Supporting Information

Biocatalytic Dynamic Kinetic Reductive Resolution with ketoreductase from *Klebsiella pneumoniae*: Asymmetric synthesis of functionalized tetrahydropyrans

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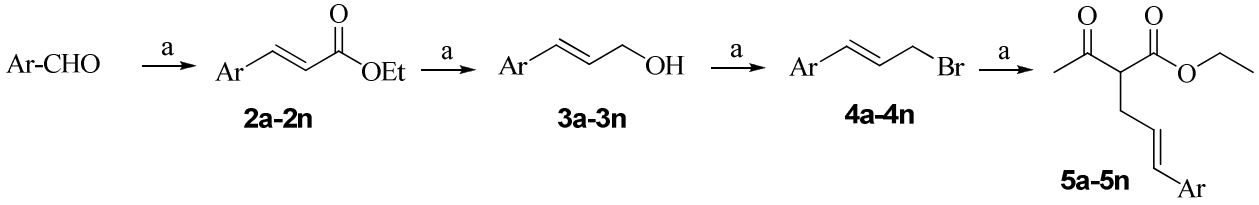
Experimental section

General procedures: All oxygen and/or moisture-sensitive reactions were carried out under N_2 atmosphere in glassware that had been flame-dried under vacuum (ca. 0.5 torr) and purged with N_2 prior to use. Unless otherwise stated, materials were obtained from commercial suppliers and used without further purification.THF and diethyl ether were distilled from sodium benzophenone ketyl. Dichloromethane (DCM) and hexane were distilled from calcium hydride. Ketoreductase strain of *K. pneumoniae* (NBRC 3319) was obtained from NBRC, Japan. Reactions were stirred magnetically using Teflon-coated magnetic stirring bars. Teflon-coated magnetic stirring bars and syringe needles were dried in an oven at 120 °C for at least 12 h prior to use, then cooled in a desiccator cabinet over Drierite. Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm silica gel plates with UV light as a visualizing agent and ethanolic anisaldehyde/heat as a developing agent. Silica gel 100–200 mesh was used for column chromatography. Yields refer to chromatographically and spectroscopically homogeneous materials unless otherwise stated. NMR spectra were recorded on 600,400,500 and 200 MHz spectrometers at 25 °C in and calibrated using residual undeuterated solvent as an internal reference. Chemical shifts are shown in δ. ^{13}C NMR spectra were recorded in a complete

proton decoupling environment. Coupling constants (*J*) are reported in hertz (Hz), and the resonance multiplicity abbreviations used are s, singlet; d, doublet; dd, doublet of doublet; t, triplet; q, quartet; m, multiplet; and comp, overlapping multiplets of magnetically non-equivalent protons. IR spectra were recorded on a Perkin Elmer IR spectrometer. The mass spectrometric analysis was performed in the CRF, IIT-Kharagpur (TOF analyzer). Chiral HPLC analysis was performed with Shimadzu 20AT prominence system with Daicel Chiral Pak OD-H, IC, IA(25 cm × 0.46 cm ∅) as the stationary phase. The racemic standard for HPLC analysis was prepared by $NaBH_4$ reduction of cprrespondingα-benzyl/cinnamyl-substituted-β-ketoesrers. In principle, the racemic compounds should provide four peaks in a chiral stationary phase. In the majority of cases, we observed four peaks, in some cases, overlapping peaks were also observed.

Substrate synthesis: (±)-α-cinnamyl-substituted-β-ketoesrers (**5a-5n**) were prepared according to the following scheme

Scheme-S1



Ethyl cinnamates (2a-2n): To a suspension of NaH (1 eq)in THF,triethylphosphonoacetate (1eq) were added sequentially at 0°C and stirred for 45 minutes, after 45 minutes the corresponding aldehydes (1eq) were added into the reaction mixture at 0°C and left the reaction 3-4 hr at room temperature. After completion of the reaction, the reaction solution was quenched with saturated ammonium chloride, and the organic phase extracted with ethylacetate. It was then washed with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure, and the product was purified by flash column chromatography (EtOAc/hexane = 1: 10) to furnish compounds**2a-2n** in good yield. R_f = approx. 0.5 (EtOAc/ hexane = 1: 10). All the synthesized compounds are reported in the literature and provide comparable spectral characteristic values.[1(a-c)]

Substituted (*E*)-cinnamyl alcohols (**3a-3n**): To a solution of compounds**2a-2n** (1eq) in dry THF, DIBAL-H in THF (2eq.) was added at 0 °C, and the reaction mixture was allowed to warm

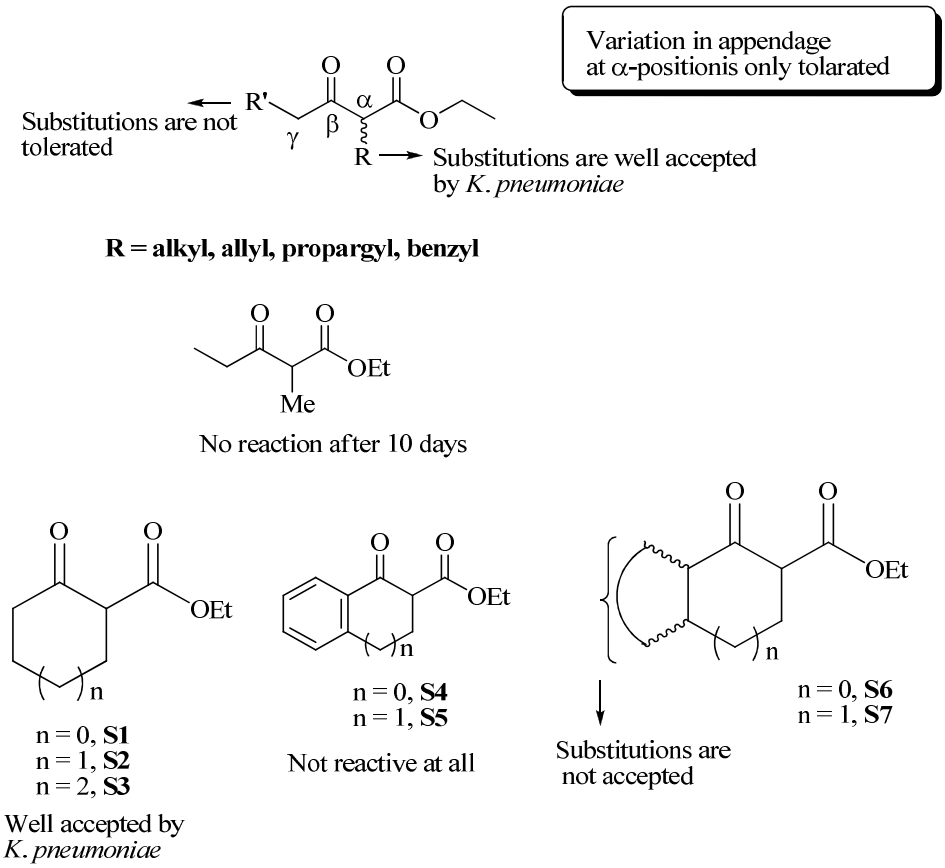
at room temperature. Subsequently, the reaction solution was stirred for 3-4 hr, and then it was quenched with saturated sodium-potassium tartrate solution and filtered through a Celite pad and washed with ethyl acetate. The combined organic layer was dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure, and the product was purified by flash column chromatography (EtOAc/hexane = 1: 10) to furnish compound **3a-3n**in approximate 85% yield. R_f = approx. 0.1 (EtOAc/ hexane = 1: 10).All the synthesized compounds are reported in the literature and provide comparable spectral characteristic values.[2(a-c)]

Substituted (*E*-cinnamyl bromides; 4a-4n): To a solution of compound **3a-3n** (1eq) in dry ether, PBr_3(0.8eq) was added at 0 °C, and the reaction mixture was stirred at the same temperature for 1hr. The reaction solution was then quenched with the careful addition of saturated $NaHCO_3$solution and extracted with ether. The organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure, and the product was used for the next step without purification. R_f = approx. 0.7(EtOAc/ hexane = 1: 10).All the synthesized compounds are reported in the literature and provide comparable spectral characteristic values.[3(a-b)]

Substrate mapping for DKRR pathway with *K. pneumoniae* : As discussed in the manuscript (Scheme 1), a detailed substrate scope was also investigated by us based on the results reported here as well as in our earlier article.[4] It was observed that the enzyme system only accepts structural variation at α-position of the parent β-ketoesters for the DKRR reaction. Different alkyl groups are well tolerated in α-position for the DKRR reaction. Allyl, homo-allyl, and propargyl appendages are also well accepted, as shown by us in the earlier paper. Substituted benzyl groups (containing ERG and EWG in the aromatic ring), thiophene moiety, 1-naphthyl and 2-naphthyl (with different substitution on the aryl ring) were also accepted by the enzyme system (Scheme 4 in the present manuscript). Any extra substitution at the γ-position was not accepted by the enzyme system. And after incubation with the growing cells of *K. pneumoniae* the starting materials remain unreacted even after 10 days. It seems that presence of the ketomethyl group (-COMe) is an essential prerequisite for successful DKRR reaction for acyclic α-substituted-β-ketoesters. For the cyclic β-ketoesters, it was found that substrates (**S1**-**S3**; commercially available) were well accepted by the enzyme systems. Cyclic β-ketoesters having 1-indanone (**S4**) and 1-tetralone framework (**S5**) seems to be not accepted by the enzyme system.

Both **S4** and **S5** are commercially available and used as obtained from the vendors without any further purification. It seems that the enzyme system does not tolerate any substitution on the γ-position. Cyclic β-ketoesters having a Me- substitution at γ-position (**S6** and **S7; S6** was commercially available and used as obtained. **S7** was prepared through a literature method [5]) were not reactive at all. Though the results are little premature, still it can be concluded that this particular enzyme system is very specific towards a certain class of α-substituted-β-ketoestrs (acyclic and cyclic). Further substrate scope is very much needed to have a final conclusion. In future we would like to explore in that direction.

Scheme S2



References:

1. (a) S. Einaru, K. Shitamichi, T. Nagano, A. Matsumoto, K. Asano and S. Matsubara, *Angew. Chem. Int. Ed.* **2018**, *57*, 13863 –13867; (b) R. Sato, K. Oyama, H. Konno, *Tetrahedron*, **2018**,*74*, 6173-6181; (c) S. Sano, K.Yokoyama, M. Fukushima, T. Yagi, and Y. Nagao, *Chem. Commun*., **1997**, 559-560.

2. (a) X. Jiang and J. F. Hartwig, *Angew. Chem. Int. Ed*. **2017**, *56*, 8887–8891. (b) S. Rao and K .R. Prabhu, *Org. Lett*.**2017**, *19*, 846–849. (c) L. Liu, X.Bao, H. Xiao,J. Li, F.Ye, C. Wang, Q. Cai, and S. Fan, *J. Org. Chem*, **2019**, *84*, 423–434.

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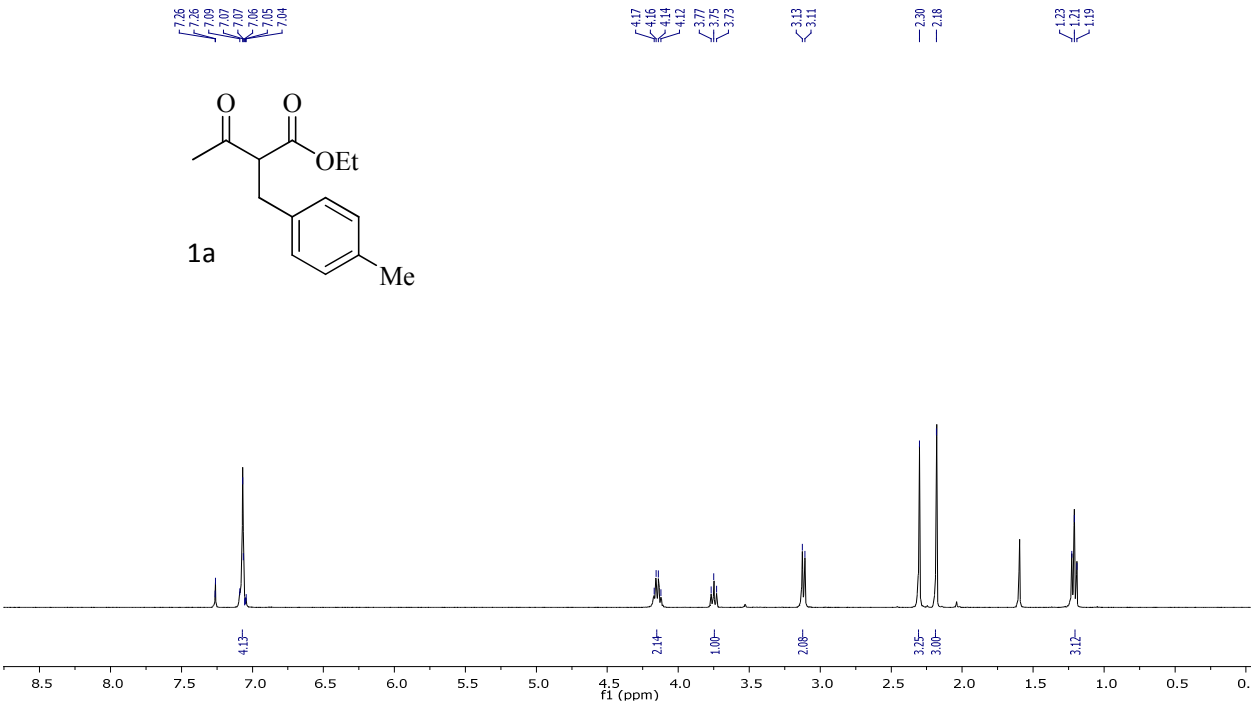
^{1}H NMR of compound (1a) (400 MHz, $CDCl_3$)



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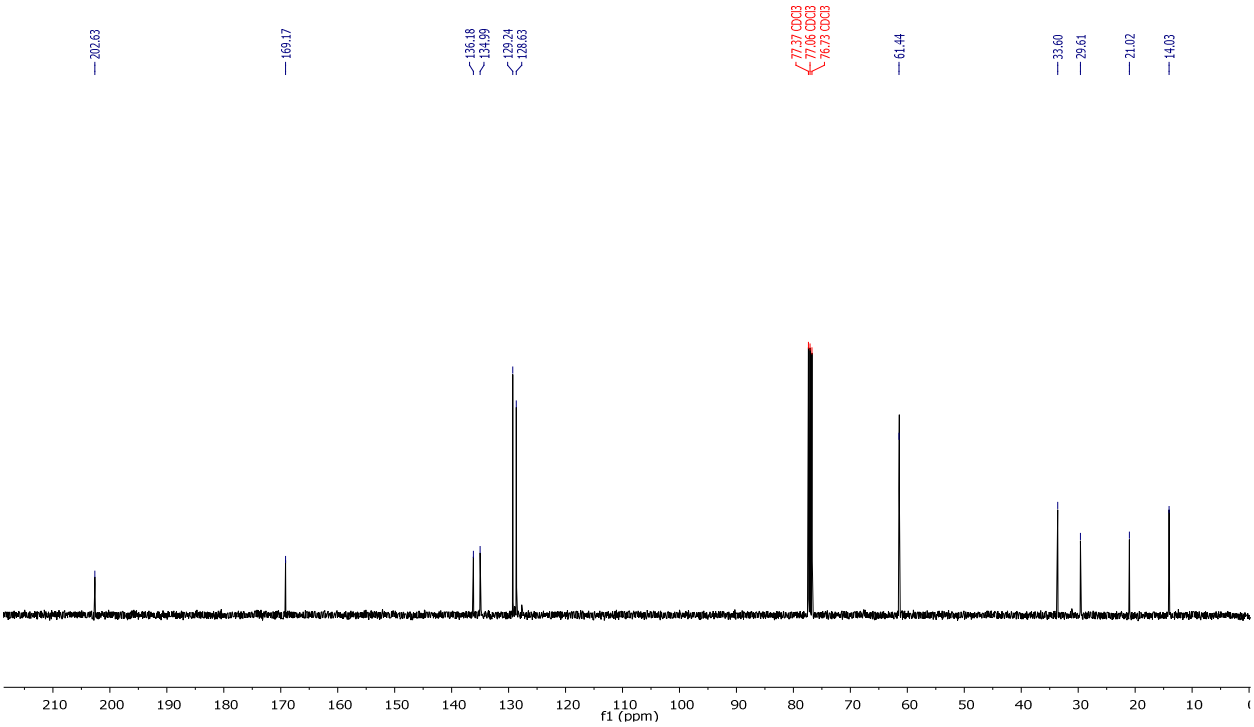

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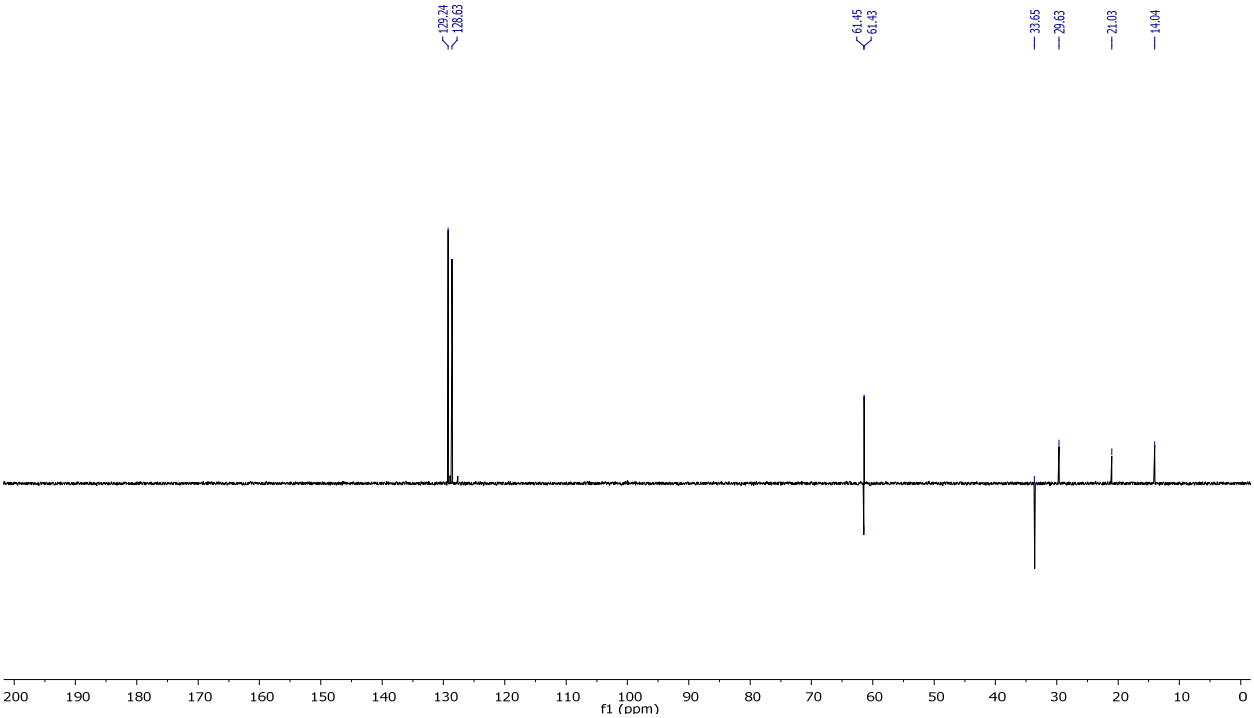

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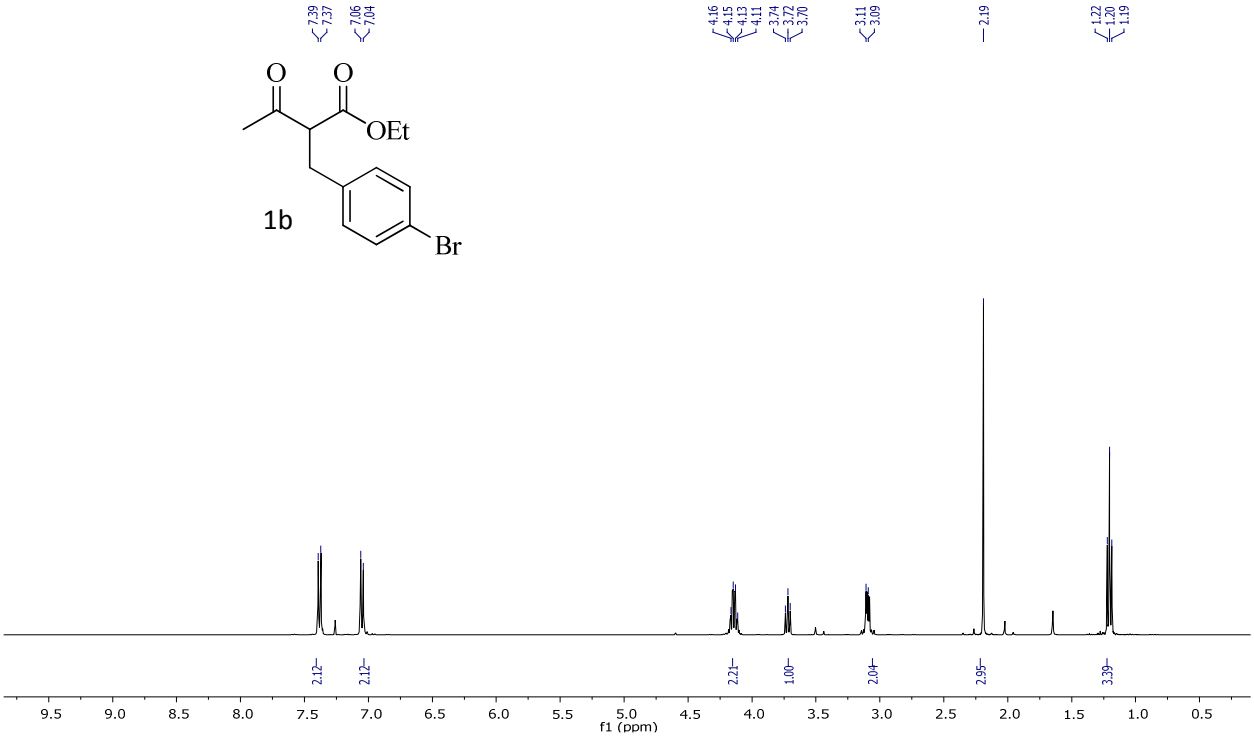

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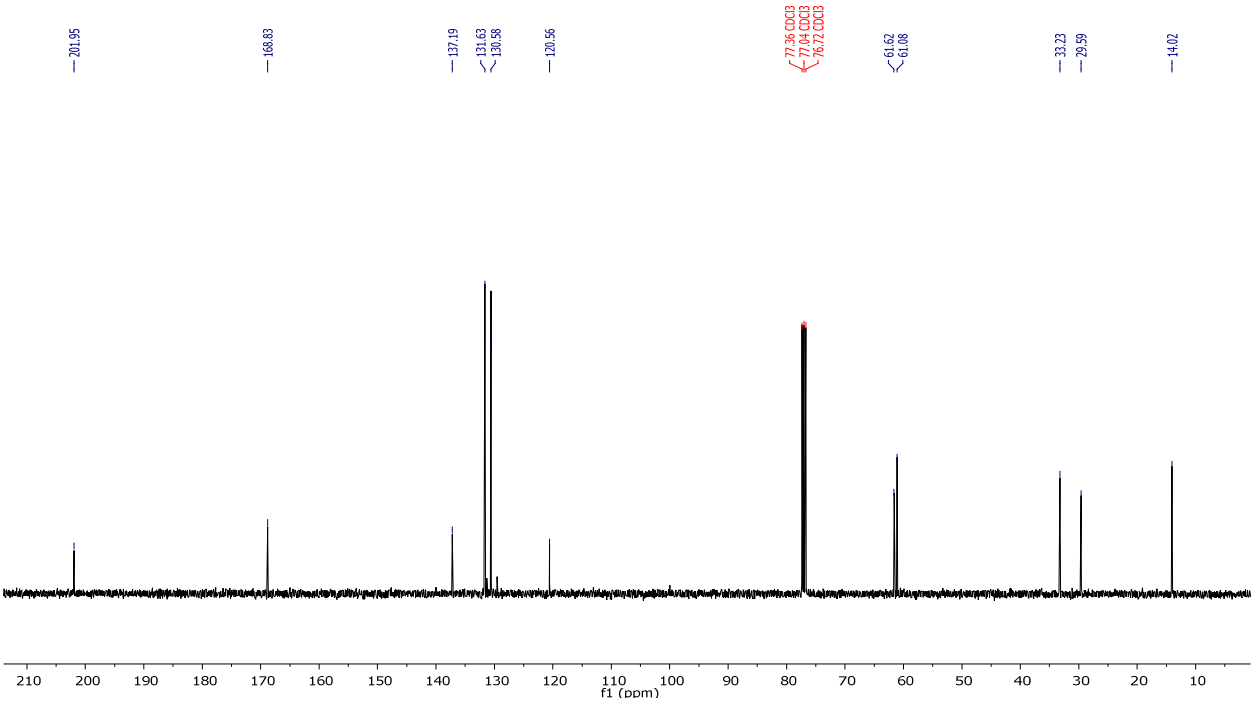

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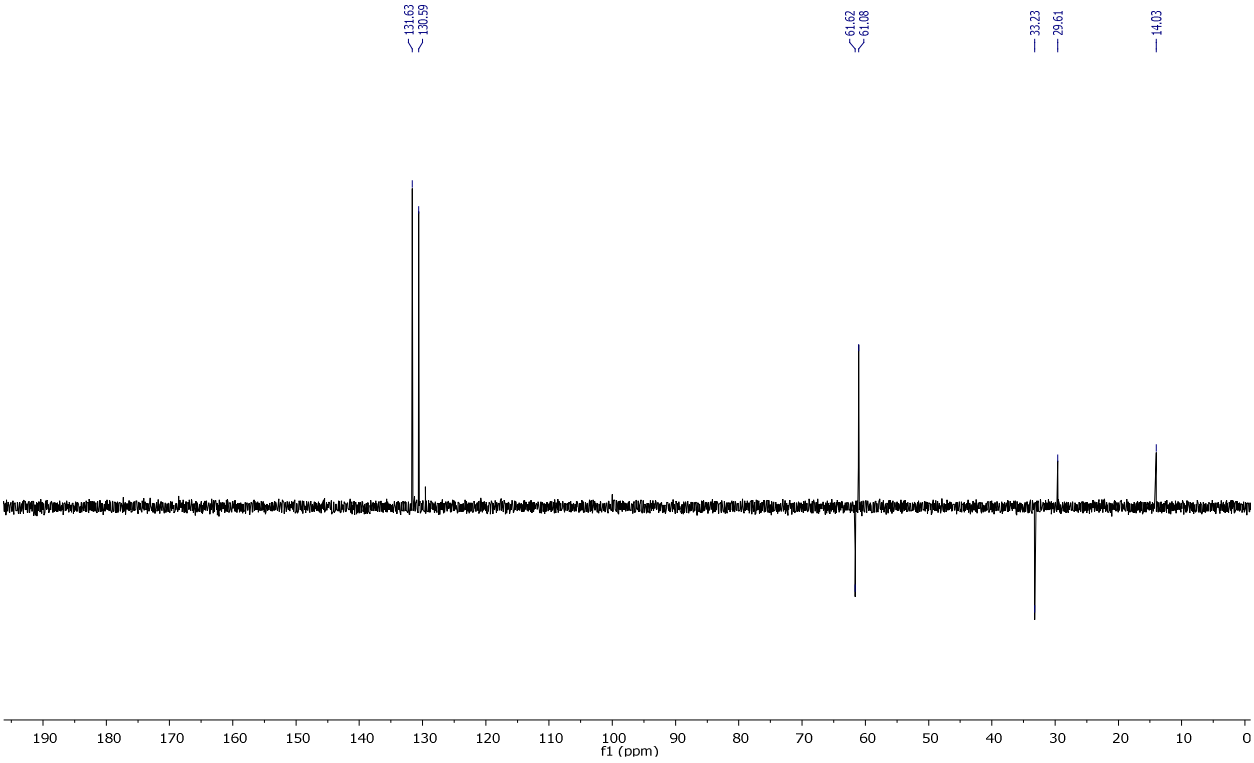

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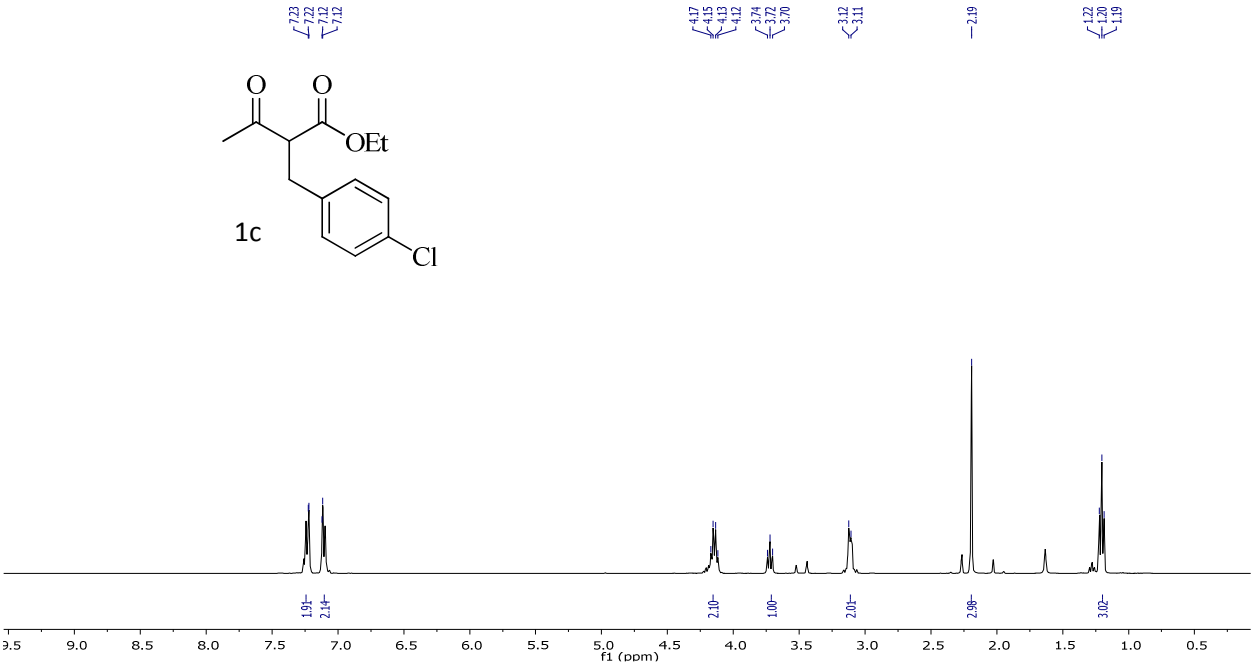

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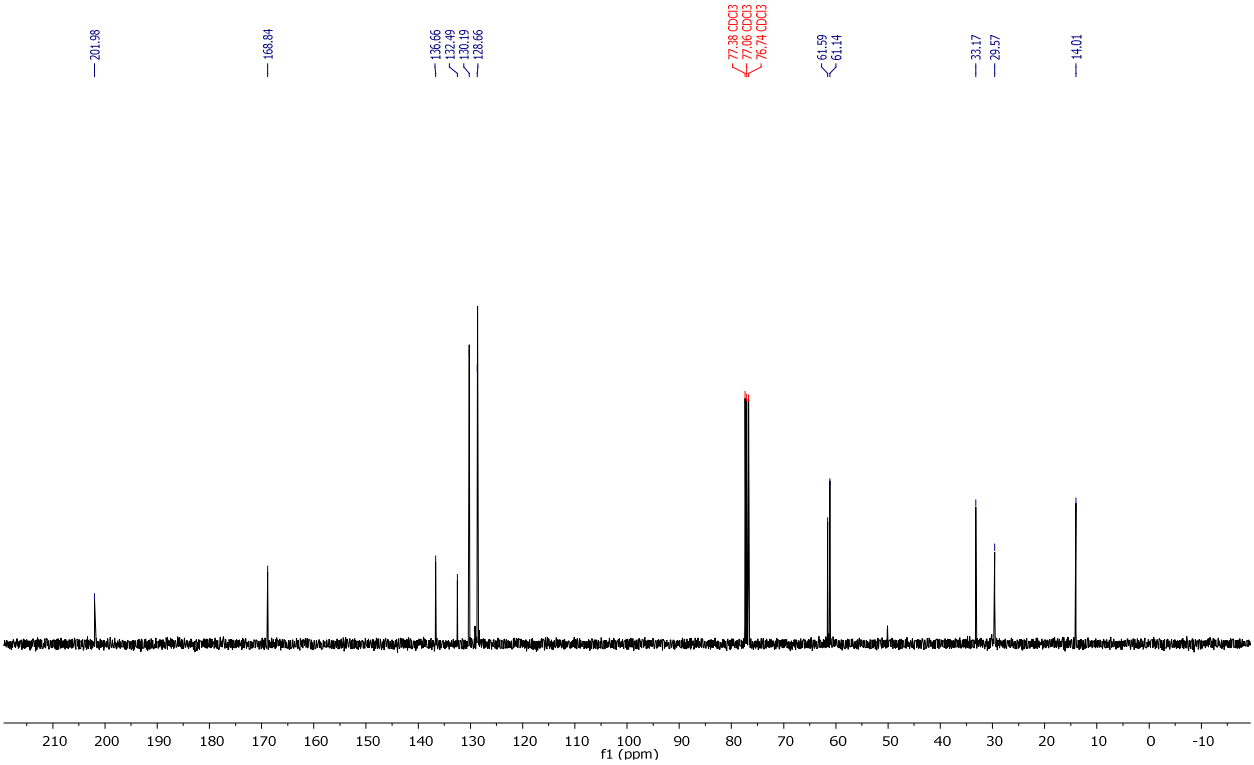

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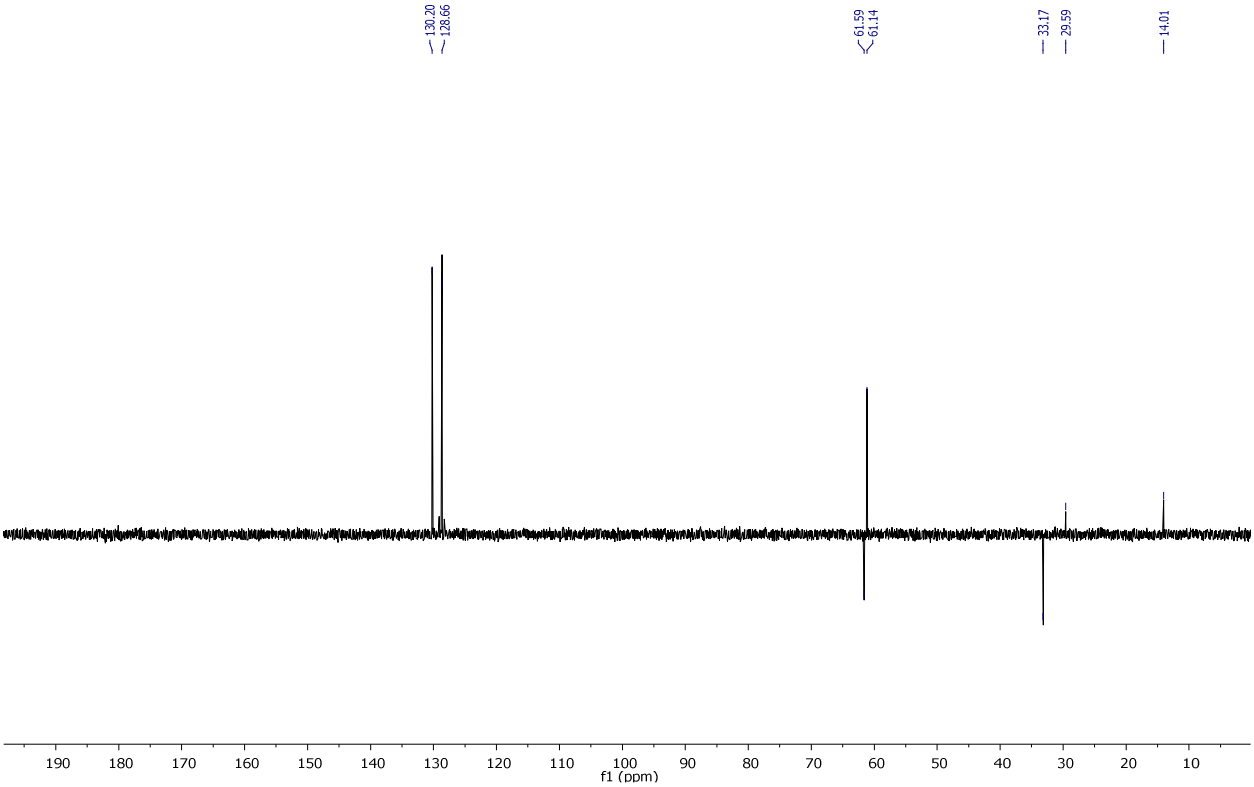

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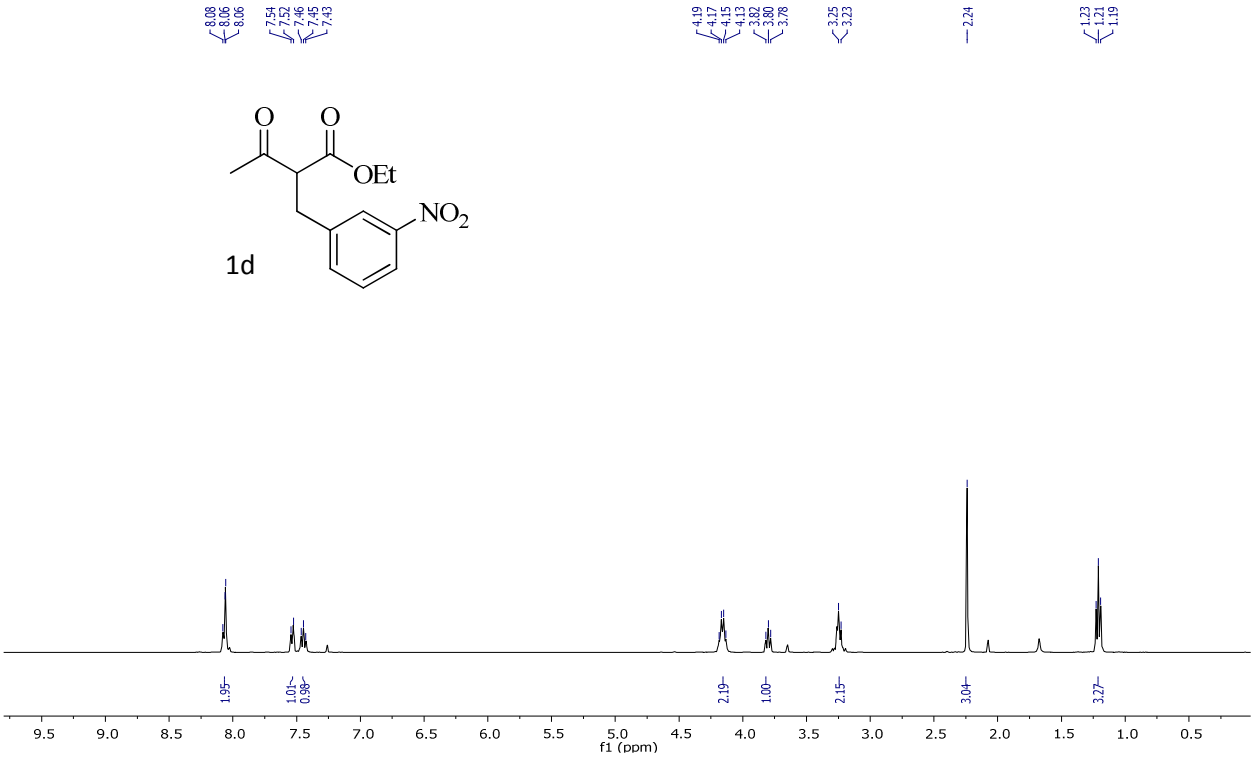

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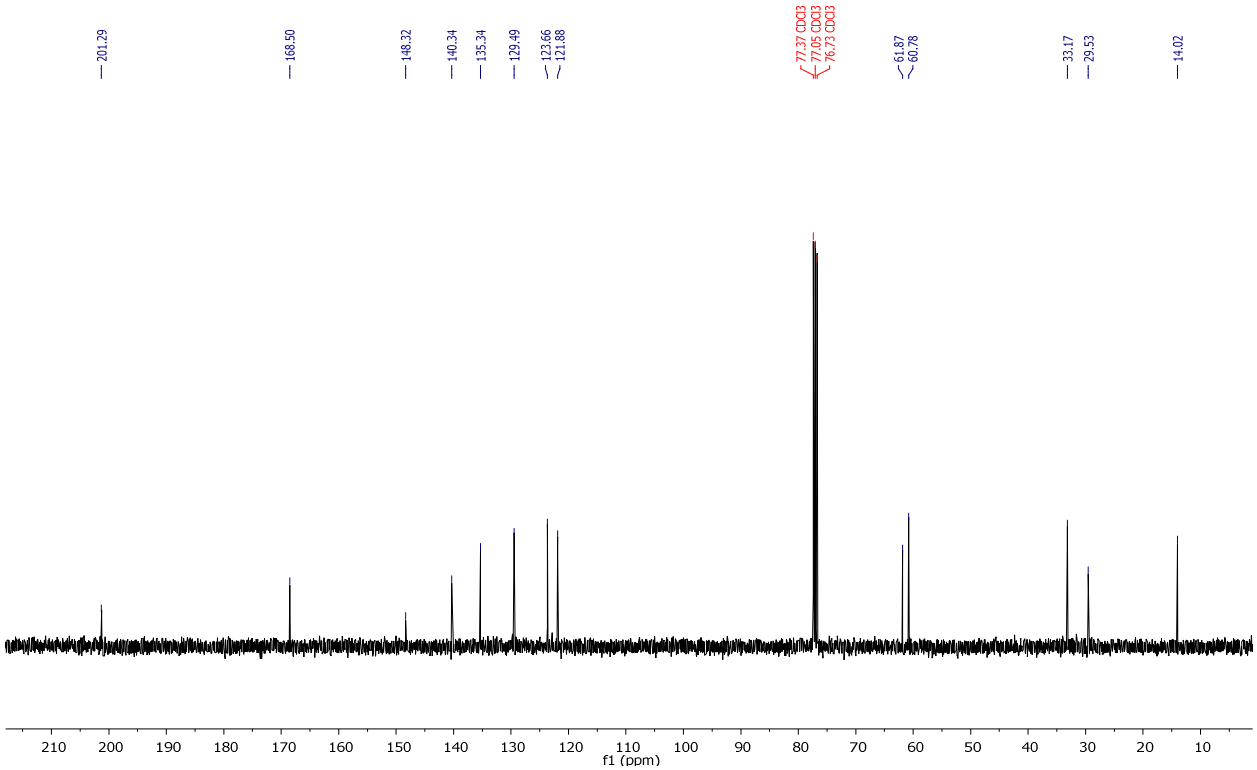

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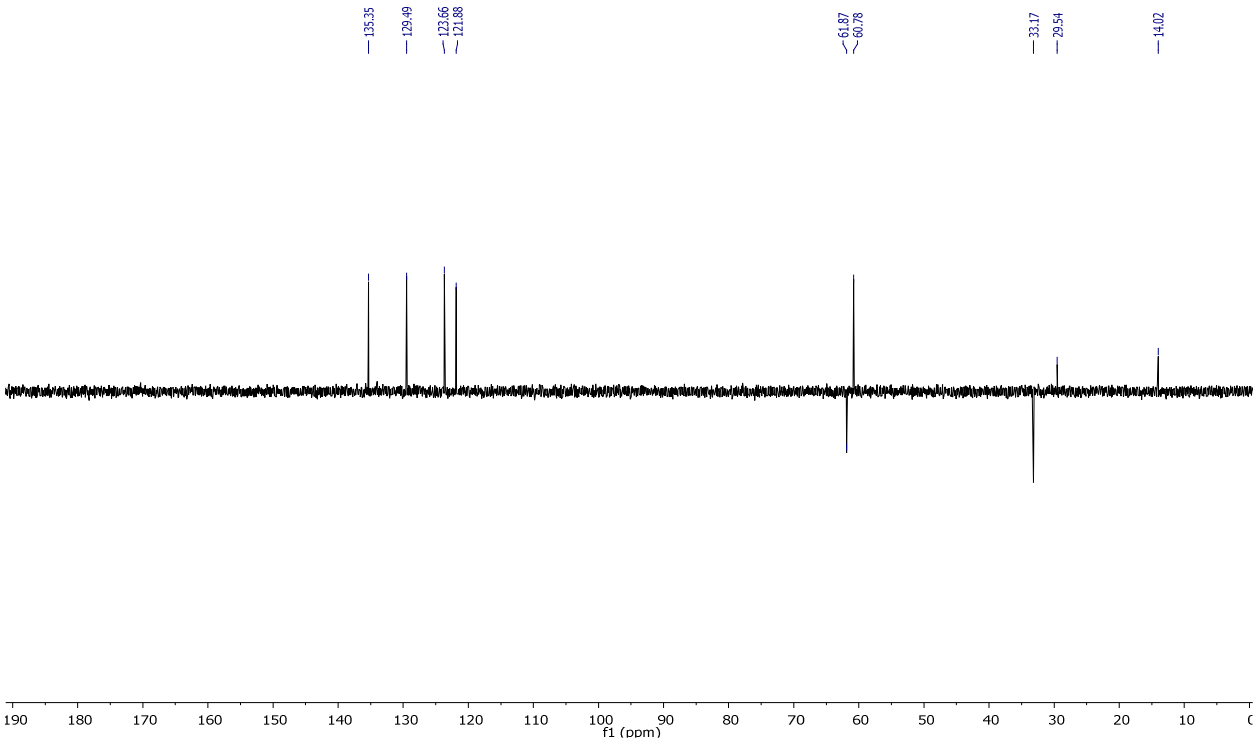

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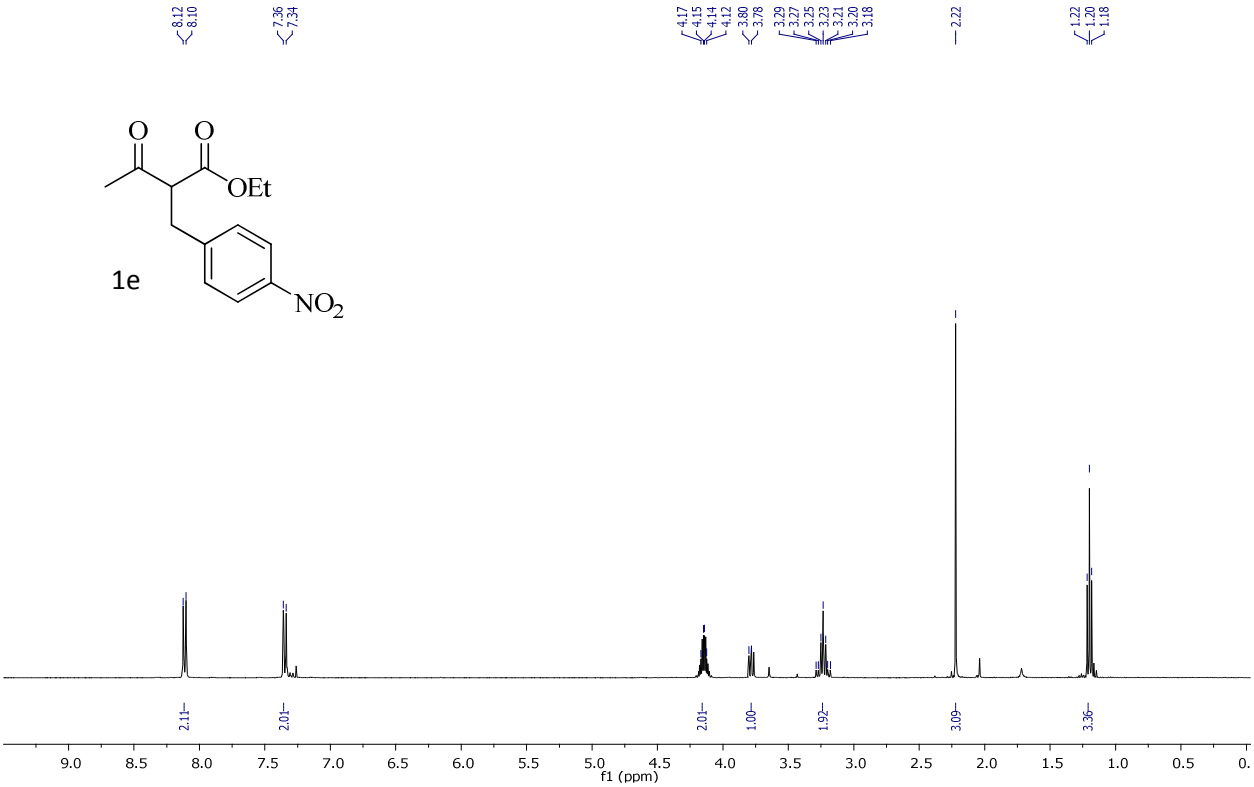

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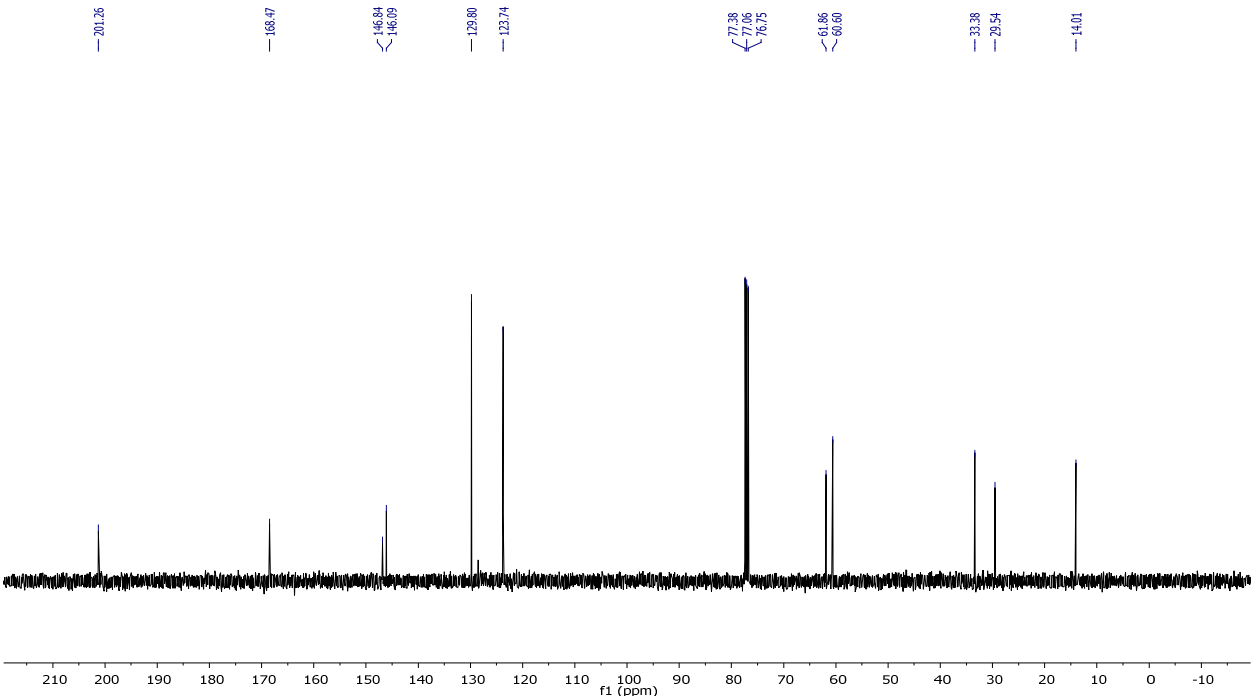

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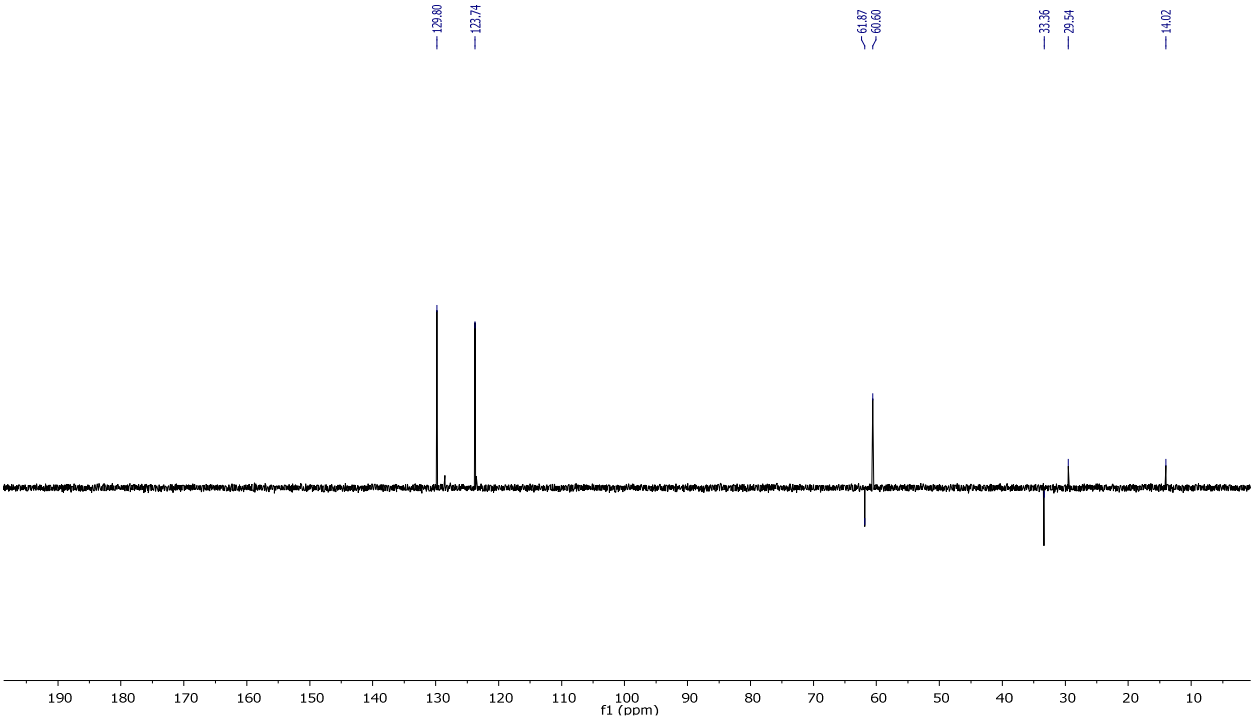

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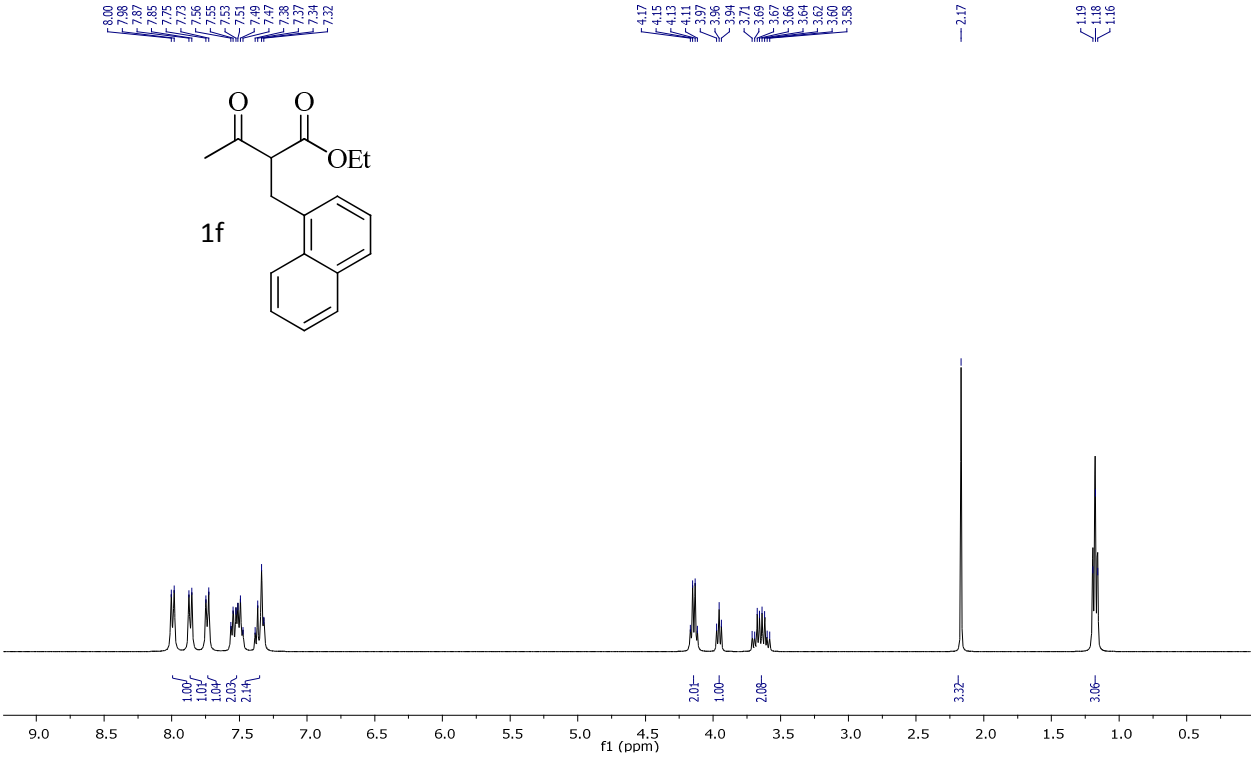

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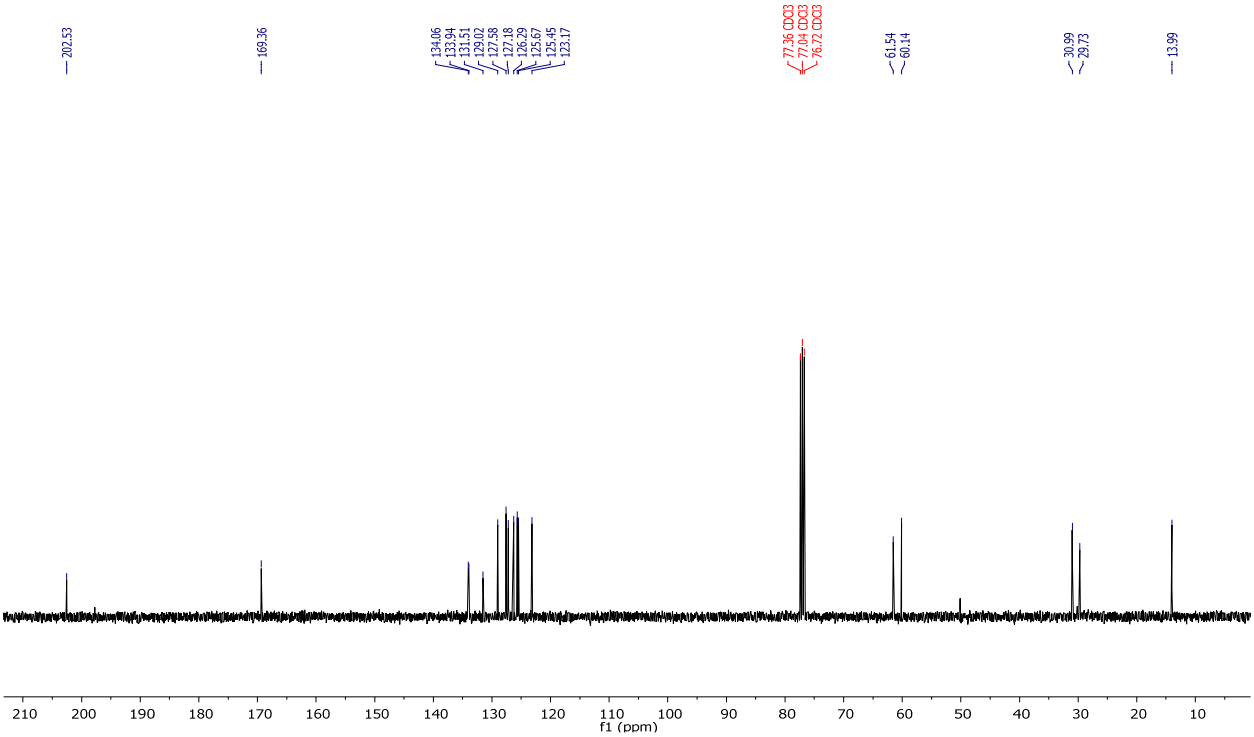

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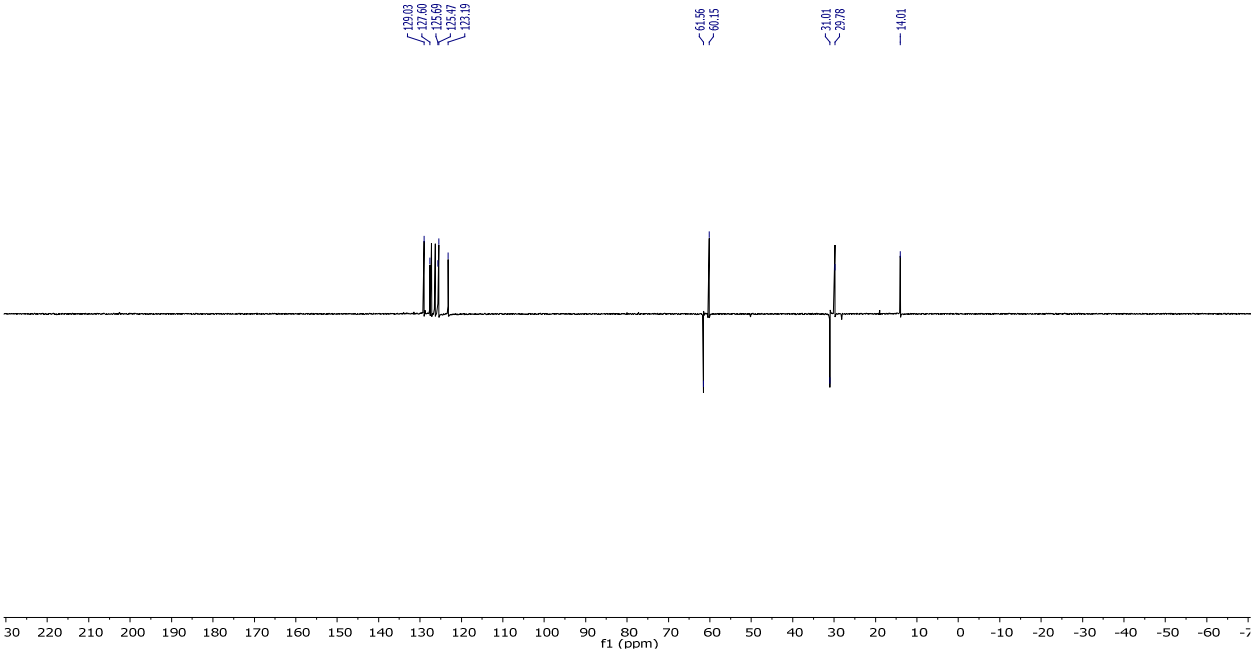

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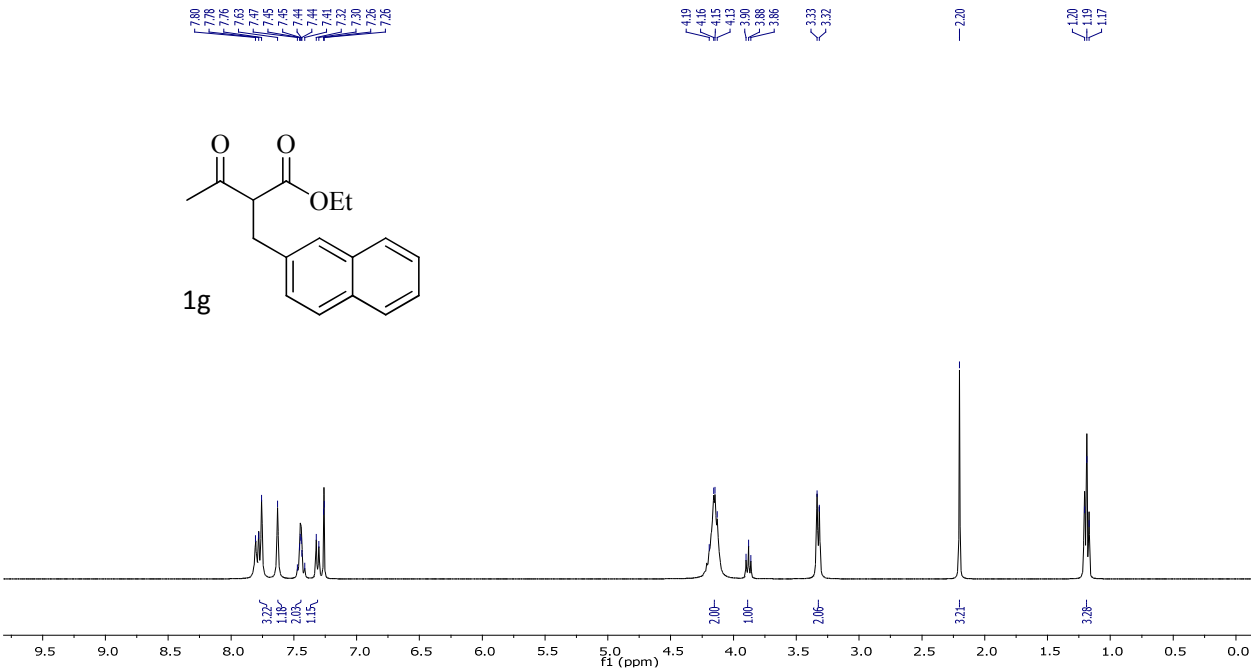

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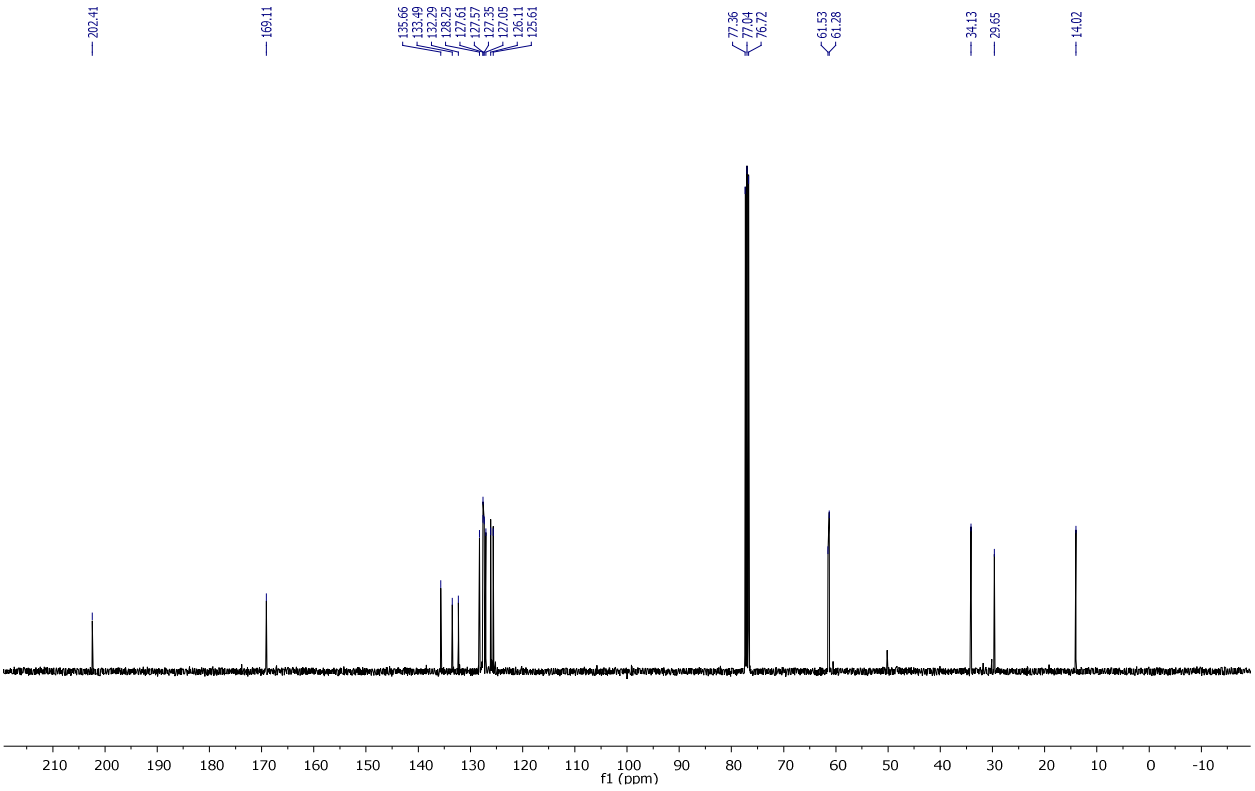

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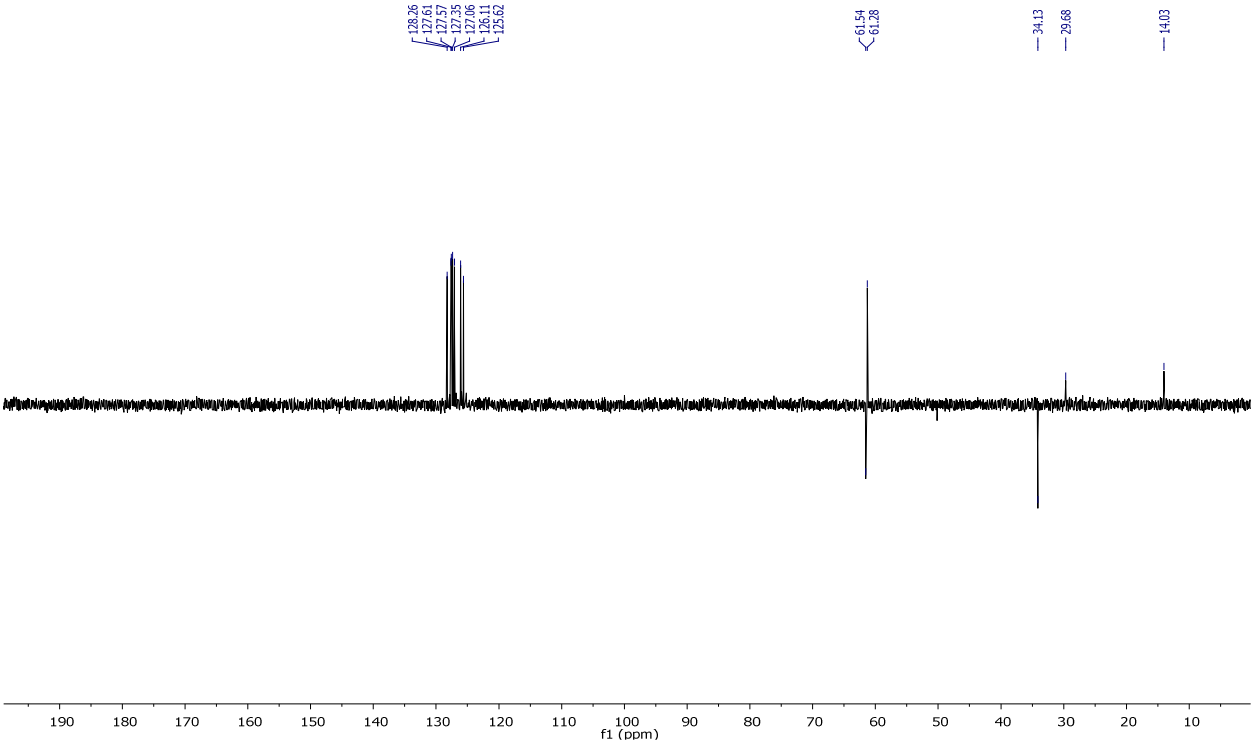

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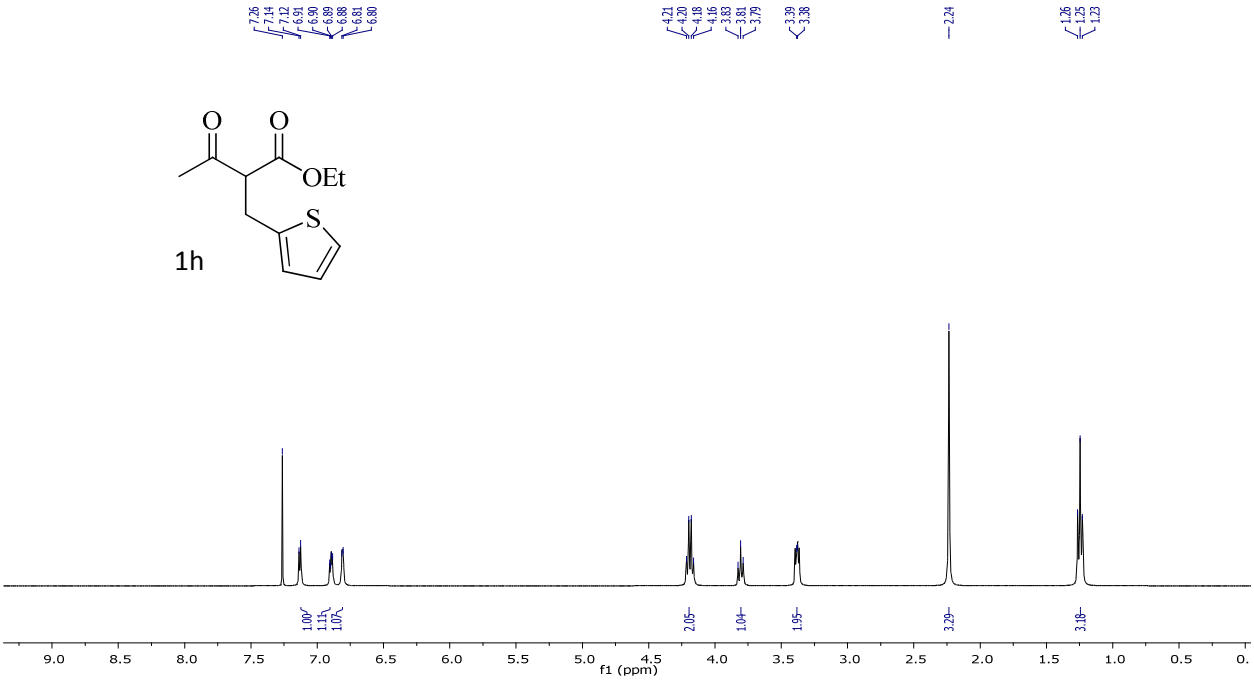

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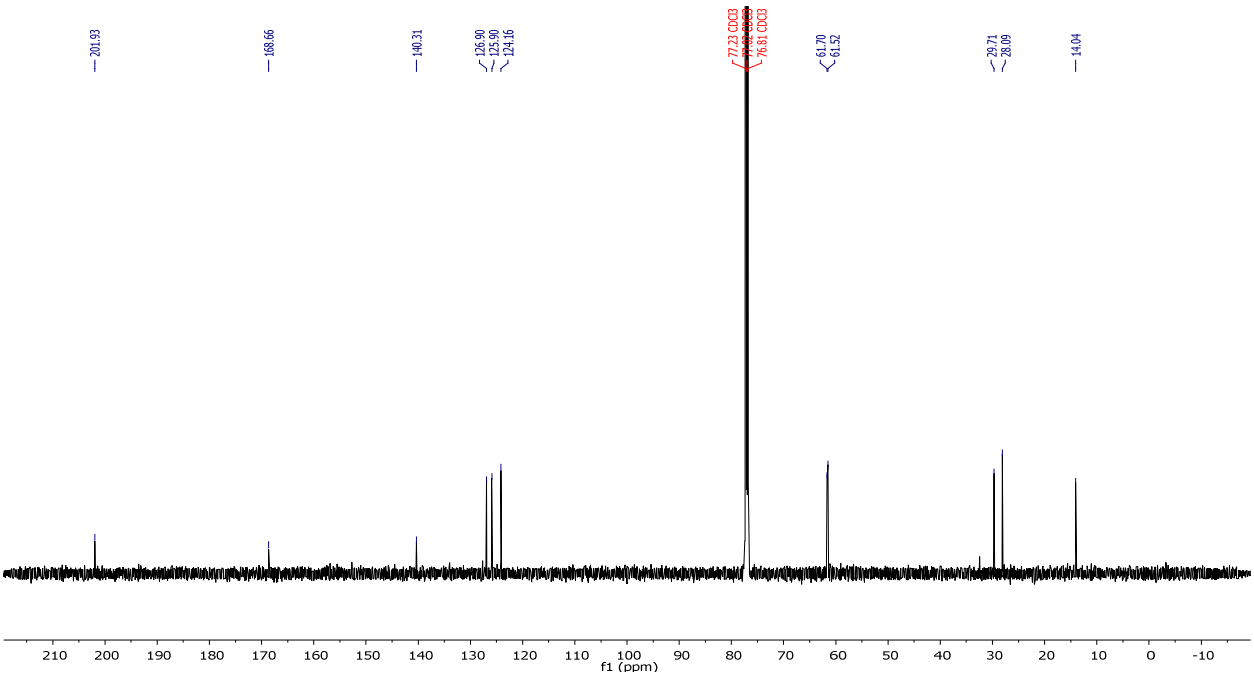
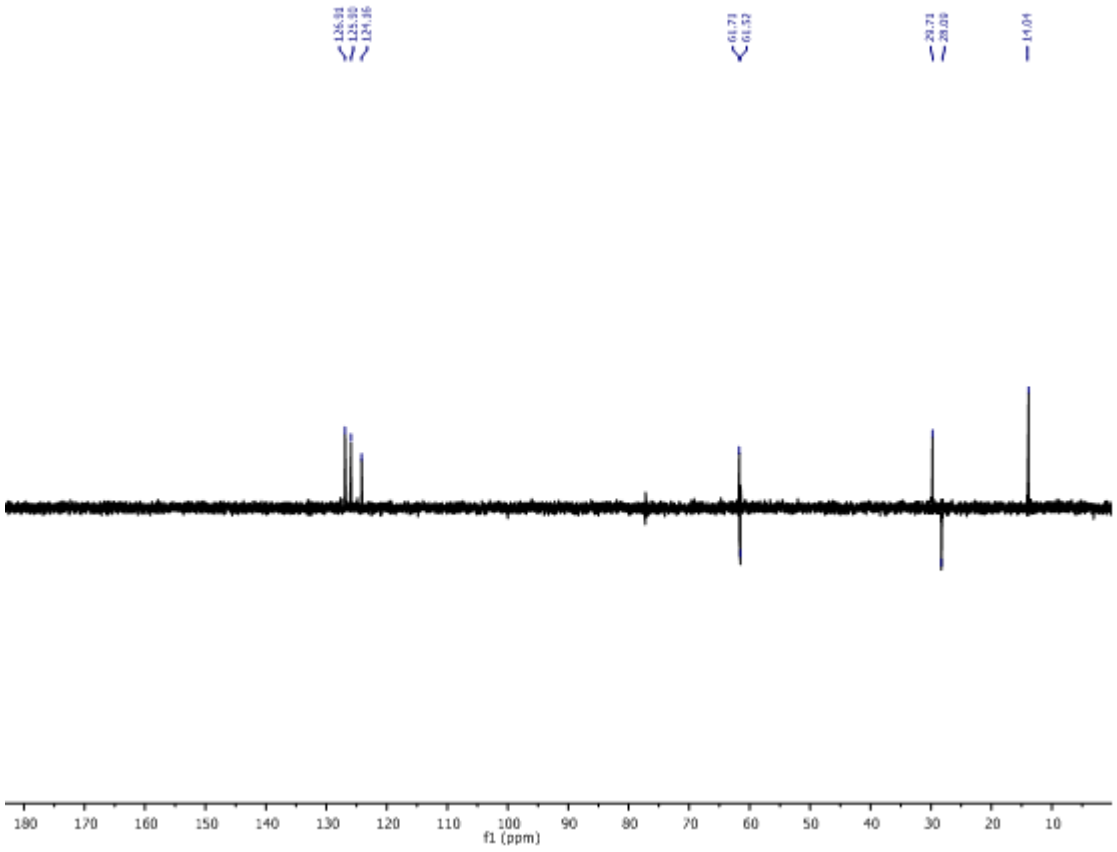
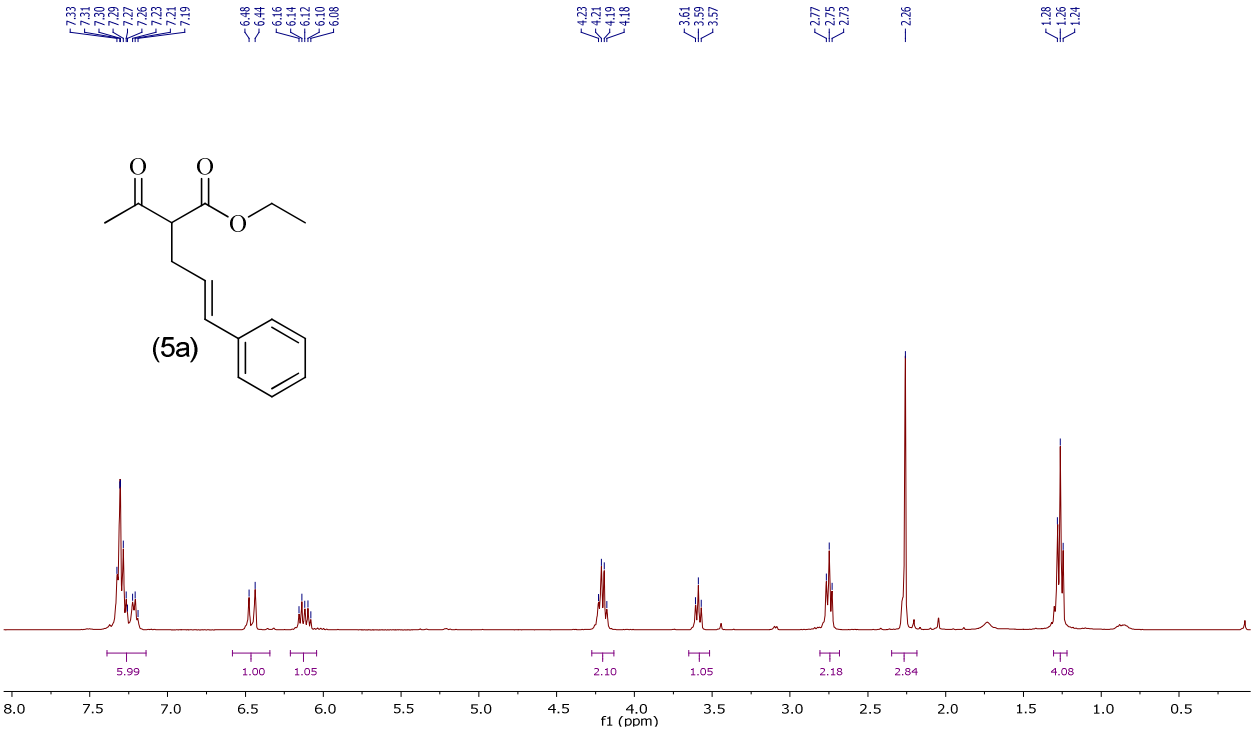


DEPT-135 of compound (1h) (150 MHz, $CDCl_3$)



^{1}H NMR of compound (5a) (400 MHz, $CDCl_3$)



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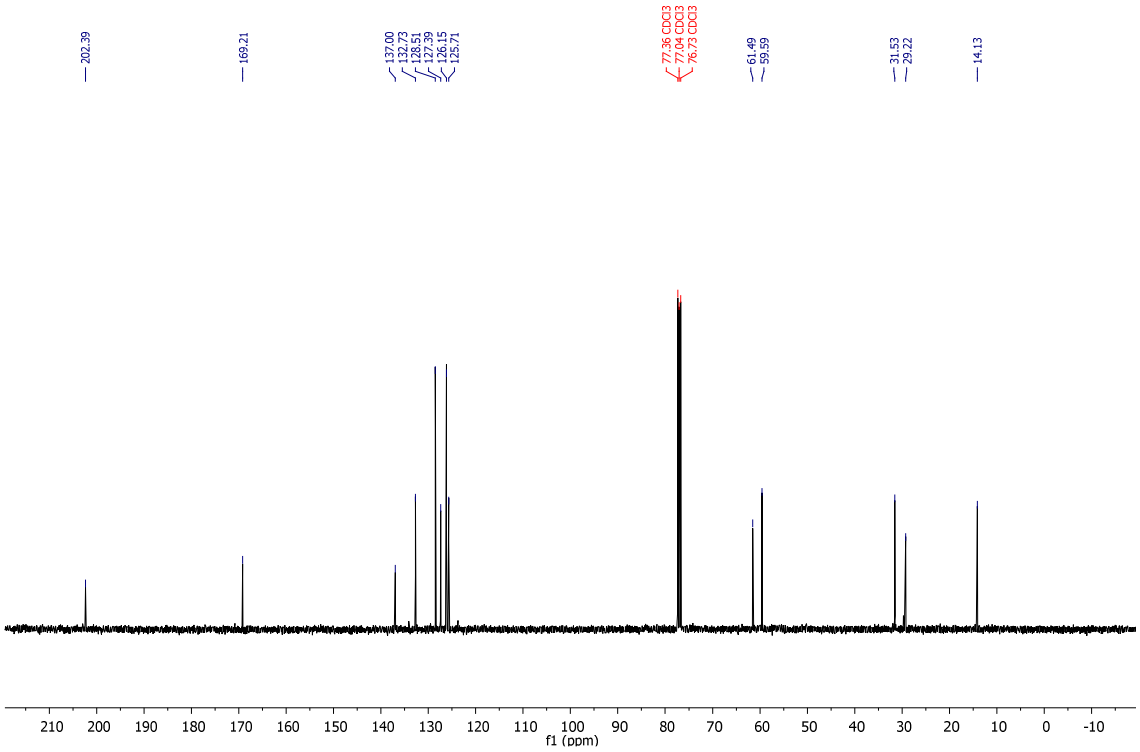

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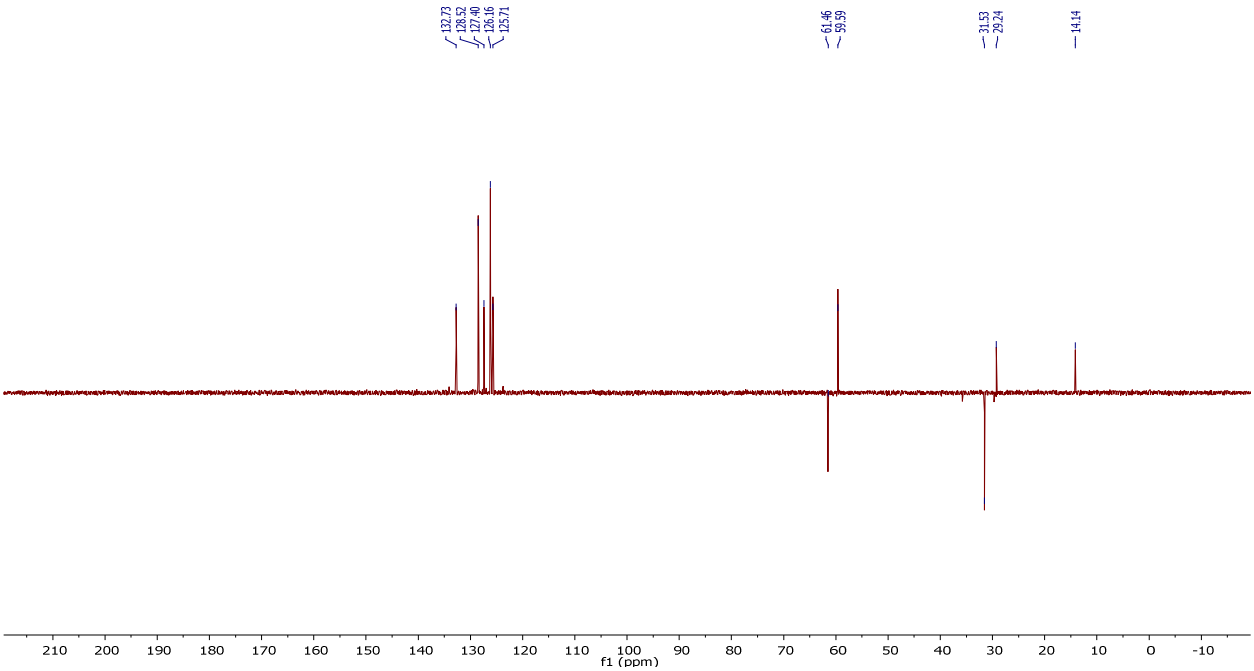

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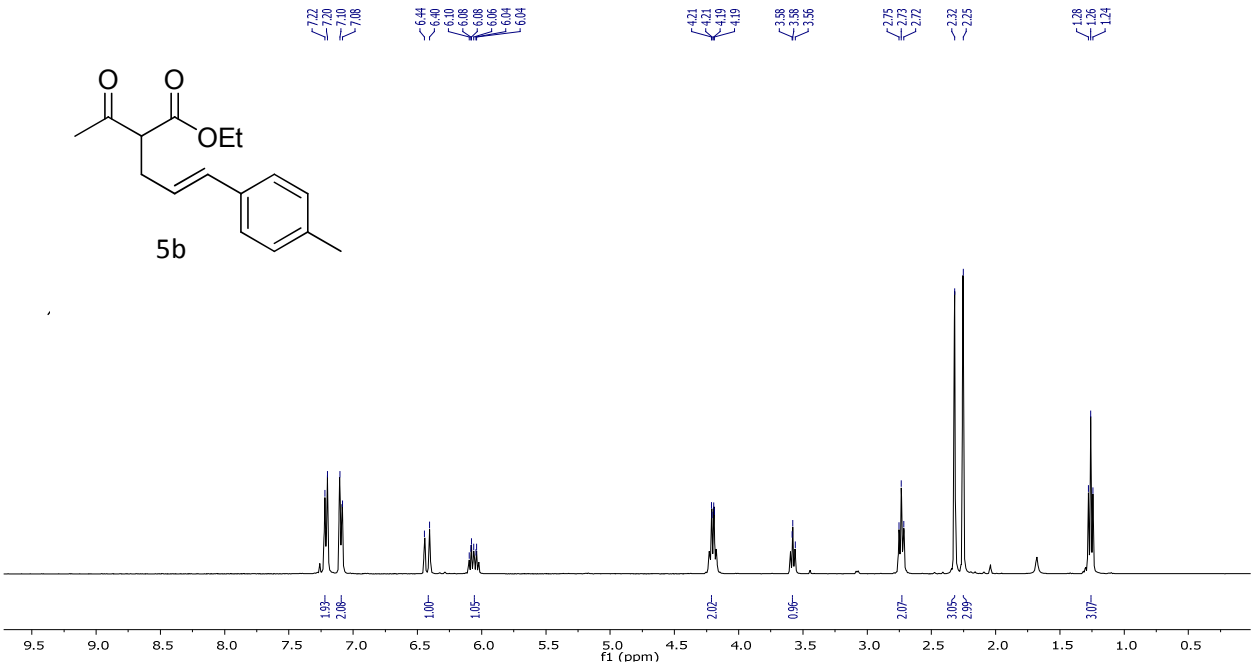

