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# Supporting Information

for

# Rhodopyran, a carboxylated hexahydrocyclopenta[*b*]pyran from *Rhodococcus*

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## NMR, HRMS, IR spectra, and HPLC chromatogram for compound 1

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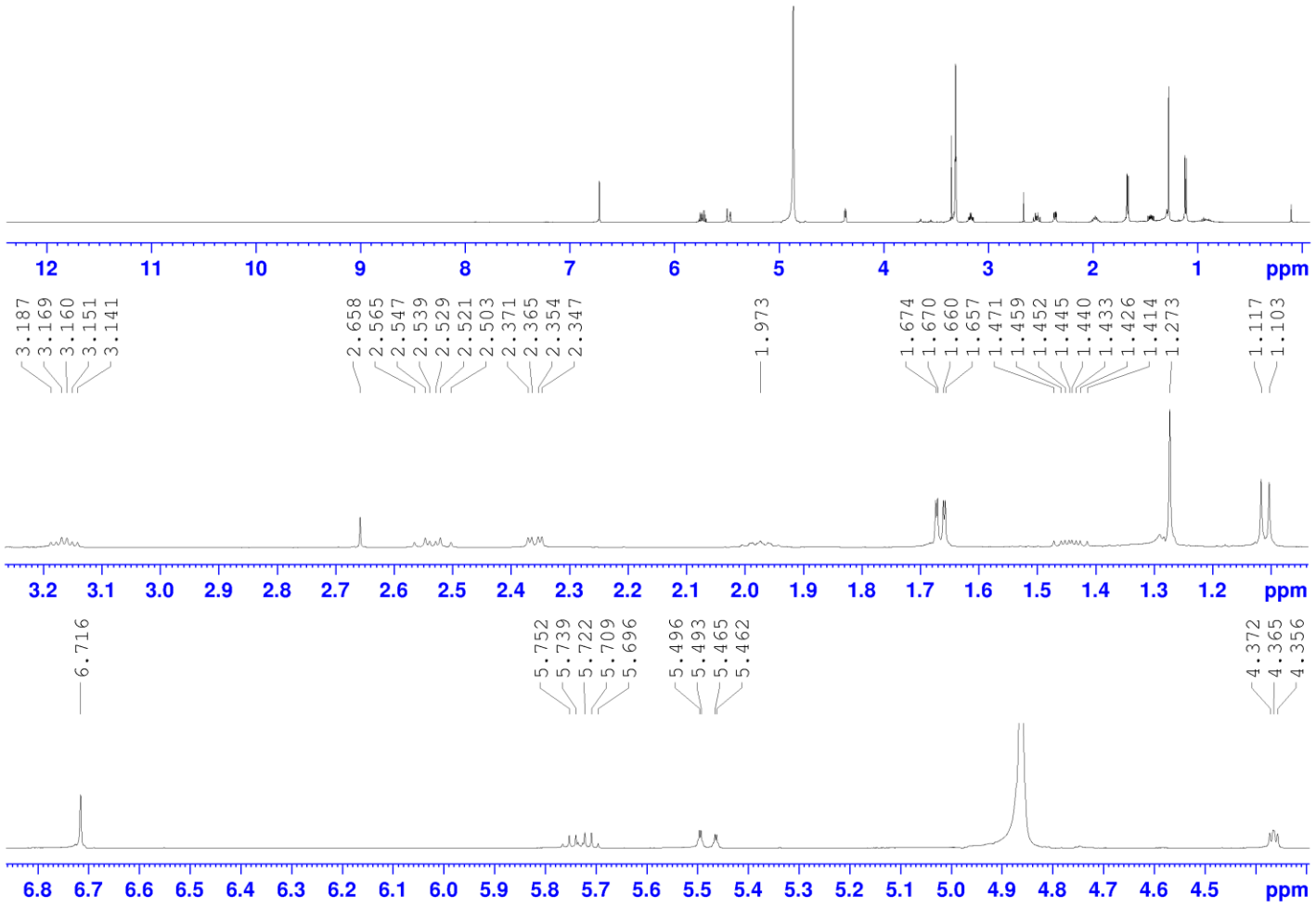
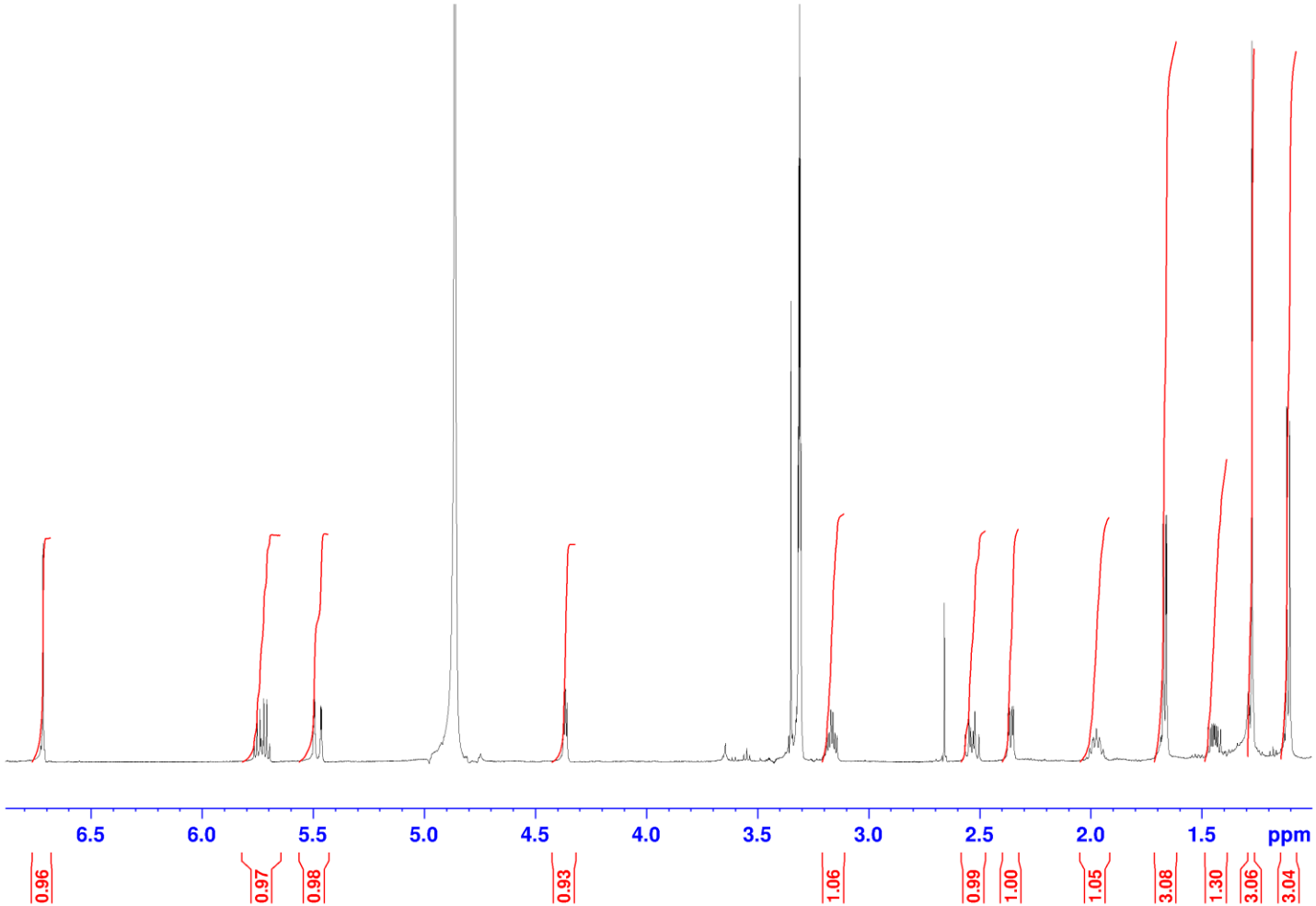
**Figure S1.** $^{1}H$ NMR spectrum of **1** (500 MHz, $CD_3OD$)




