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An Evaluation of the Chalcogen Atom Effect on the Mesomorphic and Electronic Properties in a New Homologous Series of Chalcogeno Esters

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NMR spectra of compounds

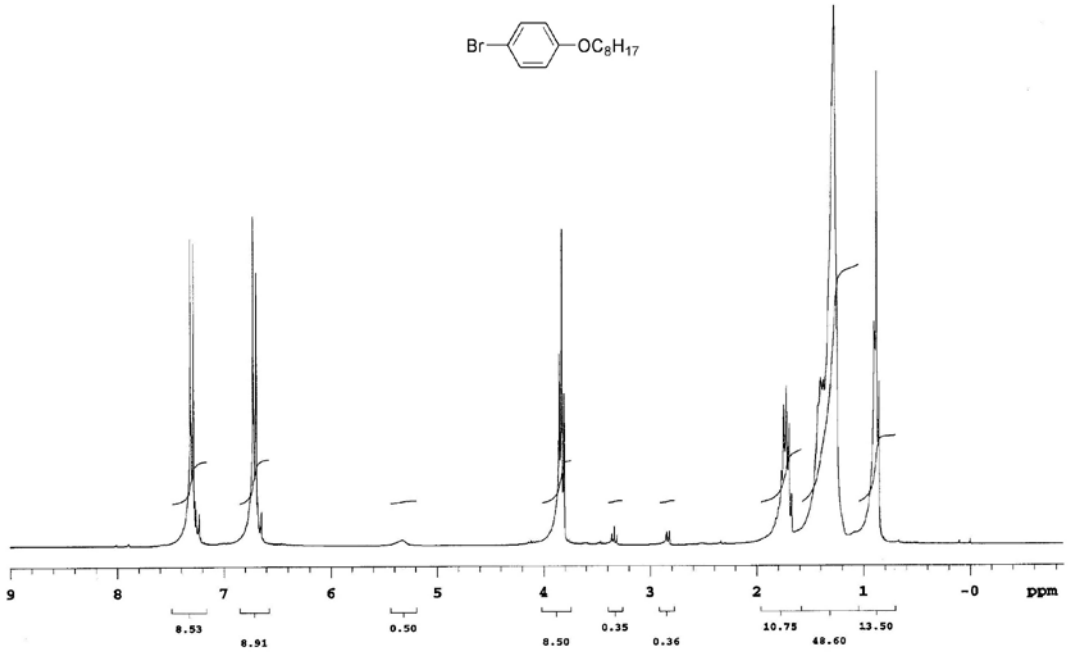

Figure S1. ^{1}H NMR spectrum of compound 1-bromo-4-octyloxybenzene (**7**) ($CDCl_3$, 300 MHz).

*e-mail: paulos@iq.ufrgs.br

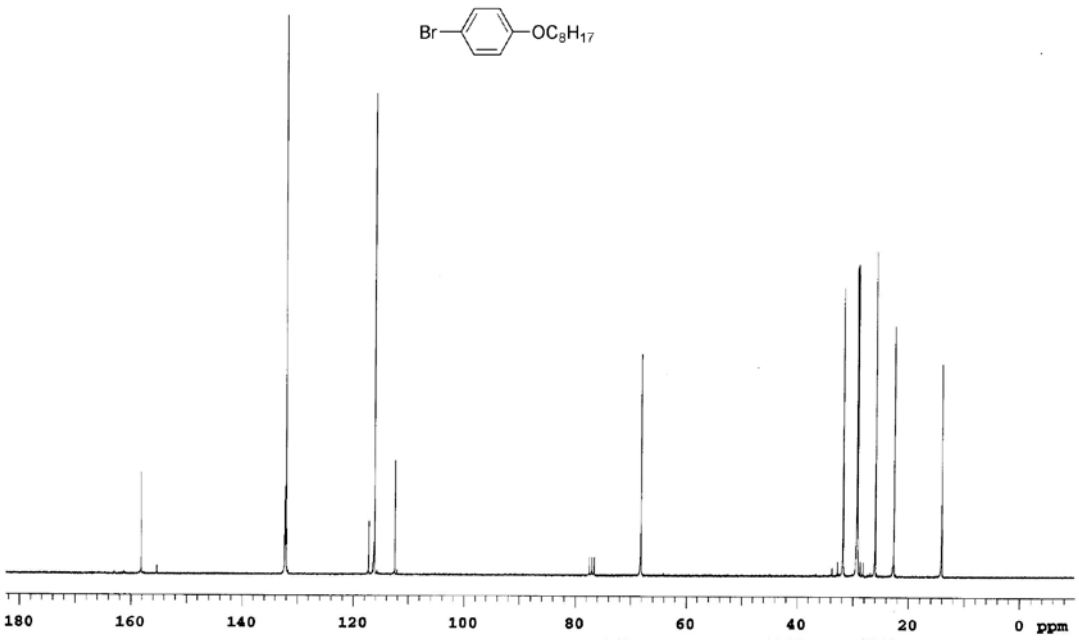

Figure S2. ^{13}C NMR spectrum of compound 1-bromo-4-octyloxybenzene (**7**) ($CDCl_3$, 75 MHz).

