

Electronic Supplementary Information

An efficient catalytic synthesis and characterization of new styryl-ferrocenes and their *trans*- π -conjugated organosilicon materials

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Procedure for the synthesis of Palladium(0) Complex

The title compound was synthesized according to the new procedure presented below.

Bis(tris(o-tolyl)phosphine)(dibenzylideneacetone)palladium(0) – $[\text{Pd}(\eta^2\text{-dba})(\text{P}(\text{o-tolyl})_3)_2]^{32}$ (**3**):
 $\text{Pd}(\text{dba})_2$ (0.3 g, 5.22×10^{-4} mol), tris(*o*-tolyl)phosphine (0.321 g, 1.054×10^{-3} mol) were placed in a Schlenk flask (25 mL) and degassed for one minute. Afterwards, 4 mL toluene (0.125M) was introduced into vigorously stirred solids of substrates and the final mixture was left for 8h at room temperature to give a yellow-orange solution. The excess of the solvent was evaporated under reduced pressure. The procedure was followed by the addition of hexane. As a result a yellow-orange precipitate was observed. Next, the precipitate was filtered ('canula' system), washed with cold hexane (4 x 10 mL) and dried in vacuum for 2h. The crude product was obtained with 93% (460 mg, yellow-orange solid) yield. Elemental analyses calcd. for $\text{C}_{60}\text{H}_{58}\text{OP}_2\text{Pd}$: C 74.80, H 6.07; found C 74.78, H 6.06.

X-Ray structure determination

Excalibur four-circle diffractometer with Eos CCD-detector, using MoK α radiation source ($\lambda = 0.7107$ Å). The data was corrected for Lorentz-polarization as well as for absorption effects.³⁸ Accurate unit-cell parameters were determined by a least-squares fit of 1984 reflections of highest intensity, chosen from the whole experiment. The structures were solved with SIR92³⁹ and refined with the full-matrix least-squares procedure on F^2 by SHELXL97.⁴⁰ All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed geometrically, in idealized positions, and refined as rigid groups with their U_{iso} 's as 1.2 times U_{eq} of the appropriate carrier atom. Crystallographic data (excluding structure factors) for the structural analysis has been deposited with the Cambridge Crystallographic Data Centre, No. CCDC 974168. Copies of this information may be obtained free of charge from: The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK. Fax: +44(1223)336-033, e-mail:deposit@ccdc.cam.ac.uk, or www: www.ccdc.cam.ac.uk.

Notes and references

38 Agilent Technologies 2010. CrysAlis PRO (Version 1.171.35.4).

39 A. Altomare, G. Cascarano, C. A. Giacovazzo, A. Gualardi, *J. Appl. Cryst.* 1993, **26**, 343-350.

40 G. M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112-122.

MS spectra

MS (m/z) spectra of **1^d** catalytic system (from Figure 1)

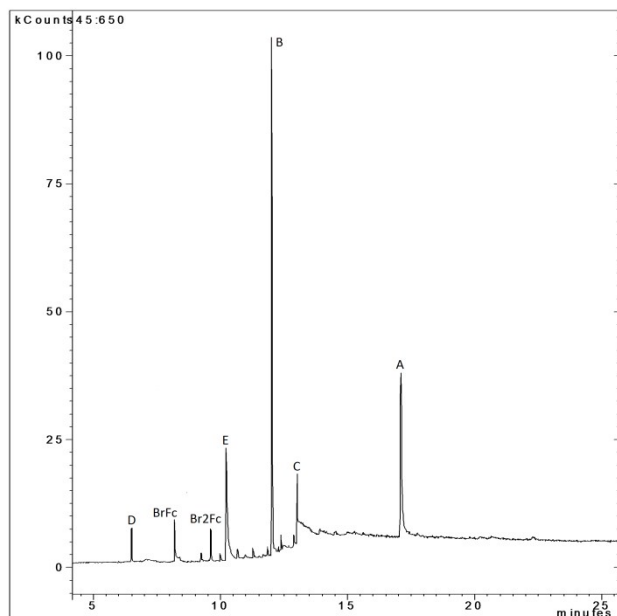
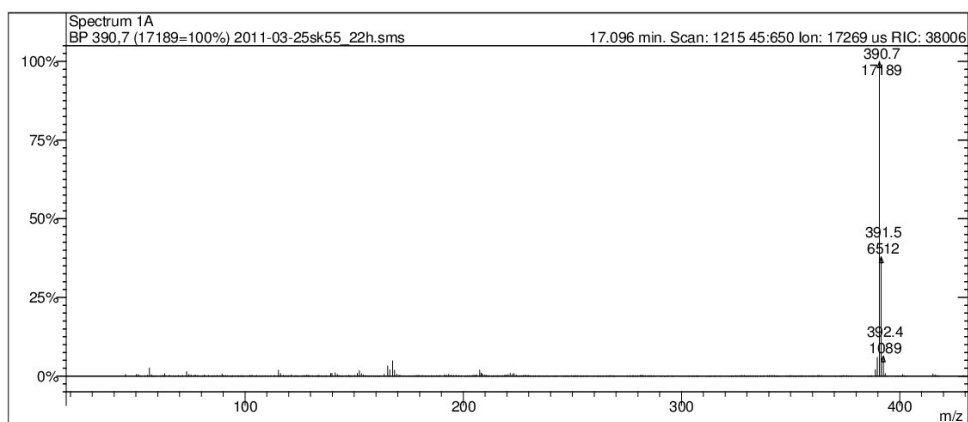
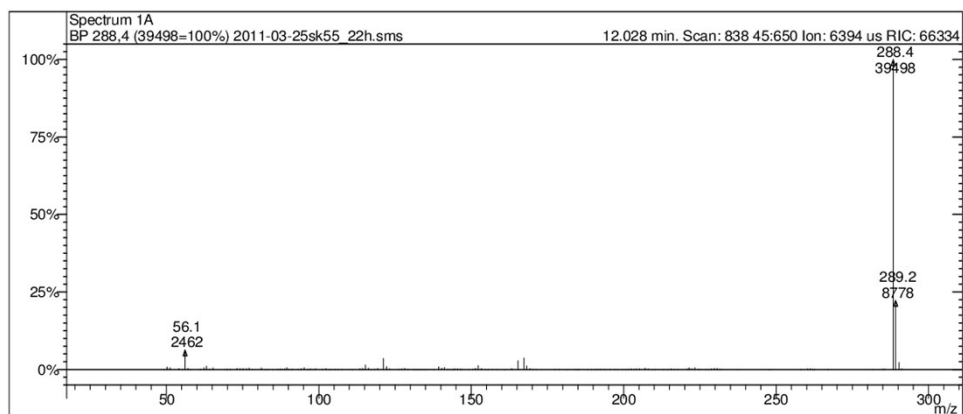


Figure 5. Sample of MS spectrum of **1^d** catalytic system.

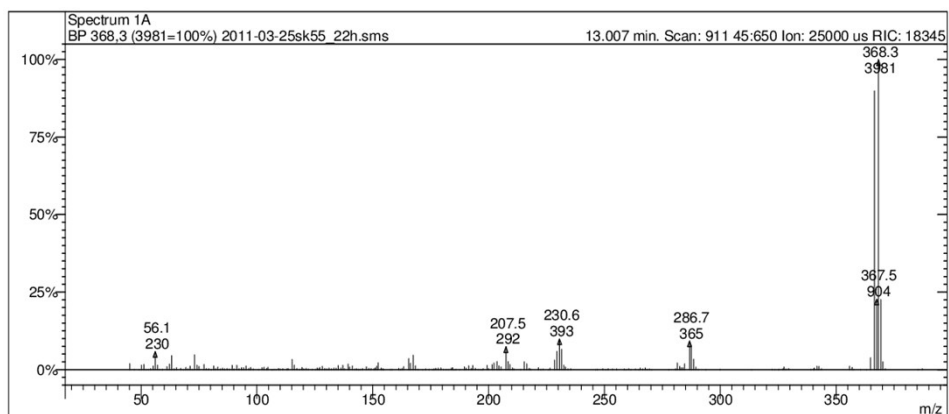
10 (A) – 1,1'-bis(4-vinylphenyl)ferrocene