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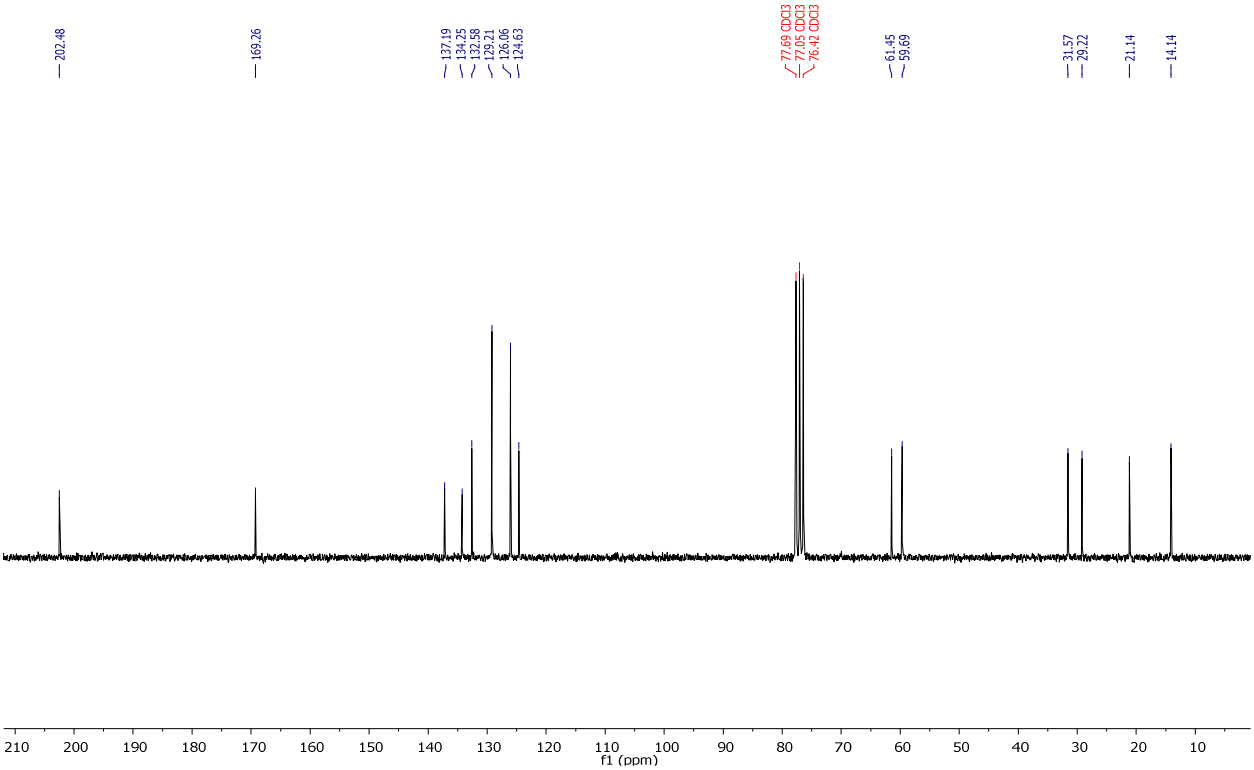
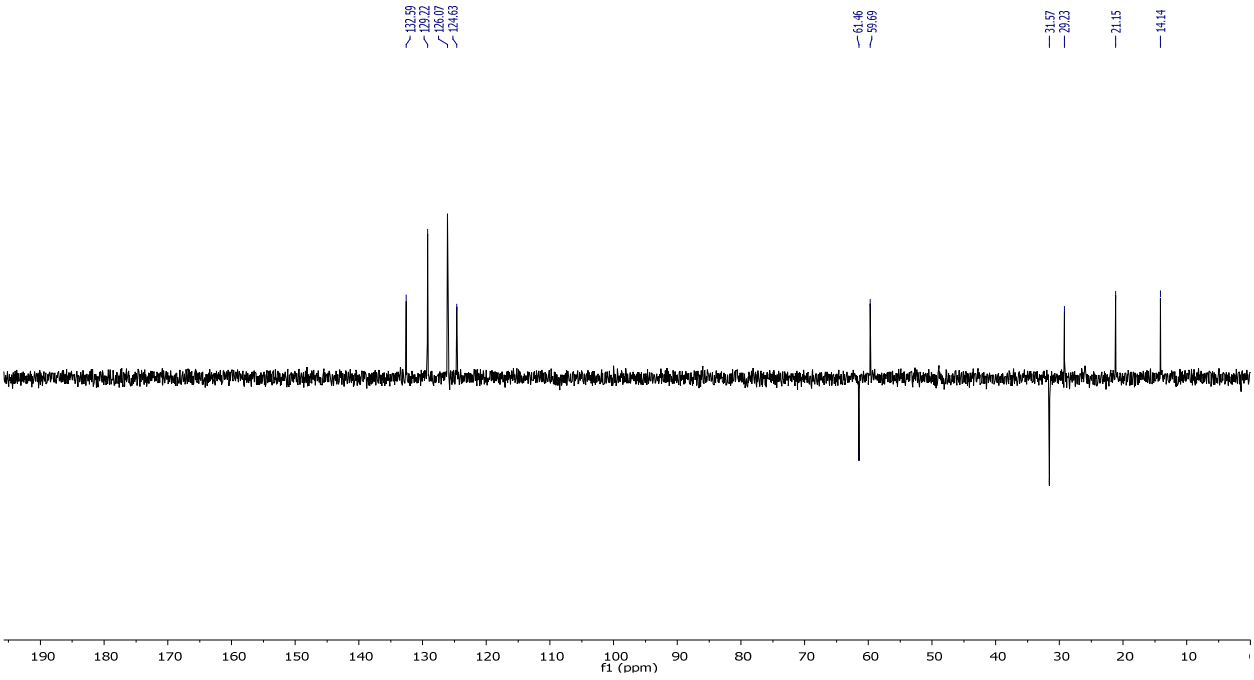


DEPT-135 of compound (5b) (50 MHz, $CDCl_3$)



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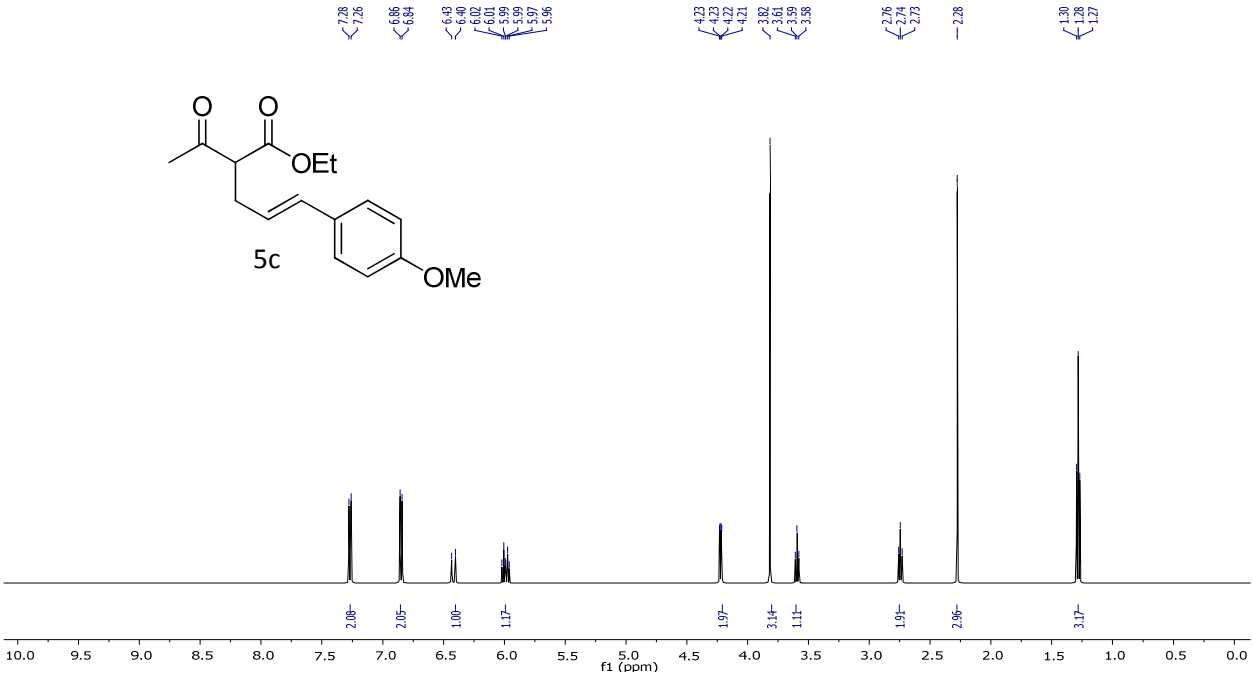

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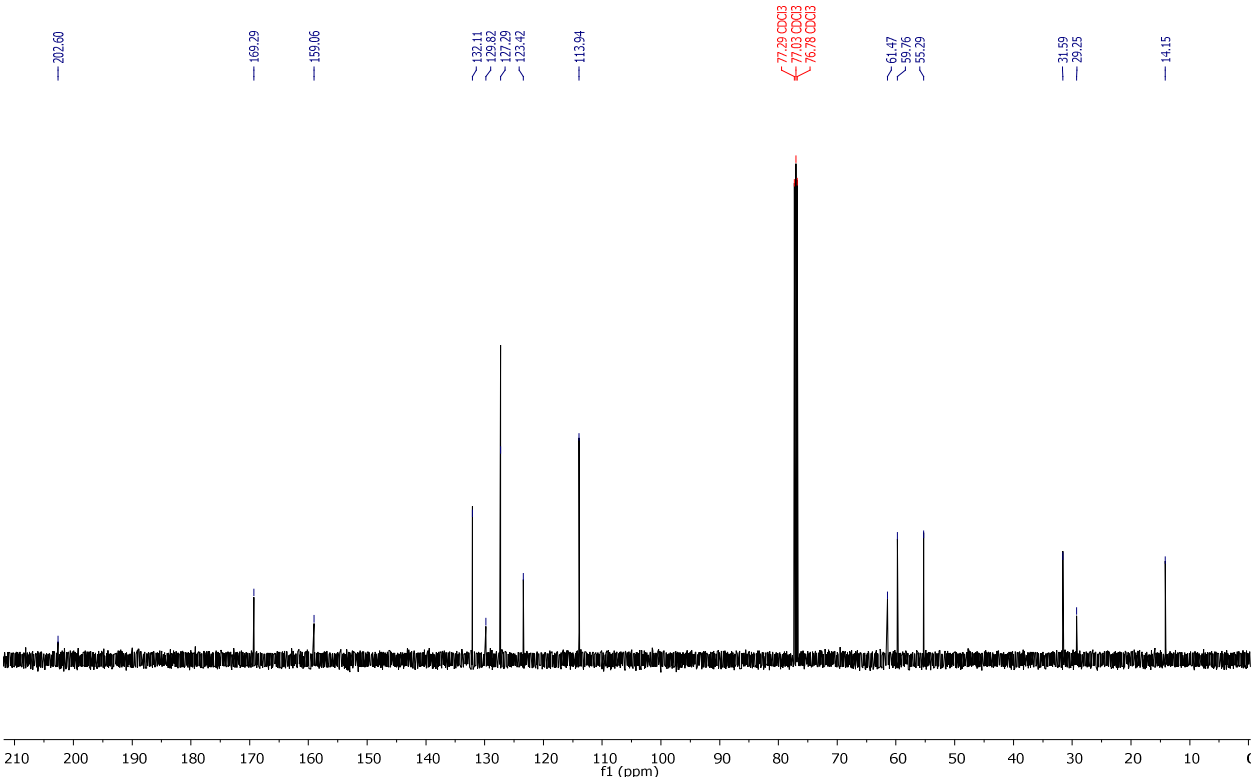
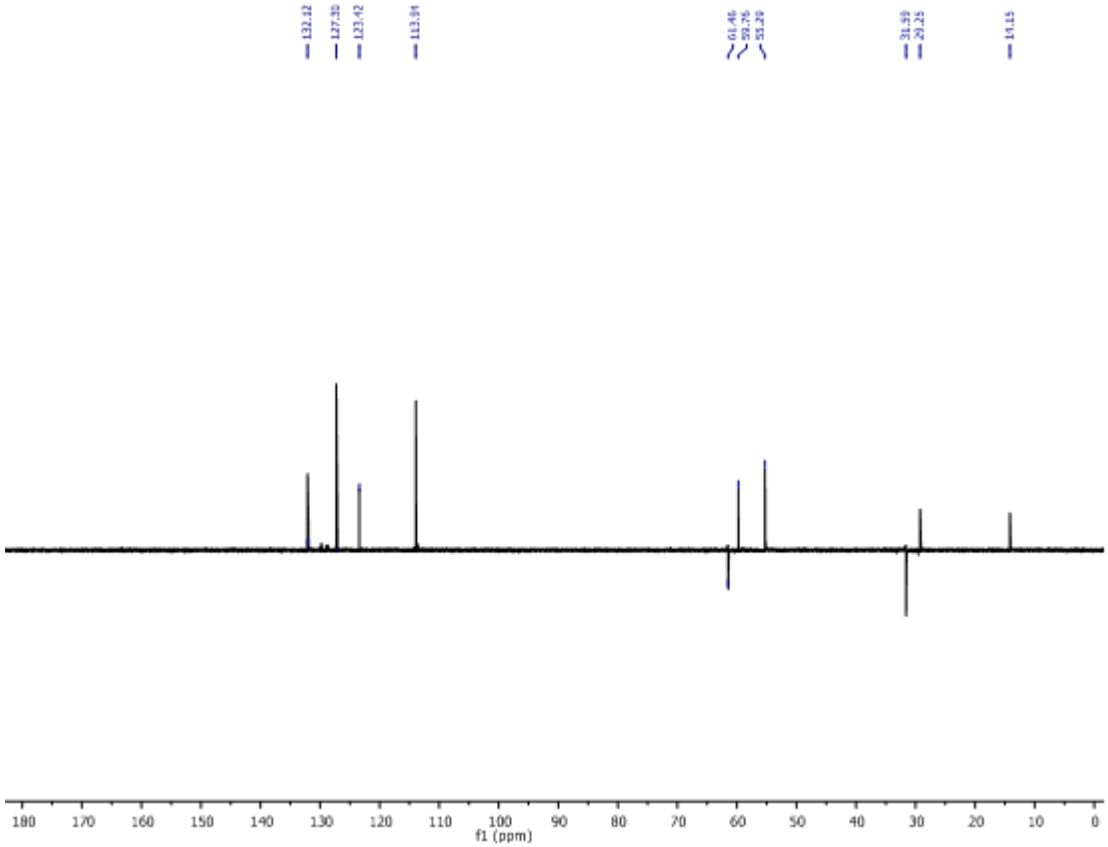


DEPT-135 of compound (5c) (125 MHz, $CDCl_3$)



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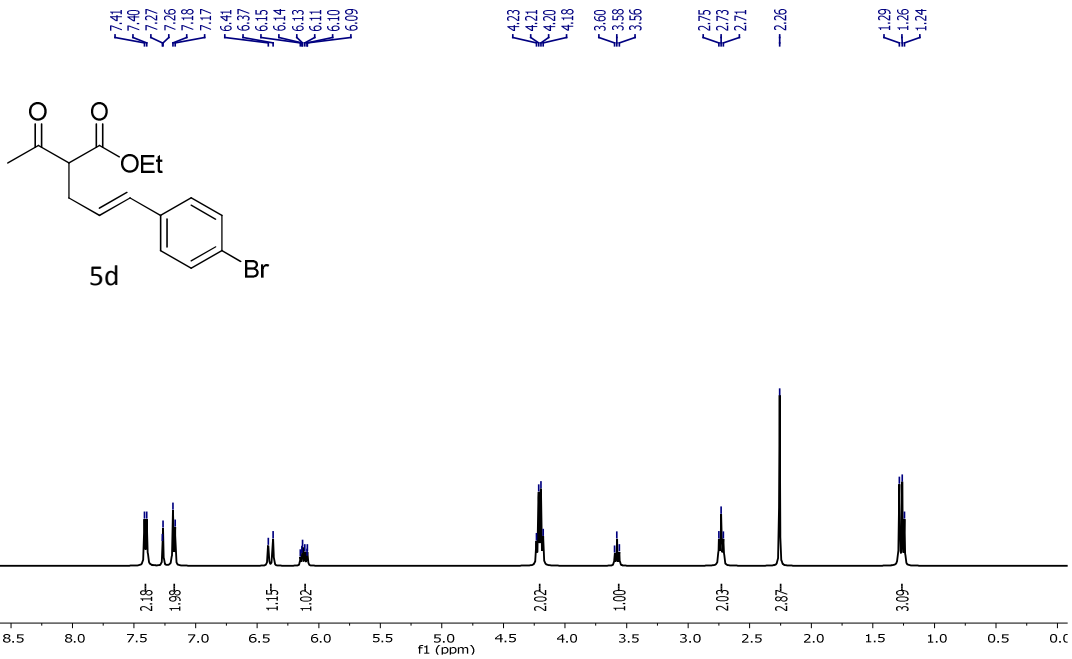

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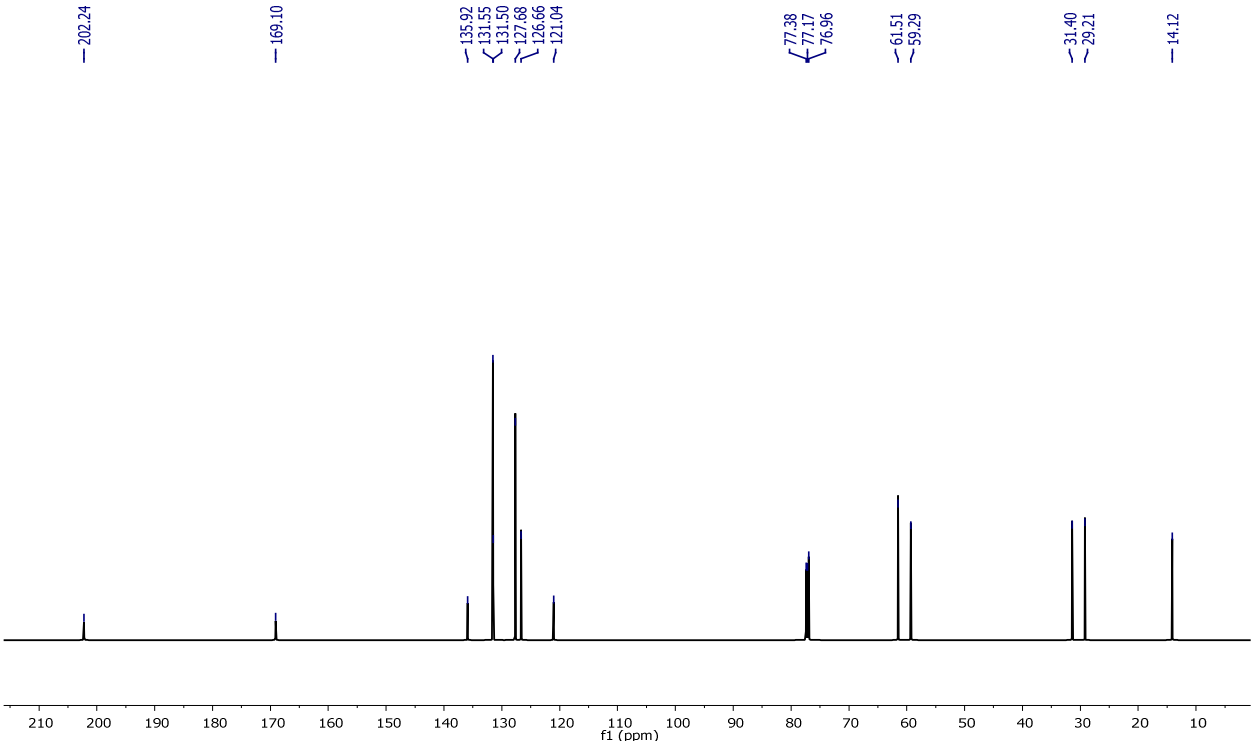
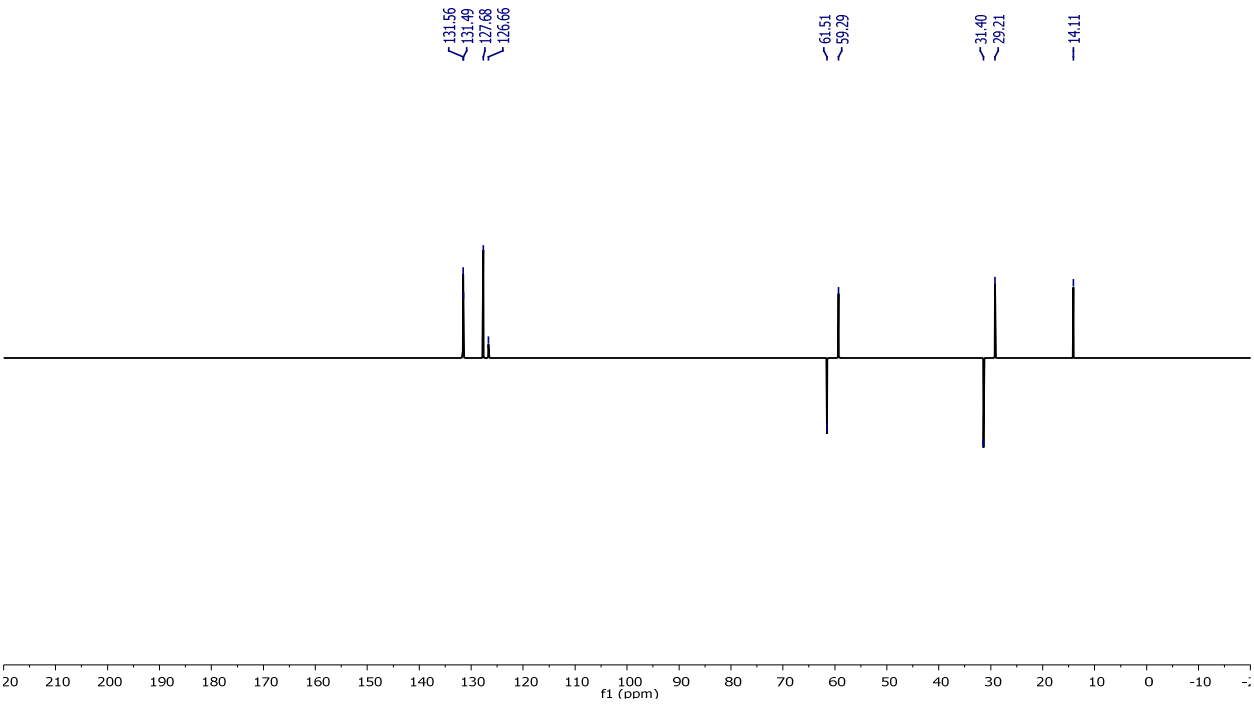
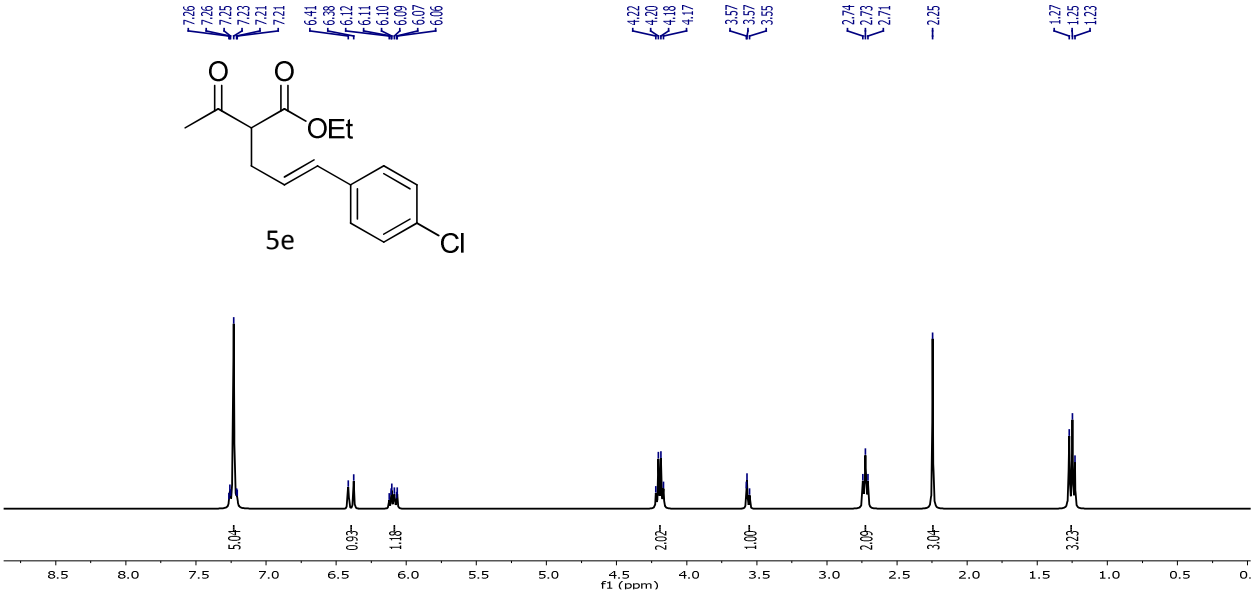


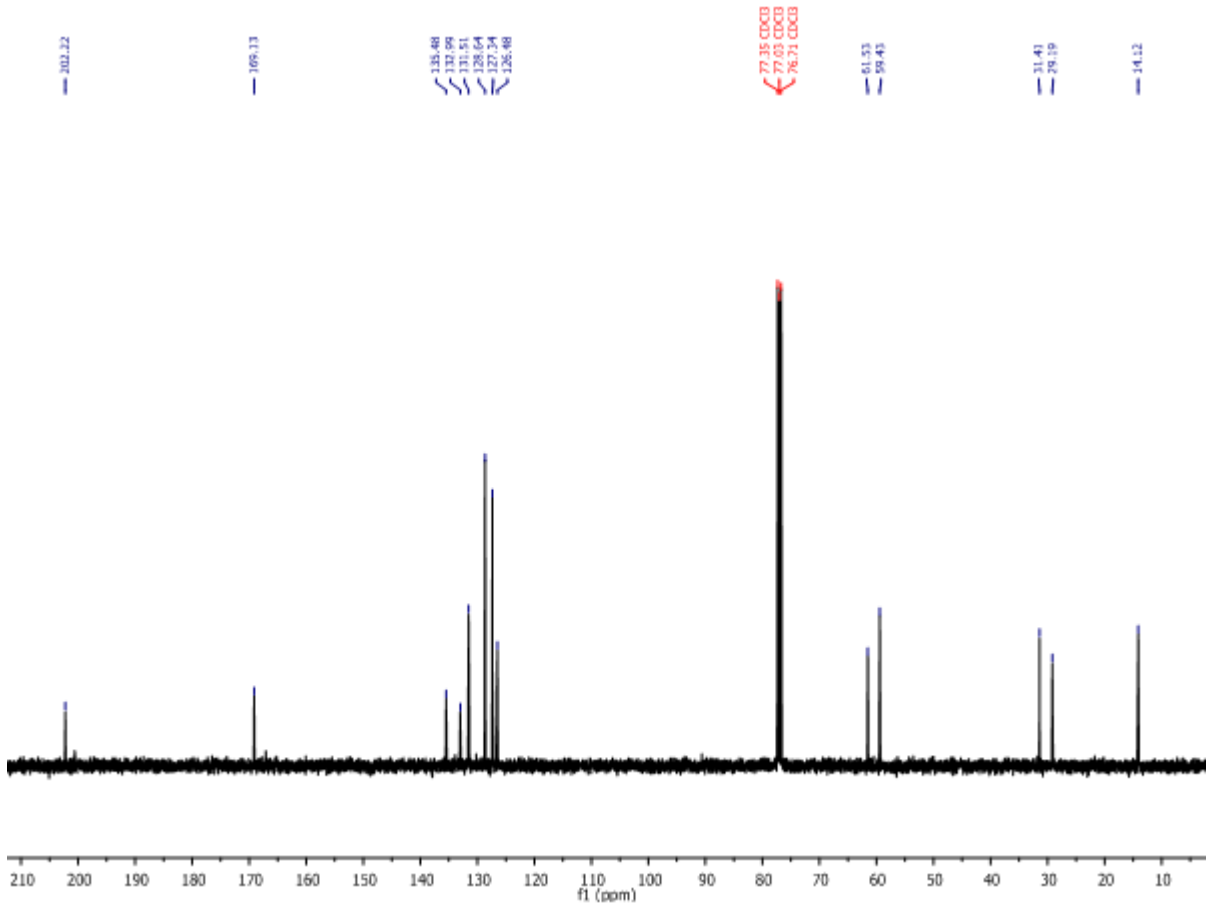
DEPT-135 of compound (5d) (150 MHz, $CDCl_3$)



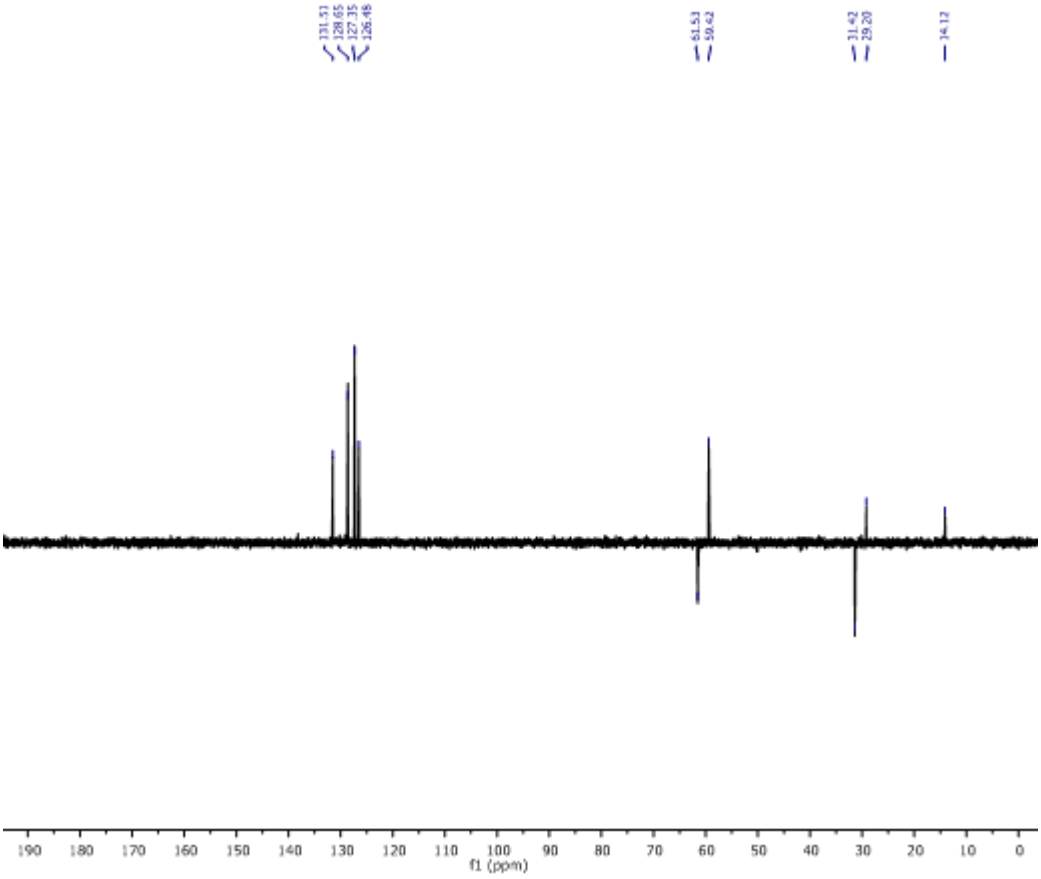
^{1}H NMR of compound (5e) (400 MHz, $CDCl_3$)



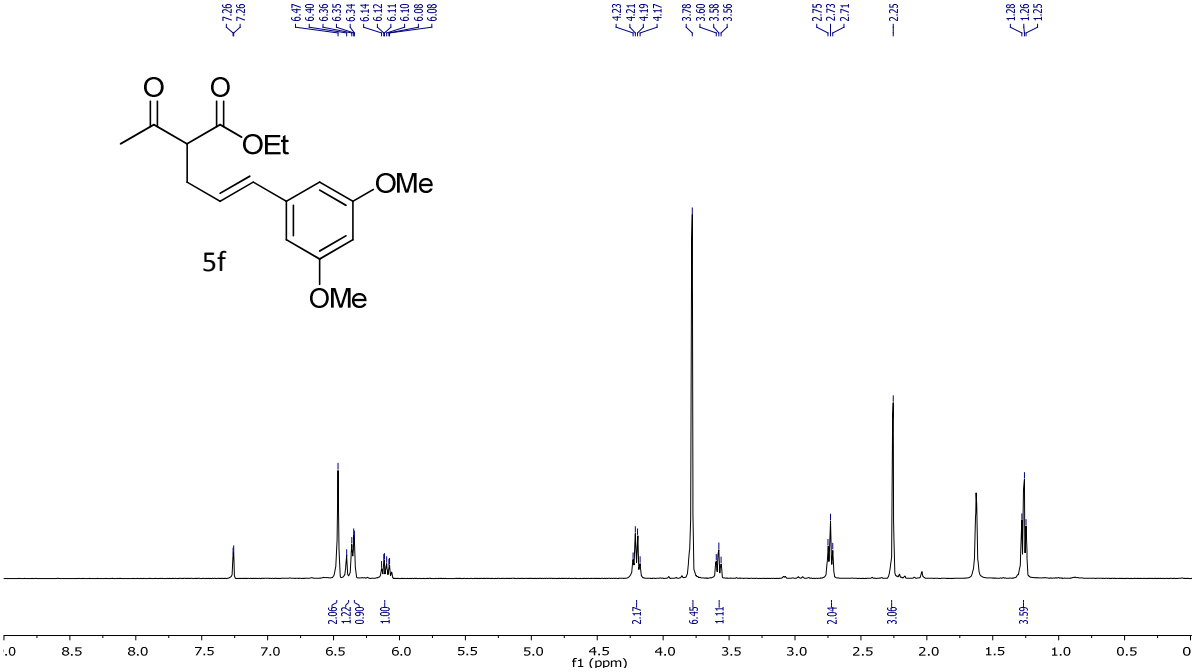
^{13}C NMR of compound (5e) (100 MHz, $CDCl_3$)



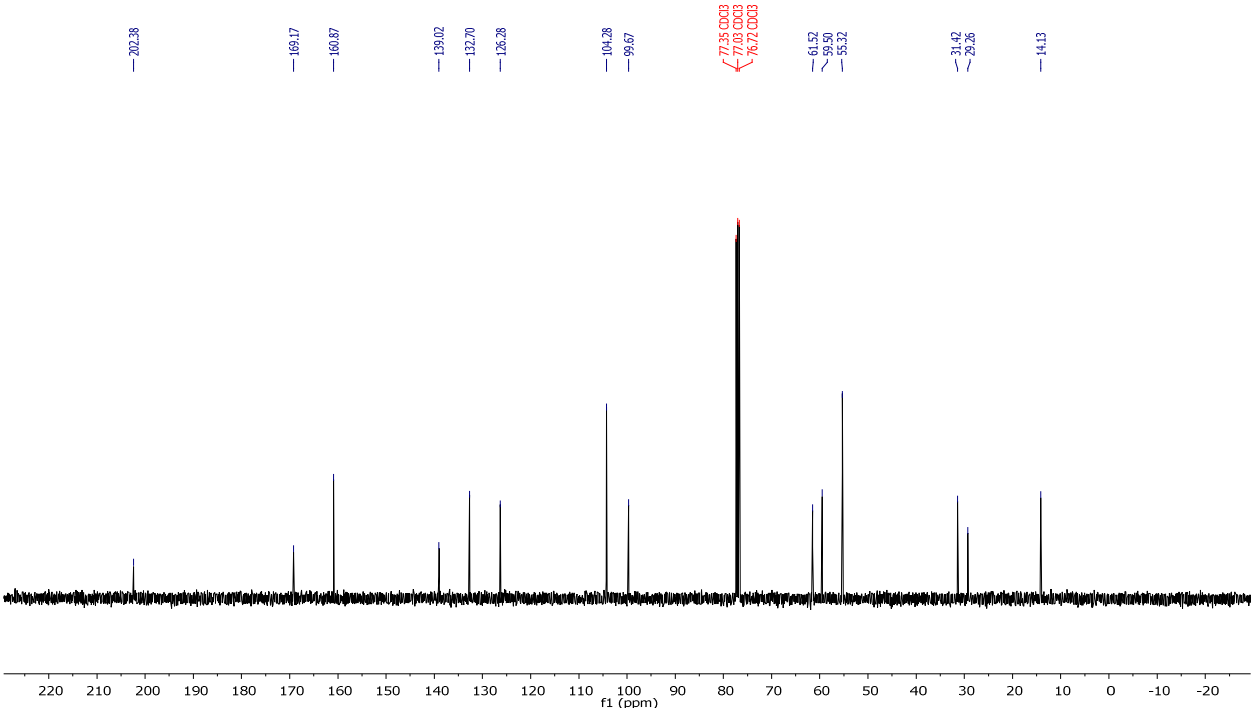
DEPT-135 of compound (5e) (100 MHz, $CDCl_3$)



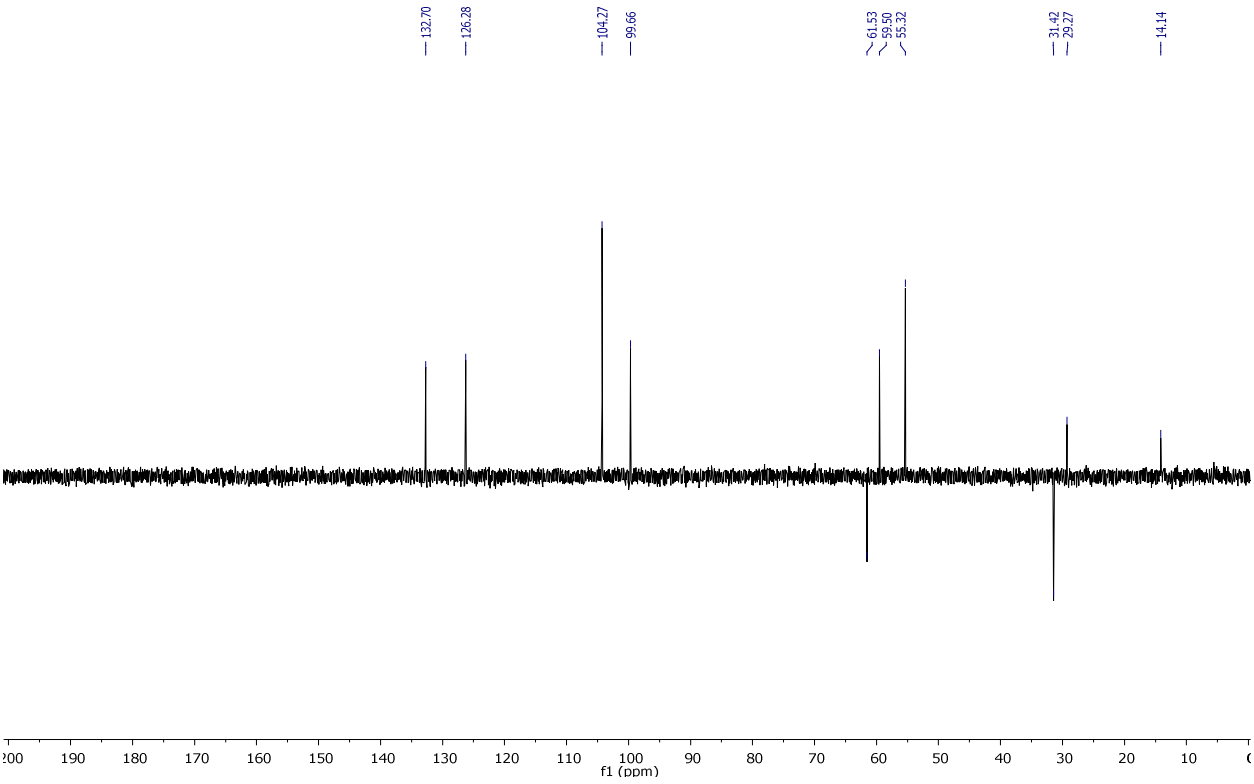
^{1}H NMR of compound (5f) (400 MHz, $CDCl_3$)



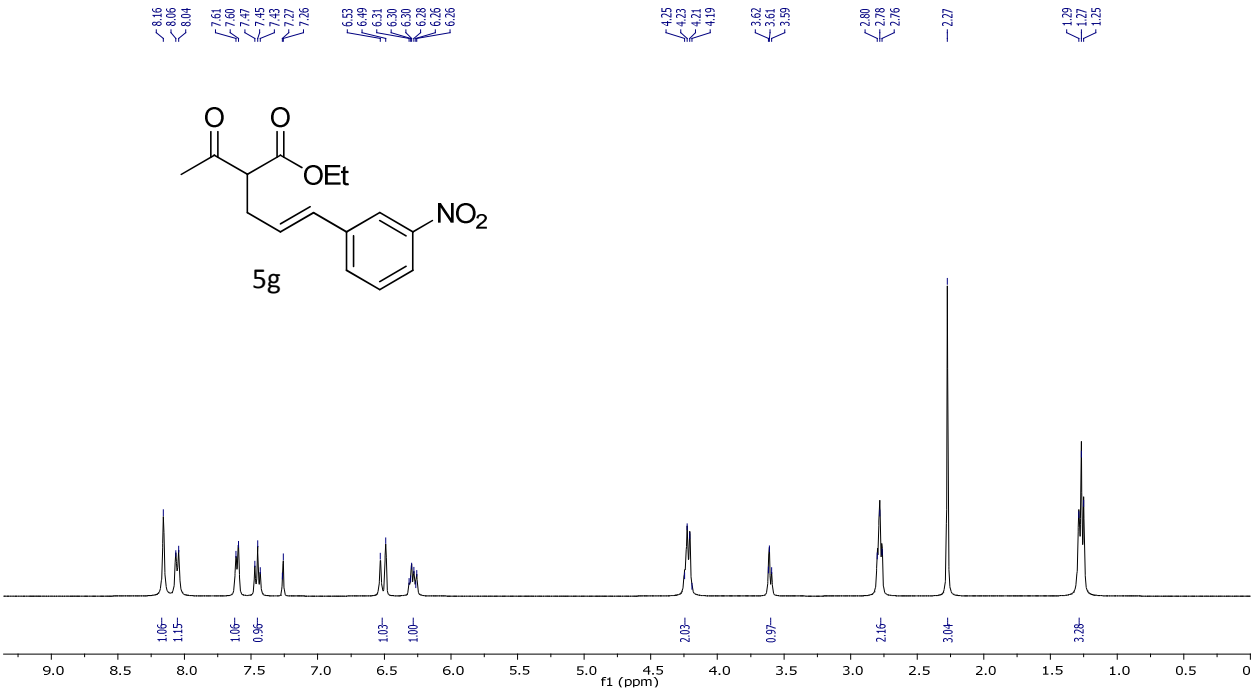
^{13}C NMR of compound (5f) (100 MHz, $CDCl_3$)



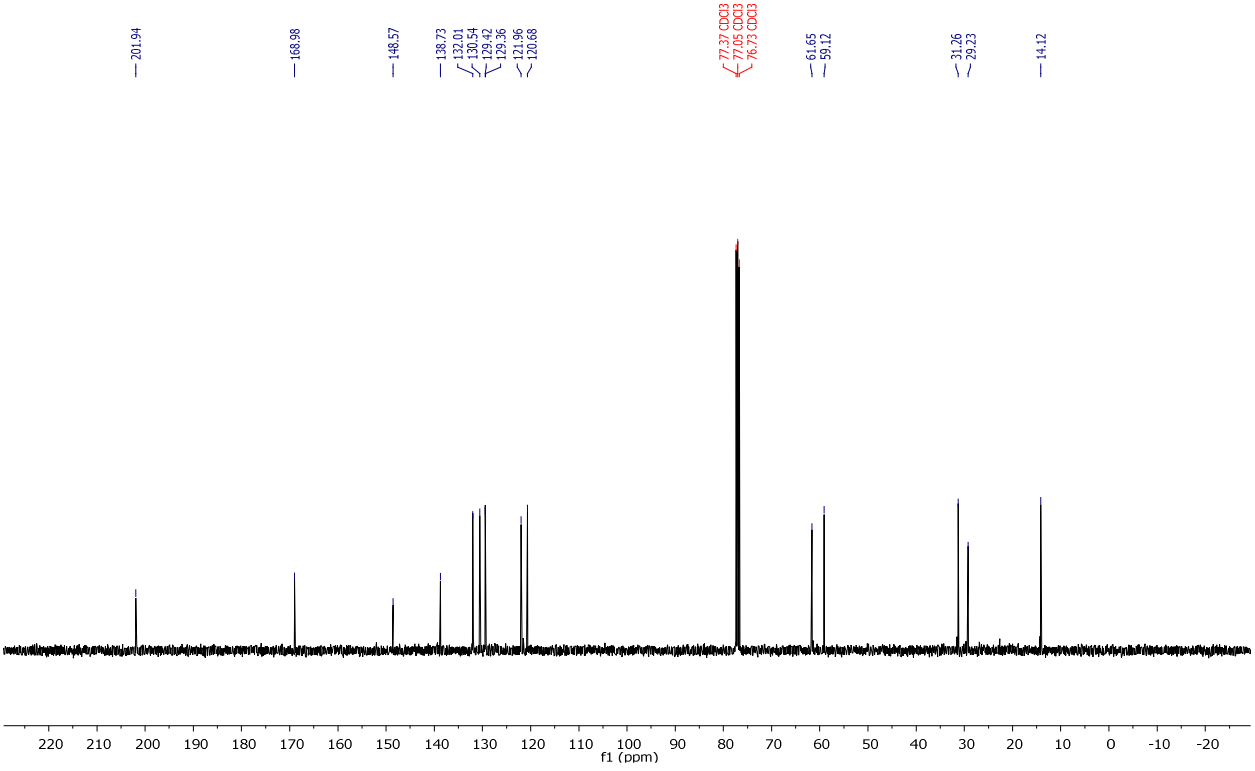
DEPT-135 of compound (5f) (100 MHz, $CDCl_3$)



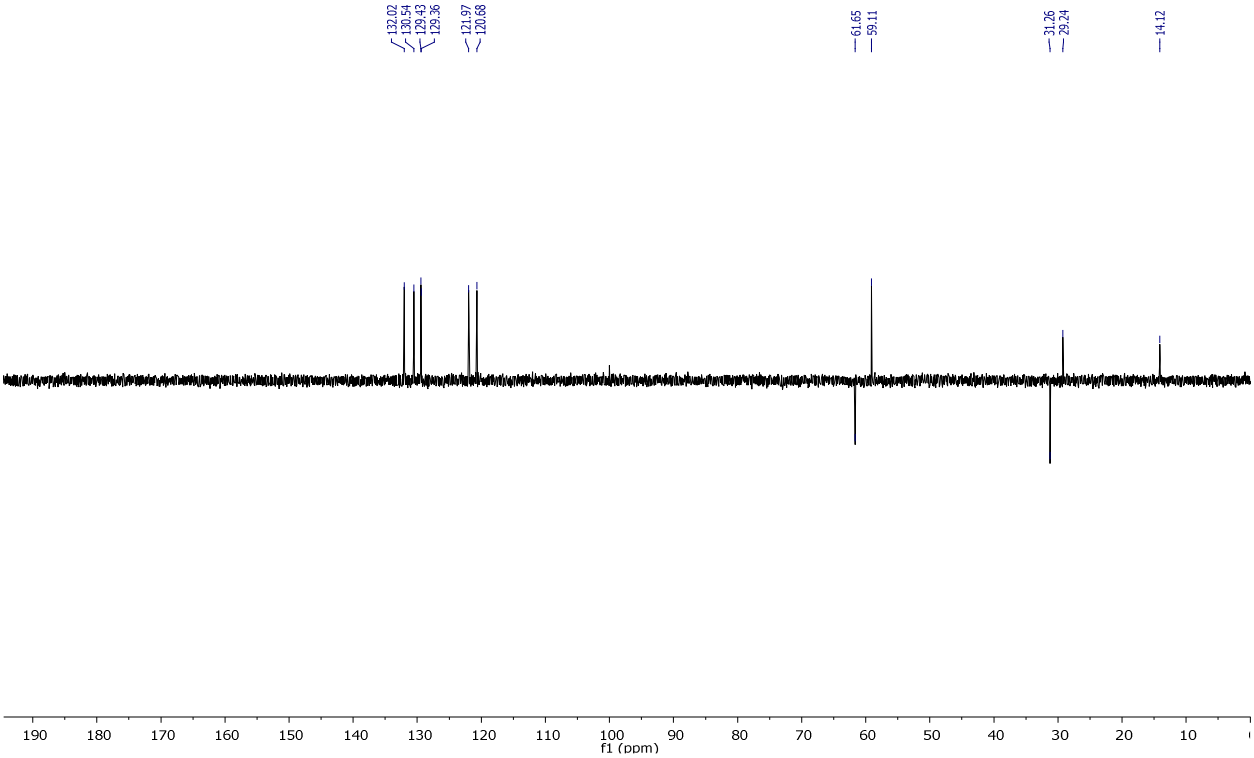
^{1}H NMR of compound (5g) (400 MHz, $CDCl_3$)



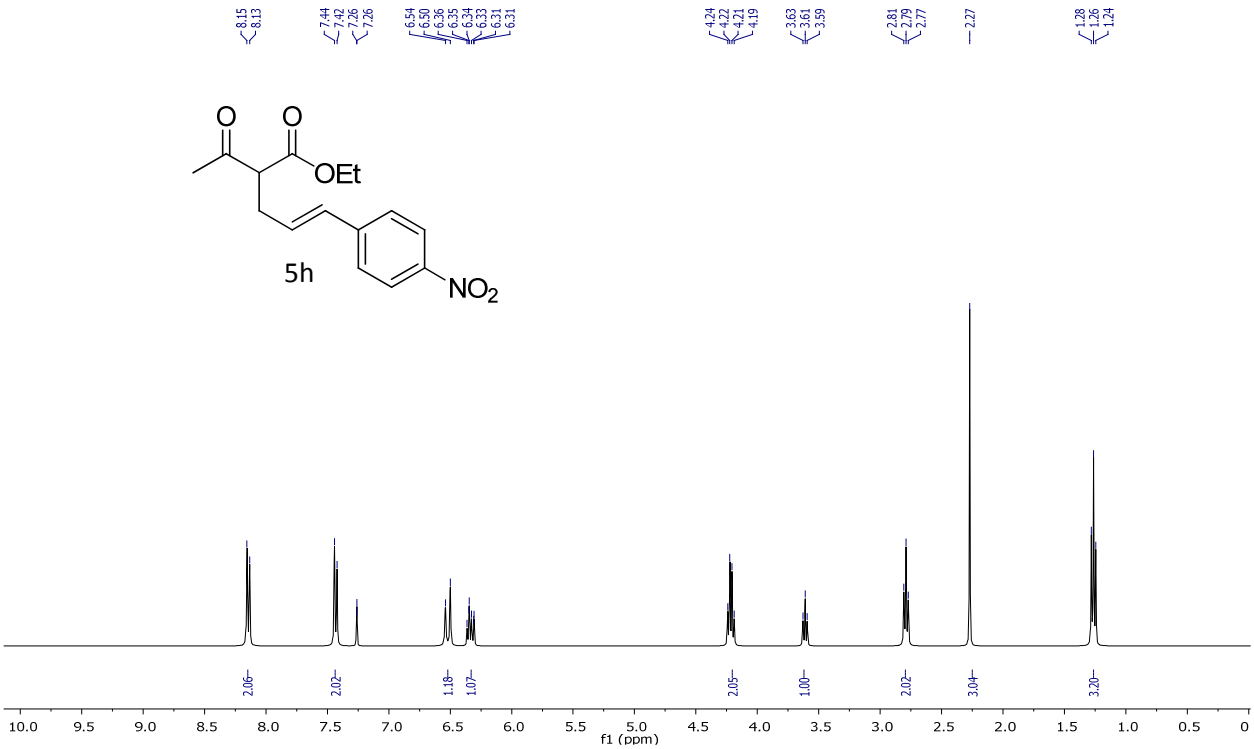
^{13}C NMR of compound (5g) (100 MHz, $CDCl_3$)



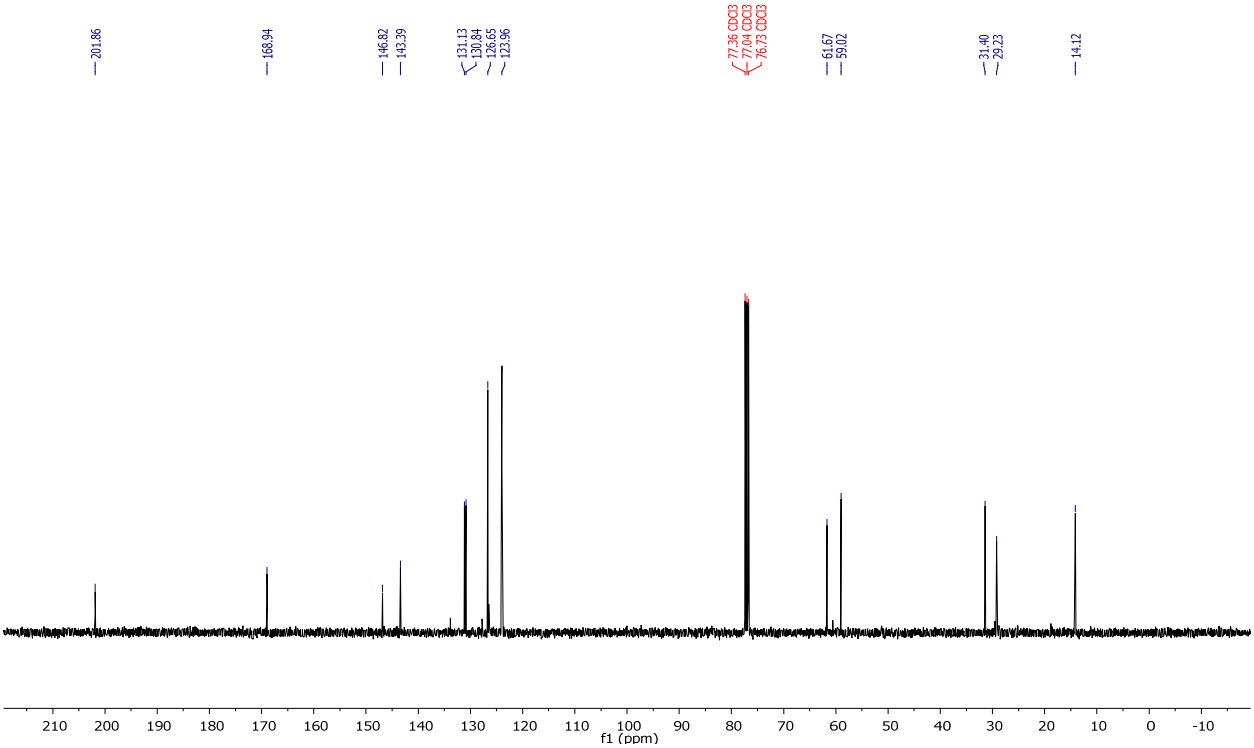
DEPT-135 of compound (5g) (100 MHz, $CDCl_3$)



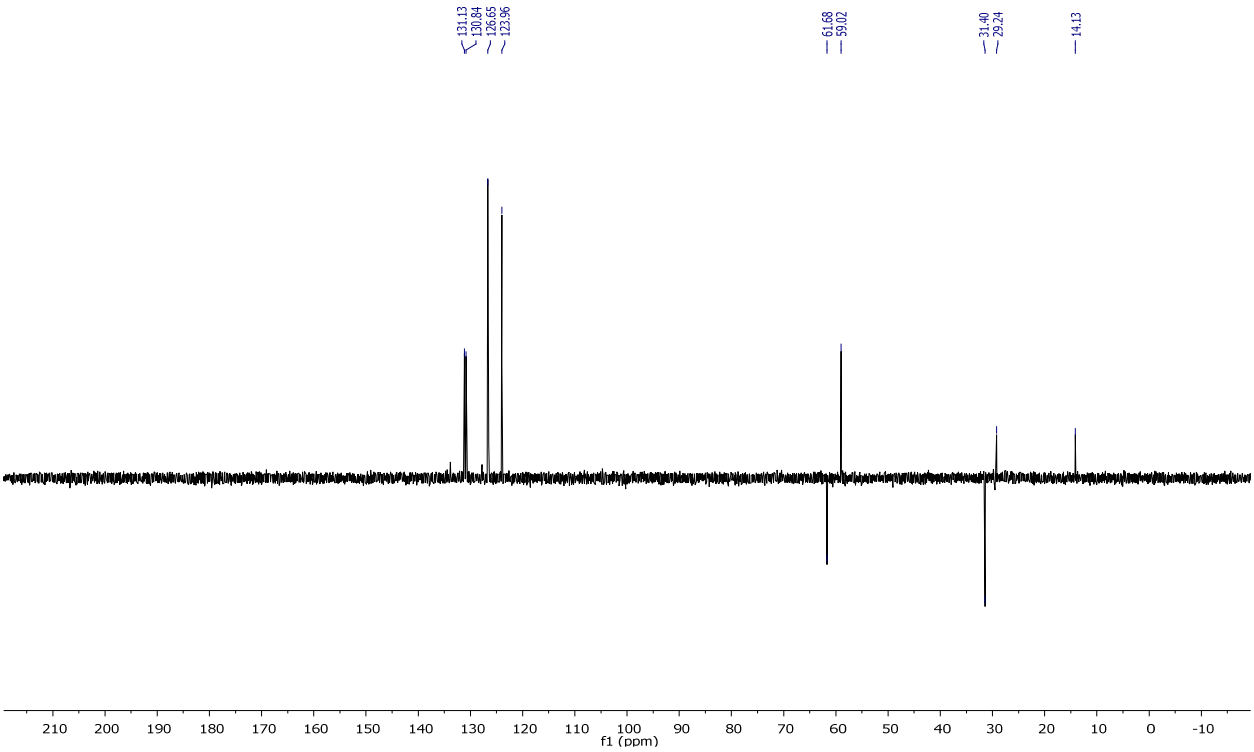
^{1}H NMR of compound (5h) (400 MHz, $CDCl_3$)



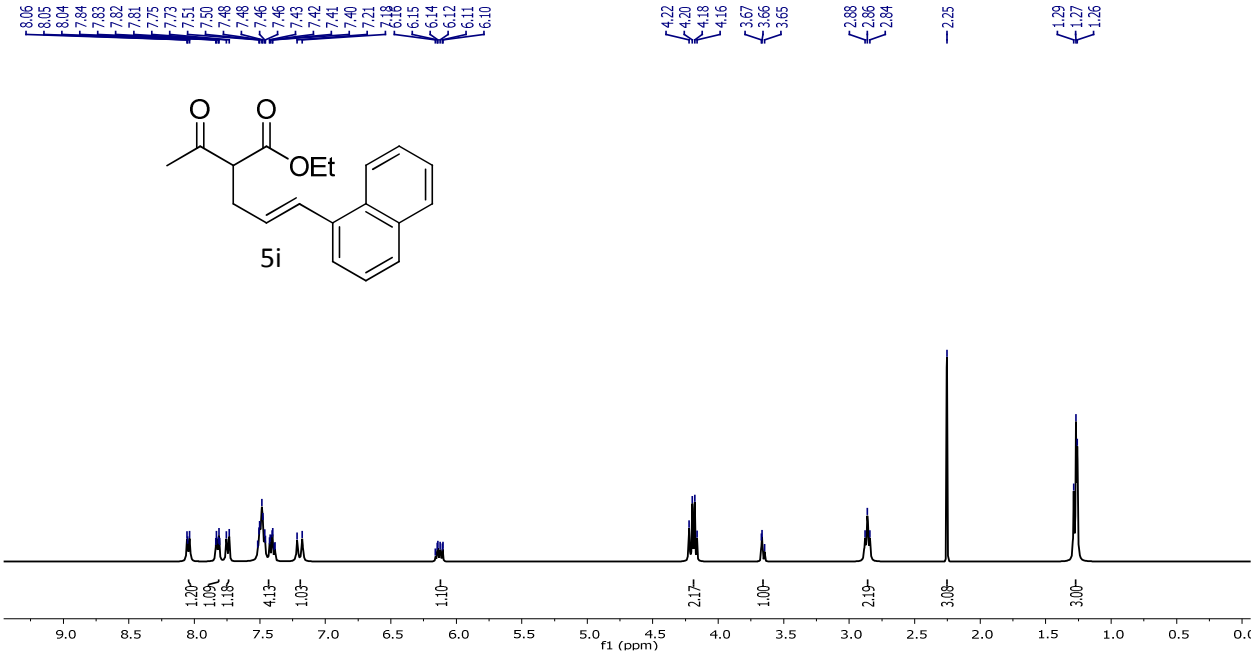
^{13}C NMR of compound (5h) (100 MHz, $CDCl_3$)



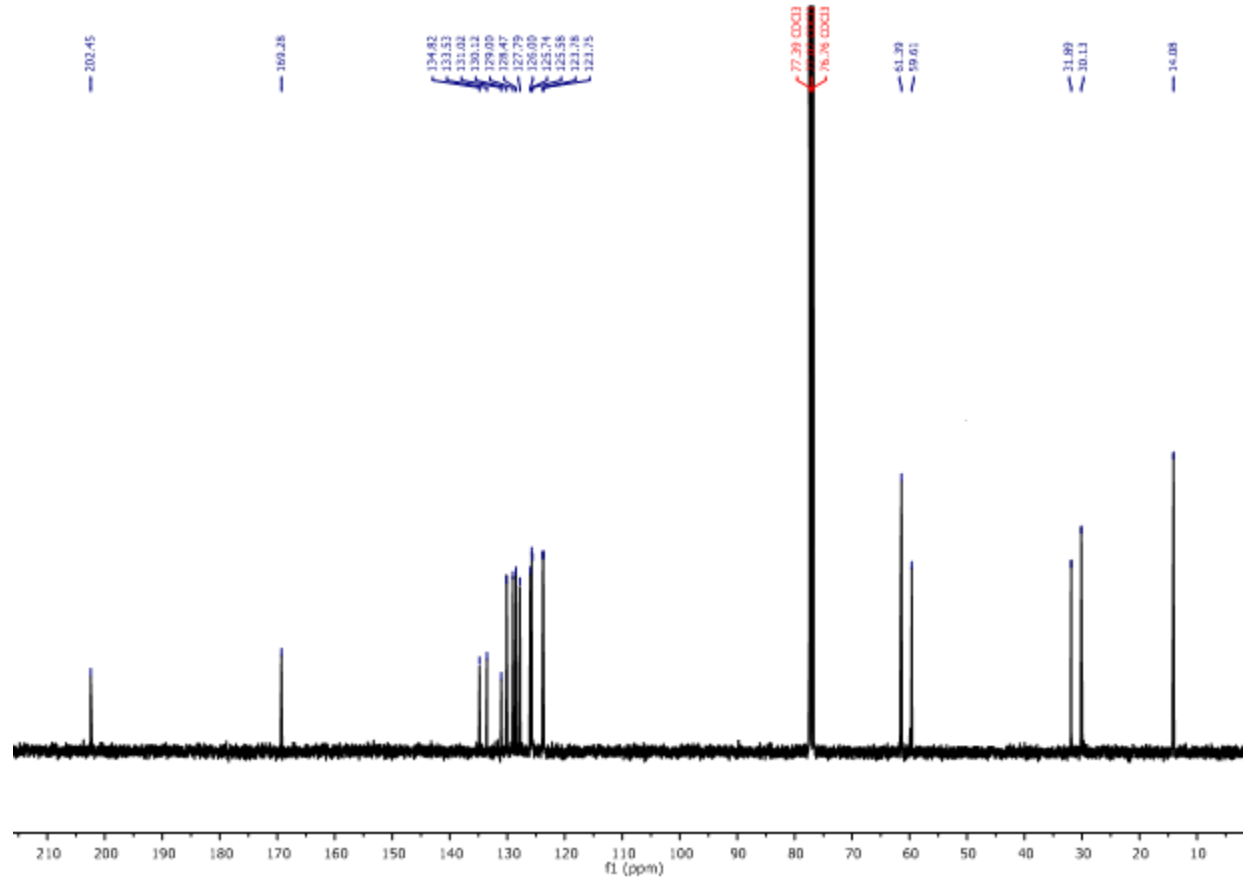
DEPT-135 of compound (5h) (100 MHz, $CDCl_3$)



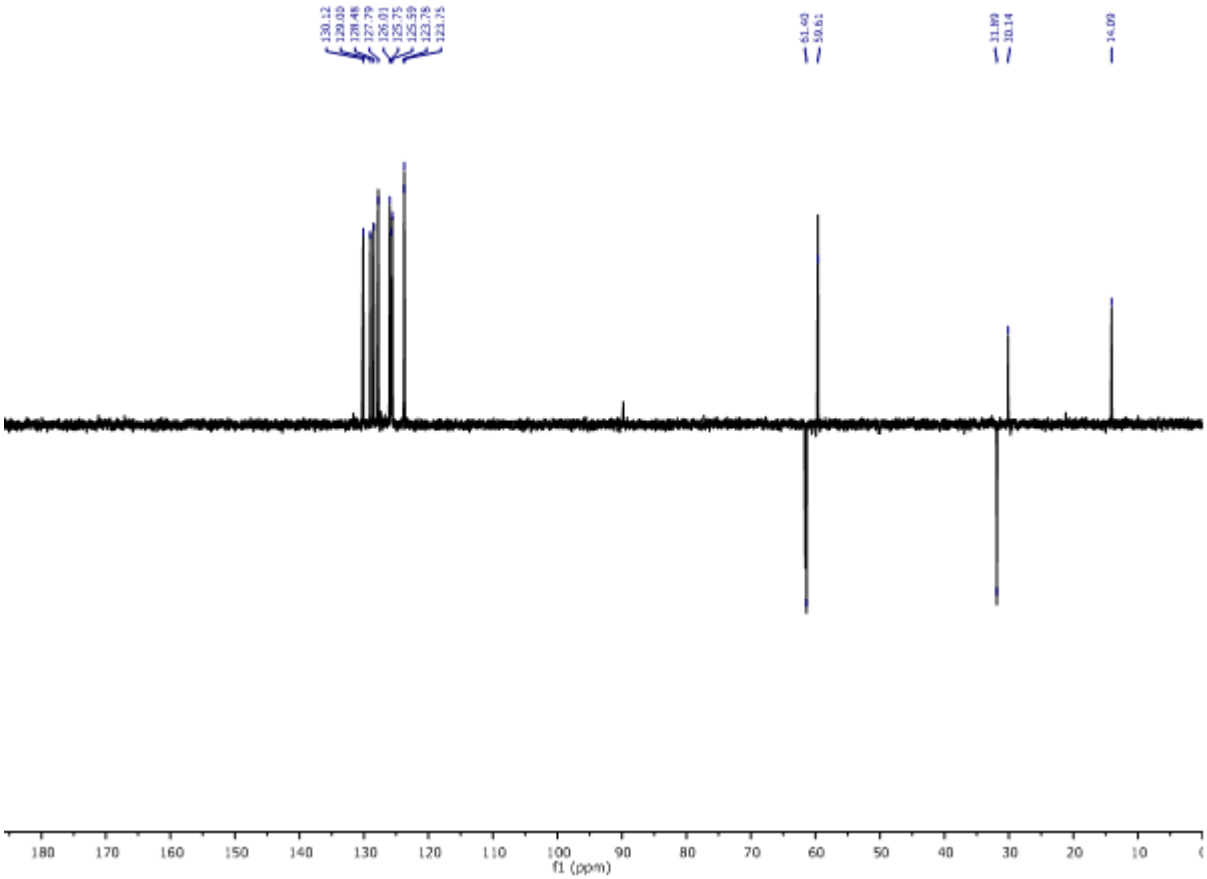
^{1}H NMR of compound (5i) (400 MHz, $CDCl_3$)



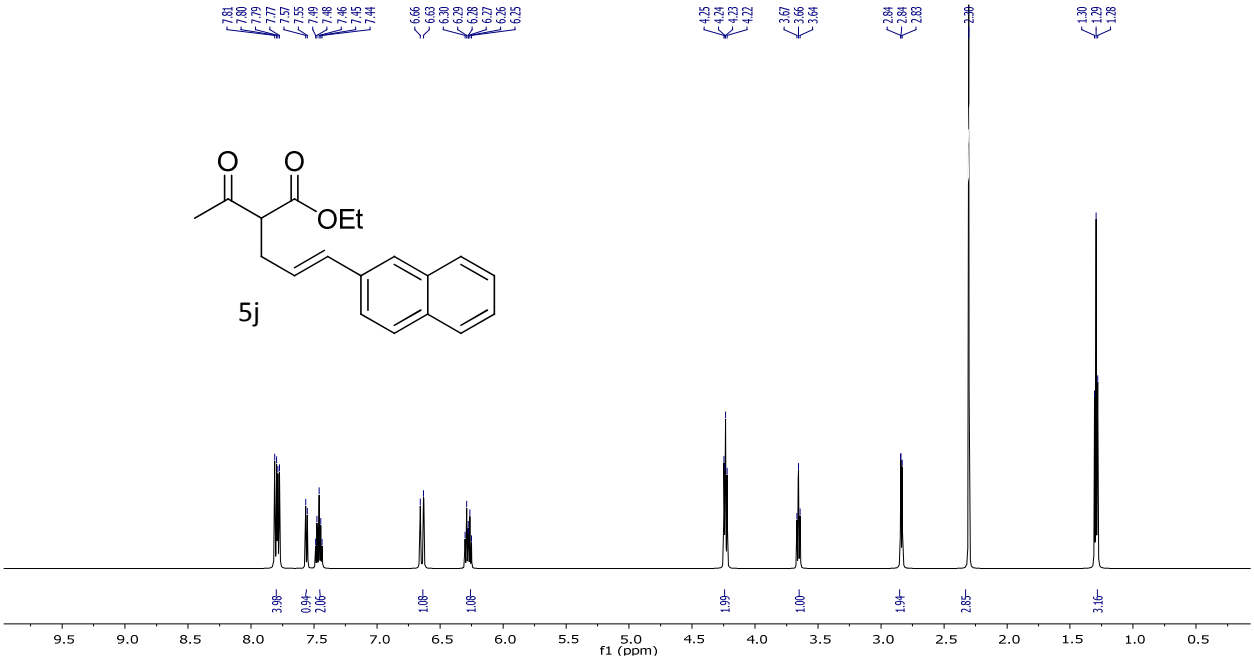
^{13}C NMR of compound (5i) (100 MHz, $CDCl_3$)



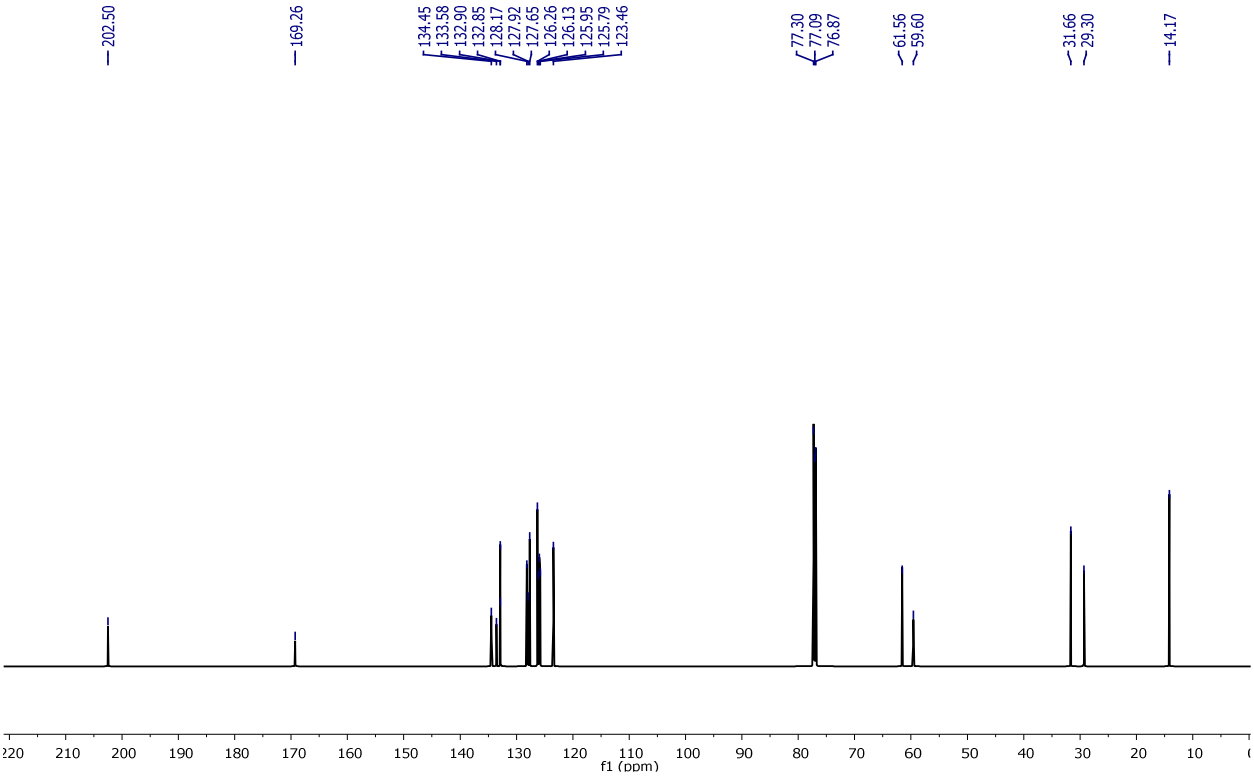
DEPT-135 of compound (5i) (100 MHz, $CDCl_3$)



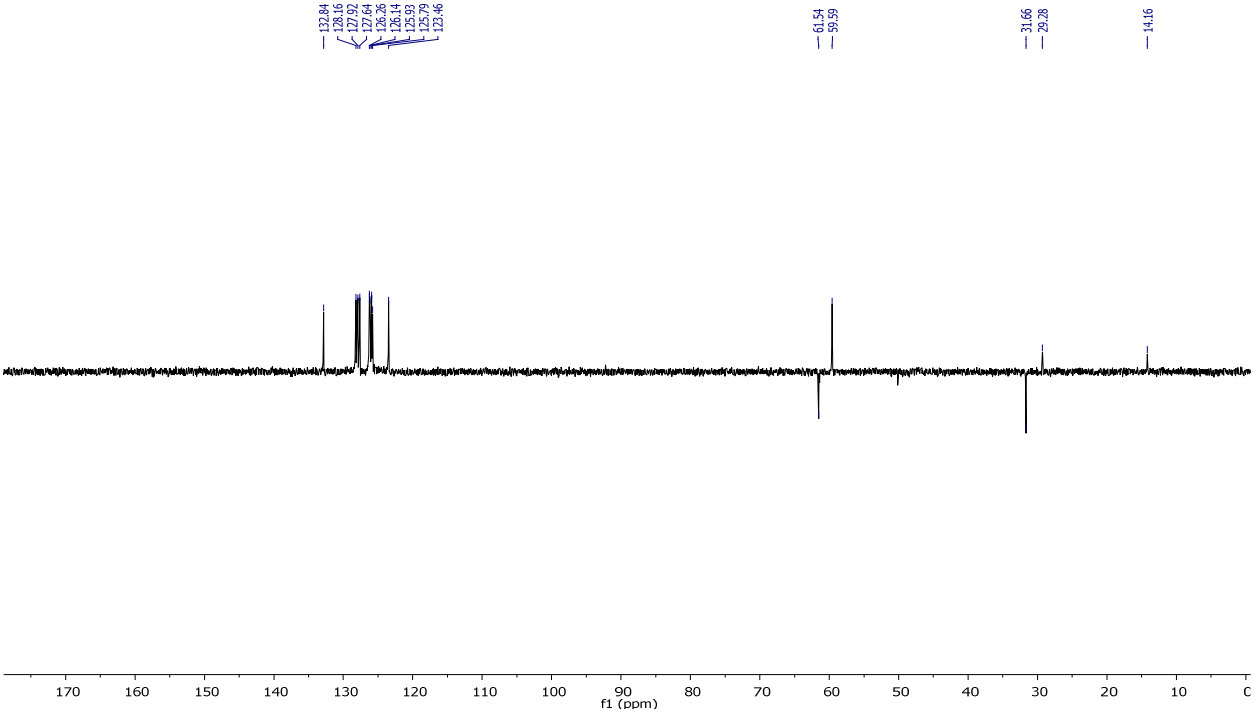
^{1}H NMR of compound (5j) (600 MHz, $CDCl_3$)



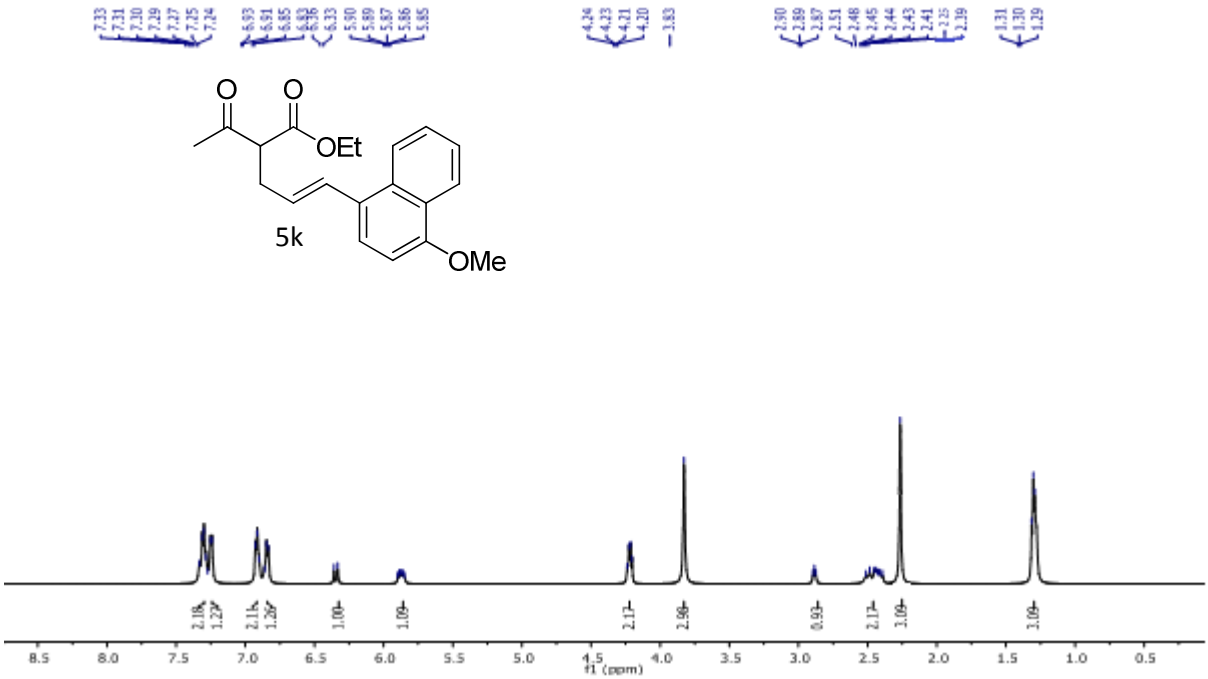
^{13}C NMR of compound (5j) (150 MHz, $CDCl_3$)



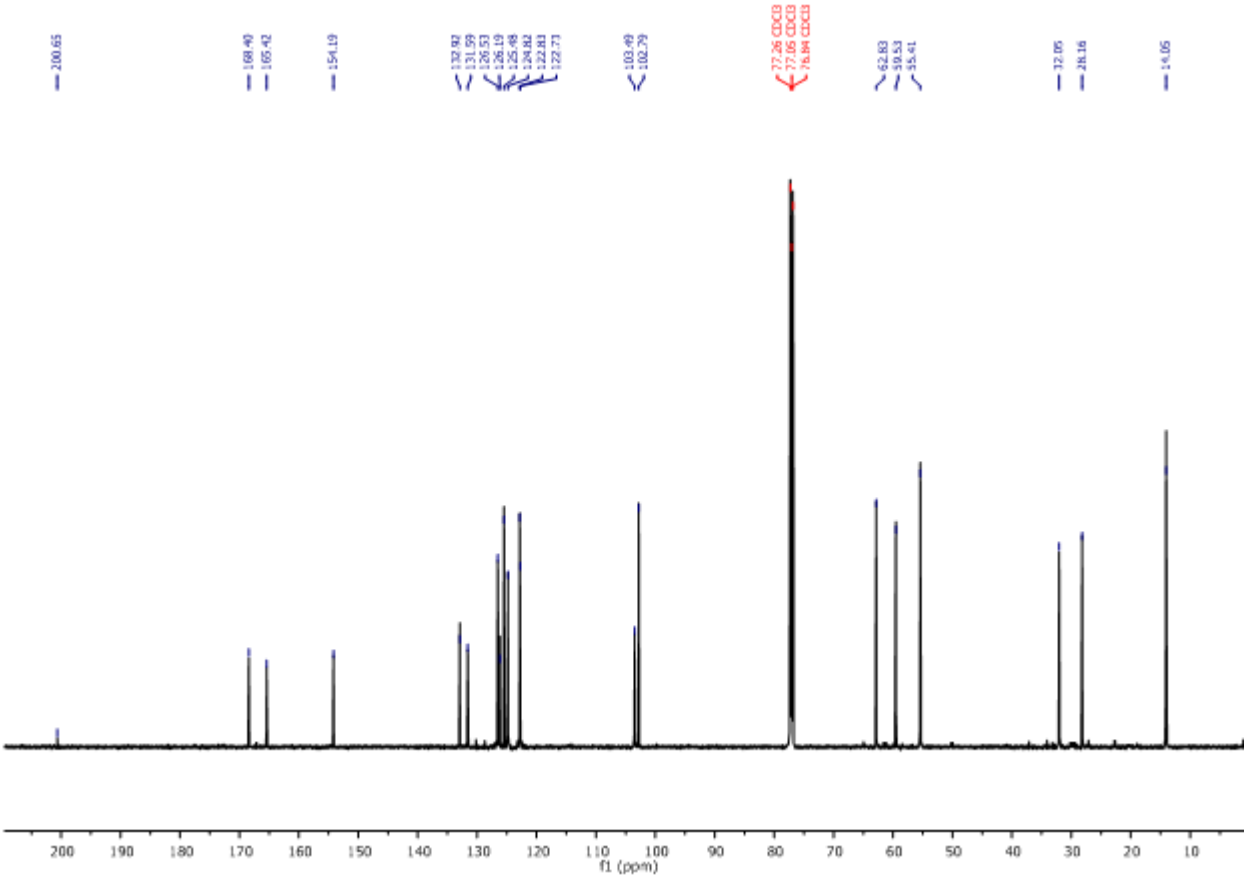
DEPT-135 of compound (5j) (150 MHz, $CDCl_3$)



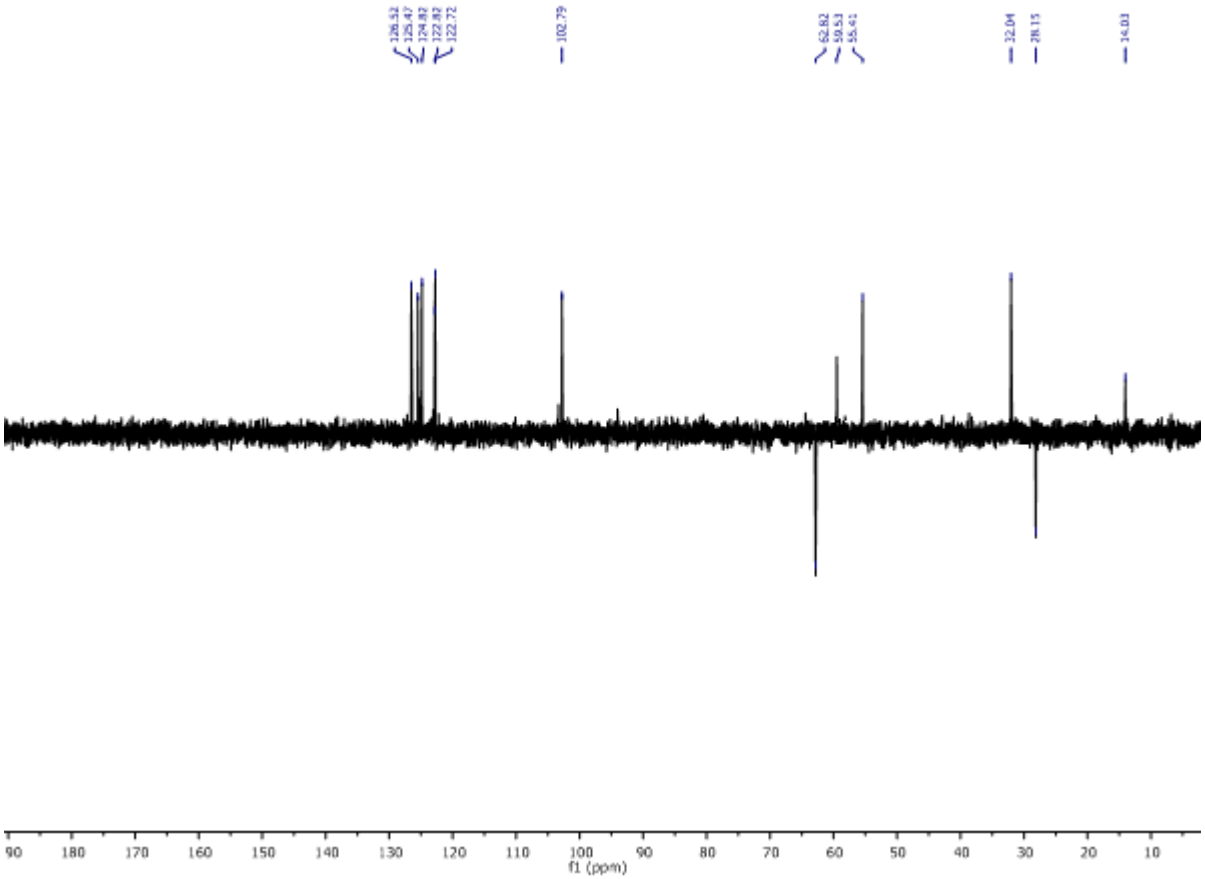
^{1}H NMR of compound (5k) (600 MHz, $CDCl_3$)



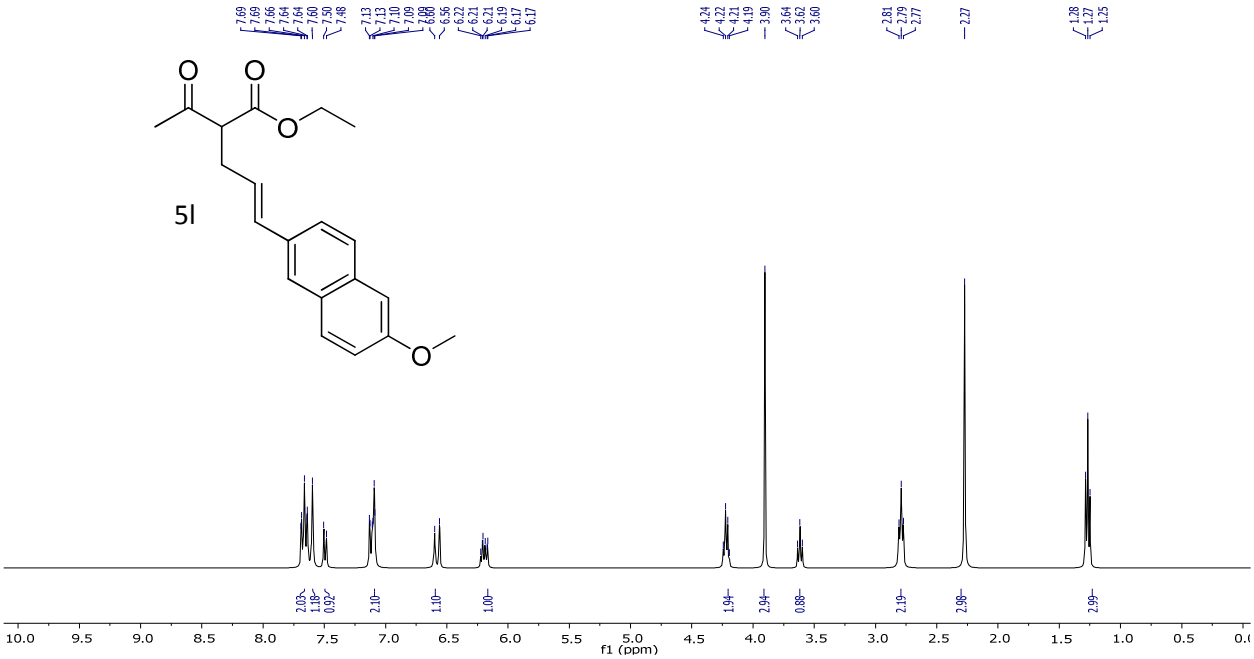
^{13}C NMR of compound (5k) (150 MHz, $CDCl_3$)



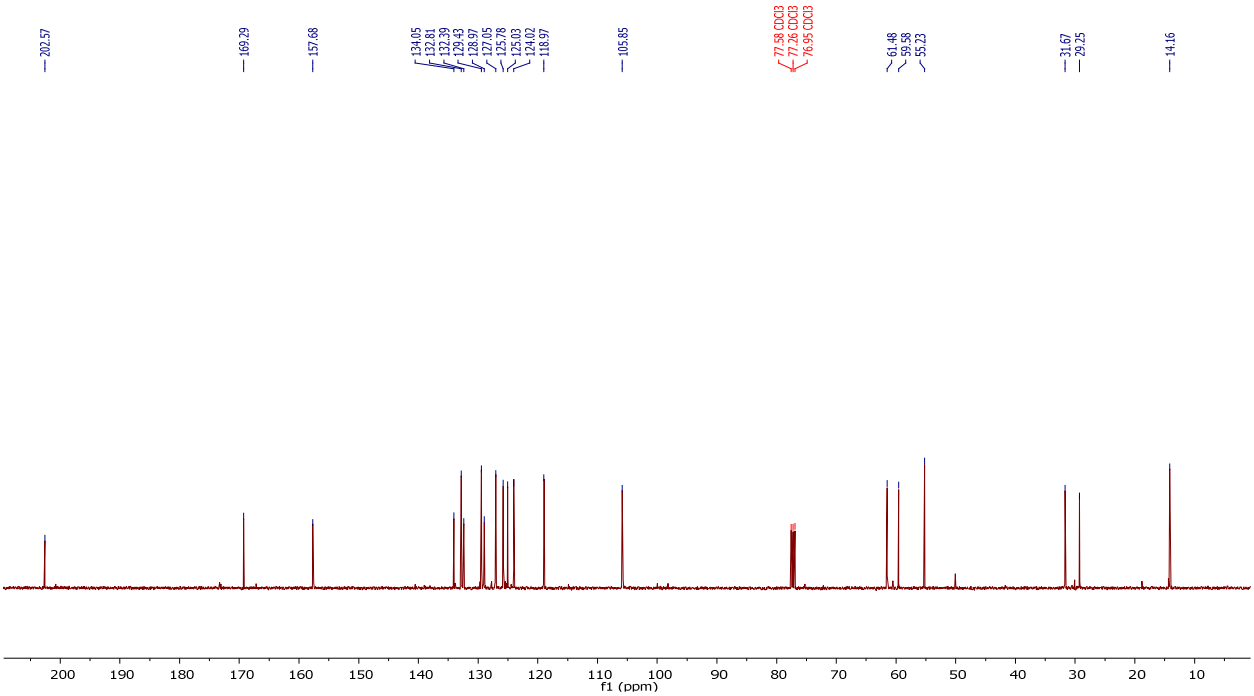
DEPT-135 of compound (5k) (100 MHz, $CDCl_3$)



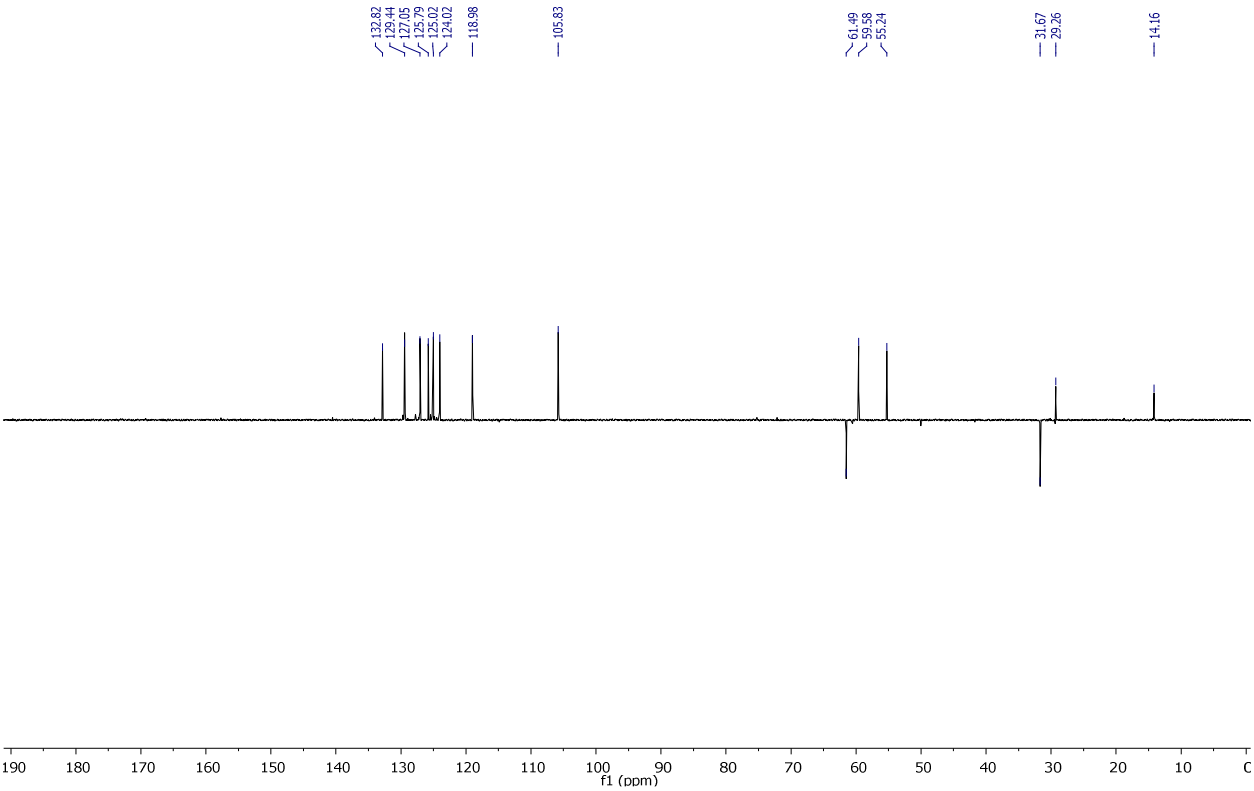
^{1}H NMR of compound (5l) (400 MHz, $CDCl_3$)



