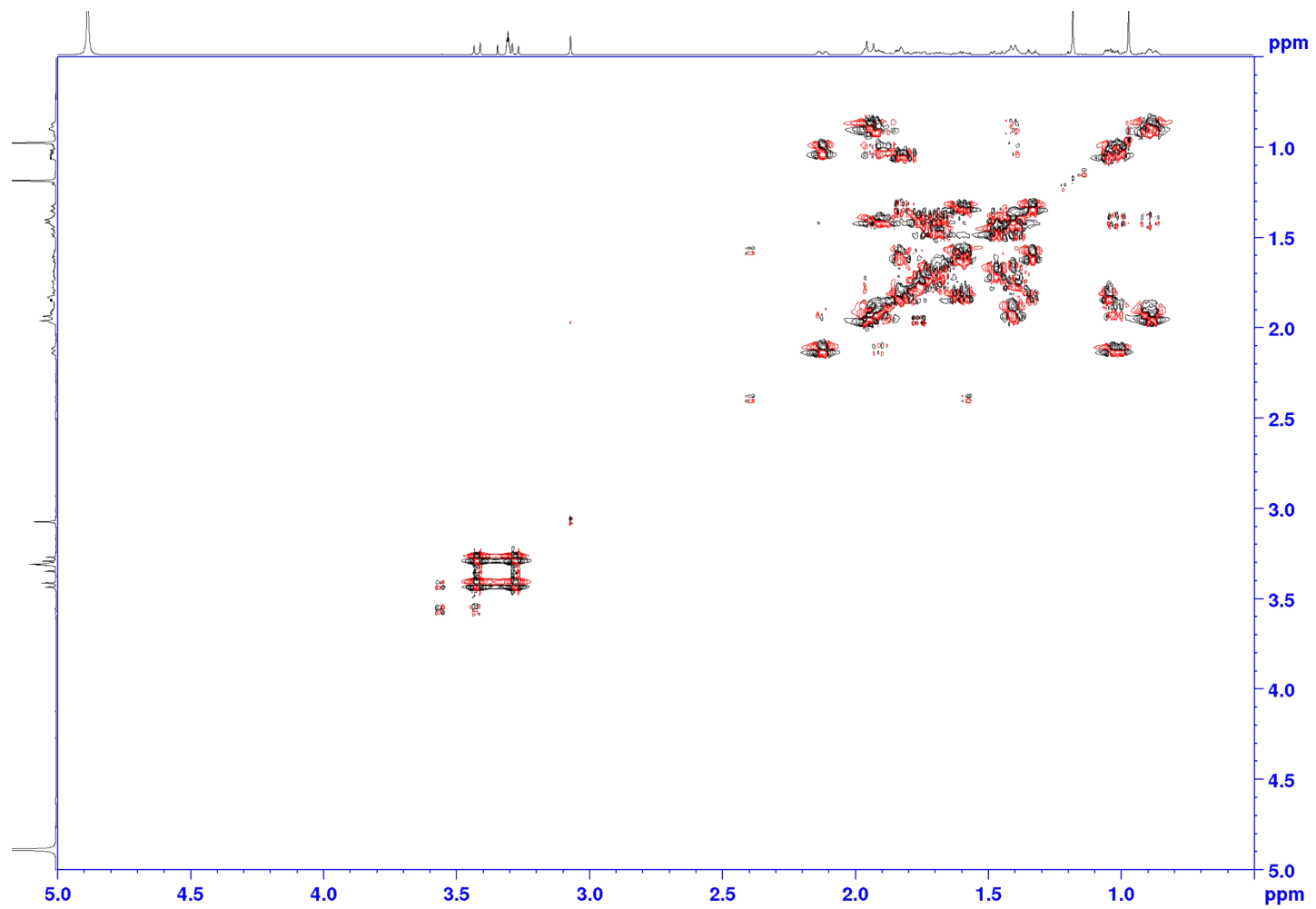


Figure S114. ^1H - ^1H COSY spectrum of Noueinsiancin J (10) in CD_3OD

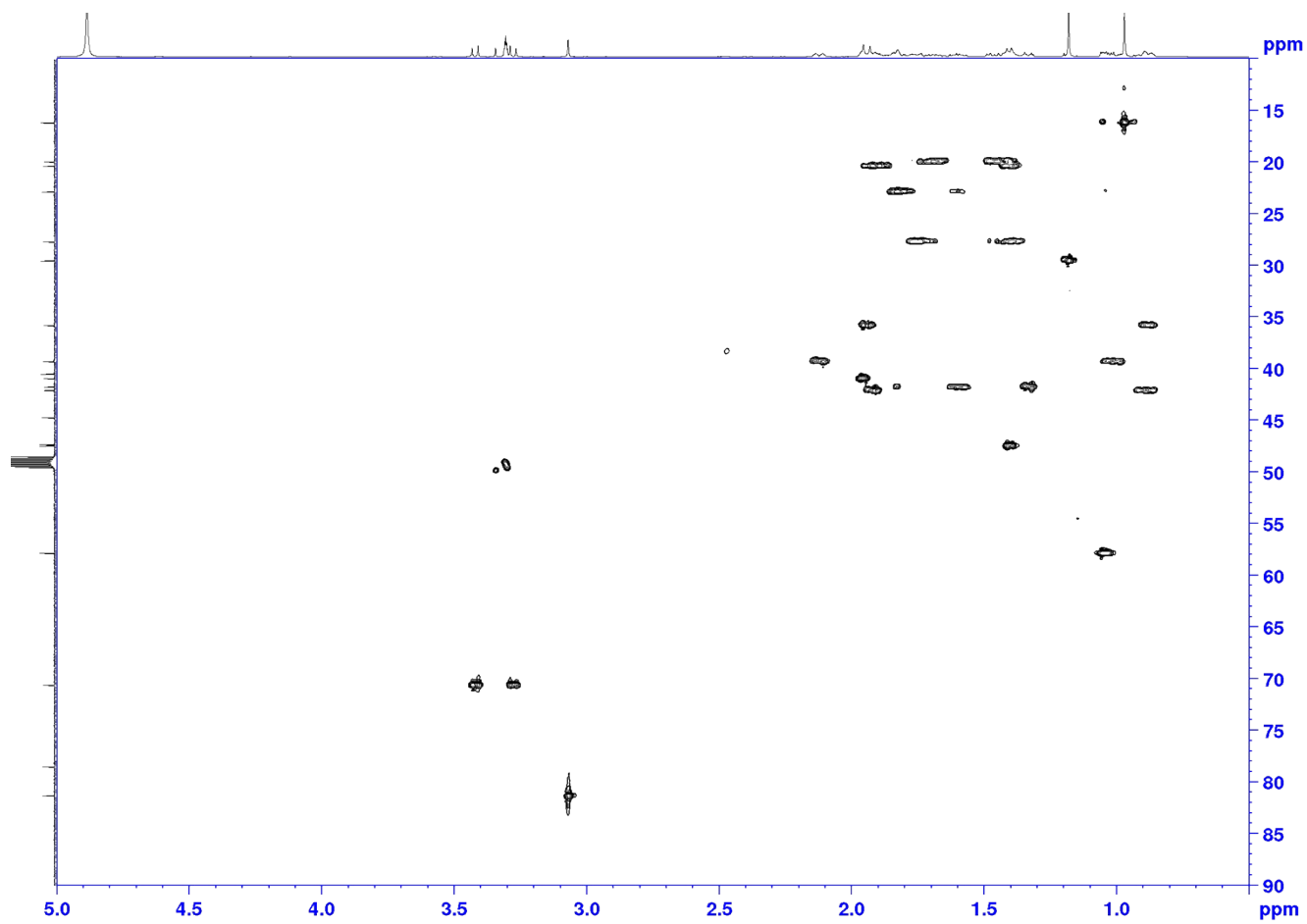


Figure S115. HSQC spectrum of Noueinsiancin J (10) in CD₃OD

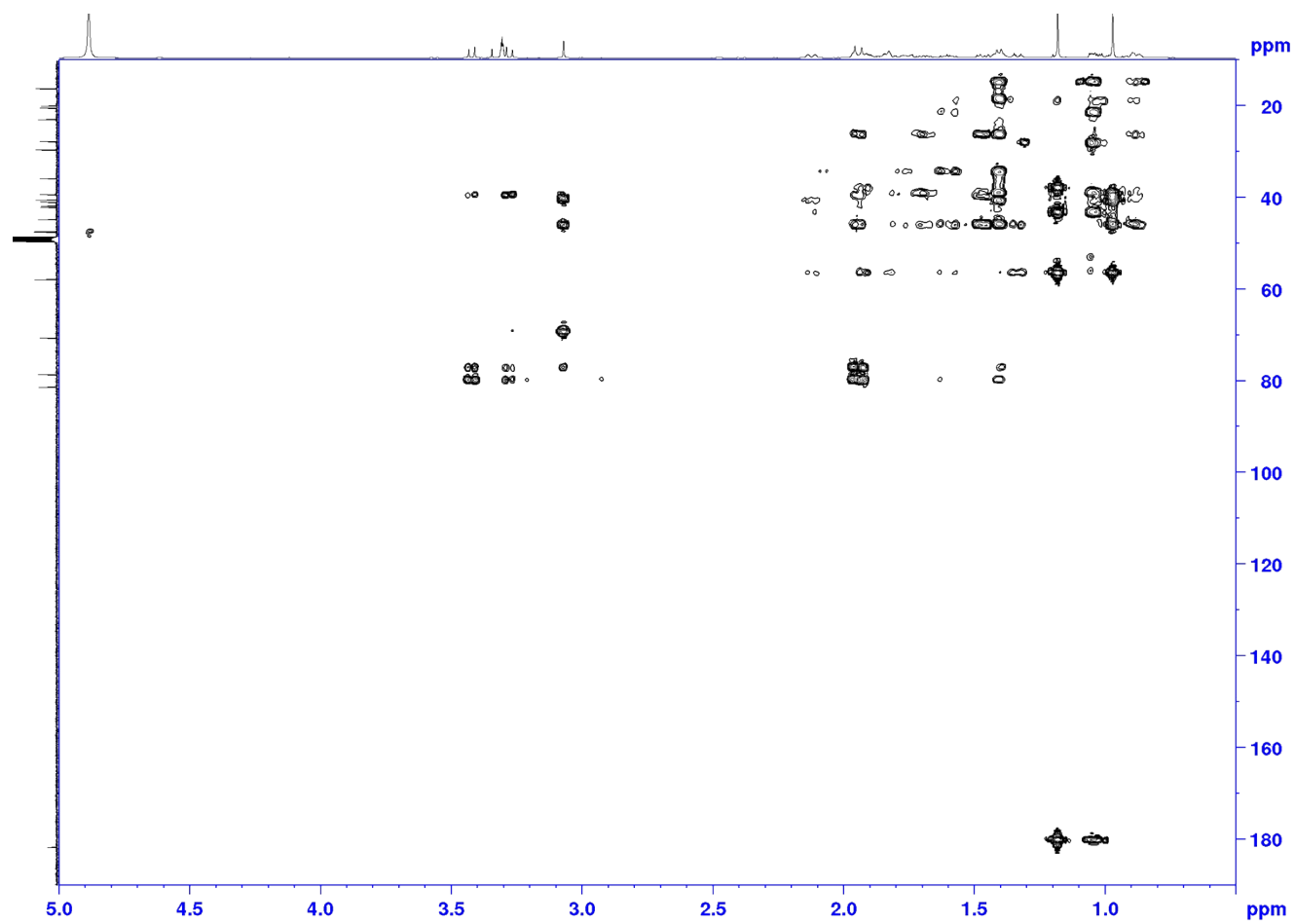


