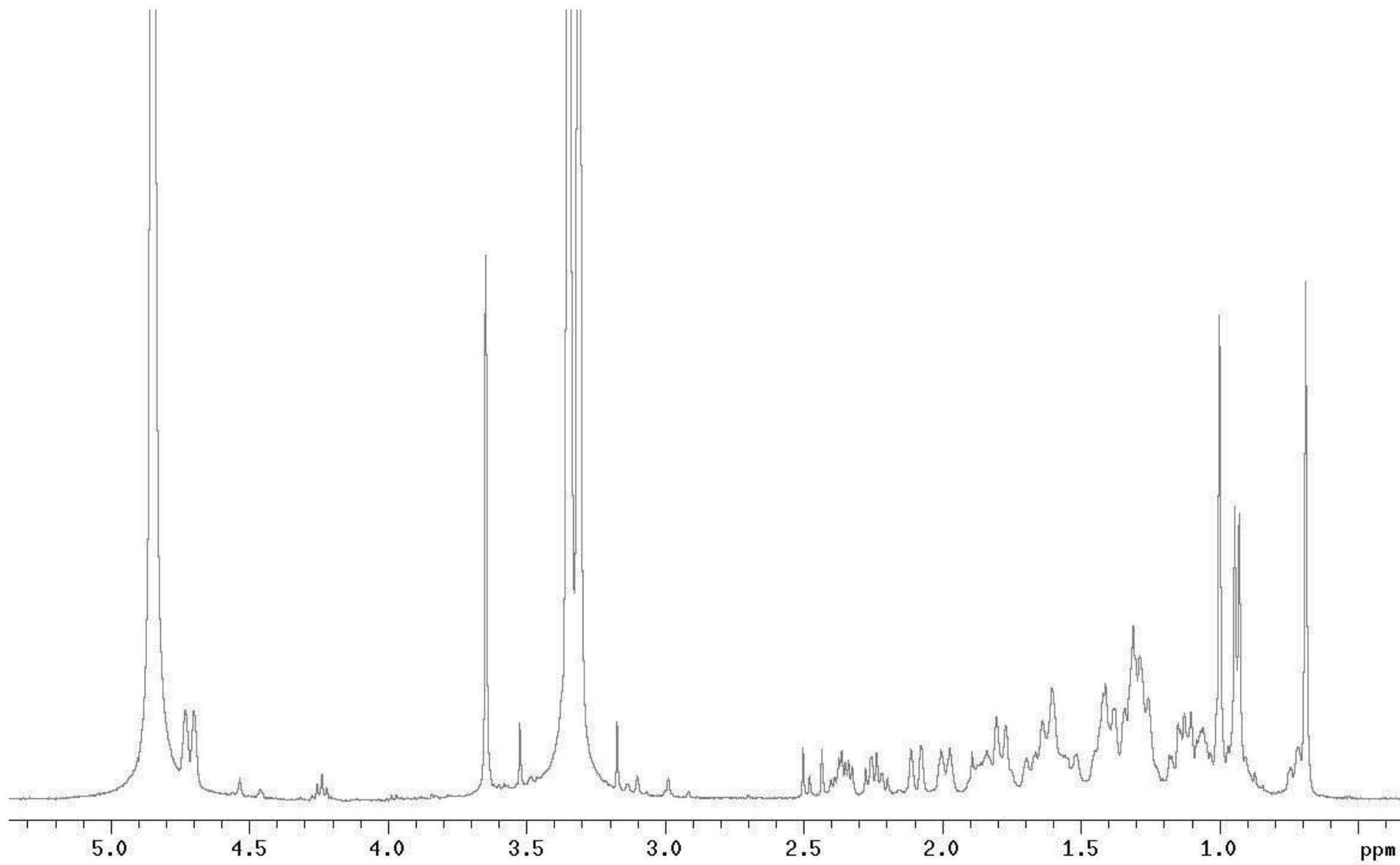


Modification in the side chain of solomonsterol A: discovery of cholestan disulfate as a potent pregnane-X-receptor agonist

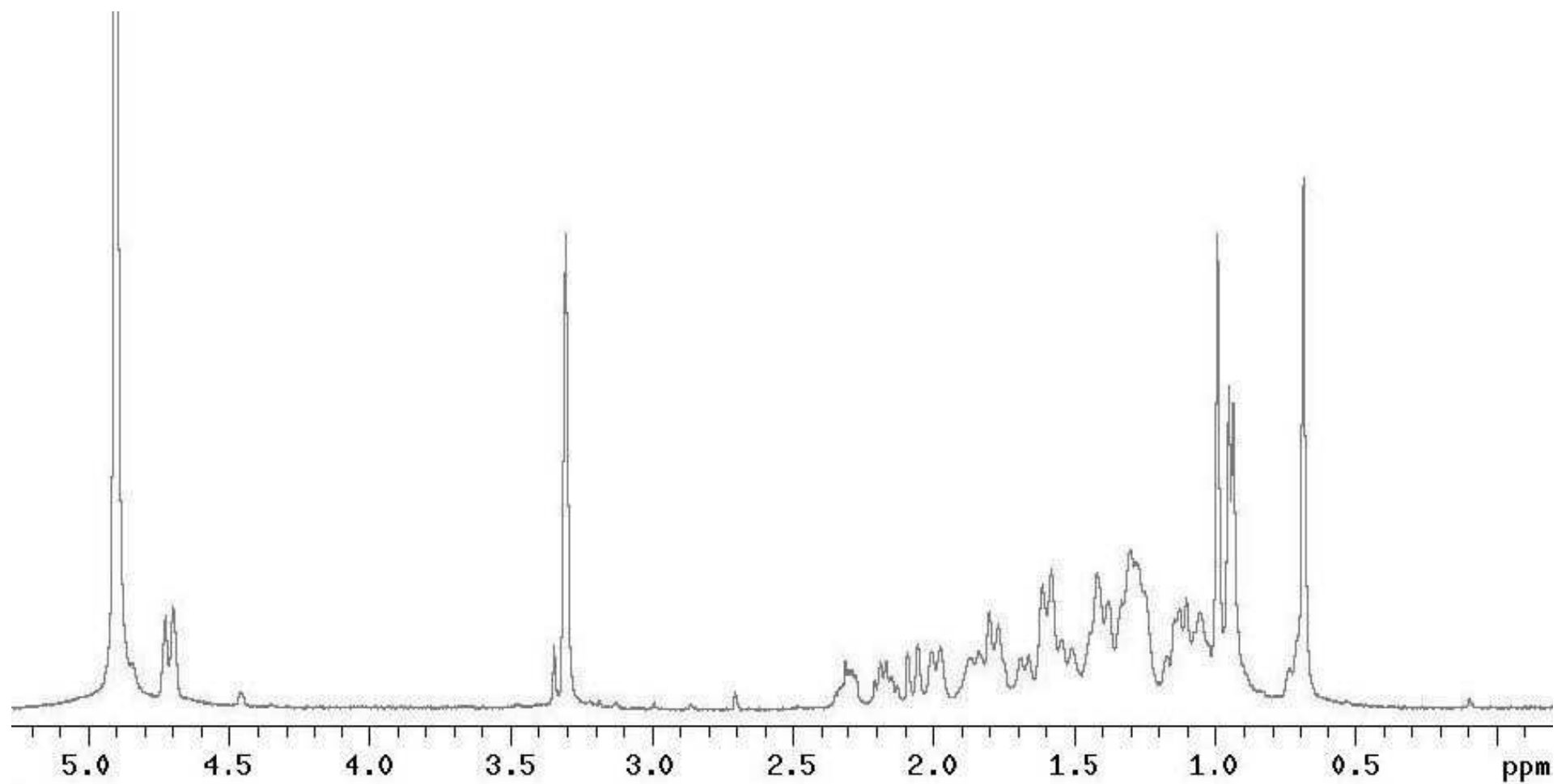
Valentina Sepe, Raffaella Ummarino, Maria Valeria D'Auria, Gianluigi Lauro, Giuseppe Bifulco, Claudio D'Amore, Barbara Renga, Stefano Fiorucci, and Angela Zampella*

