

Supporting Information of Compound 3

MS and NMR Data of Compound 3 (unpublished results)

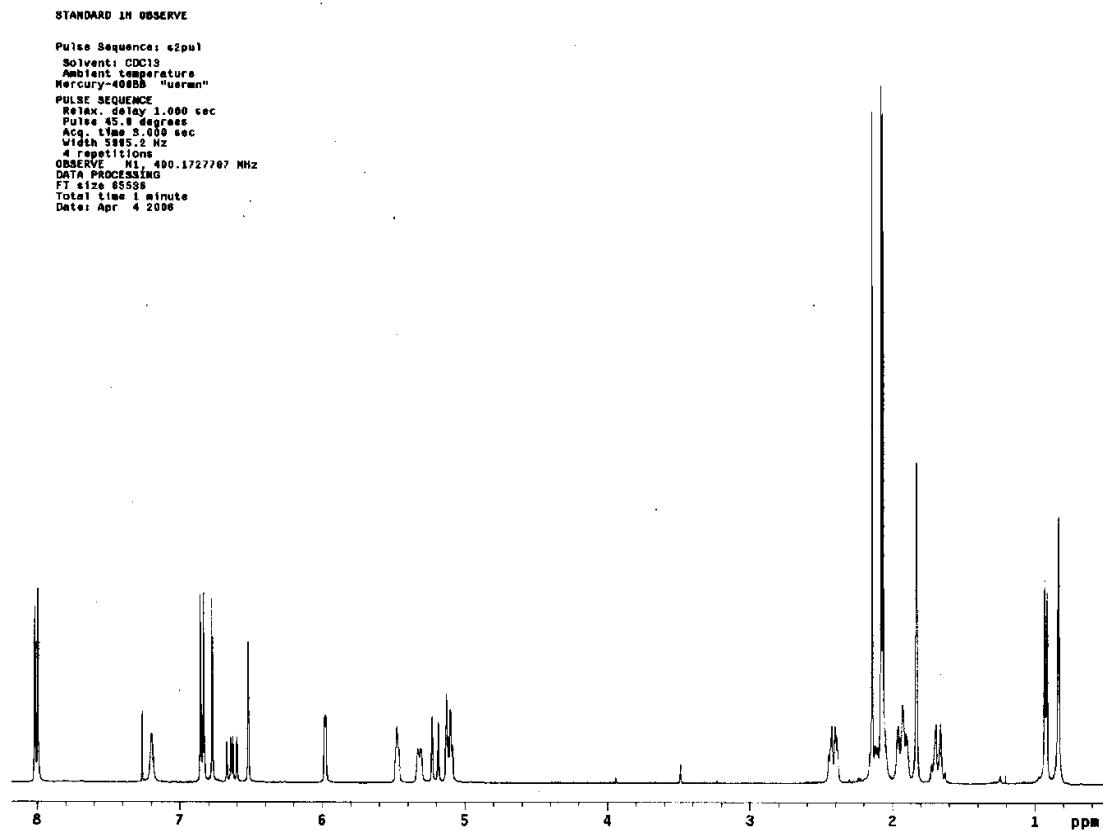
Table 1. ^{13}C (100 MHz) and ^1H (400 MHz) NMR Data of **3** in CDCl_3 (δ in ppm).

position	3	
	δ_{C}	δ_{H} (<i>J</i> in Hz)
1 α	26.8 CH ₂	2.12 m
1 β		1.95 m
2 β	66.1 CH	5.48 m
3	123.1 CH	5.98 brd (2.8)
4	144.0 C	
5	51.8 C	
6	74.2 CH	5.10 m
7 α	33.0 CH ₂	1.94 m
7 β		1.68 m
8	35.9 CH	1.95 m
9	37.2 C	
10	37.7 CH	2.40 m
11a	29.1 CH ₂	1.65 m
11b		2.40 m
12	126.5CH	5.33 brd (6.8)
13	133.6 C	
14	133.3 CH	6.63 dd (17.2, 10.8)
15a	114.5CH ₃	5.21 d (17.2)
15b		5.12d(10.8)
16	20.4 CH ₃	1.84 brs
17	15.5 CH ₃	0.93 d (6.4)
18 α	95.5 CH	6.52 brs
19 α	97.9 CH	6.78 s
20	25.0 CH ₃	0.84 s
C2-OMe		
18-OAc	170.6 C	
	21.6 CH ₃	2.08 s
19-OAc	169.7 C	
	21.2 CH ₃	2.07 s
6-OAc	170.5 C	
	21.5 CH ₃	2.14 s
C2-p-OHBz		
1'	165.5 C	
2'	121.5 C	
3'	115.5 CH	8.02 d (8.6)
4'	132.2 CH	6.85 d (8.6)
5'	160.7 C	
6'	132.2 CH	6.85 d (8.6)
7'	115.5 CH	8.02 d (8.6)

