

Small molecule purine and pseudopurine derivatives: synthesis, cytostatic evaluations and investigation of growth inhibitory effect in non-small cell lung cancer A549

Andrea Bistrović^{a#}, Petra Grbčić^{b#}, Anja Harej^b, Mirela Sedić^{b*}, Sandra Kraljević-Pavelić^b, Sanja Koštrun^c, Janez Plavec^{d,e,f}, Damjan Makuc^{d,e} and Silvana Raić-Malić^{a*}

^aUniversity of Zagreb, Department of Organic Chemistry, Faculty of Chemical Engineering and Technology, Marulićev trg 20, HR-10000 Zagreb, Croatia; ^bUniversity of Rijeka, Department of Biotechnology, Center for High-Throughput Technologies, Ulica Radmile Matejčić 2, HR-51000 Rijeka, Croatia, ^cChemistry Department, Fidelta Ltd., Prilaz baruna Filipovića 29, HR-10000 Zagreb, Croatia, ^dSlovenian NMR Centre, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia; ^eEn-FIST Centre of Excellence, Trg Osvobodilne fronte 13, SI-1000 Ljubljana, Slovenia; ^fUniversity of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000 Ljubljana, Slovenia

*Corresponding Authors:

Tel.: 00385-1-4597-213. Fax.: 00385-1-4597-224. E-mail: sraic@fkit.hr;

Tel.: 00385-51-584-574. Fax: 00385-51-584-599. E-mail: mseidic@biotech.uniri.hr

#Equally contributed

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1. *In silico* analysis of biological targets for compound 12b

Table S1. Selected biological targets as predicted by PASS^a for compound 12b

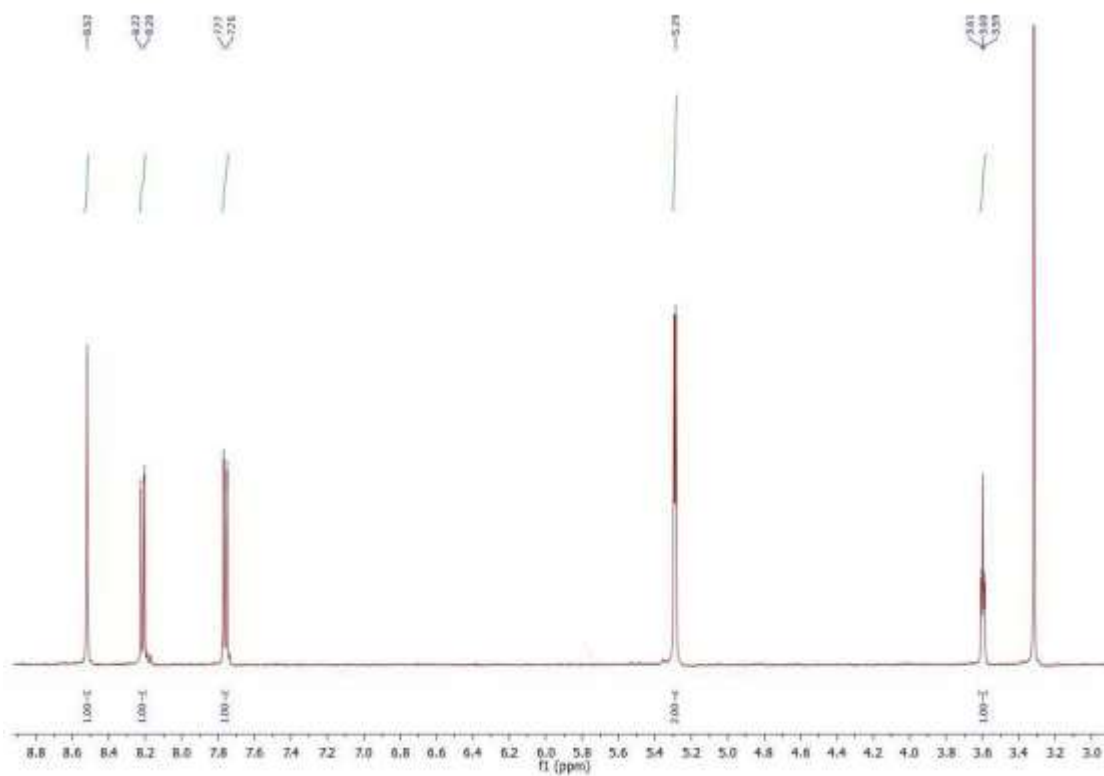
Biological targets	Pa	Pi
Glycosylphosphatidylinositol phospholipase D inhibitor	0.615	0.060
MAP kinase kinase inhibitor	0.331	0.003

^aActivity spectrum predicted by PASS is presented by the list of activities with the probabilities "to be active" (Pa) and "to be inactive" (Pi) calculated for each activity. Increased Pa and decreased Pi, the more probable is predicted activity. The list is arranged in descending order of Pa-Pi; therefore, more probable activities are at the top of the list.

2. NMR spectra of novel compounds

Fig. S2 a) ^1H NMR and b) ^{13}C NMR of compd. **2b**

a)



b)

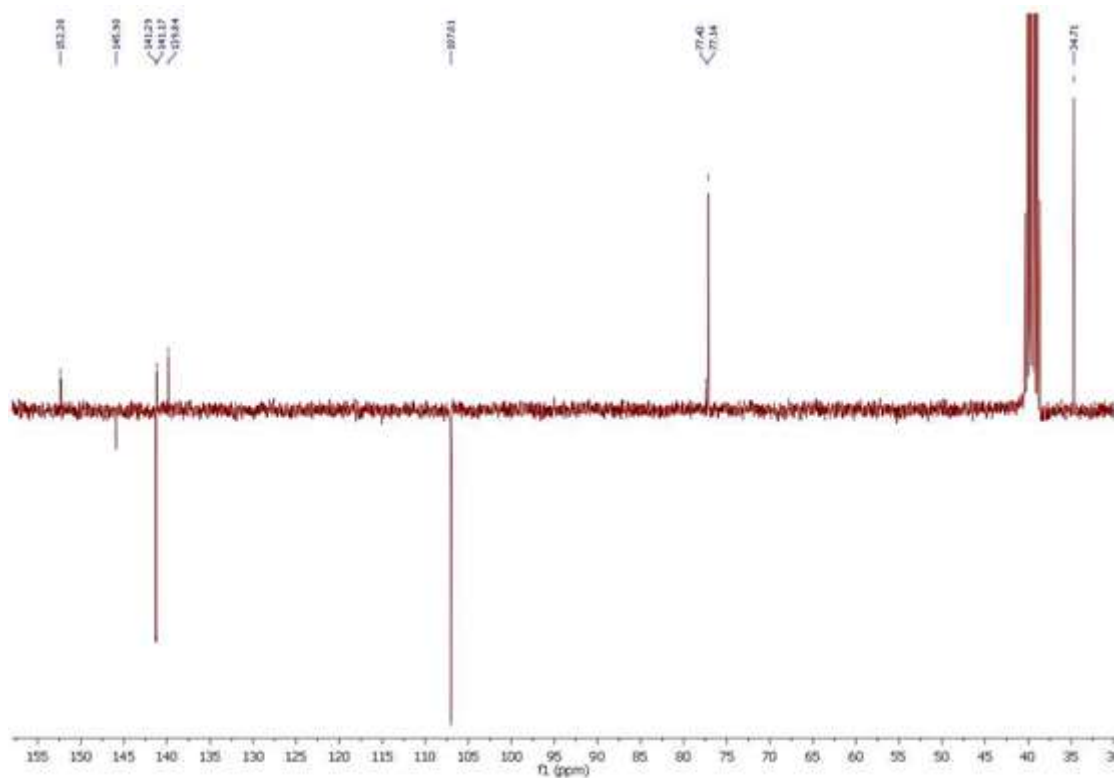
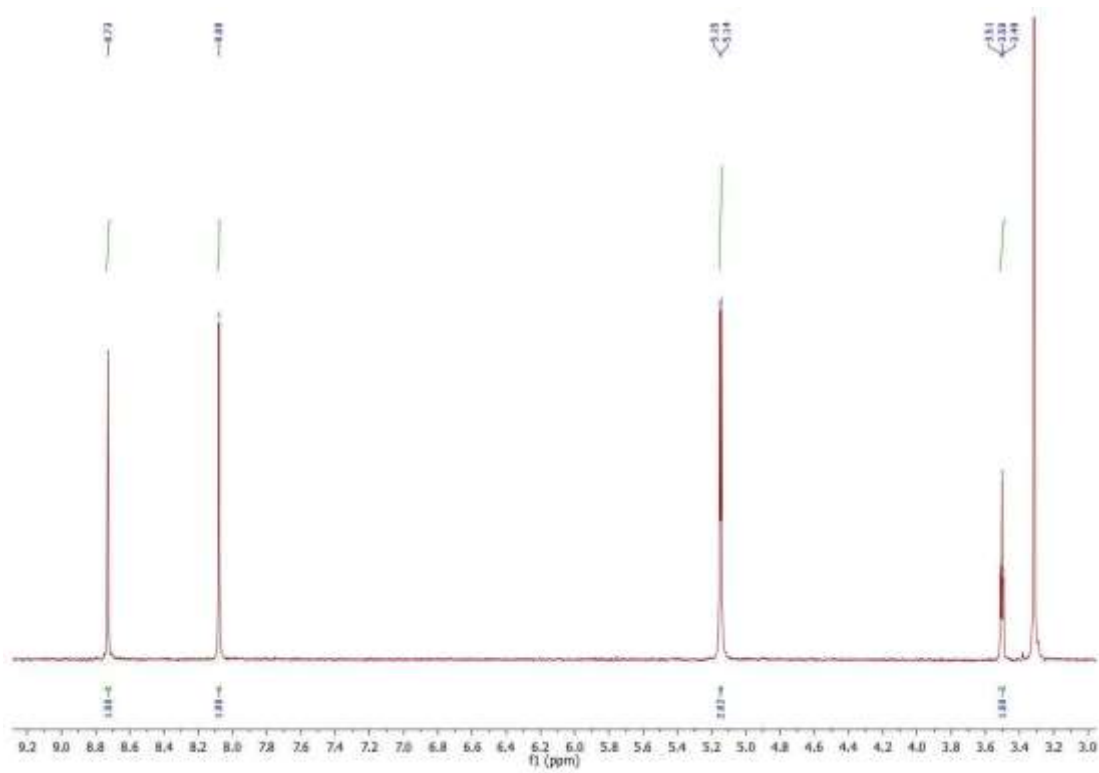


Fig. S3 a) ^1H NMR and b) ^{13}C NMR of compd. **2d**

a)



b)

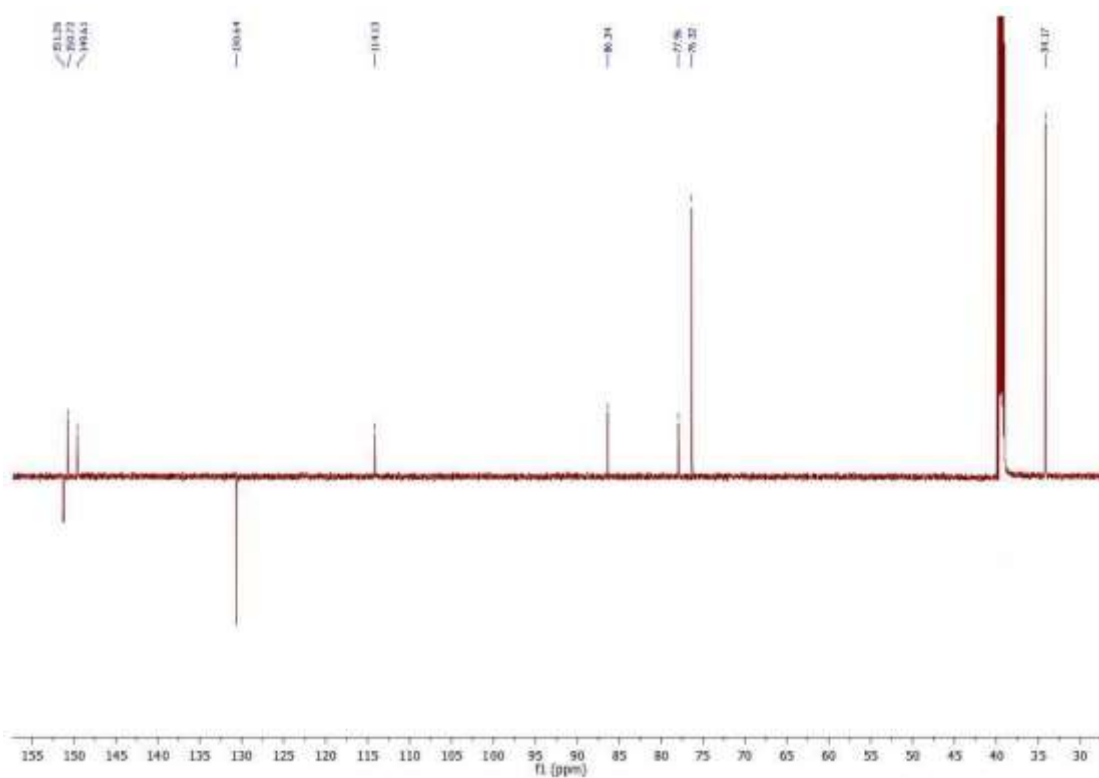
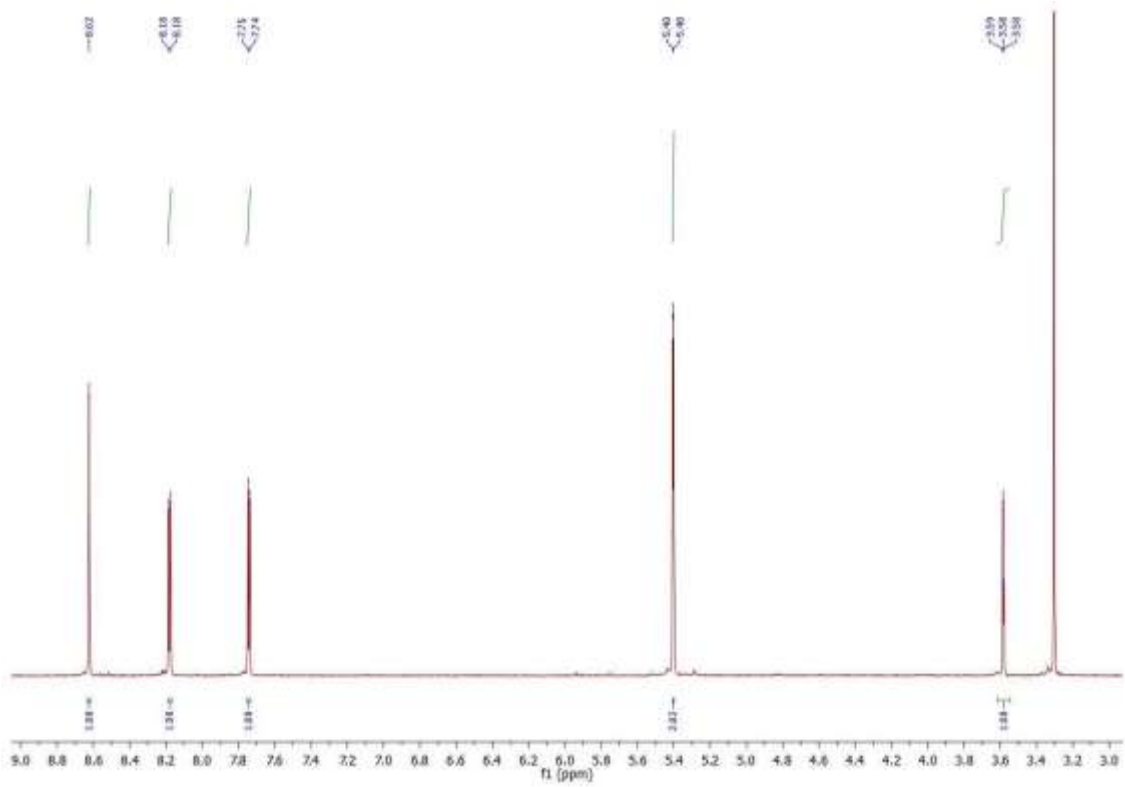


Fig. S4 a) ^1H NMR and b) ^{13}C NMR of compd. **3b**

a)



b)

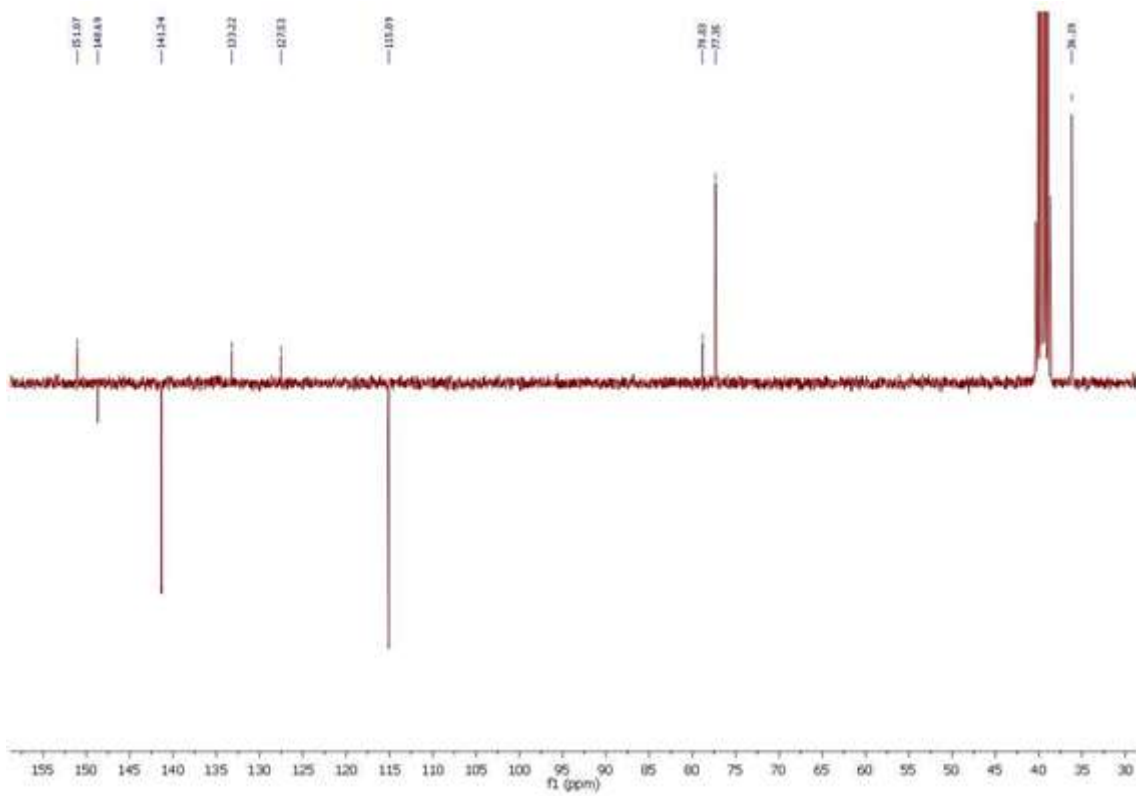
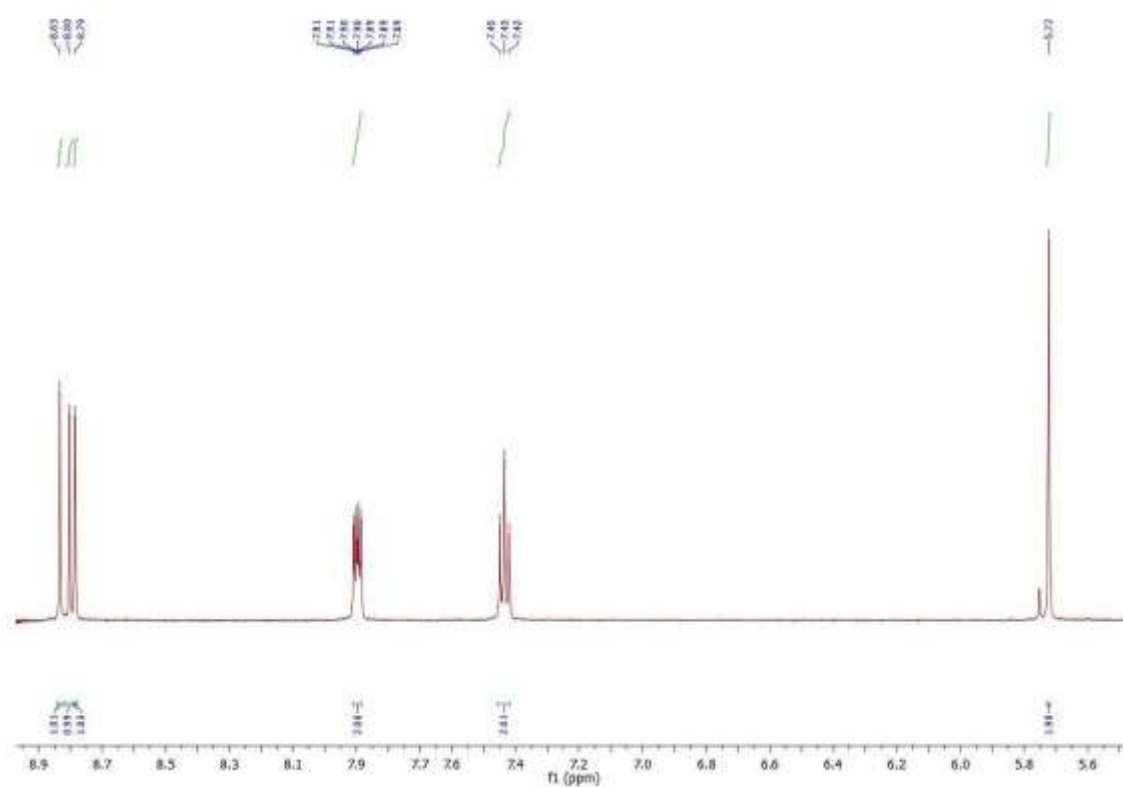


Fig. S5 a) ^1H NMR and b) ^{13}C NMR of compd. **4a**

a)



b)

