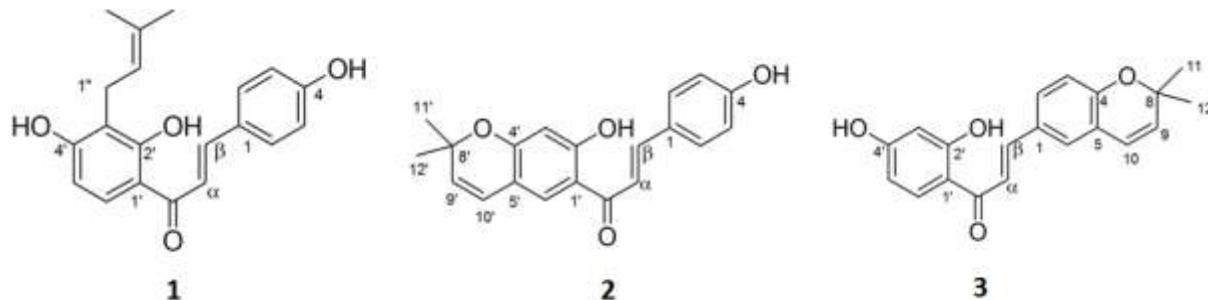


Supplementary Materials

Spectroscopic Analysis (NMR) of compounds 1 - 3



Compound 1 (isobavachalcone)

¹H NMR (CD₃OD, 400 MHz) δ: 7.82 (1H, d, *J* = 9.2, H-6'), 7.77 (1H, d, *J* = 15.6, H-β), 7.61 (1H, d, *J* = 15.6, H-α), 7.60 (2H, d, *J* = 8.4, H-2, H-6), 6.84 (2H, d, *J* = 8.4, H-3, H-5), 6.43 (1H, d, *J* = 9.2, H-5'), 5.23 (1H, m, H-2''), 3.32 (1H, m, H-1''), 1.78 (3H, s, H-4''), 1.66 (3H, s, H-5'').

¹³C NMR (CD₃OD, 100 MHz) δ: 193.7 (C=O), 165.2 (C-4'), 163.6 (C-2'), 161.5 (C-4), 145.3 (C-β), 131.9 (C-3''), 131.7 (C-2), 131.7 (C-6), 130.4 (C-6'), 123.6 (C-2''), 118.6 (C-α), 116.9 (C-3), 116.9 (C-5), 116.6 (C-3'), 114.5 (C-1), 114.5 (C-1') 108.2 (C-5'), 26.0 (C-5''), 22.5 (C-1''), 17.9 (C-4'').

Compound 2 (Bavachromene)

¹H NMR (CD₃OD + CDCl₃, 400 MHz) δ: 7.77 (1H, d, *J* = 15.2, H-β), 7.58 (1H, s, H-6'), 7.55 (2H, d, *J* = 8.8, H-2, H-6), 7.45 (1H, d, *J* = 15.2, H-α), 6.84 (2H, d, *J* = 8.8, H-3, H-5), 6.34 (1H, d, *J* = 10.0, H-10'), 6.28 (1H, s, H-3'), 5.59 (1H, d, *J* = 10.0, H-9'), 1.42 (6H, s, H-11', H-12').

¹³C NMR (CD₃OD + CDCl₃, 100 MHz) δ: 192.8 (C=O), 166.4 (C-4'), 161.0 (C-2'), 160.7 (C-4), 145.6 (C-β), 131.3 (C-2, C-6), 129.3 (C-9'), 128.3 (C-6'), 127.0 (C-1), 121.6 (C-10'), 117.5 (C- α), 116.5 (C-3, C-5), 114.8 (C-1'), 114.3 (C-5'), 104.8 (C-3'), 78.6 (C-8') 28.8 (C-11', C-12').

Compound 3 (kanzonol B)

¹H NMR (CD₃OD + CDCl₃, 400 MHz) δ: 7.84 (1H, d, *J* = 8.8, H-6'), 7.73 (1H, d, *J* = 15.2, H-β), 7.48 (1H, d, *J* = 15.2, H-α), 7.43 (1H, dd, *J* = 2.0, 8.4, H-2), 7.31 (1H, d, *J* = 2.4, H-6), 6.77 (1H, d, *J* = 8.4, H-3), 6.41 (1H, dd, *J* = 2.4, 8.8, H-5'), 6.37 (1H, d, *J* = 9.6, H-10), 6.32 (1H, d, *J* = 2.4, H-3'), 5.69 (1H, d, *J* = 9.6, H-9), 1.43 (6H, s, H-11, H-12).

¹³C NMR (CD₃OD + CDCl₃, 100 MHz) δ: 192.7 (C=O), 166.6 (C-2'), 165.5 (C-4'), 156.2 (C-4), 144.7 (C-β), 132.6 (C-6'), 132.0 (C-9), 130.7 (C-2), 128.3 (C-1), 127.2 (C-6), 122.2 (C-10), 122.1 (C-5), 118.4 (C- α), 117.5 (C-3), 114.1 (C-1'), 108.8 (C-5'), 103.6 (C-3'), 77.8 (C-8), 28.4 (C-11, C-12).

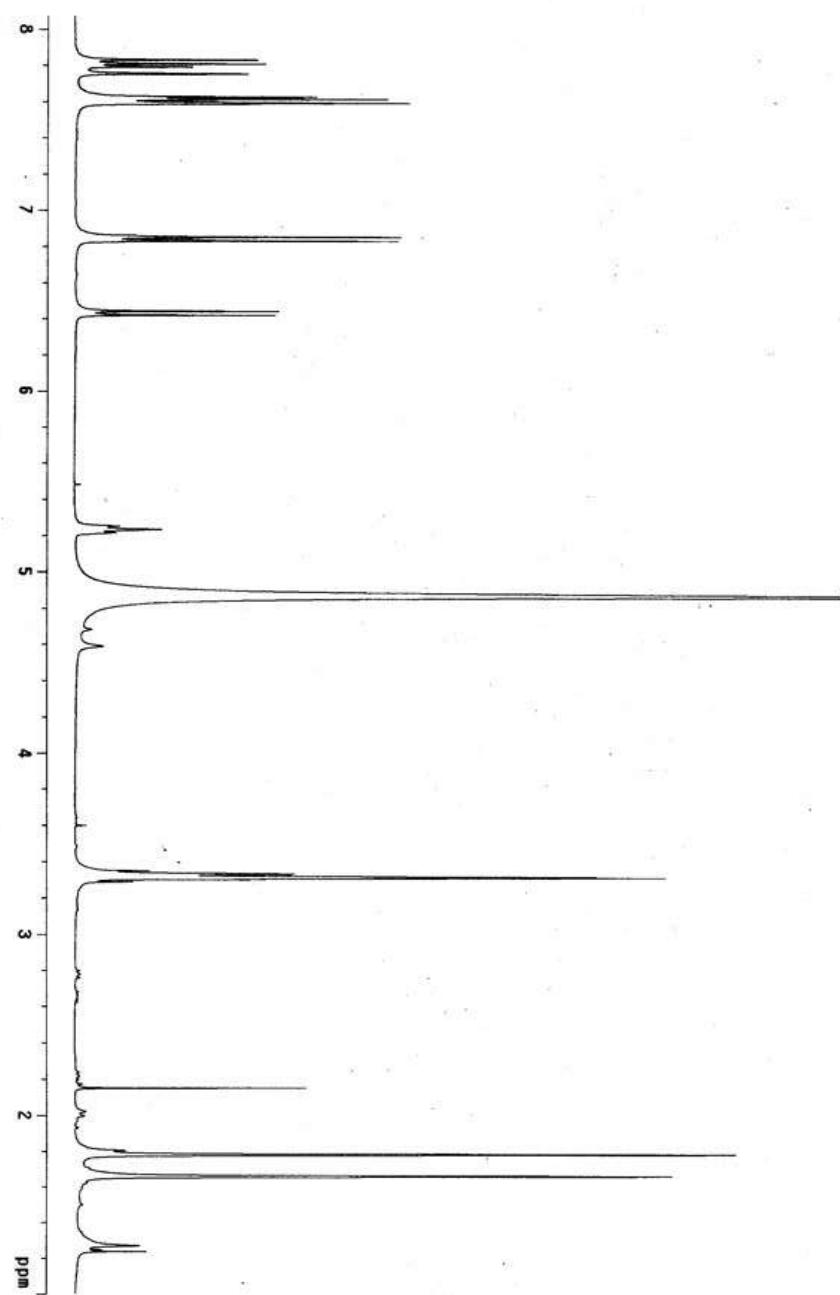


Figure S1. ^1H NMR spectrum of compound **1** (CD_3OD , 400MHz)