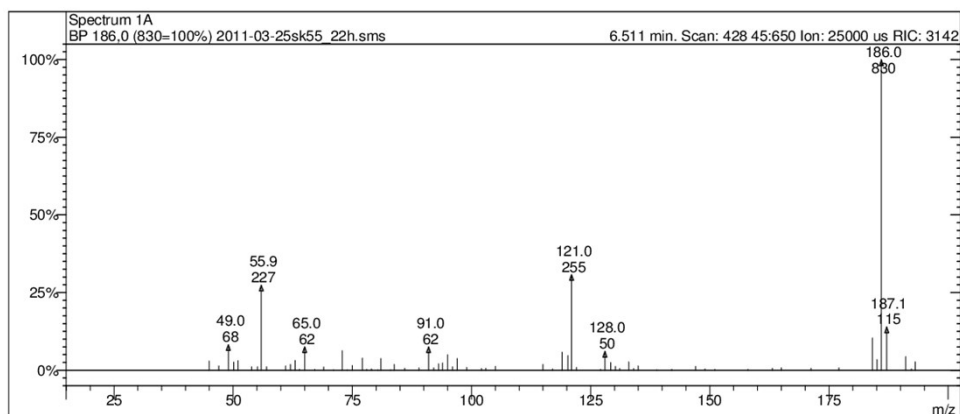
8 (B) – 1-(4-vinylphenyl)ferrocene



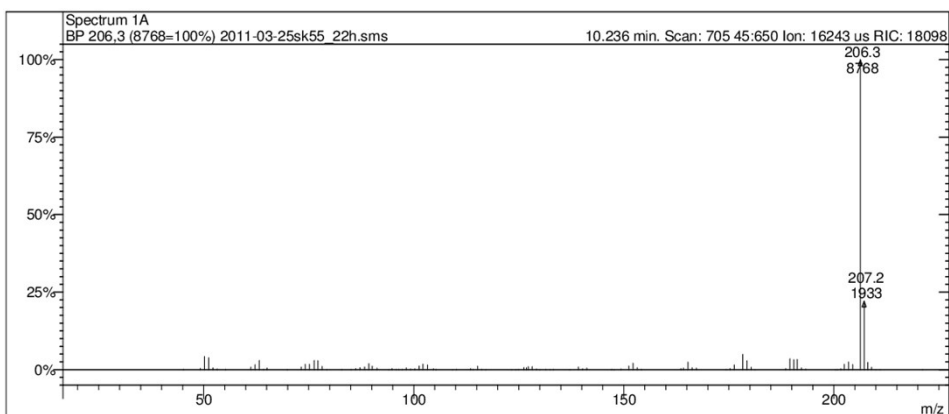
C – 1-(4-vinylphenyl)-1'-bromo-ferrocene



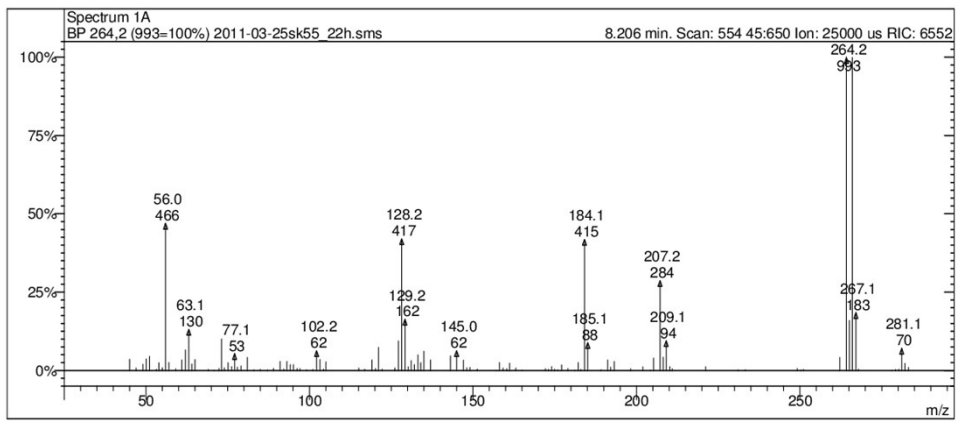
D - ferrocene



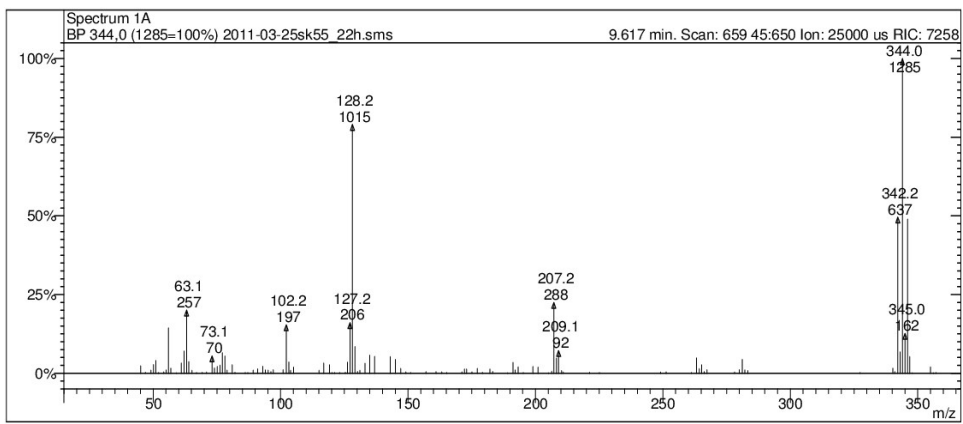
E – 4,4'-divinylbiphenyl



BrFc – 1-bromoferrocene



Br2Fc – 1,1'-dibromoferrocene



GPC chromatograms

GPC graphs of copolymers P1 and P2

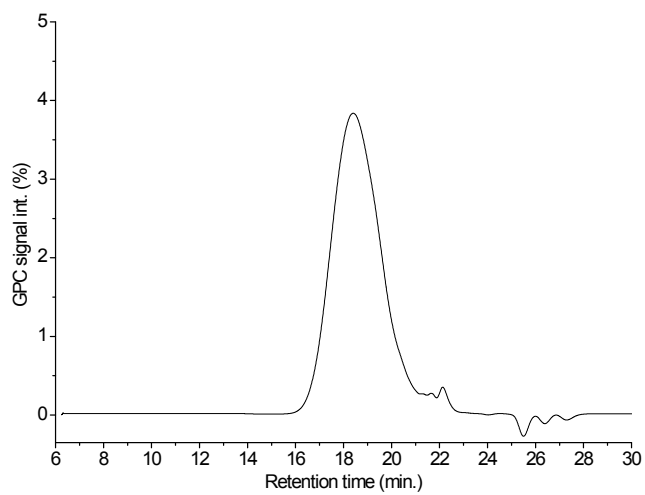


Figure 6. GPC chromatogram of copolymer **P1**.

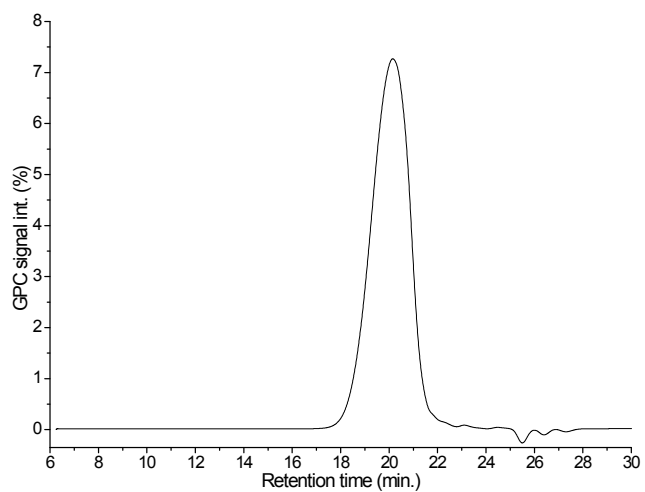
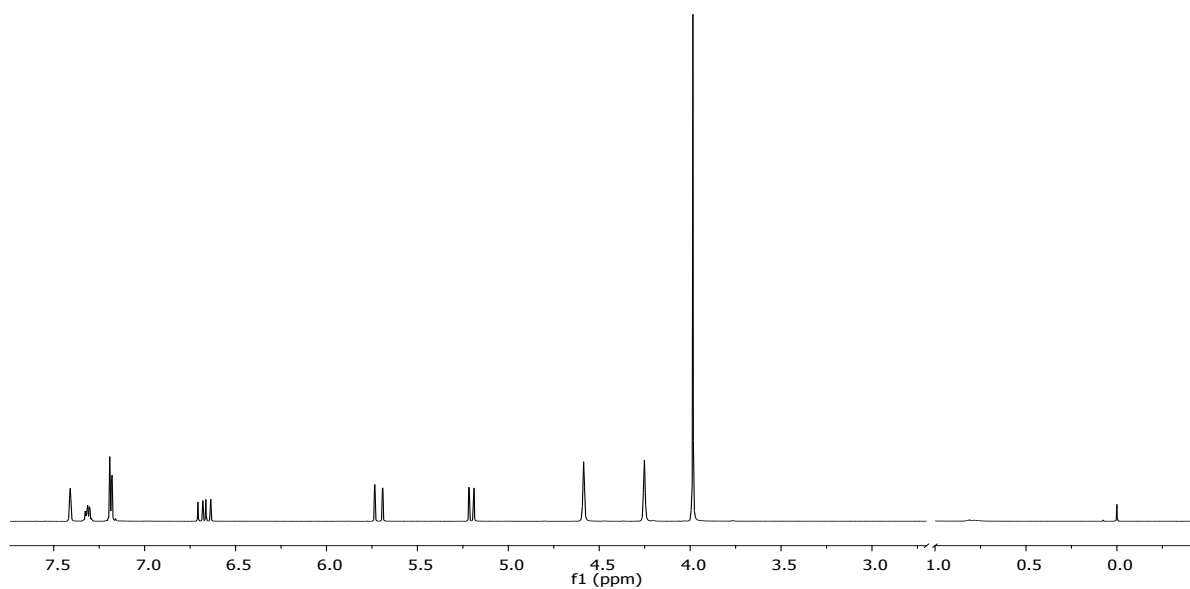


Figure 7. GPC chromatogram of copolymer **P2**.