6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
0.96
0.97
0.98
0.93
1.06
0.99
1.00
1.05
3.08
1.30
3.06
3.04

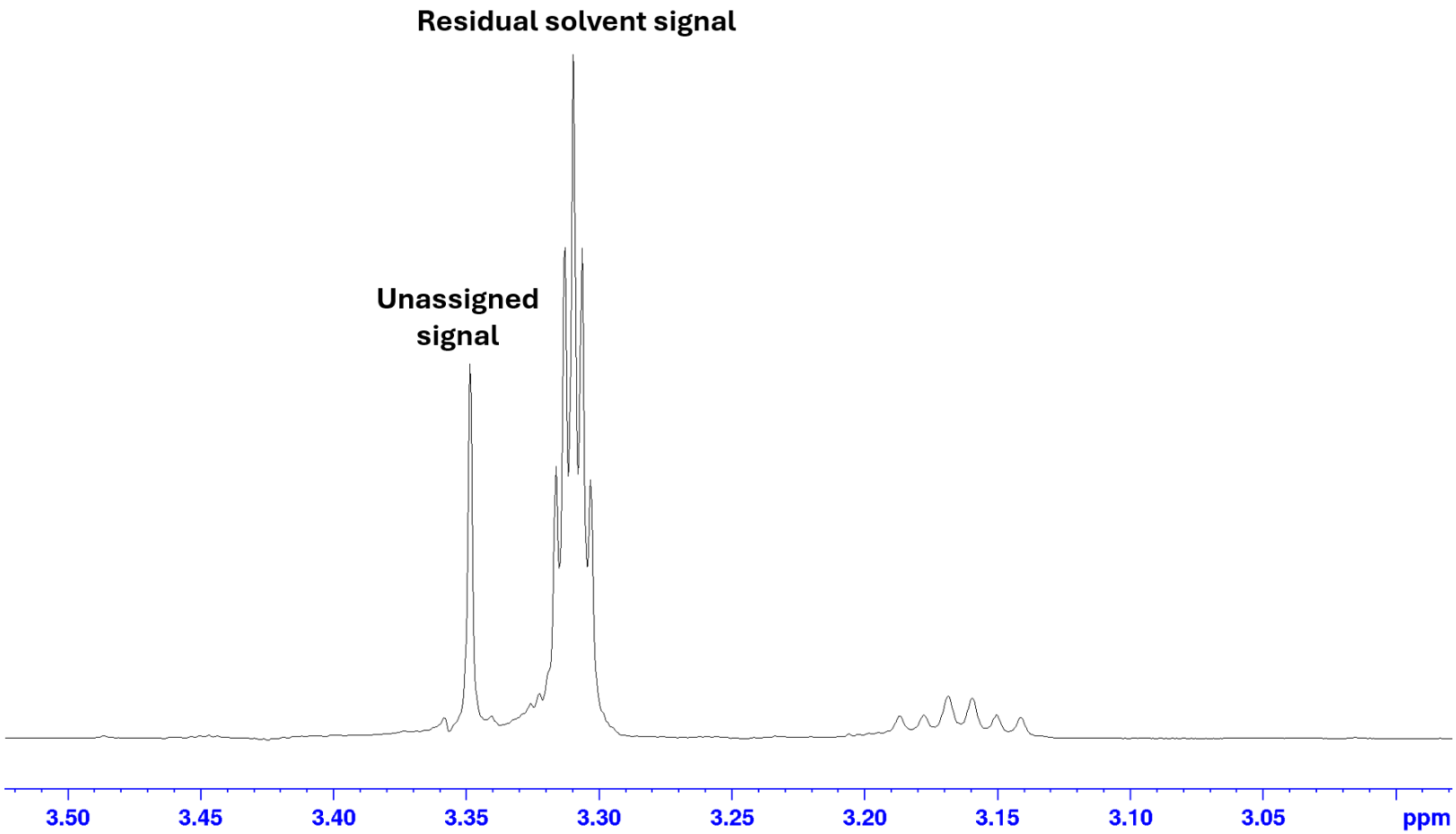

Residual solvent signal
Unassigned signal
3.50
3.45
3.40
3.35
3.30
3.25
3.20
3.15
3.10
3.05
ppm