Table of contents	page S1
¹ H-NMR spectrum of 2	page S2
¹ H-NMR spectrum of 3	page S3
¹³ C-NMR spectrum of 3	page S4
¹ H-NMR spectrum of 4	page S5
¹³ C-NMR spectrum of 4	page S6
¹ H-NMR spectrum of 5	page S7
¹³ C-NMR spectrum of 5	page S8
¹ H-NMR spectrum of 6	page S9
¹³ C-NMR spectrum of 6	page S10
¹ H-NMR spectrum of 7	page S11
¹³ C-NMR spectrum of 7	page S12
¹ H-NMR spectrum of 8	page S13
¹³ C-NMR spectrum of 8	page S14
¹ H-NMR spectrum of 9	page S15
¹ H-NMR spectrum of 10	page S16
HPLC trace of 2 and 3	page S17
HPLC trace of 4, 5, 6 and 7	page S18
HPLC trace of 8, 9 and 10	page S19
HPLC trace of 11	page S20

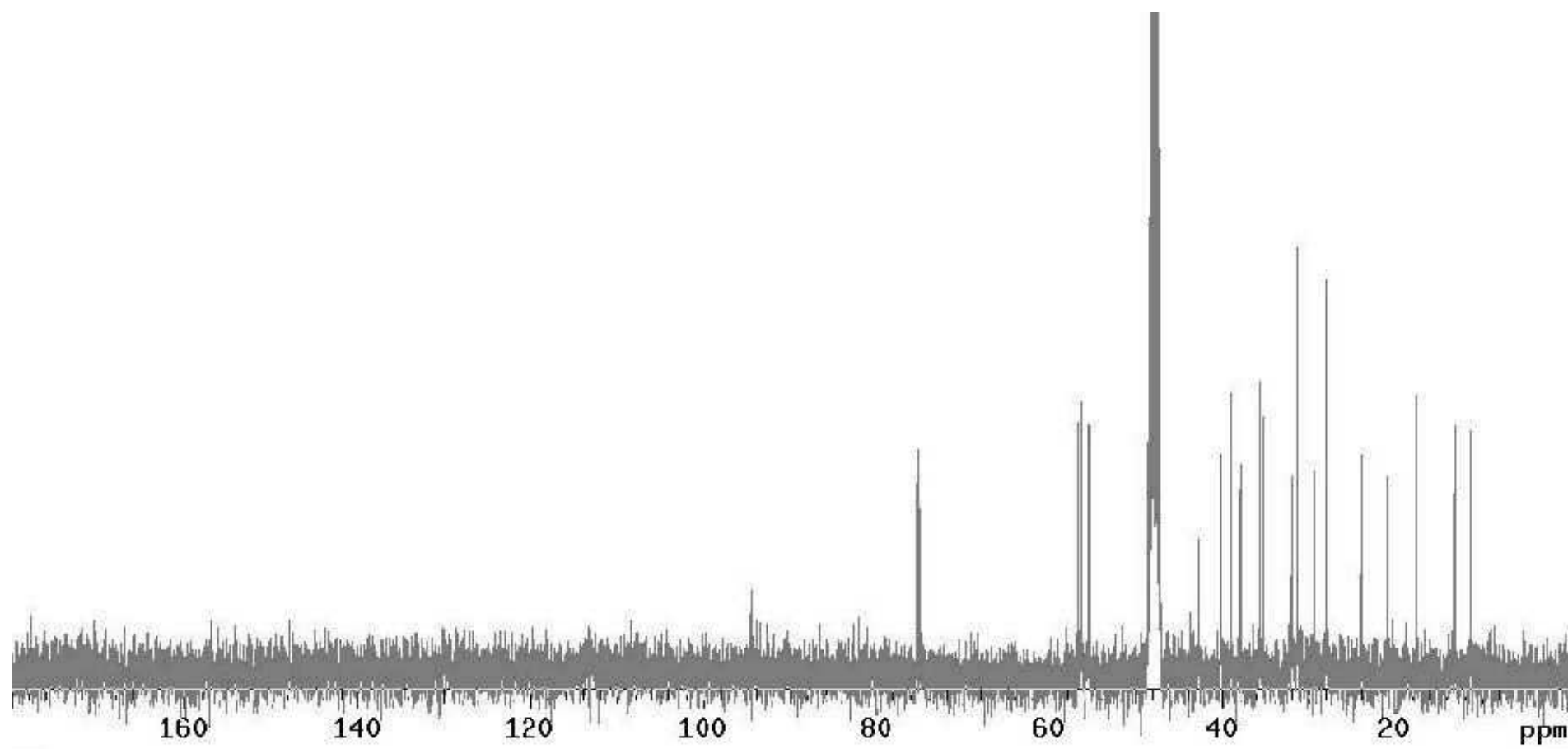
^1H NMR (400 MHz, CD_3OD) of **2**



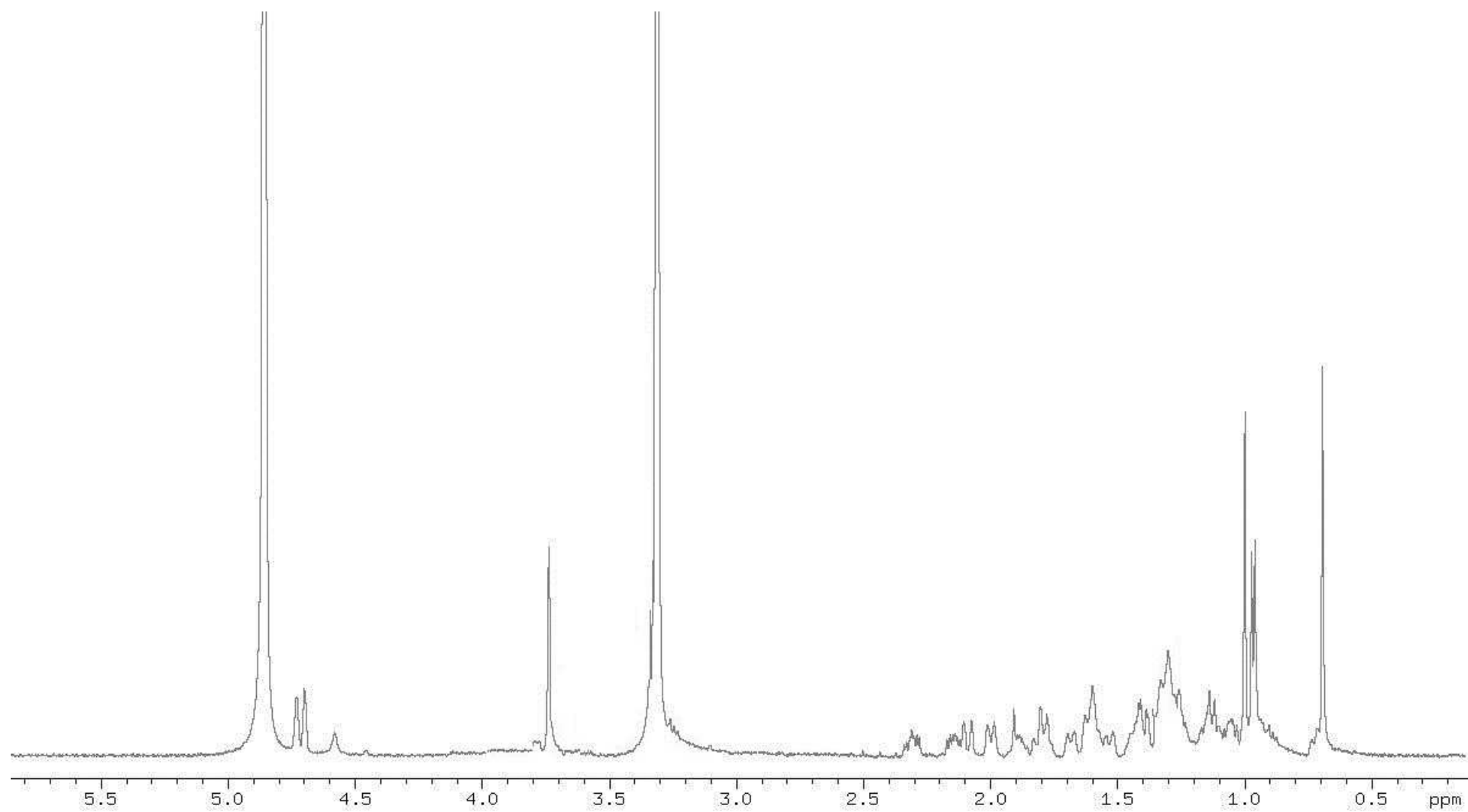
^1H NMR (400 MHz, CD_3OD) of **3**



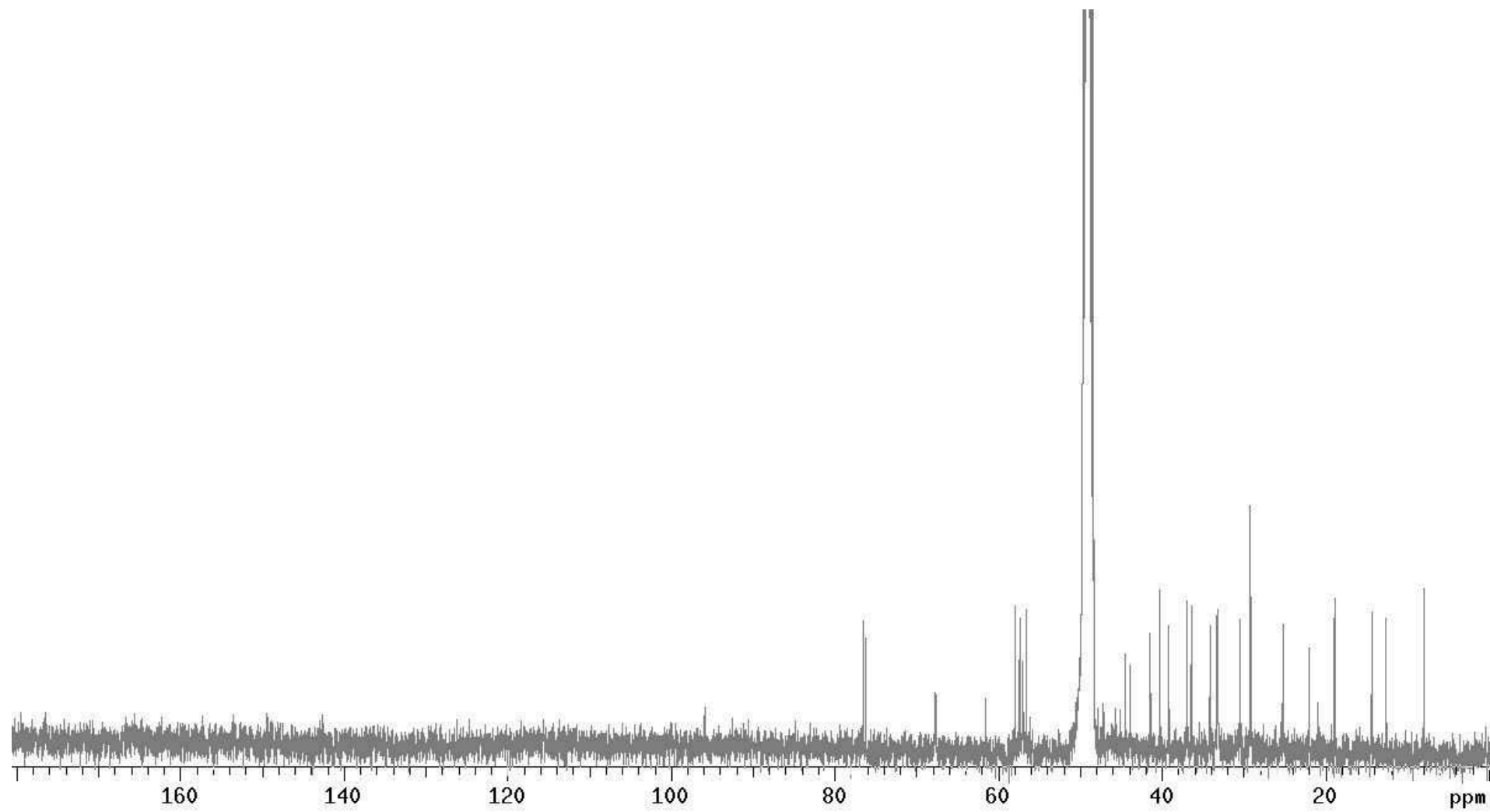
^{13}C NMR (100 MHz, CD_3OD) of **3**