NMR Spectra

Compound 7 ^1H NMR

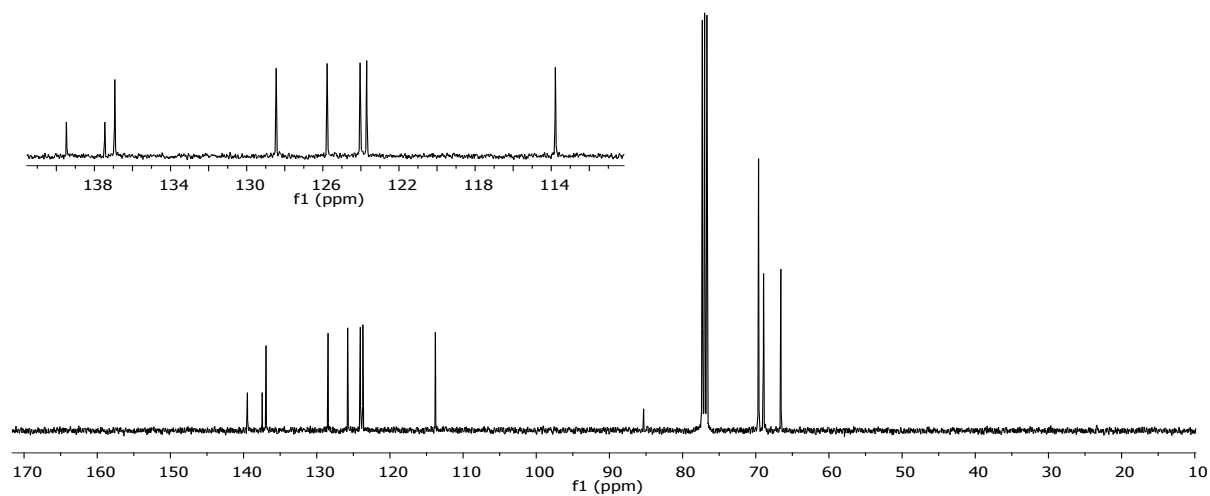
^1H NMR in CDCl_3 at 25oC Compound 7



Compound 7 ^{13}C NMR

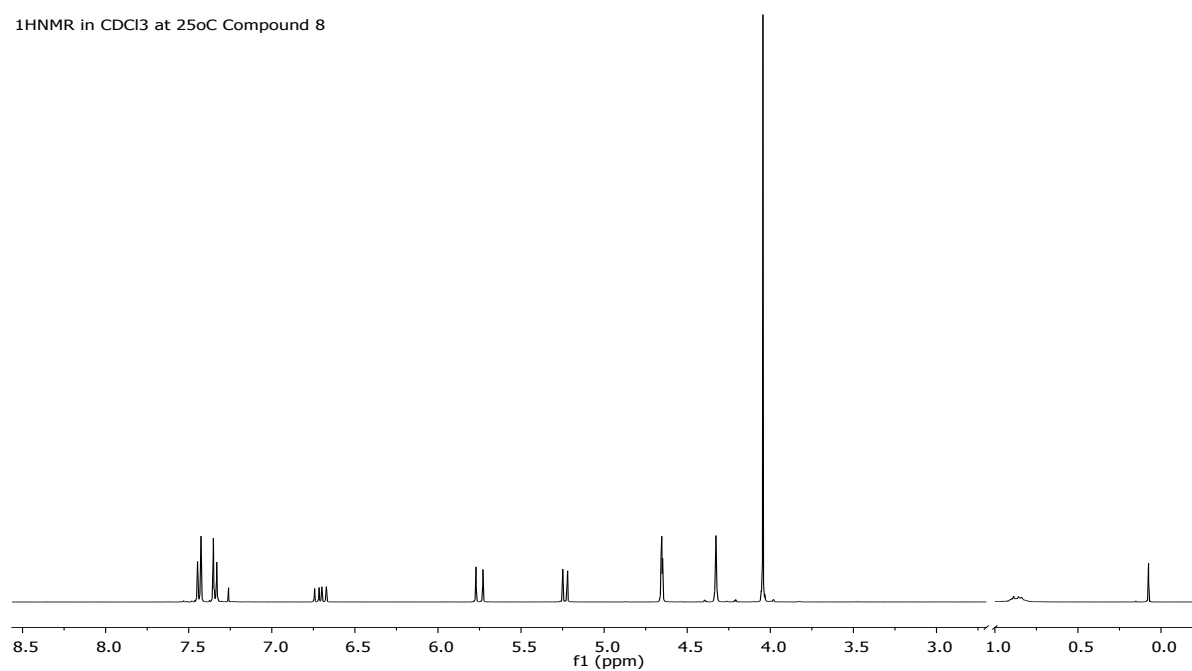
^{13}C NMR in CDCl_3 at 25oC Compound 7

^{13}C NMR in CDCl_3 at 25oC Compound 7



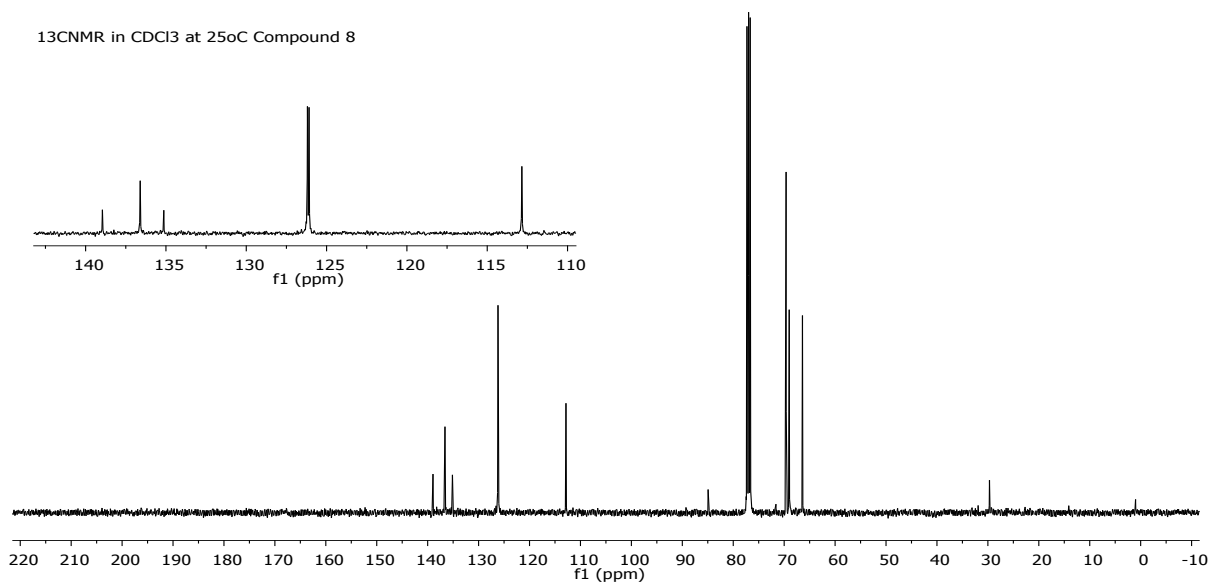
Compound **8** ^1H NMR

^1H NMR in CDCl_3 at 25oC Compound **8**



Compound **8** ^{13}C NMR

^{13}C NMR in CDCl_3 at 25oC Compound **8**

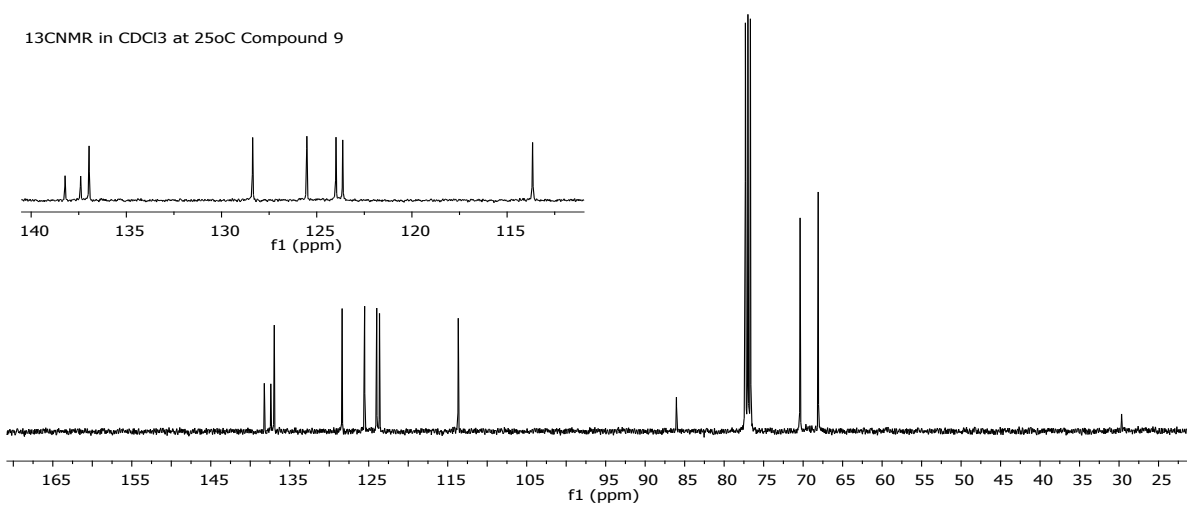


Compound **9** ^1H NMR (presence in the Article)