**Figure S2.** $^{13}C$ NMR spectrum of **1** (125 MHz, $CD_3OD$)

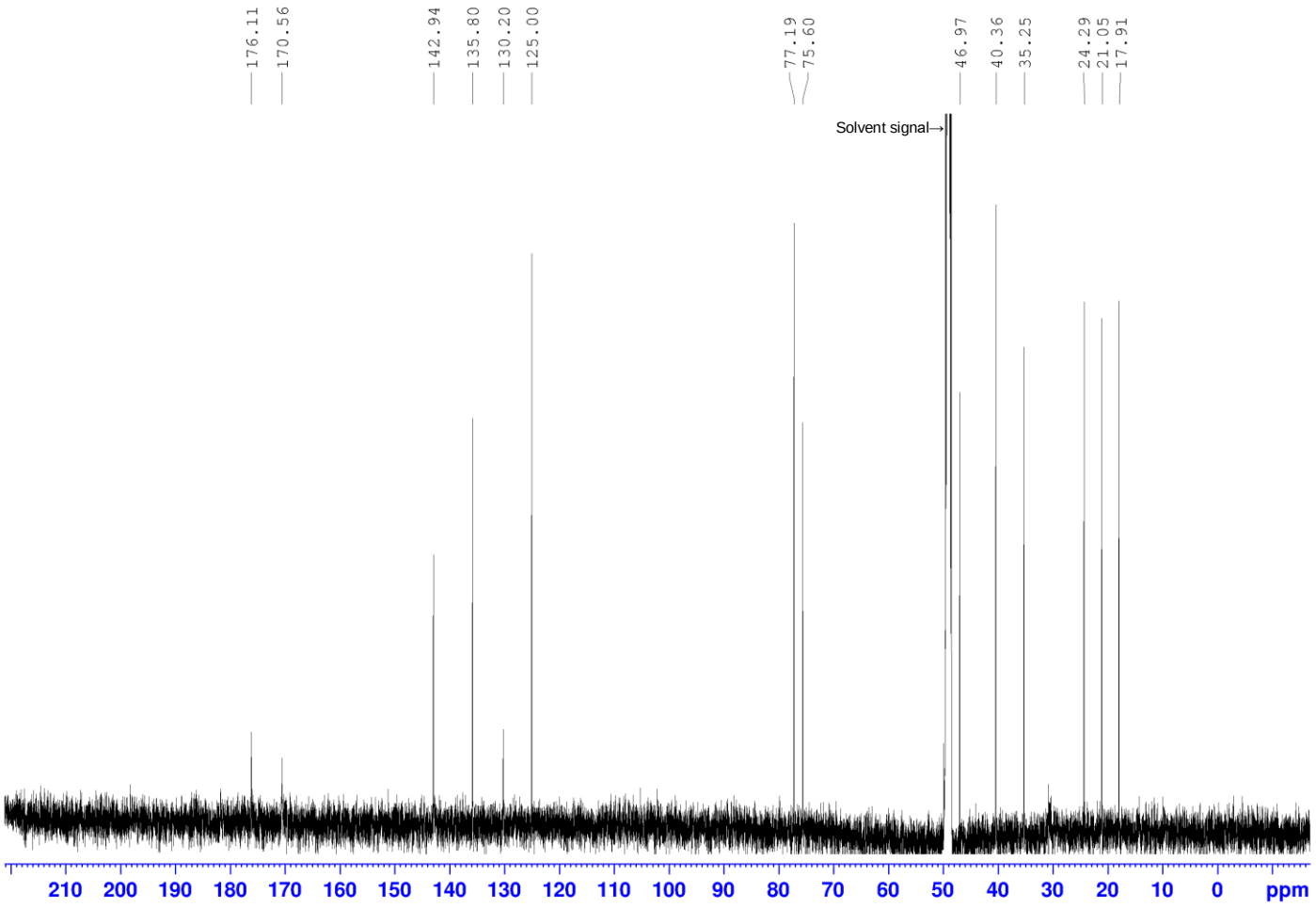