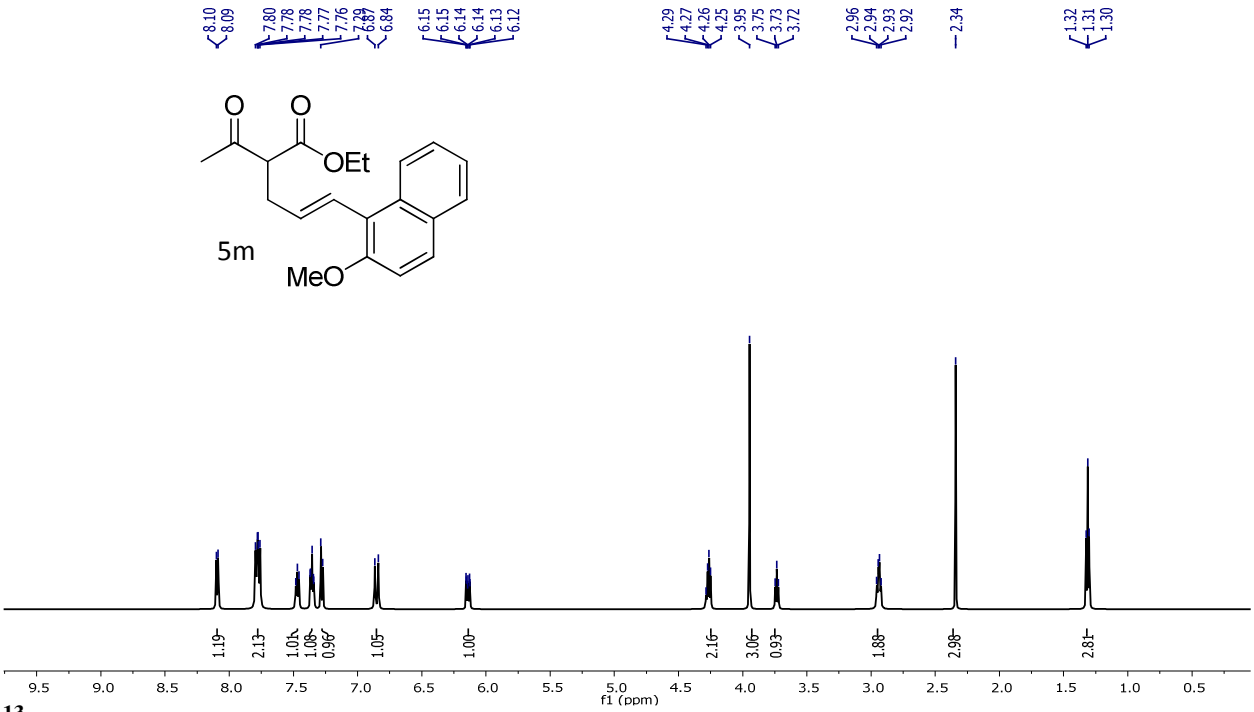
^{13}C NMR of compound (5l) (100 MHz, $CDCl_3$)



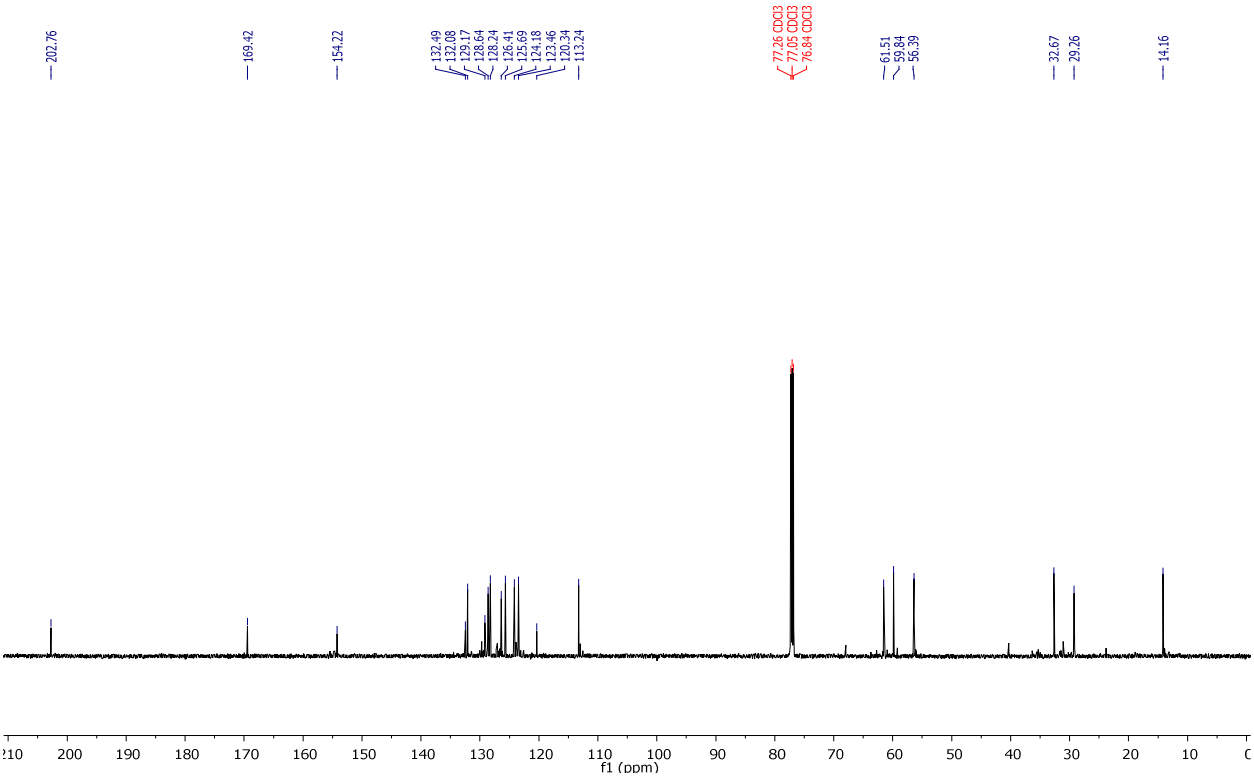
DEPT-135 of compound (5l) (100 MHz, $CDCl_3$)



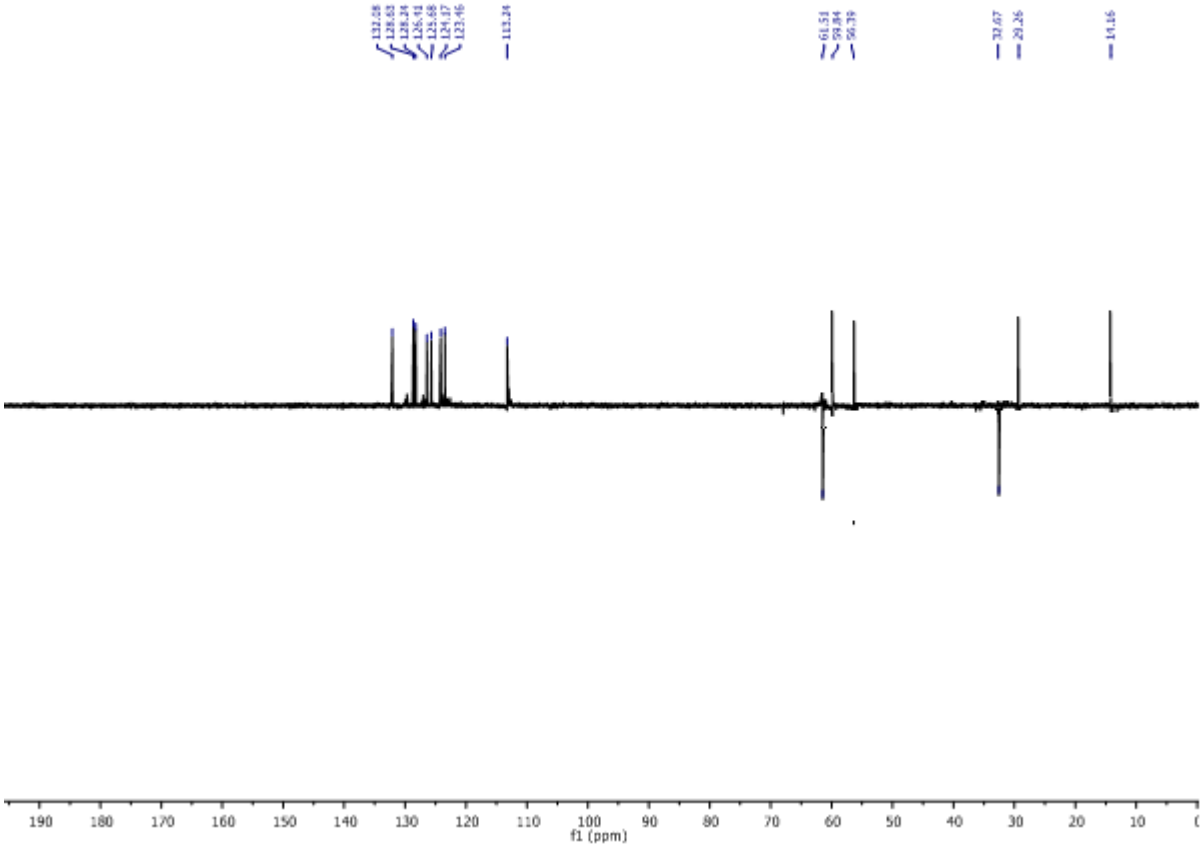
^{1}H NMR of compound (5m) (600 MHz, $CDCl_3$)



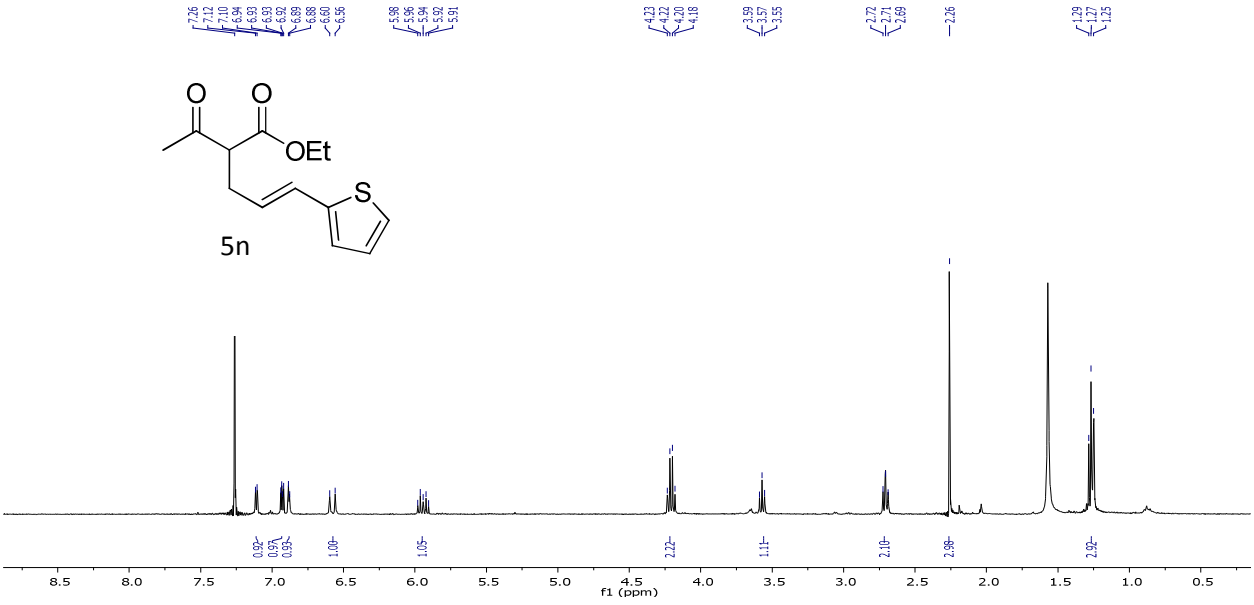
^{13}C NMR of compound (5m) (150 MHz, $CDCl_3$)



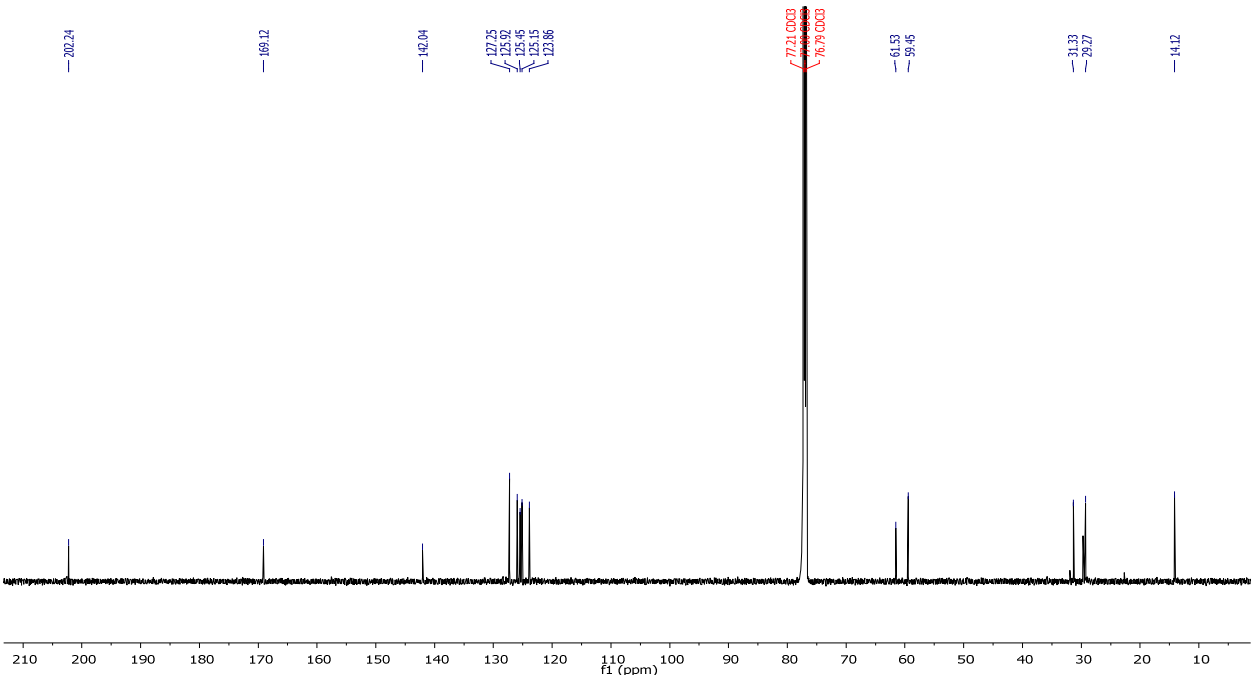
DEPT-135 of compound (5m) (150 MHz, $CDCl_3$)



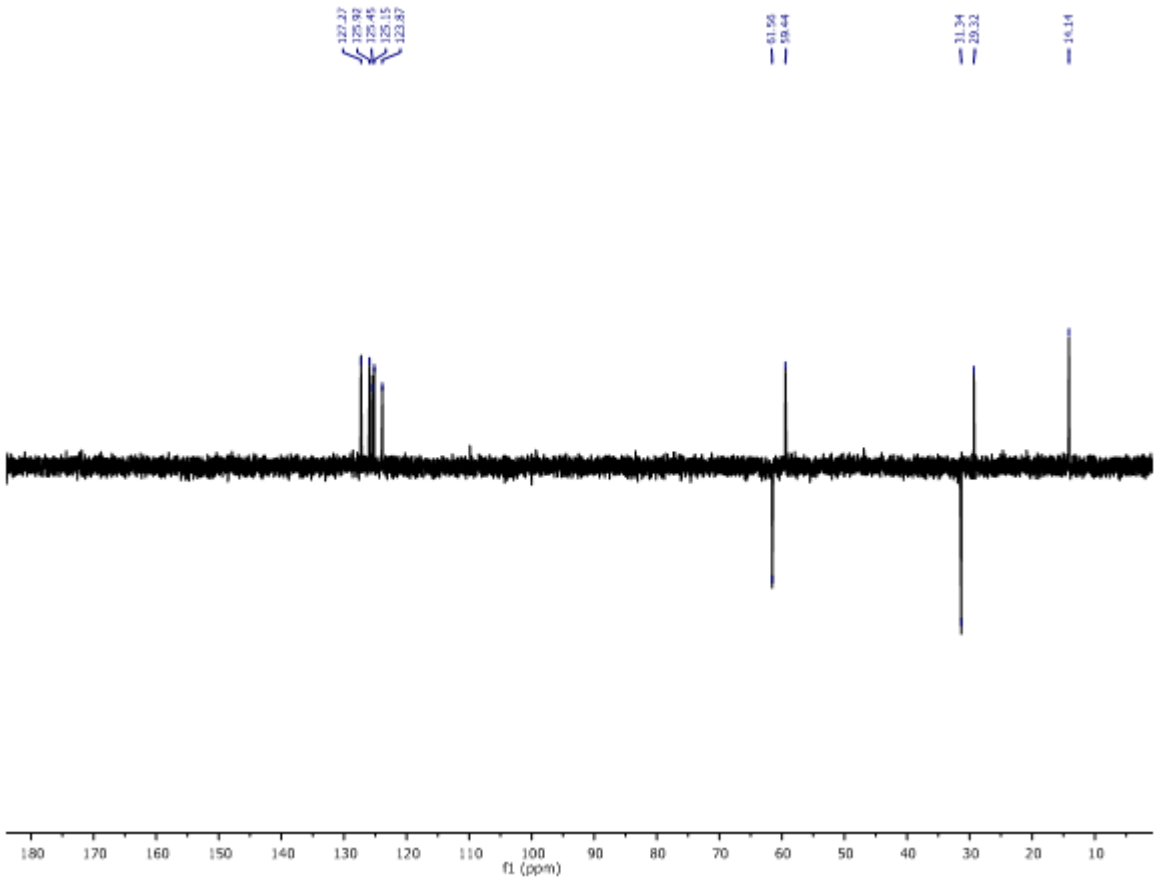
^{1}H NMR of compound (5n) (400 MHz, $CDCl_3$)



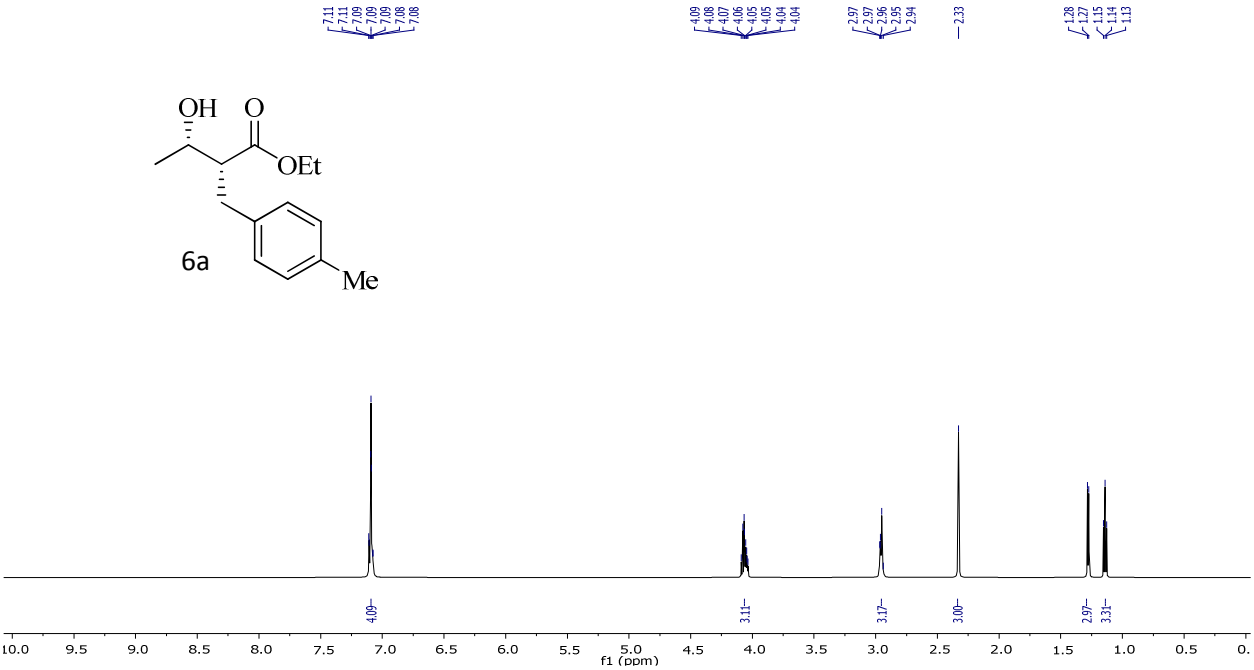
^{13}C NMR of compound (5n) (150 MHz, $CDCl_3$)



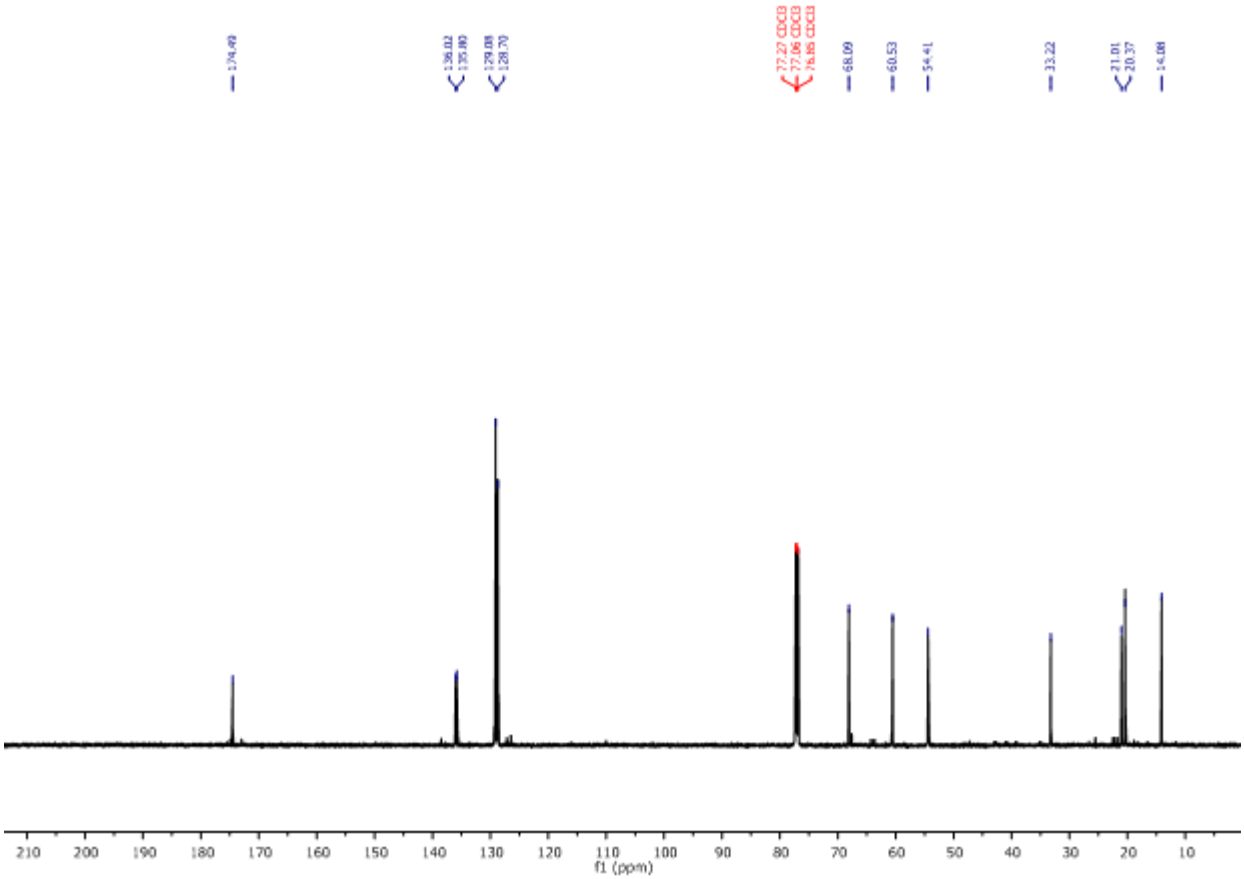
DEPT-135 of compound (5n) (150 MHz, $CDCl_3$)



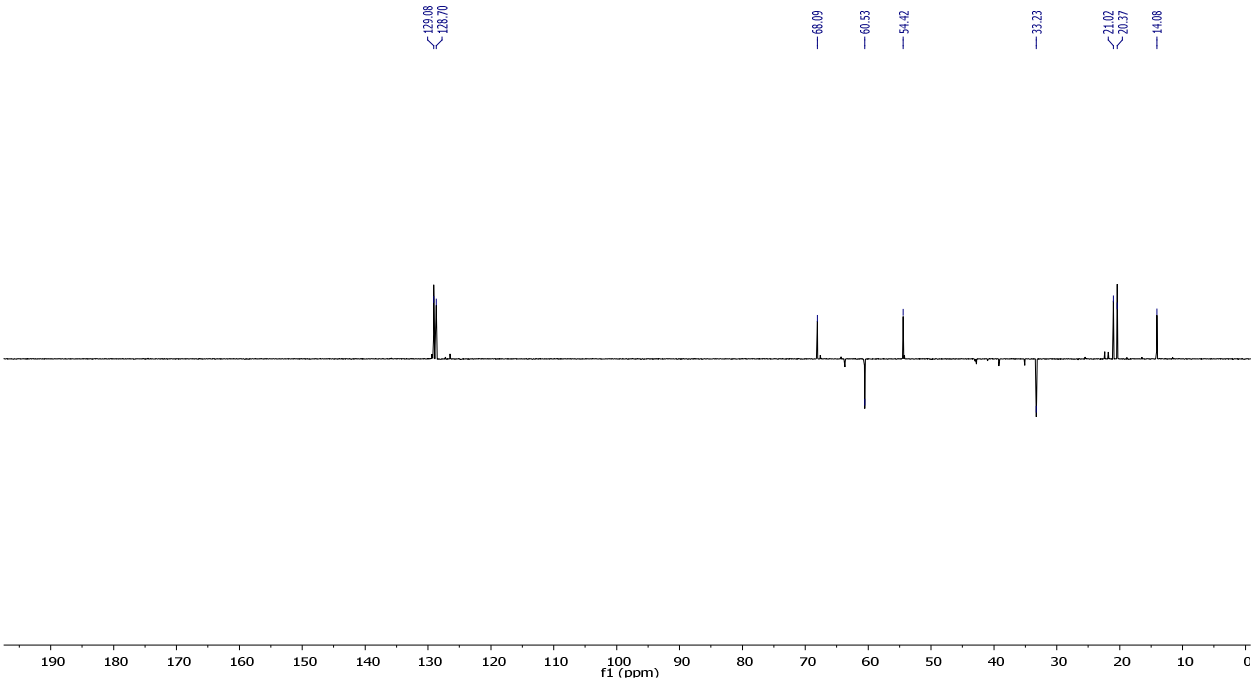
^{1}H NMR of compound (6a) (600 MHz, $CDCl_3$)



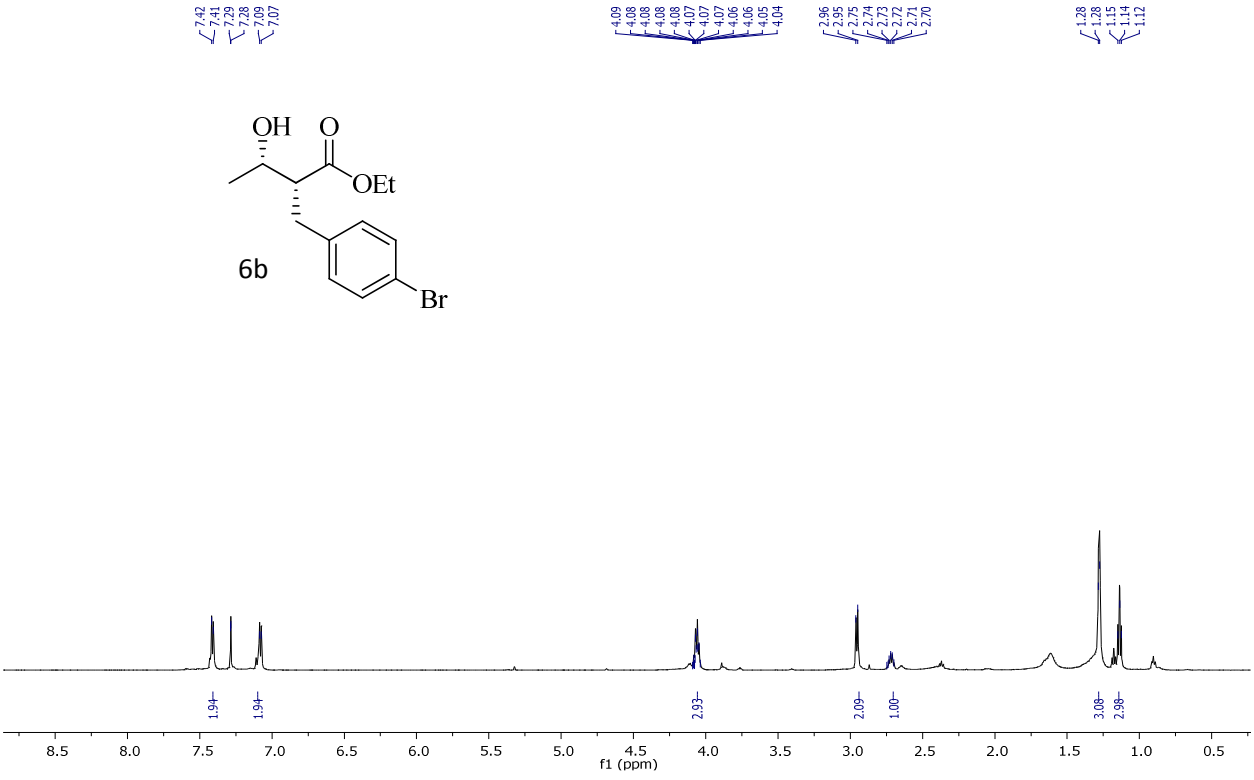
^{13}C NMR of compound (6a) (150 MHz, $CDCl_3$)



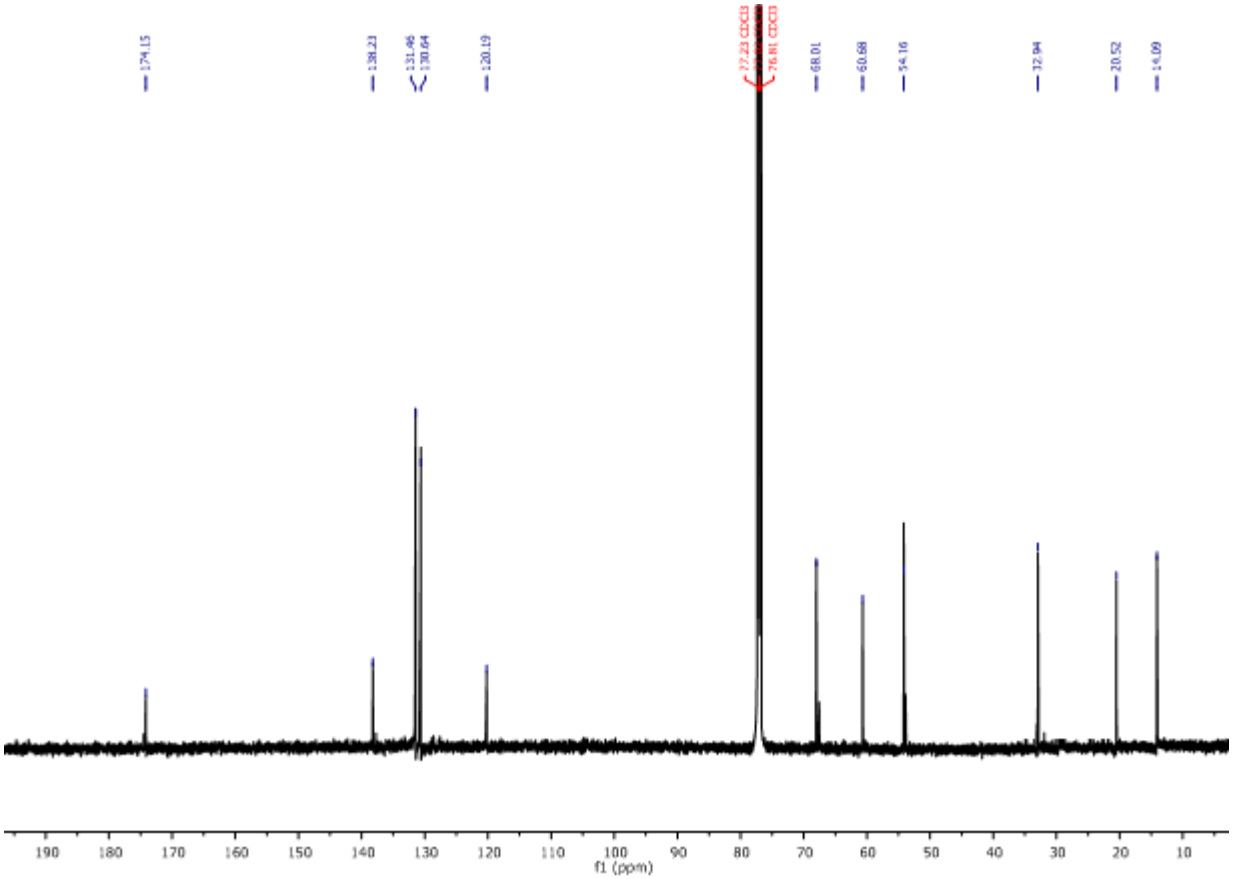
DEPT-135 of compound (6a) (150 MHz, $CDCl_3$)



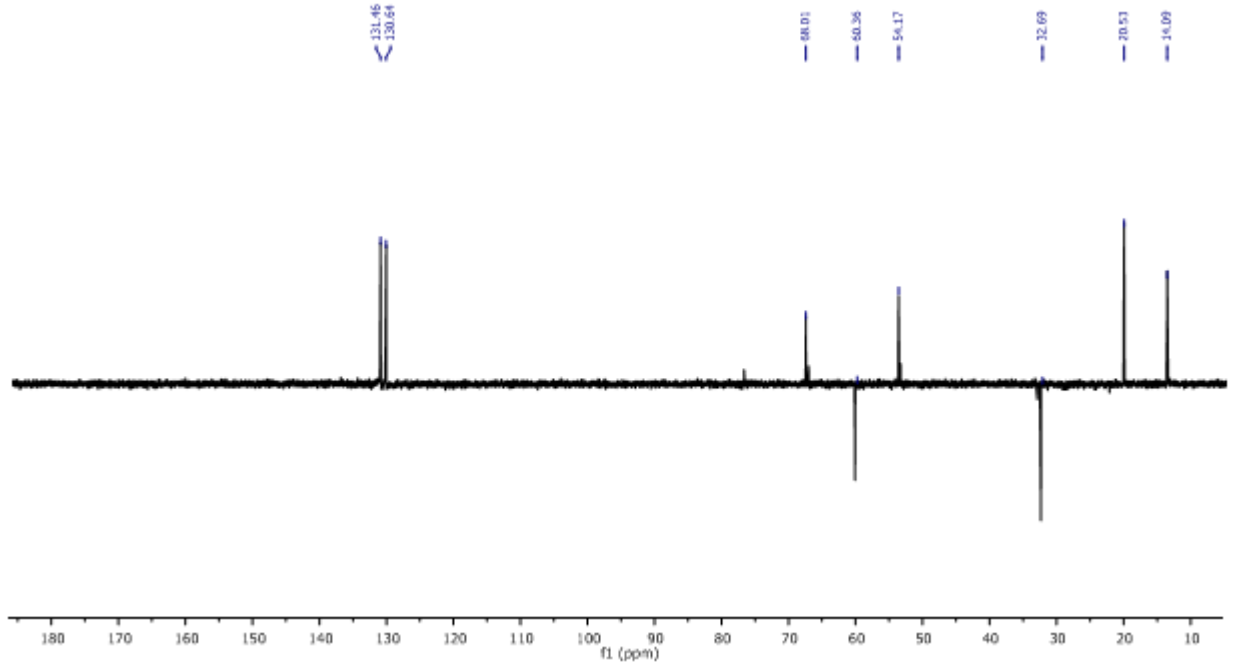
^{1}H NMR of compound (6b) (600 MHz, $CDCl_3$)



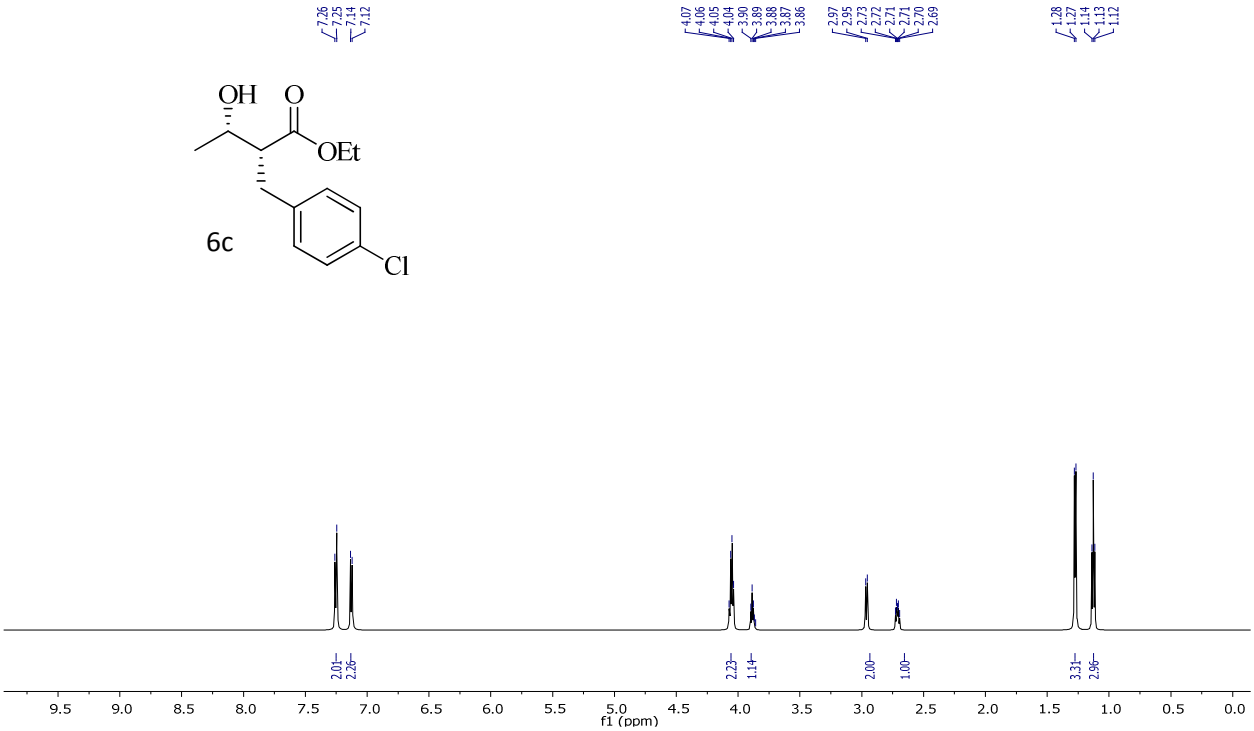
^{13}C NMR of compound (6b) (150 MHz, $CDCl_3$)



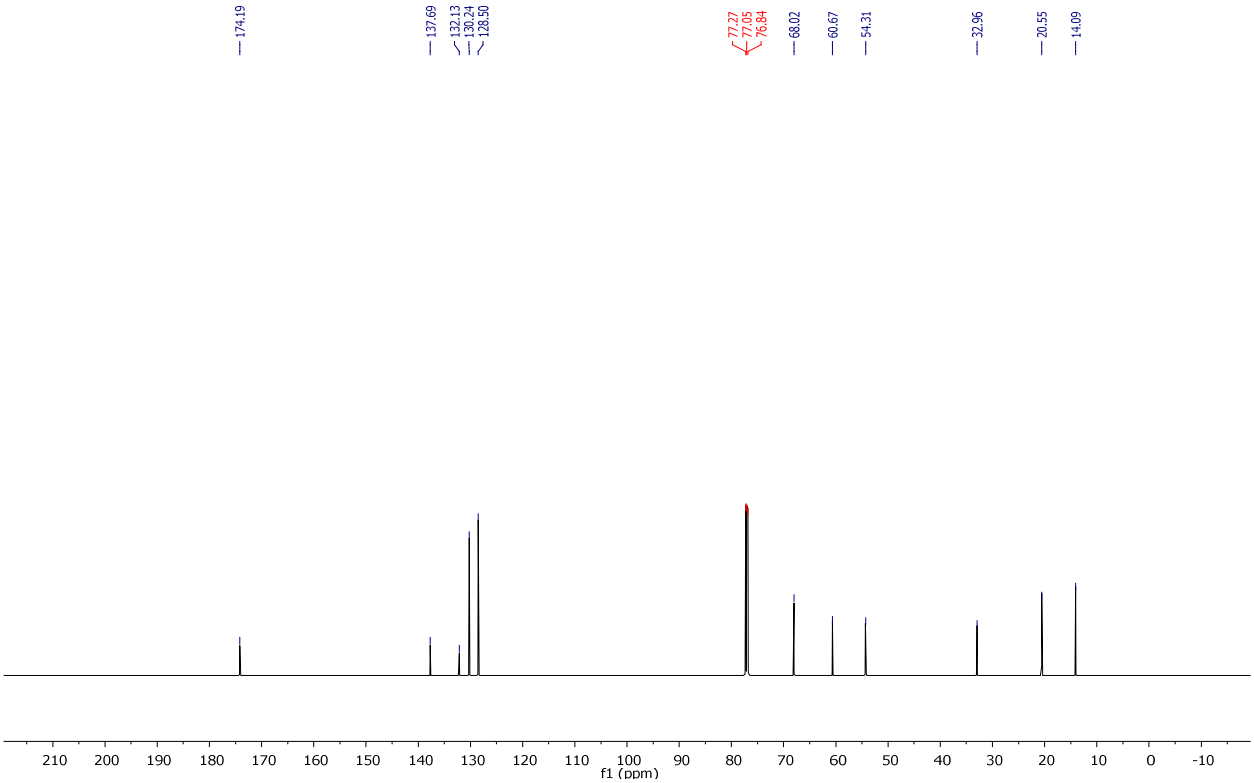
DEPT-135 of compound (6b) (150 MHz, $CDCl_3$)



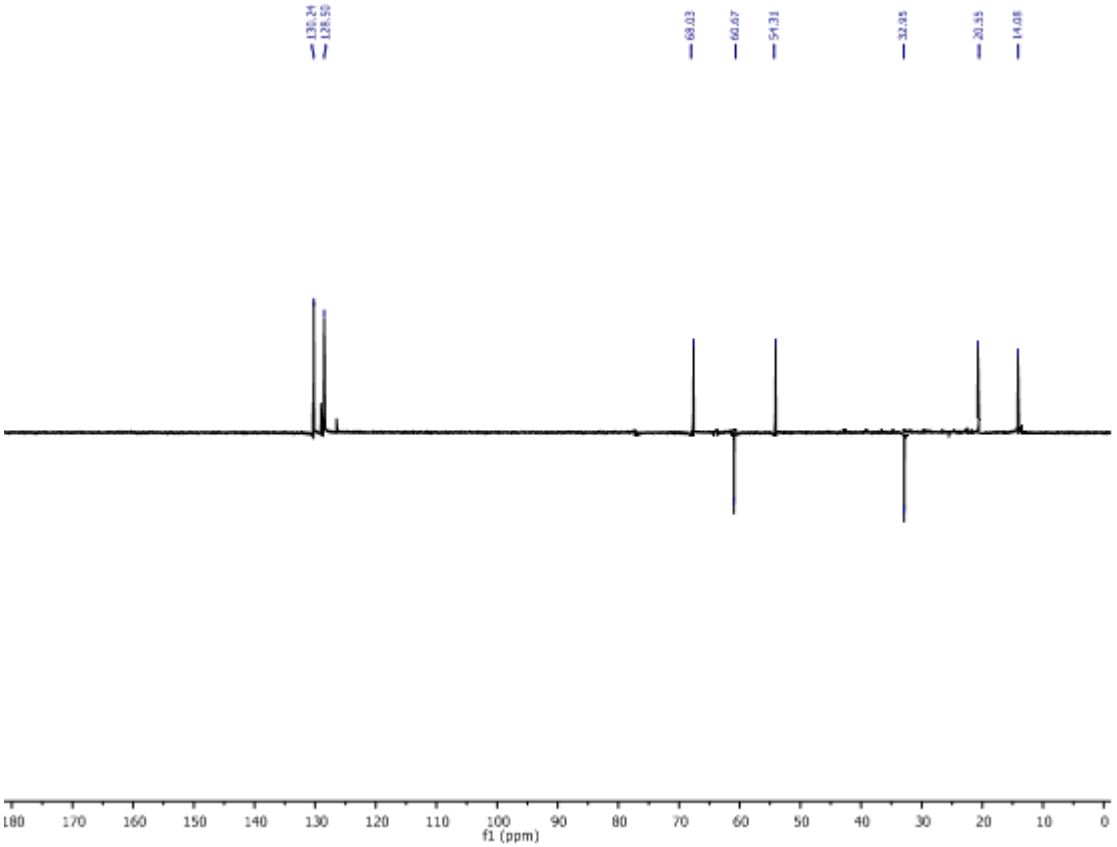
^{1}H NMR of compound (6c) (600 MHz, $CDCl_3$)



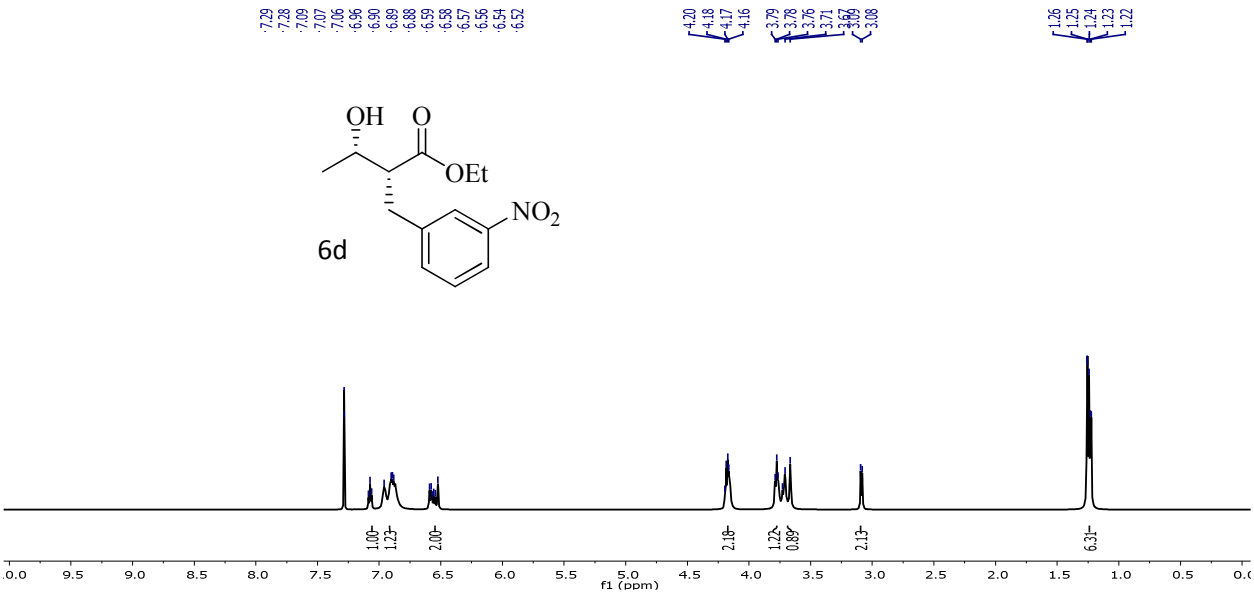
^{13}C NMR of compound (6c) (150 MHz, $CDCl_3$)



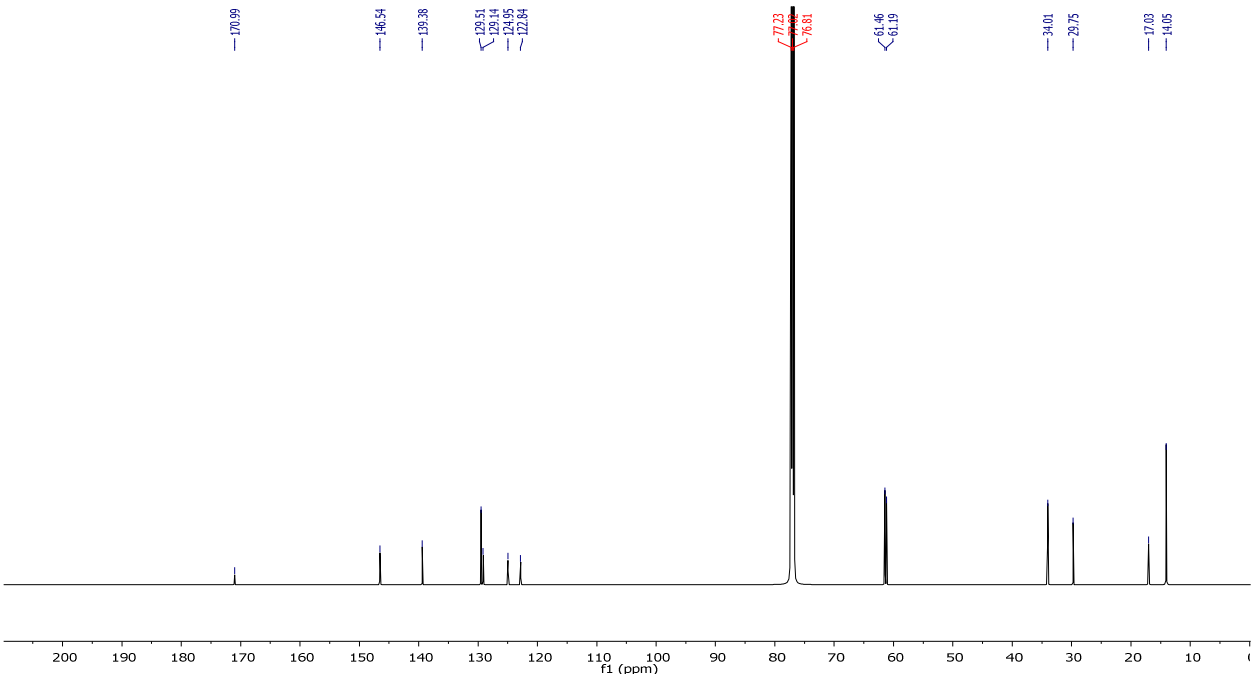
DEPT-135 of compound (6c) (150 MHz, $CDCl_3$)



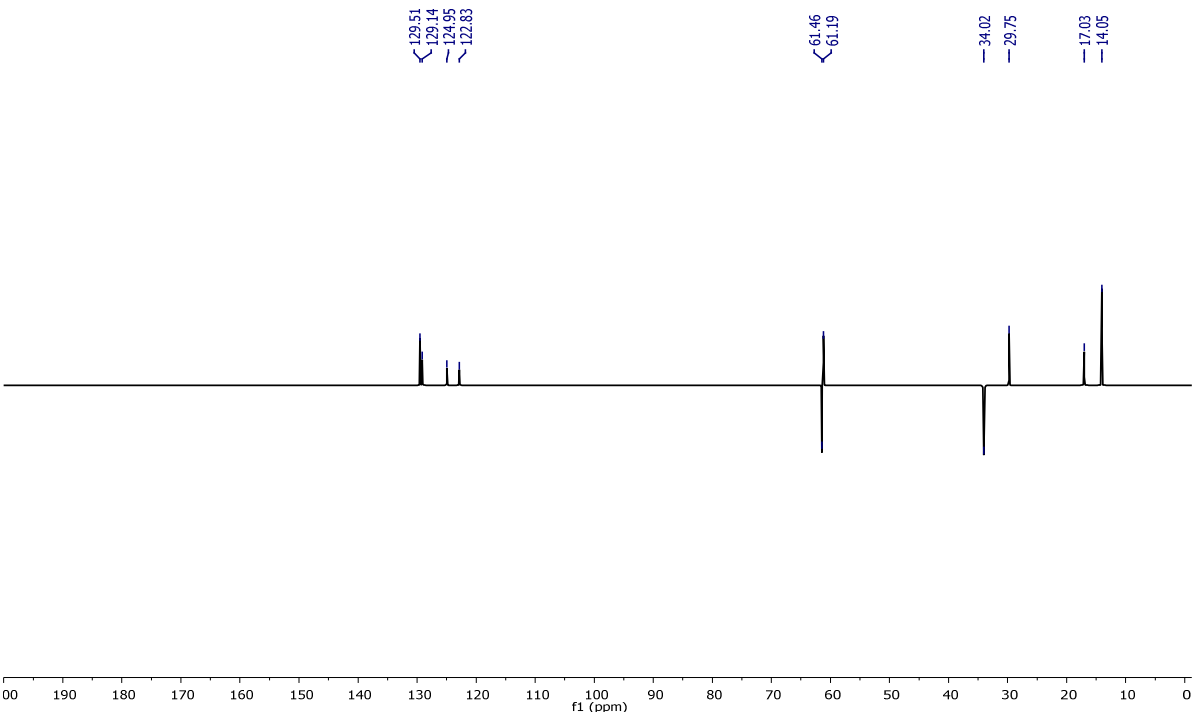
^{1}H NMR of compound (6d) (600 MHz, $CDCl_3$)



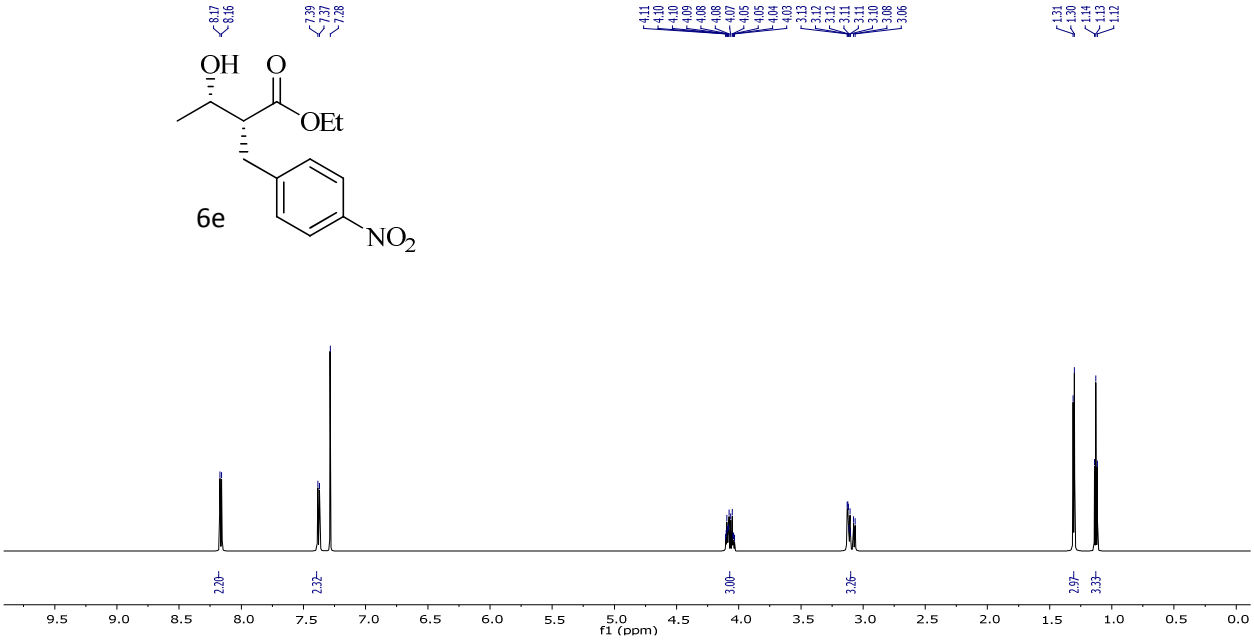
^{13}C NMR of compound (6d) (150 MHz, $CDCl_3$)



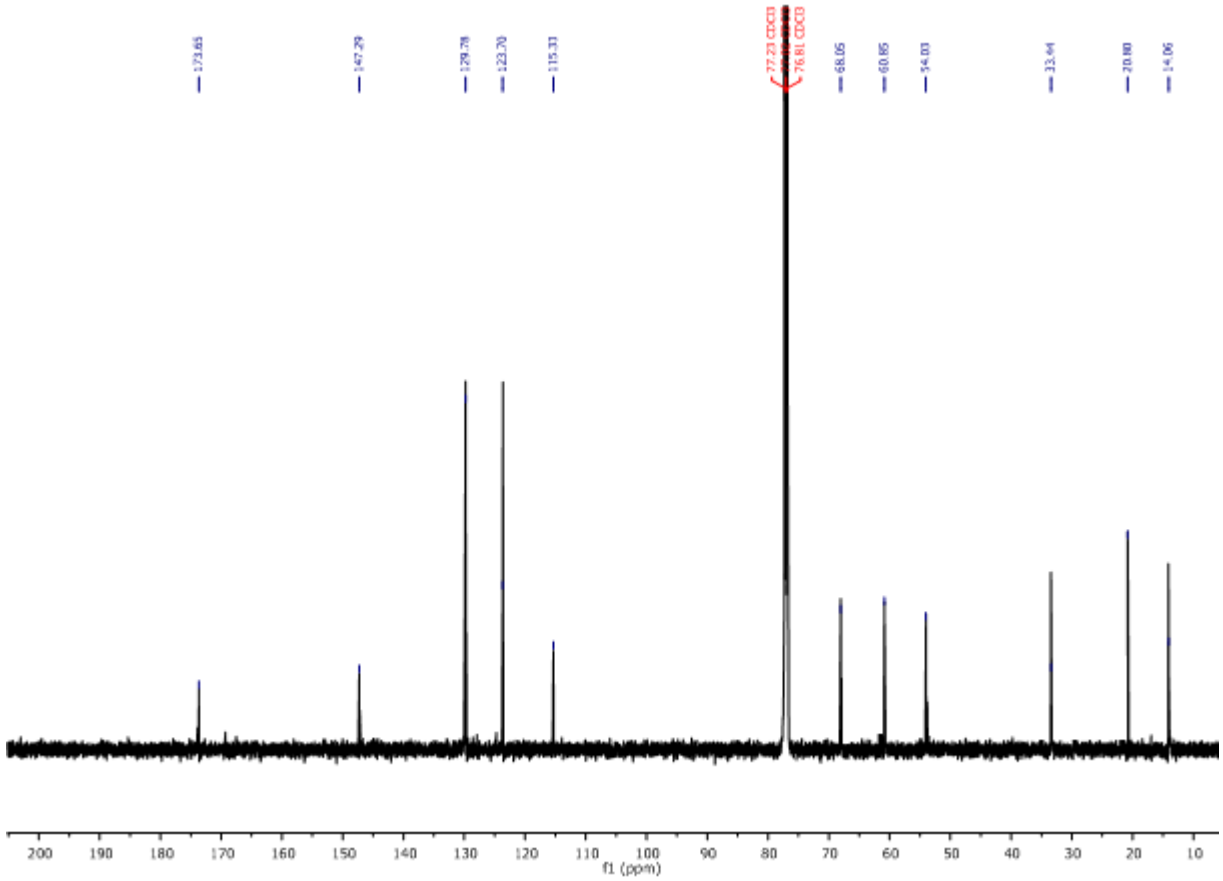
DEPT-135 of compound (6d) (150 MHz, $CDCl_3$)



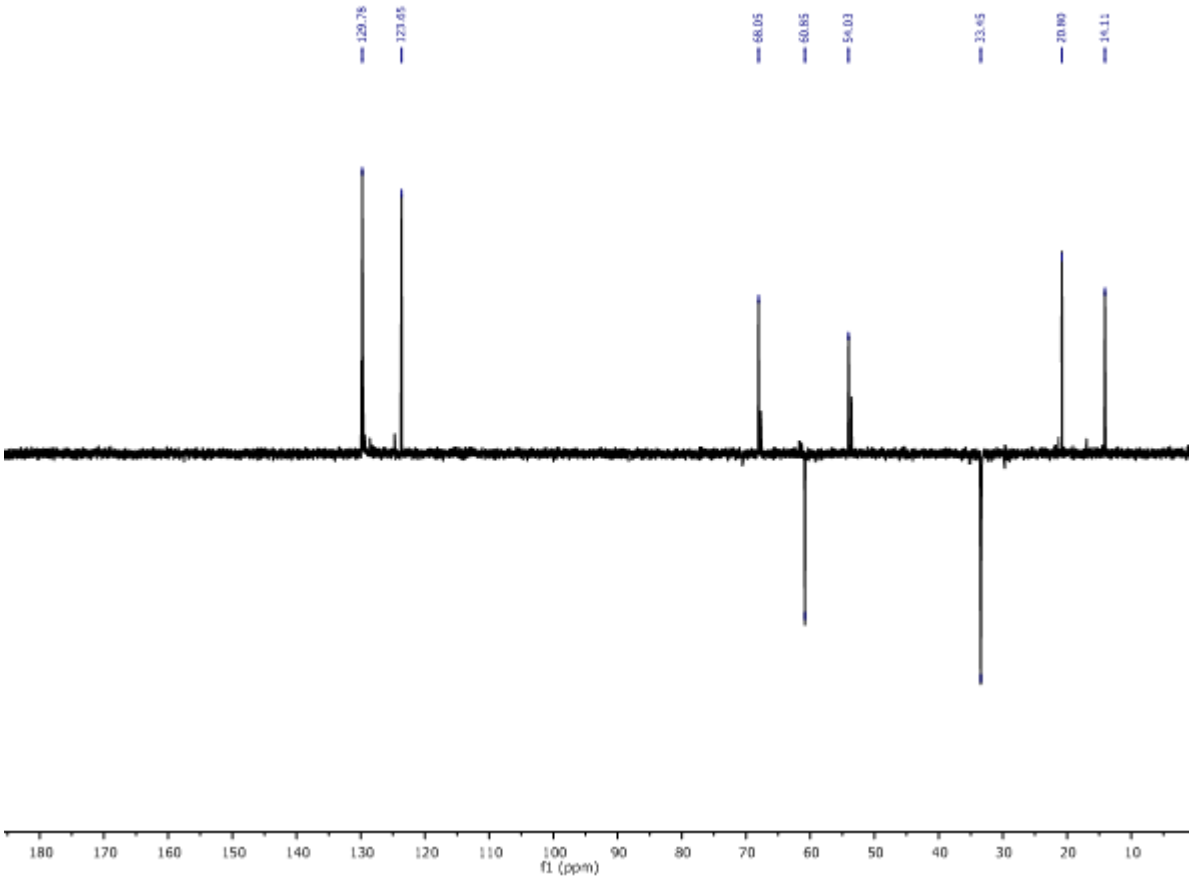
^{1}H NMR of compound (6e) (600 MHz, $CDCl_3$)



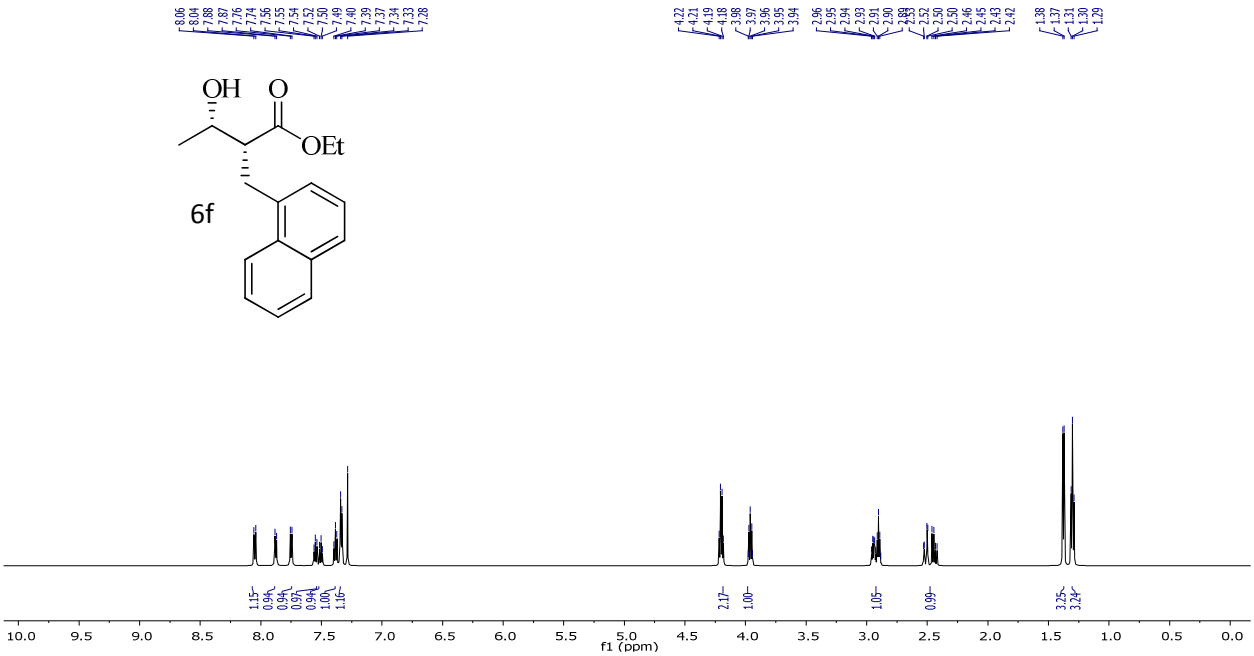
^{13}C NMR of compound (6e) (150 MHz, $CDCl_3$)



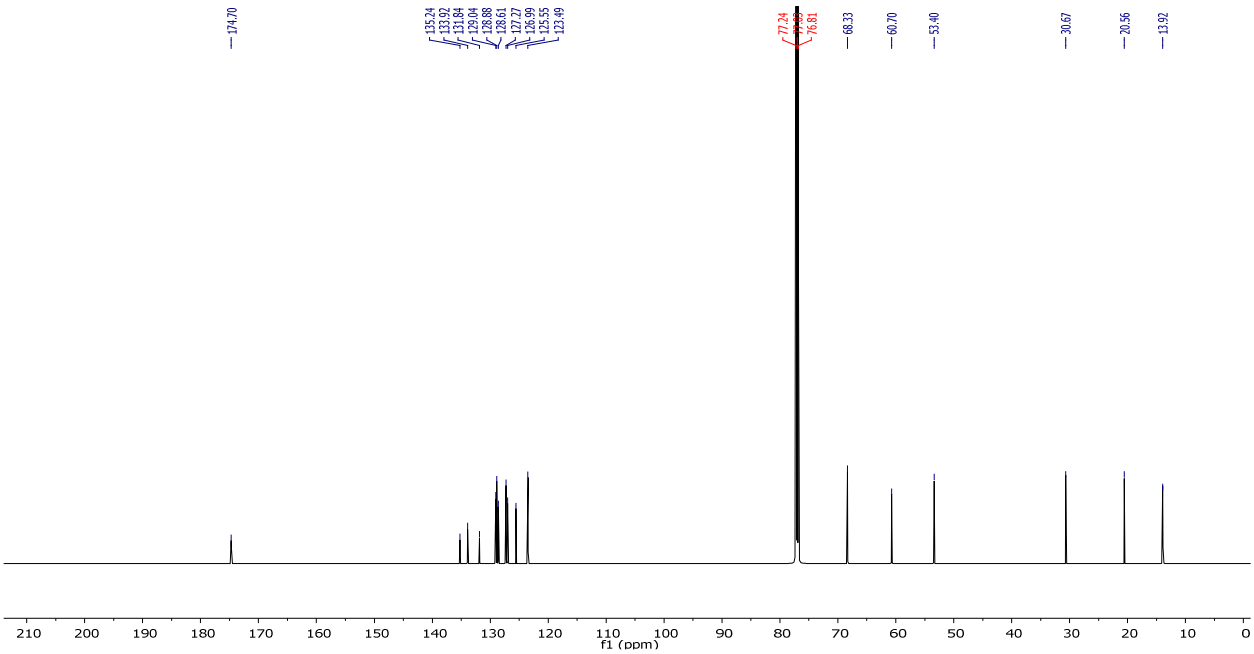
DEPT-135 of compound (6e) (150 MHz, $CDCl_3$)



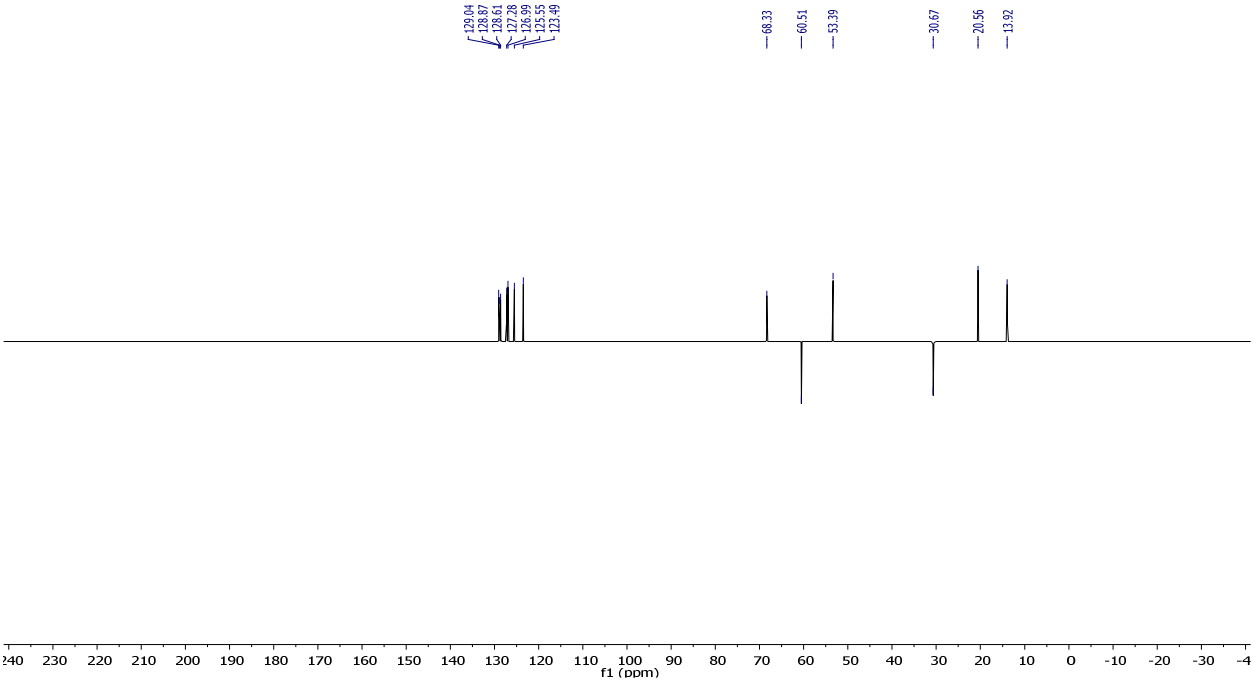
^{1}H NMR of compound (6f) (600 MHz, $CDCl_3$)



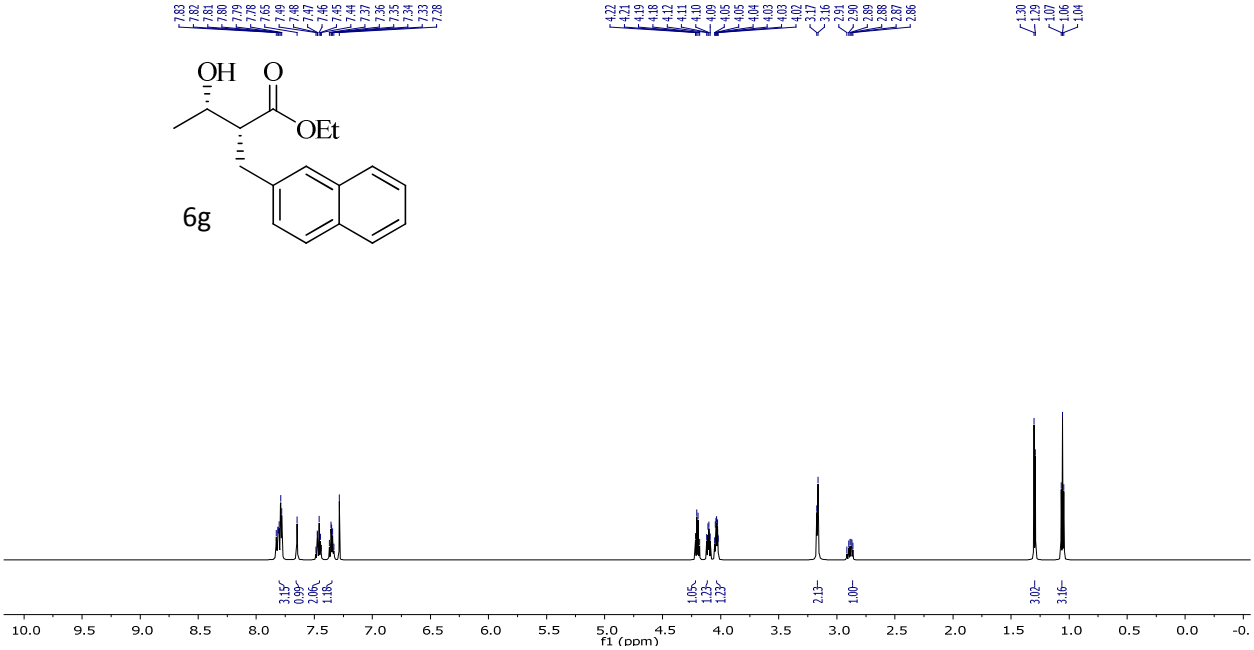
^{13}C NMR of compound (6f) (150 MHz, $CDCl_3$)



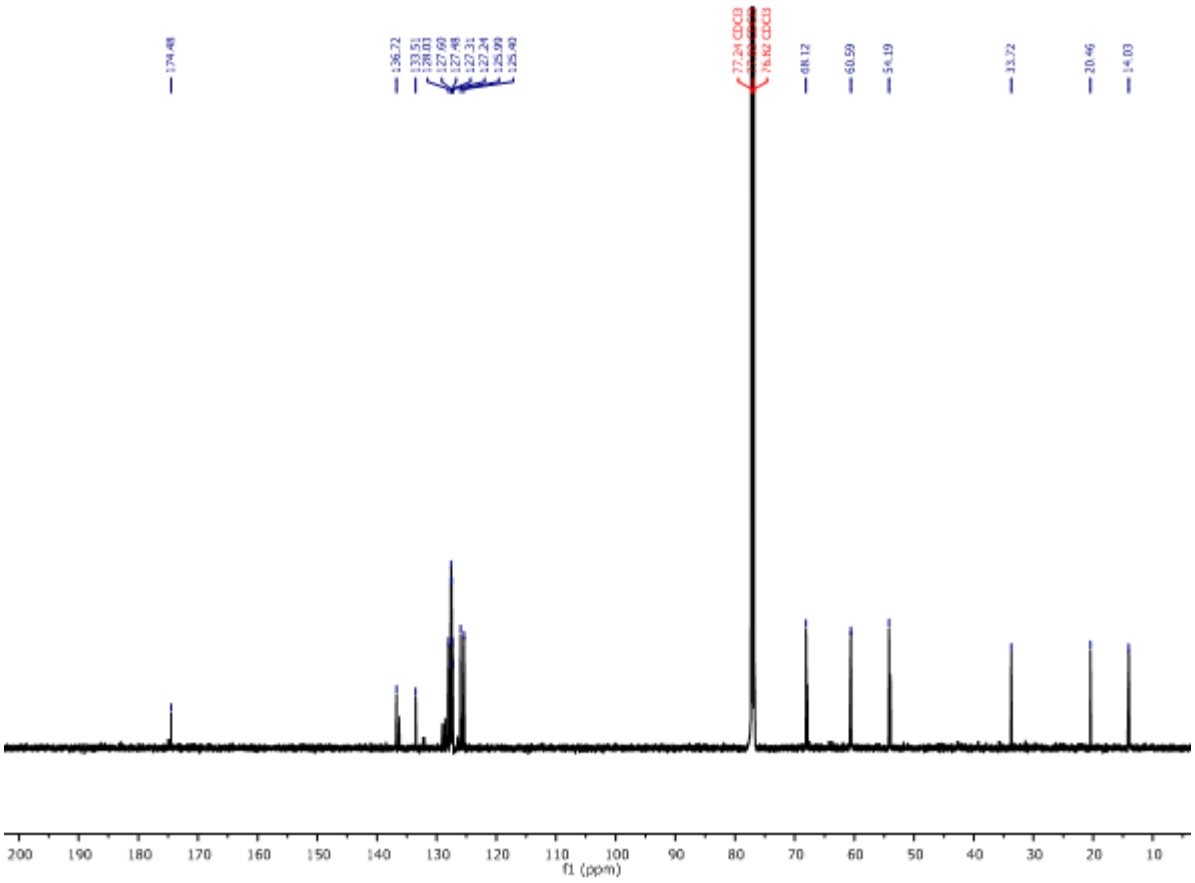
DEPT-135 of compound (6f) (150 MHz, $CDCl_3$)



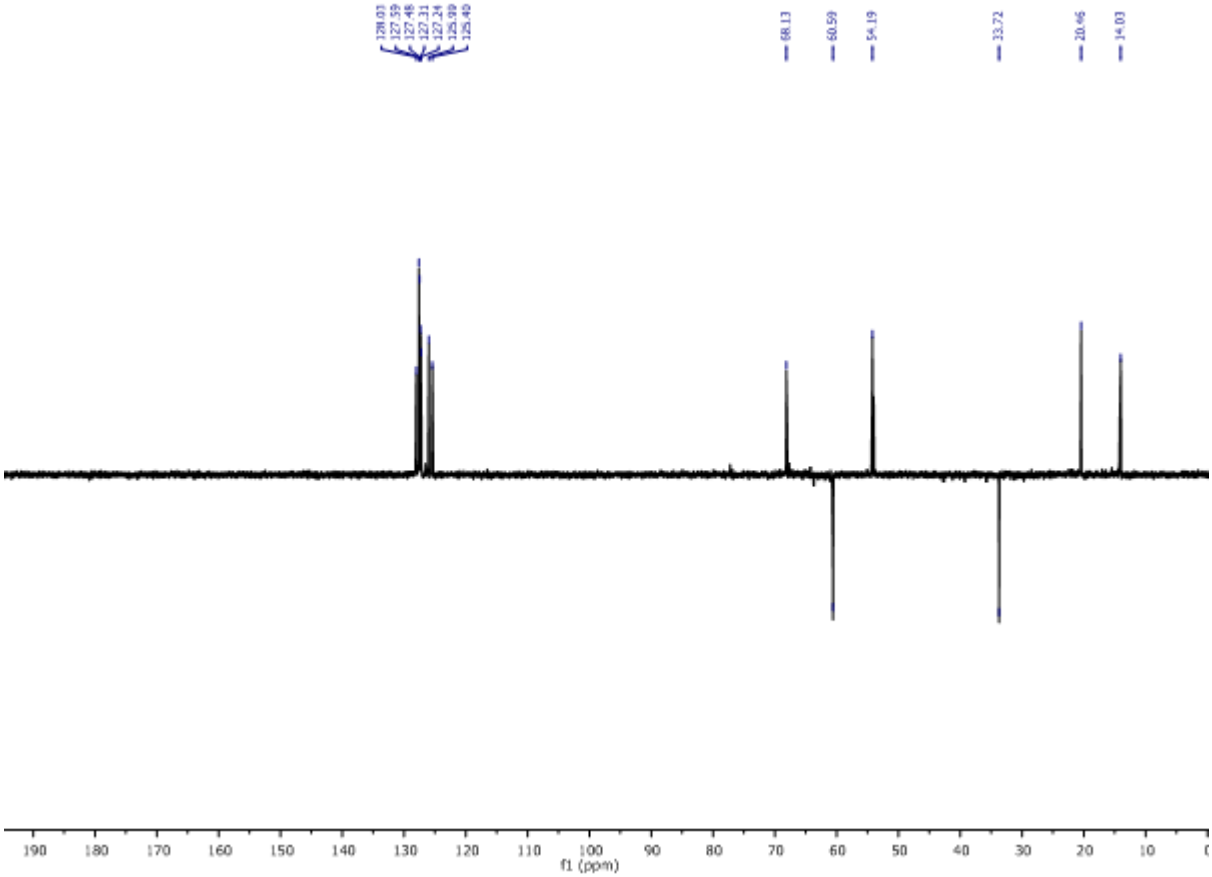
^{1}H NMR of compound (6g) (600 MHz, $CDCl_3$)



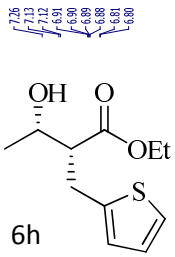
^{13}C NMR of compound (6g) (150 MHz, $CDCl_3$)



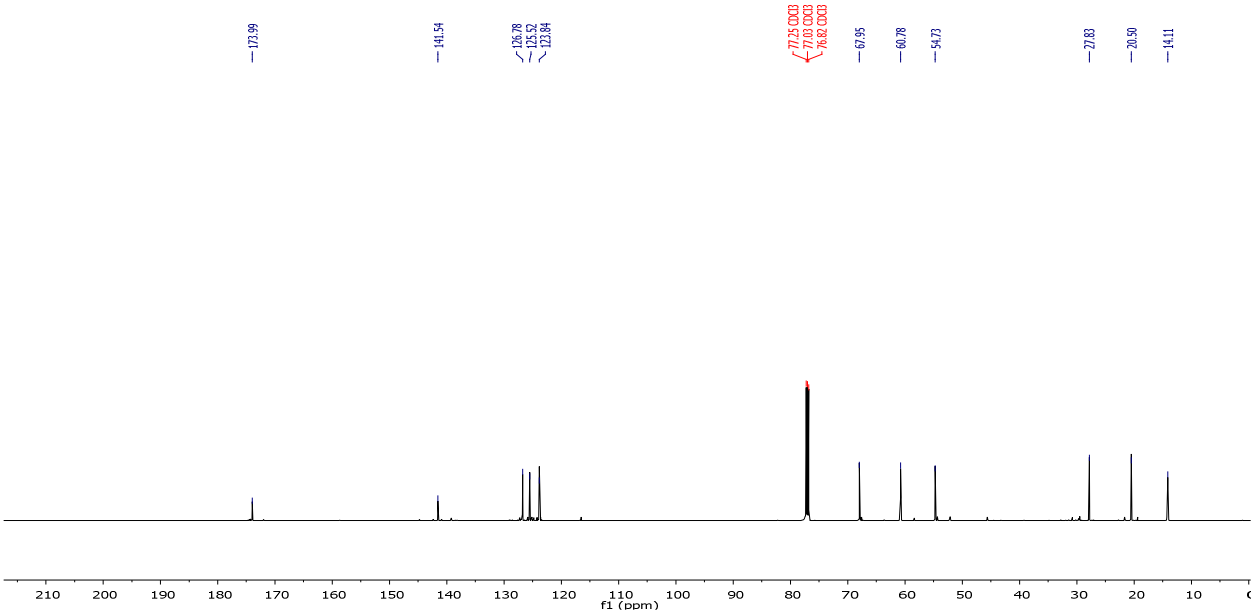
DEPT-135 of compound (6g) (150 MHz, $CDCl_3$)



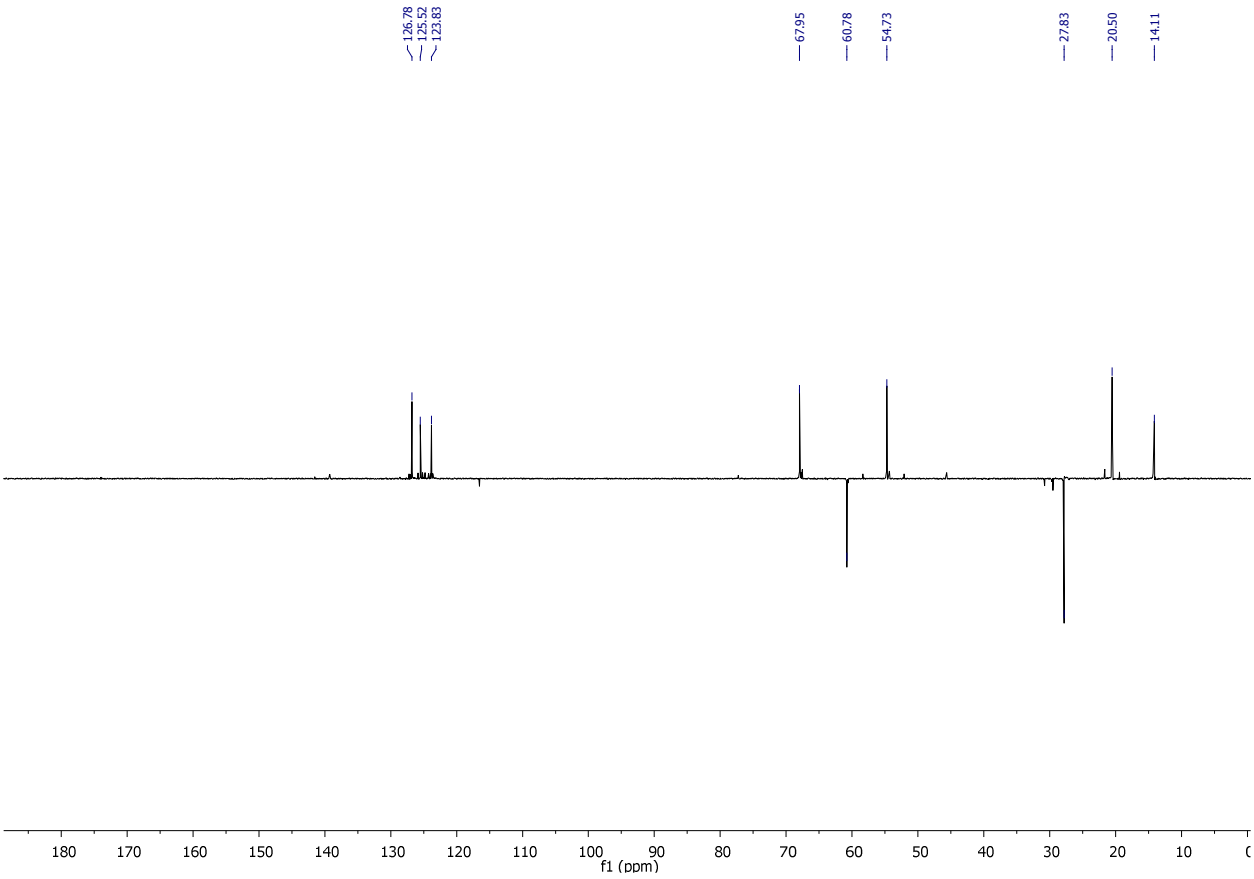
^{1}H NMR of compound (6h) (400 MHz, $CDCl_3$)



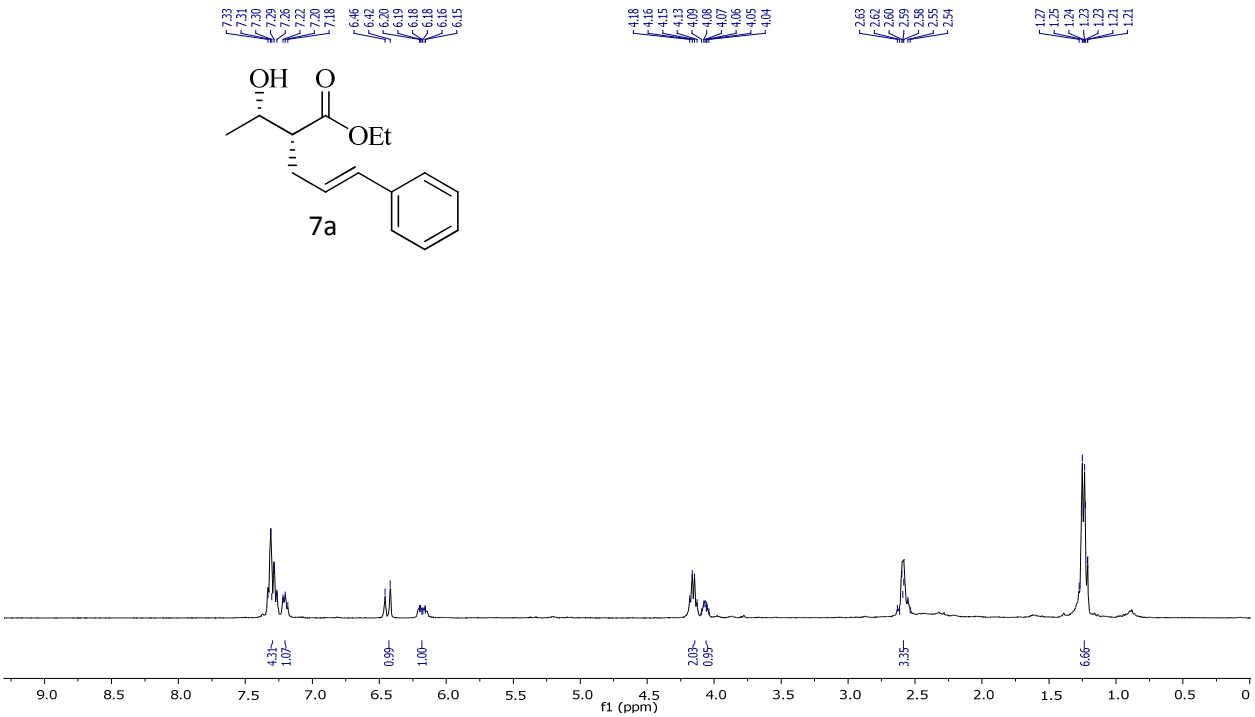
^{13}C NMR of compound (6h) (150 MHz, $CDCl_3$)



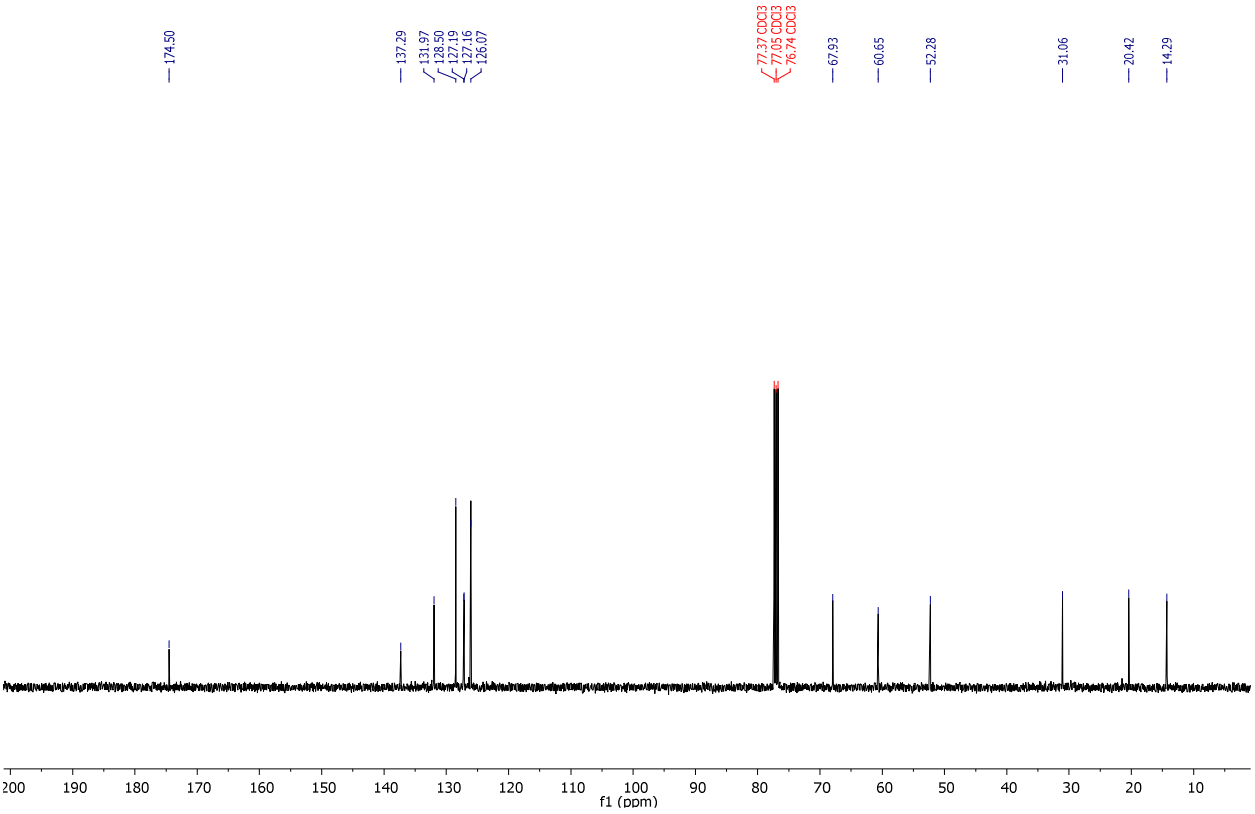
DEPT-135 of compound (6h) (150 MHz, $CDCl_3$)



