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A New Polyacetylene from *Vernonia scorpioides* (Lam.) Pers. (Asteraceae) and its *in vitro* Antitumoral Activity

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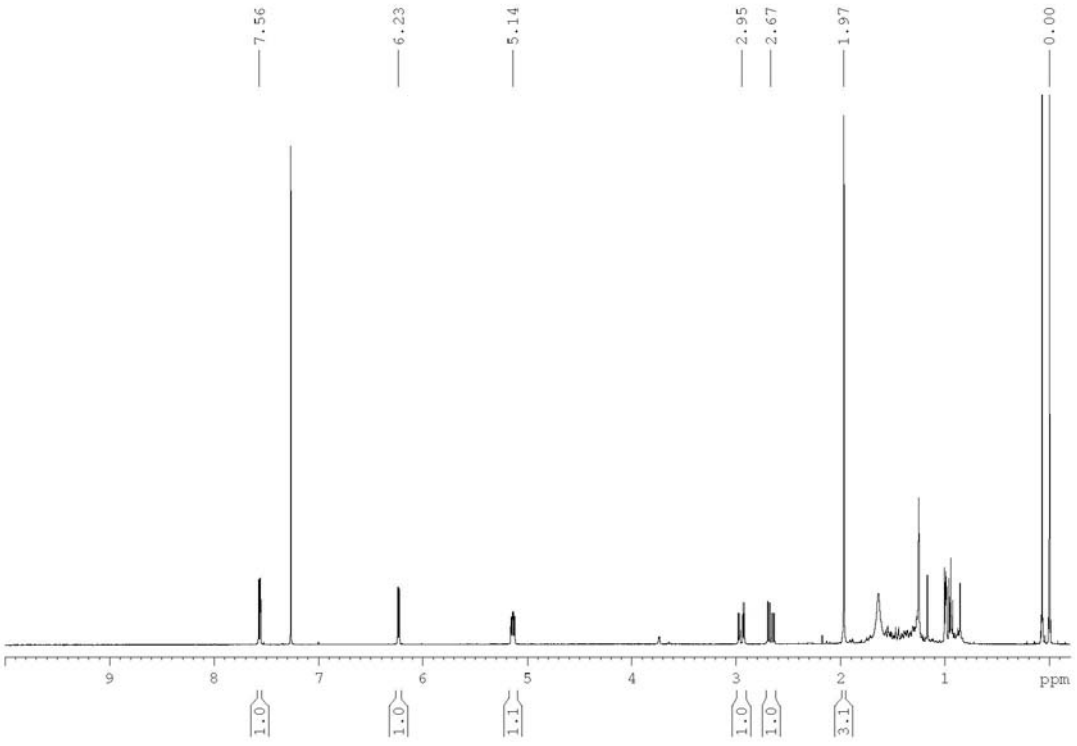

Figure S1. ^{1}H NMR spectrum of the polyacetylene (**1**) in $CDCl_3$ at 400 MHz.

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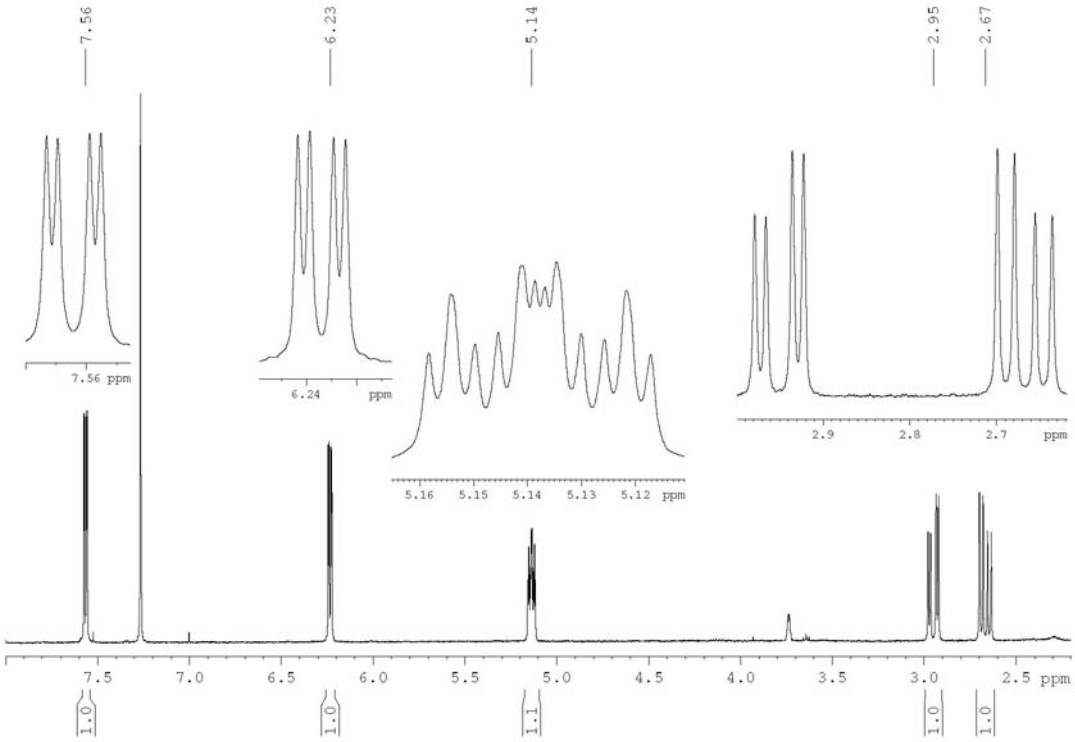

Figure S2. Expansions of the ^{1}H NMR spectrum of the polyacetylene (**1**) in $CDCl_3$ at 400 MHz.