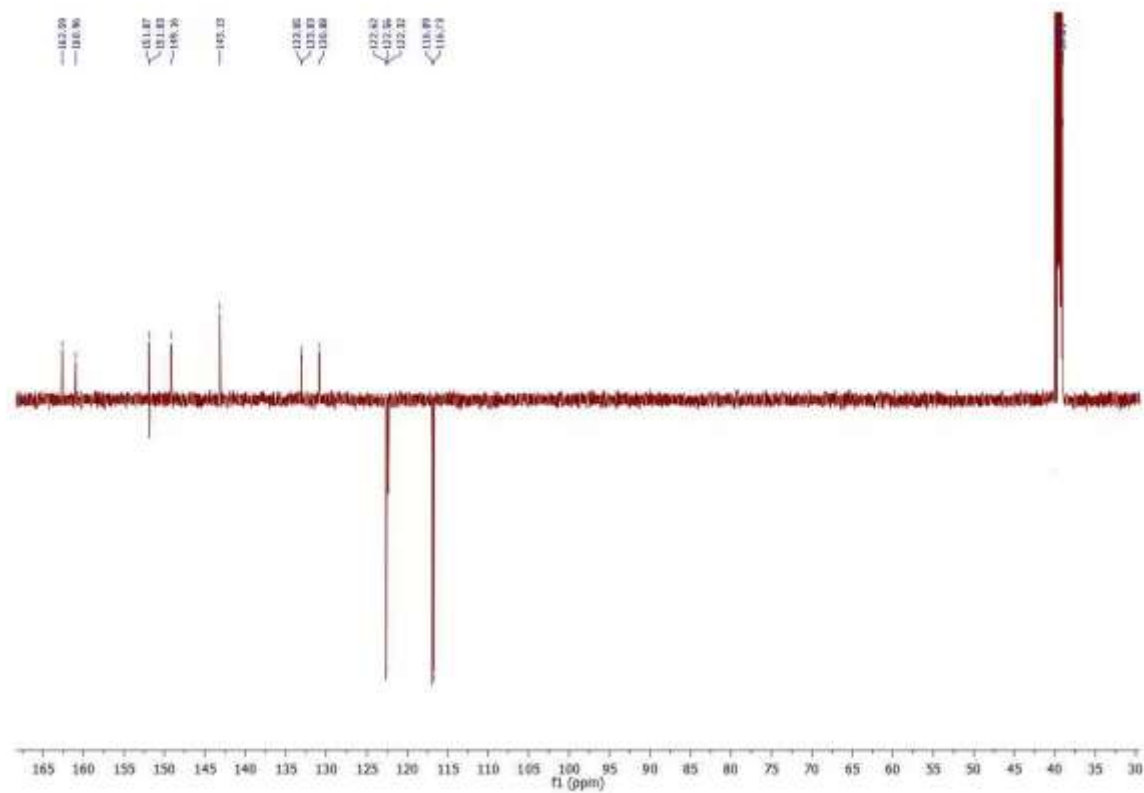
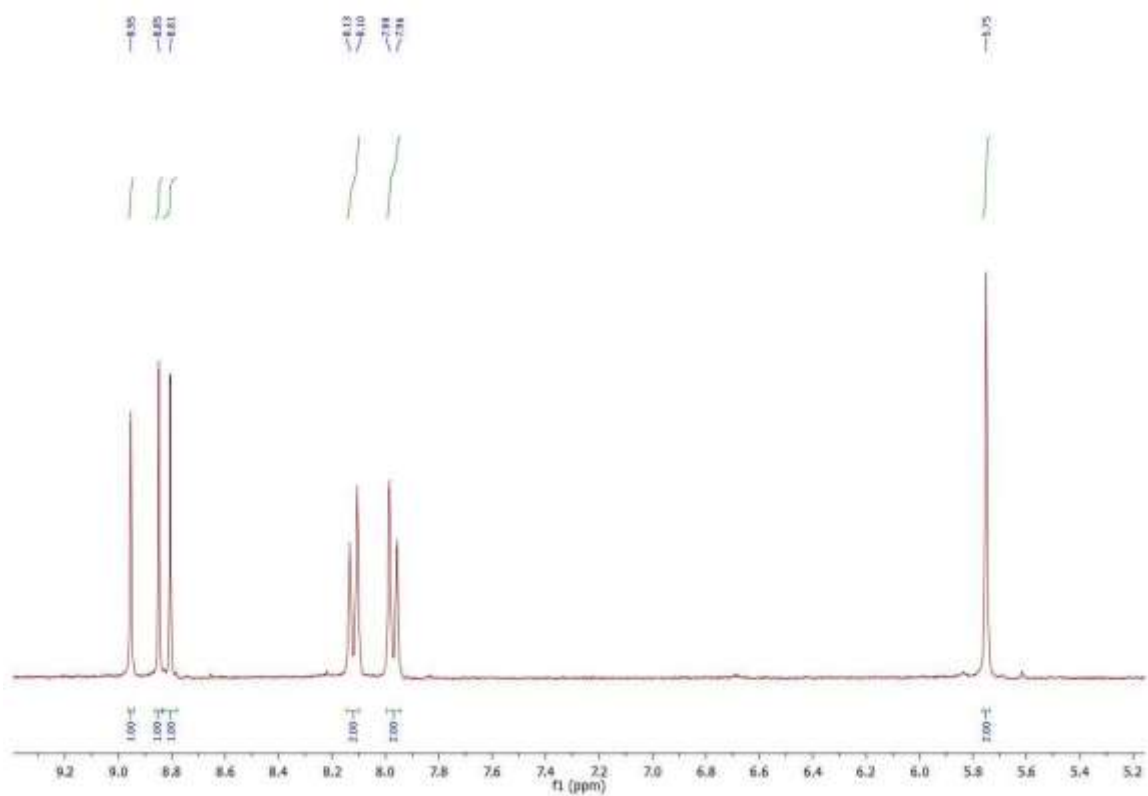


Fig. S6 a) ^1H NMR and b) ^{13}C NMR of compd. **4c**

a)



b)

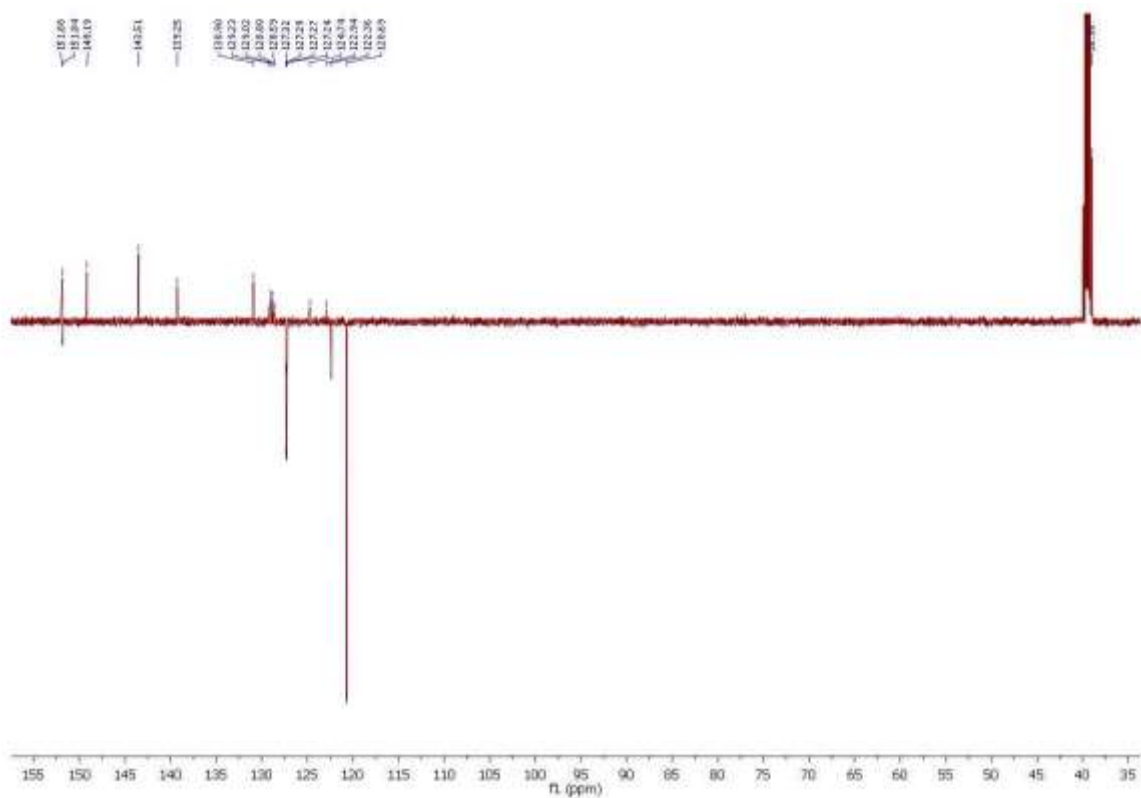
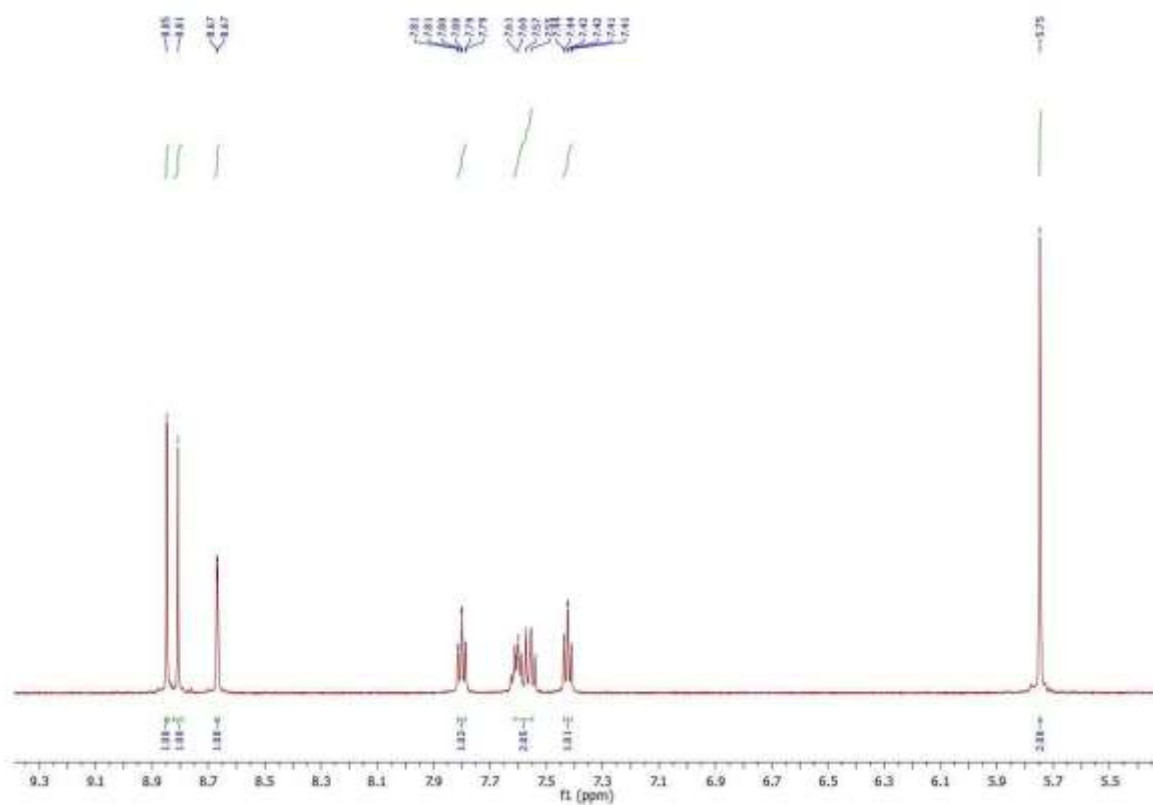


Fig. S7 a) ^1H NMR and b) ^{13}C NMR of compd. **4d**

a)



b)

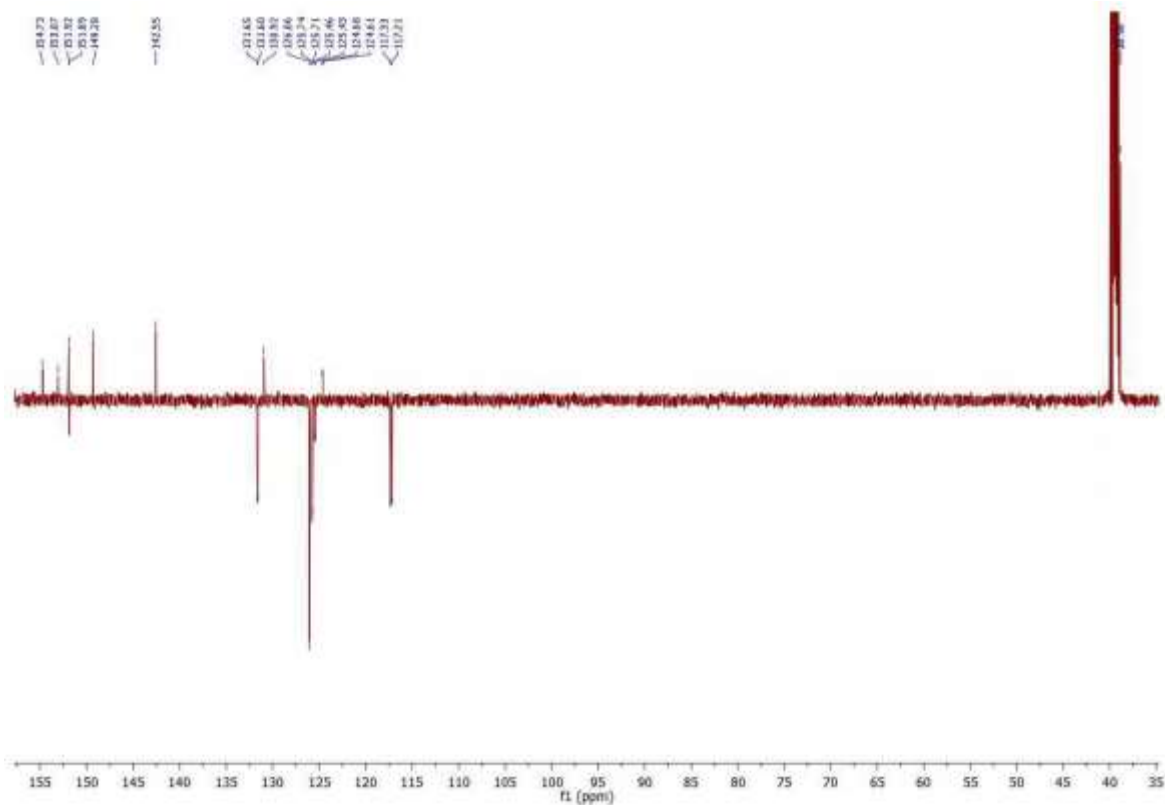
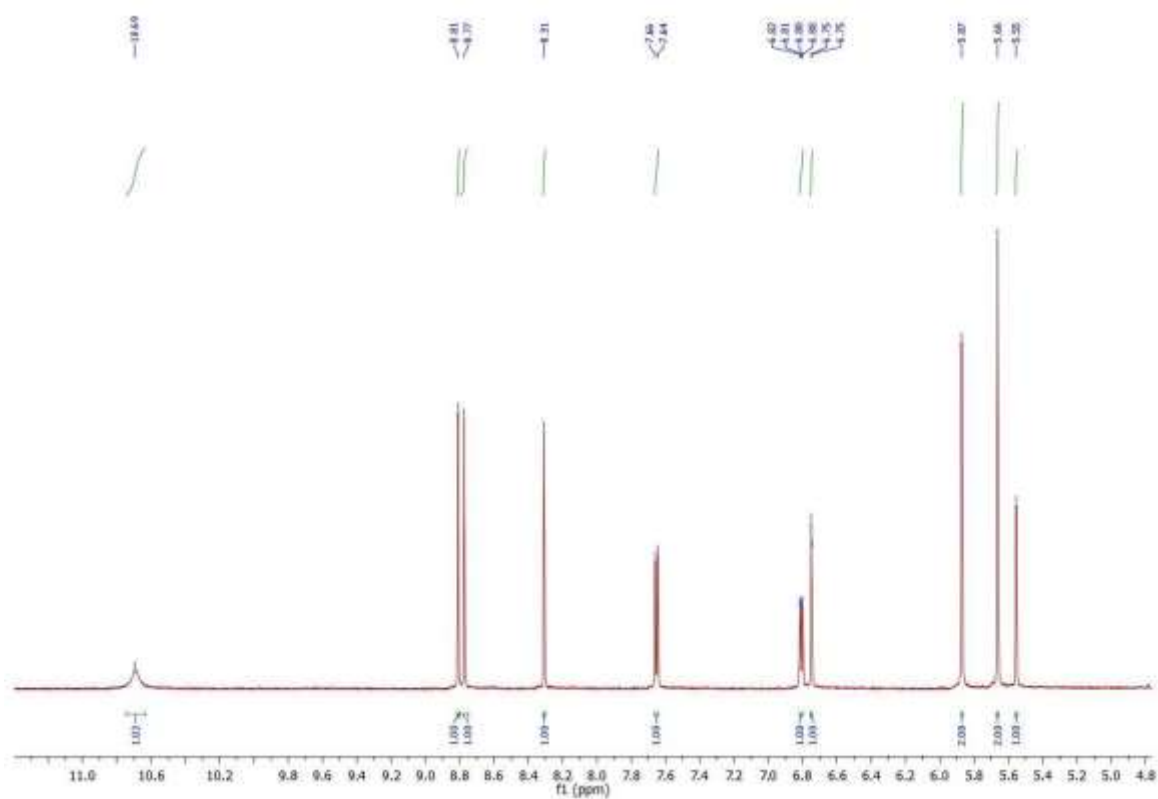


Fig. S8 a) ^1H NMR and b) ^{13}C NMR of compd. **4e**

a)



b)

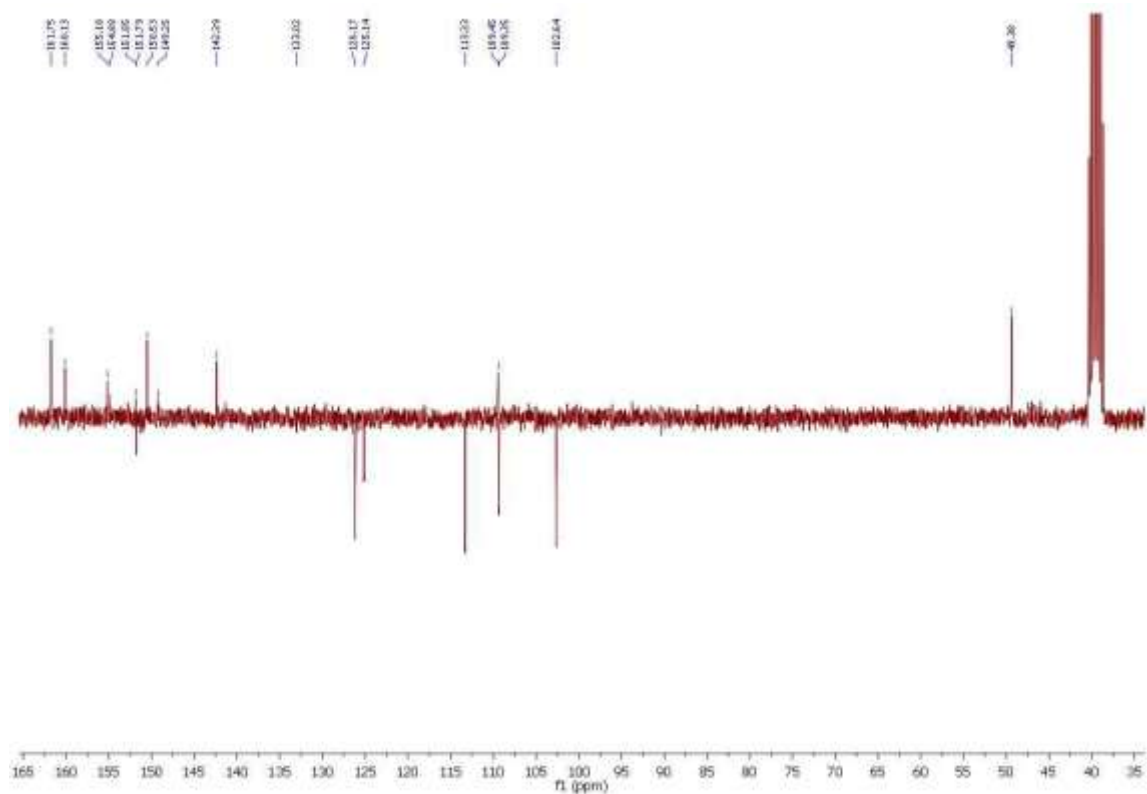
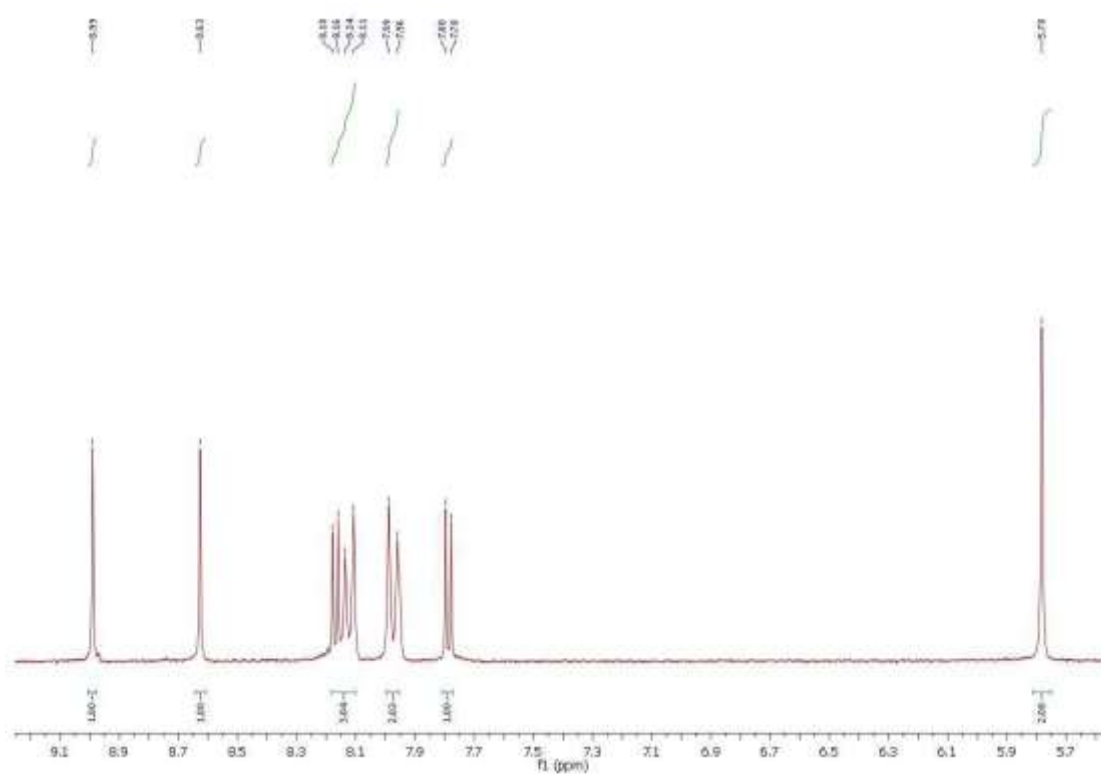