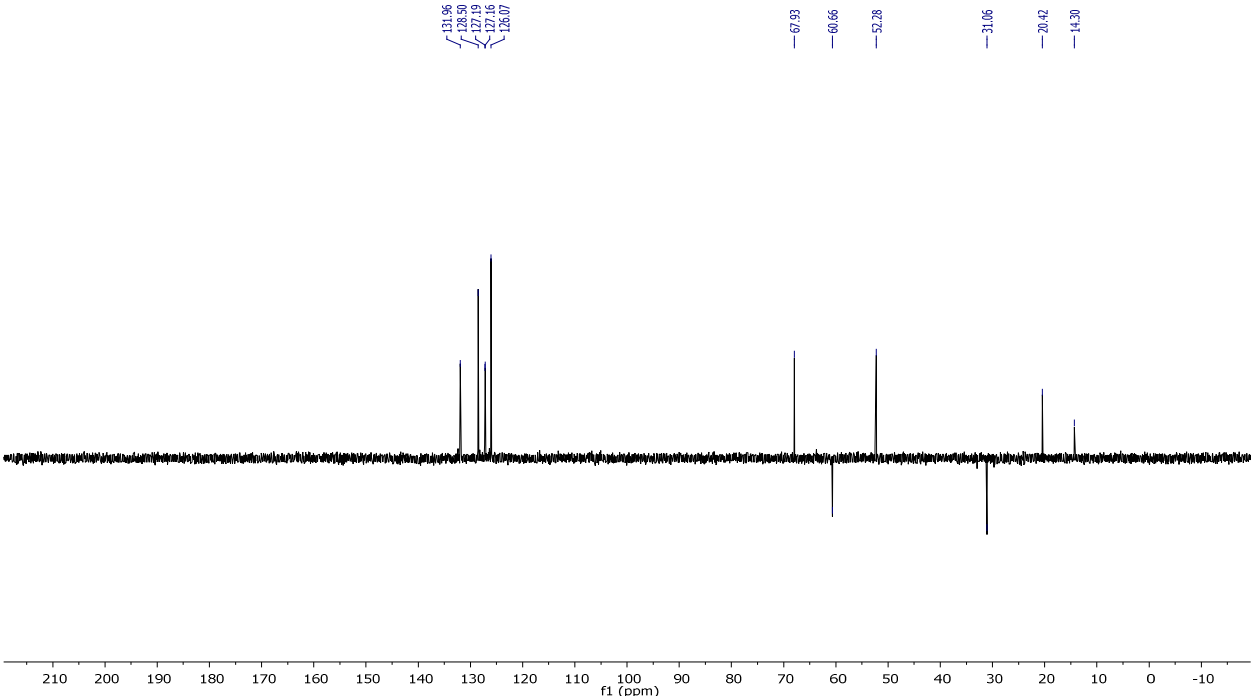
^{1}H NMR of compound (7a) (400 MHz, $CDCl_3$)



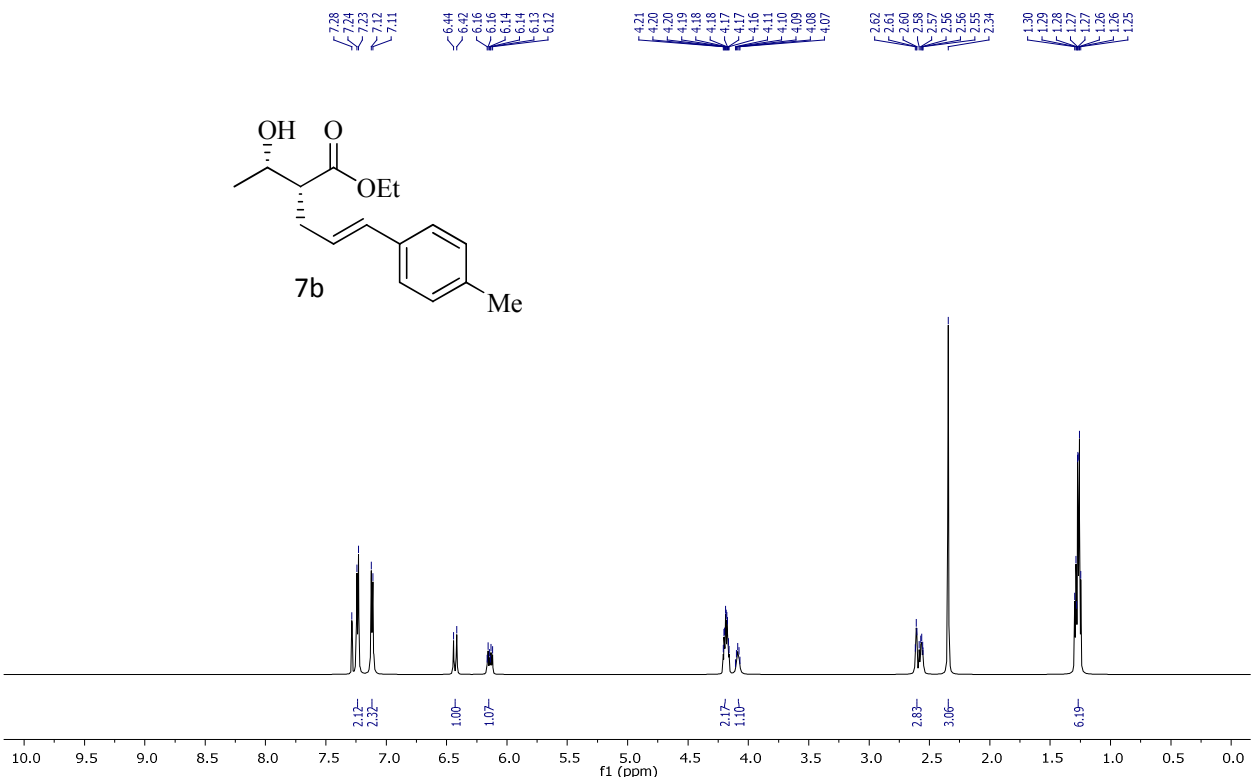
^{13}C NMR of compound (7a) (100 MHz, $CDCl_3$)



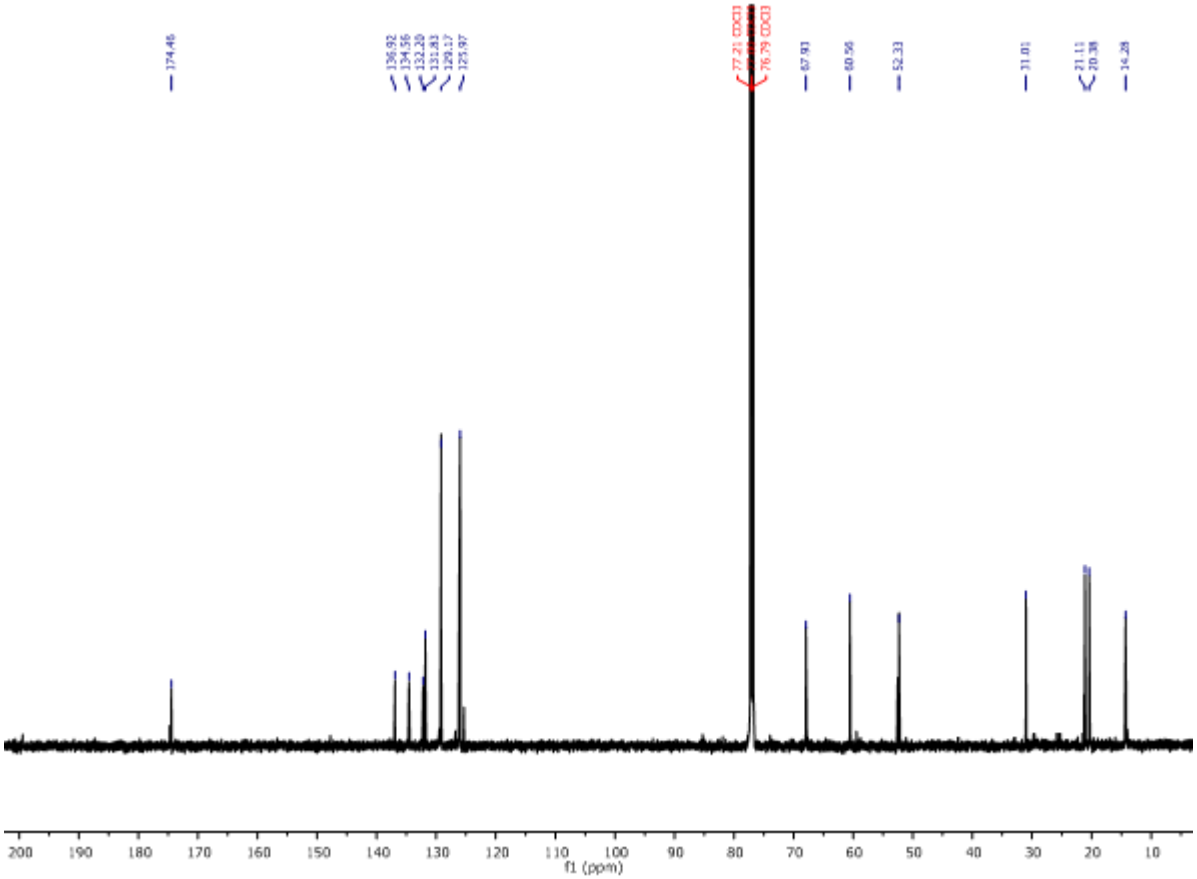
DEPT-135 of compound (7a) (100 MHz, $CDCl_3$)



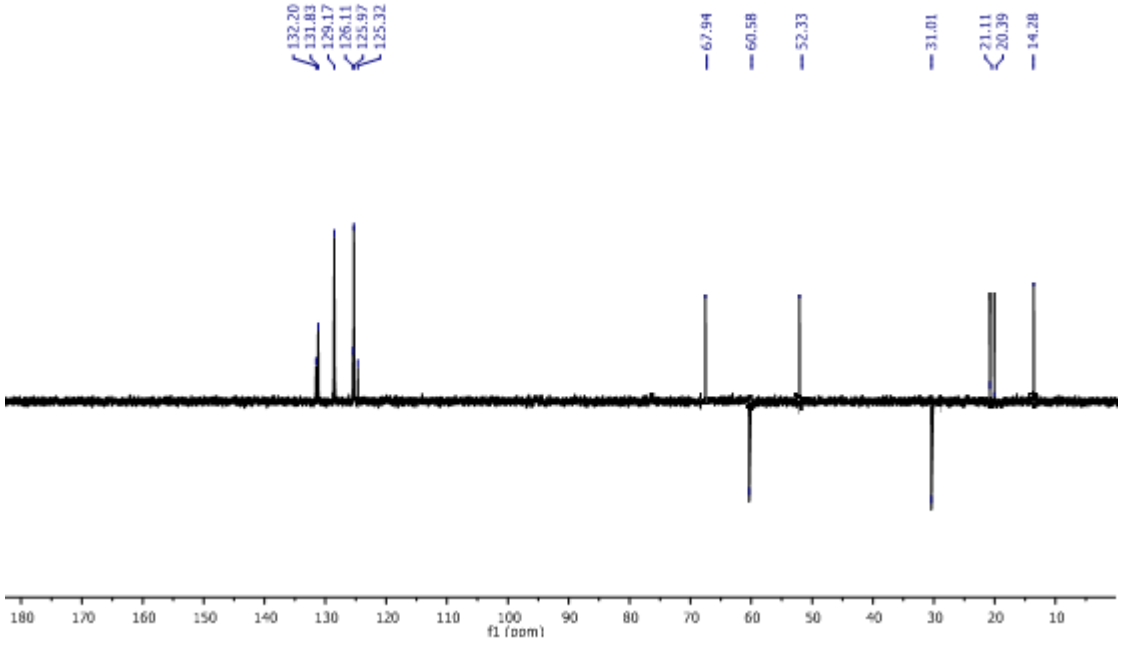
^{1}H NMR of compound (7b) (600 MHz, $CDCl_3$)



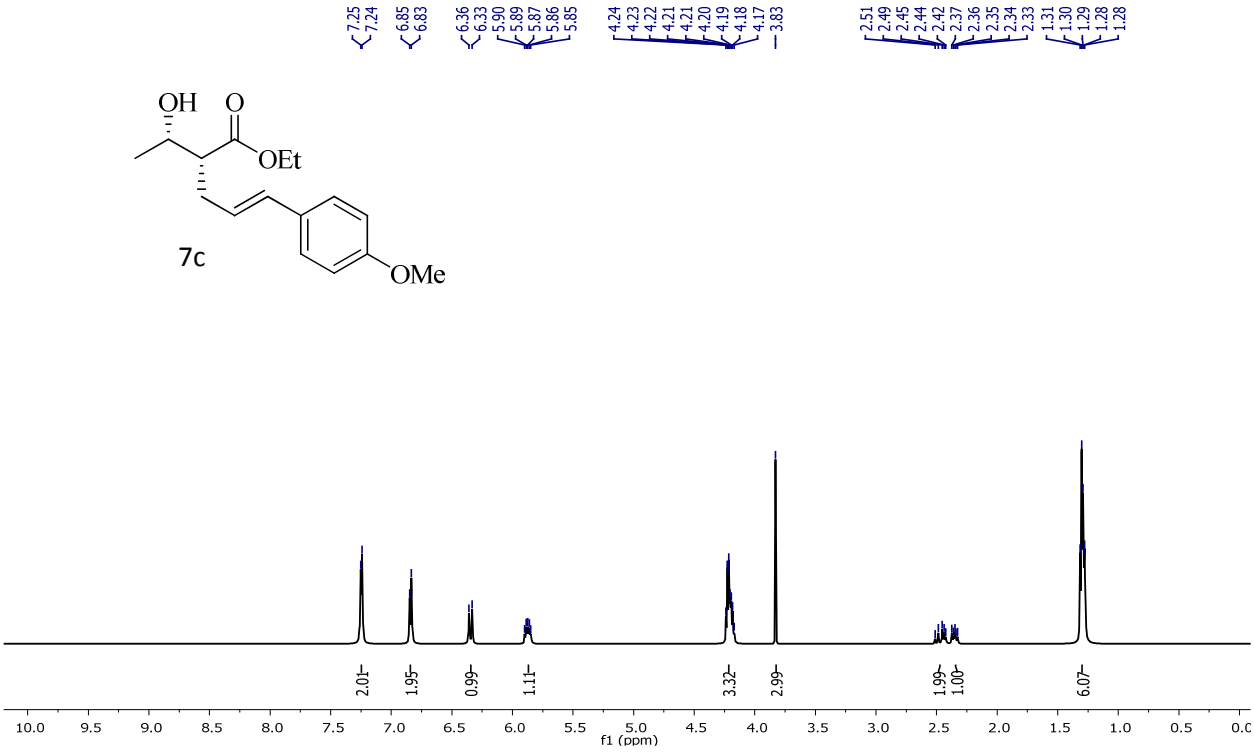
^{13}C NMR of compound (7b) (150 MHz, $CDCl_3$)



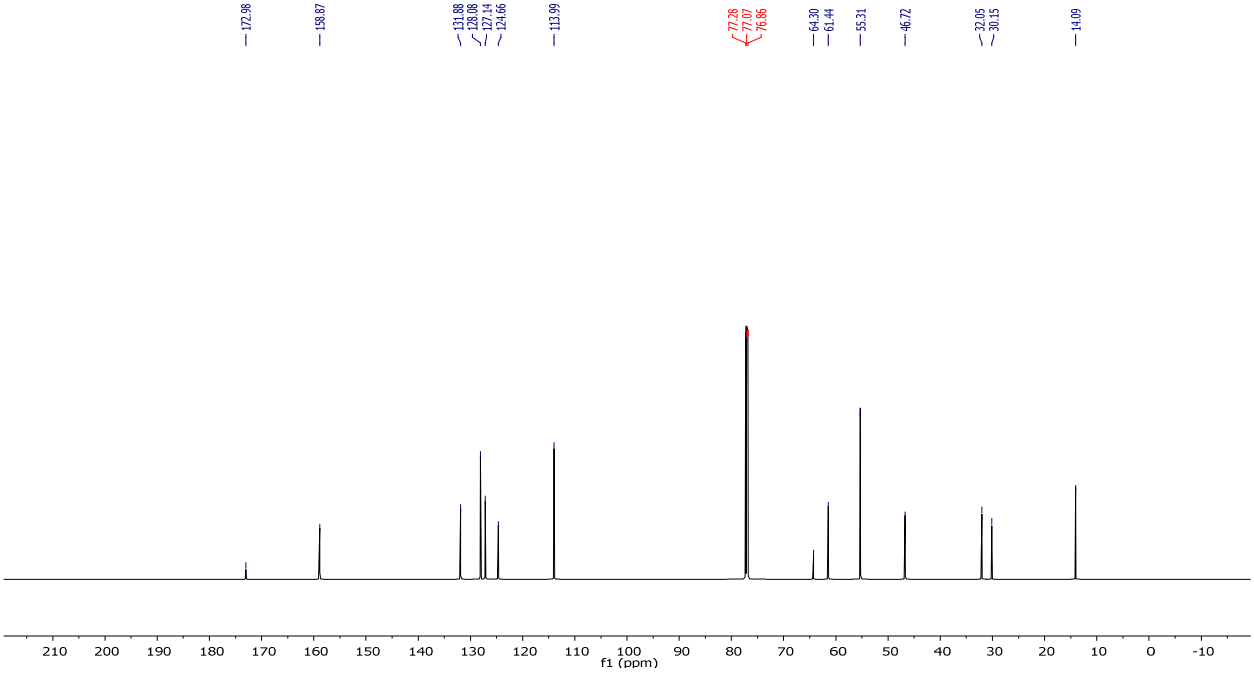
DEPT-135 of compound (7b) (150 MHz, $CDCl_33$)



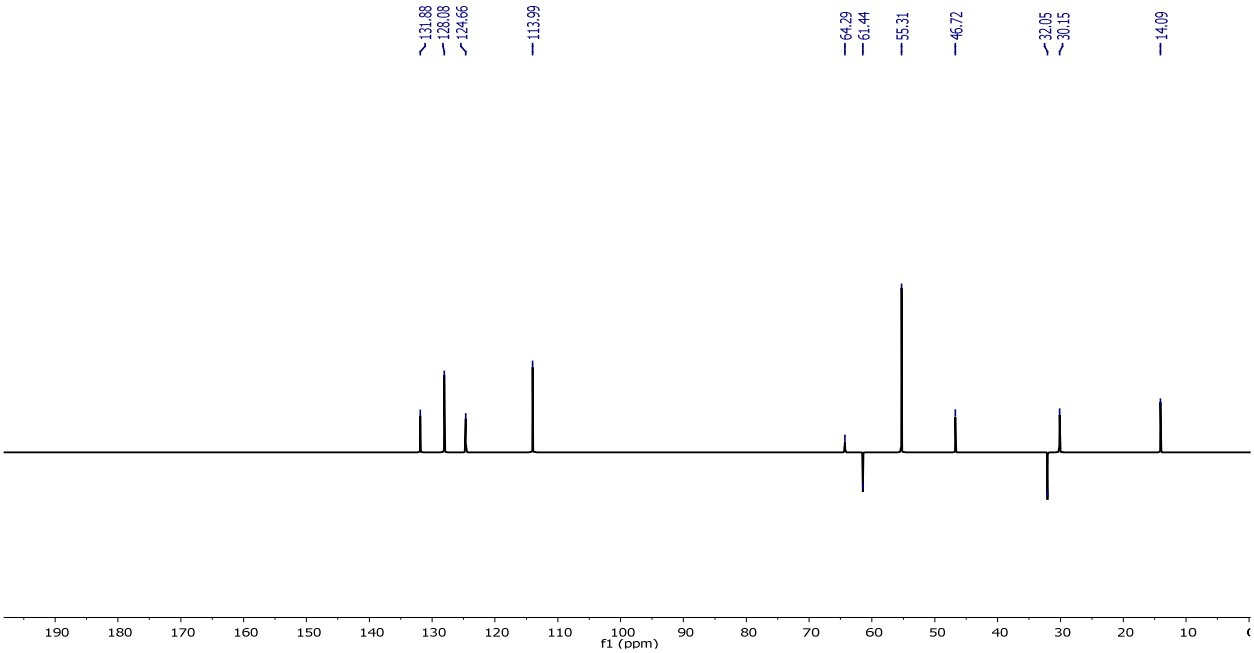
^{1}H NMR of compound (7c) (600 MHz, $CDCl_3$)



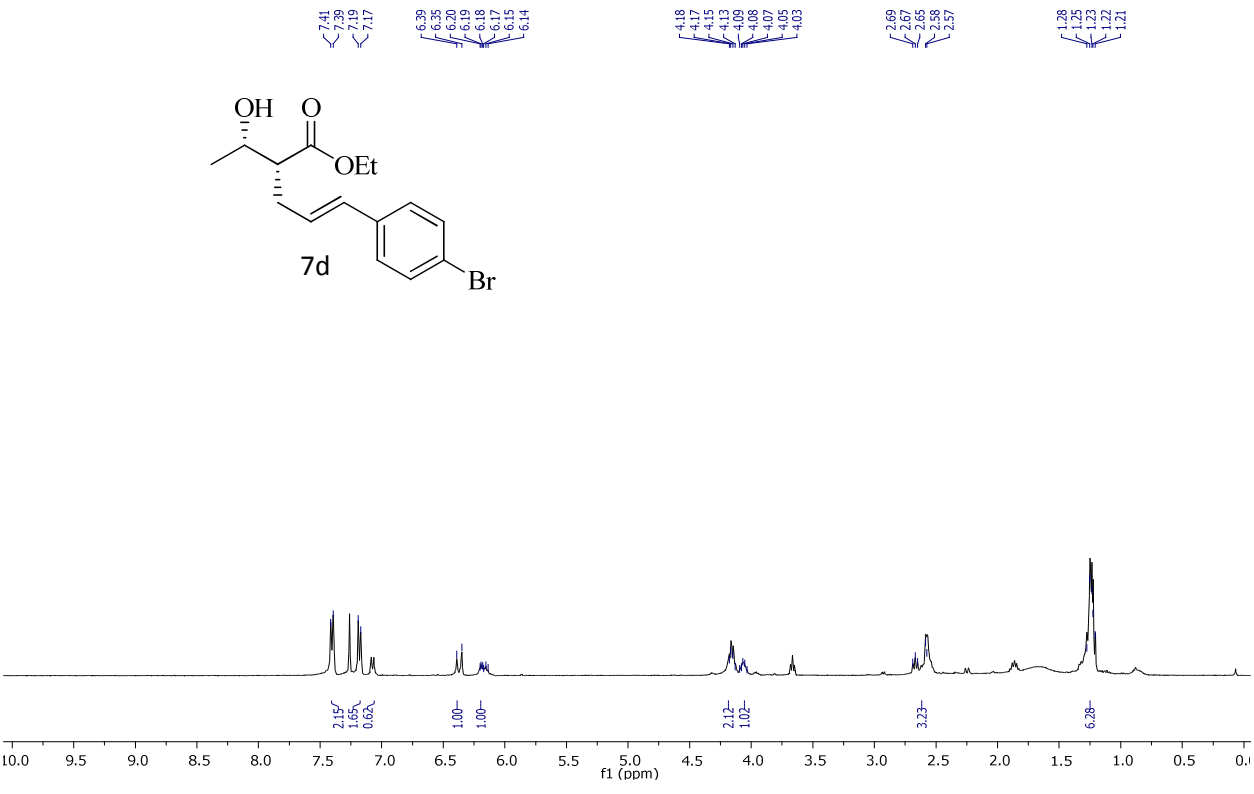
^{13}C NMR of compound (7c) (150 MHz, $CDCl_3$)



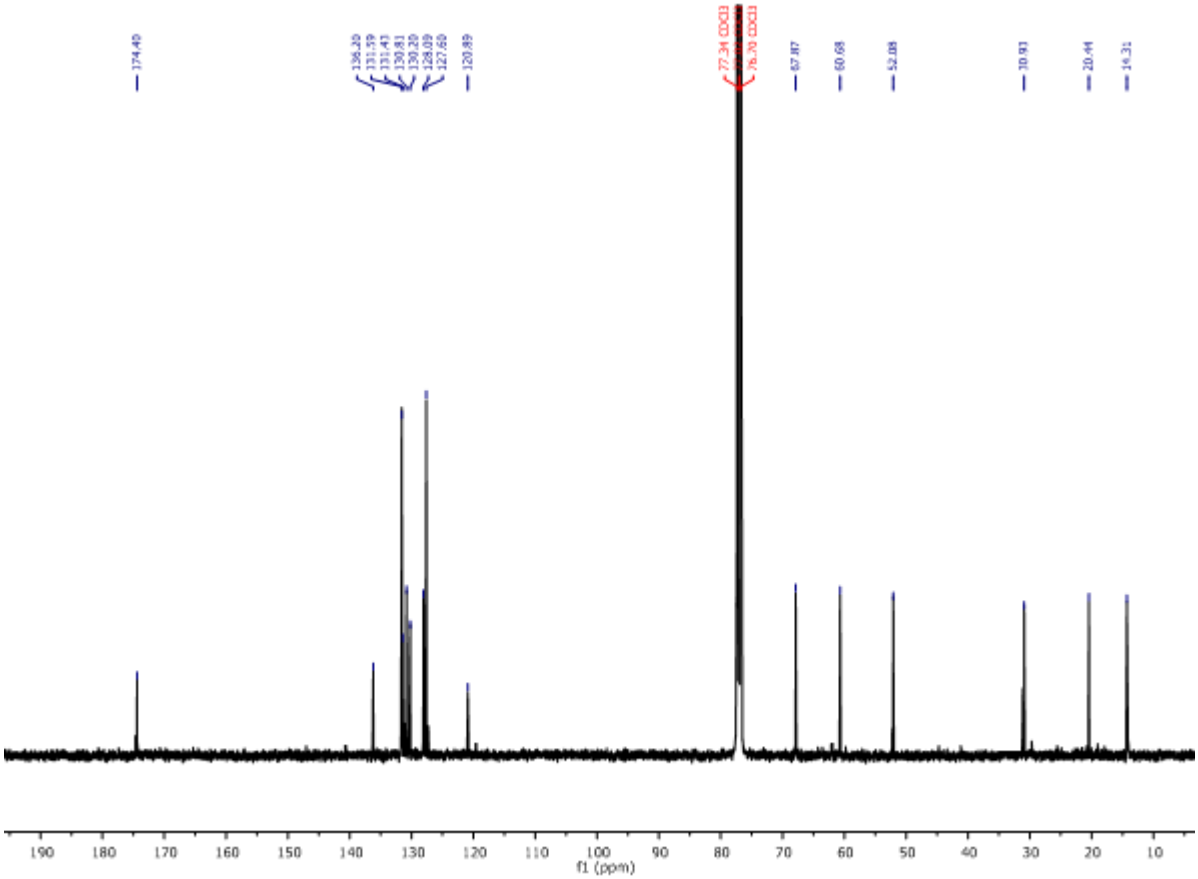
DEPT-135 of compound (7c) (150 MHz, $CDCl_3$)



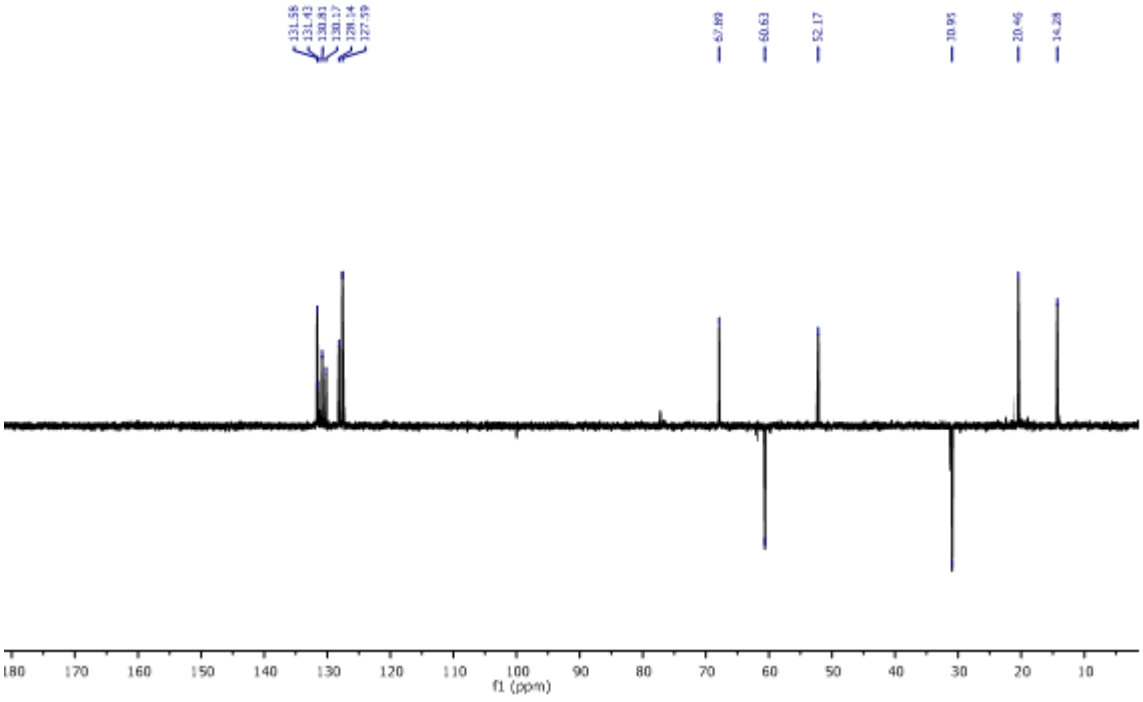
^{1}H NMR of compound (7d) (400 MHz, $CDCl_3$)



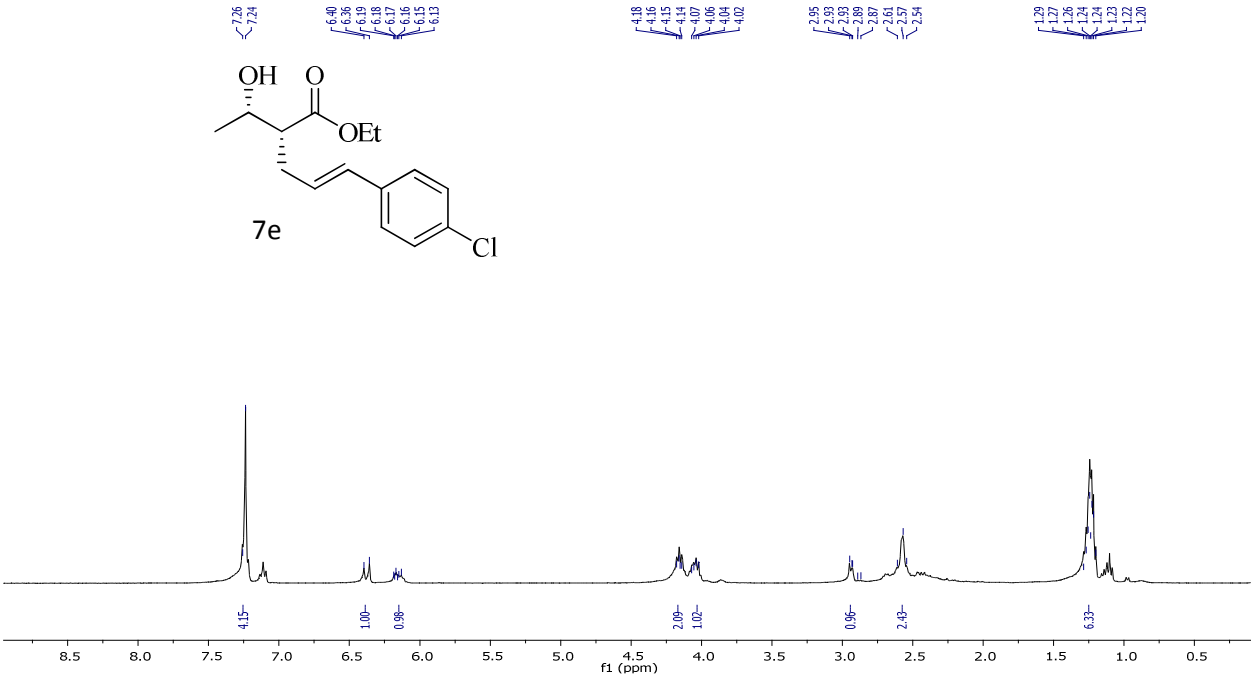
^{13}C NMR of compound (7d) (100 MHz, $CDCl_3$)



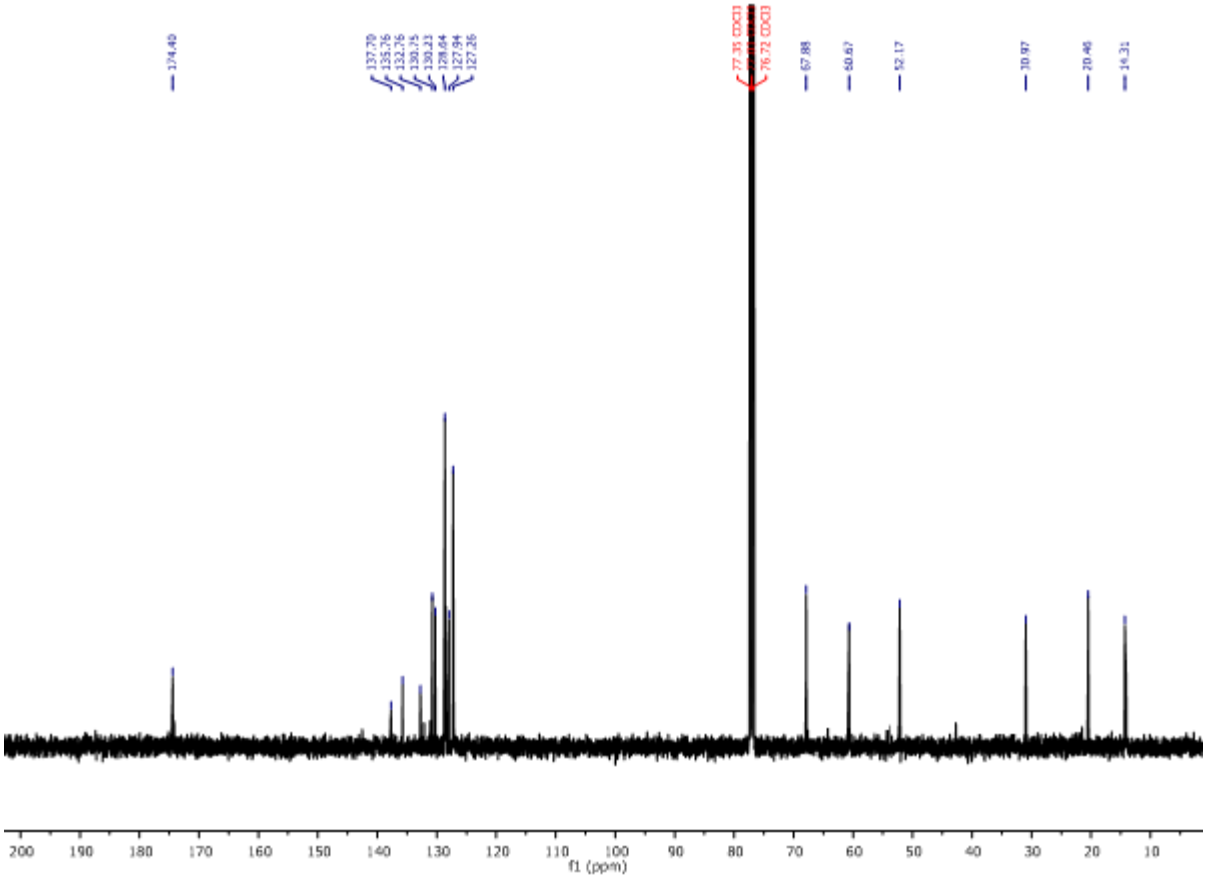
DEPT-135 of compound (7d) (100 MHz, $CDCl_3$)



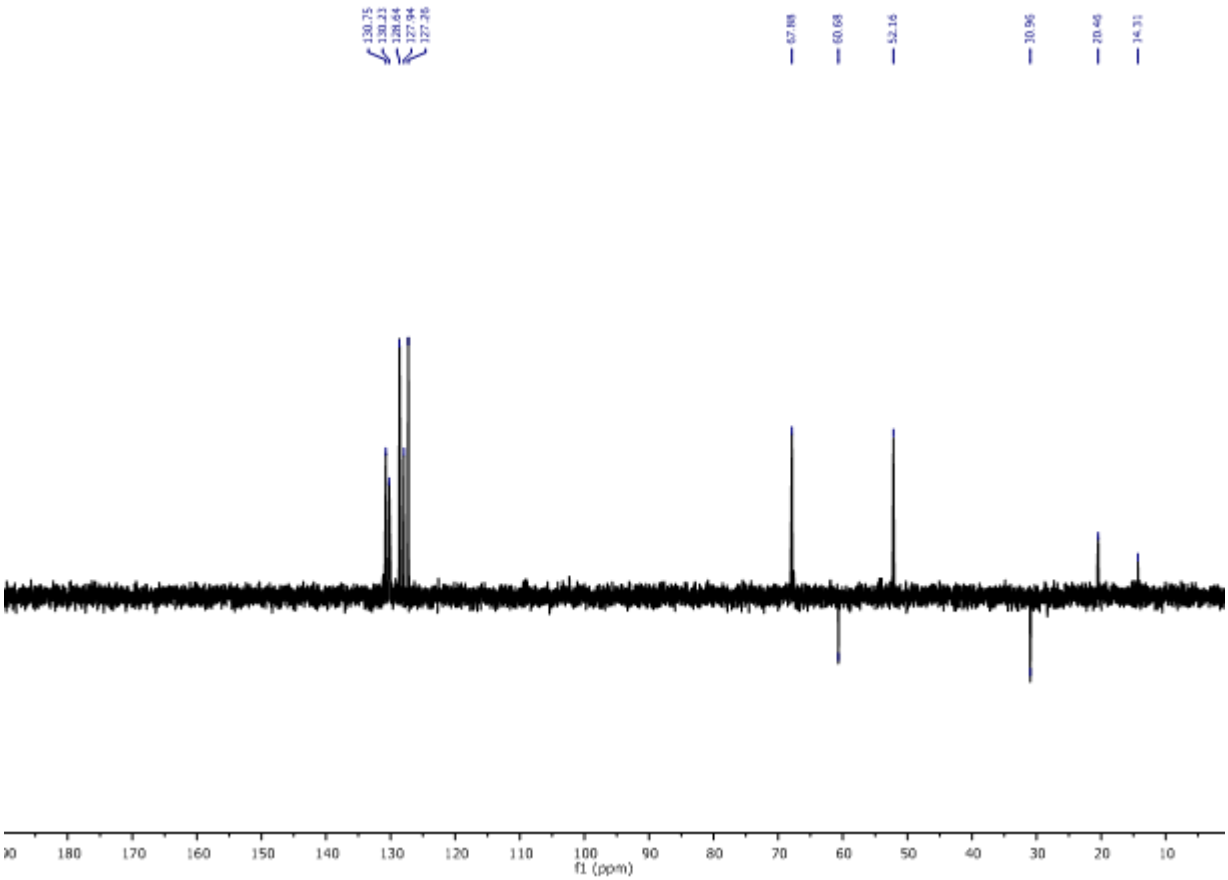
^{1}H NMR of compound (7e) (400 MHz, $CDCl_3$)



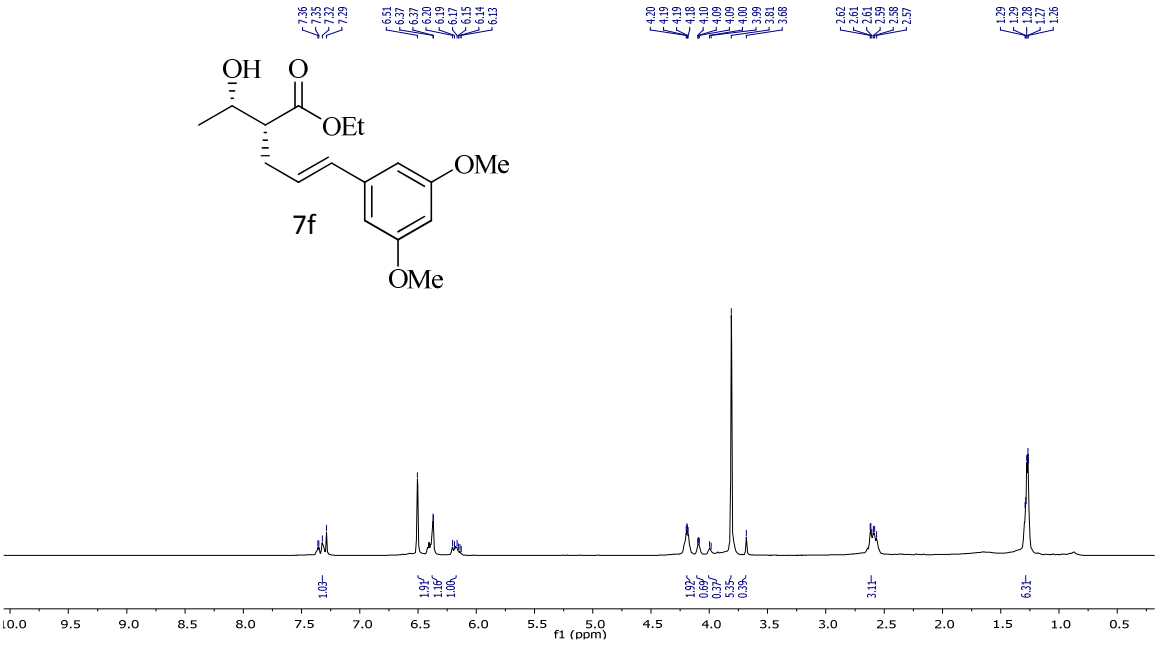
^{13}C NMR of compound (7e) (100 MHz, $CDCl_3$)



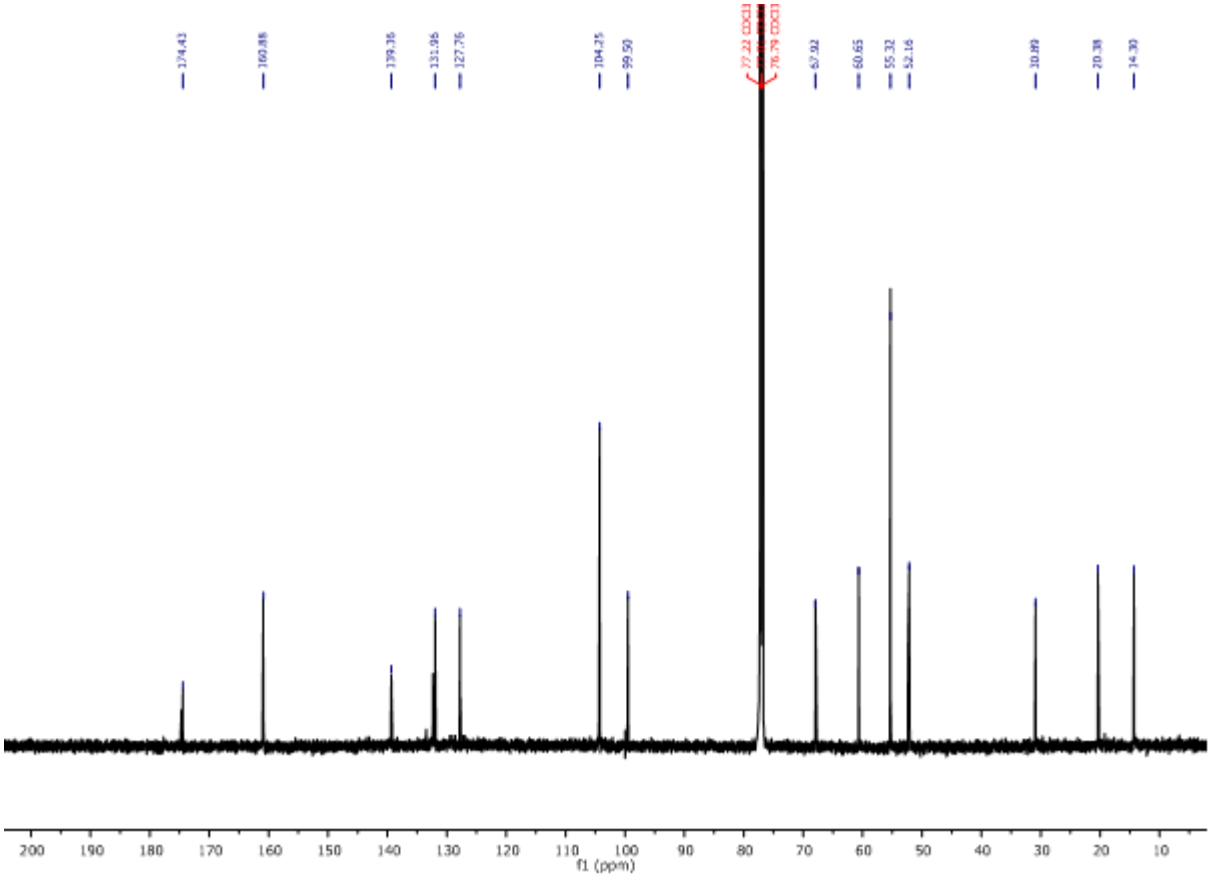
DEPT-135 of compound (7e) (50 MHz, $CDCl_3$)



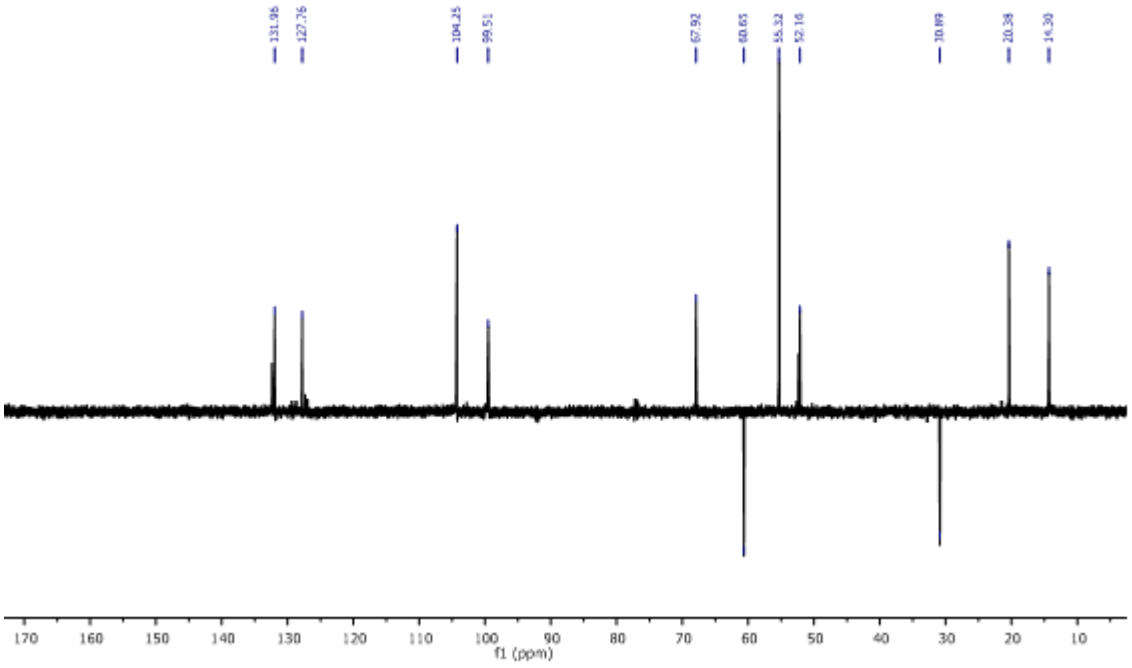
^{1}H NMR of compound (7f) (600 MHz, $CDCl_3$)



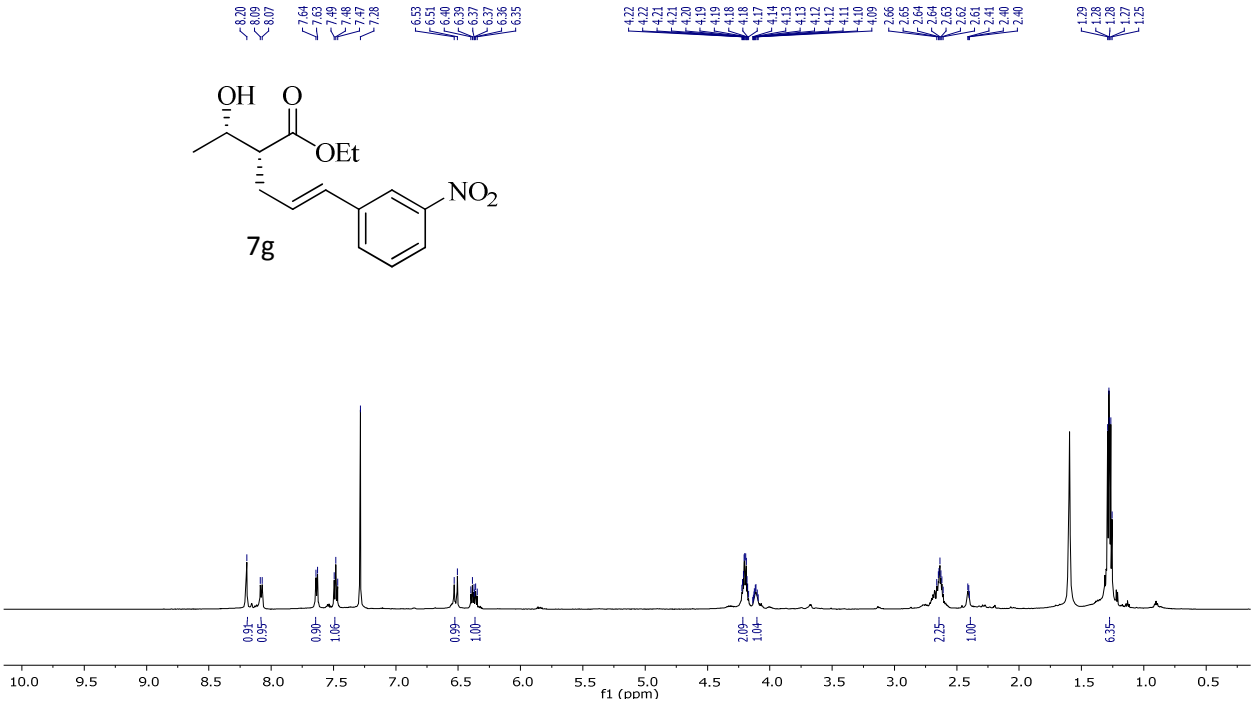
^{13}C NMR of compound (7f) (150 MHz, $CDCl_3$)



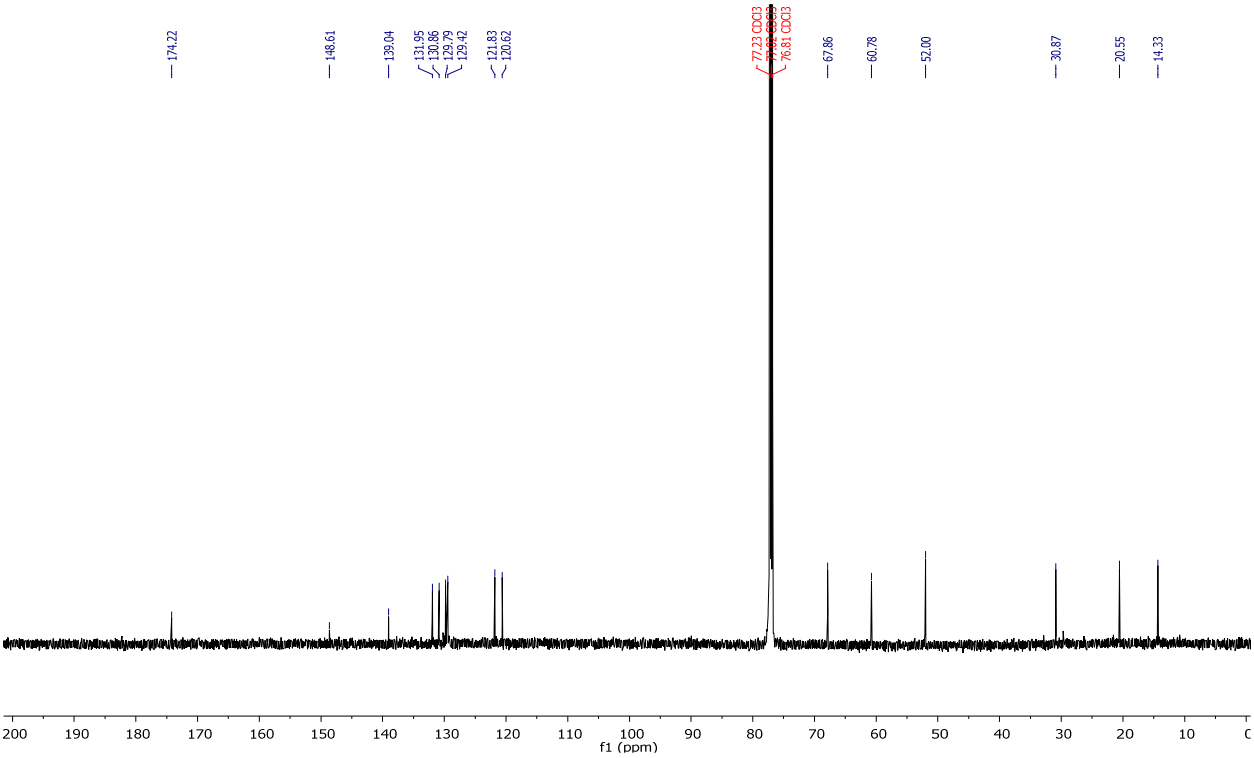
DEPT-135 of compound (7f) (150 MHz, $CDCl_3$)



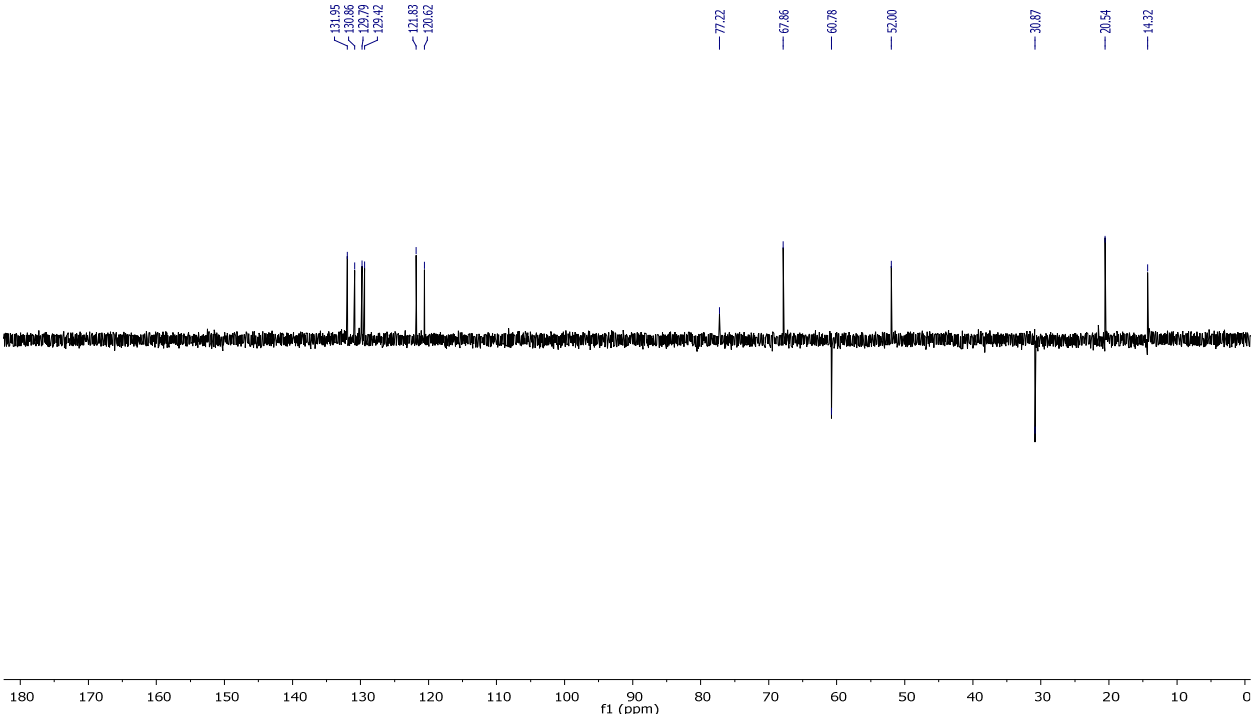
^{1}H NMR of compound (7g) (600 MHz, $CDCl_3$)



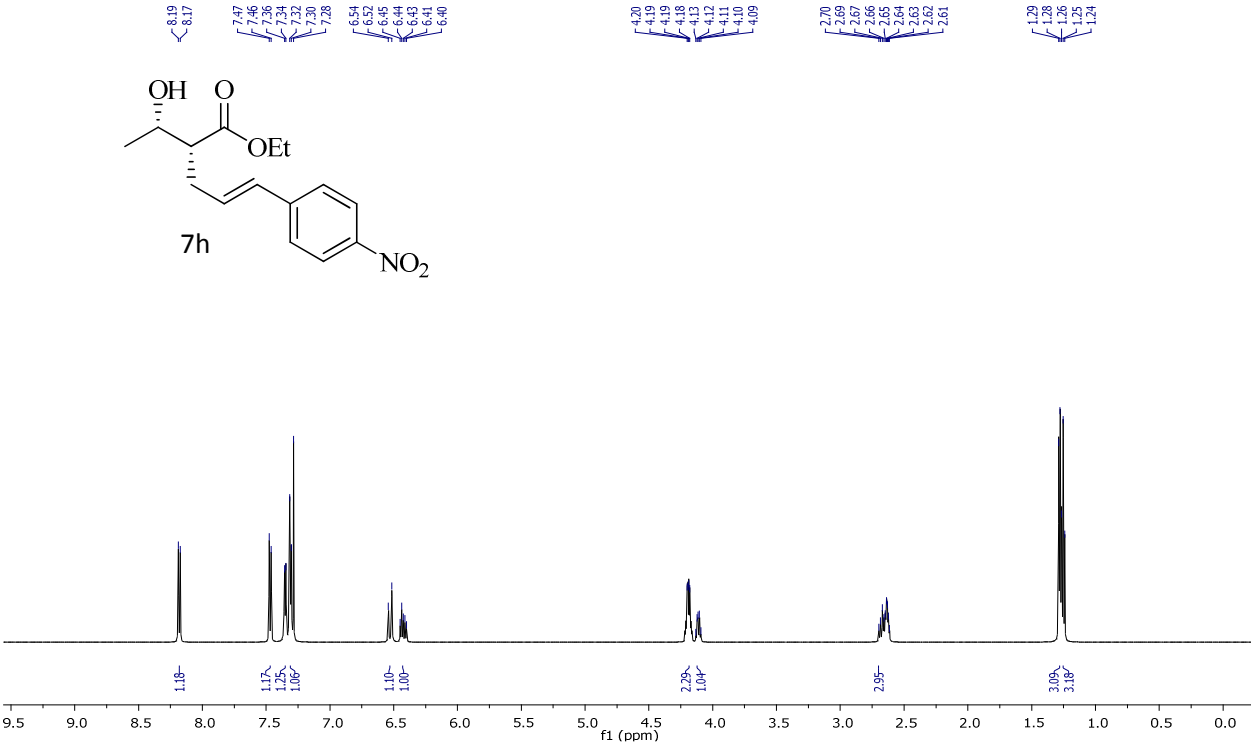
^{13}C NMR of compound (7g) (150 MHz, $CDCl_3$)



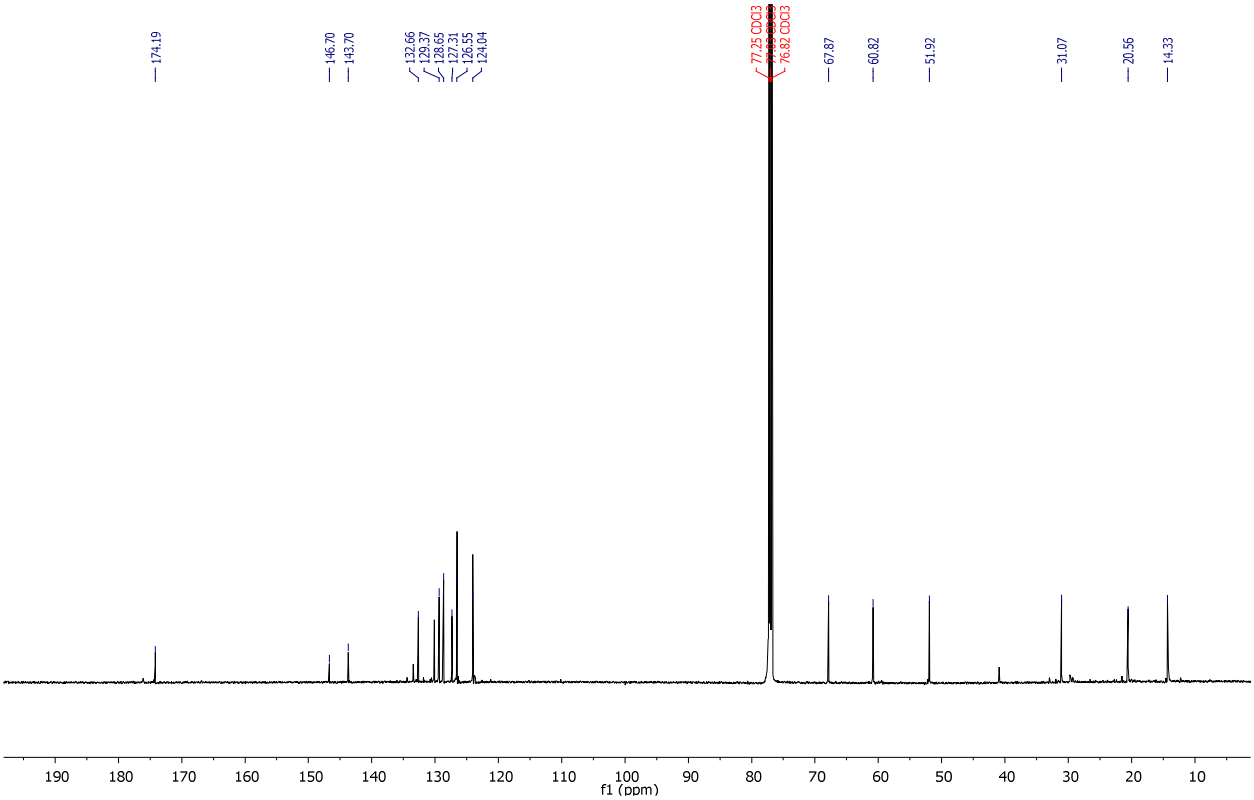
DEPT-135 of compound (7g) (150 MHz, $CDCl_3$)



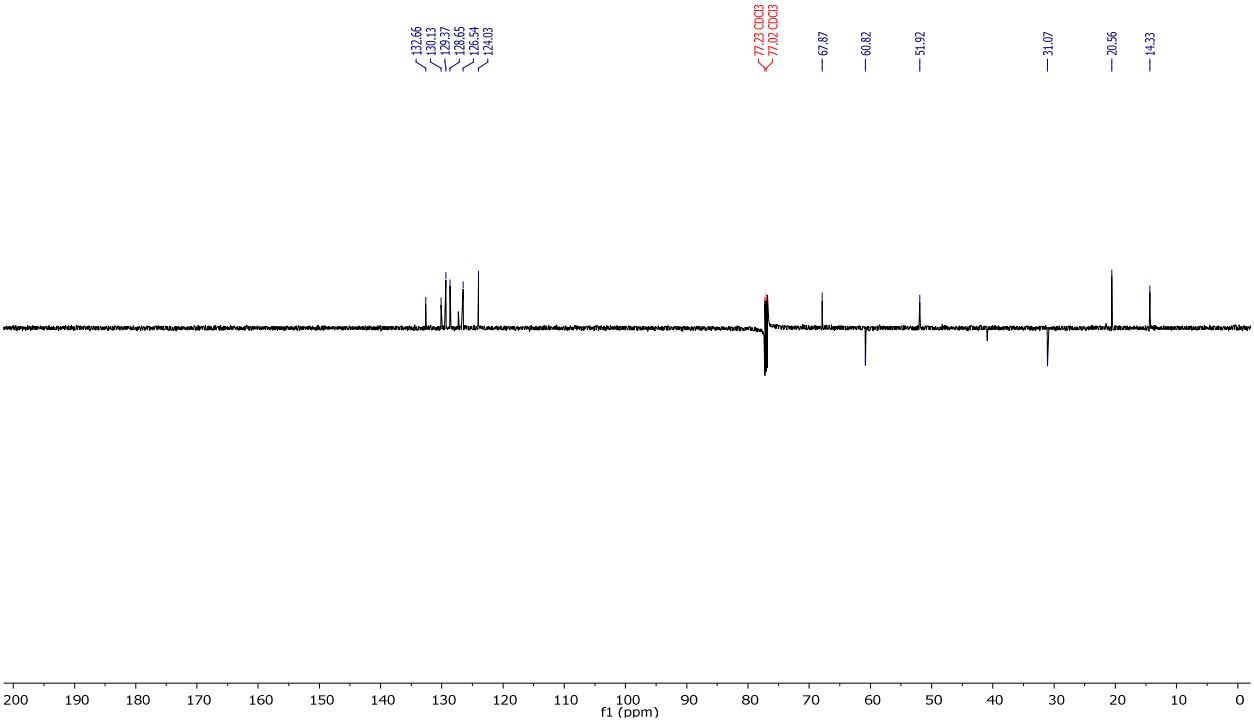
^{1}H NMR of compound (7h) (600 MHz, $CDCl_3$)



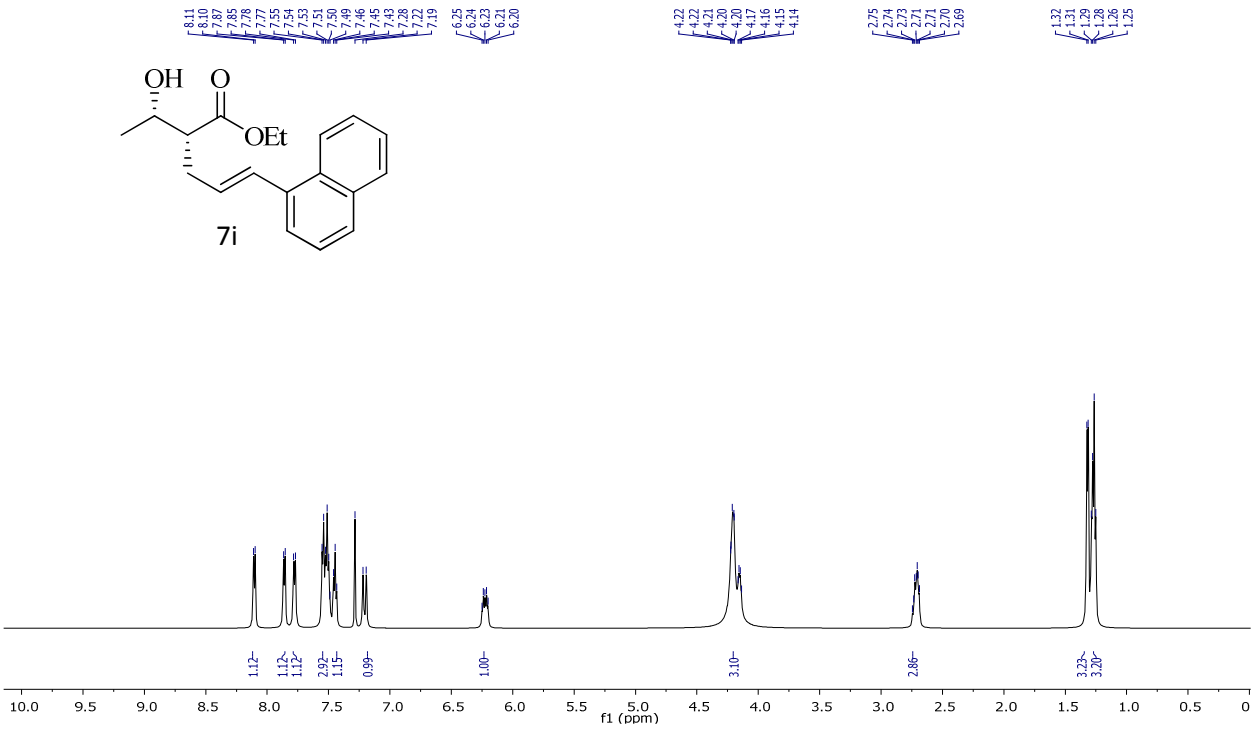
^{13}C NMR of compound (7h) (150 MHz, $CDCl_3$)



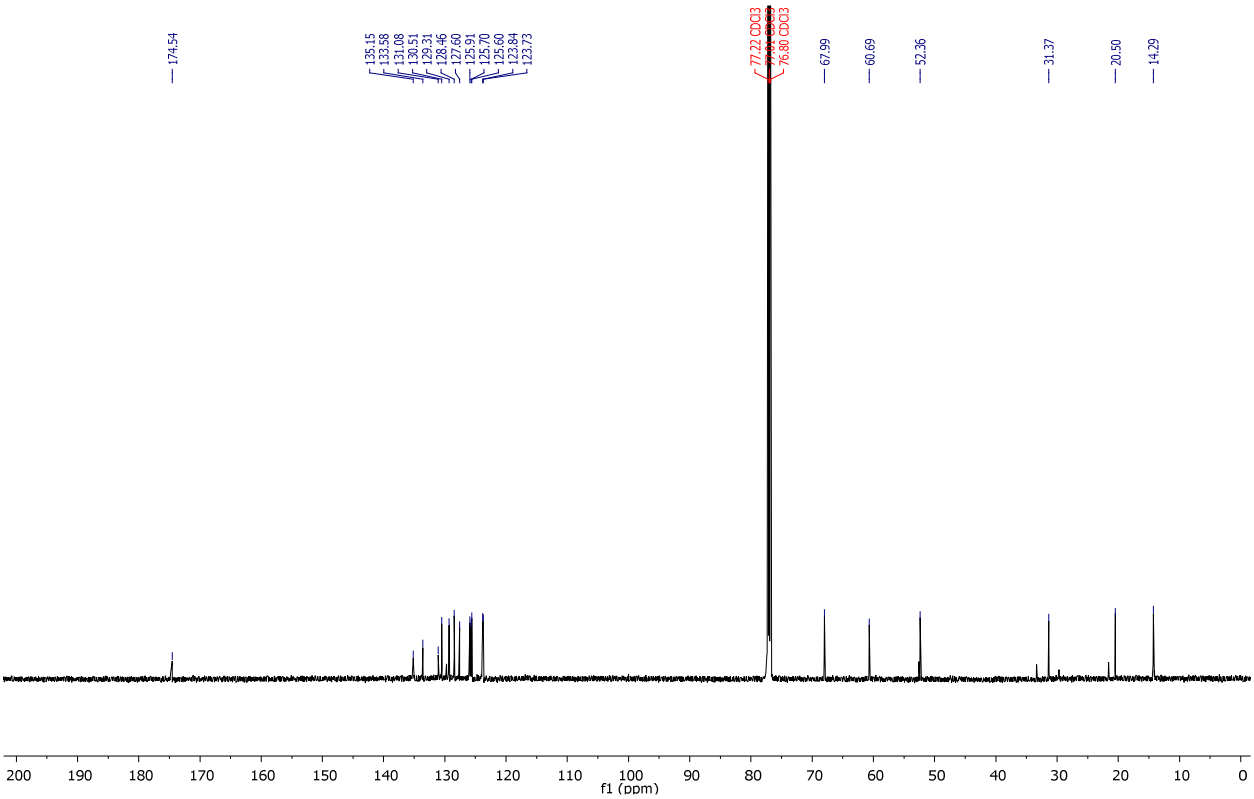
DEPT-135 of compound (7h) (150 MHz, $CDCl_3$)



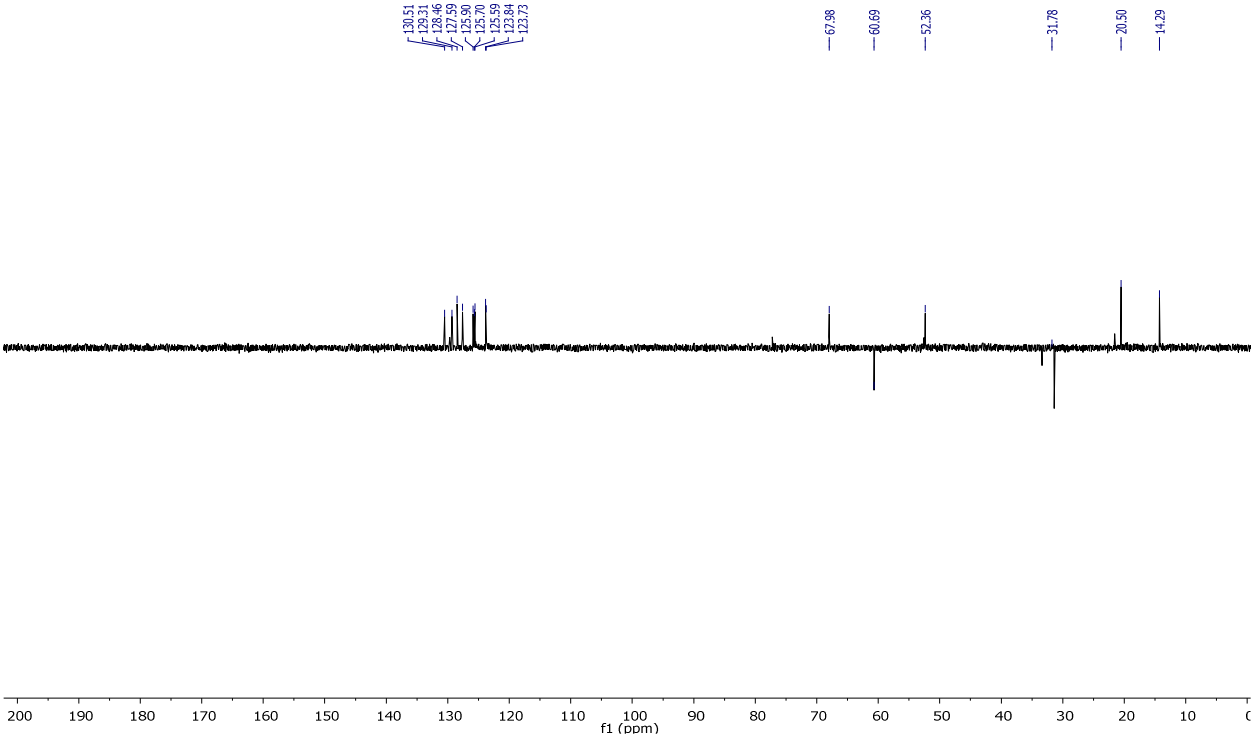
^{1}H NMR of compound (7i) (600 MHz, $CDCl_3$)



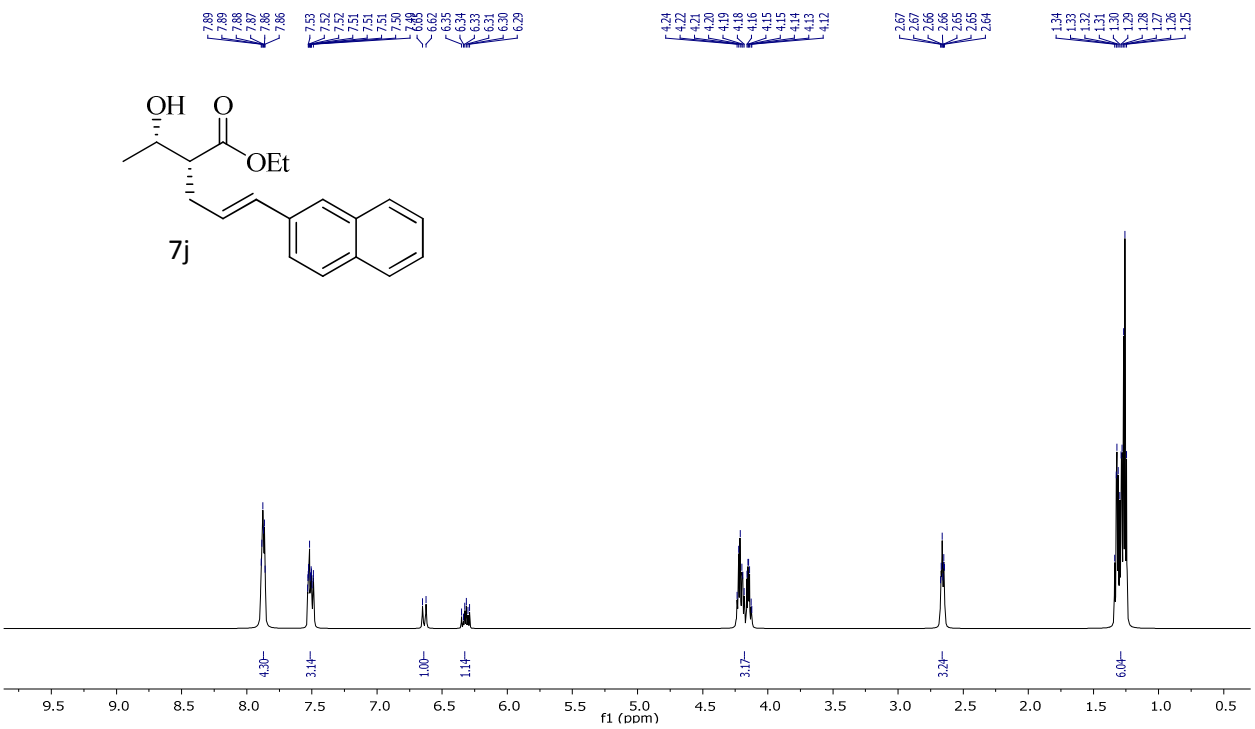
^{13}C NMR of compound (7i) (150 MHz, $CDCl_3$)



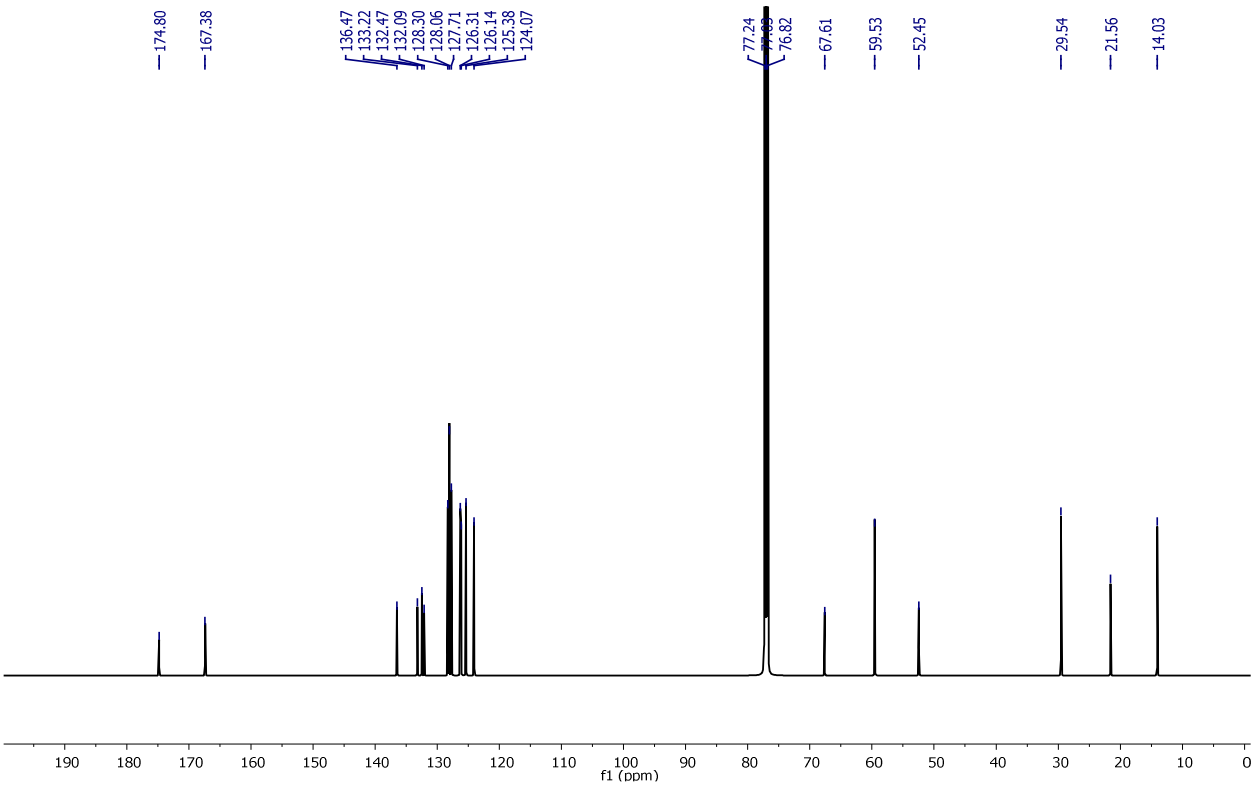
DEPT-135 of compound (7i) (150 MHz, $CDCl_3$)



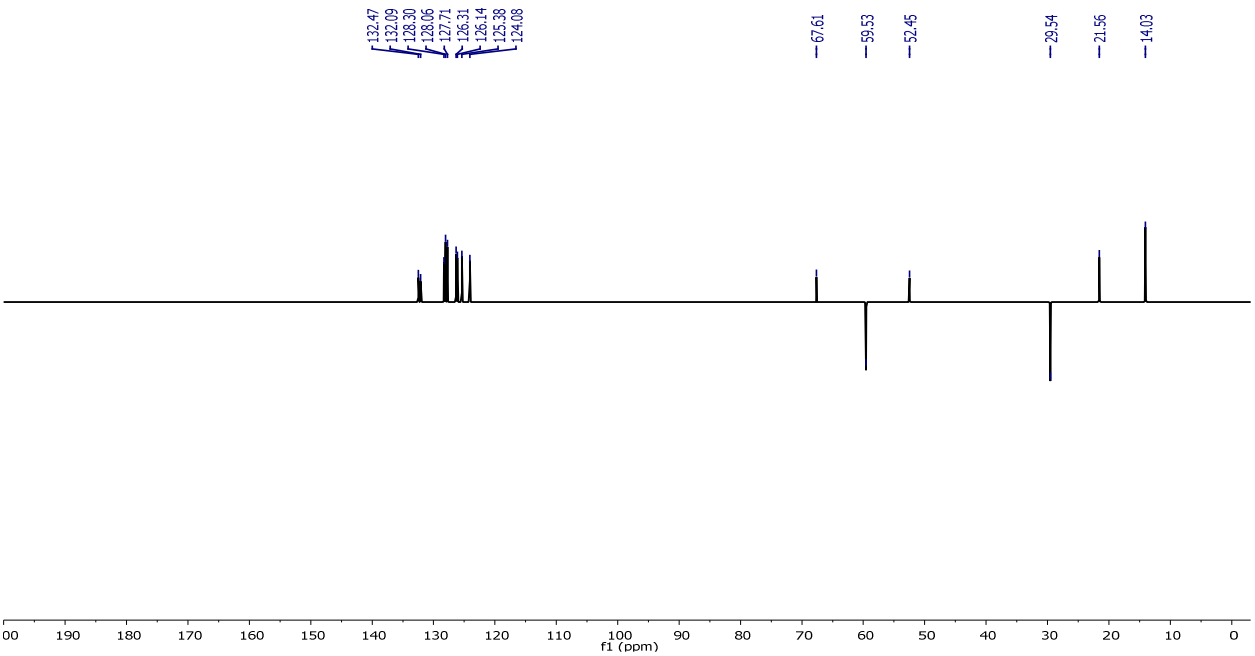
^{1}H NMR of compound (7j) (600 MHz, $CDCl_3$)



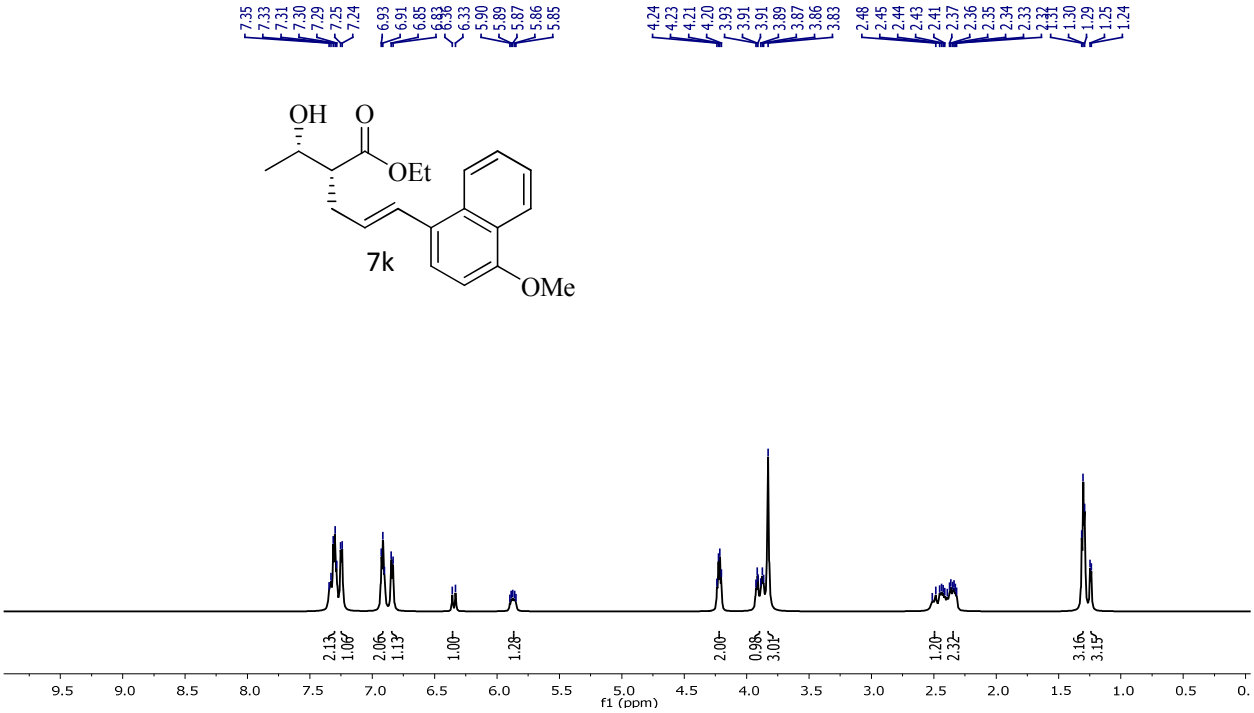
^{13}C NMR of compound (7j) (150 MHz, $CDCl_3$)



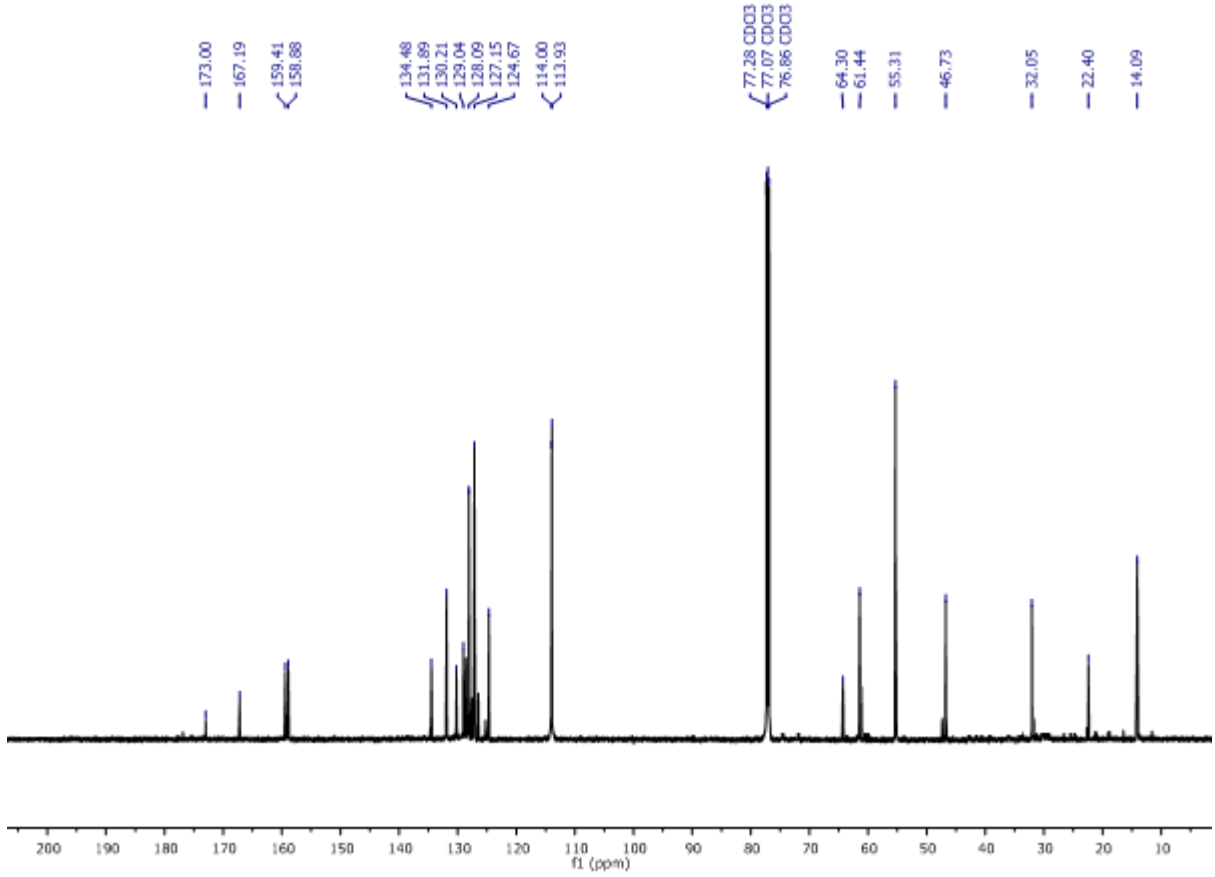
DEPT-135 of compound (7j) (150 MHz, $CDCl_3$)