Compound **9** ^{13}C NMR

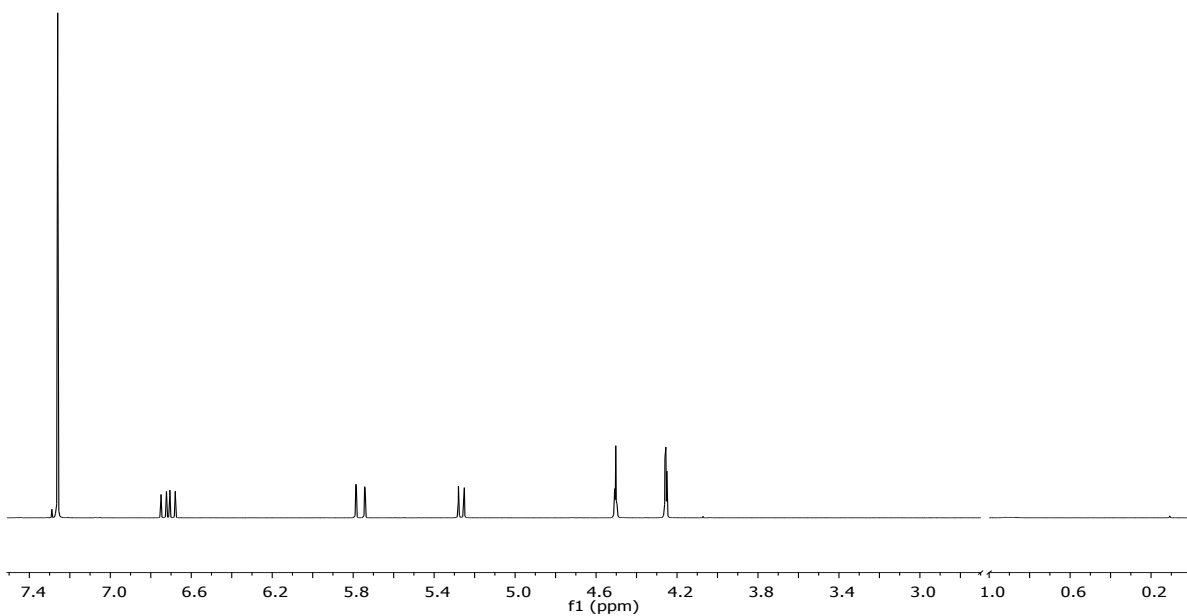
^{13}C NMR in CDCl_3 at 25oC Compound 9

^{13}C NMR in CDCl_3 at 25oC Compound 9



Compound **10** ^1H NMR

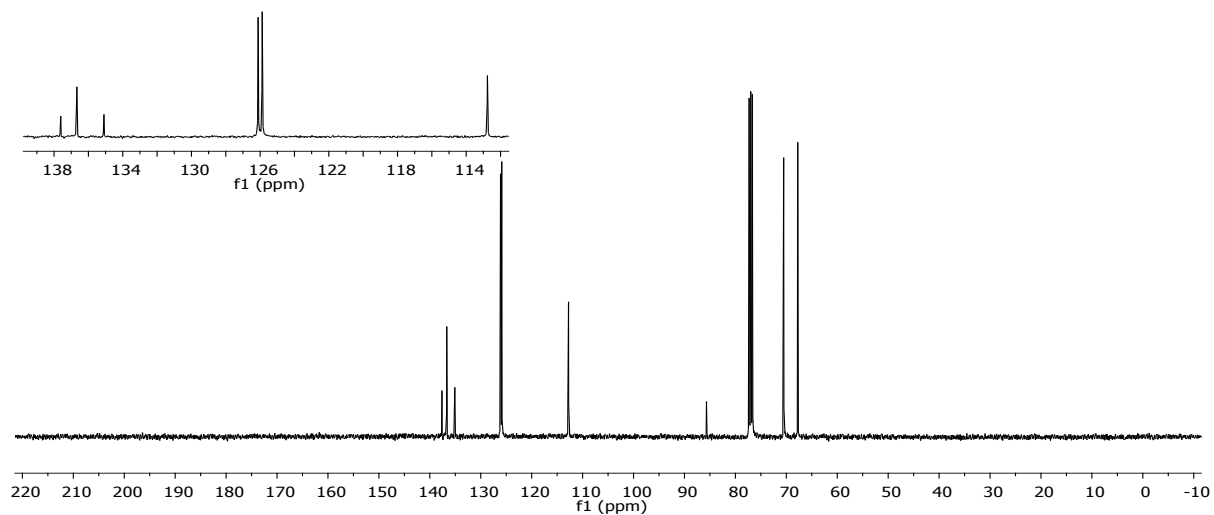
^1H NMR in CDCl_3 at 25oC Compound 10



Compound **10** ^{13}C NMR

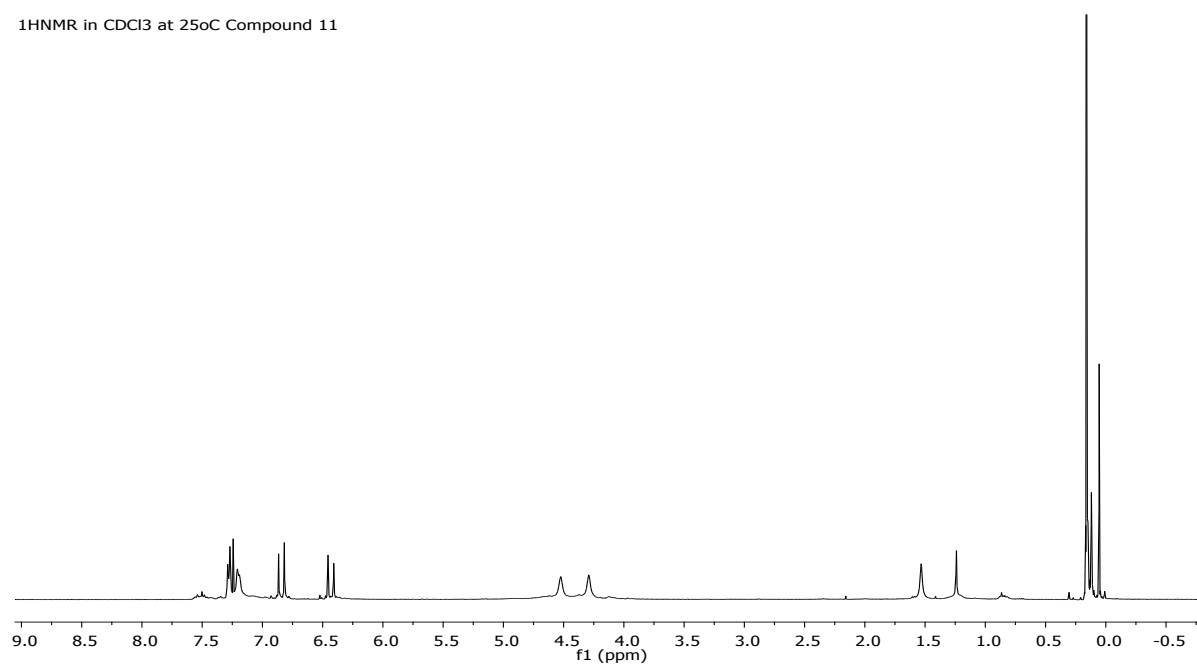
^{13}C NMR in CDCl_3 at 25°C Compound 10