Fig. S9 a) ^1H NMR and b) ^{13}C NMR of compd. **5c**

a)



b)

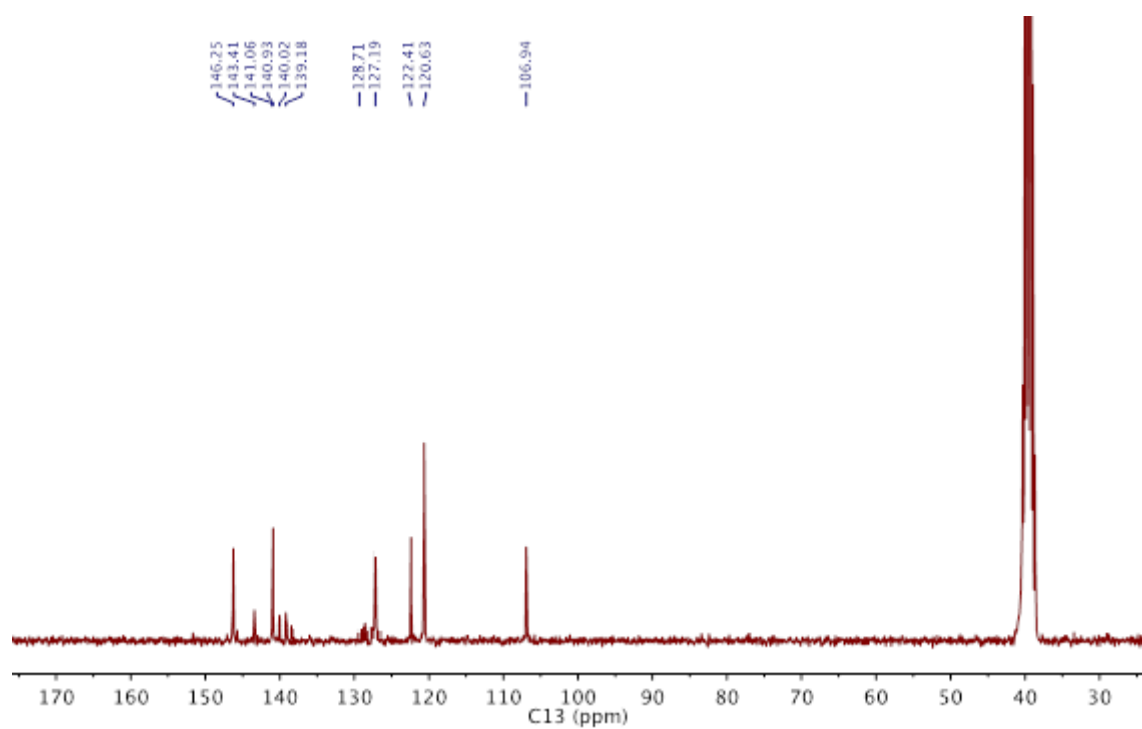
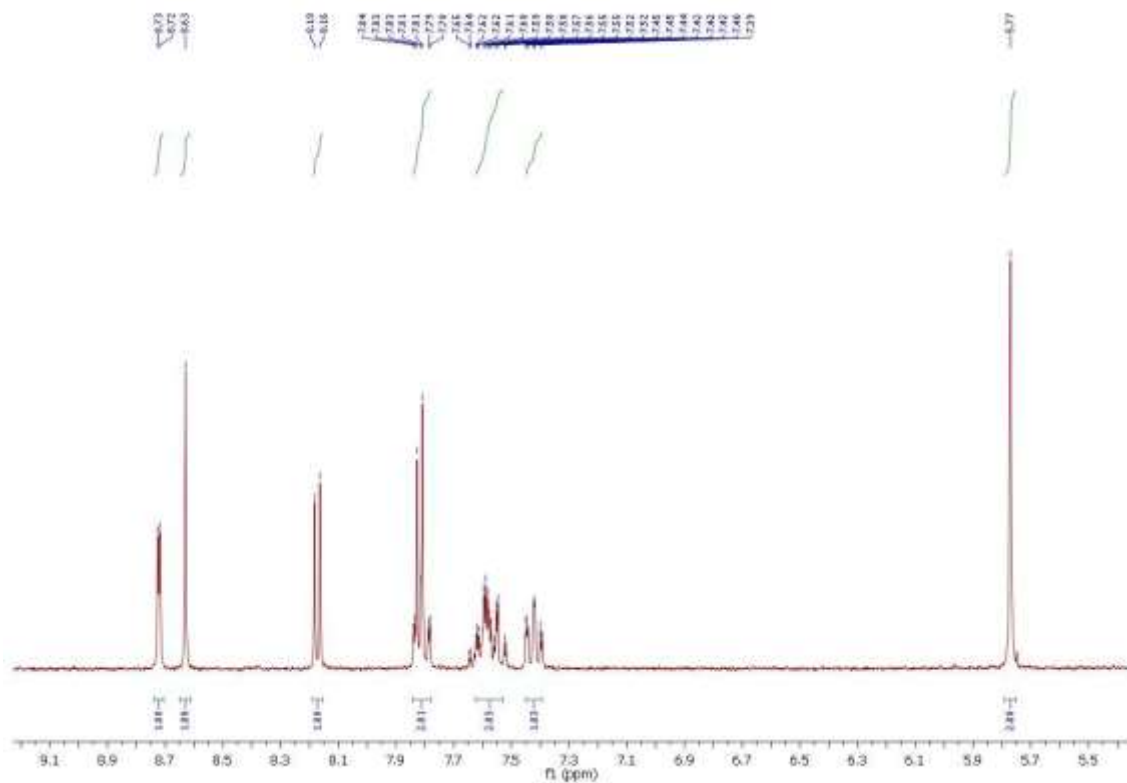


Fig. S10 a) ^1H NMR and b) ^{13}C NMR of compd. **5d**

a)



b)

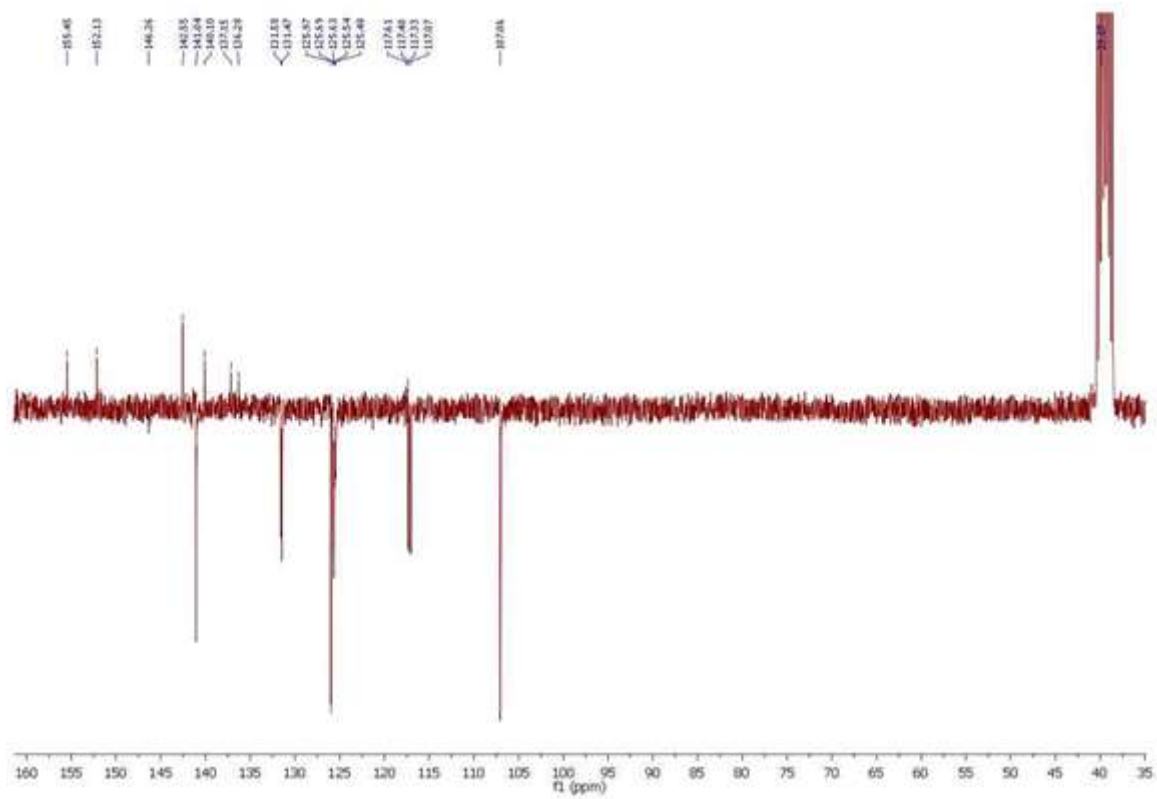
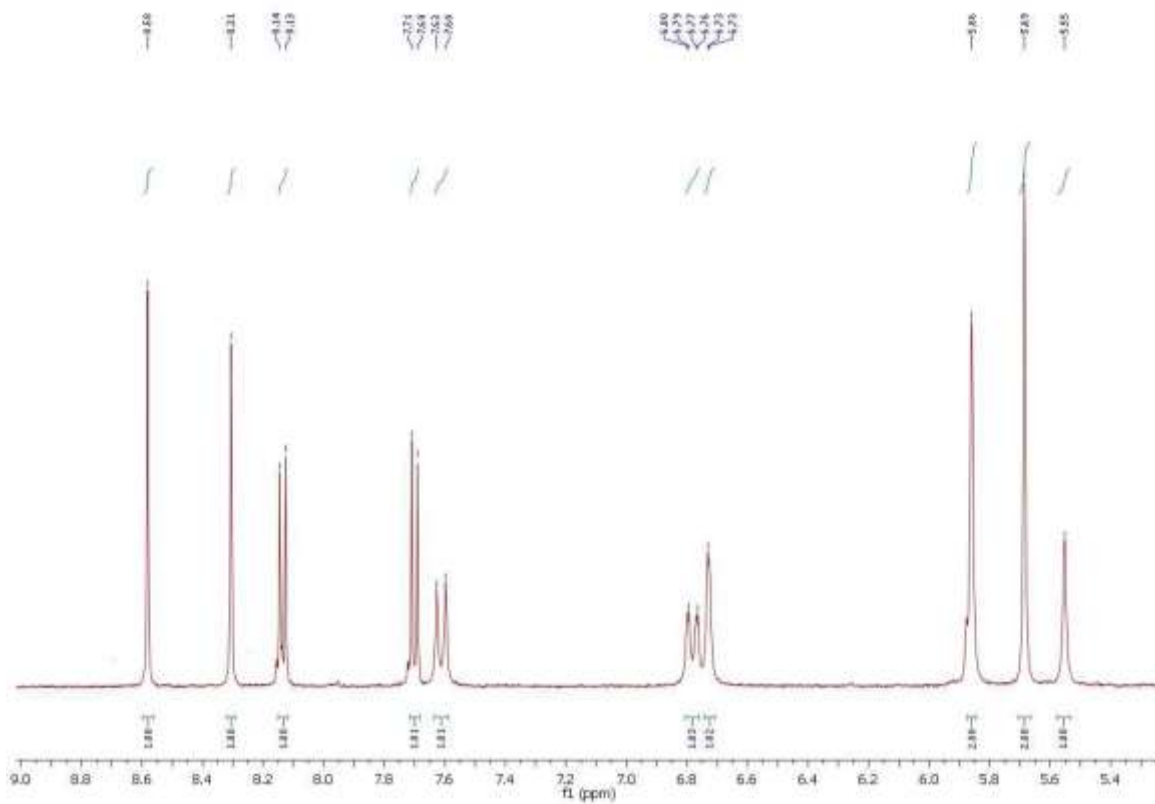


Fig. S11 a) ^1H NMR and b) ^{13}C NMR of compd. **5e**

a)



b)

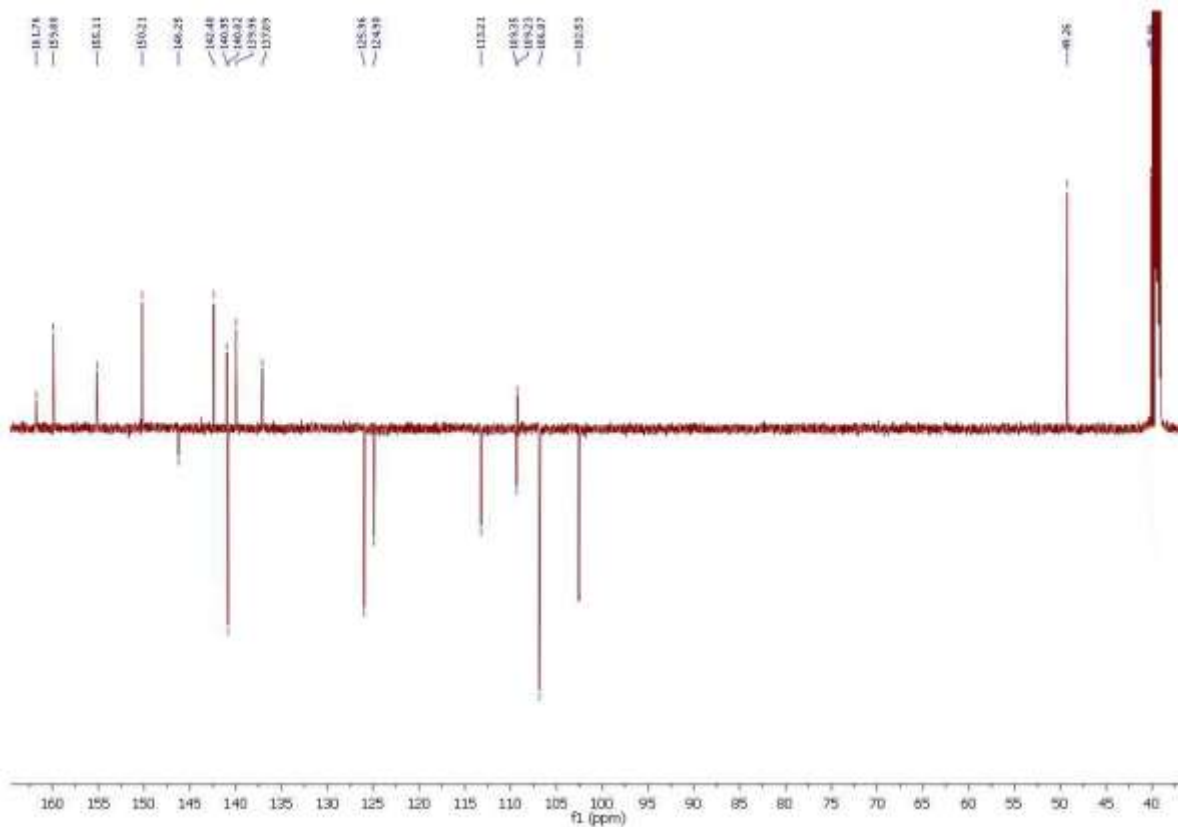
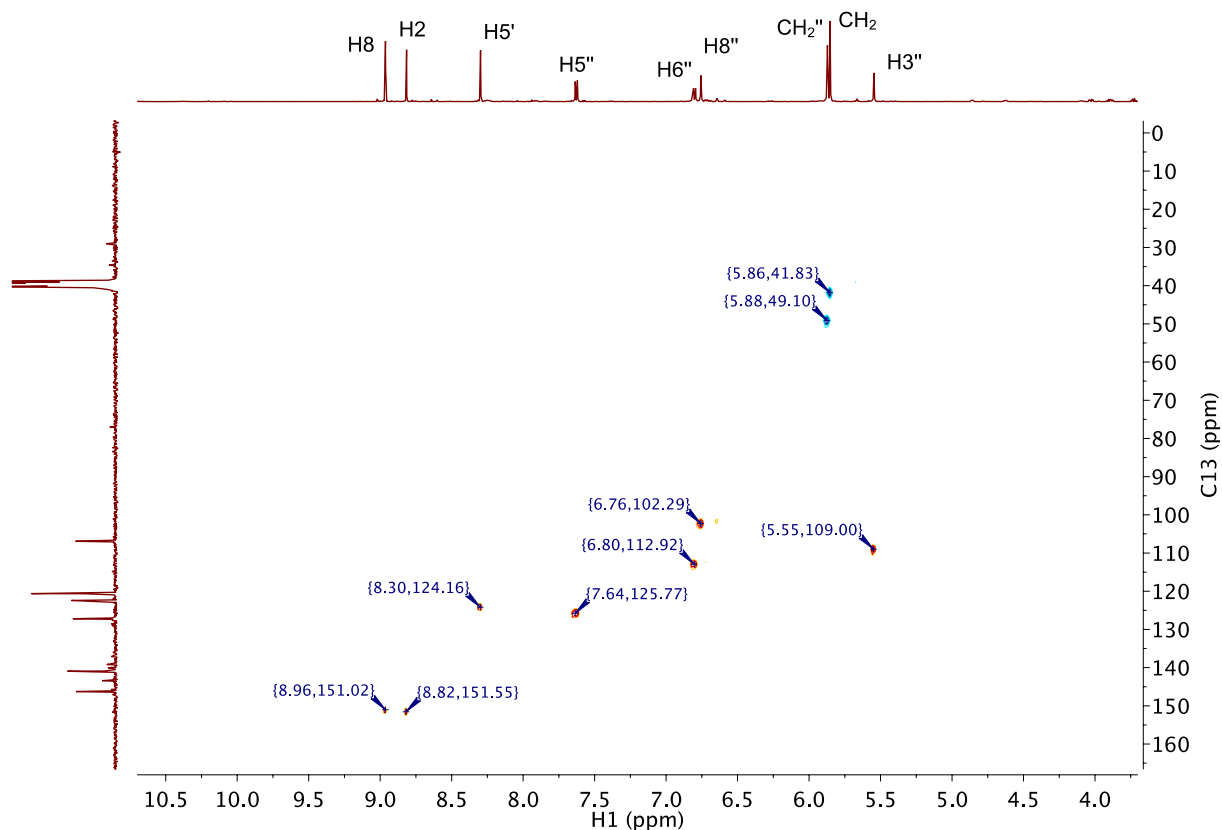


Fig. S12 a) ^1H - ^{13}C HSQC NMR and b) ^1H - ^{13}C HMBC NMR of compd. **6e**

a)



b)

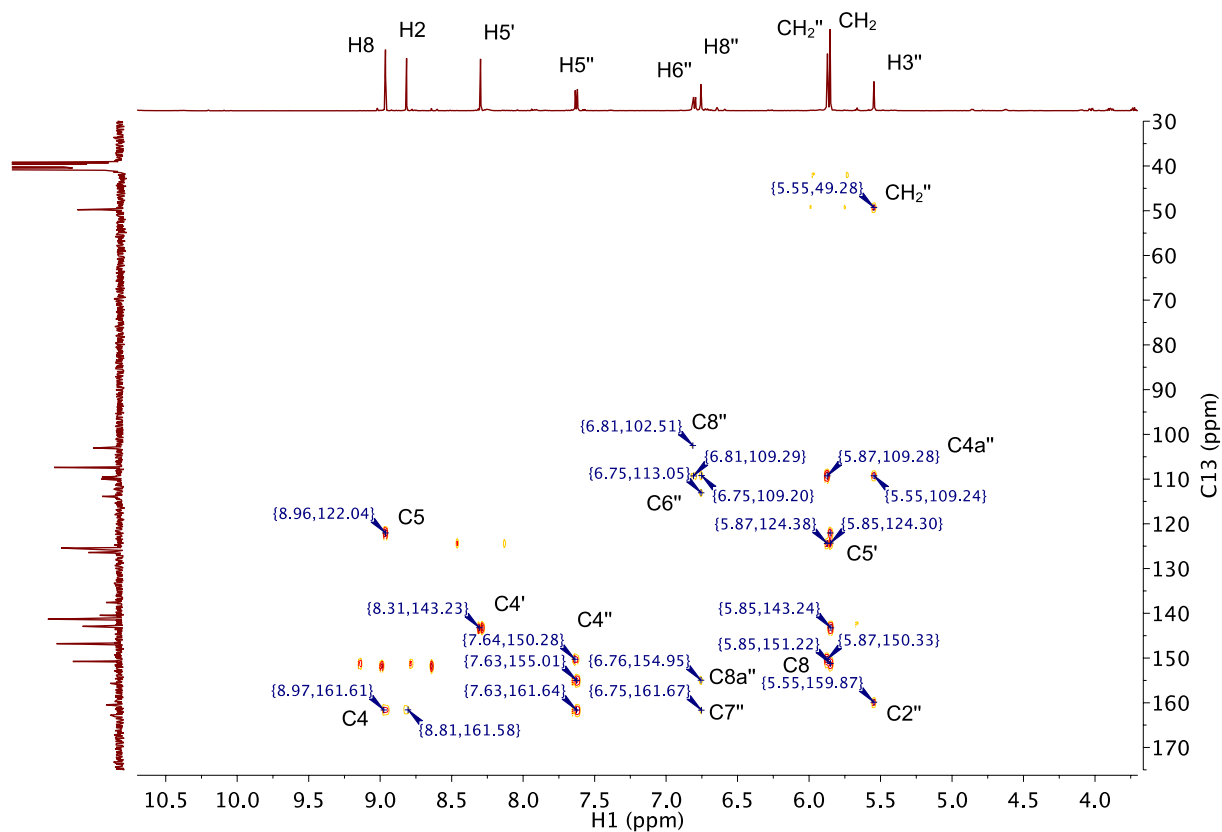
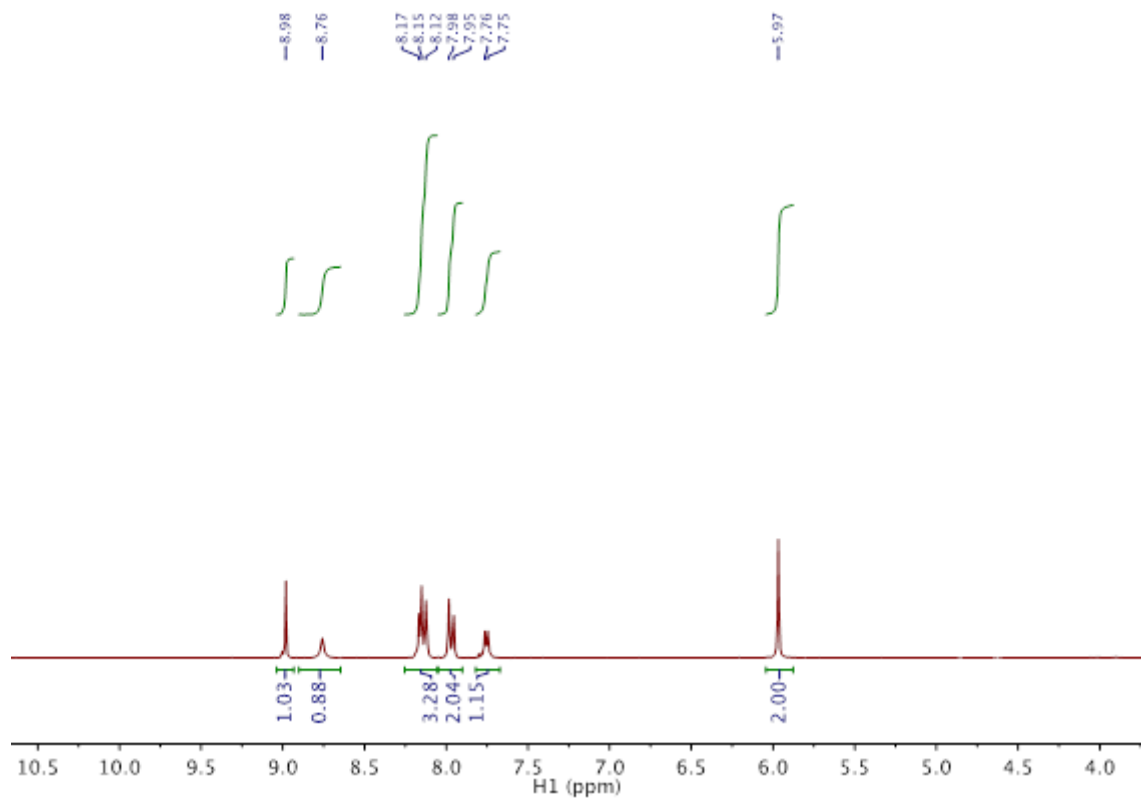