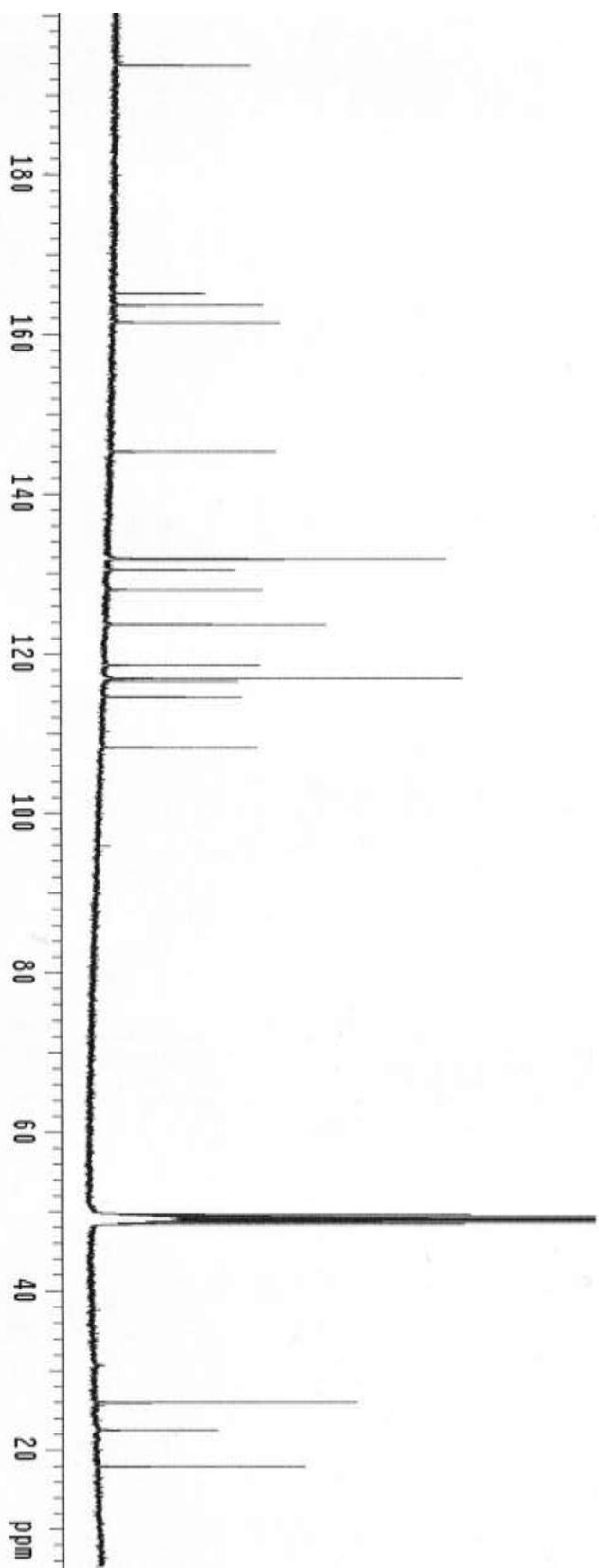


Figure S2. ^{13}C NMR spectrum of compound **1** (CD_3OD , 100MHz)

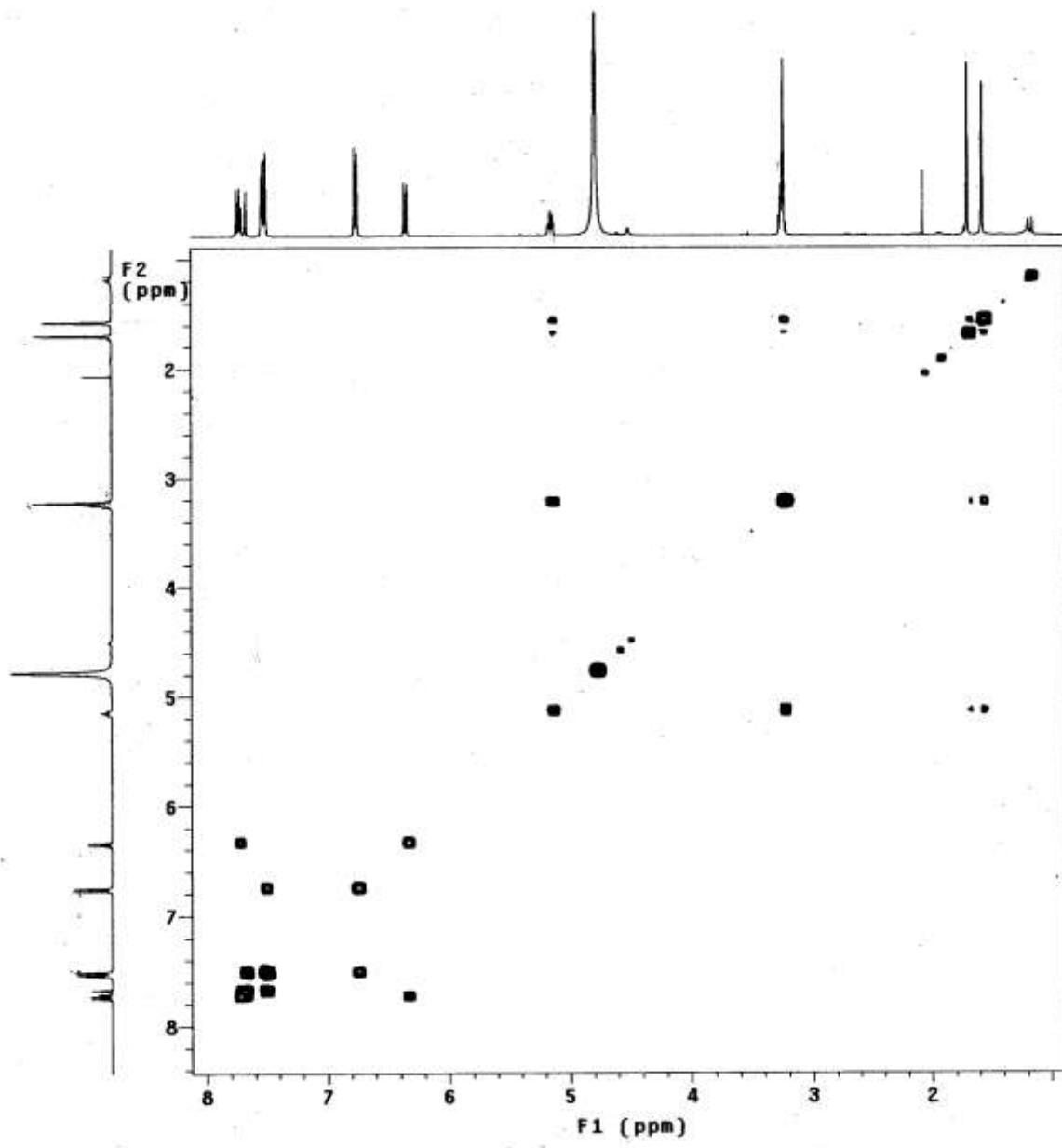


Figure S3. ^1H - ^1H COSY spectrum of compound **1** (CD_3OD , 400MHz)