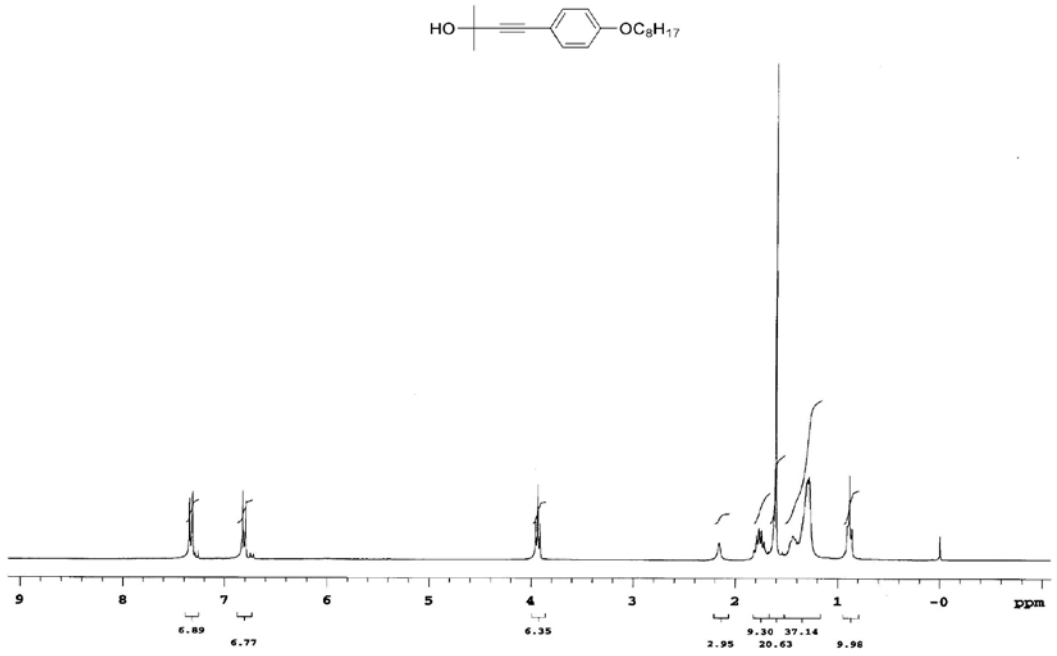

Figure S3. ^{1}H NMR spectrum of compound 4-(4-octyloxyphenyl)-2-methylbut-3-yn-2-ol (**8**) ($CDCl_3$, 300 MHz).

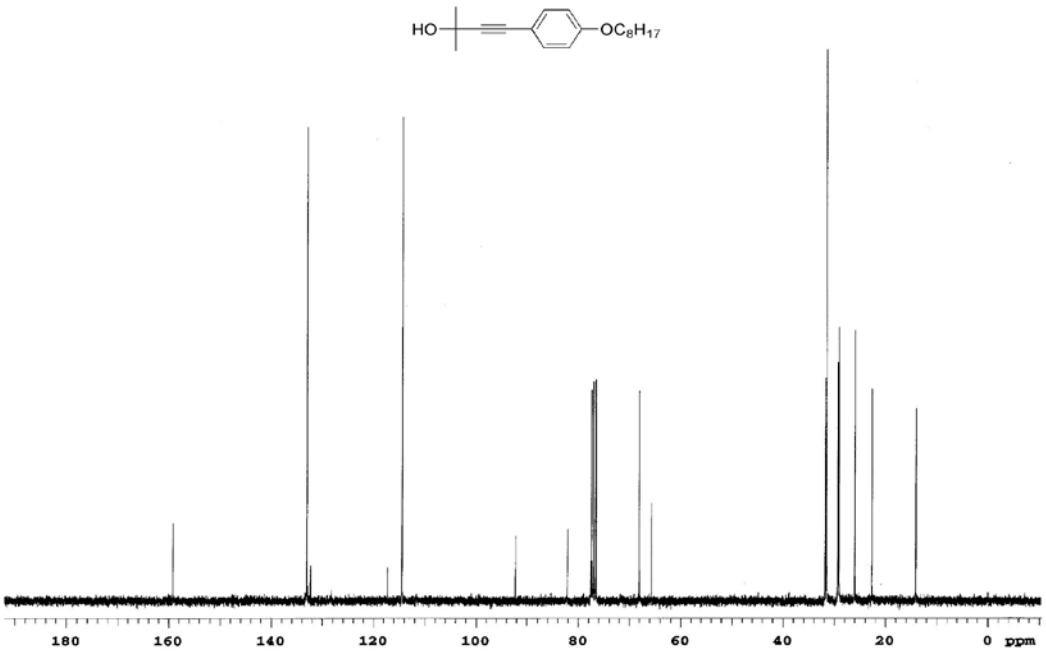

Figure S4. ^{13}C NMR spectrum of compound 4-(4-octyloxyphenyl)-2-methylbut-3-yn-2-ol (**8**) ($CDCl_3$, 75 MHz).

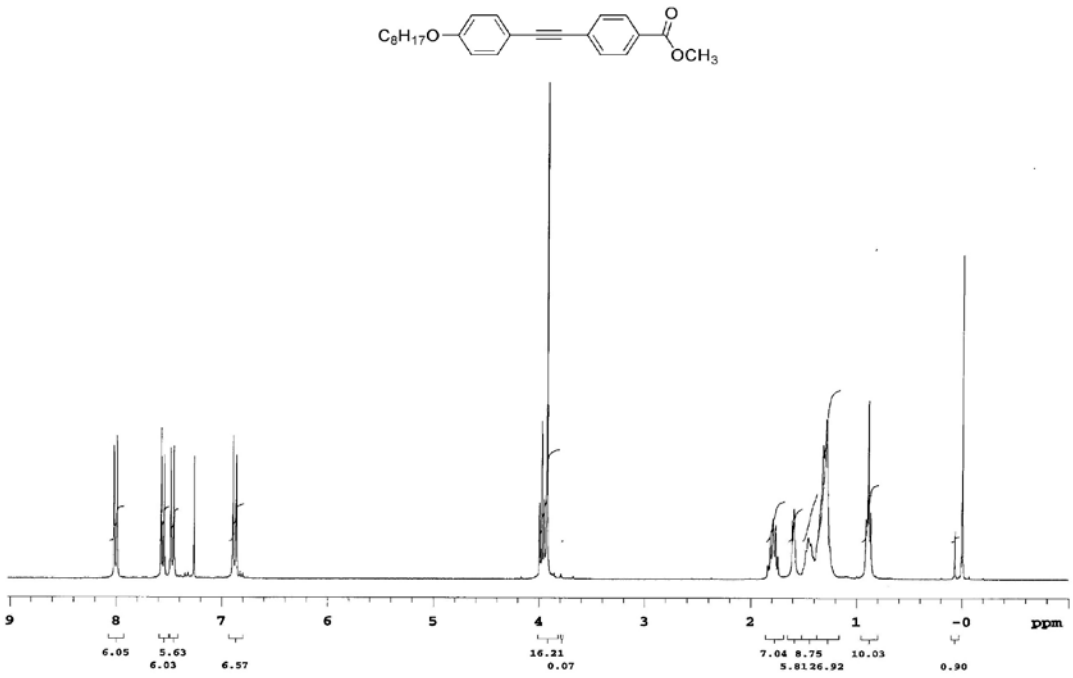

Figure S5. ^{1}H NMR spectrum of compound methyl-4-(4-octyloxyphenylethynyl)benzoate (**9**) ($CDCl_3$, 300 MHz).

