

Supporting Information

Consecutive Three-Component Suzuki-Knoevenagel Synthesis of Merocyanine Libraries and Correlation Analyses of their Oxidation Potentials and Optical Band Gaps

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3.35.	(<i>Z</i>)-5-{{10-(2-Decyltetradecyl)-7-(<i>p</i> -tolyl)-10 <i>H</i> -phenothiazin-3-yl)methylene}-2-thioxothiazolidin-4-one (12b)	132
3.36.	2-{{10-(2-Decyltetradecyl)-7-(<i>p</i> -tolyl)-10 <i>H</i> -phenothiazin-3-yl)methylene}-1 <i>H</i> -inden-1,3[2 <i>H</i>]-dione (12c)	134
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3.41.	(Z) -5-{{[10-(2-Decyltetradecyl)-7-(<i>p</i> -tolyl)-10 <i>H</i> -phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12h)	144
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3.43.	(Z) -5-{{[10-(2-Decyltetradecyl)-7-(pyridin-4-yl)-10 <i>H</i> -phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12j)	148
3.44.	(Z) -5-{{[10-(2-Decyltetradecyl)-7-(1-methyl-1 <i>H</i> -pyrazol-4-yl)-10 <i>H</i> -phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12k)	150
3.45.	(Z) -3-[10-(2-Decyltetradecyl)-7-(1-methyl-1 <i>H</i> -pyrazol-4-yl)-10 <i>H</i> -phenothiazin-3-yl]-2-(4-nitrophenyl)acrylonitrile (12l)	152
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3.50.	(Z) -5-{{[10-(2-Decyltetradecyl)-7-(4-{diphenylamino}phenyl)-10 <i>H</i> -phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12q)	162
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1. General Considerations

Reagents, catalysts, ligands, and solvents were purchased reagent grade and used without further purification. DMSO was dried and distilled from CaH_2 under argon atmosphere. Boronates/boronic acids **1** were prepared according to our previously published protocols from bromo (hetero)arenes by bromine-lithium exchange, borylation with trialkyl borates, and esterification with pinacol,¹ or from thienyl derivatives by lithiation, borylation with trialkyl borates, and esterification with pinacol.² Bromo aldehydes were prepared according to our protocol by desymmetrization of dibromo (heteroarenes)³ or thiophenes.² Column chromatography: silica gel 60, mesh 70-230. TLC: silica gel plates 60 F254.

Instrumentation: Chemical shifts δ in the ^1H NMR and ^{13}C NMR spectra are reported relative to deuterated solvents (CDCl_3 , acetone-d⁶, or DMSO-d⁶). The assignments of quaternary C, CH, CH_2 , and CH_3 signals were made by using DEPT spectra. The absorption spectra of the dyes were recorded in dichloromethane solutions on a diode array UV-vis spectrometer. Cyclic voltammetry experiments were performed under argon in dry and degassed CH_2Cl_2 at room temperature and at scan rates of 100, 250, 500 and 1000 mVs^{-1} using an electrochemical workstation. The electrolyte was Bu_4NPF_6 (0.025 m). The working electrode was a 1 mm platinum disk, the counter electrode was a platinum wire, and the reference electrode was an Ag/AgCl electrode. The potentials E_0 were corrected to the internal standard of Fc/Fc^+ in CH_2Cl_2 ($E_0^{0/+1} = 450$ mV) and calculated as $E_{1/2}$ referenced to NHE (normal hydrogen electrode) according to $E_{1/2} = E_0 + 0.20$ V. Mass spectroscopic measurements were conducted on a quadrupole (EI) analyzer (TSQ 7000, Finnigan MAT) in the Department of Mass Spectrometry of the Institute of Inorganic and Structural Chemistry, Heinrich-Heine-Universität Düsseldorf. IR spectra were measured using ATR technique (Shimadzu IR Affinity-1). The intensities of the IR bands are abbreviated as w (weak), m (medium), s (strong) and vs (very strong). Elemental analyses were carried out on a Perkin Elmer Series II Analyser 2400 in the microanalytical laboratory of the Pharmazeutisches Institut of the Heinrich-Heine-Universität Düsseldorf. Absorption spectra were recorded in various spectroscopy grade solvents at 293 K using a PerkinElmer UV/VIS/NIR Lambda 19 spectrometer. Emission spectra in solution were recorded at room temperature on a LS55 spectrometer (Perkin Elmer). Melting points and melting/softening intervals were determined on the apparatus Thermovar, Reichert-Jung/Depew using the method according to L. Kofler.⁴

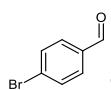
2. Syntheses

2.1. General Procedure (GP) for the Coupling-Condensation One-pot Synthesis of Chromophores 8-12

(Hetero)aryl boronic acid or boronate **6** (1.1-1.2 equivs), bromoaldehyde **1-5** (1.0 equiv), cesium fluoride or cesium carbonate (3.2 equivs), and tetrakis(triphenylphosphane)-palladium(0) (0.02-0.03 equivs) were placed in a Schlenk flask with magnetic stir bar under nitrogen and dry 1,4-dioxane (4 mL/mmol) were added (for experimental details see Tables S1-5). The solution was heated to 100 °C under reflux for 8-16 h. After cooling to room temp acetic acid (2 mL/mmol), the CH-acidic compound **7** (1.1-1.2 equivs), and a catalytic or equimolar amount of ammonium acetate was added to the reaction mixture. This mixture was heated under nitrogen to 95 °C under reflux for 3-8 h. Intensive orange, red or dark violet solutions were formed. After cooling to room temp the reaction mixture was diluted with dichloromethane (30 mL/mmol) and the organic layer was washed with distilled water until the aqueous phase did not smell like acetic acid. The combined aqueous phases were extracted with dichloromethane and the combined organic layers were dried (anhydrous magnesium sulfate) and the solvents were removed in vacuo. The residue was adsorbed on celite® and purified by flash chromatography on silica gel (*n*-hexane/acetone, toluene or ethyl acetate and gradients thereof) to furnish the chromophores **8-12**.

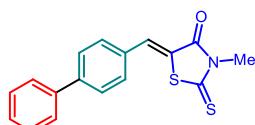
2.1.1. Consecutive Three-component Suzuki-Knoevenagel Synthesis of *p*-Phenylenedibridged Systems **8**

Table S1. Experimental details of the consecutive three-component Suzuki-Knoevenagel synthesis of *p*-phenylene bridged systems **8**.

Entry	Bromo-aldehyde 1 [mg] (mmol)	Boronic acid/ester 6 [mg] (mmol)	CsF [mg] (mmol)	Pd(PPh ₃) ₄ [mg] (mmol)	<i>t</i> ₁ [h]	methylene active compound 7 [mg] (mmol)	Organocatalyst [mg] (mmol)	<i>t</i> ₂ [h]	Product [mg] (%)
									
1	185 (1.00) of 1	134 (1.1) of 6a	CsF 487 (3.2)	24 (0.02)	6	162 (1.1) of 7a	77 (1.0) of NH ₄ OAc	6	282 (91) of 8a
2	185 (1.00) of 1	134 (1.1) of 6a	CsF 486 (3.2)	24 (0.02)	6	161 (1.1) of 7c	1 drop of Et ₂ NH	3	254 (82) of 8b
3	185 (1.00) of 1	150 (1.1) of 6b	CsF 486 (3.2)	24 (0.02)	6	160 (1.2) of 7b	78 (1.0) of NH ₄ OAc	5	254 (82) of 8c
4	185 (1.00) of 1	150 (1.1) of 6b	CsF 486 (3.2)	24 (0.02)	6	178 (1.1) of 7f	1 drop of Et ₂ NH	6	293 (86) of 8d
5	185 (1.00) of 1	150 (1.1) of 6b	CsF 486 (3.2)	24 (0.02)	6	192 (1.1) of 7e	1 drop of Et ₂ NH	4	306 (87) of 8e

6	185 (1.00) of 1	141 (1.1) of 6h	CsF 486 (3.2)	24 (0.02)	6	162 (1.1) of 7a	78 (1.0) of NH ₄ OAc	6	269 (85) of 8f
7	185 (1.00) of 1	229 (1.1) of 6l	CsF 486 (3.2)	24 (0.02)	16	161 (1.1) of 7c	1 drop of Et ₂ NH	3	223 (71) of 8g
8	93 (0.50) of 1	256 (1.2) of 6n	CsF 242 (1.6)	15 (0.013)	16	81 (0.55) of 7a	39 (0.5) of NH ₄ OAc	6	201 (79) of 8h
9	93 (0.50) of 1	256 (1.2) of 6p	CsF 242 (1.6)	18 (0.015)	16	96 (0.55) of 7e	1 drop of Et ₂ NH	4	207 (76) of 8i

2.1.1.1. 5-(Biphenyl-4-ylmethylene)-3-methyl-2-thioxothiazolidin-4-one (**8a**)

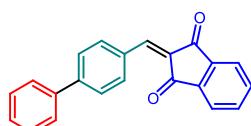


C₁₇H₁₃NOS₂ [311.42]

According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 6:1) compound **8a** (282 mg, 91%) was obtained as yellow crystals, Mp 135 °C. R_f (*n*-hexane/dichloromethane 1:1) = 0.58.

¹H NMR (300 MHz, CDCl₃): δ 3.48 (s, 3 H), 7.34–7.74 (m, 10 H). ¹³C NMR (75 MHz, CDCl₃): δ 31.4 (CH₃), 123.0 (C_{quat}), 127.2 (CH), 128.0 (CH), 128.4 (CH), 129.2 (CH), 131.4 (CH), 132.3 (C_{quat}), 132.8 (CH), 139.6 (C_{quat}), 143.5 (C_{quat}), 167.9 (C_{quat}), 193.5 (C_{quat}). MS (EI) *m/z* (%): 311 (43, [M]⁺), 235 (2, [C₁₆H₁₃NO]⁺), 210 (100, [C₁₄H₁₀S]⁺), 165 (21, [C₁₈H₉]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3013 (w), 2876 (w), 1709 (m), 1670 (w), 1589 (w), 1553 (w), 1520 (w), 1422 (m), 1352 (w), 1292 (s), 1261 (m), 1126 (s), 1098 (m), 1072 (m), 1018 (m), 993 (m), 922 (m), 829 (m), 797 (m), 762 (s), 737 (m), 716 (m), 696 (m), 679 (s), 623 (m). Anal calcd for C₁₇H₁₃NOS₂ [311.4]: C 65.56, H 4.21, N 4.50; Found: C 65.56, H 4.00, N 4.51.

2.1.1.2. 2-(Biphenyl-4-ylmethylene)-1*H*-inden-1,3[2*H*]-dione (**8b**)



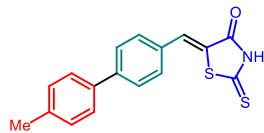
C₂₂H₁₄O₂ [310.35]

According to the GP and after purification by chromatography on silica gel (*n*-hexane/dichloromethane 15:1) and recrystallization from *n*-hexane/dichloromethane compound **8b** (254 mg, 82%) was obtained as a yellow voluminous solid, Mp 144 °C. R_f (*n*-hexane/dichloromethane 1:1) = 0.26.

¹H NMR (300 MHz, CDCl₃): δ 7.27–7.42 (m, 3 H), 7.54–7.60 (m, 2 H), 7.61–7.67 (m, 2 H), 7.67–7.74 (m, 2 H), 7.82 (s, 1 H), 7.87–7.95 (m, 2 H), 8.42–8.48 (m, 2 H). ¹³C NMR (75 MHz, CDCl₃): δ 123.4 (CH), 123.5 (CH), 127.4 (CH), 127.5 (CH), 128.5 (CH), 129.0 (C_{quat}), 129.1

(CH), 132.3 (C_{quat}), 135.0 (CH), 135.3 (CH), 135.5 (CH), 139.9 (C_{quat}), 140.2 (C_{quat}), 142.7 (C_{quat}), 145.9 (C_{quat}), 146.5 (CH), 189.3 (C_{quat}), 190.5 (C_{quat}). MS (EI) *m/z* (%): 310 (37, [M]⁺), 282 (3, [C₂₁H₁₄O]⁺), 233 (21, [C₁₆H₁₀O₂]⁺), 200 (100). IR: $\tilde{\nu}$ [cm⁻¹] = 3055 (w), 3032 (w), 1682 (s), 1616 (m), 1578 (s), 1551 (m), 1487 (w), 1450 (w), 1418 (w), 1383 (w), 1352 (m), 1335 (w), 1323 (w), 1287 (w), 1252 (w), 1219 (w), 1198 (m), 1152 (m), 1082 (m), 989 (m), 968 (w), 841 (m), 812 (w), 760 (s), 737 (s), 721 (m), 691 (m), 681 (m), 646 (w). Anal calcd for C₂₂H₁₄O₂ [310.4]: C 85.14, H 4.55; Found: C 84.93, H 4.62.

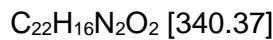
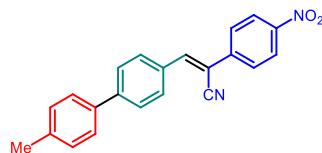
2.1.1.3. 5-{[4'-Methyl-(1,1'-biphenyl)-4-yl]methylene}-2-thioxothiazolidin-4-one (8c)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1) and recrystallization from ethanol compound **8c** (254 mg, 82%) was obtained as yellow crystals, Mp 243 °C. R_f (*n*-hexane/acetone 1:1) = 0.72.

¹H NMR (300 MHz, DMSO-d₆): δ 2.35 (s, 3 H), 7.25–7.36 (m, 2 H), 7.62–7.70 (m, 5 H), 7.81–7.86 (m, 2 H), 13.84 (br, 1 H). ¹³C NMR (75 MHz, DMSO-d₆): δ 20.8 (CH₃), 125.0 (C_{quat}), 126.7 (CH), 127.2 (CH), 129.7 (CH), 131.2 (CH), 131.3 (CH), 131.7 (C_{quat}), 135.8 (C_{quat}), 137.9 (C_{quat}), 142.0 (C_{quat}), 169.4 (C_{quat}), 195.5 (C_{quat}). MS (EI) *m/z* (%): 311 (42, [M]⁺), 224 (100, [C₁₅H₁₂S]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3098 (w), 1709 (w), 1589 (m), 1574 (w), 1500 (w), 1433 (w), 1418 (w), 1402 (w), 1344 (w), 1290 (w), 1283 (w), 1236 (w), 1167 (m), 1153 (m), 1123 (w), 1099 (w), 1059 (m), 1034 (w), 1002 (m), 980 (w), 968 (w), 932 (w), 912 (m), 851 (w), 797 (s), 745 (m), 729 (m), 721 (m), 708 (w), 677 (s), 644 (m), 627 (m). Anal calcd for C₁₇H₁₃NOS₂ [311.4]: C 65.56, H 4.21, N 4.50, S 20.59; Found: C 65.30, H 4.33, N 4.46, S 20.30.

2.1.1.4. 3-(4'-Methyl-[1,1'-biphenyl]-4-yl)-2-(4-nitrophenyl)acrylnitrile (8d)

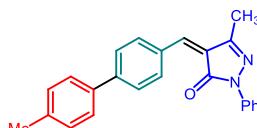


According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) compound **8d** (293 mg, 86%) was obtained as yellow voluminous crystals, Mp 158 °C. R_f (*n*-hexane/acetone 10:1) = 0.19.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 2.40 (s, 3 H), 7.31 (d, ³J = 7.9 Hz, 2 H), 7.61–7.68 (m, 2 H), 7.80–7.87 (m, 2 H), 8.03–8.10 (m, 2 H), 8.11–8.17 (m, 2 H), 8.18 (s, 1 H), 8.30–8.42

(m, 2 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 21.3 (CH₃), 109.4 (C_{quat}), 118.0 (C_{quat}), 125.1 (CH), 127.7 (CH), 127.8 (CH), 128.0 (CH), 130.6 (CH), 131.4 (CH), 133.0 (C_{quat}), 137.5 (C_{quat}), 139.0 (C_{quat}), 141.7 (C_{quat}), 144.6 (C_{quat}), 146.2 (CH), 148.7 (C_{quat}). MS (EI) m/z (%): 340 (100, [M]⁺), 294 (4, [C₂₂H₁₆N]⁺), 279 (10, [C₂₁H₁₃N]⁺), 91 (2, [C₇H₇]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3030 (w), 2968 (w), 2920 (w), 2214 (w), 1584 (m), 1506 (m), 1497 (m), 1447 (w), 1418 (w), 1387 (w), 1328 (s), 1283 (w), 1227 (w), 1196 (m), 1182 (m), 1109 (m), 1034 (w), 1002 (w), 955 (w), 912 (m), 855 (s), 806 (s), 797 (m), 775 (w), 750 (m), 733 (m), 692 (m), 673 (w). Anal calcd for C₂₂H₁₆N₂O₂ [340.4]: C 77.63, H 4.74, N 8.23; Found: C 77.66, H 4.73, N 8.13.

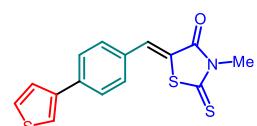
2.1.1.5. 3-Methyl-4-{{[4'-methyl-(1,1'-biphenyl)-4-yl]methylen}-1-phenyl-1*H*-pyrazol-5[4*H*]-one (8e)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) compound **8e** (306 mg, 87%) was obtained as an orange red solid, Mp 105–109 °C. R_f (*n*-hexane/acetone 10:1) = 0.18.