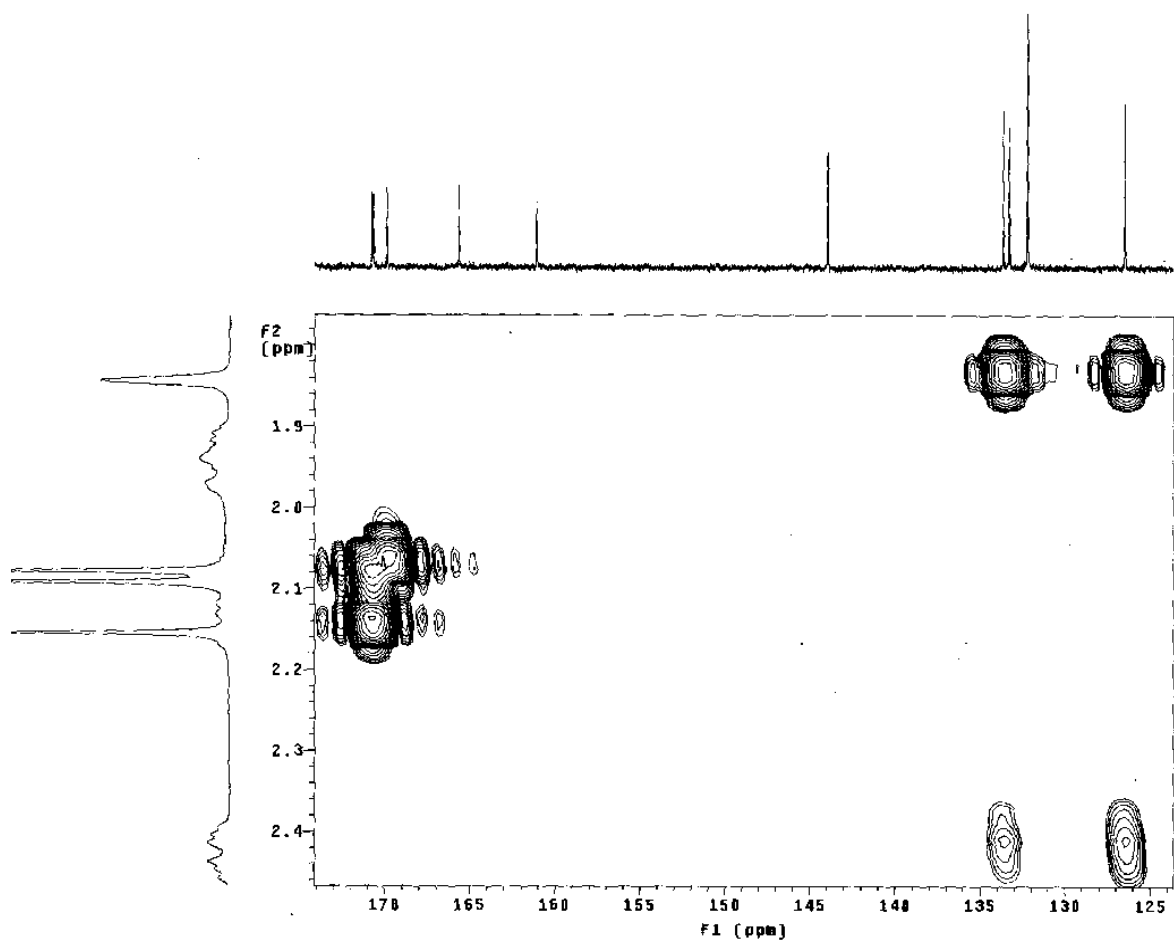
Casearborin F (**3**), white amorphous solid, isolated amount (105 mg); $[\alpha]_{\text{D}}^{20} + 98$ (*c* 0.13, MeOH); UV (MeOH) λ_{max} (log ϵ) 223 (3.97), λ_{max} (log ϵ) 280 (4.01) nm; HRESIMS (positive mode) m/z 618.24414 $[\text{M} + \text{Na}]^+$ (calcd $\text{C}_{33}\text{H}_{40}\text{O}_{10}\text{Na}$, 618.24409).

