Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

Palladium Catalyzed Synthesis of Poly-substituted and Poly-functionalised Conjugated 1,3-Dienes from Allyl Bromides and α-Diazoesters.

Hilal Ahmad Khan, Vikiho Wotsa, Lavanya. J and Chinnappan Sivasankar*

*Catalysis and Energy Laboratory, Department of Chemistry, Pondicherry University, R. V. Nagar, Puducherry 605 014, India.

Table of contents

X-Ray Crystallographic Data for 3a	3
¹ H and ¹³ C spectra	3-29

X-Ray Crystallographic Data for 3a:

The structure of **3a** was also determined by x-ray analysis. The single crystal for the analysis was grown by slow evaporation of solution of **3a** in hexane-ethylacetate mixture. X Ray Crystallography: CCDC2149586 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallographic Data Centre via <u>www.ccdc.cam.ac.uk/data_request/cif</u>.

Crystal data and structure refinement Compound 3a

Formula: C₂₀ H₁₈O₄

Formula weight: 322.34 g/mol

Wave length: = 0.71073 Å

Crystal system: triclinic

Space group: P -1

Color of crystal: colourless

Unit cell parameters: a = 9.8517(5) Å $\alpha = 86.084(2)^{\circ}$ b = 10.0871(5) Å $\beta = 71.973(2)^{\circ}$ c = 10.0861(5) Å $\gamma = 64.392(2)^{\circ}$

Temperature of data collection: 300(2) K

Values of Z, R, GOF:

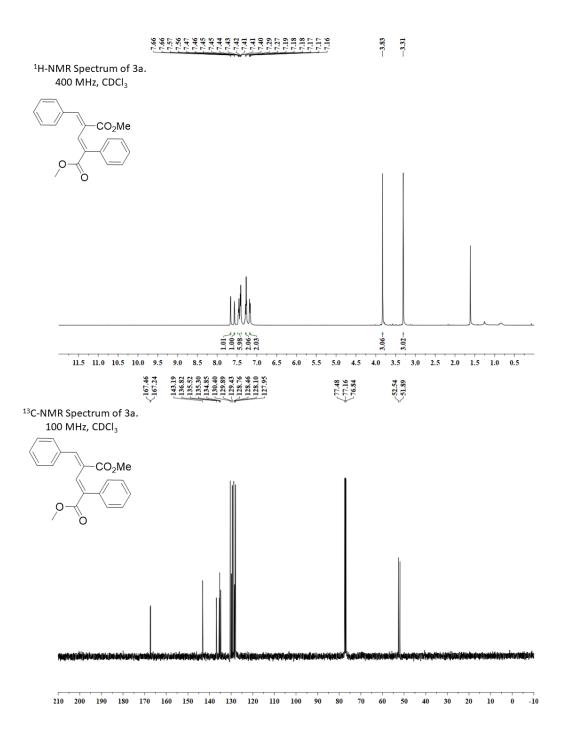
$$Z = 2$$

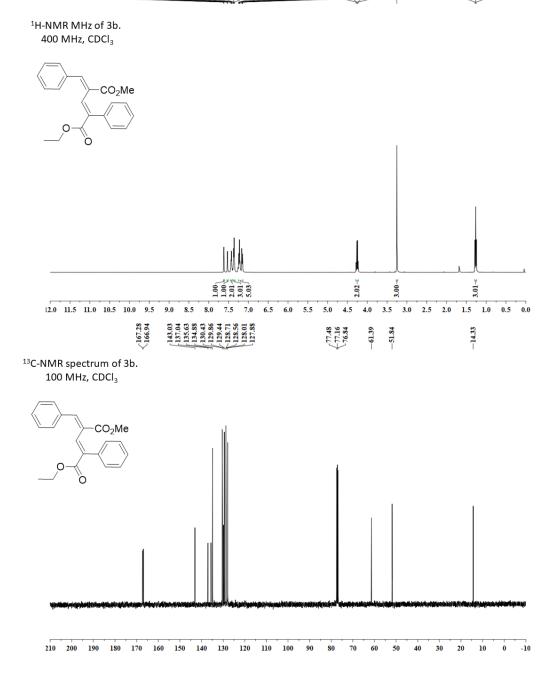
R(reflections) = 0.0443(2849), wR2(reflections) = 0.1151(3478)
GOF = 1.035