Figure S116. HMBC spectrum of Noueinsiaincin J (10) in CD₃OD

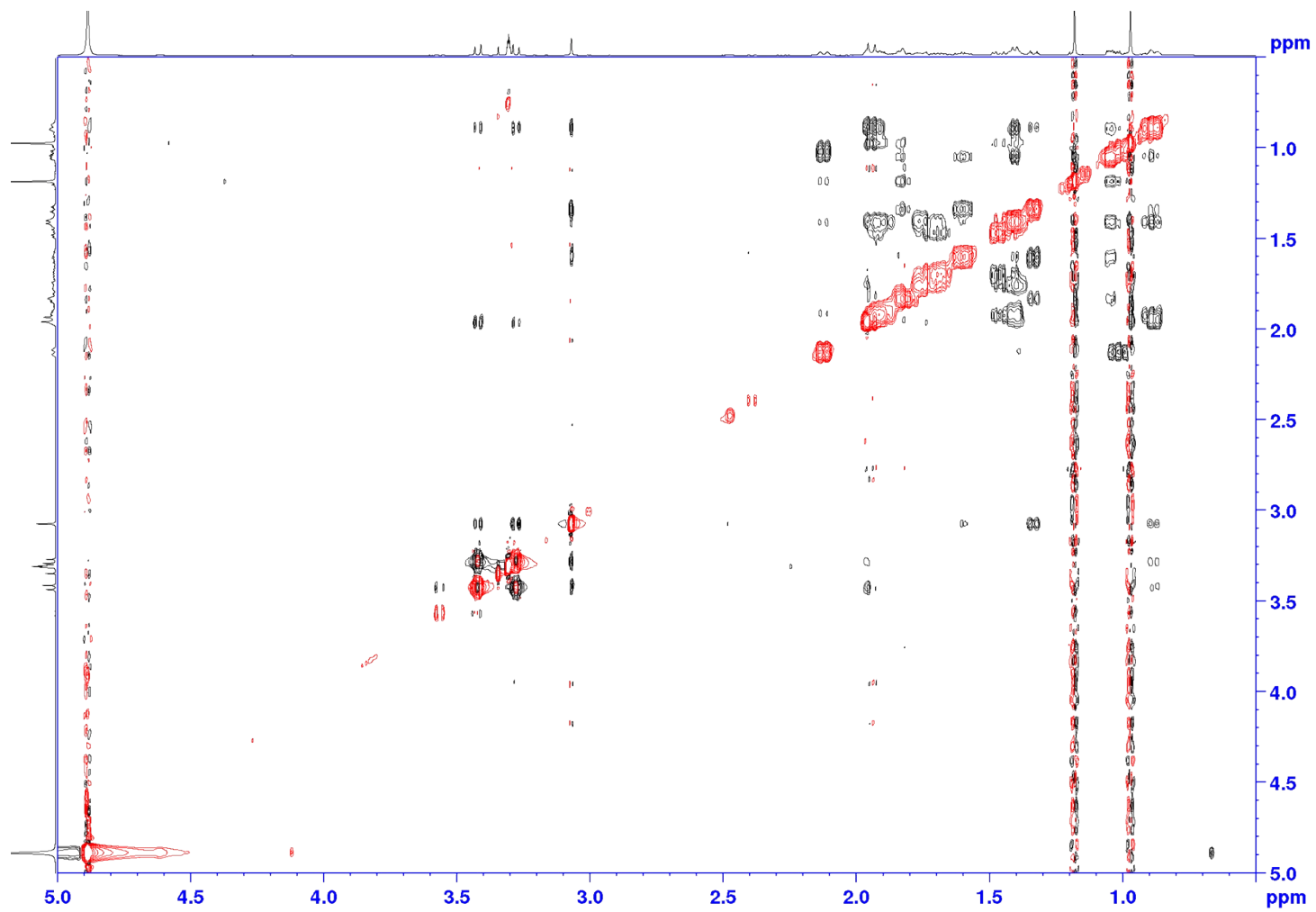
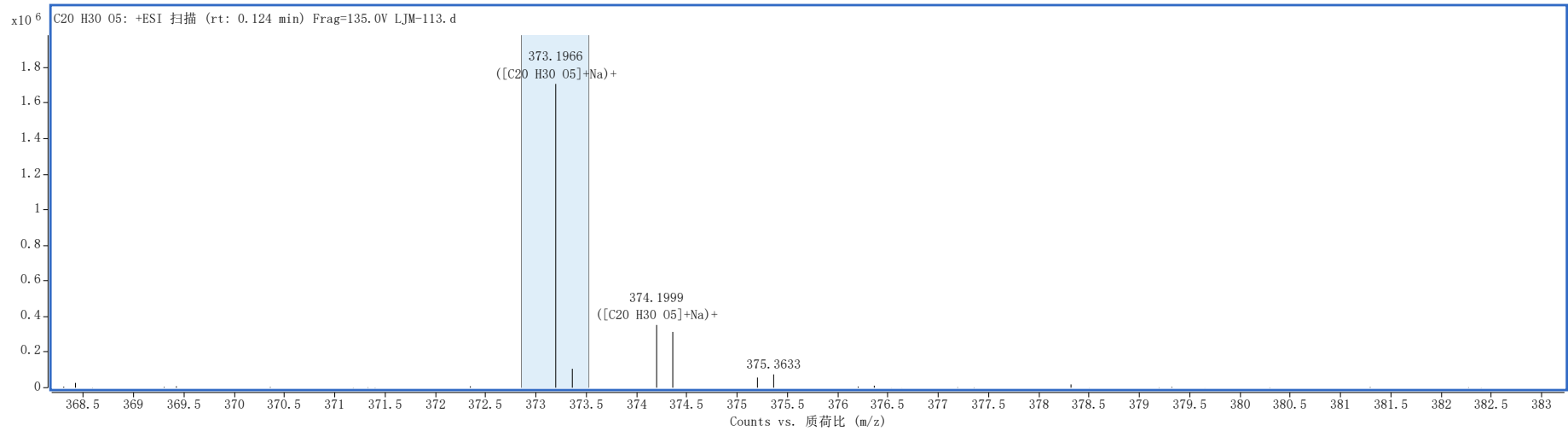


Figure S117. NOESY spectrum of Noueinsiancin J (10) in CD₃OD



最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H30 O5	(M+Na)+	373.1966	89.33	5.71	89.33

峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数 (计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.7	1686932.3	100	373.1985	2	1708077.2	100	80.7	373.1966	5.28

Figure S118. HRESIMS spectrum of Nouveinsiancin K (11)