NMR data

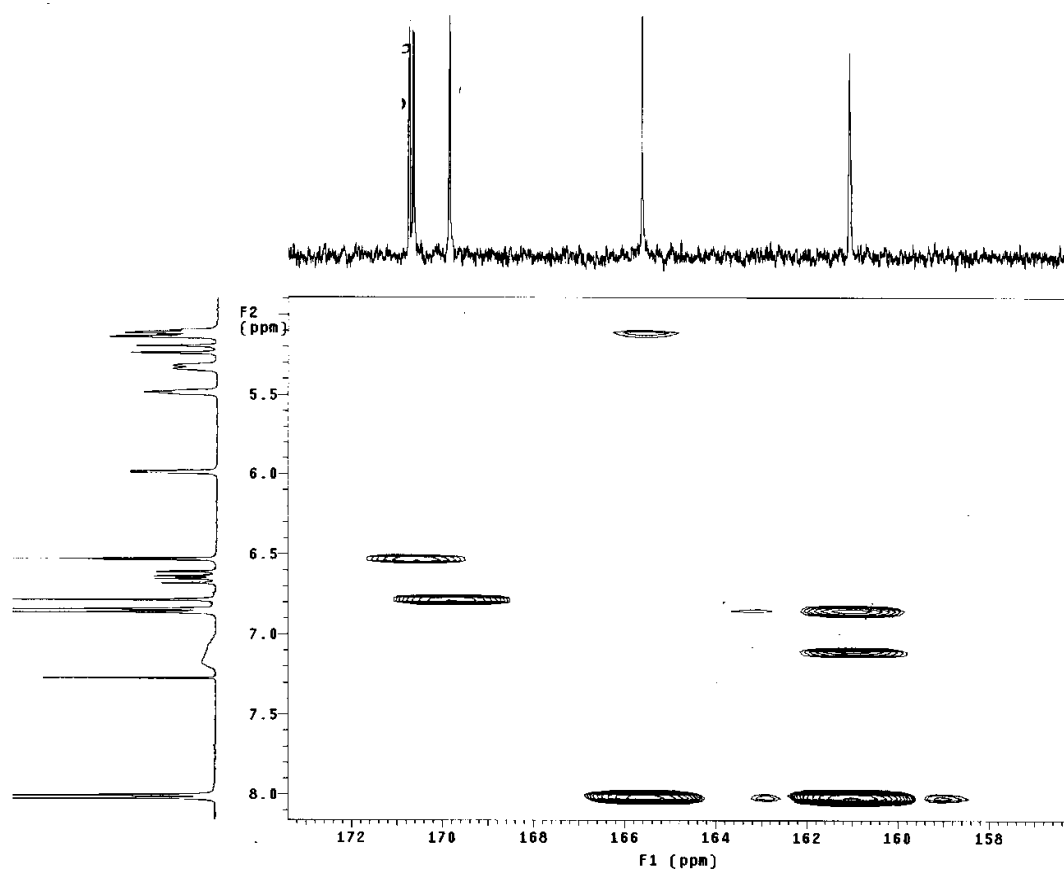
Compound 3 (casearborin F)