Fig. S13 a) ^1H NMR and b) ^{13}C NMR of compd. **7c**

a)



b)

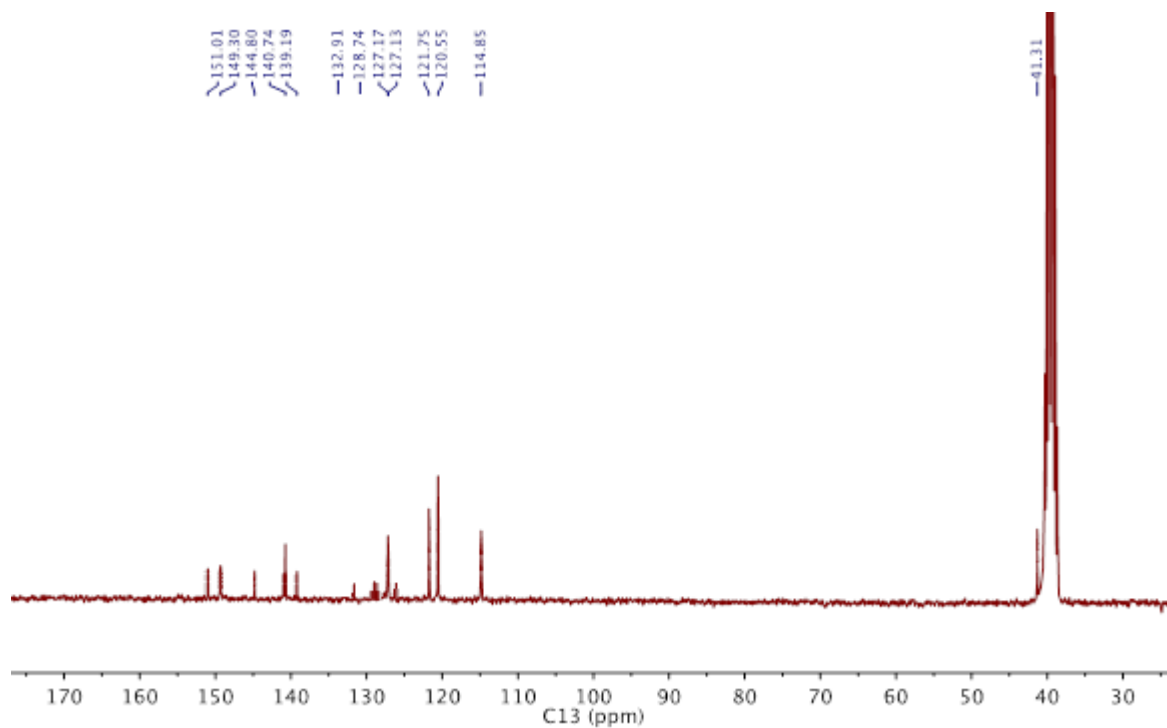
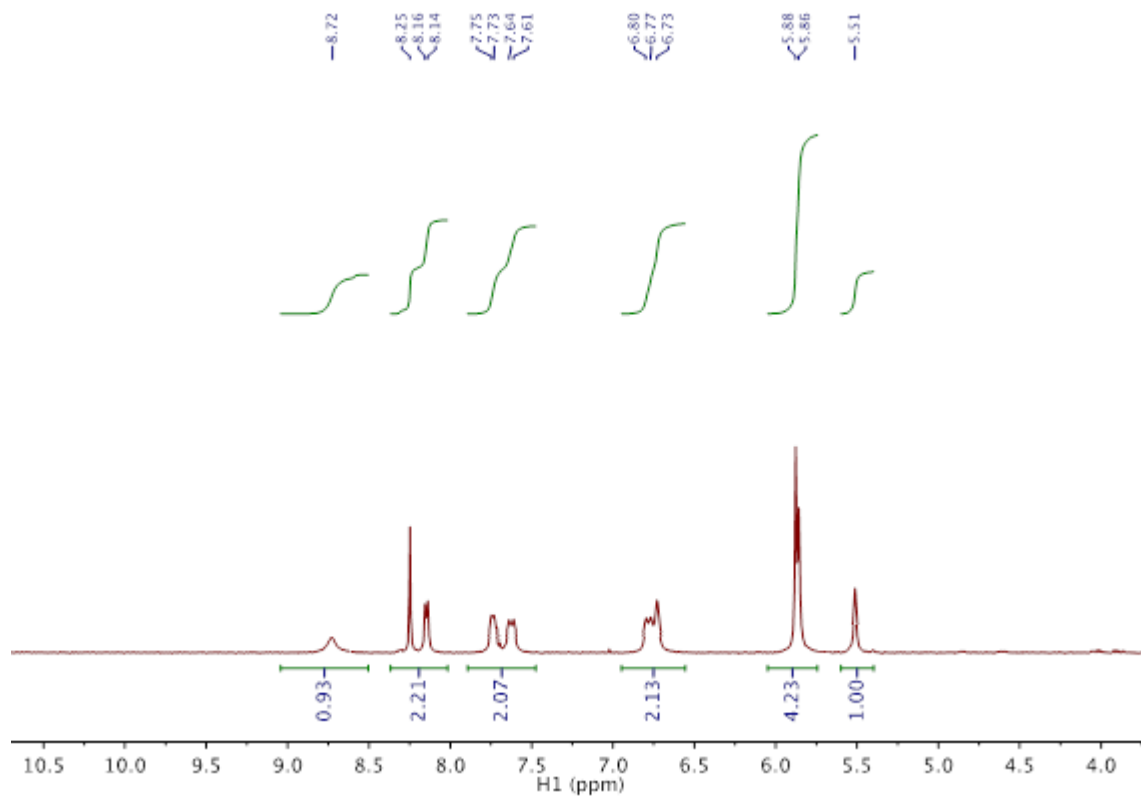


Fig. S14 a) ^1H NMR and b) ^{13}C NMR of compd. **7e**

a)



b)

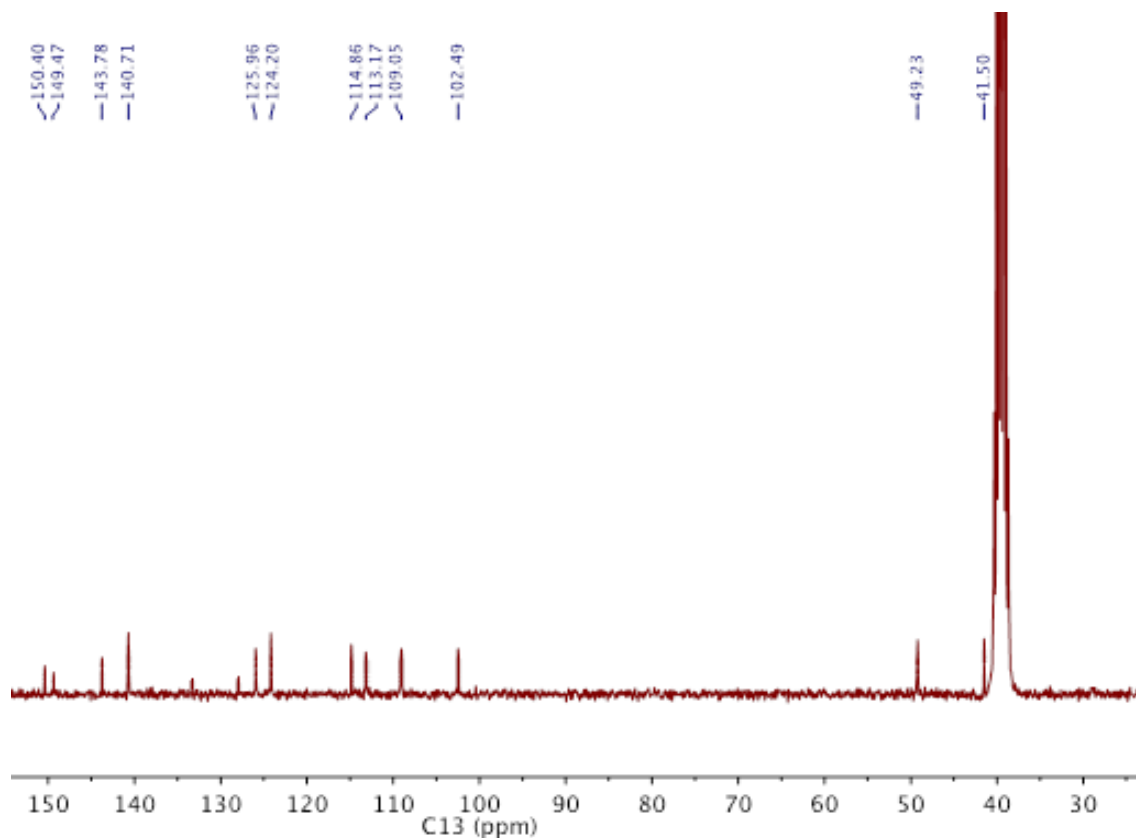
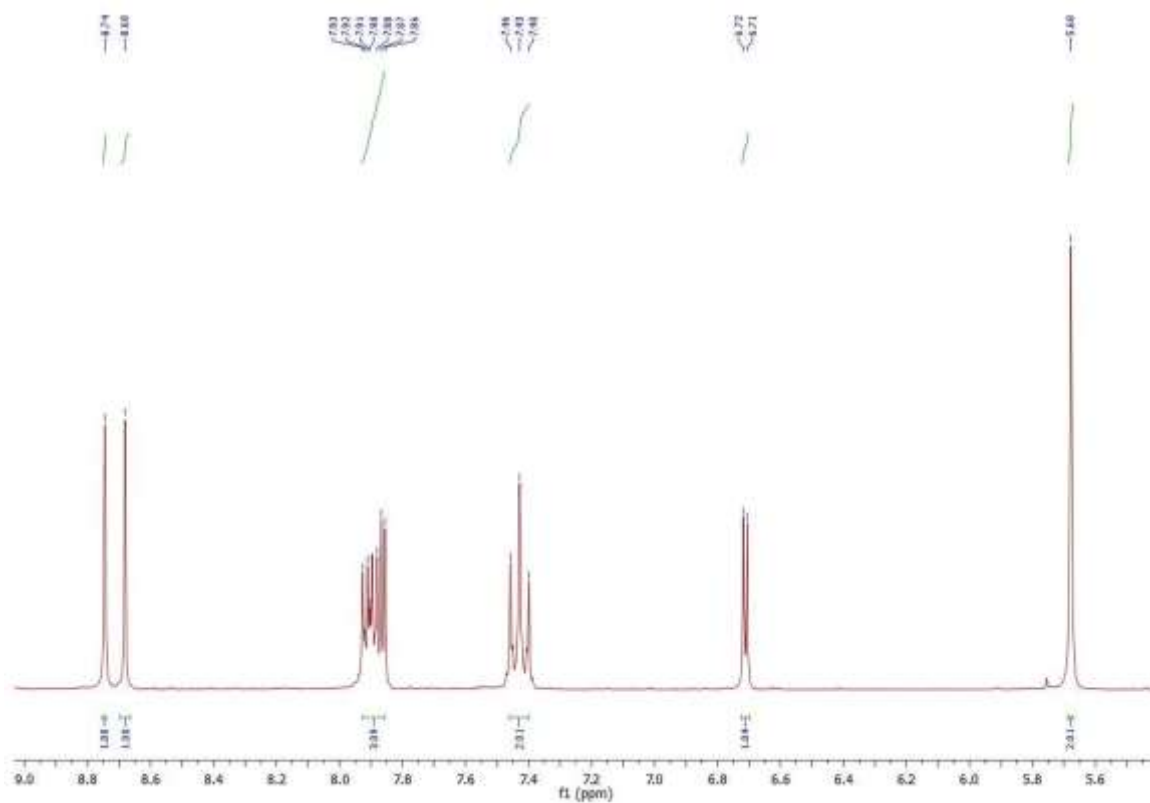


Fig. S15 a) ^1H NMR and b) ^{13}C NMR of compd. **8a**

a)



b)

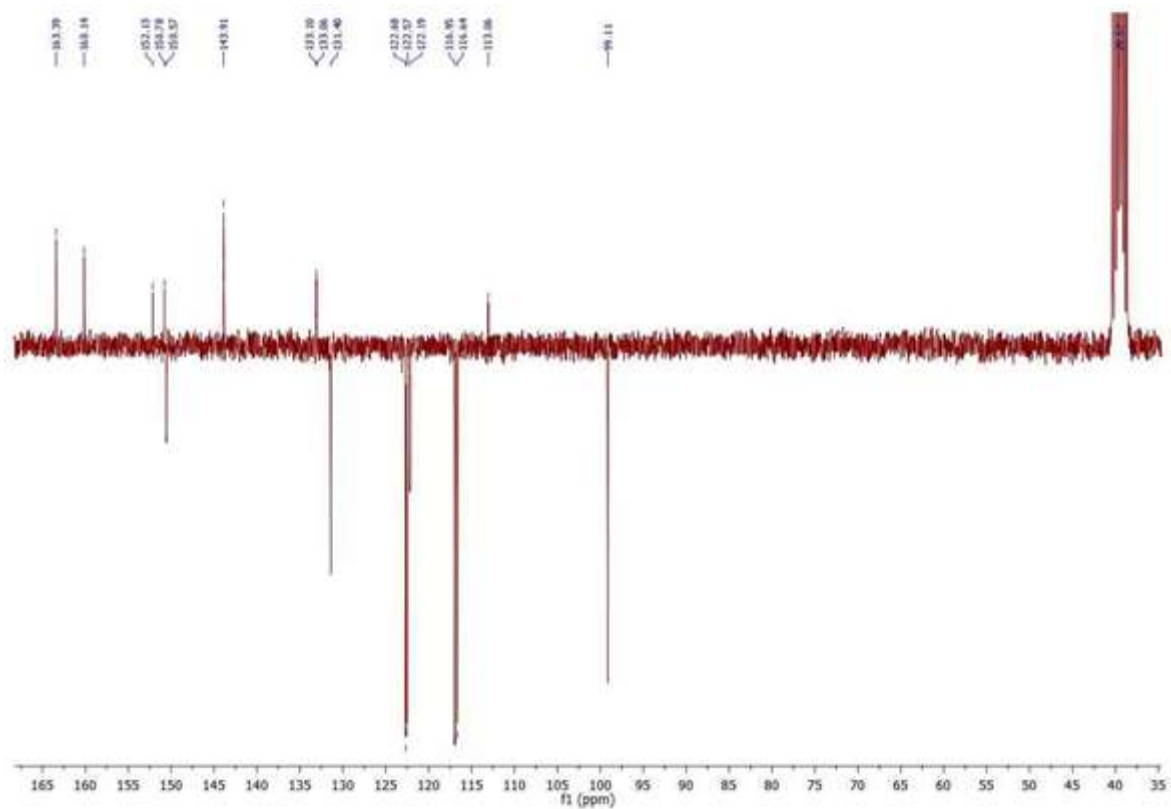
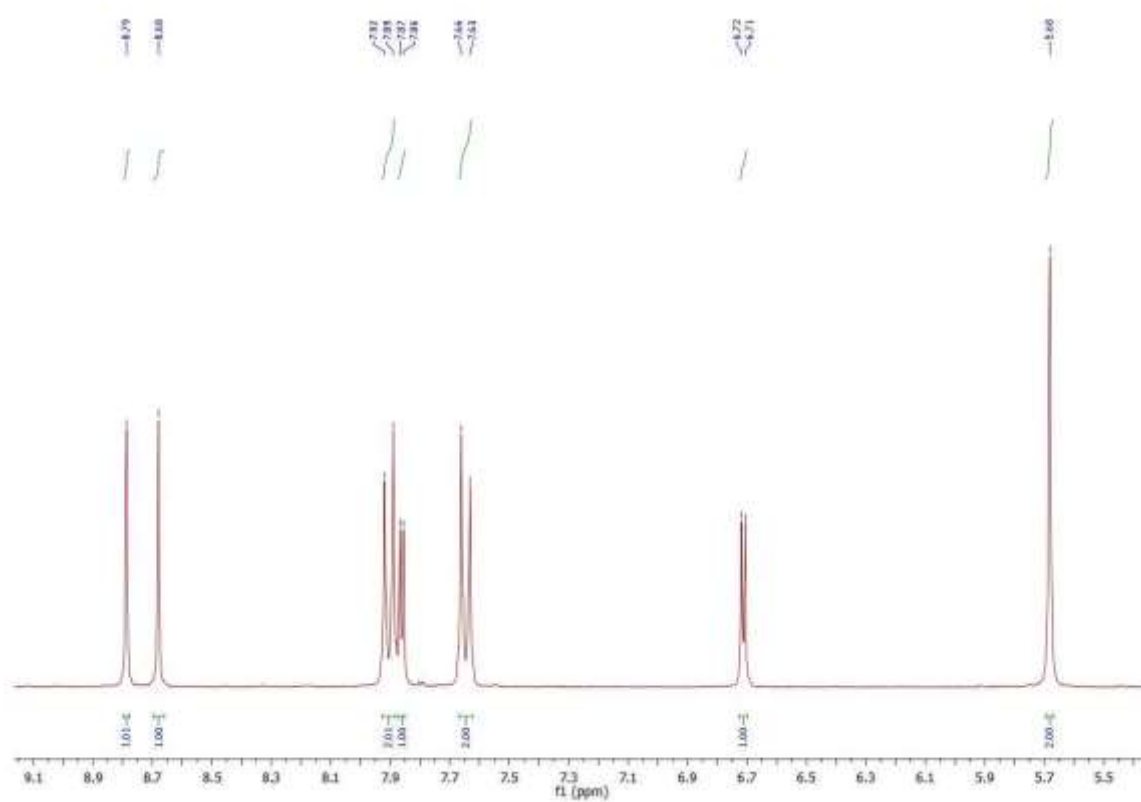


Fig. S16 a) ^1H NMR and b) ^{13}C NMR of compd. **8b**

a)



b)

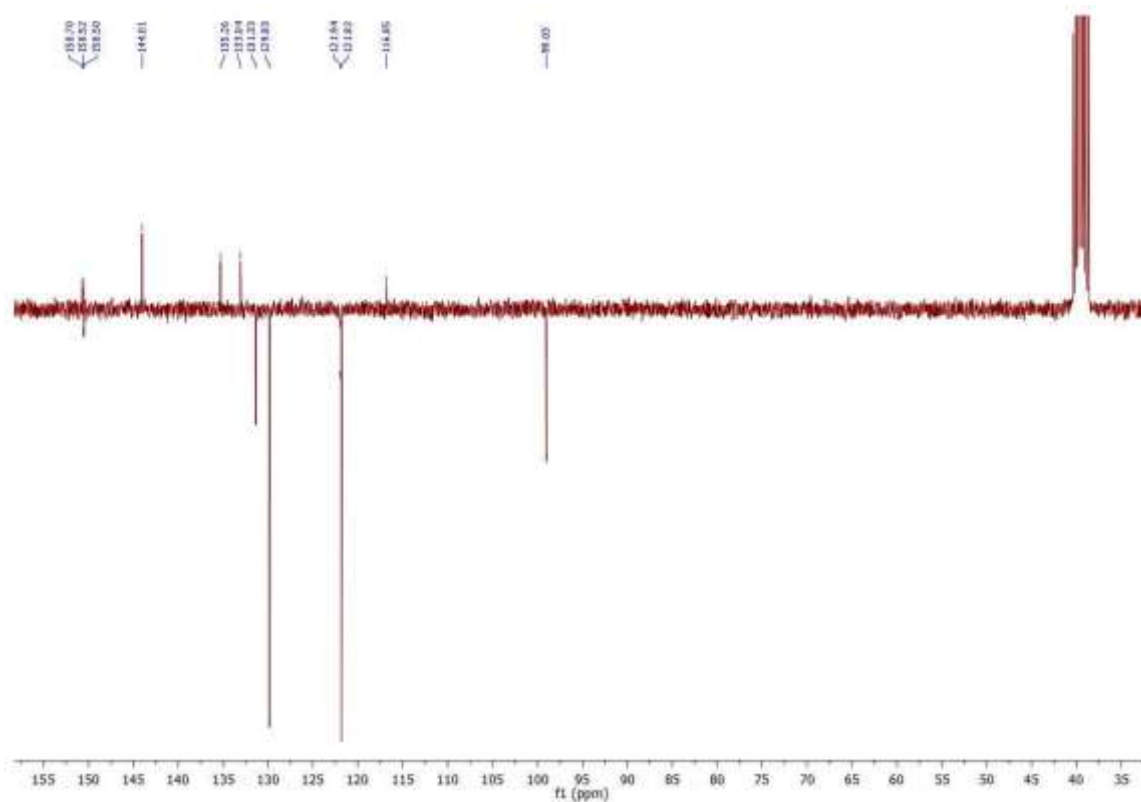
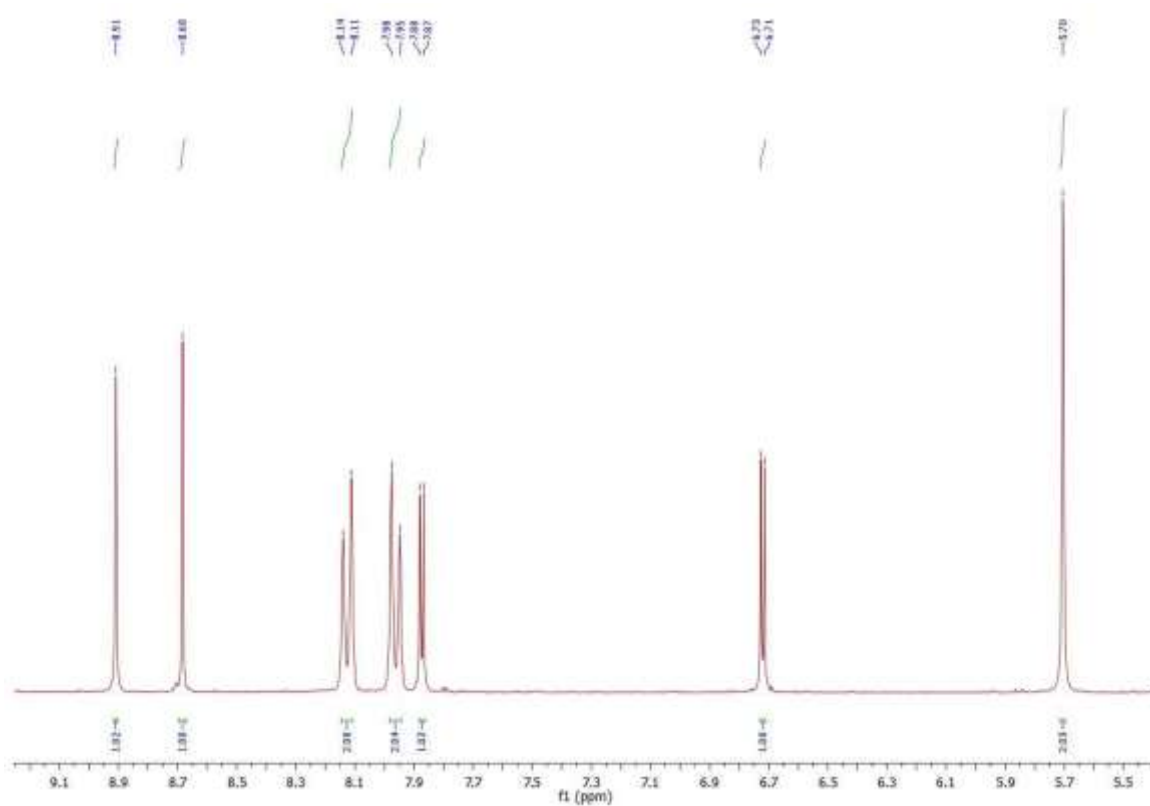


