Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Eleven new highly oxygenated triterpenoids from the leaves and stems of *Schisandra chinensis*

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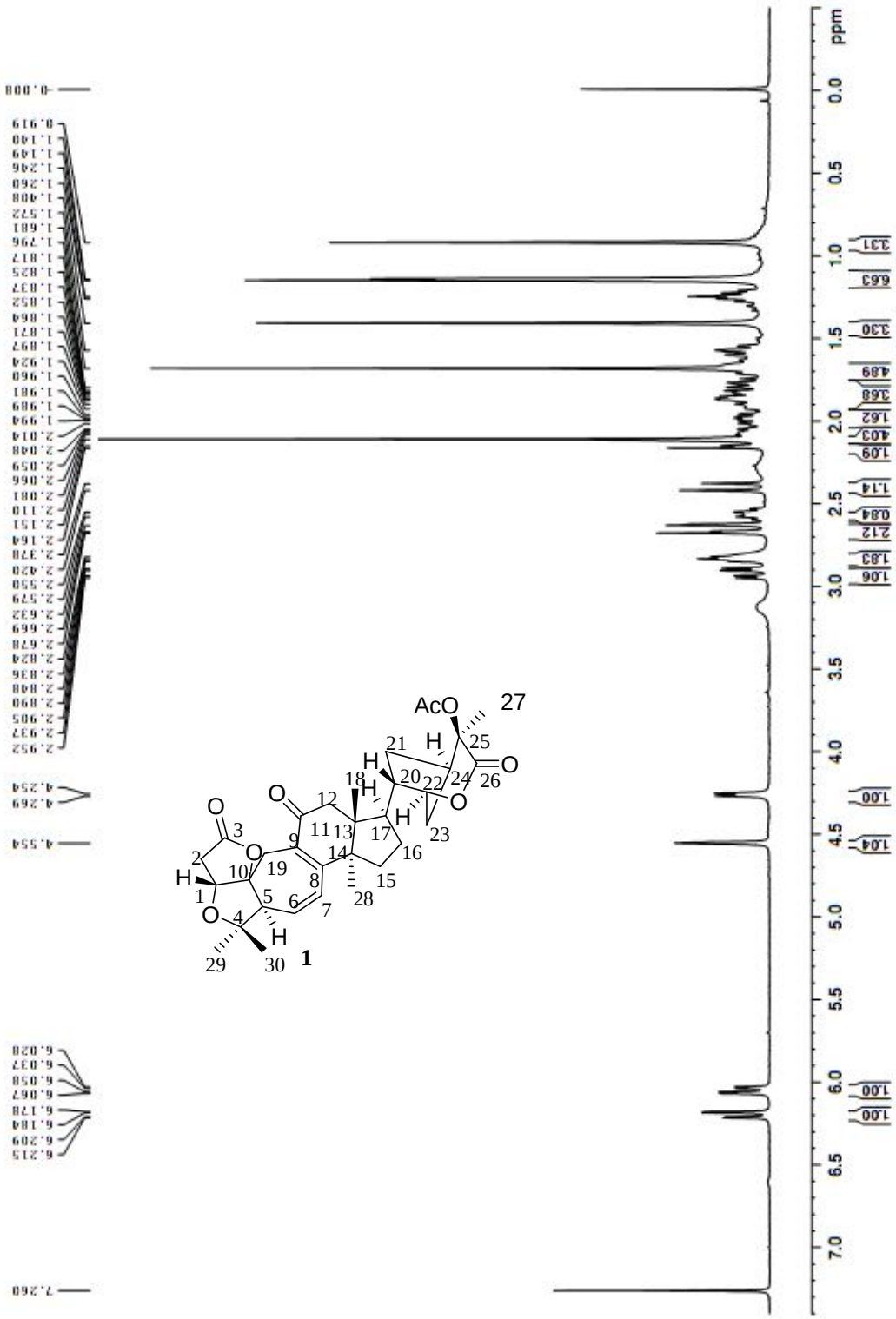
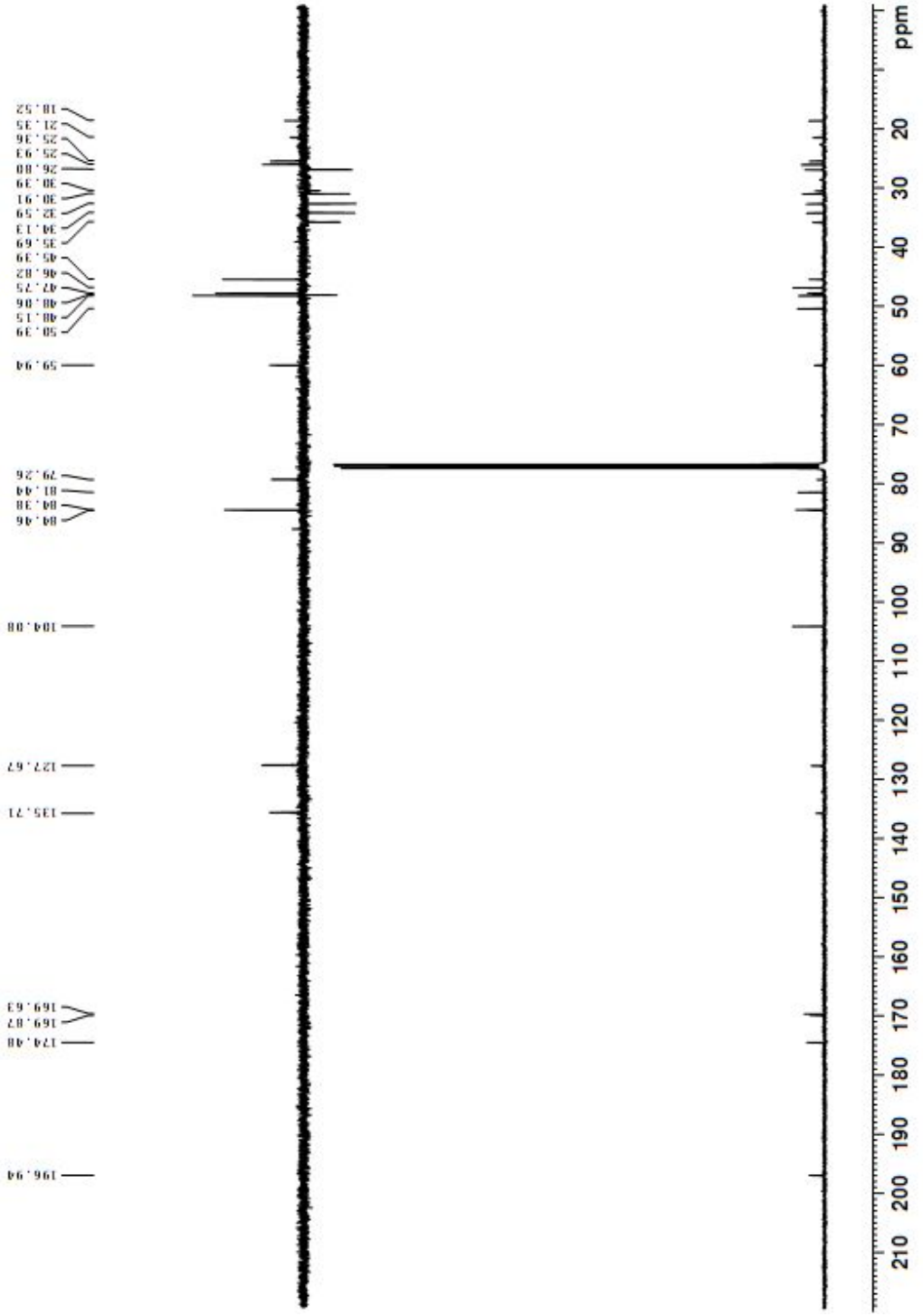
Contents of supporting information:

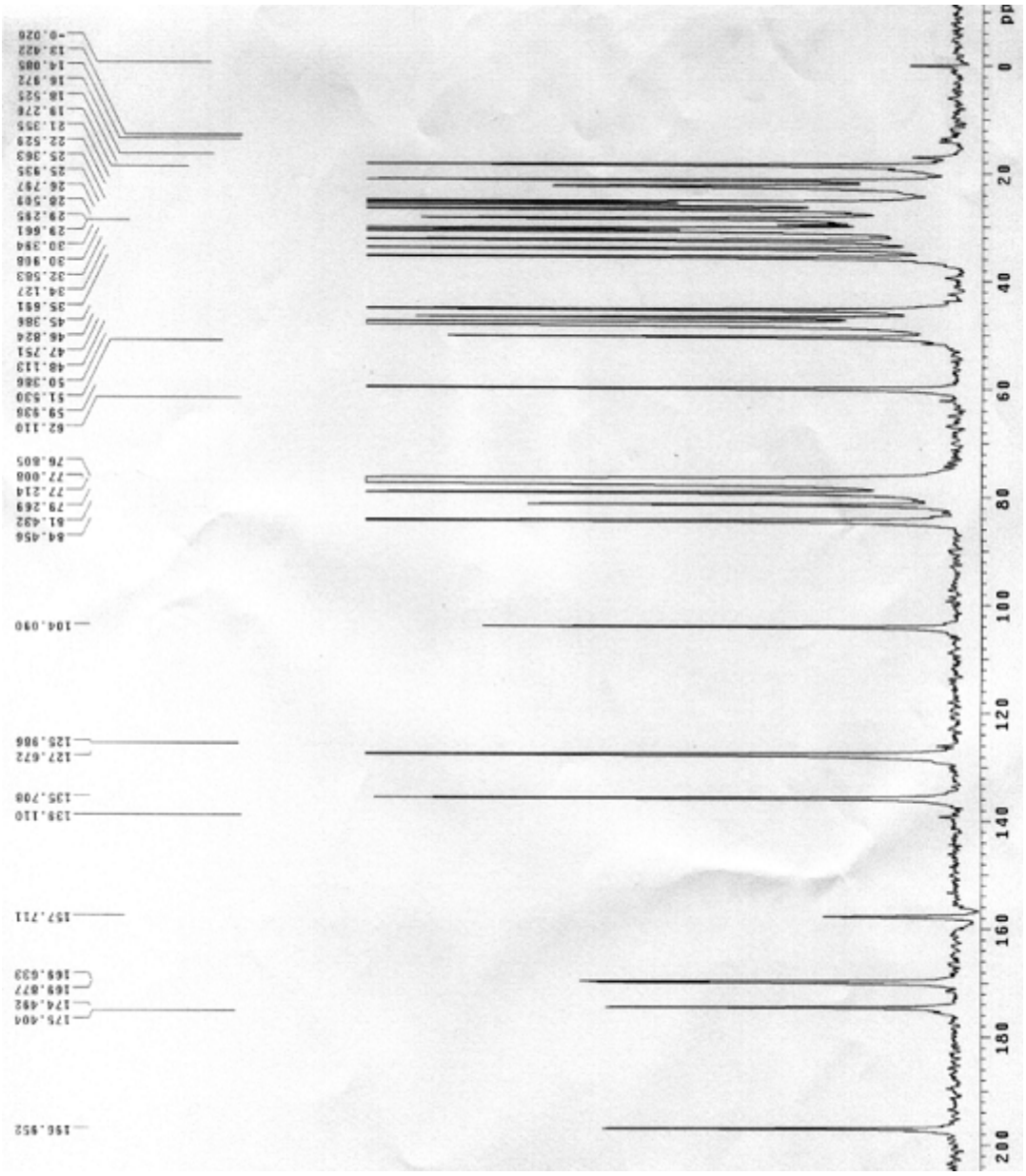
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of schinchinenin A.



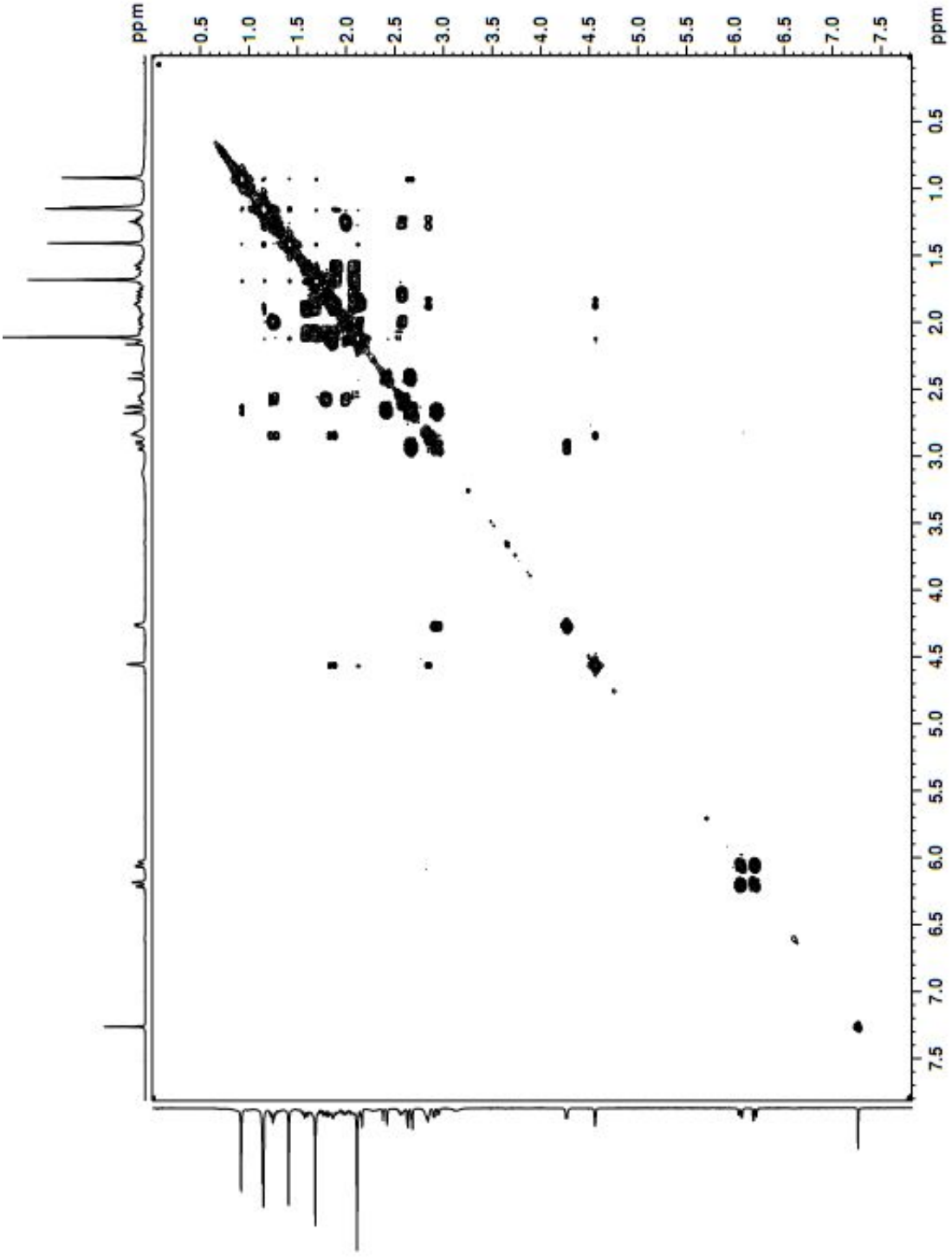
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenin A.



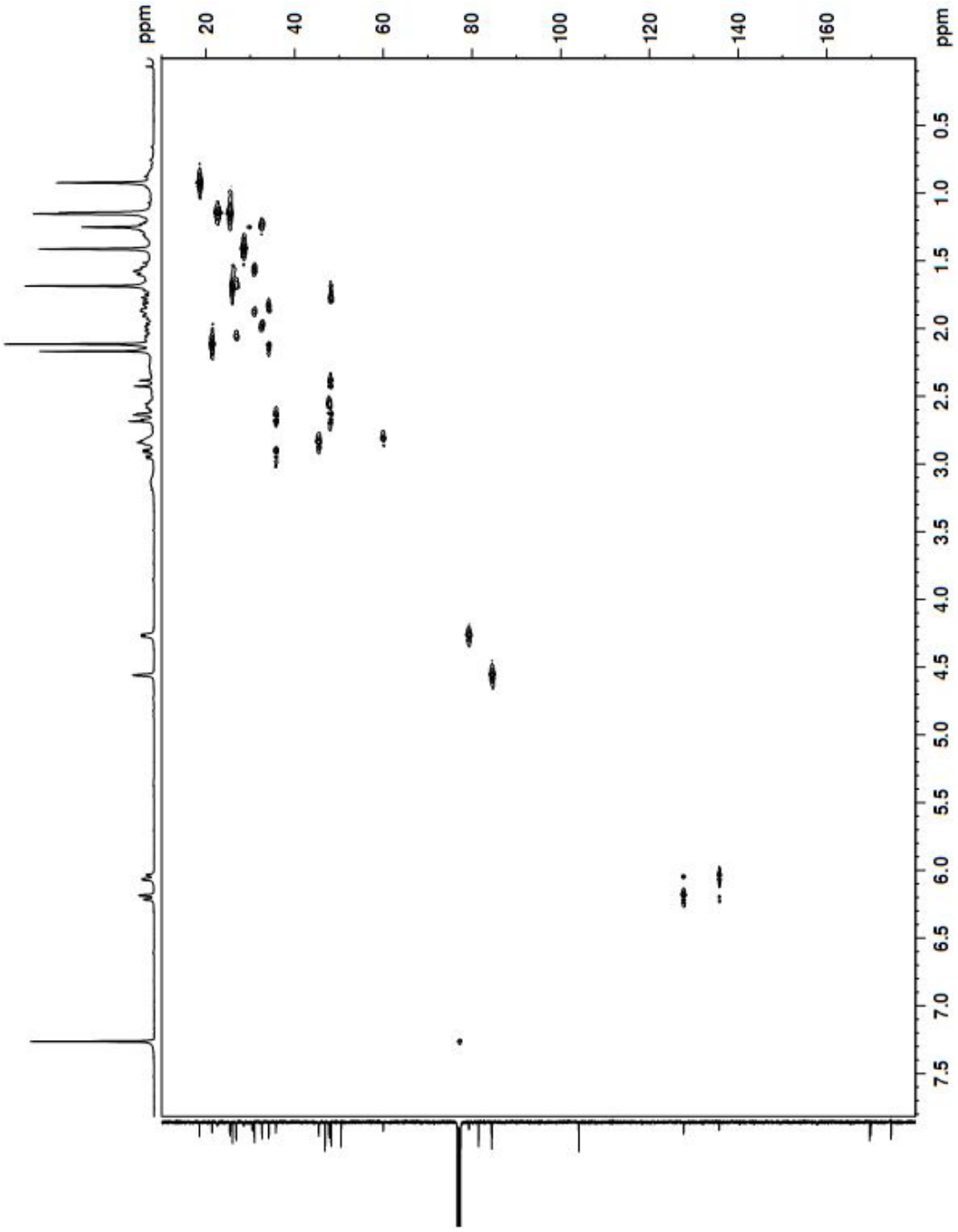
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of schinchinenin A.