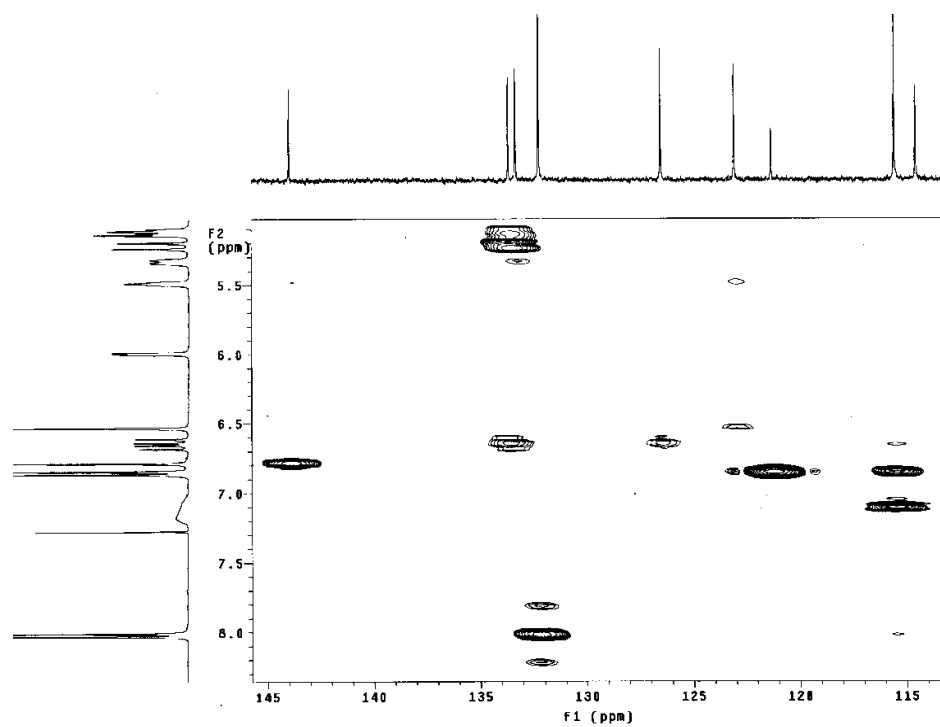
¹H-NMR spectrum of TCD 3. The measure was carried out in CDCl₃ at 400 MHz.



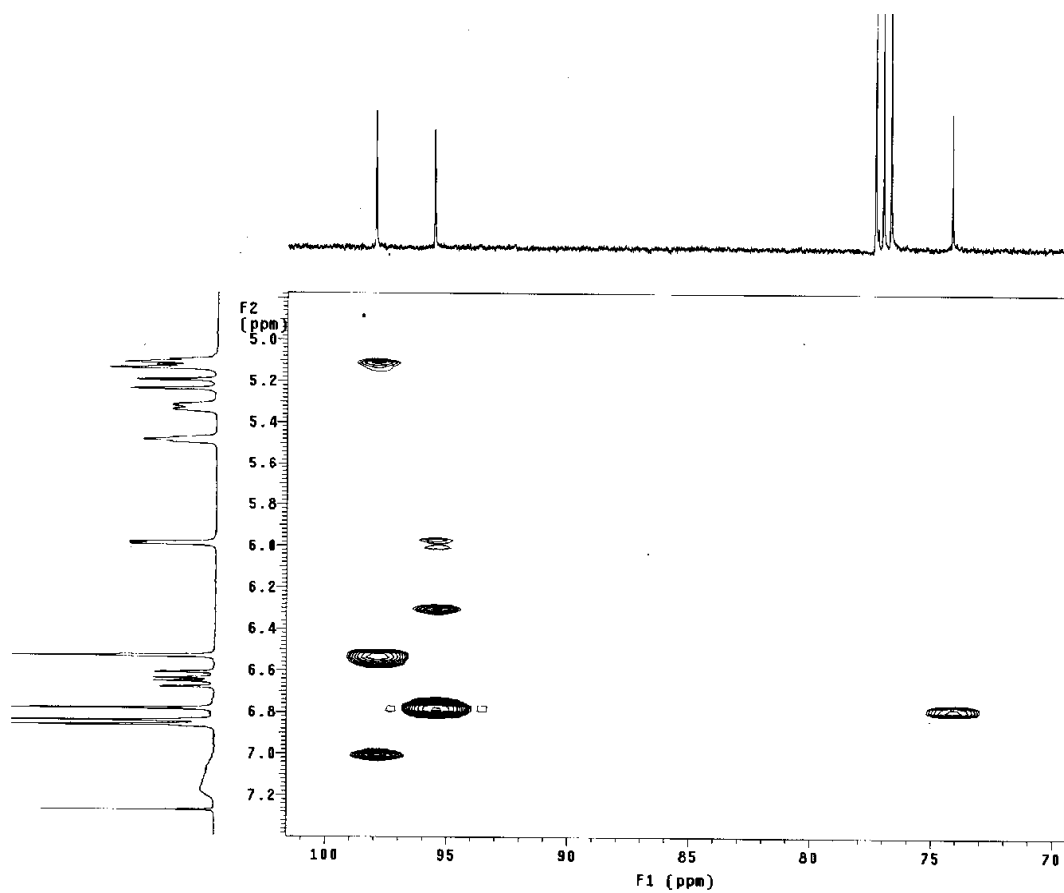
gHMBC spectrum of compound 3.