Fig. S17 a) ^1H NMR and b) ^{13}C NMR of compd. **8c**

a)



b)

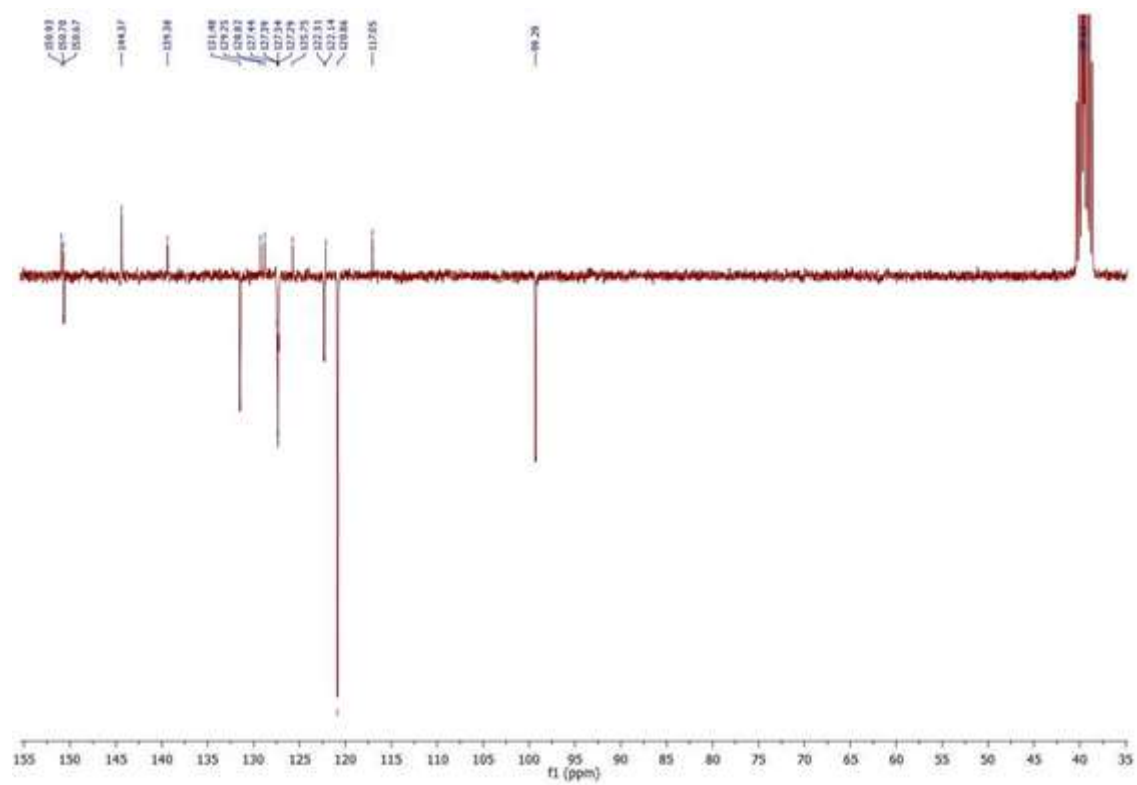
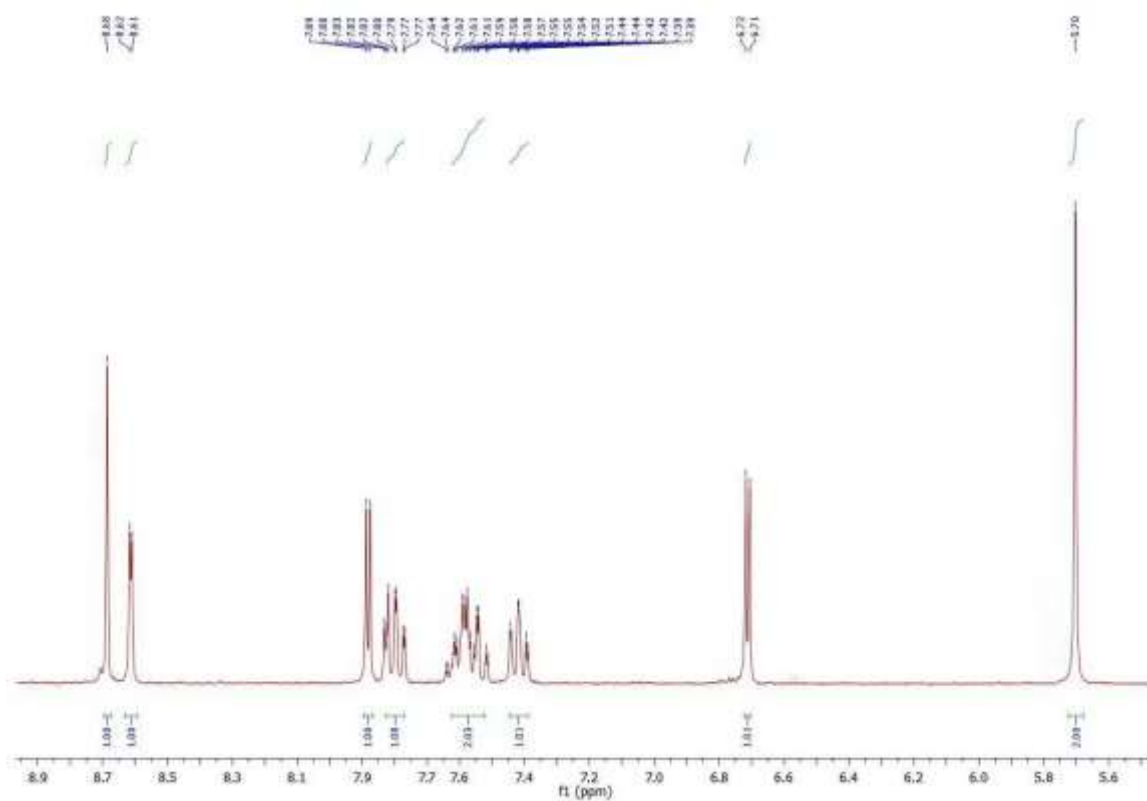


Fig. S18 a) ^1H NMR and b) ^{13}C NMR of compd. **8d**

a)



b)

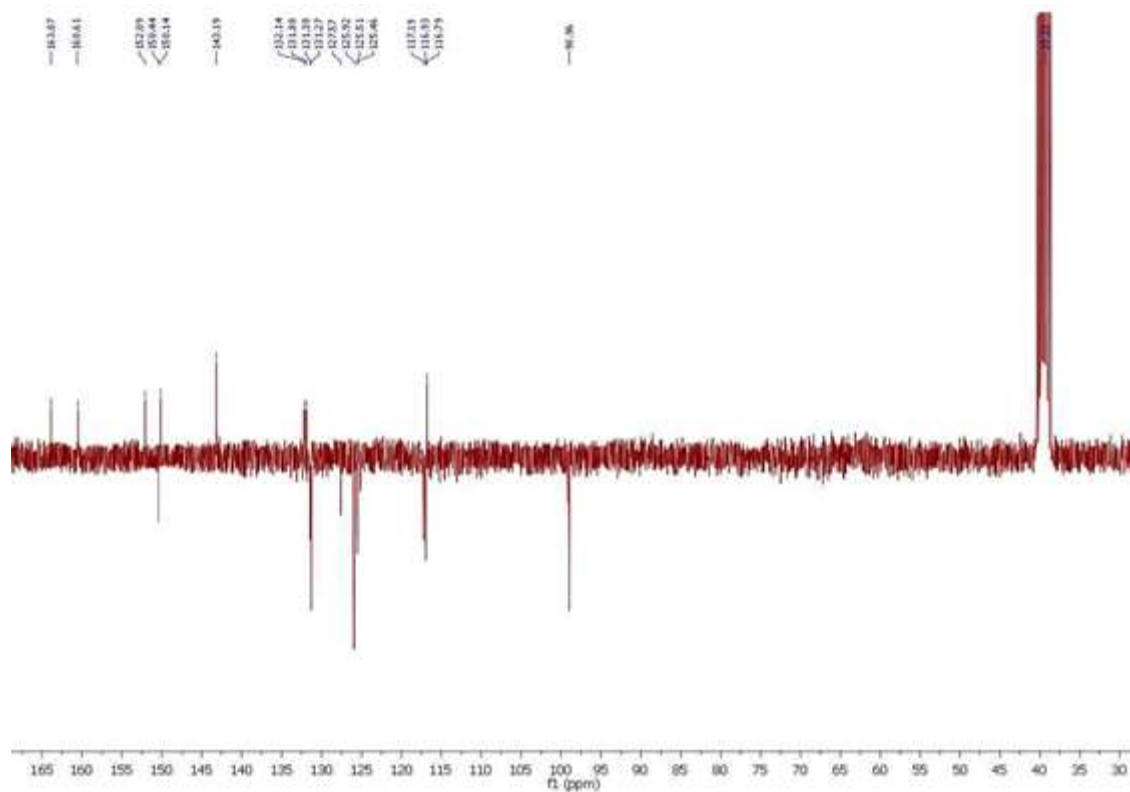
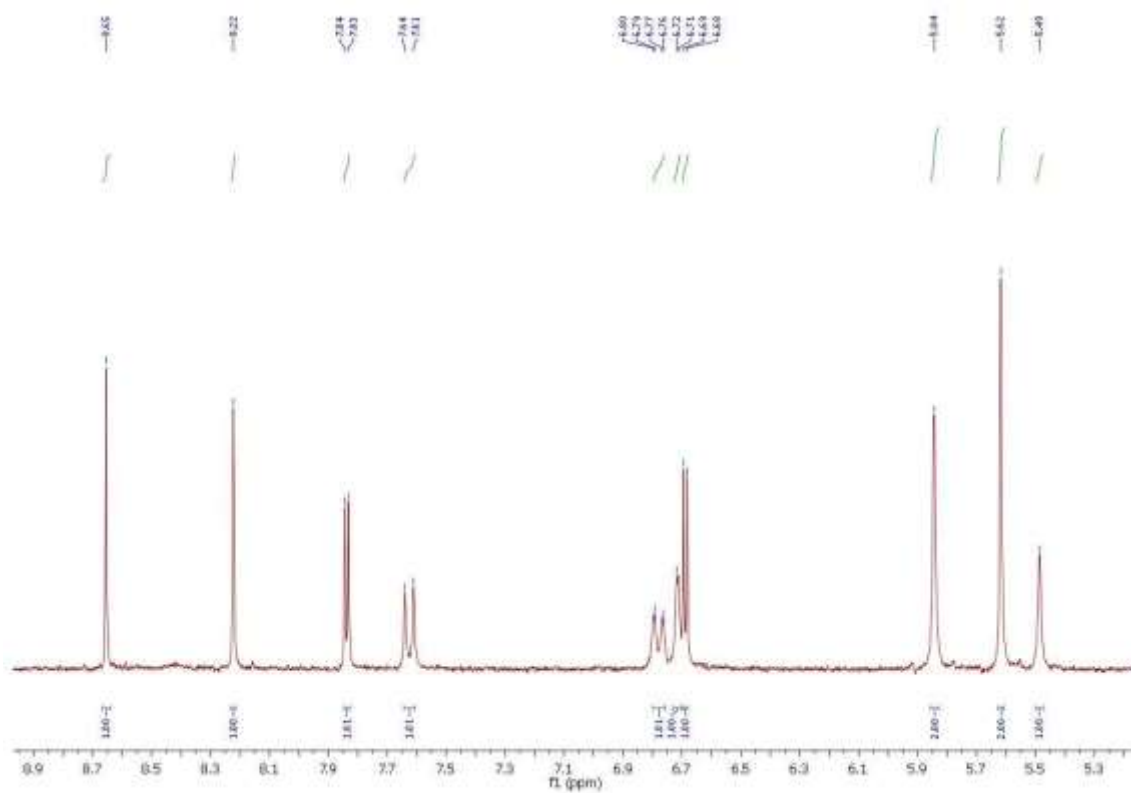


Fig. S19 a) ^1H NMR and b) ^{13}C NMR of compd. **8e**

a)



b)

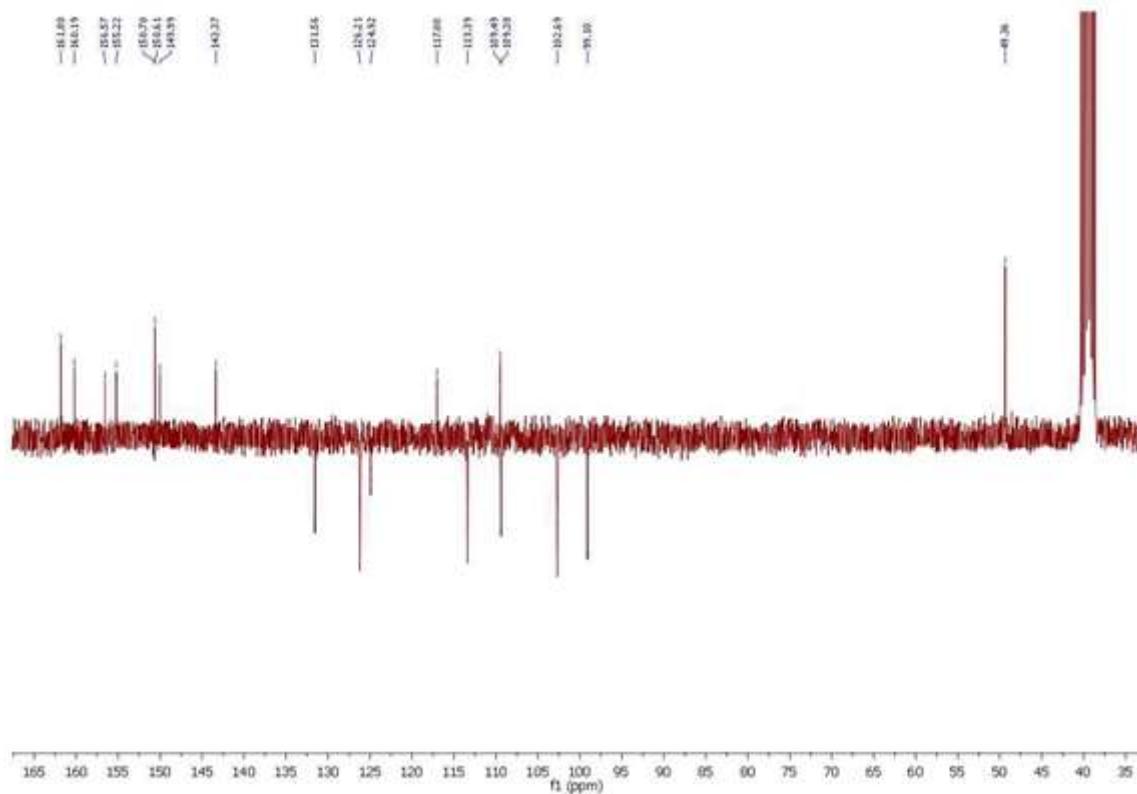
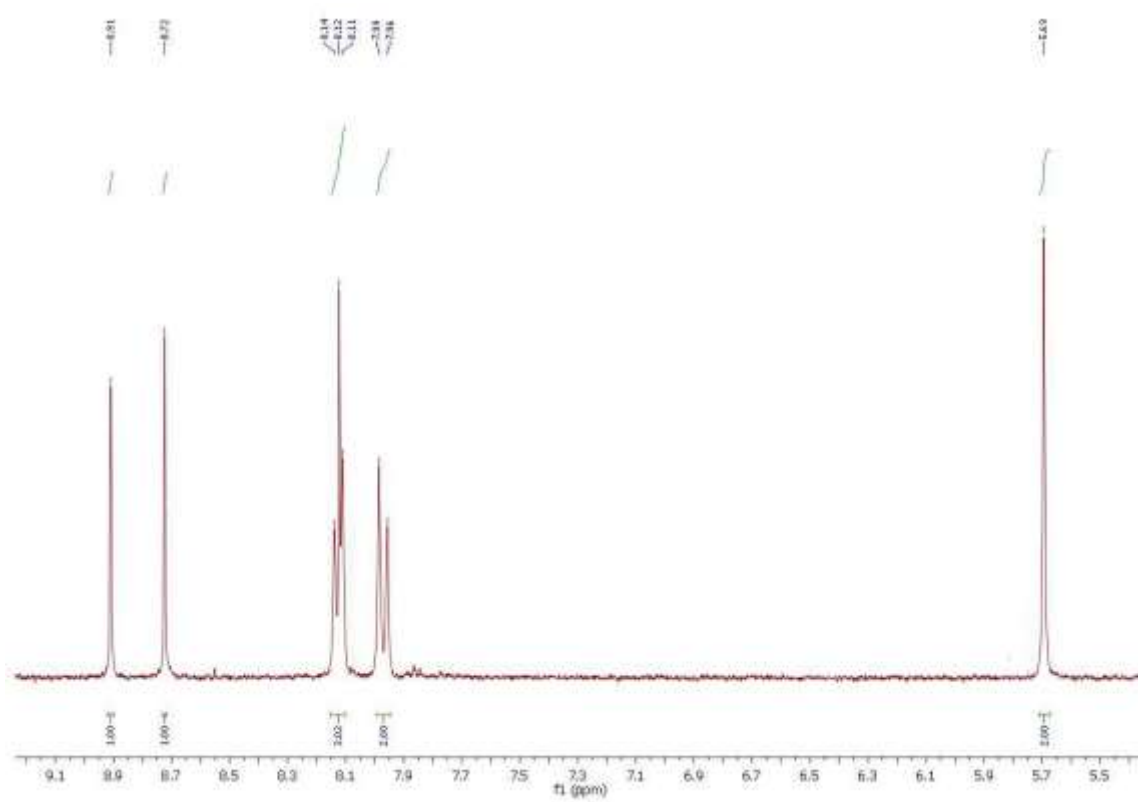


Fig. S20 a) ^1H NMR and b) ^{13}C NMR of compd. **9c**

a)



b)