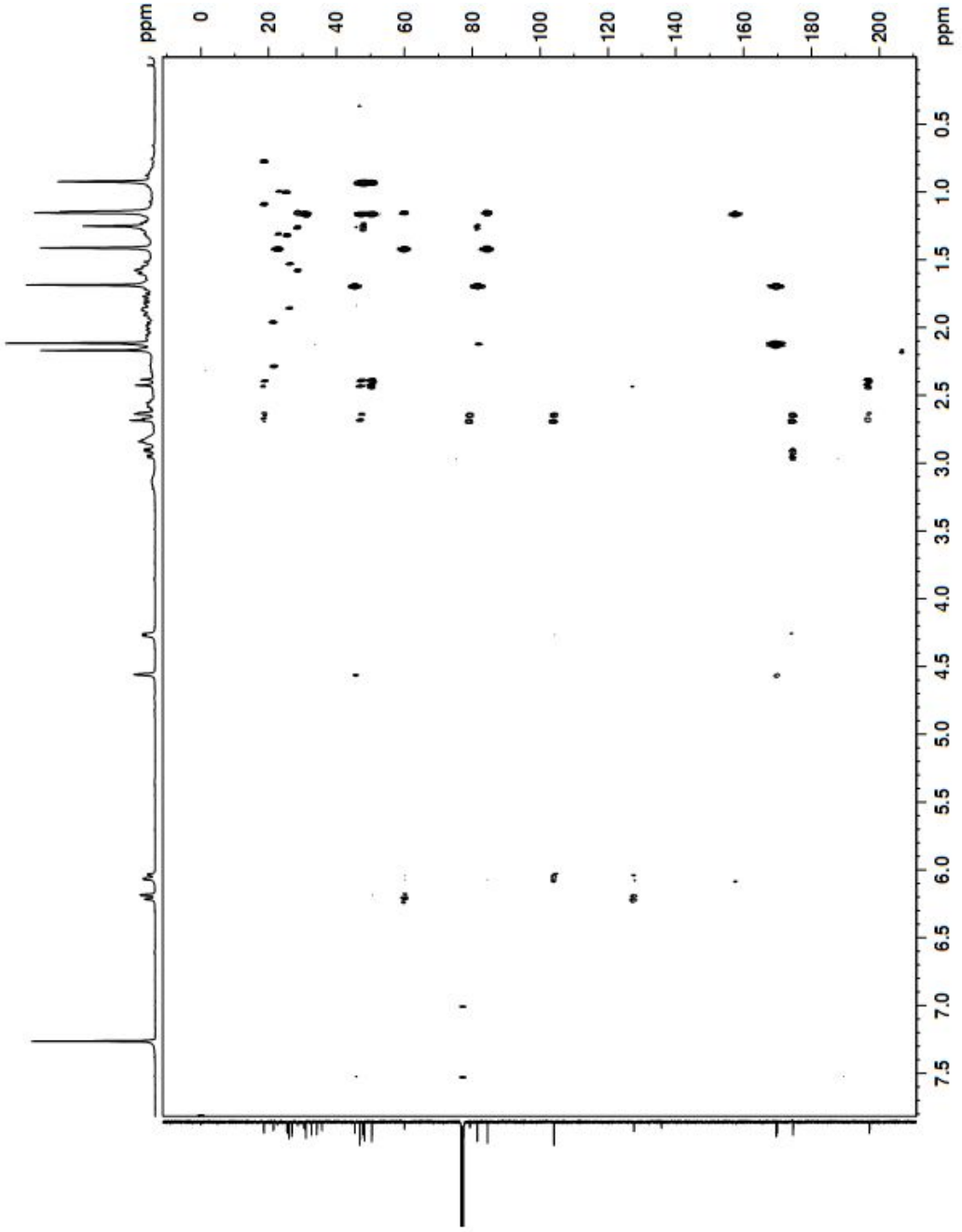
COSY spectrum (400 MHz, $CDCl_3$) of schinchinenin A.



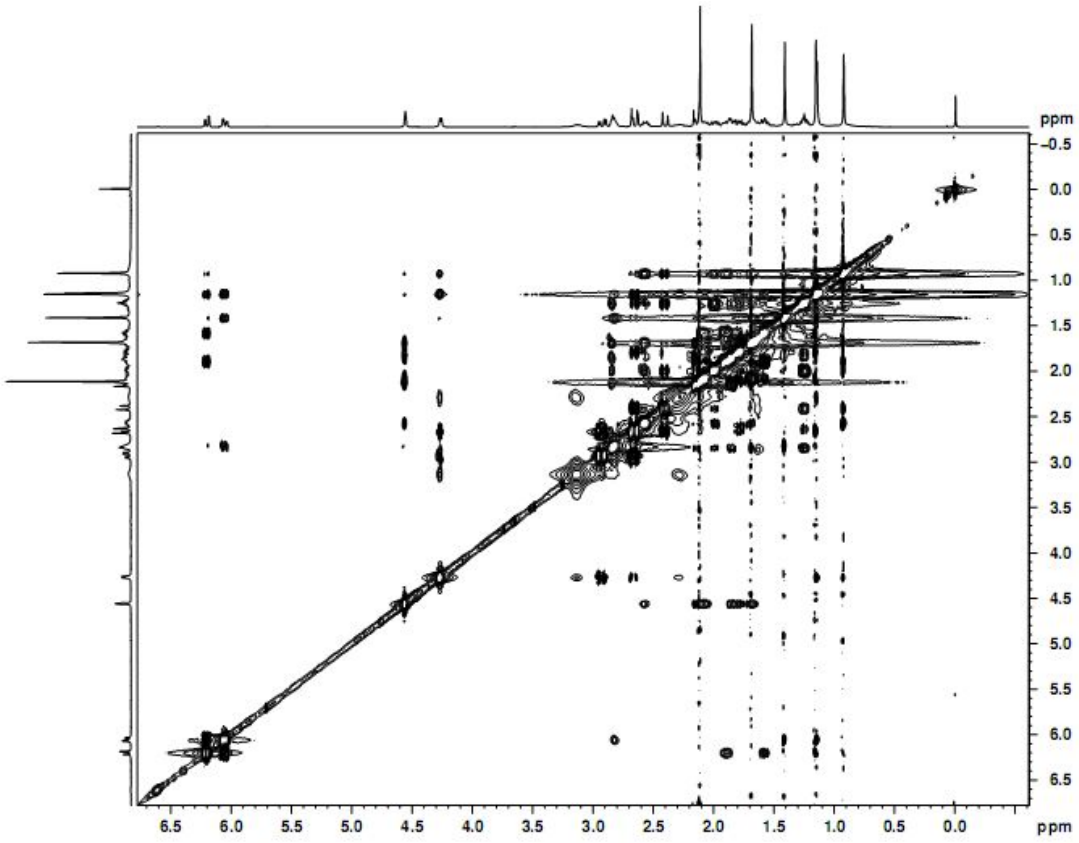
HSQC spectrum (400 MHz, $CDCl_3$) of schinchinenin A.



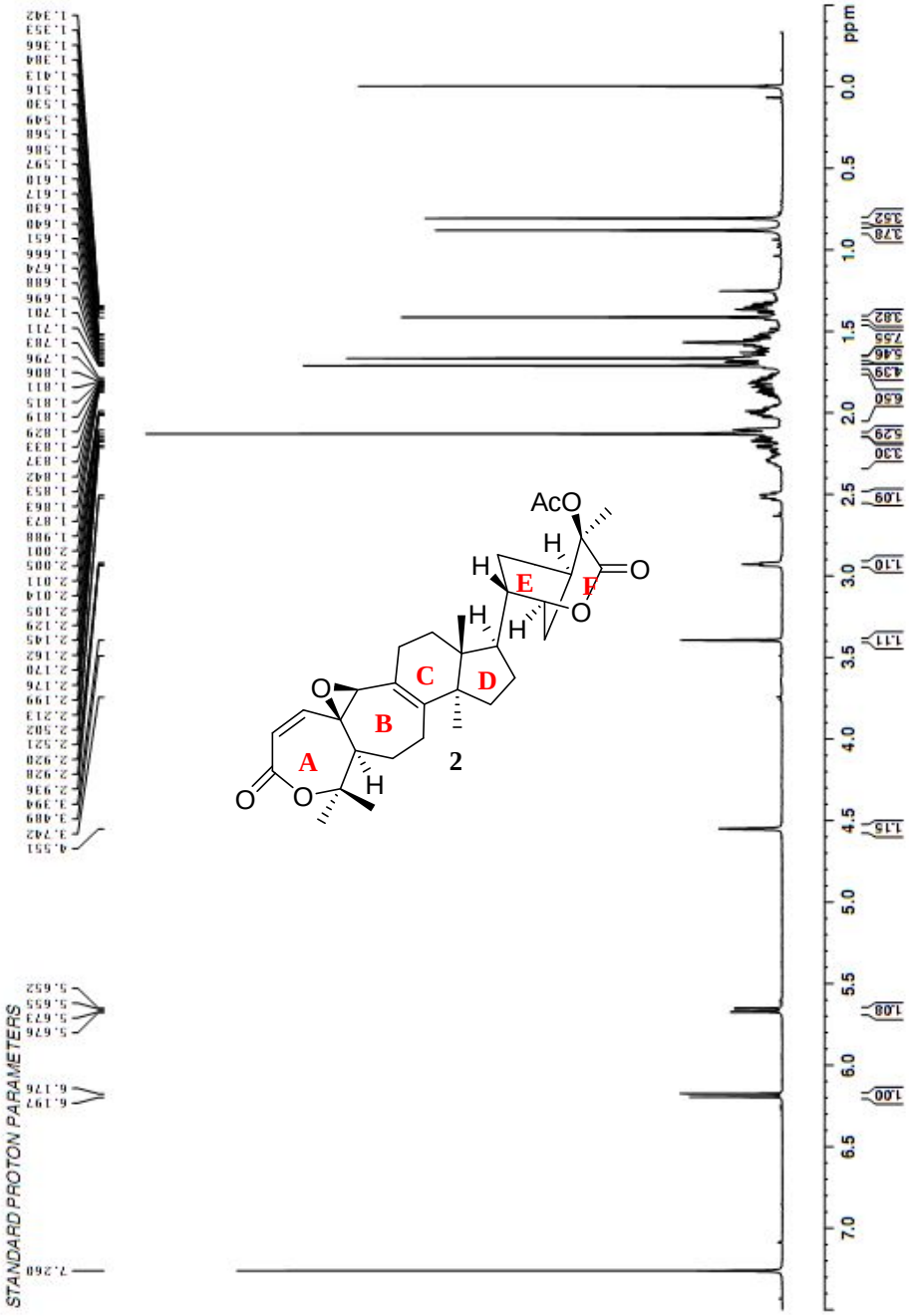
HMBC spectrum (400 MHz, $CDCl_3$) of schinchinenin A.



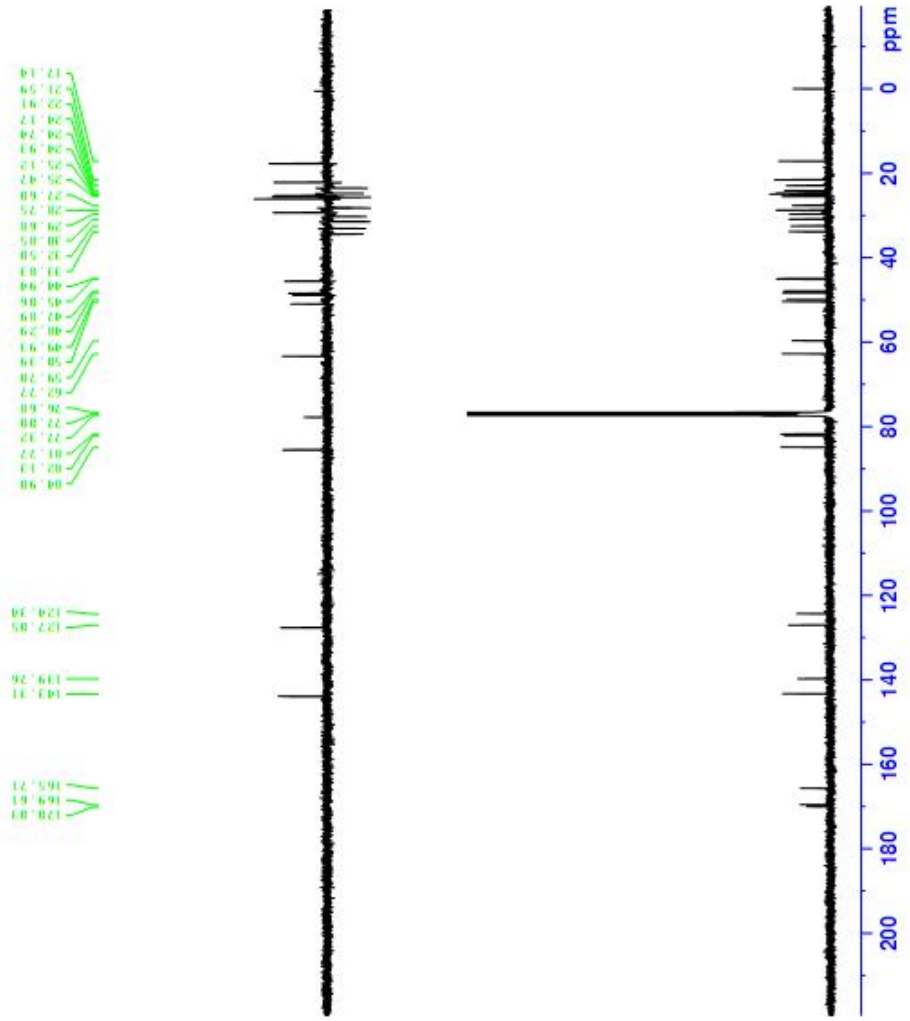
NOESY spectrum (400 MHz, $CDCl_3$) of schinchinenin A.



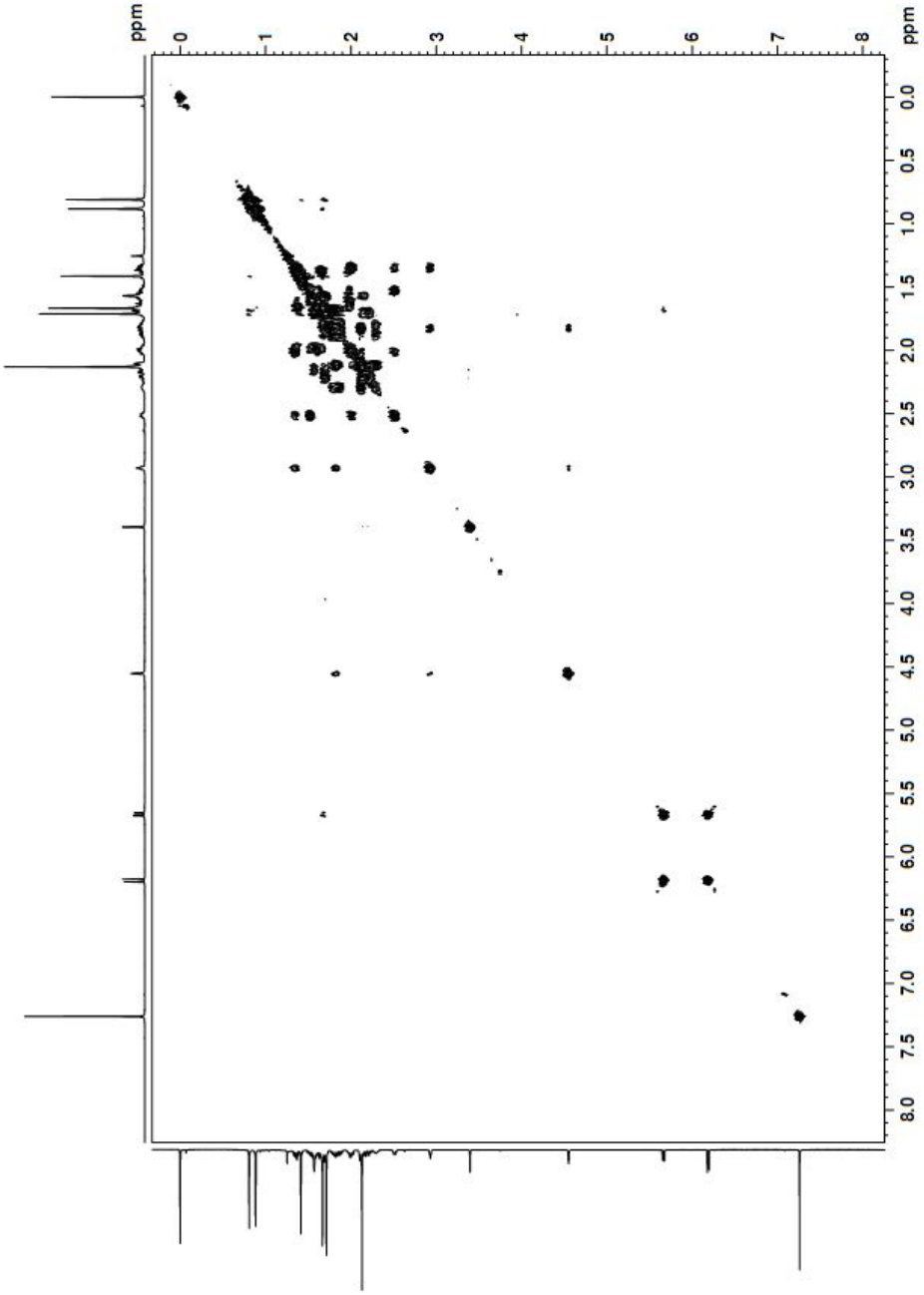
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of schinchinenin B.