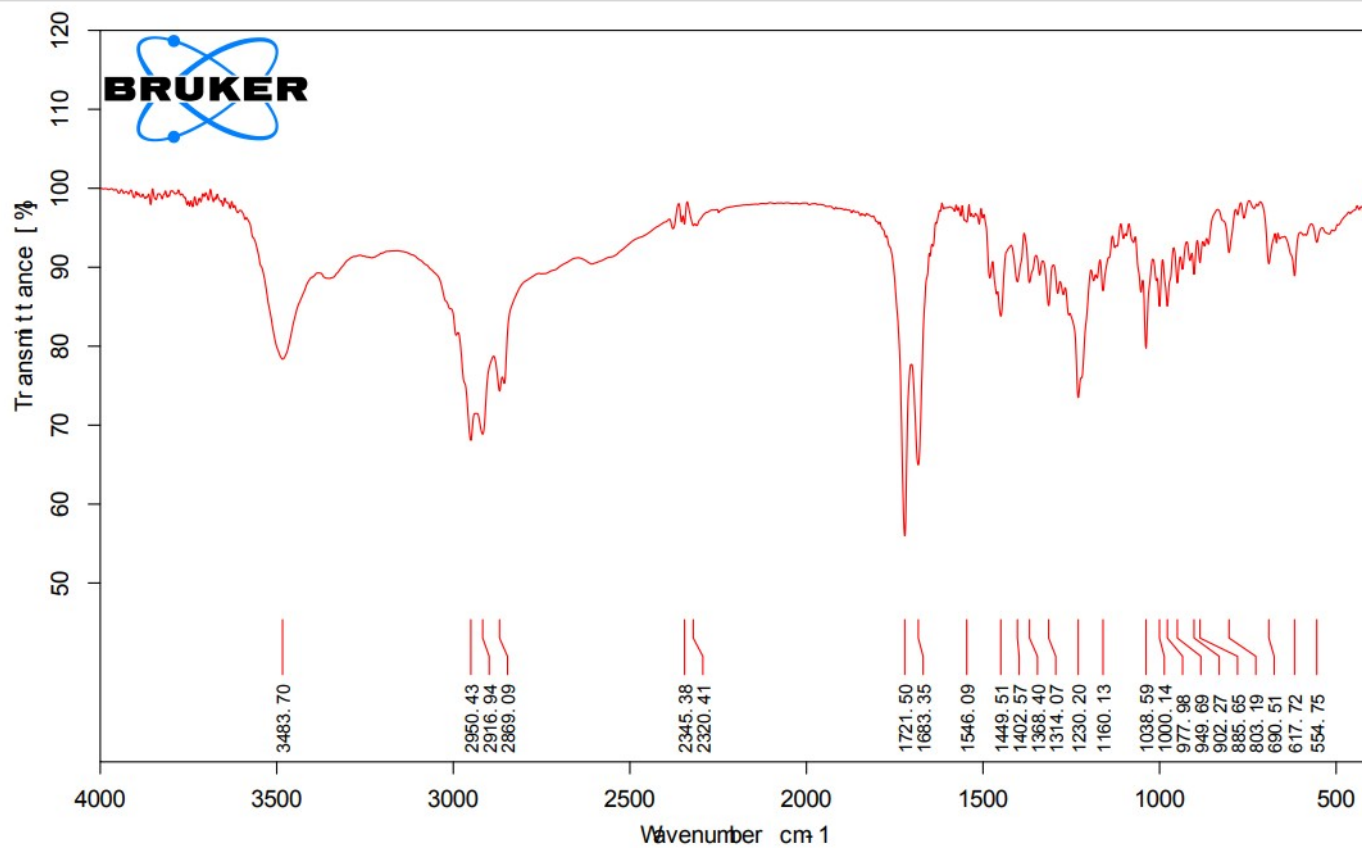


Figure S119. IR spectrum of Noueinsiancin K (11)

Rudolph Research Analytical

Thursday, 02/10/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : LJM-113
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-96.000	0.0000	-96.000	-96.000

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	LJM-113	08:12:00 PM	-96.000	SR	-0.048	589	100.00	0.050	20.3	
2	LJM-113	08:12:05 PM	-96.000	SR	-0.048	589	100.00	0.050	20.2	
3	LJM-113	08:12:11 PM	-96.000	SR	-0.048	589	100.00	0.050	20.2	
4	LJM-113	08:12:16 PM	-96.000	SR	-0.048	589	100.00	0.050	20.2	
5	LJM-113	08:12:21 PM	-96.000	SR	-0.048	589	100.00	0.050	20.2	
6	LJM-113	08:12:27 PM	-96.000	SR	-0.048	589	100.00	0.050	20.1	