Measurement device type: Bruker D8 goniometer

Computing structure solution: SHELXT 2018/2 (Sheldrick, 2018)

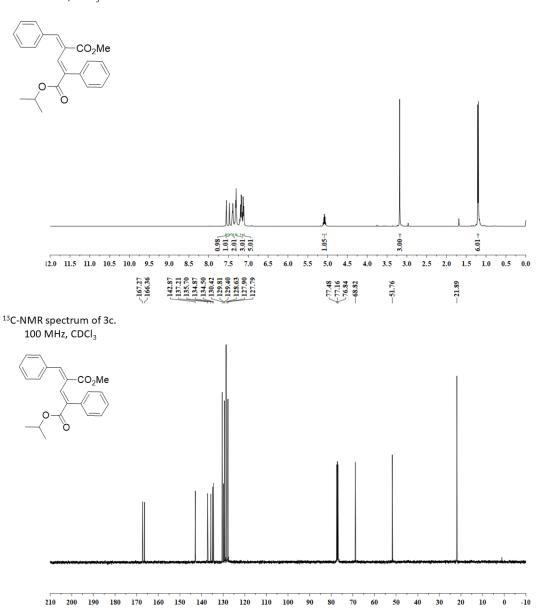
Computing structure refinement: SHELXL-2018/3 (Sheldrick, 2018)