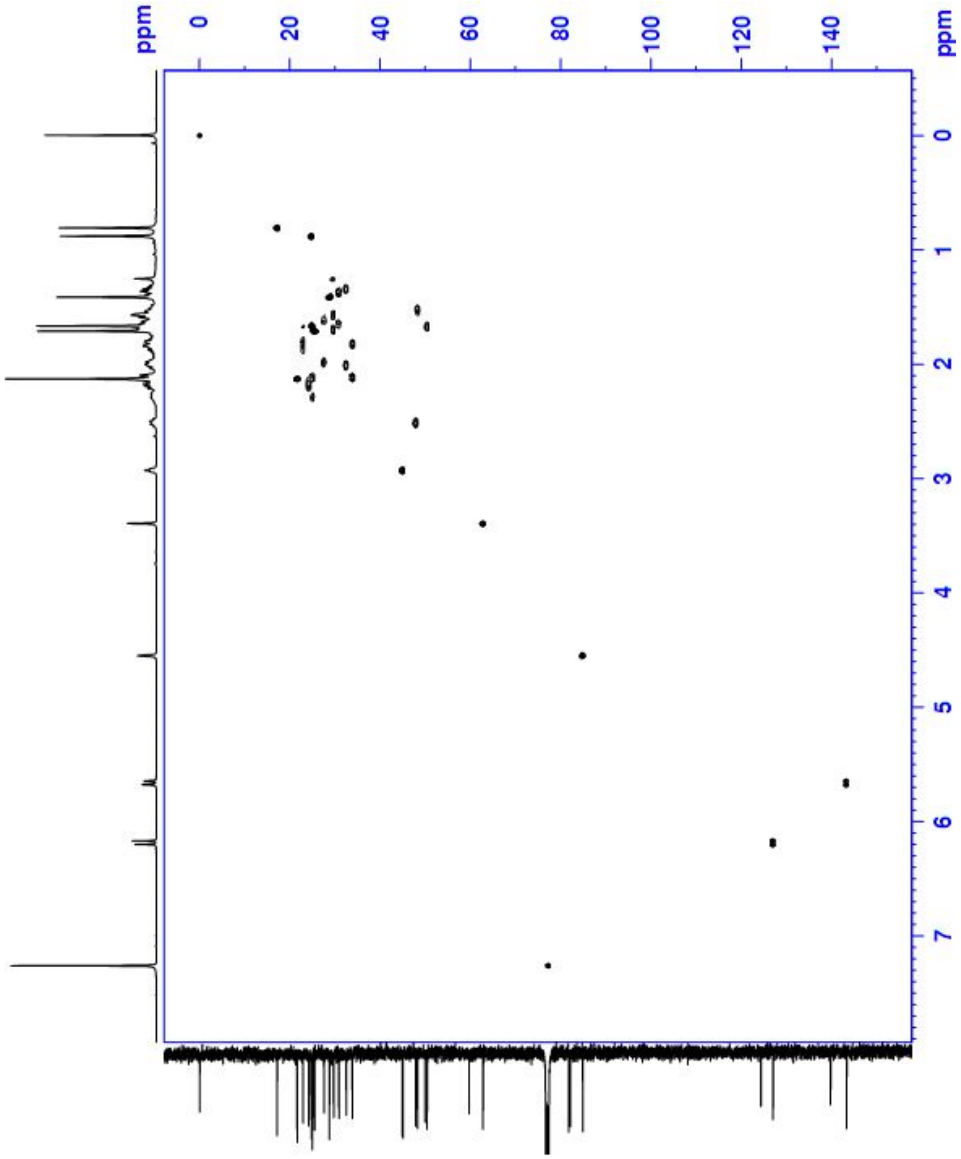
^{13}C NMR spectrum (100, $CDCl_3$) of schinchinenin B.



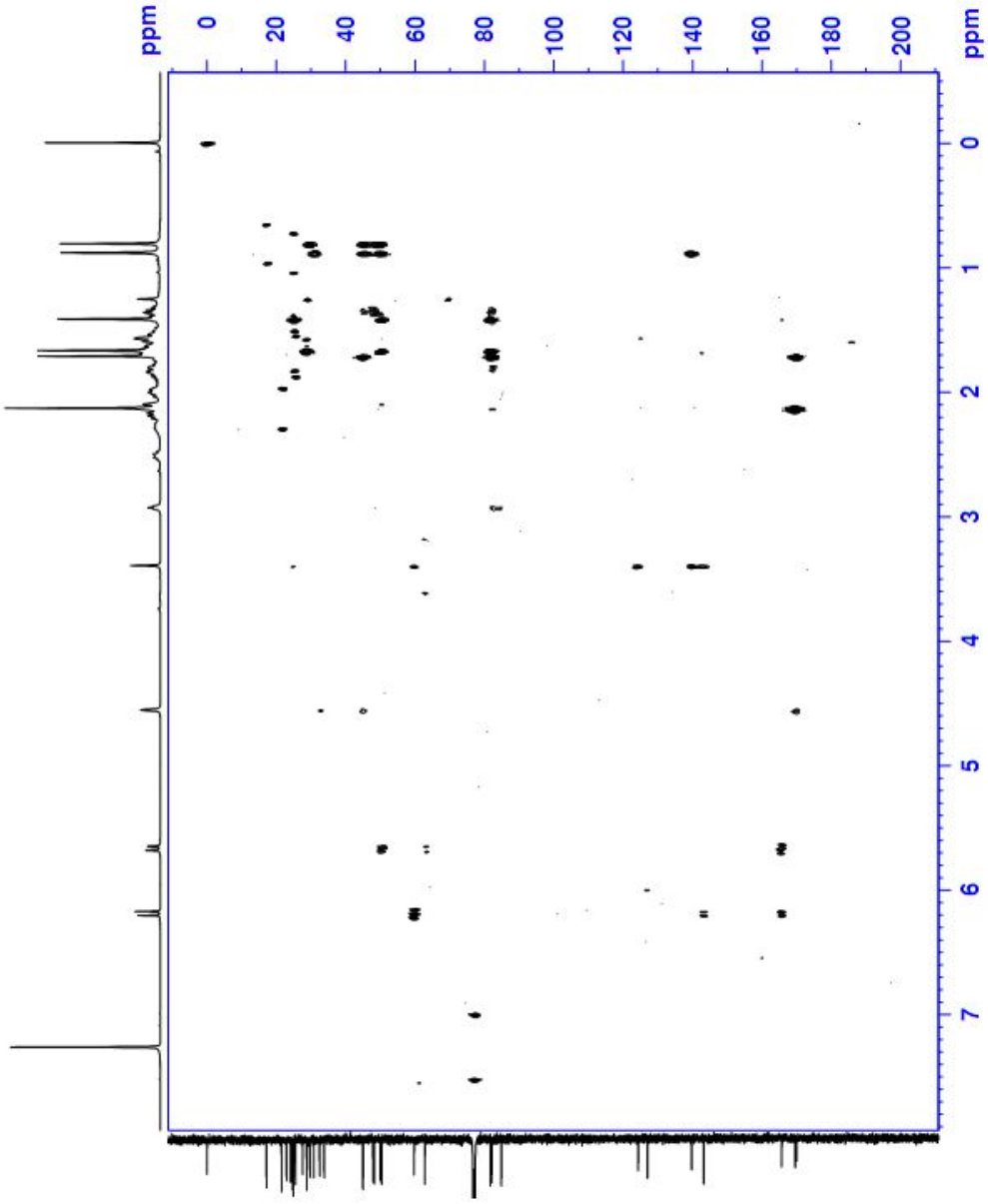
COSY spectrum (400 MHz, $CDCl_3$) of schinchinenin B.



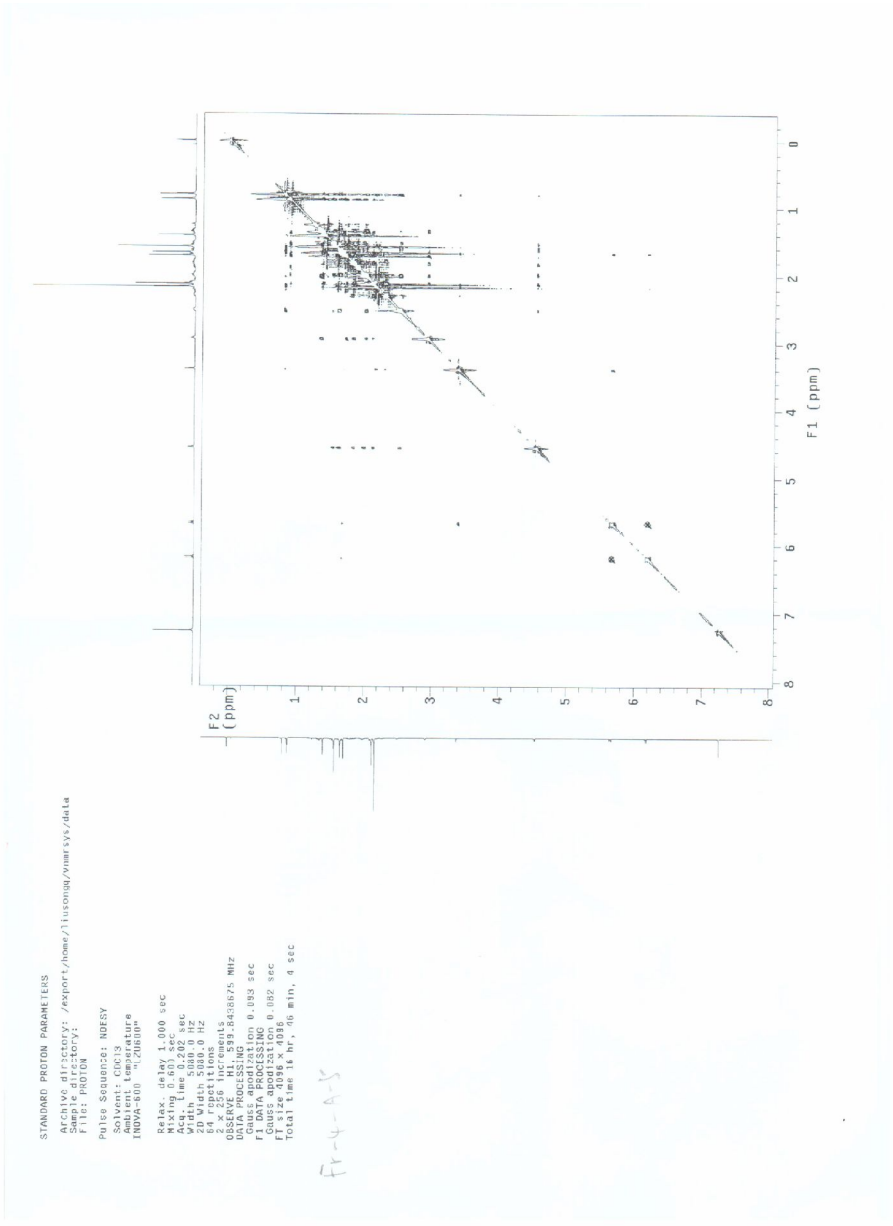
HSQC spectrum (400 MHz, $CDCl_3$) of schinchinenin B.



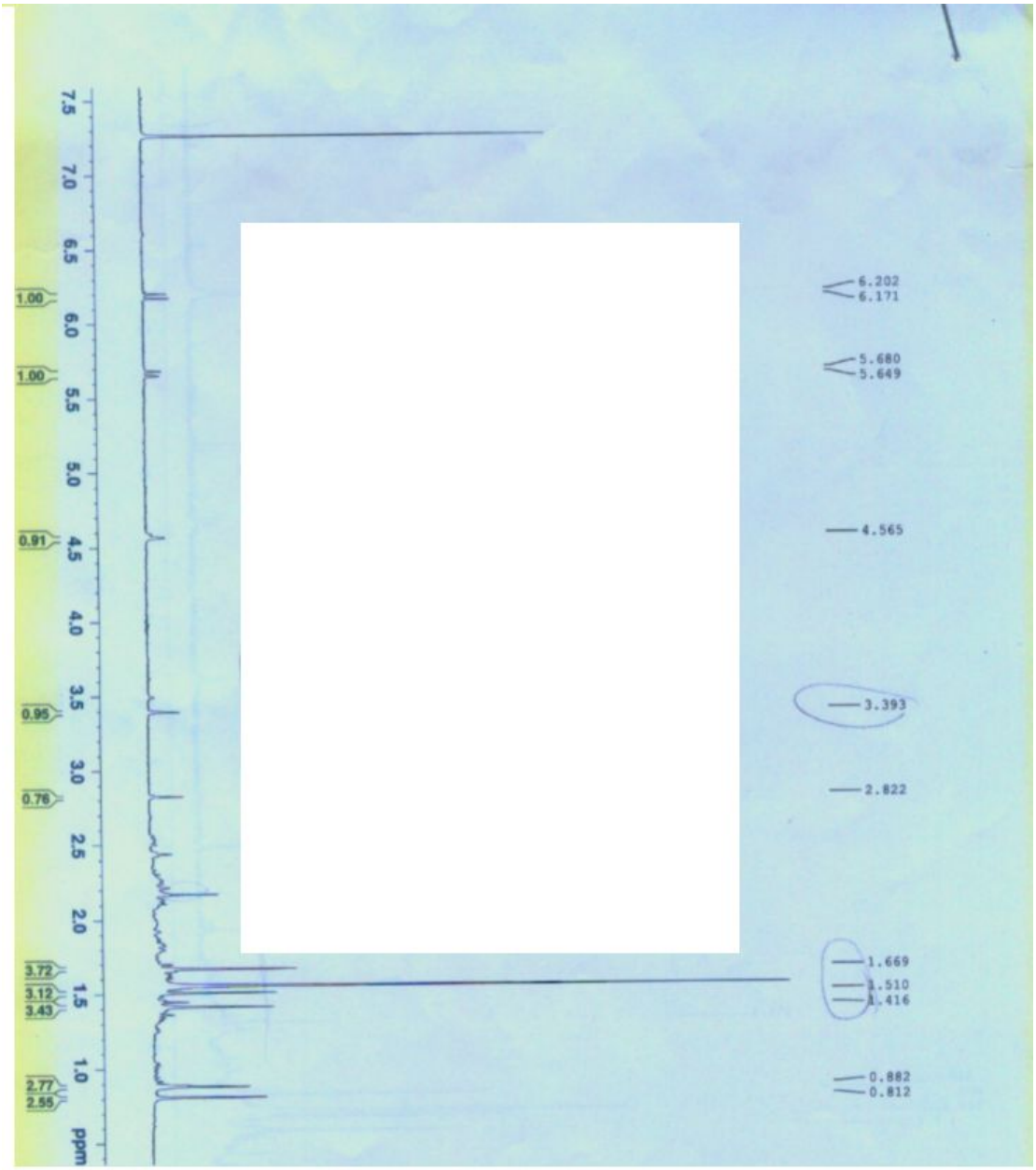
HMBC spectrum (400 MHz, $CDCl_3$) of schinchinenin B.



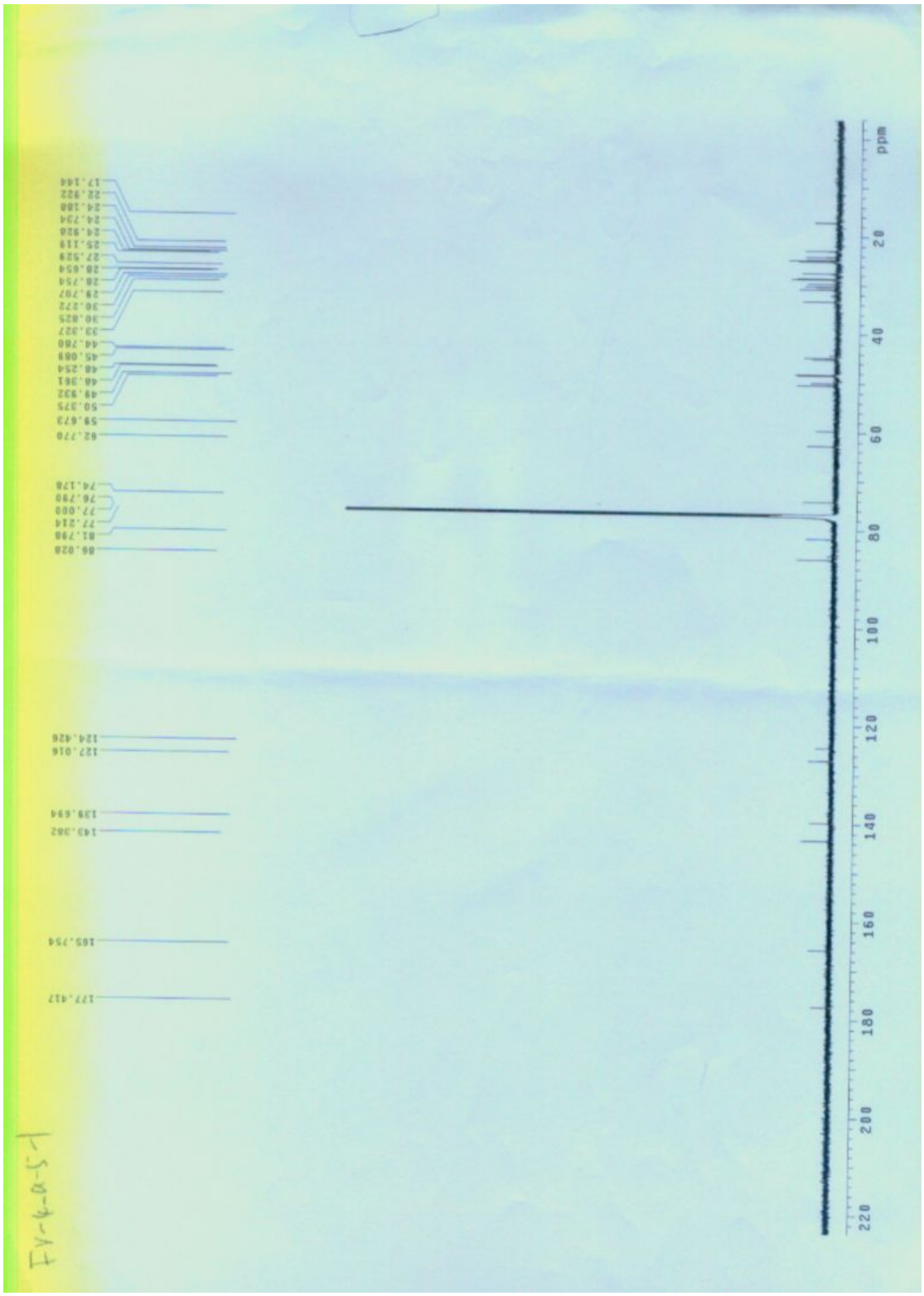
NOESY spectrum (600 MHz, $CDCl_3$) of schinchinenin B.



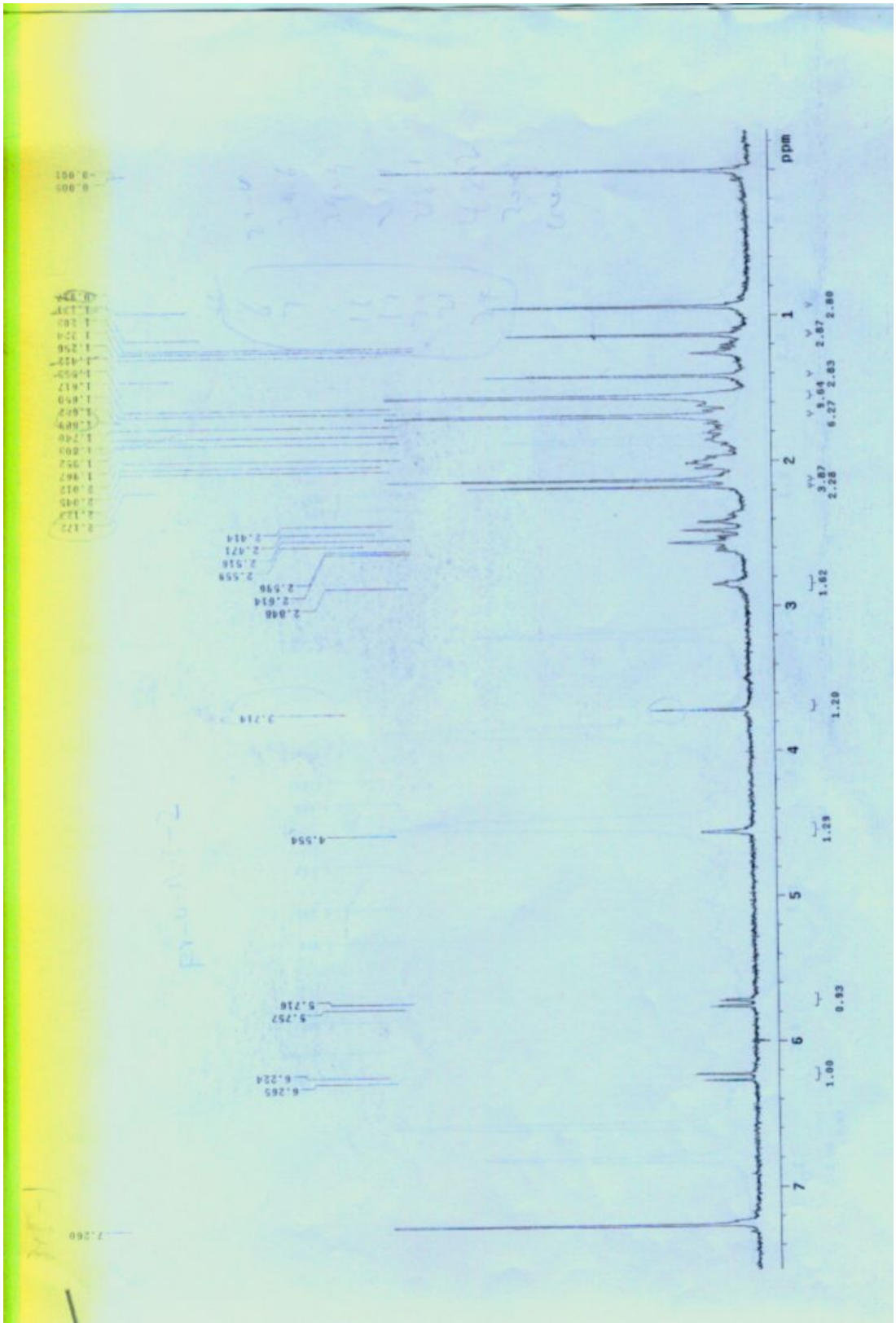
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of schinchinenin C.