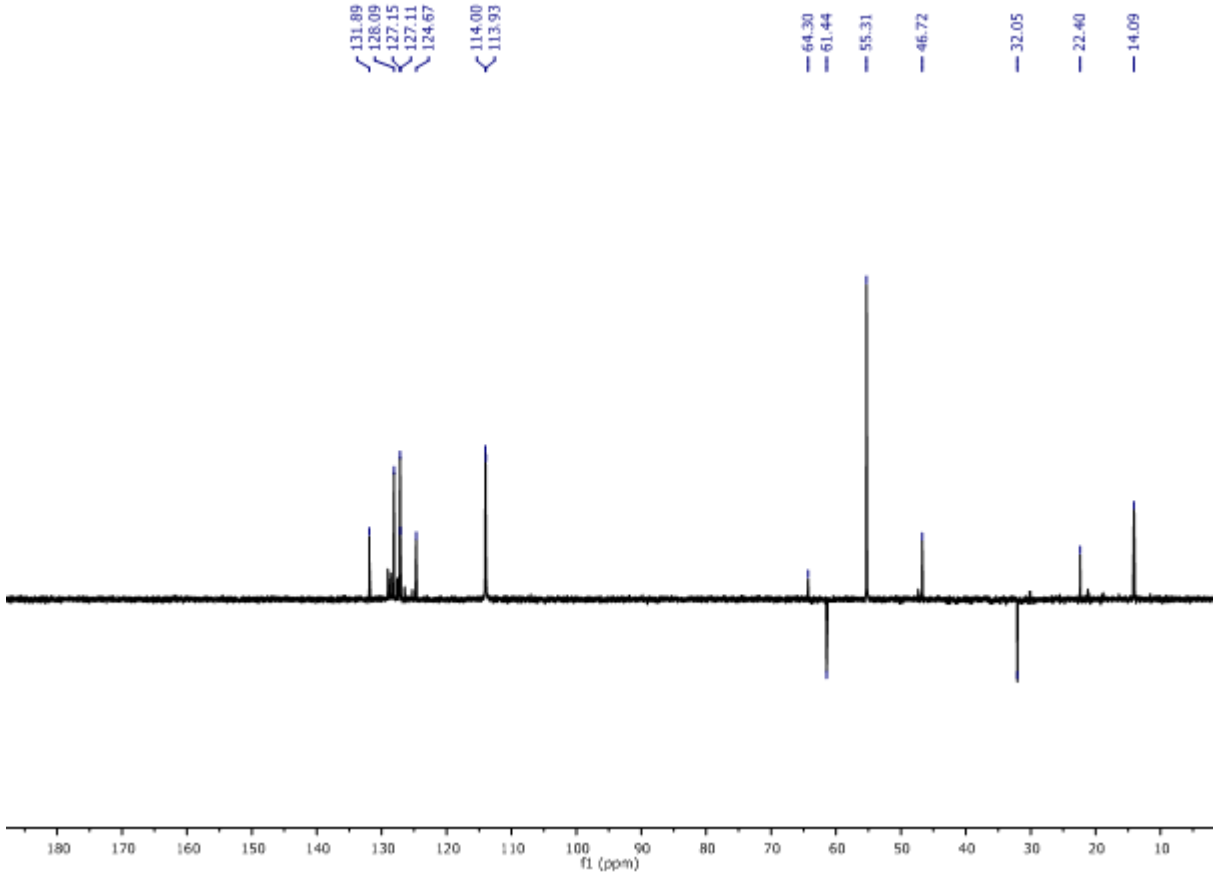
^{1}H NMR of compound (7k) (600 MHz, $CDCl_3$)



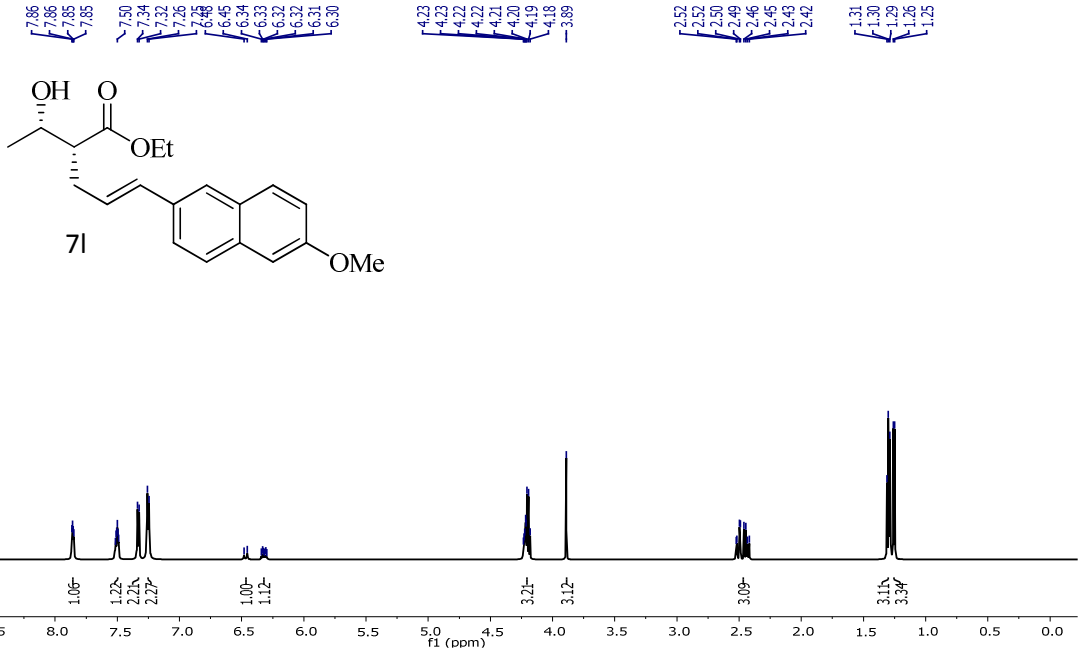
^{13}C NMR of compound (7k) (150 MHz, $CDCl_3$)



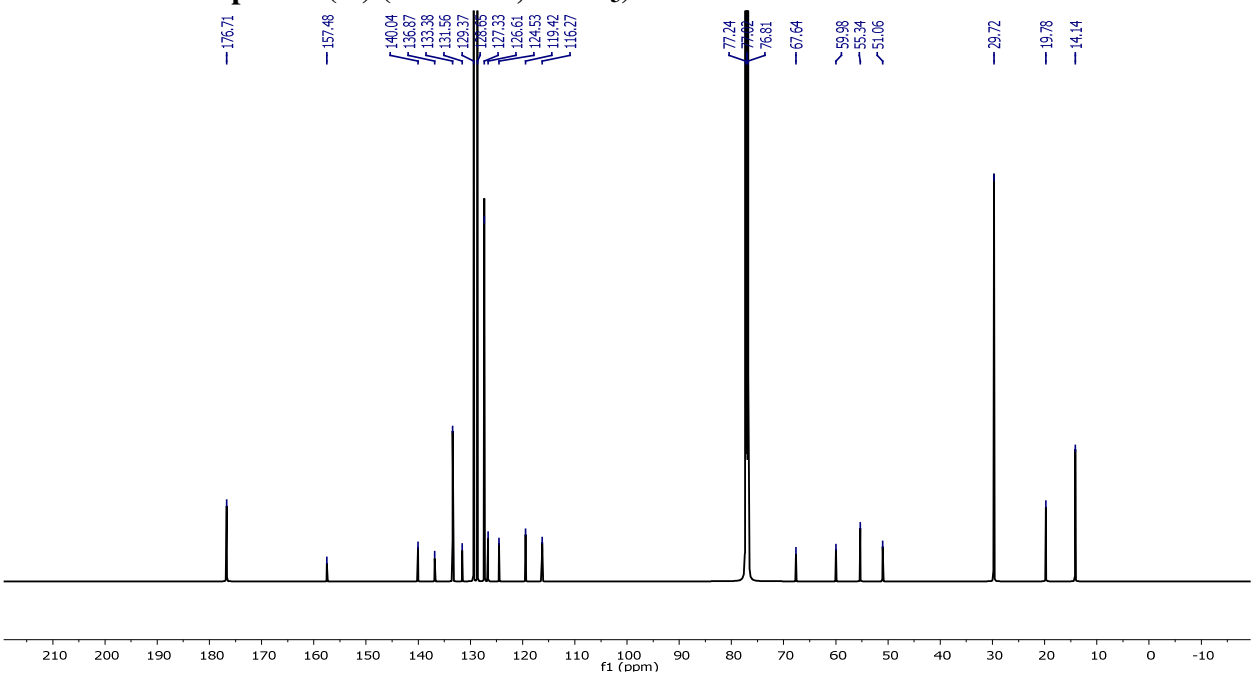
DEPT-135 of compound (7k) (150 MHz, $CDCl_3$)



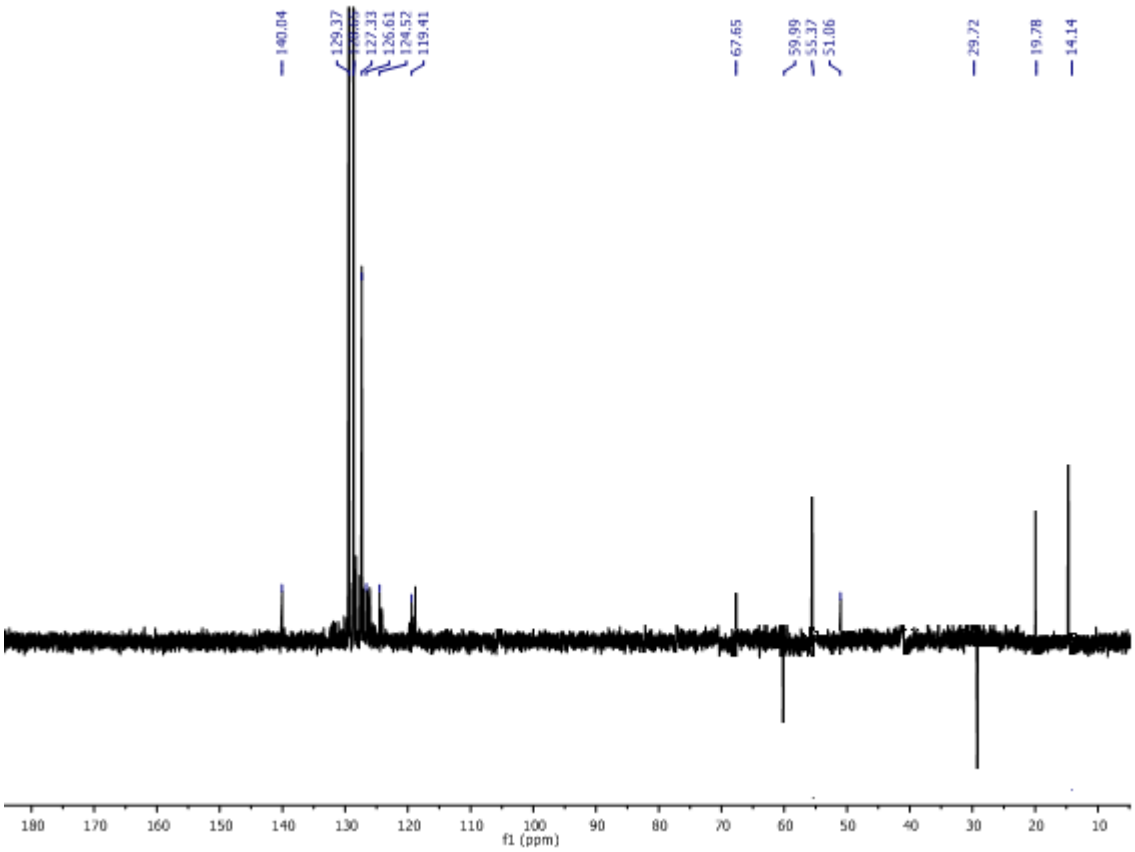
^{1}H NMR of compound (7l) (600 MHz, $CDCl_3$)



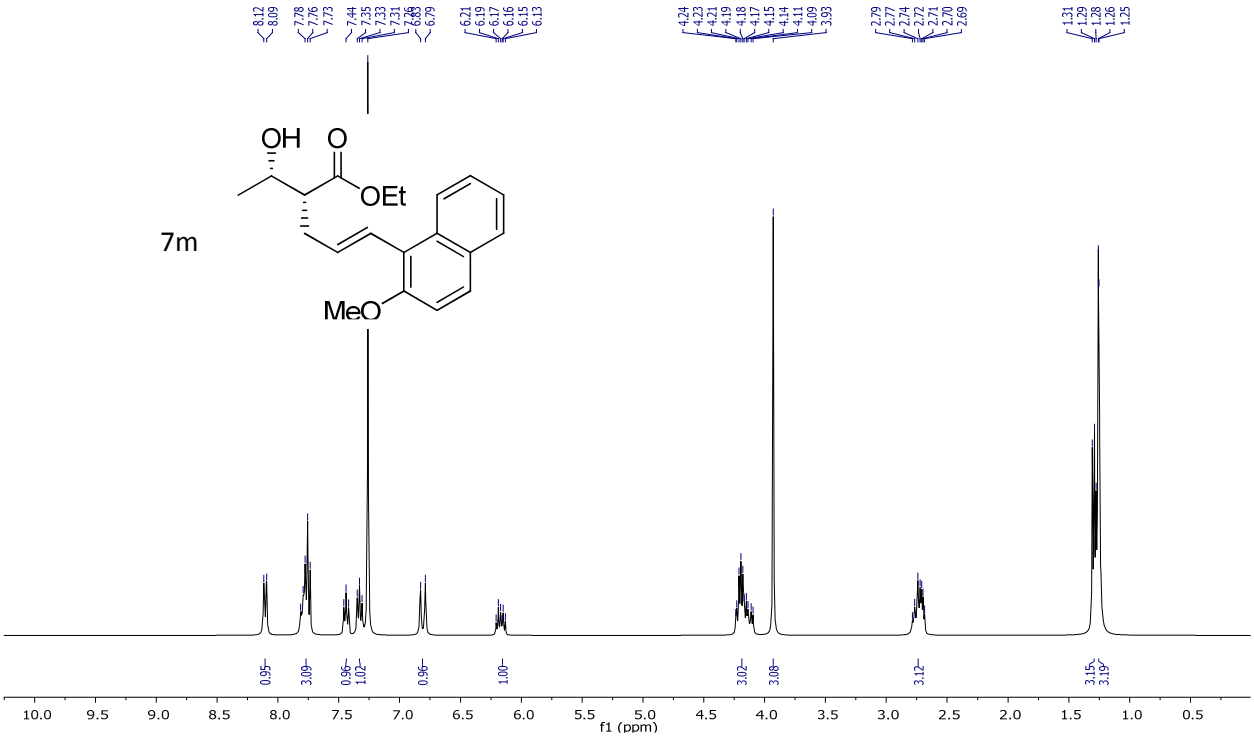
^{13}C NMR of compound (7l) (150 MHz, $CDCl_3$)



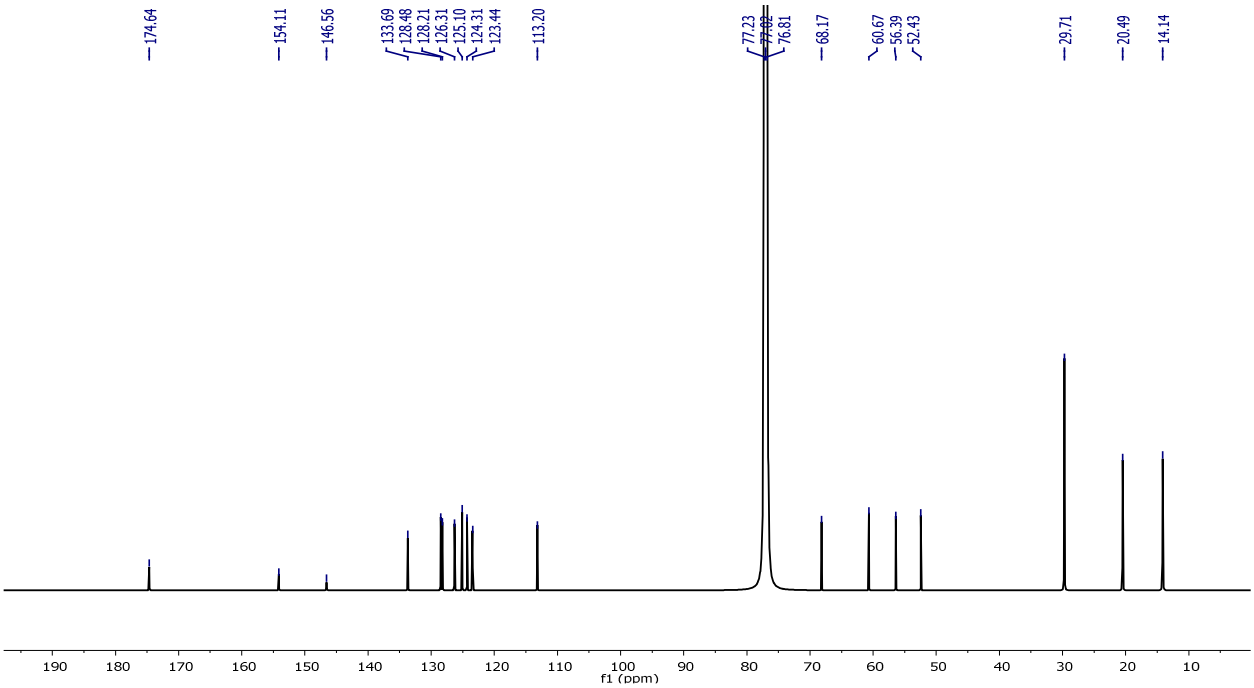
DEPT-135 of compound (7l) (150 MHz, $CDCl_3$)



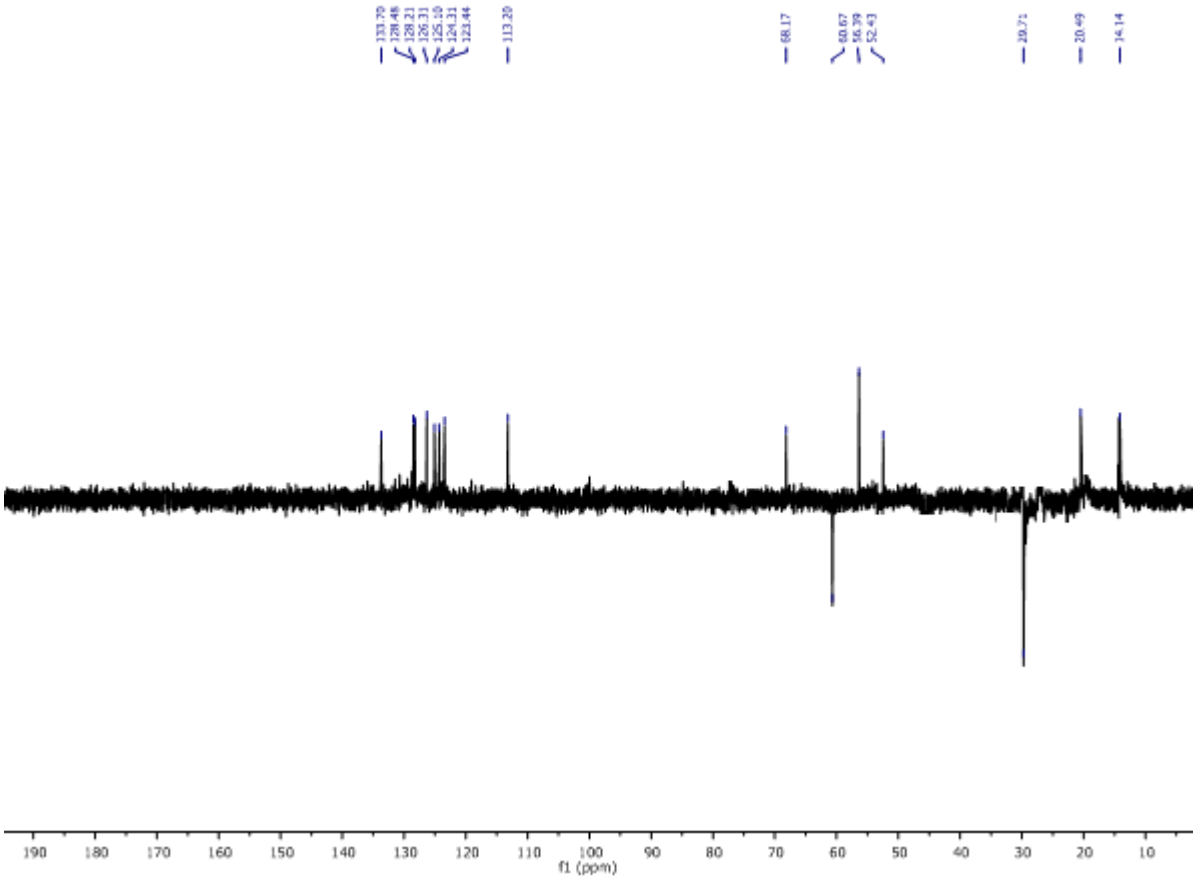
^{1}H NMR of compound (7m) (400 MHz, $CDCl_3$)



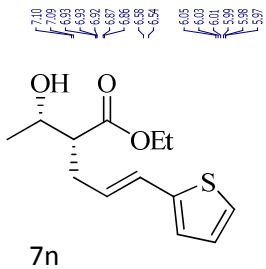
^{13}C NMR of compound (7m) (150 MHz, $CDCl_3$)



DEPT-135 of compound (7m) (100 MHz, $CDCl_3$)

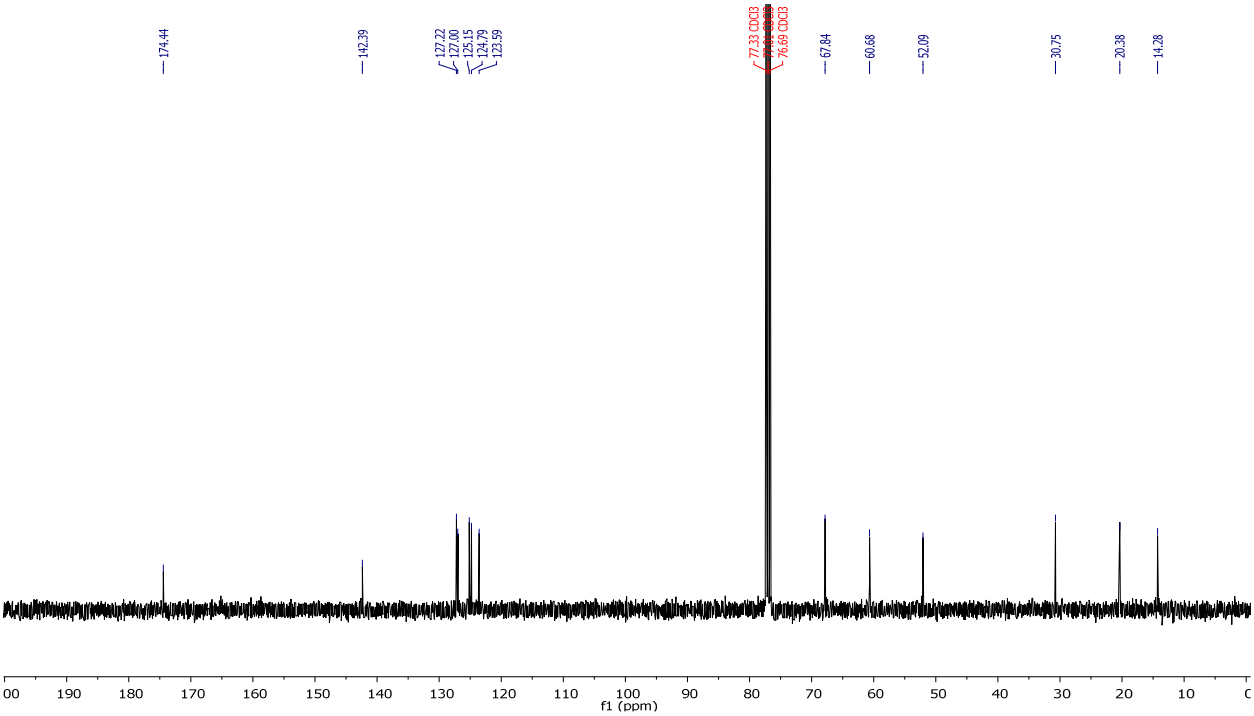


^{1}H NMR of compound (7n) (400 MHz, $CDCl_3$)

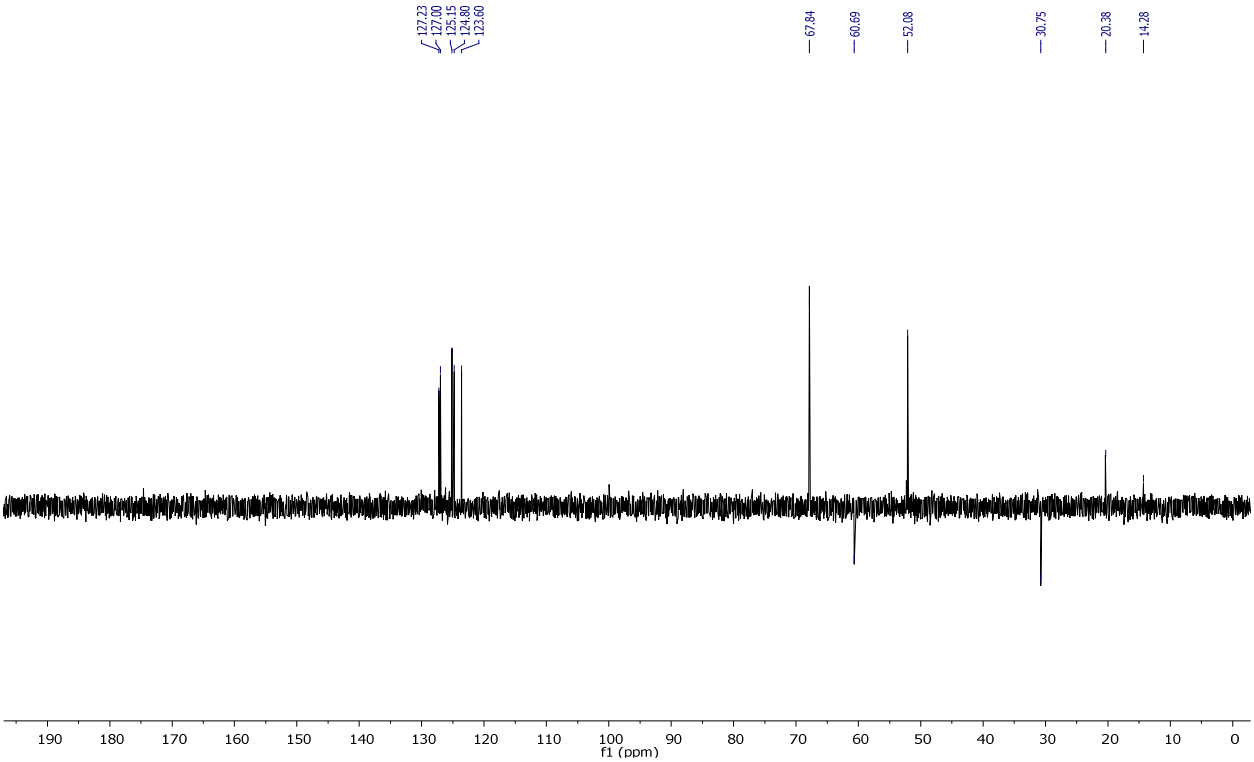


7n

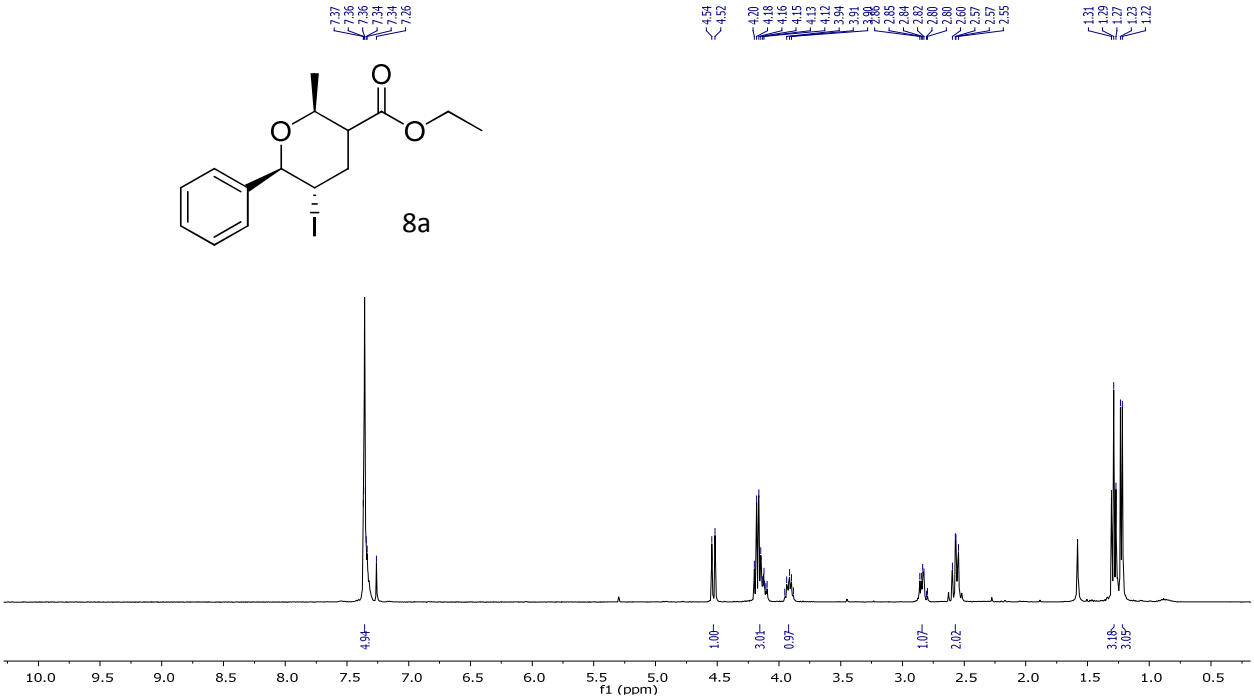
^{13}C NMR of compound (7n) (100 MHz, $CDCl_3$)



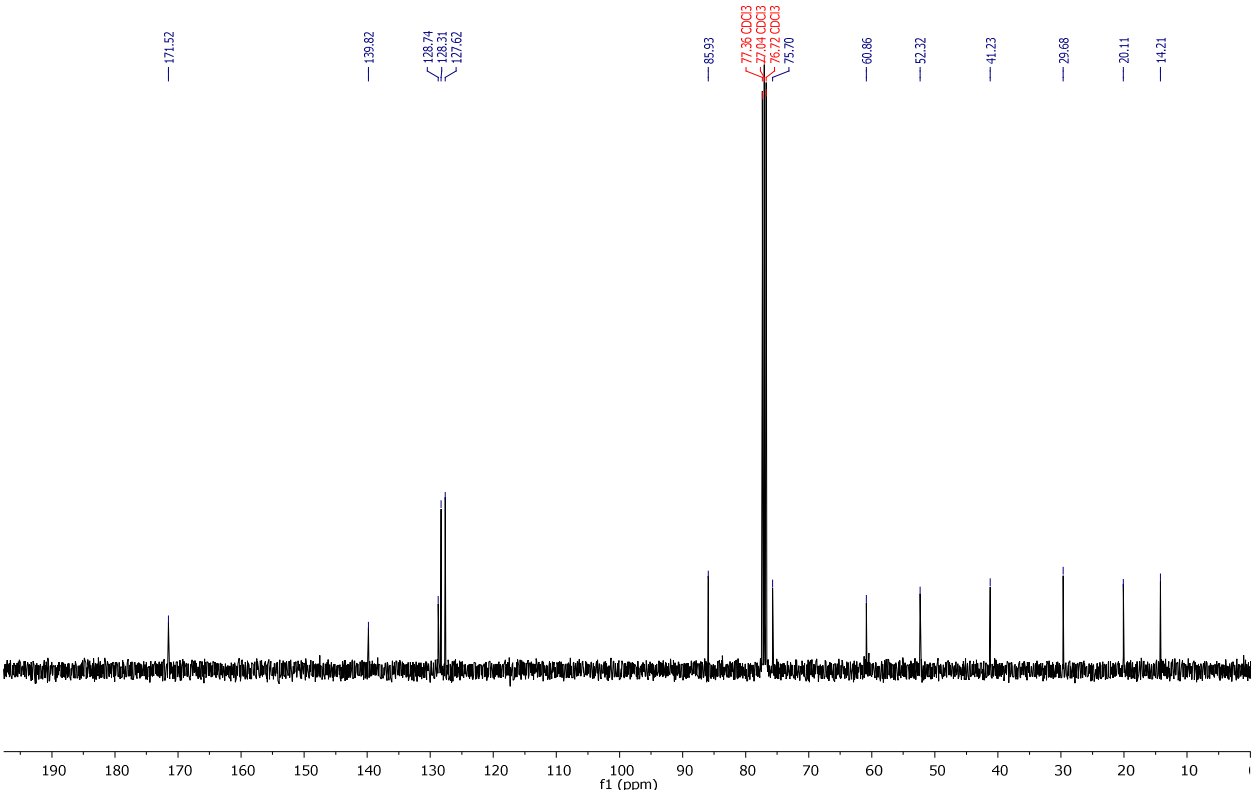
DEPT-135 of compound (7n) (100 MHz, $CDCl_3$)



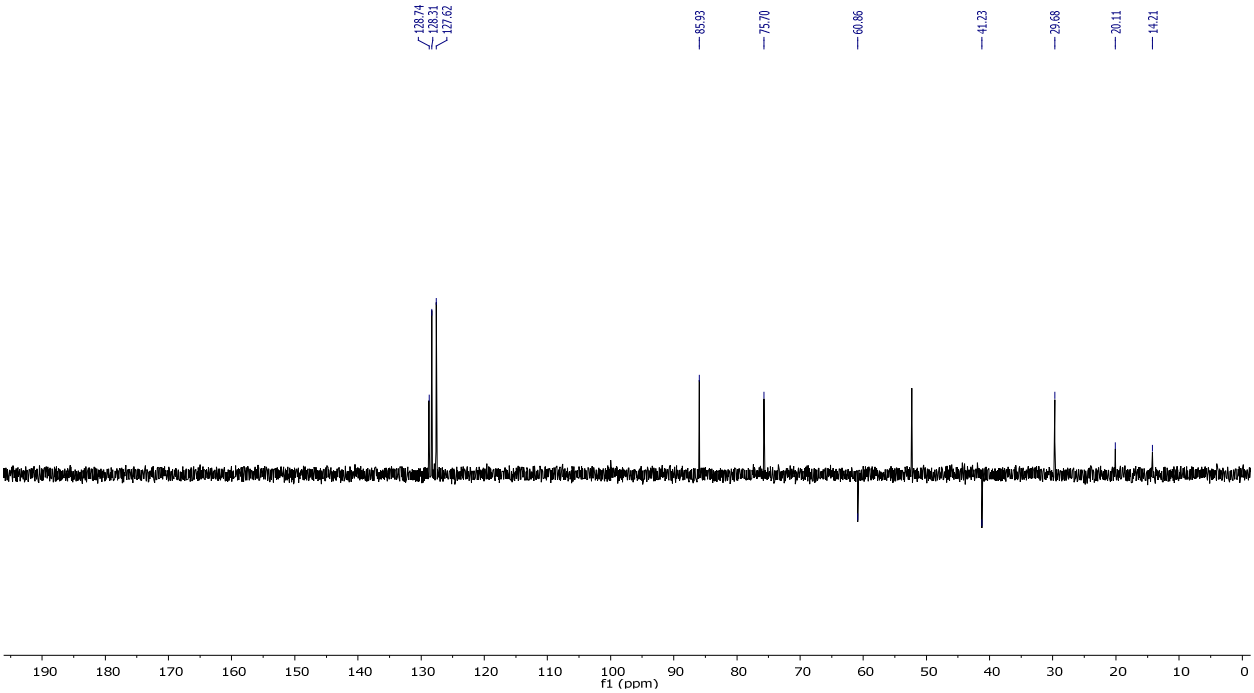
^{1}H NMR of compound (8a) (400 MHz, $CDCl_3$)



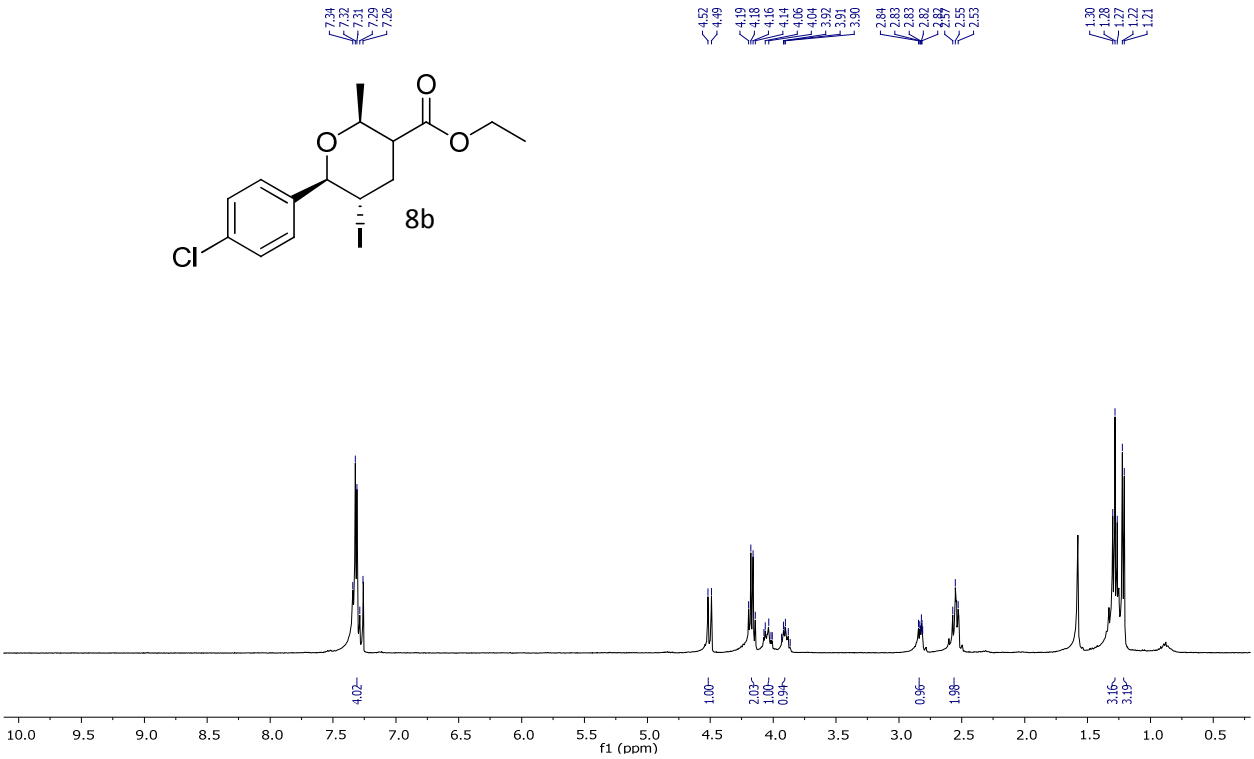
^{13}C NMR of compound (8a) (100 MHz, $CDCl_3$)



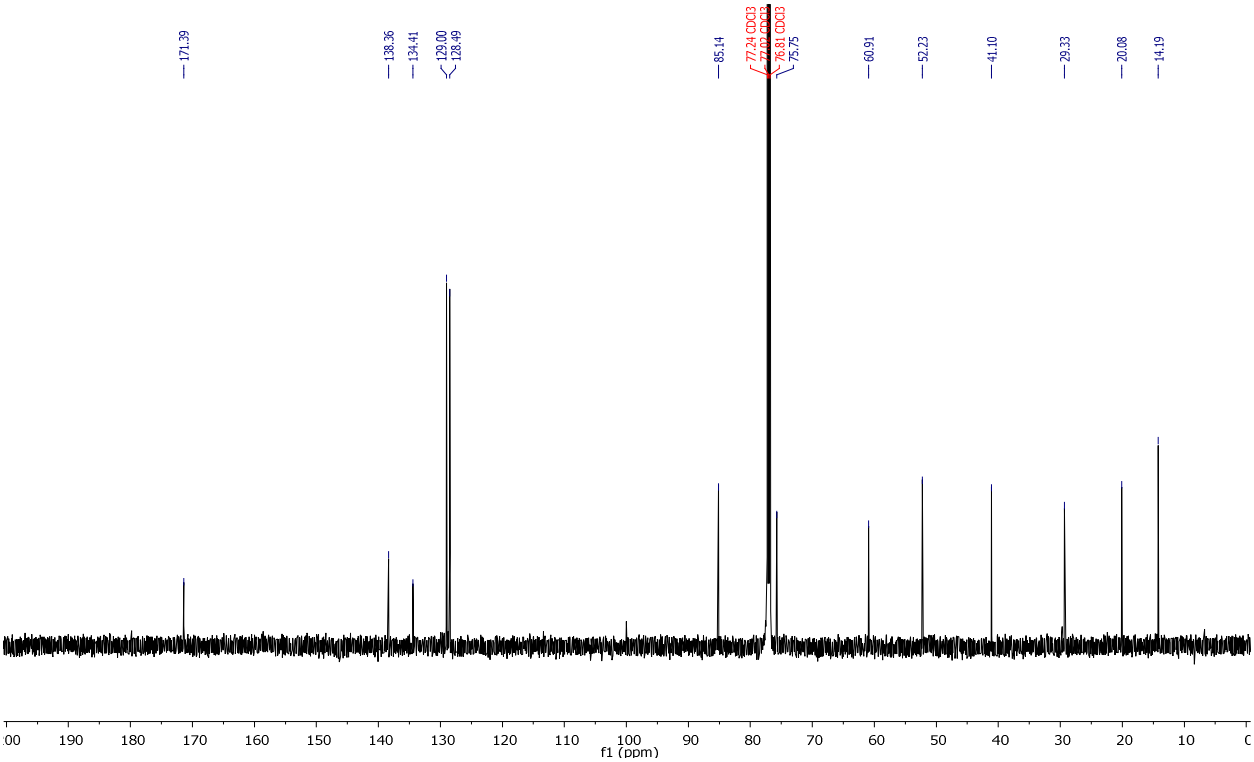
DEPT-135 of compound (8a) (100 MHz, $CDCl_3$)



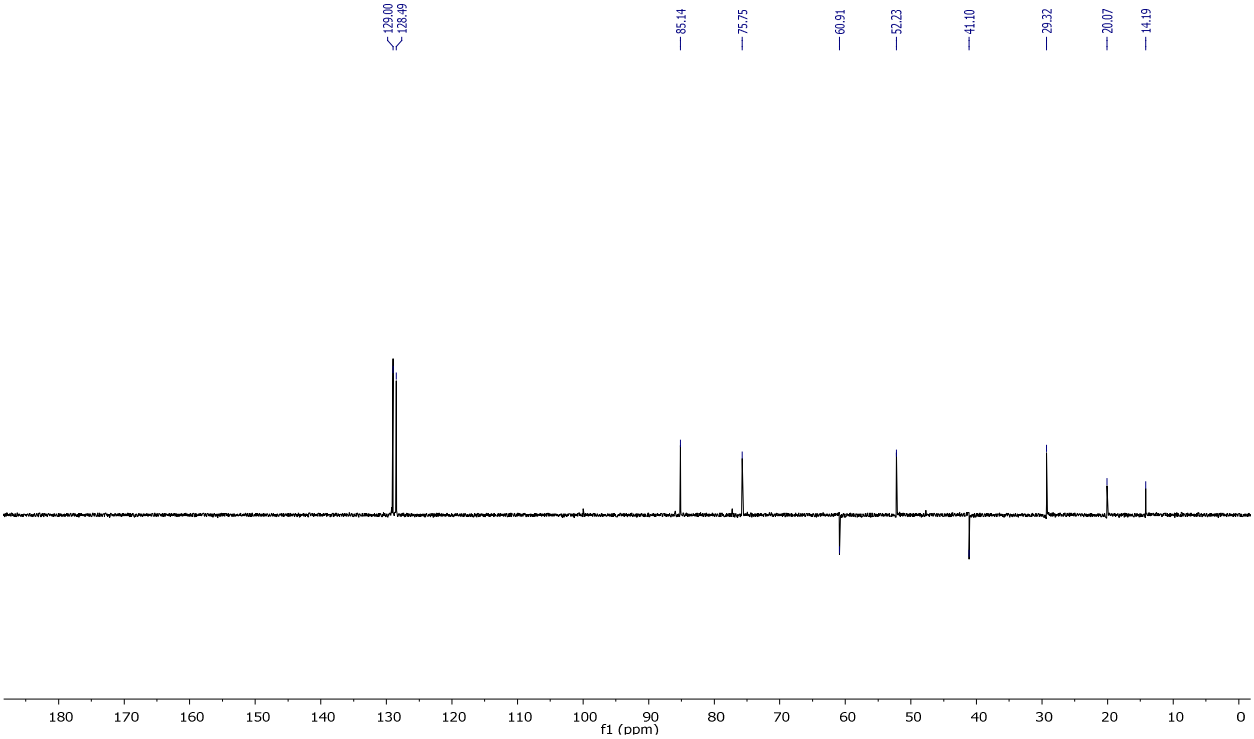
^{1}H NMR of compound (8b) (400 MHz, $CDCl_3$)



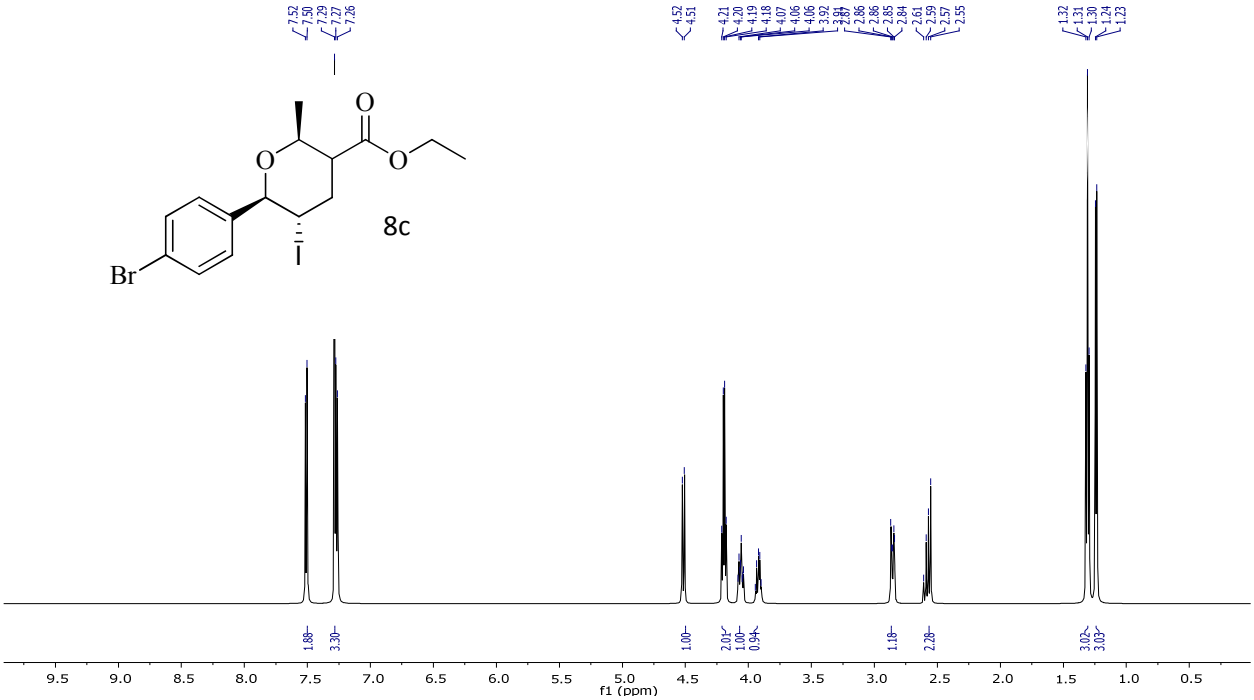
^{13}C NMR of compound (8b) (150 MHz, $CDCl_3$)



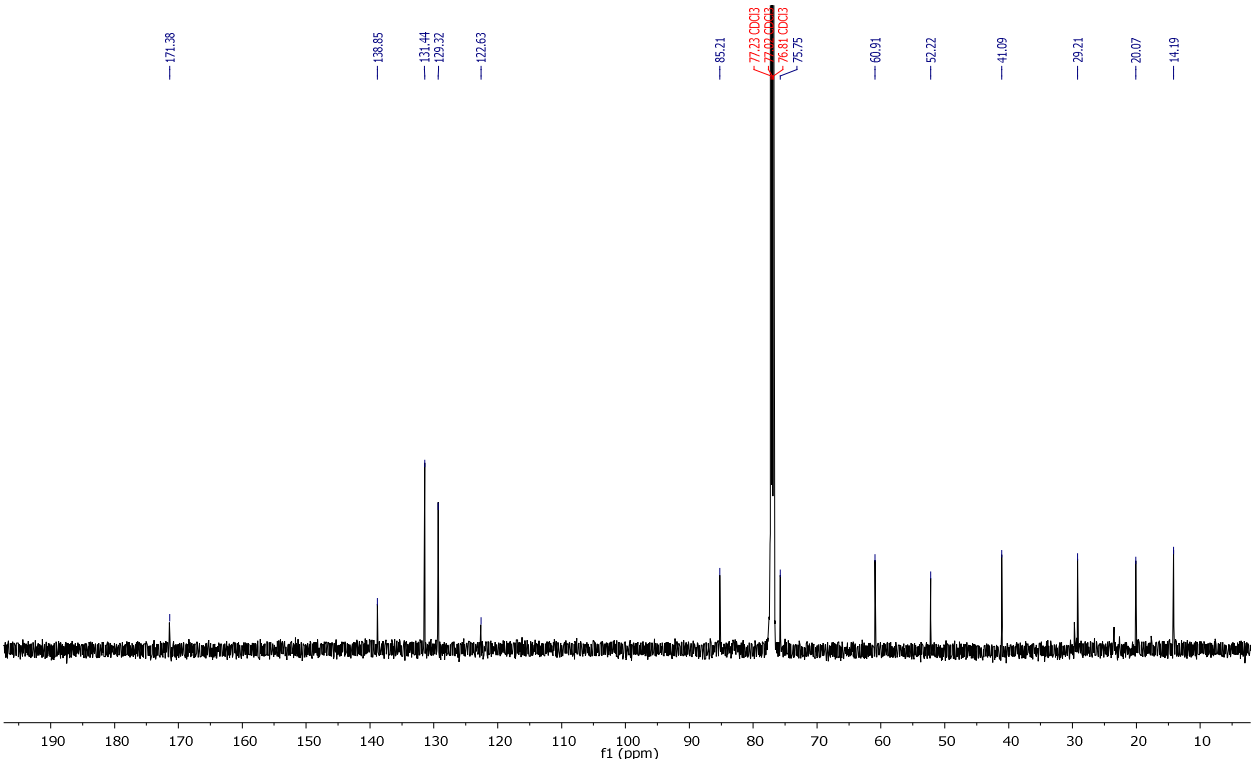
DEPT-135 of compound (8b) (150 MHz, $CDCl_3$)



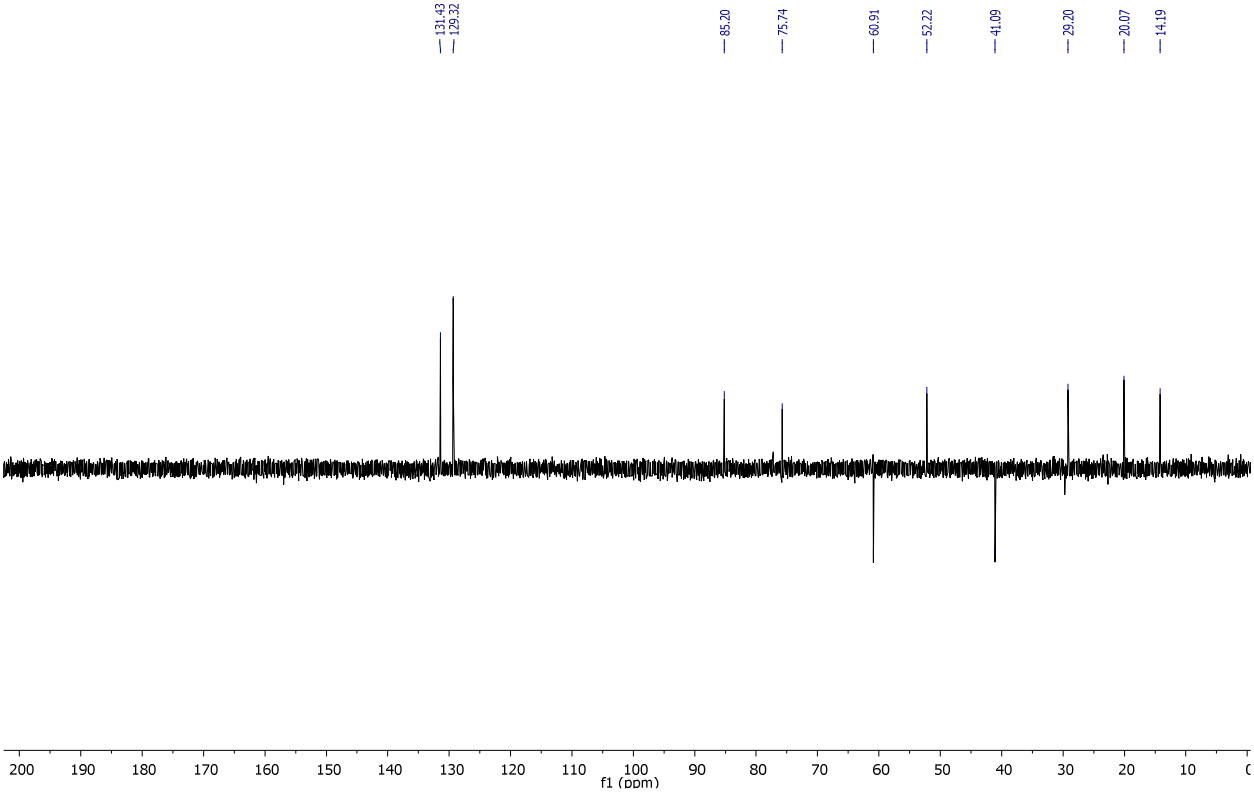
^{1}H NMR of compound (8c) (600 MHz, $CDCl_3$)



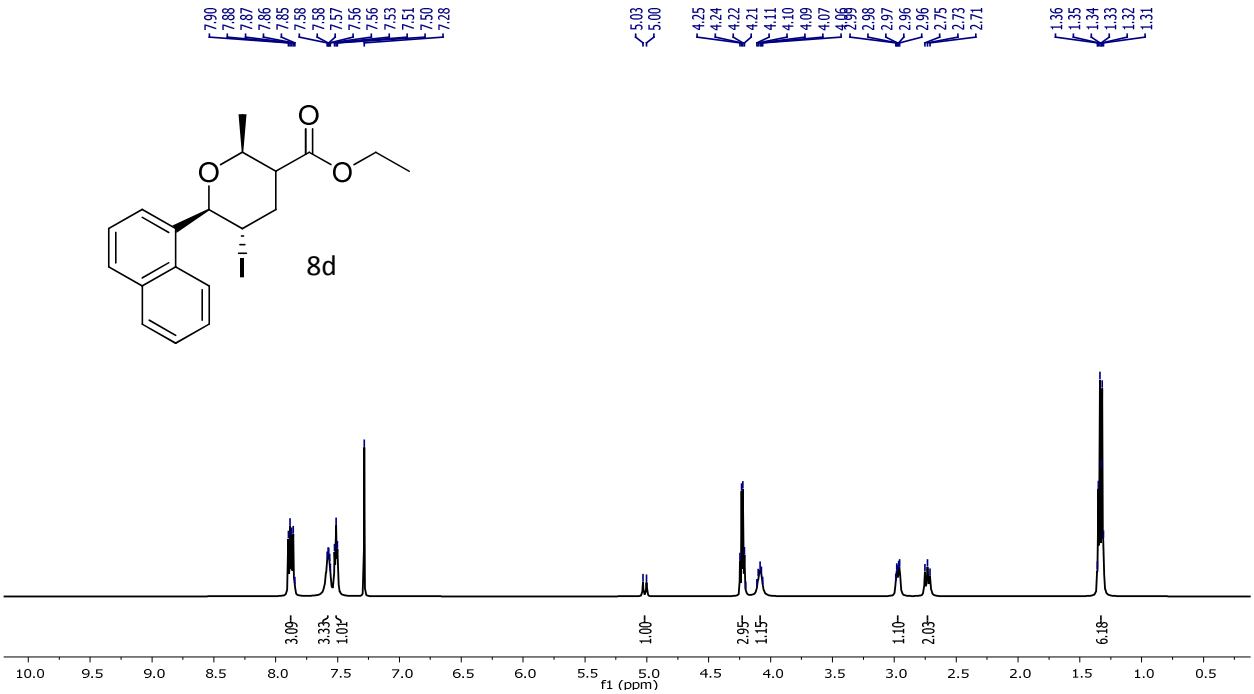
^{13}C NMR of compound (8c) (150 MHz, $CDCl_3$)



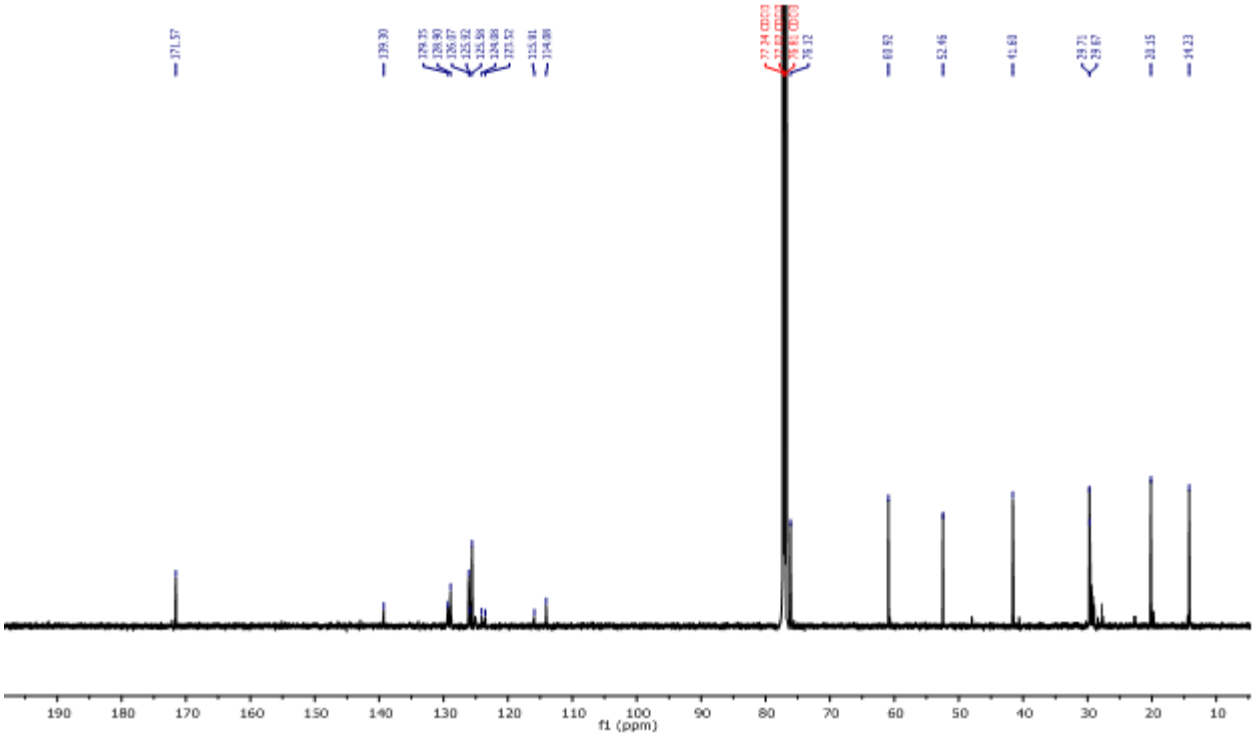
DEPT-135 of compound (8c) (150 MHz, $CDCl_3$)



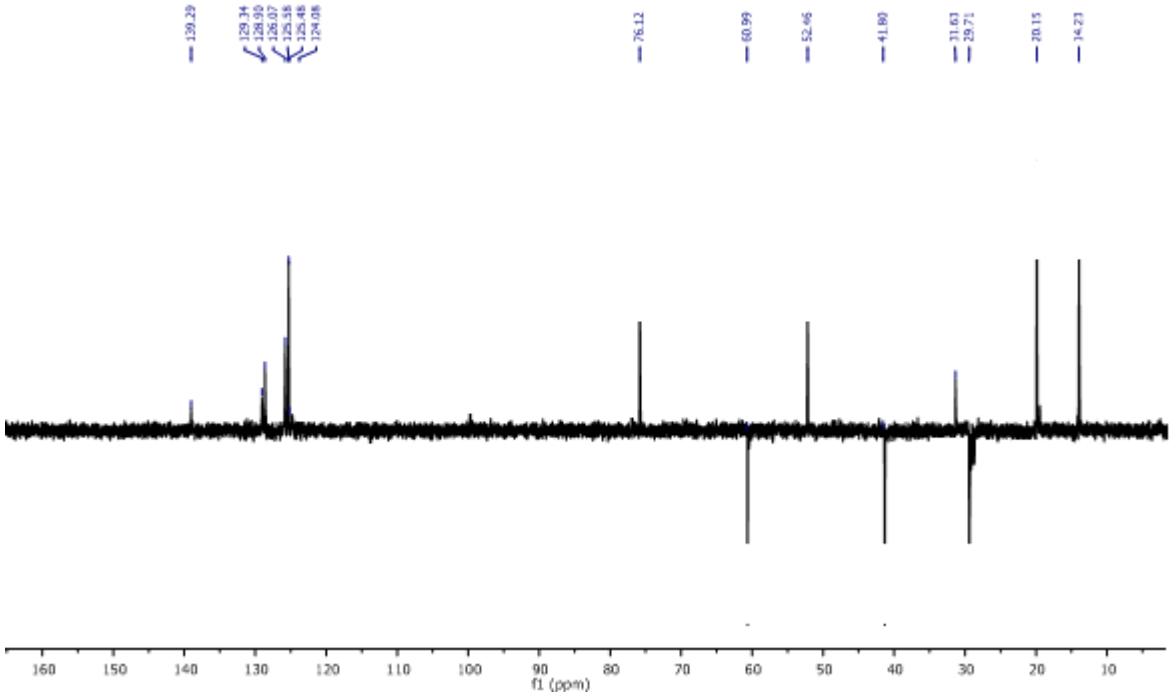
^{1}H NMR of compound (8d) (600 MHz, $CDCl_3$)



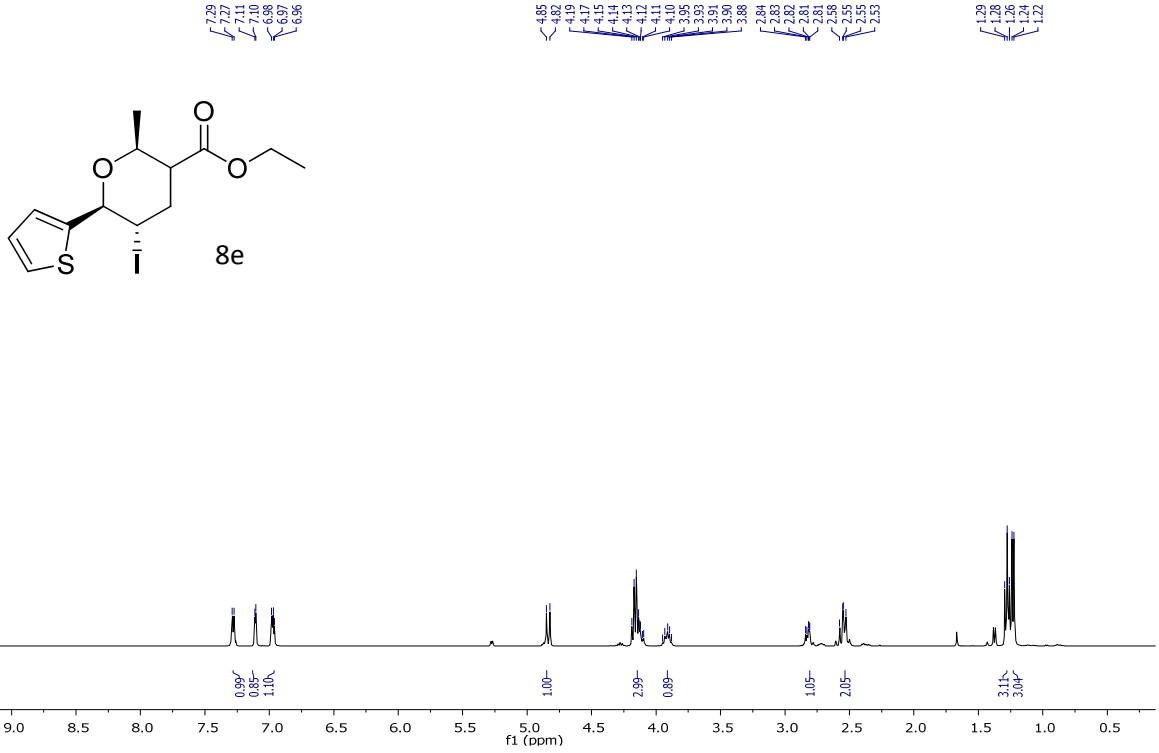
^{13}C NMR of compound (8d) (150 MHz, $CDCl_3$)



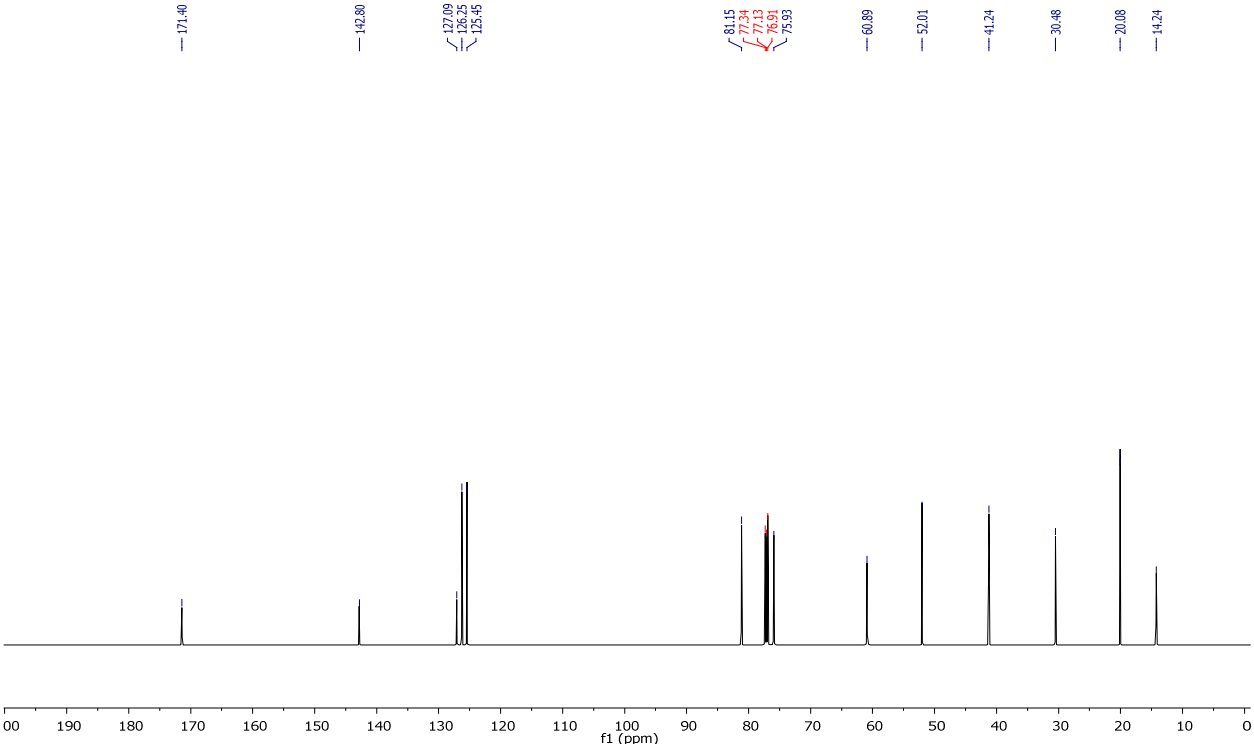
DEPT-135 of compound (8d) (150 MHz, $CDCl_3$)



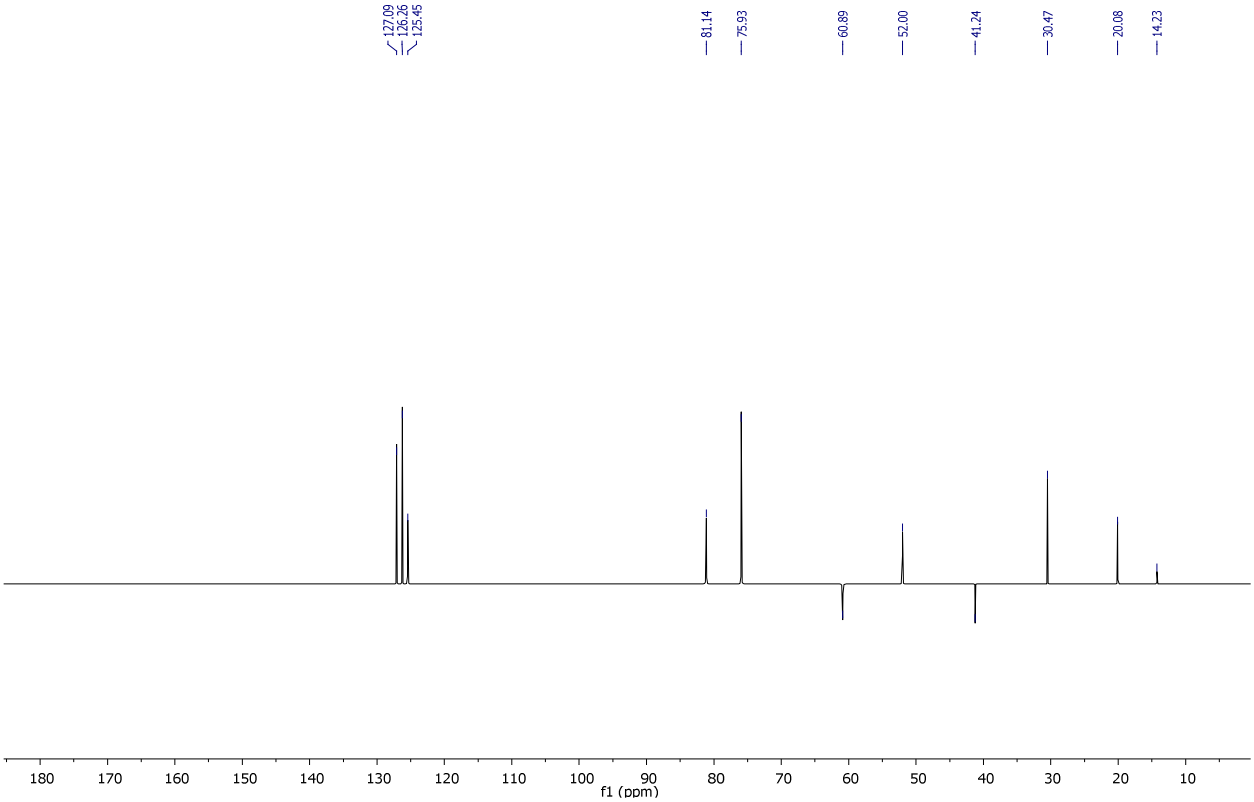
^{1}H NMR of compound (8e) (400 MHz, $CDCl_3$)



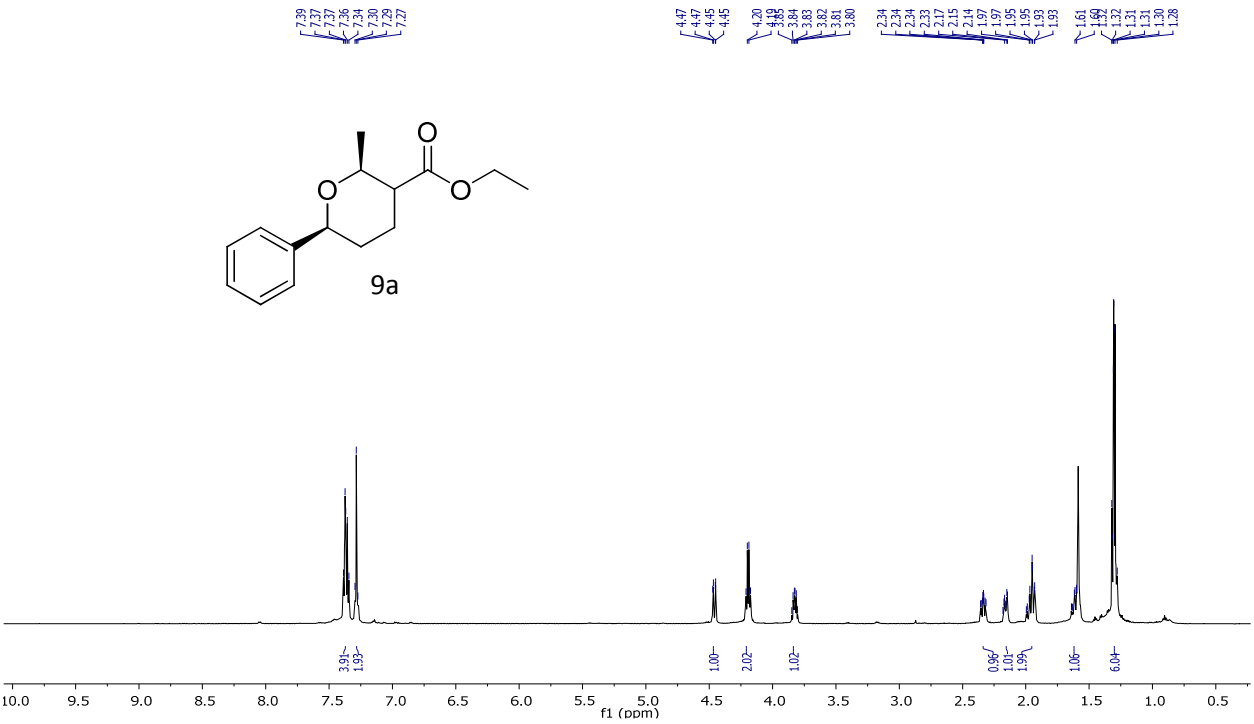
^{13}C NMR of compound (8e) (150 MHz, $CDCl_3$)



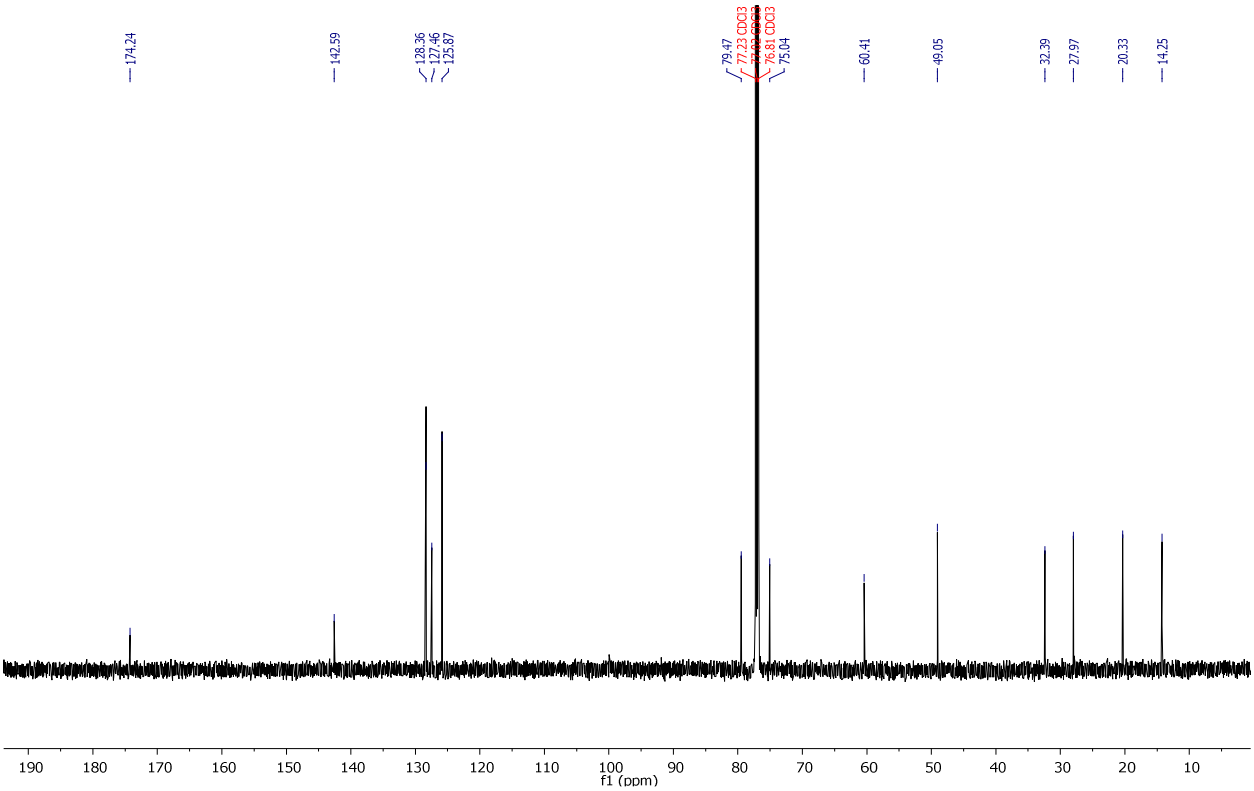
DEPT-135 of compound (8e) (150 MHz, $CDCl_3$)



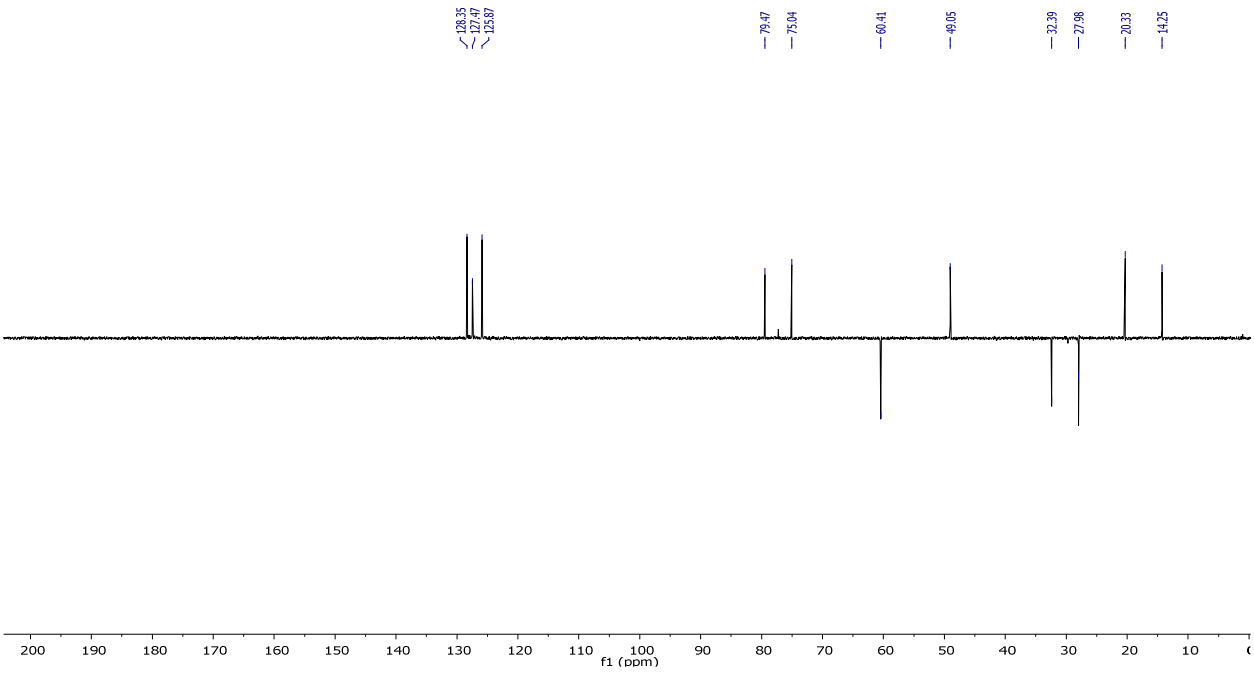
^{1}H NMR of compound (9a) (600 MHz, $CDCl_3$)



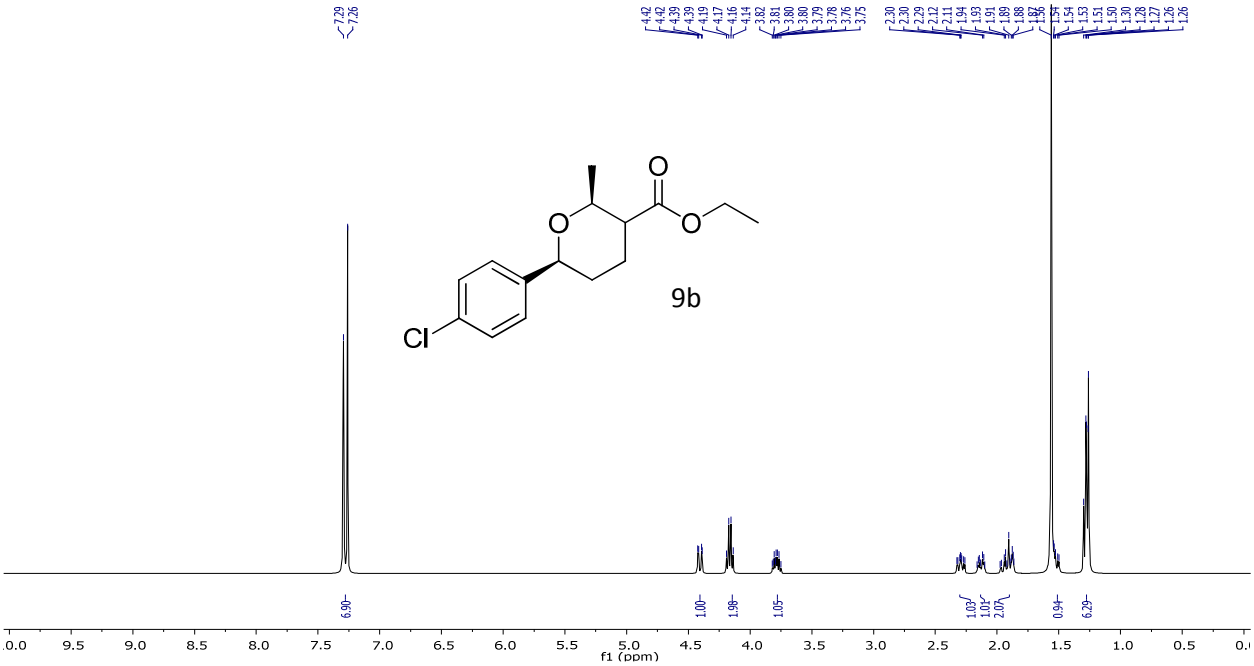
^{13}C NMR of compound (9a) (150 MHz, $CDCl_3$)



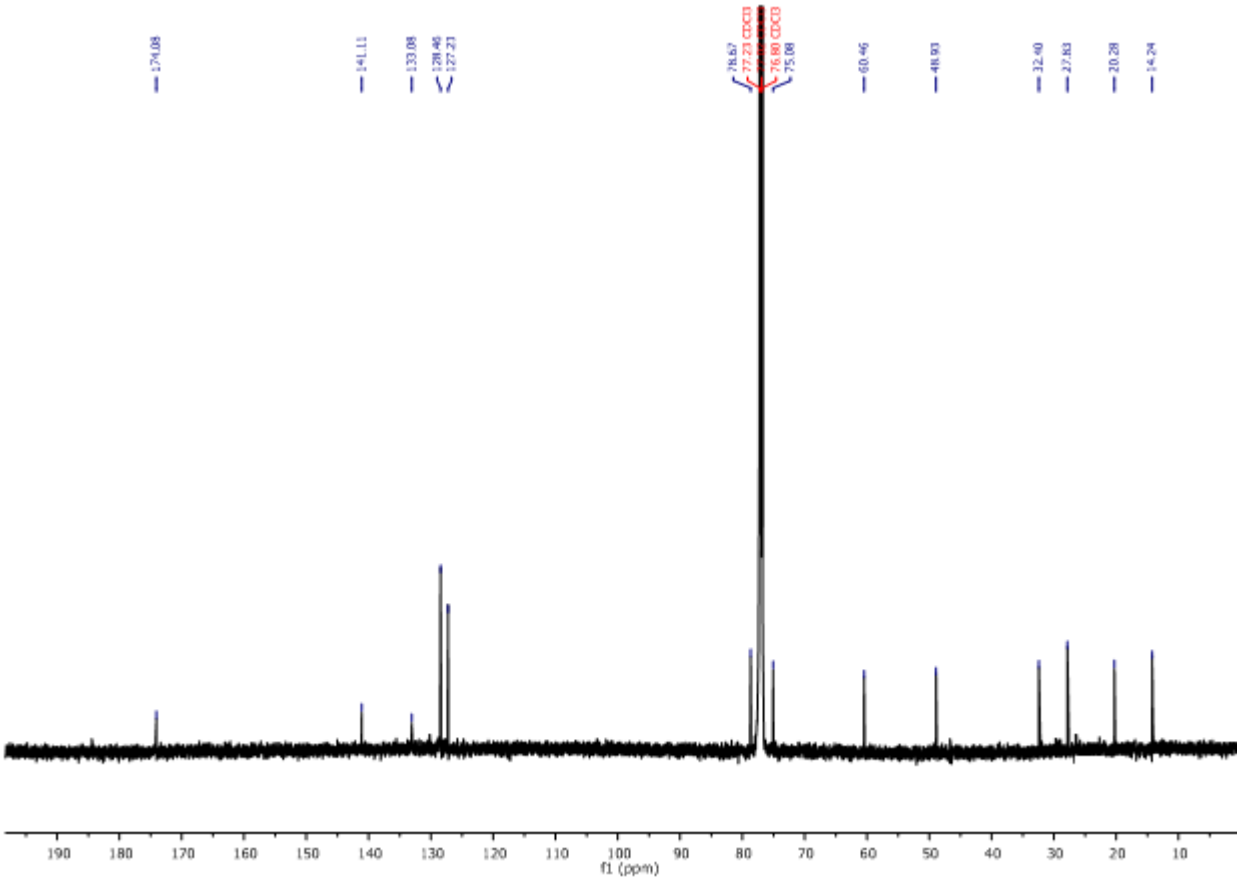
DEPT-135 of compound (9a) (150 MHz, $CDCl_3$)



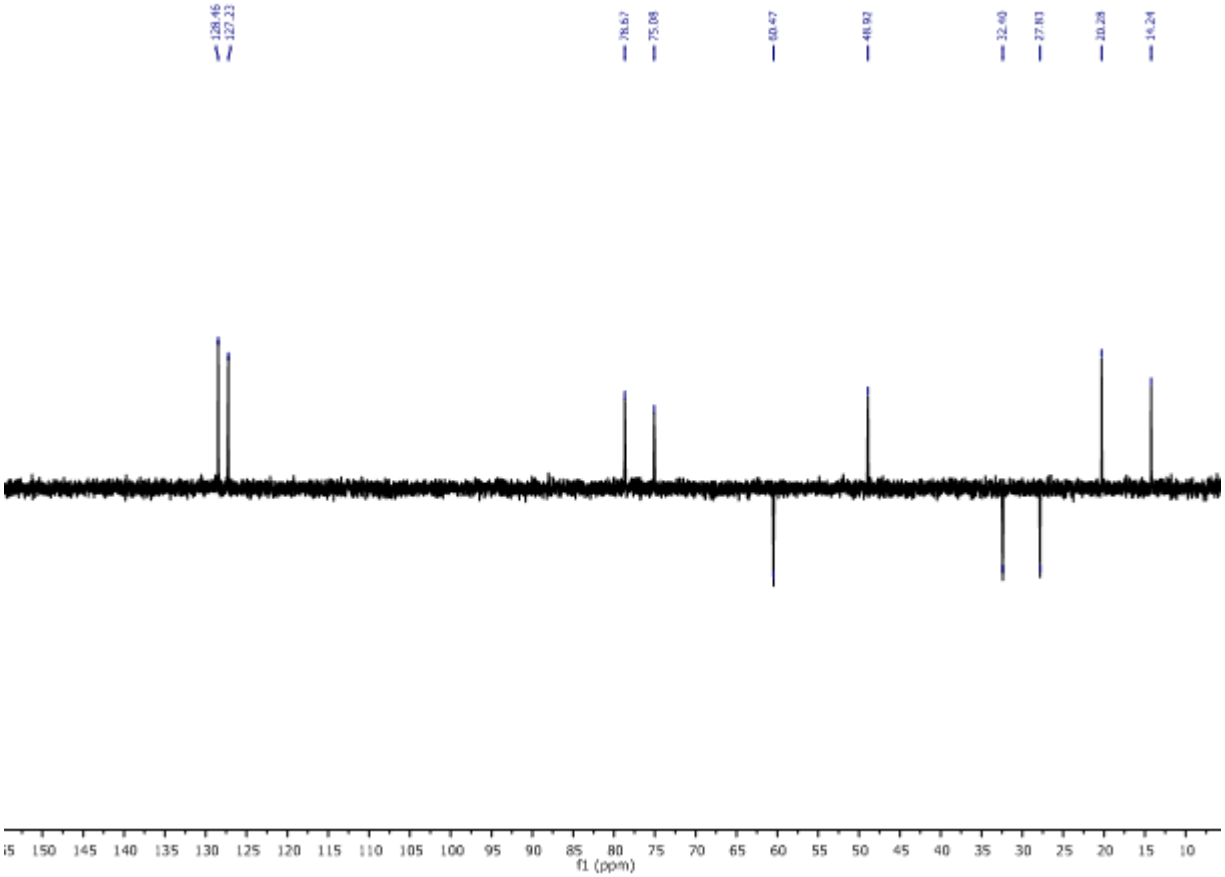
^{1}H NMR of compound (9b) (400 MHz, $CDCl_3$)



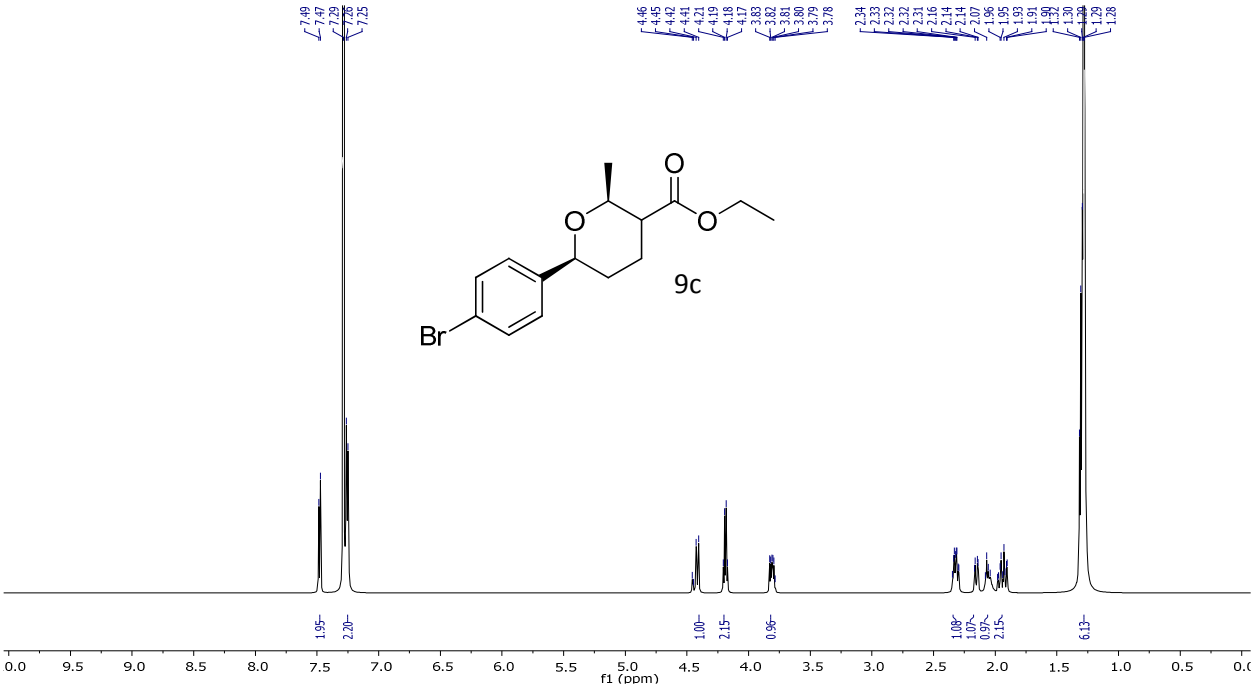
^{13}C NMR of compound (9b) (150 MHz, $CDCl_3$)



