

Supplementary Information

Catalyst- and metal-free C(sp²)-H bond selenylation of (N-hetero)-arenes using diselenides and trichloroisocyanuric acid at room temperature.

José S. S. Neto¹, Isis J. A. Granja², Marcos R. Scheide¹, Marcelo S. Franco¹, Cassio A. O. Moraes³, Adilson Beatriz³, Dênis P. de Lima³, Giancarlo V. Botteselle⁴, Tiago E. A. Frizon⁵, Sumbal Saba², Jamal Rafique^{2,3*}, and Antonio L. Braga^{1,*}

¹ Departamento de Química, Universidade Federal de Santa Catarina - UFSC, Florianópolis, 88040-970, SC-Brazil. <http://labselen.ufsc.br>; E-mail: braga.antonio@ufsc.br

² Instituto de Química, Universidade Federal de Goiás - UFG, Goiânia, 74690-900, GO-Brazil

³ Instituto de Química, Universidade Federal do Mato Grosso do Sul - UFMS, Campo Grande, 79074-460, MS-Brazil. <https://sintmol.ufms.br/>; E-mail: jamal.rafique@ufms.br, jamal.chm@gmail.com

⁴ Departamento de Química, Universidade Estadual do Centro-Oeste - UNICENTRO, 85819110, Guarapuava, PR - Brazil

⁵ Universidade Federal de Santa Catarina – UFSC, Campus Araranguá, 88905120 Araranguá, SC-Brazil

*Corresponding author: jamal.chm@gmail.com (J.R.), braga.antonio@ufsc.br (A.L.B.)

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General Remarks

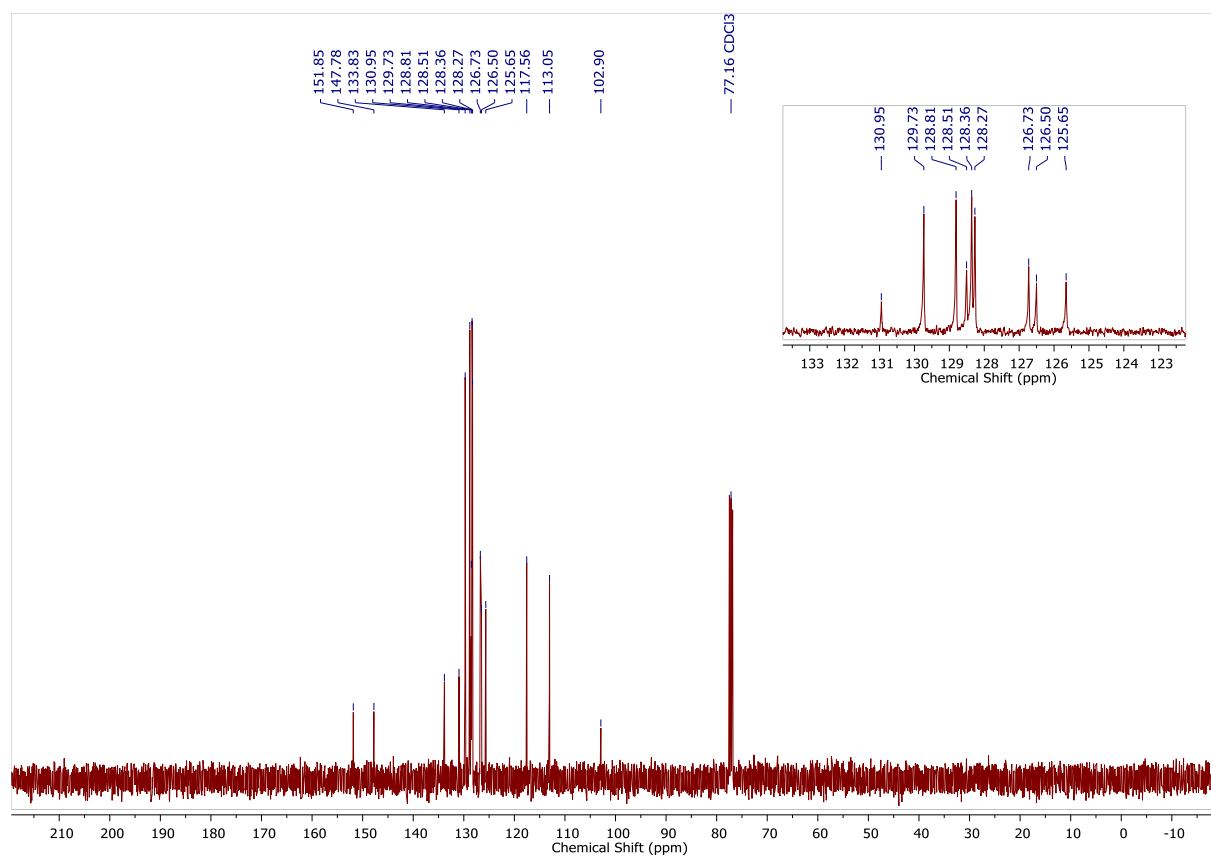
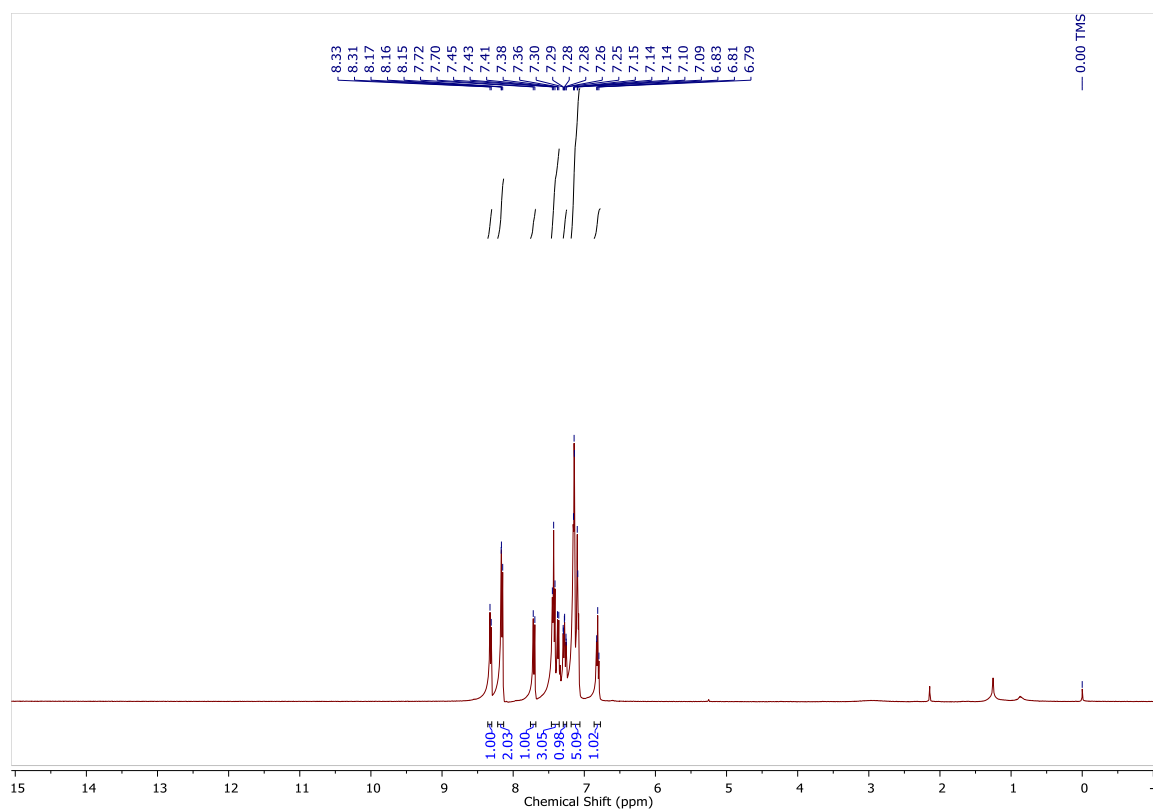
Starting materials obtained from commercial suppliers were used unless otherwise stated. Column chromatography was performed using silica gel 60 (diameter 0.05 - 0.10 mm) Macherey-Nagel. Thin layer chromatography (TLC) was performed using Macherey-Nagel pre-coated TLC sheets ALUGRAM[®] Xtra SIL with layer of 0.20 mm. Visualization was achieved by UV fluorescence, iodine chamber and acidic vanillin.

Synthesis of Starting Materials

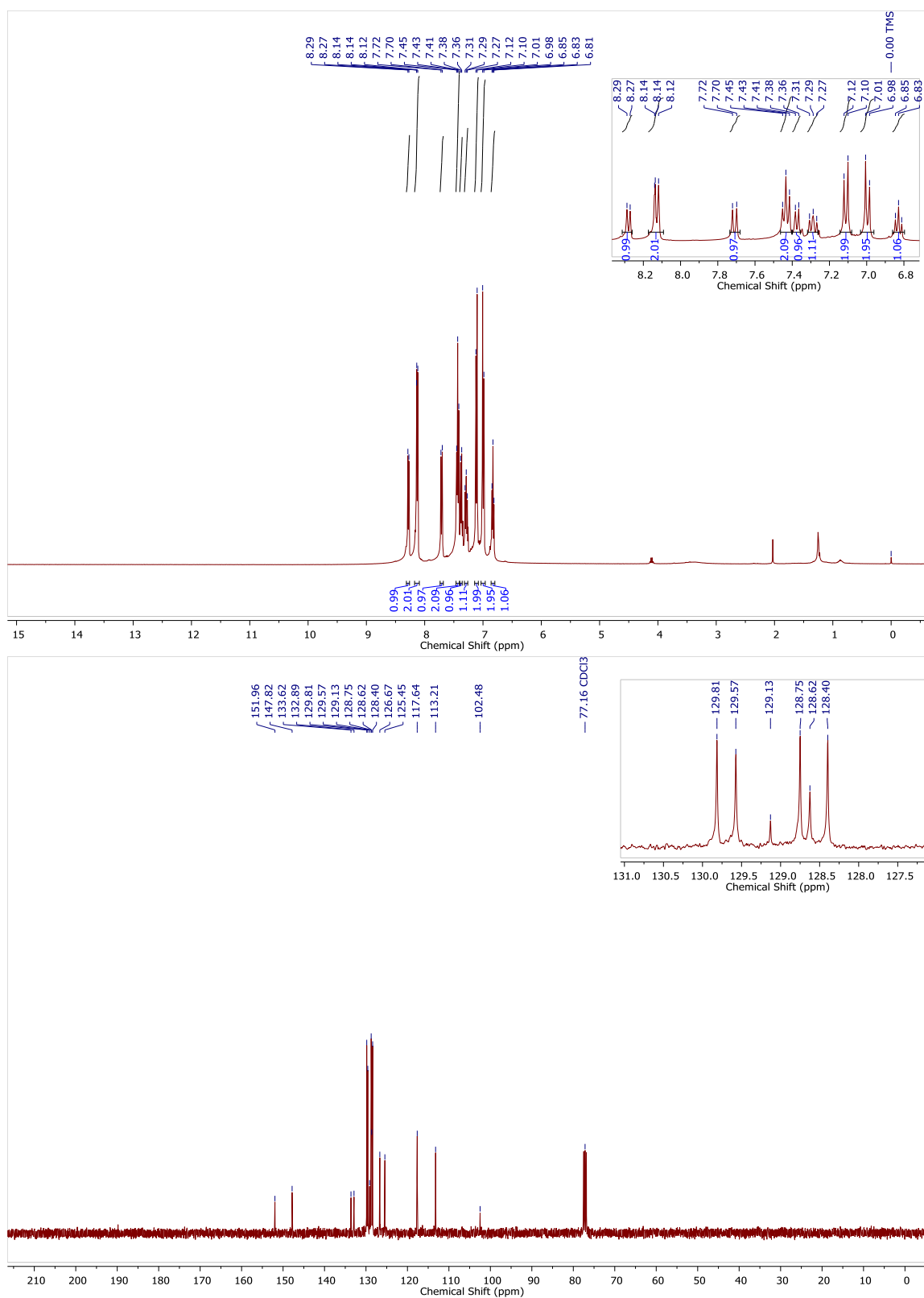
The substrates imidazo[1,2-*a*]pyridines, imidazo[1,2-*a*]pyrimidines and imidazo[2,1-*b*]thiazoles were prepared according to the literature reports.^[1-12]

Characterization Data Products

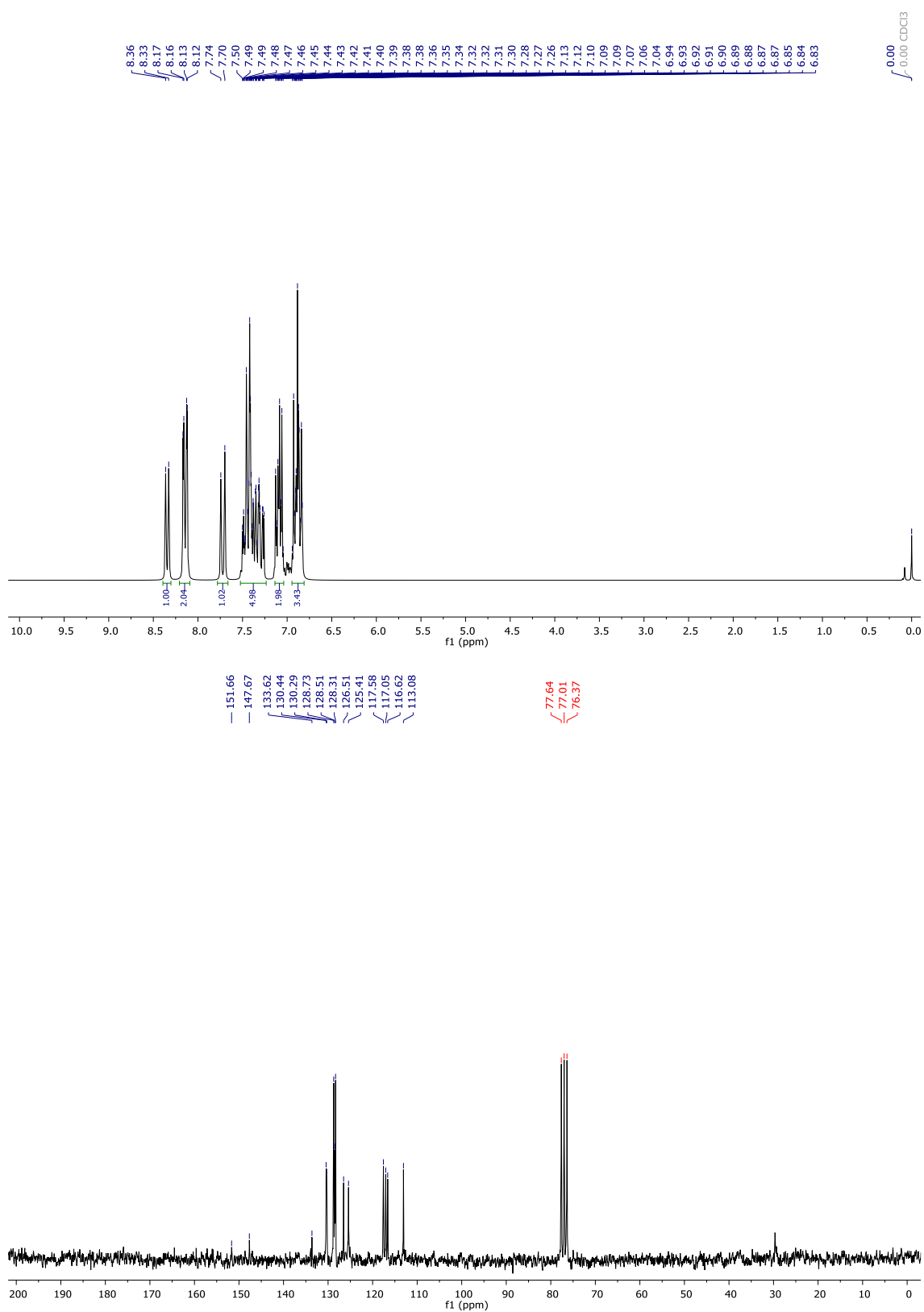
General considerations: The melting points were taken on a MQAPF-301 melting point apparatus, uncorrected. ¹H and ¹³C NMR spectra were recorded on Varian NMR AS 400 spectrometer and Bruker NMR AC 200, with the samples dissolved in CDCl₃. Chemical shifts are informed in ppm downfield from the signal of TMS, used as internal standard, and the coupling constants (*J*) are expressed in Hertz (Hz). High-resolution mass spectral data were obtained on a Bruker microTOF-Q IIT instrument and Xevo G2-S QTOF (Waters) on ESI⁺ mode. Infrared spectra were recorded on Bruker Alpha using KBr pellets.