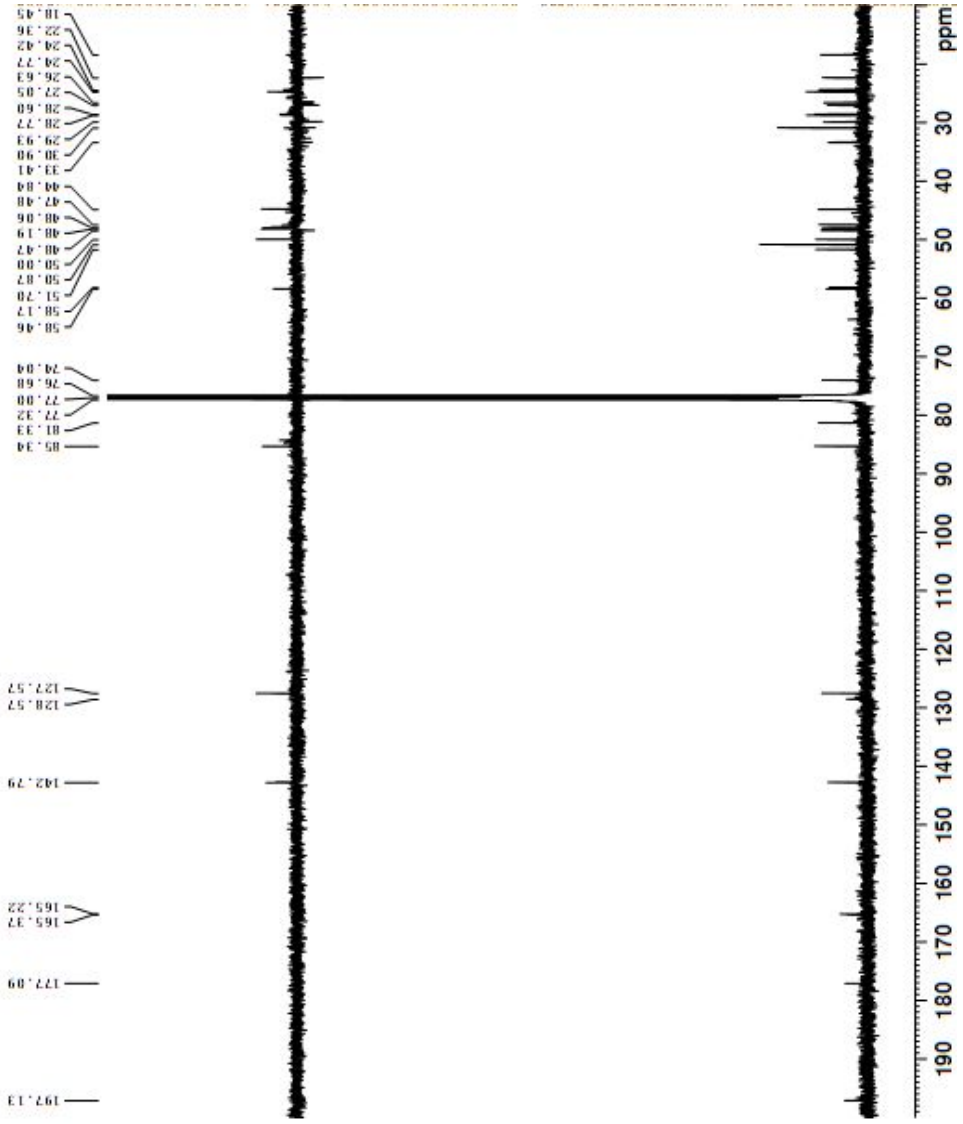
^{13}C NMR spectrum (600 MHz, $CDCl_3$) of schinchinenin C.



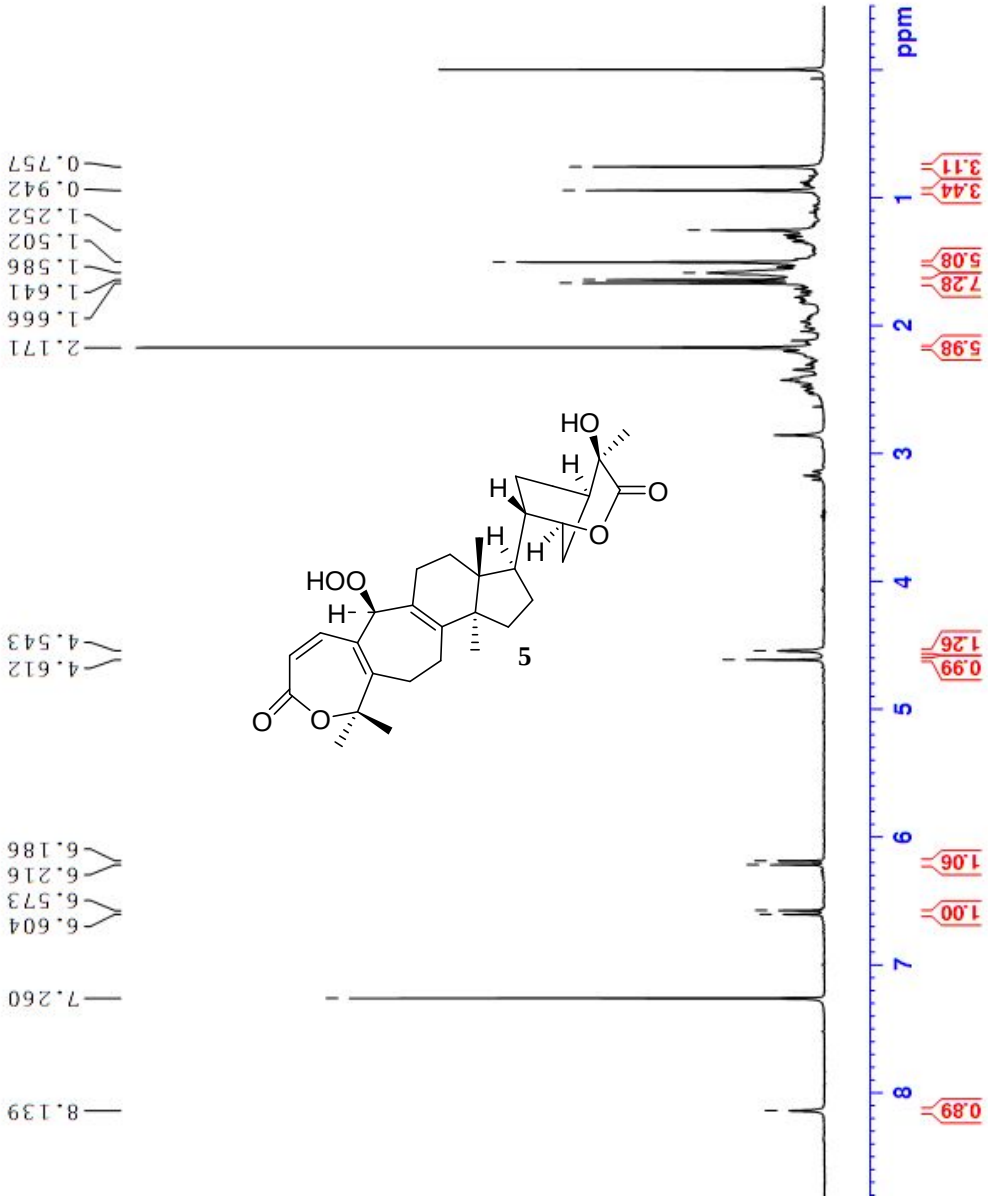
^{1}H NMR spectrum (300 MHz, $CDCl_3$) of schinchinenin D.



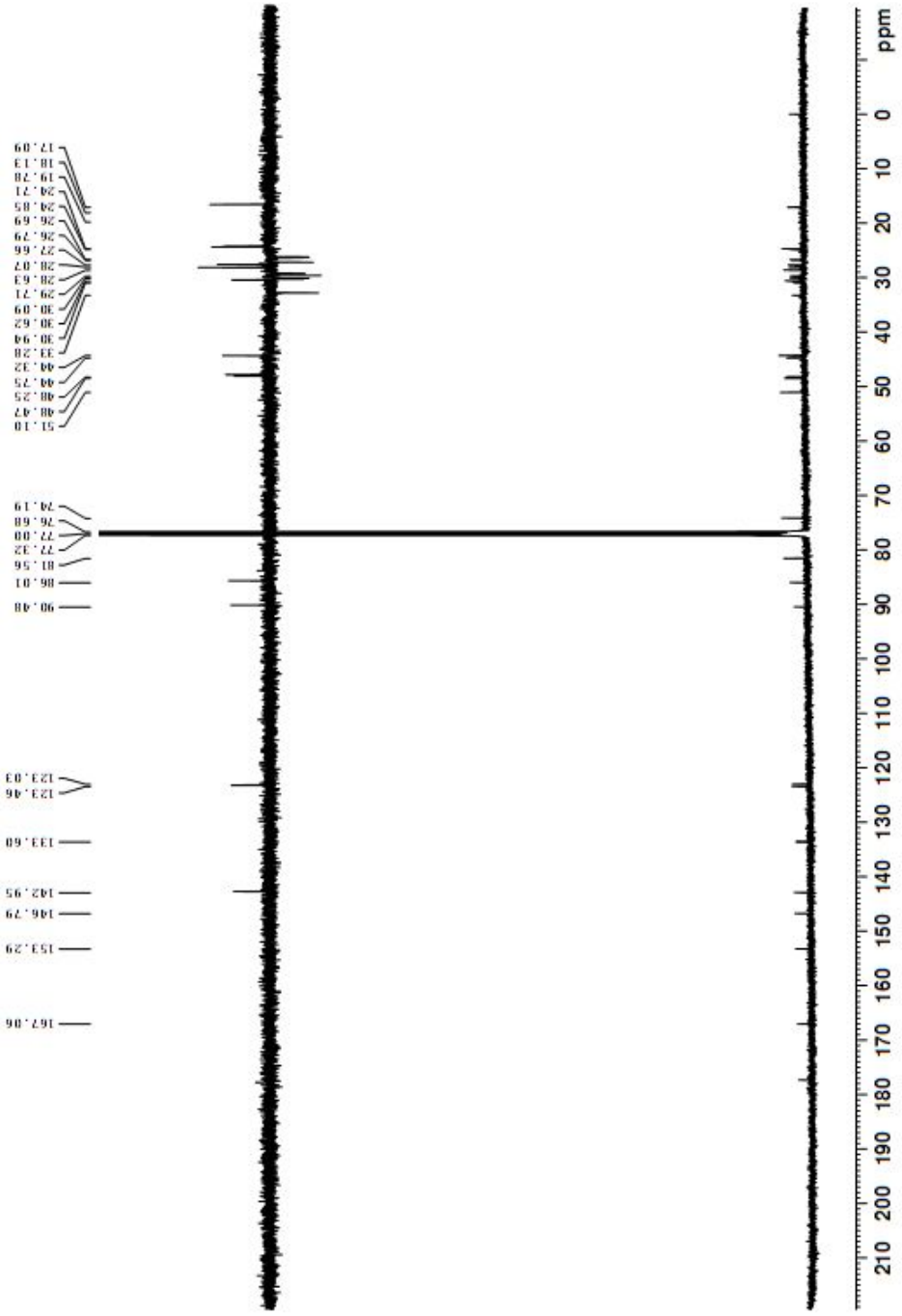
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenin D.



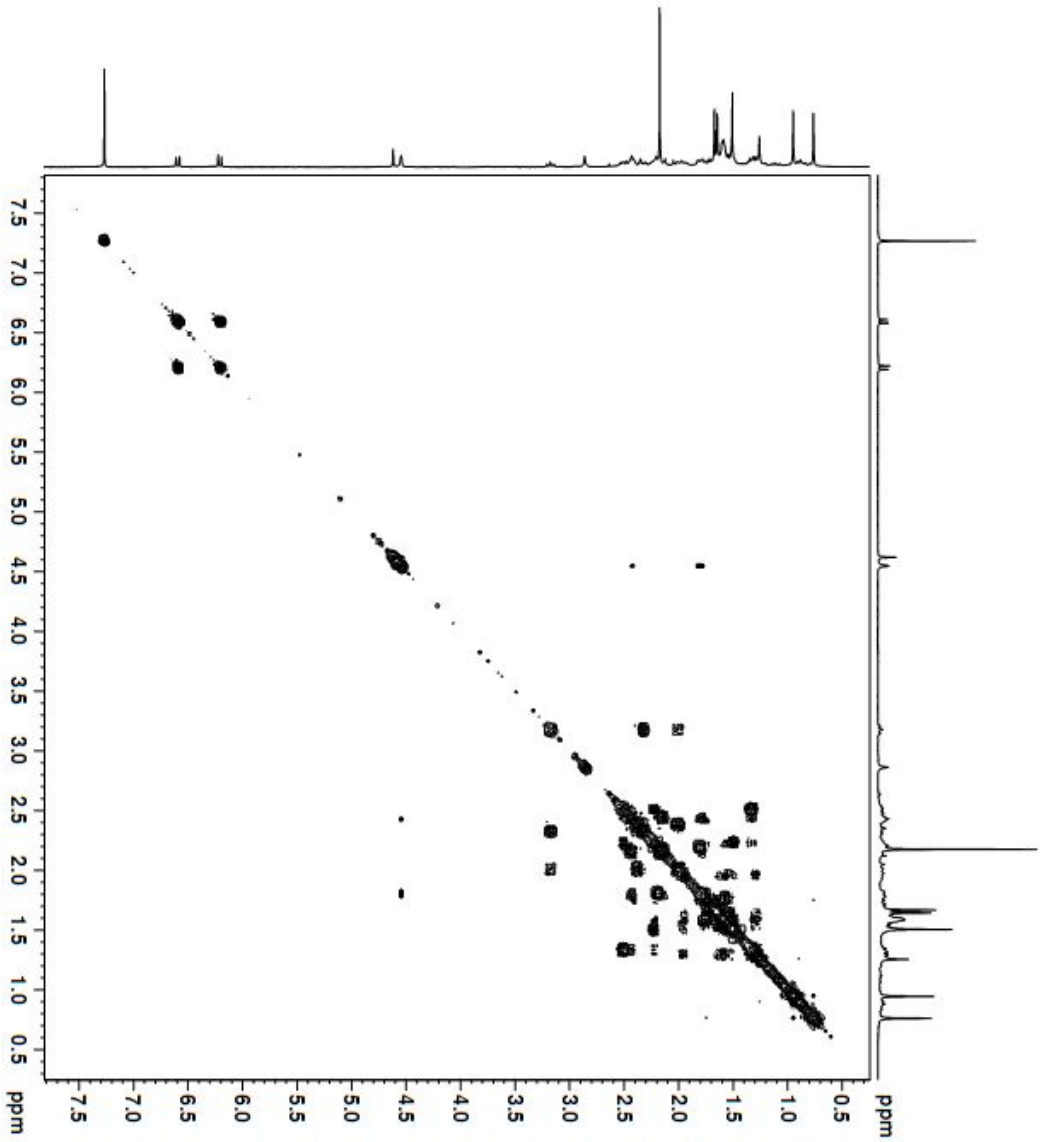
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of schinchinenin E.



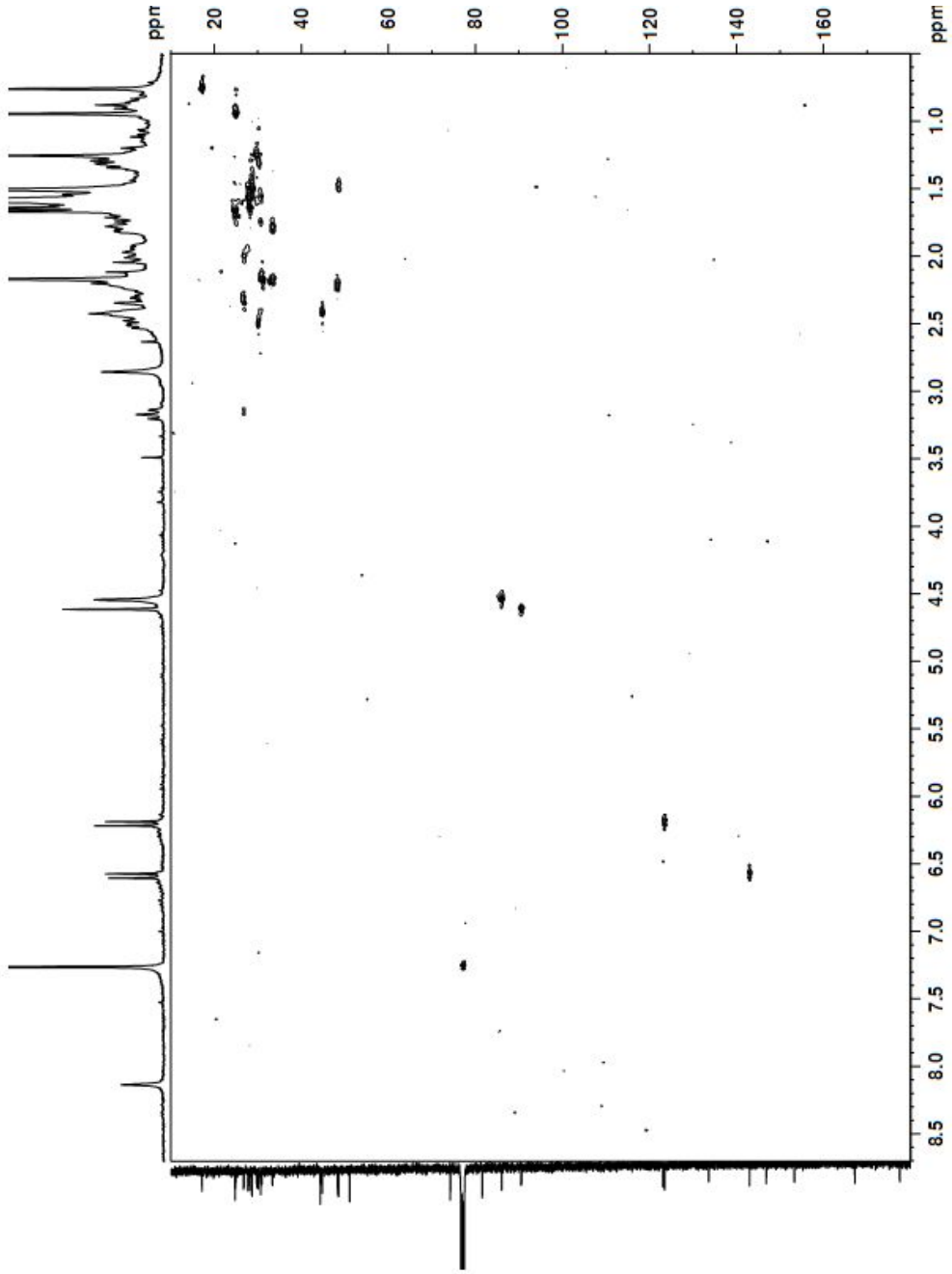
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenin E.