Signature

Figure S120. OR Value of Noueinsiancin K (11) in CH₃OH

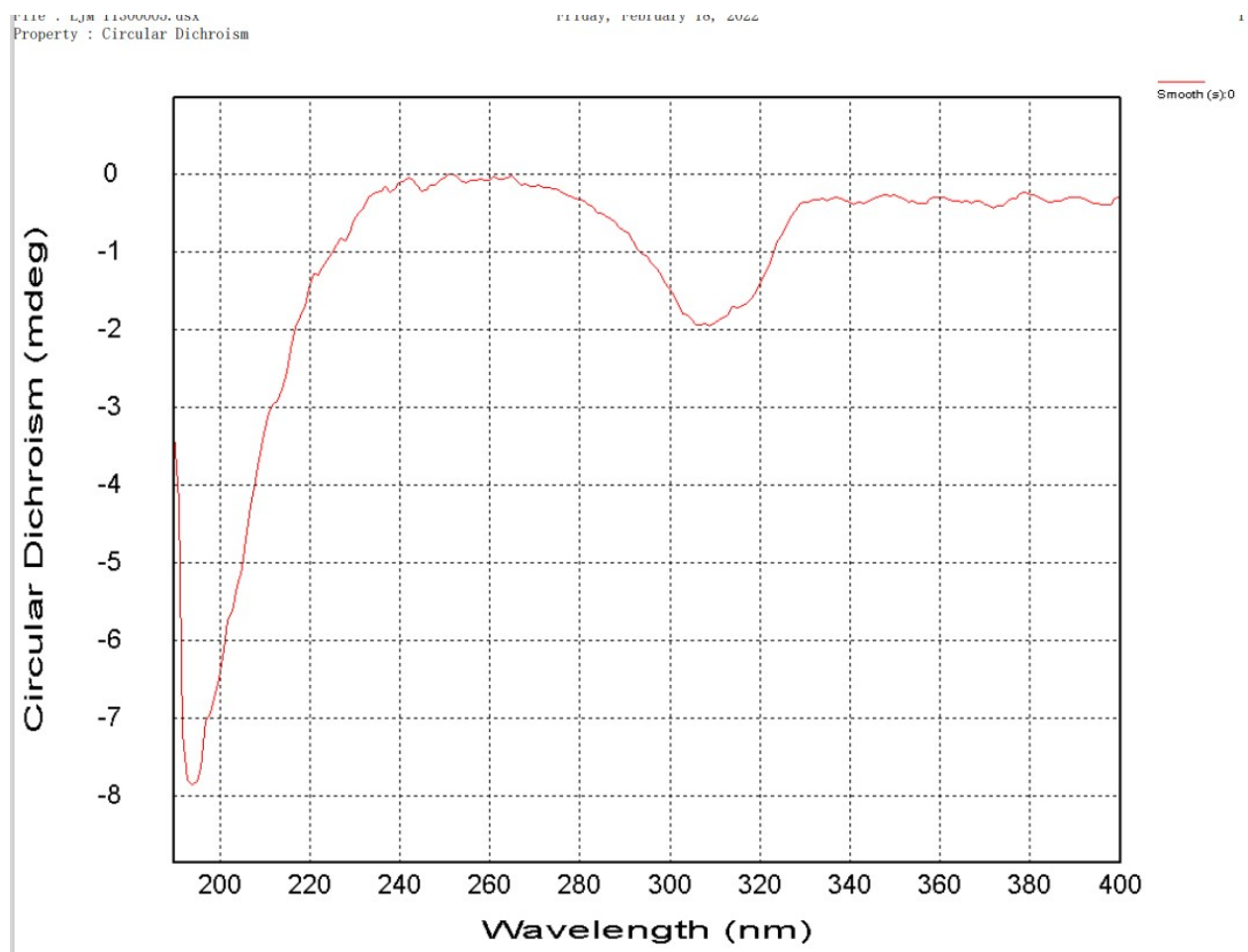


Figure S121. CD Value of Noueinsiancin K (11) in CH₃OH

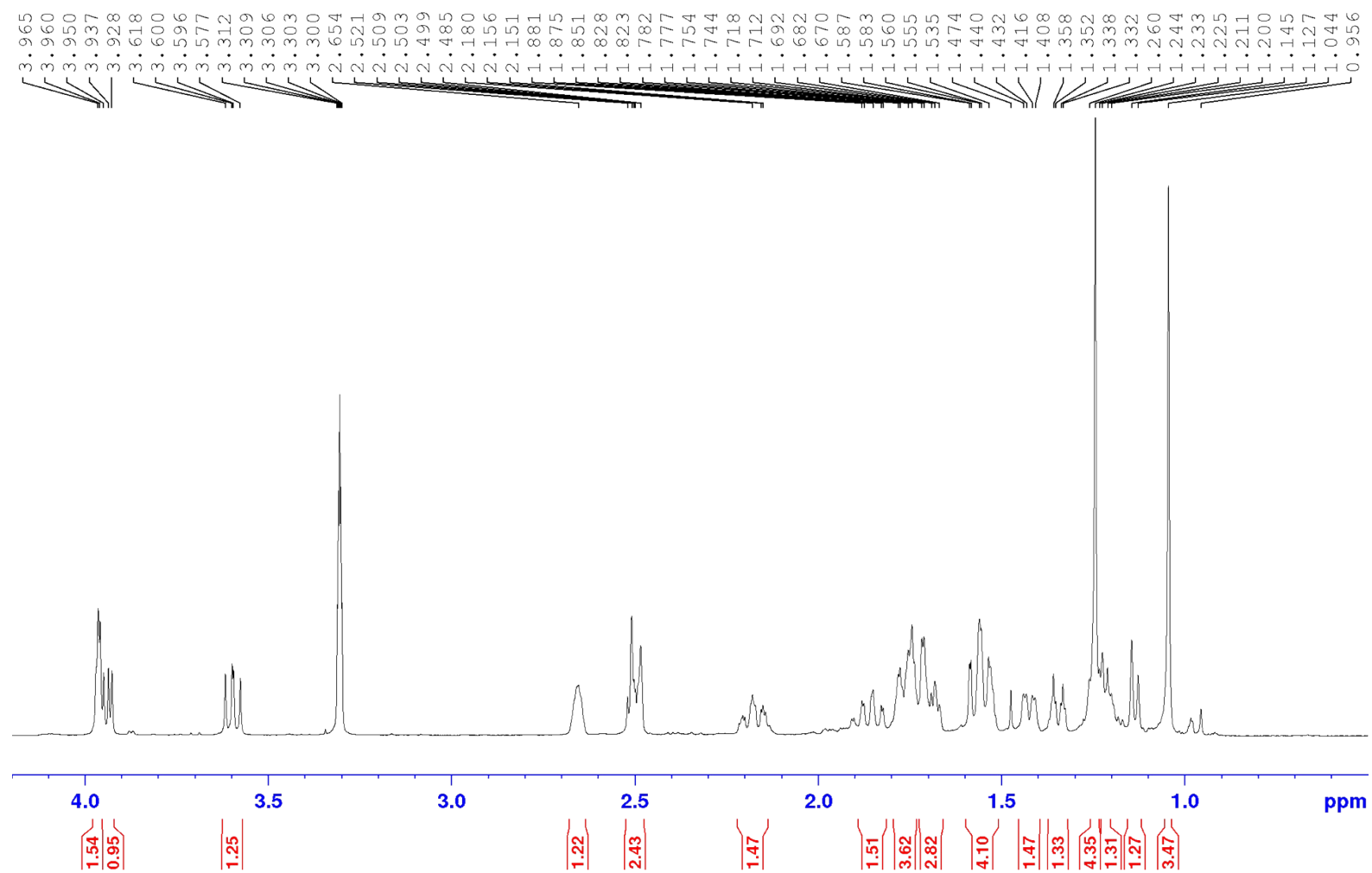