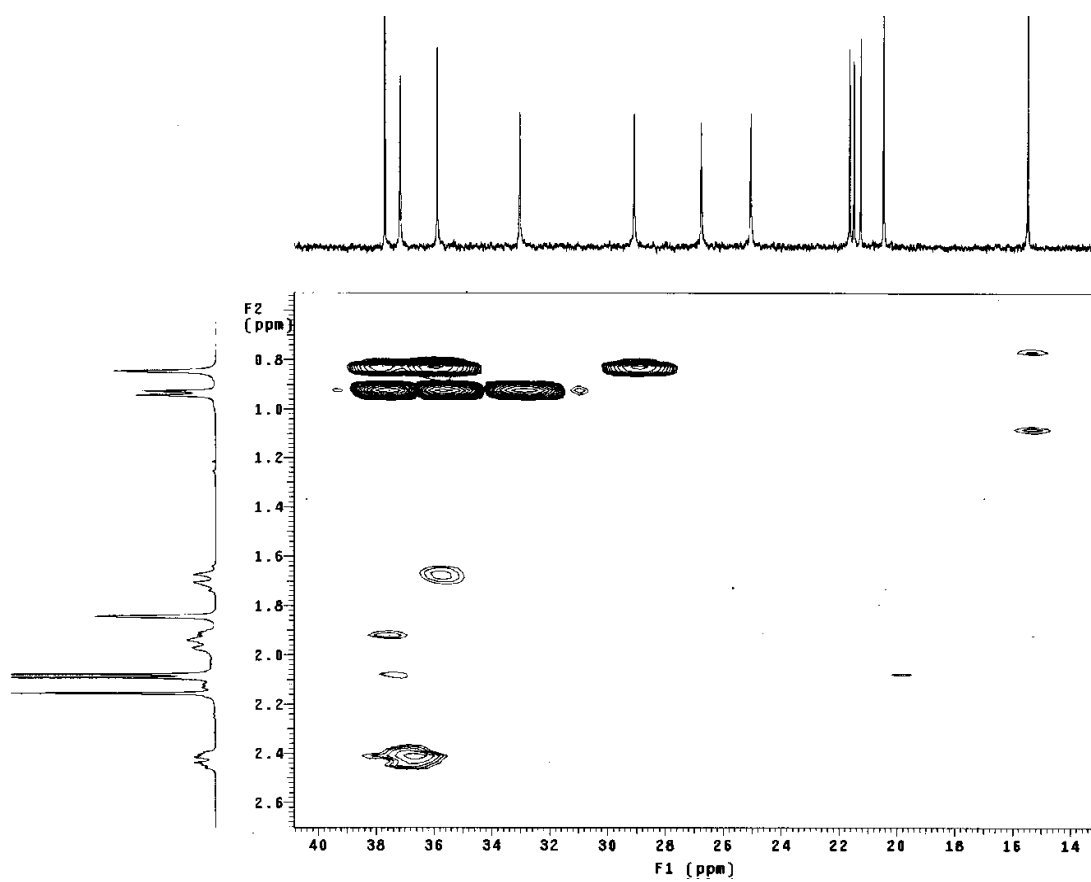
gHMBC spectrum of compound 3.