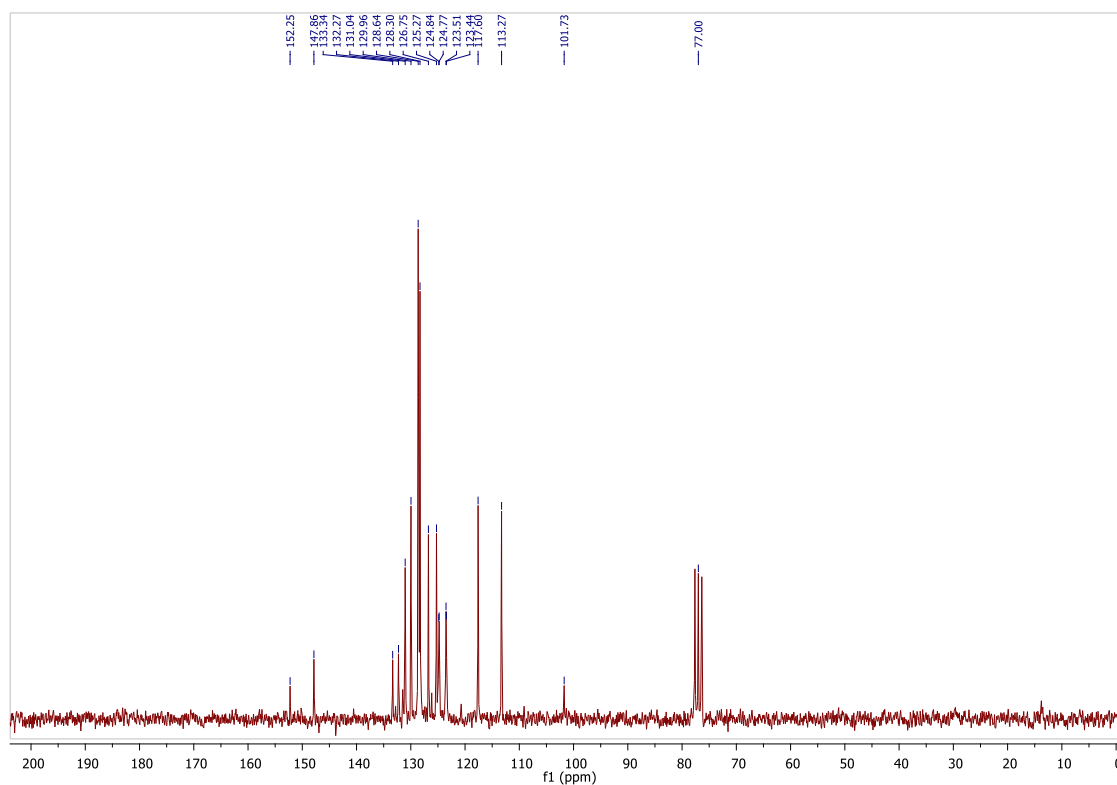
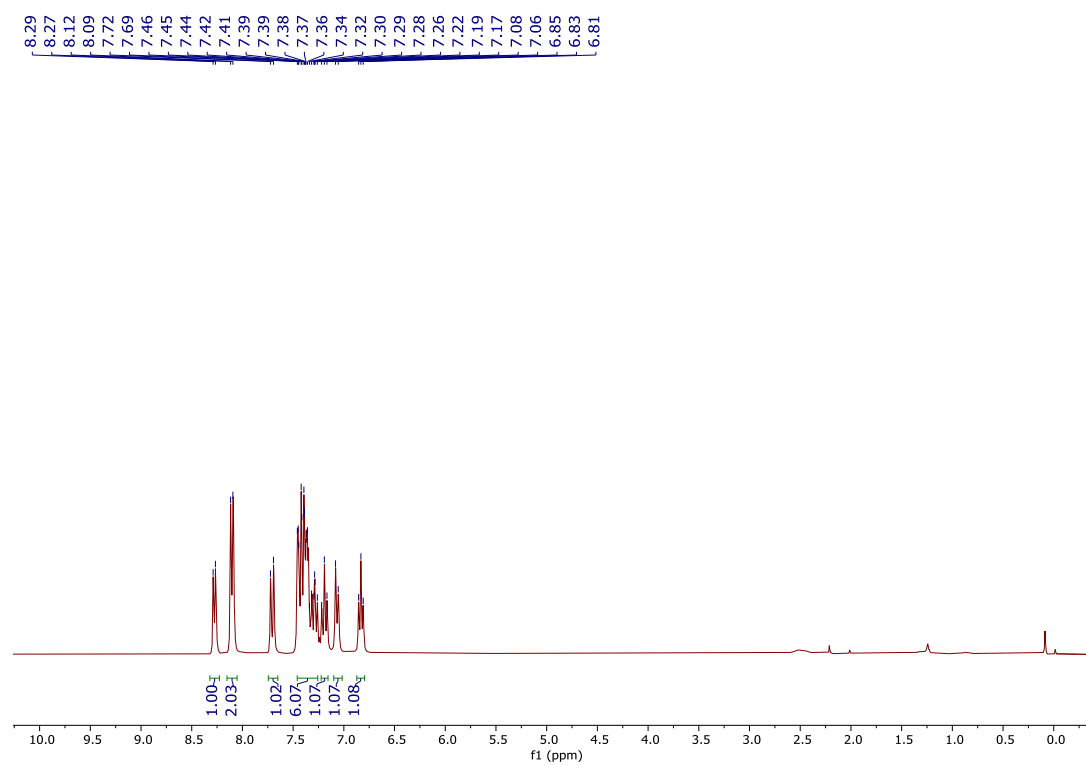


¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **3a**

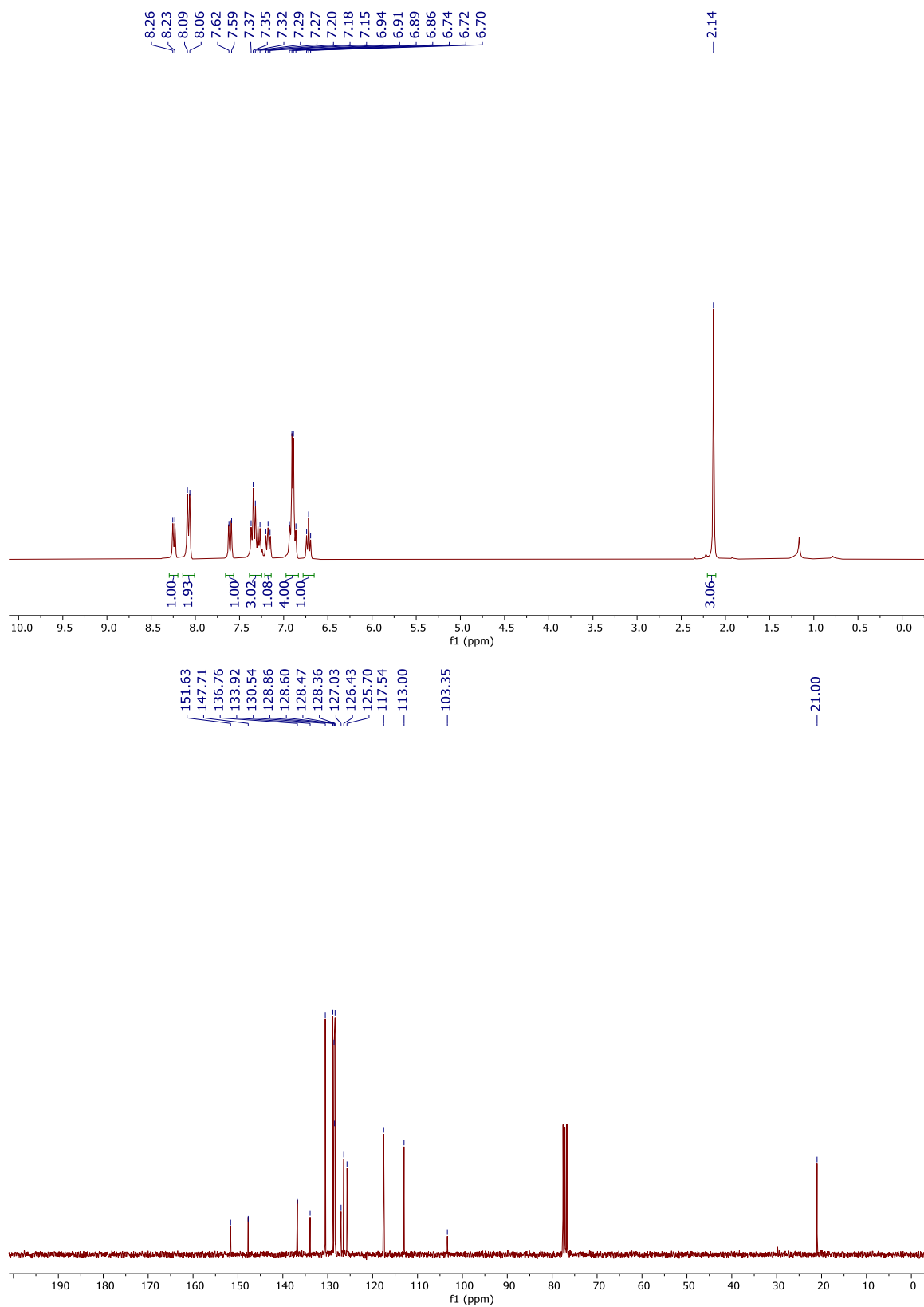


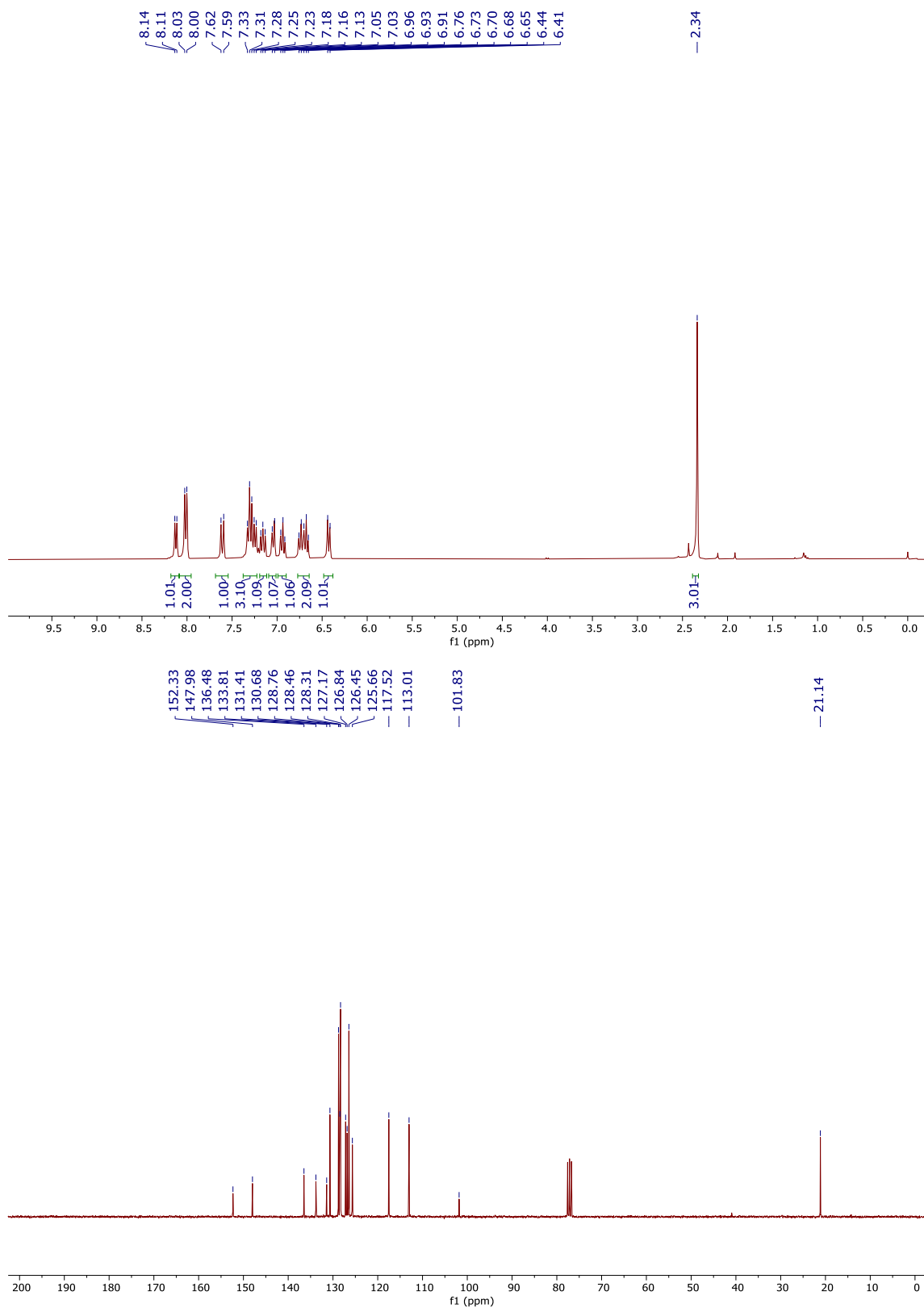
^1H NMR (top) ^{13}C NMR (bottom) CDCl_3 spectra of compound **3b**

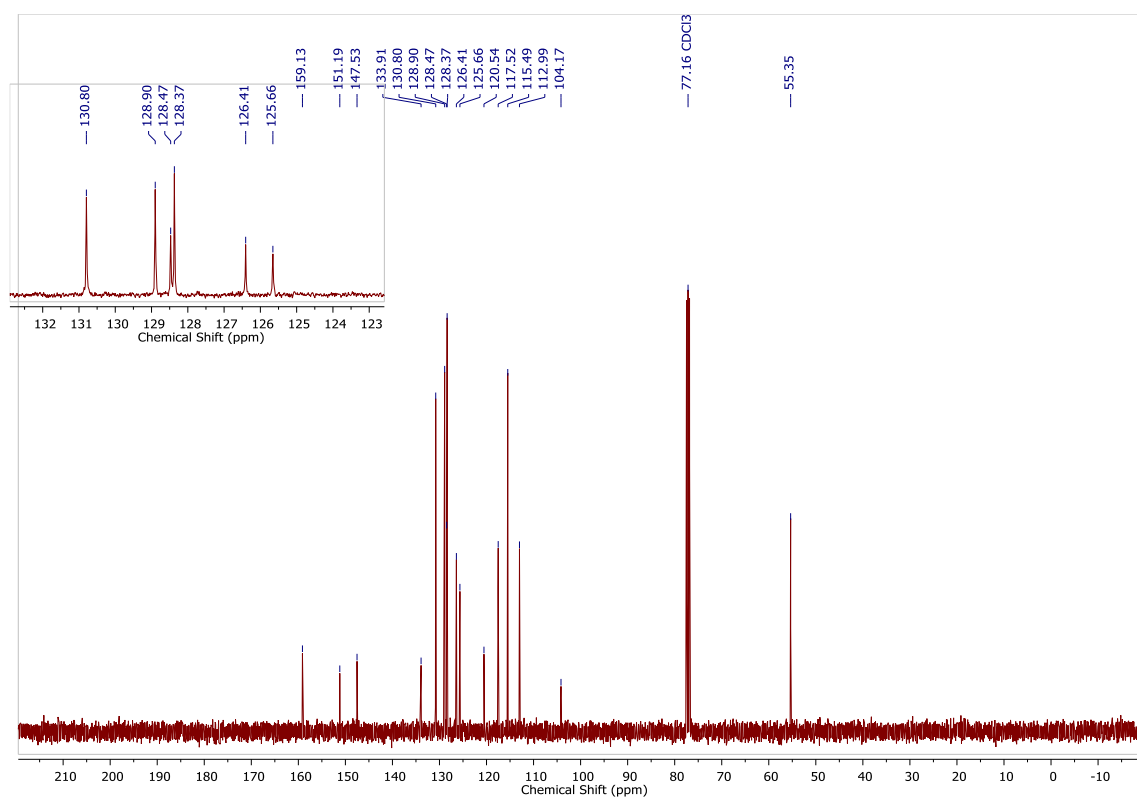
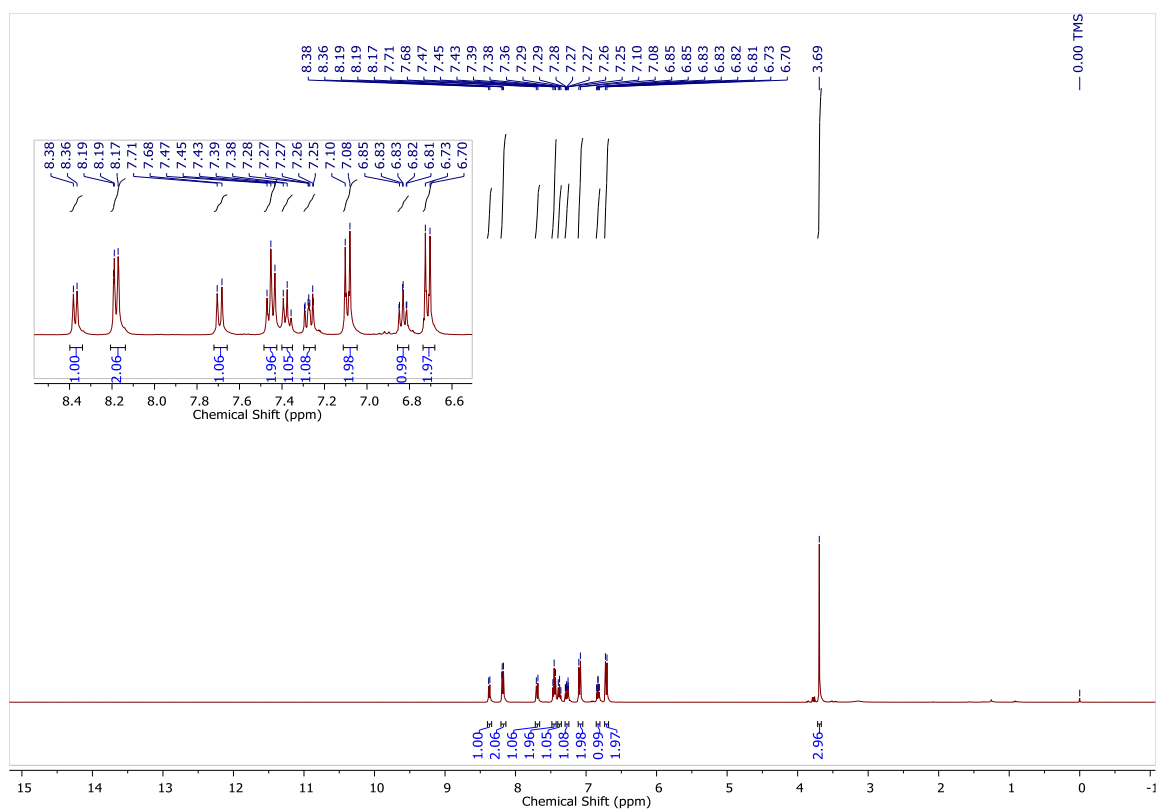




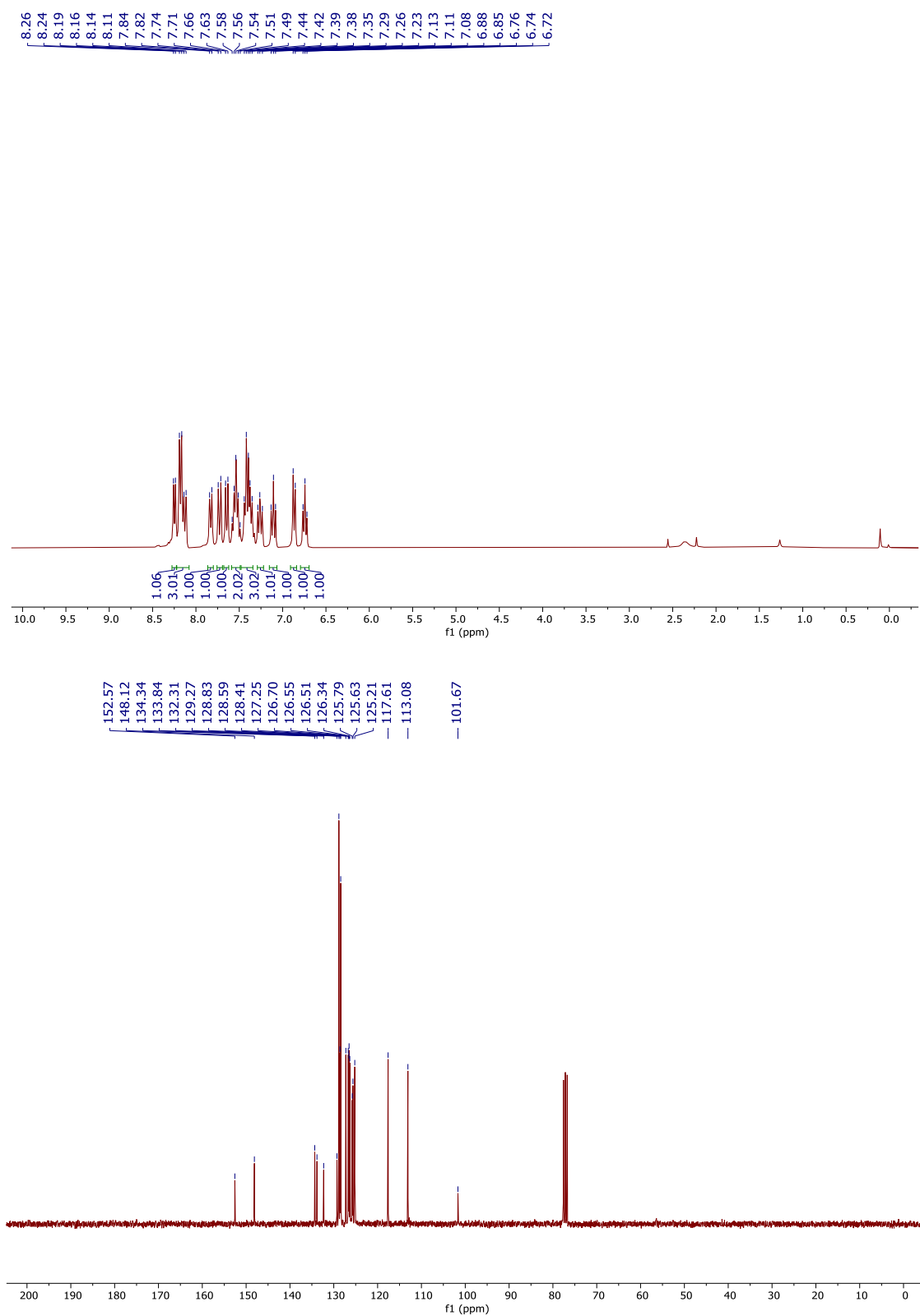
¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **3d**