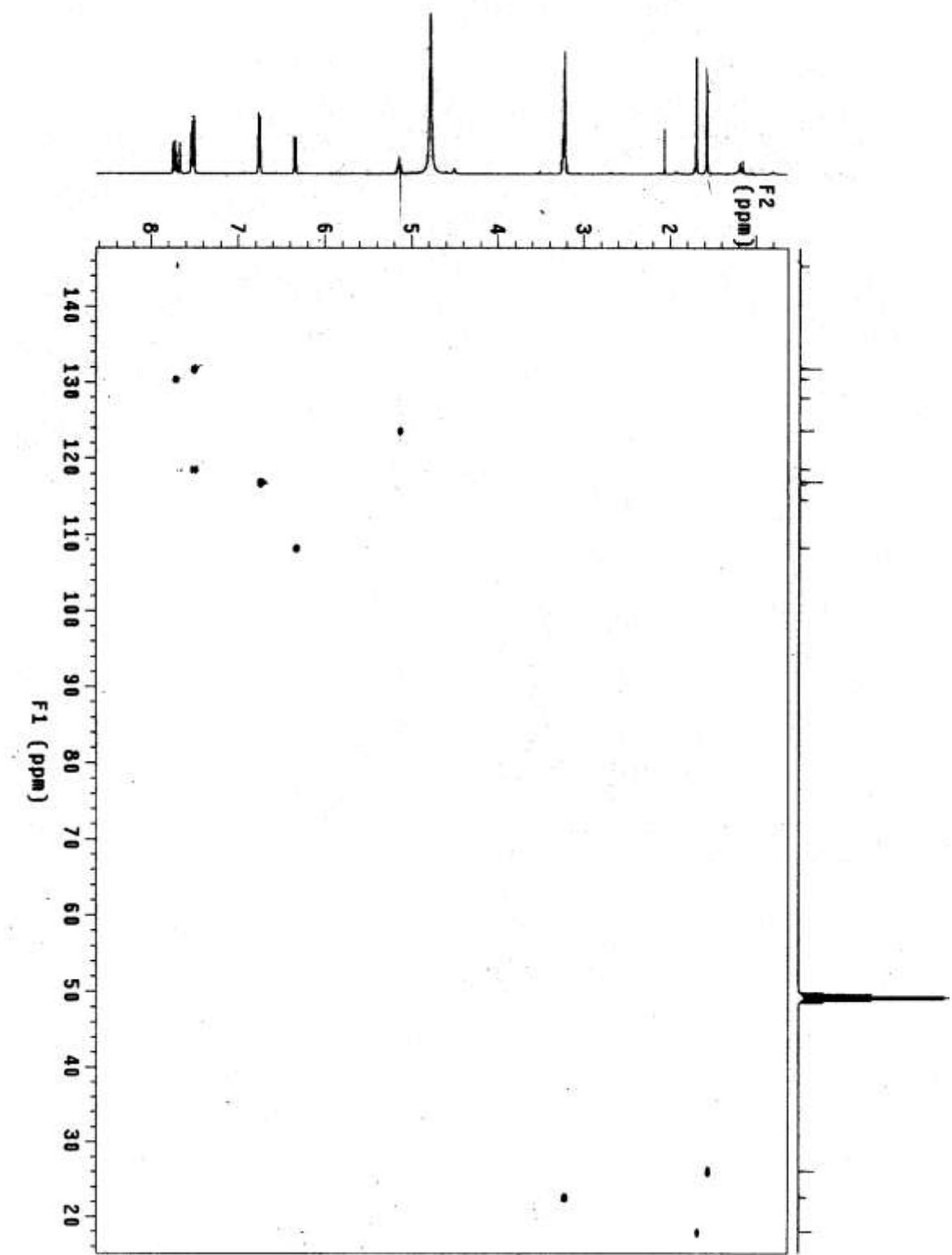


Figure S4. HSQC spectrum of compound **1** (CD_3OD , 400MHz)

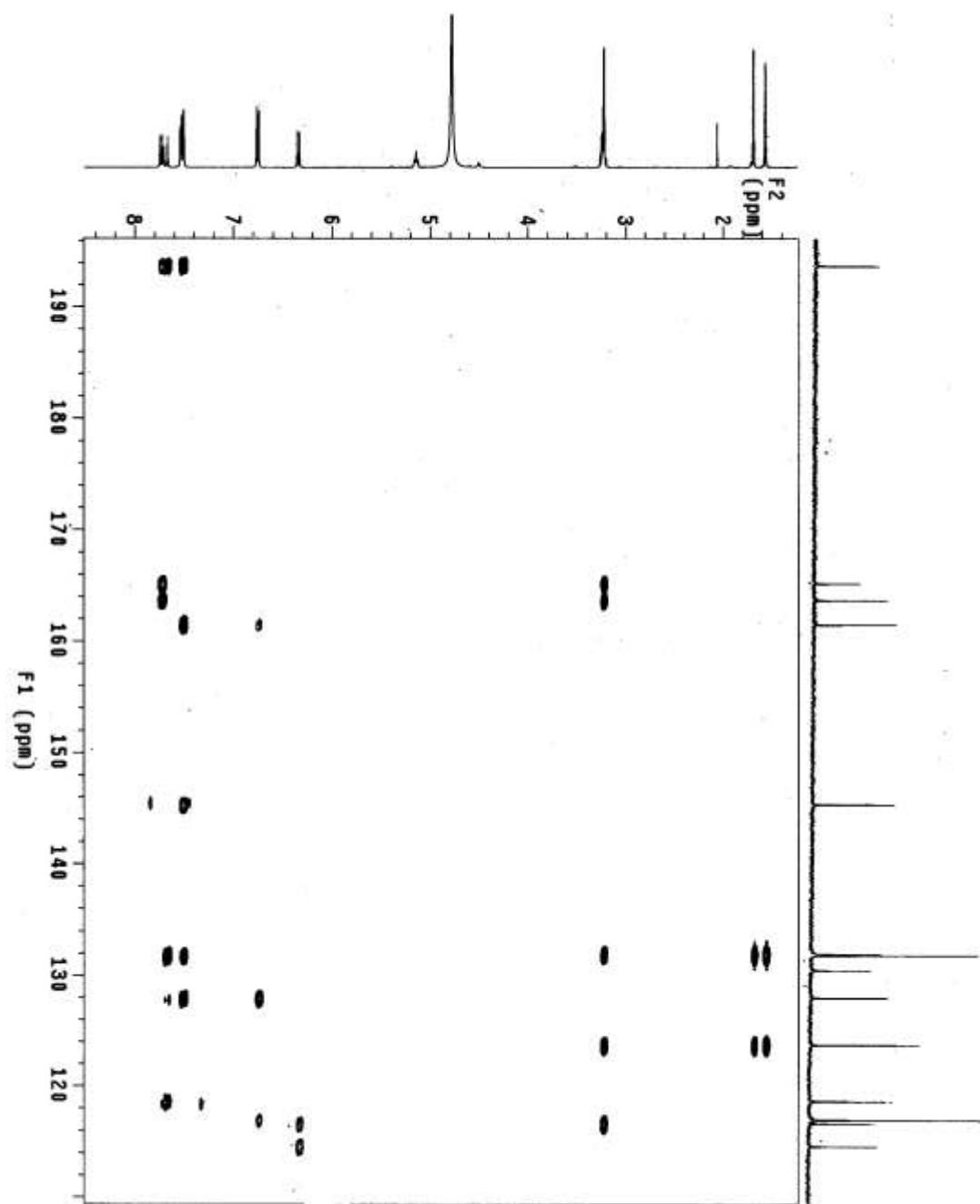


Figure S5. HMBC spectrum of compound **1** (CD_3OD , 400MHz)