**Figure S3.** $^{1}H$-$^{1}H$ COSY spectrum of **1** (500 MHz, $CD_3OD$)

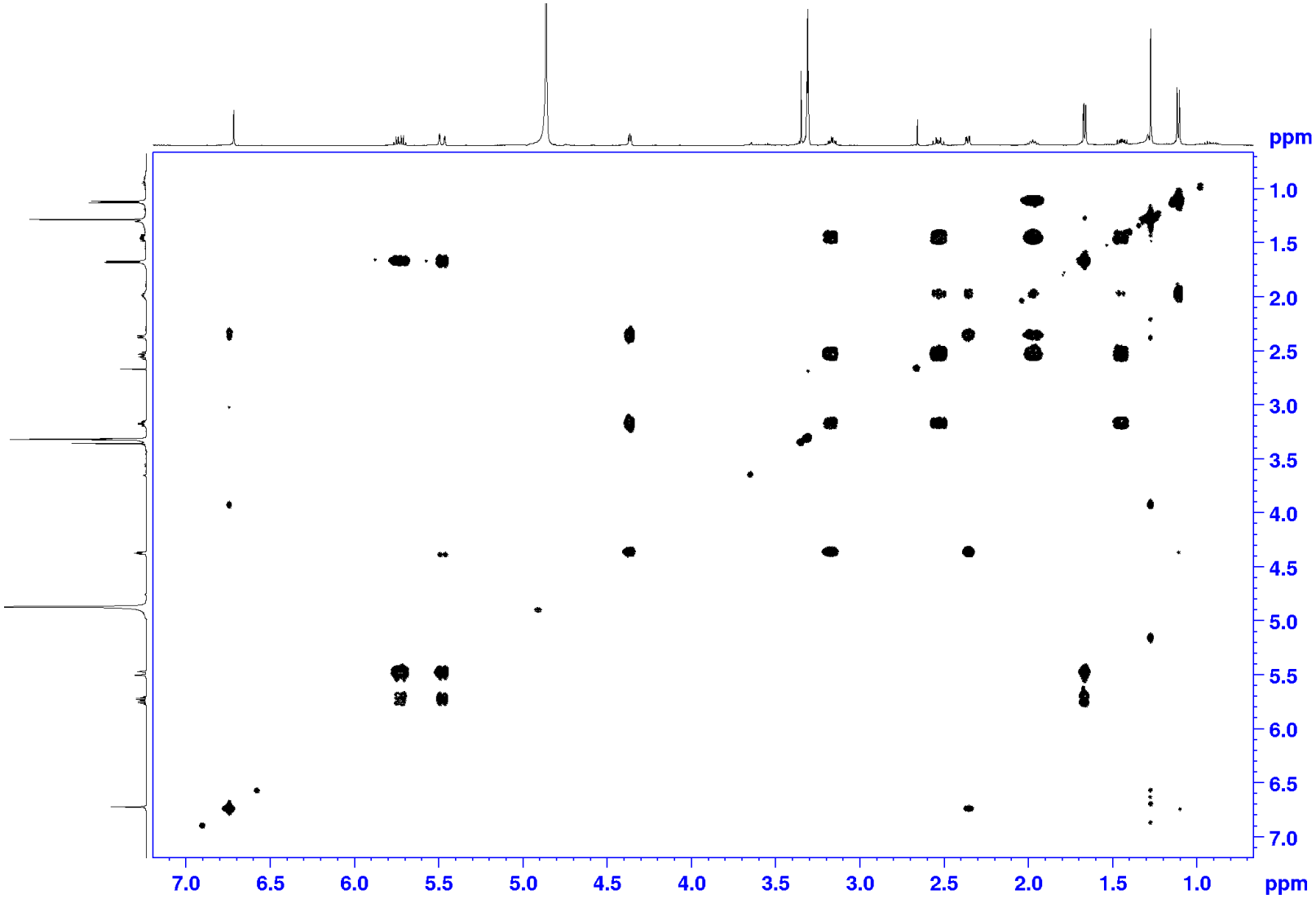


**Figure S4.