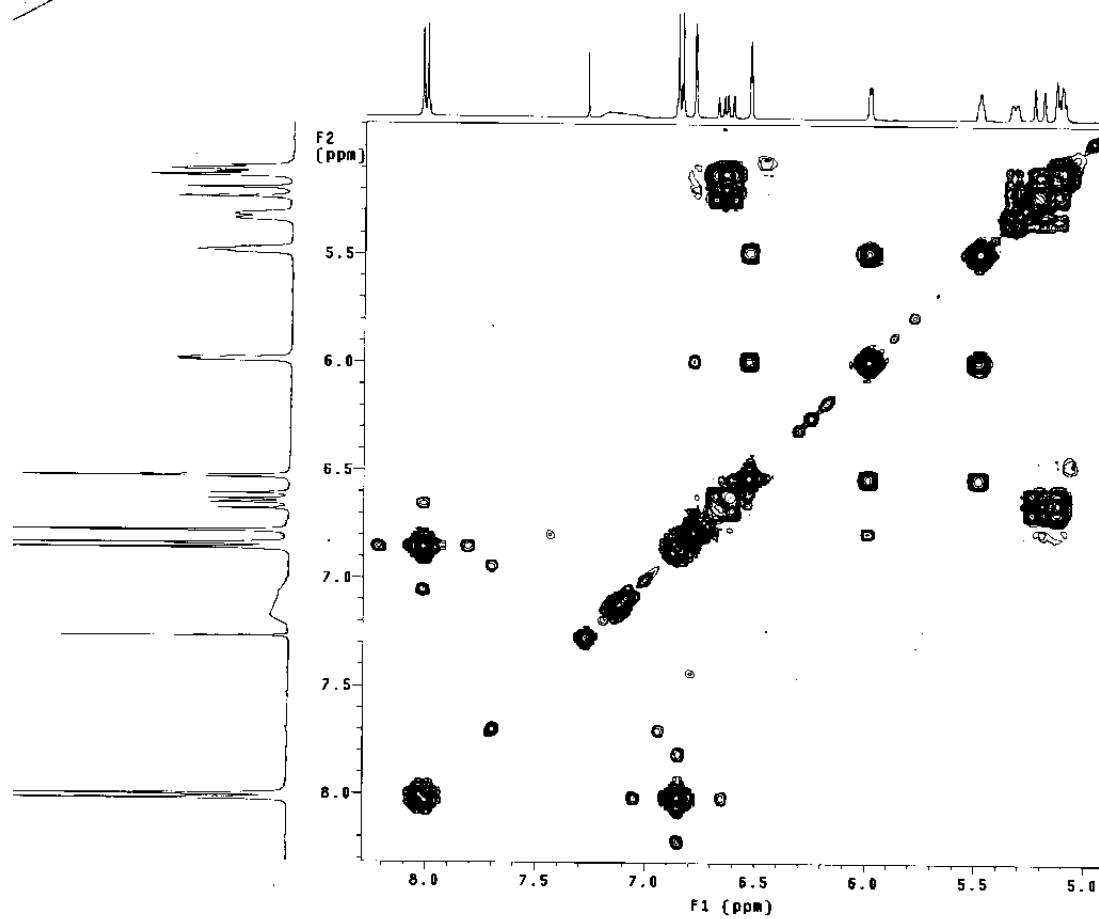
. gHMBC spectrum of compound 3.



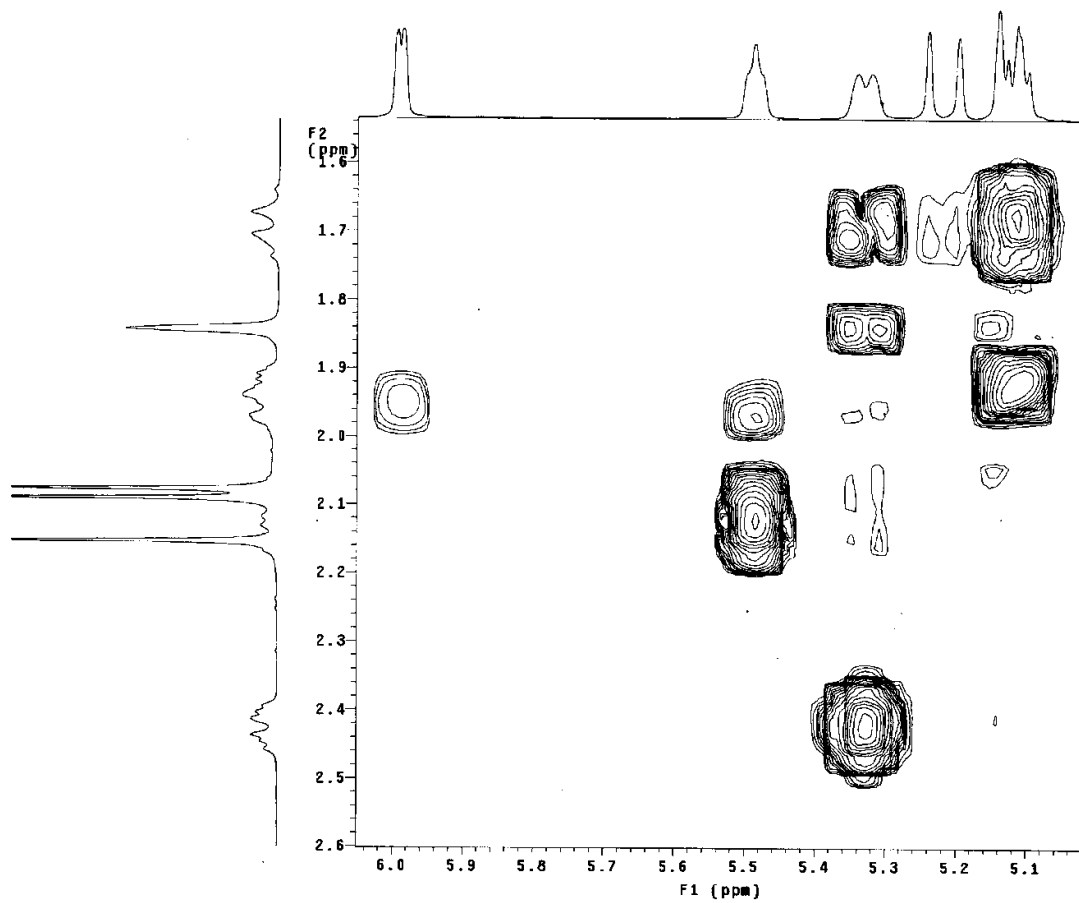
gHMBC spectrum of compound 3.