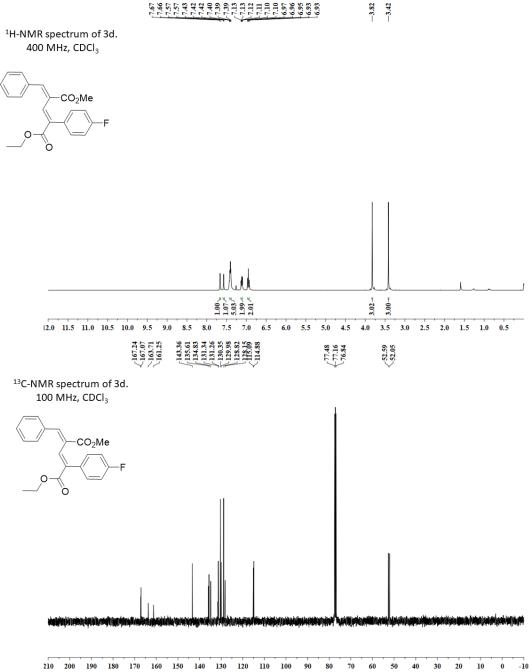


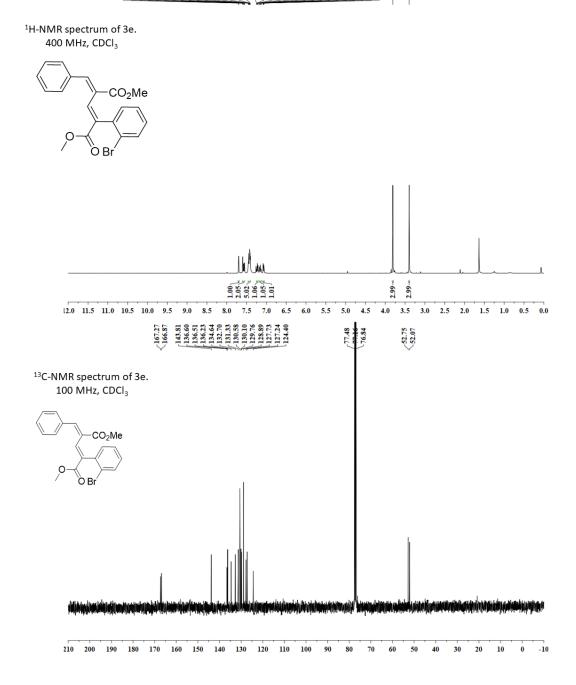


 $<^{1.21}_{1.20}$

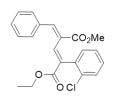
¹H-NMR spectrum of 3c. 400 MHz, CDCl₃

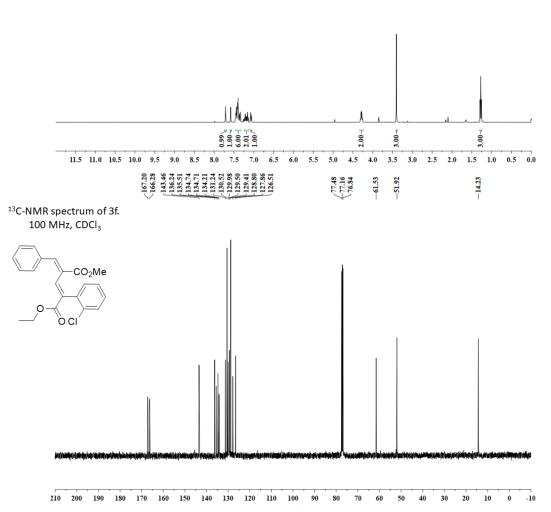


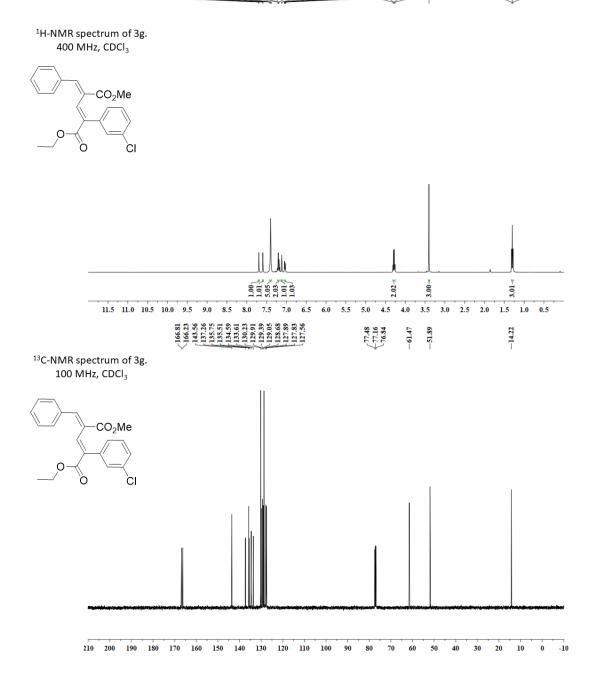


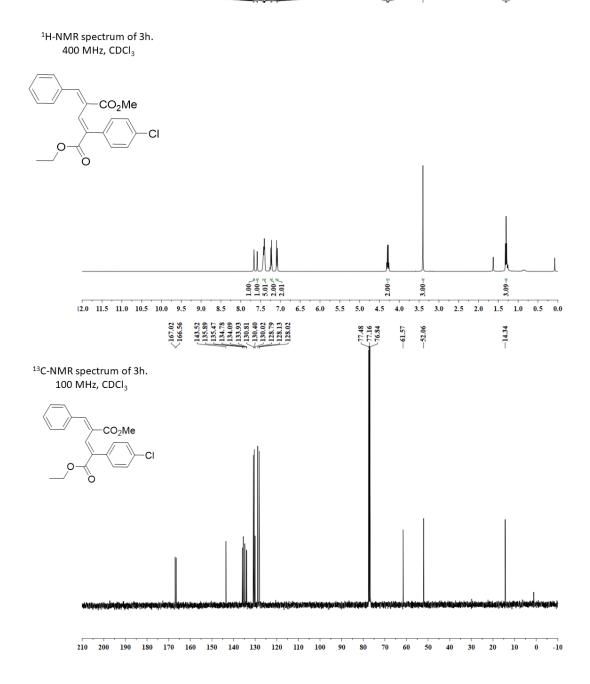


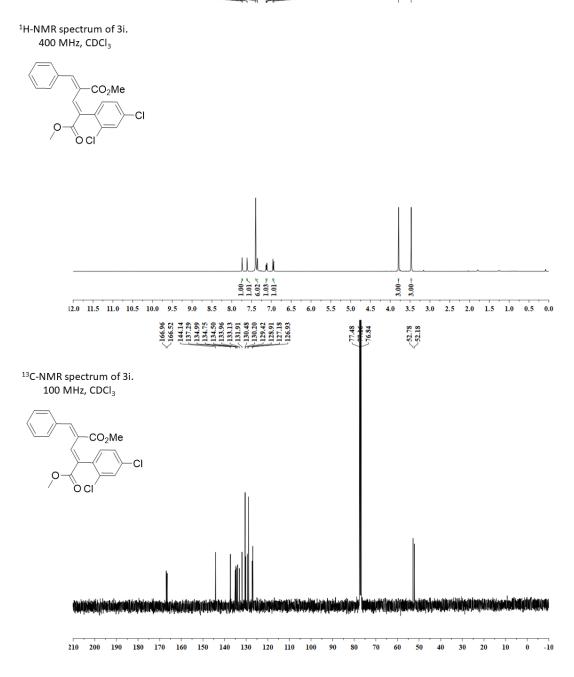