^1H NMR (600 MHz, acetone-d₆/CS₂ 4:1): δ 2.38 (s, 3 H), 2.41 (s, 3 H), 7.16 (dt, 3J = 7.4 Hz, 4J = 1.1 Hz, 1 H), 7.31 (d, 3J = 7.8 Hz, 2 H), 7.40 (t, 3J = 8.0 Hz, 2 H), 7.65 (d, 3J = 7.7 Hz, 2 H), 7.69 (s, 1 H), 7.79 (d, 3J = 8.5 Hz, 2 H), 8.04 (d, 3J = 8.7 Hz, 2 H), 8.73 (d, 3J = 8.1 Hz, 2 H). ^{13}C NMR (150 MHz, acetone-d₆/CS₂ 4:1): δ 13.6 (CH₃), 21.4 (CH₃), 119.1 (CH), 125.0 (CH), 127.4 (CH), 127.8 (CH), 129.4 (CH), 130.6 (CH), 133.1 (C_{quat}), 135.1 (C_{quat}), 135.6 (CH), 137.5 (C_{quat}), 139.1 (C_{quat}), 139.7 (C_{quat}), 145.9 (C_{quat}), 147.3 (CH), 151.8 (C_{quat}), 162.5 (C_{quat}). MS (EI) m/z (%): 352 (100, [M]⁺), 261 (13, [C₁₇H₁₃N₂O]⁺), 185 (45, [C₁₁H₉N₂O]⁺), 91 (6, [C₇H₇]⁺), 77 (8, [C₆H₅]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3030 (w), 2914 (w), 1680 (m), 1614 (w), 1591 (m), 1560 (w), 1547 (m), 1493 (m), 1410 (w), 1366 (w), 1314 (s), 1196 (m), 1148 (m), 1136 (m), 1111 (w), 1099 (w), 1034 (w), 995 (m), 922 (w), 855 (m), 806 (s), 768 (m), 747 (s), 689 (m), 665 (m), 646 (w). Anal calcd for C₂₄H₂₀N₂O [352.4]: C 81.79, H 5.72, N 7.95; Found: C 81.68, H 5.81, N 7.85.

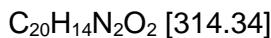
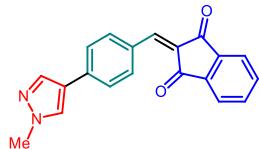
2.1.1.6. 3-Methyl-5-(4-(thiophen-3-yl)benzylidene)-2-thioxothiazolidin-4-one (8f)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/dichloromethane 3:2) and crystallization from *n*-hexane/dichloromethane compound **8f** (269 mg, 85%) was obtained as yellow orange crystals, Mp 205 °C. R_f (*n*-hexane/dichloromethane 1:1) = 0.45.

^1H NMR (300 MHz, CD_2Cl_2): δ 3.50 (s, 3 H), 7.45–7.48 (m, 2 H), 7.54–7.59 (m, 2 H), 7.63 (dd, 4J = 2.6 Hz, 4J = 1.7 Hz, 1 H), 7.73–7.75 (m, 3 H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 31.7 (CH_3), 122.6 (CH), 123.2 (C_{quat}), 126.5 (CH), 127.4 (CH), 127.6 (CH), 131.9 (CH), 132.6 (C_{quat}), 133.1 (CH), 138.4 (C_{quat}), 141.4 (C_{quat}), 168.3 (C_{quat}), 194.2 (C_{quat}). MS (EI) m/z (%): 317 (51, [M] $^+$), 301 (11, $[\text{C}_{14}\text{H}_8\text{NOS}_3]^+$), 216 (100, $[\text{C}_{12}\text{H}_8\text{S}_2]^+$). IR: $\tilde{\nu}$ [cm^{-1}] = 3094 (w), 3007 (w), 2938 (w), 1707 (m), 1678 (m), 1587 (w), 1557 (w), 1530 (w), 1497 (w), 1452 (w), 1422 (m), 1352 (w), 1290 (s), 1229 (w), 1198 (w), 1125 (m), 1099 (m), 1088 (m), 1014 (w), 993 (w), 922 (w), 864 (w), 842 (m), 781 (s), 718 (s), 681 (m), 646 (w), 621 (w). Anal calcd for $\text{C}_{15}\text{H}_{11}\text{NOS}_3$ [317.5]: C 56.75, H 3.49, N 4.41; Found: C 56.95, H 3.34, N 4.37.

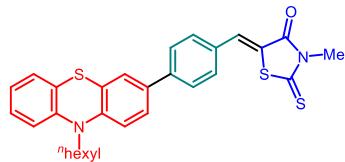
2.1.1.7. 2-[4-(1-Methyl-1*H*-pyrazol-4-yl)benzylidene]-1*H*-inden-1,3[2*H*]-dione (8g)



According to the GP and after purification by chromatography on silica gel (dichloromethane/dichloromethane/methanol 40:1) and crystallization from *n*-hexane/dichloromethane compound **8g** (223 mg, 71%) was obtained as a yellow orange voluminous solid, Mp 209 °C. R_f (dichloromethane/methanol 15:1) = 0.65.

^1H NMR (600 MHz, CD_2Cl_2): δ 3.94 (s, 3 H), 7.62–7.67 (m, 2 H), 7.79 (s, 1 H), 7.80–7.87 (m, 4 H), 7.94–8.03 (m, 2 H), 8.48–8.54 (m, 2 H). ^{13}C NMR (150 MHz, CD_2Cl_2): δ 39.7 (CH_3), 122.6 (C_{quat}), 123.5 (CH), 123.6 (CH), 125.7 (CH), 128.4 (CH), 128.9 (C_{quat}), 131.8 (C_{quat}), 135.65 (CH), 135.73 (CH), 135.8 (CH), 137.5 (CH), 138.4 (C_{quat}), 140.6 (C_{quat}), 143.1 (C_{quat}), 146.5 (CH), 189.7 (C_{quat}), 190.7 (C_{quat}). MS (EI) m/z (%): 314 (97, [M] $^+$), 313 (100, [M-H] $^+$), 286 (6, $[\text{C}_{19}\text{H}_{14}\text{N}_2\text{O}]^+$), 233 (3, $[\text{C}_{16}\text{H}_9\text{O}_2]^+$), 157 (5, $[\text{C}_{10}\text{H}_9\text{N}_2]^+$), 129 (2, $[\text{C}_9\text{H}_5\text{O}]^+$), 104 (3, $[\text{C}_7\text{H}_4\text{O}]^+$), 76 (4, $[\text{C}_6\text{H}_4]^+$). IR: $\tilde{\nu}$ [cm^{-1}] = 3107 (w), 3084 (w), 1717 (w), 1672 (s), 1626 (w), 1593 (w), 1578 (m), 1556 (s), 1541 (s), 1510 (m), 1469 (w), 1439 (m), 1415 (w), 1379 (m), 1354 (m), 1339 (m), 1321 (m), 1310 (w), 1285 (w), 1256 (w), 1213 (w), 1190 (s), 1159 (m), 1088 (m), 1074 (m), 1059 (w), 993 (m), 982 (w), 949 (s), 833 (m), 810 (m), 743 (s), 733 (w). Anal calcd for $\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_2$ [314.3]: C 76.42, H 4.49, N 8.91; Found: C 76.24, H 4.45, N 8.83.

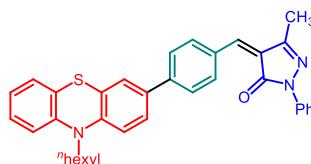
2.1.1.8. 5-[4-(10-Hexyl-10*H*-phenothiazin-3-yl)benzylidene]-3-methyl-2-thioxothiazolidin-4-one (8h)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) and drying und vacuo compound **8h** (201 mg, 79%) was obtained as orange red crystal needles, Mp 130 °C. R_f (*n*-hexane/acetone 10:1) = 0.42.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86–0.97 (m, 3 H), 1.29–1.39 (m, 4 H), 1.45–1.57 (m, 2 H), 1.85 (quin, ³J = 7.6 Hz, 2 H), 3.49 (s, 3 H), 3.95 (d, ³J = 7.1 Hz, 2 H), 6.88–6.98 (m, 2 H), 7.02 (d, ³J = 8.5 Hz, 1 H), 7.10 (dd, ³J = 7.6 Hz, ⁴J = 1.6 Hz, 1 H), 7.17 (ddd, ³J = 8.2 Hz, ³J = 7.2 Hz, ⁴J = 1.6 Hz, 1 H), 7.43 (d, ⁴J = 2.2 Hz, 1 H), 7.52 (dd, ³J = 8.5 Hz, ⁴J = 2.2 Hz, 1 H), 7.61–7.67 (m, 2 H), 7.72–7.79 (m, 3 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃), 23.7 (CH₂), 27.5 (CH₂), 27.7 (CH₂), 31.6 (CH₃), 32.5 (CH₂), 48.1 (CH₂), 116.4 (CH), 116.6 (CH), 123.3 (C_{quat}), 123.4 (CH), 124.8 (C_{quat}), 126.1 (CH), 126.2 (C_{quat}), 126.8 (CH), 127.7 (CH), 128.0 (CH), 128.2 (CH), 132.2 (CH), 132.7 (C_{quat}), 133.0 (CH), 134.1 (C_{quat}), 142.6 (C_{quat}), 145.3 (C_{quat}), 146.1 (C_{quat}), 167.7 (C_{quat}), 193.6 (C_{quat}). MS (MALDI-TOF) calcd for C₂₉H₂₈N₂OS₃ m/z: 516.14; Found: 516.2 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3063 (w), 2957 (w), 2924 (w), 2853 (w), 1713 (s), 1587 (m), 1572 (M), 1545 (w), 1493 (w), 1464 (s), 1441 (m), 1425 (m), 1395 (w), 1358 (m), 1290 (s), 1277 (s), 1248 (s), 1223 (w), 1194 (m), 1180 (w), 1128 (m), 1123 (s), 1101 (m), 1047 (w), 1038 (w), 991 (w), 955 (w), 907 (w), 878 (w), 872 (w), 813 (w), 808 (s), 721 (s), 718 (m), 716 (m), 667 (w). Anal calcd for C₂₉H₂₈N₂OS₃ [516.7]: C 67.41, H 5.46, N 5.42, S 18.62; Found: C 67.17, H 5.42, N 5.28, S 18.33.

2.1.1.9. 4-[4-(10-Hexyl-10*H*-phenothiazin-3-yl)benzylidene]-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (8i)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **8i** (207 mg, 76%) was obtained as a crystalline black red solid, Mp 58–61 °C. R_f (*n*-hexane/acetone 10:1) = 0.29.

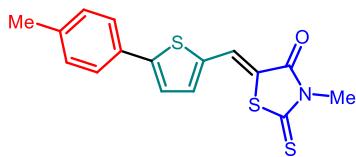
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86–0.94 (m, 3 H), 1.28–1.41 (m, 4 H), 1.43–1.56 (m, 2 H), 1.84 (quin, ³J = 7.6 Hz, 2 H), 2.37 (s, 3 H), 3.96 (d, ³J = 7.0 Hz, 2 H), 6.94 (dt, ³J = 7.4 Hz, ⁴J = 1.2 Hz, 1 H), 6.99 (d, ³J = 7.7 Hz, 1 H), 7.06 (d, ³J = 8.5 Hz, 1 H), 7.11 (d, ⁴J = 1.6 Hz, 1 H), 7.12–7.22 (m, 2 H), 7.36–7.45 (m, 2 H), 7.51 (d, ⁴J = 2.2 Hz, 1 H), 7.59 (dd, ³J = 8.5 Hz, ⁴J = 2.2 Hz, 1 H), 7.67 (s, 1 H), 7.73–7.80 (m, 2 H), 8.01–8.08 (m, 2 H), 8.68–8.75 (m, 2 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.6 (CH₃), 14.5 (CH₃), 23.5 (CH₂), 27.4 (CH₂), 27.6 (CH₂), 32.4 (CH₂), 48.1 (CH₂), 116.6 (CH), 116.7 (CH), 119.1 (CH), 123.5 (CH), 124.9 (C_{quat}), 125.0 (CH), 126.1 (C_{quat}), 126.3 (CH), 126.8 (CH), 127.1 (CH), 127.6 (C_{quat}), 128.0 (CH), 128.3 (CH), 129.4 (CH), 133.0 (C_{quat}), 134.3 (C_{quat}), 135.7 (CH), 139.8 (C_{quat}), 144.7 (C_{quat}), 145.4 (C_{quat}), 146.4 (C_{quat}), 147.3 (CH), 151.9 (C_{quat}), 162.6 (C_{quat}). MS (MALDI-TOF) calcd for C₃₅H₃₃N₃OS *m/z*: 543.72; Found: 543.2 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2953 (w), 2924 (w), 2855 (w), 1680 (w), 1616 (w), 1586 (m), 1574 (m), 1559 (m), 1541 (w), 1497 (m), 1460 (s), 1443 (m), 1427 (w), 1395 (w), 1362 (m), 1316 (s), 1289 (m), 1250 (m), 1225 (w), 1192 (m), 1142 (m), 1119 (m), 1111 (w), 1040 (w), 995 (m), 963 (w), 922 (w), 899 (w), 883 (w), 851 (w), 808 (m), 753 (m), 748 (s), 691 (m), 667 (m), 640 (w). Anal calcd for C₃₅H₃₃N₃OS [543.7]: C 77.31, H 6.12, N 7.73, S 5.90; Found: C 77.38, H 6.05, N 7.68, S 5.75.

2.1.2. Consecutive Three-component Suzuki-Knoevenagel Synthesis of Thienylene-bridged Systems 9

Table S2. Experimental details of the consecutive three-component Suzuki-Knoevenagel synthesis of thienylene-bridged systems 9

Entry	Bromo-aldehyde 2 [mg] (mmol)	Boronic acid/ester 6 [mg] (mmol)	CsF [mg] (mmol)	Pd(PPh ₃) ₄ [mg] (mmol)	t ₁ [h]	methylene active compound 7 [mg] (mmol)	Organocatalyst [mg] (mmol)	t ₂ [h]	Product [mg] (%)
1	191 (1.00) of 2	150 (1.1) of 6b	486 (3.2)	24 (0.02)	6	162 (1.10) of 7a	78 (1.0) of NH ₄ OAc	5	251 (76) of 9a
2	190 (1.00) of 2	150 (1.1) of 6b	486 (3.2)	24 (0.02)	8	161 (1.10) of 7c	1 drop of Et ₂ NH	3	264 (80) of 9b
3	190 (1.00) of 2	150 (1.1) of 6b	486 (3.2)	24 (0.02)	6	254 (1.20) of 7d	1 drop of Et ₂ NH	8	337 (85) of 9c
4	190 (1.00) of 2	150 (1.1) of 6b	486 (3.2)	24 (0.02)	8	192 (1.10) of 7e	1 drop of Et ₂ NH	4	290 (81) of 9d
5	115 (0.60) of 2	90 (1.1) of 6b	292 (3.2)	21 (0.02)	8	178 (0.66) of 7f	46 (0.6) of NH ₄ OAc	6	94 (45) of 9e
6	115 (0.60) of 2	267 (1.2) of 6d	291 (3.2)	21 (0.02)	8	98 (0.66) of 7a	46 (0.6) of NH ₄ OAc	5	174 (60) of 9f
7	95 (0.50) of 2	256 (1.2) of 6n	242 (3.2)	15 (0.013)	16	96 (0.55) of of 7e	1 drop of Et ₂ NH	4	218 (79) of 9g

2.1.2.1. 3-Methyl-2-thioxo-5-{[5-(*p*-tolyl)thiophen-2-yl]methylene}thiazolidin-4-one (**9a**)

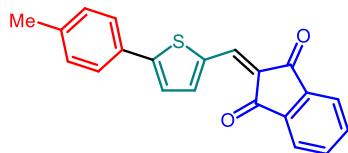


$C_{16}H_{13}NOS_3$ [331.48]

According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1) and drying under vacuo compound **9a** (251 mg, 76%) was obtained as a crystalline orange brown solid, Mp 212 °C. R_f (*n*-hexane/acetone 7:1) = 0.38.

1H NMR (300 MHz, DMSO-d₆/CS₂ 8:1): δ 2.38 (s, 3 H), 3.43 (s, 3 H), 7.24–7.31 (m, 2 H), 7.63–7.69 (m, 3 H), 7.74 (dd, 3J = 4.0 Hz, 4J = 0.7 Hz, 1 H), 8.07 (d, 4J = 0.7 Hz, 1 H). ^{13}C NMR (75 MHz, DMSO-d₆/CS₂ 8:1): δ 20.9 (CH₃), 31.1 (CH₃), 119.4 (C_{quat}), 125.1 (CH), 125.7 (CH), 125.9 (CH), 129.7 (CH), 129.8 (C_{quat}), 136.1 (C_{quat}), 137.4 (CH), 138.8 (C_{quat}), 152.0 (C_{quat}), 166.4 (C_{quat}), 191.7 (C_{quat}). MS (EI) *m/z* (%): 331 (59, [M]⁺), 230 (100, [C₁₃H₁₀S]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3007 (w), 2914 (w), 1694 (s), 1578 (s), 1435 (m), 1421 (m), 1350 (m), 1289 (s), 1265 (s), 1175 (m), 1120 (m), 1117 (m), 1053 (m), 991 (m), 951 (m), 936 (w), 905 (w), 882 (w), 819 (w), 810 (w), 785 (s), 731 (m), 706 (w), 631 (m). Anal calcd for $C_{16}H_{13}NOS_3$ [331.5]: C 57.97, H 3.95, N 4.23, S 29.02; Found: C 57.73, H 3.89, N 4.26, S 28.75.