^{13}C NMR in CDCl_3 at 25°C Compound 10



Compound **11** ^1H NMR

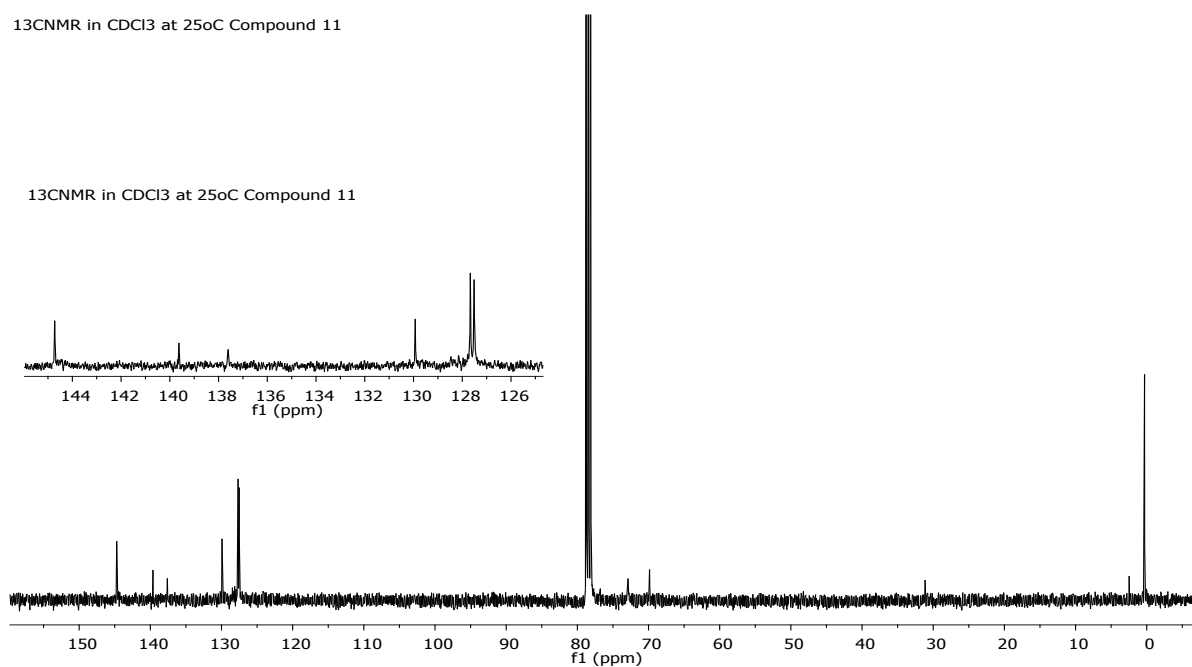
^1H NMR in CDCl_3 at 25°C Compound 11



Compound **11** ^{13}C NMR

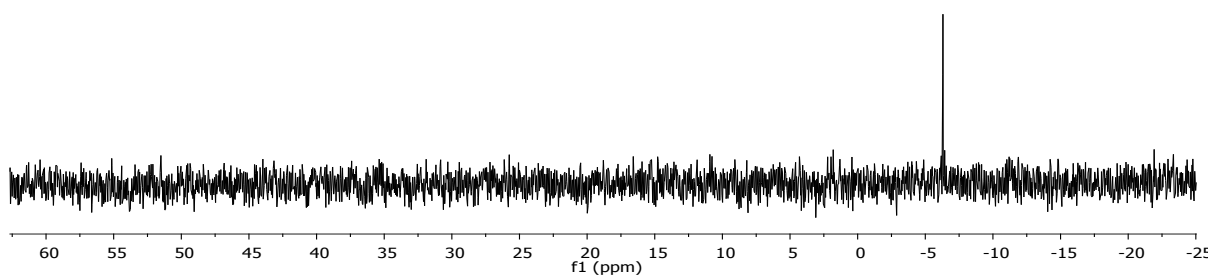
^{13}C NMR in CDCl_3 at 25oC Compound 11

^{13}C NMR in CDCl_3 at 25oC Compound 11



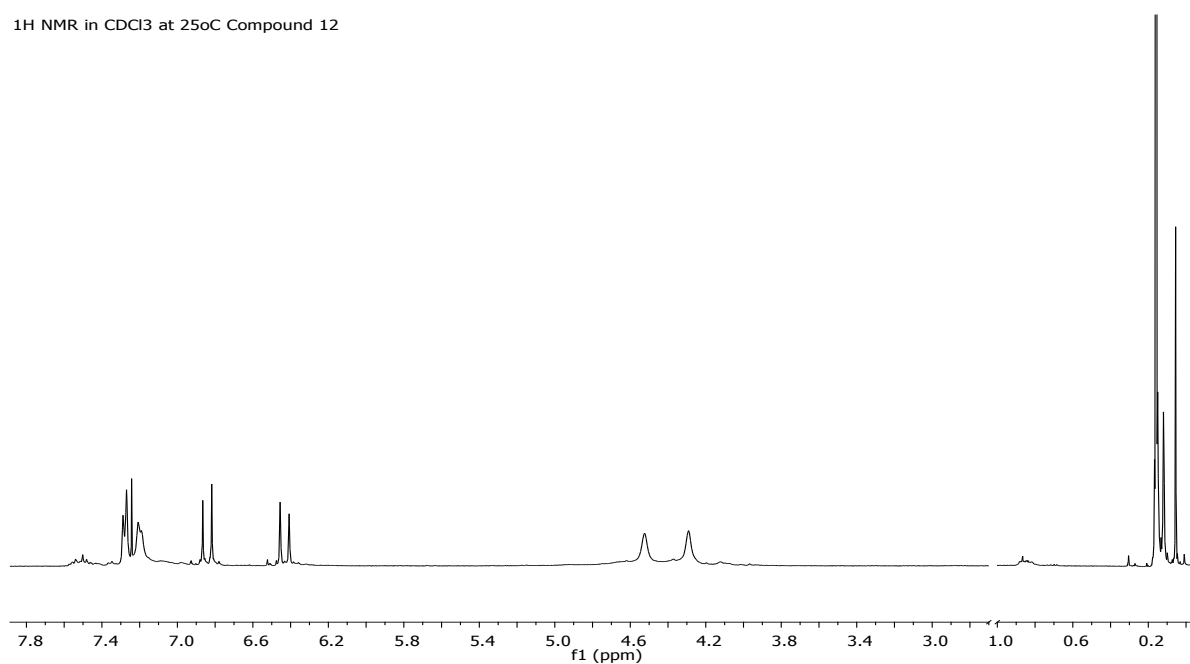
Compound **11** ^{29}Si NMR

^{29}Si NMR in CDCl_3 at 25oC compound 11



Compound **12** ^1H NMR

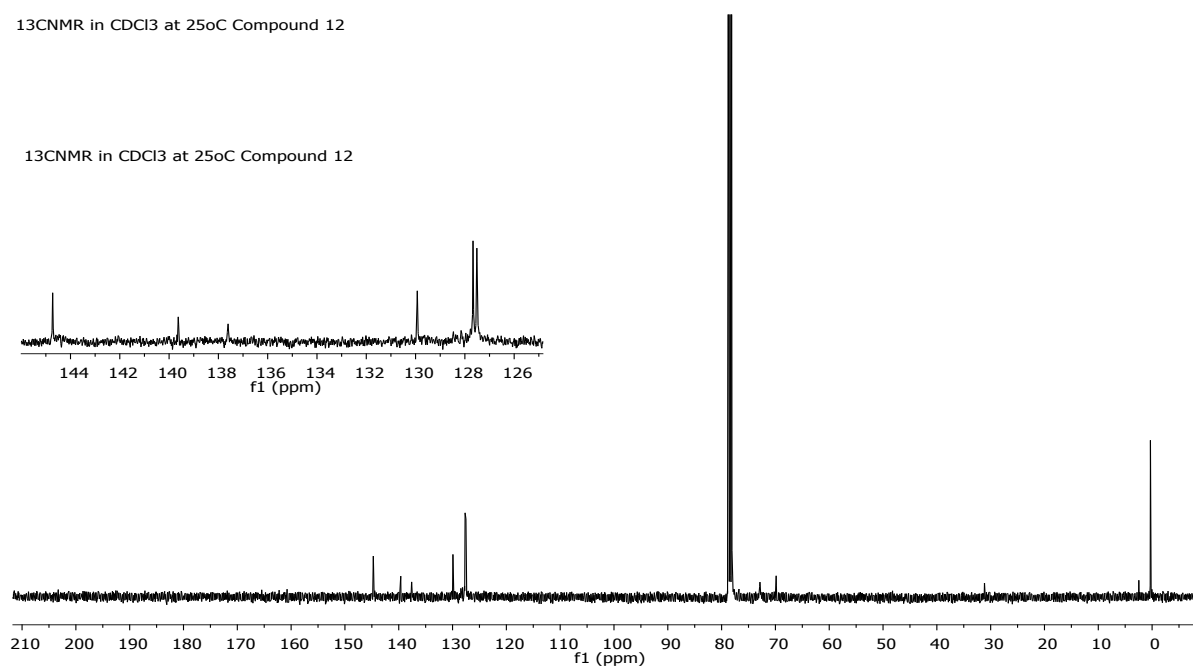
^1H NMR in CDCl_3 at 25°C Compound 12



Compound **12** ^{13}C NMR

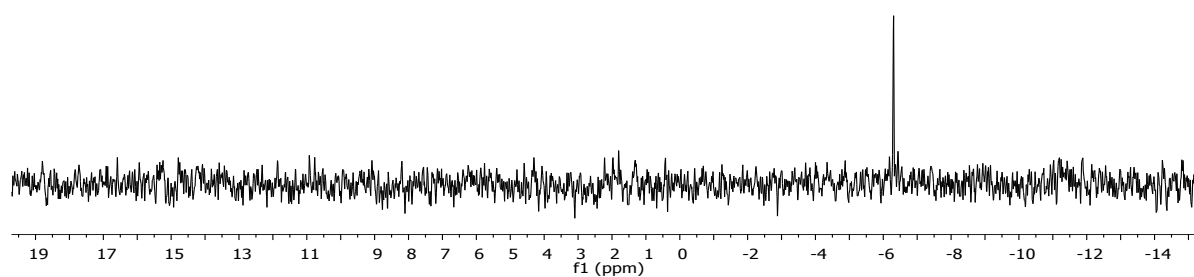
^{13}C NMR in CDCl_3 at 25°C Compound 12