¹H-NMR spectrum of 3f. 400 MHz, CDCl₃

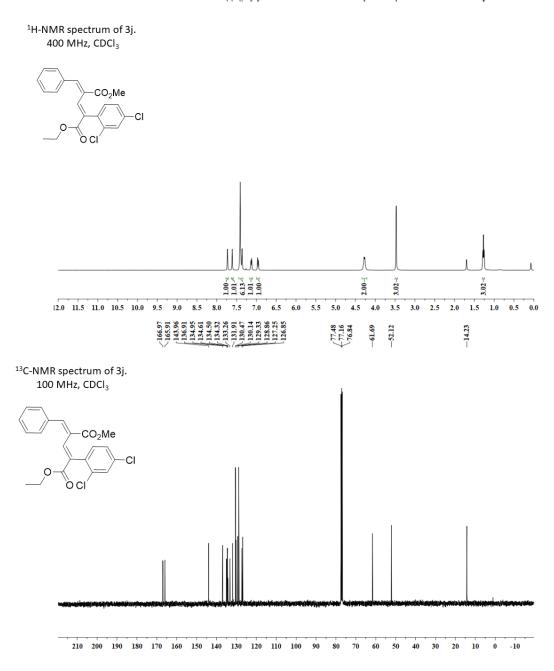






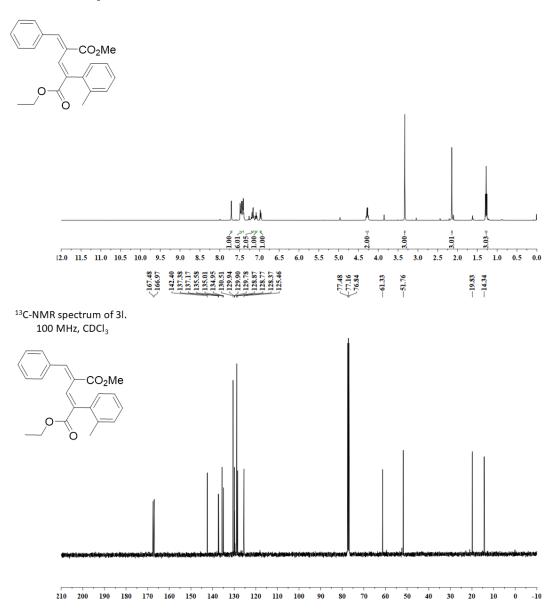


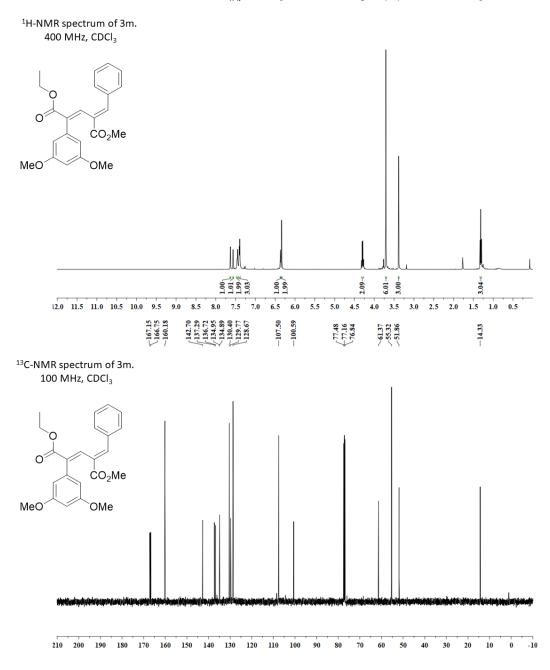


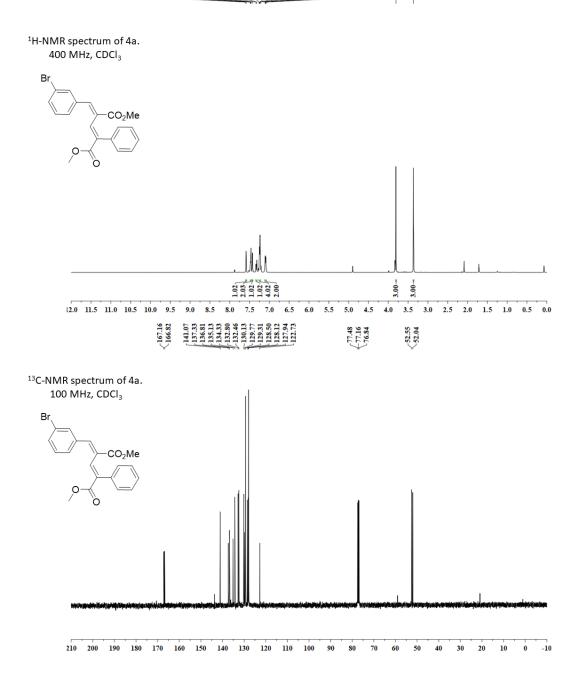


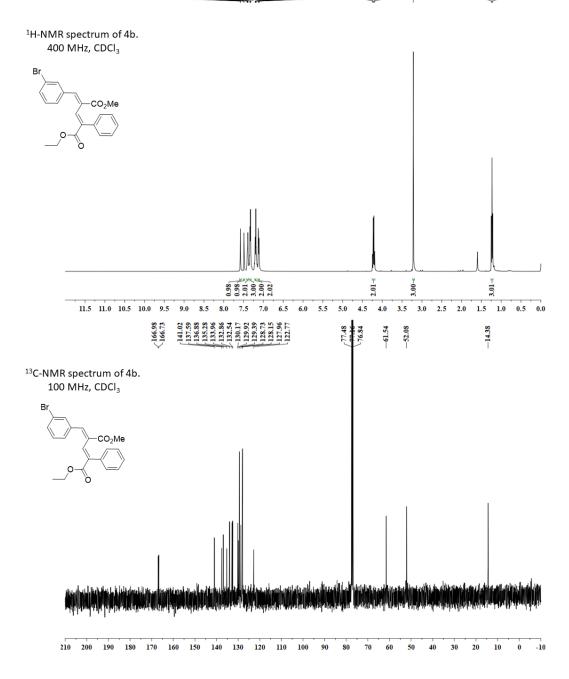
¹H-NMR spectrum of 3k. 400 MHz, CDCl_3 -CO₂Me 0 1.04 ∼ 5.99 ∀ 2.03 \ 1.06 ≪ 3.00--2.99--12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -167.52 142.61 137.16 135.92 135.93 135.93 135.93 135.93 135.93 135.93 129.84 129.54 129.54 129.54 128.45 125.51 77.48 77.16 76.84 <52.50 <51.77 -19.76 ¹³C-NMR spectrum of 3k. 100 MHz, CDCl₃ -CO₂Me 0 210 200 190 180 170 160 150 140 130 120 110 100 90 60 50 30 10 0 -10 80 70 40 20