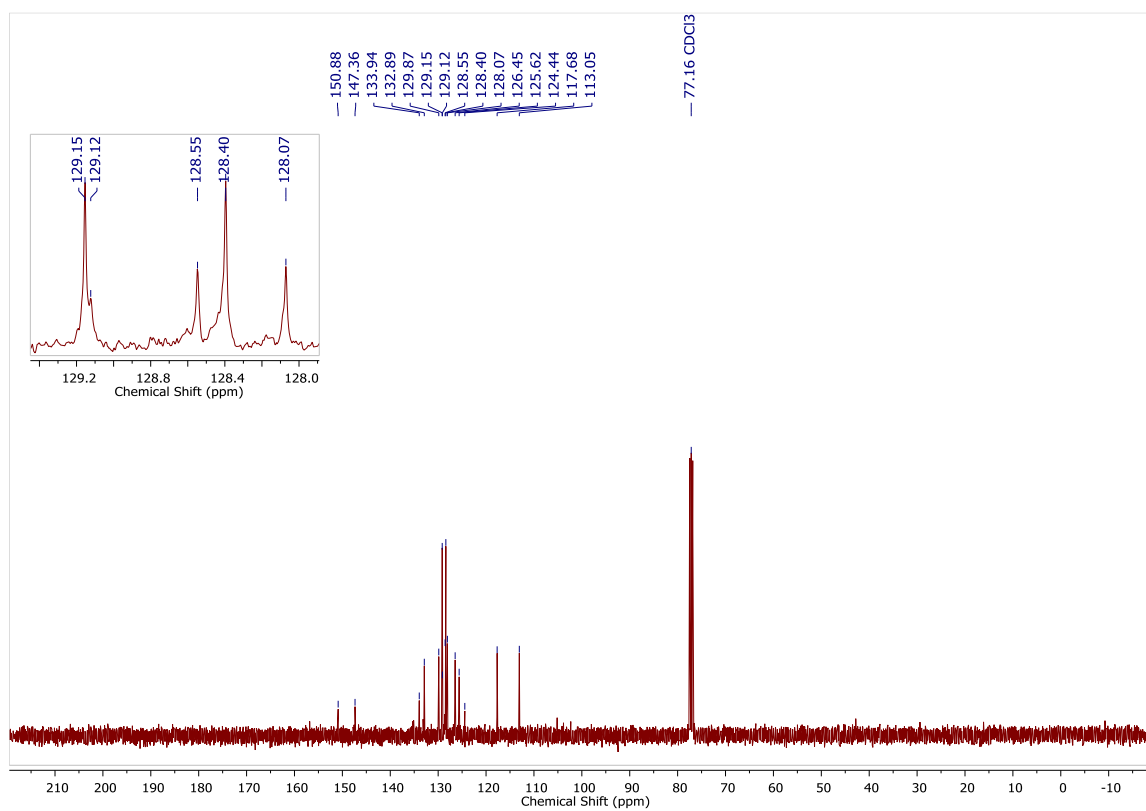
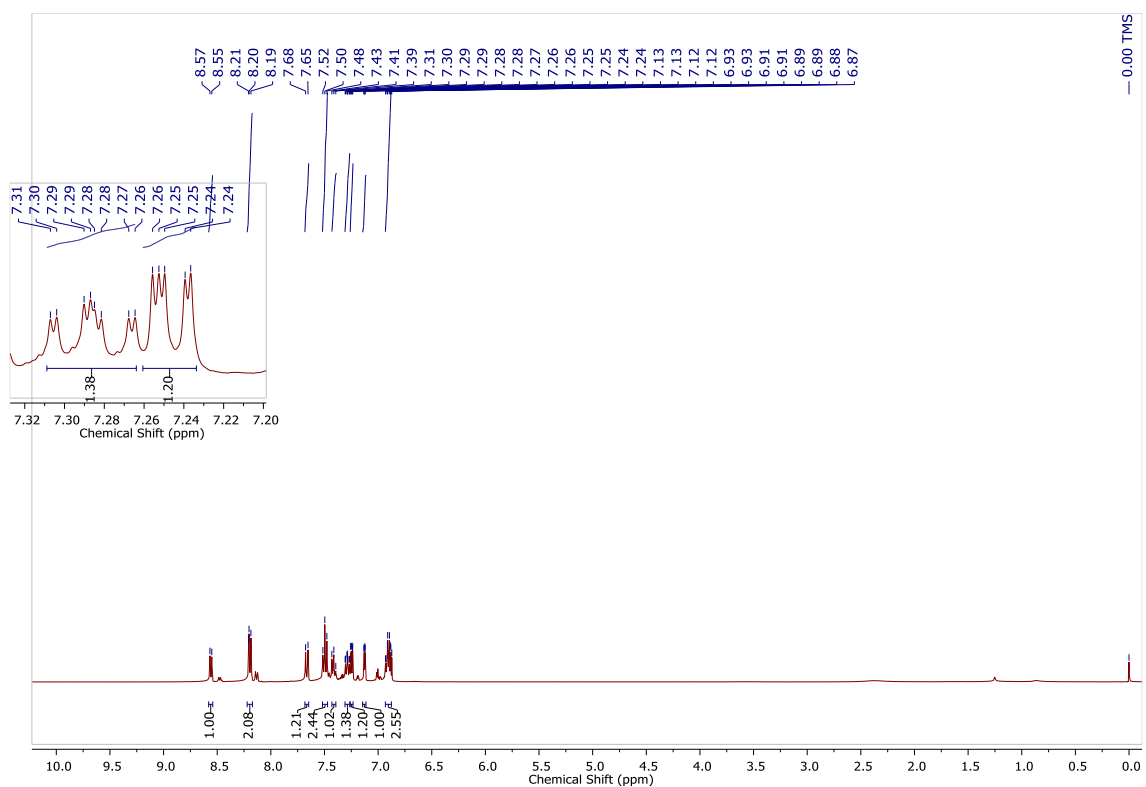




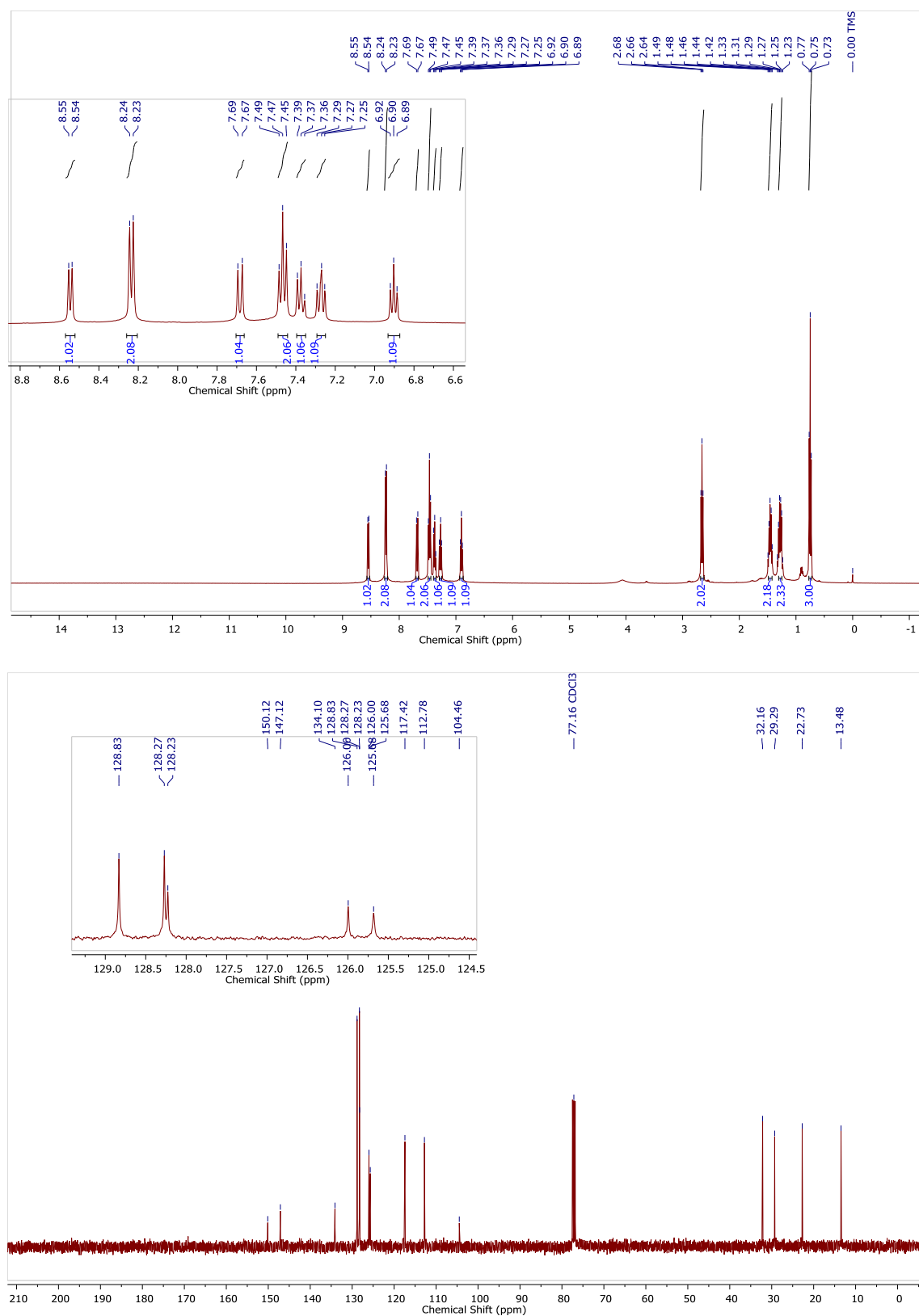


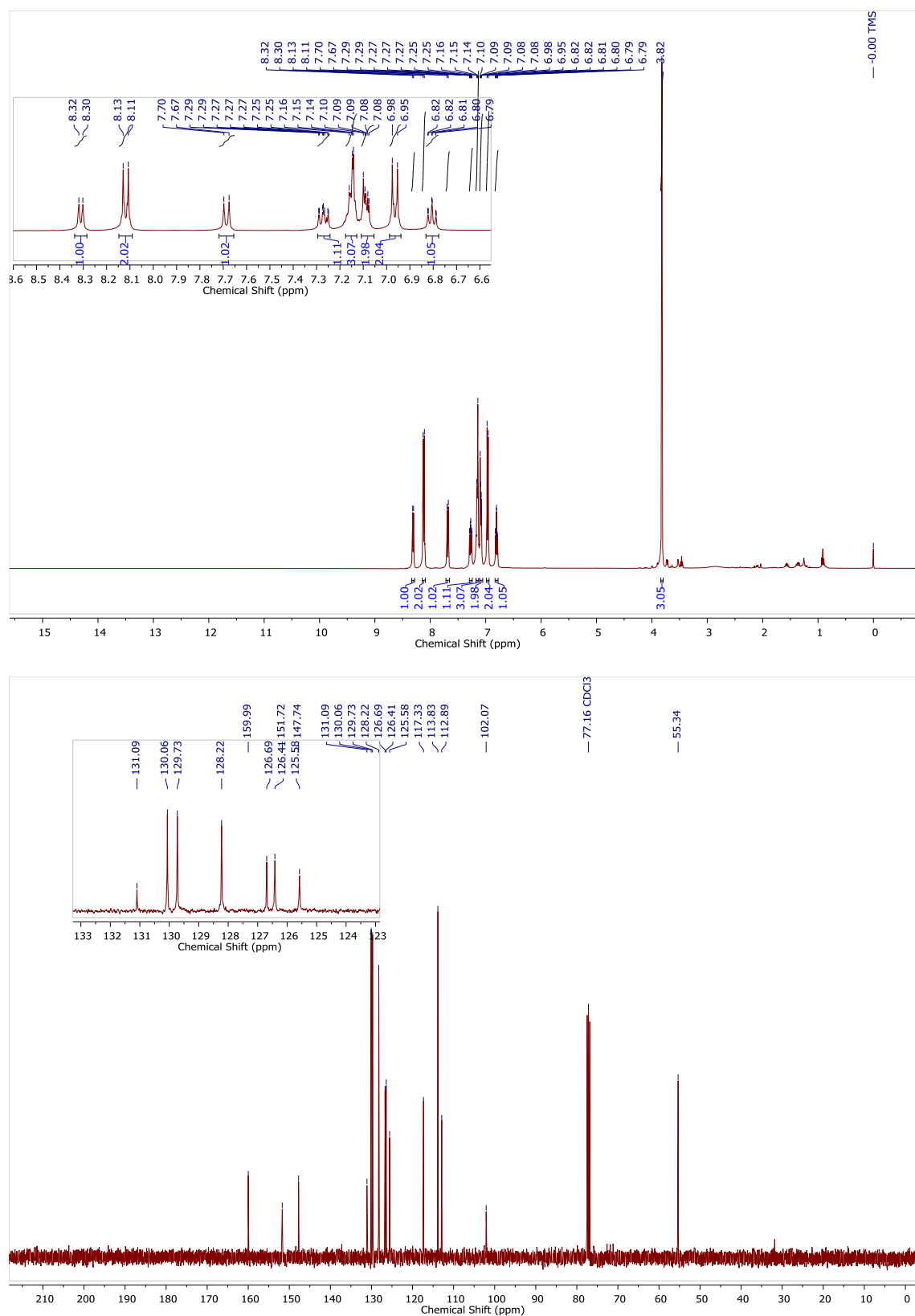
¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **3g**



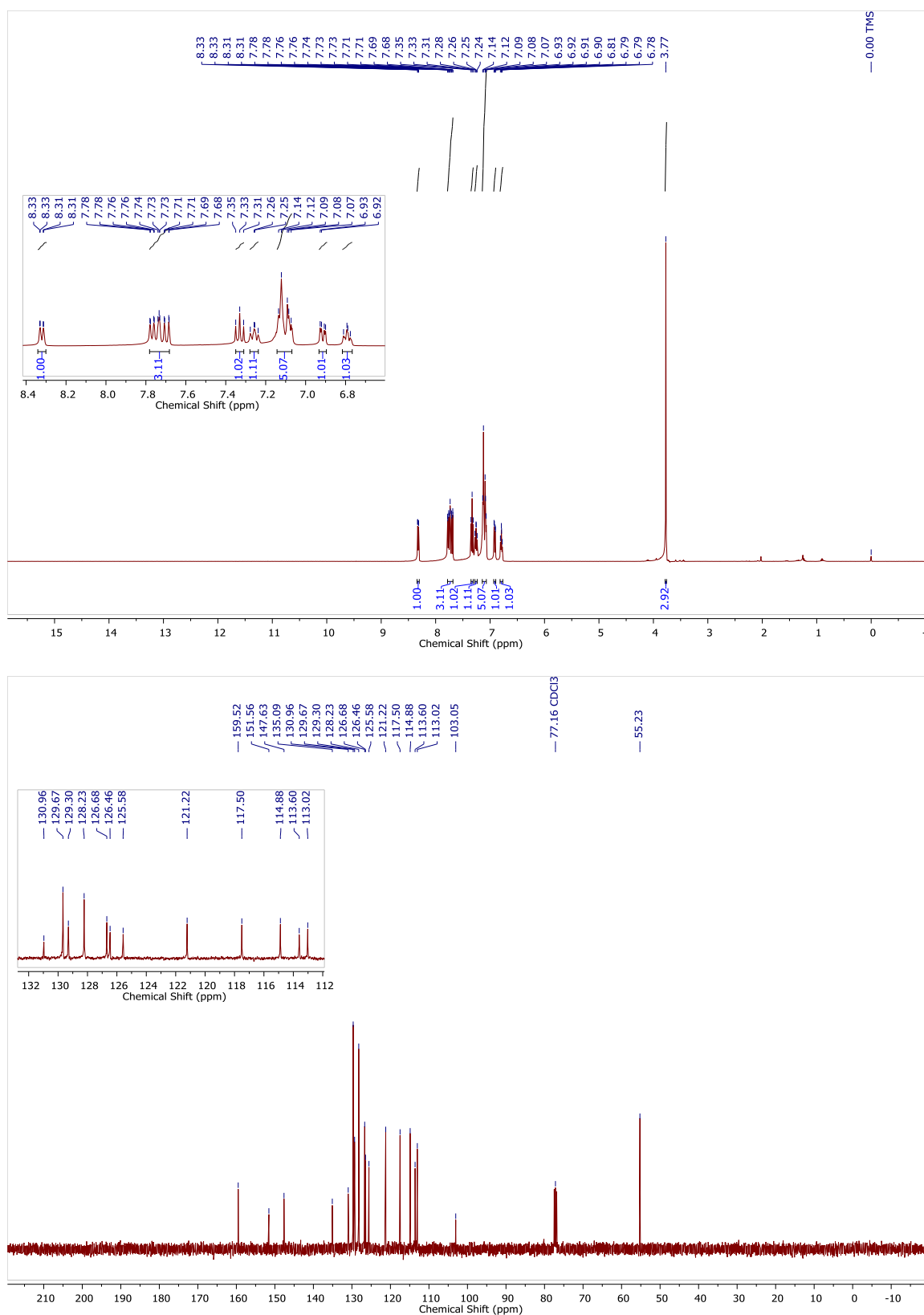


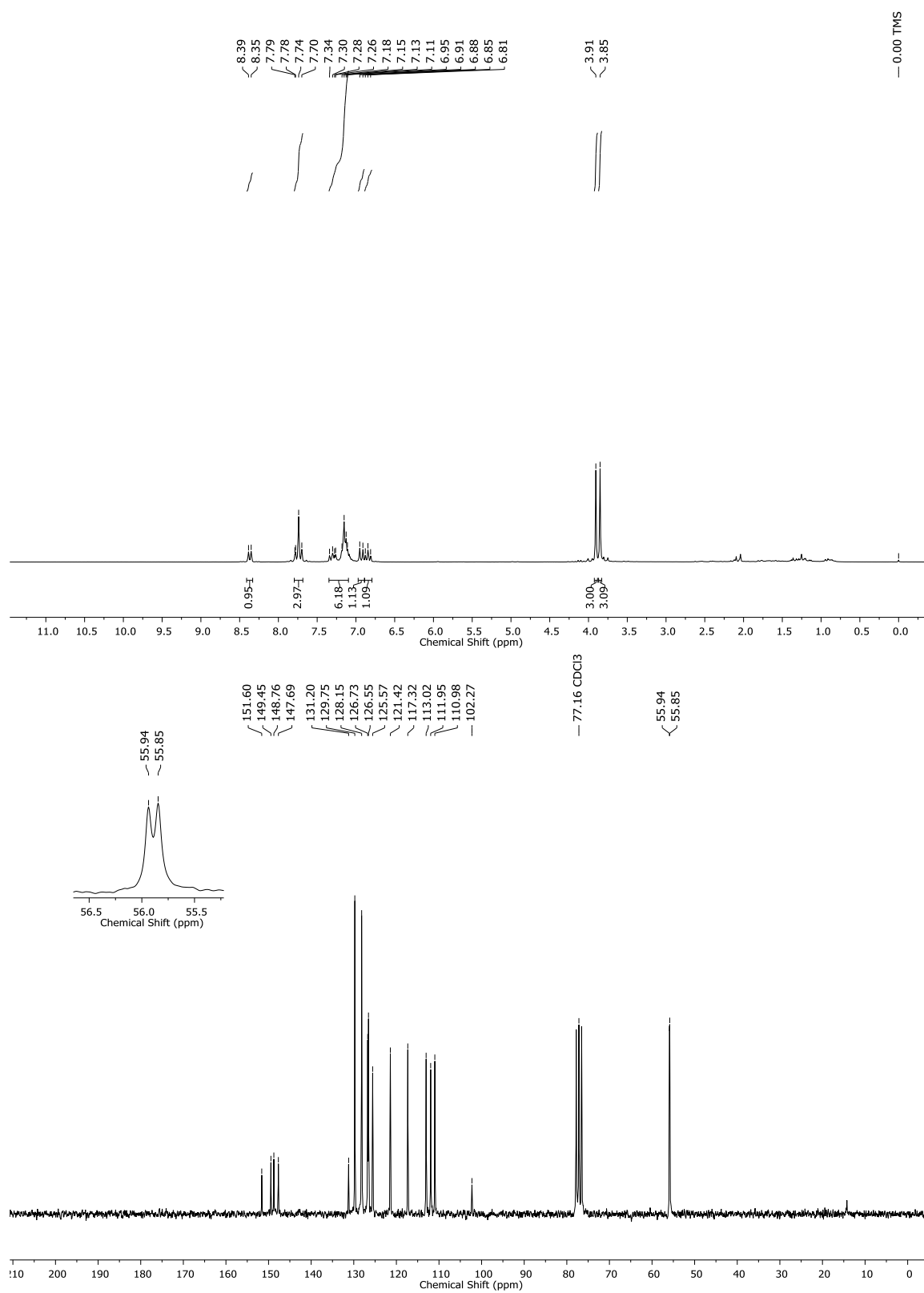
¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **3j**