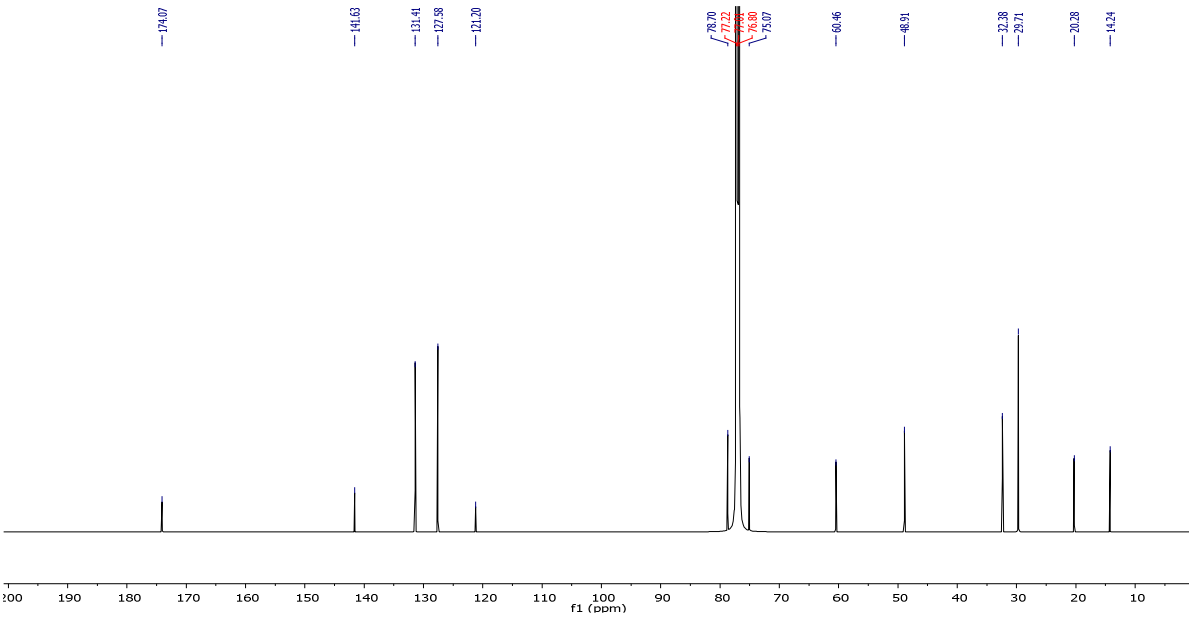
DEPT-135 of compound (9b) (150 MHz, $CDCl_3$)



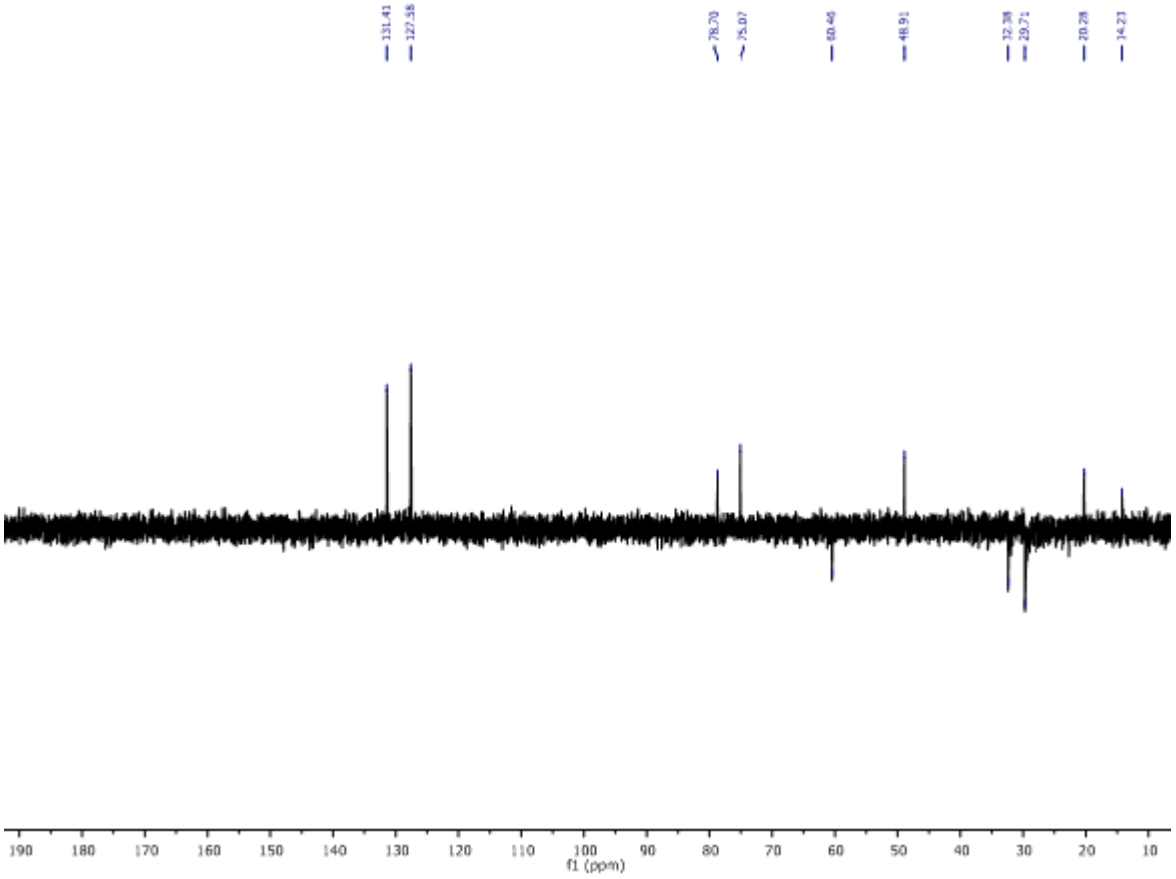
^{1}H NMR of compound (9c) (600 MHz, $CDCl_3$)



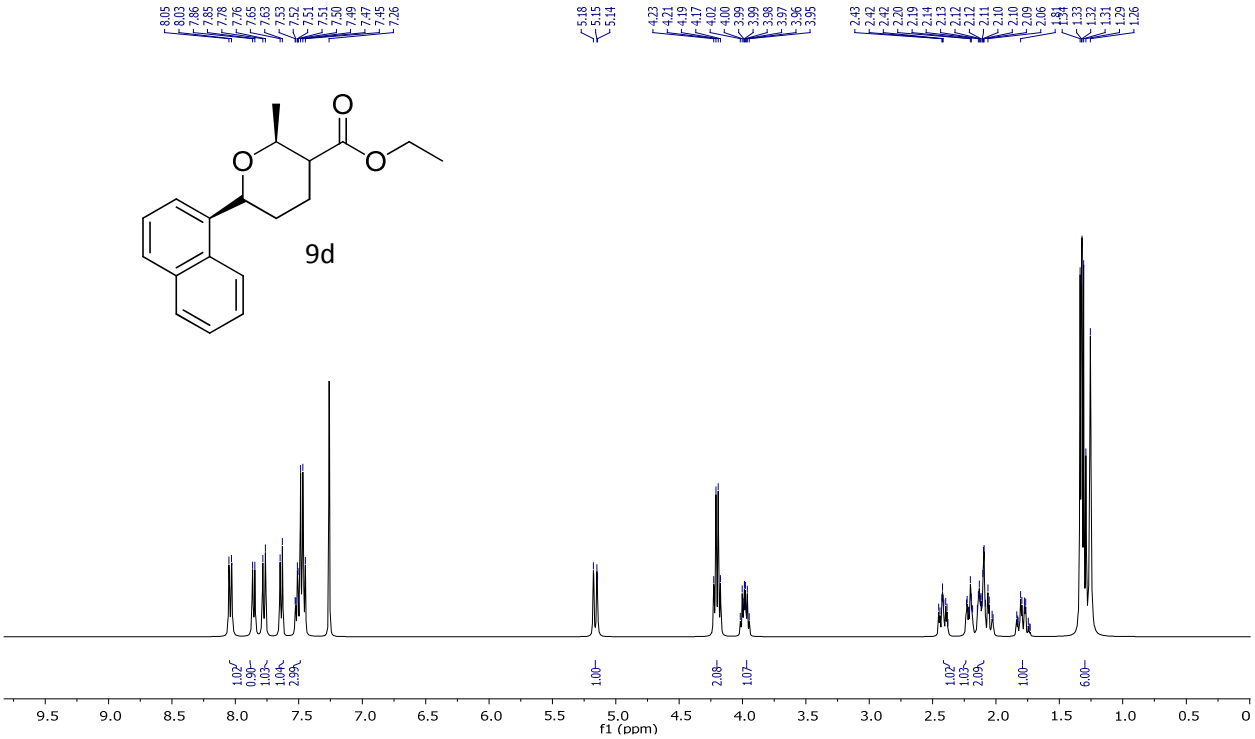
^{13}C NMR of compound (9c) (150 MHz, $CDCl_3$)



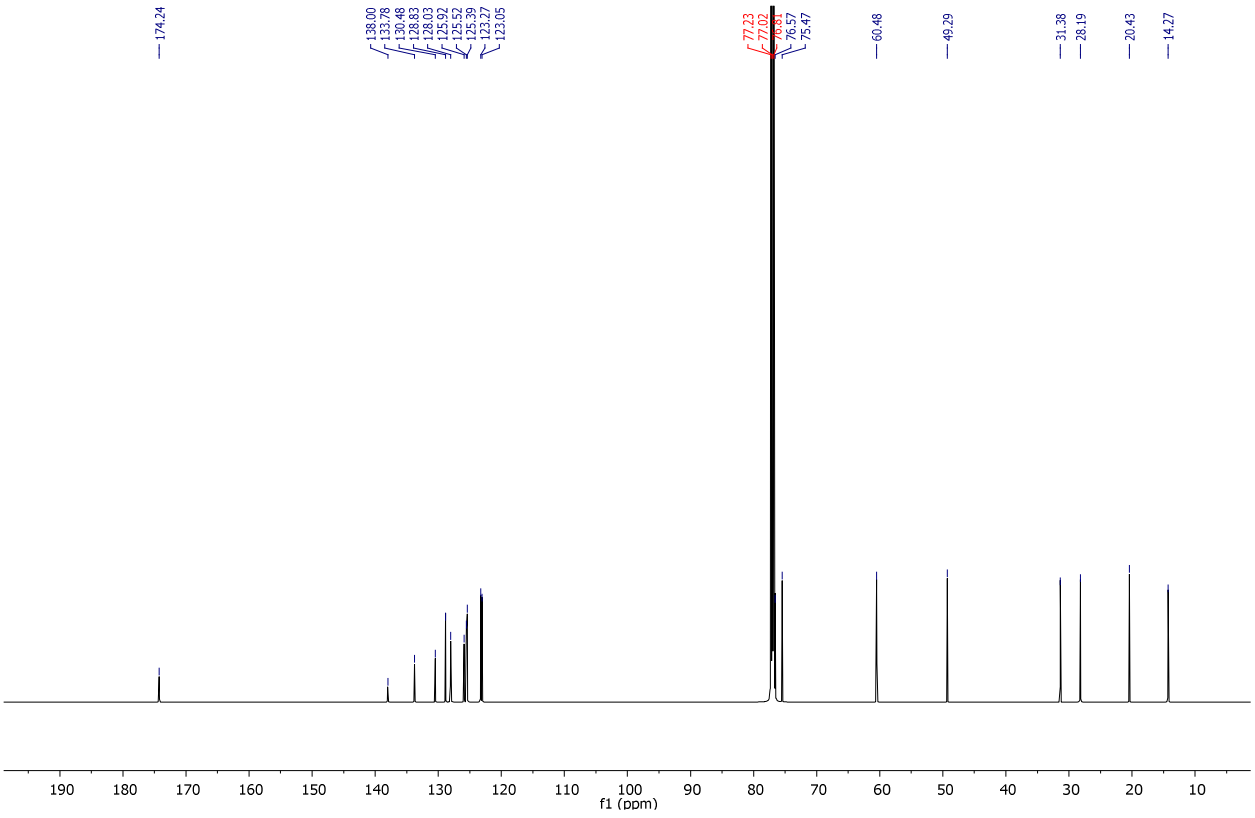
DEPT-135 of compound (9c) (150 MHz, $CDCl_3$)



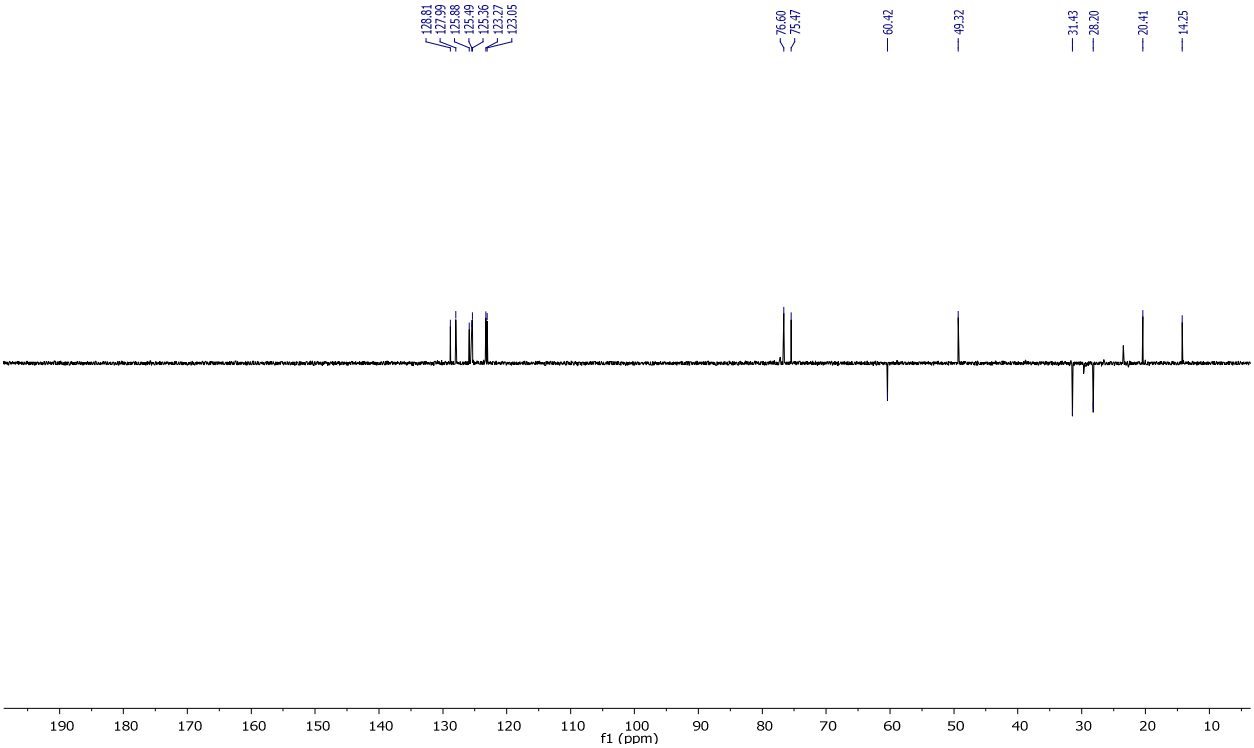
^{1}H NMR of compound (9d) (400 MHz, $CDCl_3$)



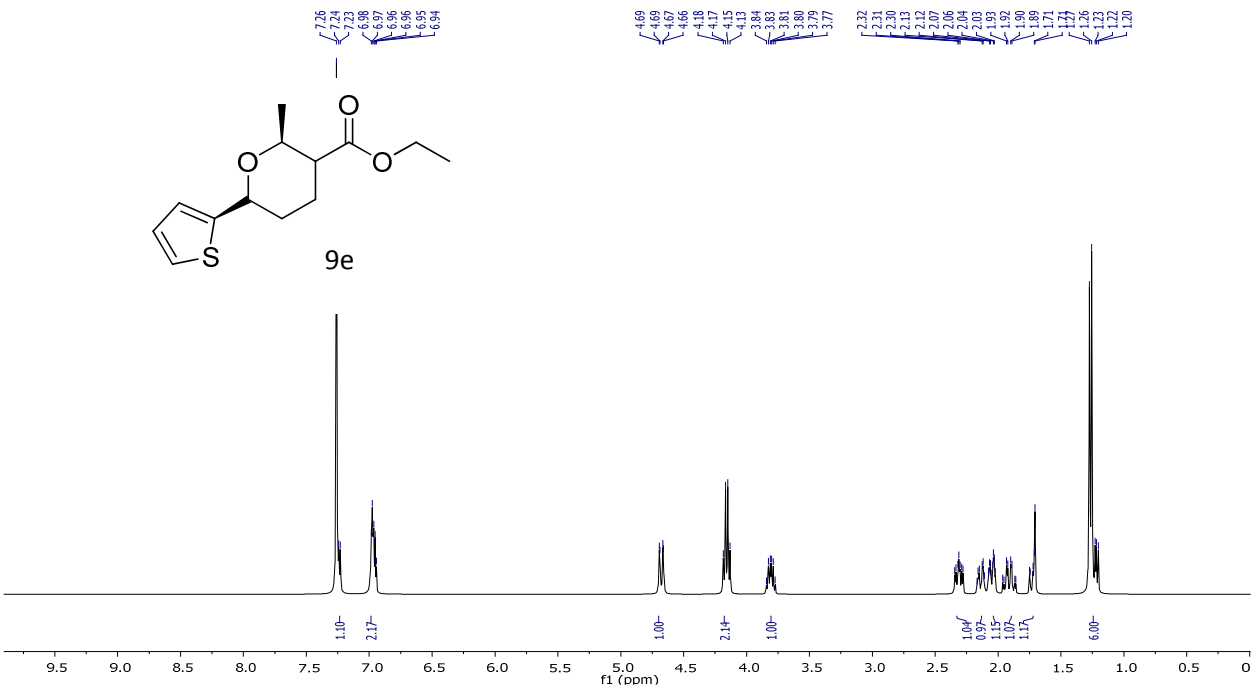
^{13}C NMR of compound (9d) (150 MHz, $CDCl_3$)



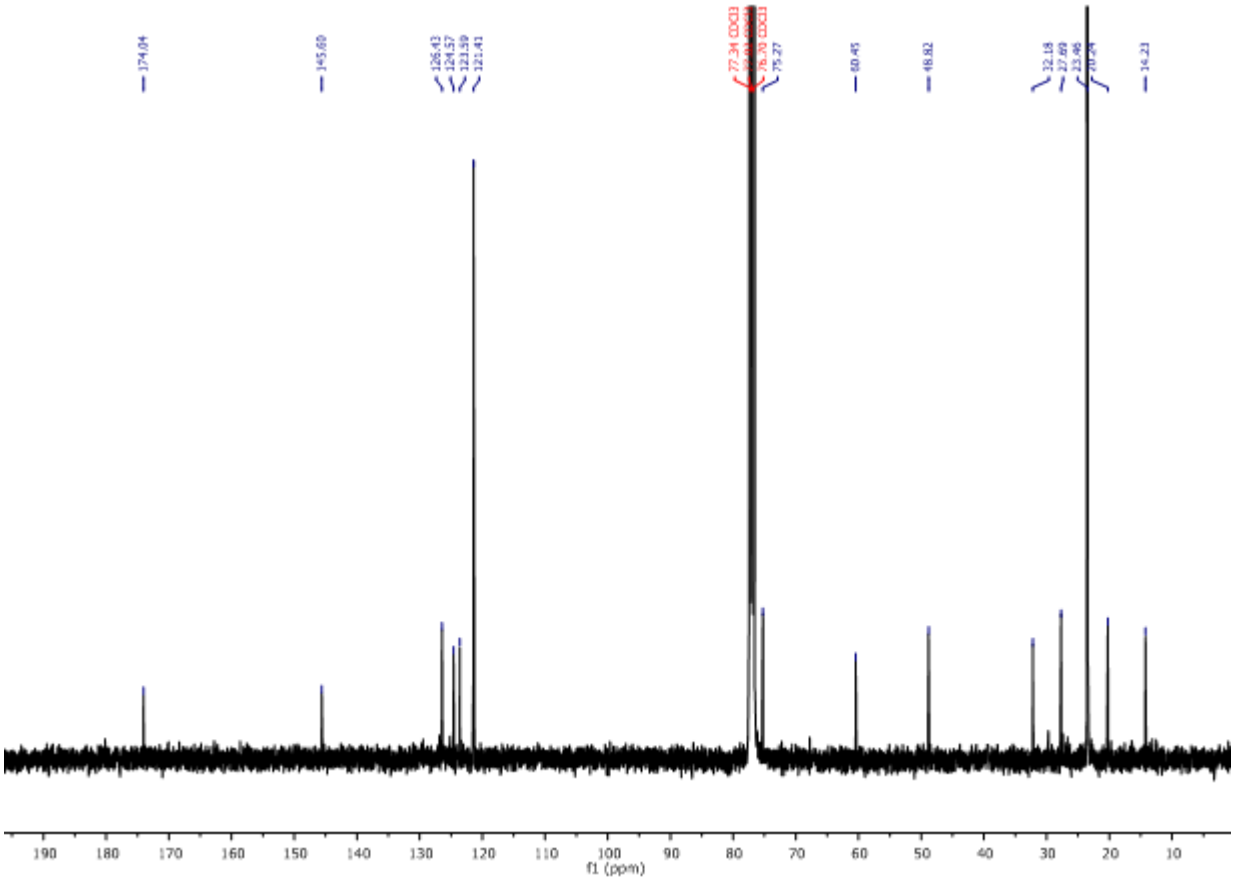
DEPT-135 of compound (9d) (150 MHz, $CDCl_3$)



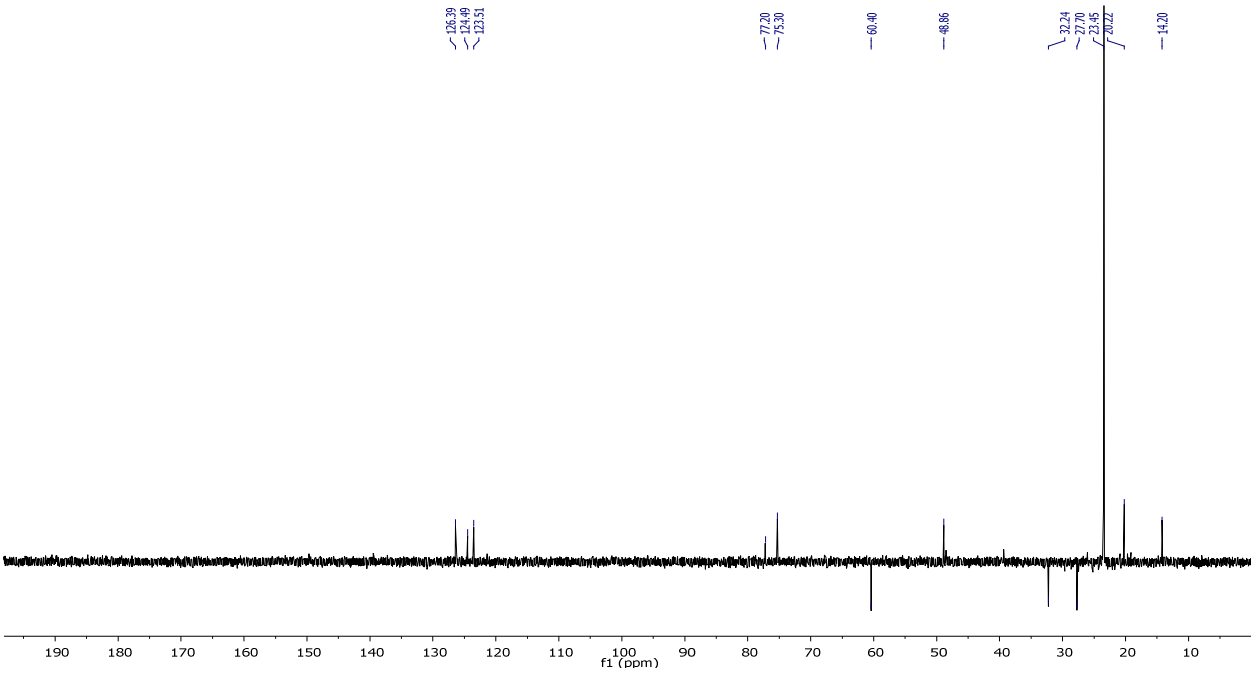
^{1}H NMR of compound (9e) (400 MHz, $CDCl_3$)



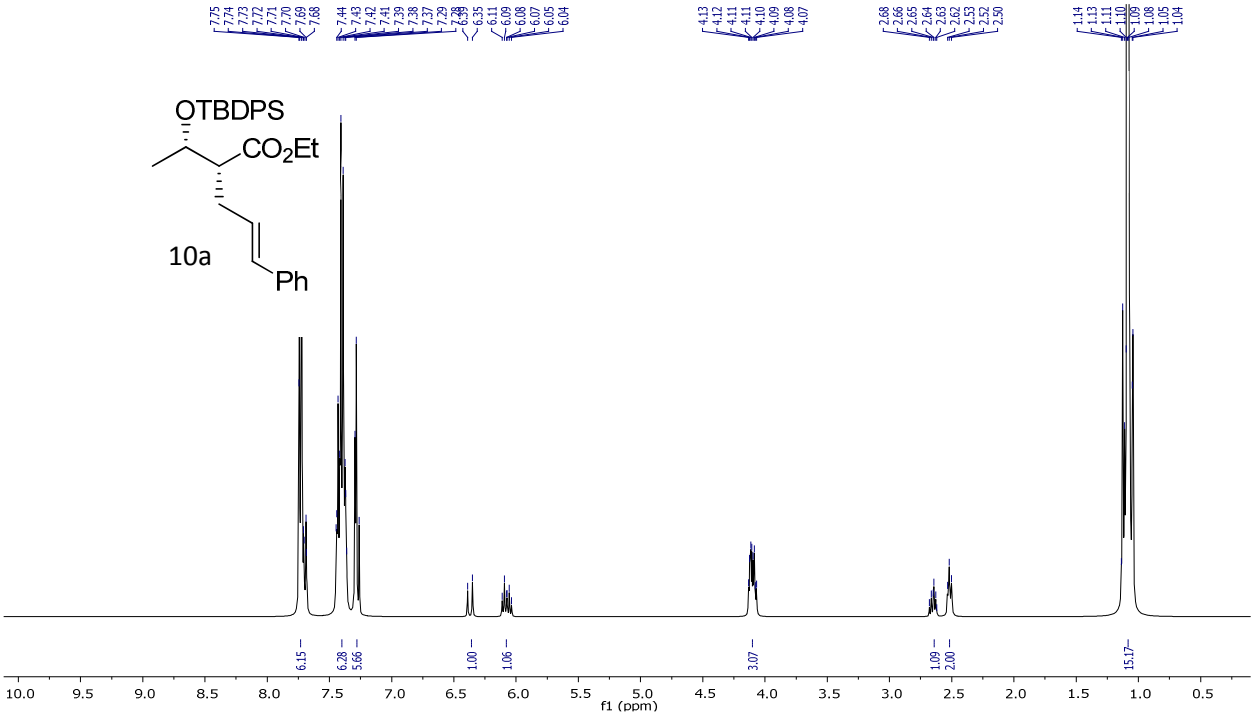
^{13}C NMR of compound (9e) (100 MHz, $CDCl_3$)



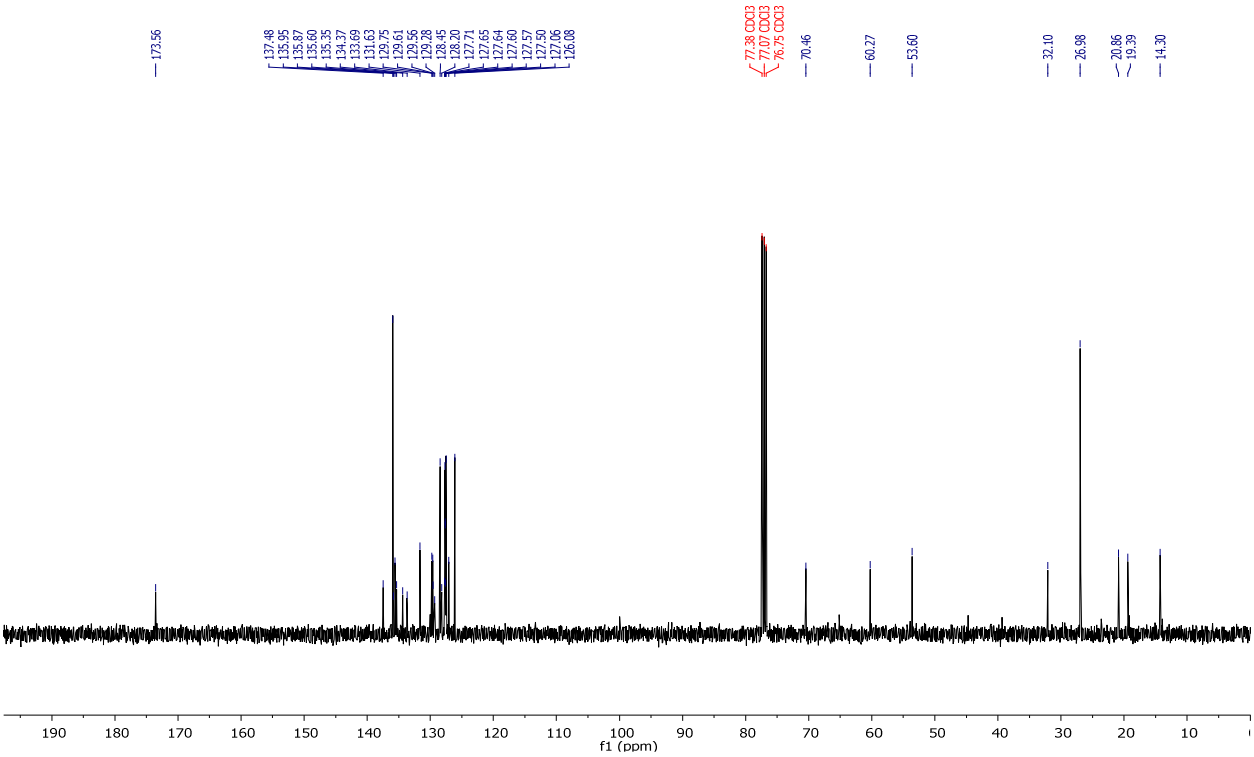
DEPT-135 of compound (9e) (150 MHz, $CDCl_3$)



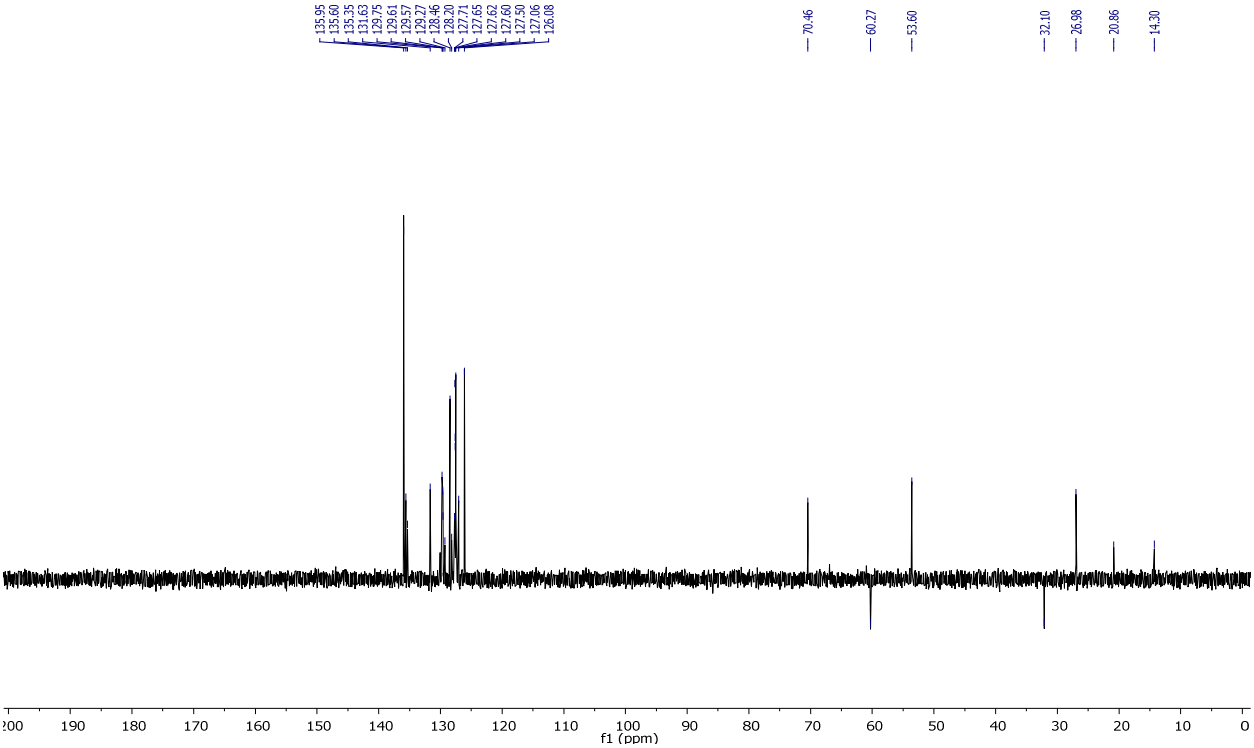
^{1}H NMR of compound (10a) (400 MHz, $CDCl_3$)



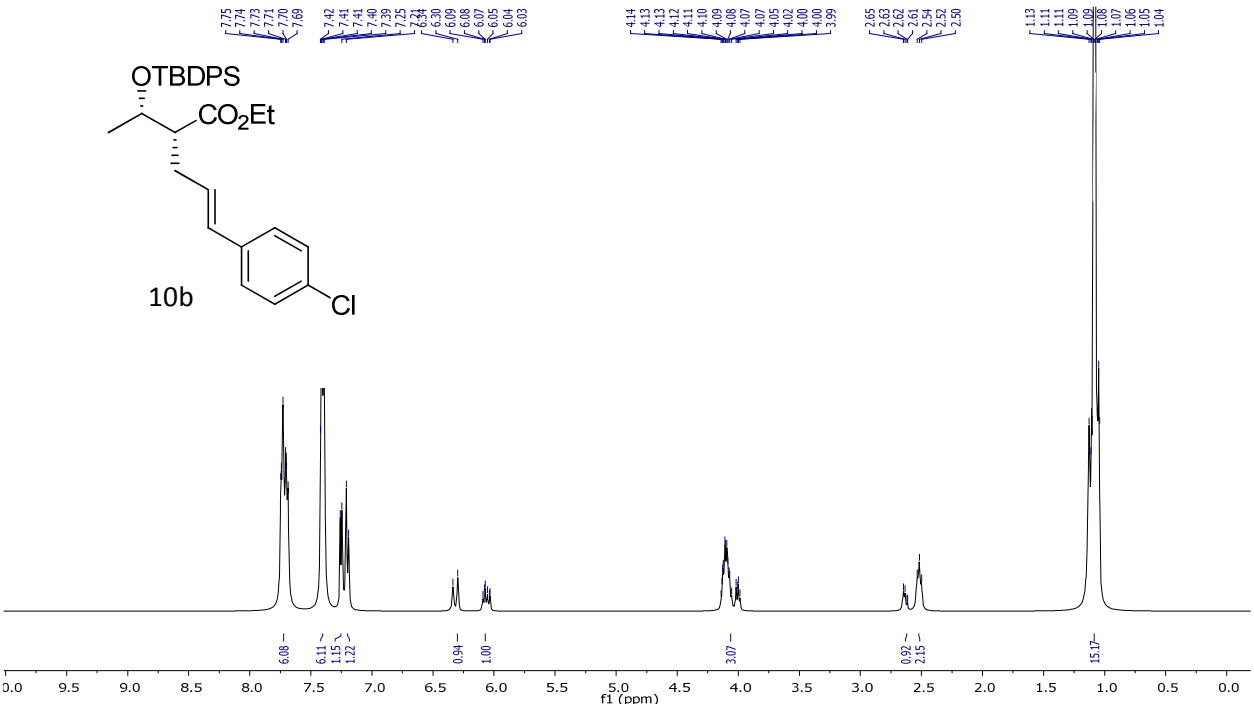
^{13}C NMR of compound (10a) (100 MHz, $CDCl_3$)



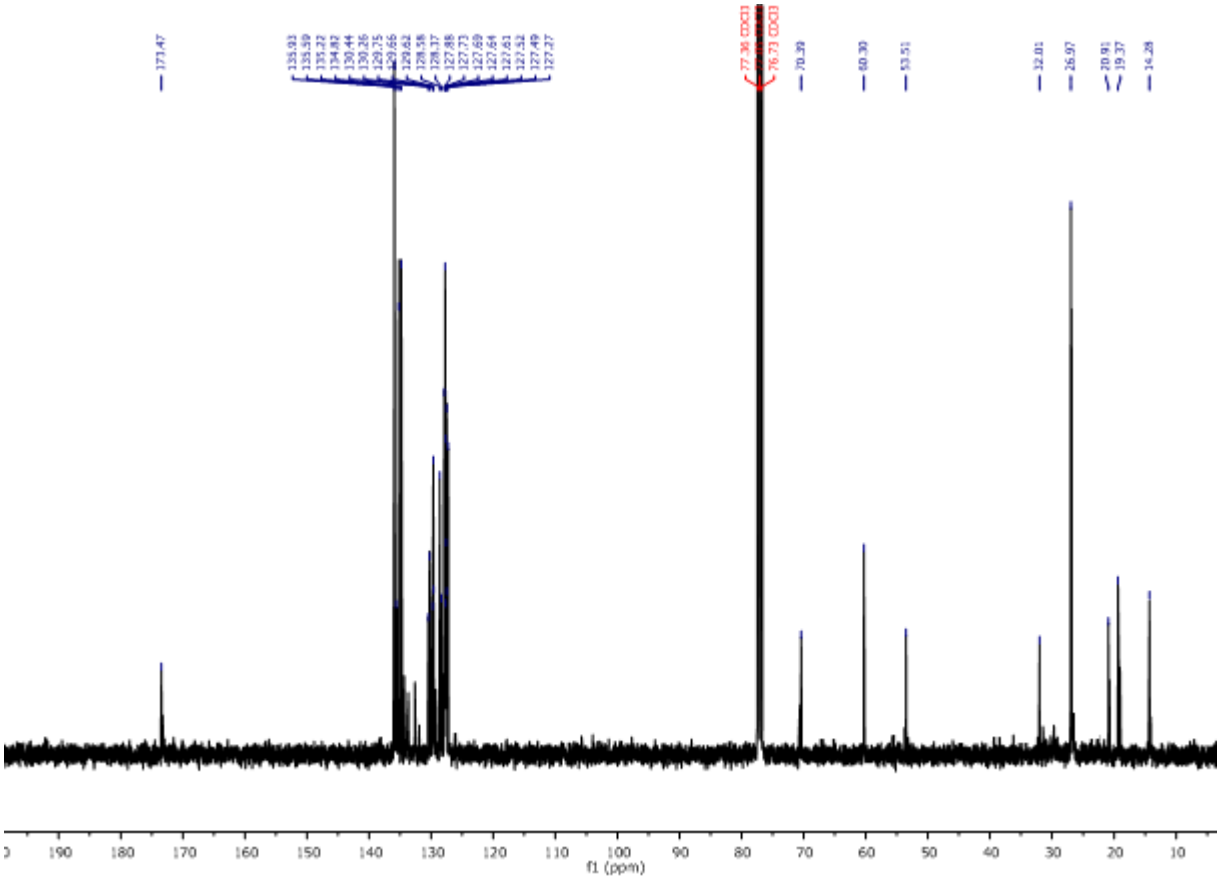
DEPT-135 of compound (10a) (100 MHz, $CDCl_3$)



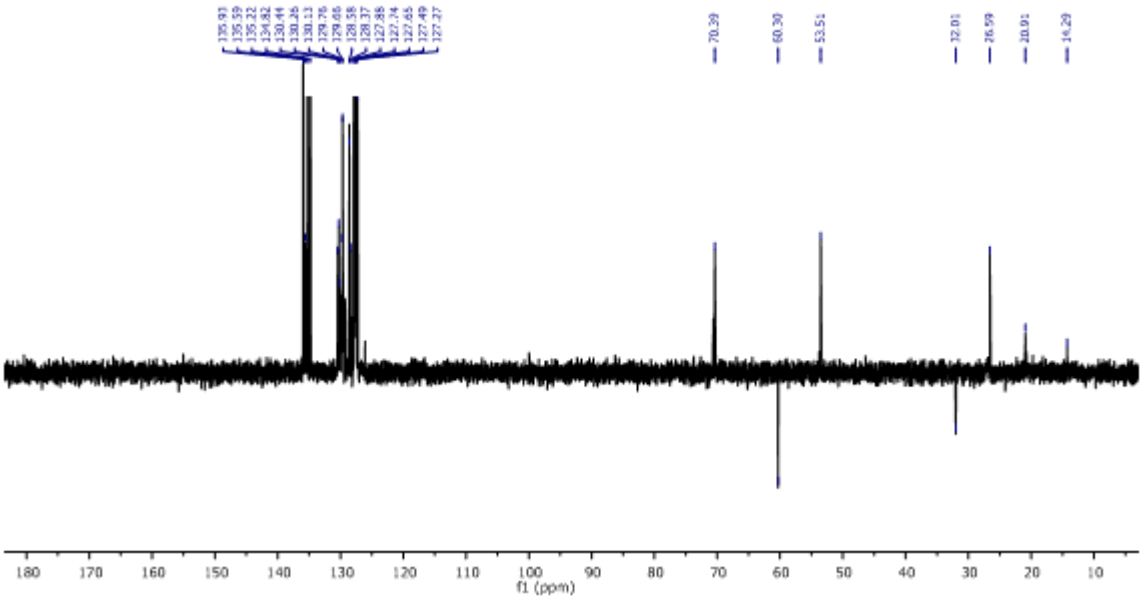
^{1}H NMR of compound (10b) (400 MHz, $CDCl_3$)



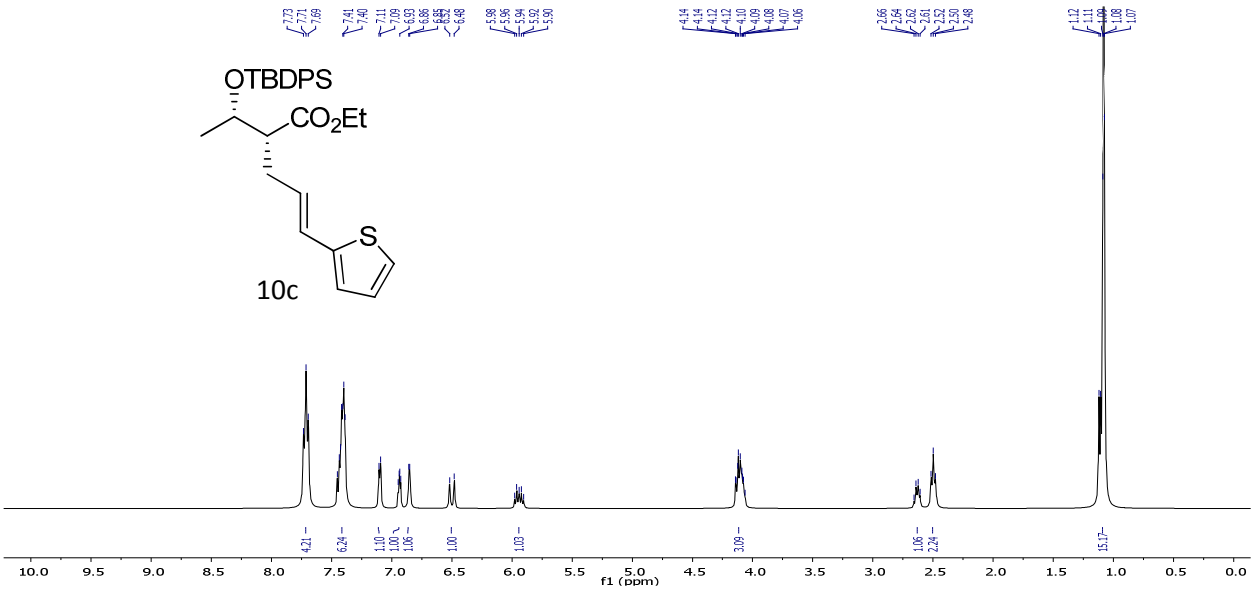
^{13}C NMR of compound (10b) (100 MHz, $CDCl_3$)



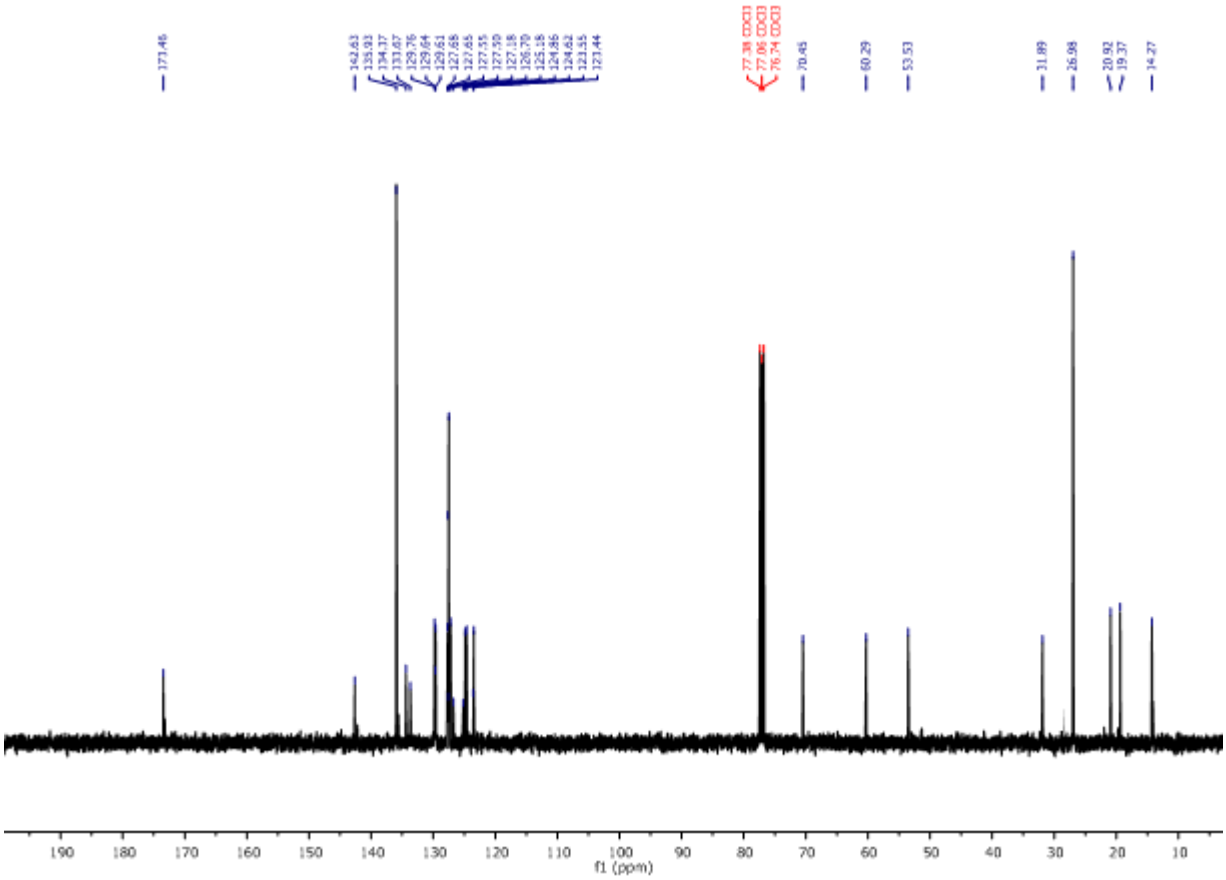
DEPT-135 of compound (10b) (100 MHz, $CDCl_3$)



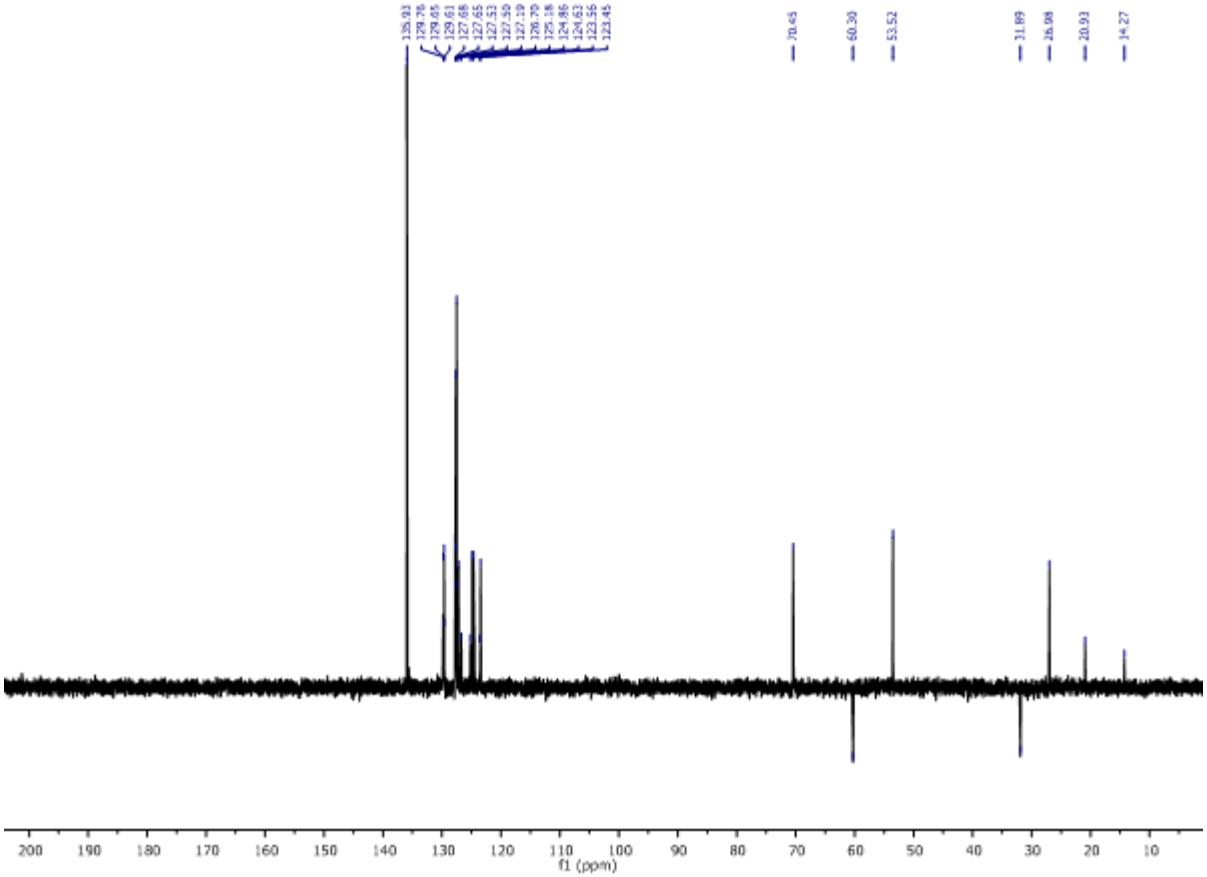
^{1}H NMR of compound (10c) (400 MHz, $CDCl_3$)



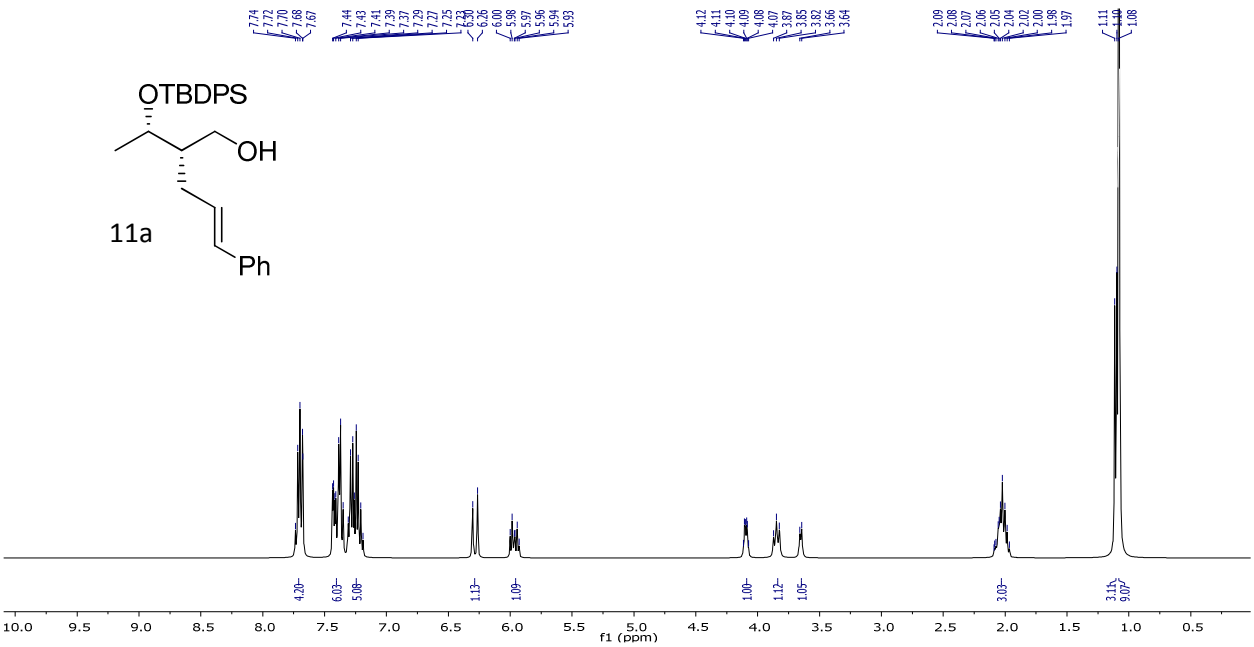
^{13}C NMR of compound (10c) (100 MHz, $CDCl_3$)



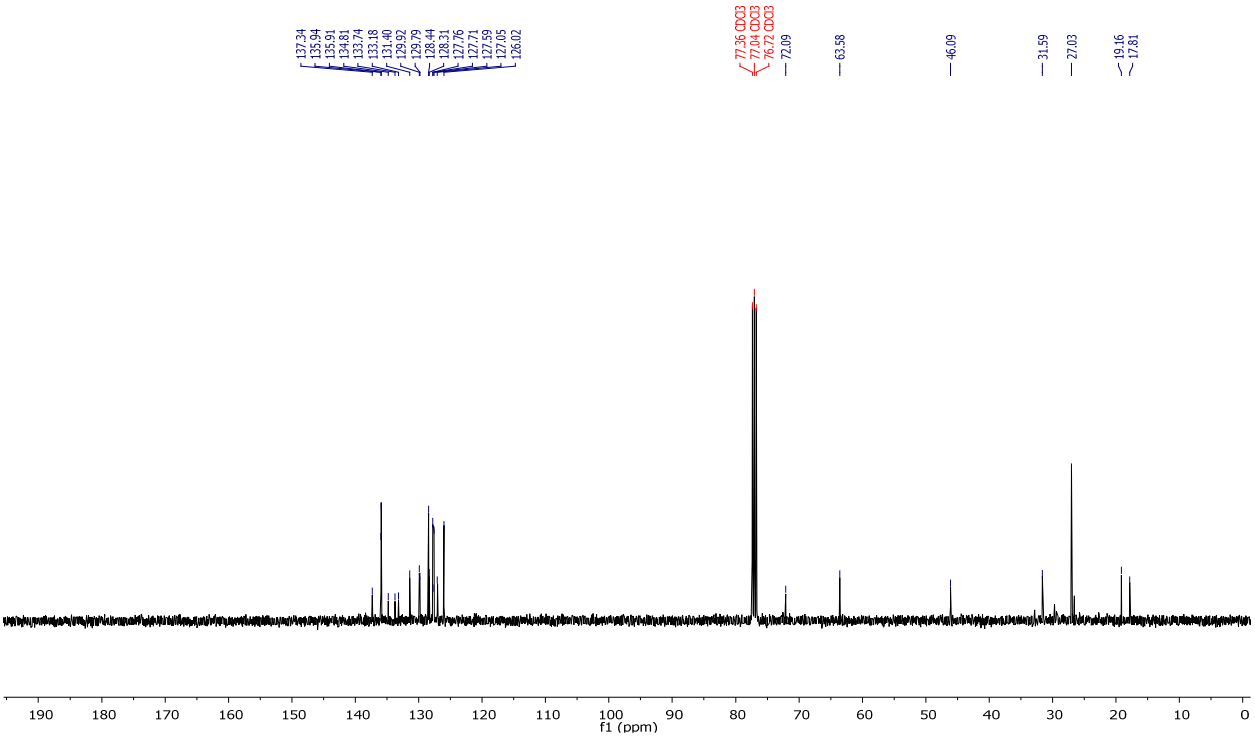
DEPT-135 of compound (10c) (100 MHz, $CDCl_3$)



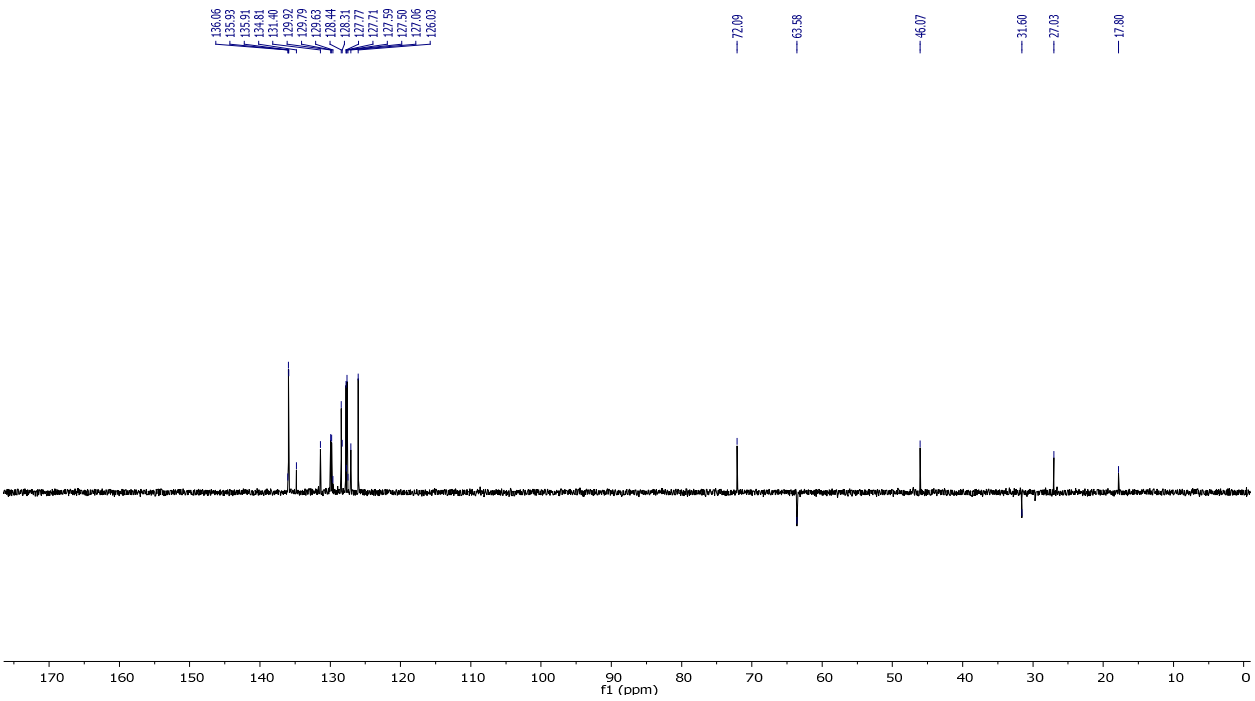
^{1}H NMR of compound (11a) (400 MHz, $CDCl_3$)



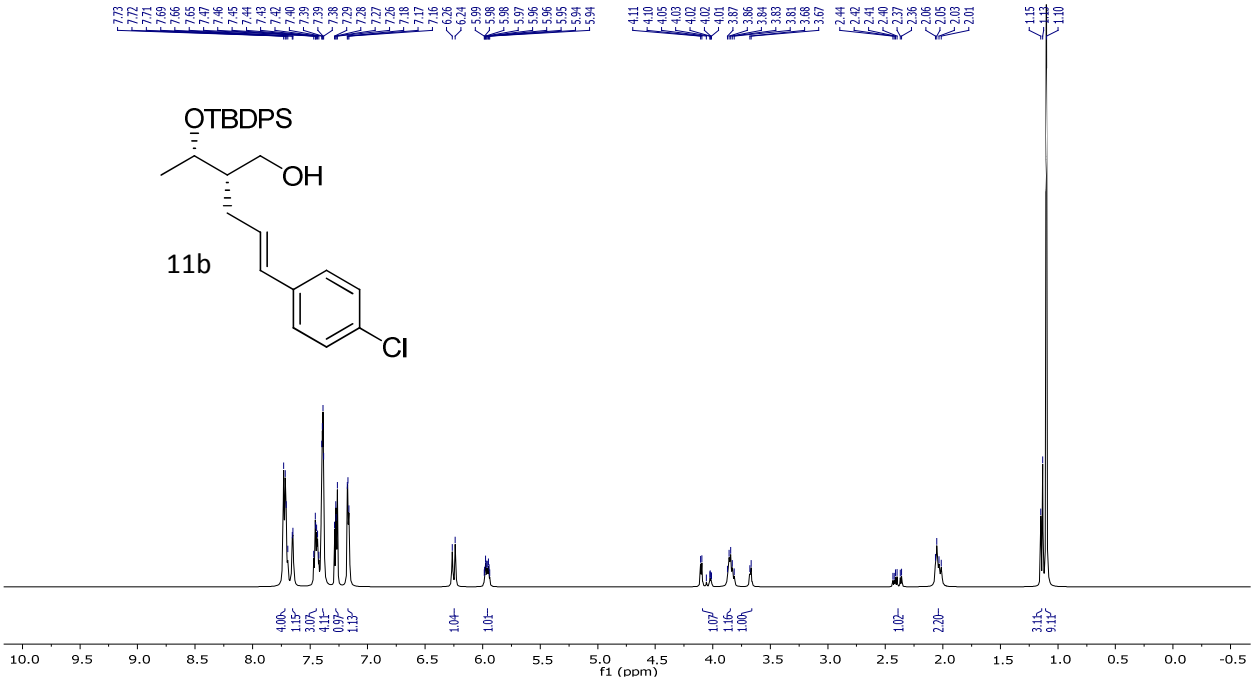
^{13}C NMR of compound (11a) (100 MHz, $CDCl_3$)



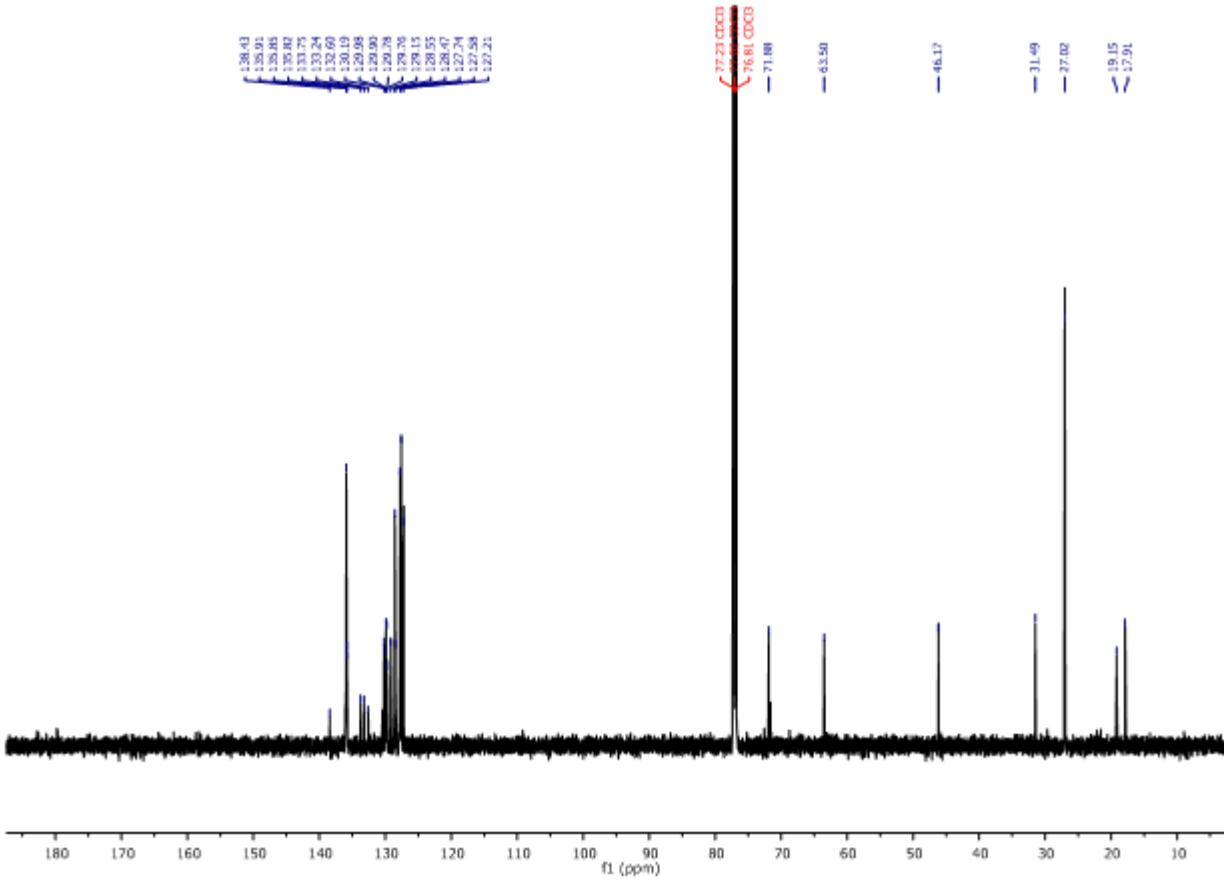
DEPT-135 of compound (11a) (100 MHz, $CDCl_3$)



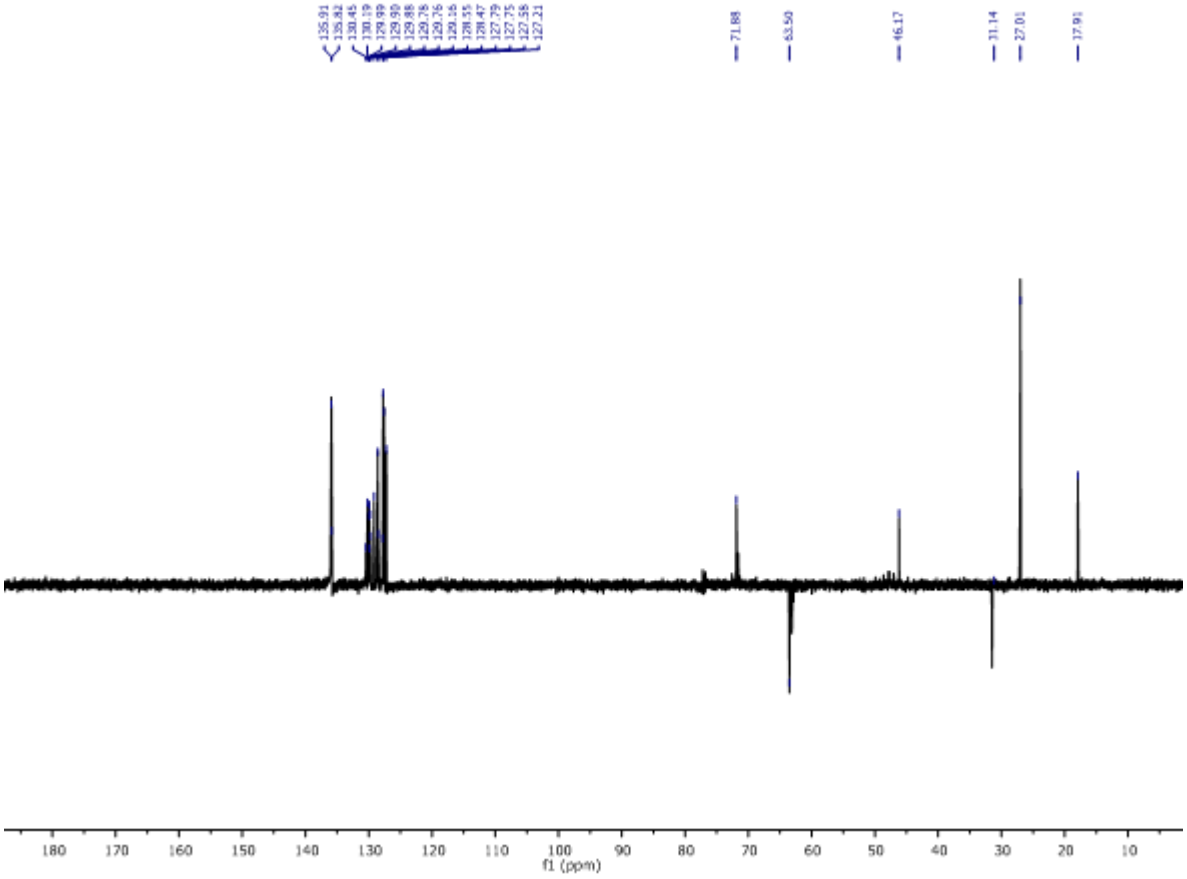
^{1}H NMR of compound (11b) (600 MHz, $CDCl_3$)



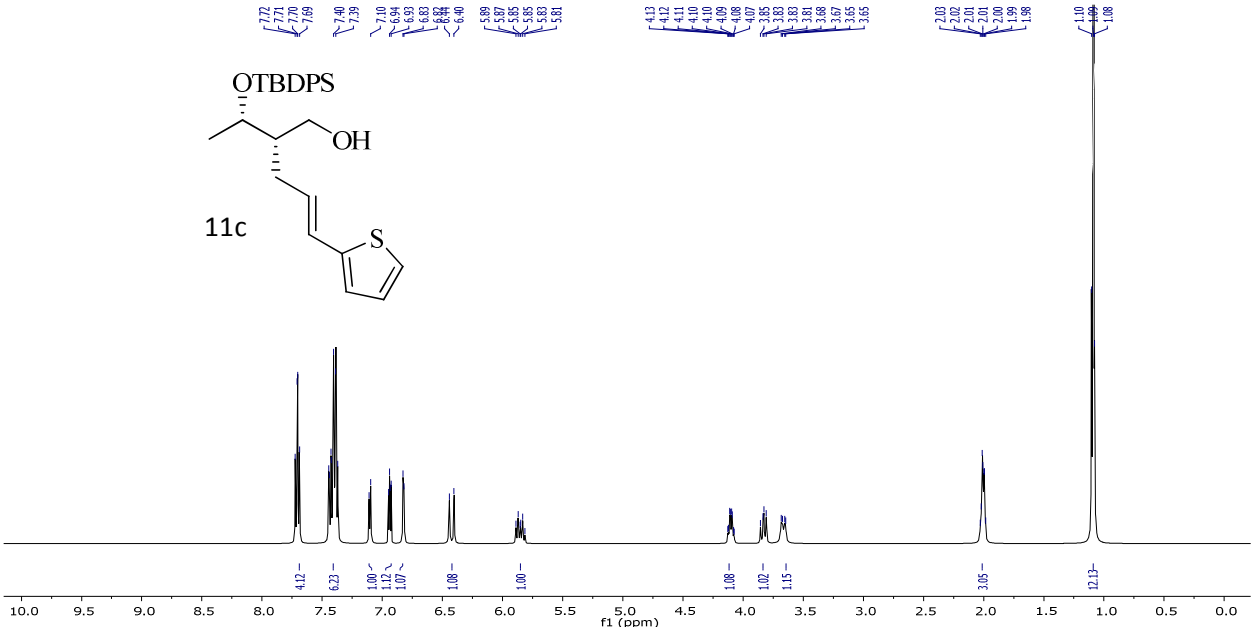
^{13}C NMR of compound (11b) (150 MHz, $CDCl_3$)



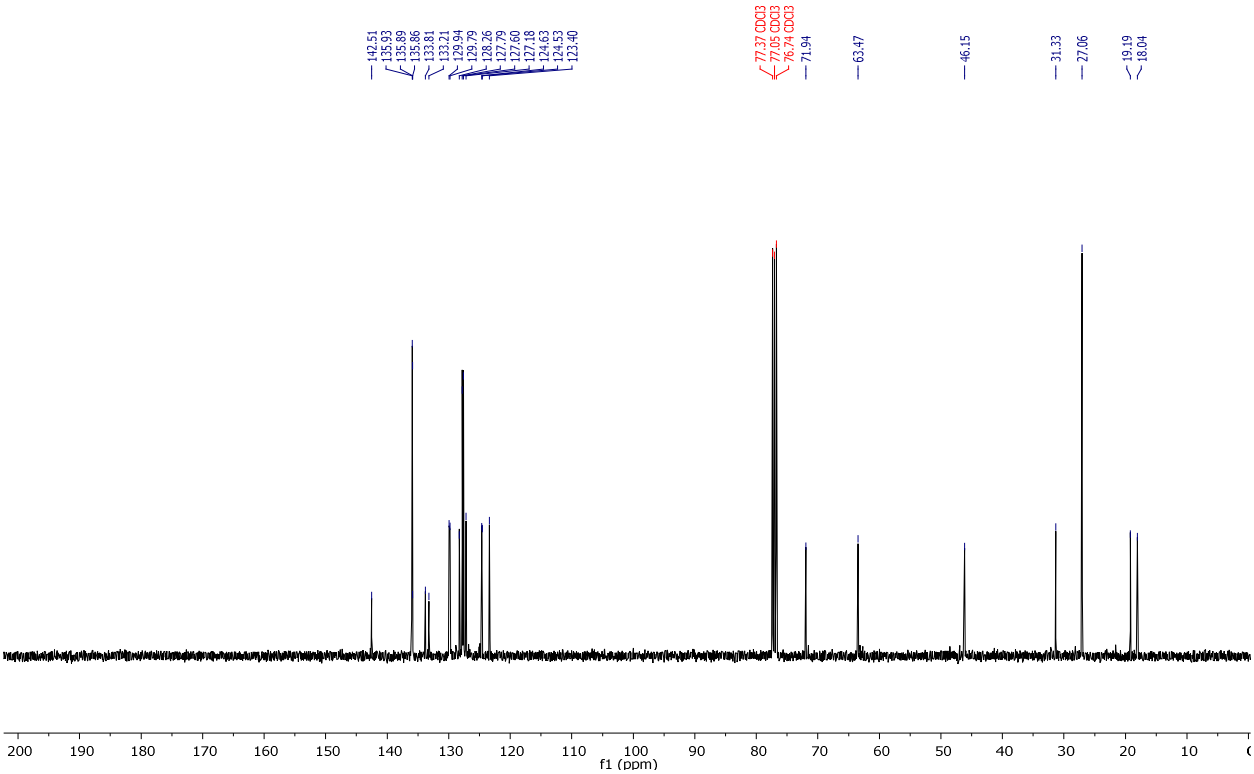
DEPT-135 of compound (11b) (150 MHz, $CDCl_3$)



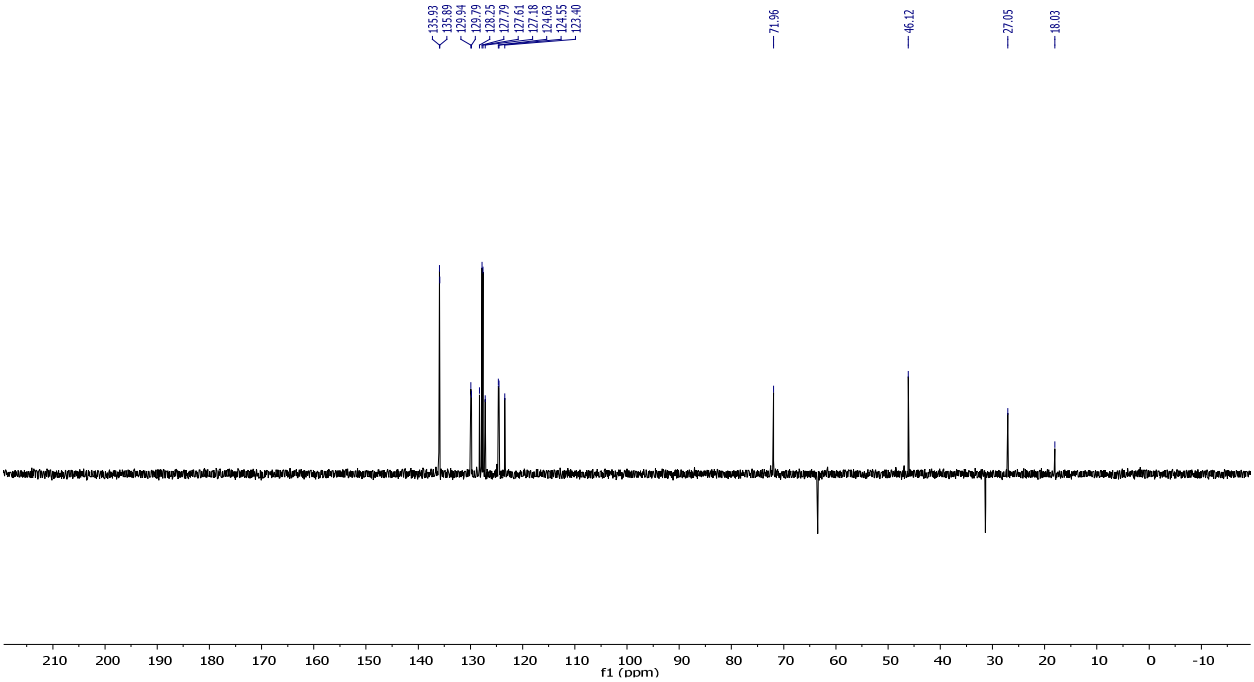
^{1}H NMR of compound (11c) (400 MHz, $CDCl_3$)



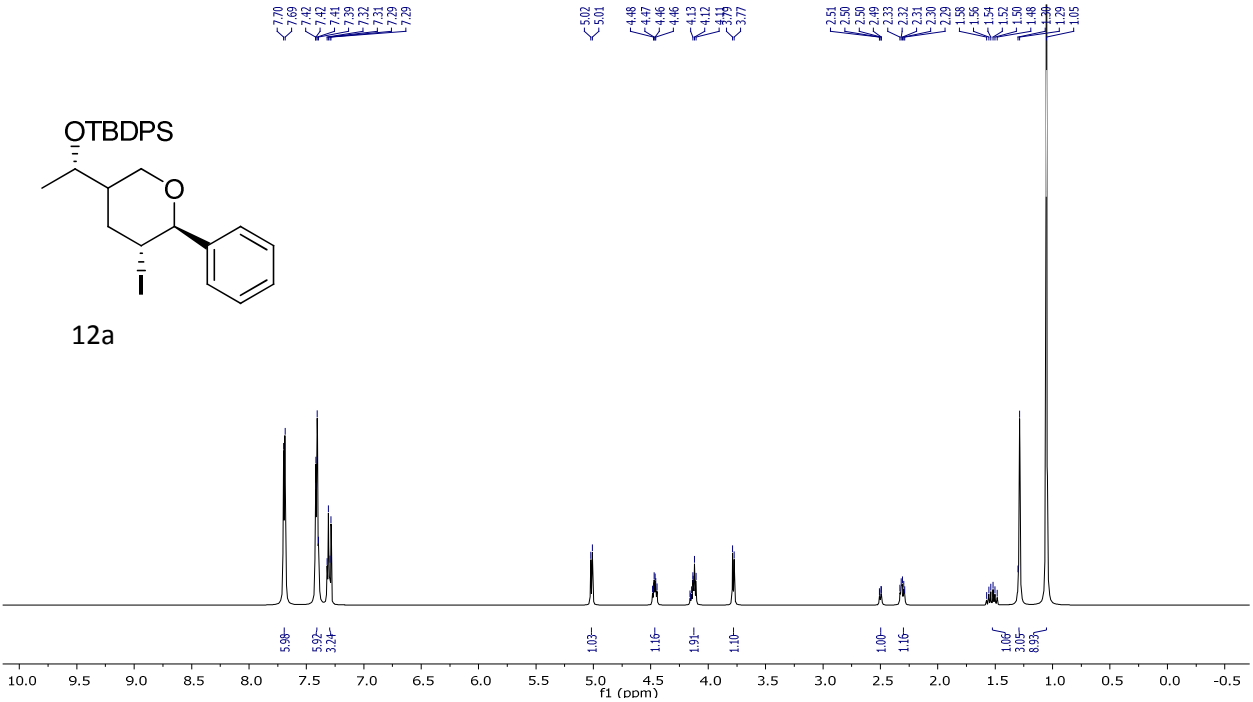
^{13}C NMR of compound (11c) (100 MHz, $CDCl_3$)



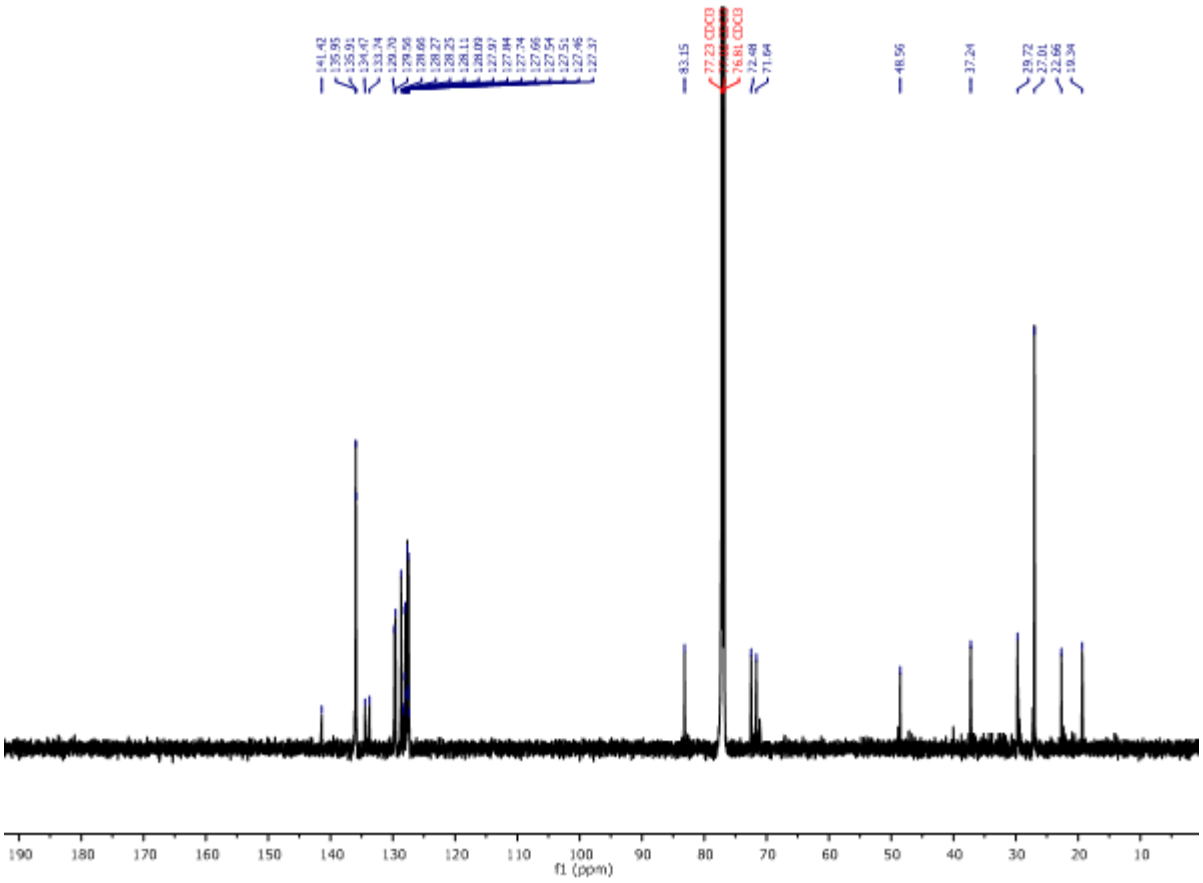
DEPT-135 of compound (11c) (100 MHz, $CDCl_3$)



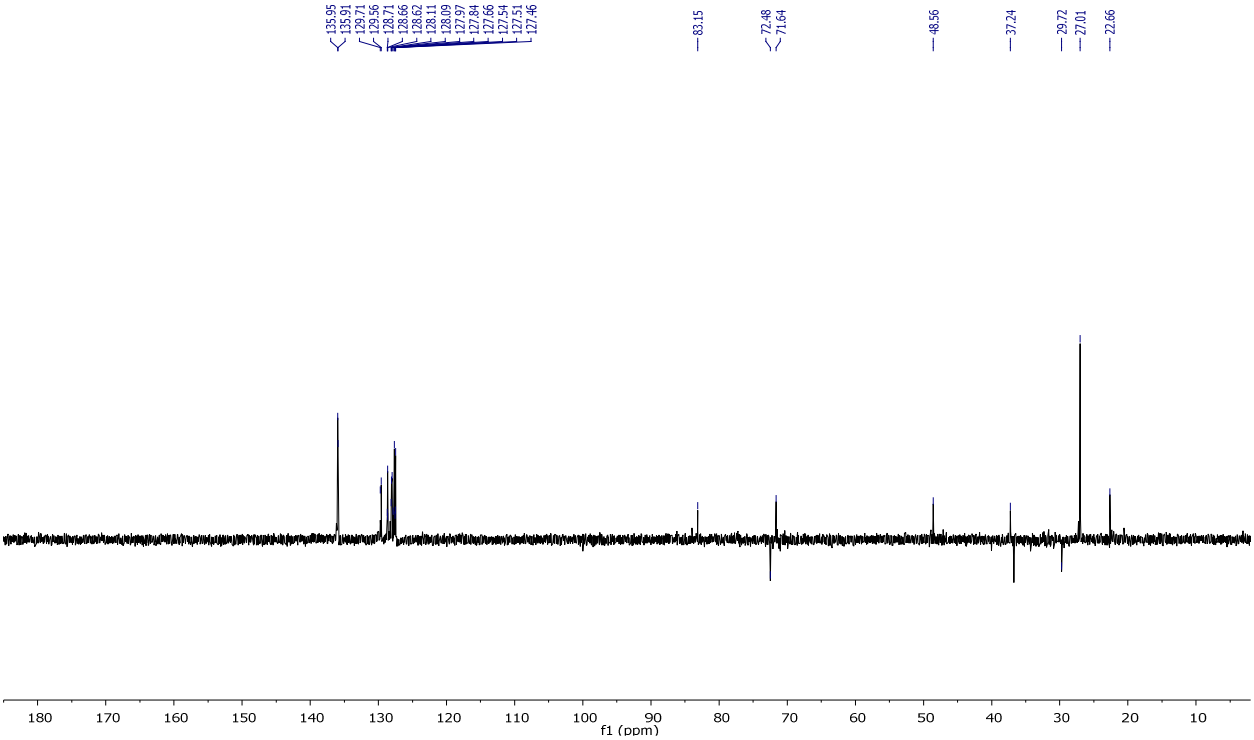
^{1}H NMR of compound (12a) (600 MHz, $CDCl_3$)



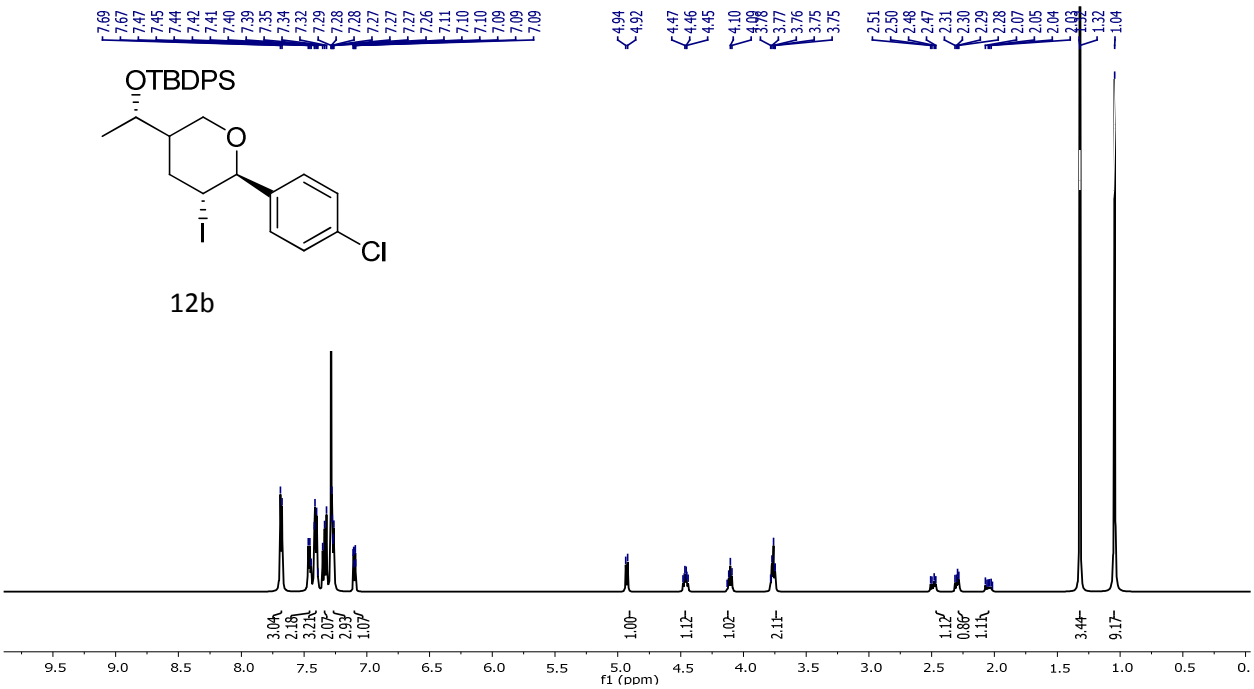
^{13}C NMR of compound (12a) (150 MHz, $CDCl_3$)



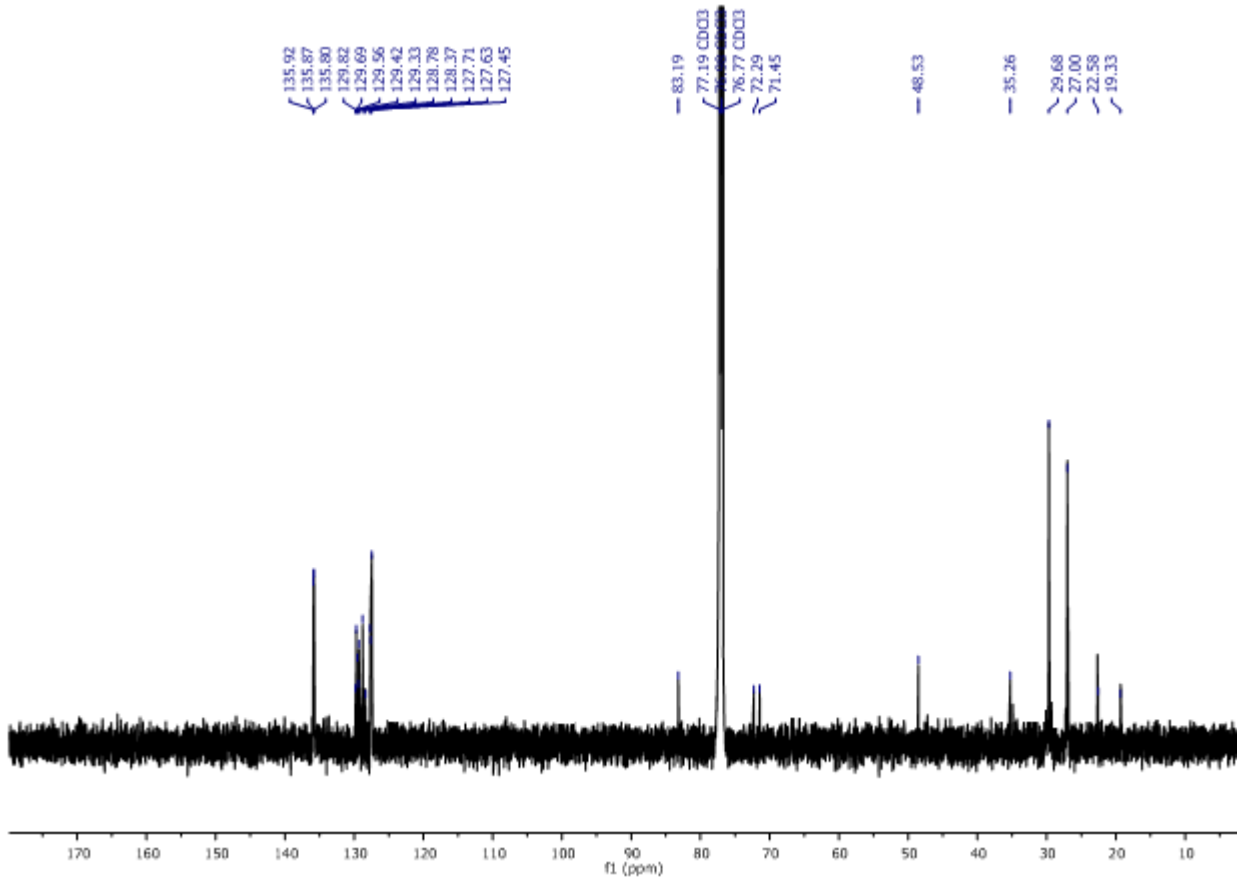
DEPT-135 of compound (12a) (150 MHz, $CDCl_3$)