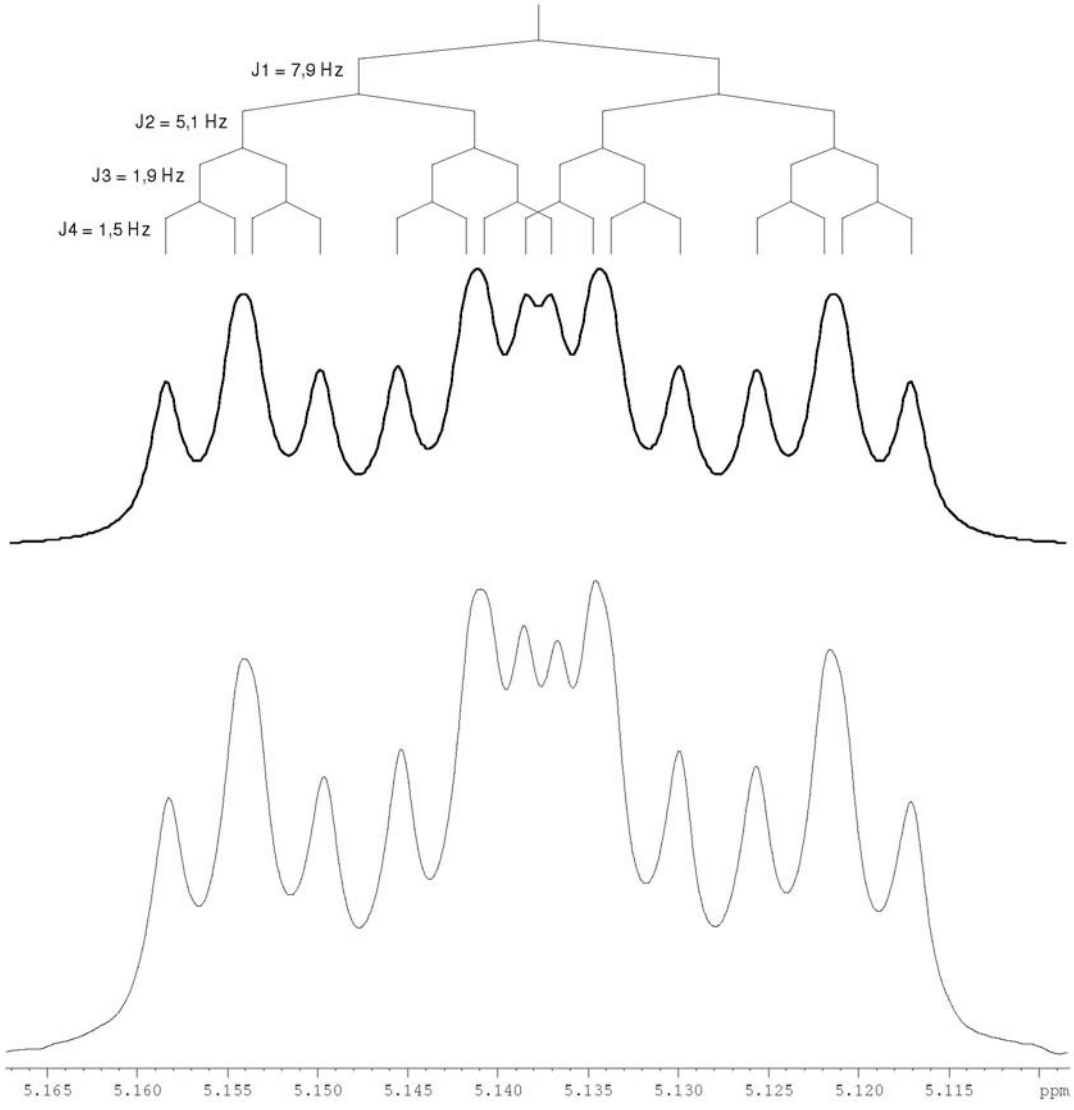

Figure S3. Simulated (Top) and experimental (Bottom, $CDCl_3$ at 400 MHz) ^1H NMR signal in order to understand the multiplicity of H-5 at 5.14 ppm (*dddd* 7.9, 5.1, 1.9, 1.5) of the polyacetylene (**1**). The signal was simulated with aid of the FOMSC-3 software (http://artemis.ffclrp.usp.br/NMR.htm).