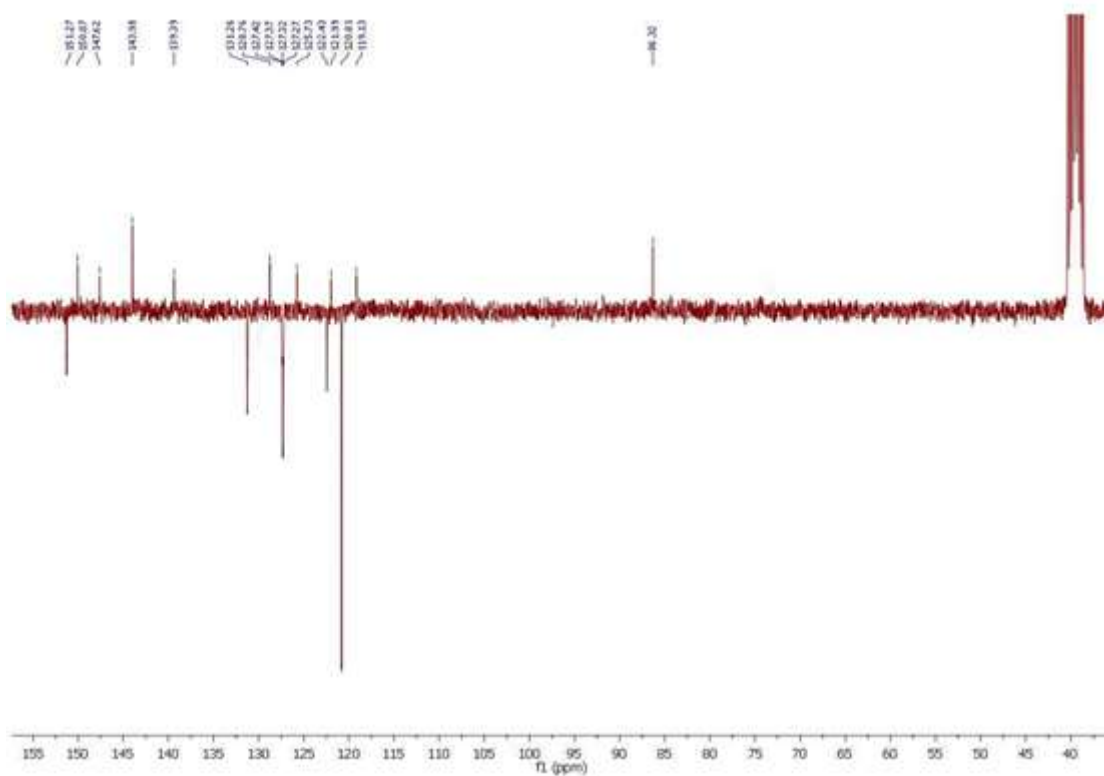
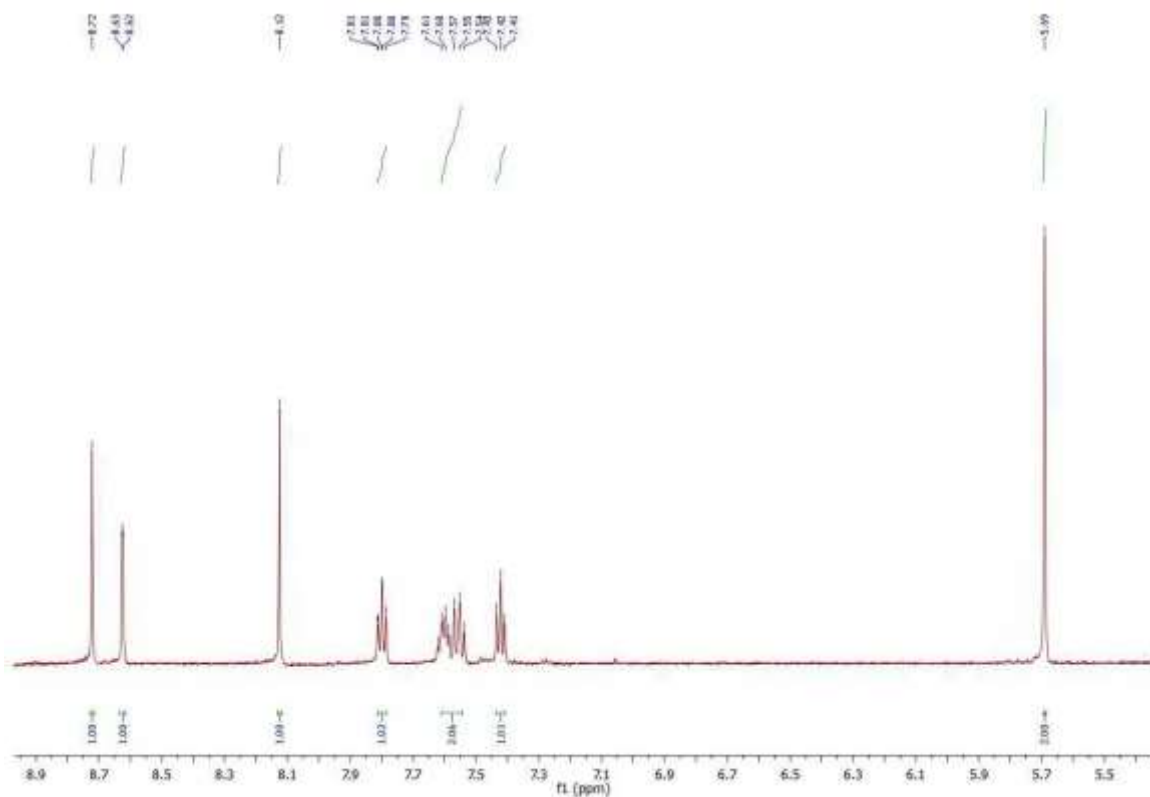


Fig. S21 a) ^1H NMR and b) ^{13}C NMR of compd. **9d**

a)



b)

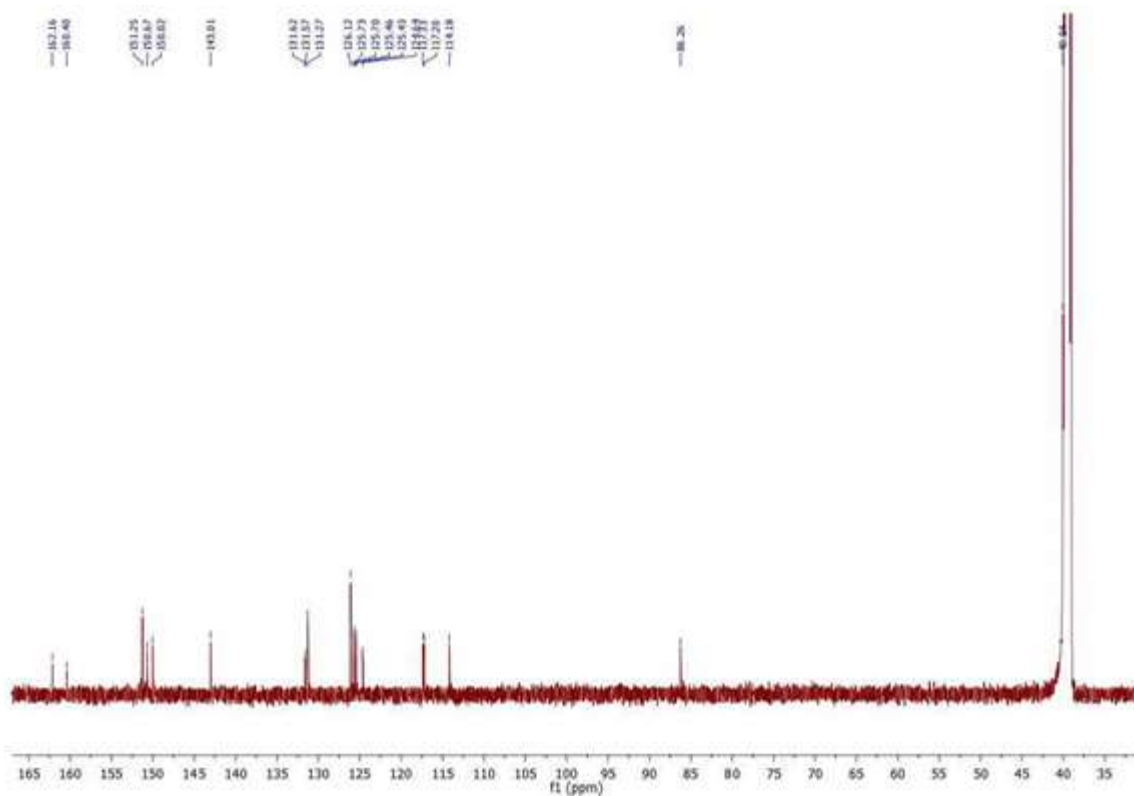
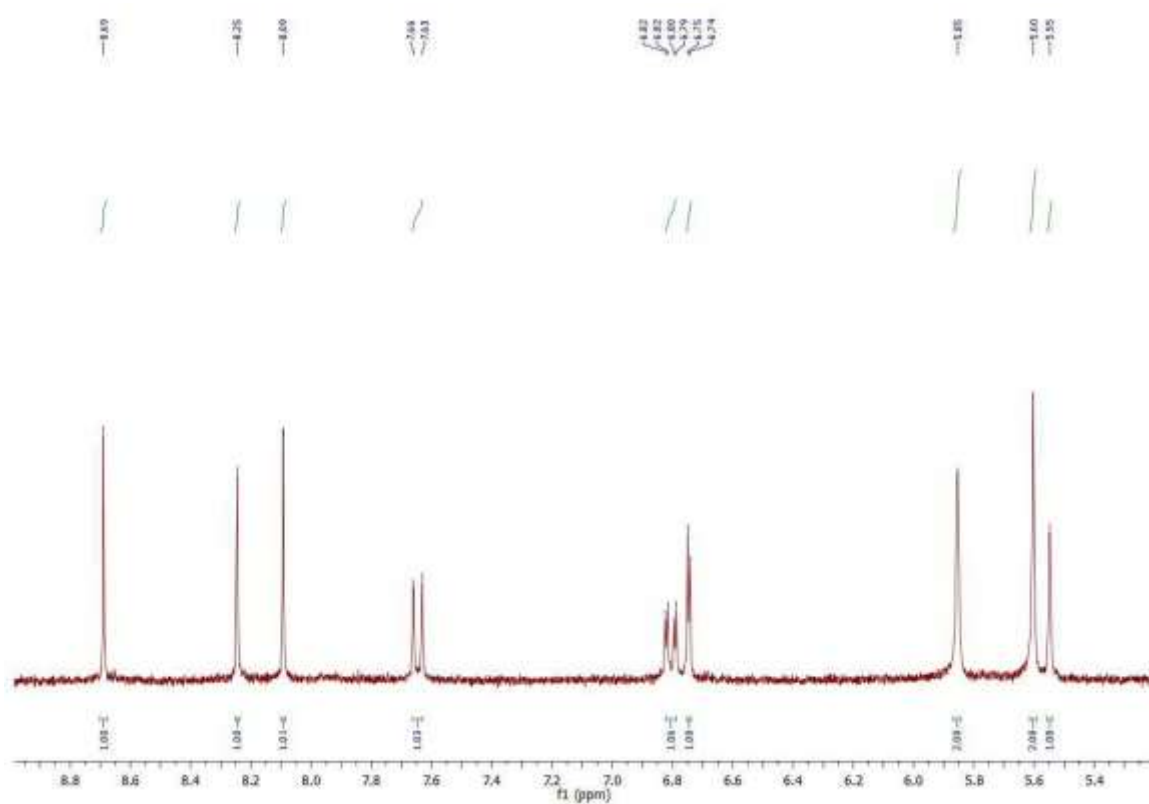


Fig. S22 a) ^1H NMR and b) ^{13}C NMR of compd. **9e**

a)



b)

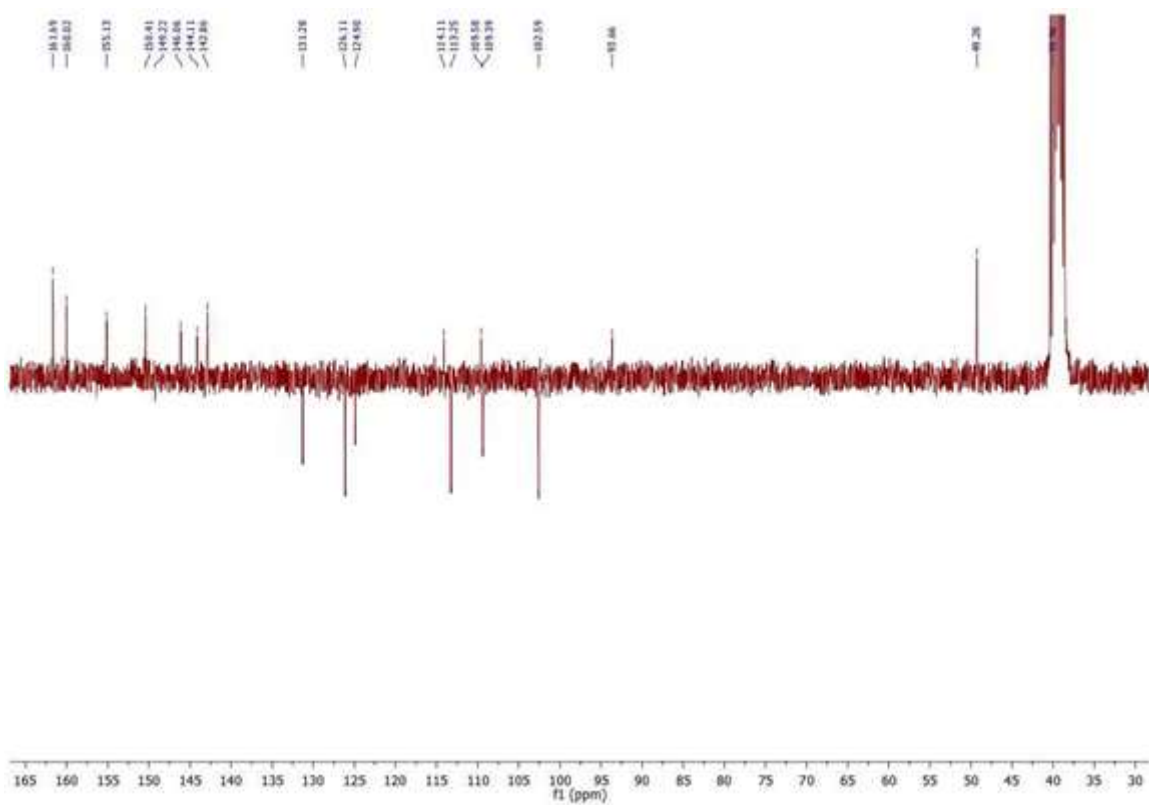
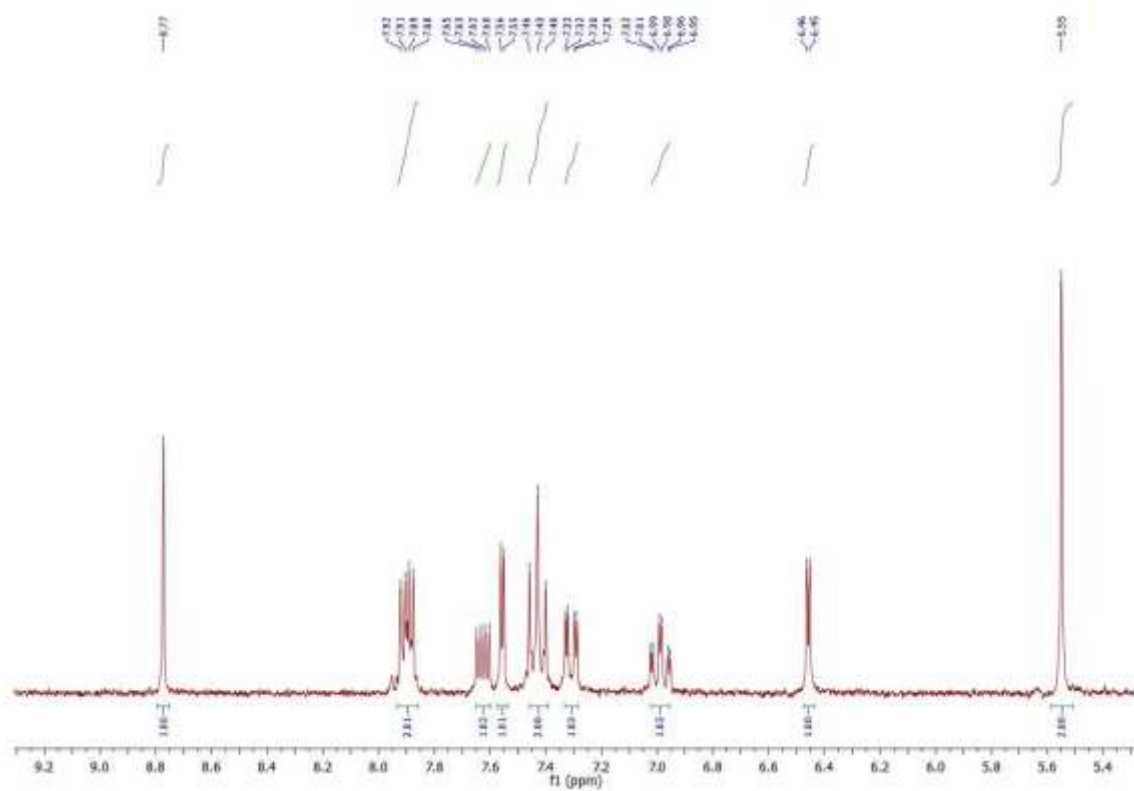


Fig. S23 a) ^1H NMR and b) ^{13}C NMR of compd. **10a**

a)



b)

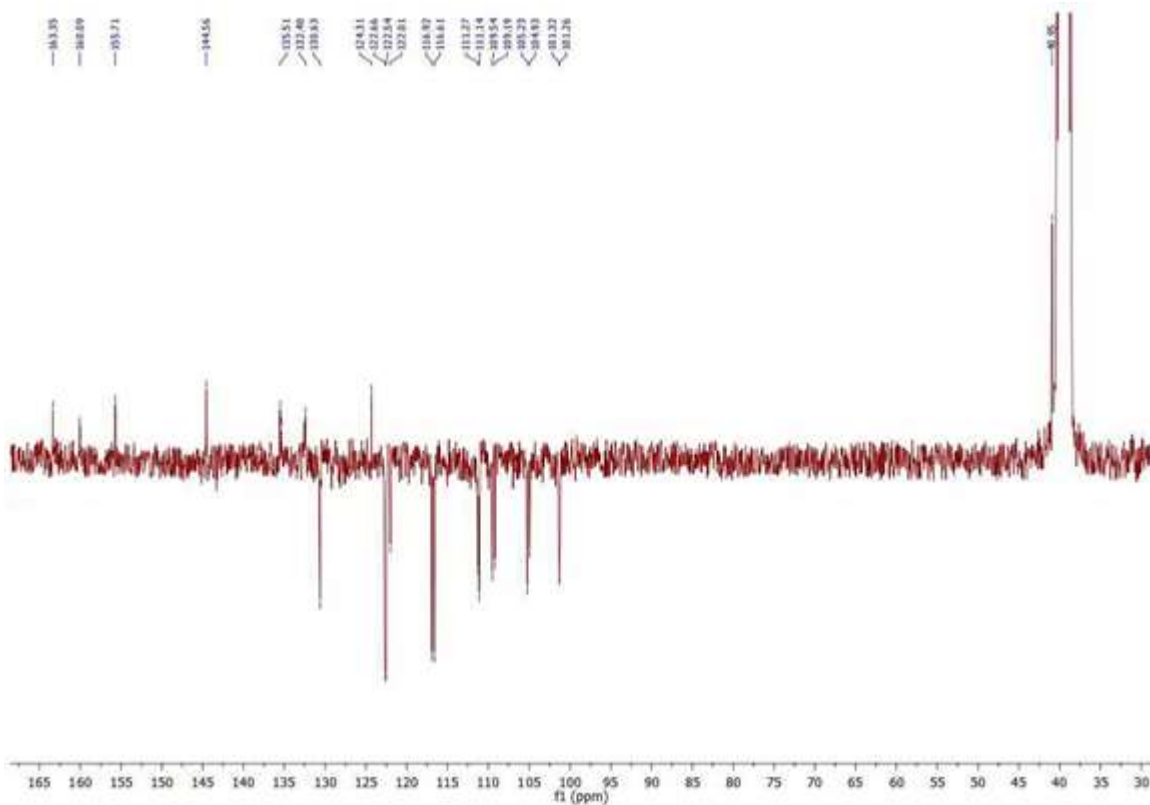
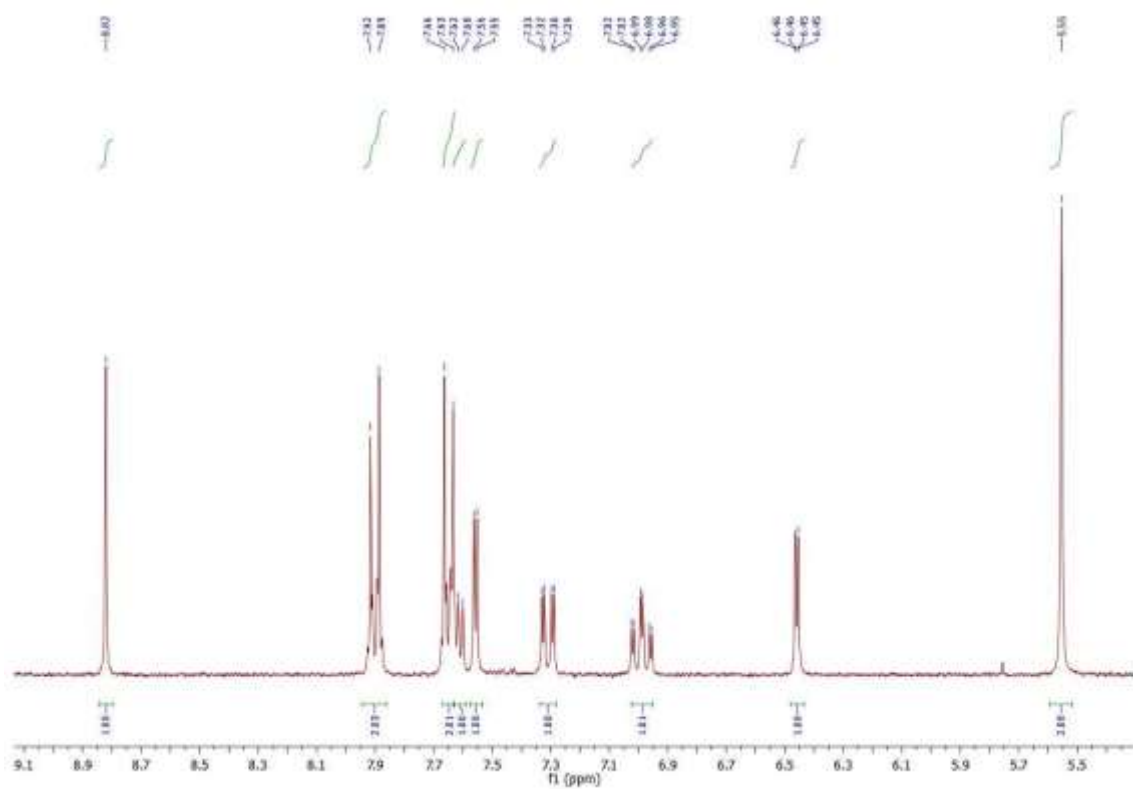


Fig. S24 a) ^1H NMR and b) ^{13}C NMR of compd. **10b**

a)



b)