^{13}C NMR in CDCl_3 at 25°C Compound 12



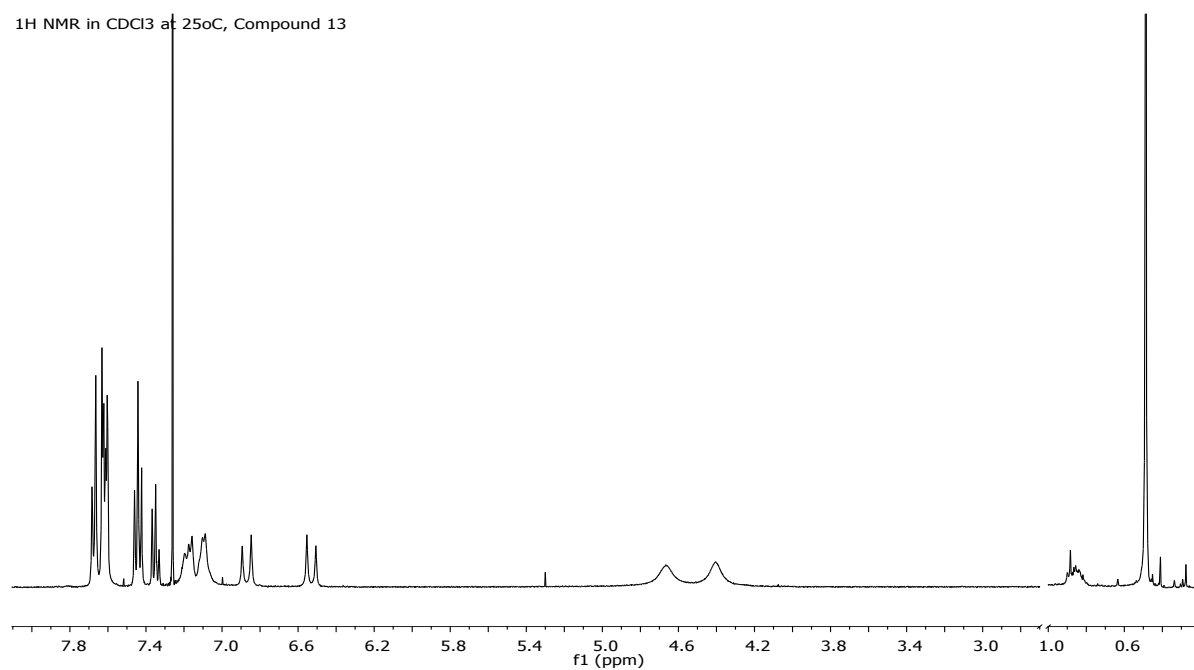
Compound **12** ^{29}Si NMR

^{29}Si NMR in CDCl_3 at 25°C compound 12



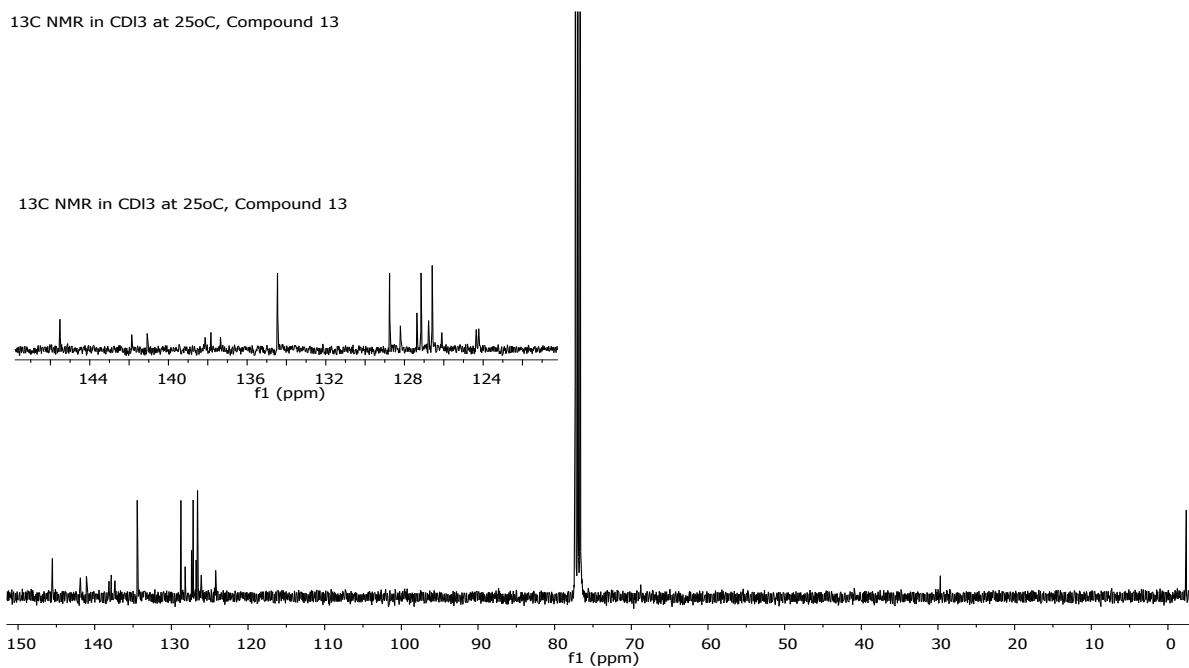
Compound **13** ^1H NMR

^1H NMR in CDCl_3 at 25°C, Compound 13



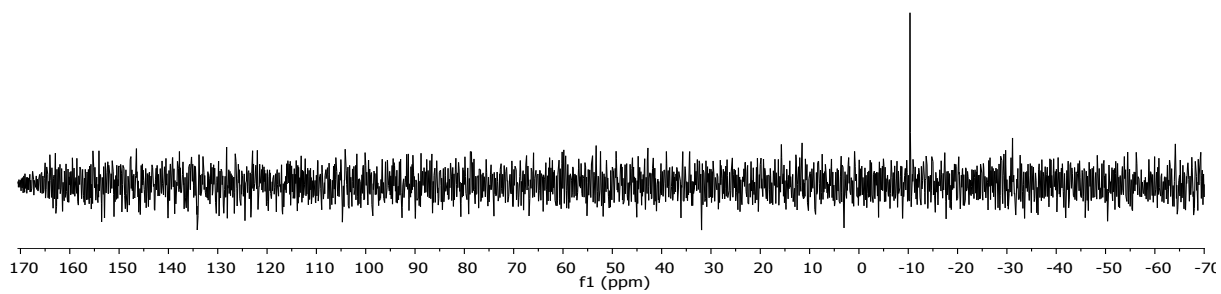
Compound **13** ^{13}C NMR

^{13}C NMR in CDCl_3 at 25°C, Compound 13



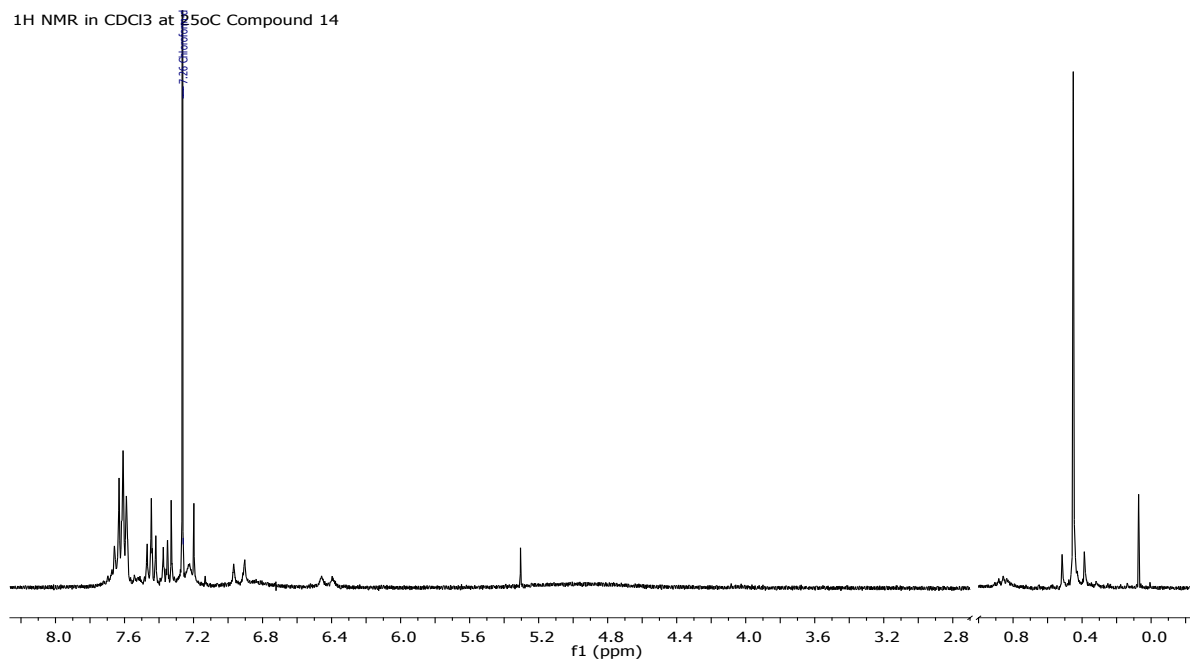
Compound **13** ^{29}Si NMR