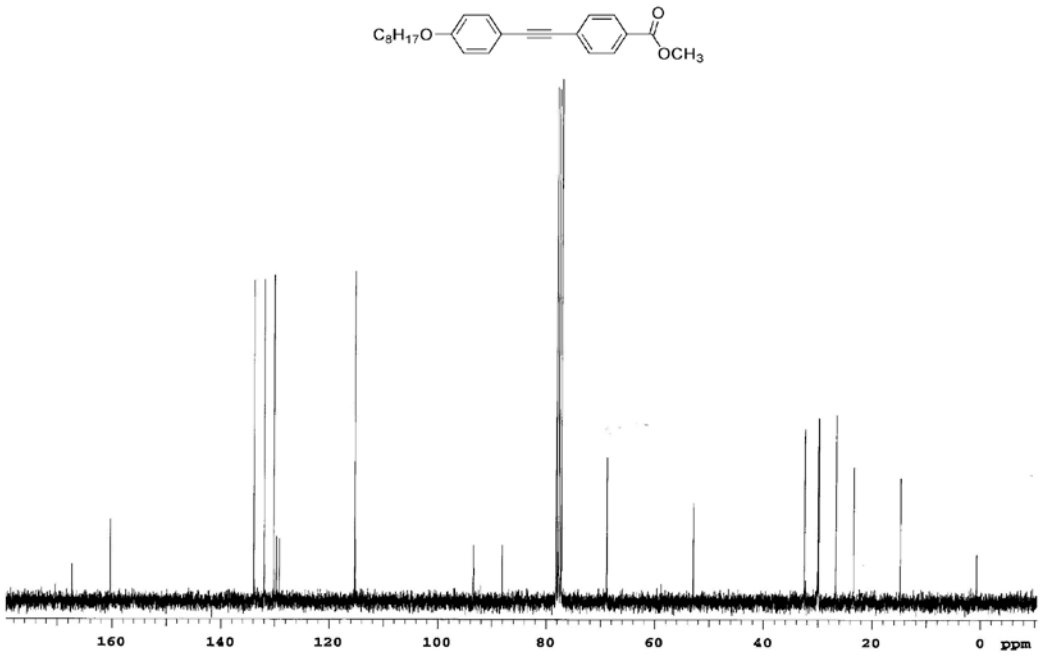

Figure S6. ^{13}C NMR spectrum of compound methyl-4-(4-octyloxyphenylethynyl)benzoate (**9**) ($CDCl_3$, 75 MHz).

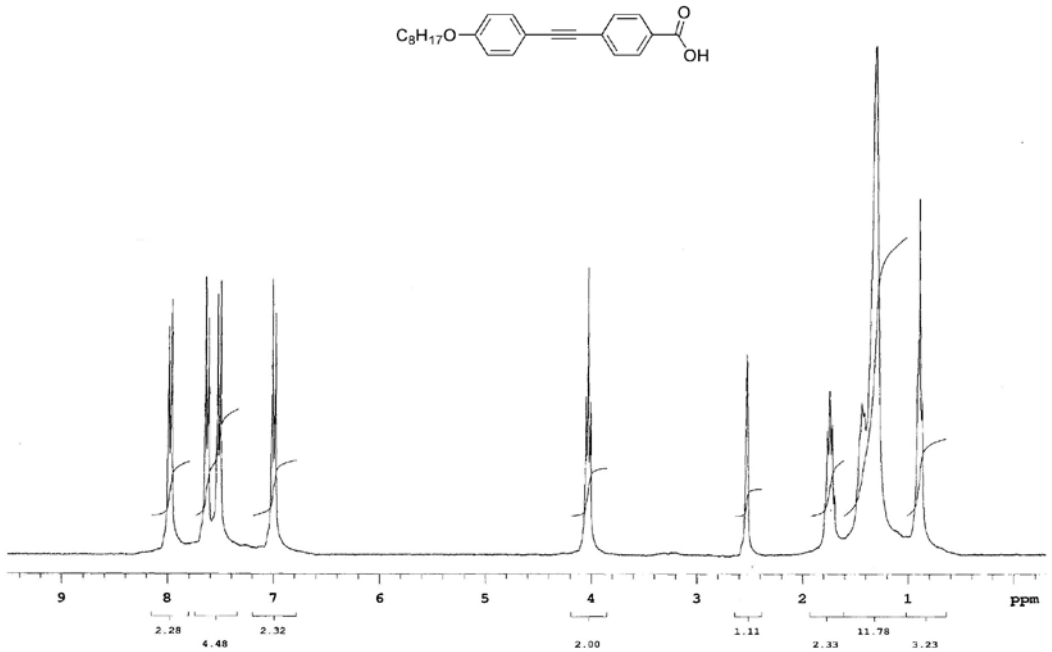

Figure S7. ^{1}H NMR spectrum of compound 4-[4-(octyloxyphenylethynyl)]benzoic acid (**4**) (DMSO-d_6, 300 MHz).

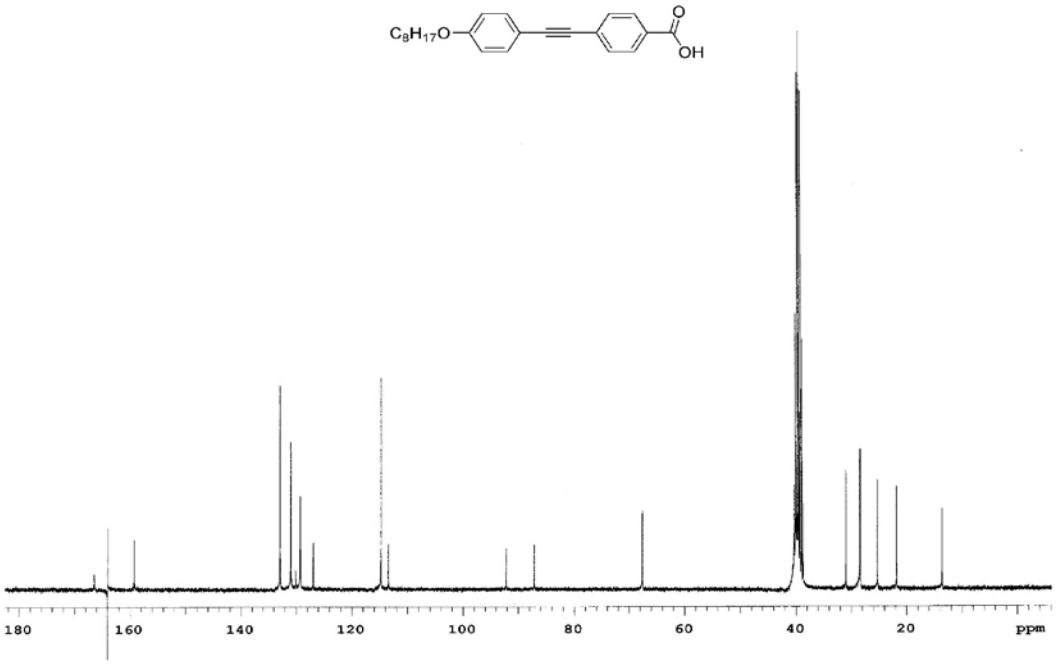

Figure S8. ^{13}C NMR spectrum of compound 4-[4-(octyloxyphenylethynyl)]benzoic acid (**4**) (DMSO-d_6, 75 MHz).