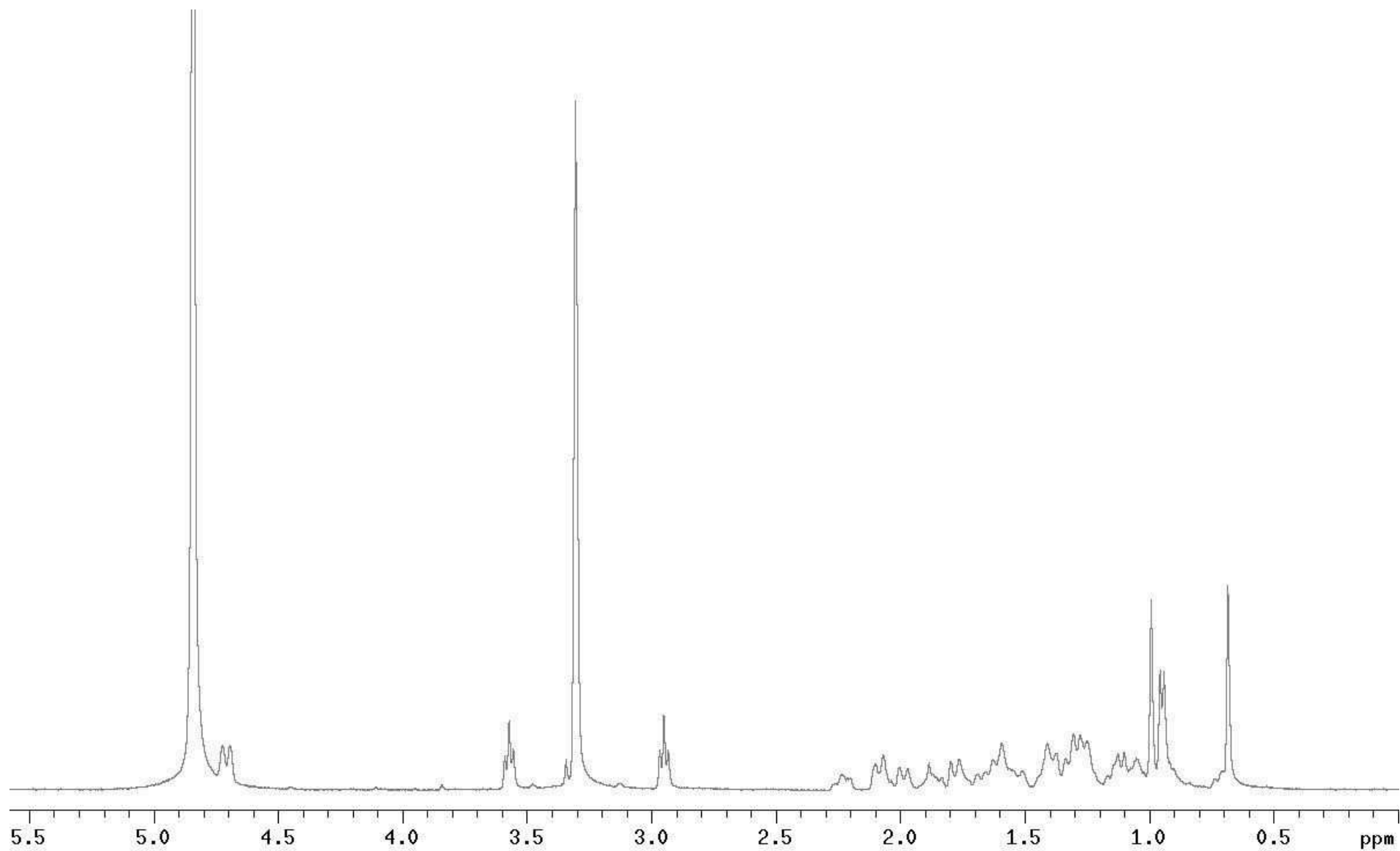
^1H NMR (400 MHz, CD_3OD) of **4**



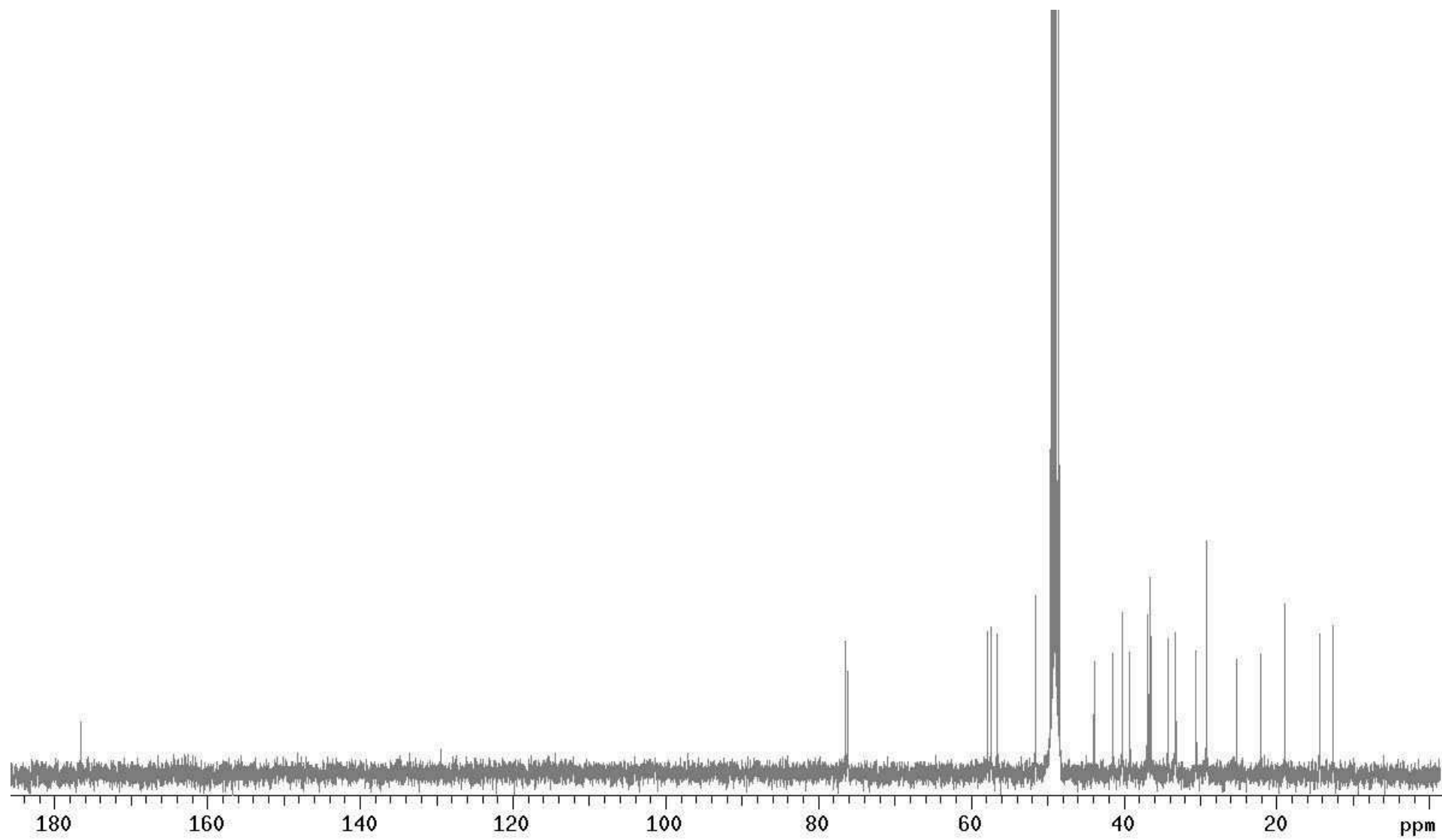
^{13}C NMR (100 MHz, CD_3OD) of **4**



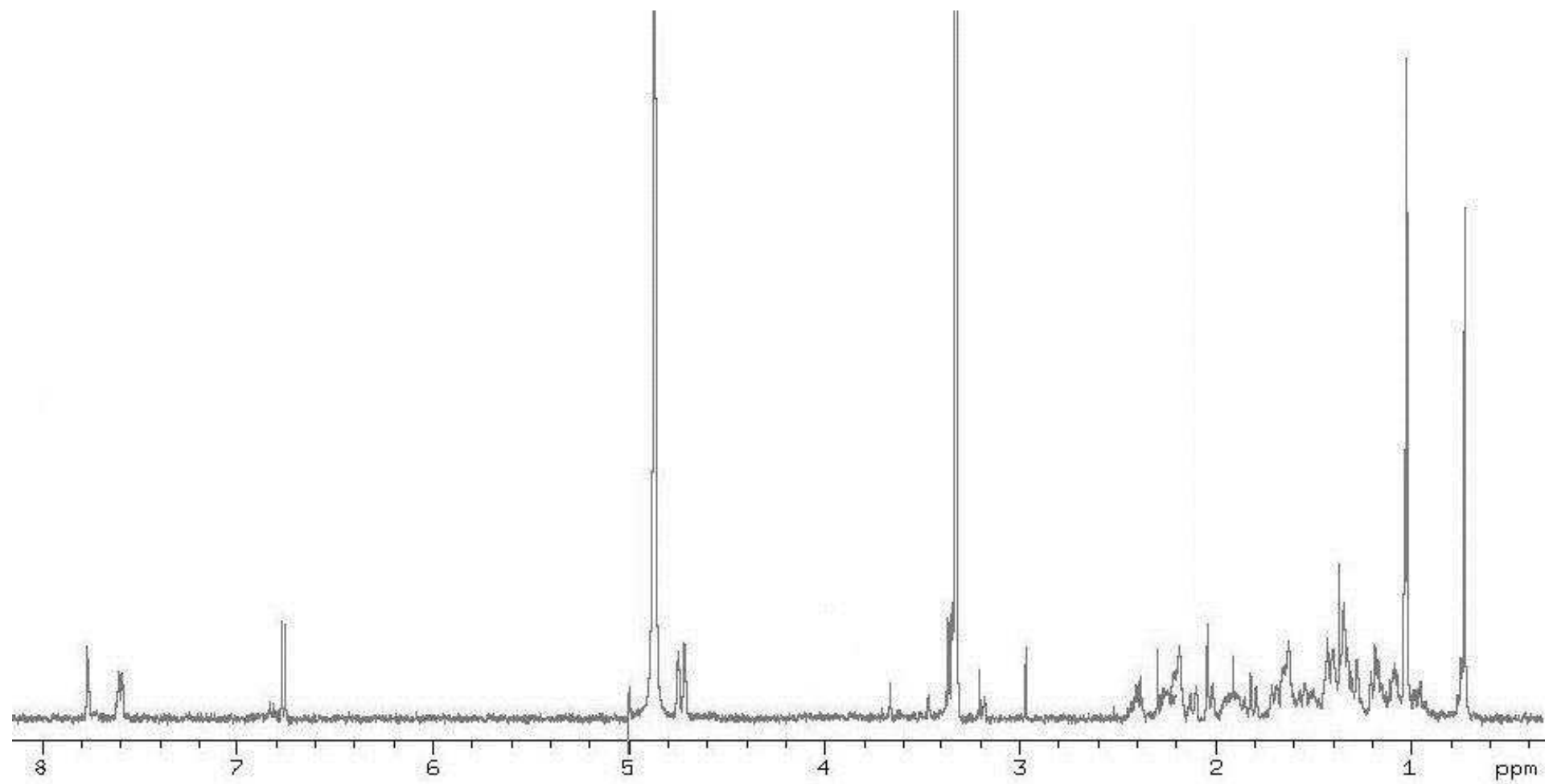
^1H NMR (400 MHz, CD_3OD) of **5**



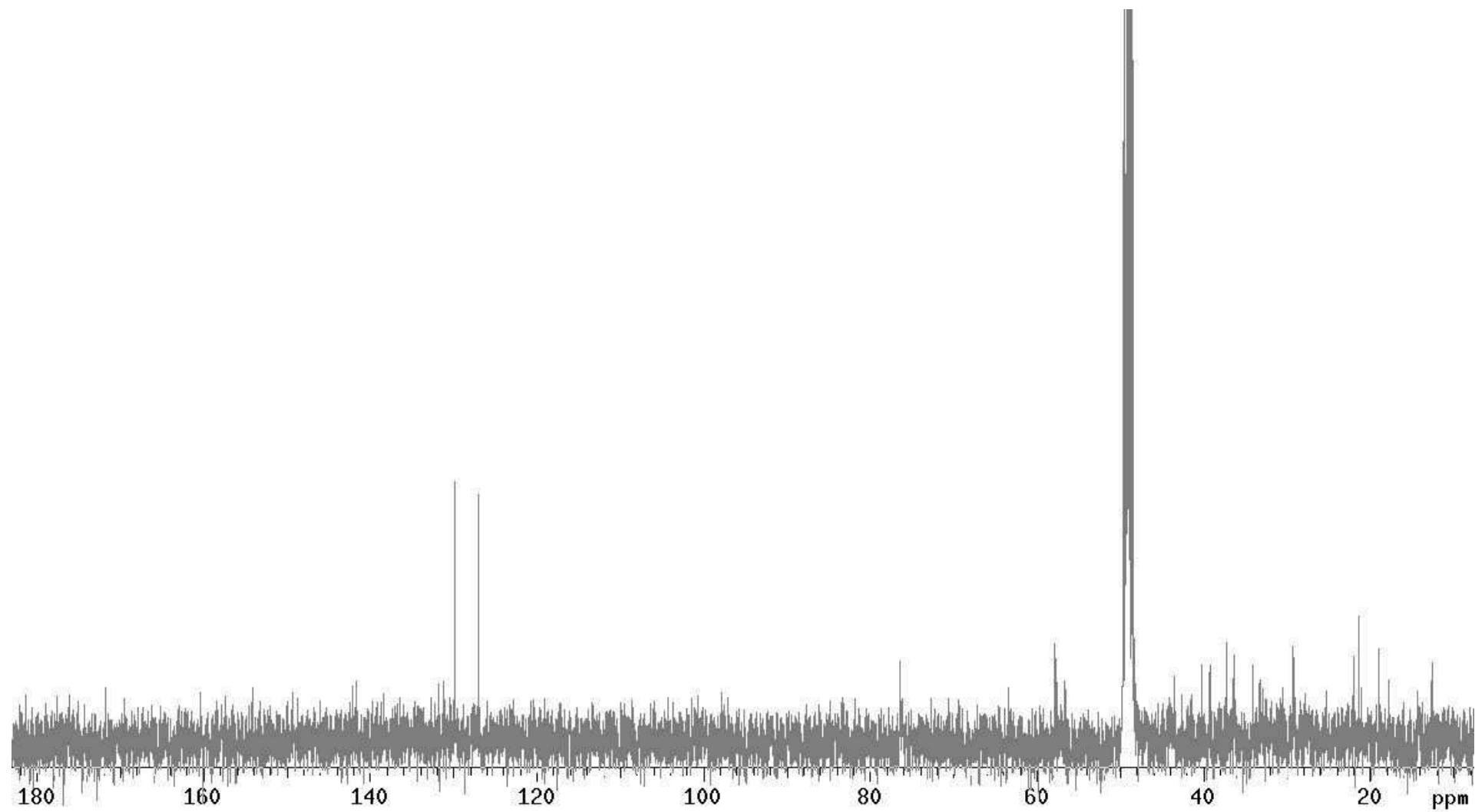
^{13}C NMR (100 MHz, CD_3OD) of **5**



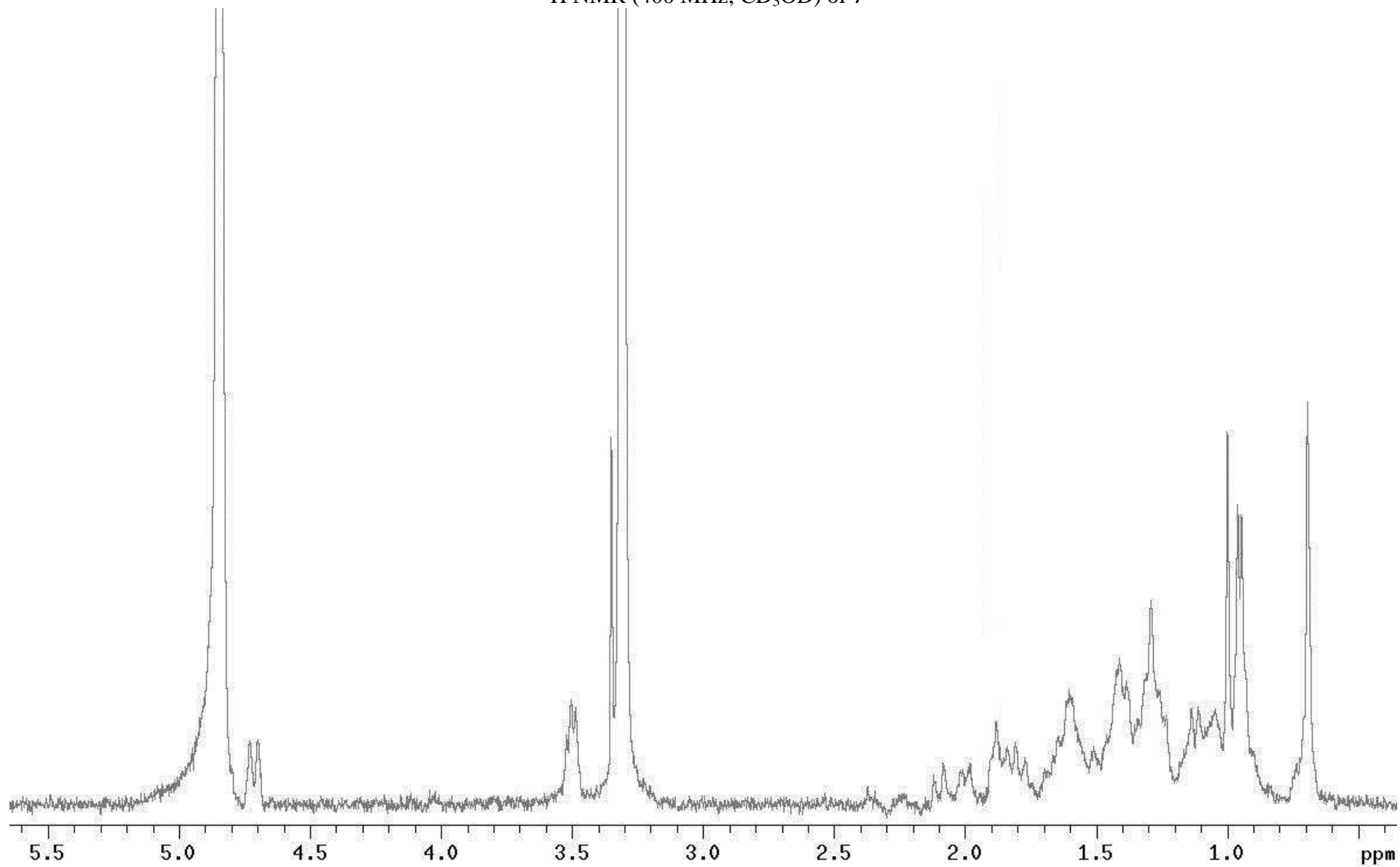
^1H NMR (400 MHz, CD_3OD) of **6**

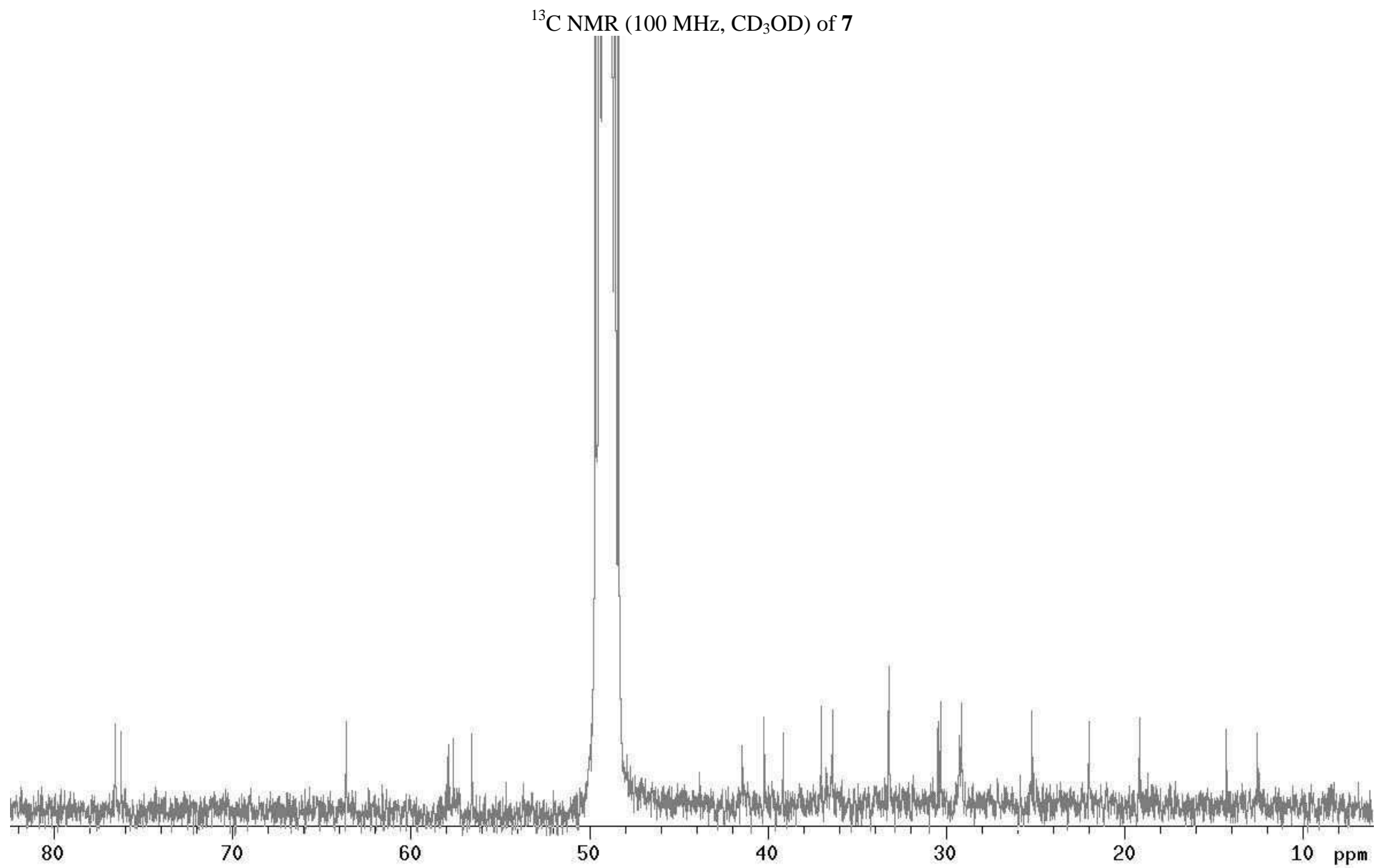