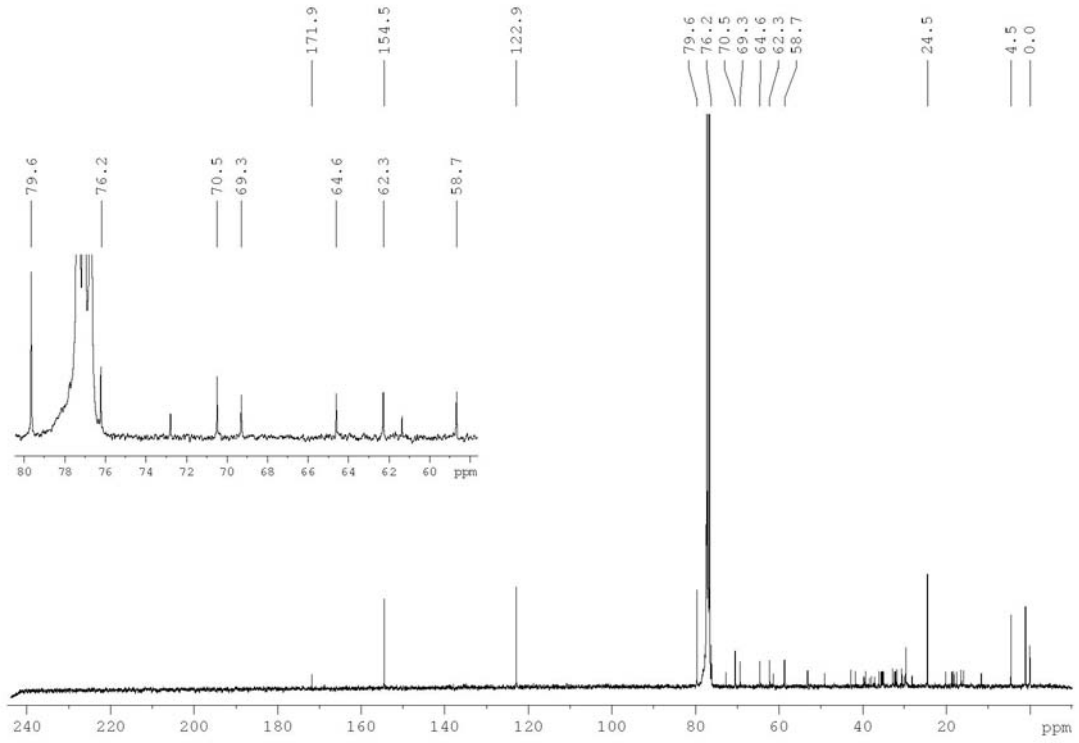

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of the polyacetylene (**1**) in $CDCl_3$ at 100 MHz. Insert is an expansion showing the signal from C-2' to C-7'.

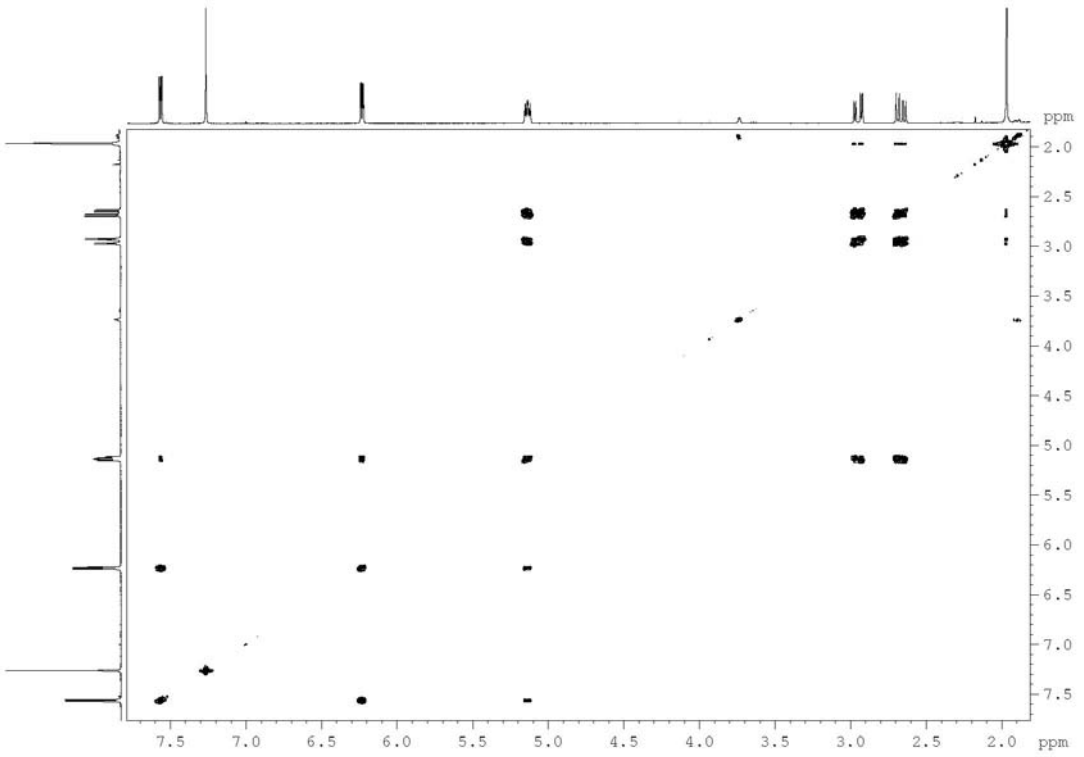

Figure S5. ^{1}H-^{1}H correlation map from COSY NMR experiment of the polyacetylene (**1**) in $CDCl_3$ at 400 MHz.