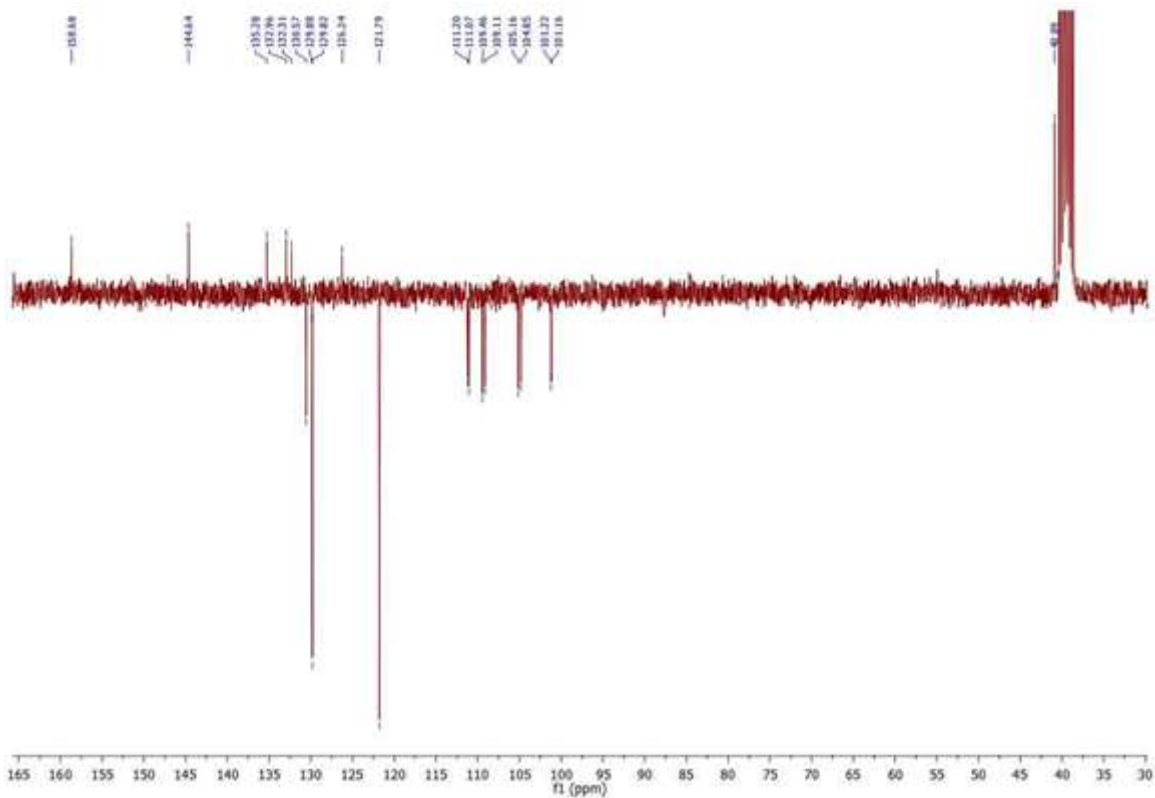
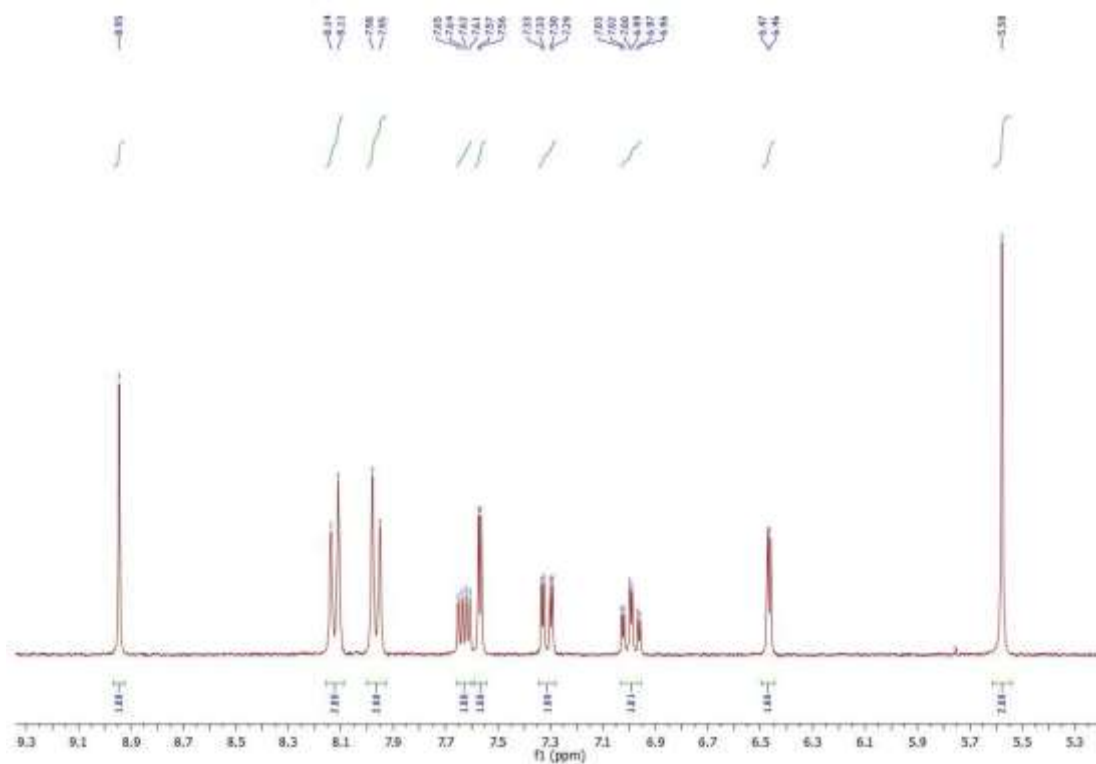


Fig. S25 a) ^1H NMR and b) ^{13}C NMR of compd. **10c**

a)



b)

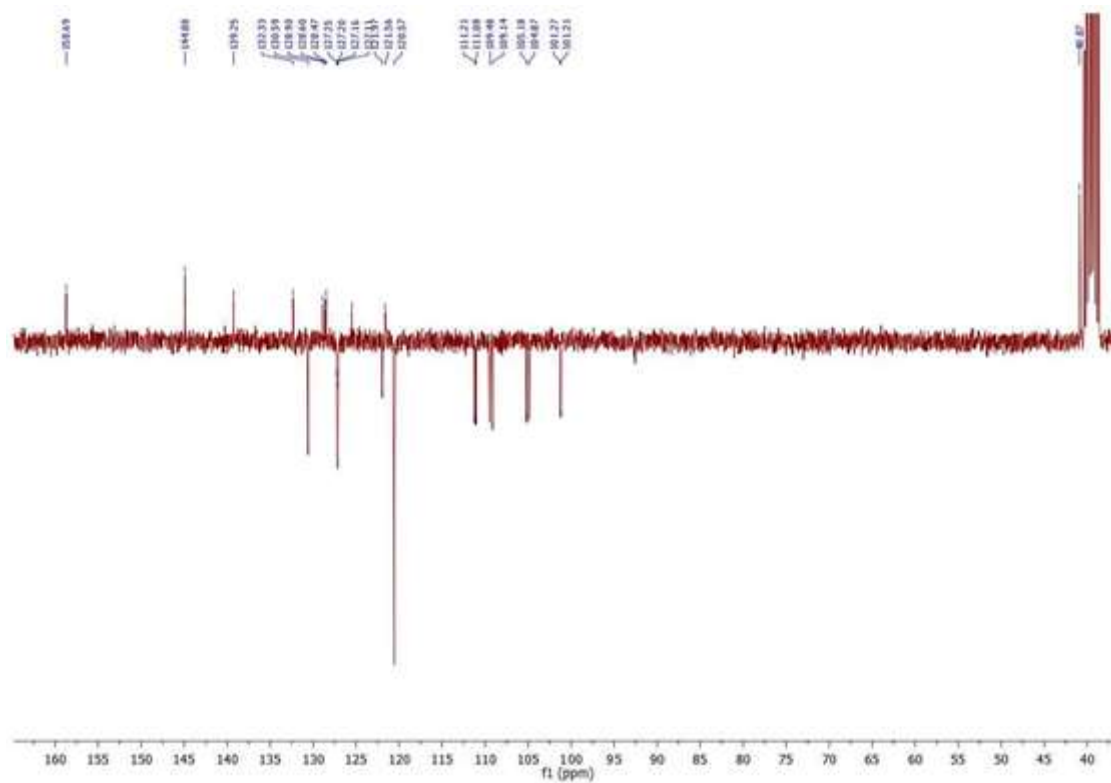
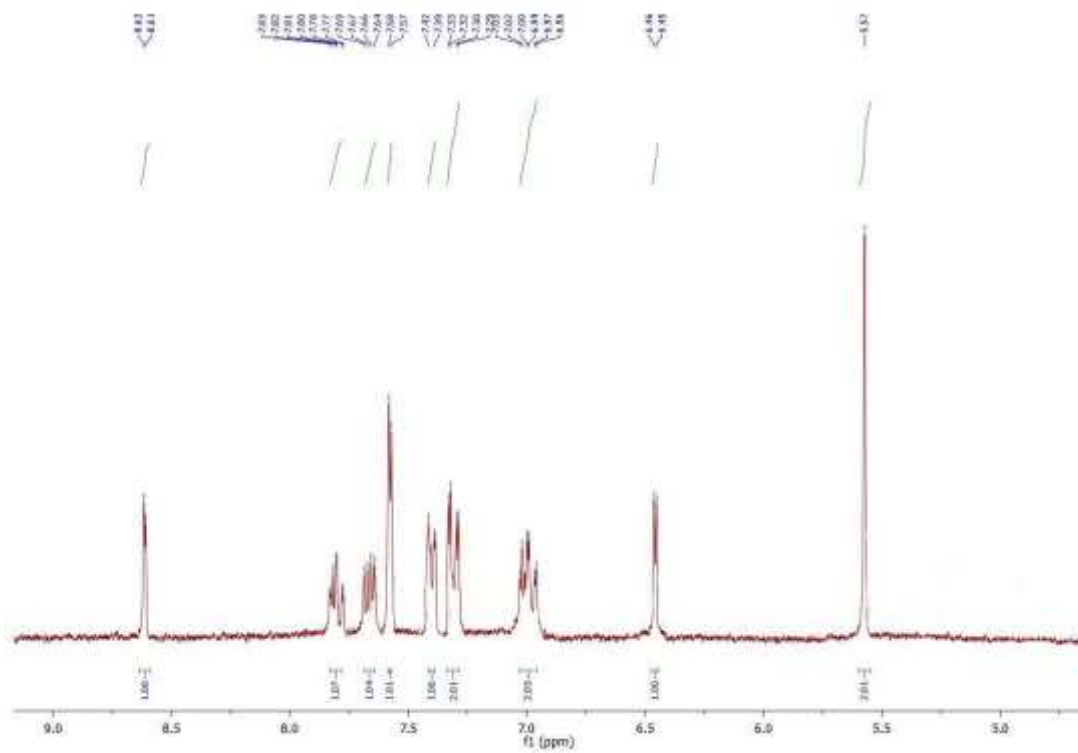


Fig. S26 a) ^1H NMR and b) ^{13}C NMR of compd. 10d

a)



b)

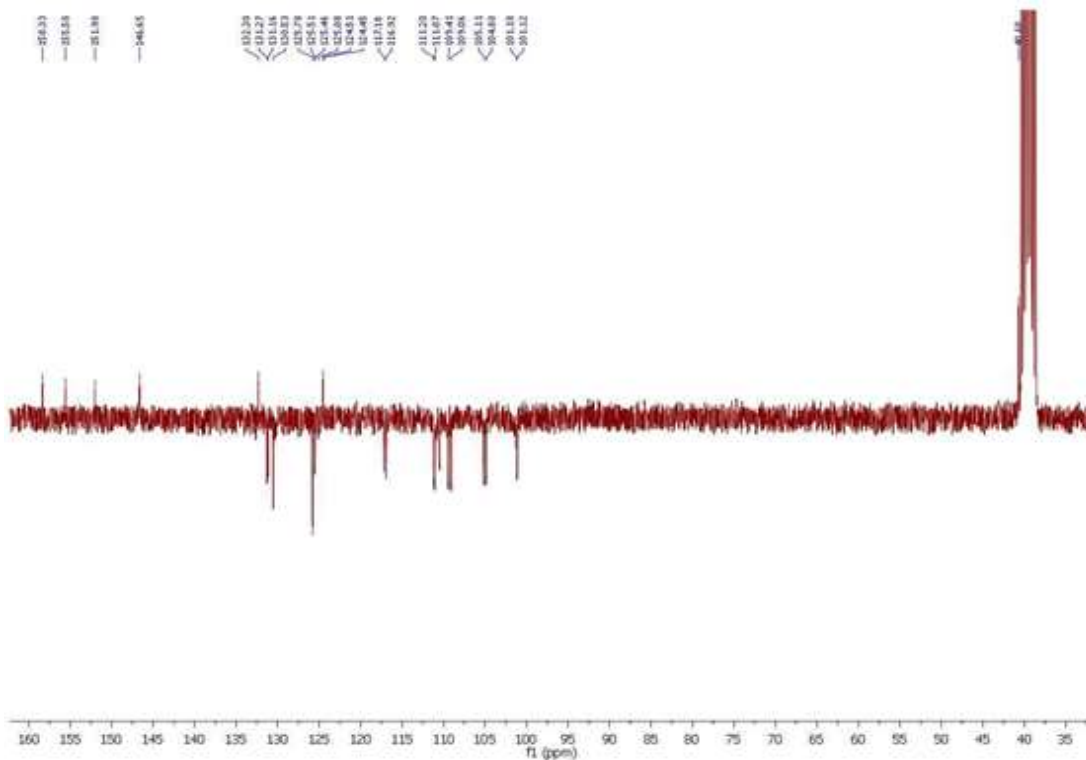
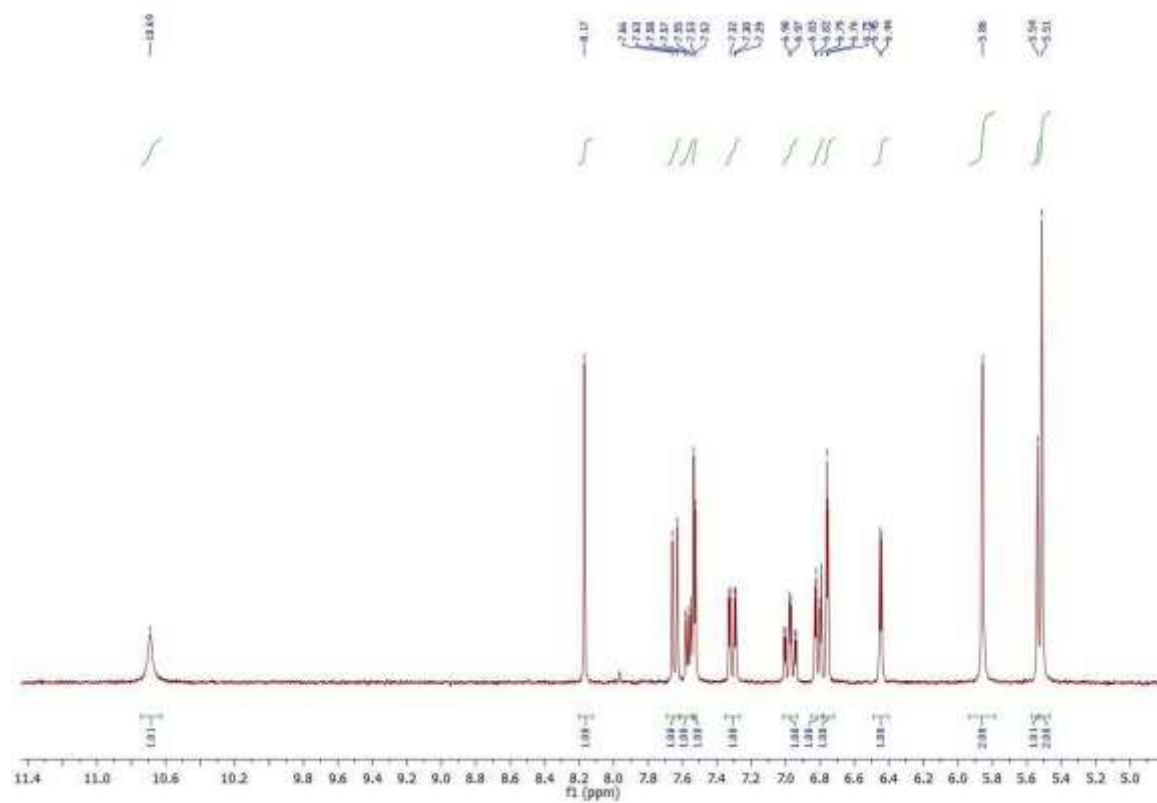


Fig. S27 a) ^1H NMR and b) ^{13}C NMR of compd. **10e**

a)



b)

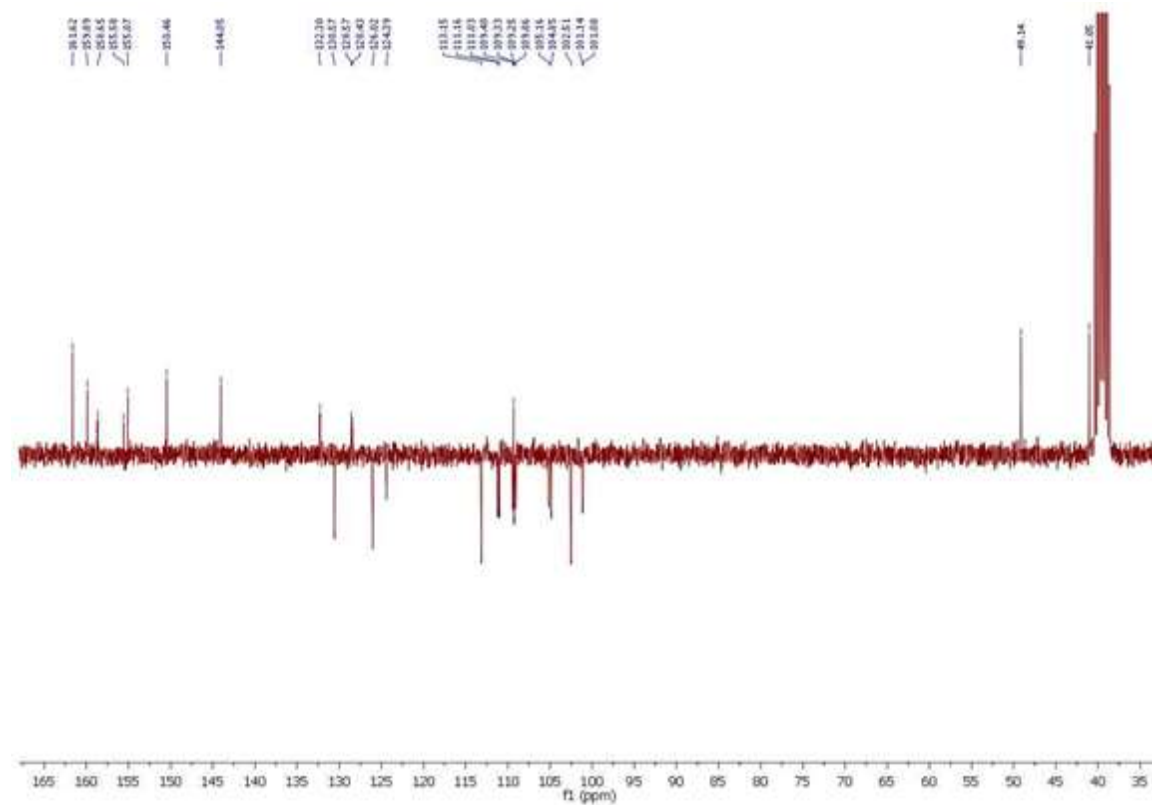
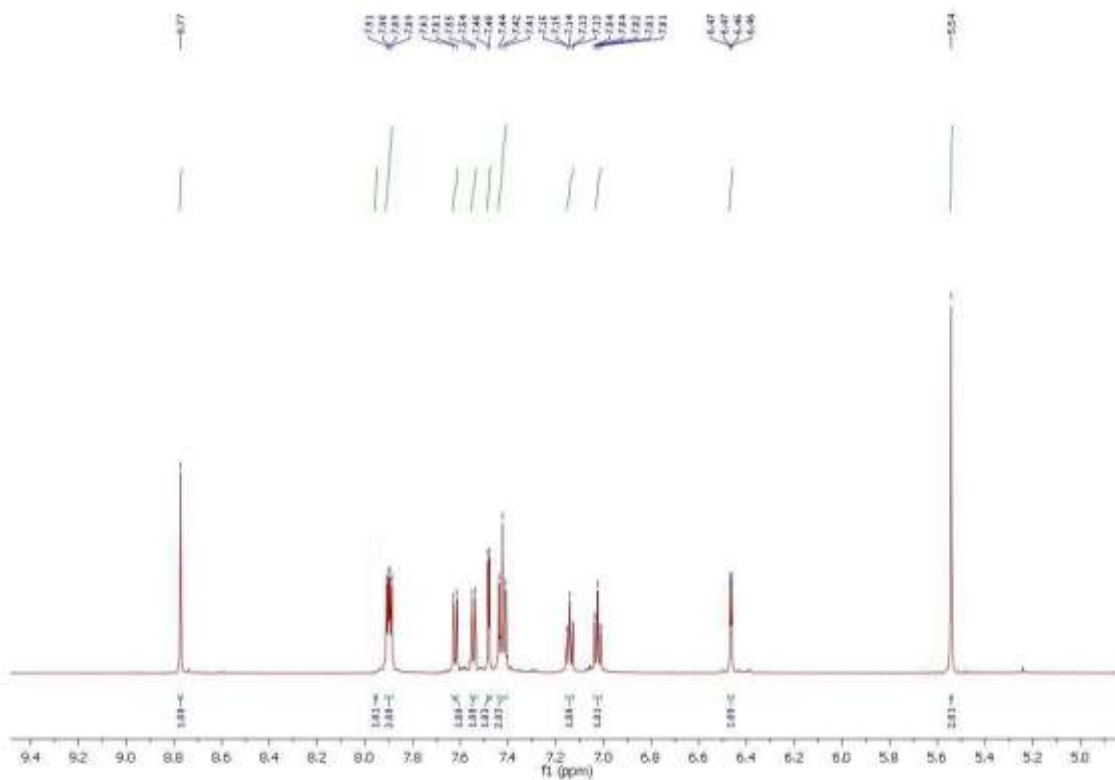


Fig. S28 a) ^1H NMR and b) ^{13}C NMR of compd. **11a**

a)



b)