2.1.2.2. 2-{[5-(*p*-Tolyl)thiophen-2-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (**9b**)



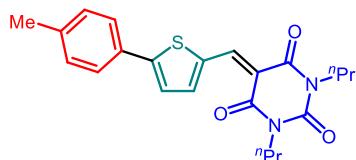
$C_{21}H_{14}O_2S$ [330.40]

According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1) and drying under vacuo compound **9b** (264 mg, 80%) was obtained as an orange voluminous solid, Mp 154 °C. R_f (*n*-hexane/acetone 4:1) = 0.20.

1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 2.43 (s, 3 H), 7.28–7.34 (m, 2 H), 7.58 (d, 3J = 4.1 Hz, 1 H), 7.69–7.75 (m, 2 H), 7.85–7.97 (m, 5 H), 8.17 (dd, 3J = 4.1 Hz, 4J = 0.6 Hz, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 21.7 (CH₃), 123.37 (CH), 123.43 (CH), 124.8 (C_{quat}), 125.4 (CH), 127.2 (CH), 130.8 (CH), 131.5 (C_{quat}), 135.6 (CH), 135.8 (CH), 136.1 (CH), 137.2 (C_{quat}), 140.4 (C_{quat}), 141.2 (C_{quat}), 142.8 (C_{quat}), 144.5 (CH), 157.7 (C_{quat}), 189.3 (C_{quat}), 189.6 (C_{quat}). MS (MALDI-TOF) calcd for $C_{21}H_{14}O_2S$ *m/z*: 330.07; Found: 330.7 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 1719 (w), 1678 (s), 1628 (w), 1600 (m), 1580 (s), 1524 (w), 1493 (w), 1437 (m), 1416 (w), 1379 (m), 1356 (w), 1341 (w), 1325 (w), 1233 (w), 1211 (m), 1198 (w), 1179 (w), 1159 (w), 1126 (w),

1098 (m), 1076 (w), 1026 (w), 993 (w), 947 (w), 824 (w), 799 (s), 783 (w), 733 (s), 642 (w). Anal calcd for C₂₁H₁₄O₂S [330.4]: C 76.34, H 4.27; Found: C 76.07, H 4.38.

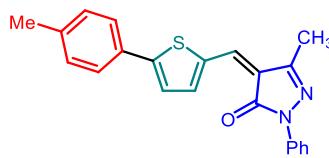
2.1.2.3. 1,3-Dipropyl-5-{{[5-(*p*-tolyl)thiophen-2-yl]methylene}pyrimidin-2,4,6[1*H*,3*H*,5*H*]-trione (9c)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 25:1) and drying under vacuo compound **9c** (337 mg, 85%) was obtained as yellow crystalline needles, Mp 155 °C. R_f (*n*-hexane/acetone 10:1) = 0.32.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.95 (t, ³J = 7.5 Hz, 3 H), 0.99 (t, ³J = 7.5 Hz, 3 H), 1.58–1.77 (m, 4 H), 2.42 (s, 3 H), 3.84–3.95 (m, 4 H), 7.30 (d, ³J = 8.1 Hz, 2 H), 7.60 (d, ³J = 4.1 Hz, 1 H), 7.68–7.76 (m, 2 H), 7.99 (d, ³J = 4.1 Hz, 1 H), 8.55 (s, 1 H). ¹³C NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 11.8 (CH₃), 11.9 (CH₃), 21.7 (CH₃), 22.17 (CH₂), 22.21 (CH₂), 43.4 (CH₂), 44.0 (CH₂), 110.9 (C_{quat}), 125.0 (CH), 127.2 (CH), 130.8 (CH), 131.5 (C_{quat}), 136.8 (C_{quat}), 140.7 (C_{quat}), 147.5 (CH), 148.1 (CH), 151.3 (C_{quat}), 160.3 (C_{quat}), 162.1 (C_{quat}), 162.5 (C_{quat}). MS (MALDI-TOF) calcd for C₂₂H₂₄N₂O₃S m/z: 396.15; Found: 397.0 ([MH]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2973 (w), 2970 (m), 2901 (w), 1649 (s), 1551 (m), 1520 (w), 1490 (w), 1452 (w), 1441 (w), 1398 (s), 1368 (m), 1340 (w), 1310 (m), 1255 (w), 1238 (m), 1201 (w), 1153 (m), 1107 (m), 1074 (s), 1057 (m), 1005 (w), 893 (w), 800 (m), 790 (m), 660 (w), 600 (w). Anal calcd for C₂₂H₂₄N₂O₃S [396.5]: C 66.64, H 6.10, N 7.07, S 8.09; Found: C 66.57, H 5.92, N 7.15, S 7.99.

2.1.2.4. 3-Methyl-1-phenyl-4-{{[5-(*p*-tolyl)thiophen-2-yl]methylene}-1*H*-pyrazol-5[4*H*]-one (9d)

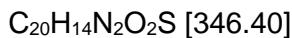
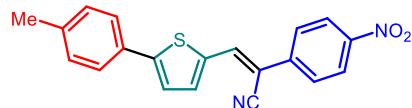


According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 10:1) and drying under vacuo compound **9d** (290 mg, 81%) was obtained as a red solid, Mp 133 °C. R_f (*n*-hexane/acetone 4:1) = 0.27.

¹H NMR (600 MHz, acetone-d₆/CS₂): δ 2.35 (s, 3 H), 2.41 (s, 3 H), 7.41 (tt, ³J = 7.4 Hz, ⁴J = 1.1 Hz, 1 H), 7.27–7.31 (m, 2 H), 7.37–7.42 (m, 2 H), 7.56 (d, ³J = 4.0 Hz, 1 H), 7.68–7.72 (m,

2 H), 7.86 (s, 1 H), 8.05–8.08 (m, 2 H), 8.11 (d, $^3J = 4.0$ Hz, 1 H). ^{13}C NMR (150 MHz, acetone-d₆/CS₂): δ 13.3 (CH₃), 21.6 (CH₃), 118.7 (CH), 122.1 (C_{quat}), 124.7 (CH), 124.9 (CH), 127.1 (CH), 129.3 (CH), 130.7 (CH), 131.6 (C_{quat}), 136.7 (C_{quat}), 137.2 (CH), 139.9 (C_{quat}), 140.3 (C_{quat}), 143.7 (CH), 150.7 (C_{quat}), 157.4 (C_{quat}), 162.9 (C_{quat}). MS (MALDI-TOF) calcd for C₂₂H₁₈N₂OS *m/z*: 358.11; Found: 359.1 ([MH]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2980 (w), 2972 (w), 2918 (w), 2851 (w), 1678 (s), 1653 (w), 1593 (m), 1557 (m), 1500 (m), 1489 (m), 1431 (m), 1410 (m), 1375 (m), 1360 (m), 1335 (w), 1314 (m), 1304 (m), 1255 (w), 1213 (m), 1142 (m), 1096 (w), 1078 (m), 1024 (m), 1001 (m), 957 (w), 926 (m), 912 (w), 891 (w), 804 (s), 797 (s), 762 (m), 756 (s), 729 (w), 689 (s), 673 (m), 658 (m), 619 (w). Anal calcd for C₂₂H₁₈N₂OS [358.5]: C 73.71, H 5.06, N 7.82, S 8.95; Found: C 73.63, H 5.09, N 7.86, S 8.98.

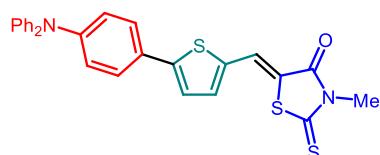
2.1.2.5. 2-(4-Nitrophenyl)-3-[5-(*p*-tolyl)thiophen-2-yl]acrylonitrile (**9e**)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1) and crystallization from a *n*-hexane/dichloromethane solution compound **9e** (94 mg, 45%) was obtained as a yellow golden amorphous voluminous solid, Mp 245 °C. R_f (*n*-hexane/acetone 10:1) = 0.13.

^1H NMR (300 MHz, DMSO-d₆): δ 2.37 (s, 3 H), 7.30 (d, $^3J = 7.7$ Hz, 2 H), 7.63–7.73 (m, 3 H), 7.86 (d, $^3J = 3.9$ Hz, 1 H), 8.00 (d, $^3J = 8.5$ Hz, 2 H), 8.34 (d, $^3J = 8.5$ Hz, 2 H), 8.56 (s, 1 H). ^{13}C NMR (75 MHz, DMSO-d₆): δ 20.9 (CH₃), 103.2 (C_{quat}), 117.5 (C_{quat}), 124.3 (CH), 124.35 (CH), 124.39 (C_{quat}), 125.9 (CH), 126.3 (CH), 129.86 (C_{quat}), 129.91 (CH), 135.9 (C_{quat}), 138.4 (CH), 138.9 (CH), 139.0 (C_{quat}), 140.0 (C_{quat}), 146.8 (C_{quat}). MS (MALDI-TOF) calcd for C₂₀H₁₄N₂O₂S *m/z*: 346.07; Found: 346.3 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3674 (w), 2988 (m), 2972 (m), 2901 (m), 1600 (w), 1572 (w), 1512 (m), 1502 (m), 1493 (m), 1443 (m), 1410 (m), 1373 (w), 1339 (m), 1269 (w), 1236 (m), 1165 (w), 1111 (m), 1067 (s), 1057 (m), 1044 (m), 1013 (w), 902 (m), 820 (w), 801 (s), 748 (m), 687 (m). Anal calcd for C₂₀H₁₄N₂O₂S [346.4]: C 69.35, H 4.07, N 8.09, S 9.26; Found: C 69.13, H 4.02, N 8.04, S 9.46.

2.1.2.6. 5-{[5-(4-{Diphenylamino}phenyl)thiophen-2-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (**9f**)

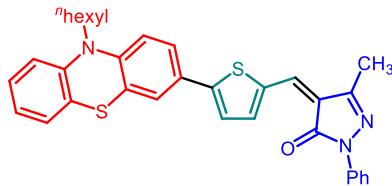




According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) and drying under vacuo compound **9f** (174 mg, 60%) was obtained as a red amorphous solid, Mp 150–154 °C. R_f (*n*-hexane/acetone 10:1) = 0.39.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 3.46 (s, 3 H), 7.03–7.08 (m, 2 H), 7.09–7.15 (m, 6 H), 7.28–7.35 (m, 4 H), 7.44 (d, 3J = 4.0 Hz, 1 H), 7.56 (dd, 3J = 4.0 Hz, 4J = 0.7 Hz, 1 H), 7.58–7.62 (m, 2 H), 7.87 (d, 4J = 0.6 Hz, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 31.6 (CH₃), 120.5 (C_{quat}), 123.1 (CH), 124.7 (CH), 124.8 (CH), 125.8 (CH), 126.1 (CH), 127.1 (C_{quat}), 127.7 (CH), 130.3 (CH), 136.9 (C_{quat}), 137.2 (CH), 147.6 (C_{quat}), 149.4 (C_{quat}), 153.3 (C_{quat}), 167.2 (C_{quat}), 192.5 (C_{quat}). MS (MALDI-TOF) calcd for C₂₇H₂₀N₂OS₃ *m/z*: 484.07; Found: 484.1 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3063 (w), 3030 (w), 3011 (w), 1697 (s), 1578 (s), 1526 (w), 1485 (m), 1431 (m), 1420 (m), 1389 (w), 1348 (m), 1329 (m), 1289 (s), 1283 (s), 1269 (s), 1196 (w), 1173 (m), 1126 (m), 1076 (w), 1051 (m), 1030 (w), 989 (w), 951 (w), 883 (w), 826 (w), 806 (w), 783 (m), 747 (s), 729 (m), 694 (s), 631 (m), 621 (w). Anal calcd for C₂₇H₂₀N₂OS₃ [484.7]: C 66.91, H 4.16, N 5.78, S 19.85; Found: C 66.69, H 4.26, N 5.61, S 19.87.

2.1.2.7. 4-{{[5-(10-Hexyl-10*H*-phenothiazin-3-yl)thiophen-2-yl]methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (9g)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **9g** (218 mg, 79%) was obtained as a dark brown amorphous solid, Mp 61 °C. R_f (*n*-hexane/acetone 10:1) = 0.23.

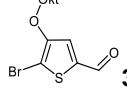
^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86–0.94 (m, 3 H), 1.28–1.42 (m, 4 H), 1.43–1.57 (m, 2 H), 1.84 (quin, 3J = 7.6 Hz, 2 H), 2.33 (s, 3 H), 3.96 (t, 3J = 7.1 Hz, 2 H), 6.95 (dt, 3J = 7.5 Hz, 4J = 1.2 Hz, 1 H), 6.98–7.05 (m, 2 H), 7.12 (dd, 3J = 7.5 Hz, 4J = 1.5 Hz, 2 H), 7.15–7.22 (m, 1 H), 7.36–7.44 (m, 2 H), 7.52 (d, 4J = 1.3 Hz, 1 H), 7.53 (d, 3J = 0.7 Hz, 1 H), 7.61 (dd, 3J = 8.5 Hz, 4J = 2.2 Hz, 1 H), 7.85 (d, 3J = 0.6 Hz, 1 H), 8.05–8.10 (m, 3 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.3 (CH₃), 14.5 (CH₃), 23.5 (CH₂), 27.3 (CH₂), 27.6 (CH₂), 32.4 (CH₂), 48.2 (CH₂), 116.7 (CH)¹, 118.7 (CH), 121.8 (C_{quat}), 123.7 (CH), 124.49 (C_{quat}), 124.54 (CH), 124.7 (CH), 125.4 (CH), 126.2 (C_{quat}), 126.6 (CH), 128.1 (CH), 128.4 (CH), 128.6 (C_{quat}), 129.4 (CH), 136.4 (C_{quat}), 137.2 (CH), 140.0 (C_{quat}), 144.0 (CH), 145.1 (C_{quat}), 147.0 (C_{quat}), 150.8

¹ Two CH signals coincide.

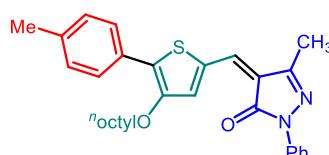
(C_{quat}), 156.6 (C_{quat}), 163.0 (C_{quat}). MS (MALDI-TOF) calcd for C₃₃H₃₁N₃OS₂ *m/z*: 549.19; Found: 550.2 ([MH]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2953 (w), 2924 (w), 2853 (w), 1674 (m), 1591 (s), 1574 (m), 1557 (w), 1497 (m), 1466 (m), 1425 (s), 1404 (m), 1364 (m), 1333 (m), 1312 (s), 1271 (m), 1252 (m), 1219 (m), 1196 (w), 1140 (m), 1109 (w), 1074 (m), 1057 (w), 1024 (w), 999 (m), 918 (w), 905 (w), 892 (w), 876 (w), 797 (m), 748 (s), 691 (m), 665 (w), 662 (w). Anal calcd for C₃₃H₃₁N₃OS₂ [549.8]: C 72.10, H 5.68, N 7.64, S 11.67; Found: C 72.24, H 5.82, N 7.52, S 11.53.

2.1.3. Consecutive Three-component Suzuki-Knoevenagel Synthesis of 4-*n*Ocytyloxy-substituted Thienylene-bridged Systems 9

Table S3. Experimental details of the consecutive three-component Suzuki-Knoevenagel synthesis of 4-*n*Ocytyloxy-substituted thienylene-bridged systems 10.