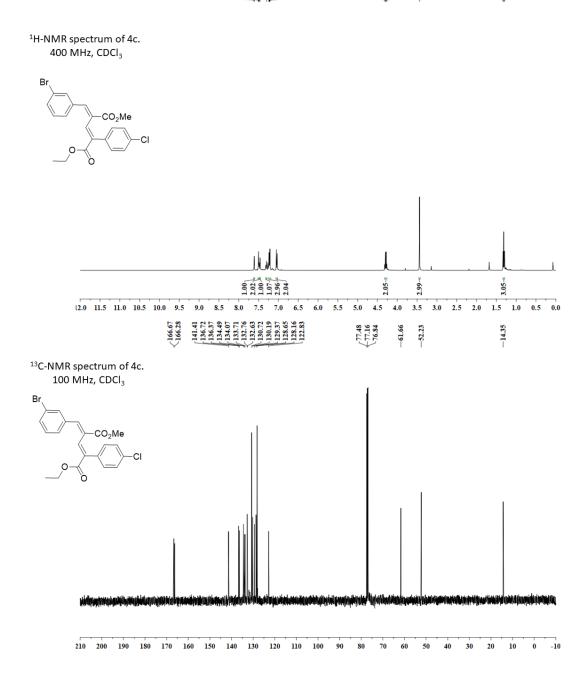
¹H-NMR spectrum of 3I. 400 MHz, CDCl₃



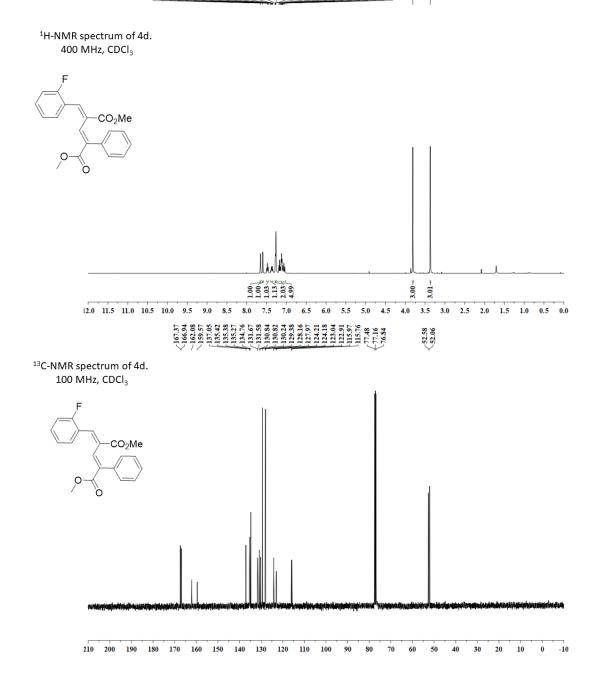


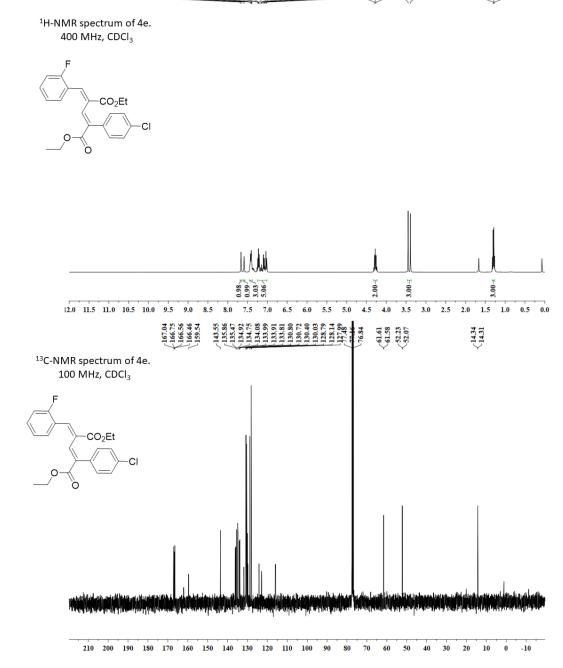