Figure S122. ¹H NMR spectrum of Noueinsiancin K (11) in CD₃OD

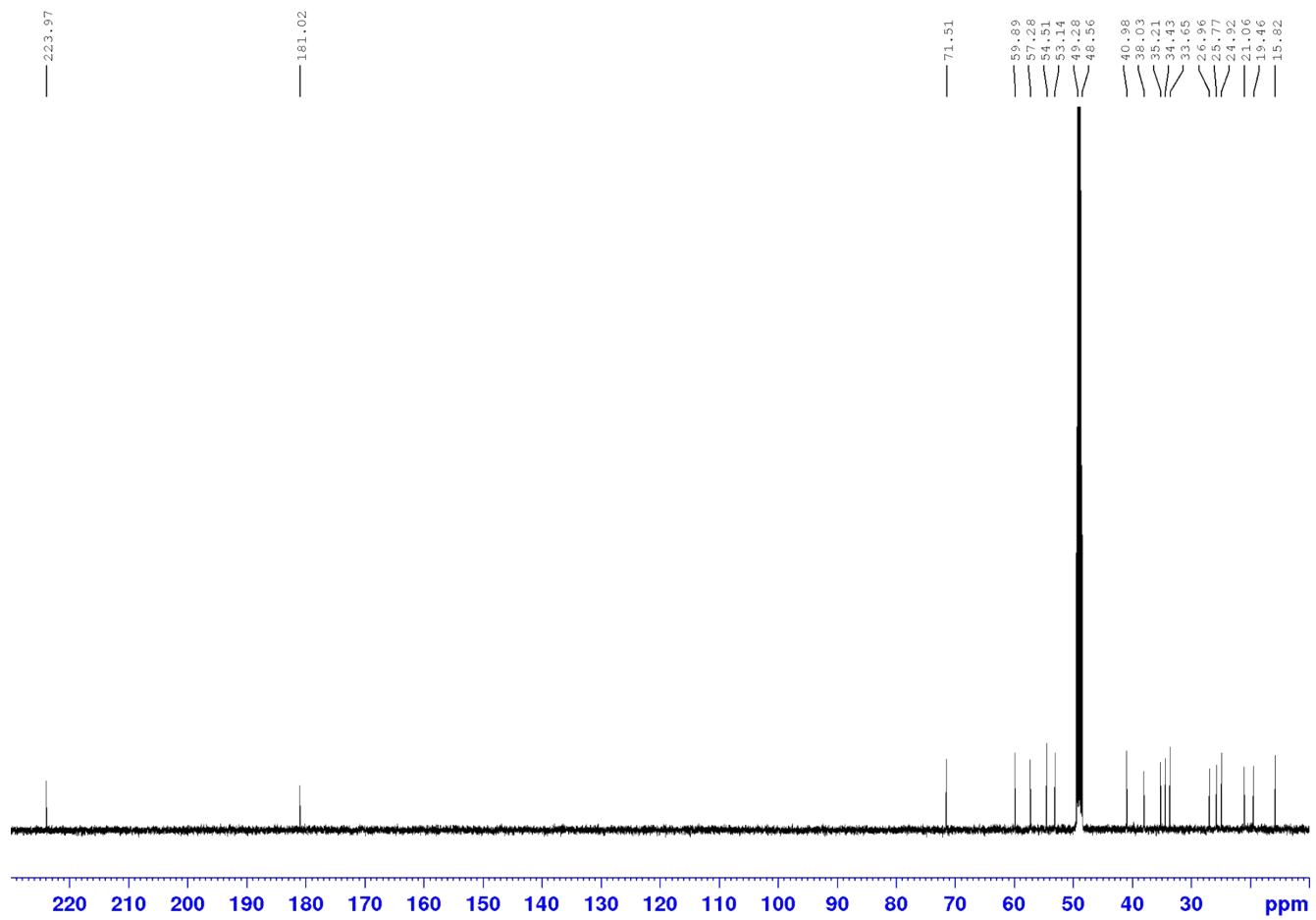


Figure S123. ¹³C NMR spectrum of Noueinsiancin K (11) in CD₃OD

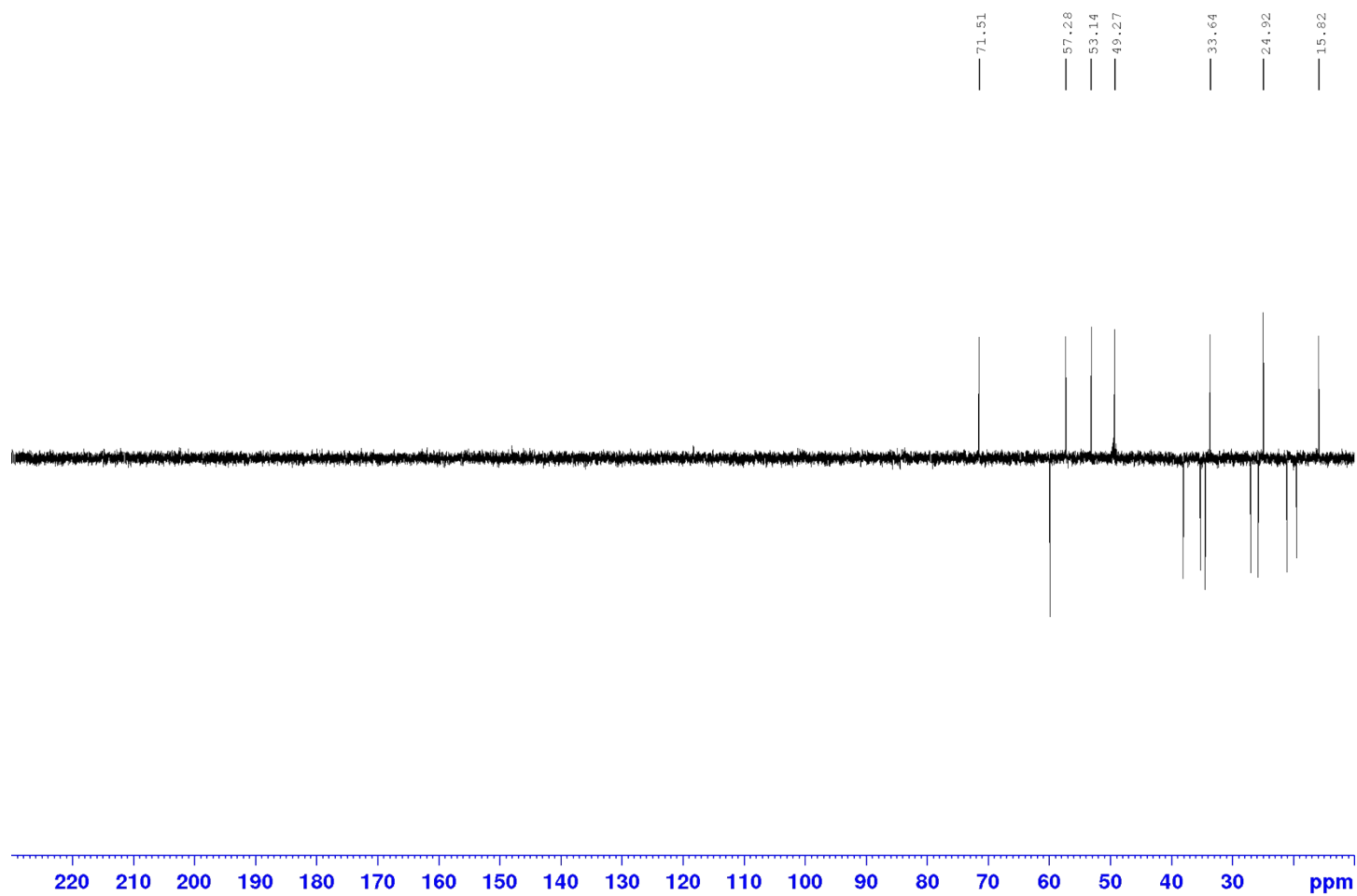


Figure S124. DEPT-135 NMR spectrum of Noueinsiancin K (11) in CD₃OD