Entry	Bromo-aldehyde 3 [mg] (mmol)	Boronic acid/ester 6 [mg] (mmol)	CsF [mg] (mmol)	Pd(PPh ₃) ₄ [mg] (mmol)	t ₁ [h]	methylene active compound 7 [mg] (mmol)	Organocatalyst [mg] (mmol)	t ₂ [h]	Product [mg] (%)
									
31	256 (0.80) of 3	131 (0.96) of 6b	389 (2.56)	28 (0.024)	16	167 (0.96) of 7e	1 drop of Et ₂ NH 46 (0.60) of NH ₄ OAc 39 (0.50) of NH ₄ OAc	4	268 (69) of 10a
37	192 (0.60) of 3	98 (0.72) of 6b	292 (1.92)	21 (0.018)	16	156 (0.78) of 7g	46 (0.60) of NH ₄ OAc	5	169 (55) of 10b
25	160 (0.50) of 3	276 (0.60) of 6f	243 (1.60)	17 (0.015)	16	80 (0.60) of 7b	39 (0.50) of NH ₄ OAc	5	204 (59) of 10c
26	192 (0.60) of 3	311 (0.72) of 6e	292 (1.92)	21 (0.018)	16	96 (0.72) of 7b	46 (0.60) of NH ₄ OAc	5	355 (90) of 10d
32	320 (1.00) of 3	519 (1.20) of 6e	486 (3.20)	35 (0.030)	16	209 (1.20) of 7e	1 drop of Et ₂ NH 46 (0.60) of NH ₄ OAc	4	545 (78) of 10e
27	192 (0.60) of 3	478 (0.72) of 6o	292 (1.92)	21 (0.018)	16	96 (0.72) of 7b	46 (0.60) of NH ₄ OAc	5	470 (88) of 10f
28	192 (0.60) of 3	360 (0.72) of 6p	292 (1.92)	21 (0.018)	16	96 (0.72) of 7b	46 (0.60) of NH ₄ OAc	5	350 (80) of 10g
33	300 (0.94) of 3	563 (1.13) of 6p	457 (3.01)	33 (0.028)	16	197 (1.13) of 7e	1 drop of Et ₂ NH	4	431 (60) of 10h

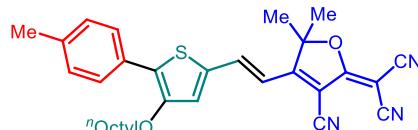
2.1.3.1. (*Z*-5-methyl-4-((4-(octyloxy)-5-(*p*-tolyl)thiophen-2-yl)methylene)-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (10a)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) and drying under vacuo compound **10a** (268 mg, 69%) was obtained as a red brown amorphous solid, Mp 102–104 °C. R_f (*n*-hexane/acetone 10:1) = 0.19.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.87–0.98 (m, 3 H), 1.30–1.47 (m, 8 H), 1.55 (quin, 3J = 7.1 Hz, 2 H), 1.87 (quin, 3J = 6.4 Hz, 2 H), 2.33 (s, 3 H), 2.40 (s, 3 H), 4.21 (t, 3J = 6.4 Hz, 2 H), 7.13 (t, 3J = 7.4 Hz, 1 H), 7.24 (d, 3J = 8.1 Hz, 2 H), 7.34–7.42 (m, 2 H), 7.64 (s, 1 H), 7.78–7.85 (m, 2 H), 8.03–8.09 (m, 2 H), 8.28 (s, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.3 (CH₃), 14.7 (CH₃), 21.7 (CH₃), 23.7 (CH₂), 27.0 (CH₂), 30.2 (CH₂), 30.3 (CH₂), 30.4 (CH₂), 32.8 (CH₂), 72.4 (CH₂), 118.8 (CH), 122.6 (C_{quat}), 124.7 (CH), 128.3 (CH), 129.3 (CH), 129.5 (CH), 130.2 (CH), 130.8 (C_{quat}), 132.6 (C_{quat}), 135.3 (C_{quat}), 136.5 (CH), 139.0 (C_{quat}), 139.9 (C_{quat}), 150.5 (C_{quat}), 155.2 (C_{quat}), 162.9 (C_{quat}). MS (MALDI-TOF) calcd for C₃₀H₃₄N₂O₂S *m/z*: 486.23; Found: 487.0 ([MH]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2988 (w), 2953 (w), 2924 (w), 2855 (w), 1672 (m), 1595 (m), 1559 (w), 1535 (w), 1497 (m), 1429 (w), 1412 (m), 1383 (w), 1366 (w), 1306 (s), 1271 (w), 1242 (m), 1213 (w), 1188 (w), 1142 (m), 1130 (w), 1109 (w), 1080 (m), 1061 (w), 1026 (w), 1001 (w), 978 (w), 943 (w), 909 (w), 889 (w), 810 (m), 791 (w), 766 (w), 748 (s), 716 (w), 689 (m), 662 (m). Anal calcd for C₃₀H₃₄N₂O₂S [486.7]: C 74.04, H 7.04, N 5.76, S 6.59; Found: C 74.17, H 7.11, N 6.01, S 6.25.

2.1.3.2. (*E*)-2-(3-cyano-5,5-dimethyl-4-(2-(4-(*n*-octyloxy)-5-(*p*-tolyl)thiophen-2-yl)vinyl)furan-2(5*H*)-ylidene)malononitrile (**10b**)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) and drying under vacuo compound **10b** (169 mg, 55%) was obtained as a black amorphous solid, Mp 164–167 °C. R_f (*n*-hexane/acetone 3:1) = 0.34.

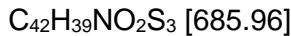
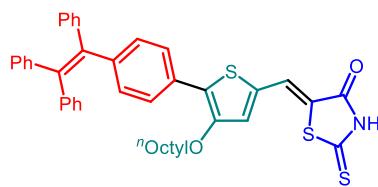
^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.91 (t, 3J = 6.7 Hz, 3 H), 1.25–1.45 (m, 8 H), 1.52 (quin, 3J = 7.5 Hz, 2 H), 1.87 (m, 8 H), 2.38 (s, 3 H), 4.20 (t, 3J = 6.6 Hz, 2 H), 6.94 (d, 3J = 15.7 Hz, 1 H), 7.24 (d, 3J = 7.6 Hz, 2 H), 7.70–7.80 (m, 3 H), 8.05 (d, 3J = 15.8 Hz, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.6 (CH₃), 21.5 (CH₃), 23.5 (CH₂), 26.2 (CH₃), 26.9 (CH₂), 30.1 (CH₂),² 30.2 (CH₂), 32.7 (CH₂), 72.7 (CH₂), 98.8 (C_{quat}), 98.8 (C_{quat}),³ 111.4 (C_{quat}), 112.2 (C_{quat}), 112.9 (C_{quat}), 113.5 (CH), 125.0 (CH), 128.0 (CH), 130.3 (CH), 130.5 (C_{quat}), 130.7 (C_{quat}), 135.6 (C_{quat}), 139.1 (C_{quat}), 140.2 (CH), 155.7 (C_{quat}), 174.5 (C_{quat}), 176.9 (C_{quat}). MS

² Two CH₂ signals coincide.

³ Two C_{quat} signals coincide.

(MALDI-TOF) calcd for $C_{31}H_{33}N_3O_2S$ m/z : 511.23; Found: 511.2 ([M] $^+$). IR: $\tilde{\nu}$ [cm $^{-1}$] = 3672 (w), 2987 (w), 2922 (w), 2866 (w), 2228 (m), 1599 (w), 1565 (s), 1559 (s), 1545 (s), 1522 (w), 1470 (w), 1439 (m), 1410 (w), 1395 (w), 1360 (s), 1306 (w), 1275 (m), 1256 (s), 1213 (w), 1188 (w), 1171 (m), 1105 (m), 1078 (m), 976 (w), 955 (m), 941 (w), 858 (w), 841 (w), 817 (m), 750 (w), 714 (w), 652 (w), 625 (w). Anal calcd for $C_{31}H_{33}N_3O_2S$ [511.2]: C 72.77, H 6.50, N 8.21, S 6.27; Found: C 72.60, H 6.55, N 7.99, S 6.38.

2.1.3.3. (*Z*-5-((4-(octyloxy)-5-(4-(1,2,2-triphenylvinyl)phenyl)thiophen-2-yl)methylene)-2-thioxothiazolidin-4-one (10c)



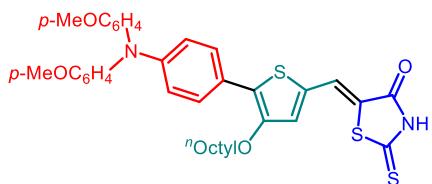
According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 10:1), precipitation from a *n*-hexane/dichloromethane solution and drying under vacuo compound **10c** (204 mg, 59%) was obtained as orange red crystal platelets, Mp 154–157 °C. R_f (*n*-hexane/ethyl acetate 5:1) = 0.24.

1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.87–0.95 (m, 3 H), 1.25–1.56 (m, 10 H), 1.82 (quin, 3J = 6.5 Hz, 2 H), 4.20 (t, 3J = 6.4 Hz, 2 H), 7.01–7.17 (m, 17 H), 7.49 (s, 1 H), 7.62–7.67 (m, 2 H), 7.68 (s, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃), 23.6 (CH₂), 26.9 (CH₂), 30.1 (CH₂),⁴ 30.3 (CH₂), 32.7 (CH₂), 72.7 (CH₂), 123.7 (C_{quat}), 124.9 (CH), 124.9 (CH), 126.9 (CH), 127.3 (CH), 127.4 (CH), 127.5 (CH), 128.5 (CH), 128.6 (CH), 128.7 (CH), 129.5 (C_{quat}), 131.6 (C_{quat}), 131.96 (CH), 131.98 (CH), 132.1 (CH), 132.4 (CH), 133.7 (C_{quat}), 141.2 (C_{quat}), 142.3 (C_{quat}), 144.0 (C_{quat}), 144.2 (C_{quat}),⁵ 144.4 (2 C_{quat}), 155.7 (C_{quat}), 168.9 (C_{quat}), 194.1 (C_{quat}). MS (MALDI-TOF) calcd for $C_{42}H_{39}NO_2S_3$ m/z : 685.21; Found: 685.2 ([M] $^+$). IR: $\tilde{\nu}$ [cm $^{-1}$] = 3138 (w), 3005 (w), 2922 (w), 2847 (w), 1686 (m), 1649 (w), 1572 (s), 1545 (m), 1530 (m), 1491 (w), 1431 (m), 1406 (m), 1379 (w), 1296 (m), 1263 (m), 1213 (s), 1167 (m), 1153 (m), 1126 (w), 1078 (m), 1063 (m), 1014 (w), 977 (w), 965 (w), 941 (w), 891 (w), 850 (w), 826 (m), 751 (m), 696 (s), 665 (s), 652 (m), 619 (w). Anal calcd for $C_{42}H_{39}NO_2S_3$ [686.0]: C 73.54, H 5.73, N 2.04, S 14.02; Found: C 73.62, H 5.89, N 1.92, S 13.98.

⁴ Two CH₂ signals coincide.

⁵ Two C_{quat} signals coincide.

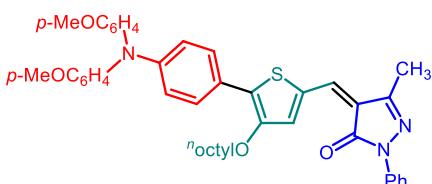
2.1.3.4. 5-{[5-(4-{Bis[4-methoxyphenyl]amino}phenyl)-3-(octyloxy)thiophen-2-yl]methylene}-2-thioxothiazolidin-4-one (10d)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1) and drying under vacuo compound **10d** (355 mg, 90%) was obtained as a dark red amorphous solid, Mp 92–94 °C. R_f (*n*-hexane/acetone 1:1) = 0.74.

1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.84–0.97 (m, 3 H), 1.22–1.47 (m, 8 H), 1.51 (quin, 3J = 7.1 Hz, 2 H), 1.84 (quin, 3J = 6.5 Hz, 2 H), 3.80 (s, 6 H), 4.19 (t, 3J = 6.4 Hz, 2 H), 6.83–6.93 (m, 6 H), 7.04–7.12 (m, 4 H), 7.44 (s, 1 H), 7.65 (s, 1 H), 7.66–7.71 (m, 2 H), 12.06 (br, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃), 23.6 (CH₂), 27.0 (CH₂), 30.2 (CH₂),⁶ 30.4 (CH₂), 32.7 (CH₂), 55.7 (CH₃), 72.6 (CH₂), 115.6 (CH), 119.9 (CH), 122.4 (C_{quat}), 124.8 (C_{quat}), 125.08 (CH), 125.11 (CH), 127.9 (CH), 128.6 (CH), 131.2 (C_{quat}), 132.0 (C_{quat}), 140.7 (C_{quat}), 149.3 (C_{quat}), 154.6 (C_{quat}), 157.4 (C_{quat}), 168.8 (C_{quat}), 194.0 (C_{quat}). MS (MALDI-TOF) calcd for $C_{36}H_{38}N_2O_4S_3$ *m/z*: 658.20; Found: 658.1 ([M]⁺). IR: IR: $\tilde{\nu}$ [cm⁻¹] = 3671 (w), 2988 (w), 2955 (w), 2922 (w), 2901 (w), 2853 (w), 1697 (w), 1574 (m), 1533 (w), 1501 (s), 1462 (w), 1433 (m), 1416 (m), 1412 (m), 1400 (m), 1381 (m), 1319 (w), 1289 (m), 1263 (m), 1238 (s), 1207 (s), 1196 (s), 1161 (s), 1126 (m), 1105 (m), 1076 (m), 1057 (m), 1036 (s), 1013 (m), 974 (w), 947 (w), 891 (w), 822 (s), 779 (m), 764 (w), 729 (w), 710 (m), 675 (m), 648 (m), 617 (w). Anal calcd for $C_{36}H_{38}N_2O_4S_3$ [658.9]: C 65.62, H 5.81, N 4.25, S 14.60; Found: C 65.63, H 5.91, N 4.11, S 14.30.

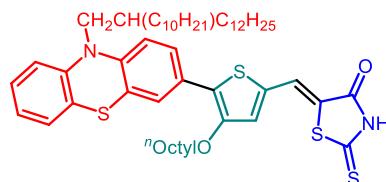
2.1.3.5. (Z)-4-((5-(4-(bis(4-methoxyphenyl)amino)phenyl)-4-(octyloxy)thiophen-2-yl)methylene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (10e)



⁶ Two CH₂ signals coincide.

According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **10e** (545 mg, 78%) was obtained as a dark violet amorphous solid, Mp softening >60 °C, melting >90 °C. R_f (*n*-hexane/acetone 10:1) = 0.15. ^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.83–0.94 (m, 3 H), 1.24–1.46 (m, 8 H), 1.51 (quin, 3J = 7.2 Hz, 2 H), 1.84 (quin, 3J = 6.5 Hz, 2 H), 2.30 (s, 3 H), 3.80 (s, 6 H), 4.19 (t, 3J = 6.4 Hz, 2 H), 6.83–6.95 (m, 6 H), 7.07–7.16 (m, 5 H), 7.33–7.42 (m, 2 H), 7.60–7.63 (s, 1 H), 7.72–7.80 (m, 2 H), 8.03–8.09 (m, 2 H), 8.24 (s, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.3 (CH₃), 14.6 (CH₃), 23.5 (CH₂), 27.0 (CH₂), 30.1 (CH₂), 30.2 (CH₂), 30.3 (CH₂), 32.7 (CH₂), 55.8 (CH₃), 72.4 (CH₂), 115.7 (CH), 118.8 (CH), 119.5 (CH), 121.5 (C_{quat}), 124.6 (CH), 124.9 (C_{quat}), 128.2 (CH), 129.2 (CH), 129.3 (CH), 129.7 (CH), 131.5 (C_{quat}), 136.5 (CH), 136.7 (C_{quat}), 140.1 (C_{quat}), 140.6 (C_{quat}), 149.9 (C_{quat}), 150.6 (C_{quat}), 154.8 (C_{quat}), 157.6 (C_{quat}), 163.1 (C_{quat}). MS (MALDI-TOF) calcd for C₄₃H₄₅N₃O₄S *m/z*: 699.31; Found: 699.3 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2924 (w), 2833 (w), 1670 (w), 1580 (m), 1557 (w), 1530 (w), 1499 (s), 1464 (w), 1433 (w), 1406 (m), 1364 (m), 1317 (m), 1302 (m), 1275 (m), 1238 (s), 1194 (m), 1179 (m), 1165 (w), 1123 (m), 1109 (w), 1078 (w), 1029 (m), 1026 (m), 997 (w), 976 (w), 951 (w), 909 (w), 880 (w), 826 (m), 793 (w), 779 (w), 752 (m), 721 (w), 704 (w), 691 (m), 660 (m), 633 (w). Anal calcd for C₄₃H₄₅N₃O₄S [699.9]: C 73.79, H 6.48, N 6.00, S 4.58; Found: C 74.03, H 6.66, N 6.03, S 4.70.

2.1.3.6. (*Z*)-5-((5-(10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl)-4-(octyloxy)thiophen-2-yl)methylene)-2-thioxothiazolidin-4-one (**10f**)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) and drying under vacuo compound **10f** (470 mg, 88%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.14.

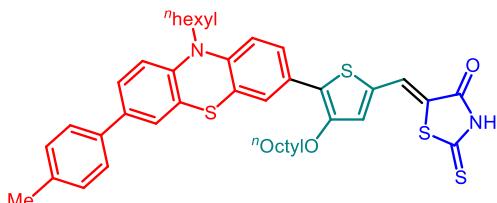
^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.87–0.98 (m, 9 H), 1.20–1.65 (m, 50 H), 1.81–1.97 (m, 2 H), 1.97–2.05 (m, 1 H), 3.85 (d, 3J = 7.0 Hz, 2 H), 4.23 (t, 3J = 6.3 Hz, 2 H), 6.91–7.02 (m, 3 H), 7.13 (dd, 3J = 7.7 Hz, 4J = 1.5 Hz, 1 H), 7.12–7.24 (m, 1 H), 7.47 (s, 1 H), 7.64 (dd, 3J = 8.6 Hz, 4J = 2.2 Hz, 1 H), 7.67 (s, 1 H), 7.70 (d, 4J = 2.2 Hz, 1 H), 12.10 (br, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.76 (CH₃)⁷, 14.78 (CH₃), 23.7 (CH₂)⁸, 27.1 (CH₂), 27.16 (CH₂), 27.18 (CH₂), 30.29 (CH₂), 30.32 (CH₂), 30.4 (CH₂)⁸, 30.45 (CH₂), 30.48 (CH₂)⁸, 30.6

⁷ Two CH₃ signals coincide.