gHMBC spectrum of compound 3.



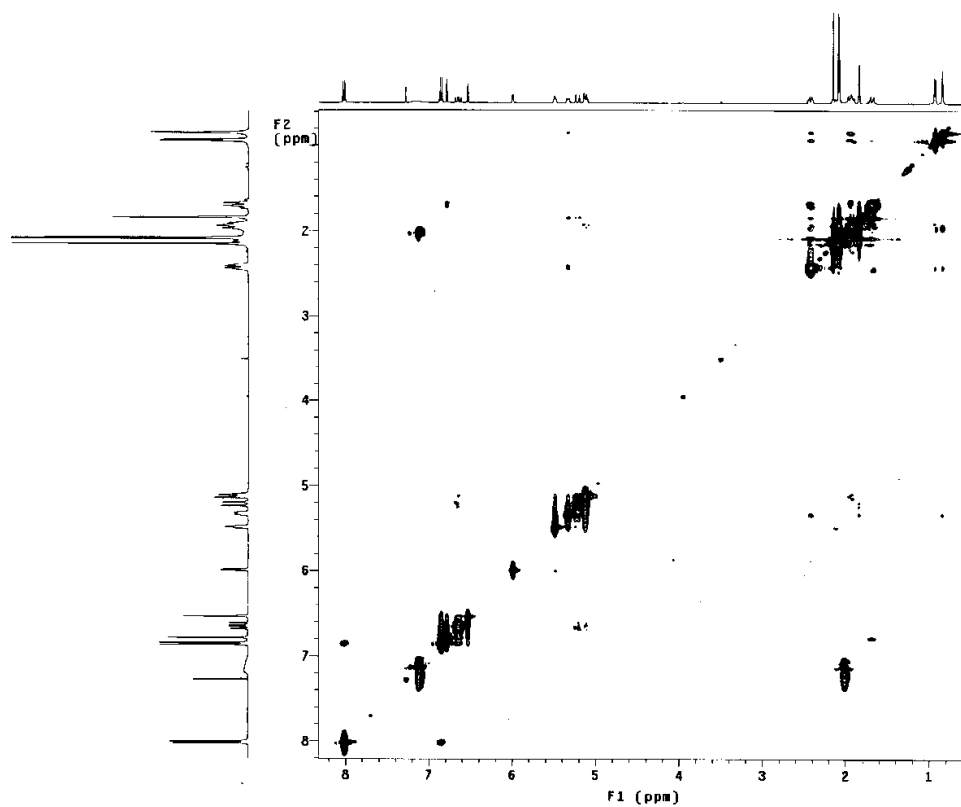
^1H , ^1H -COSY spectrum of compound **3**.



$^1\text{H},^1\text{H}$ -COSY spectrum of compound **3**.



^1H , ^1H -COSY spectrum of compound 3.



NOESY spectrum of compound **3**. The measurement was carried out in CDCl₃ at 400 MHz.