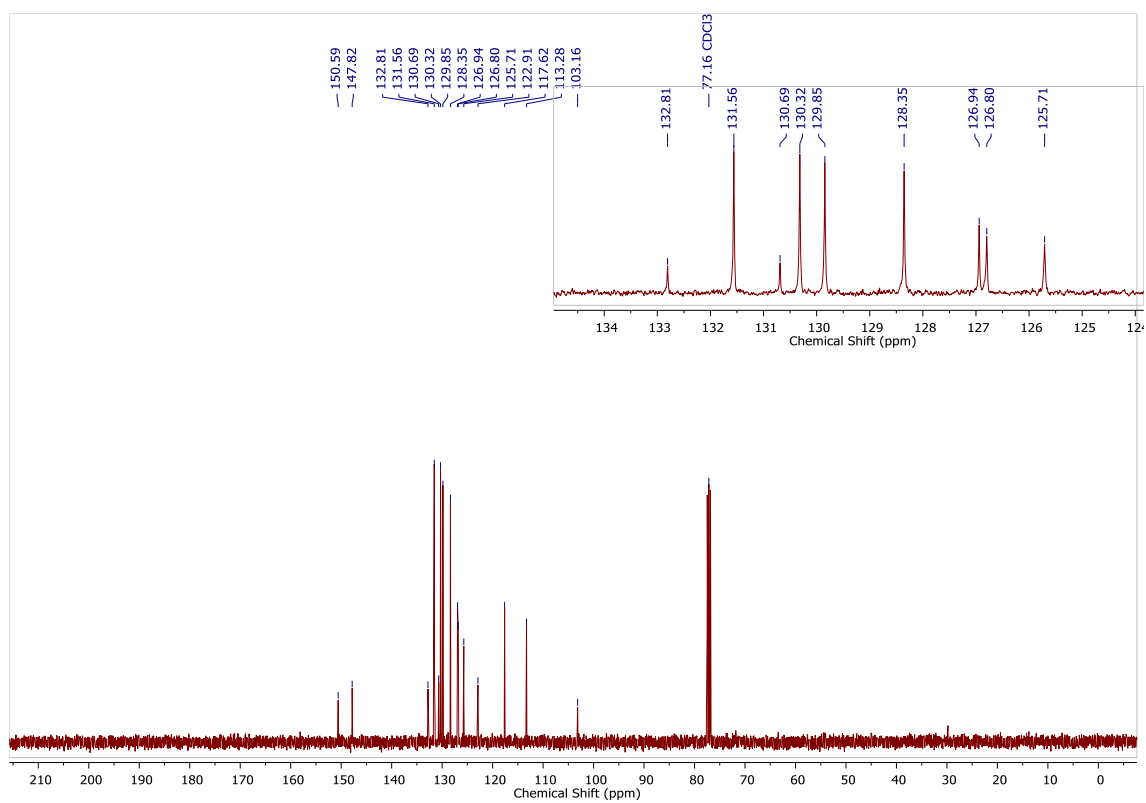
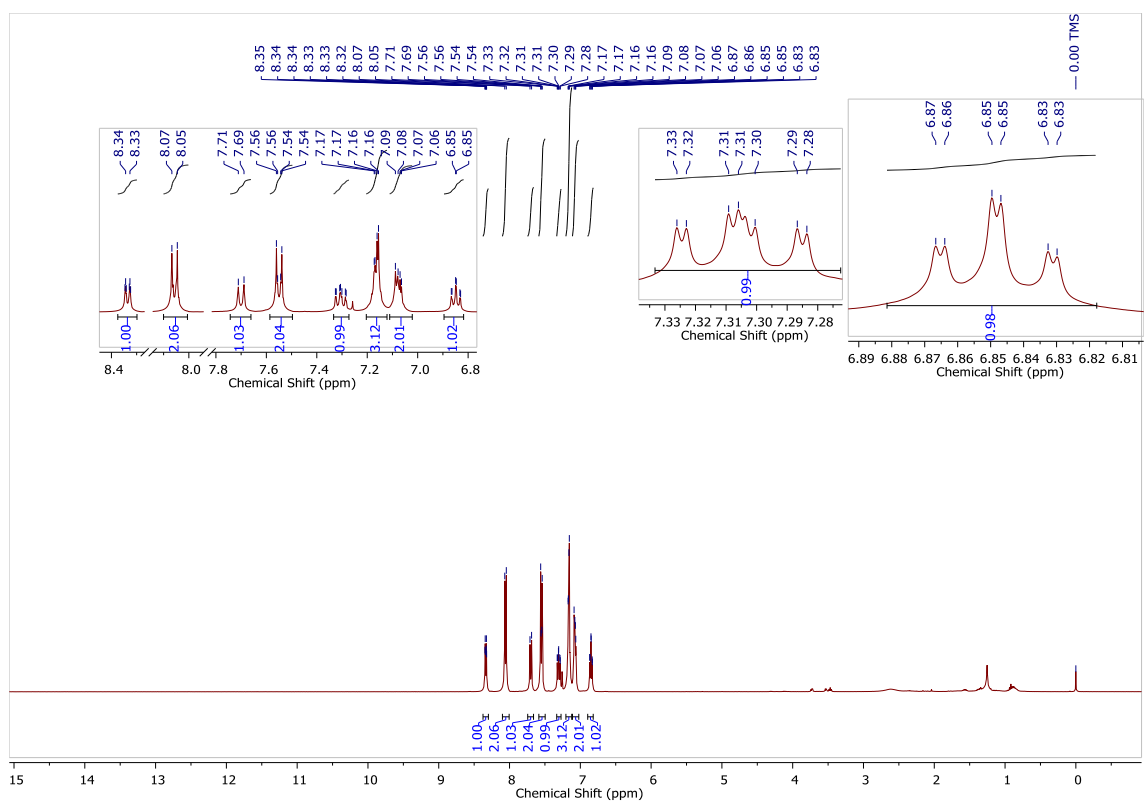




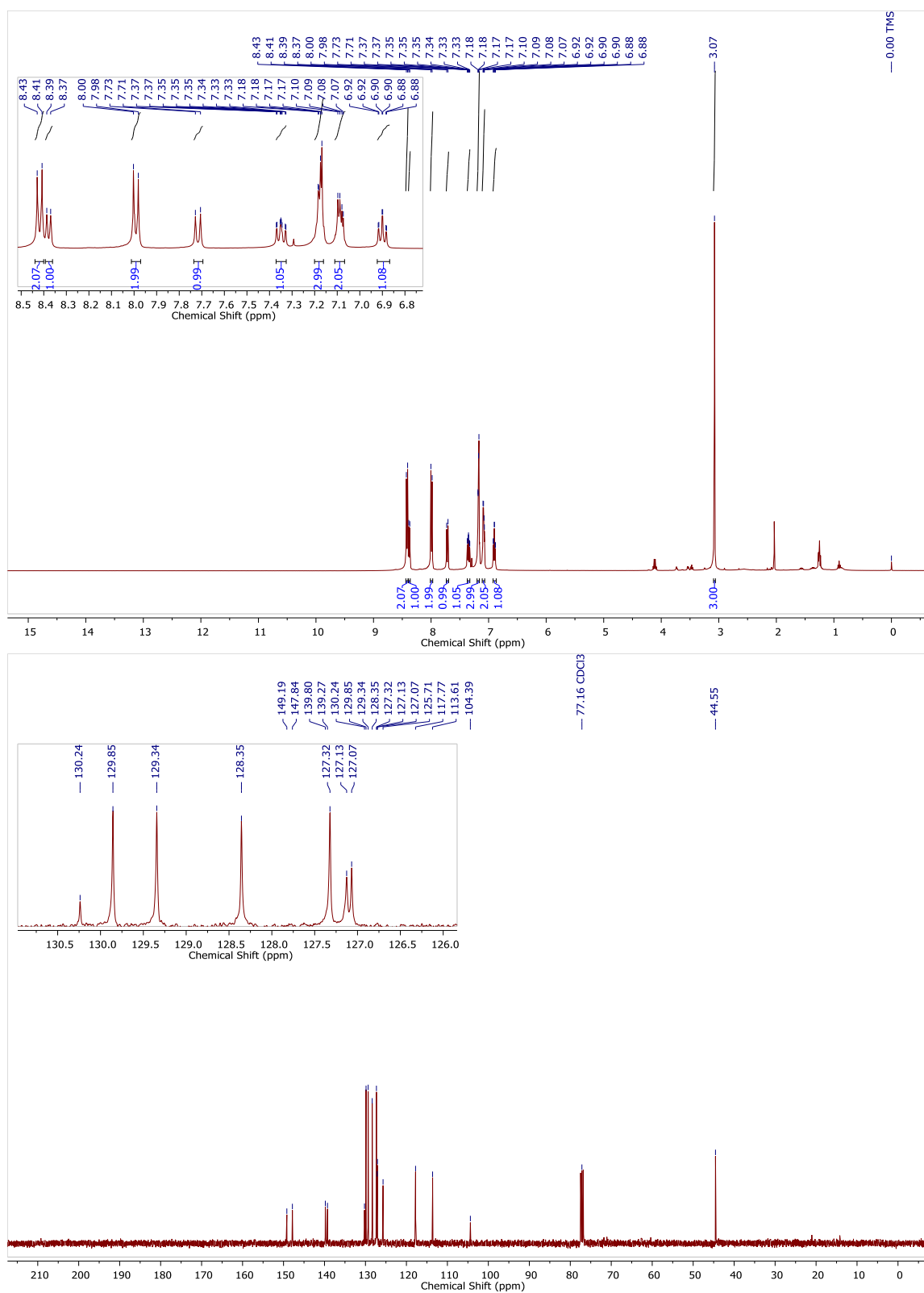
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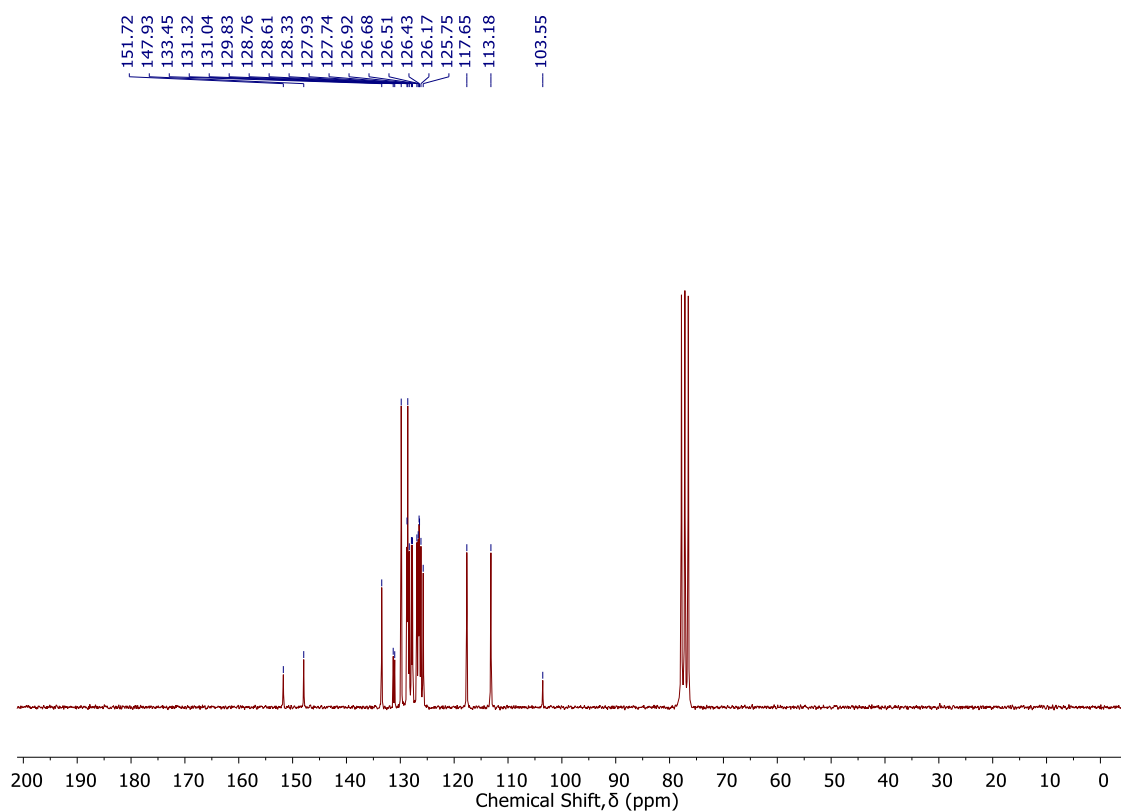
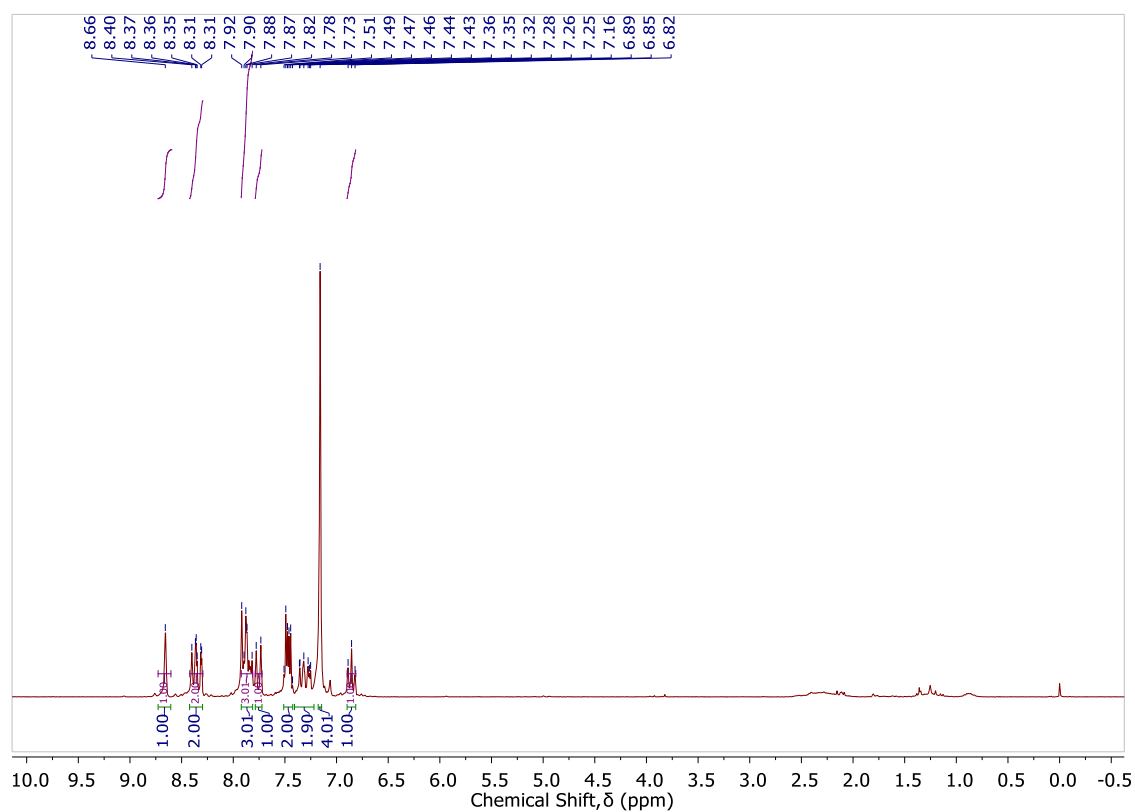