⁸ Two CH₂ signals coincide.

(CH₂)⁹ 30.65 (CH₂)⁸ 30.66 (CH₂), 30.69 (CH₂), 31.0 (CH₂)⁸ 32.4 (CH₂)⁸ 32.8 (CH₂), 32.9 (CH₂)⁸ 35.5 (CH), 52.2 (CH₂), 72.7 (CH₂), 116.9 (CH), 117.1 (CH), 123.2 (C_{quat}), 123.6 (CH), 124.9 (CH)¹⁰ 125.8 (C_{quat}), 126.3 (CH), 126.77 (C_{quat}), 126.81 (CH), 127.8 (C_{quat}), 128.2 (CH)¹⁰ 129.4 (C_{quat}), 132.9 (C_{quat}), 145.9 (C_{quat}), 146.0 (C_{quat}), 155.0 (C_{quat}), 168.8 (C_{quat}), 193.9 (C_{quat}). MS (MALDI-TOF) calcd for C₅₂H₇₆N₂O₂S₄ *m/z*: 888.48; Found: 888.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3150 (w), 3090 (w), 3071 (w), 2953 (w), 2920 (m), 2851 (m), 1699 (m), 1581 (m), 1572 (m), 1533 (w), 1495 (w), 1464 (m), 1427 (s), 1395 (w), 1377 (w), 1331 (w), 1294 (m), 1277 (m), 1250 (m), 1213 (s), 1165 (m), 1132 (w), 1107 (w), 1084 (w), 1063 (w), 1037 (w), 1003 (w), 949 (w), 926 (w), 889 (w), 870 (w), 816 (w), 791 (w), 768 (w), 745 (m), 729 (w), 673 (m), 656 (w), 611 (w). Anal calcd for C₅₂H₇₆N₂O₂S₄ [889.4]: C 70.22, H 8.61, N 3.15, S 14.42; Found: C 70.05, H 8.38, N 3.09, S 14.33.

2.1.3.7. (*Z*)-5-((5-(10-hexyl-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl)-4-(octyloxy)thiophen-2-yl)methylene)-2-thioxothiazolidin-4-one (10g)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1), precipitation from a *n*-hexane/acetone solution, and drying under vacuo compound **10g** (350 mg, 80%) was obtained as a black amorphous solid, Mp 121–123 °C. R_f (*n*-hexane/acetone 1:1) = 0.77.

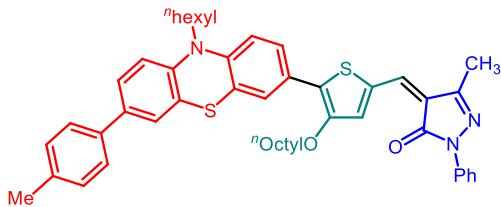
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.85–0.95 (m, 6 H), 1.27–1.57 (m, 16 H), 1.70–1.88 (m, 4 H), 2.36 (s, 3 H), 3.88 (t, ³J = 7.0 Hz, 2 H), 4.13 (t, ³J = 6.3 Hz, 2 H), 6.90 (d, ³J = 8.5 Hz, 1 H), 6.96 (d, ³J = 8.6 Hz, 1 H), 7.19 (d, ³J = 8.0 Hz, 2 H), 7.26 (d, ⁴J = 2.1 Hz, 1 H), 7.37 (dd, ³J = 8.5 Hz, ⁴J = 2.2 Hz, 1 H), 7.39–7.44 (m, 2 H), 7.50–7.58 (m, 3 H), 7.71 (s, 1 H), 13.63 (br, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃), 14.8 (CH₃), 21.5 (CH₃), 23.29 (CH₂), 23.31 (CH₂), 26.7 (CH₂), 27.0 (CH₂), 27.1 (CH₂), 29.8 (CH₂), 29.9 (CH₂), 30.0 (CH₂), 32.0 (CH₂), 32.3 (CH₂), 47.6 (CH₂), 72.1 (CH₂), 115.8 (CH), 116.3 (CH), 122.9 (C_{quat}), 124.2 (C_{quat}), 124.4 (C_{quat}), 124.7 (CH), 125.3 (CH), 125.4 (CH), 125.4 (CH), 126.1 (CH), 126.4 (CH), 126.5 (CH), 127.1 (C_{quat}), 128.4 (C_{quat}), 130.0 (CH), 132.5 (C_{quat}), 135.4 (C_{quat}), 136.75 (C_{quat}), 136.81 (C_{quat}), 143.4 (C_{quat}), 144.3 (C_{quat}), 154.4 (C_{quat}), 169.4 (C_{quat}), 194.2 (C_{quat}). MS (MALDI-TOF) calcd for C₄₁H₄₆N₂O₂S₄ *m/z*: 726.24; Found: 726.2 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3078 (w), 2951

⁹ Three CH₂ signals coincide.

¹⁰ Two CH signals coincide.

(w), 2868 (w), 2835 (w), 1692 (m), 1570 (m), 1532 (m), 1474 (m), 1422 (m), 1389 (m), 1364 (m), 1298 (w), 1265 (w), 1245 (w), 1206 (s), 1163 (m), 1100 (w), 1078 (m), 1061 (m), 1005 (m), 982 (w), 947 (w), 885 (w), 820 (w), 795 (m), 745 (w), 675 (s), 648 (m). Anal calcd for C₄₁H₄₆N₂O₂S₄ [727.1]: C 67.73, H 6.38, N 3.85, S 17.64; Found: C 67.44, H 6.28, N 3.86, S 17.53.

2.1.3.8. (*Z*)-4-((5-(10-hexyl-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl)-4-(octyloxy)thiophen-2-yl)methylene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (10h)



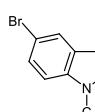
According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **10h** (431 mg, 60%) was obtained as a dark violet amorphous solid, Mp softening >60 °C, melting >95 °C. R_f (*n*-hexane/acetone 10:1) = 0.23.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.87–0.97 (m, 6 H), 1.30–1.60 (m, 16 H), 1.79–1.97 (m, 4 H), 2.30 (s, 3 H), 2.37 (s, 3 H), 3.96 (t, ³J = 7.1 Hz, 2 H), 4.21 (t, ³J = 6.3 Hz, 2 H), 7.00 (t, ³J = 8.9 Hz, 2 H), 7.09–7.18 (m, 1 H), 7.22 (d, ³J = 8.0 Hz, 2 H), 7.32–7.50 (m, 6 H), 7.63 (s, 1 H), 7.70 (dd, ³J = 8.6 Hz, ⁴J = 2.2 Hz, 1 H), 7.76 (d, ⁴J = 2.1 Hz, 1 H), 8.04–8.11 (m, 2 H), 8.21 (s, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.3 (CH₃), 14.6 (CH₃), 14.7 (CH₃), 21.4 (CH₃), 23.6 (CH₂), 23.7 (CH₂), 27.2 (CH₂), 27.4 (CH₂), 27.6 (CH₂), 30.30 (CH₂), 30.34 (CH₂), 30.40 (CH₂), 30.44 (CH₂), 32.8 (CH₂), 48.2 (CH₂), 72.5 (CH₂), 116.2 (CH), 116.7 (CH), 118.8 (CH), ¹¹ 122.2 (C_{quat}), 124.7 (CH), 124.97 (CH), 125.04 (C_{quat}), 126.0 (C_{quat}), 126.6 (CH), 127.0 (CH), 127.5 (CH), 127.9 (C_{quat}), 129.3 (CH), 129.6 (CH), 130.3 (CH), 132.2 (C_{quat}), 134.5 (C_{quat}), 136.35 (C_{quat}), 136.40 (CH), 137.4 (C_{quat}), 137.6 (C_{quat}), 140.0 (C_{quat}), 144.0 (C_{quat}), 145.6 (C_{quat}), 150.6 (C_{quat}), 155.1 (C_{quat}), 163.0 (C_{quat}). MS (MALDI-TOF) calcd for C₄₈H₅₃N₃O₂S₂ m/z: 767.36; Found: 767.3 ([M]⁺). IR: ν [cm⁻¹] = 3026 (w), 2951 (w), 2922 (w), 2853 (w), 1672 (w), 1593 (m), 1578 (m), 1557 (w), 1532 (w), 1497 (m), 1472 (m), 1416 (s), 1396 (m), 1362 (s), 1319 (m), 1306 (s), 1277 (s), 1262 (m), 1238 (m), 1173 (w), 1136 (m), 1121 (m), 1111 (m), 1086 (w), 1026 (w), 997 (s), 949 (w), 907 (w), 880 (w), 802 (s), 754 (m), 752 (m), 712 (w), 691 (m), 660 (m). Anal calcd for C₄₈H₅₃N₃O₂S₂ [768.1]: C 75.06, H 6.96, N 5.47, S 8.35; Found: C 74.99, H 6.83, N 5.65, S 8.08.

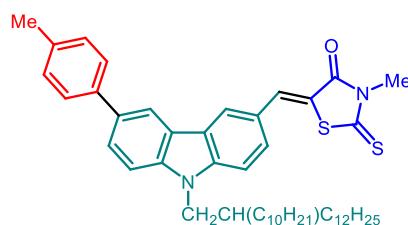
¹¹ Two CH signals coincide.

2.1.4. Consecutive Three-component Suzuki-Knoevenagel Synthesis of Carbazole-bridged Systems 11

Table S4. Experimental details of the consecutive three-component Suzuki-Knoevenagel synthesis of carbazole-bridged systems 11.

Entry	Bromo-aldehyde 4 [mg] (mmol)	Boronic acid/ester 6 [mg] (mmol)	CsX [mg] (mmol)	Pd(PPh ₃) ₄ [mg] (μmol)	t ₁ [h]	methylene active compound 7 [mg] (mmol)	Organocatalyst [mg] (mmol)	t ₂ [h]	Product [mg] (%)
	 4 C _{14,10}								
1	300 (0.492) of 4	81 (0.59) of 6b	239 (1.57) of CsF	17 (15)	16	80 (0.54) of 7a	38 (0.49) of NH ₄ OAc	6	332 (90) of 11a
2	325 (0.532) of 4	87 (0.64) of 6b	259 (1.70) of CsF	18 (16)	16	78 (0.585) of 7b	41 (0.53) of NH ₄ OAc	5	337 (86) of 11b
3	302 (0.495) of 4	81 (0.59) of 6b	516 (0.79) of Cs ₂ CO ₃	17 (15)	16	87 (0.59) of 7c	1 drop of Et ₂ NH	4	293 (59) of 11c
4	318 (0.521) of 4	85 (0.63) of 6b	253 (1.67) of CsF	18 (16)	16	109 (0.63) of 7e	1 drop of Et ₂ NH	5	320 (79) of 11d
5	330 (0.54) of 4	88 (0.648) of 6b	262 (1.73) of CsF	19 (16)	16	101 (0.62) of 7f	1 drop of Et ₂ NH	8	287 (73) of 11e
6	330 (0.540) of 4	88 (0.648) of 6b	262 (1.73) of CsF	19 (16)	16	140 (0.70) of 7g	42 (0.54) of NH ₄ OAc	6	395 (91) of 11f
7	300 (0.492) of 4	123 (0.59) of 6l	512 (0.77) of Cs ₂ CO ₃	17 (15)	16	86 (0.59) of 7c	1 drop of Et ₂ NH	4	292 (60) of 11g
8	315 (0.516) of 4	267 (0.62) of 6e	538 (1.65) of Cs ₂ CO ₃	18 (16)	16	108 (0.63) of 7e	1 drop of Et ₂ NH	5	289 (57) of 11h
9	315 (0.516) of 4	309 (0.62) of 6p	538 (1.65) of Cs ₂ CO ₃	18 (16)	16	109 (0.63) of 7e	1 drop of Et ₂ NH	5	334 (61) of 11i

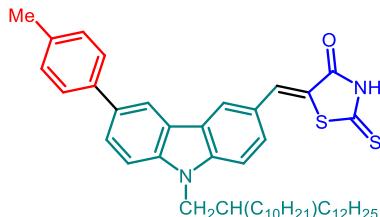
2.1.4.1. 5-[{9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (**11a**)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 40:1) and drying under vacuo compound **11a** (332 mg, 90%) was obtained as a viscous orange red oil. R_f (*n*-hexane/acetone 10:1) = 0.43.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86 (t, ³J = 6.7 Hz, 3 H), 0.87 (t, ³J = 6.7 Hz, 3 H), 1.14–1.45 (m, 40 H), 2.09–2.21 (m, 1 H), 2.40 (s, 3 H), 3.44 (s, 3 H), 4.21 (d, ³J = 7.5 Hz, 2 H), 7.26–7.33 (m, 2 H), 7.52–7.60 (m, 3 H), 7.64–7.70 (m, 2 H), 7.77 (dd, ³J = 8.5 Hz, ⁴J = 1.8 Hz, 1 H), 7.83 (s, 1 H), 8.32 (d, ⁴J = 1.3 Hz, 1 H), 8.46 (d, ⁴J = 1.7 Hz, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.5 (CH₃)¹² 21.2 (CH₃), 23.5 (CH₂)¹³ 27.26 (CH₂), 27.29 (CH₂), 30.18 (CH₂), 30.20 (CH₂), 30.23 (CH₂), 30.3 (CH₂), 30.39 (CH₂), 30.42 (CH₂), 30.44 (CH₂), 30.47 (CH₂), 30.49 (CH₃), 30.51 (CH₂), 30.65 (CH₂), 30.69 (CH₂), 31.5 (CH₂), 32.55 (CH₂), 32.58 (CH₂), 32.7 (2 CH₂), 38.6 (CH), 48.5 (CH₂), 111.1 (CH), 111.2 (CH), 119.4 (C_{quat}), 119.5 (CH), 124.0 (C_{quat}), 124.7 (C_{quat}), 125.0 (CH), 125.2 (C_{quat}), 126.6 (CH), 127.7 (CH), 129.6 (CH), 130.4 (CH), 134.1 (C_{quat}), 135.3 (CH), 137.0 (C_{quat}), 139.4 (C_{quat}), 141.7 (C_{quat}), 143.3 (C_{quat}), 168.1 (C_{quat}), 194.4 (C_{quat}). MS (MALDI-TOF) calcd for C₄₈H₆₆N₂OS₂·H⁺ *m/z*: 750.5; Found: 750.5. IR: $\tilde{\nu}$ [cm⁻¹] = 2920 (m), 2851 (w), 1705 (m), 1578 (m), 1479 (m), 1464 (w), 1424 (w), 1389 (w), 1350 (w), 1287 (s), 1260 (m), 1233 (w), 1207 (w), 1157 (w), 1125 (s), 1099 (s), 1065 (w), 990 (w), 955 (w), 899 (w), 887 (w), 824 (w), 799 (s), 729 (m), 718 (w), 687 (w), 631 (w). Anal calcd for C₄₈H₆₆N₂OS₂ [751.2]: C 76.75, H 8.86, N 3.73, S 8.54; Found: C 76.53, H 8.79, N 3.69, S 8.69.

2.1.4.2. 5-[{[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9H-carbazol-3-yl]methylene}-2-thioxothiazolidin-4-one (11b)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **11b** (337 mg, 86%) was obtained as a yellow orange amorphous solid, Mp 110–115 °C. R_f (*n*-hexane/acetone 5:1) = 0.51.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.90 (t, ³J = 6.7 Hz, 3 H), 0.94 (t, ³J = 6.7 Hz, 3 H), 1.21–1.47 (m, 40 H), 2.19 (hep, ³J = 6.9 Hz, 1 H), 2.42 (s, 3 H), 4.32 (d, ³J = 7.5 Hz, 2 H), 7.25–7.31 (m, 2 H), 7.55–7.69 (m, 5 H), 7.77 (dd, ³J = 8.6 Hz, ⁴J = 1.8 Hz, 1 H), 7.79 (s, 1 H), 8.39 (d, ⁴J = 1.6 Hz, 1 H), 8.46 (d, ⁴J = 1.7 Hz, 1 H), 12.08 (s, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃)¹² 21.4 (CH₃), 23.6 (CH₂)¹⁵ 27.5 (CH₂),¹⁵ 30.31 (CH₂), 30.33 (CH₂), 30.5 (CH₂),¹⁵ 30.59 (CH₂),¹⁶ 30.61 (CH₂),¹⁵ 30.64 (CH₂), 30.87 (CH₂), 30.88 (CH₂), 32.7 (CH₂),¹⁵

¹² Two CH₃ signals coincide.

¹³ Two CH₂ signals coincide.

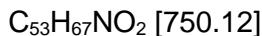
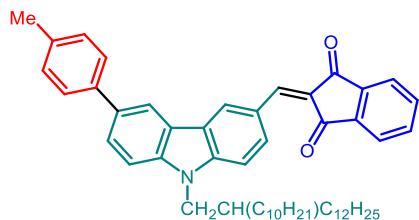
¹⁴ Two CH₃ signals coincide.

¹⁵ Two CH₂ signals coincide.

¹⁶ Three CH₂ signals coincide.