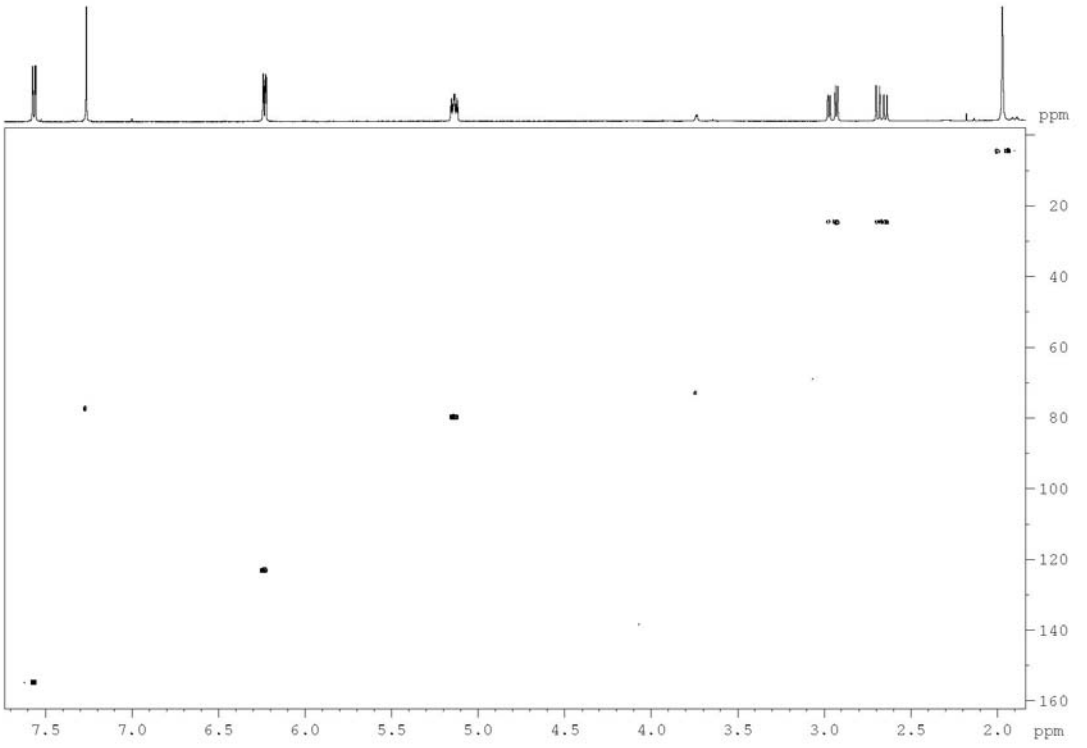

Figure S6. ^{1}H-^{13}C one-bond correlation map from HSQC NMR experiment of the polyacetylene (**1**) in $CDCl_3$ at 400 and 100 MHz.

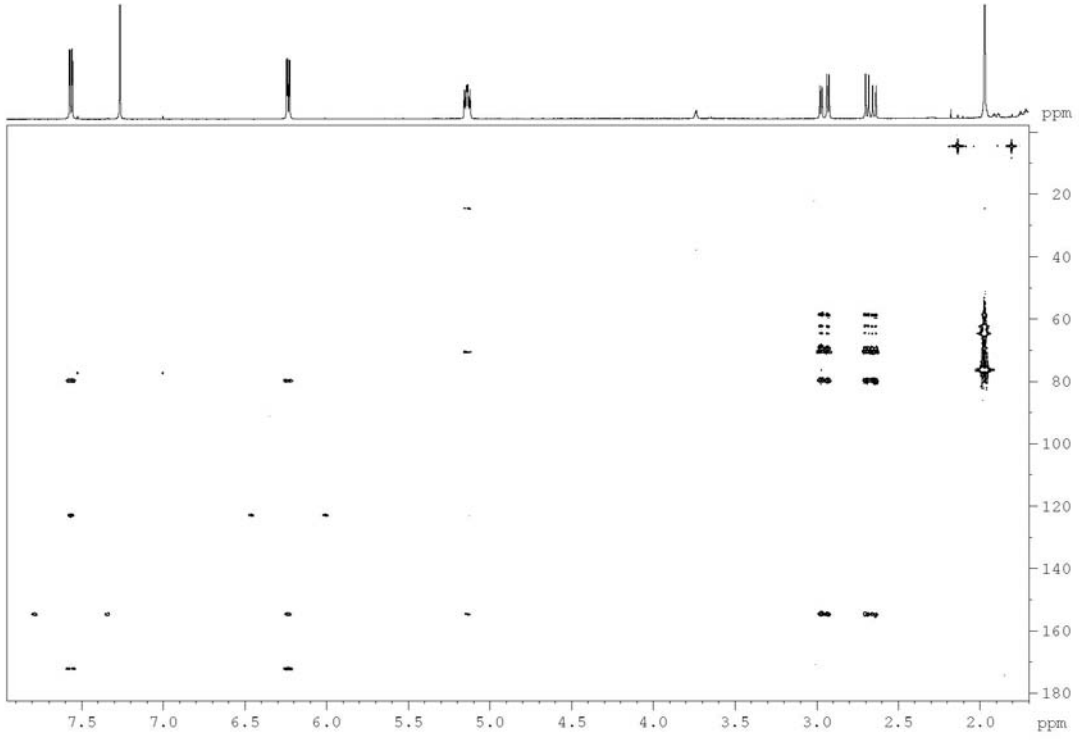

Figure S7. ^{1}H-^{13}C long-range correlation map from HMBC NMR experiment of the polyacetylene (**1**) in $CDCl_3$ at 400 and 100 MHz.