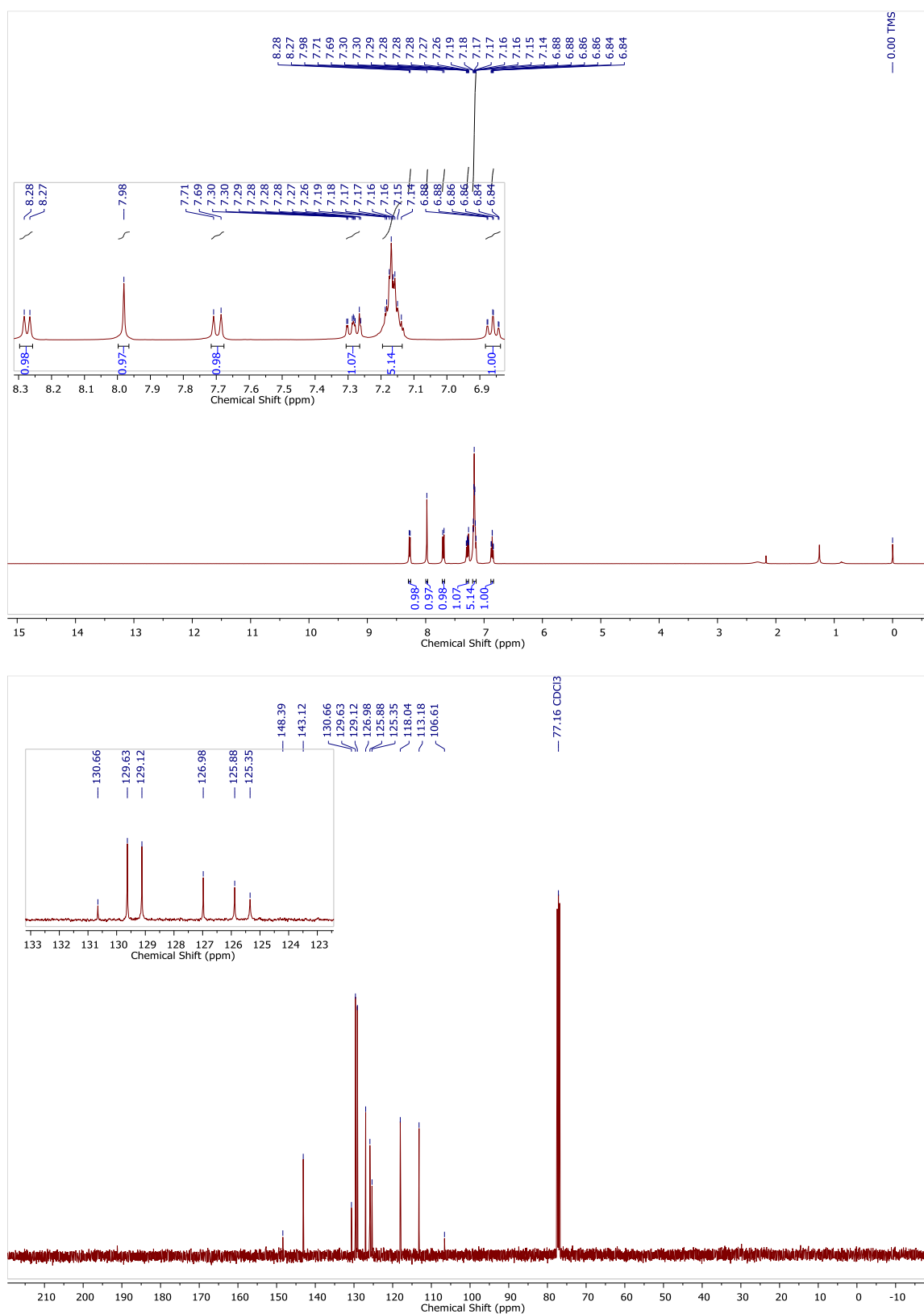


¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **4d**

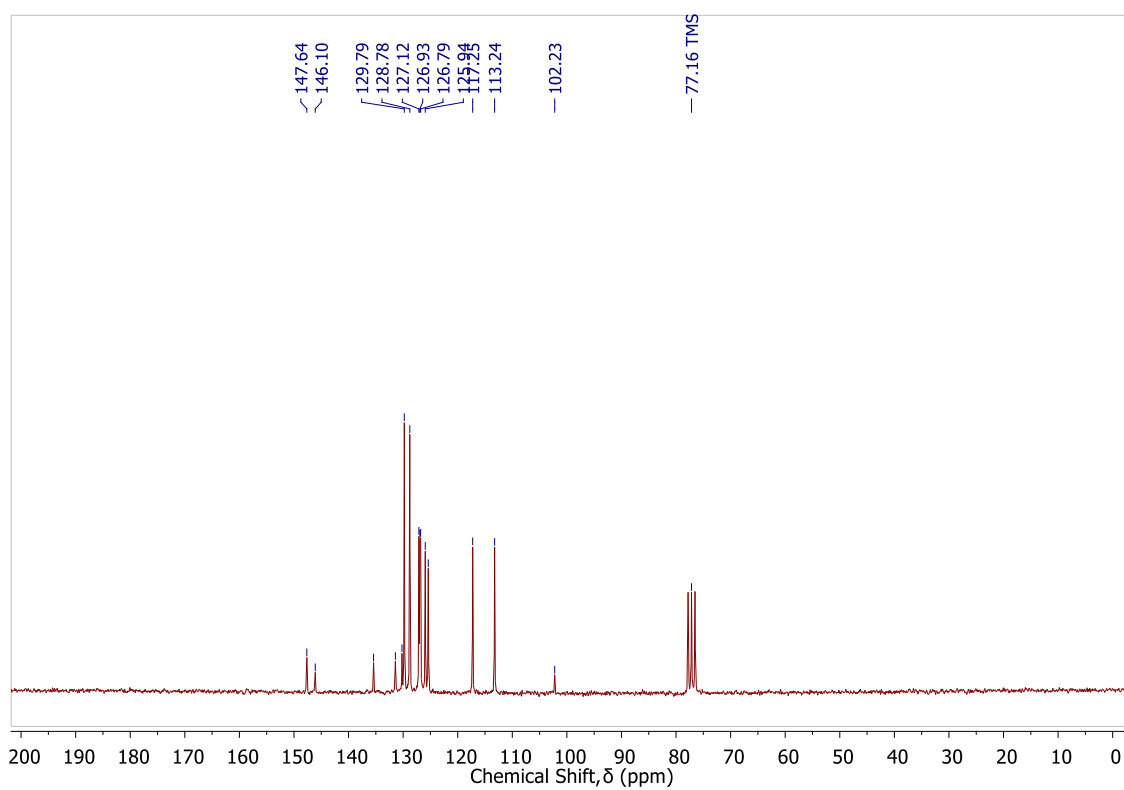
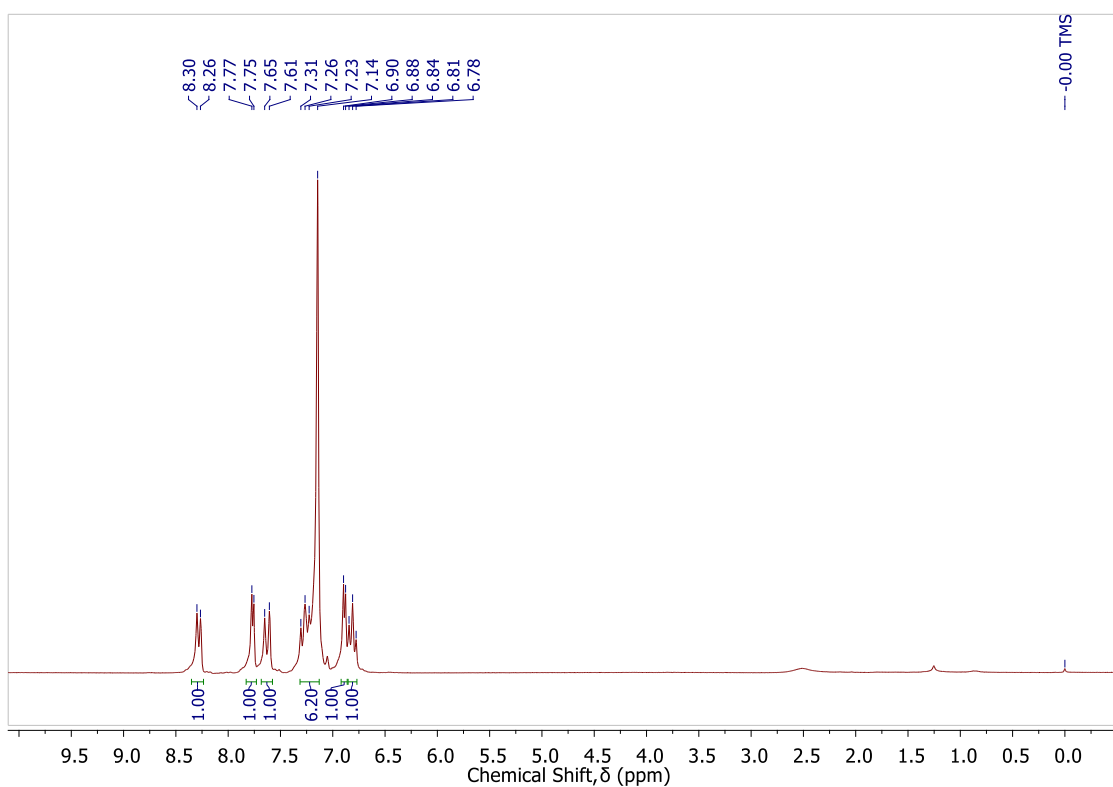




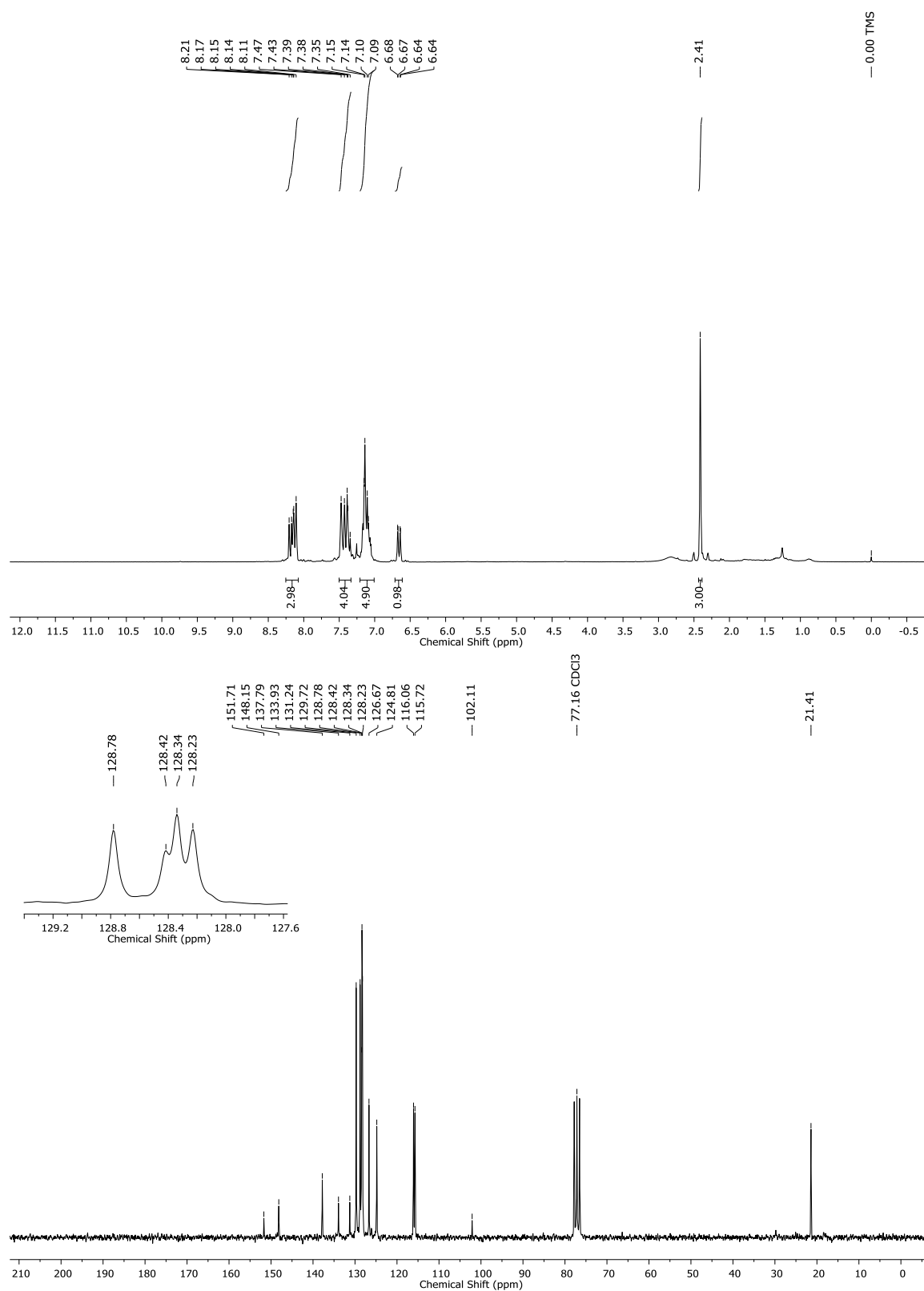
¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **4f**

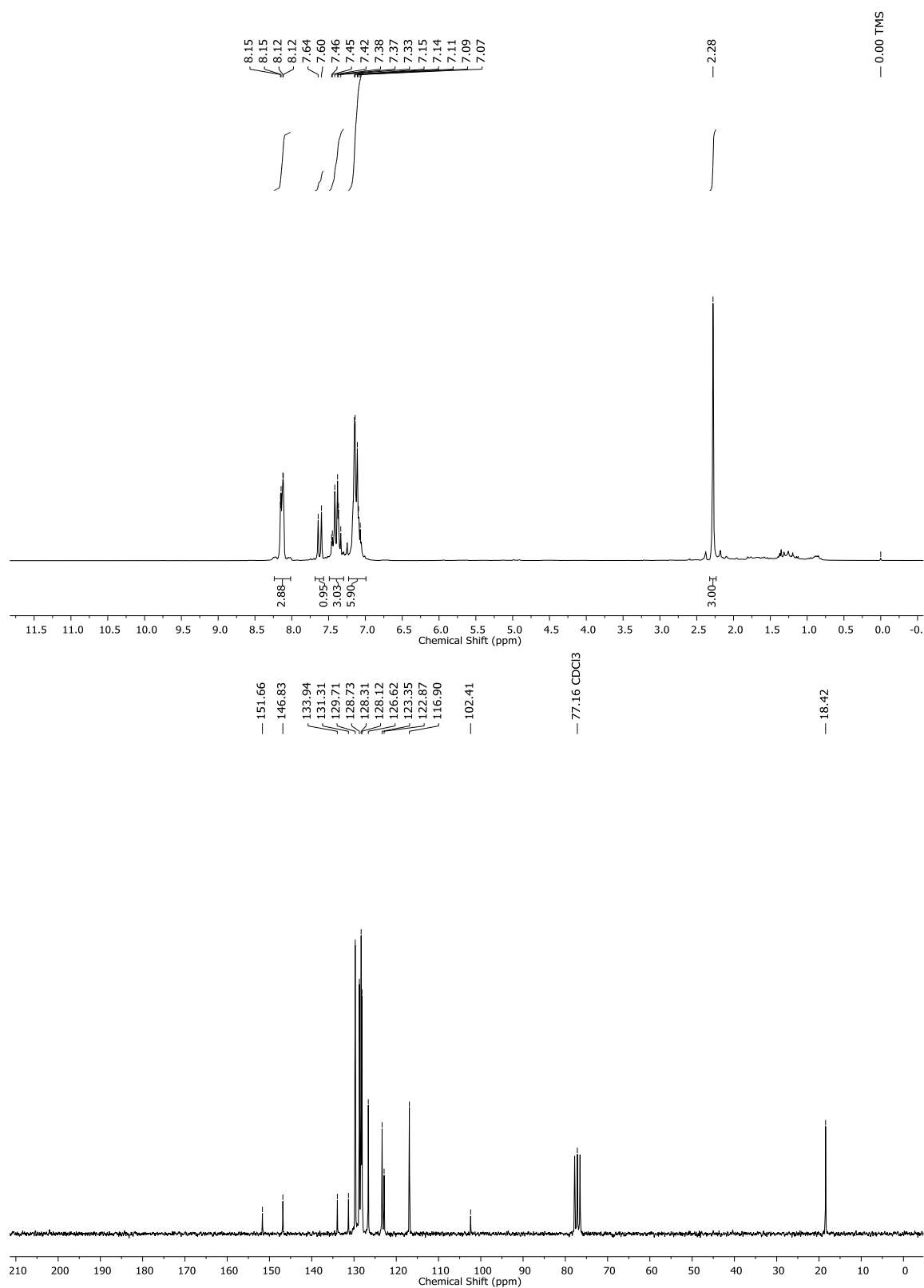


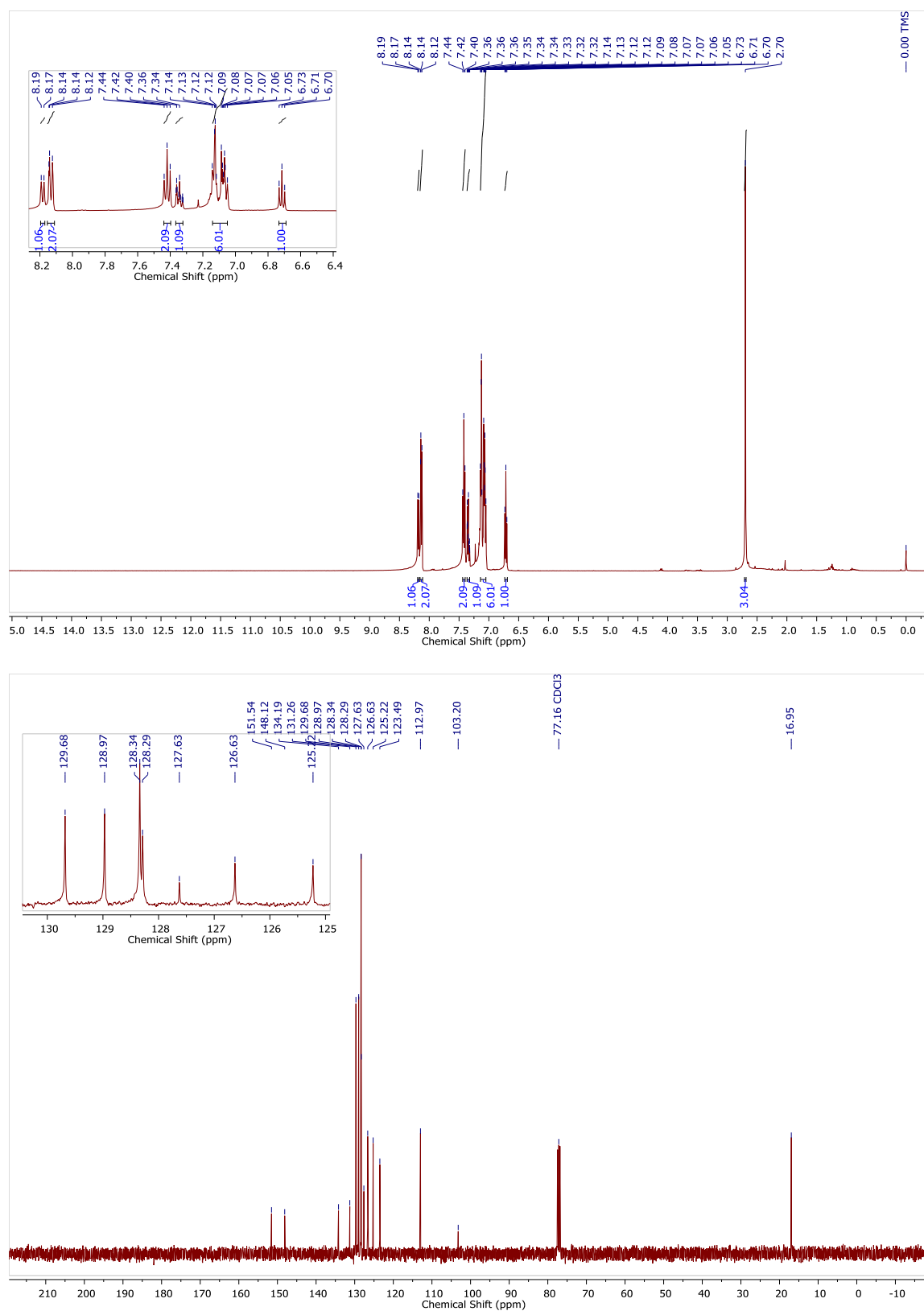
¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **4g**