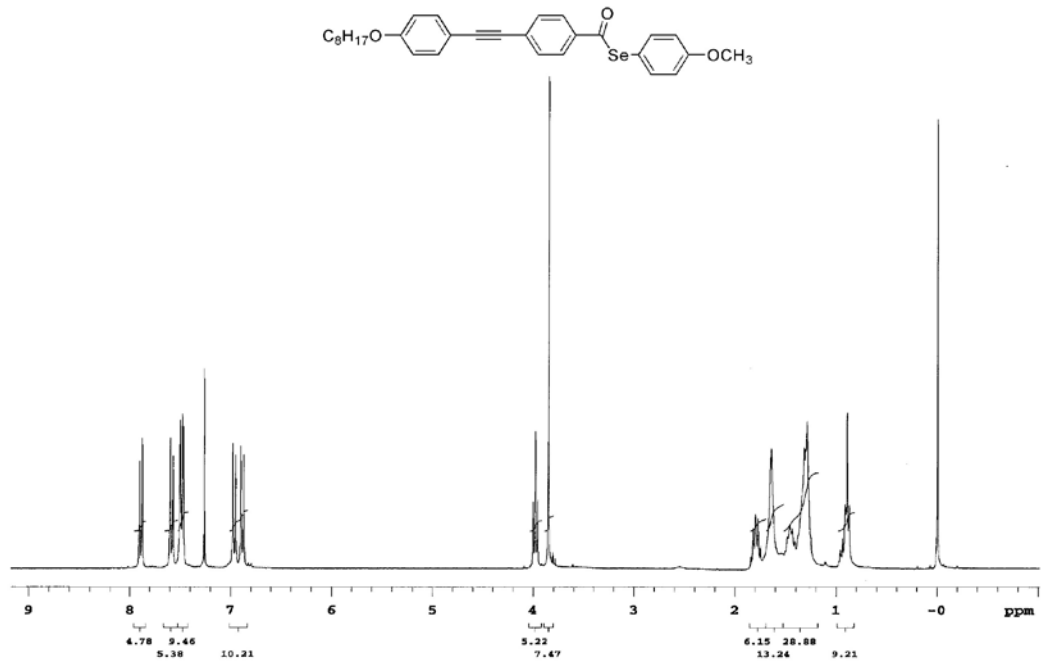

Figure S9. ^{1}H NMR spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate (**1a**) ($CDCl_3$, 300 MHz).

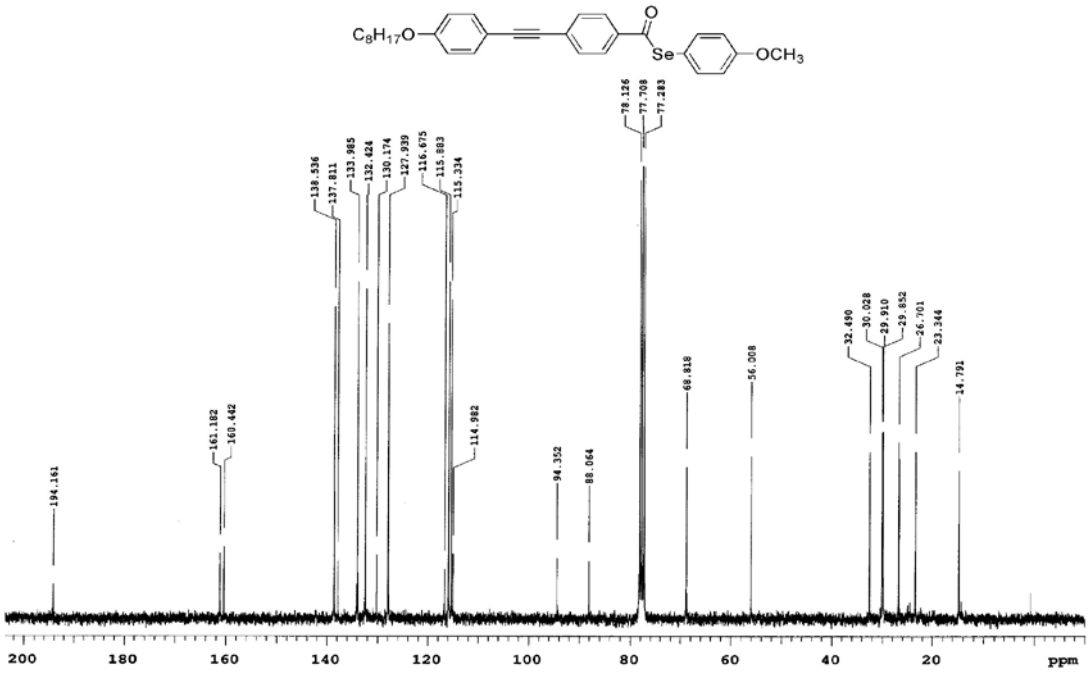

Figure S10. ^{13}C NMR spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate (**1a**) ($CDCl_3$, 75 MHz).