32.9 (CH₂)¹⁵ 38.8 (CH), 48.6 (CH₂), 111.0 (CH), 111.2 (CH), 119.7 (CH), 122.4 (C_{quat}), 124.0 (C_{quat}), 124.7 (C_{quat}), 124.8 (CH), 125.2 (C_{quat}), 126.7 (CH), 127.8 (CH), 129.5 (CH), 130.3 (CH), 134.2 (C_{quat}), 134.4 (CH), 136.8 (C_{quat}), 139.4 (C_{quat}), 141.6 (C_{quat}), 143.2 (C_{quat}), 169.3 (C_{quat}), 195.2 (C_{quat}). MS (MALDI-TOF) calcd for C₄₇H₆₄N₂OS₂ *m/z*: 736.45; Found: 736.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3686 (w), 3669 (w), 3138 (w), 2988 (w), 2957 (m), 2918 (s), 2851 (m), 1694 (s), 1576 (s), 1559 (m), 1485 (m), 1451 (m), 1445 (m), 1393 (w), 1344 (w), 1310 (w), 1285 (w), 1258 (w), 1238 (m), 1209 (s), 1171 (m), 1159 (m), 1140 (m), 1098 (w), 1067 (m), 1020 (w), 899 (w), 862 (w), 824 (w), 795 (m), 721 (w), 677 (m), 646 (w). Anal calcd for C₄₇H₆₄N₂OS₂ [737.2]: C 76.58, H 8.75, N 3.80, S 8.70; Found: C 76.43, H 8.61, N 3.70, S 8.63.

2.1.4.3. 2-{{[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (11c)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **11c** (220 mg, 57%) was obtained as an orange red amorphous solid, Mp 65–67 °C. R_f (*n*-hexane/acetone 10:1) = 0.31.

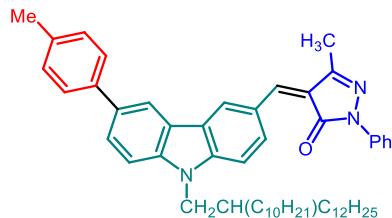
¹H NMR (600 MHz, acetone-d₆/CS₂ 4:1): δ 0.87 (t, ³J = 7.0 Hz, 3 H), 0.88 (t, ³J = 7.0 Hz, 3 H), 1.18–1.49 (m, 40 H), 2.21 (hep, ³J = 6.6 Hz, 1 H), 2.42 (s, 3 H), 4.32 (d, ³J = 7.6 Hz, 2 H), 7.31 (d, ³J = 7.8 Hz, 2 H), 7.60 (t, ³J = 9.1 Hz, 2 H), 7.65–7.69 (m, 2 H), 7.77 (dd, ³J = 8.4 Hz, ⁴J = 1.8 Hz, 1 H), 7.86–7.94 (m, 3 H), 7.86–7.94 (m, 2 H), 8.46 (d, ⁴J = 1.7 Hz, 1 H), 8.80 (dd, ³J = 8.7 Hz, ⁴J = 1.7 Hz, 1 H), 9.53 (d, ⁴J = 1.8 Hz, 1 H). ¹³C NMR (150 MHz, acetone-d₆/CS₂ 4:1): δ 14.6 (CH₃)¹⁷ 21.4 (CH₃), 23.6 (CH₂)¹⁸ 27.4 (CH₂), 27.5 (CH₂), 30.27 (CH₂), 30.29 (CH₂), 30.40 (CH₂), 30.41 (CH₂), 30.51 (CH₂), 30.53 (CH₂)¹⁸ 30.58 (CH₂)¹⁸ 30.60 (CH₂), 30.81 (CH₂), 30.84 (CH₂), 32.65 (CH₂), 32.67 (CH₂), 32.8 (CH₂)¹⁸ 38.7 (CH), 48.6 (CH₂), 110.6 (CH), 111.2 (CH), 119.6 (CH), 123.4 (CH), 123.6 (CH), 124.4 (C_{quat}), 124.6 (C_{quat}), 126.0 (C_{quat}), 126.5 (C_{quat}), 126.6 (CH), 127.8 (CH), 129.6 (CH), 130.4 (CH), 133.9 (CH), 134.7 (C_{quat}), 135.6 (CH), 135.8 (CH), 137.0 (C_{quat}), 139.4 (C_{quat}), 140.7 (C_{quat}), 141.7 (C_{quat}), 143.3 (C_{quat}), 145.2 (C_{quat}), 148.5 (CH), 189.7 (C_{quat}), 190.5 (C_{quat}). MS (MALDI-TOF) calcd for C₅₃H₆₇NO₂-H⁺ *m/z*: 750.52; Found: 750.5. IR: $\tilde{\nu}$ [cm⁻¹] = 2953 (w), 2920 (m), 2851 (m), 1719 (w), 1678 (s), 1595 (w), 1566 (m), 1551 (s), 1487 (m), 1462 (m), 1435 (w), 1383 (m), 1333 (m), 1302 (m), 1256 (w), 1209

¹⁷ Two CH₃ signals coincide.

¹⁸ Two CH₂ signals coincide.

(m), 1180 (m), 1152 (m), 1092 (w), 1067 (w), 1016 (w), 993 (m), 963 (w), 926 (w), 887 (w), 824 (w), 806 (m), 793 (m), 785 (w), 760 (w), 729 (s), 677 (w), 650 (w), 602 (w). Anal calcd for C₅₃H₆₇NO₂ [782.2]: C 84.86, H 9.00, N 1.87; Found: C 85.03, H 8.88, N 1.84.

2.1.4.4. 4-{[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]methylen}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (11d)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 40:1) and drying under vacuo compound **11d** (329 mg, 81%) was obtained as an orange red amorphous solid, Mp 95–99 °C. R_f (*n*-hexane/acetone 10:1) = 0.41.

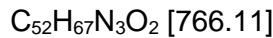
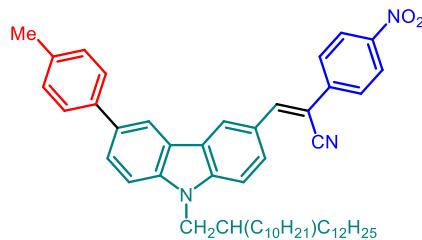
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.89 (t, ³J = 6.6 Hz, 3 H), 0.90 (t, ³J = 6.6 Hz, 3 H), 1.20–1.50 (m, 40 H), 2.14–2.27 (m, 1 H), 2.37 (s, 3 H), 2.43 (s, 3 H), 4.30 (d, ³J = 7.5 Hz, 2 H), 7.15 (tt, ³J = 7.4 Hz, ⁴J = 1.2 Hz, 1 H), 7.30 (d, ³J = 8.0, 2 H), 7.37–7.45 (m, 2 H), 7.55 (d, ³J = 8.7 Hz, 1 H), 7.56 (d, ³J = 8.7 Hz, 1 H), 7.62–7.67 (m, 2 H), 7.73–7.78 (m, 2 H), 8.09–8.17 (m, 2 H), 8.39 (d, ⁴J = 1.7 Hz, 1 H), 8.87 (dd, ³J = 8.8 Hz, ⁴J = 1.7 Hz, 1 H), 9.63 (d, ⁴J = 1.7 Hz, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.7 (CH₃), 14.7 (CH₃),¹⁹ 21.4 (CH₃), 23.6 (CH₂),²⁰ 27.48 (CH₂),²⁰ 30.30 (CH₂), 30.01 (CH₂), 30.5 (CH₂),²⁰ 30.6 (CH₂),²¹ 30.61 (CH₂),²⁰ 30.63 (CH₂), 30.87 (CH₂), 30.88 (CH₂), 32.68 (CH₂),²⁰ 32.84 (CH₂),²⁰ 38.8 (CH), 48.6 (CH₂), 110.3 (CH), 111.1 (CH), 119.1 (CH), 119.5 (CH), 124.2 (C_{quat}), 124.4 (C_{quat}), 124.6 (C_{quat}), 124.7 (CH), 126.1 (C_{quat}), 126.6 (CH), 127.8 (CH), 129.2 (CH), 129.3 (CH), 130.4 (CH), 133.8 (CH), 134.6 (C_{quat}), 136.9 (C_{quat}), 139.4 (C_{quat}), 140.1 (C_{quat}), 141.6 (C_{quat}), 144.9 (C_{quat}), 149.0 (CH), 151.7 (C_{quat}), 163.0 (C_{quat}). MS (MALDI-TOF) calcd for C₅₄H₇₁N₃O-H⁺ m/z: 777.56; Found: 778.6. IR: $\tilde{\nu}$ [cm⁻¹] = 2951 (w), 2920 (m), 2851 (m), 1678 (m), 1582 (s), 1557 (m), 1499 (m), 1479 (s), 1464 (m), 1456 (m), 1389 (w), 1358 (w), 1314 (m), 1309 (m), 1261 (w), 1229 (m), 1134 (s), 997 (m), 926 (w), 870 (w), 808 (m), 795 (s), 764 (m), 747 (m), 721 (w), 689 (m), 669 (s). Anal calcd for C₅₄H₇₁N₃O [778.2]: C 83.35, H 9.20, N 5.40; Found: C 83.12, H 9.09, N 5.17.

¹⁹ Two CH₃ signals coincide.

²⁰ Two CH₂ signals coincide.

²¹ Three CH₂ signals coincide.

2.1.4.5. 3-[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]-2-(4-nitrophenyl)acrylonitrile (11e)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under *vacuo* compound **11e** (287 mg, 69%) was obtained as an orange amorphous solid, Mp 87–96 °C. R_f (*n*-hexane/acetone 10:1) = 0.26.

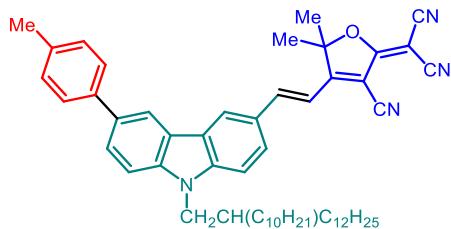
¹H NMR (600 MHz, acetone-d₆/CS₂ 4:1): δ 0.89 (t, ³J = 7.0 Hz, 3 H), 0.90 (t, ³J = 7.0 Hz, 3 H), 1.22–1.49 (m, 40 H), 2.21 (hep, ³J = 6.9 Hz, 1 H), 2.42 (s, 3 H), 4.33 (d, ³J = 7.5 Hz, 2 H), 7.28 (d, ³J = 7.8 Hz, 2 H), 7.59 (d, ³J = 8.5 Hz, 1 H), 7.60–7.64 (m, 3 H), 7.76 (dd, ³J = 8.5 Hz, ⁴J = 1.8 Hz, 1 H), 8.00–8.04 (m, 2 H), 8.21 (s, 1 H), 8.29 (dd, ³J = 8.7 Hz, ⁴J = 1.9 Hz, 1 H), 8.30–8.33 (m, 2 H), 8.34 (d, ⁴J = 1.8 Hz, 1 H), 8.84 (d, ⁴J = 1.8 Hz, 1 H). ¹³C NMR (150 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (2 CH₃),²² 21.4 (CH₃), 23.6 (2 CH₂),²³ 27.50 (CH₂), 27.51 (CH₂), 30.31 (CH₂), 30.33 (CH₂), 30.5 (2 CH₂),²³ 30.58 (3 CH₂),²⁴ 30.61 (CH₂), 30.62 (CH₂), 30.7 (CH₂), 30.91 (CH₂), 39.92 (CH₂), 32.7 (2 CH₂),²³ 32.9 (2 CH₂),²³ 38.8 (CH), 48.6 (CH₂), 105.3 (C_{quat}), 110.8 (CH), 111.0 (CH), 118.8 (C_{quat}), 119.4 (CH), 124.1 (C_{quat}), 124.2 (C_{quat}), 124.7 (CH), 125.0 (CH), 125.4 (C_{quat}), 126.7 (CH), 127.1 (CH), 127.8 (CH), 128.3 (CH), 130.4 (CH), 134.3 (C_{quat}), 136.9 (C_{quat}), 139.4 (C_{quat}), 141.6 (C_{quat}), 142.4 (C_{quat}), 143.8 (C_{quat}), 147.3 (CH), 148.0 (C_{quat}). MS (MALDI-TOF) calcd for C₅₂H₆₇N₃O₂ m/z: 765.52; Found: 765.5. IR: $\tilde{\nu}$ [cm⁻¹] = 2980 (w), 2953 (w), 2920 (m), 2851 (w), 2210 (w), 1680 (w), 1632 (w), 1599 (w), 1576 (m), 1560 (m), 1514 (m), 1493 (m), 1478 (m), 1458 (w), 1437 (w), 1393 (m), 1377 (w), 1337 (s), 1263 (w), 1227 (m), 1196 (w), 1163 (m), 1148 (m), 1109 (m), 1067 (w), 997 (w), 932 (w), 891 (w), 845 (m), 822 (w), 810 (m), 795 (s), 750 (m), 720 (w), 689 (m), 635 (w), 617 (w). Anal calcd for C₅₂H₆₇N₃O₂ [766.1]: C 81.52, H 8.81, N 5.48; Found: C 81.46, H 8.66, N 5.43.

²² Two CH₃ signals coincide.

²³ Two CH₂ signals coincide.

²⁴ Three CH₂ signals coincide.

2.1.4.6. (*E*)-2-{3-Cyano-4-[2-(9-{2-decyltetradecyl}-6-{*p*-tolyl}-9*H*-carbazol-3-yl)vinyl]-5,5-dimethylfuran-2[5*H*]-yliden}malonitrile (11f)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **11f** (355 mg, 82%) was obtained as a dark red amorphous solid, Mp 156–161 °C. R_f (*n*-hexane/acetone 10:1) = 0.23.

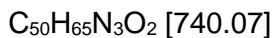
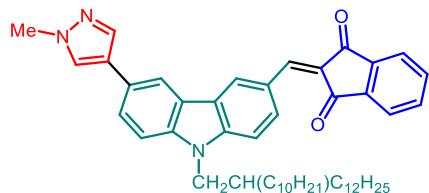
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.82–0.93 (m, 6 H), 1.16–1.49 (m, 40 H), 1.93 (s, 6 H), 2.14–2.26 (m, 1 H), 2.40 (s, 3 H), 4.34 (d, ³J = 7.5 Hz, 2 H), 7.27–7.36 (m, 3 H), 7.61–7.68 (m, 4 H), 7.80 (dd, ³J = 8.6 Hz, ⁴J = 1.8 Hz, 1 H), 8.01 (dd, ³J = 8.8 Hz, ⁴J = 1.7 Hz, 1 H), 8.23 (d, ³J = 16.3 Hz, 1 H), 8.45 (d, ⁴J = 1.7 Hz, 1 H), 8.84 (d, ⁴J = 1.7 Hz, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.5 (CH₃)²⁵ 21.2 (CH₃), 23.4 (CH₂)²⁶ 26.3 (CH₃), 27.3 (CH₂)²⁶ 30.15 (CH₂), 30.18 (CH₂), 30.3 (CH₂)²⁶ 30.39 (CH₂)²⁶ 30.4 (CH₂), 30.46 (CH₂)²⁶ 30.49 (CH₂), 30.7 (CH₂)²⁶ 32.6 (CH₂)²⁶ 32.71 (CH₂), 32.73 (CH₂), 38.6 (CH), 48.6 (CH₂), 97.8 (C_{quat}), 99.1 (C_{quat})²⁷ 111.36 (CH), 111.38 (CH), 111.8 (C_{quat}), 112.5 (C_{quat}), 112.8 (CH), 113.2 (C_{quat}), 119.6 (CH), 124.3 (C_{quat}), 124.4 (CH), 124.8 (C_{quat}), 126.7 (CH), 126.8 (C_{quat}), 127.7 (CH), 128.4 (CH), 130.4 (CH), 134.4 (C_{quat}), 137.1 (C_{quat}), 139.3 (C_{quat}), 141.7 (C_{quat}), 144.9 (C_{quat}), 150.4 (CH), 176.1 (C_{quat}), 177.5 (C_{quat}). MS (MALDI-TOF) calcd for C₅₅H₇₀N₄O *m/z*: 802.56; Found: 802.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2922 (m), 2851 (w), 2228 (w), 1565 (m), 1559 (s), 1557 (s), 1528 (s), 1476 (m), 1462 (m), 1433 (w), 1381 (m), 1343 (w), 1283 (s), 1262 (w), 1227 (m), 1209 (w), 1192 (w), 1155 (w), 1138 (m), 1107 (m), 1063 (w), 1024 (w), 1011 (w), 974 (w), 939 (w), 899 (w), 885 (w), 858 (w), 835 (w), 799 (s), 737 (w), 719 (w), 706 (w), 660 (w), 610 (w). Anal calcd for C₅₅H₇₀N₄O [803.2]: C 82.25, H 8.78, N 6.98; Found: C 82.09, H 8.52, N 6.85.

²⁵ Two CH₃ signals coincide.

²⁶ Two CH₂ signals coincide.

²⁷ Two C_{quat} signals coincide.