^{13}C NMR (100 MHz, CD_3OD) of **6**

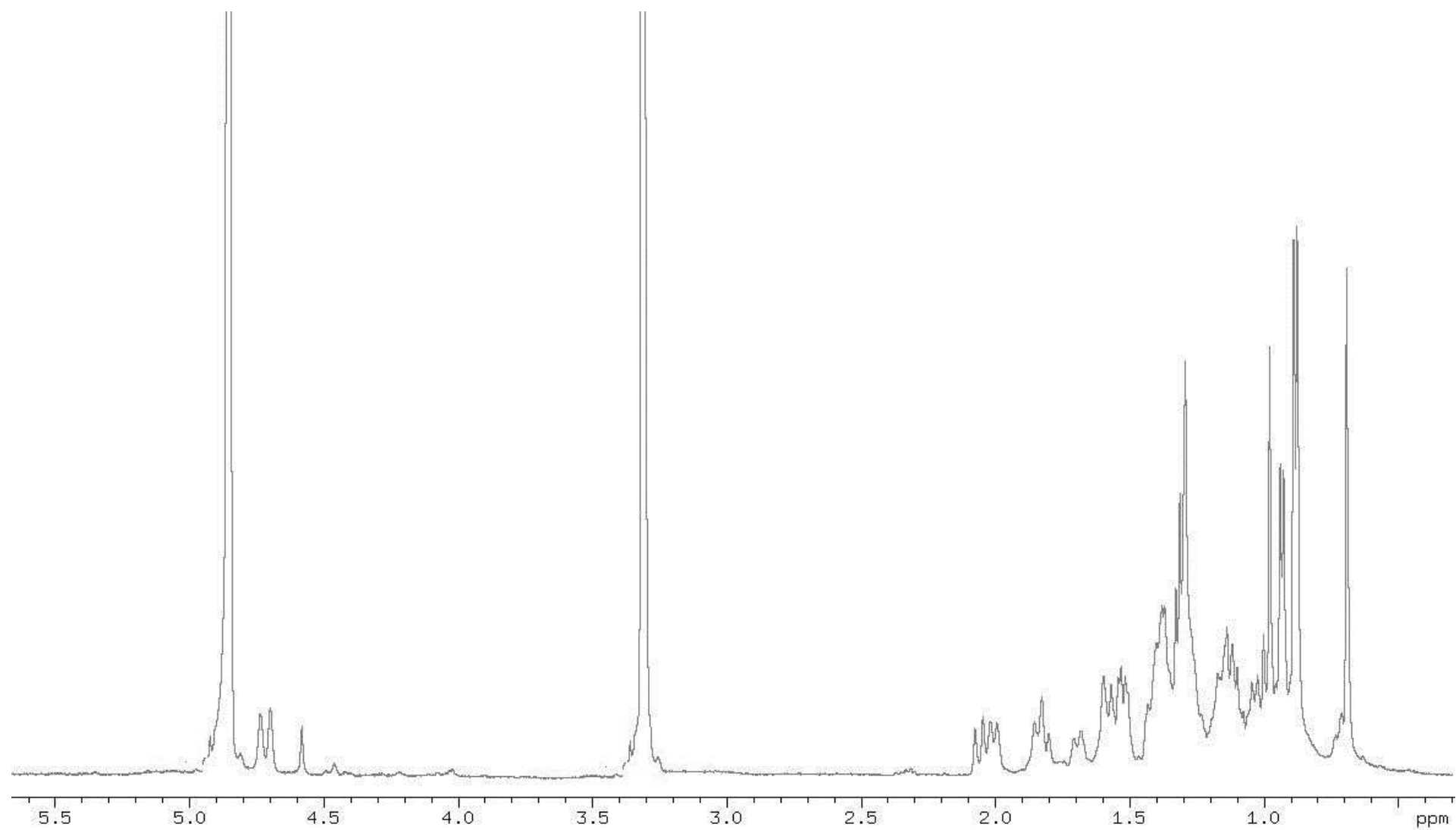


^1H NMR (400 MHz, CD_3OD) of **7**

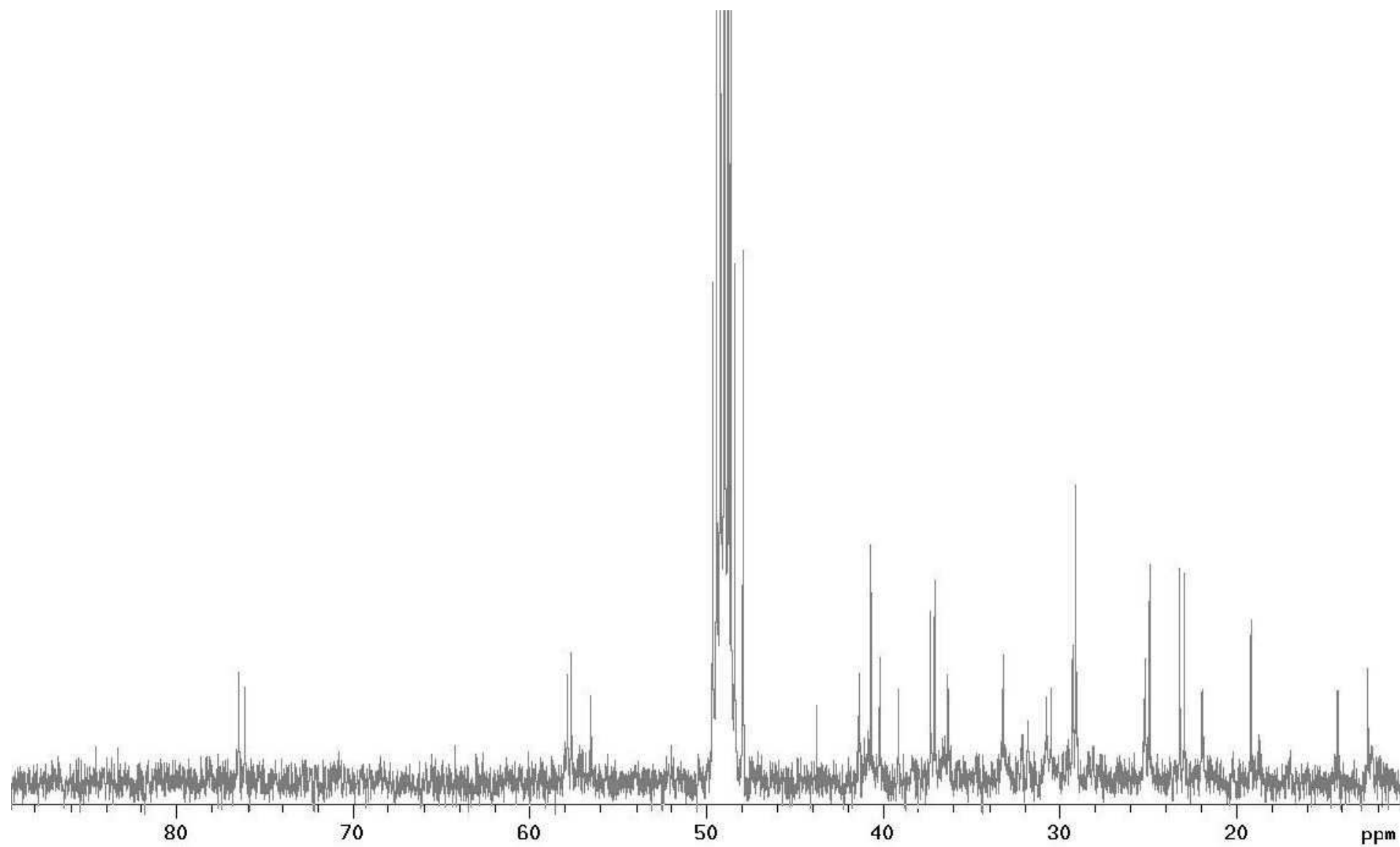




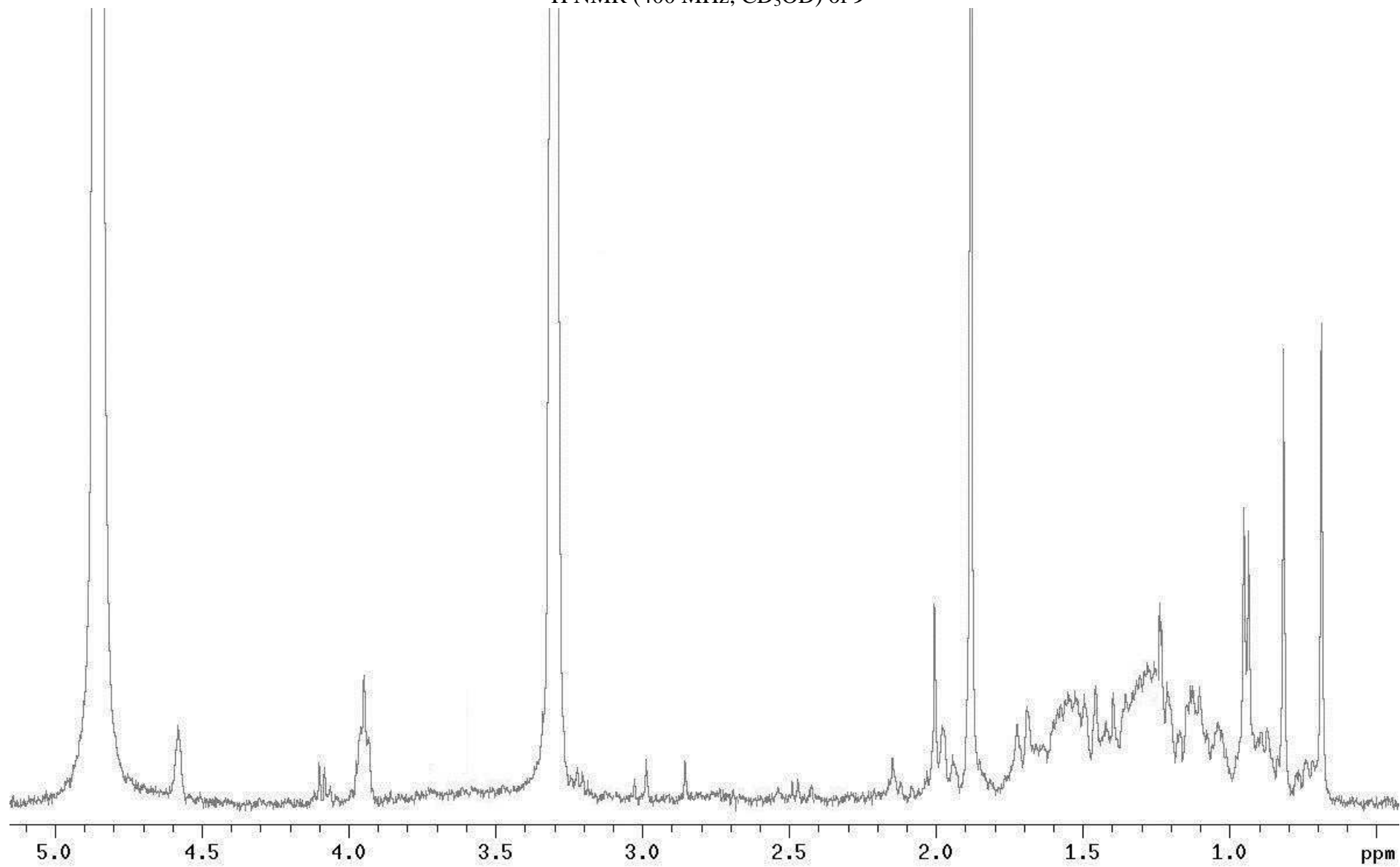
^1H NMR (400 MHz, CD_3OD) of **8**



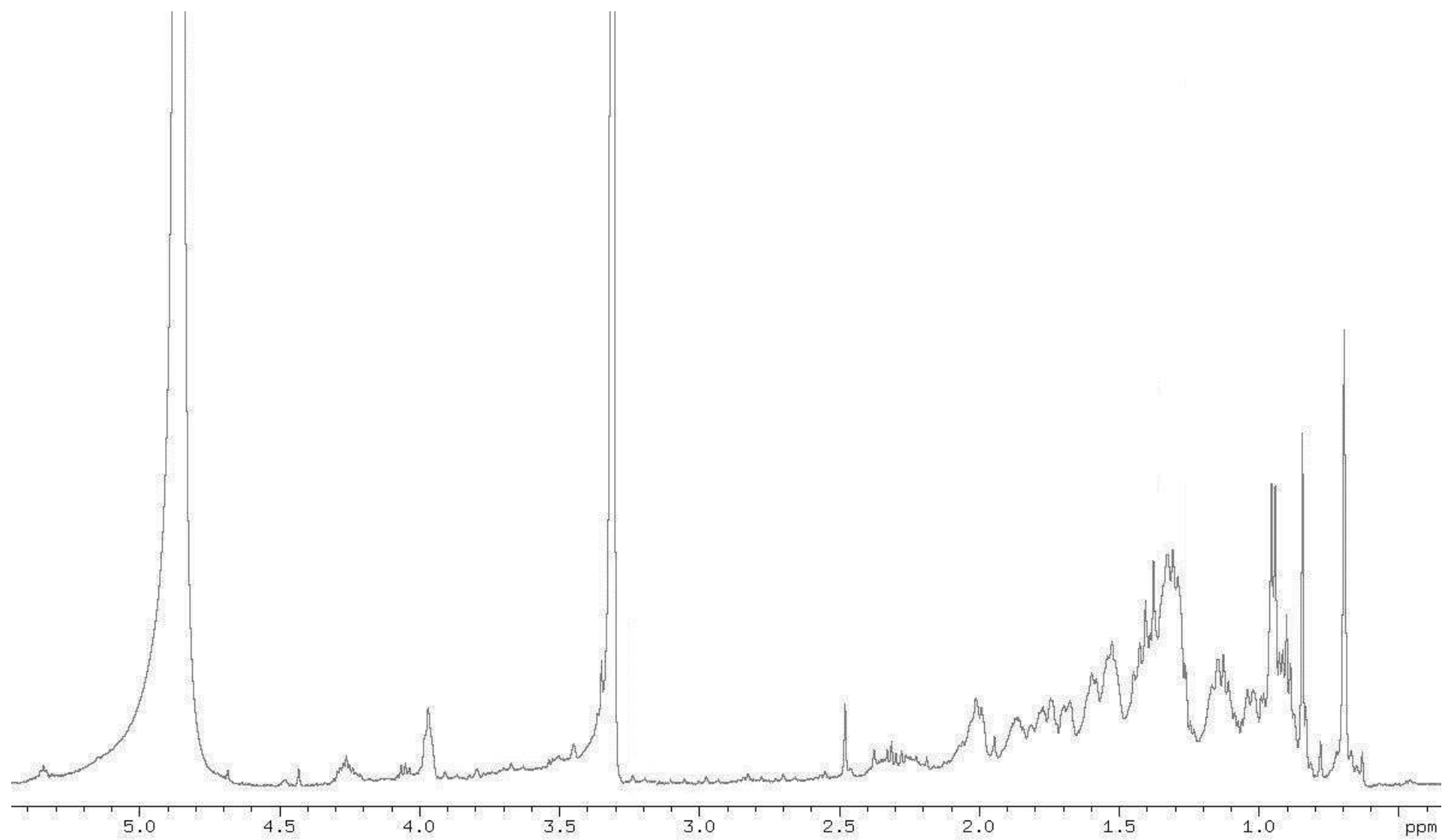
^{13}C NMR (100 MHz, CD_3OD) of **8**



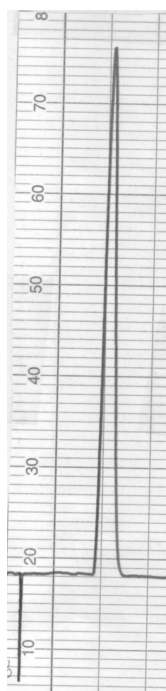
^1H NMR (400 MHz, CD_3OD) of **9**