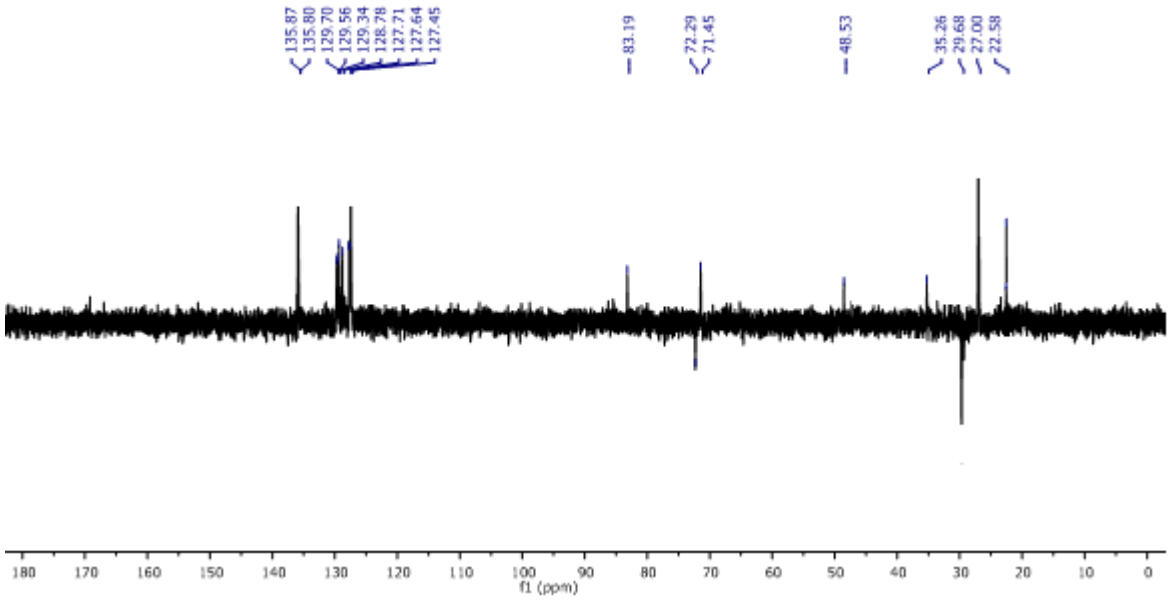
^{1}H NMR of compound (12b) (600 MHz, $CDCl_3$)



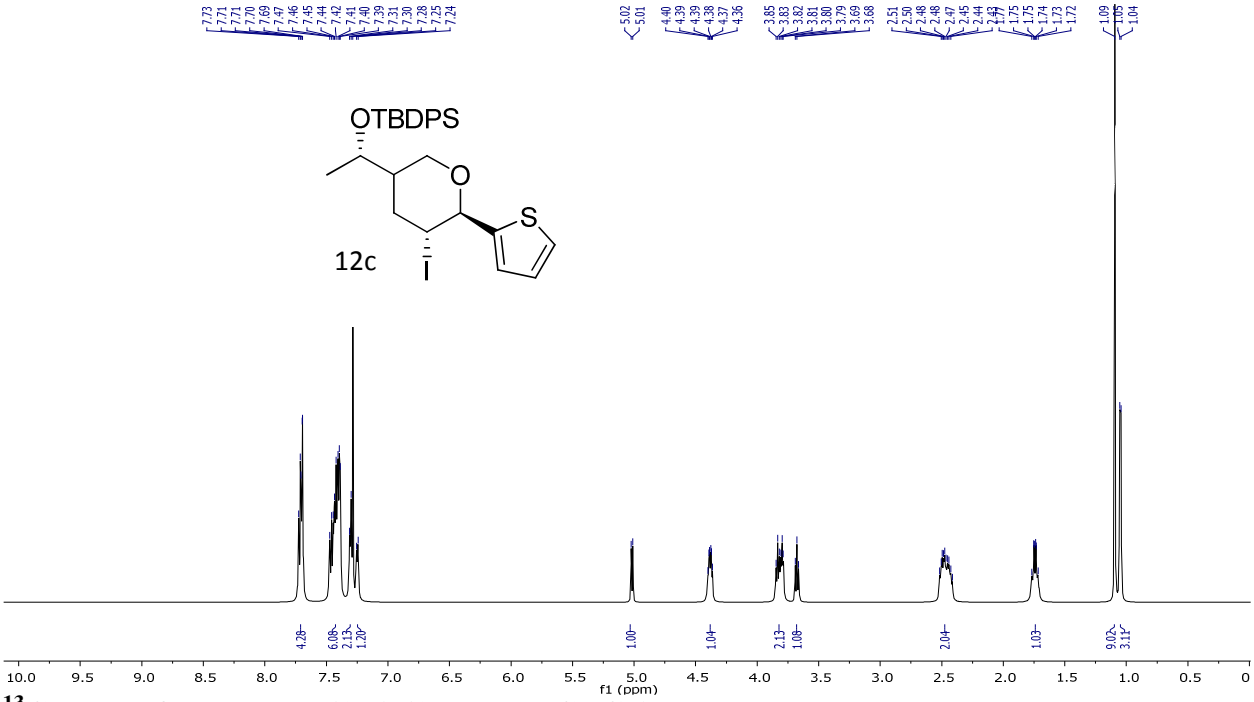
^{13}C NMR of compound (12b) (150 MHz, $CDCl_3$)



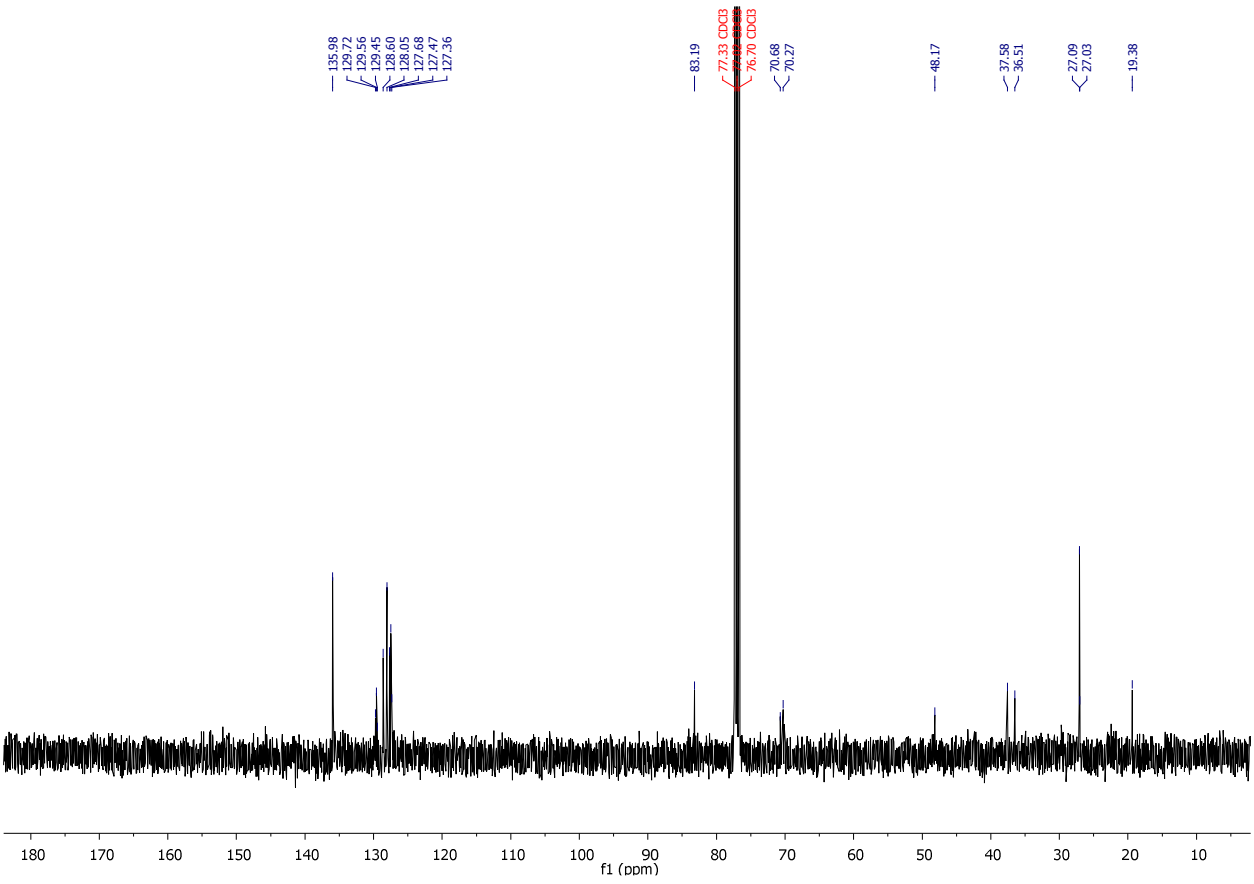
DEPT-135 of compound (12b) (150 MHz, $CDCl_3$)



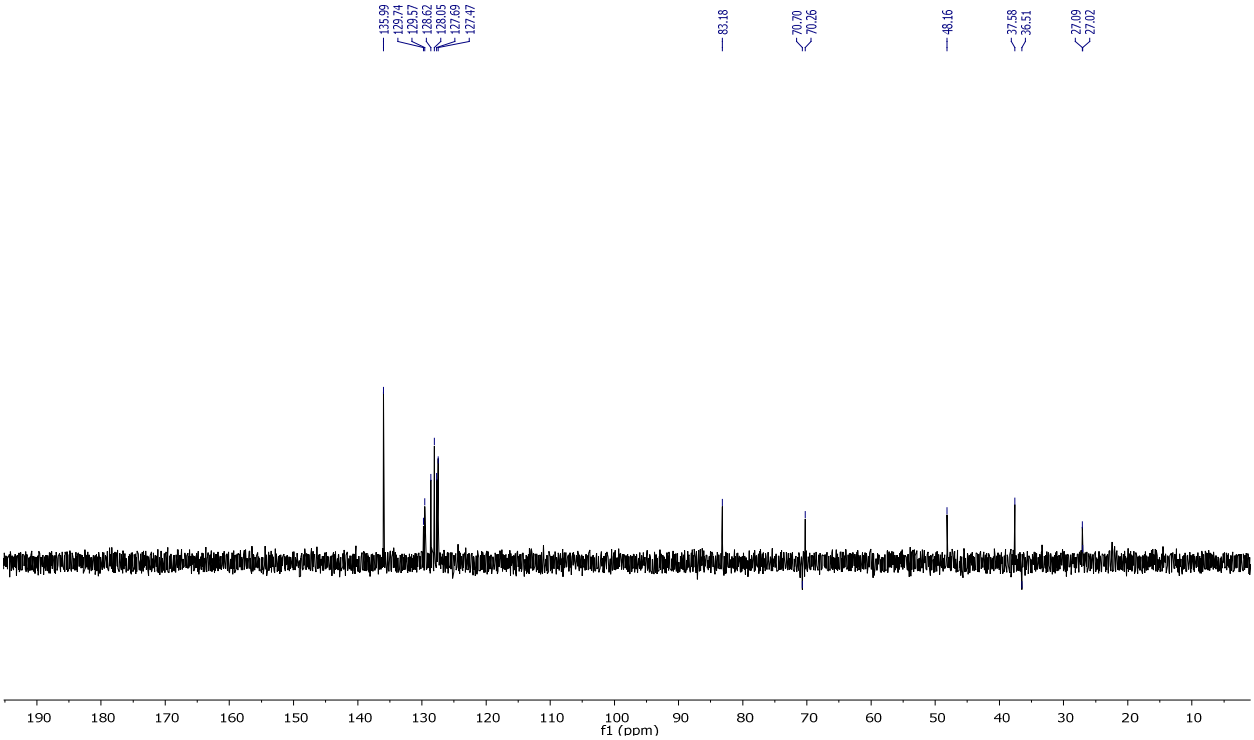
^{1}H NMR of compound (12c) (600 MHz, $CDCl_3$)



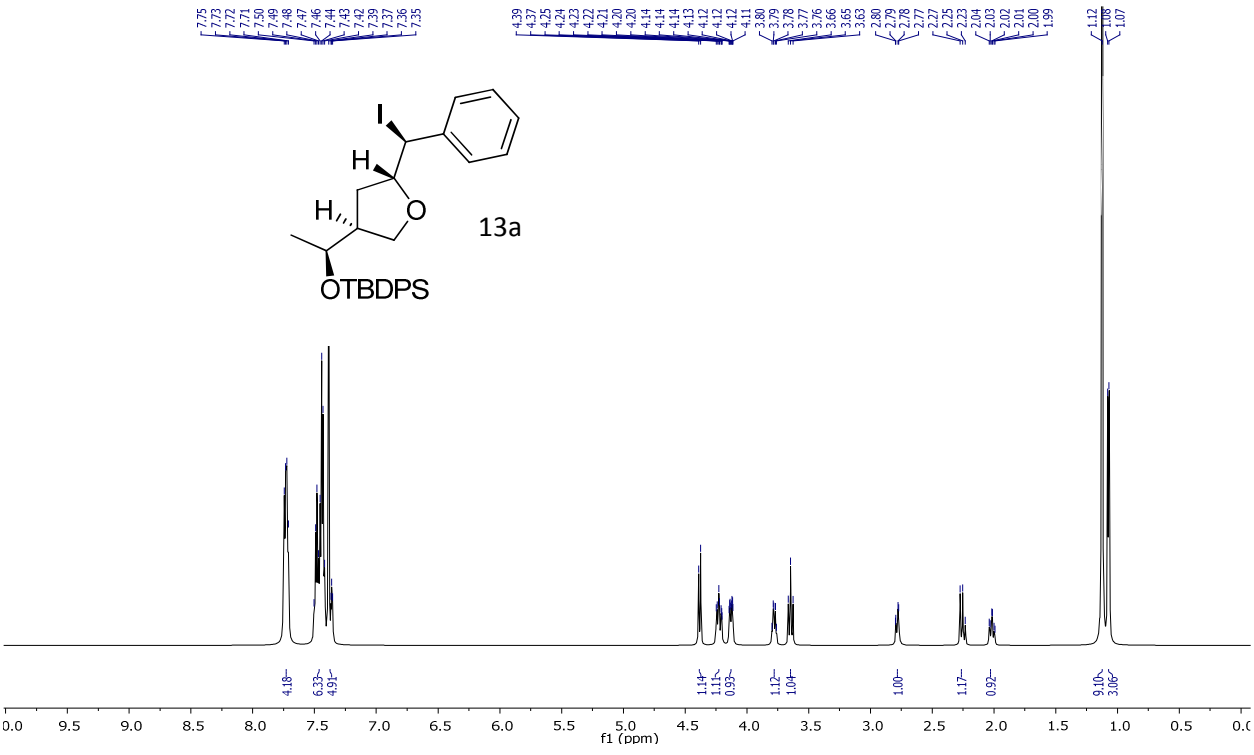
^{13}C NMR of compound (12c) (100 MHz, $CDCl_3$)



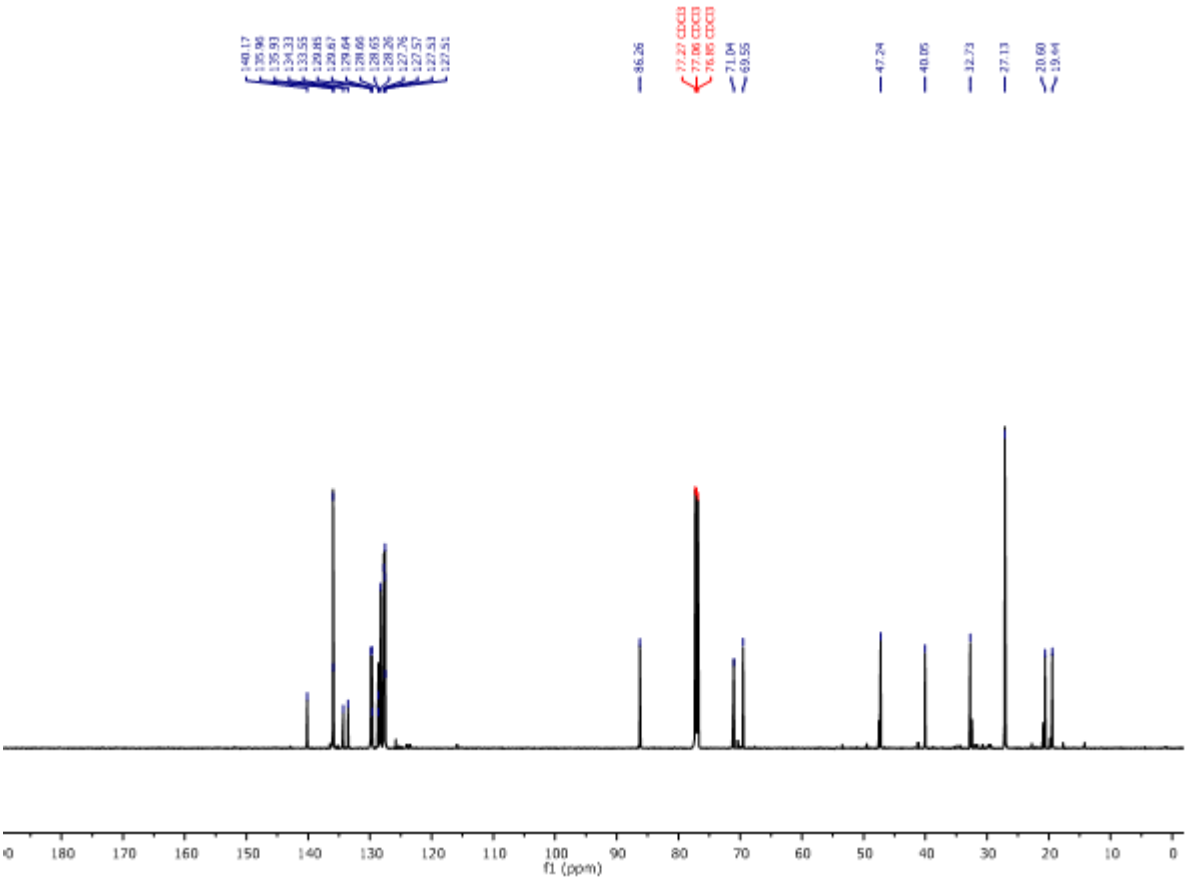
DEPT-135 of compound (12c) (100 MHz, $CDCl_3$)



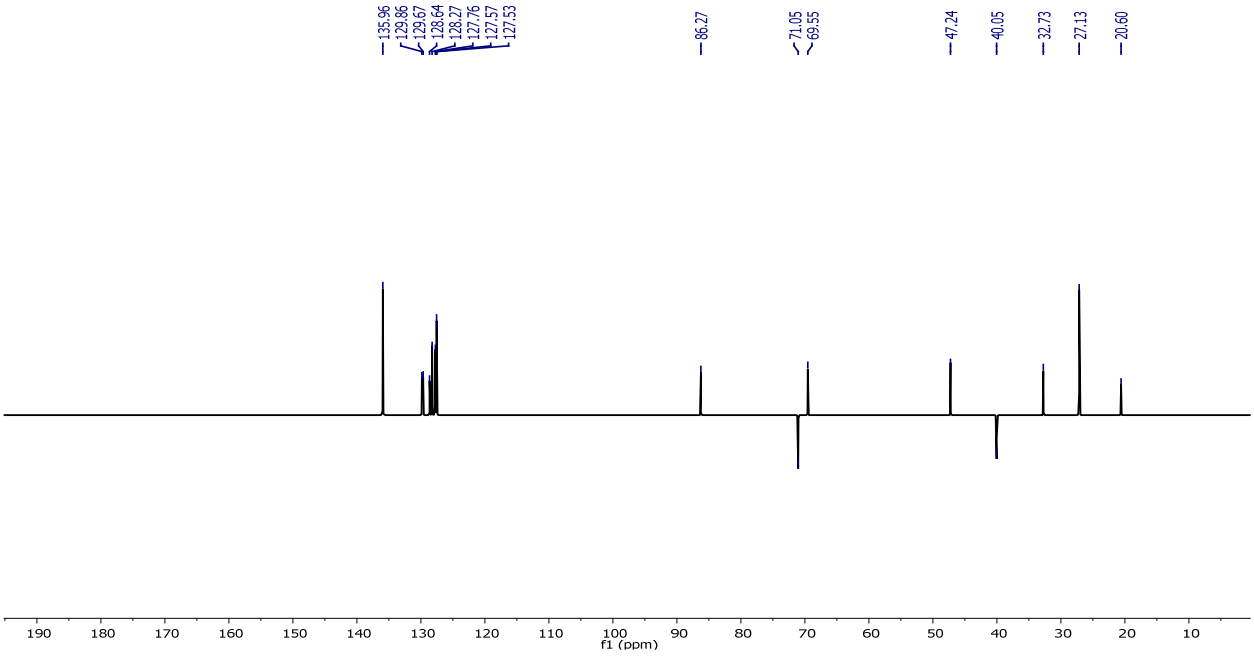
^{1}H NMR of compound (13a) (600 MHz, $CDCl_3$)



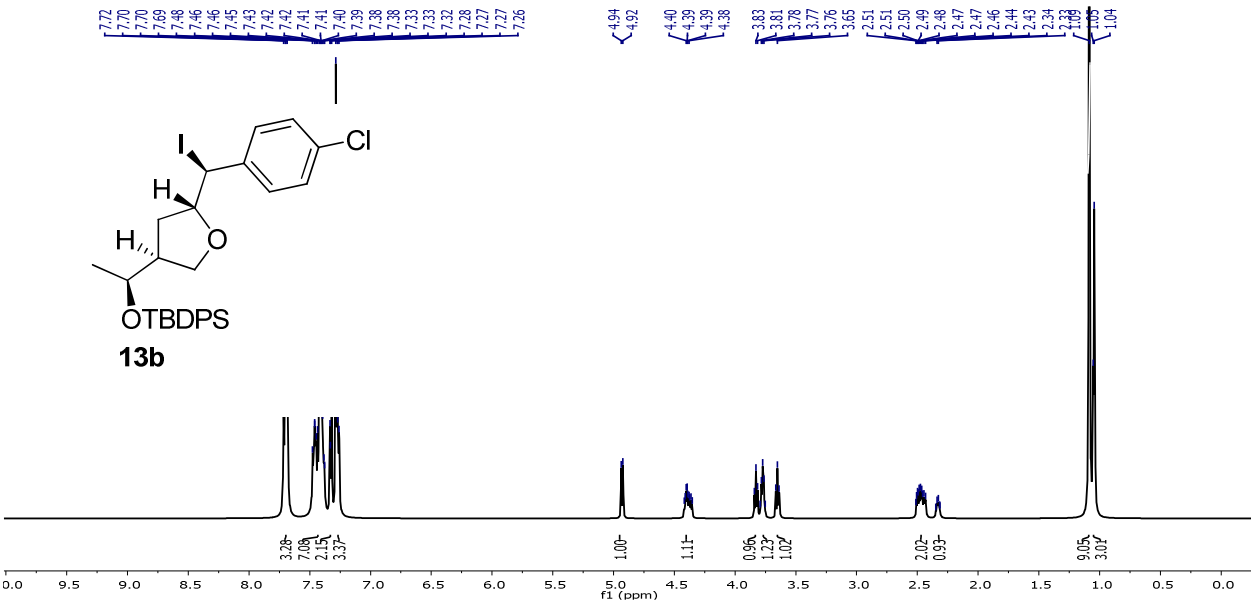
^{13}C NMR of compound (13a) (150 MHz, $CDCl_3$)



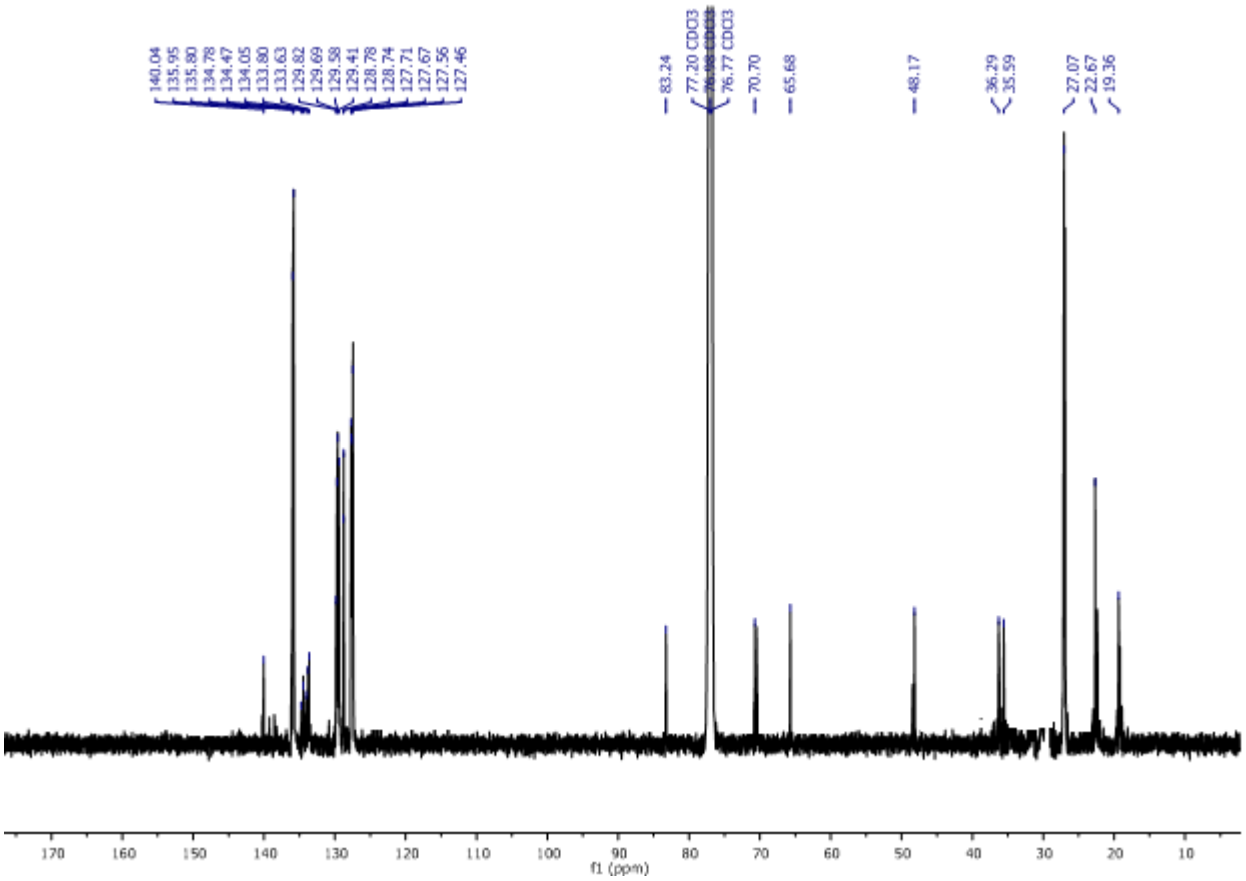
DEPT-135 of compound (13a) (150 MHz, $CDCl_3$)



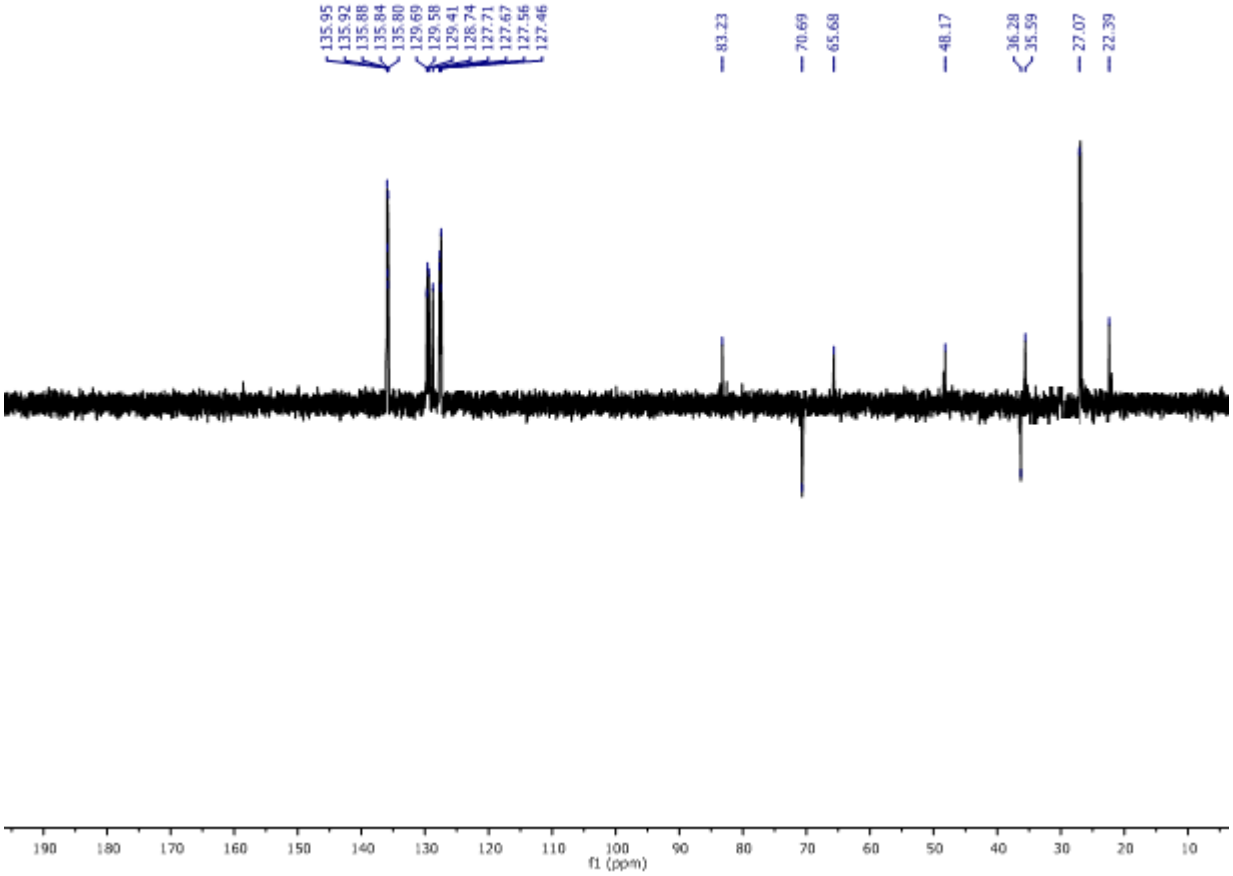
^{1}H NMR of compound (13b) (600 MHz, $CDCl_3$)



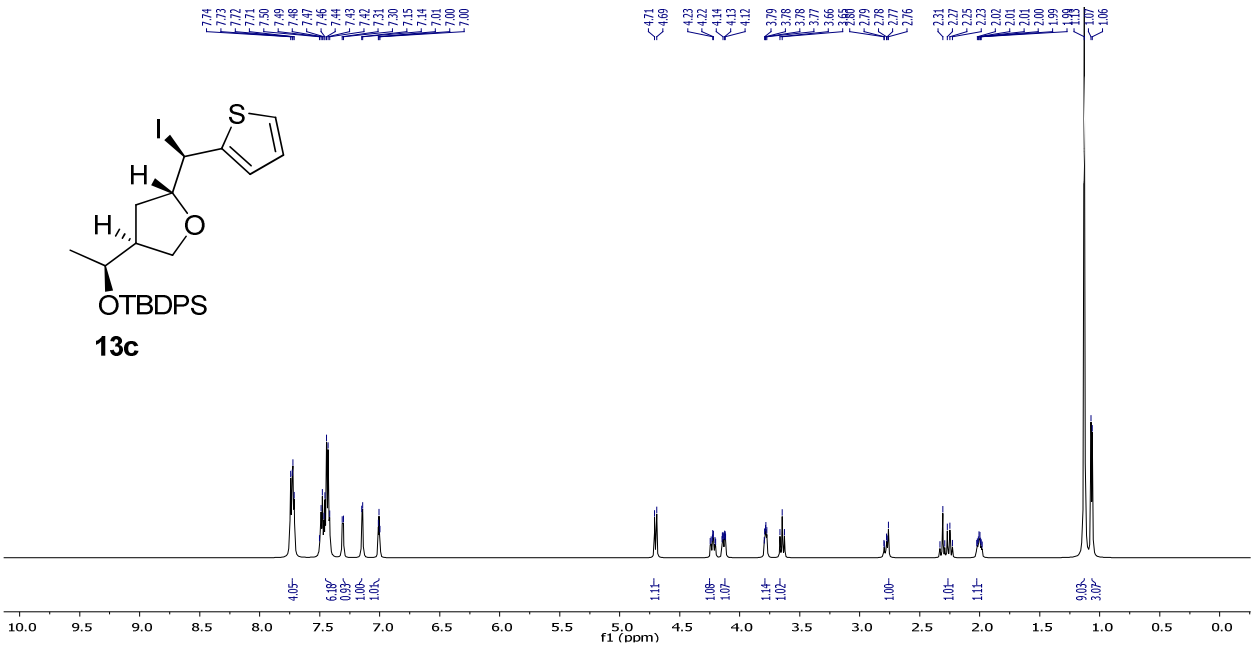
^{13}C NMR of compound (13b) (150 MHz, $CDCl_3$)



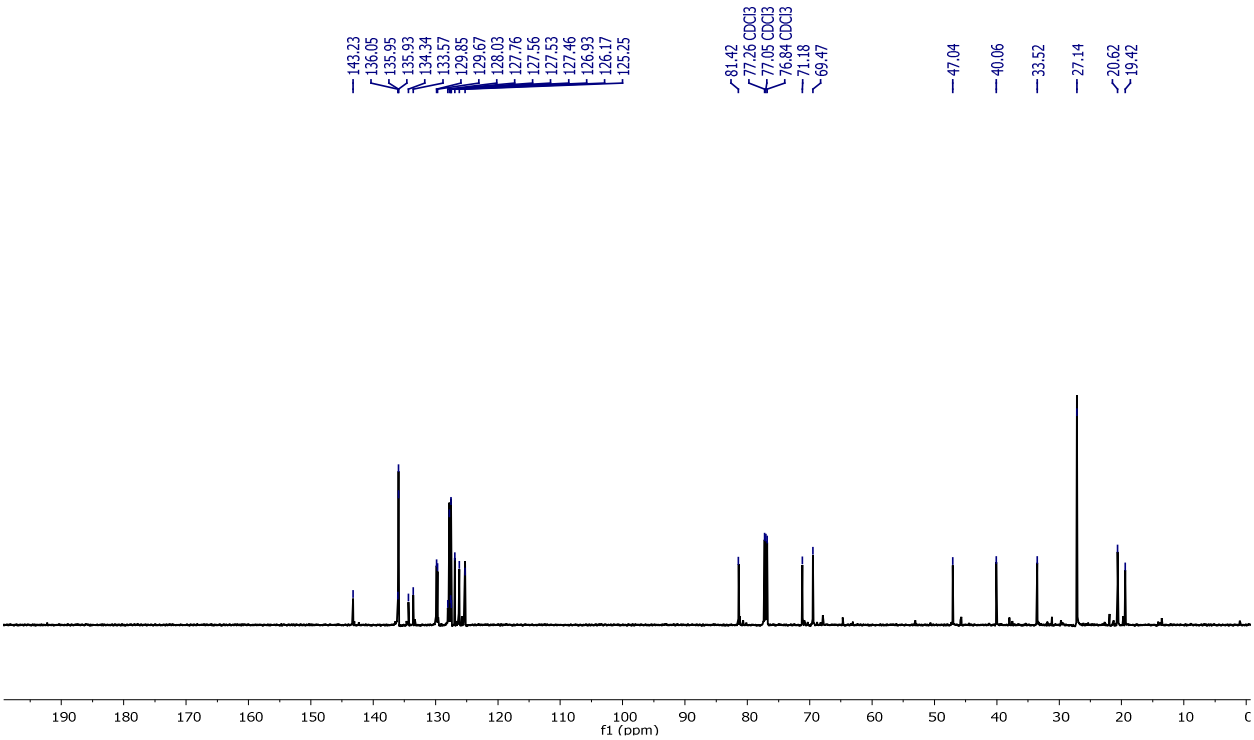
DEPT-135 of compound (13b) (150 MHz, $CDCl_3$)



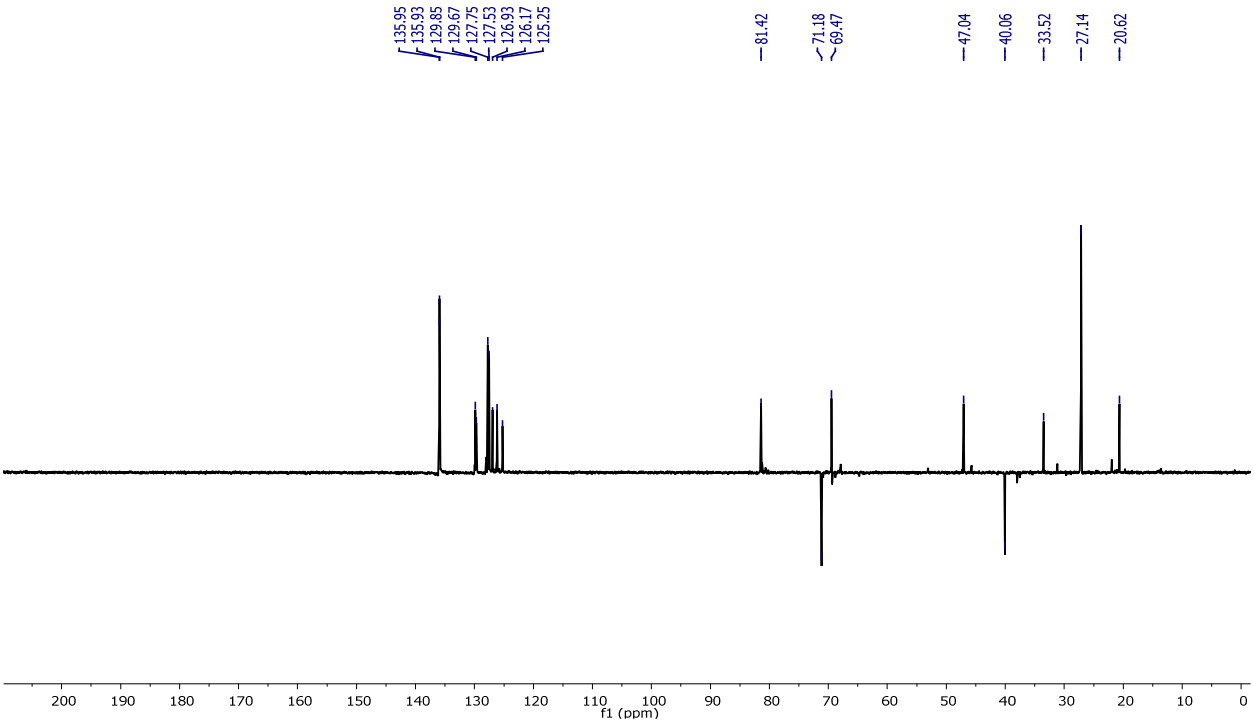
^{1}H NMR of compound (13c) (600 MHz, $CDCl_3$)



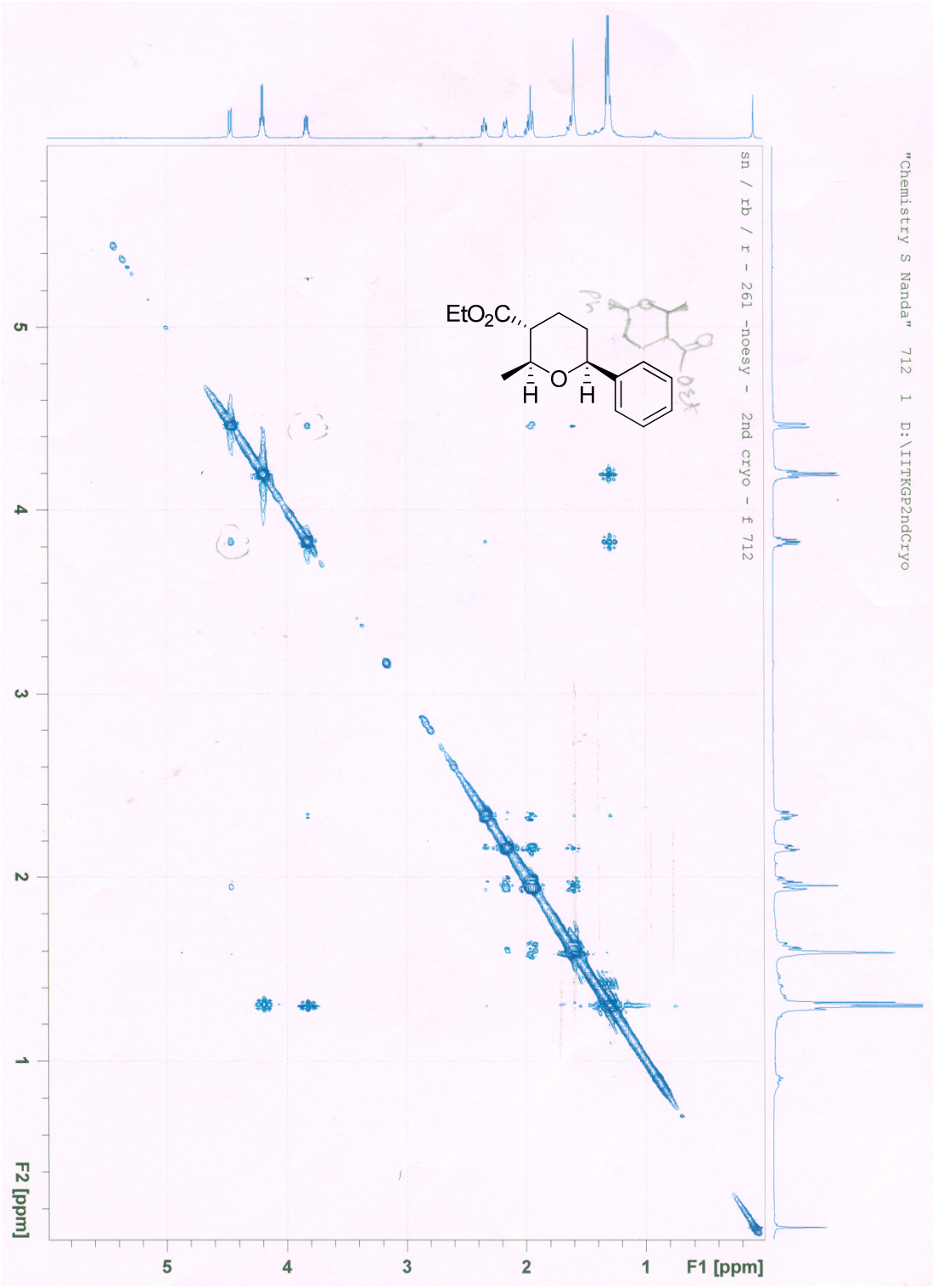
^{13}C NMR of compound (13c) (150 MHz, $CDCl_3$)



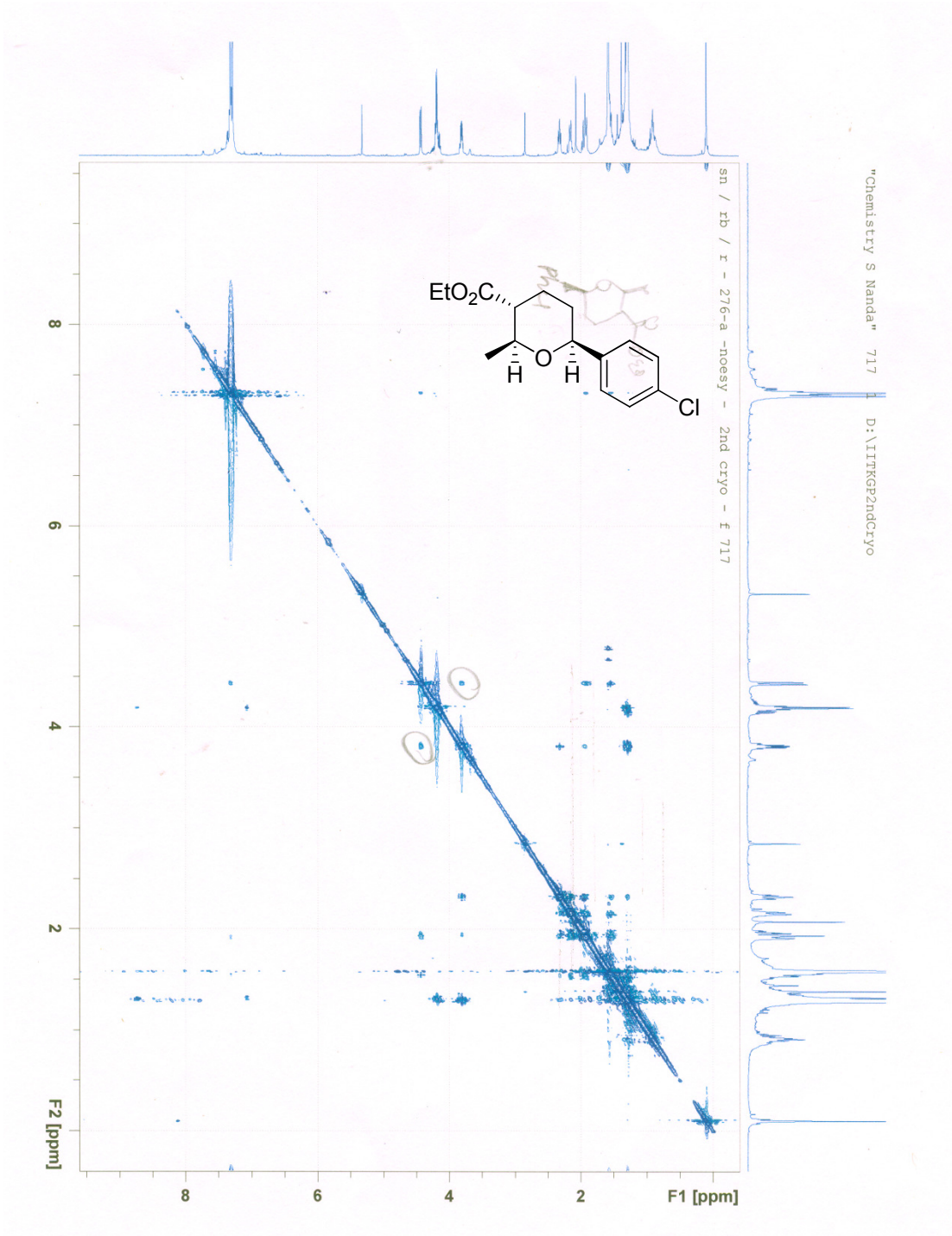
DEPT-135 of compound (13c) (150 MHz, $CDCl_3$)



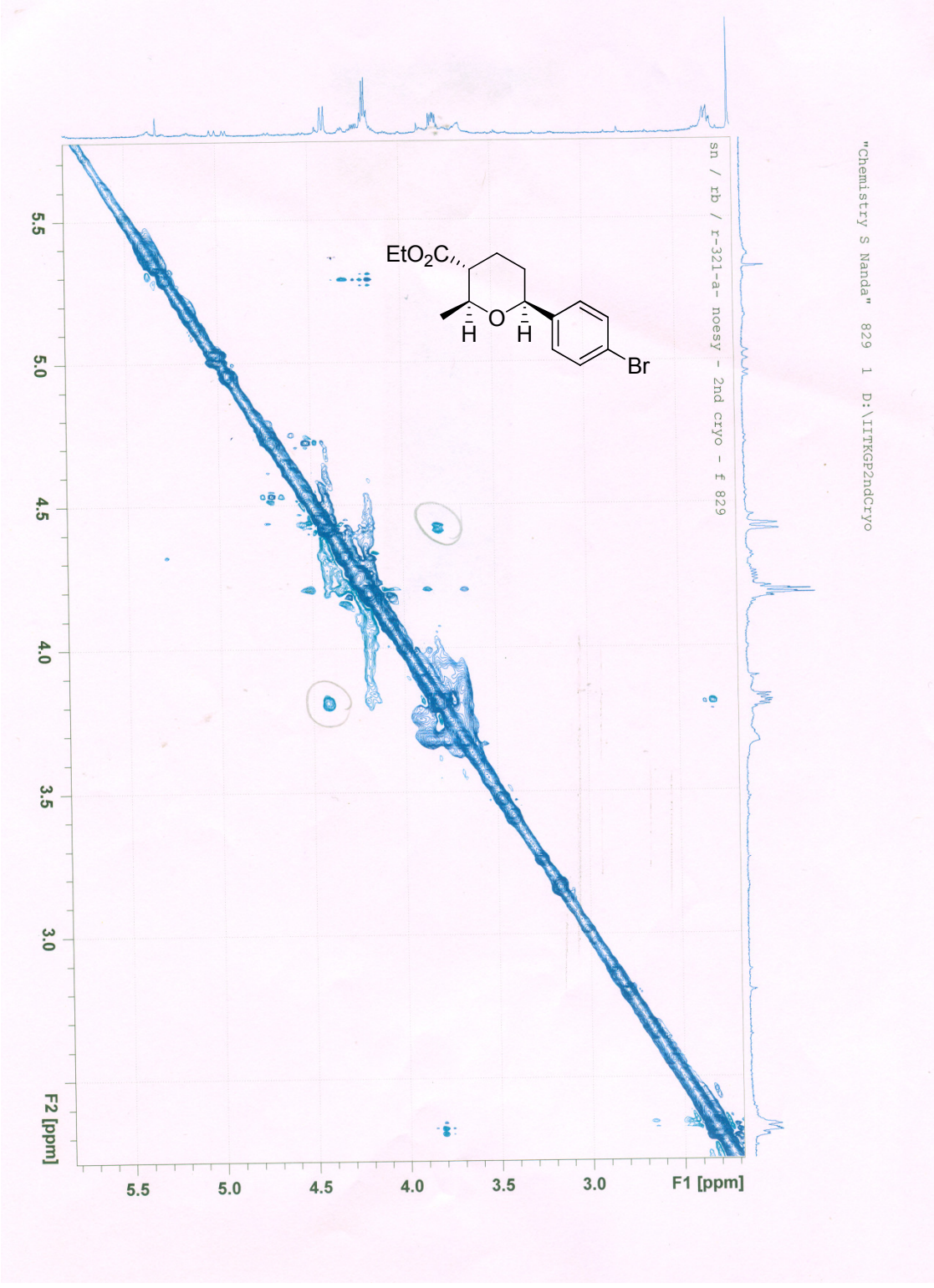
2D-NOESY spectrum of 9a (600 MHz, $CDCl_3$)



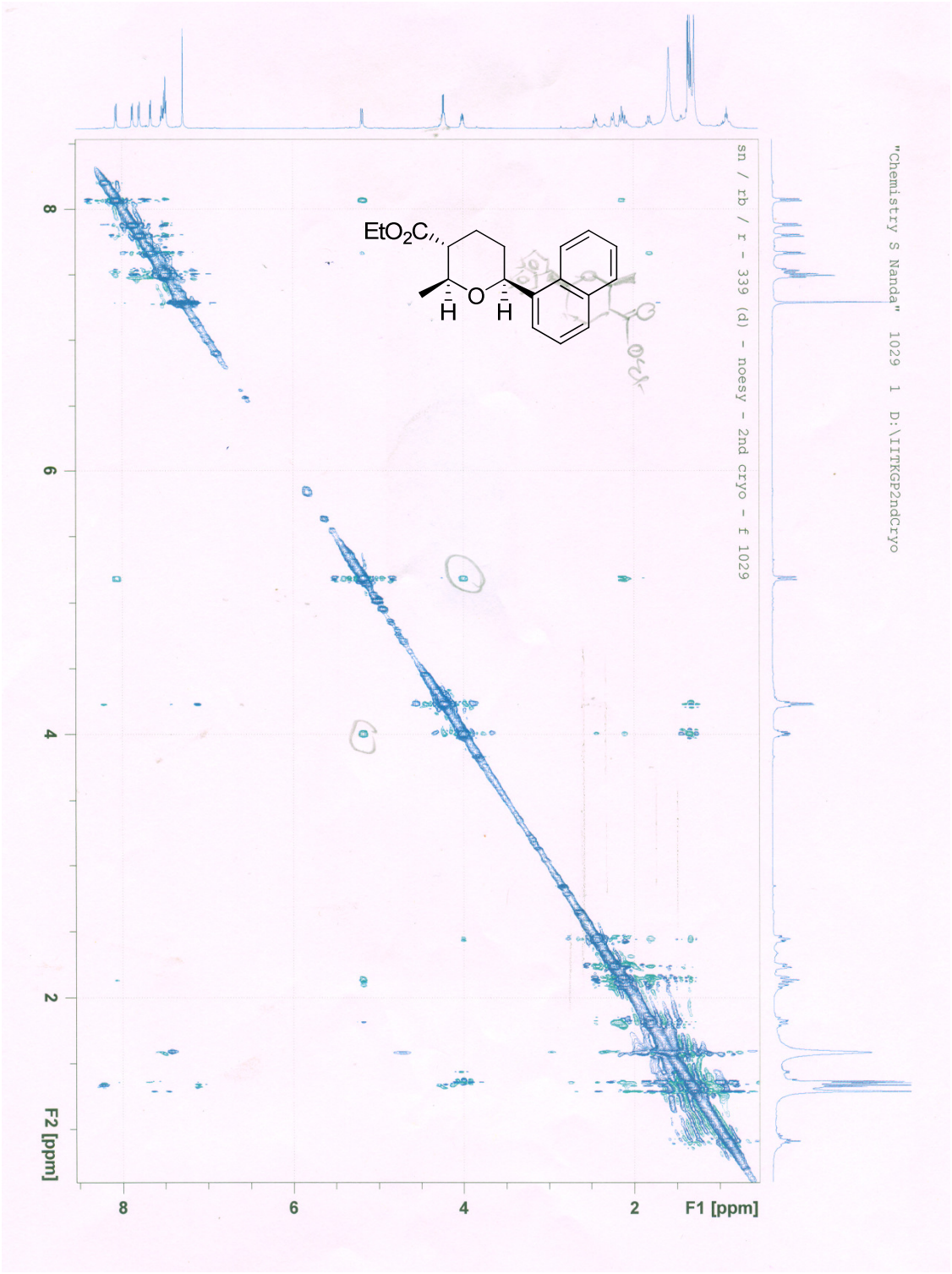
2D-NOESY spectrum of 9b (600 MHz, $CDCl_3$)



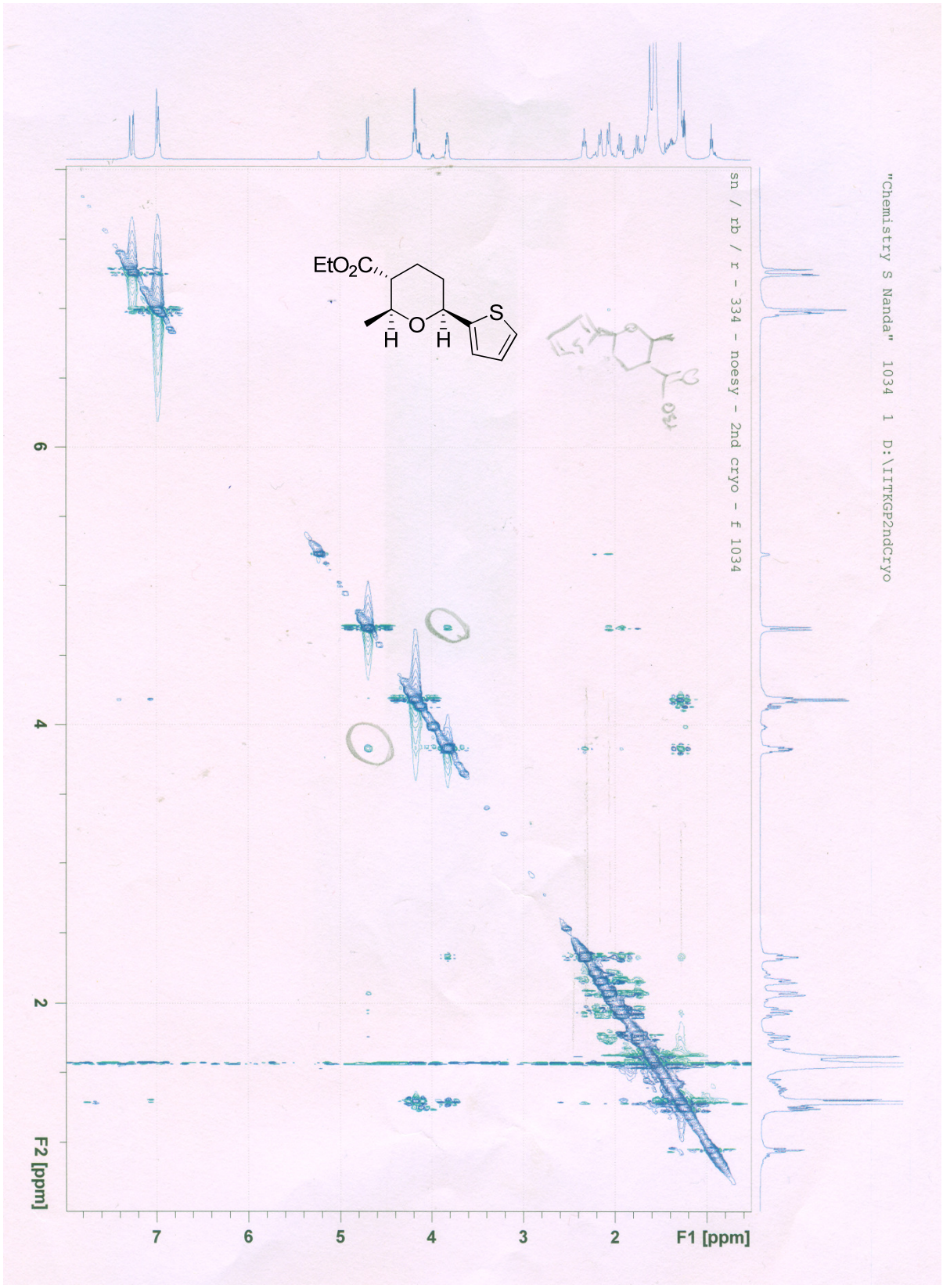
2D-NOESY spectrum of 9c (600 MHz, $CDCl_3$)



2D-NOESY spectrum of 9d (600 MHz, $CDCl_3$)



2D-NOESY spectrum of 9e (600 MHz, $CDCl_3$)

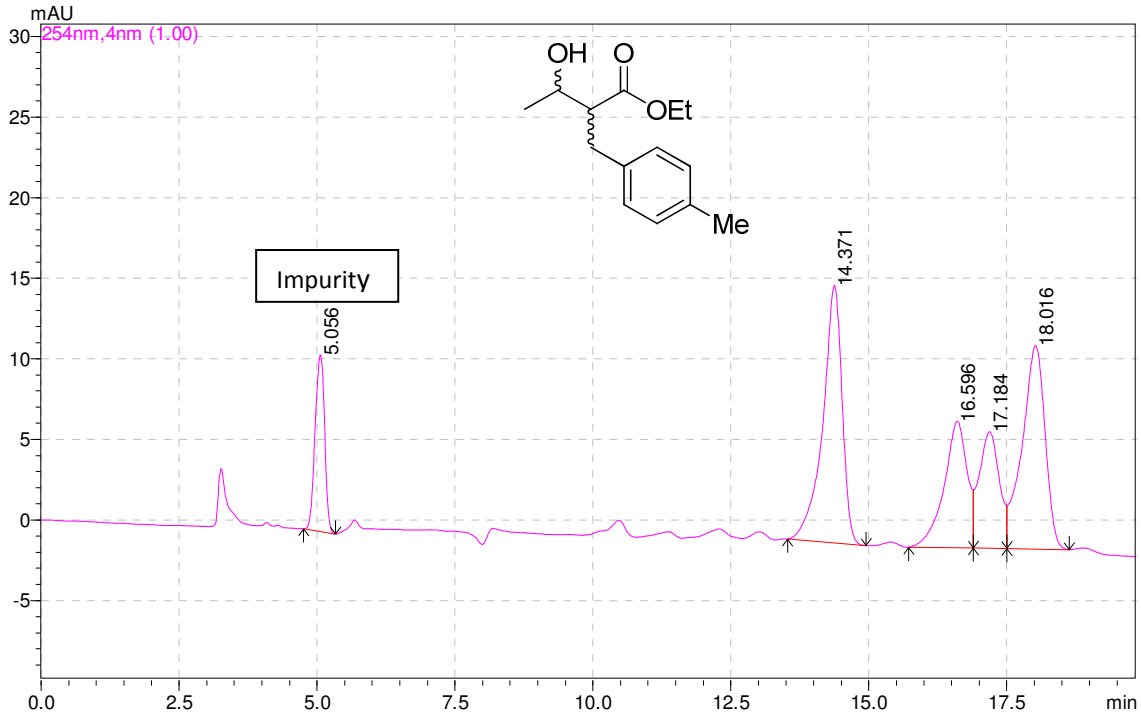


Sample name: Rashmita racemic 4-tolyl with $NaBH_4$

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



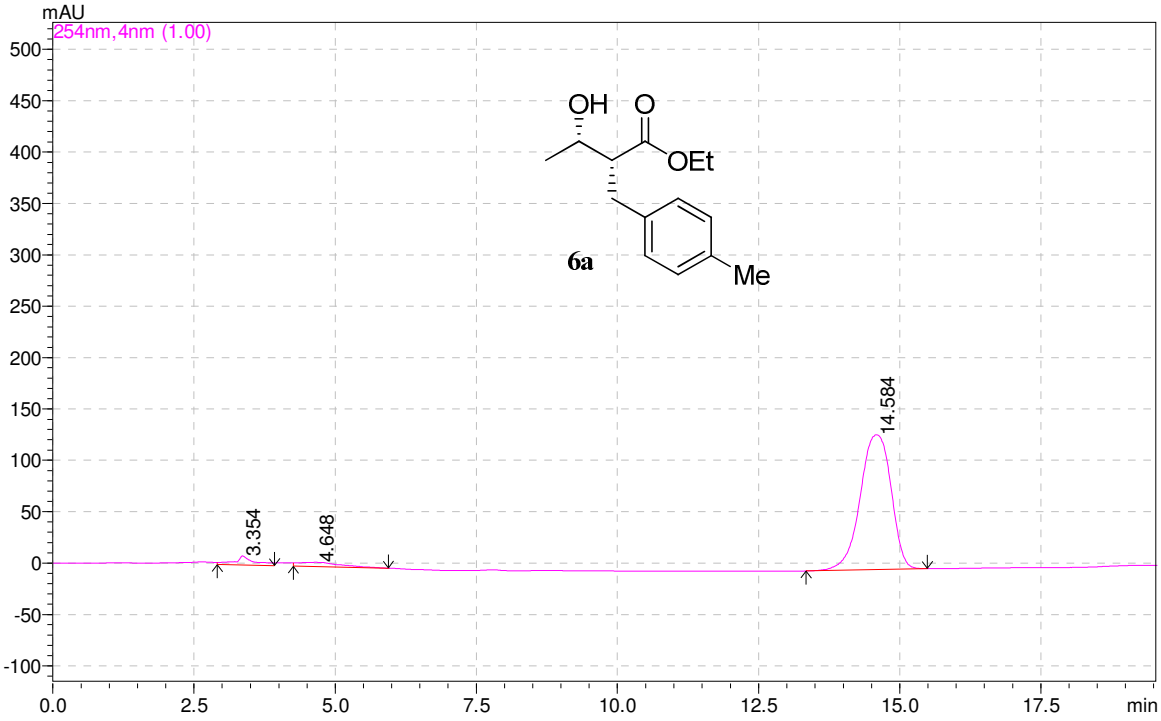
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	5.056	10.10	131631	10943	10.1
2	14.371	29.86	388884	15956	29.86
3	16.596	16.68	230247	7853	16.68
4	17.184	15.25	185318	7237	15.25
5	18.016	28.11	366114	12635	28.11

Sample name: Rashmitabioreduction 4-tolyl with NBRC3319

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

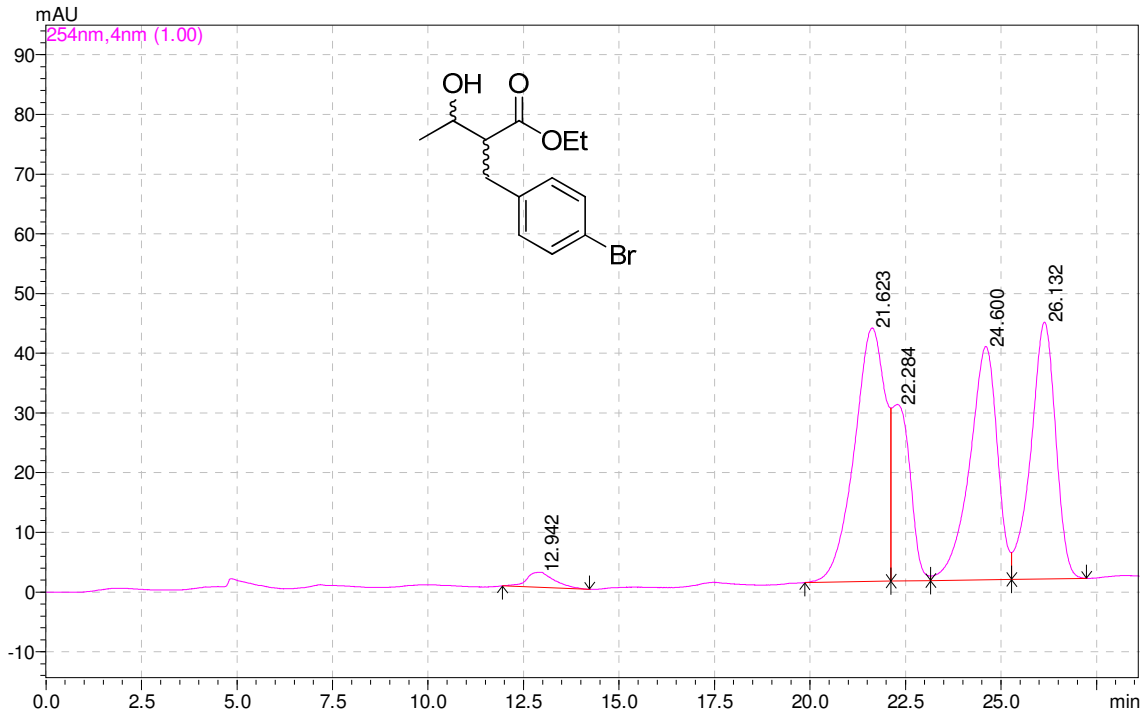
Peak#	Ret time	Conc	area	Height	Area (%)
1	3.354	3.91	212675	8650	3.91
2	4.648	3.97	215802	4239	3.98
3	14.584	92.11	5003250	131182	92.11

Sample name: Rashmita 4-bromobenzyl with $NaBH_4$

Column: CHIRALPAK IC; Flow rate: 0.8 ml/min

Mobile phase: 99:1; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



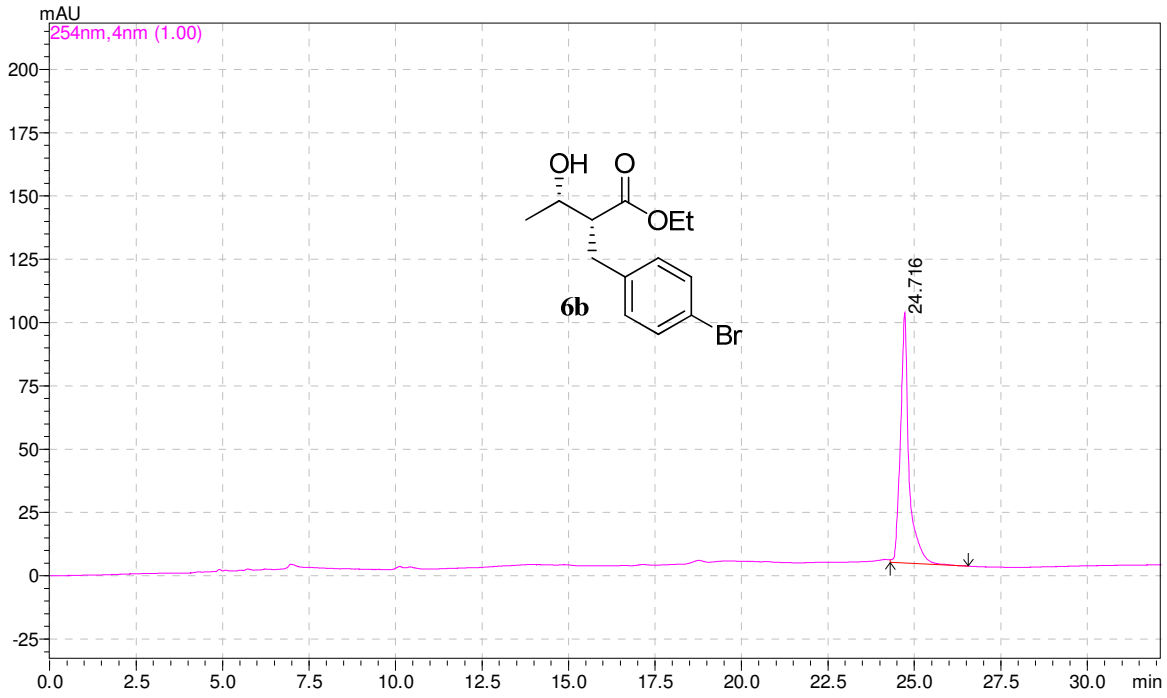
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	12.942	1.53	126526	2551	1.53
2	21.623	32.25	2435674	42462	32.25
3	22.284	13.10	977384	29586	13.1
4	24.600	26.58	1981800	39082	26.58
5	26.132	26.54	1933953	42992	25.94

Sample name: Rashmita 4-bromobenzyl bioreduction with NBRC 3319

Column: CHIRALPAK IC; Flow rate: 0.8 ml/min

Mobile phase: 99:1; hexane:IPA; Injection volume: 5µL



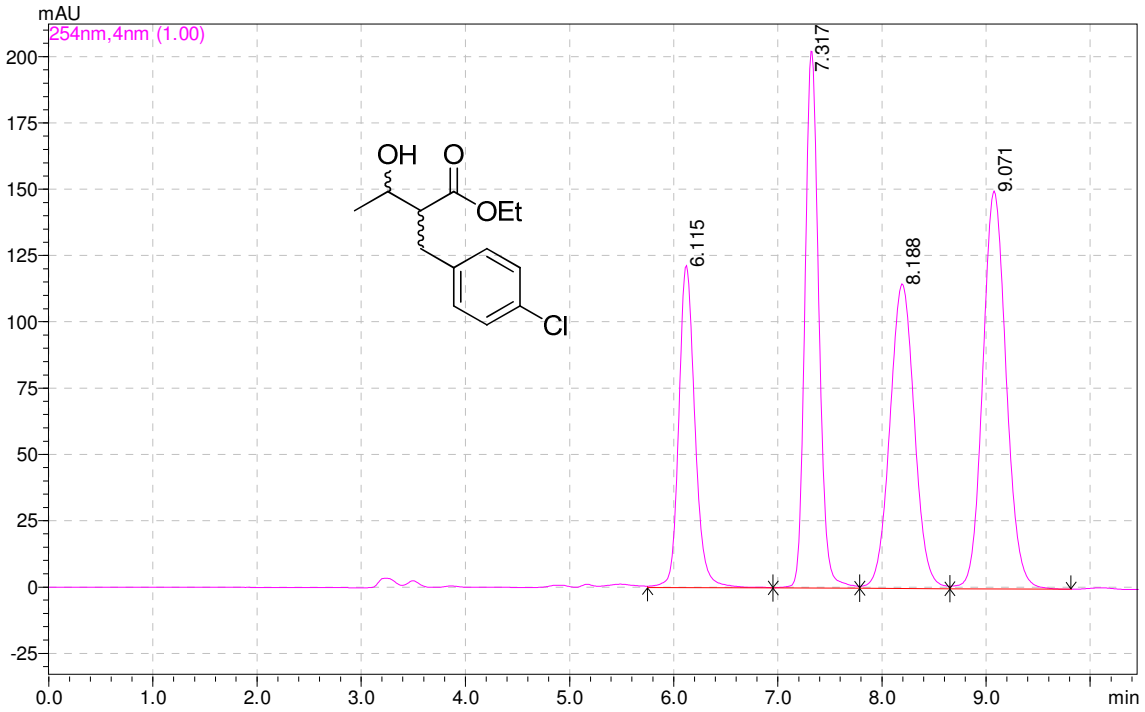
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	24.716	100.00	1693663	98877	100

Sample name: Rashmita 4-Cl benzyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

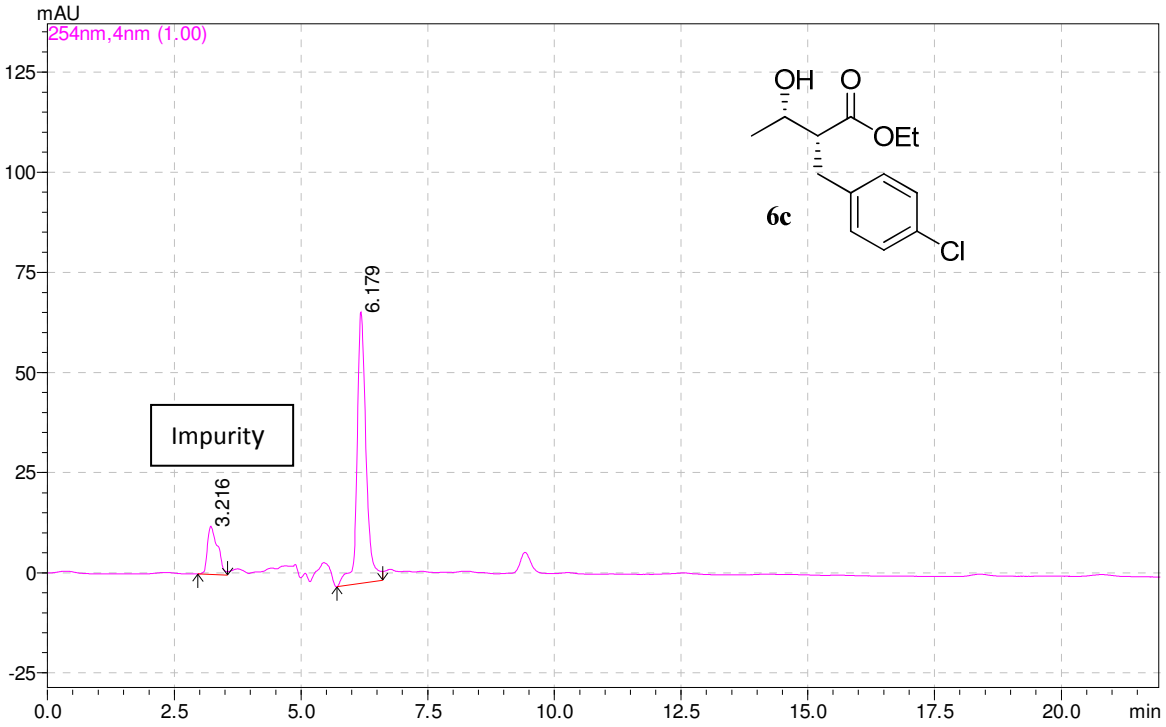
Peak#	Ret time	Conc	area	Height	Area (%)
1	6.115	22.73	1312258	121586	22.73
2	7.317	27.28	1870850	202499	27.28
3	8.188	22.33	1874582	114803	22.33
4	9.071	27.66	2341010	149913	27.66

Sample name: Rashmita 4-Cl benzyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 10µL

PDA Ch1 254nm 4nm

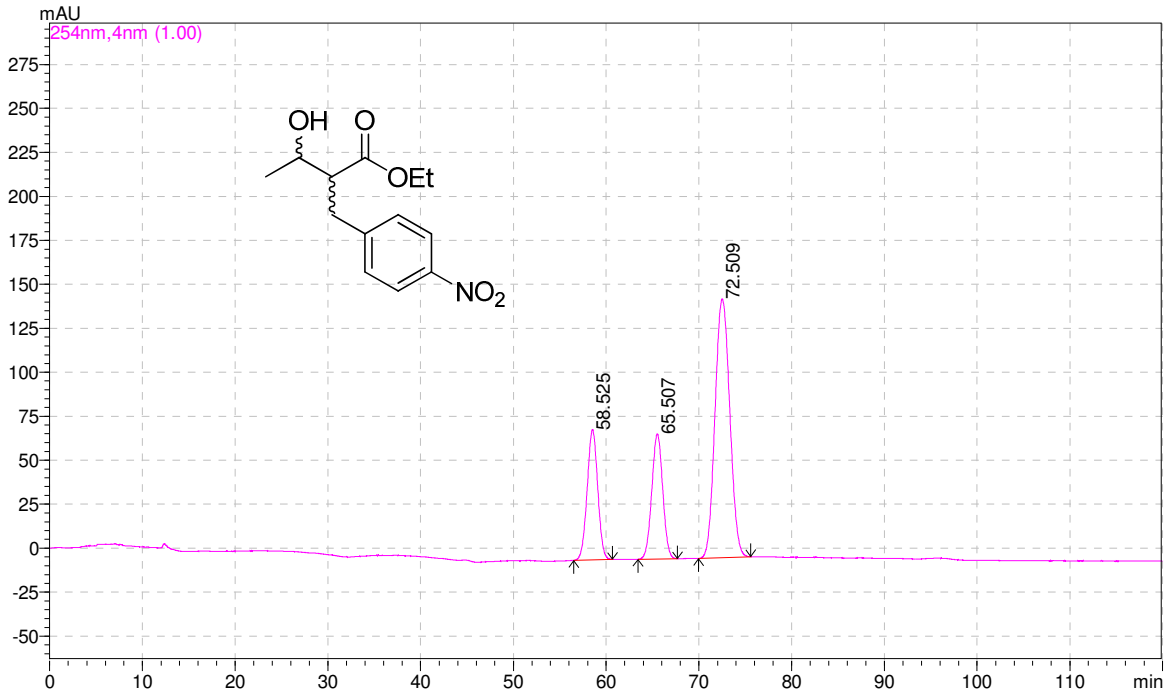


Peak#	Ret time	Conc	area	Height	Area (%)
1	3.218	16.76513	252484	15872	16.76
2	6.179	83.23487	1263001	79379	83.24

Sample name: Rashmita 4-nitrobenzyl with $NaBH_4$

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

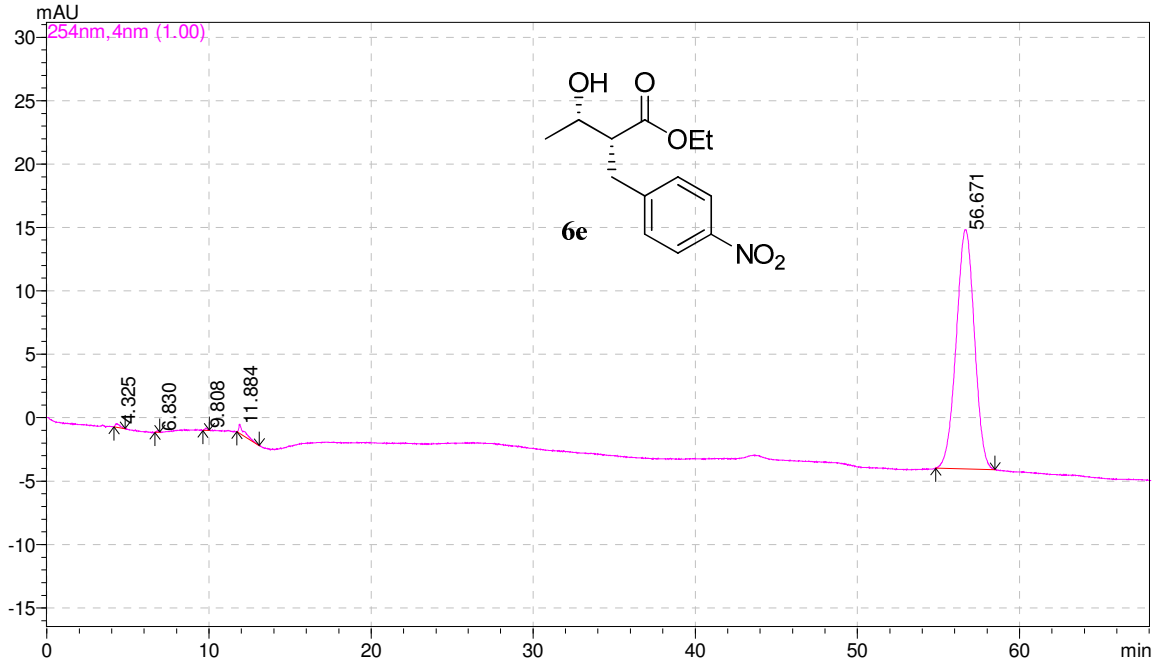
Peak#	Ret time	Conc	area	Height	Area (%)
1	58.525	20.9498	5869241	74306	20.94
2	65.507	20.8751	5848298	71078	20.87
3	72.509	58.175	16298109	147078	58.17

The peak at 72.509 corresponds to two stereoisomers, and we are unable to separate it (Chiral pak IA, IB, IC, OD, OB, OJ, AD, AS and Lux cellulose-1, cellulose-2, cellulose-3, cellulose-4, amylose-1 was used as a stationary phase).