2.1.4.7. 2-{{[9-(2-Decyltetradecyl)-6-(1-methyl-1H-pyrazol-4-yl)-9H-carbazol-3-yl]methylene}-1H-inden-1,3[2H]-dione (11g)}



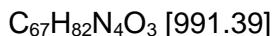
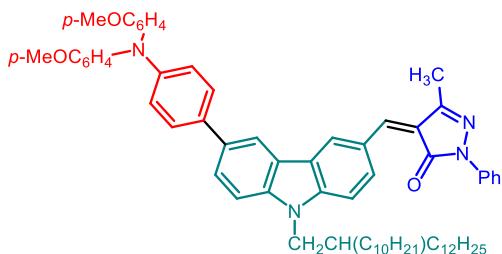
According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1) and drying under vacuo compound **11g** (216 mg, 59%) was obtained as a red amorphous solid, Mp 121–125 °C. R_f (*n*-hexane/acetone 10:1) = 0.05.

¹H NMR (600 MHz, acetone-d₆/CS₂ 4:1): δ 0.88 (t, ³J = 7.0 Hz, 3 H), 0.89 (t, ³J = 7.0 Hz, 3 H), 1.16–1.49 (m, 40 H), 2.18 (hep, ³J = 6.8 Hz, 1 H), 3.96 (s, 3 H), 4.28 (d, ³J = 7.6 Hz, 2 H), 7.49 (d, ³J = 8.3 Hz, 1 H), 7.56 (d, ³J = 8.8 Hz, 1 H), 7.67 (d, ³J = 8.4 Hz, 1 H), 7.82 (s, 1 H), 7.85–8.01 (m, 6 H), 8.35 (s, 1 H), 8.77 (d, ³J = 8.6 Hz, 1 H), 9.44 (s, 1 H). ¹³C NMR (150 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃)²⁸ 23.6 (CH₂)²⁹ 27.5 (CH₂)²⁹ 30.29 (CH₂), 30.30 (CH₂), 30.4 (CH₂)²⁹ 30.55 (CH₂)²⁹ 30.59 (CH₂)²⁹ 30.62 (CH₂), 30.85 (CH₂), 30.86 (CH₂), 32.7 (CH₂)²⁹ 32.8 (CH₂)²⁹ 38.7 (CH), 39.2 (CH₃), 48.6 (CH₂), 110.4 (CH), 111.2 (CH), 118.0 (CH), 123.3 (CH), 123.5 (CH), 124.2 (C_{quat}), 124.3 (C_{quat}), 124.5 (C_{quat}), 125.4 (CH), 125.8 (C_{quat}), 126.3 (C_{quat}), 126.9 (C_{quat}), 127.5 (CH), 129.6 (CH), 133.9 (CH), 135.6 (CH), 135.7 (CH), 136.8 (CH), 140.7 (C_{quat}), 141.0 (C_{quat}), 143.2 (C_{quat}), 145.0 (C_{quat}), 148.5 (CH), 189.6 (C_{quat}), 190.4 (C_{quat}). MS (MALDI-TOF) calcd for C₅₀H₆₅N₃O₂·H⁺ m/z: 740.5; Found: 740.5. ESI-HRMS calcd for C₅₀H₆₅N₃O₂·H⁺: 740.51495; Found: 740.51514 ([MH]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3065 (w), 2951 (w), 2918 (m), 2851 (w), 1717 (w), 1678 (s), 1622 (w), 1595 (w), 1566 (m), 1549 (s), 1491 (m), 1468 (w), 1435 (w), 1383 (m), 1343 (m), 1325 (m), 1294 (w), 1210 (w), 1190 (m), 1175 (w), 1150 (m), 1142 (m), 1092 (w), 1072 (w), 1049 (w), 1018 (w), 993 (m), 970 (w), 963 (w), 924 (w), 845 (w), 808 (m), 791 (m), 760 (w), 733 (s), 721 (m), 708 (w), 685 (w), 648 (w), 665 (w). UV/VIS (CH₂Cl₂) λ_{max} (ε 10³ [M⁻¹cm⁻¹]) [nm] = 281 (34), 303 (21), 352 (19), 467 (43).

²⁸ Two CH₃ signals coincide.

²⁹ Two CH₂ signals coincide.

2.1.4.8. 4-{{6-(4-{Bis[4-methoxyphenyl]amino}phenyl)-9-(2-decytetradecyl)-9*H*-carbazol-3-yl)methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (11h)



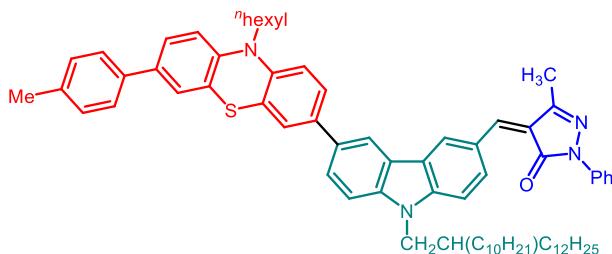
According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 25:1) and drying under vacuo compound **11h** (289 mg, 57%) was obtained as a dark red amorphous solid, Mp softening >40 °C, melting >65 °C. R_f (*n*-hexane/acetone 10:1) = 0.22.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.83 (t, ³J = 6.8 Hz, 3 H), 0.84 (t, ³J = 6.8 Hz, 3 H), 1.09–1.36 (m, 40 H), 2.07–2.12 (m, 1 H), 2.28 (s, 3 H), 3.79 (s, 6 H), 4.13 (d, ³J = 6.2 Hz, 2 H), 6.87–7.00 (m, 6 H), 7.03–7.10 (m, 4 H), 7.15 (t, ³J = 7.5 Hz, 1 H), 7.36–7.51 (m, 4 H), 7.52–7.59 (m, 2 H), 7.22–7.63 (m, 2 H), 8.09–8.16 (m, 2 H), 8.28–8.35 (m, 1 H), 8.82 (d, ³J = 8.7 Hz, 1 H), 9.48 (s, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.5 (CH₃), 14.4 (CH₃),³⁰ 23.4 (CH₂),³¹ 27.16 (CH₂), 27.18 (CH₂), 30.12 (CH₂),³¹ 30.14 (CH₂), 30.2 (CH₂), 30.3 (CH₂), 30.35 (CH₂), 30.37 (CH₂), 30.41 (CH₂),³¹ 30.44 (CH₂), 30.5 (CH₂), 30.6 (CH₂), 32.49 (CH₂), 32.51 (CH₂), 32.7 (CH₂),³¹ 38.5 (CH), 48.5 (CH₂), 55.7 (CH₃), 110.3 (CH), 111.2 (CH), 115.6 (CH), 118.8 (CH), 119.1 (CH), 121.5 (CH), 124.1 (C_{quat}), 124.2 (C_{quat}), 124.5 (C_{quat}), 124.8 (CH), 126.0 (C_{quat}), 126.1 (CH), 127.5 (CH), 128.3 (CH), 129.2 (CH), 129.4 (CH), 133.6 (CH), 134.2 (C_{quat}), 134.3 (C_{quat}), 140.3 (C_{quat}), 141.4 (C_{quat}), 141.7 (C_{quat}), 144.9 (C_{quat}), 148.7 (C_{quat}), 149.4 (CH), 152.1 (C_{quat}), 157.1 (C_{quat}), 163.3 (C_{quat}). MS (MALDI-TOF) calcd for C₆₇H₈₂N₄O₃ m/z: 990.64; Found: 990.7 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2922 (m), 2851 (w), 1678 (w), 1582 (m), 1551 (m), 1505 (s), 1478 (m), 1462 (m), 1441 (w), 1418 (w), 1387 (w), 1379 (w), 1360 (w), 1317 (m), 1277 (w), 1238 (s), 1179 (w), 1159 (w), 1132 (m), 1105 (w), 1065 (w), 1036 (m), 995 (m), 934 (w), 903 (w), 872 (w), 828 (m), 802 (m), 768 (w), 752 (m), 725 (w), 706 (w), 691 (m), 669 (m), 646 (w), 631 (w). Anal calcd for C₆₇H₈₂N₄O₃ [991.4]: C 81.17, H 8.34, N 5.65; Found: C 81.08, H 8.23, N 5.57.

³⁰ Two CH₃ signals coincide.

³¹ Two CH₂ signals coincide.

2.1.4.9. 4-{{[9-(2-Decyltetradecyl)-6-(10-hexyl-7-{*p*-tolyl}-10*H*-phenothiazin-3-yl)-9*H*-carbazol-3-yl)methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (11i)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **11i** (334 mg, 61%) was obtained as a red amorphous solid, Mp softening >47 °C, melting >60 °C. R_f (*n*-hexane/acetone 10:1) = 0.38.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86–0.96 (m, 9 H), 1.18–1.59 (m, 46 H), 1.89 (quin, ³J = 6.6 Hz, 2 H), 2.12–2.23 (m, 1 H), 2.37 (s, 6 H), 3.98 (t, ³J = 7.1 Hz, 2 H), 4.27 (d, ³J = 7.4 Hz, 2 H), 7.01 (d, ³J = 8.4 Hz, 1 H), 7.05 (d, ³J = 8.4 Hz, 1 H), 7.11–7.18 (m, 1 H), 7.22 (d, ³J = 8.0 Hz, 2 H), 7.36–7.57 (m, 10 H), 7.72 (dd, ³J = 8.4 Hz, ⁴J = 1.9 Hz, 1 H), 7.73 (s, 1 H), 8.09–8.17 (m, 2 H), 8.36 (d, ⁴J = 1.7 Hz, 1 H), 8.88 (dd, ³J = 8.8 Hz, ⁴J = 1.7 Hz, 1 H), 9.59 (d, ⁴J = 1.6 Hz, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.7 (CH₃), 14.68 (CH₃), 14.73 (CH₃),³² 21.4 (CH₃), 23.6 (CH₂),³³ 23.7 (CH₂), 27.49 (CH₂),³³ 27.52 (CH₂), 27.7 (CH₂), 30.3 (CH₂),³³ 30.5 (CH₂),³³ 30.57 (CH₂),³⁴ 30.61 (CH₂),³³ 30.64 (CH₂), 30.9 (CH₂),³³ 32.5 (CH₂), 32.7 (CH₂),³³ 32.9 (CH₂),³³ 38.8 (CH), 48.1 (CH₂), 48.6 (CH₂), 110.3 (CH), 111.1 (CH), 116.5 (CH), 116.6 (CH), 119.1 (CH),³⁵ 124.2 (C_{quat}), 124.5 (C_{quat}), 124.6 (C_{quat}), 124.7 (CH), 125.55 (C_{quat}), 125.62 (C_{quat}), 126.0 (CH), 126.1 (C_{quat}), 126.2 (CH), 126.3 (CH), 126.4 (CH), 126.8 (CH), 127.0 (CH), 129.3 (CH),³⁵ 130.3 (CH), 133.4 (C_{quat}), 133.8 (CH), 136.0 (C_{quat}), 136.6 (C_{quat}), 137.2 (C_{quat}), 137.7 (C_{quat}), 140.1 (C_{quat}), 141.6 (C_{quat}), 144.5 (C_{quat}), 144.8 (C_{quat}), 144.9 (C_{quat}), 149.0 (CH), 151.7 (C_{quat}), 163.0 (C_{quat}). MS (MALDI-TOF) calcd for C₇₂H₉₀N₄OS m/z: 1058.68; Found: 1058.7 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2951 (w), 2920 (m), 2851 (w), 1676 (w), 1578 (m), 1551 (m), 1495 (w), 1461 (m), 1458 (m), 1389 (w), 1377 (w), 1356 (w), 1317 (m), 1298 (w), 1275 (w), 1256 (m), 1229 (m), 1215 (w), 1190 (w), 1130 (s), 1067 (w), 1018 (w), 995 (m), 932 (w), 901 (w), 874 (w), 802 (s), 785 (w), 768 (m), 752 (m), 720 (w), 704 (w), 691 (m), 669 (w), 646 (w), 615 (w). Anal calcd for C₇₂H₉₀N₄OS [1060]: C 81.61, H 8.56, N 5.29; Found: C 81.55, H 8.53, N 5.21.

³² Two CH₃ signals coincide.

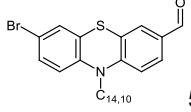
³³ Two CH₂ signals coincide.

³⁴ Three CH₃ signals coincide.

³⁵ Two CH signals coincide.

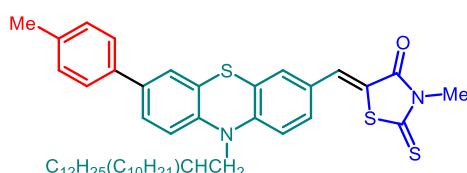
2.1.5. Consecutive Three-component Suzuki-Knoevenagel Synthesis of Phenothiazine-bridged Systems 12

Table S5. Experimental details of the consecutive three-component Suzuki-Knoevenagel synthesis of phenothiazine-bridged systems **12**.

Entry	Bromo-aldehyde 5 [mg] (mmol)	Boronic acid/ester 6 [mg] (mmol)	CsF [mg] (mmol)	Pd(PPh_3) ₄ [mg] (μmol)	t_1 [h]	methylene active compound 7 [mg] (mmol)	Organocatalyst [mg] (mmol)	t_2 [h]	Product [mg] (%)
	 5								
59	340 (0.530) of 5	87 (0.636) of 6b	258 (1.70)	18 (16)	14	94 (0.636) of 7a	41 (0.53) of NH_4OAc	6	365 (88) of 12a
56	324 (0.504) of 5	82 (0.605) of 6b	245 (1.61)	18 (15)	16	81 (0.605) of 7b	39 (0.50) of NH_4OAc	6	335 (87) of 12b
74	327 (0.509) of 5	83 (0.611) of 6b	248 (1.63)	18 (16)	16	89 (0.61) of 7c	1 drop of Et_2NH	4	314 (79) of 12c
75	324 (0.504) of 5	82 (0.605) of 6b	245 (1.61)	18 (16)	16	188 (1.06) of 7c	47 (0.605) of NH_4OAc	8	134 (32) of 12d
82	335 (0.521) of 5	85 (0.625) of 6b	253 (1.68)	18 (16)	14	109 (0.625) of 7e	1 drop of Et_2NH	4	325 (77) of 12e
77	452 (0.703) of 5	115 (0.843) of 6b	342 (2.25)	24 (21)	14	137 (0.843) of 7f	54 (0.70) of NH_4OAc	8	490 (87) of 12f
88	340 (0.529) of 5	86 (0.635) of 6b	257 (1.69)	18 (16)	14	127 (0.635) of 7g	41 (0.53) of NH_4OAc	6	358 (81) of 12g
60	321 (0.499) of 5	137 (0.599) of 6c	241 (1.60)	17 (15)	16	88 (0.599) of 7a	39 (0.50) of NH_4OAc	6	375 (95) of 12h
76	310 (0.482) of 5	133 (0.578) of 6c	236 (1.54)	17 (15)	16	85 (0.578) of 7c	1 drop of Et_2NH	4	309 (81) of 12i
64	330 (0.513) of 5	76 (0.616) of 6m	250 (1.65)	18 (16)	16	91 (0.616) of 7a	40 (0.51) of NH_4OAc	6	308 (78) of 12j
65	345 (0.537) of 5	134 (0.644) of 6l	261 (1.72)	19 (17)	16	95 (0.644) of 7a	41 (0.53) of NH_4OAc	6	333 (80) of 12k
78	331 (0.515) of 5	129 (0.618) of 6l	250 (1.65)	18 (16)	16	100 (0.618) of 7f	40 (0.51) of NH_4OAc	8	288 (71) of 12l
83	331 (0.515) of 5	129 (0.618) of 6l	250 (1.65)	17 (15)	16	108 (0.618) of 7e	1 drop of Et_2NH	4	288 (69) of 12m
61	310 (0.482) of 5	130 (0.578) of 6i	234 (1.54)	17 (15)	14	85 (0.578) of 7a	37 (0.48) of NH_4OAc	6	322 (85) of 12n
62	371 (0.577) of 5	247 (0.692) of 6k	281 (1.85)	20 (17)	16	102 (0.692) of 7a	45 (0.58) of NH_4OAc	6	355 (67) of 12o
63	363 (0.565) of 5	255 (0.678) of 6j	275 (1.81)	20 (17)	16	100 (0.678) of 7a	44 (0.57) of NH_4OAc	6	391 (74) of 12p

66	315 (0.490) of 5	218 (0.588) of 6d	238 (1.57)	17 (15)	16	7a 87 (0.59)	38 (0.49) of NH ₄ OAc	6	383 (84) of 12q
79	326 (0.507) of 5	226 (0.608) of 6d	247 (1.62)	18 (16)	16	99 (0.608) of 7f	39 (0.50) of NH ₄ OAc	8	394 (82) of 12r
67	322 (0.501) of 5	259 (0.601) of 6e	244 (1.60)	17 (15)	16	89 (0.60) of 7a	39 (0.50) of NH ₄ OAc	6	417 (83) of 12s
57	332 (0.516) of 5	267 (0.619) of 6e	251 (1.65)	18 (16)	16	83 (0.62) of 7b	40 (0.51) of NH ₄ OAc	6	400 (79) of 12t
80	323 (0.502) of 5	260 (0.602) of 6e	245 (1.61)	17 (15)	16	98 (0.602) of 7f	39 (0.50) of NH ₄ OAc	8	411 (81) of 12u
84	330 (0.513) of 5	266 (0.616) of 6e	249 (1.64)	18 (16)	16	107 (0.616) of 7e	1 drop of Et ₂ NH	4	376 (72) of 12v
68	338 (0.526) of 5	315 (0.631) of 6p	256 (1.68)	18 (16)	16	93 (0.63) of 7a	41 (0.53) of NH ₄ OAc	6	446 (80) of 12w
58	356 (0.554) of 5	332 (0.665) of 6p	269 (1.77)	19 (17)	16	89 (0.665) of 7b	43 (0.55) of NH ₄ OAc	6	520 (89) of 12x
81	330 (0.513) of 5	308 (0.616) of 6p	250 (1.65)	18 (16)	16	100 (0.616) of 7f	40 (0.51) of NH ₄ OAc	8	436 (79) of 12y
85	320 (0.498) of 5	299 (0.598) of Cs ₂ CO ₃	500 (1.59) of Cs ₂ CO ₃	17 (15)	16	104 (0.598) of 7e	1 drop of Et ₂ NH	4	371 (68) of 12z