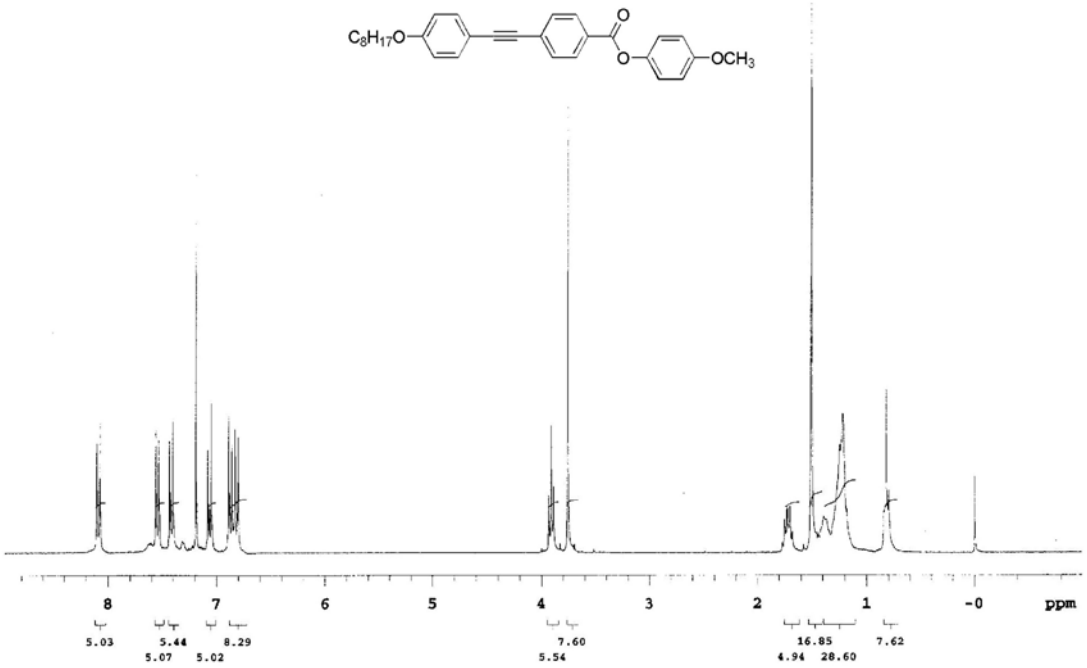

Figure S11. ^{1}H NMR spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoate (**6a**) ($CDCl_3$, 300 MHz).

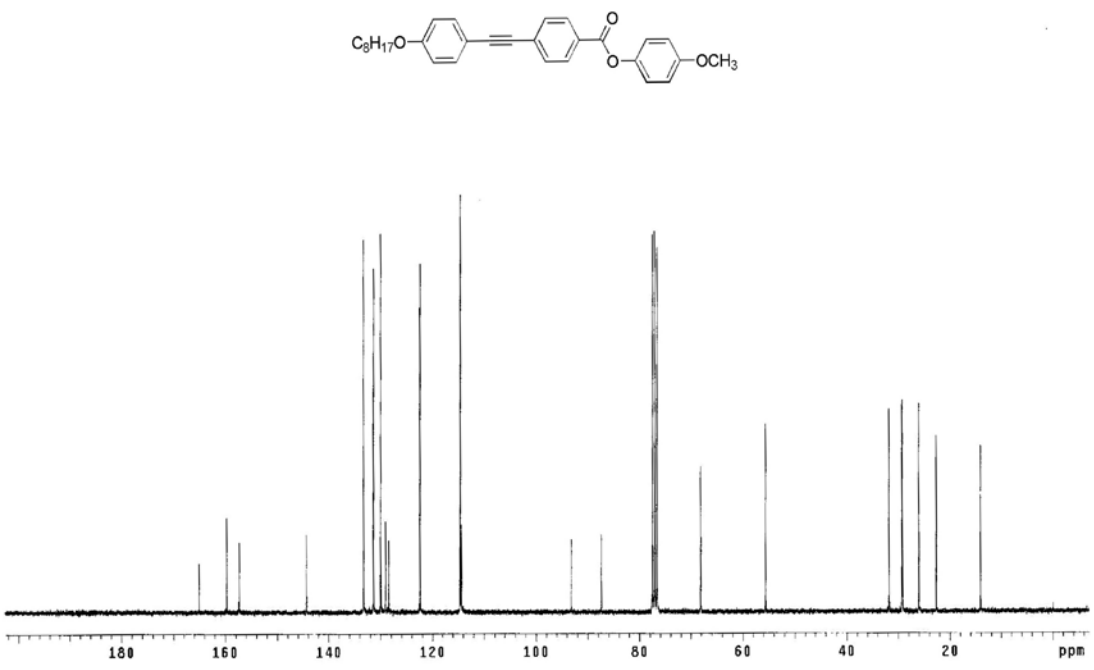

Figure S12. ^{13}C NMR spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoate (**6a**) ($CDCl_3$, 75 MHz).

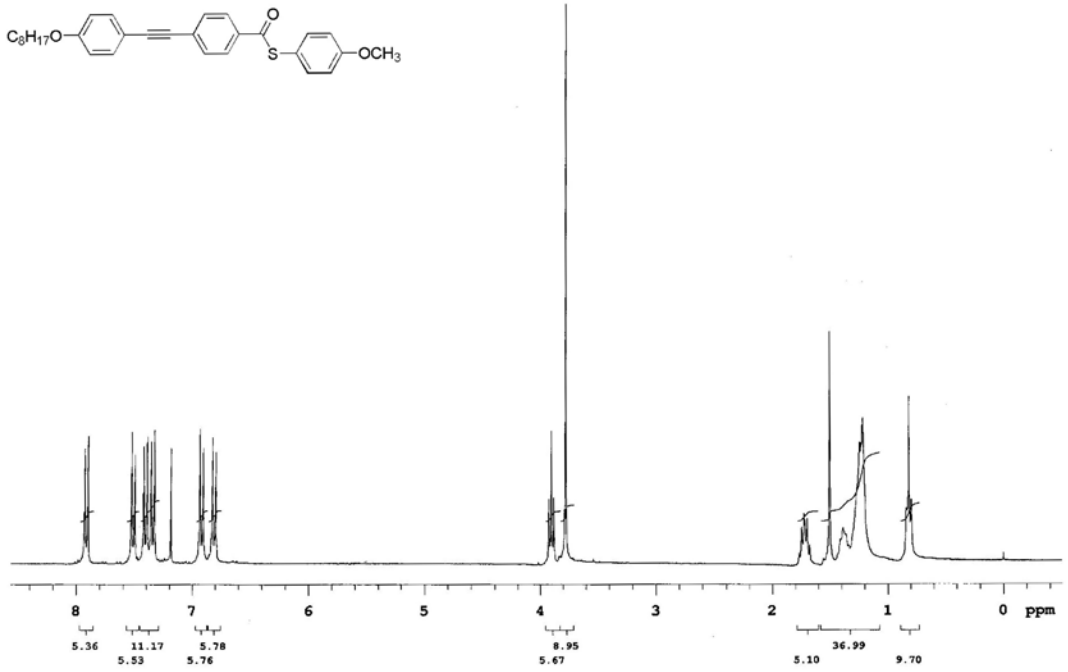

Figure S13. ^{1}H NMR spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzothioate (**6b**) ($CDCl_3$, 300 MHz).