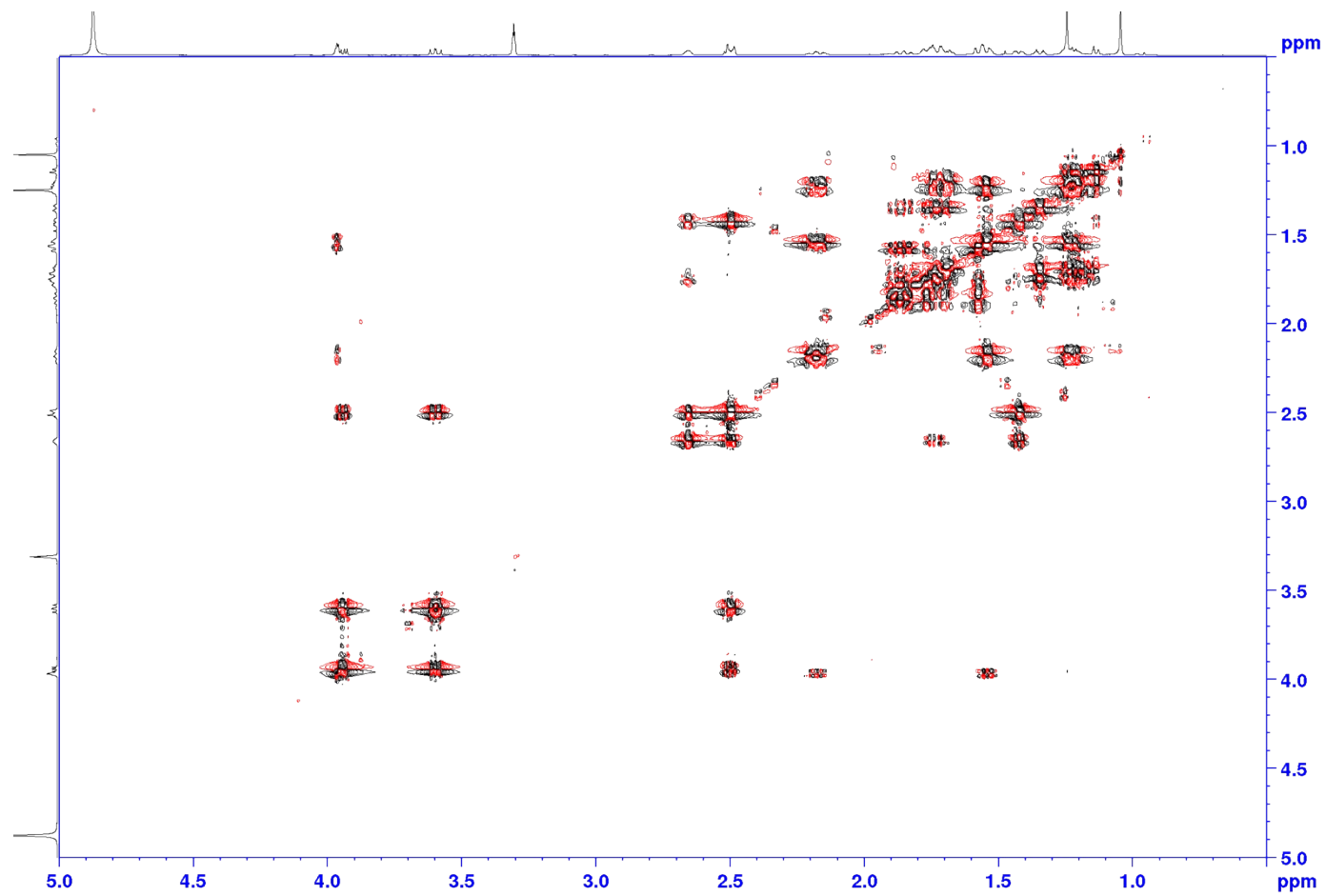


Figure S125. ^1H - ^1H COSY spectrum of Noueinsiancin K (11) in CD_3OD

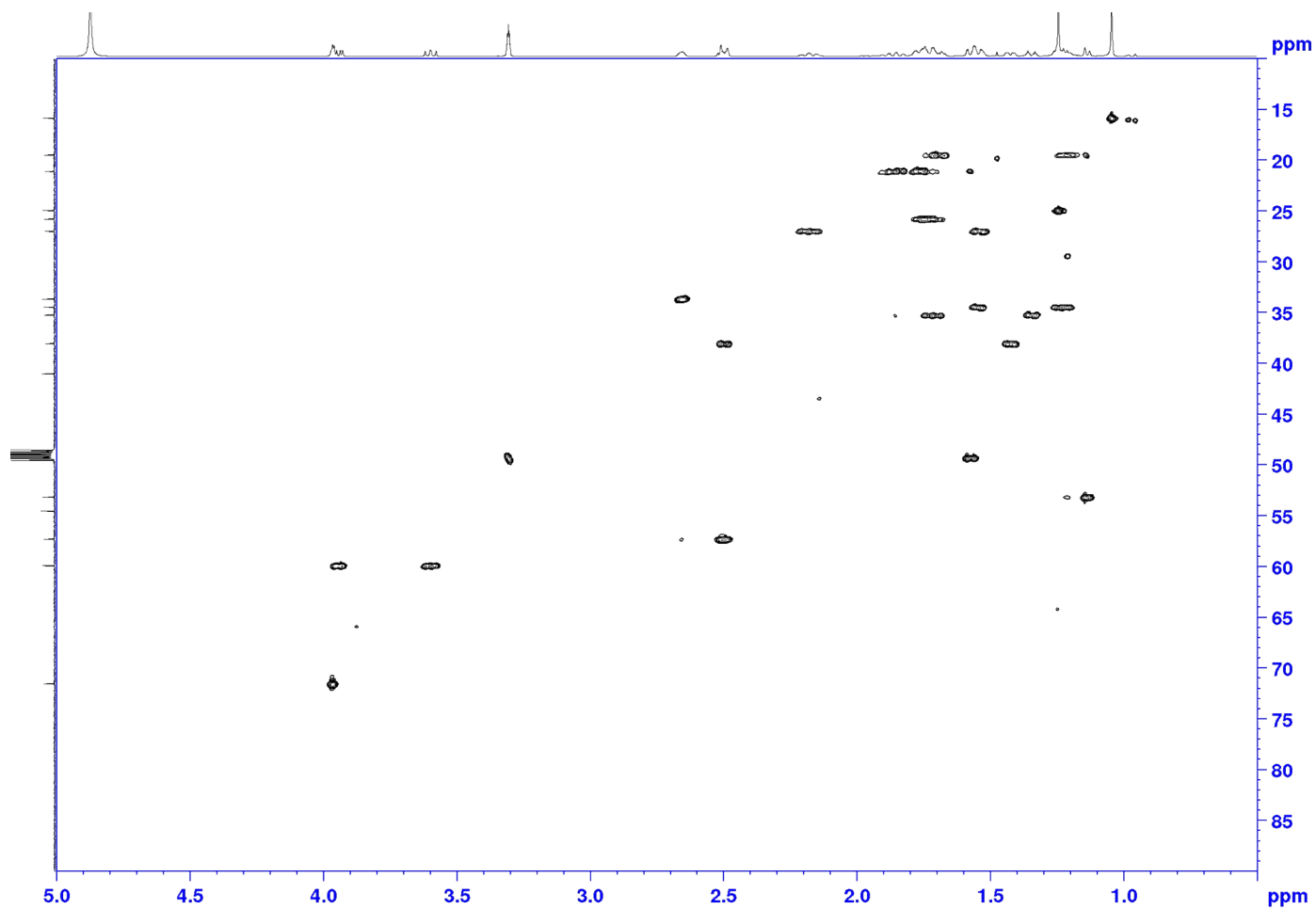


Figure S126. HSQC spectrum of Noueinsiancin K (11) in CD₃OD