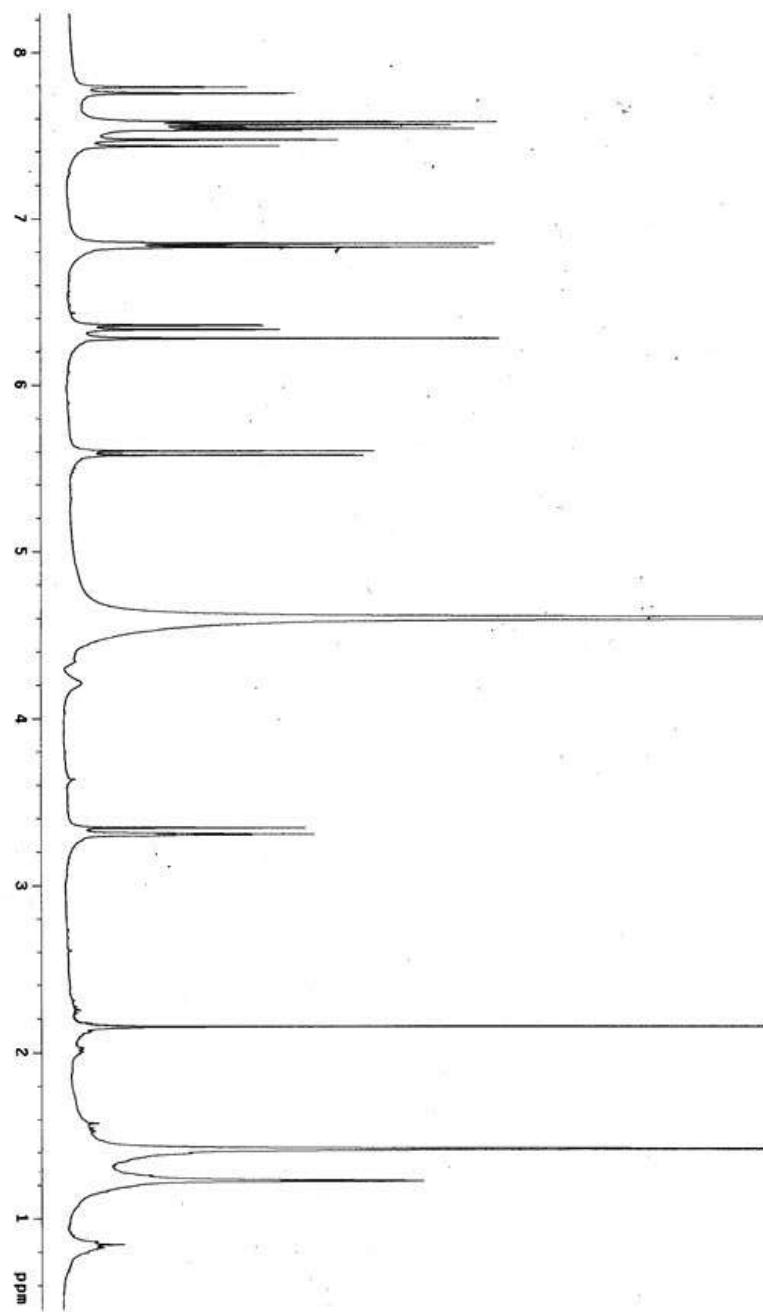


Figure S6. ¹H NMR spectrum of compound 2 (CD₃OD + CDCl₃, 400MHz)

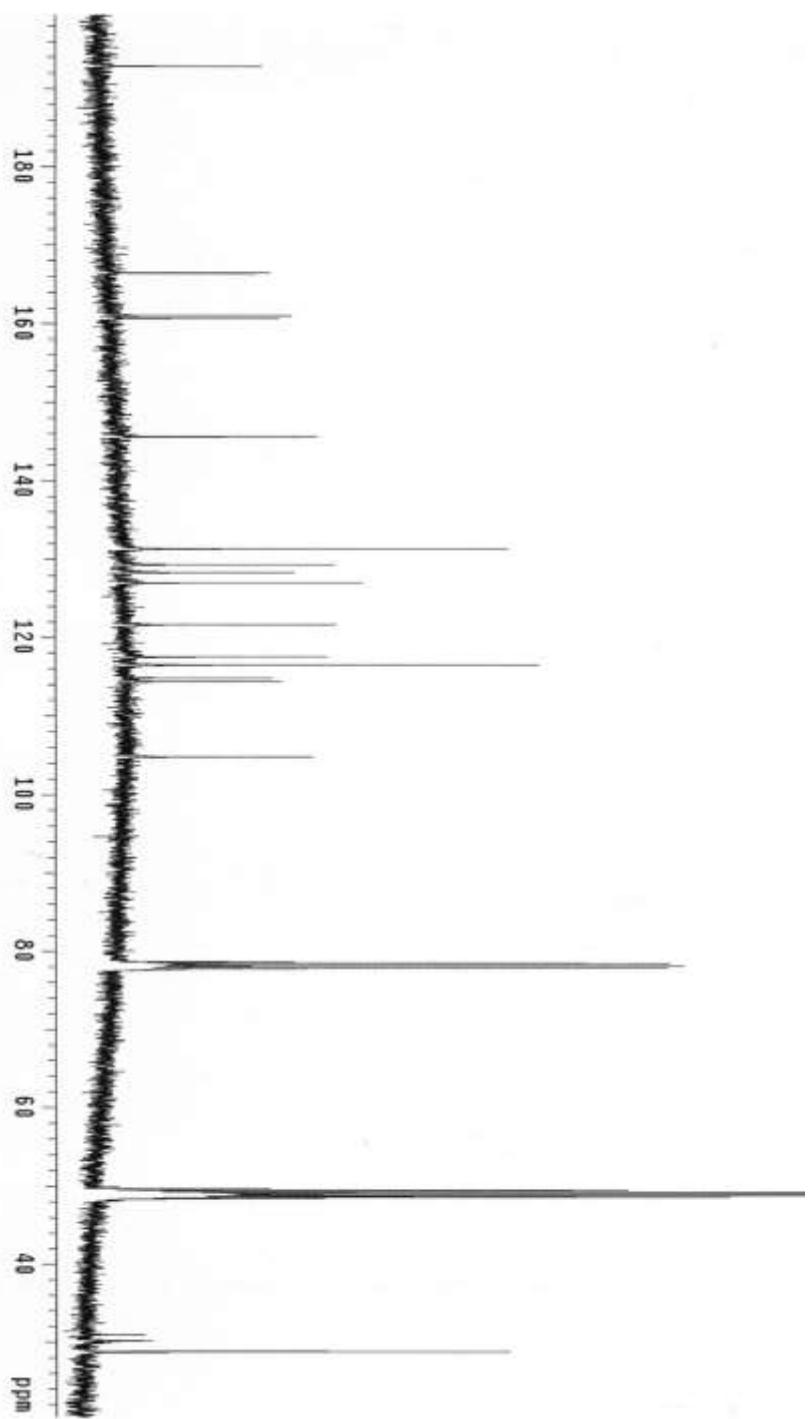


Figure S7. ^{13}C NMR spectrum of compound 2 ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 100MHz)