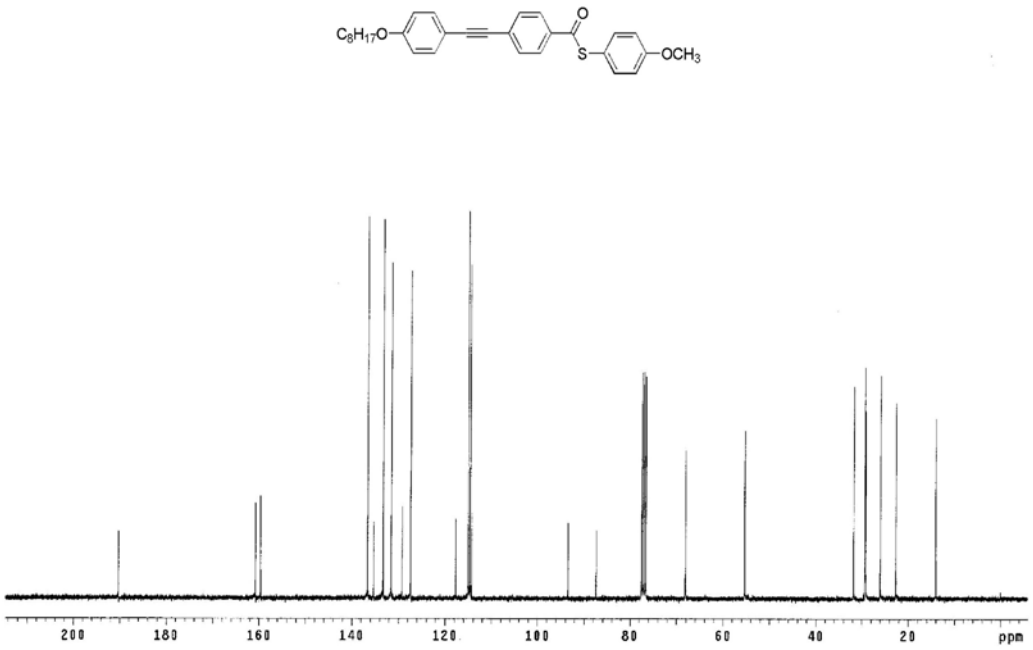

Figure S14. ^{13}C NMR spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzothioate (**6b**) ($CDCl_3$, 75 MHz).

Infrared spectra of compounds

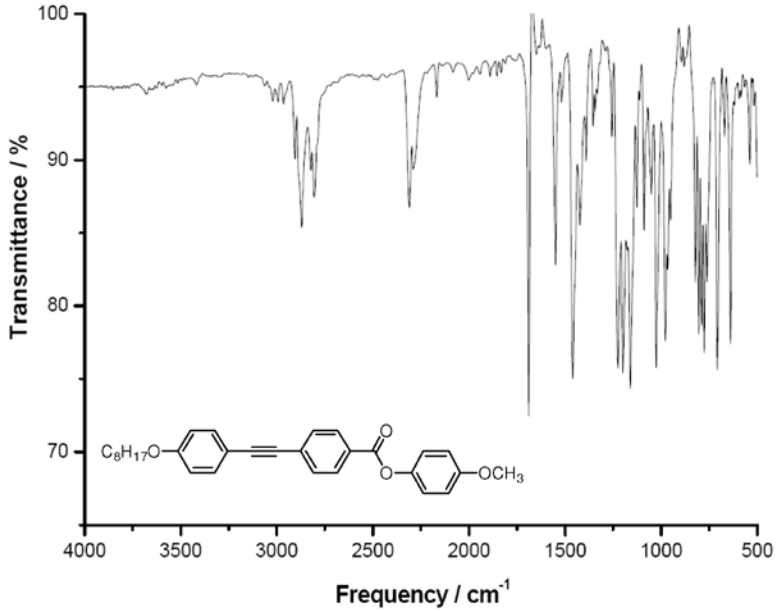

Figure S15. Infrared spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoate (**6a**).

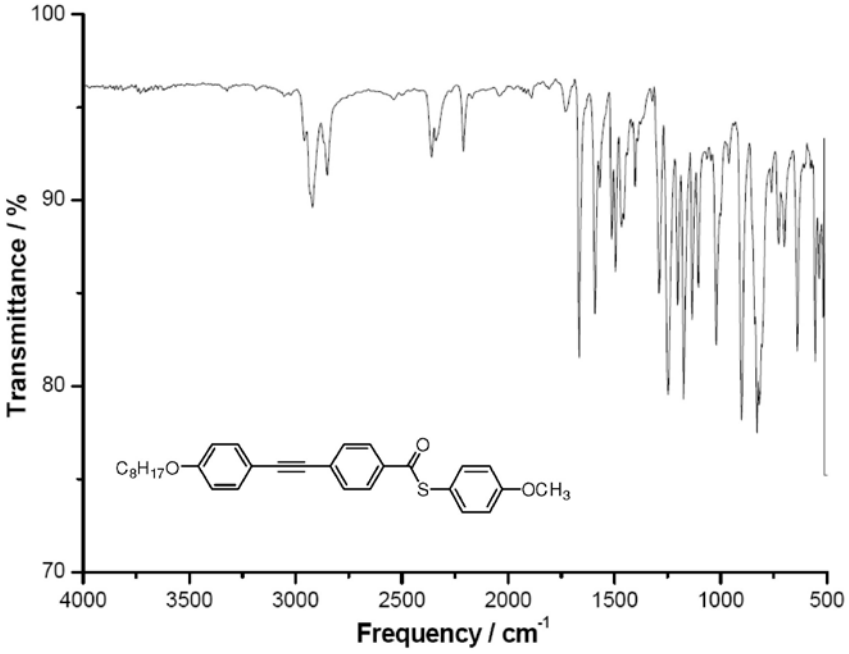

Figure S16. Infrared spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzothioate (**6b**).

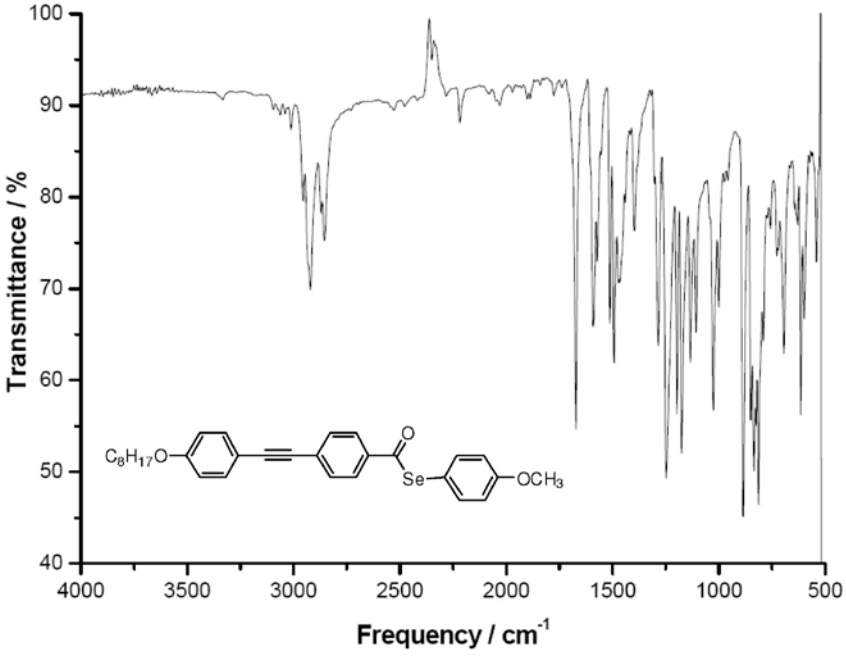

Figure S17. Infrared spectrum of compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate (**1a**).