** HSQC spectrum of **1** (500 MHz, $CD_3OD$)

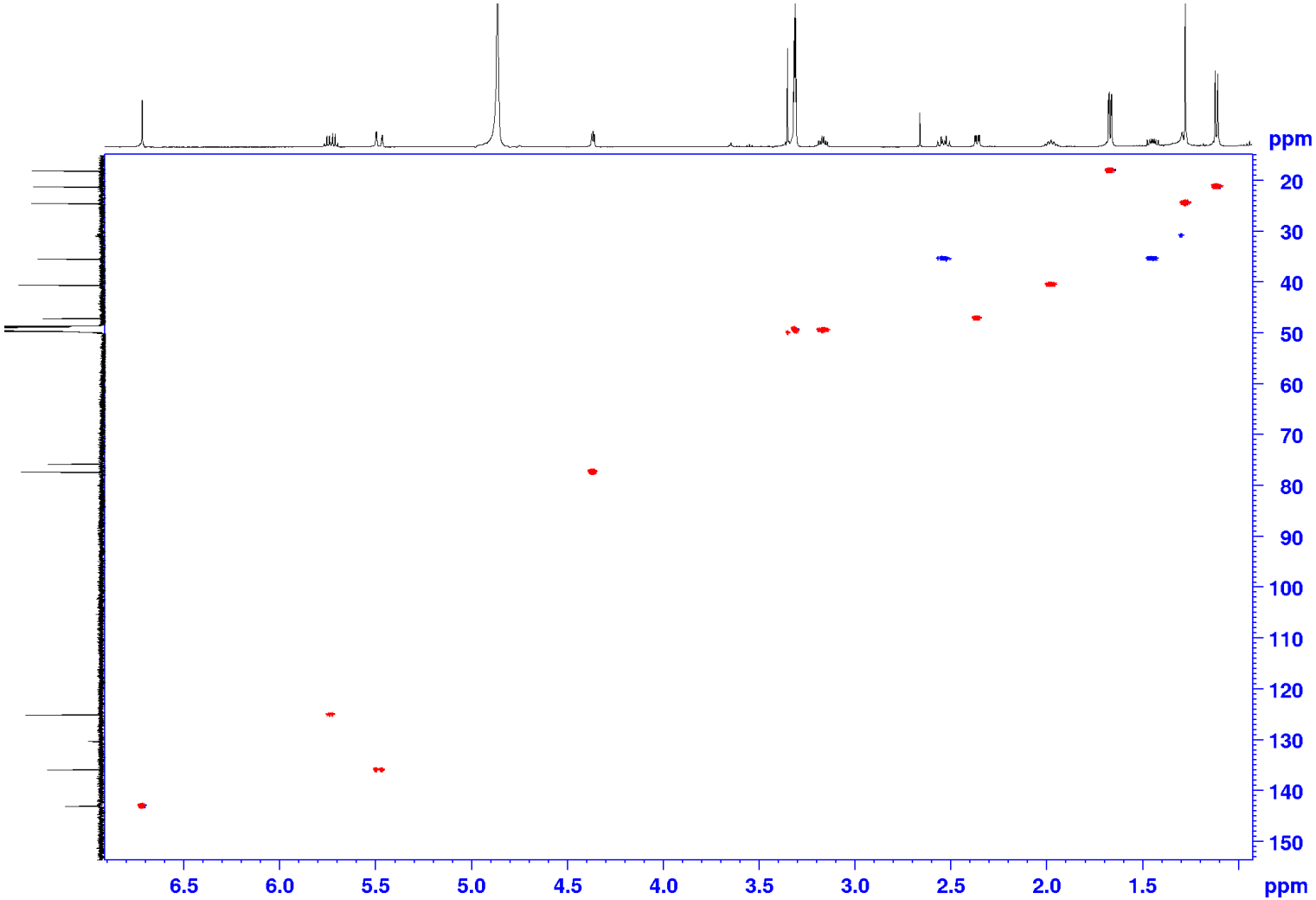
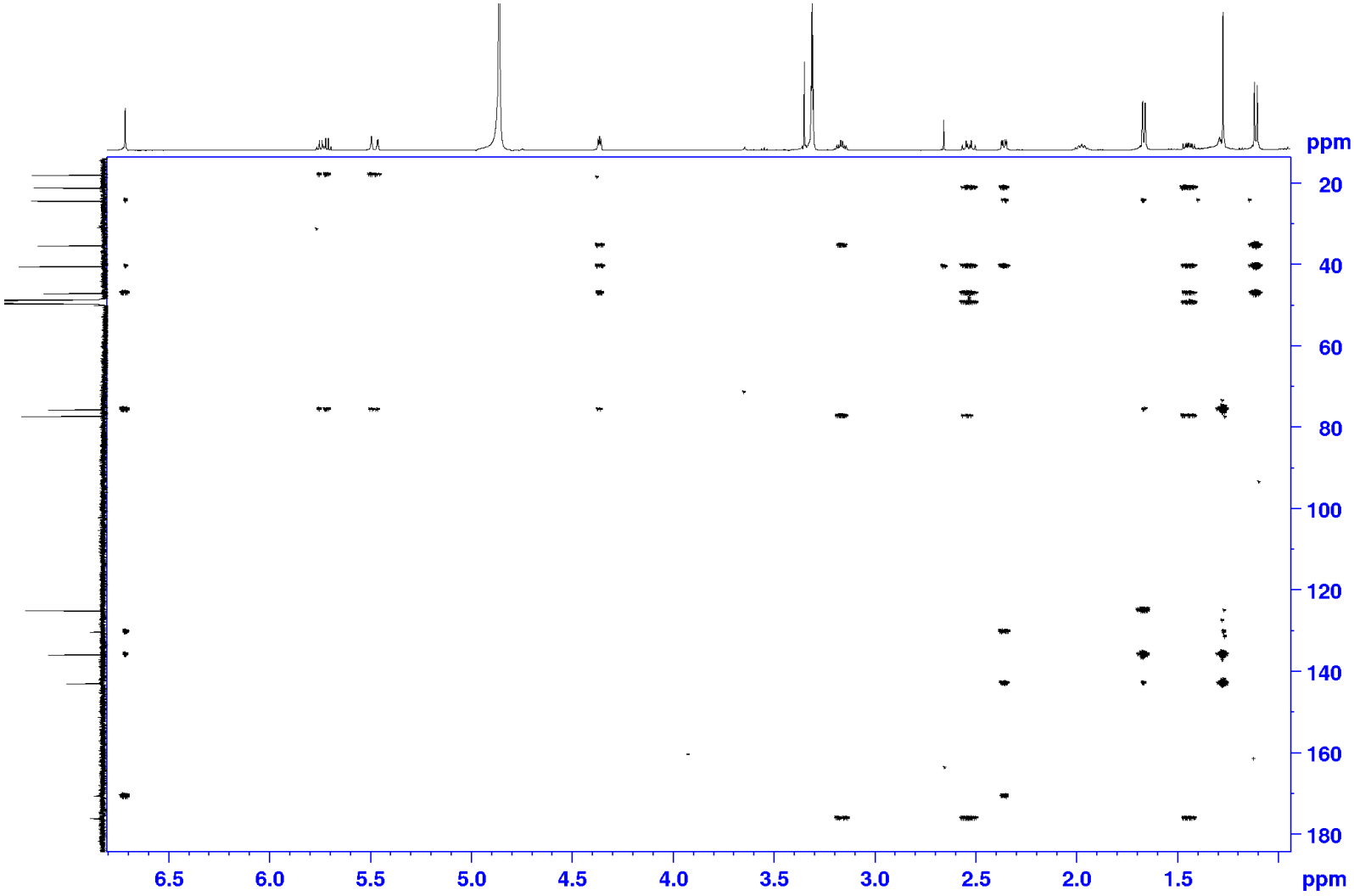