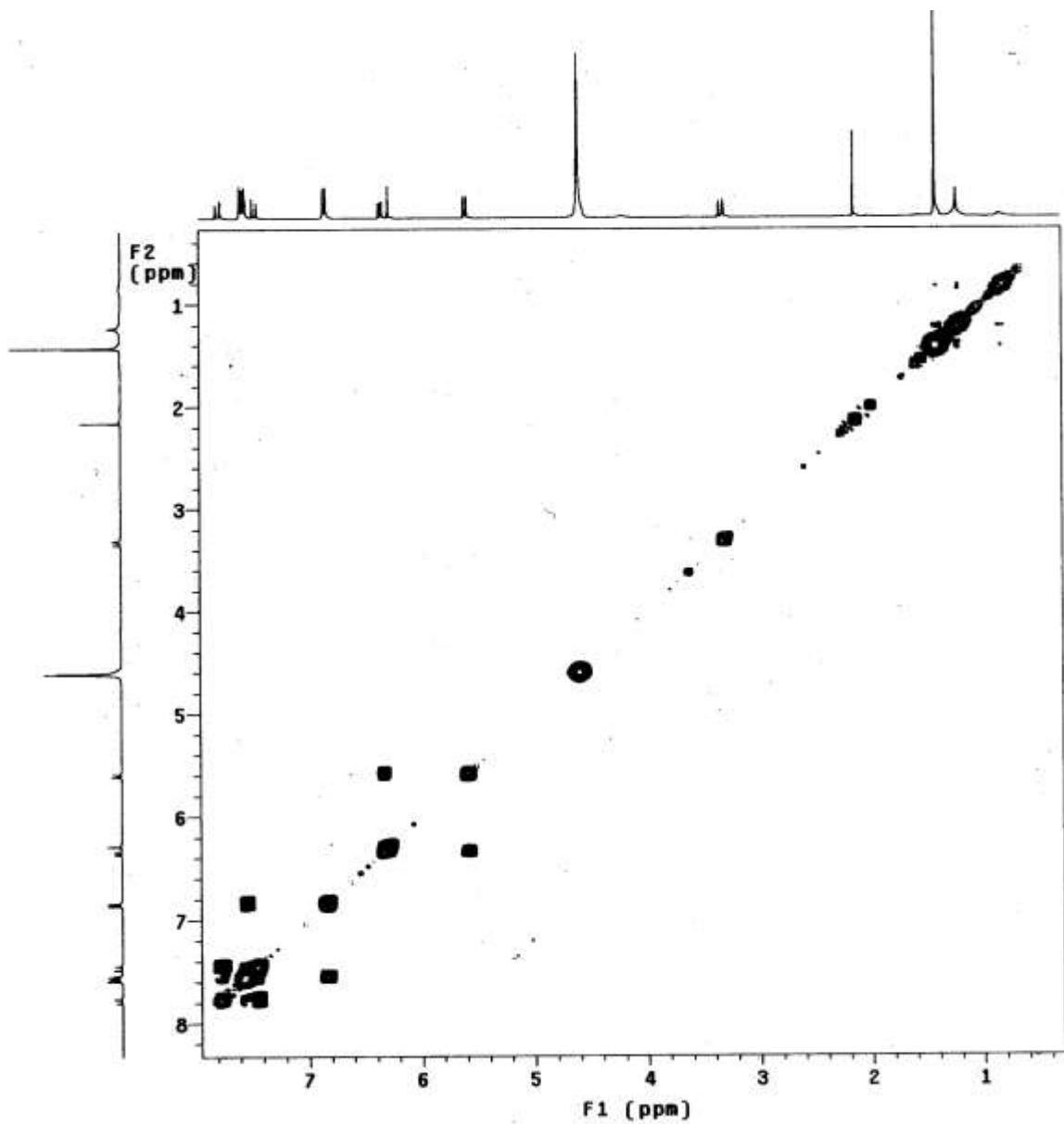


Figure S8. ^1H - ^1H COSY spectrum of compound **2** ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 400MHz)

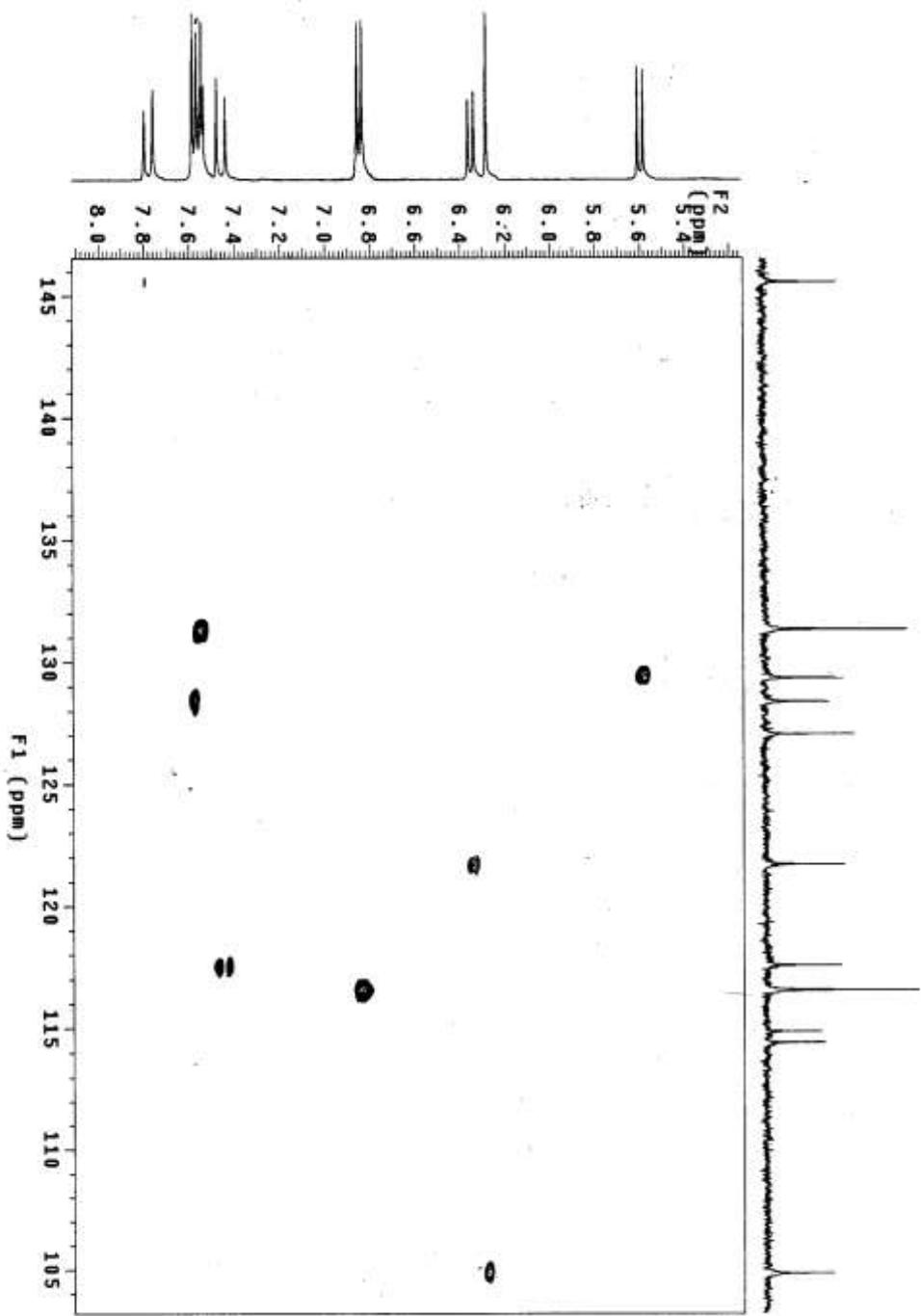


Figure S9. HSQC spectrum of compound **2** ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 400MHz)