Sample name: Rashmita 4-nitrobenzyl with NBRC 3319

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 10µL



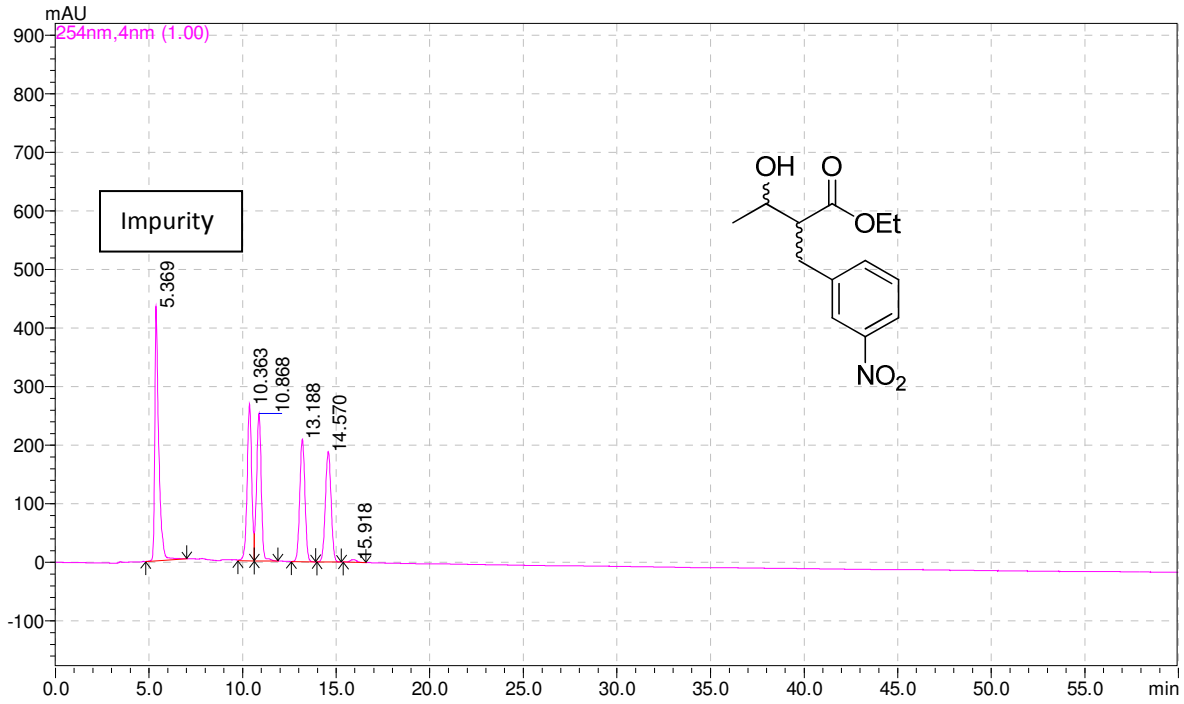
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	4.325	0.1836	3806	244	0.18
2	6.83	0.1245	526379	6592	.12
3	9.80	0.1038	2152	203	0.1
4	11.884	2.1532	3176	394	2.15
5	56.671	97.435	1537432	19023	97.43

Sample name: Rashmita 3-nitrobenzyl with $NaBH_4$

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



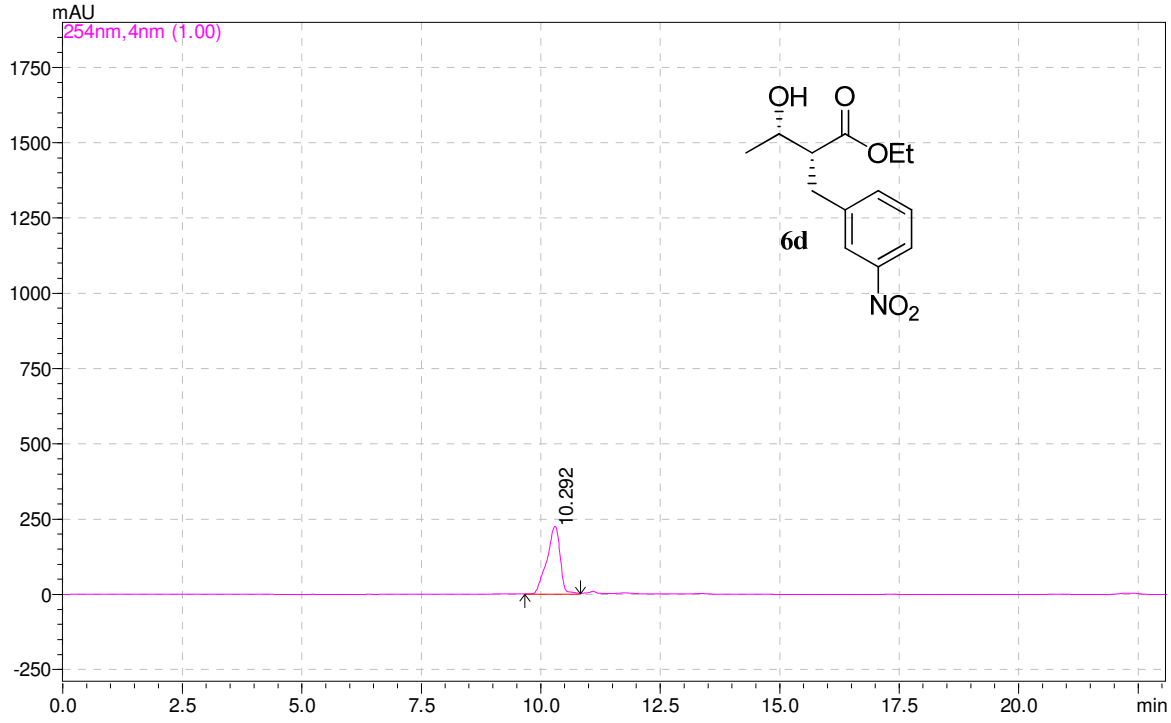
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	5.369	27.12	6329891	434488	27.12
2	10.363	19.30	4504012	268034	19.30
3	10.868	18.69	4362127	252076	18.69
4	13.188	17.24	4024332	209134	17.24
5	14.570	17.15	4003849	188678	17.15
6	15.918	0.50	112398	4563	0.50

Sample name: Rashmita 3-nitrobenzyl with NBRC3319

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 10µL



PDA Ch1 254nm 4nm

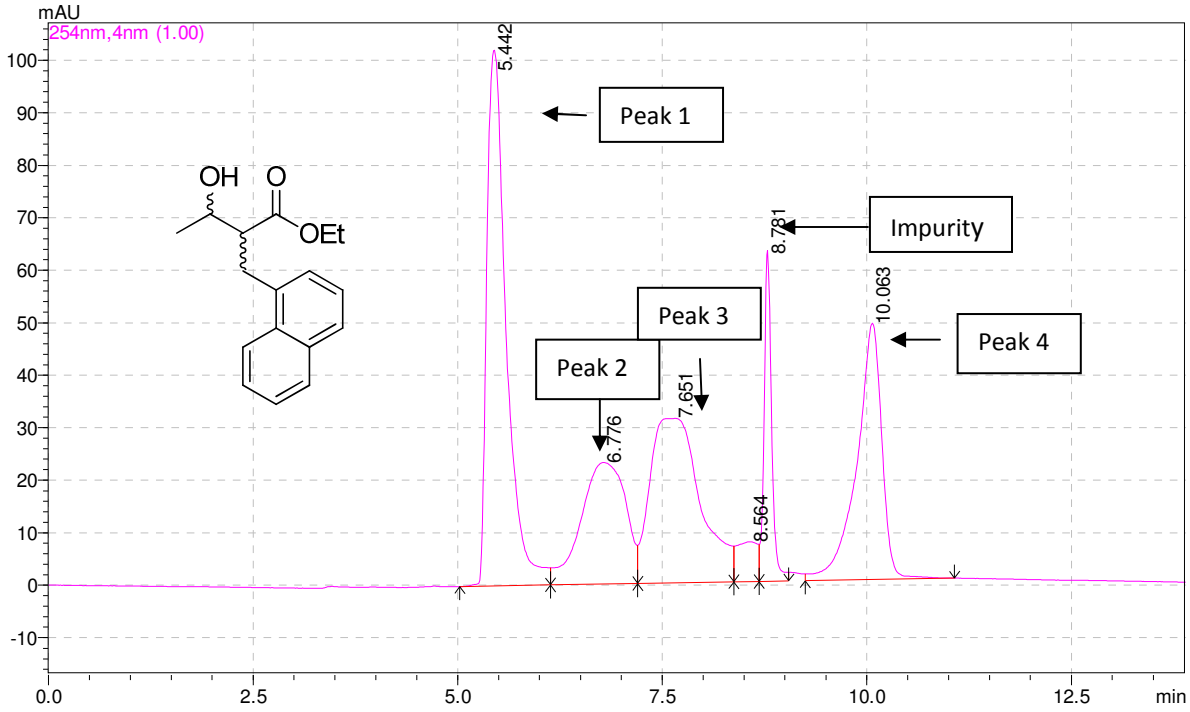
Peak#	Ret time	Conc	area	Height	Area (%)
1	10.292	100.00	519444	38347	100

Sample name: Rashmita 1-naphthyl with $NaBH_4$

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



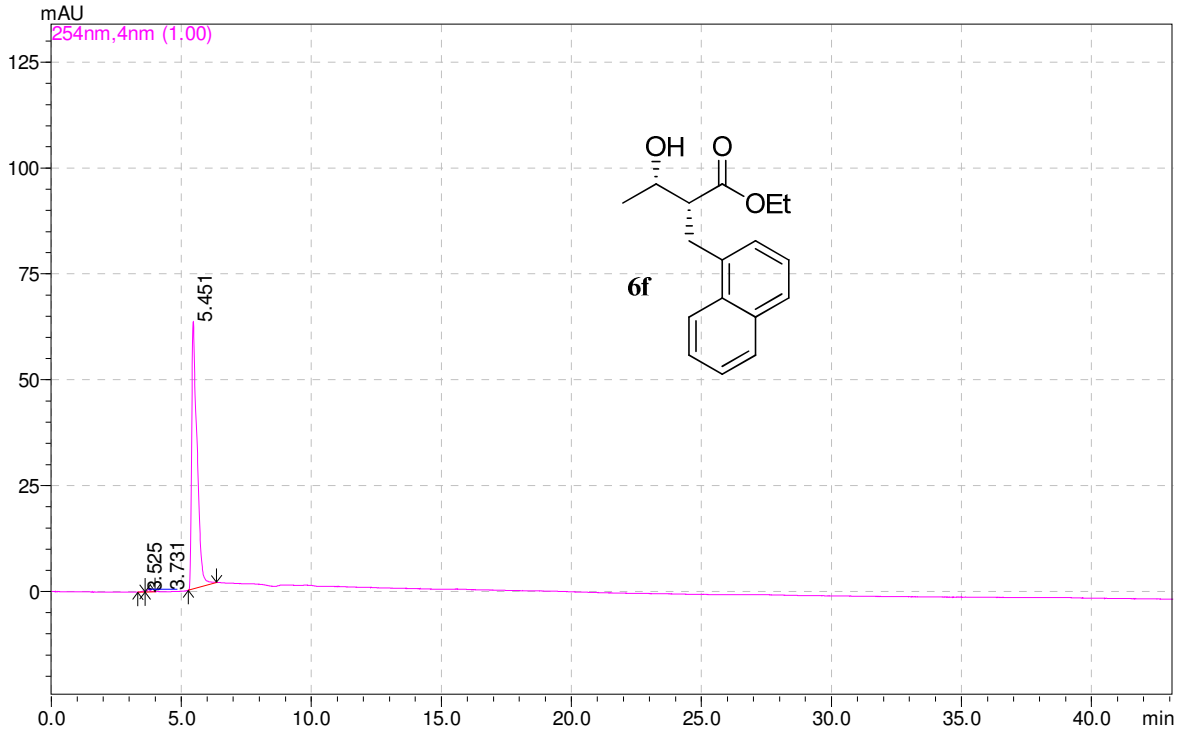
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	5.442	26.74	1689678	102055	28.74
2	6.776	19.04	881786	23186	19.04
3	7.651	26.88	1344230	31344	26.88
4	8.564	2.05	134847	7555	2.05
5	8.781	6.26	399108	63067	6.26
6	10.063	19.03	1046378	48814	19.03

Sample name: Rashmita 1-naphthyl with NBRC3319

Column: CHIRALPAK IC; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

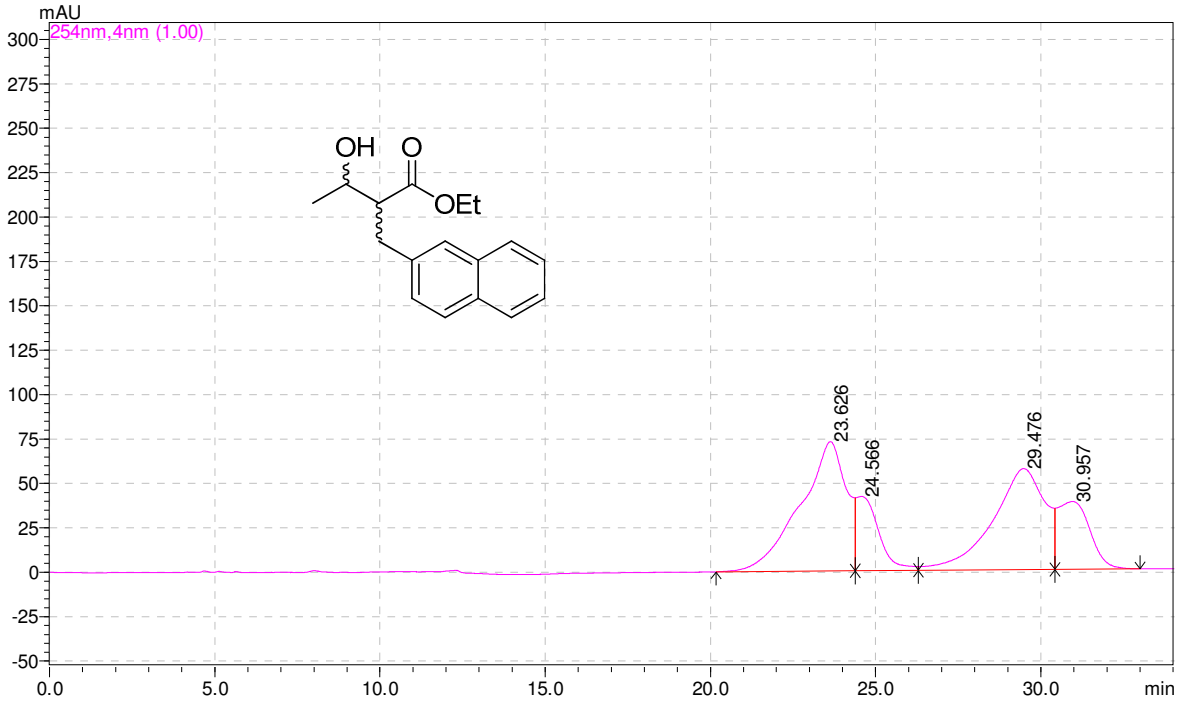
Peak#	Ret time	Conc	area	Height	Area (%)
1	3.525	0.20562	1914	221	0.2056
2	3.731	0.58544	5450	592	0.5854
3	5.451	99.20894	923552	63098	99.2089

Sample name: Rashmita 2-naphthyl with $NaBH_4$

Column: CHIRALCEL OD-H; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



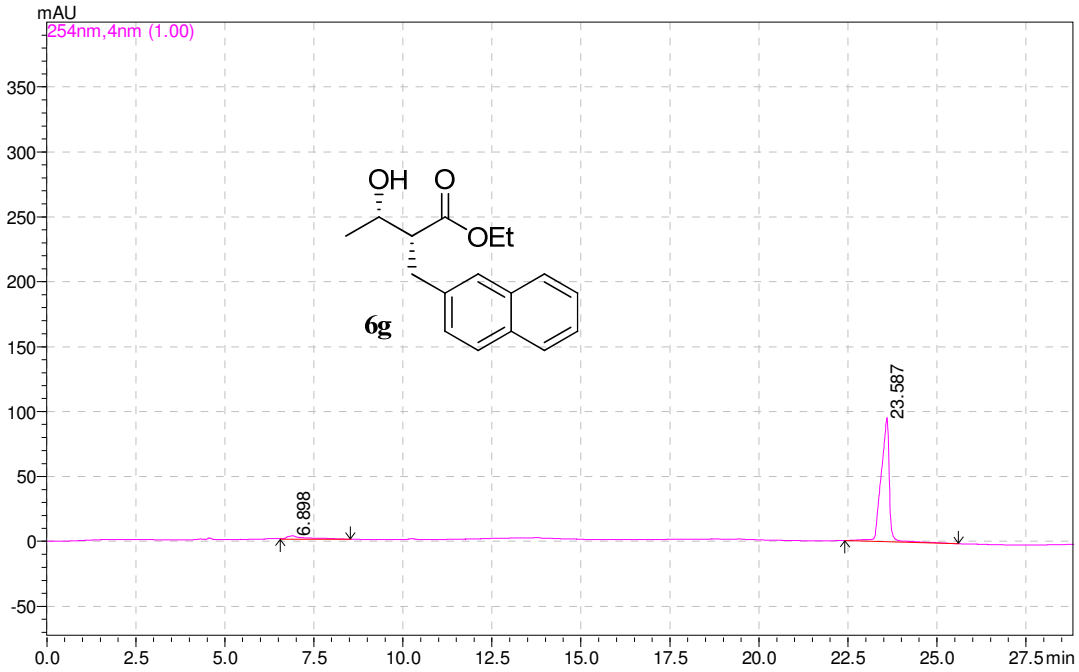
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	23.626	37.49	7060234	72863	37.49
2	24.566	12.16	1997034	41760	12.16
3	29.476	35.87	6236982	56924	35.87
4	30.957	14.48	2590327	38186	14.48

Sample name: Rashmita 2-naphthyl with NBRC3319

Column: CHIRALCEL OD-H; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



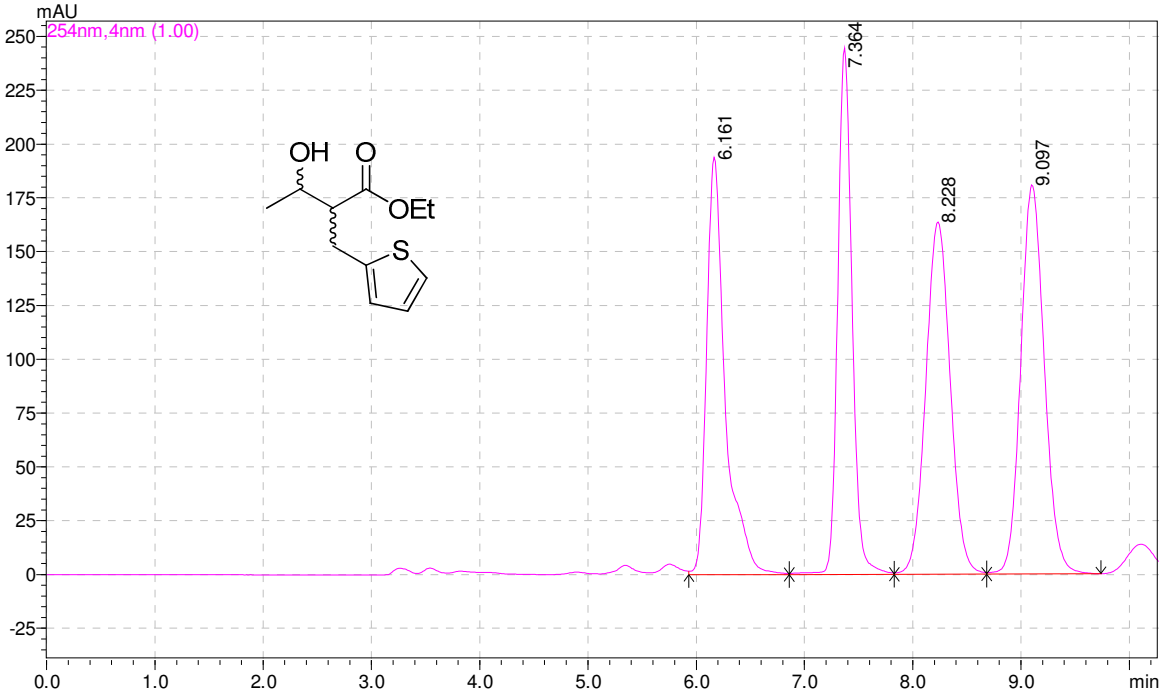
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	6.898	6.20	101159	2647	6.20
2	23.587	93.80	1529949	95268	93.80

Sample name: Rashmita 2-thienyl benzyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



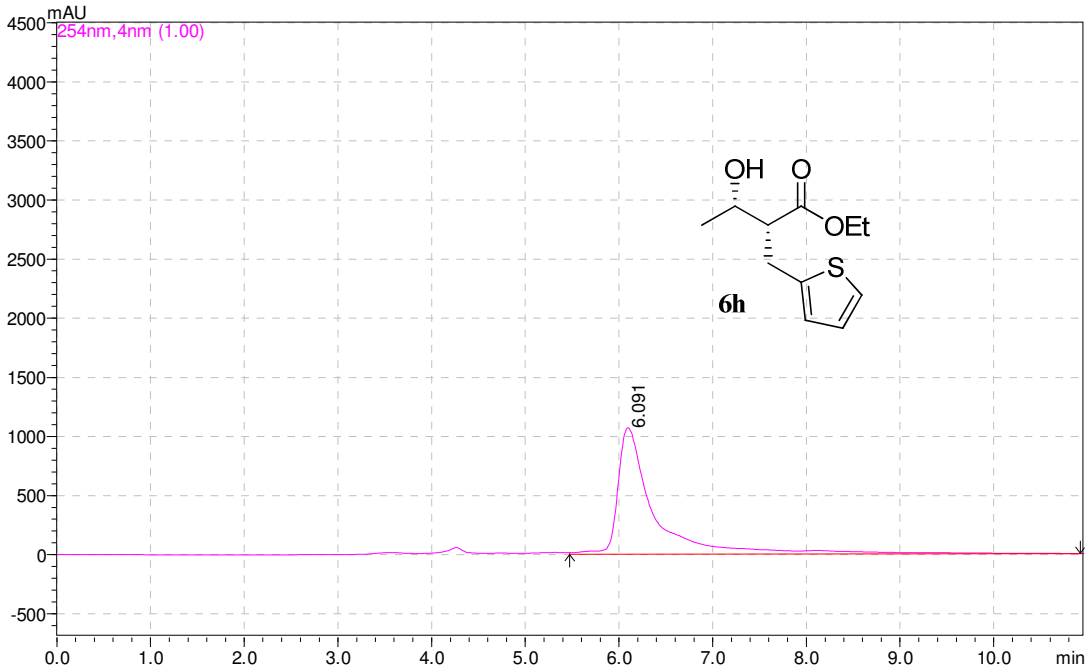
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	6.161	23.48	2320215	193747	23.48
2	7.364	23.05	2247770	244608	23.05
3	8.228	26.33	2569260	163562	26.33
4	9.097	27.14	2740691	180652	27.14

Sample name: Rashmita 2-thienyl benzyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

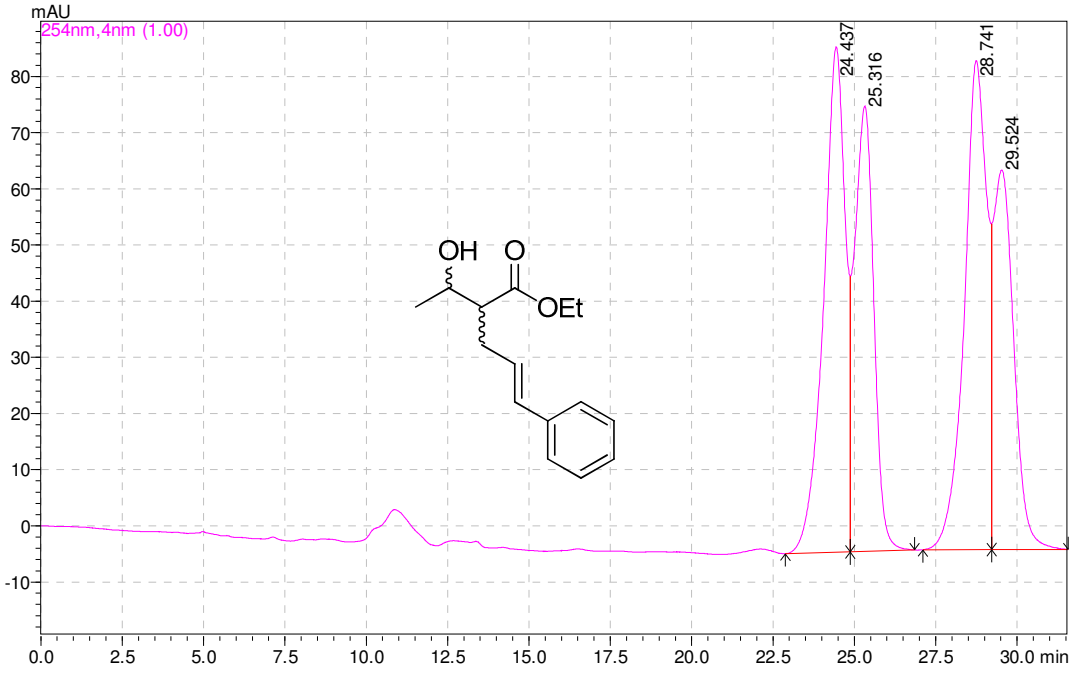
Peak#	Ret time	Conc	area	Height	Area (%)
1	6.091	100.00000	29274898	1069543	100

Sample name: Rashmitacinnamyl with $NaBH_4$

Column: CHIRALCEL OD-H; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



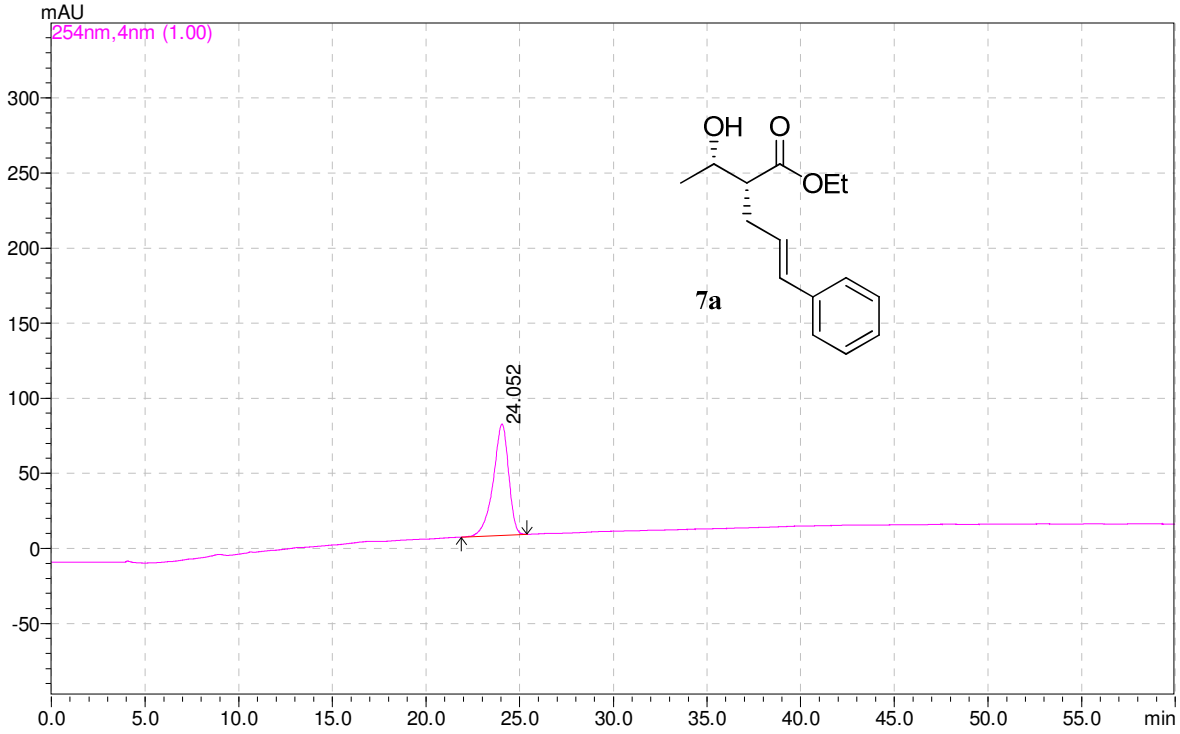
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	24.437	28.63	4198134	89974	28.63
2	25.316	21.29	3267973	79247	21.29
3	28.741	28.92	4241355	87088	28.92
4	29.524	21.16	2953383	67620	21.16

Sample name: Rashmitacinnamyl with NBRC3319

Column: CHIRALCEL OD-H; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

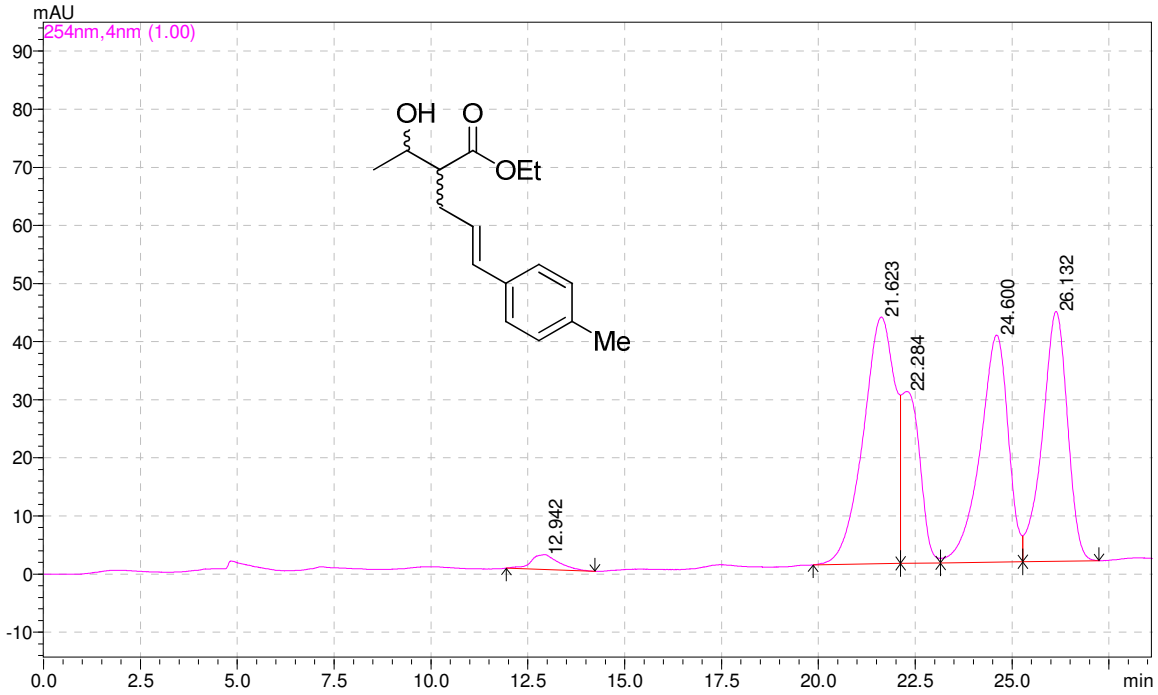
Peak#	Ret time	Conc	area	Height	Area (%)
1	24.052	100.00000	4246210	74158	100

Sample name: Rashmita 4-Me-cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



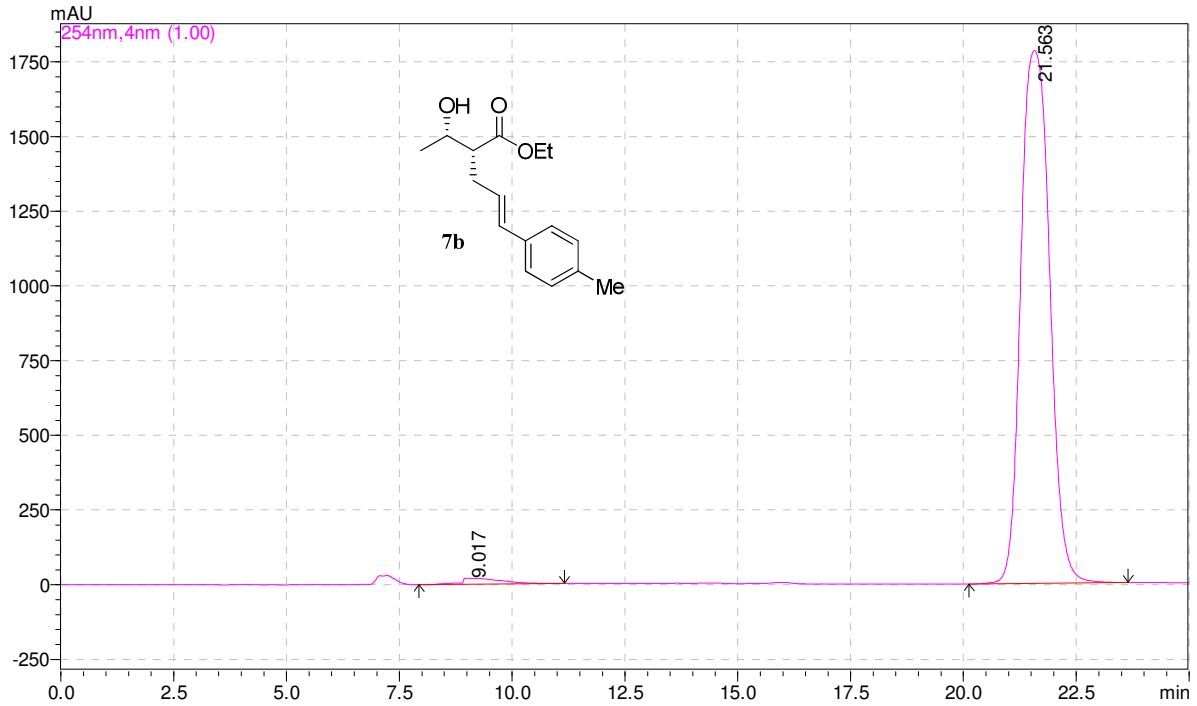
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	12.942	1.69	126526	2551	1.69
2	21.623	31.87	2435674	42462	31.87
3	22.284	13.88	977384	29586	13.88
4	24.6	25.95	1981800	39082	25.95
5	26.132	26.61	1933953	42992	26.61

Sample name: Rashmita 4-Me-cinnamyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

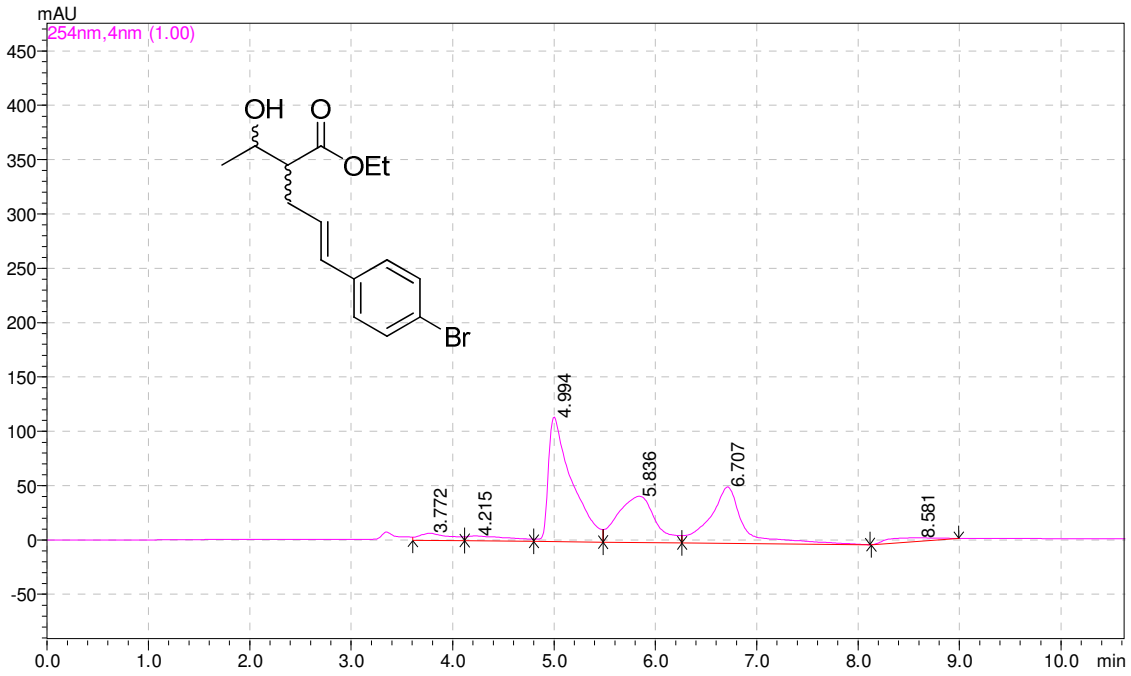
Peak#	Ret time	Conc	area	Height	Area (%)
1	9.017	1.54191	1243162	20177	1.5
2	21.563	98.45809	79381747	79381747	98.5

Sample name: Rashmita 4-Br-cinnamyl with $NaBH_4$

Column: CHIRALCEL OD-H; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



PDA Ch1 254nm 4nm

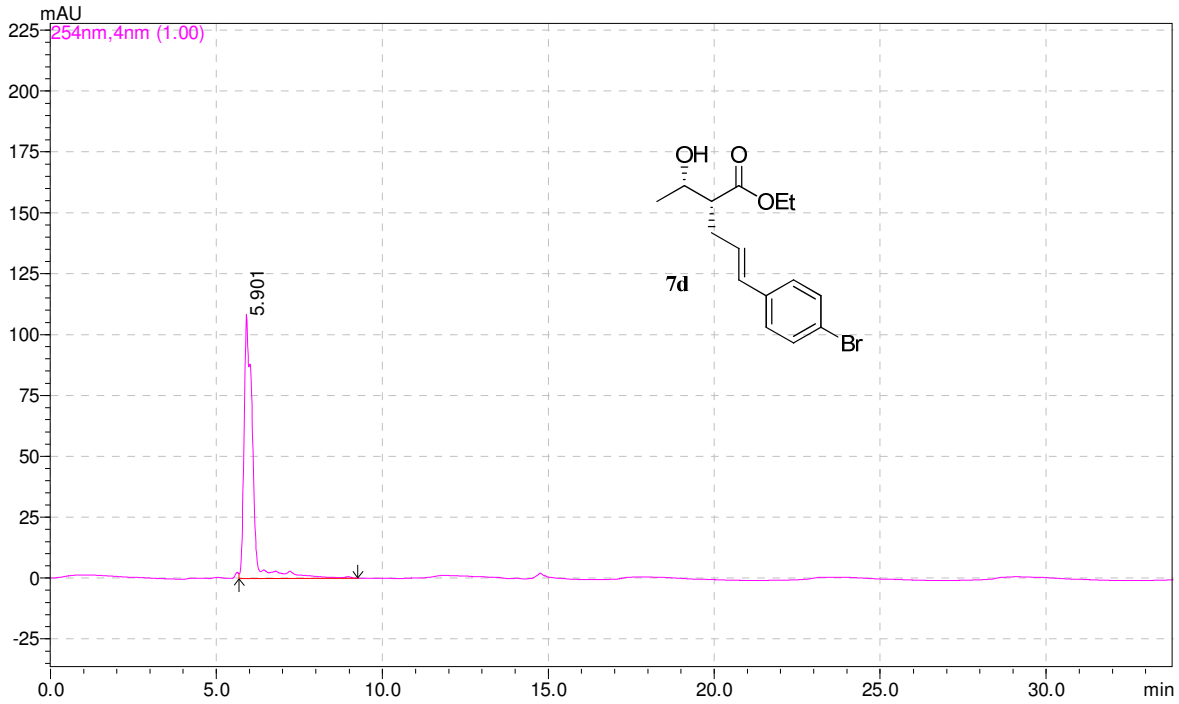
Peak#	Ret time	Conc	area	Height	Area (%)
1	3.772	2.04	137056	6566	2.04
2	4.215	1.98	134457	4589	1.98
3	4.994	44.11	1851594	114323	44.11
4	5.836	24.99	1088009	42381	24.99
5	6.707	25.00	117093	51745	25.00
6	8.581	1.88	121006	3108	1.88

The peak at 4.994 corresponds to two stereoisomers, and we are unable to separate it (Chiral pak IA, IB, IC, OD, OB, OJ, AD, AS and Lux cellulose-1, cellulose-2, cellulose-3, cellulose-4, amylose-1 was used as a stationary phase).

Sample name: Rashmita 4-Br-cinnamyl with NBRC3319

Column: CHIRALCEL OD-H; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



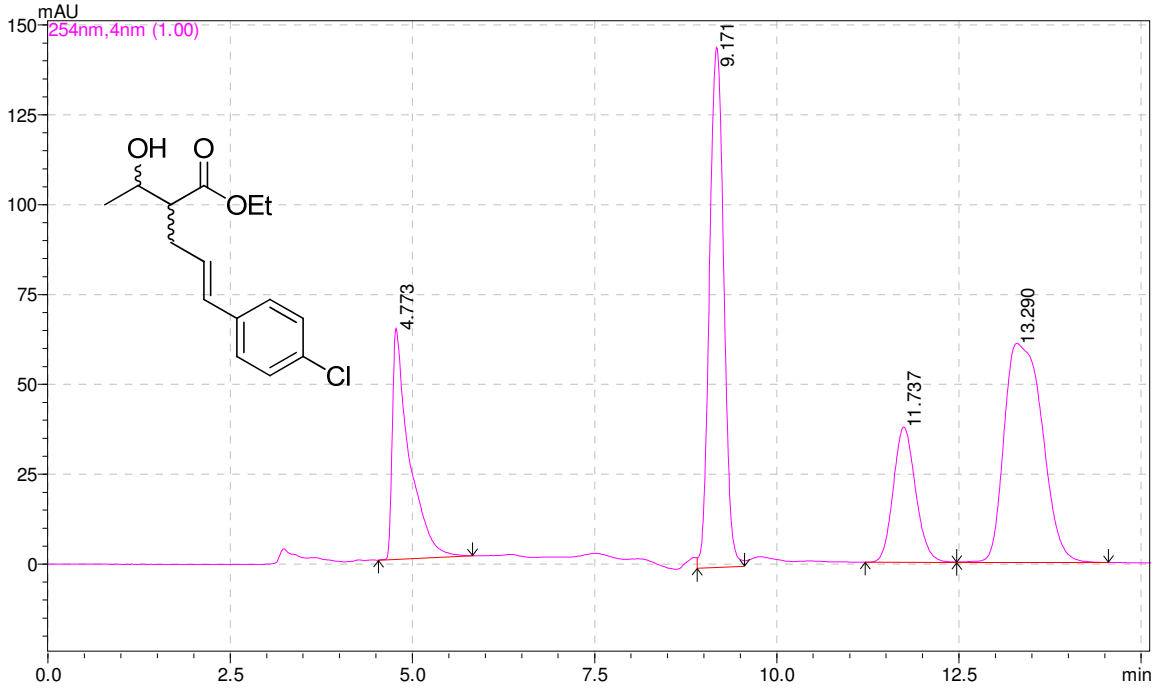
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	5.901	100.00	1943435	108484	100

Sample name: Rashmita 4-Cl cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



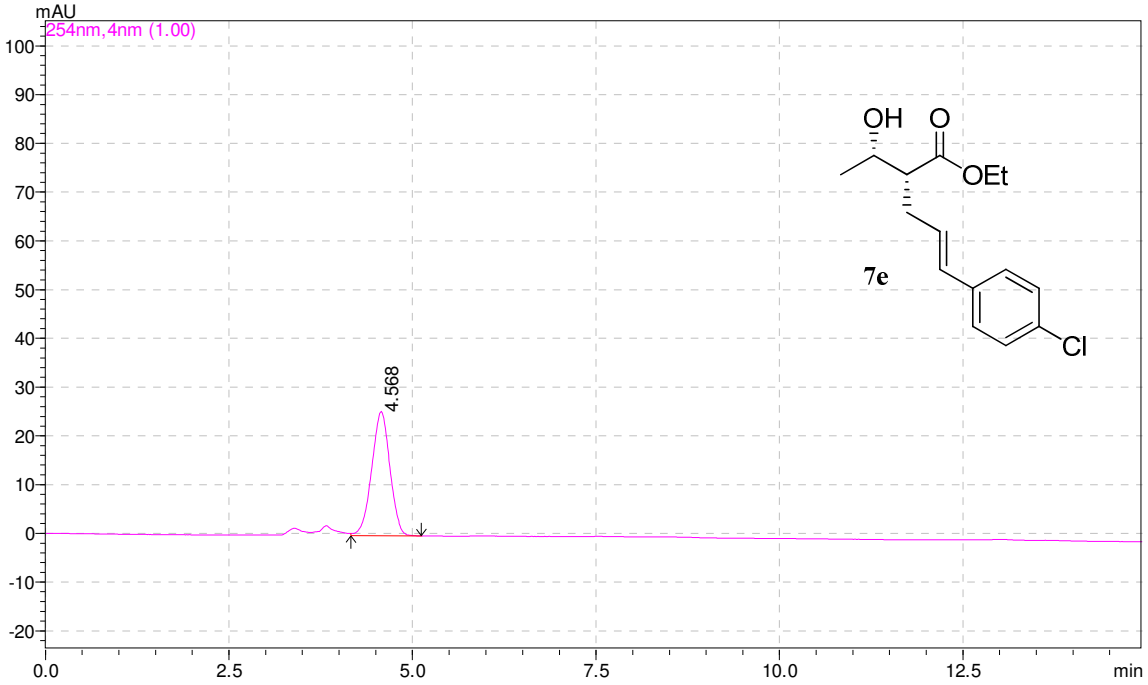
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	4.773	15.21	1038279	64218	15.21
2	9.171	34.42	1979160	144725	9.171
3	11.737	14.68	801259	37629	14.68
4	13.290	35.69	2213526	60932	35.69

Sample name: Rashmita 4-Cl cinnamyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



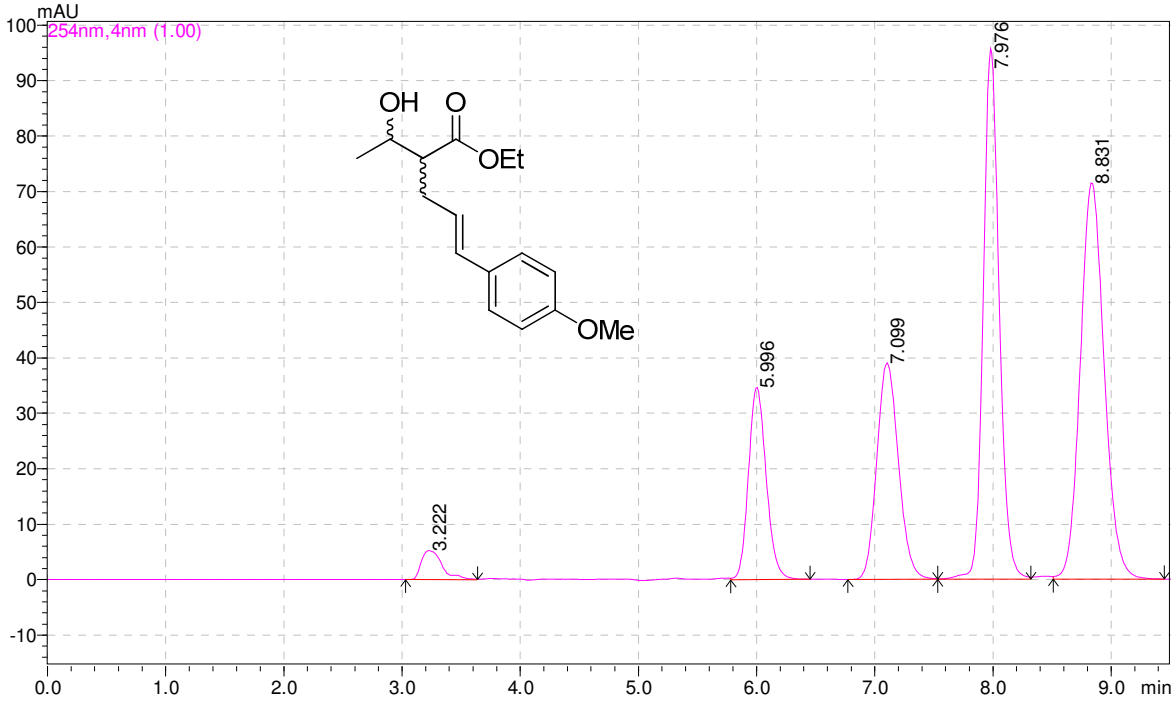
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	4.568	100.00000	440960	25425	100

Sample name: Rashmita 4-OMe cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



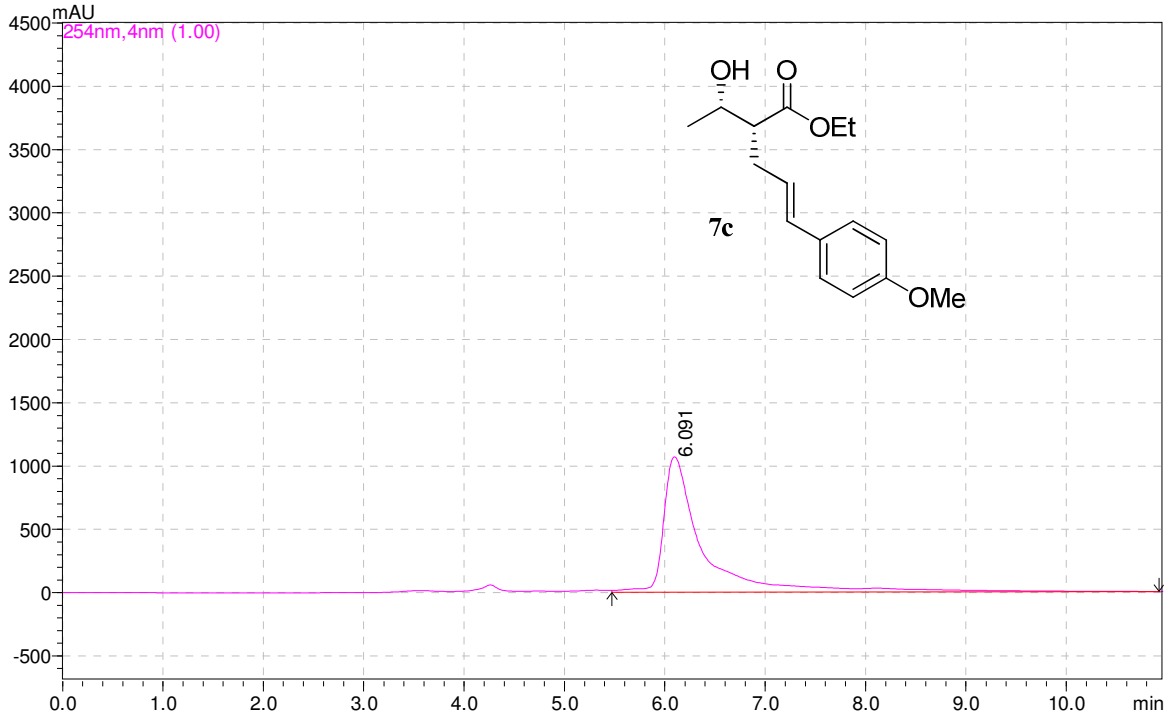
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	3.222	2.81	65555	5245	2.81
2	5.996	14.98	363466	34676	14.98
3	7.099	16.75	498664	39037	16.75
4	7.977	32.78	900928	95732	32.78
5	8.831	32.68	1005636	71450	32.68

Sample name: Rashmita 4-OMe cinnamyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

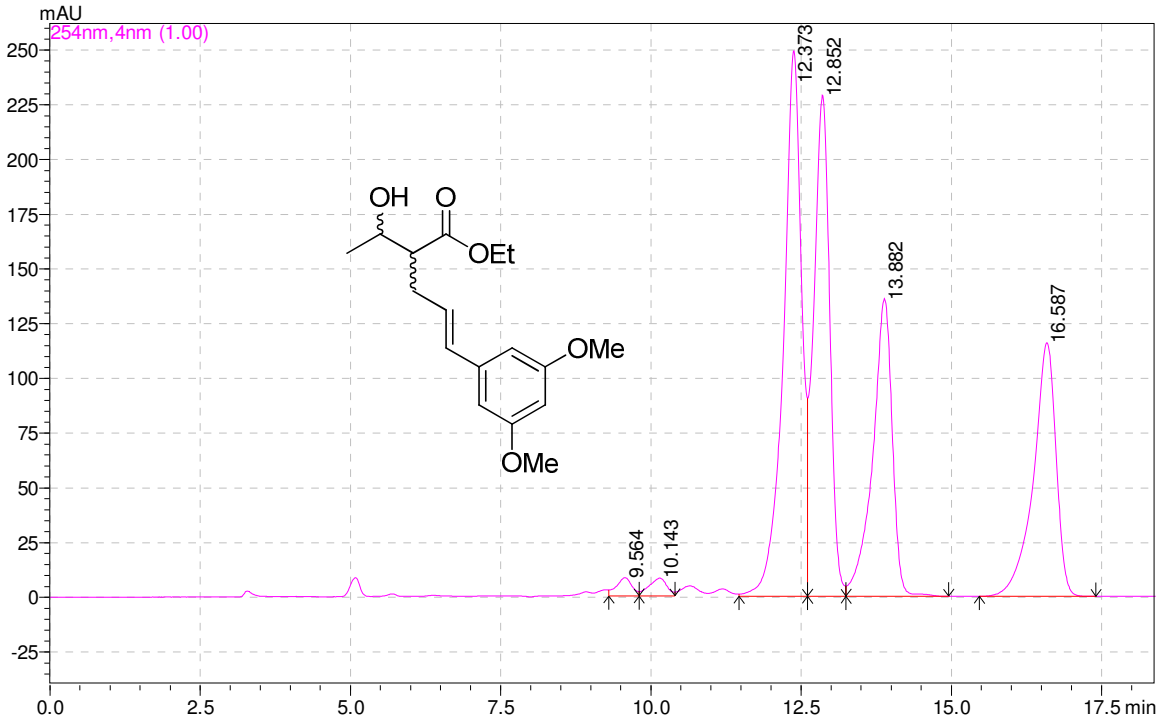
Peak#	Ret time	Conc	area	Height	Area (%)
1	6.091	100.00000	29274898	1069543	100

Sample name: Rashmita 3,5-diOMe cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



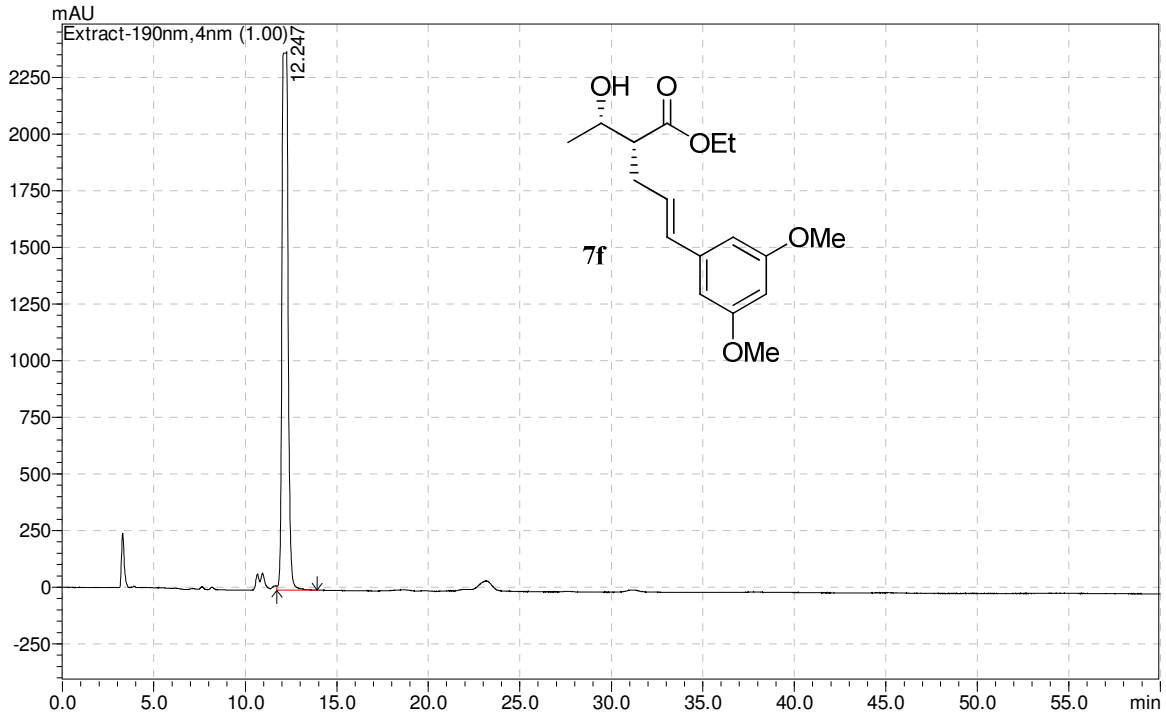
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	9.564	0.94	148394	8315	0.94
2	10.143	1.22	169182	8124	1.22
3	12.373	29.88	5243338	248962	29.88
4	12.852	29.62	4243615	228780	29.62
5	13.882	19.22	3049582	116237	19.22
5	16.587	19.12	3048565	115816	19.12

Sample name: Rashmita 3,5-diOMe cinnamyl with NBRC 3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 190nm 4nm

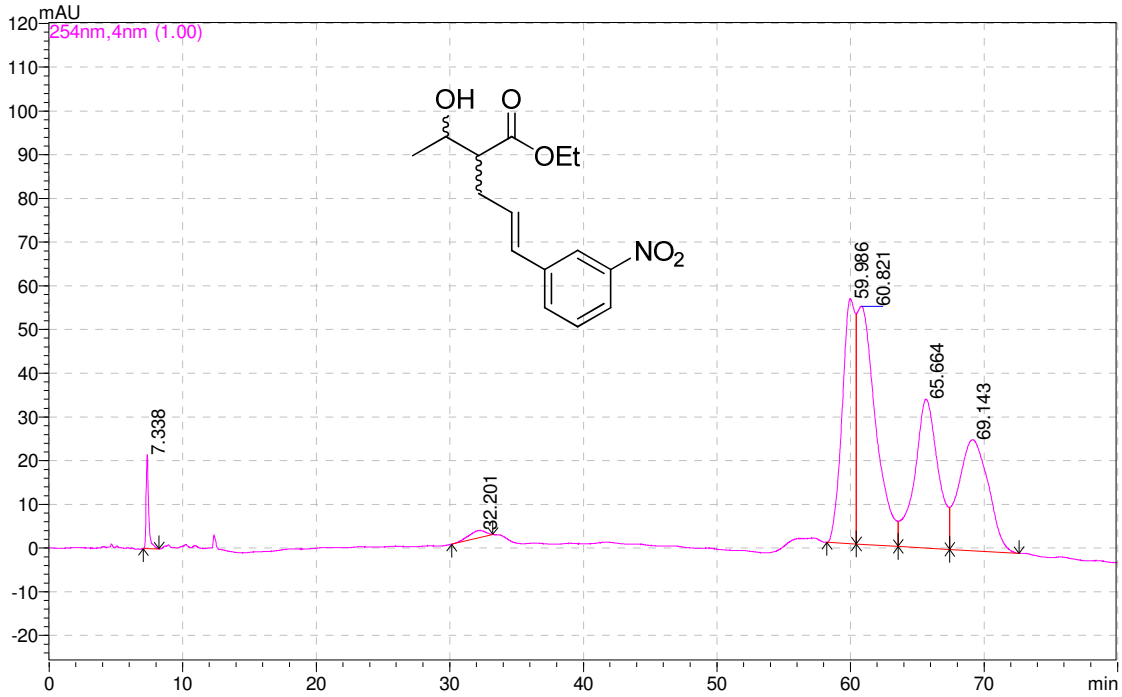
Peak#	Ret time	Conc	area	Height	Area (%)
1	12.247	100.00000	55318232	2377239	100

Sample name: Rashmita 3-NO_2-cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



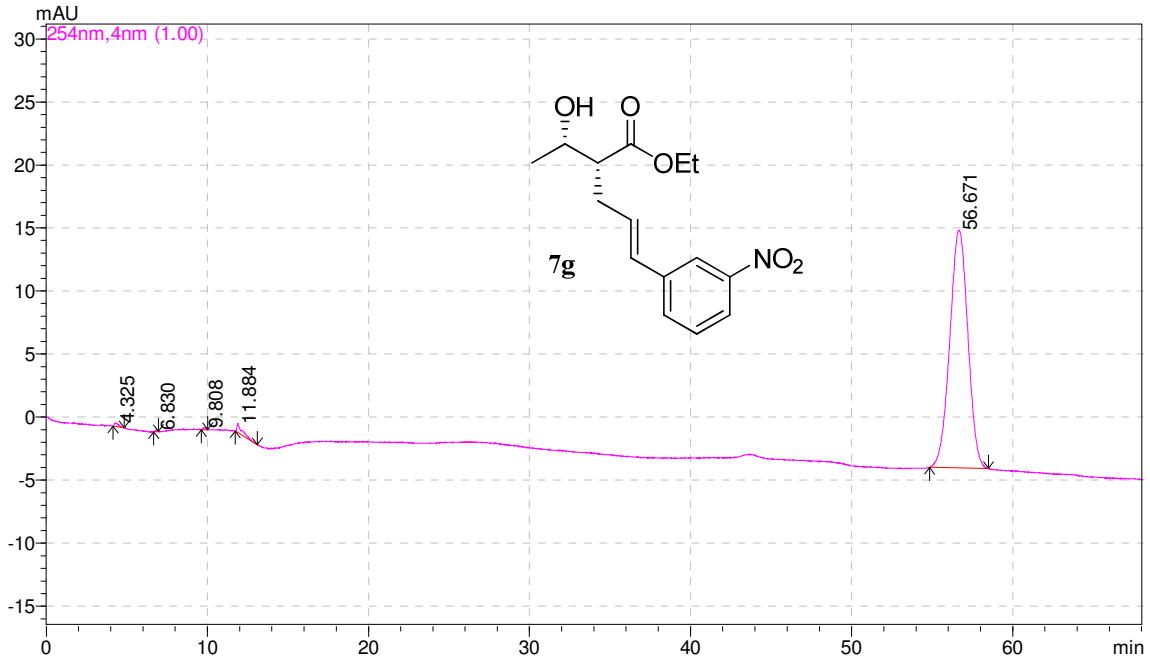
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	7.338	1.62	286509	21508	1.62
2	32.201	0.83	147320	1661	0.83
3	59.986	22.59	3812370	56096	22.59
4	60.821	28.60	5335049	54461	28.60
5	65.664	23.22	4174629	34037	23.22
6	69.143	23.14	3912073	25427	23.14

Sample name: Rashmita 3-NO_2-cinnamyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

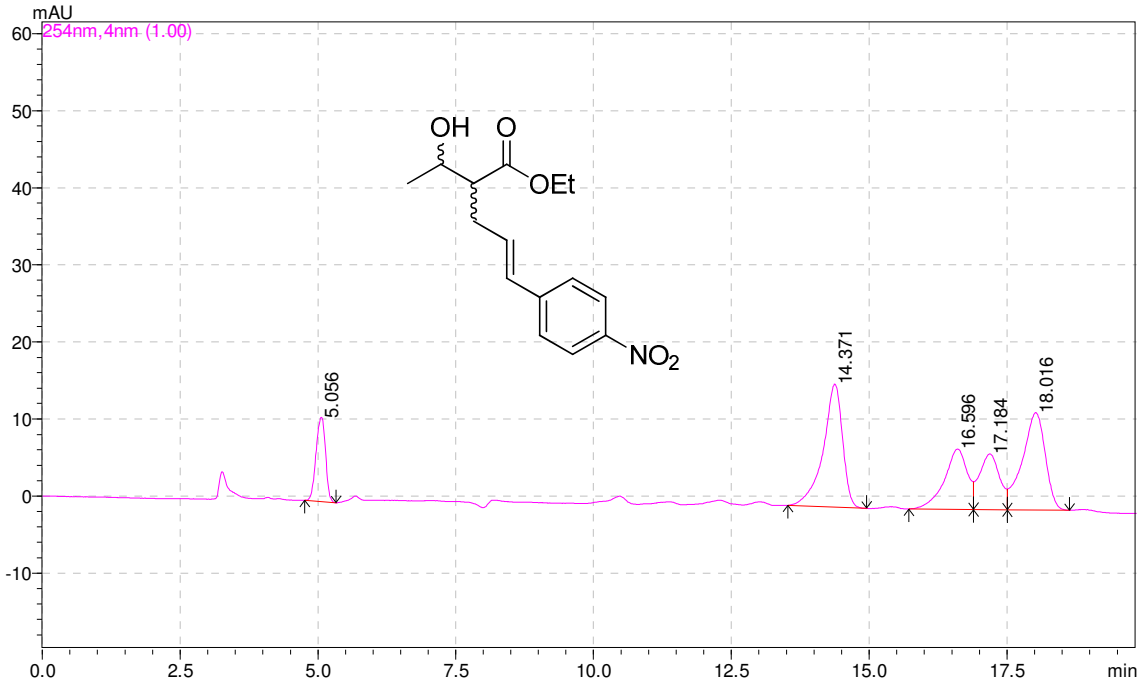
Peak#	Ret time	Conc	area	Height	Area (%)
1	4.325	0.25	5136	277	0.25
2	6.830	0.06	1280	145	0.06
3	9.808	0.09	1997	183	0.09
4	11.884	0.85	17085	702	0.85
5	56.671	98.75	1471685	18868	98.75

Sample name: Rashmita 4- NO_2-cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



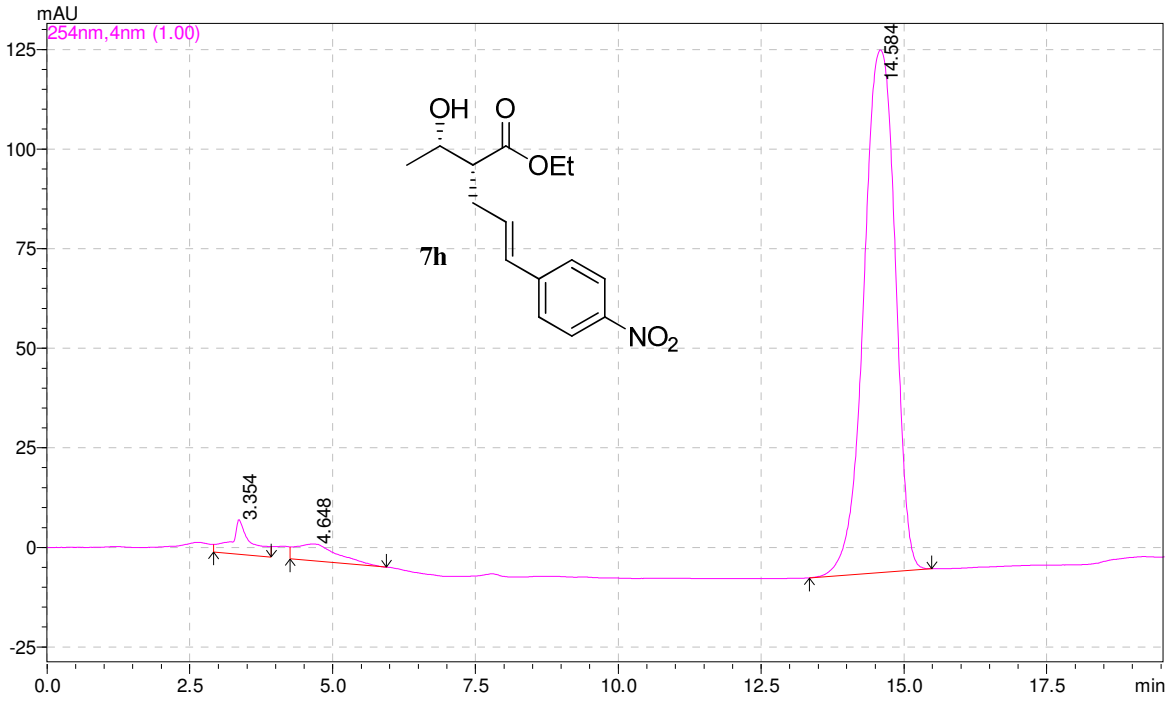
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	5.056	10.12	131631	10943	10.12
2	14.371	29.86	388884	15956	29.86
3	16.596	15.68	230247	7853	15.68
4	17.184	15.23	18531	7237	15.23
5	18.016	29.11	366114	12635	29.11

Sample name: Rashmita 4- NO_2-cinnamyl with NBRC 3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

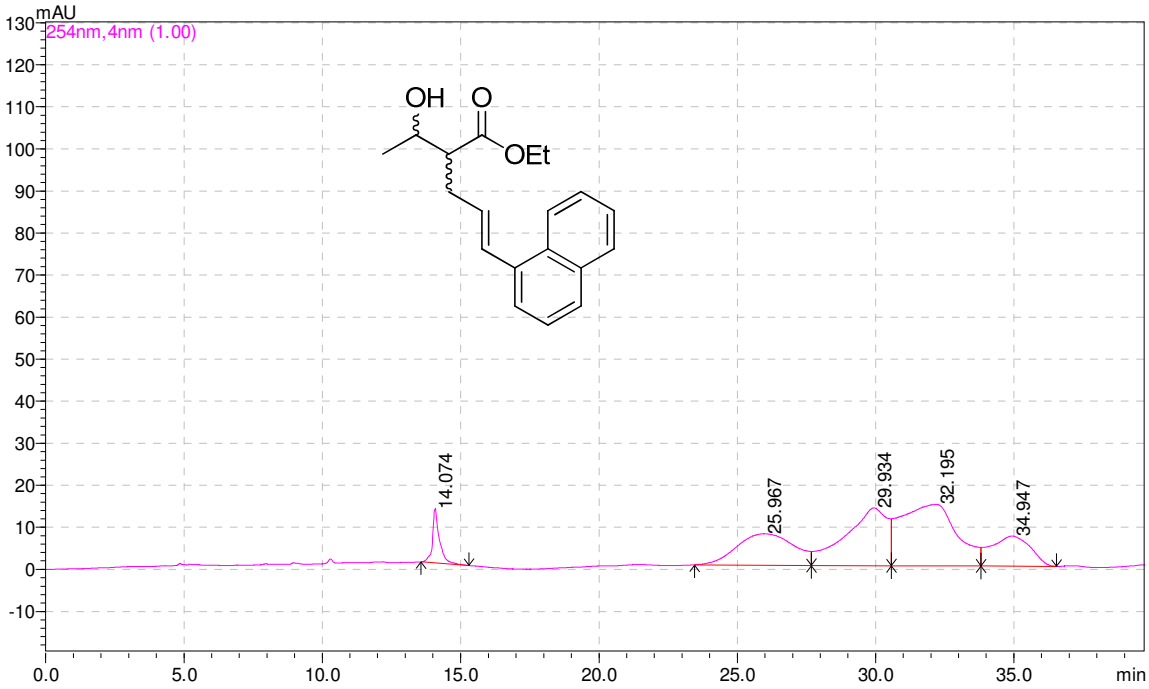
Peak#	Ret time	Conc	area	Height	Area (%)
1	3.354	3.92	212675	8650	3.92
2	4.648	3.97	215802	4239	3.97
3	14.584	92.11	5003250	131182	92.11

Sample name: Rashmita 1-naphthyl cinnamyl with $NaBH_4$

Column: CHIRALPAK IC; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



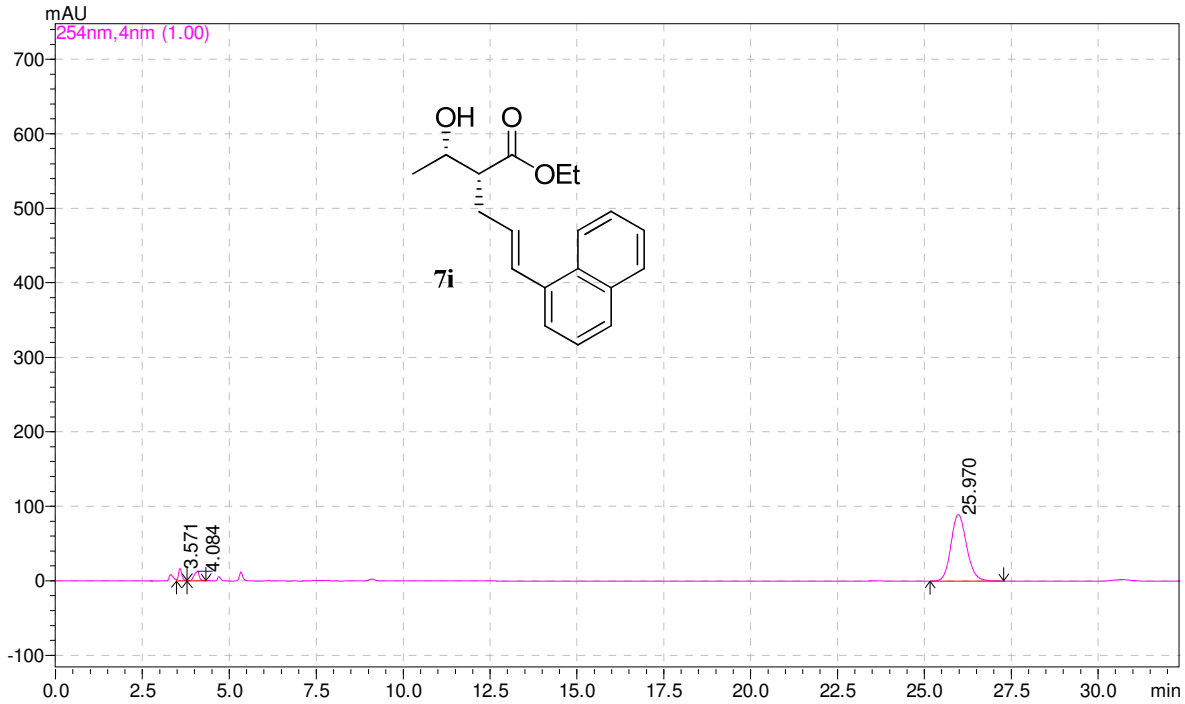
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	14.074	4.12	226853	12903	4.12
2	25.967	17.40	1073158	7459	17.40
3	29.934	27.25	1451666	13724	27.25
4	32.195	34.34	2064785	14679	34.34
5	34.947	16.89	713073	7208	16.89

Sample name: Rashmita 1-naphthyl cinnamyl with NBRC 3319

Column: CHIRALPAK IC; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

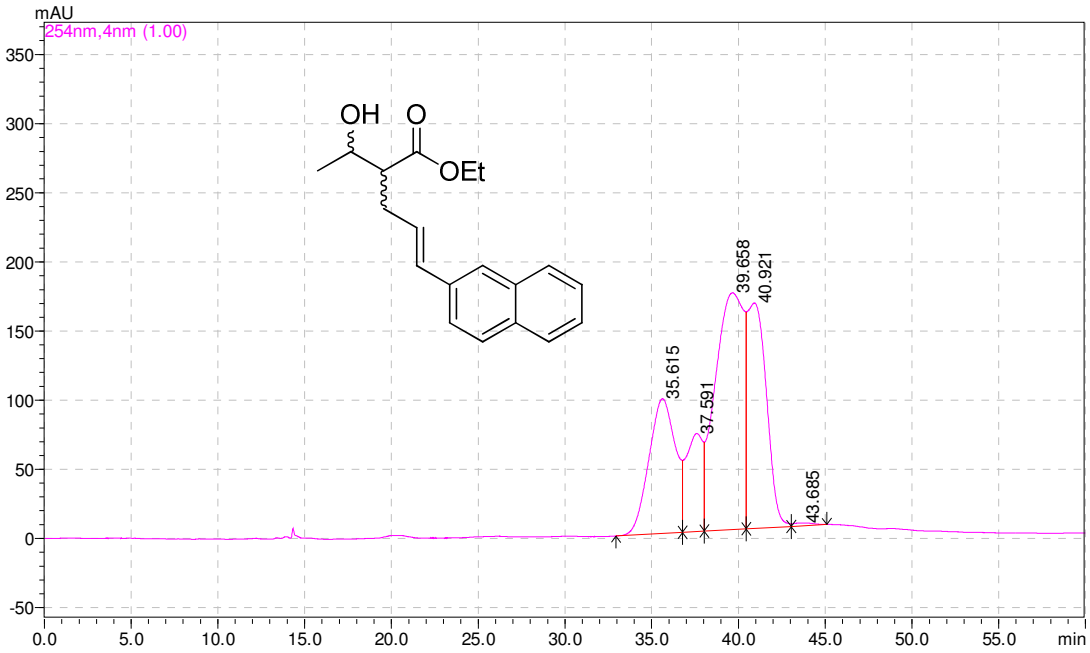
Peak#	Ret time	Conc	area	Height	Area (%)
1	3.571	3.69	111221	16563	3.69
2	4.084	4.41	133103	12884	4.41
3	25.970	91.90	2768238	89113	91.90

Sample name: Rashmita 2-naphthyl cinnamyl with $NaBH_4$

Column: CHIRALPAK IC; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



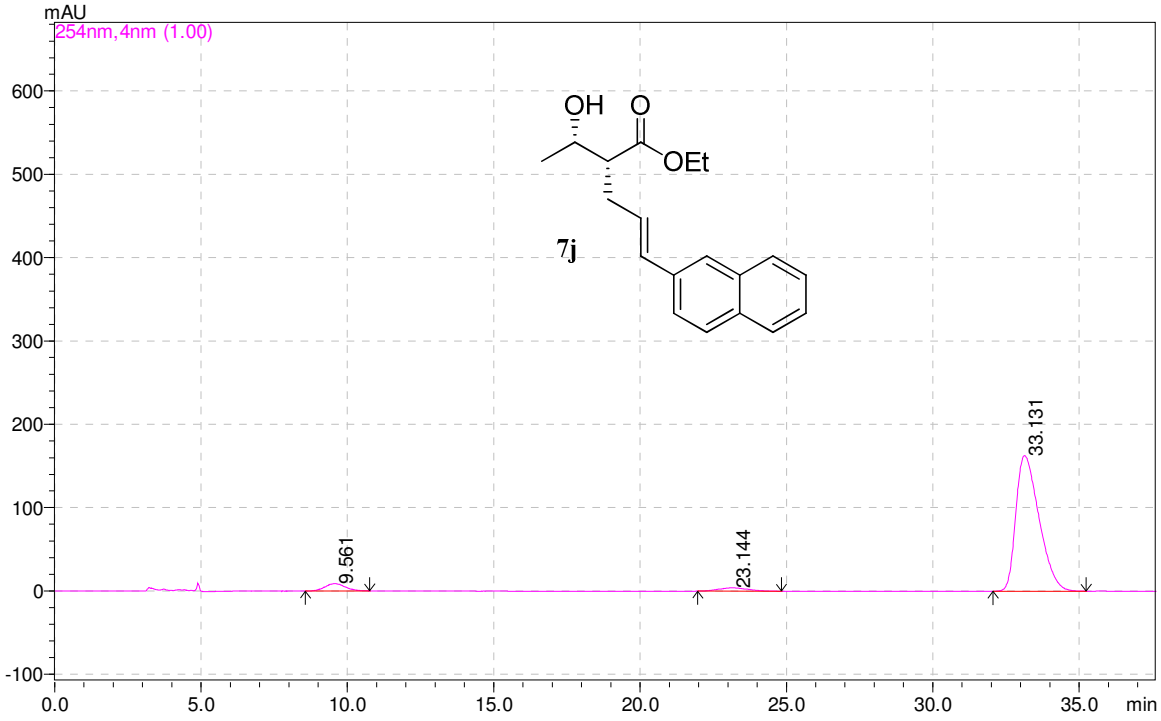
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	35.615	21.83	10390352	97437	21.83
2	37.591	12.98	4749236	70967	12.98
3	39.658	36.37	19687025	171268	36.37
4	40.921	28.45	12586259	163067	28.45
5	43.685	0.37	163327	2069	0.37

Sample name: Rashmita 2-naphthyl cinnamyl with NBRC 3319

Column: CHIRALPAK IC; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

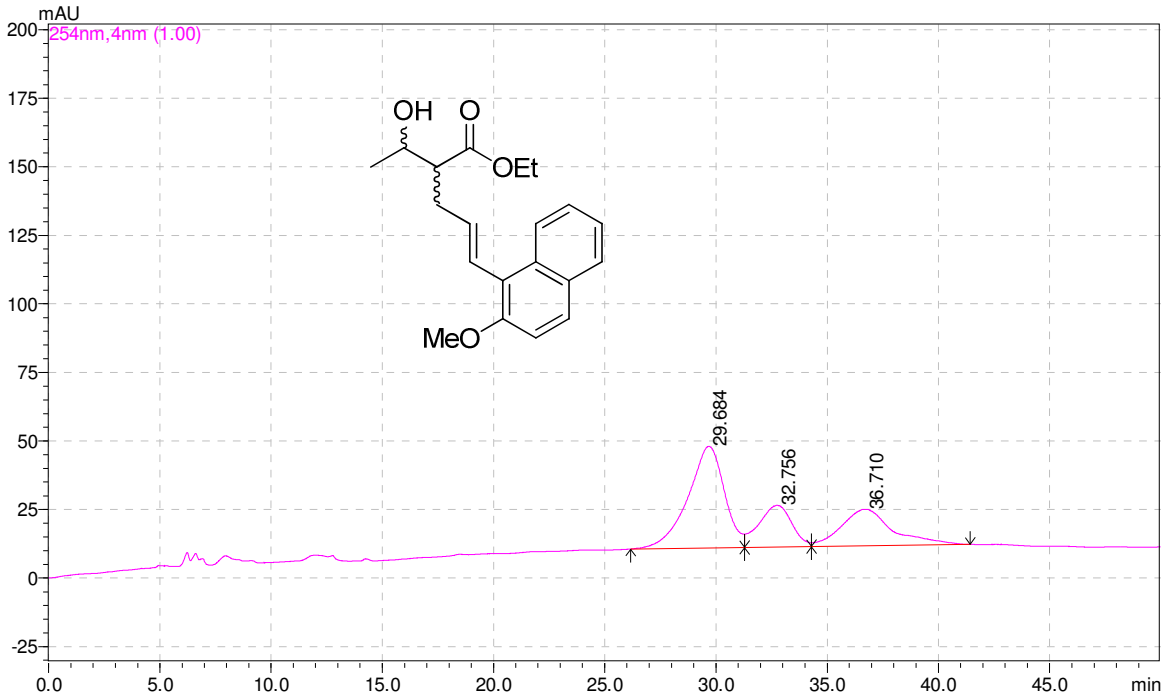
Peak#	Ret time	Conc	area	Height	Area (%)
1	9.561	4.31	415415	8747	4.31
2	23.144	2.69	259332	3834	2.69
3	33.131	93.0	8951592	162548	93.0

Sample name: Rashmita 2OMe-1-naphthyl cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



PDA Ch1 254nm 4nm

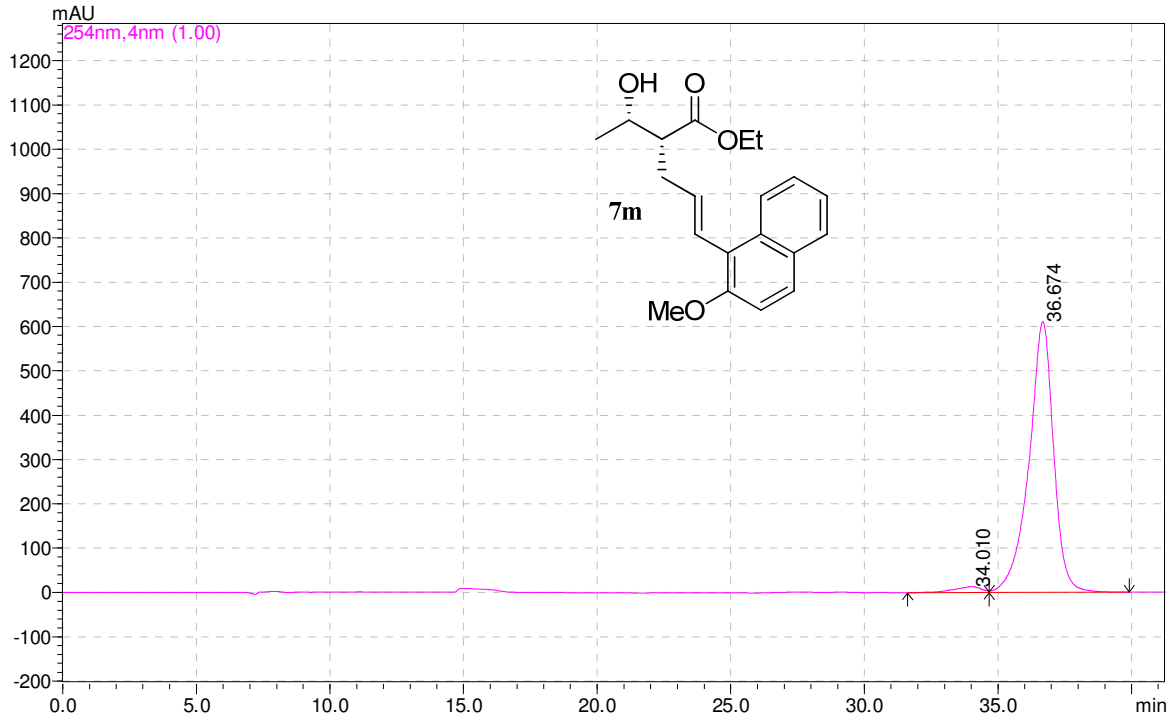
Peak#	Ret time	Conc	area	Height	Area (%)
1	29.684	50.26	4238799	37085	50.26
2	32.756	22.72	1568345	15235	22.72
3	36.710	27.02	2151060	13362	27.02

The peak at 29.684 corresponds to two stereoisomers, and we are unable to separate it (Chiral pak IA, IB, IC, OD, OB, OJ, AD, AS and Lux cellulose-1, cellulose-2, cellulose-3, cellulose-4, amylose-1 was used as a stationary phase).

Sample name: Rashmita 2OMe-1-naphthyl cinnamyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



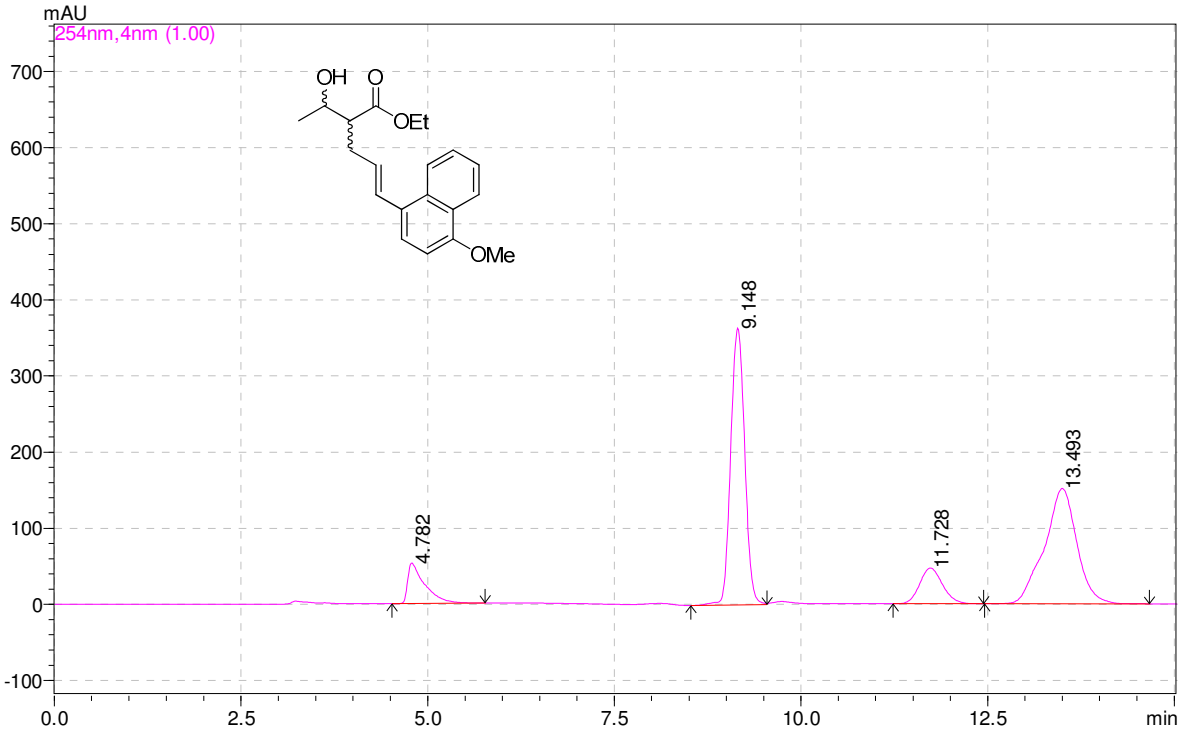
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	34.010	1.51	1013364	13885	1.31
2	36.674	98.49	39343638	610981	98.49

Sample name: Rashmita 4-OMe-1-naphthyl cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



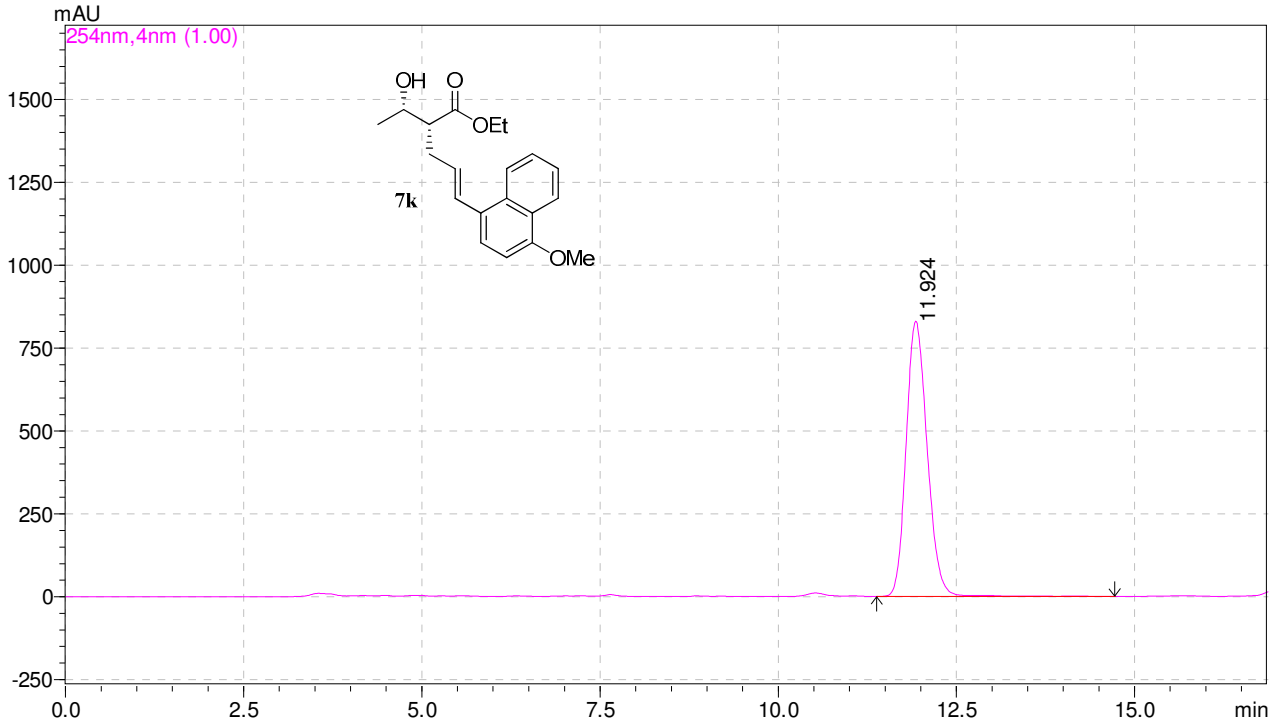
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	4.782	10.51	840183	53200	10.56
2	9.148	39.77	4747524	363624	39.77
3	11.728	10.55	1001133	46823	10.55
4	13.493	39.17	4588379	151534	39.17

Sample name: Rashmita 4-OMe-1-naphthyl cinnamyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



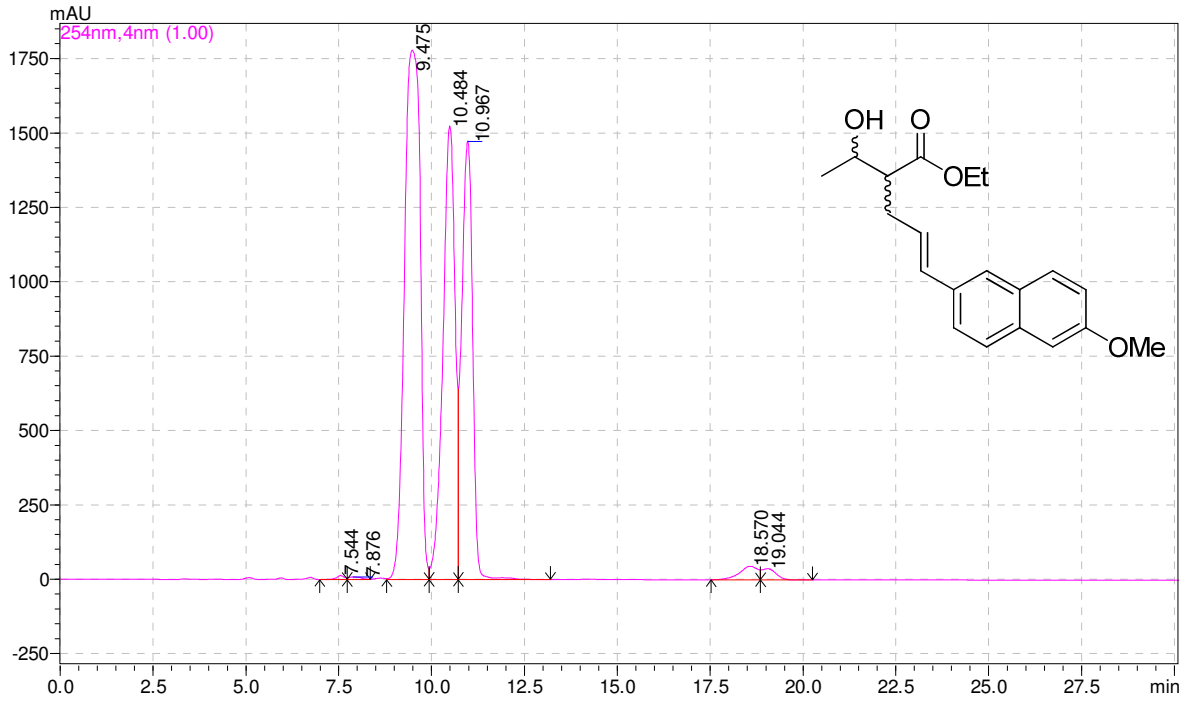
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	11.924	100.00000	17137545	830224	100

Sample name: Rashmita 6-OMe-2-naphthyl cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

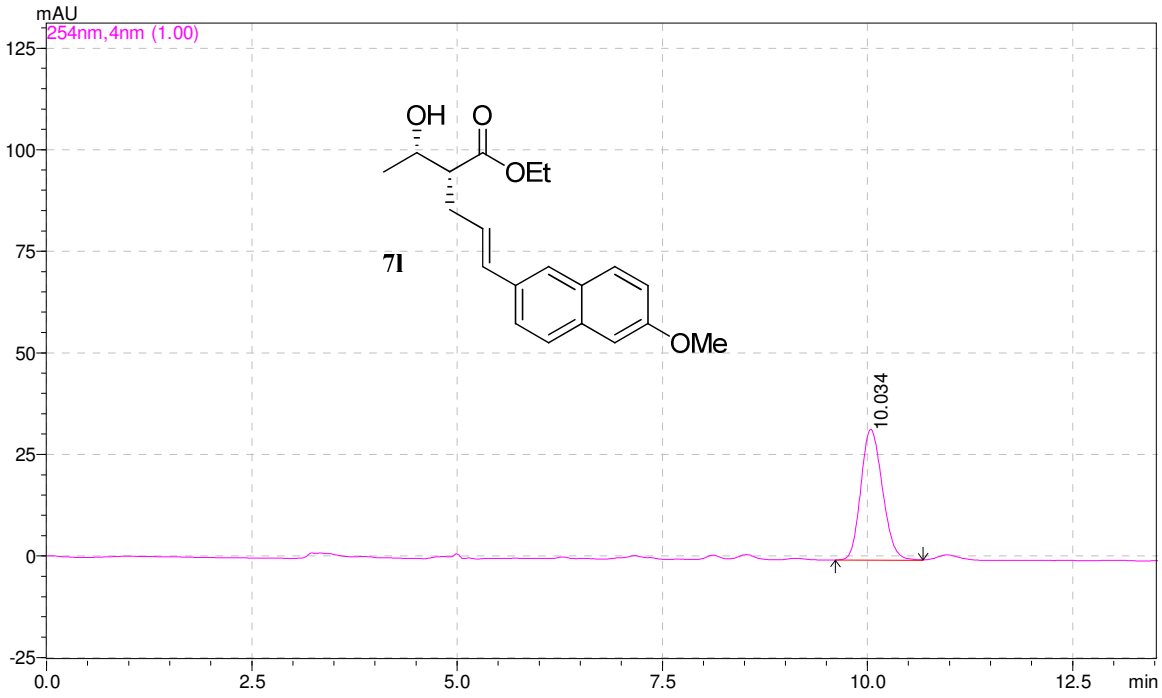
Peak#	Ret time	Conc	area	Height	Area (%)
1	7.544	0.15	187795	13243	0.15
2	7.876	0.16	194941	8272	0.16
3	9.475	43.81	52667194	1778996	43.81
4	10.484	26.90	34745520	1523359	26.90
5	10.967	26.81	29827442	1472695	26.81
6	18.570	1.33	1605532	45890	1.33
7	19.044	0.84	985941	37294	0.84

The peak at 9.475 corresponds to two stereoisomers, and we are unable to separate it (Chiral pak IA, IB, IC, OD, OB, OJ, AD, AS and Lux cellulose-1, cellulose-2, cellulose-3, cellulose-4, amylose-1 was used as a stationary phase).

Sample name: Rashmita 6-OMe-2-naphthyl cinnamyl with NBRC3319

Column: CHIRALPAK IA; Flow rate: 1.0 ml/min

Mobile phase: 90:10; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

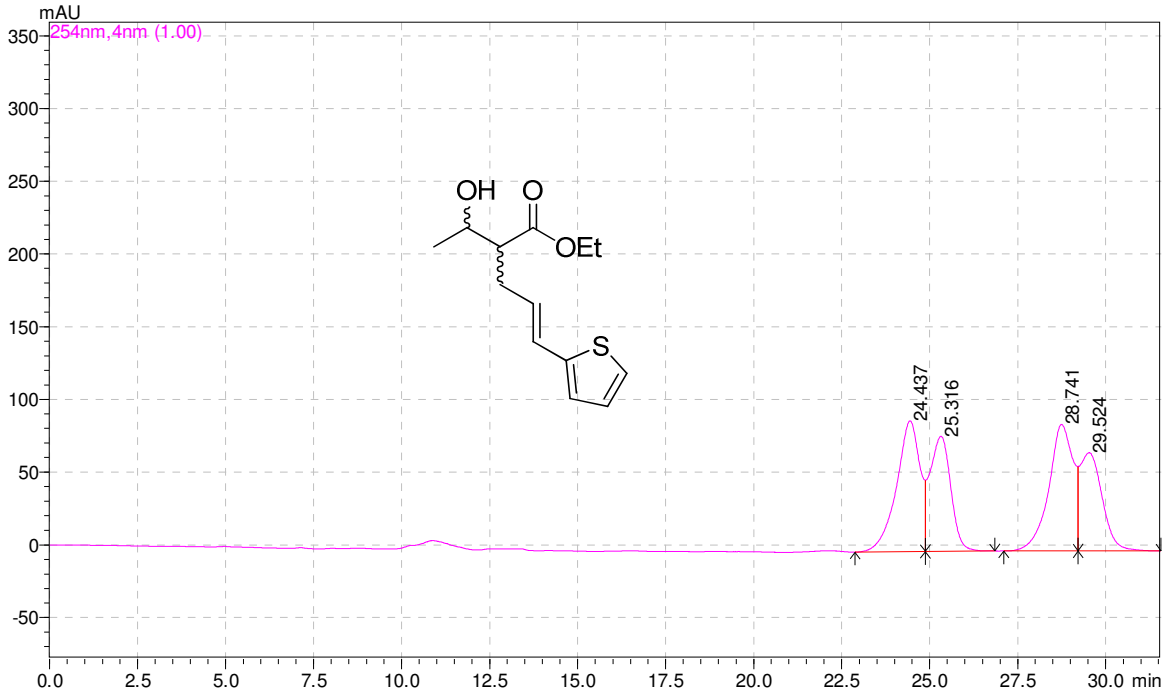
Peak#	Ret time	Conc	area	Height	Area (%)
1	10.034	100.00000	589356	32155	100

Sample name: Rashmita 2-thienyl cinnamyl with $NaBH_4$

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL

Additional information: Manually integrated



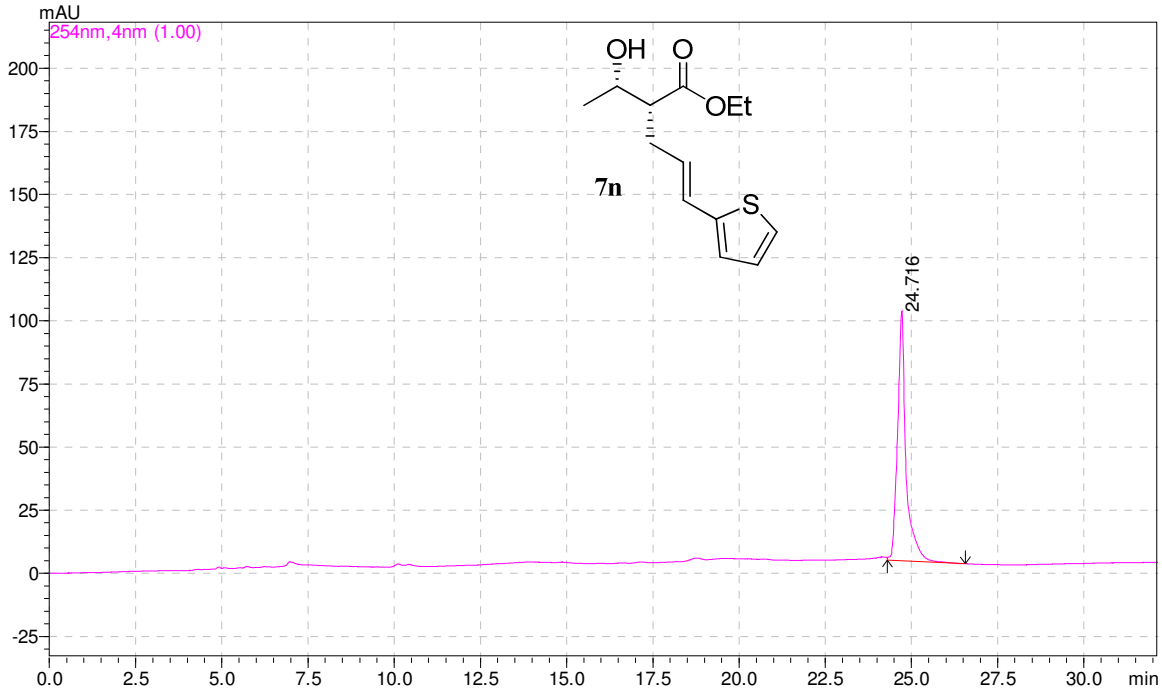
PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	24.437	26.63	4198134	89974	26.63
2	25.316	24.29	3867973	79247	24.29
3	28.741	26.92	4241355	87088	26.92
4	29.524	22.16	3453383	67620	22.16

Sample name: Rashmita 2-thienyl cinnamyl with NBRC 3319

Column: CHIRALPAK IA; Flow rate: 0.8 ml/min

Mobile phase: 98:2; hexane:IPA; Injection volume: 5µL



PDA Ch1 254nm 4nm

Peak#	Ret time	Conc	area	Height	Area (%)
1	24.716	100.00	1693663	98877	100