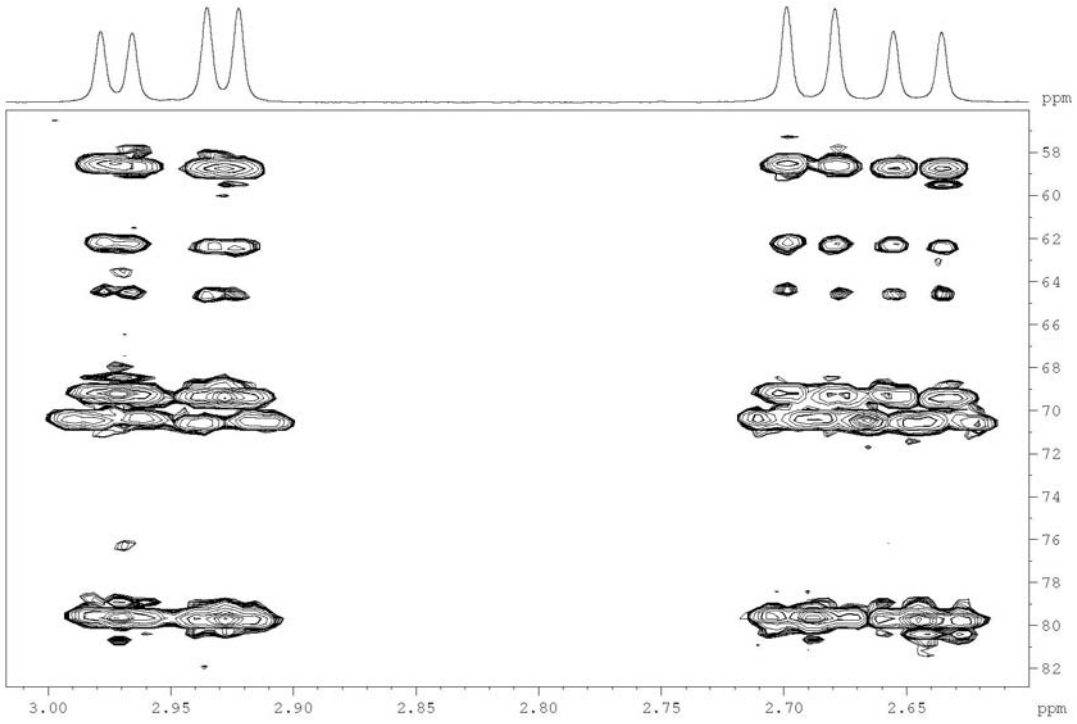

Figure S8. Expansion of the ^{1}H-^{13}C long-range correlation map from HMBC NMR experiment of the polyacetylene (**1**) in $CDCl_3$ at 400 and 100 MHz, showing the correlations for both H-1' at 2.67 and 2.95 ppm.

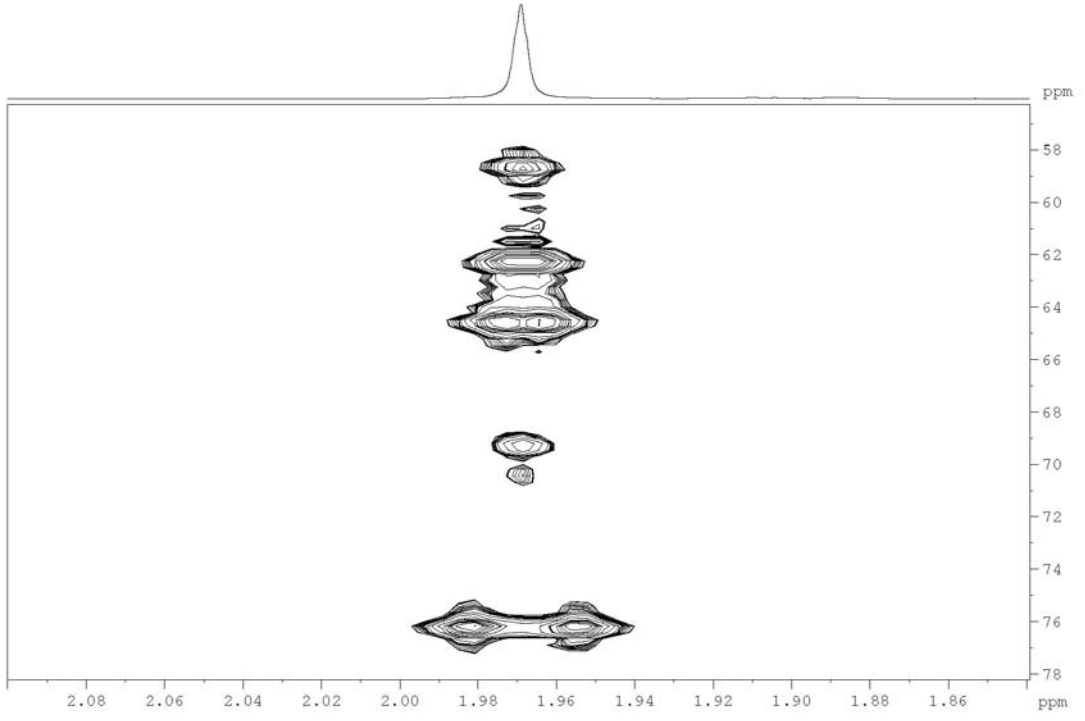

Figure S9. Expansion of the ^{1}H-^{13}C long-range correlation map from HMBC NMR experiment of the polyacetylene (**1**) in $CDCl_3$ at 400 and 100 MHz, showing the correlations for H-8' at 2.97 ppm.