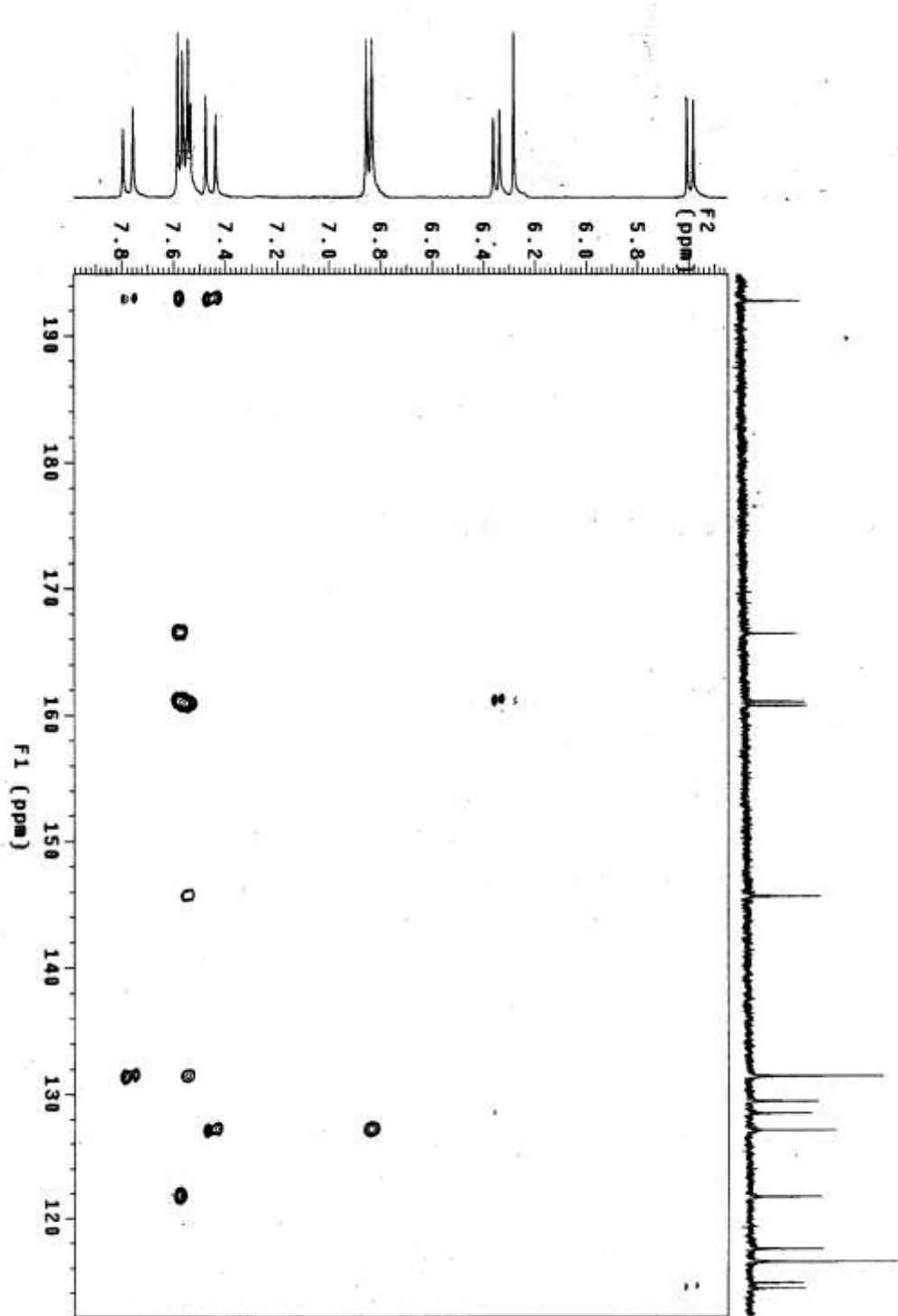


Figure S10. HMBC spectrum of compound 2 ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 400MHz)

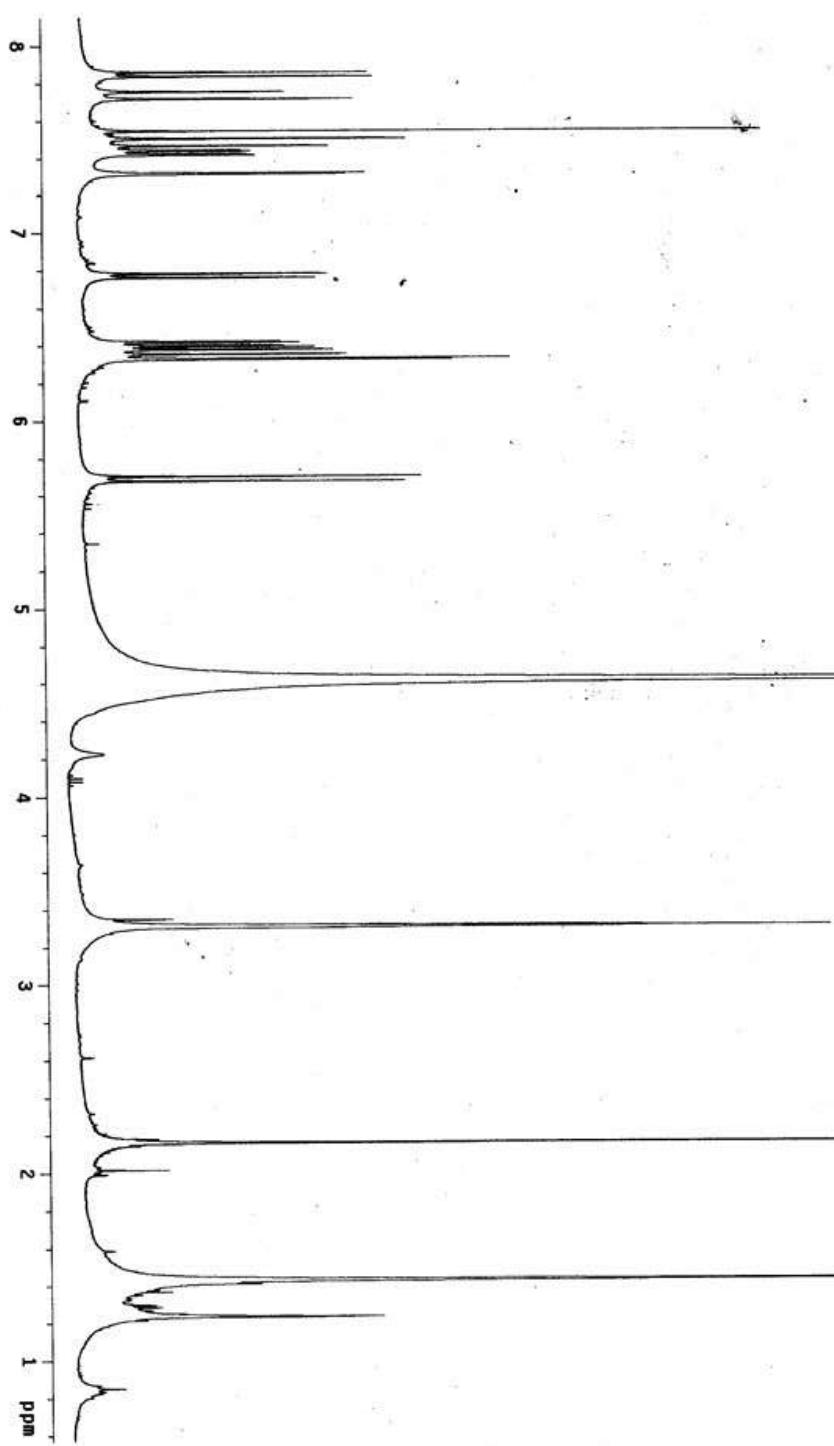


Figure S11. ¹H NMR spectrum of compound 3 ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 400MHz)