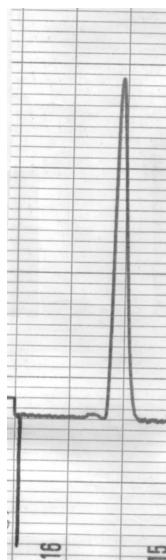
^1H NMR (400 MHz, CD_3OD) of **10**



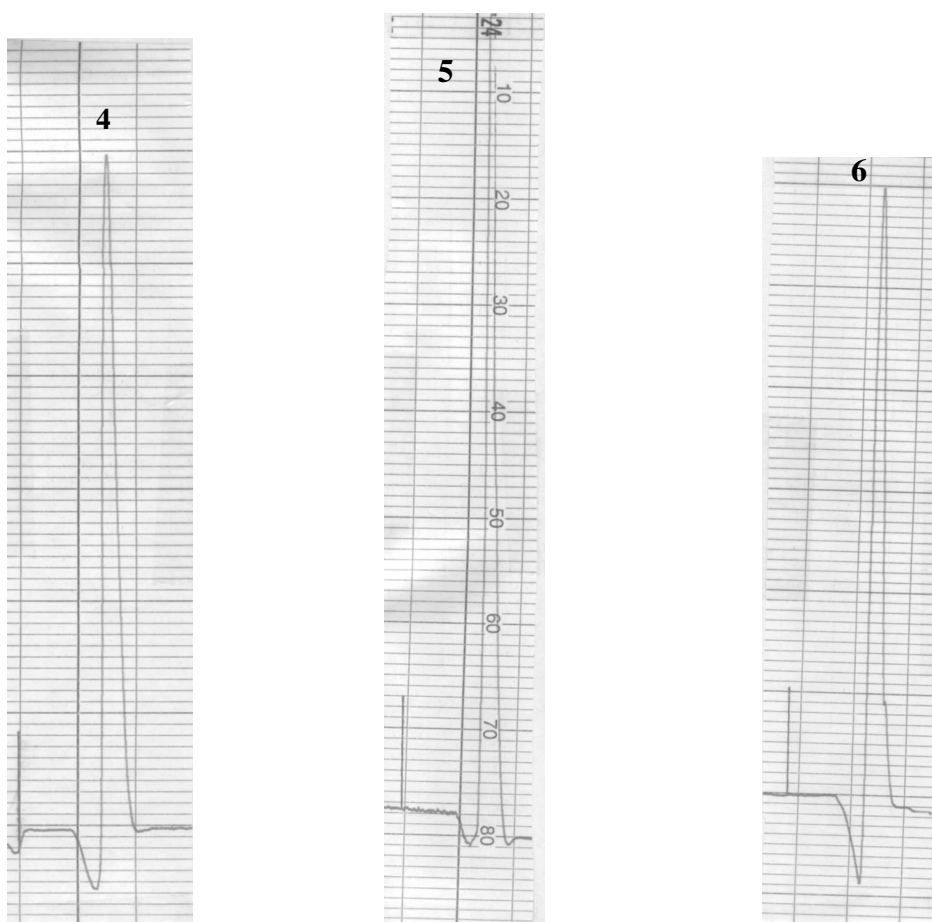
HPLC trace of **2** on a Nucleodur 100-5 C18 (5 μ m; 4.6 mm i.d. x 250 mm) with MeOH:H₂O (34:66) as eluent (flow rate 1.5 mL/min) t_R =3.6 min.



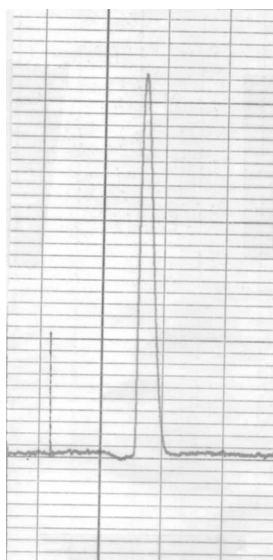
HPLC trace of **3** on a Nucleodur 100-5 C18 (5 μ m; 4.6 mm i.d. x 250 mm) with MeOH:H₂O (30:70) as eluent (flow rate 1.5 mL/min) t_R =3.6 min.