^{29}Si NMR in CDCl_3 at 25°C Compound 13



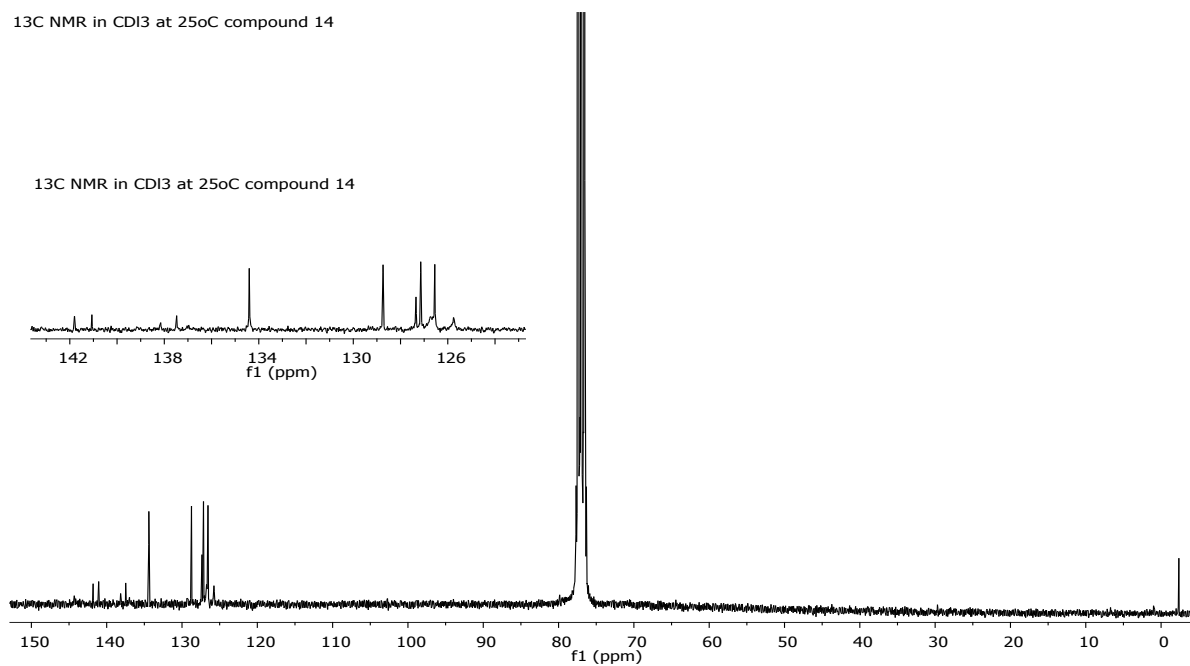
Compound **14** ^1H NMR

^1H NMR in CDCl_3 at 25°C Compound 14



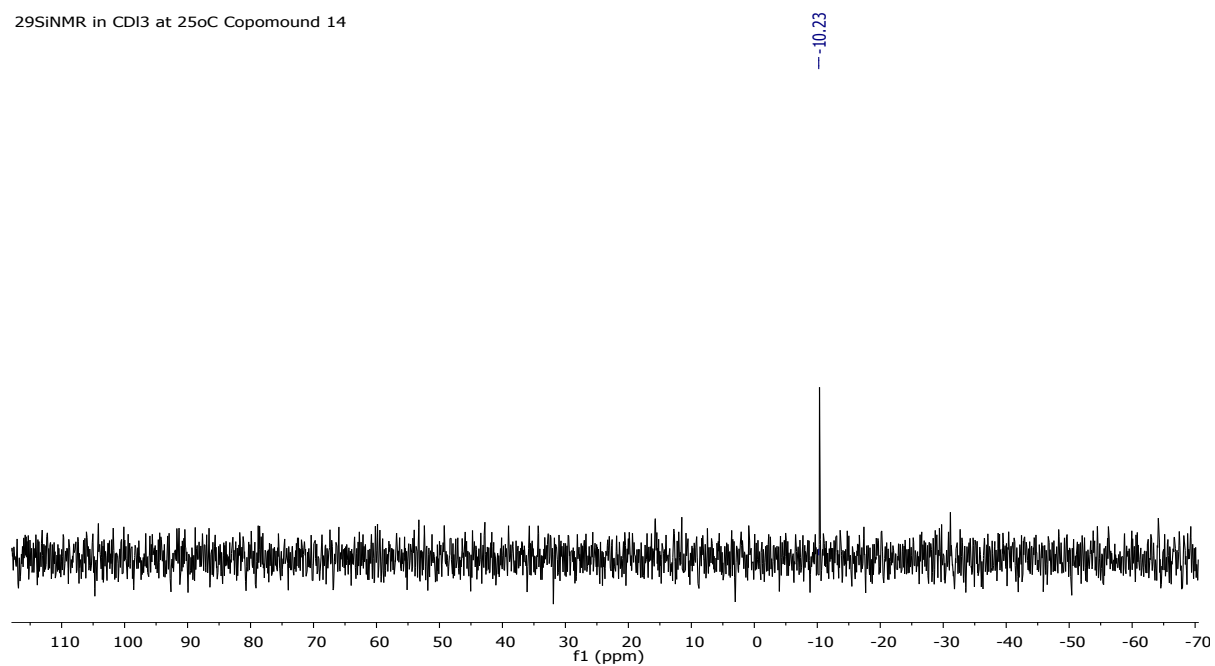
Compound **14** ^{13}C NMR

^{13}C NMR in CDCl_3 at 25°C compound 14



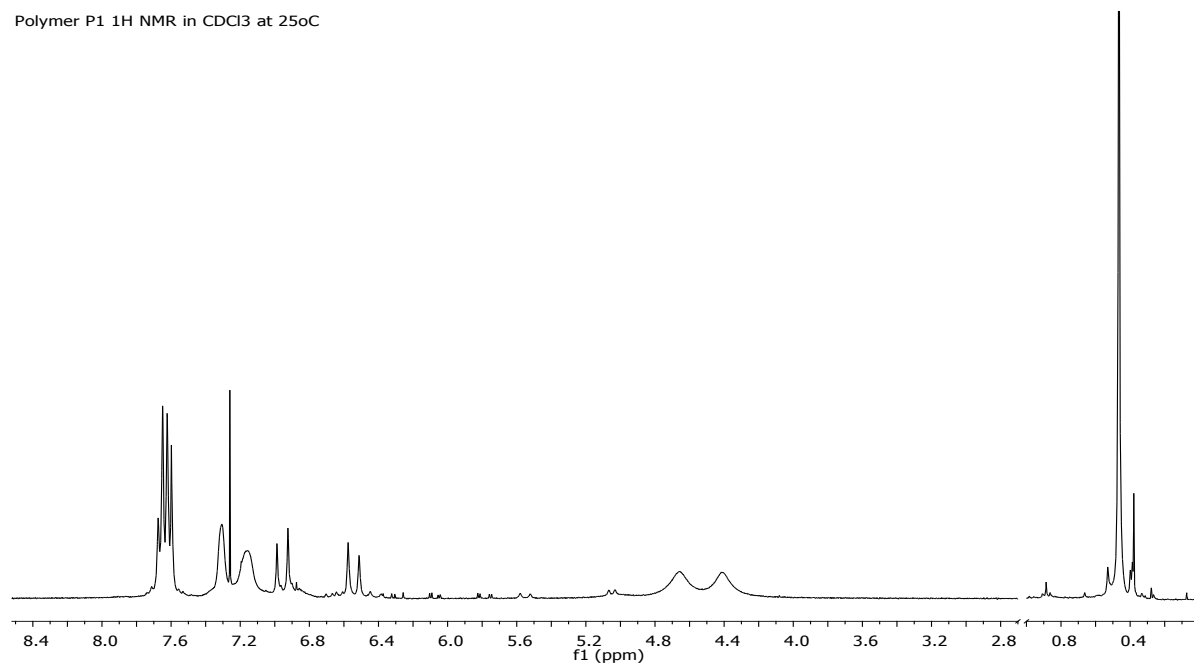
Compound **14** ^{29}Si NMR

^{29}Si NMR in CDCl_3 at 25°C Copomound 14



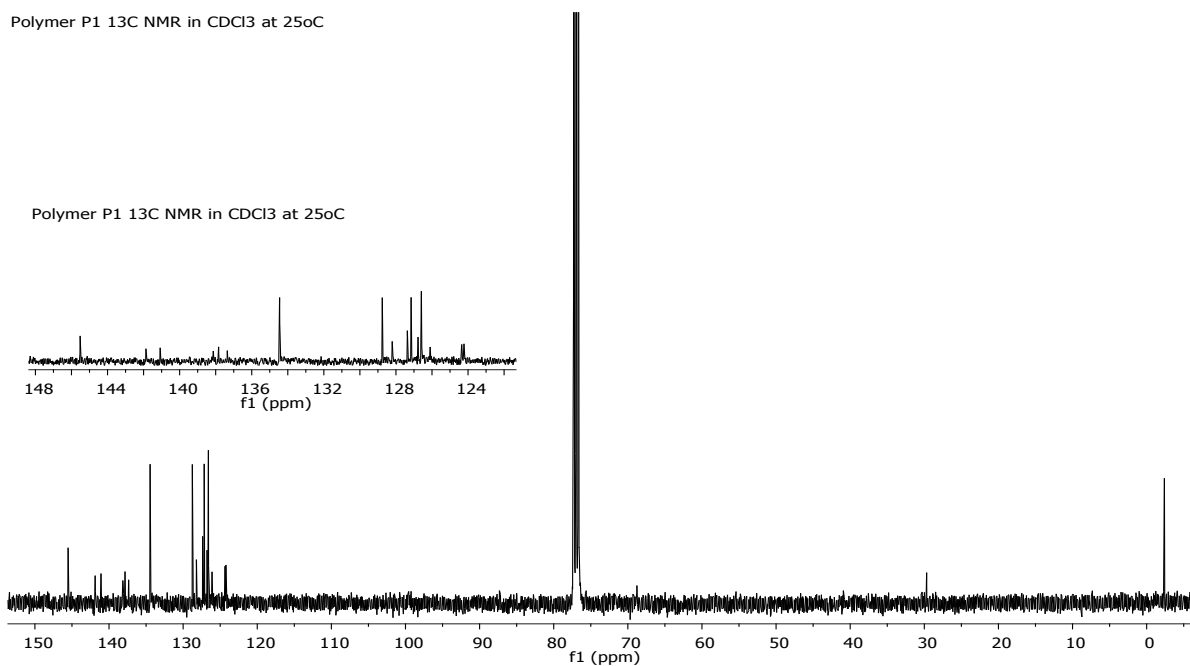
Polymer **P1** ^1H NMR

Polymer P1 ^1H NMR in CDCl_3 at 25°C