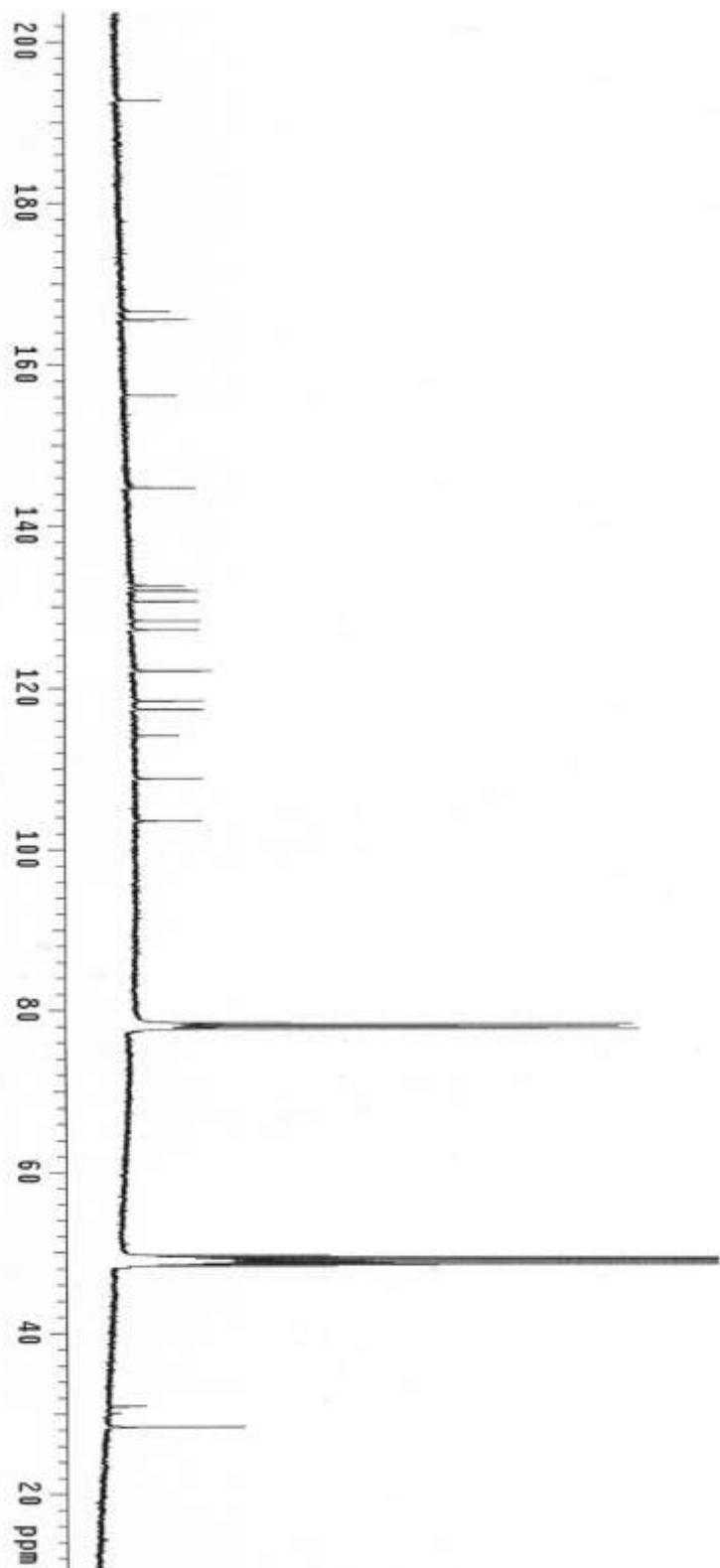


Figure S12. ^{13}C NMR spectrum of compound 3 ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 100MHz)

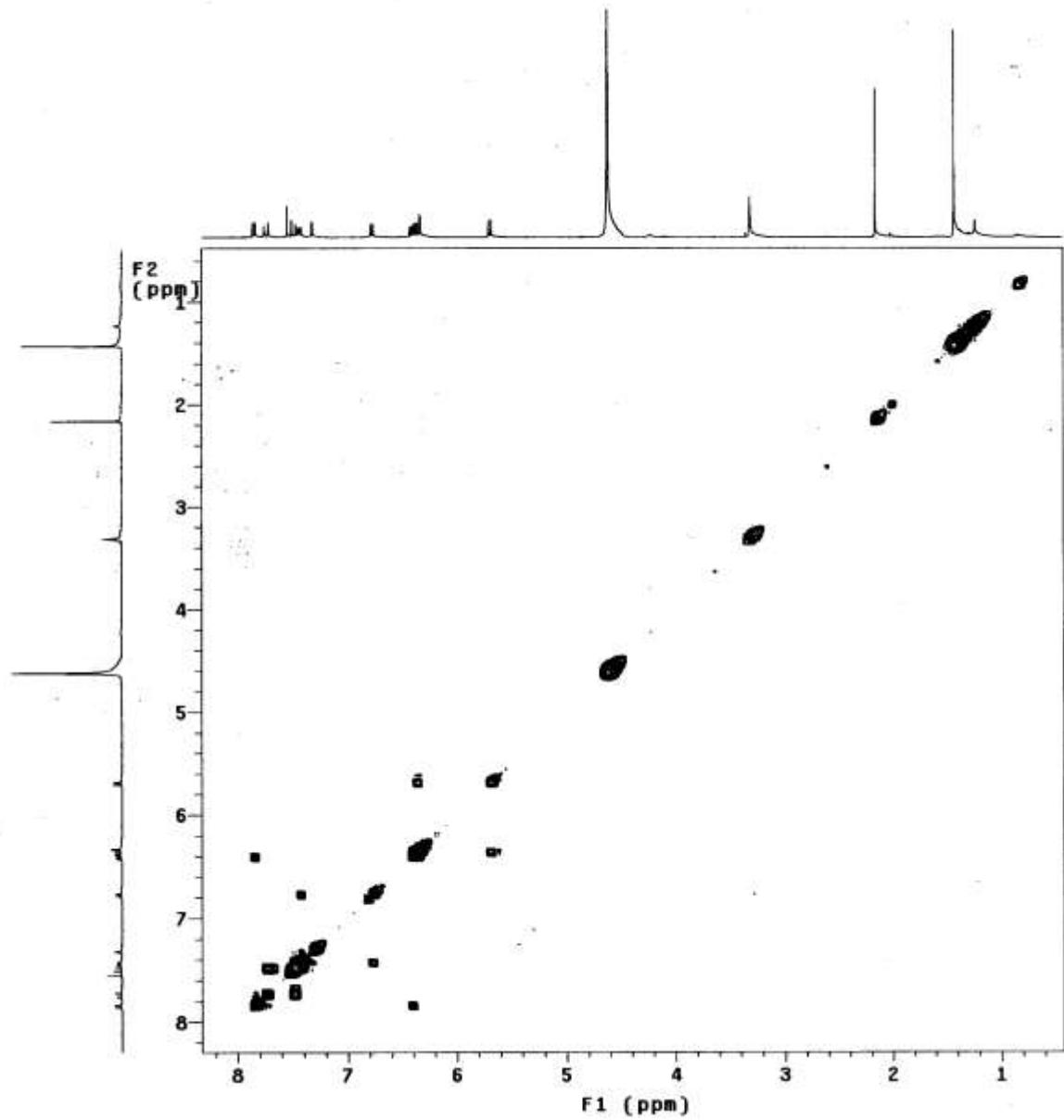


Figure S13. ^1H - ^1H COSY spectrum of compound **3** ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 400MHz)