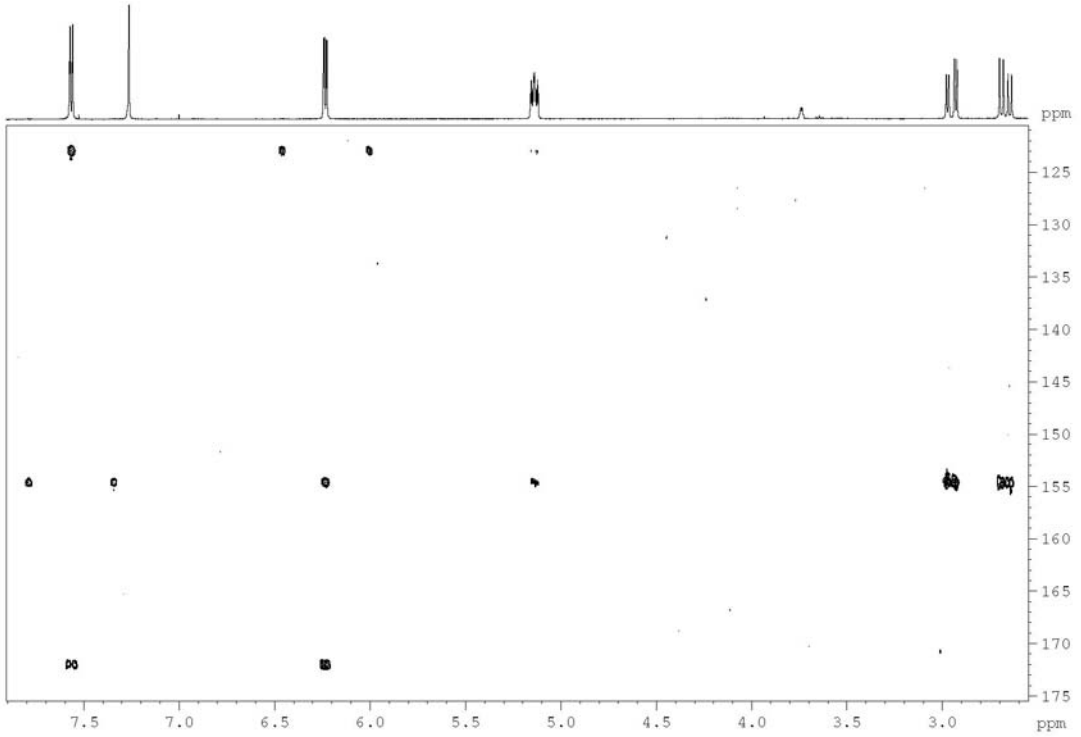

Figure S10. Expansion of the ^{1}H-^{13}C long-range correlation map from HMBC NMR experiment of the polyacetylene (**1**) in $CDCl_3$ at 400 and 100 MHz, showing the correlations with the olefinic C-2 and C-3 and the carbonyl C-4.

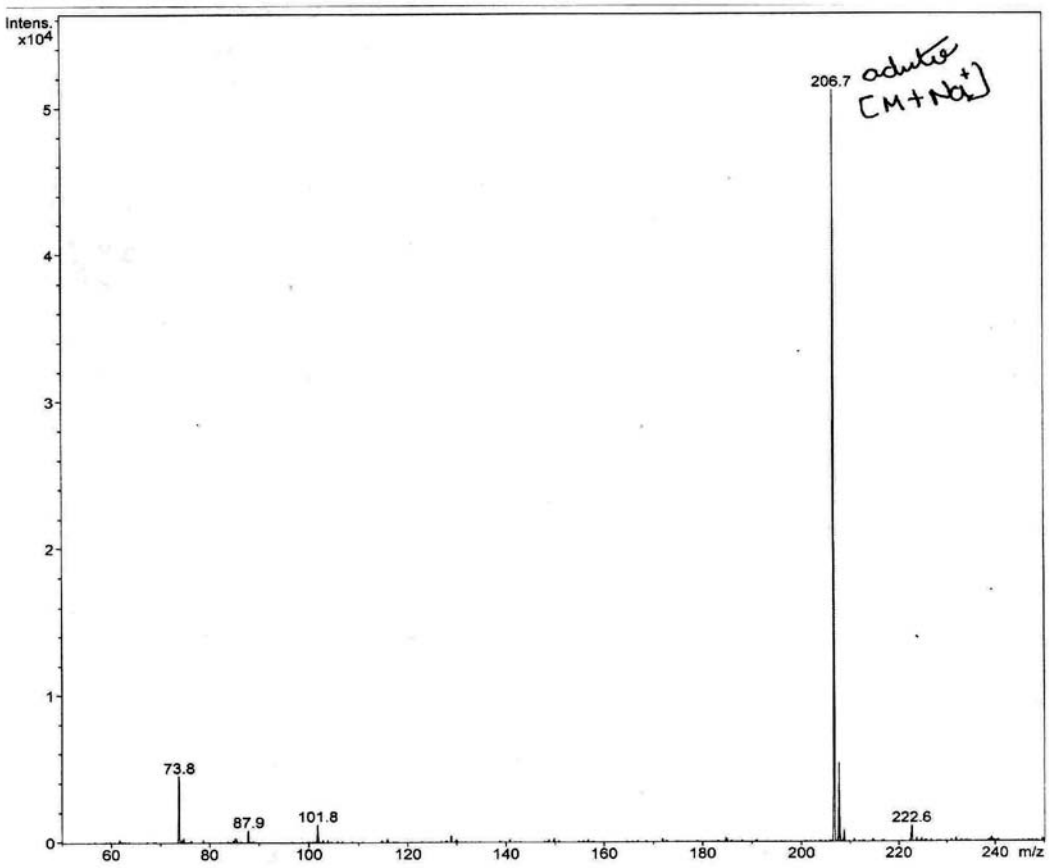

Figure S11. ESI-MS of the polyacetylene (**1**) in MeOH, positive mode.