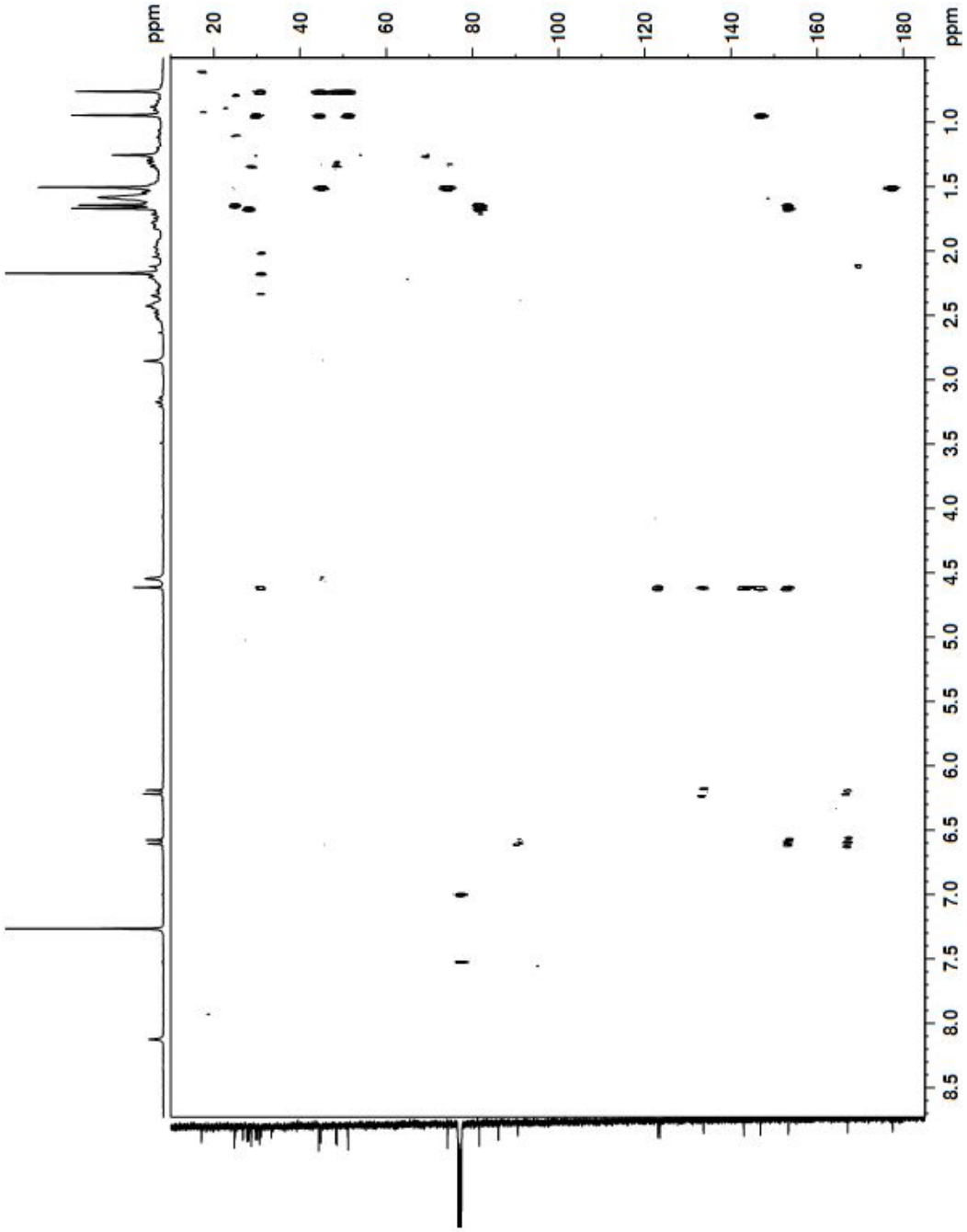
COSY spectrum (400 MHz, $CDCl_3$) of schinchinenin E.



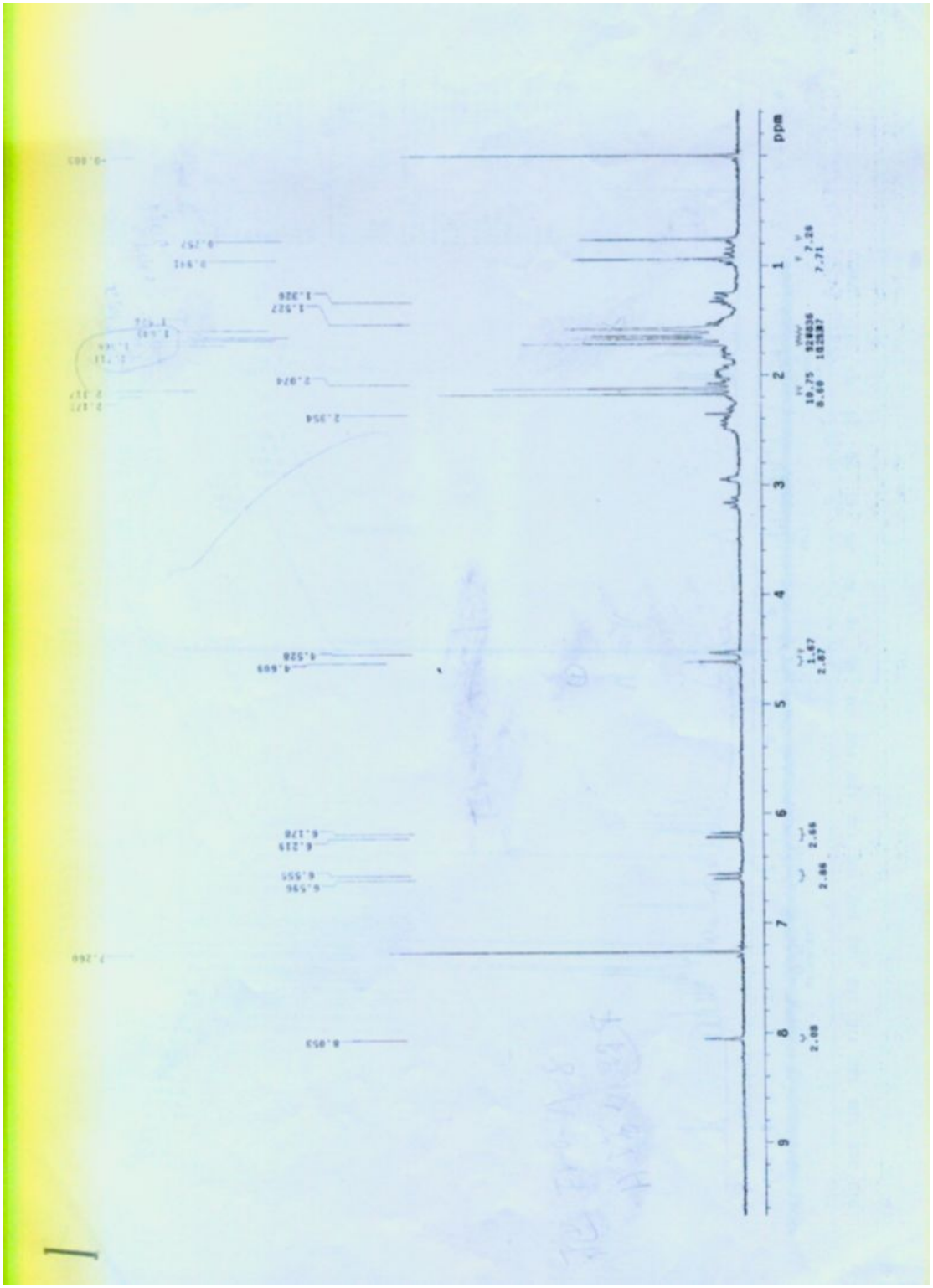
HSQC spectrum (400 MHz, $CDCl_3$) of schinchinenin E.



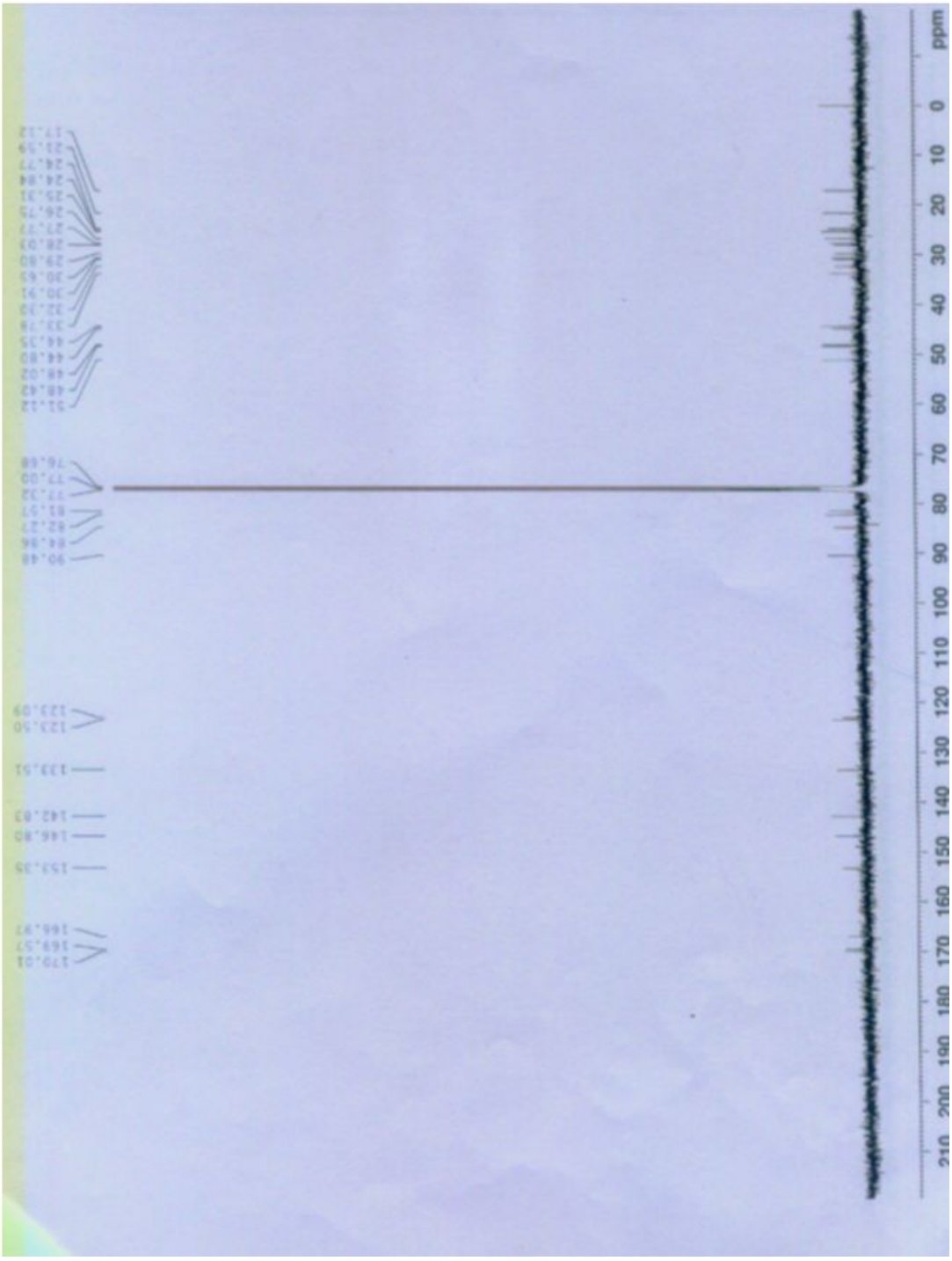
HMBC spectrum (400 MHz, $CDCl_3$) of schinchinenin E.



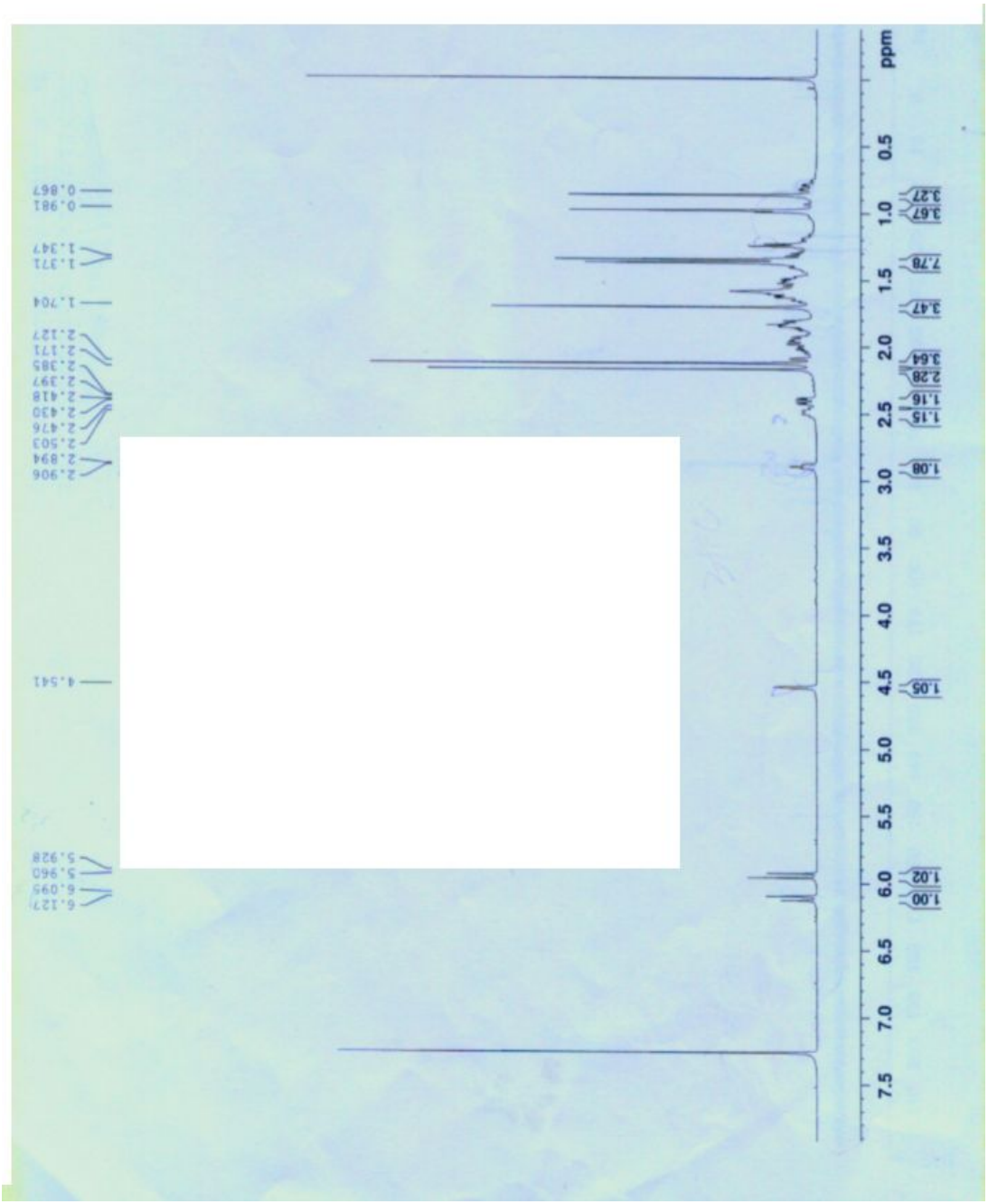
^{1}H NMR spectrum (300 MHz, $CDCl_3$) of schinchinenlactone F.



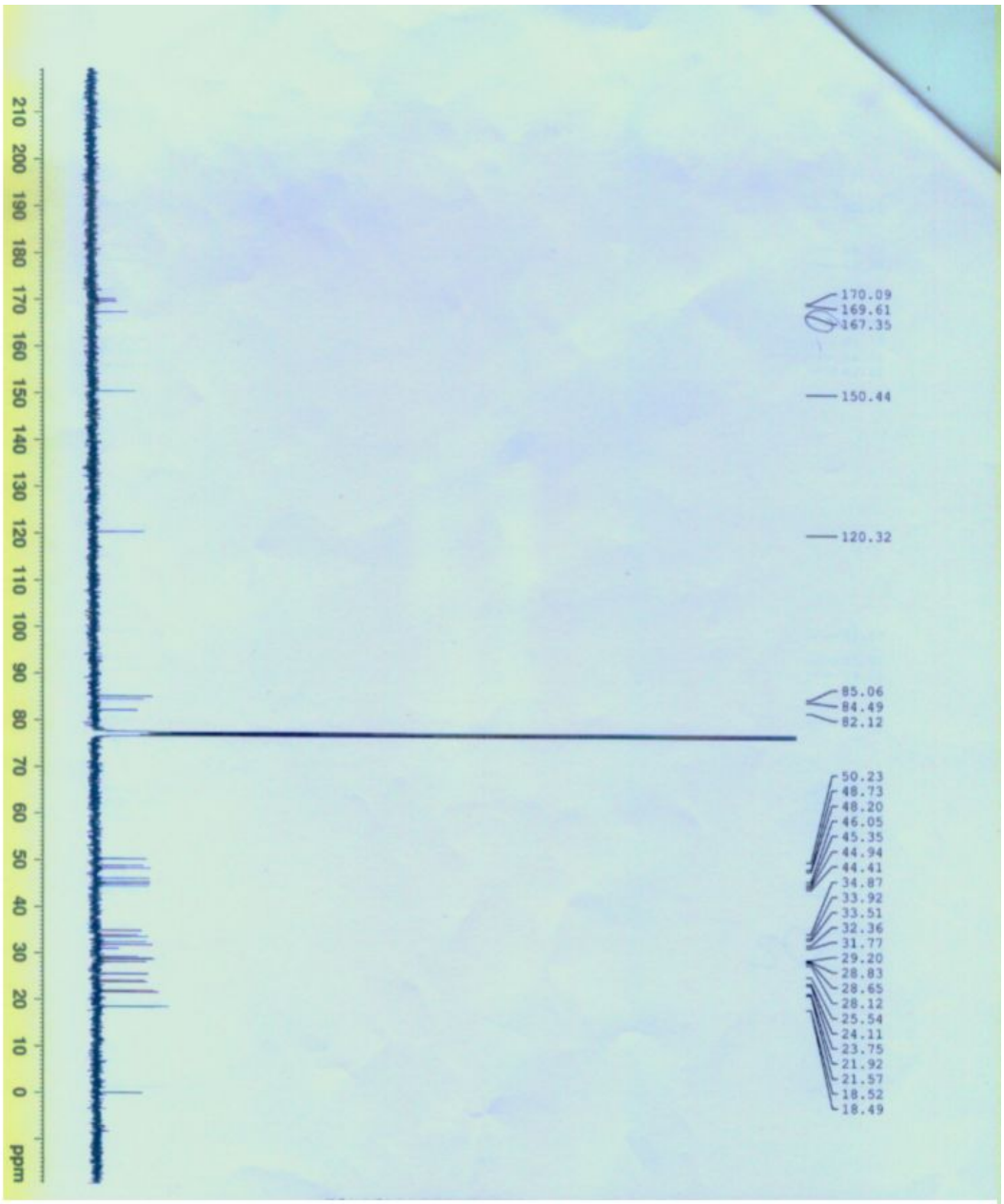
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenlactone F.