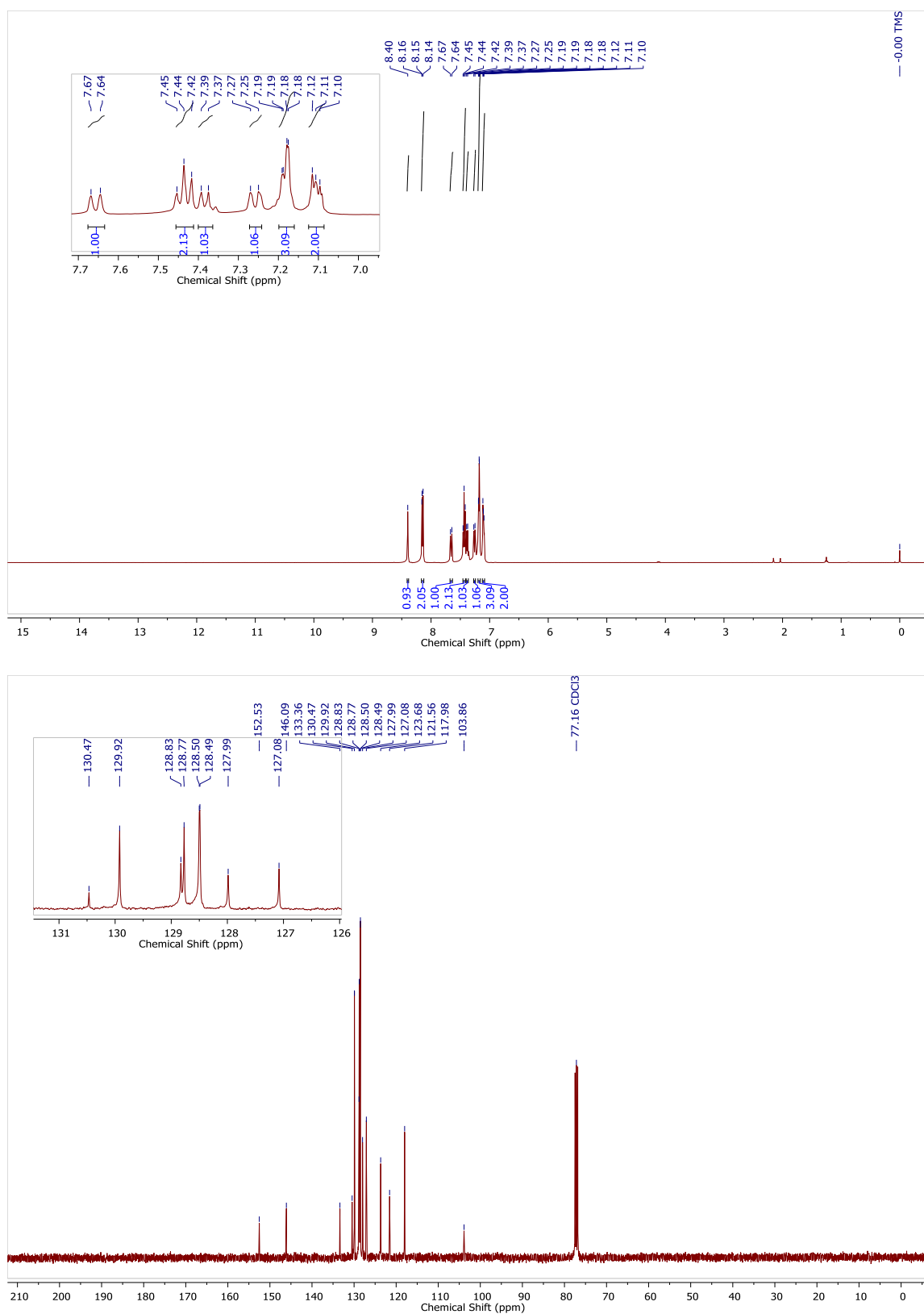
^1H NMR (top) ^{13}C NMR (bottom) CDCl_3 spectra of compound **4h**



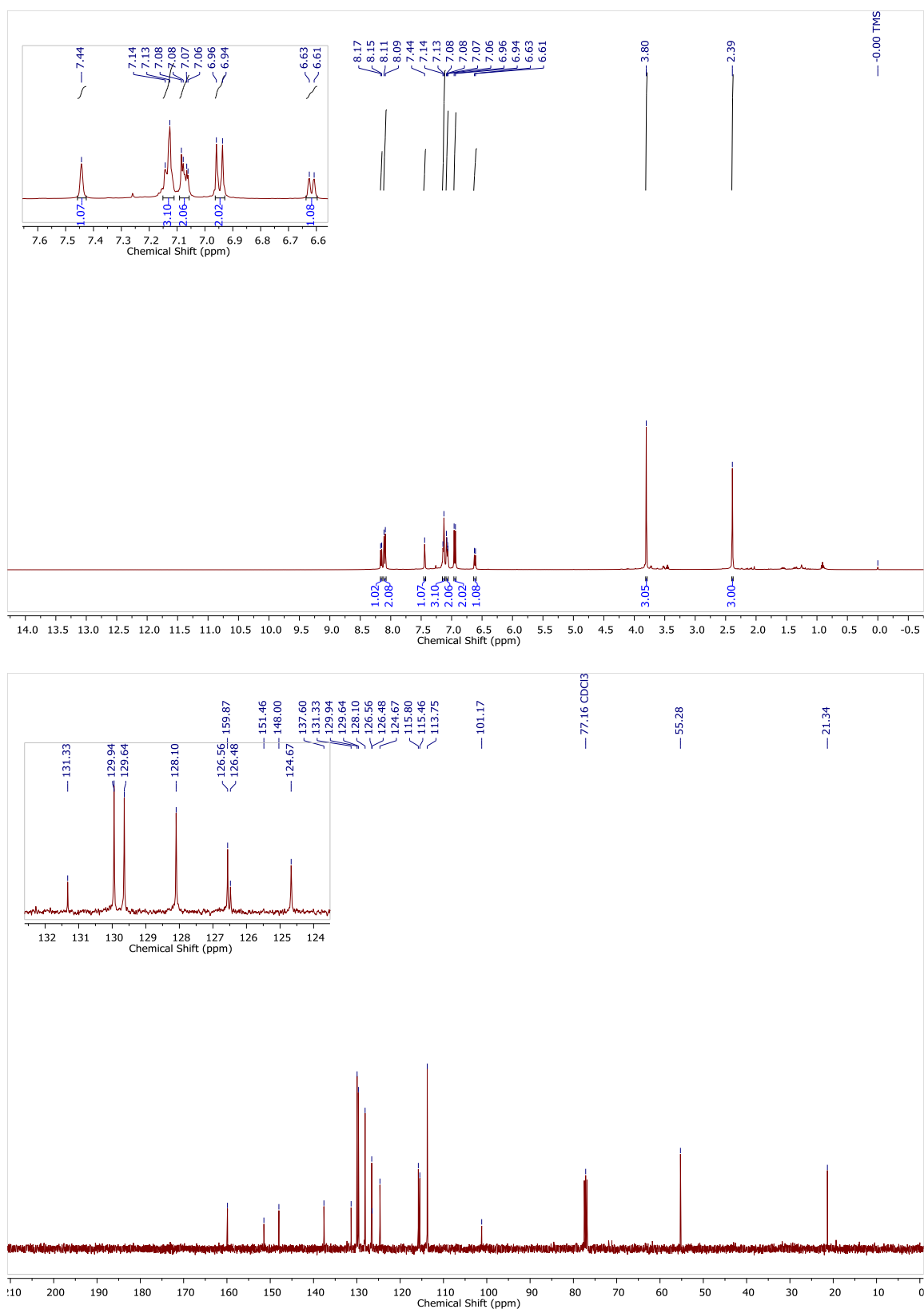


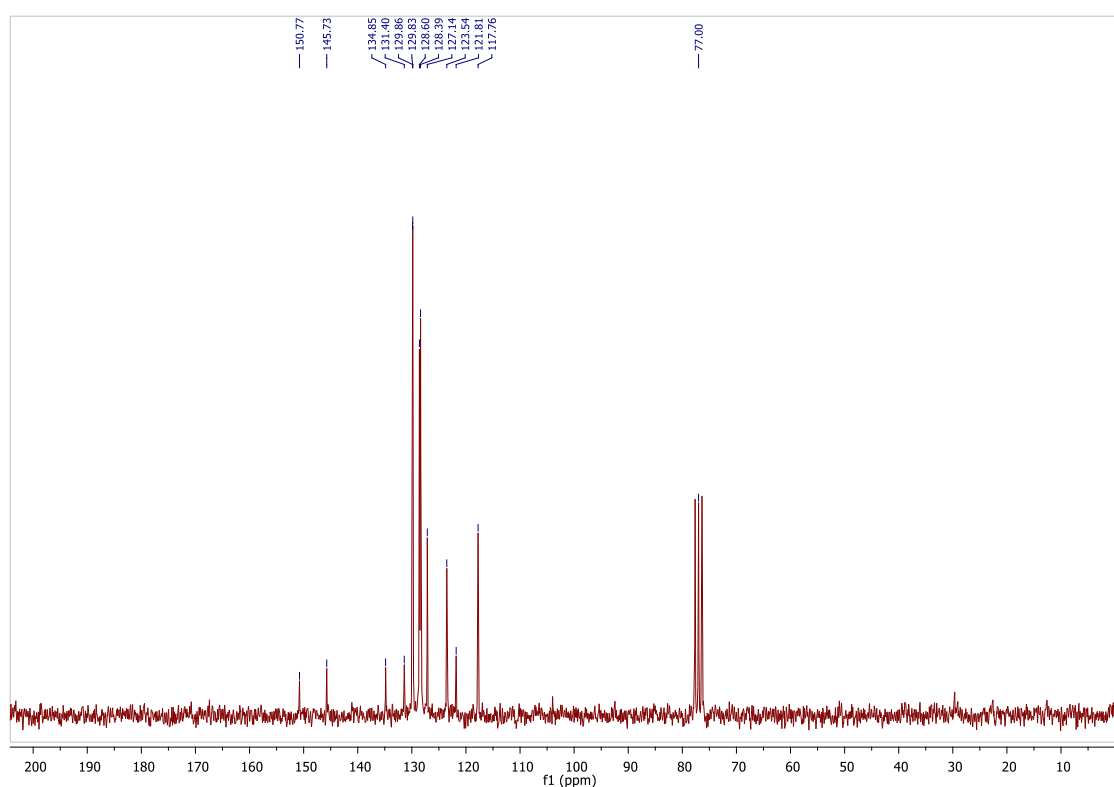
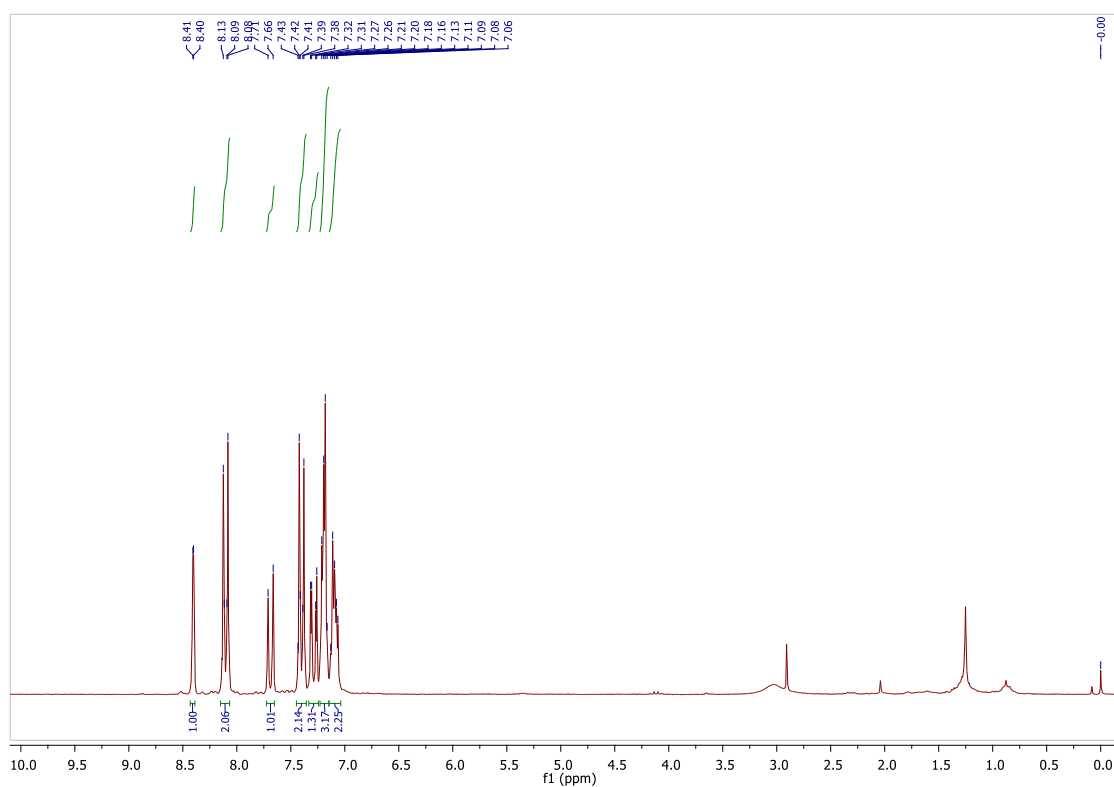


¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **4k**

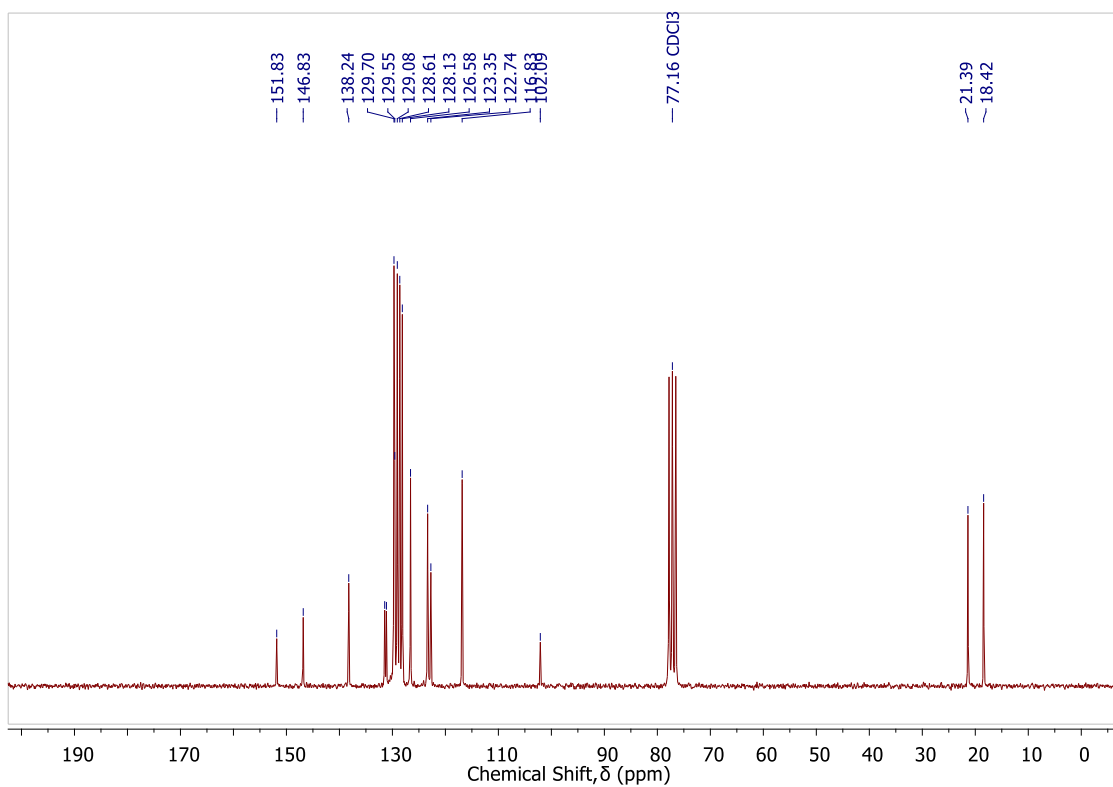
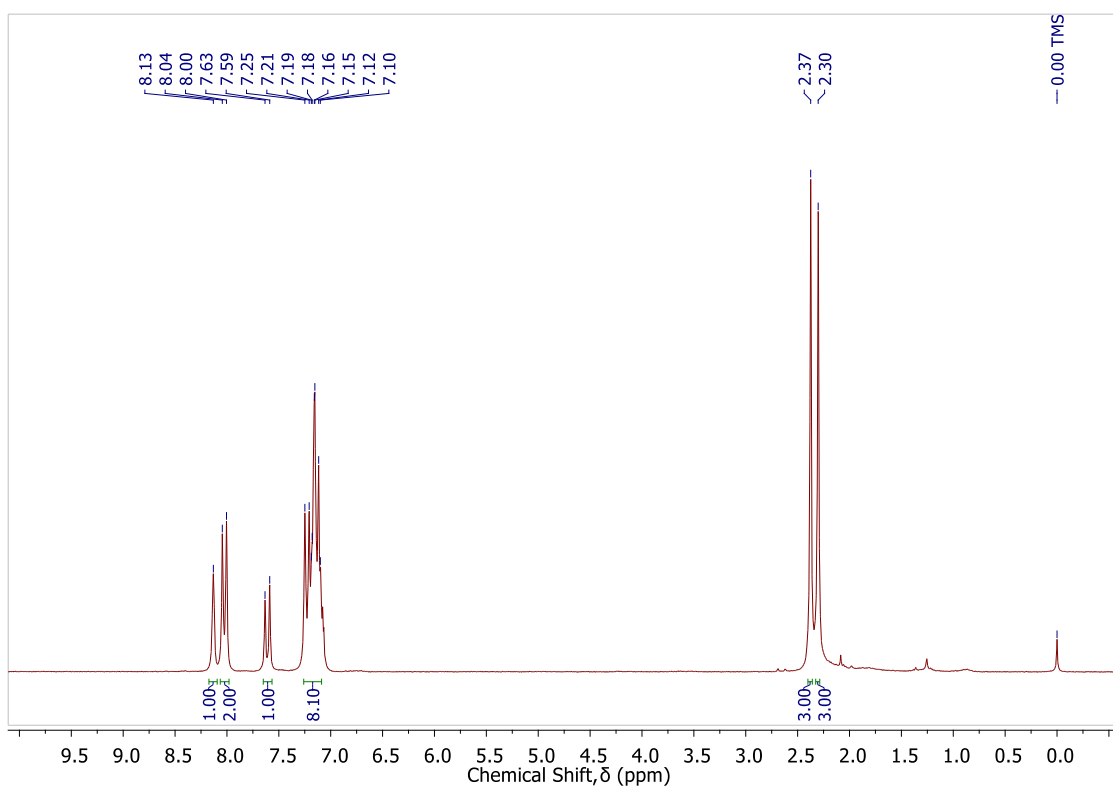


¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **4l**

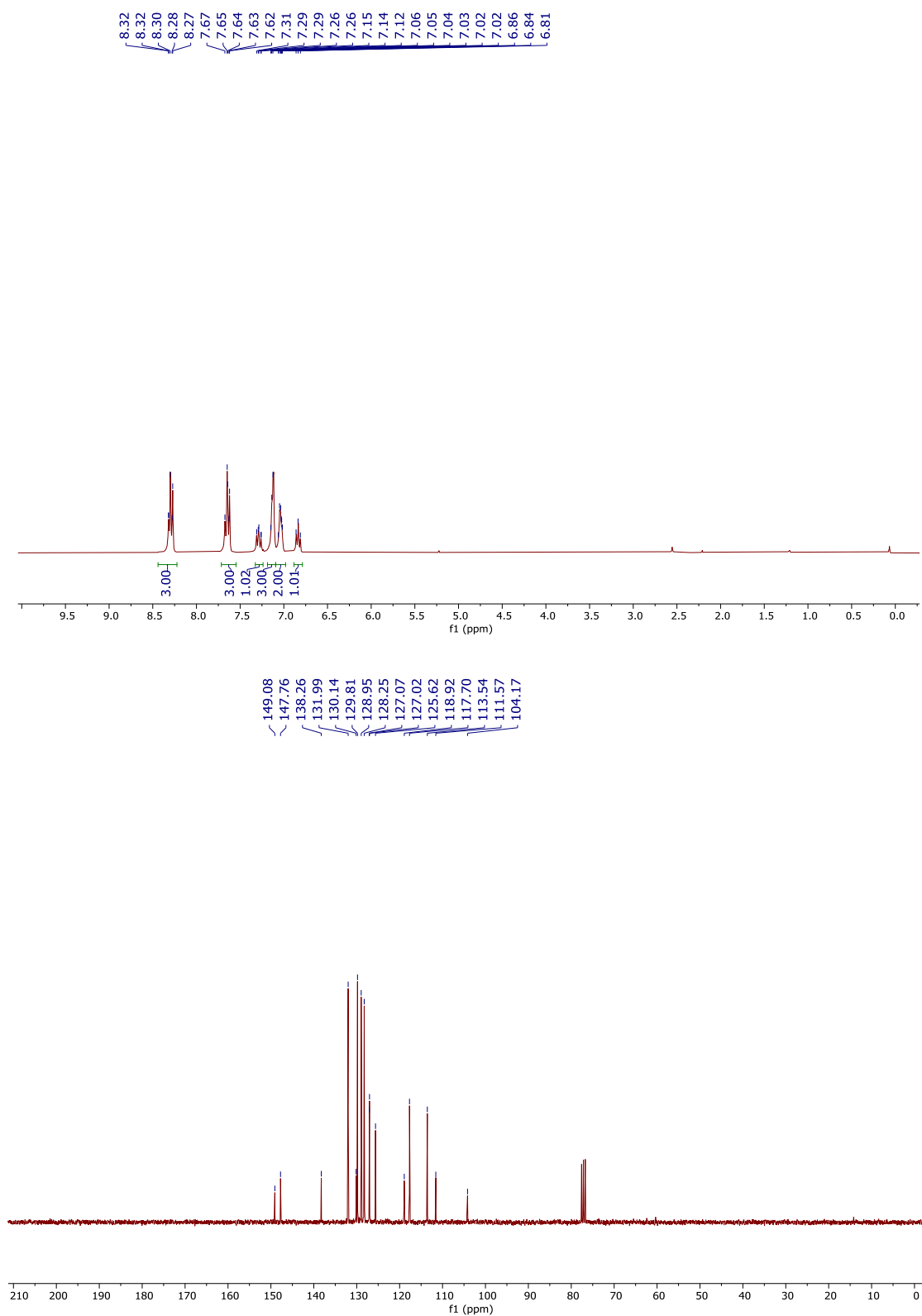


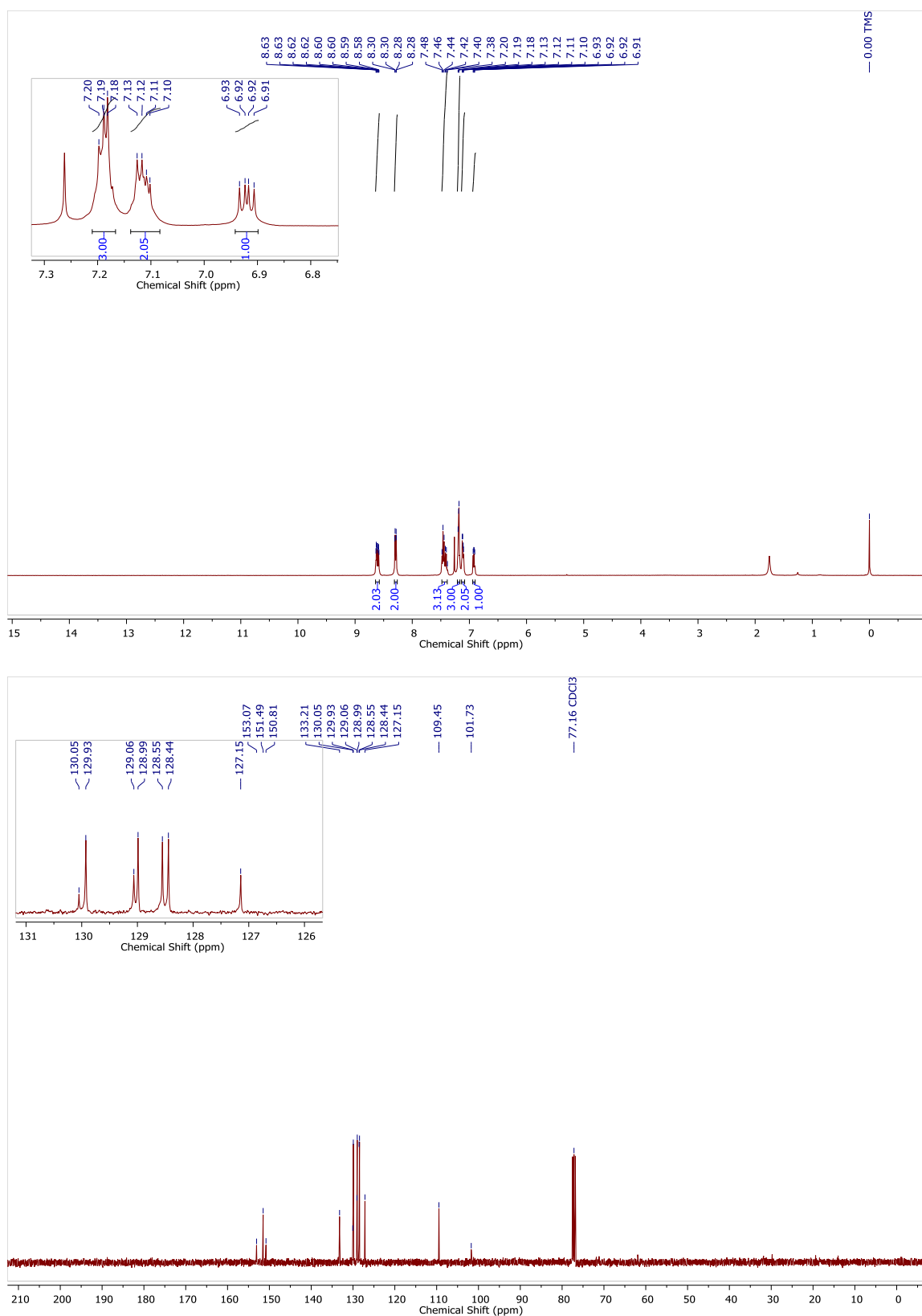


¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **4n**

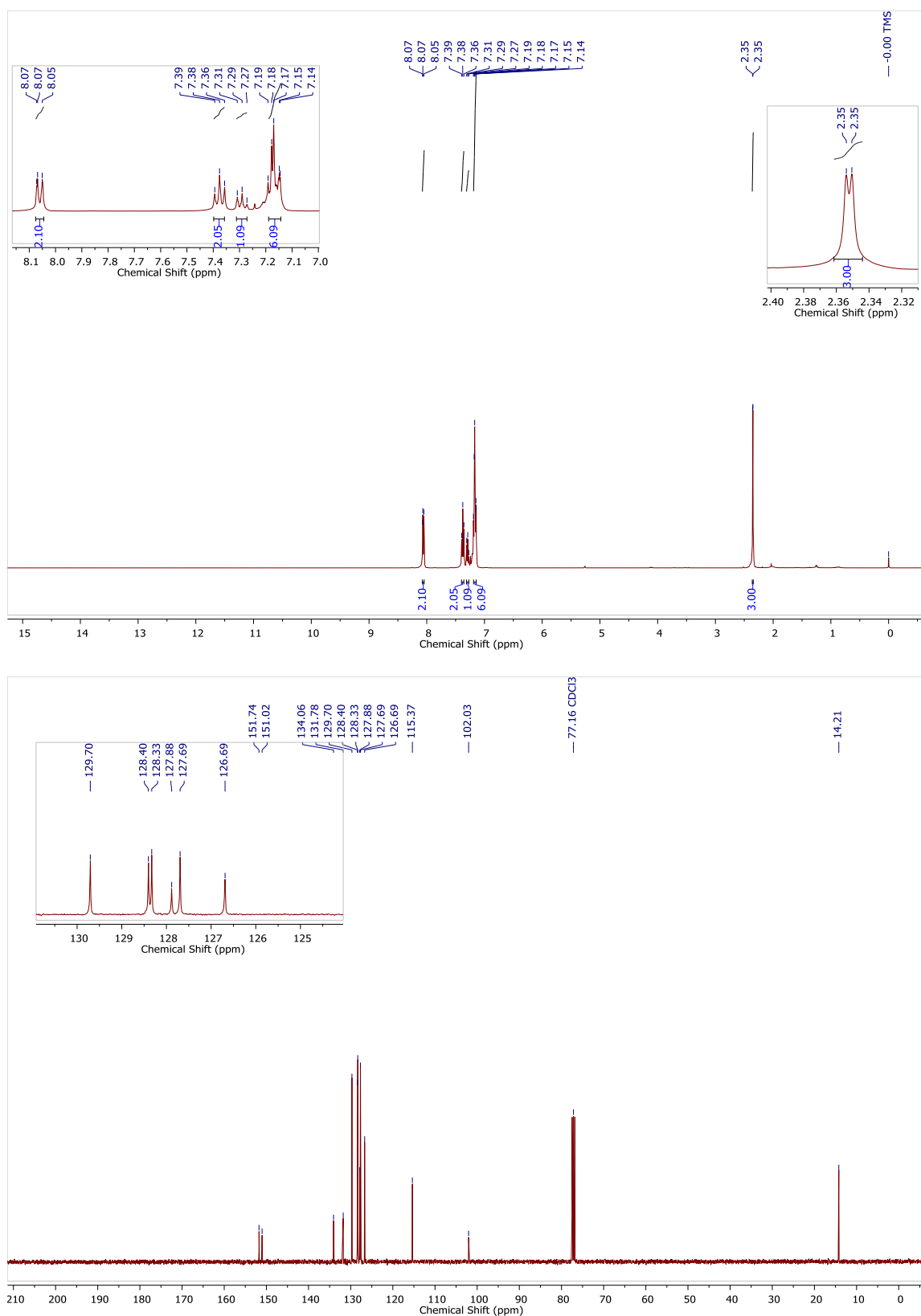


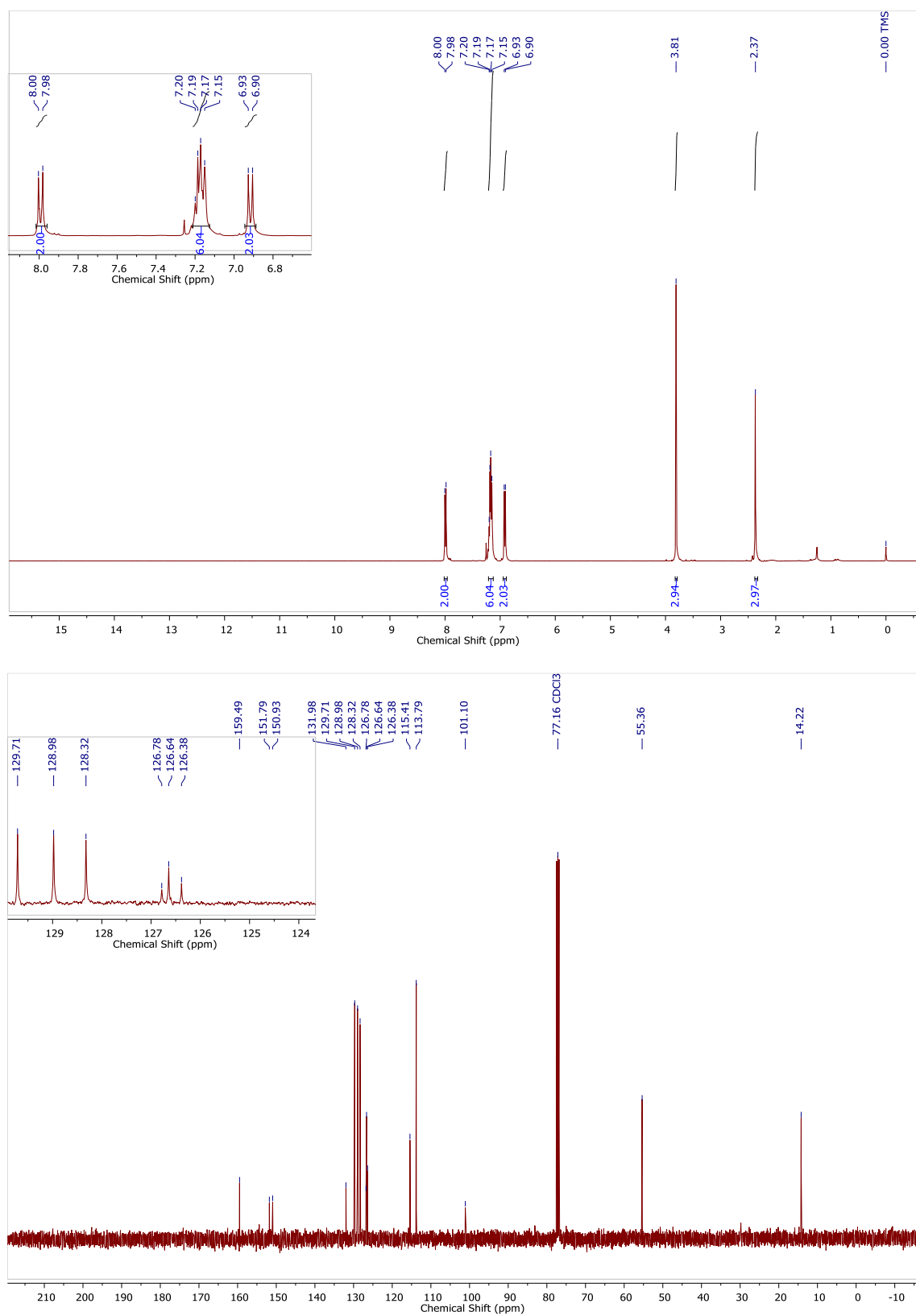
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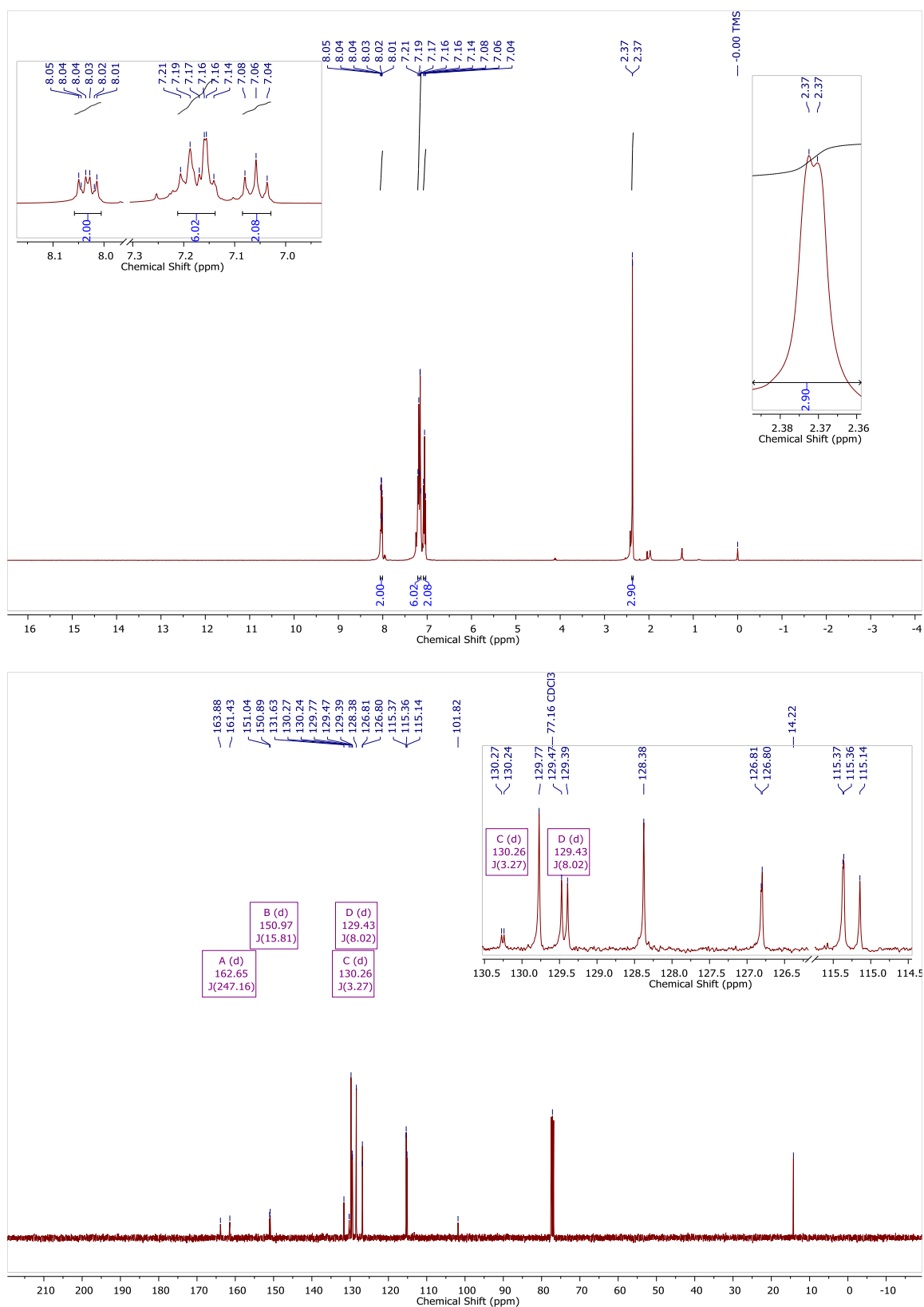