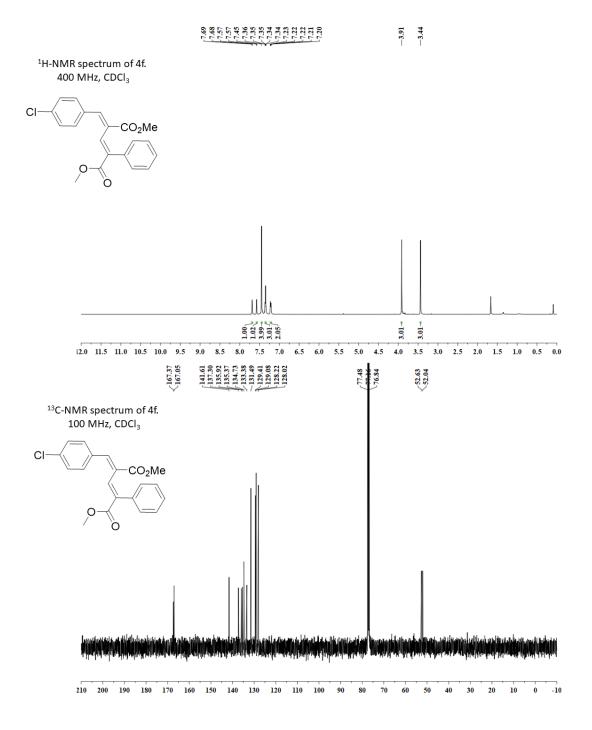


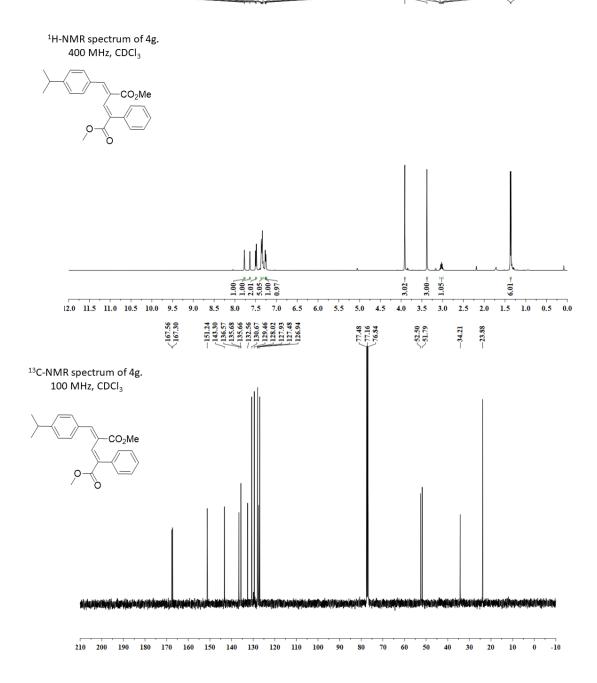


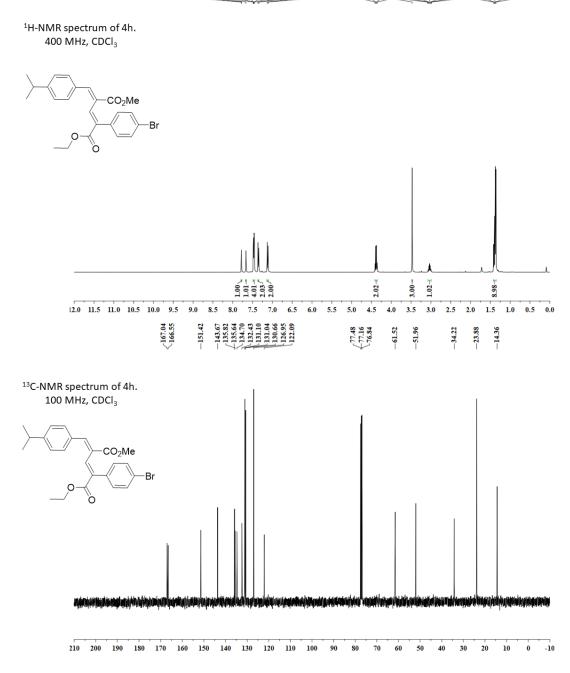
7,055 7,165 7,165 7,166 7,166 7,166 7,166 7,178