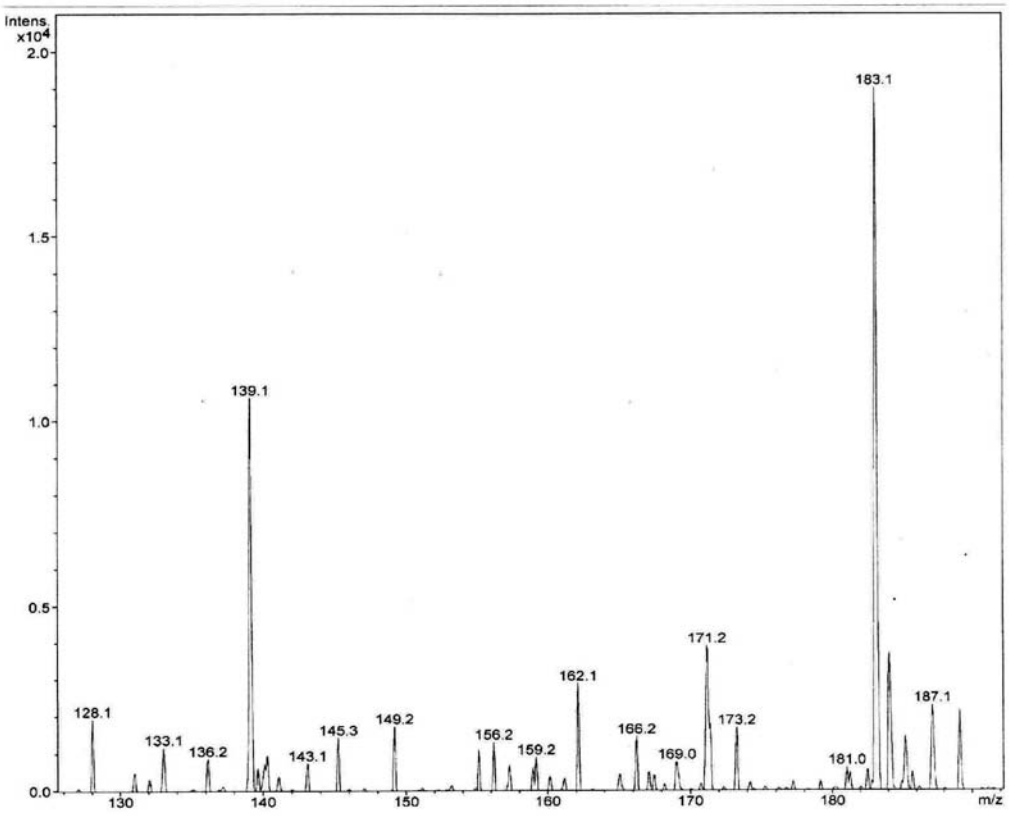

Figure S12. ESI-MS of the polyacetylene (**1**) in MeOH, negative mode.

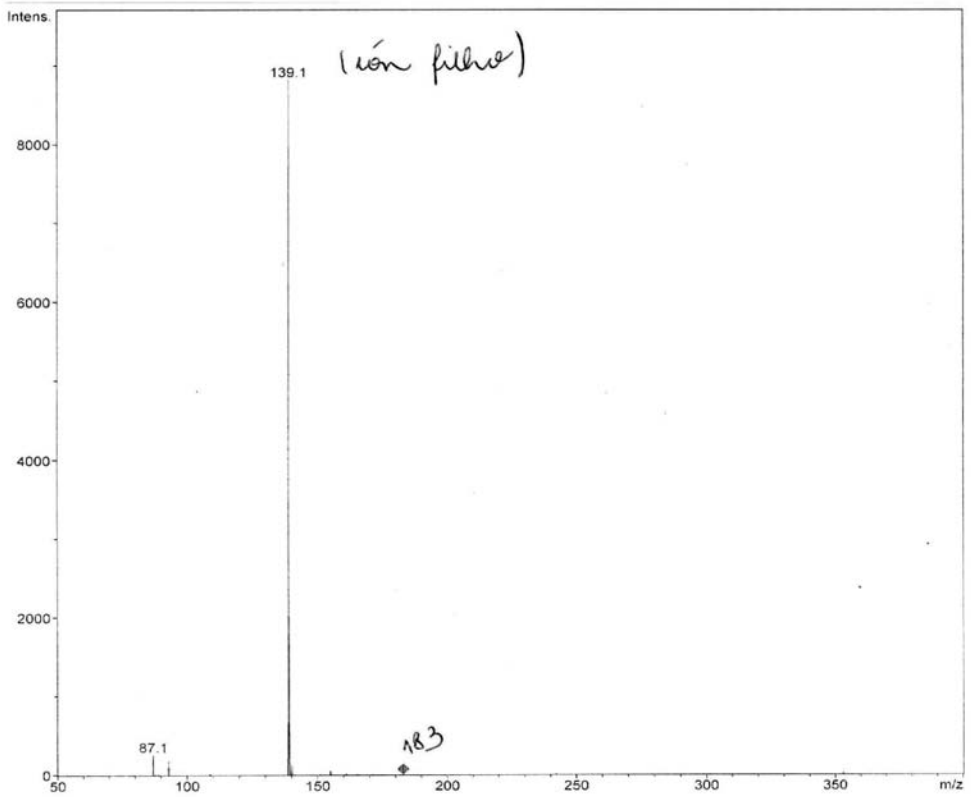

Figure S13. ESI-MS/MS of the polyacetylene (**1**) in MeOH, negative mode at 40 eV.

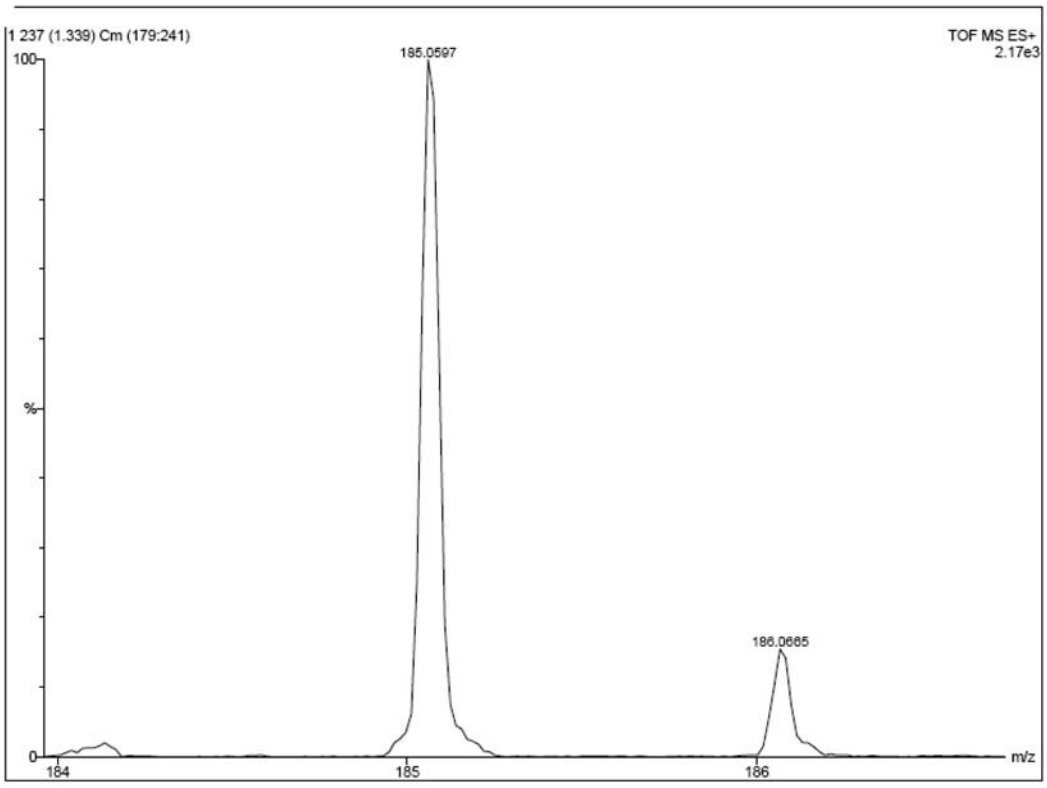

Figure S14. HR-ESI-TOF-MS of the polyacetylene (**1**), positive mode.