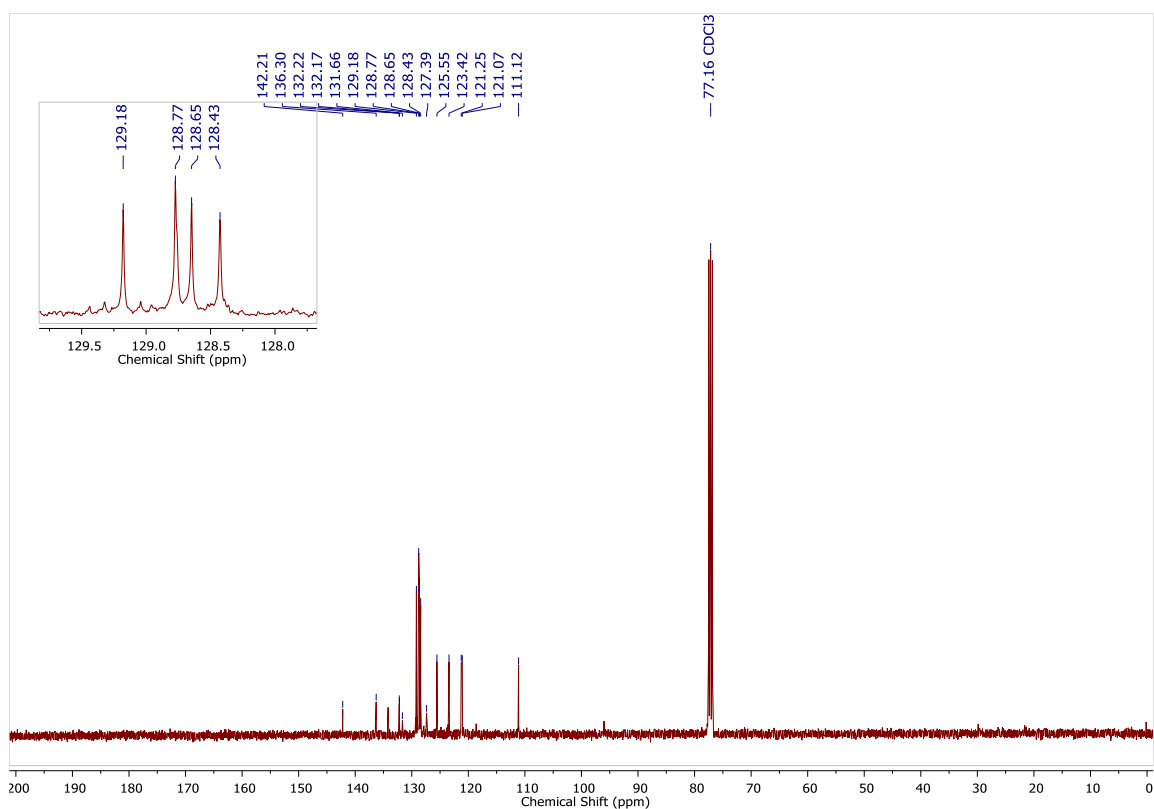
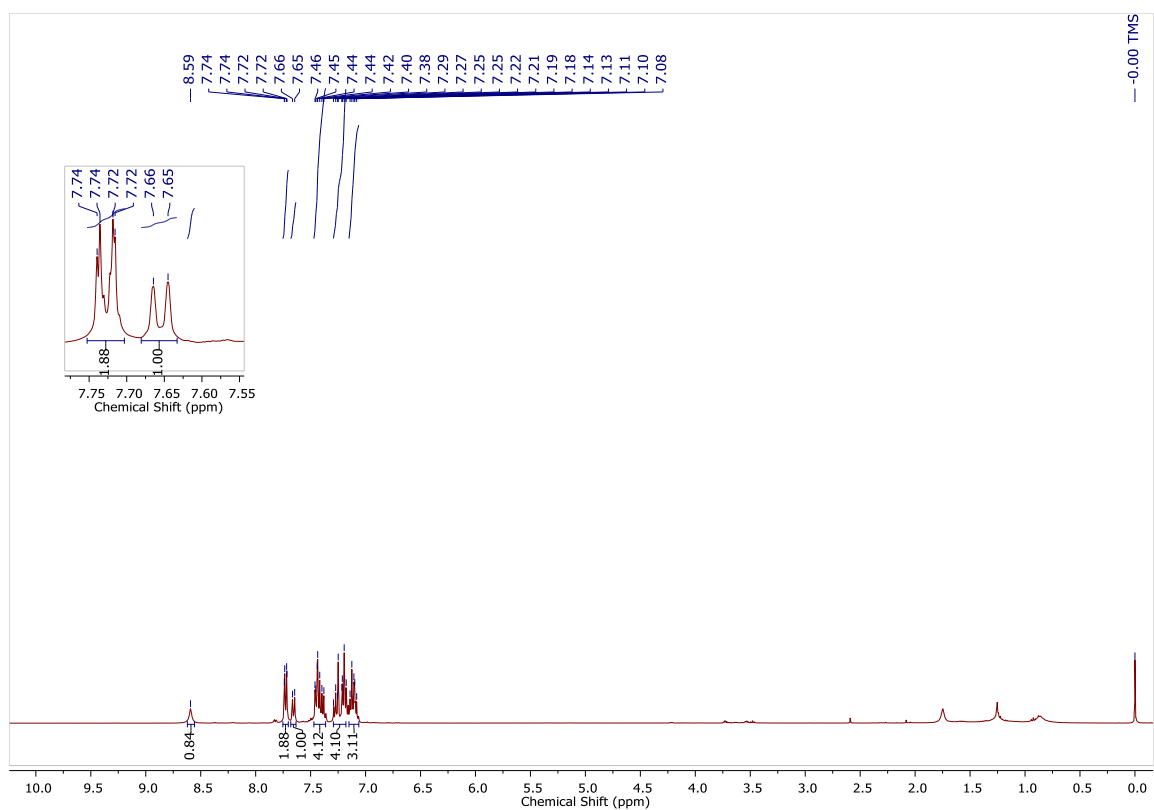


¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **6a**

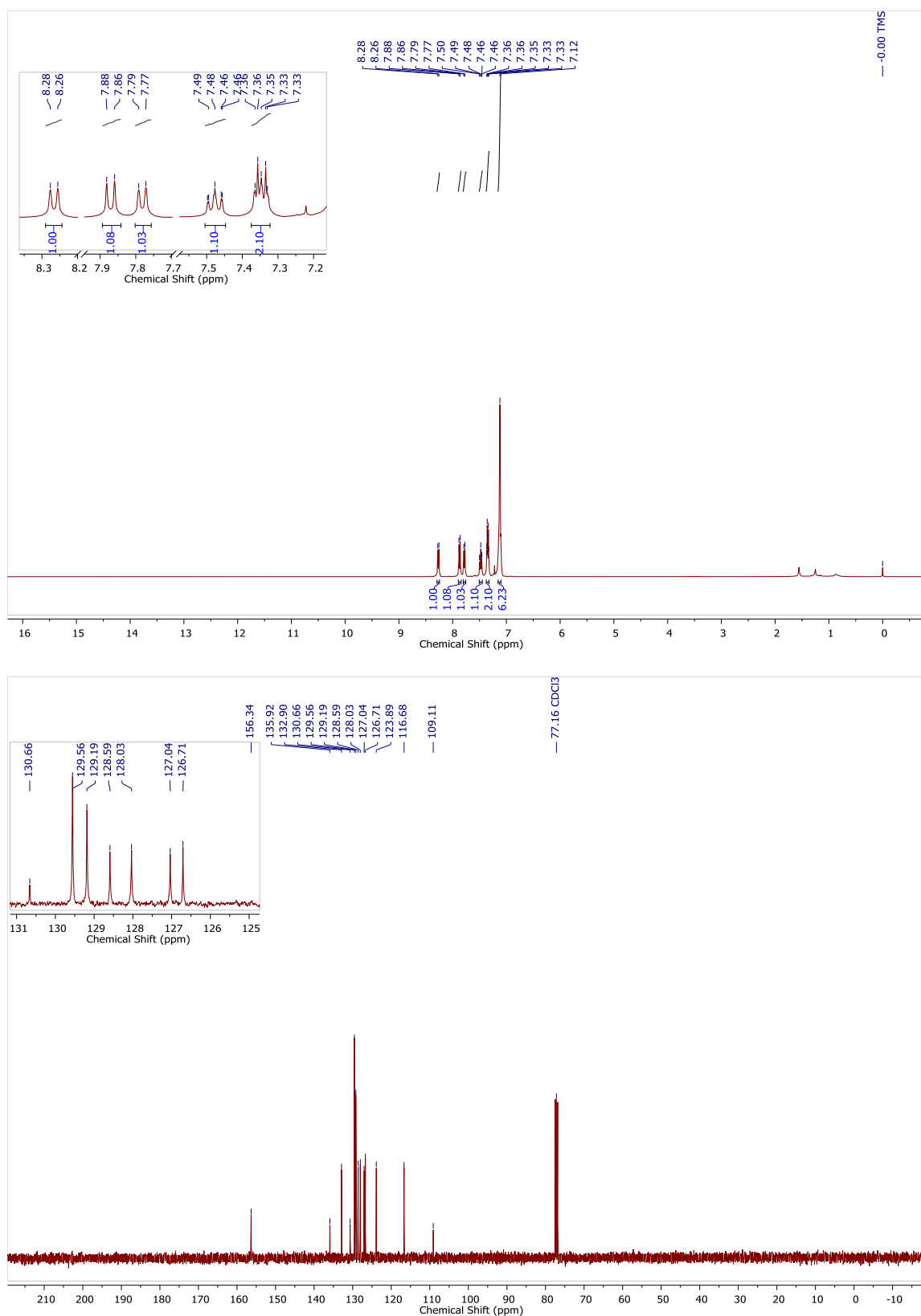


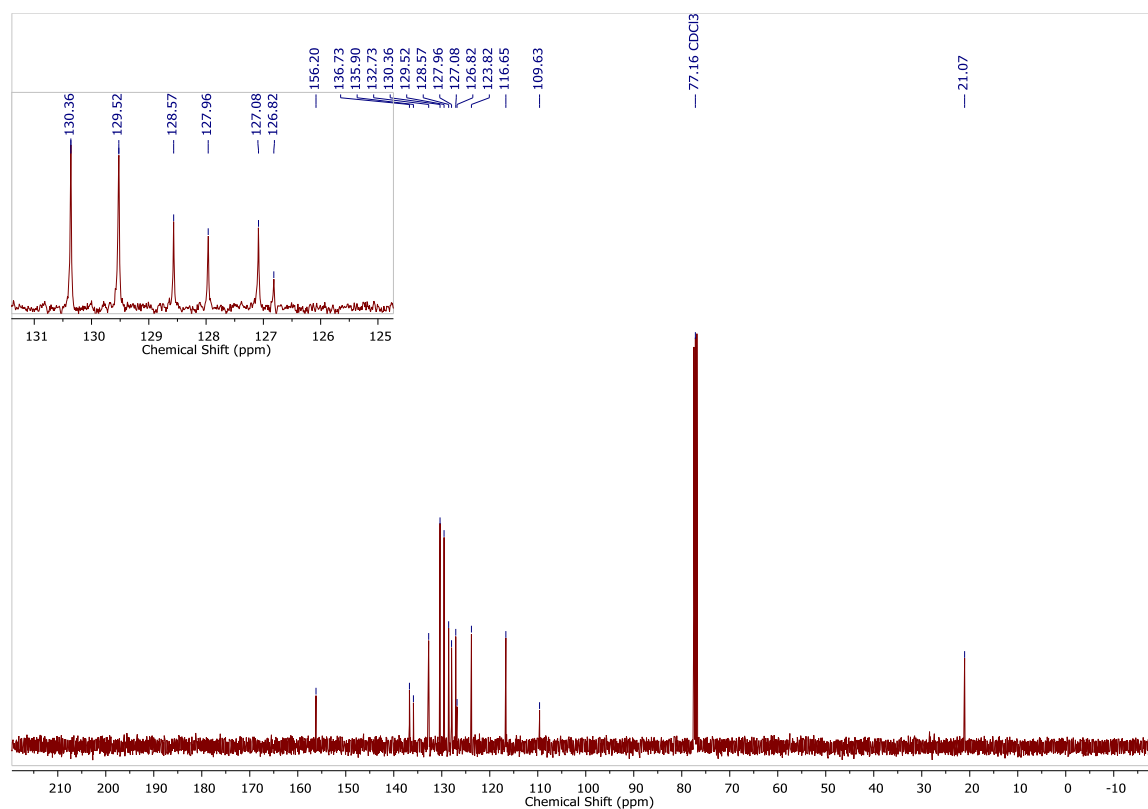
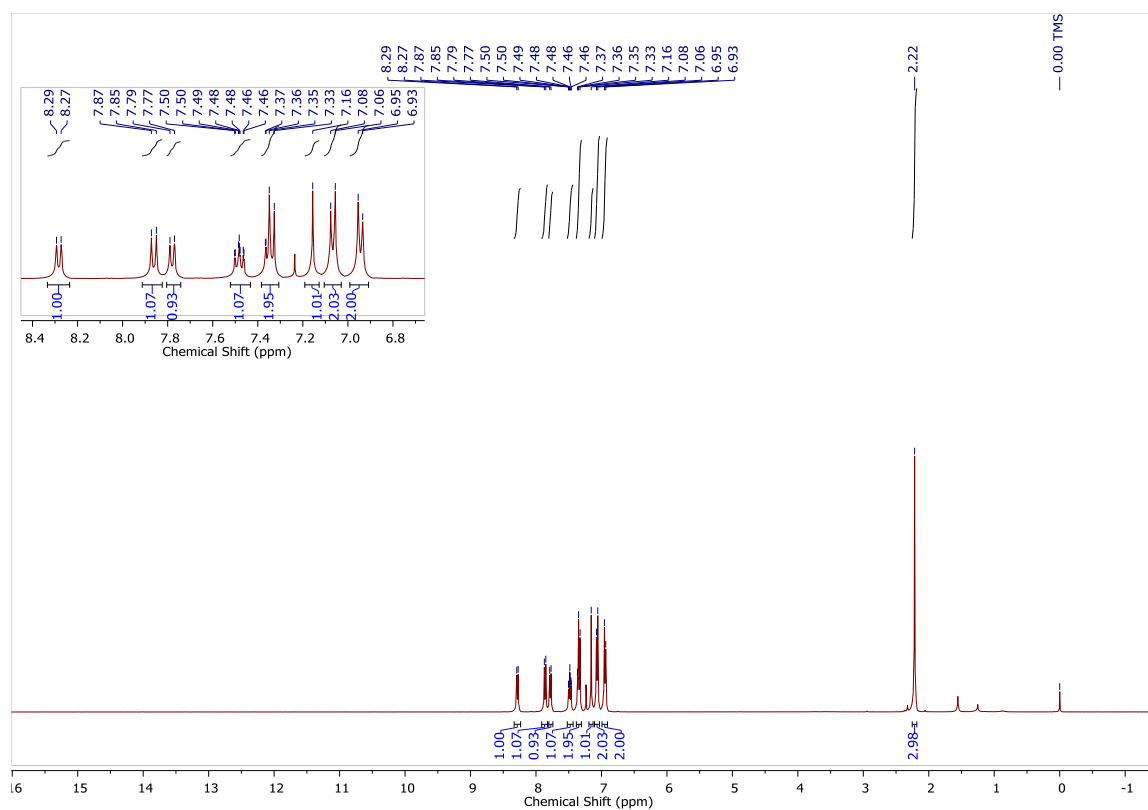




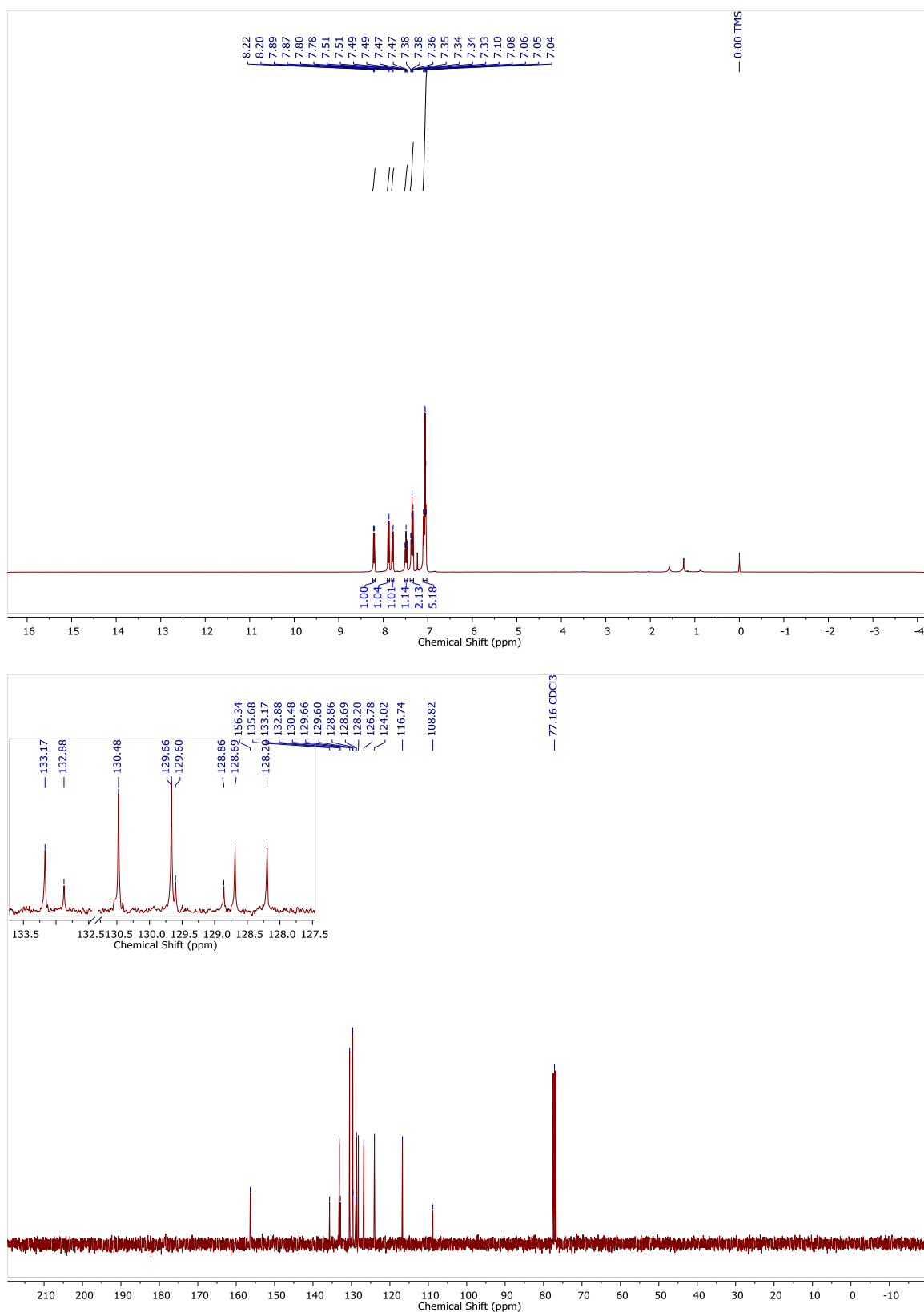


¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **6e**





¹H NMR (top) ¹³C NMR (bottom) CDCl₃ spectra of compound **6g**



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