**Figure S5.** HMBC spectrum of **1** (500 MHz, $CD_3OD$)



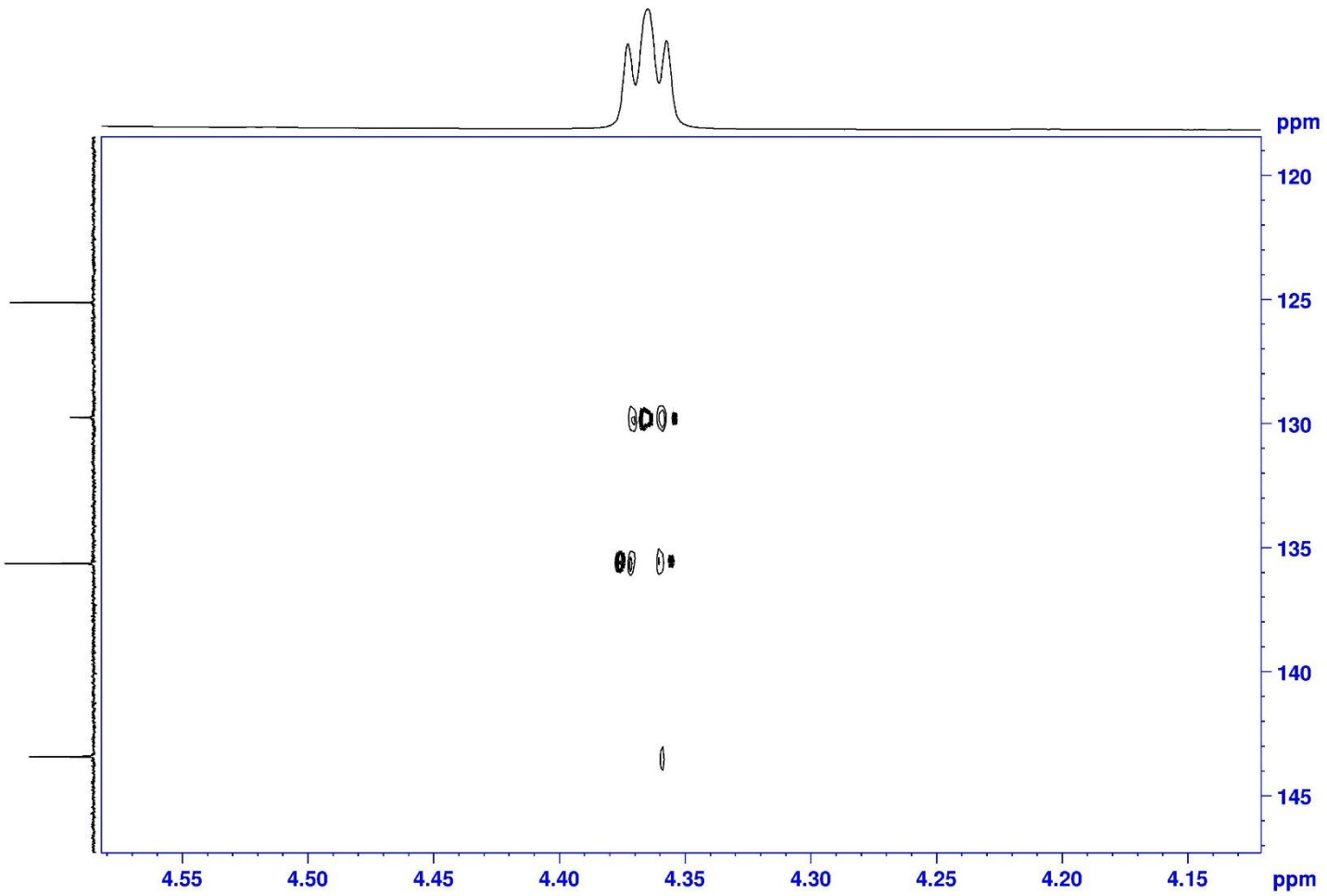

ppm
120
125
130
135
140
145
4.55
4.50
4.45
4.40
4.35
4.30
4.25
4.20
4.15
ppm

**Figure S6.