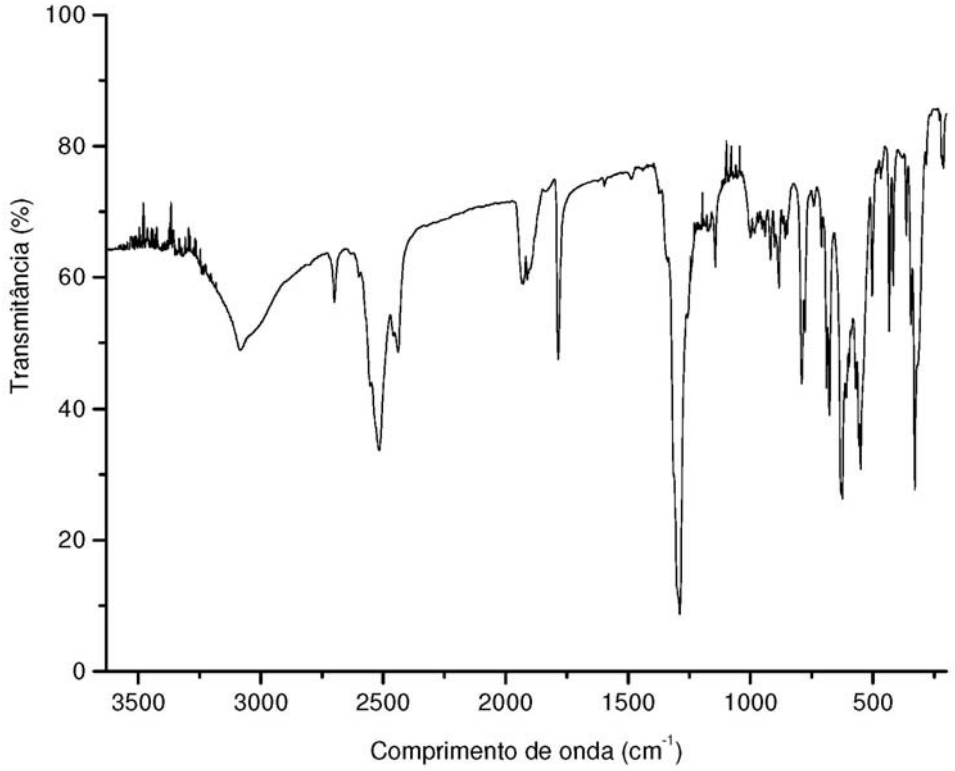

Figure S15. FT-IR spectrum of the polyacetylene (**1**) in KBr pellets.

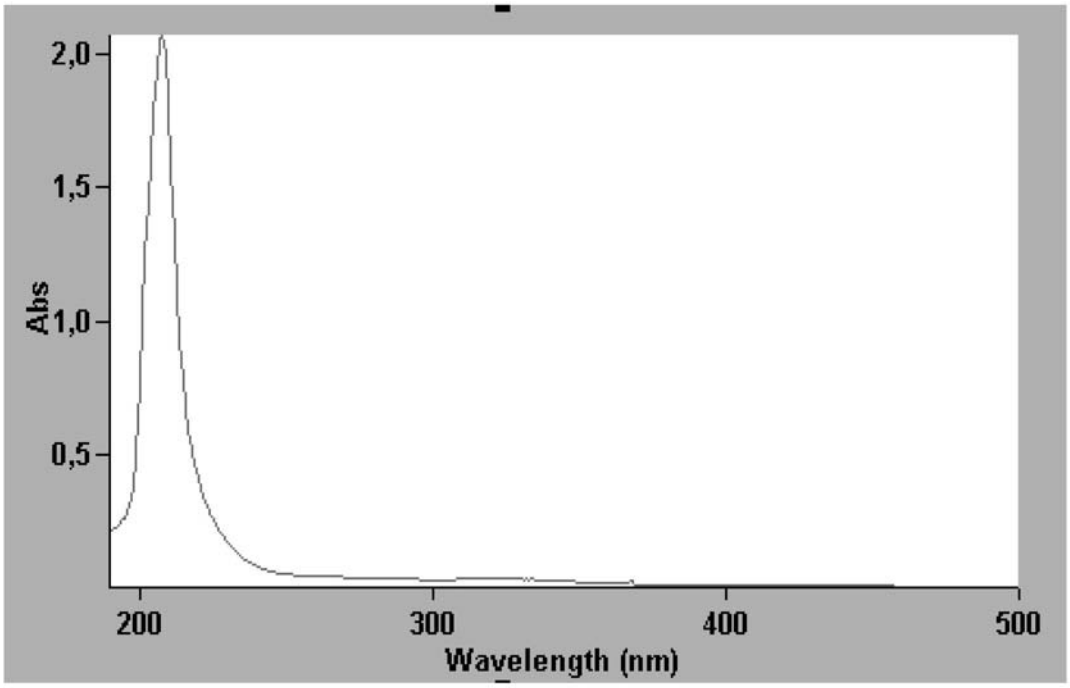

Figure S16. UV spectrum of the polyacetylene (**1**) in MeOH.