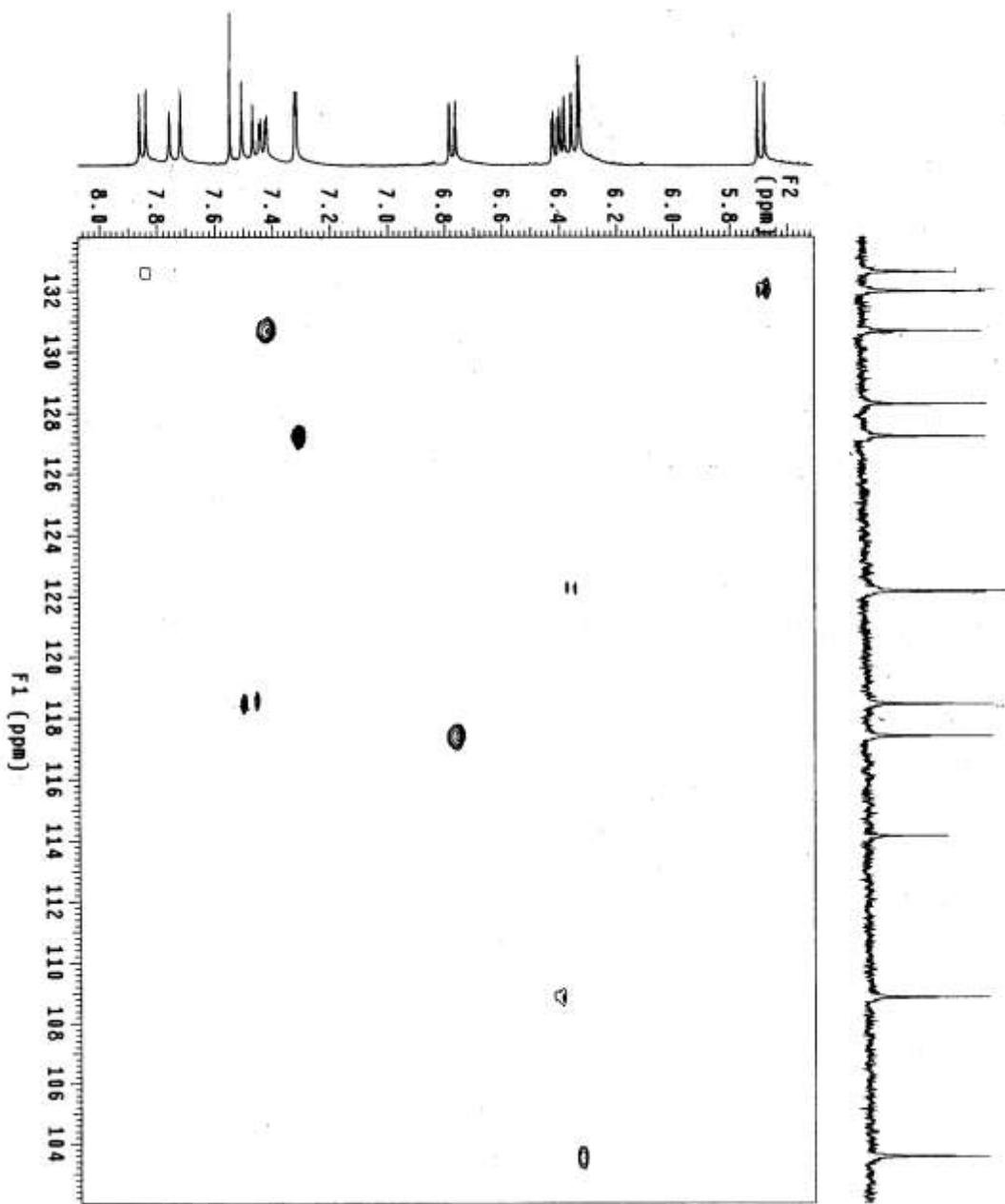


Figure S14. HSQC spectrum of compound 3 ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 400MHz)

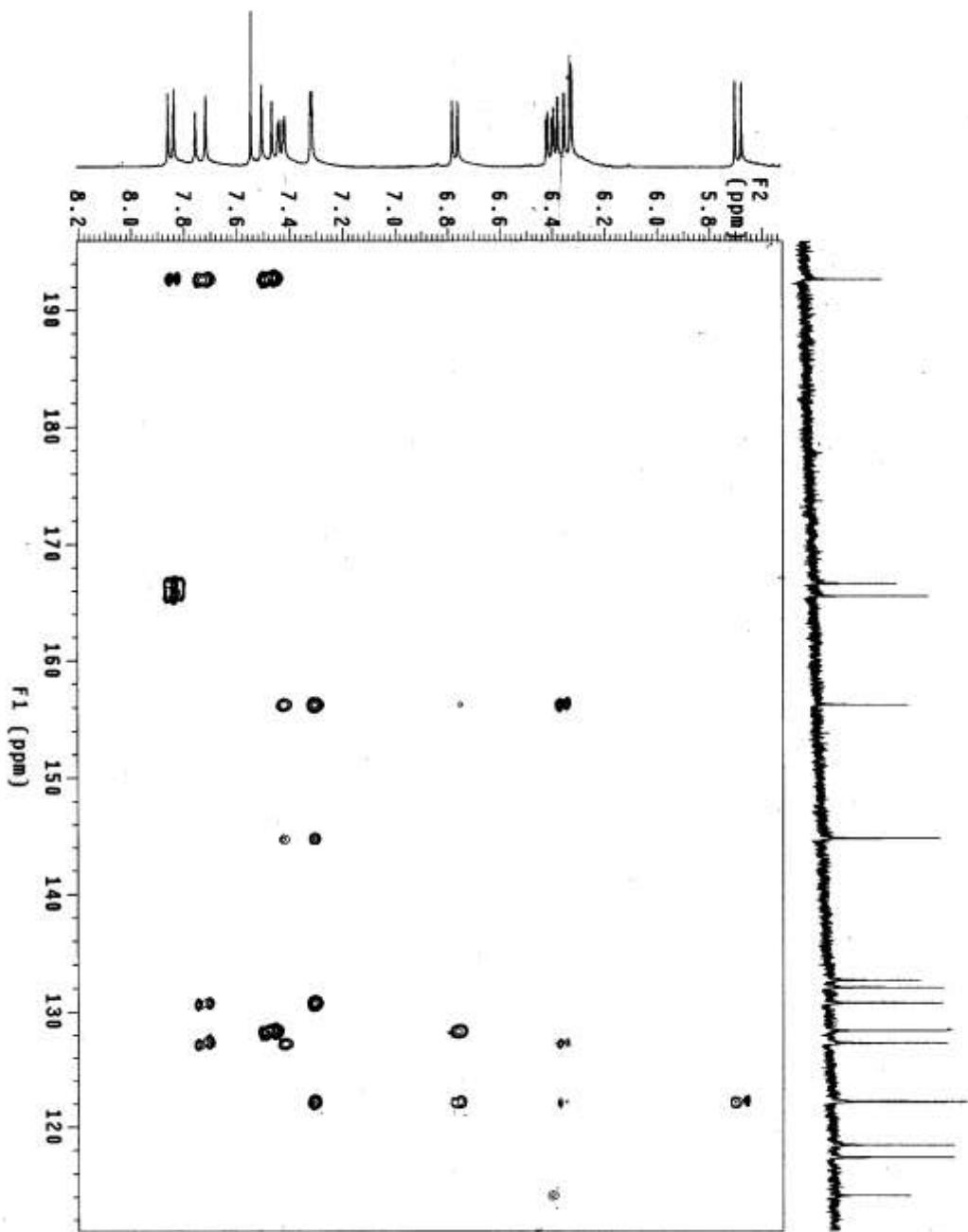


Figure S15. HMBC spectrum of compound 3 ($\text{CD}_3\text{OD} + \text{CDCl}_3$, 400MHz)