** NOESY spectrum of **1** (500 MHz, $CD_3OD$)

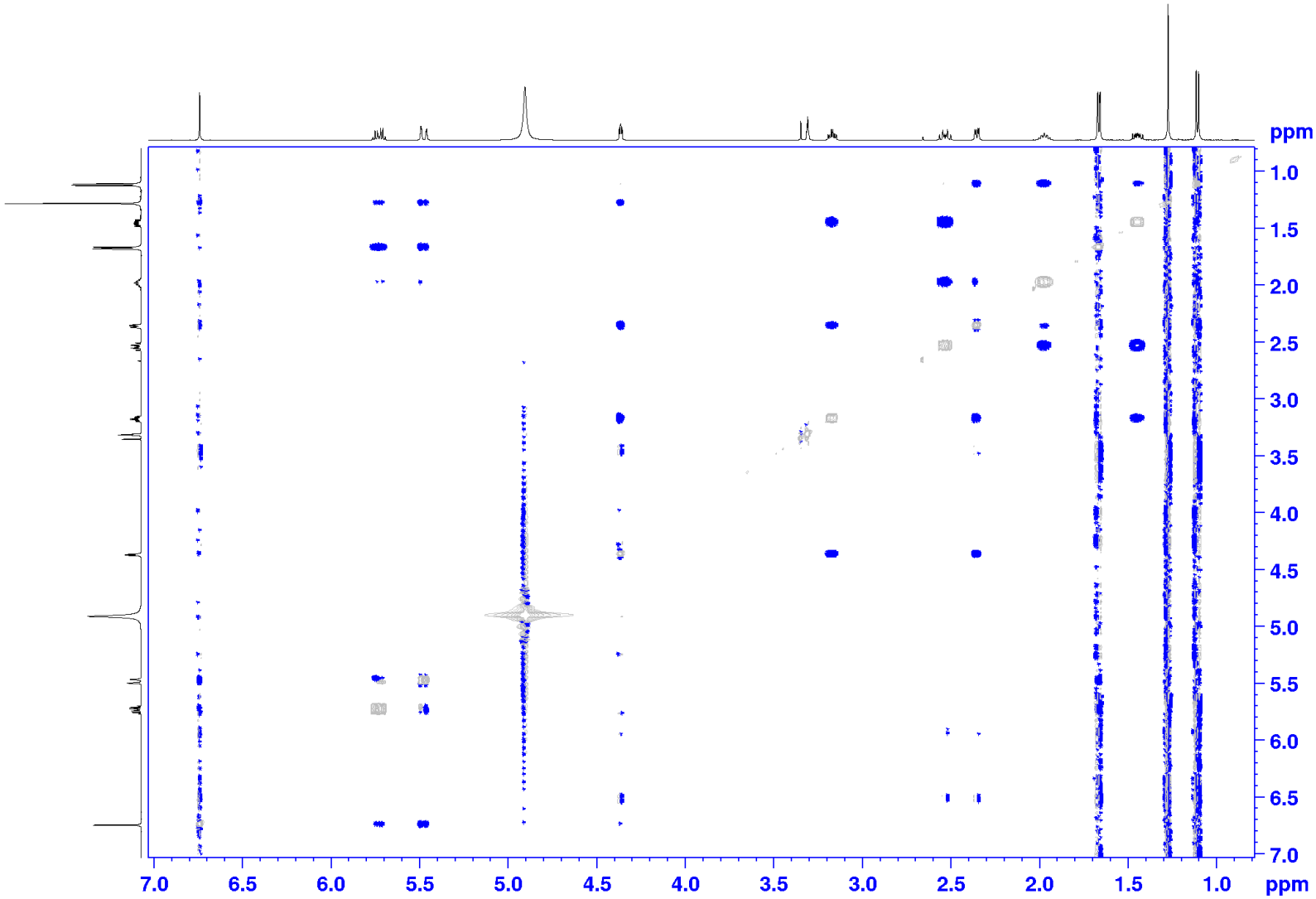


**Figure S7.** HRMS spectrum of **1**. The ion at *m*/*z* 279.1237 corresponds to $[M–H]^-$ of 1; other intense ions are attributable to background/impurity ions.