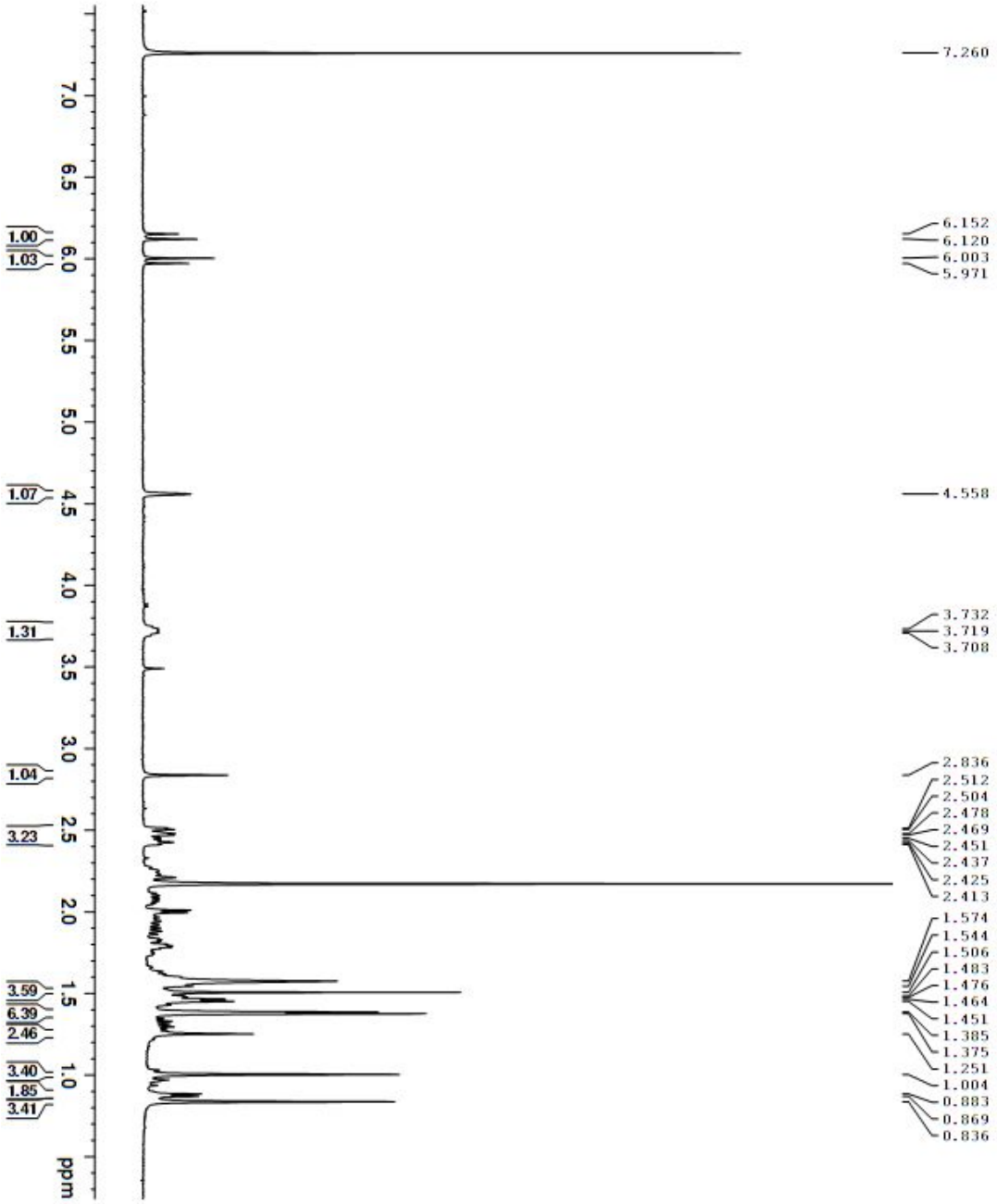
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of schinchinenlactone G.



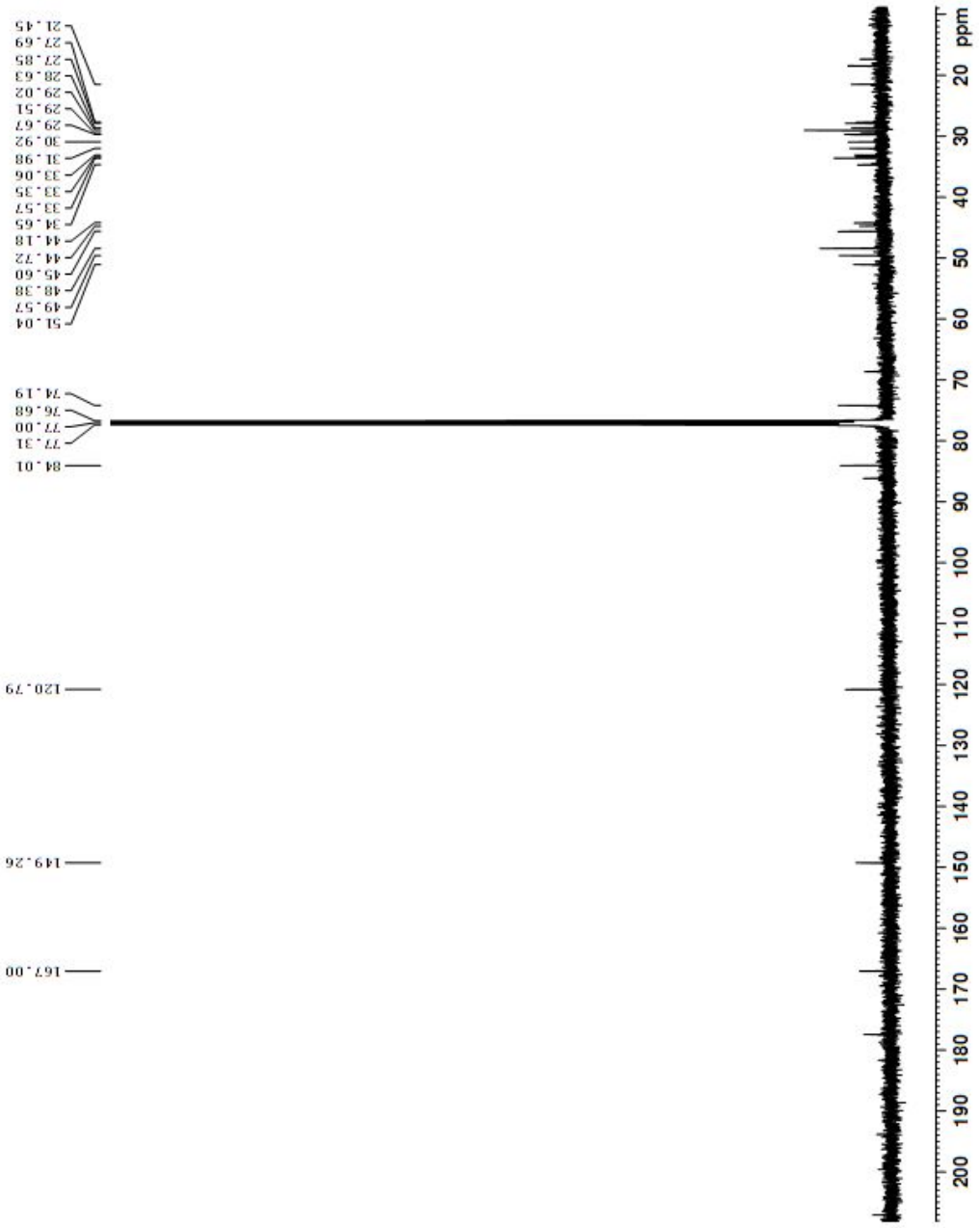
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenlactone G.



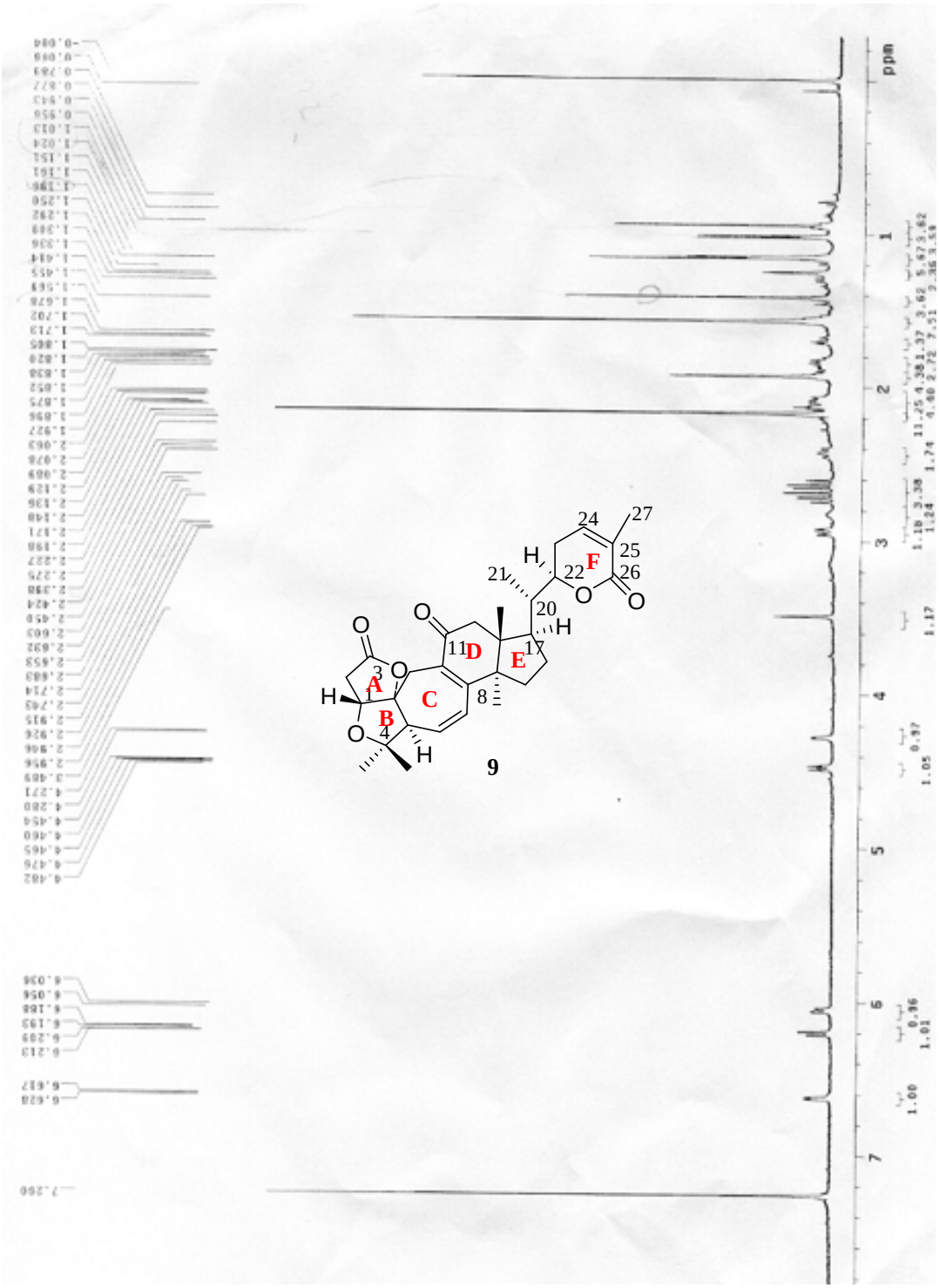
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of schinchinenlactone H.



^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenlactone H.



^{1}H NMR spectrum (600 MHz, $CDCl_3$) of schinchinenlactone A.



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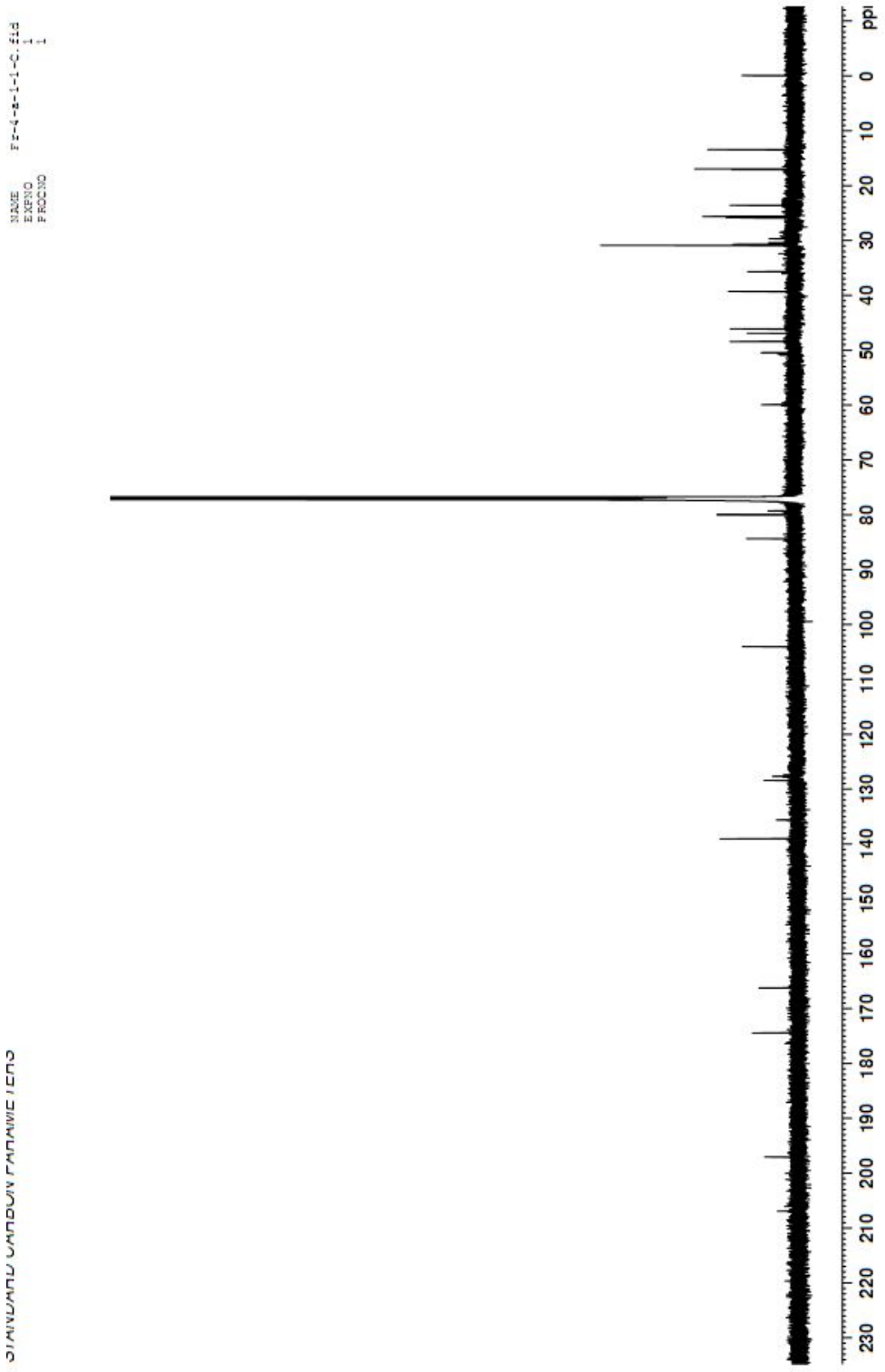
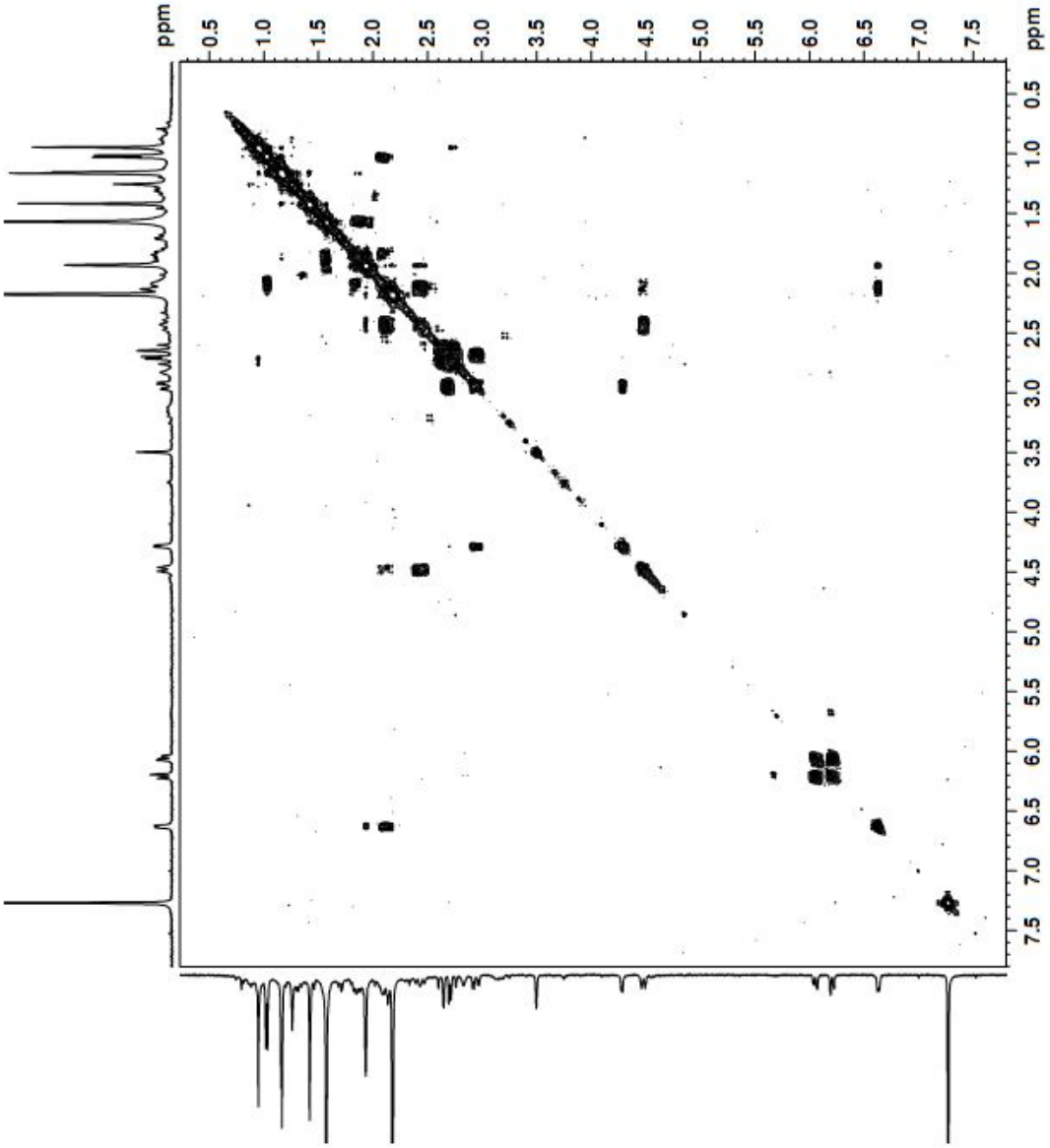
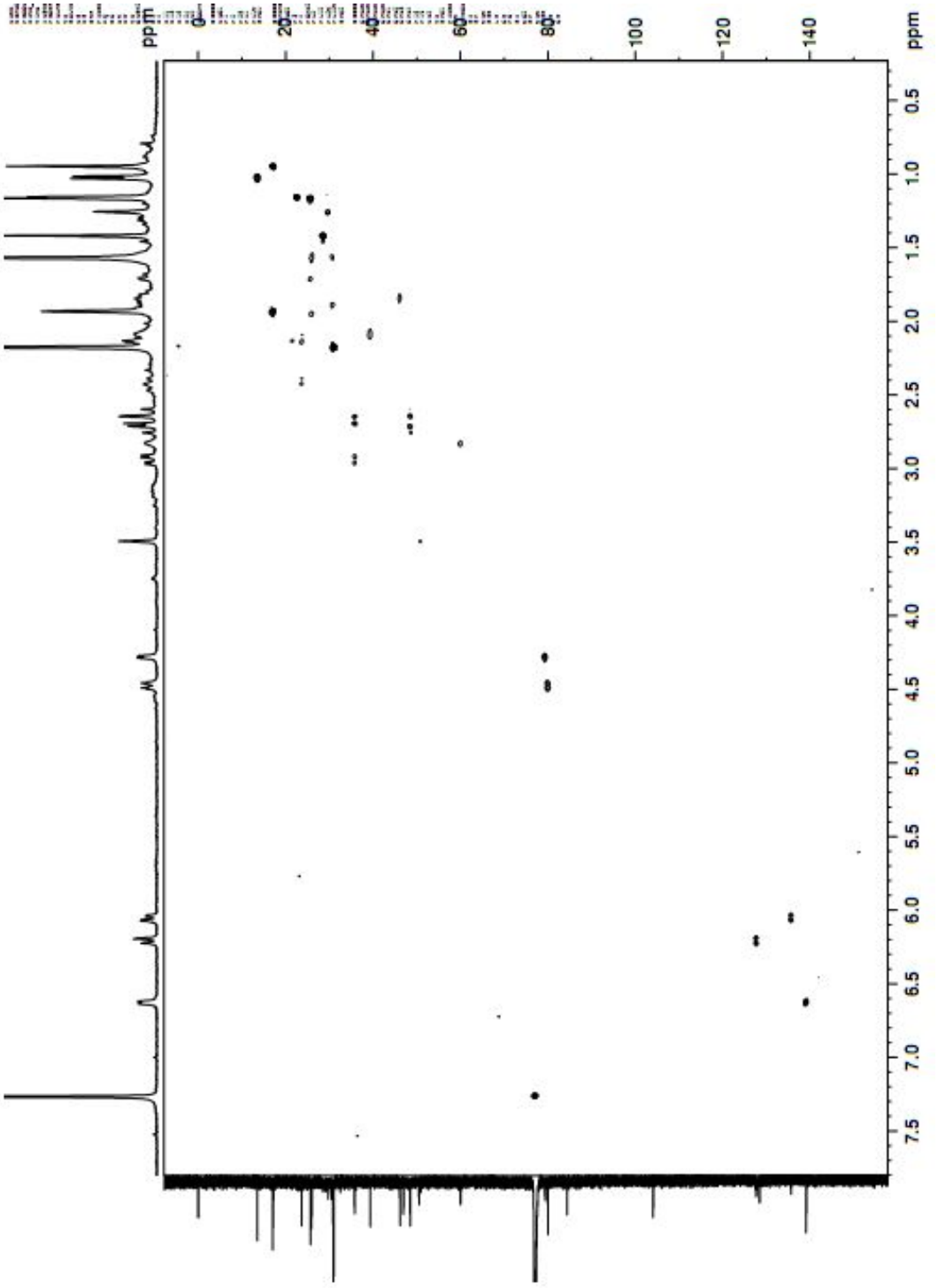
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of schinchinenlactone A.