UV-Vis absorption spectra of compounds

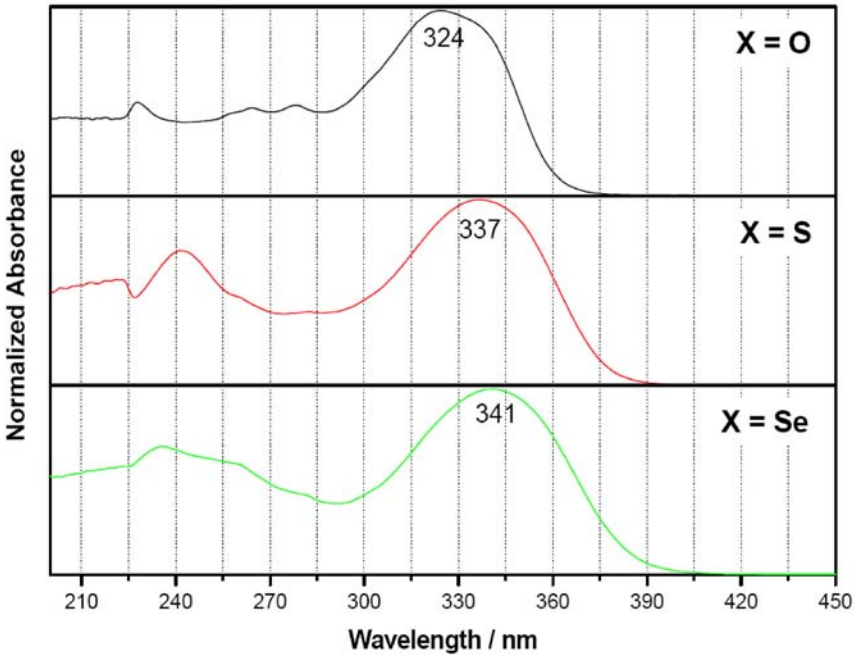

Figure S18. Normalized absorption spectra of the dyes **6a**, **6b** and **1a**, where X = O, S and Se, respectively.

DSC thermograms

Thermograms set for compounds **6a**, **6b** and **1a** on heating at 10 ºC min^{-1}.

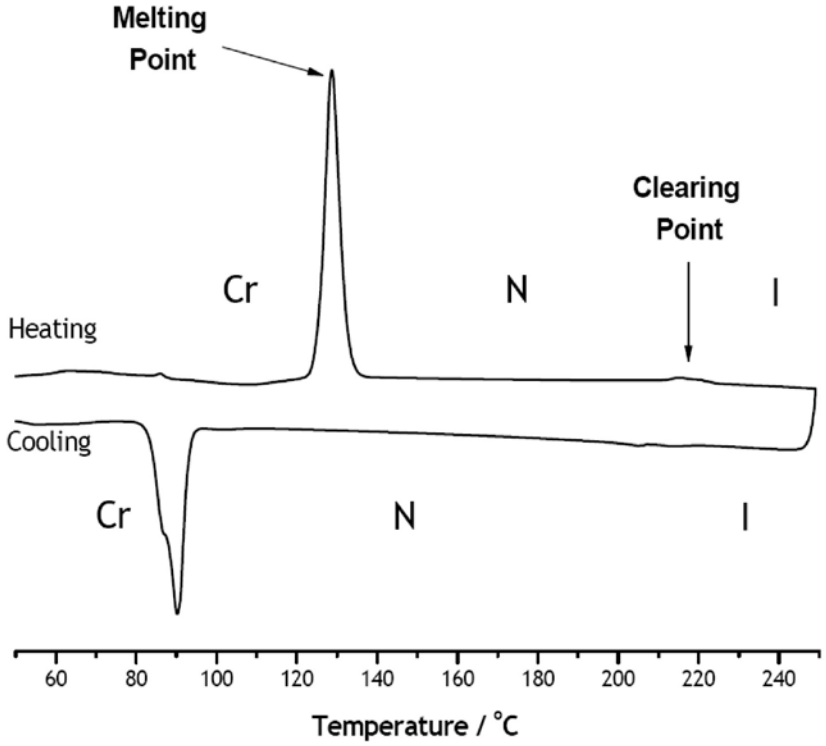

Figure S19. Thermogram for compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoate (**6a**).