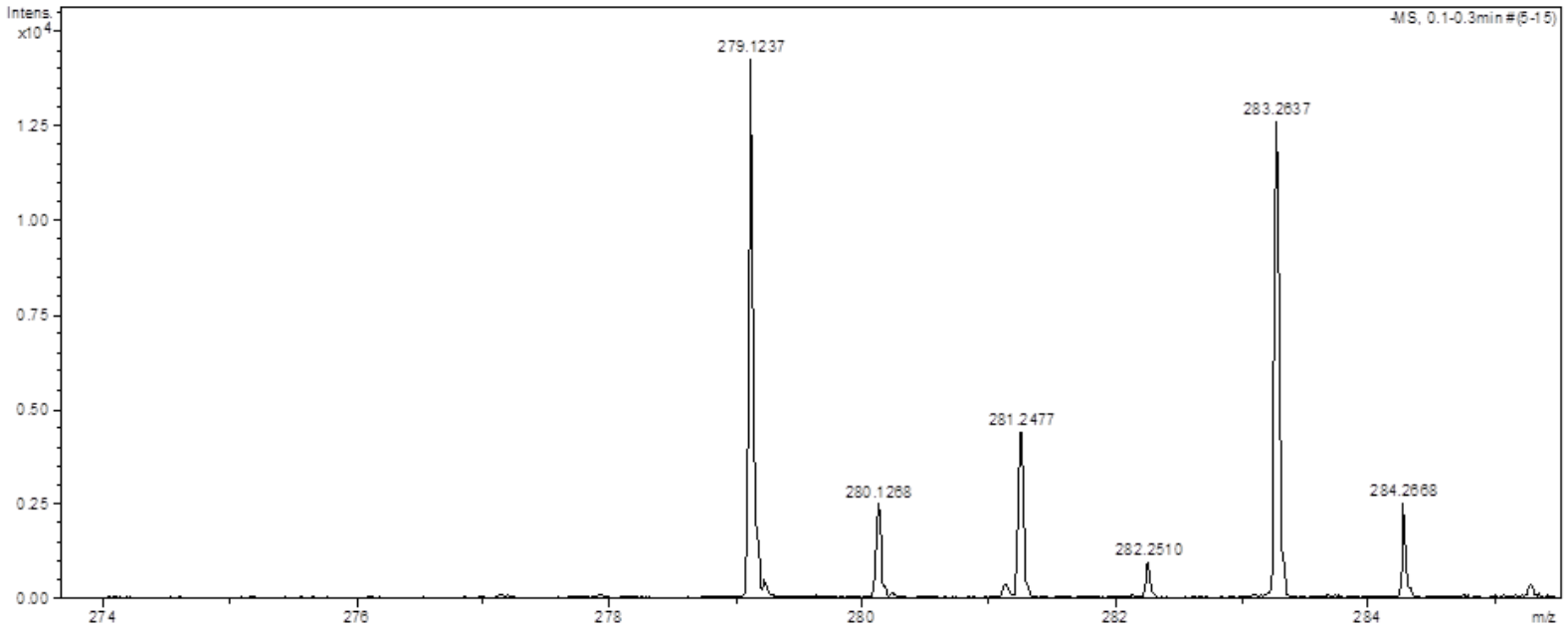


**Figure S8.** IR spectrum of **1**.

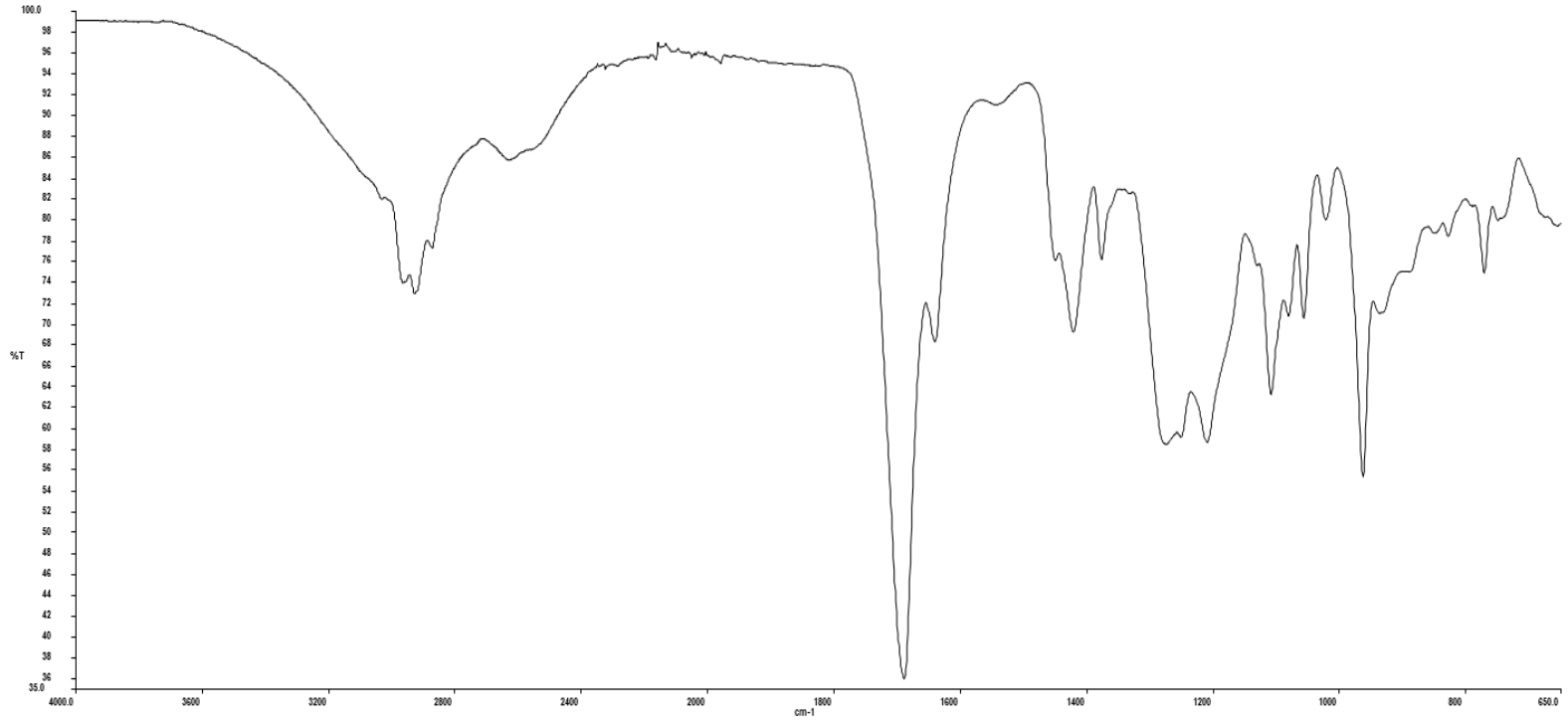


**Figure S9.** HPLC chromatograms of BuOH extracts from the RD066637 culture and the uninoculated A-3M medium control.
(A) *Rhodococcus* sp. RD066637 cultured in A-3M medium for 5 days. (B) Uninoculated A-3M medium incubated for 5 days under identical conditions. Both samples were processed in the same manner, including 1-BuOH extraction. The red arrow indicates rhodopyran (**1**). No peak corresponding to **1** was detected in the medium control. The HPLC analysis was performed using a C18-AR II column (4.6 × 100 mm) with water and acetonitrile as the mobile phases at a flow rate of 1.2 mL/min. The gradient program was as follows: 15% MeCN from 0 to 3 min, a linear increase to 85% MeCN from 3 to 25 min, 85% MeCN from 25 to 28 min, and a return to 15% MeCN by 32 min. UV detection was performed at 230 nm.