HPLC trace of **4**, **5** and **6** on a Nucleodur 100-5 C18 (5 μ m; 4.6 mm i.d. x 250 mm) with MeOH:H₂O (30:70) as eluent (flow rate 1.5 mL/min) $t_R=3.4$ min.



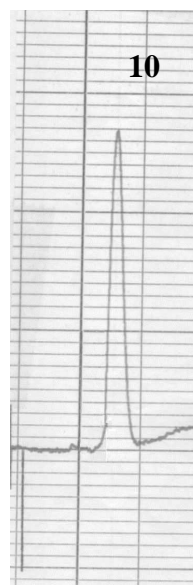
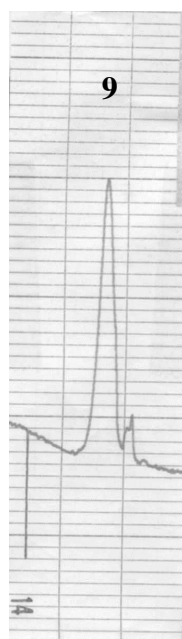
HPLC trace of **7** on a Nucleodur 100-5 C18 (5 μ m; 4.6 mm i.d. x 250 mm) with MeOH:H₂O (32:68) as eluent (flow rate 1.5 mL/min) $t_R=3.2$ min.



HPLC trace of **8** on a Nucleodur 100-5 C18 (5 μ m; 4.6 mm i.d. x 250 mm) with MeOH:H₂O (87:13) as eluent (flow rate 1.5 mL/min) t_R =2.6 min.



HPLC trace of **9** and **10** on a Nucleodur 100-5 C18 (5 μ m; 4.6 mm i.d. x 250 mm) with MeOH:H₂O (25:75) as eluent (flow rate 1.5 mL/min) t_R =2.4 min).



HPLC trace of **11** on a Nucleodur 100-5 C18 (5 μ m; 4.6 mm i.d. x 250 mm) with MeOH:H₂O
(87:13) as eluent (flow rate 1.5 mL/min) t_R =2.6 min.