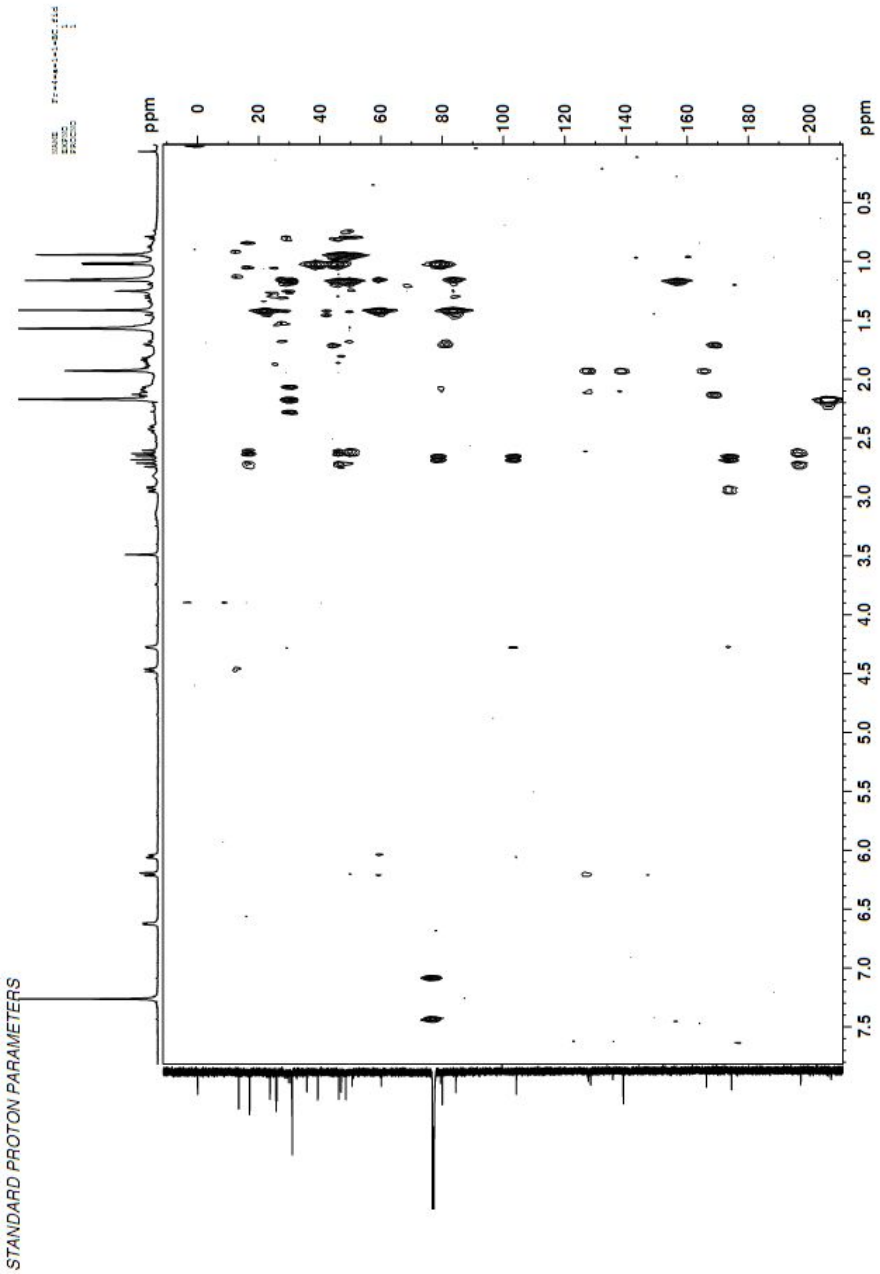
COSY spectrum (400 MHz, $CDCl_3$) of schinchinenlactone A.



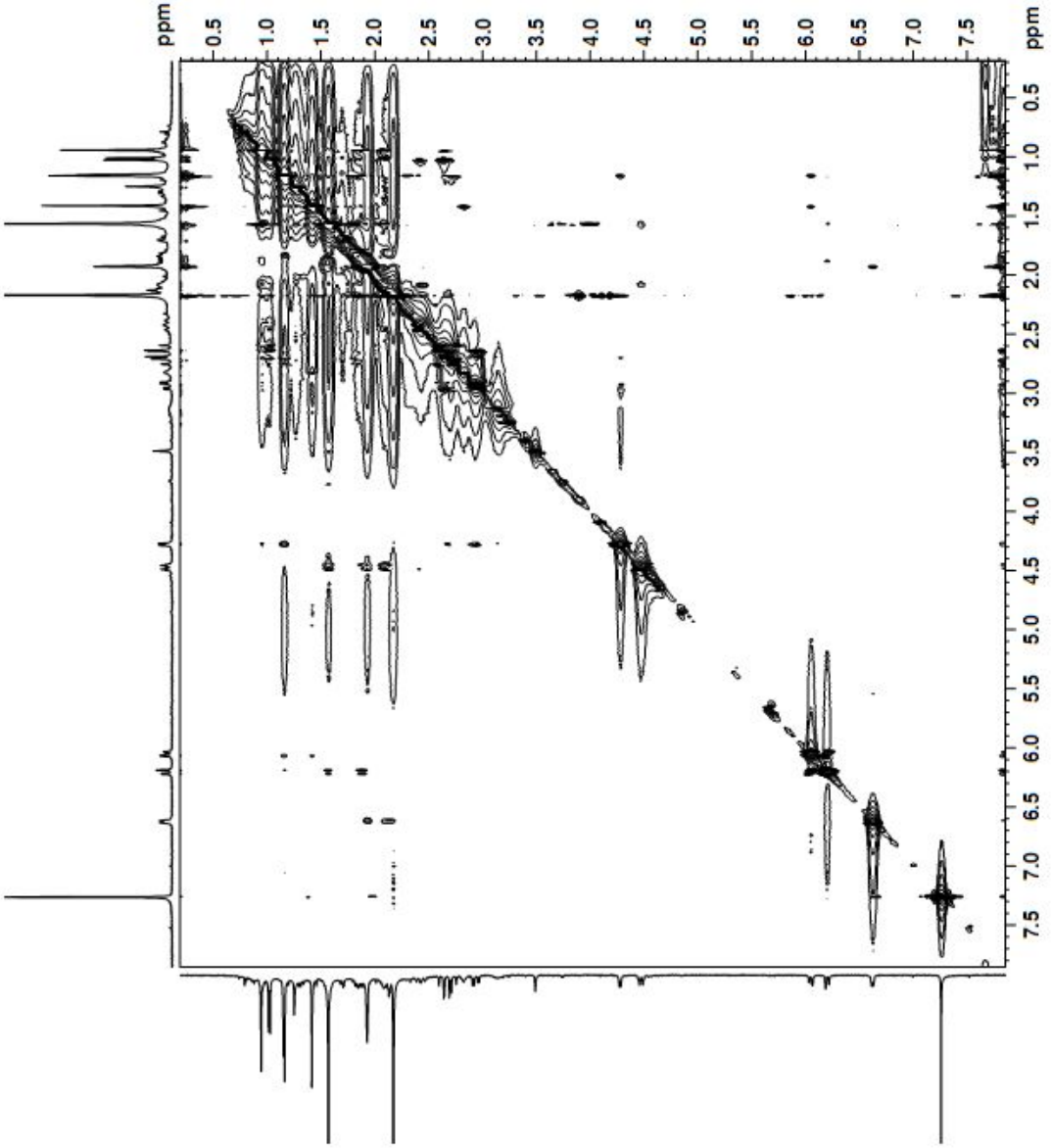
HMQC spectrum (400 MHz, $CDCl_3$) of schinchinenlactone A.



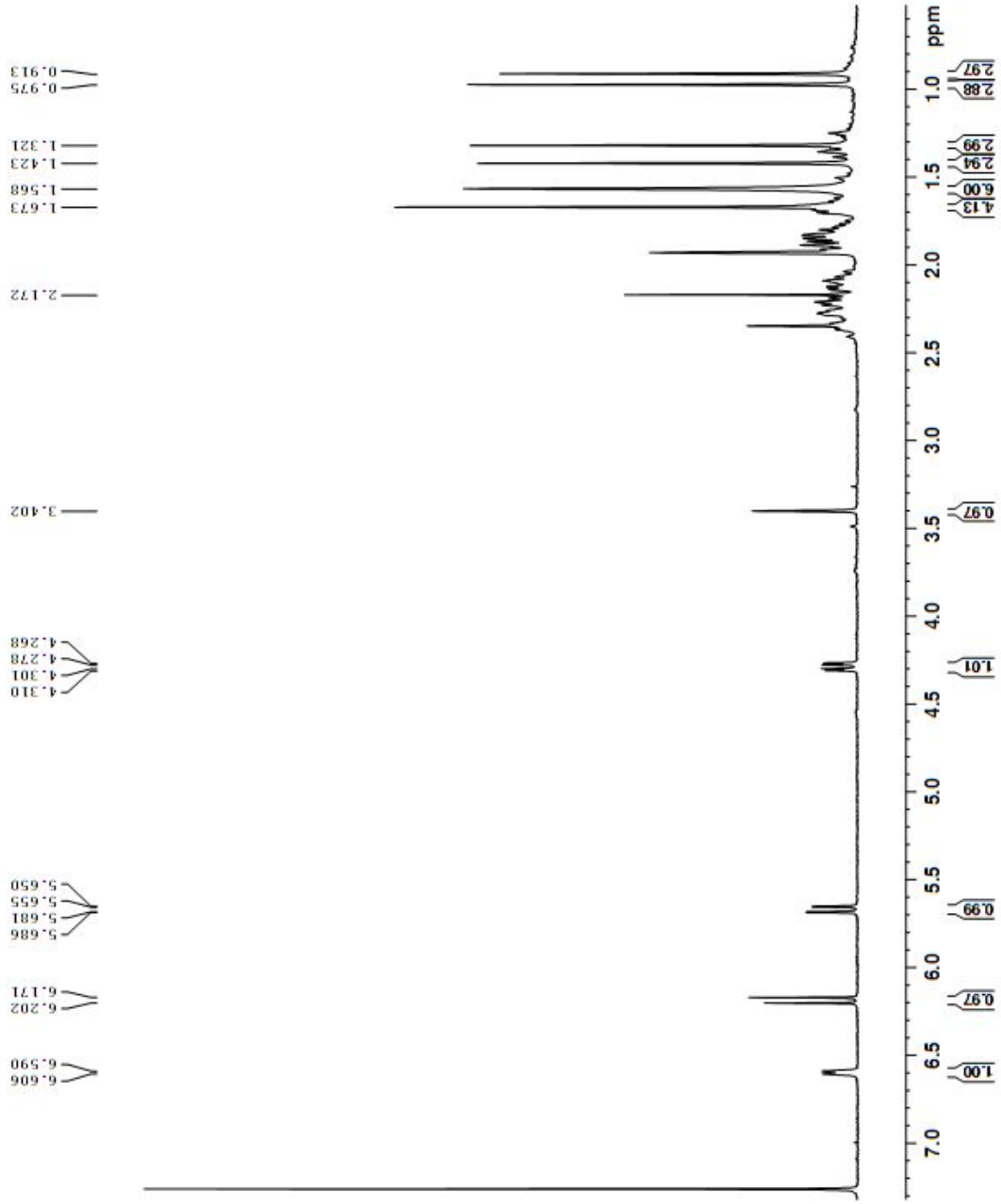
HMBC spectrum (600 MHz, $CDCl_3$) of schinchinenlactone A.



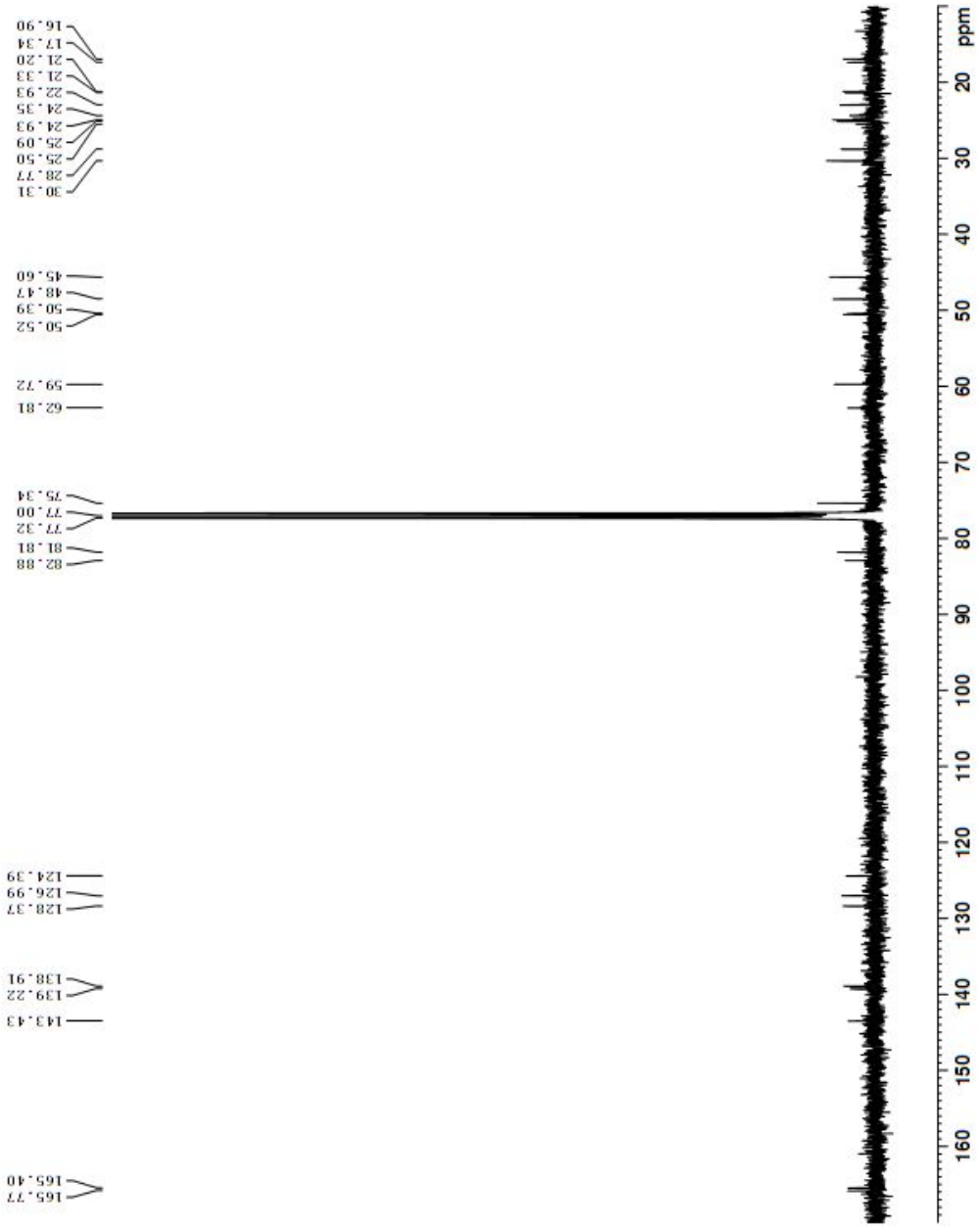
NOESY spectrum (400 MHz, $CDCl_3$) of schinchinenlactone A.