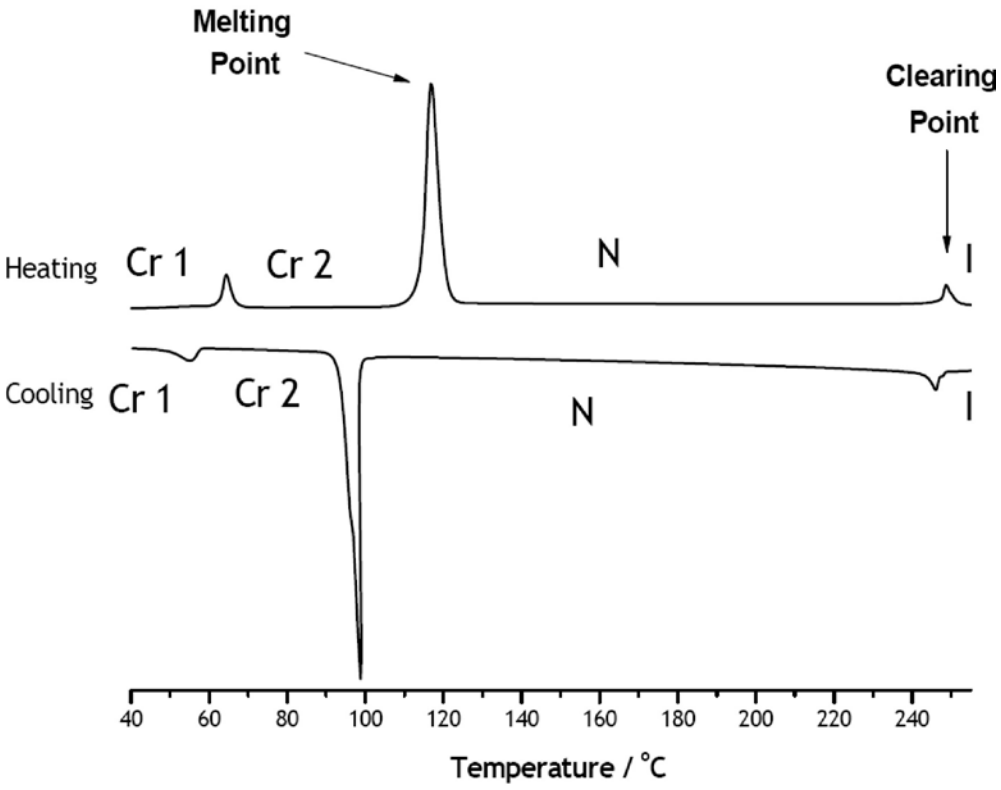

Figure S20. Thermogram for compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzothioate (**6b**).

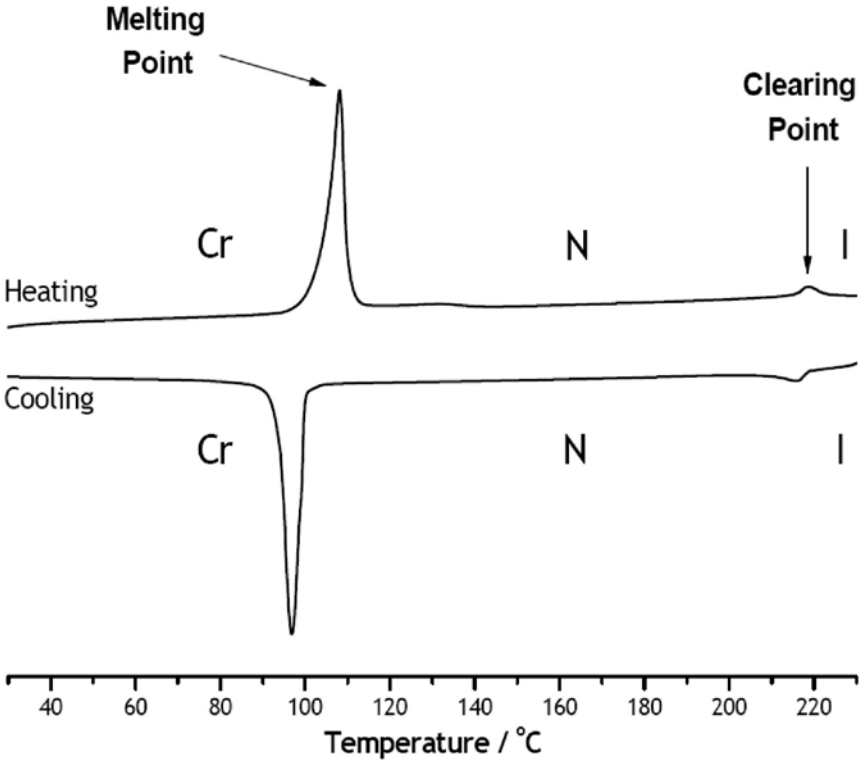

Figure S21. Thermogram for compound methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate (**1a**).

Microscopic analysis

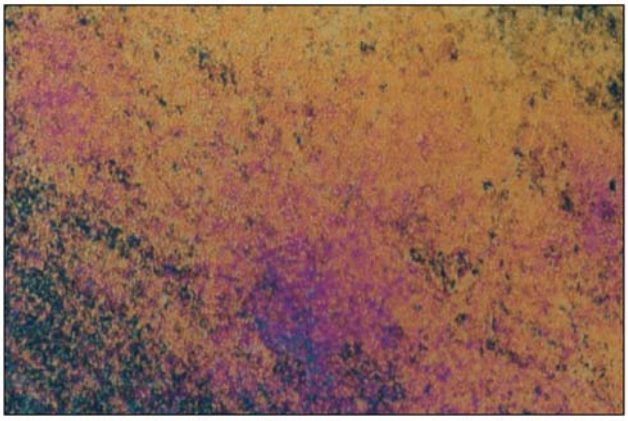

Figure S22. Schlieren texture grainy of methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoate (**6a**) occurring at 150 ºC.

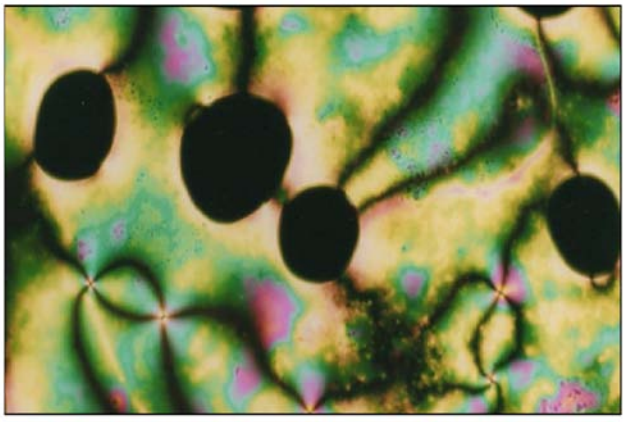

Figure S23. Planar thread-like nematic texture of methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzothioate (**6b**) occurring at 220 ºC.

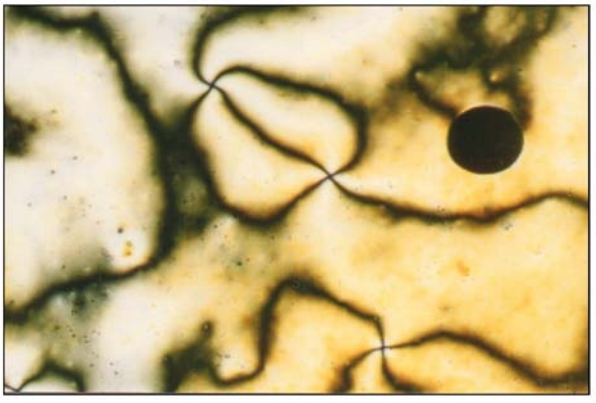

Figure S24. Planar thread-like nematic texture of methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate (**1a**) occurring at 174 ºC.