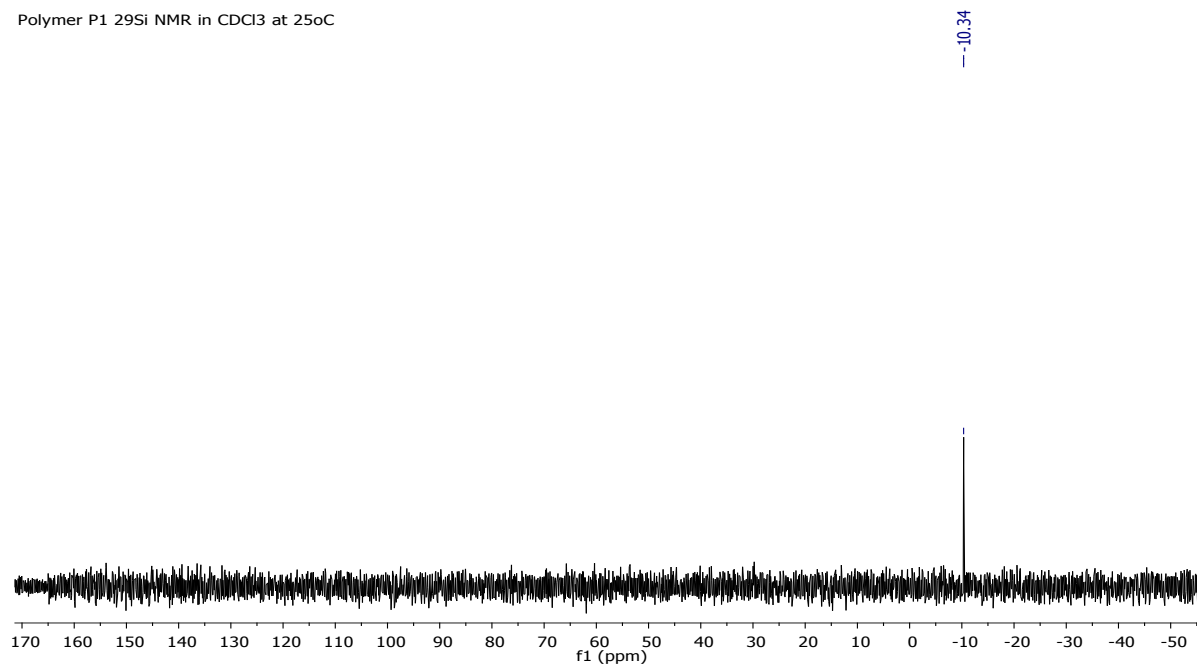
Polymer P1 ^{13}C NMR

Polymer P1 ^{13}C NMR in CDCl_3 at 25oC



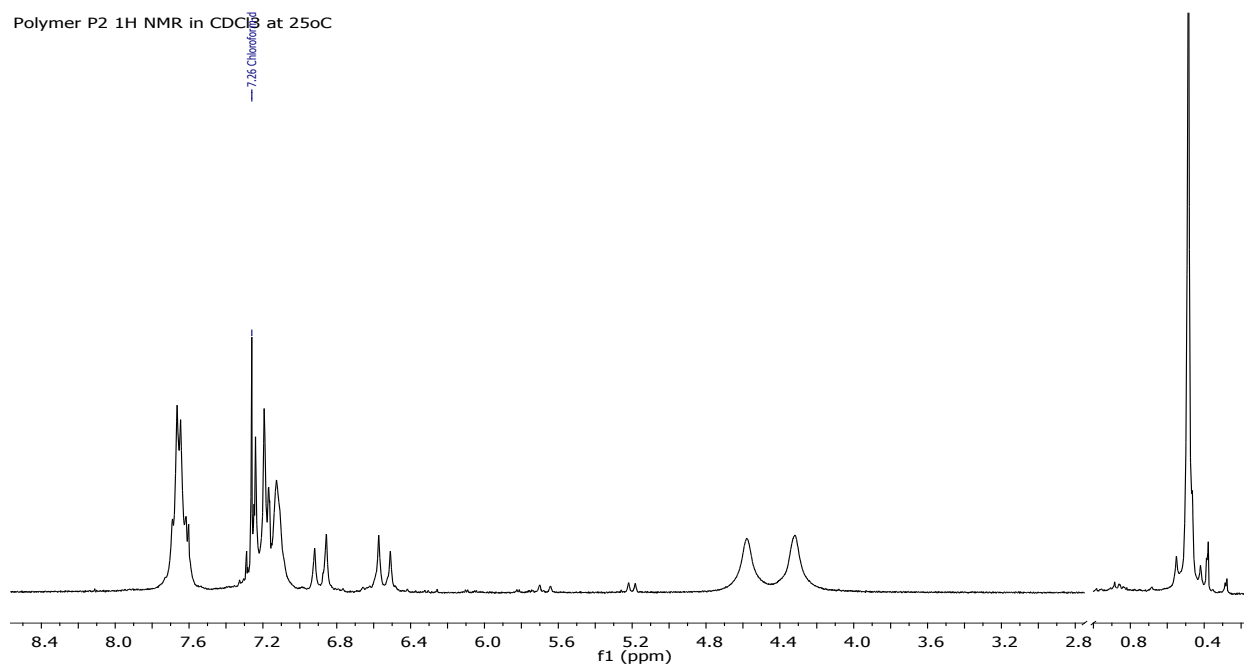
Polymer P1 ^{29}Si NMR

Polymer P1 ^{29}Si NMR in CDCl_3 at 25oC



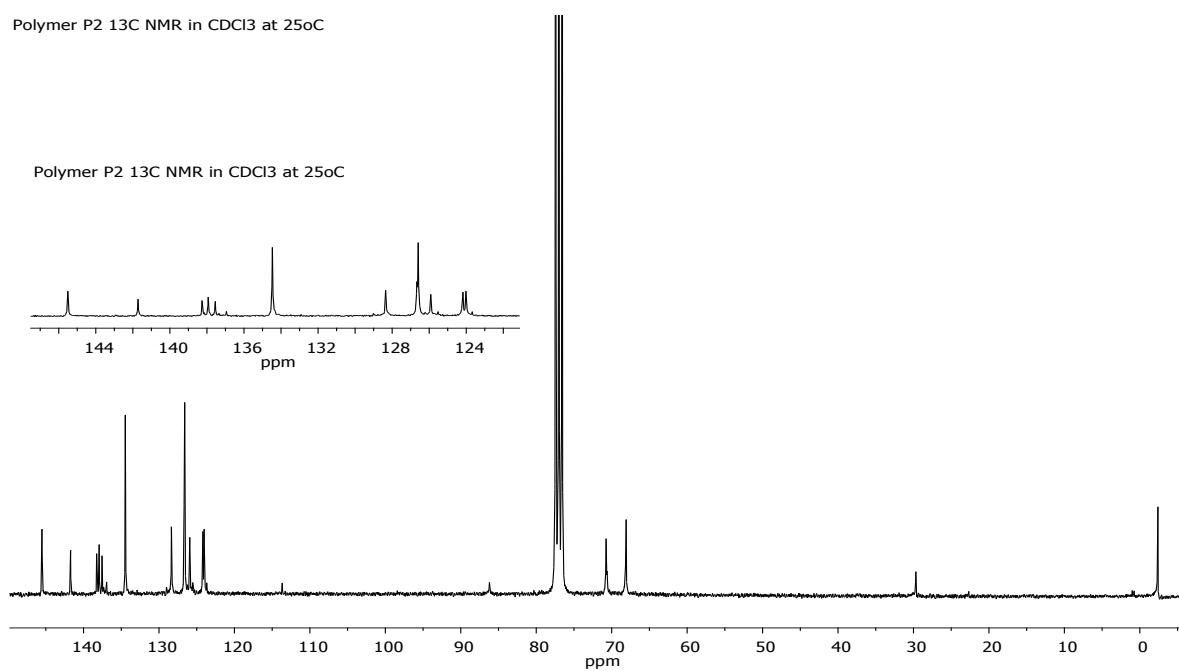
Polymer P2 ^1H NMR (presence in the Article)

Polymer P2 1H NMR in CDCl₃ at 25oC



Polymer P2 ¹³C NMR

Polymer P2 13C NMR in CDCl₃ at 25oC



Polymer P2 ²⁹Si NMR

Polymer 2 ²⁹SiNMR in CDCl₃ at 25oC