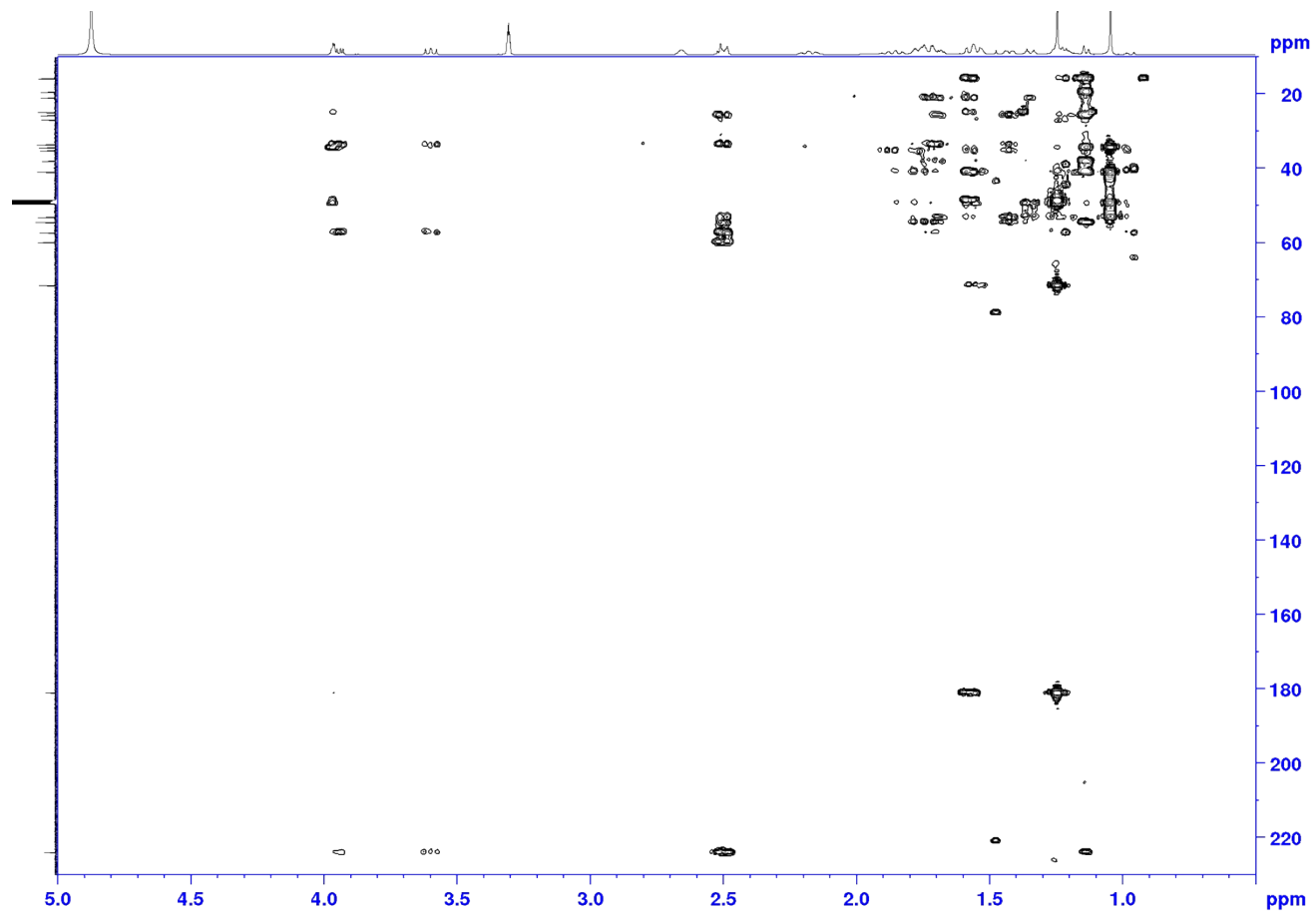


Figure S127. HMBC spectrum of Noueinsiancin K (11) in CD₃OD

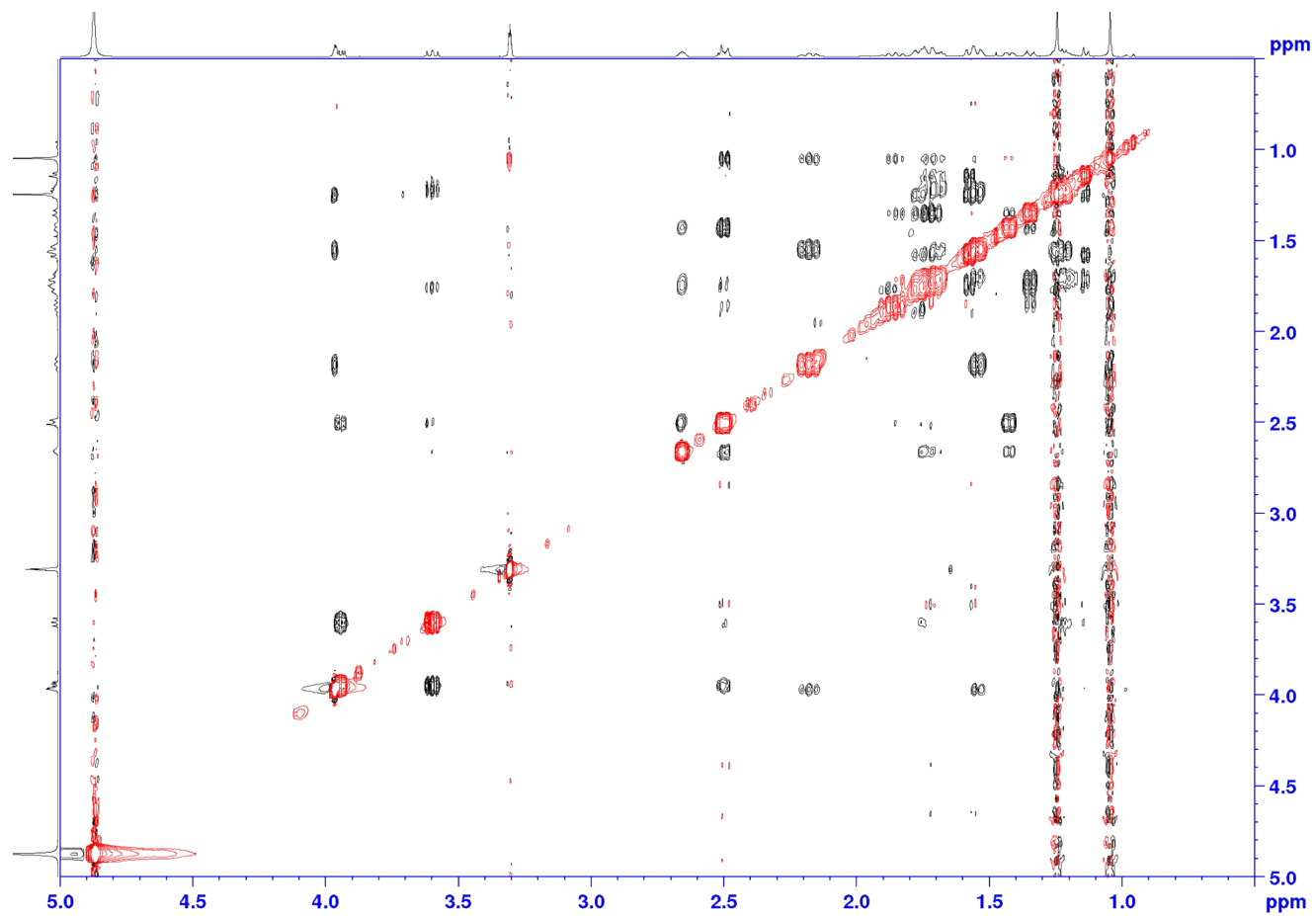


Figure S128. NOESY spectrum of Noueinsiancin K (11) in CD₃OH