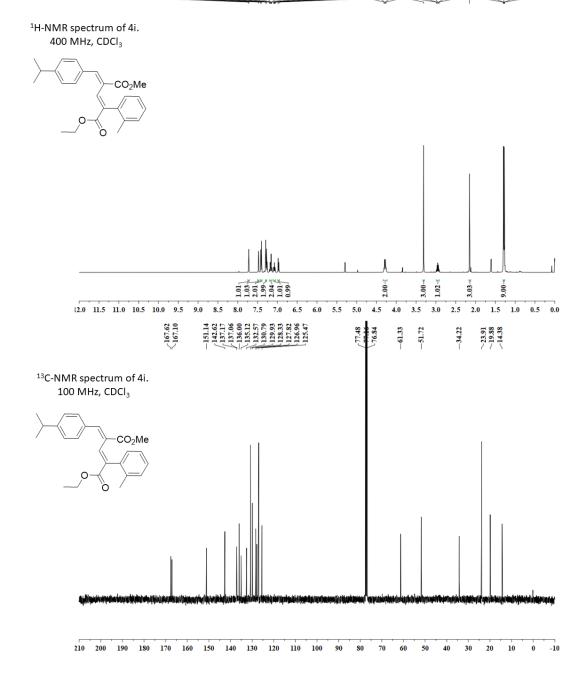


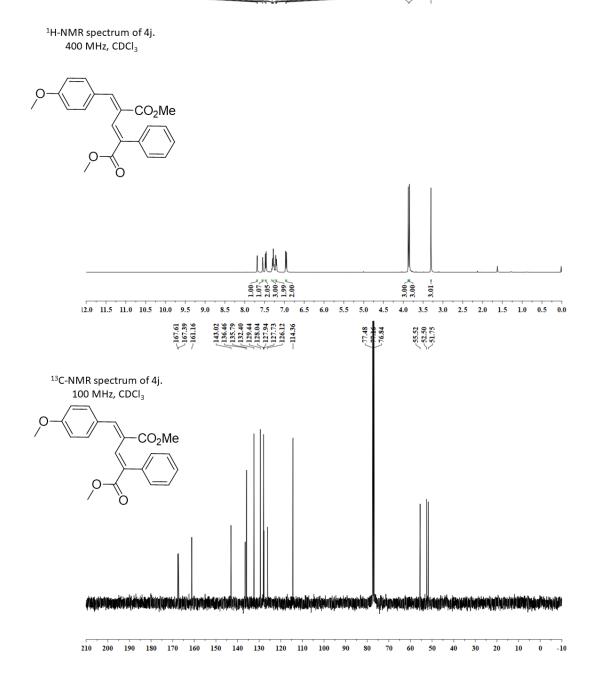






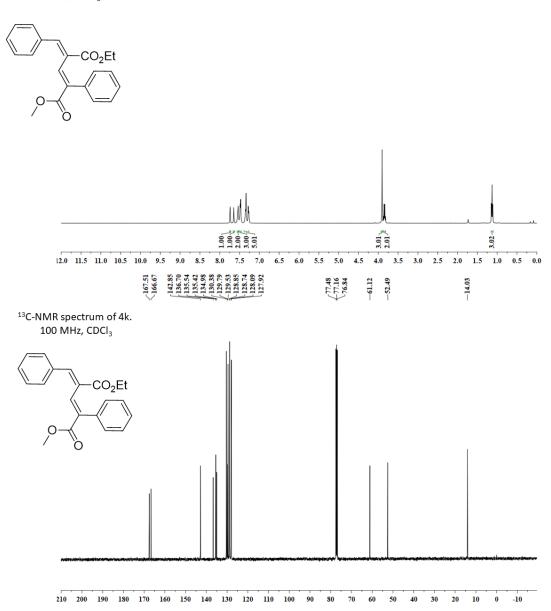






1.15 1.13 1.11

¹H-NMR spectrum of 4k. 400 MHz, CDCl₃



¹H-NMR spectrum of 4I. 400 MHz, CDCl₃