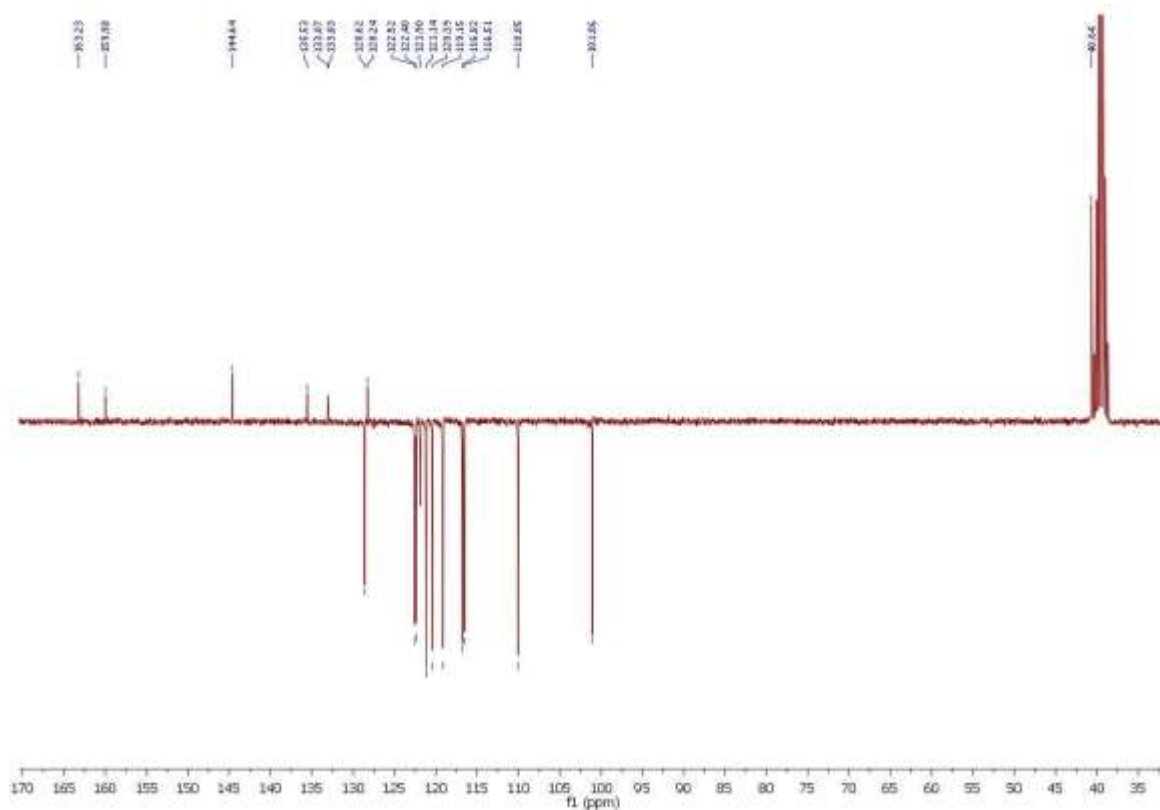
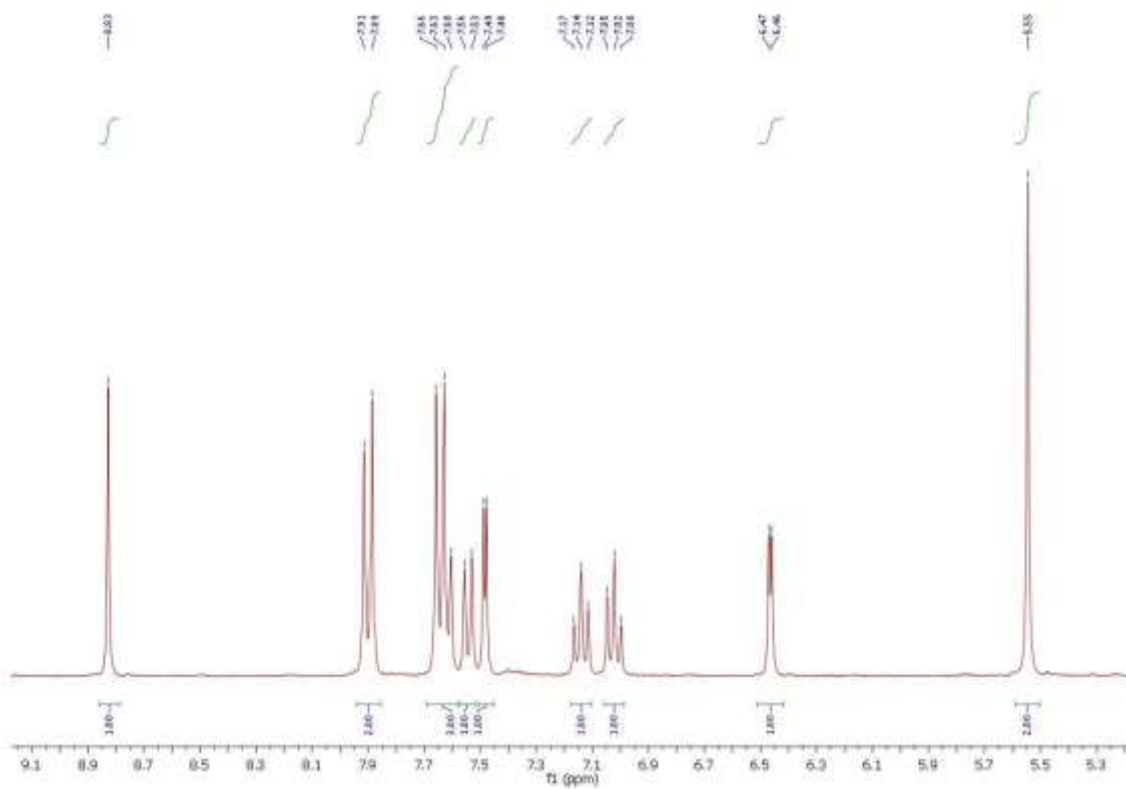


Fig. S29 a) ^1H NMR and b) ^{13}C NMR of compd. **11b**

a)



b)

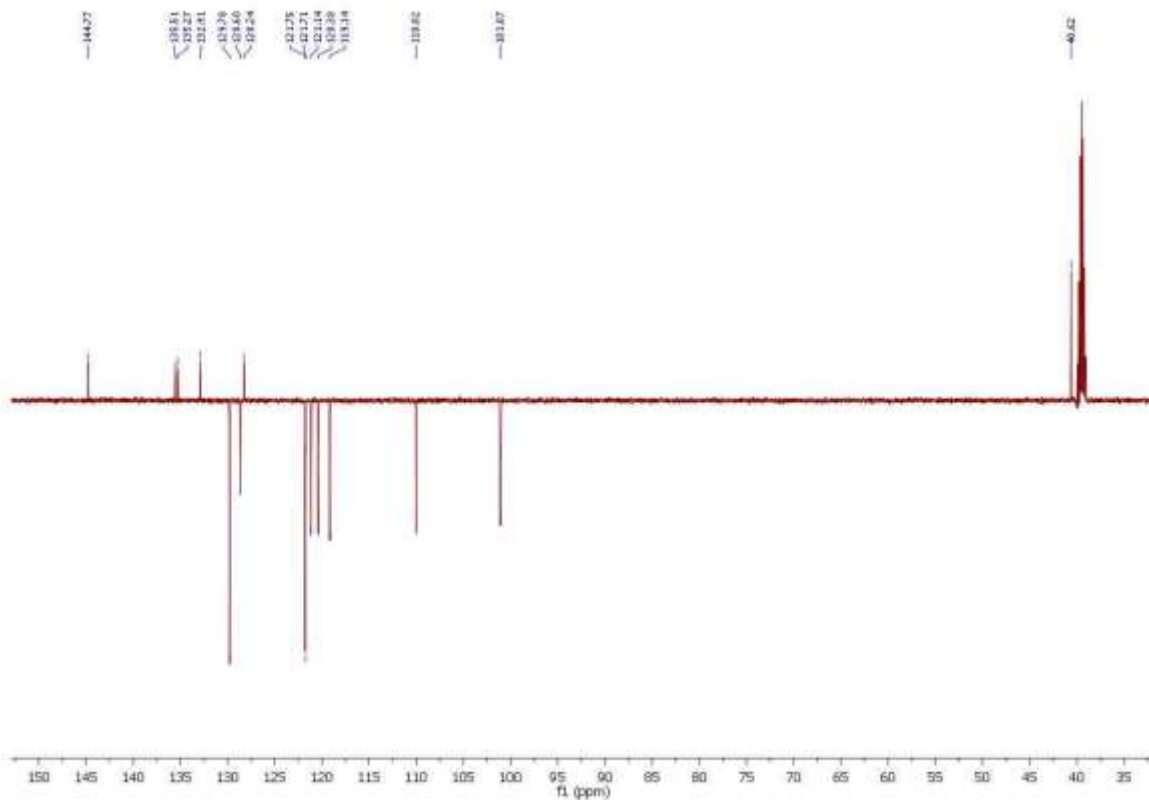
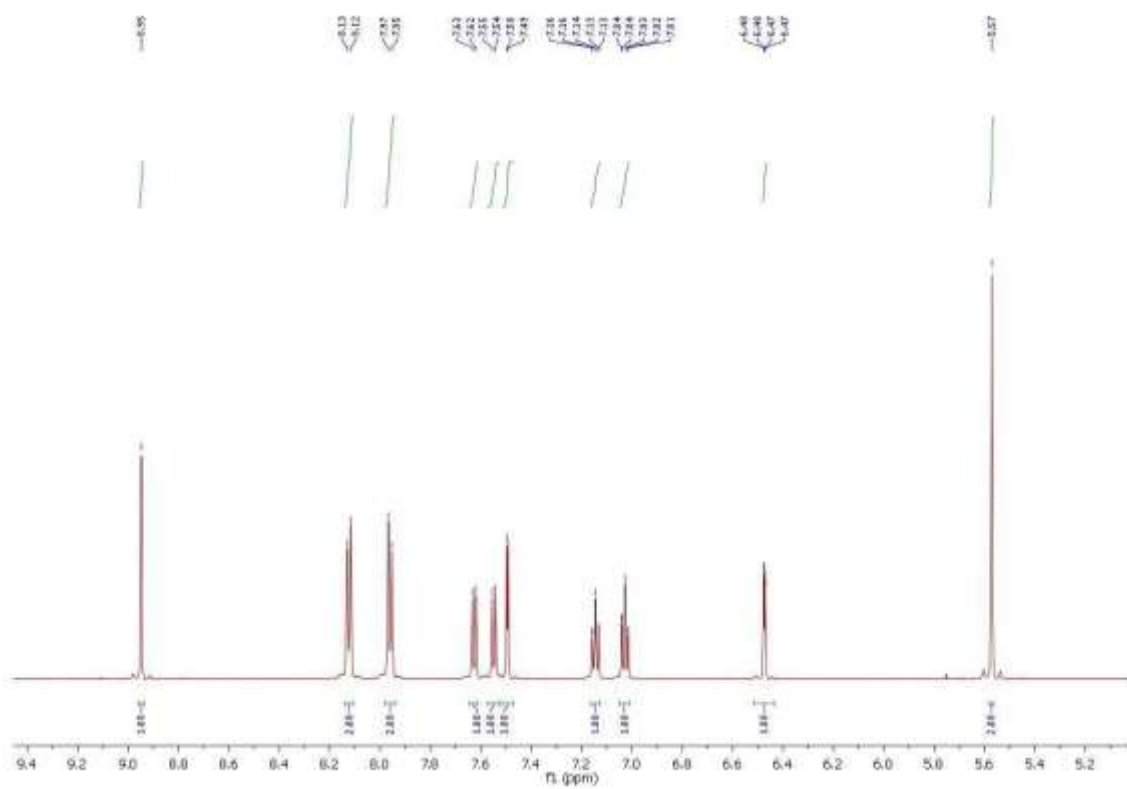


Fig. S30 a) ^1H NMR and b) ^{13}C NMR of compd. **11c**

a)



b)

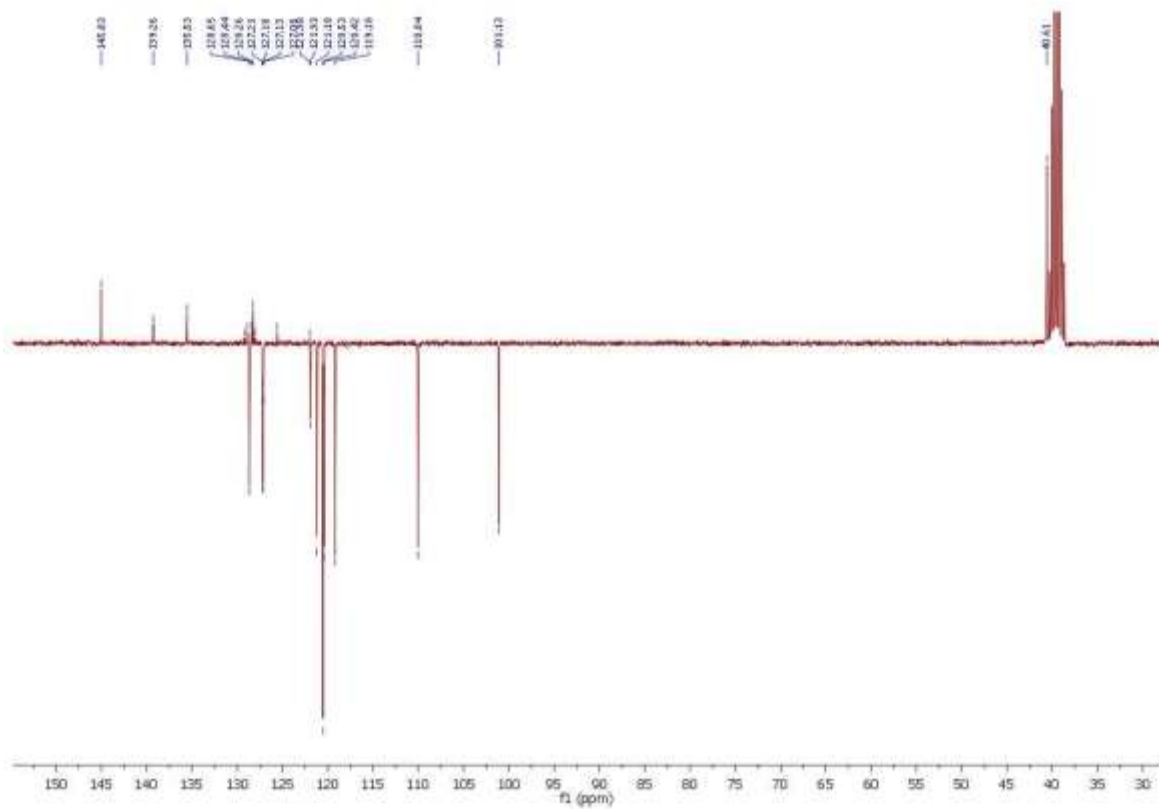
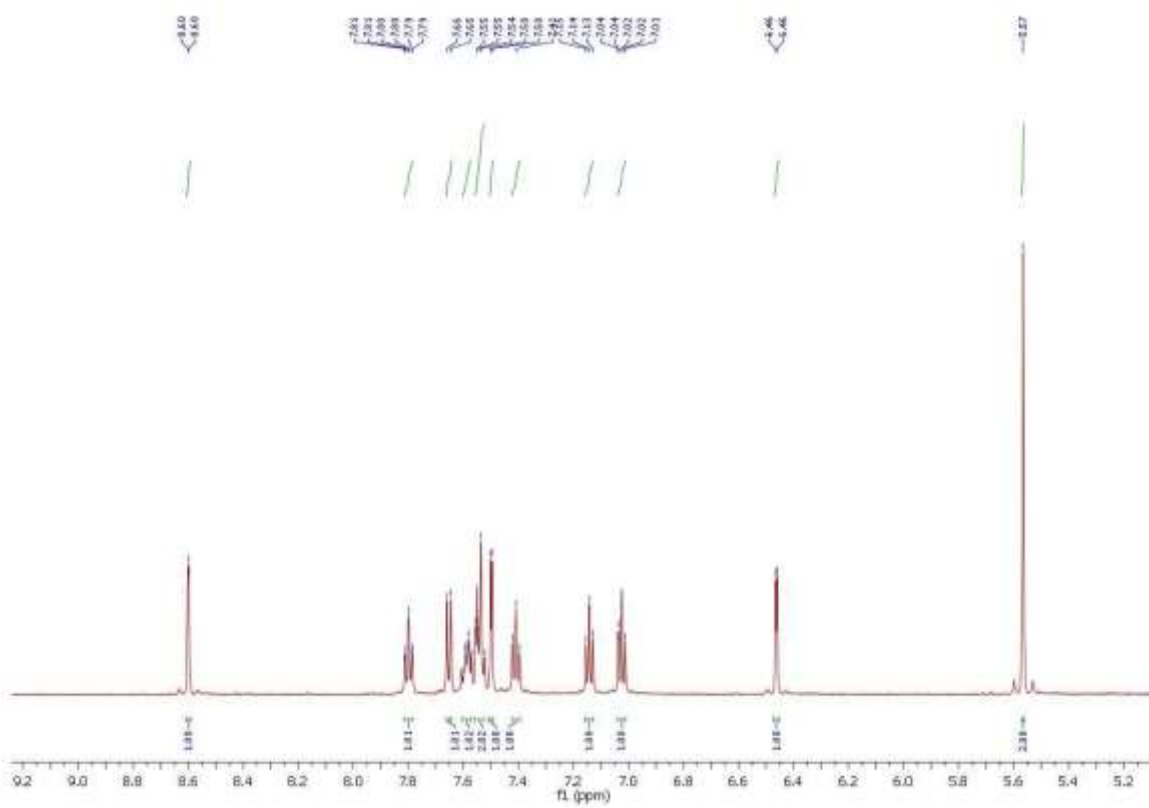


Fig. S31 a) ^1H NMR and b) ^{13}C NMR of compd. **11d**

a)



b)

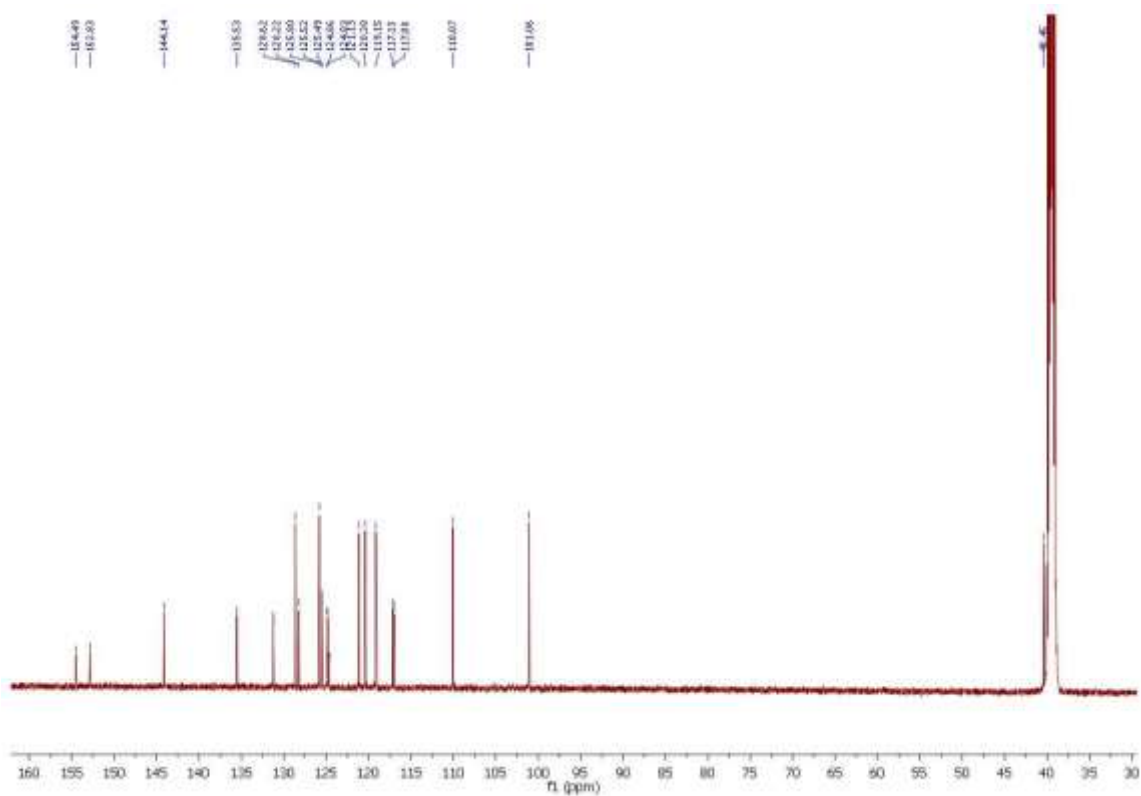
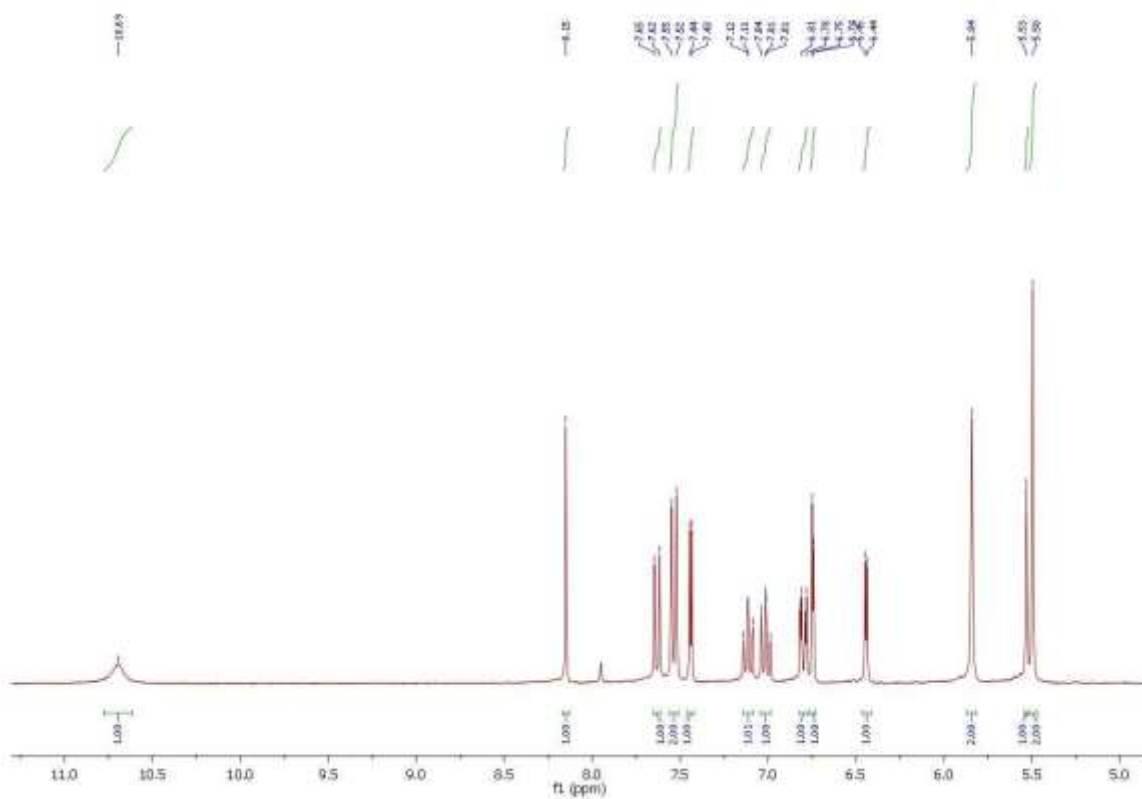


Fig. S32 a) ^1H NMR and b) ^{13}C NMR of compd. **11e**

a)



b)