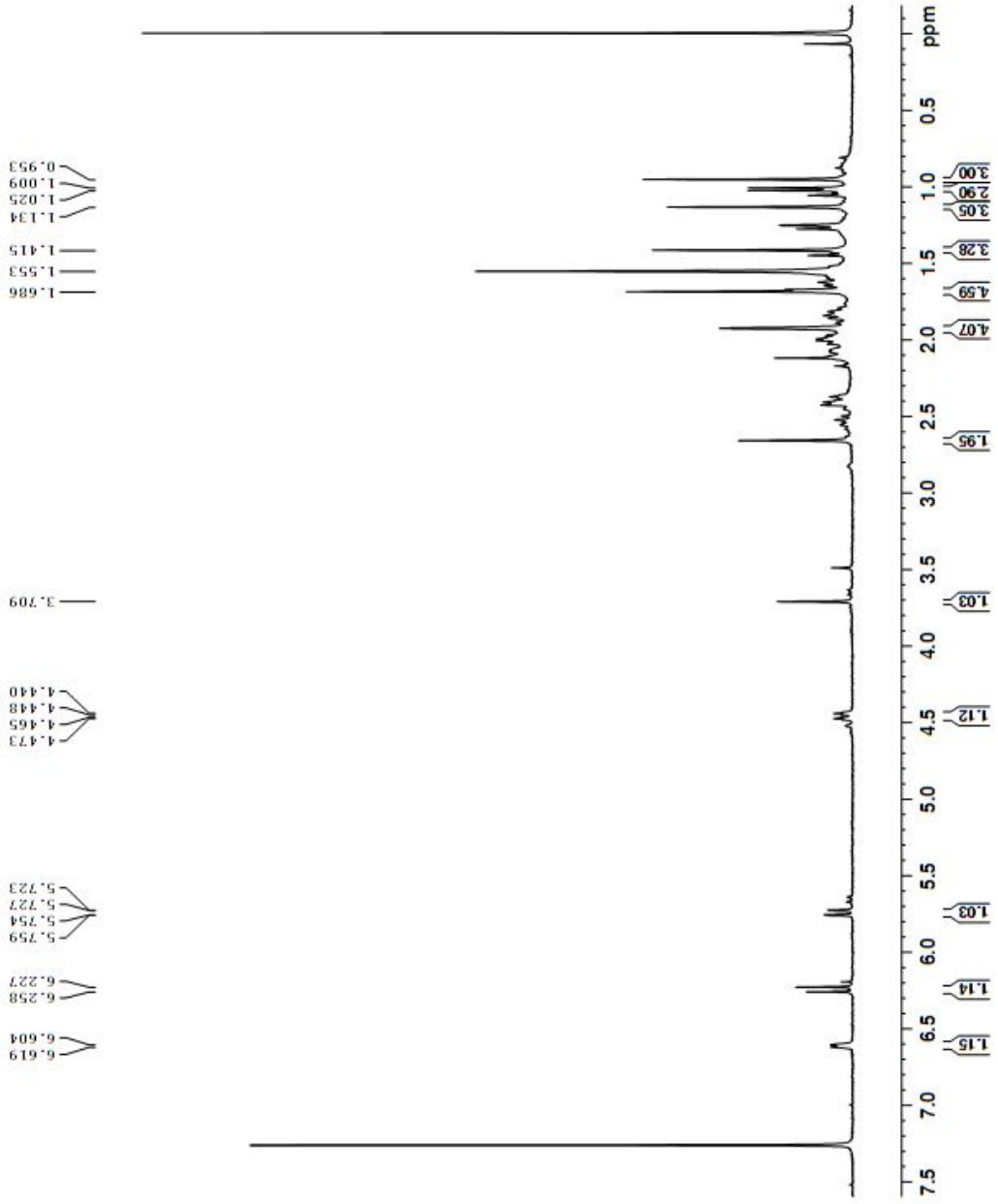
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of schinchinenlactone B.



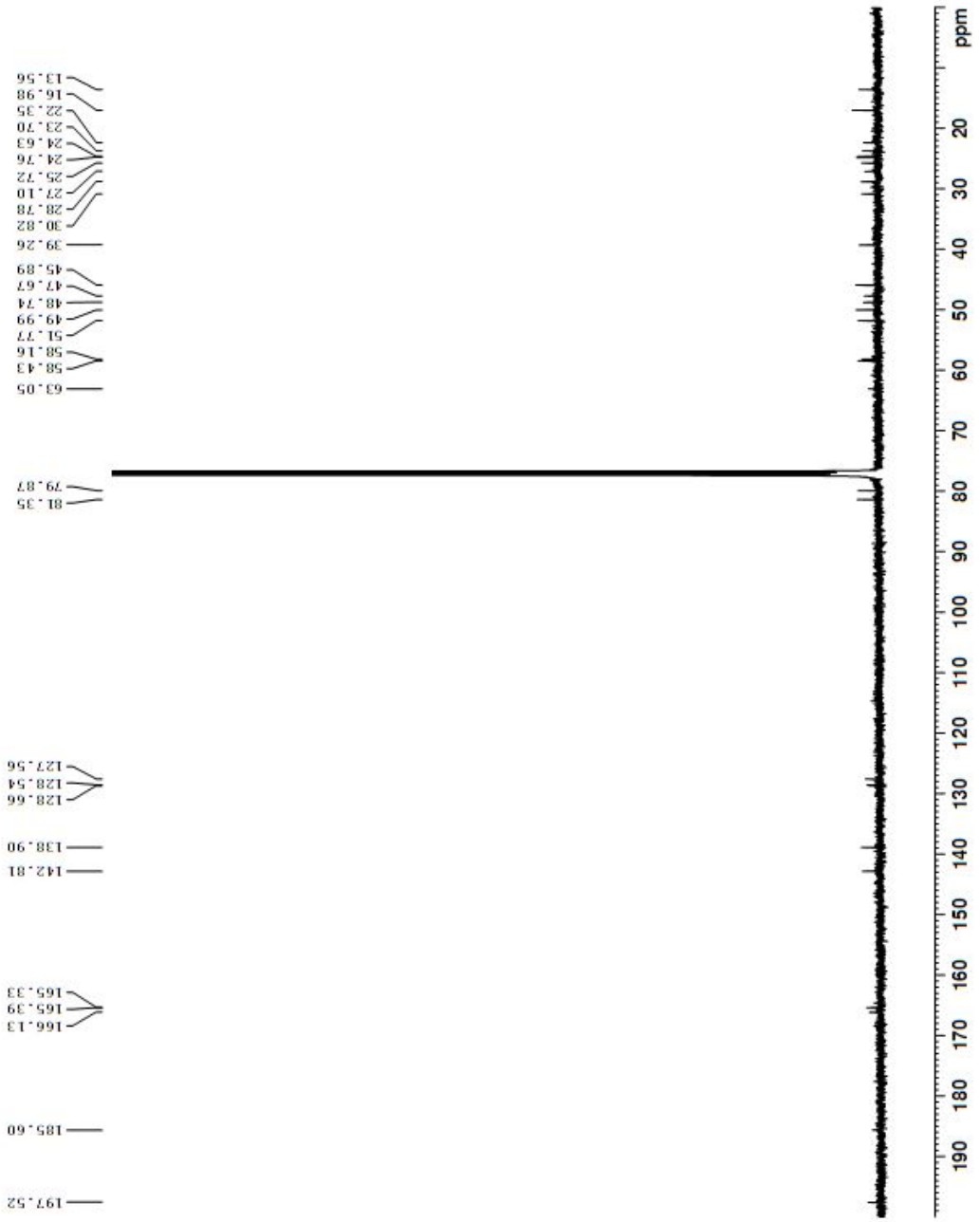
^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenlactone B.



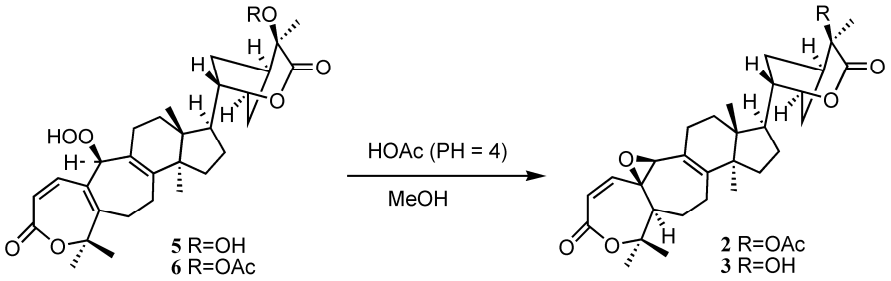
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of schinchinenlactone C.



^{13}C NMR spectrum (100 MHz, $CDCl_3$) of schinchinenlactone C.

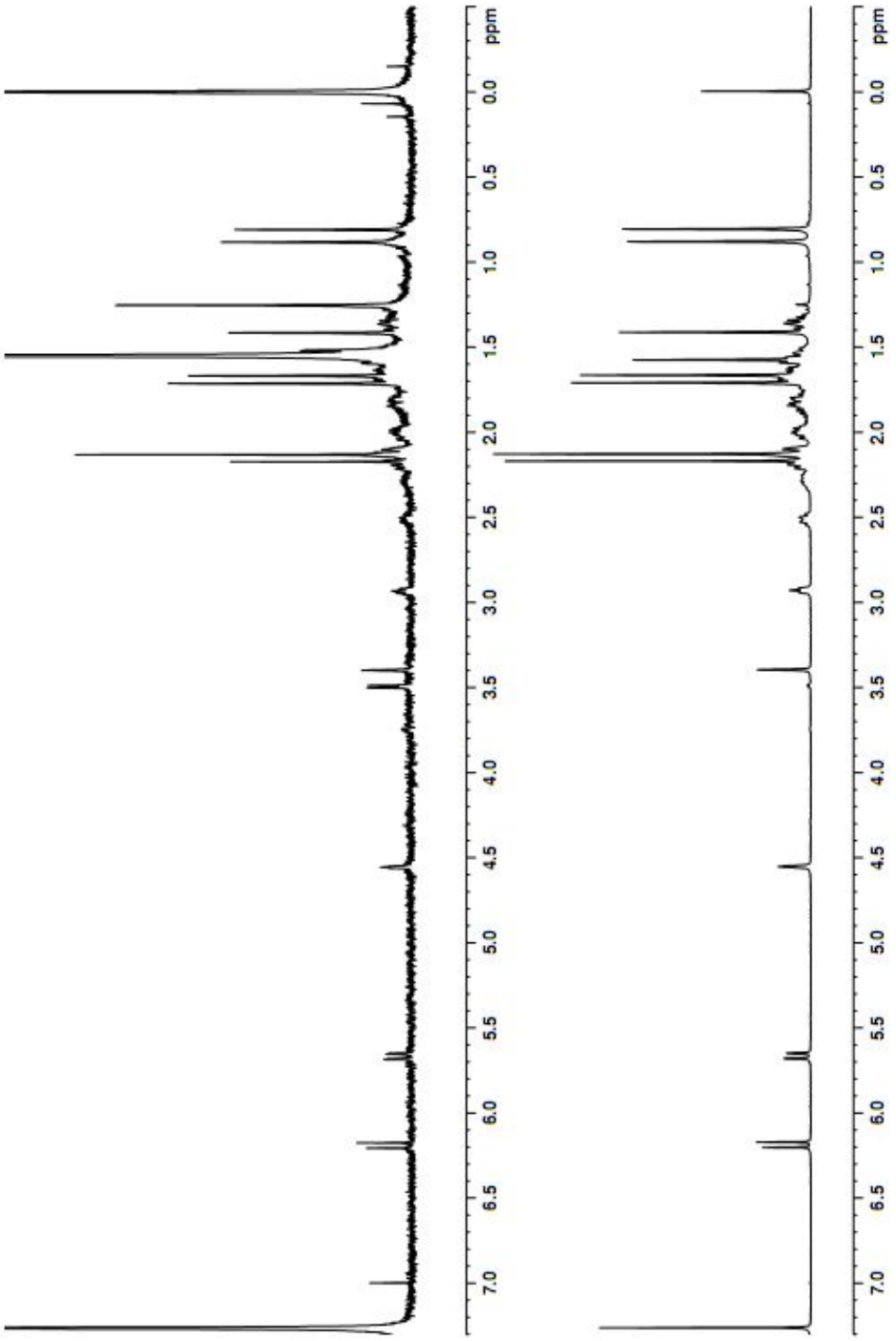


Partial conversion between schinchinenins D/E and B/C.

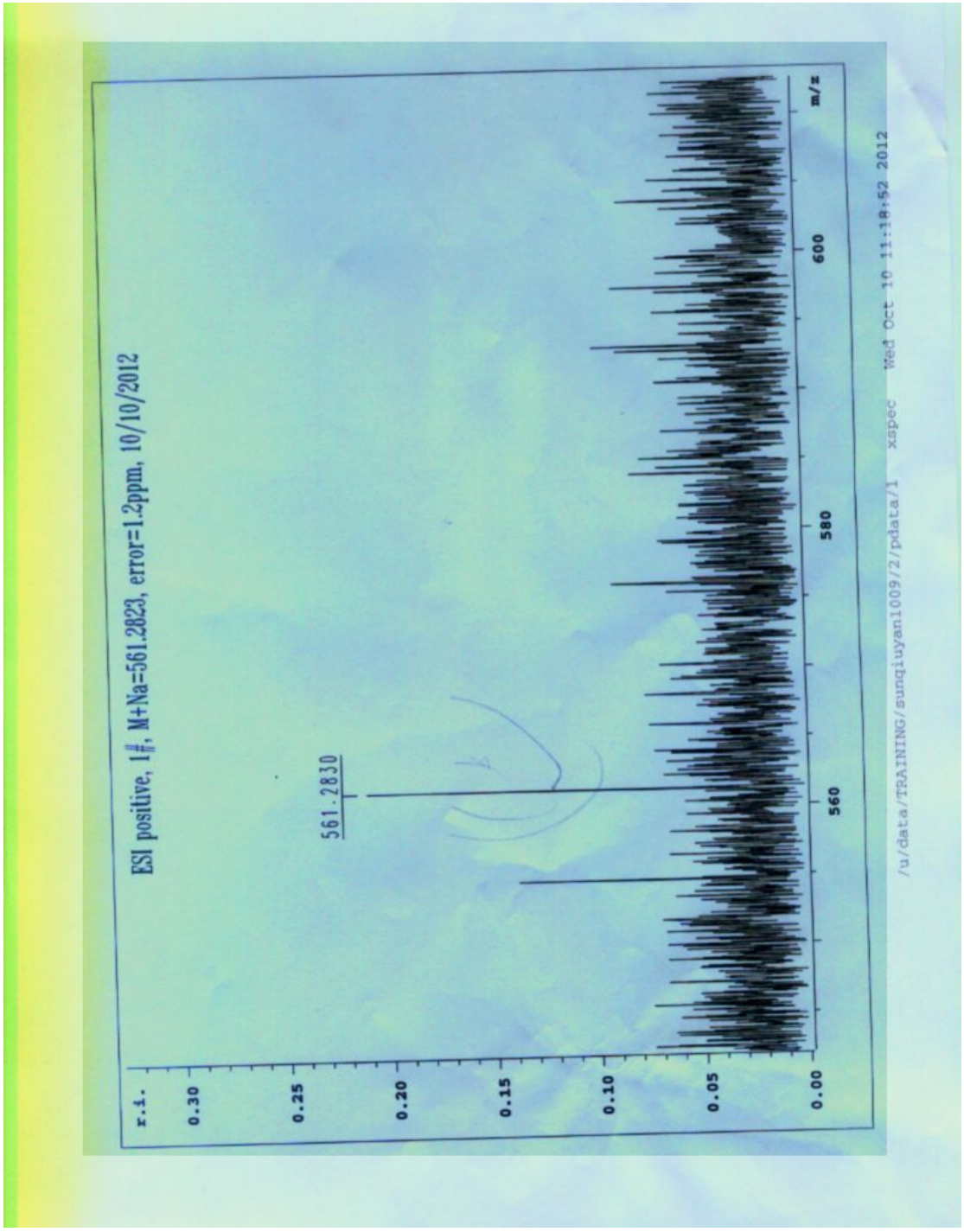


The main product obtained from the reaction of **5**/**6** in the presence of acetic acid (pH = 5) was the compound (**3**/**2**) isolated from the EtOAc extract of *S. chinensis* (scheme see above), another two minor products were also isolated from this reaction. Nevertheless, further establishment the structures of these minor products were prohibited due to the limited amount, one of their molecular formula exhibited a more oxygen atom than the main product as demonstrated via the Mass Spectra. Thus, this reaction was proposed to be a disproportionation reaction. In the case of compound **6**, the main product was **2**, which was confirmed by the ^{1}H NMR spectrum (page 41) and HRESIMS (page 42). And the molecular formula of one of the minor products showed a more oxygen atom than the main product as demonstrated via the Mass Spectra (page 43). Therefore, the relative configuration of the hydroperoxyl group of schinchinenin E/F could be determinated as *β*-orientation from the relative configuration of epoxide group of schinchinenin C/B.

^{1}H NMR spectrum (400 MHz, $CDCl_3$) of the main product obtained from the disproportionation reaction of **6** (the left) and **2** isolated from the EtOAc (the rignt) extract of *S. chinensis*.



HRESIMS spectrum of the main product obtained from the disproportionation reaction of **6**. The peak at 561.2830 $[M+Na]^+$ was assigned to the main product of this disproportionation reaction.



ESIMS spectrum of one of the two minor products obtained from the disproportionation reaction of **6**. The peak at 555.4 $[M+H]^+$ and 557.4 $[M+Na]^+$ was assigned to one of the minor product of this disproportionation reaction, which exhibited a more oxygen atom than the main product (M = 538).