2.1.5.1. (*Z*)-5-{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (**12a**)



C₄₈H₆₆N₂OS₃ [783.25]

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 40:1) and drying under vacuo compound **12a** (365 mg, 88%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.63.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.91 (t, ³J = 6.5 Hz, 3 H), 0.92 (t, ³J = 6.5 Hz, 3 H), 1.21–1.52 (m, 40 H), 1.99–2.04 (m, 1 H), 2.38 (s, 3 H), 3.47 (s, 3 H), 3.92 (d, ³J = 7.1 Hz, 2 H), 7.06 (d, ³J = 8.5 Hz, 1 H), 7.10 (d, ³J = 8.6 Hz, 1 H), 7.19–7.25 (m, 2 H), 7.33 (d, ⁴J = 2.1 Hz, 1 H), 7.37 (d, ⁴J = 2.1 Hz, 1 H), 7.40–7.48 (m, 4 H), 7.61 (s, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.8 (2 CH₃),³⁶ 21.5 (CH₃), 23.7 (2 CH₂),³⁷ 27.12 (CH₂), 27.14 (CH₂), 30.4 (2 CH₂),³⁷ 30.5 (2 CH₂),³⁷ 30.6 (3 CH₂),³⁸ 30.65 (CH₂), 30.68 (CH₂), 30.70 (CH₂), 30.99 (2 CH₂),³⁷ 31.5 (CH₃), 32.3 (2 CH₂),³⁷ 32.9 (2 CH₂),³⁷ 35.7 (CH), 52.3 (CH₂), 117.2 (CH), 117.7 (CH),

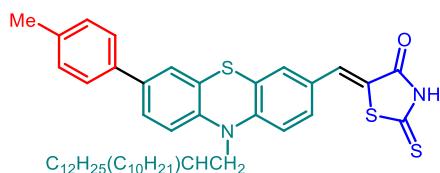
³⁶ Two CH₃ signals coincide.

³⁷ Two CH₂ signals coincide.

³⁸ Three CH₂ signals coincide.

121.1 (C_{quat}), 125.8 (C_{quat}), 126.3 (CH), 126.7 (CH), 126.9 (C_{quat}), 127.0 (CH), 128.5 (C_{quat}), 130.2 (CH), 130.3 (CH), 131.5 (CH), 132.6 (CH), 137.2 (C_{quat}), 137.4 (C_{quat}), 137.5 (C_{quat}), 143.8 (C_{quat}), 148.7 (C_{quat}), 167.6 (C_{quat}), 193.3 (C_{quat}). MS (MALDI-TOF) calcd for C₄₈H₆₆N₂OS₃ *m/z*: 782.43; Found: 782.4 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3023 (w), 2920 (m), 2851 (m), 1709 (m), 1595 (w), 1574 (m), 1543 (w), 1495 (w), 1460 (s), 1424 (m), 1402 (m), 1348 (m), 1285 (s), 1250 (m), 1221 (m), 1167 (w), 1126 (s), 1099 (s), 1057 (w), 1017 (w), 990 (w), 959 (w), 901 (w), 885 (w), 804 (s), 781 (w), 762 (w), 725 (w), 721 (w), 692 (w), 673 (w), 652 (w), 613 (w). Anal calcd for C₄₈H₆₆N₂OS₃ [783.3]: C 73.61, H 8.49, N 3.58, S 12.28; Found: C 73.65, H 8.41, N 3.51, S 12.34.

2.1.5.2. (*Z*)-5-{{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-2-thioxothiazolidin-4-one (12b)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 15:1) and drying under vacuo compound **12b** (337 mg, 87%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.18.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.905 (t, ³J = 6.8 Hz, 3 H), 0.914 (t, ³J = 6.8 Hz, 3 H), 1.20–1.55 (m, 40 H), 2.05–2.09 (m, 1 H), 2.38 (s, 3 H), 3.93 (d, ³J = 7.1 Hz, 2 H), 7.07 (d, ³J = 8.6 Hz, 1 H), 7.12 (d, ³J = 8.7 Hz, 1 H), 7.22 (d, ³J = 7.9 Hz, 2 H), 7.32 (d, ⁴J = 2.1 Hz, 1 H), 7.38 (d, ⁴J = 2.0 Hz, 1 H), 7.38–7.49 (m, 5 H), 12.03 (br, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.8 (CH₃)³⁹ 21.4 (CH₃), 23.7 (CH₂),⁴⁰ 27.13 (CH₂),⁴⁰ 30.4 (CH₂),⁴⁰ 30.5 (CH₂),⁴⁰ 30.6 (CH₂),⁴¹ 30.70 (CH₂),⁴⁰ 31.0 (CH₂),⁴⁰ 32.3 (CH₂),⁴⁰ 32.9 (CH₂),⁴⁰ 35.7 (CH), 52.3 (CH₂), 117.2 (CH), 117.7 (CH), 123.8 (C_{quat}), 125.8 (C_{quat}), 126.3 (CH), 126.7 (CH), 126.9 (C_{quat}), 127.1 (CH), 128.5 (C_{quat}), 130.1 (CH), 130.3 (CH), 131.3 (CH), 131.7 (CH), 137.1 (C_{quat}), 137.4 (C_{quat}), 137.5 (C_{quat}), 143.9 (C_{quat}), 148.6 (C_{quat}), 169.1 (C_{quat}), 194.6 (C_{quat}). MS (MALDI-TOF) calcd for C₄₇H₆₄N₂OS₃ *m/z*: 768.42; Found: 768.4 ([M]⁺). ESI-HRMS calcd for C₄₇H₆₄N₂OS₃: 768.41808; Found: 768.4183 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3066 (w), 3026 (w), 2922 (m), 2851 (m), 1686 (m), 1595 (w), 1570 (m), 1499 (w), 1458 (s), 1437 (w), 1404 (m), 1389 (w), 1375 (w), 1341 (w), 1319 (w), 1289 (w), 1279 (w), 1258 (w), 1234 (m), 1217 (w), 1192 (s), 1179 (s), 1126 (w), 1107 (w), 1063

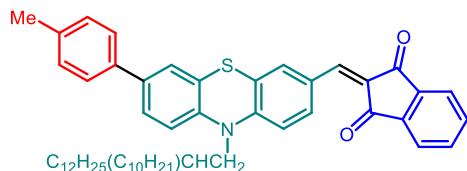
³⁹ Two CH₃ signals coincide.

⁴⁰ Two CH₂ signals coincide.

⁴¹ Four CH₂ signals coincide.

(w), 1018 (w), 997 (w), 922 (w), 883 (w), 856 (w), 806 (m), 770 (w), 741 (w), 718 (w), 700 (w), 660 (w).

2.1.5.3. 2-{{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (12c)



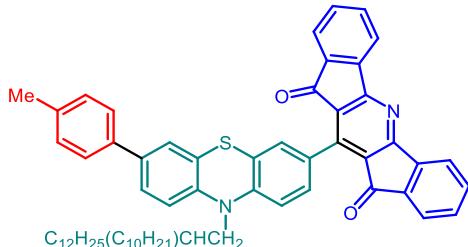
According to the GP and after purification by chromatography on silica gel (*n*-hexane/ethyl acetate 25:1) and drying under vacuo compound **12c** (314 mg, 79%) was obtained as a dark red resin. R_f (*n*-hexane/ethyl acetate 10:1) = 0.28.

1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.82 (t, 3J = 6.7 Hz, 3 H), 0.84 (t, 3J = 6.7 Hz, 3 H), 1.13–1.46 (m, 40 H), 1.98–2.04 (m, 1 H), 2.34 (s, 3 H), 3.93 (d, 3J = 7.1 Hz, 2 H), 7.09 (t, 3J = 8.4 Hz, 2 H), 7.23 (d, 3J = 8.0 Hz, 2 H), 7.40 (d, 4J = 2.2 Hz, 1 H), 7.47 (dd, 3J = 8.4 Hz, 4J = 2.2 Hz, 1 H), 7.51 (d, 3J = 8.1 Hz, 2 H), 7.66 (s, 1 H), 7.83–7.98 (m, 4 H), 8.33 (dd, 3J = 8.7 Hz, 4J = 2.1 Hz, 1 H), 8.59 (d, 4J = 2.1 Hz, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.4 (CH₃)⁴², 21.3 (CH₃), 23.4 (CH₂)⁴³, 26.7 (CH₂), 26.8 (CH₂), 30.12 (CH₂), 30.14 (CH₂)⁴³, 30.36 (CH₂), 30.39 (CH₂), 30.40 (CH₂)⁴³, 30.43 (CH₂)⁴³, 30.5 (CH₂), 30.58 (CH₂), 30.63 (CH₂), 31.87 (CH₂), 31.91 (CH₂), 32.66 (CH₂), 32.67 (CH₂), 35.5 (CH), 52.3 (CH₂), 116.7 (CH), 118.2 (CH), 123.5 (CH), 123.6 (CH), 125.3 (C_{quat}), 125.8 (C_{quat}), 126.1 (CH), 126.6 (CH), 127.0 (CH), 127.5 (C_{quat}), 128.9 (C_{quat}), 130.4 (CH), 133.6 (CH), 135.9 (CH), 136.1 (CH), 136.6 (CH), 137.3 (C_{quat}), 137.4 (C_{quat}), 137.7 (C_{quat}), 140.8 (C_{quat}), 143.2 (C_{quat}), 143.5 (C_{quat}), 145.5 (CH), 151.2 (C_{quat}), 189.8 (C_{quat}), 190.4 (C_{quat}). MS (MALDI-TOF) calcd for $C_{53}H_{67}NO_2S$ *m/z*: 781.49; Found: 781.5 ([M]⁺). ESI-HRMS calcd for $C_{53}H_{67}NO_2S$: 781.48925; Found: 781.48968 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3061 (w), 2955 (w), 2920 (m), 2851 (m), 1724 (w), 1678 (m), 1597 (w), 1562 (m), 1537 (m), 1497 (w), 1460 (s), 1412 (m), 1377 (w), 1331 (m), 1317 (m), 1277 (w), 1258 (m), 1198 (s), 1173 (m), 1153 (m), 1018 (m), 997 (m), 961 (w), 922 (w), 909 (w), 882 (w), 804 (s), 735 (s), 694 (w), 675 (w), 602 (w).

⁴² Two CH₃ signals coincide.

⁴³ Two CH₂ signals coincide.

2.1.5.4. 11-[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]diindeno[1,2-*b*:2',1'-*e*]pyridin-10,12-dione (12d)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under *vacuo* compound **12d** (143 mg, 32%) was obtained as a red brown resin. R_f (*n*-hexane/ethyl acetate 20:1) = 0.20.

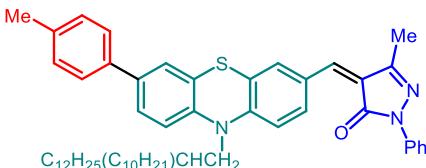
¹H NMR (300 MHz, CD₂Cl₂): δ 0.75–0.96 (m, 6 H), 1.09–1.58 (m, 40 H), 2.09 (hep, ³J = 6.1 Hz, 1 H), 2.38 (s, 3 H), 3.86 (d, ³J = 7.1 Hz, 2 H), 6.99 (dd, ³J = 8.8 Hz, ⁴J = 2.9 Hz, 2 H), 7.23 (d, ³J = 7.8 Hz, 2 H), 7.39–7.55 (m, 6 H), 7.58–7.70 (m, 3 H), 7.73 (d, ³J = 7.3 Hz, 1 H), 7.87 (d, ⁴J = 2.1 Hz, 1 H), 7.91 (dd, ³J = 7.7 Hz, ⁴J = 3.3 Hz, 2 H), 8.81 (d, ³J = 7.5 Hz, 1 H). ¹³C NMR (75 MHz, CD₂Cl₂): δ 14.5 (CH₃),⁴⁴ 21.4 (CH₃), 23.3 (CH₂),⁴⁵ 26.86 (CH₂), 26.89 (CH₂), 30.0 (CH₂),⁴⁵ 30.1 (CH₂),⁴⁵ 30.27 (CH₂),⁴⁶ 30.30 (CH₂), 30.32 (CH₂), 30.62 (CH₂), 30.63 (CH₂), 32.15 (CH₂), 32.16 (CH₂), 32.5 (CH₂),⁴⁵ 35.4 (CH), 52.3 (CH₂), 115.2 (CH), 117.1 (CH), 121.0 (C_{quat}), 122.4 (CH), 124.1 (C_{quat}), 124.25 (CH), 124.30 (CH), 124.6 (C_{quat}), 126.1 (CH), 126.3 (C_{quat}), 126.7 (CH), 128.3 (CH), 130.0 (2 CH), 130.1 (CH), 130.9 (CH), 131.1 (C_{quat}), 132.7 (CH), 133.0 (CH), 135.4 (C_{quat}), 135.5 (CH), 135.7 (CH), 136.3 (C_{quat}), 137.1 (C_{quat}), 137.4 (C_{quat}), 137.5 (C_{quat}), 140.0 (C_{quat}), 143.3 (C_{quat}), 144.4 (C_{quat}), 148.7 (C_{quat}), 152.2 (C_{quat}), 160.0 (C_{quat}), 168.8 (C_{quat}), 191.1 (C_{quat}), 191.3 (C_{quat}). MS (MALDI-TOF) calcd for C₆₂H₇₀N₂O₂S m/z: 906.52; Found: 906.5 ([M]⁺). ESI-HRMS calcd for C₆₂H₇₀N₂O₂S: 906.51580; Found: 906.51602 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3030 (w), 2922 (m), 2851 (m), 2220 (w), 1686 (w), 1597 (w), 1572 (m), 1541 (w), 1460 (s), 1402 (m), 1395 (m), 1377 (m), 1339 (m), 1308 (m), 1277 (m), 1252 (m), 1207 (s), 1173 (m), 1105 (w), 1076 (w), 1022 (w), 999 (w), 957 (w), 939 (w), 883 (m), 816 (m), 789 (w), 760 (s), 741 (w), 720 (m), 696 (s), 629 (w), 611 (m).

⁴⁴ Two CH₃ signals coincide.

⁴⁵ Two CH₂ signals coincide.

⁴⁶ Four CH₂ signals coincide.

2.1.5.5. (*Z*)-4-[(10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl)methylene]-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (12e)

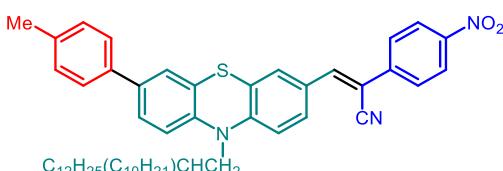


$\text{C}_{54}\text{H}_{71}\text{N}_3\text{OS}$ [810.23]

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/ethyl acetate 30:1) and drying under vacuo compound **12e** (325 mg, 77%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.22.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.90 (t, ${}^3J = 6.7$ Hz, 3 H), 0.91 (t, ${}^3J = 6.7$ Hz, 3 H), 1.23–1.52 (m, 40 H), 2.06–2.12 (m, 1 H), 2.43 (s, 3 H), 2.39 (s, 3 H), 3.97 (d, ${}^3J = 7.1$ Hz, 2 H), 7.08 (dd, ${}^3J = 8.6$ Hz, ${}^4J = 2.5$ Hz, 2 H), 7.12–7.17 (m, 1 H), 7.23 (d, ${}^3J = 7.9$ Hz, 2 H), 7.34–7.49 (m, 7 H), 8.00–8.10 (m, 2 H), 8.50 (dd, ${}^3J = 8.7$ Hz, ${}^4J = 2.1$ Hz, 1 H), 8.67 (d, ${}^4J = 2.1$ Hz, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.6 (CH₃), 14.8 (CH₃),⁴⁷ 21.5 (CH₃), 23.7 (CH₂),⁴⁸ 27.1 (CH₂),⁴⁸ 30.4 (CH₂),⁴⁸ 30.5 (CH₂),⁴⁸ 30.6 (CH₂),⁴⁹ 30.67 (CH₂), 30.69 (CH₂), 31.0 (CH₂),⁴⁸ 32.2 (CH₂),⁴⁸ 32.9 (CH₂),⁴⁸ 35.8 (CH), 52.4 (CH₂), 116.3 (CH), 117.9 (CH), 119.0 (CH), 124.8 (CH), 125.4 (C_{quat}), 125.5 (C_{quat}), 126.1 (C_{quat}), 126.3 (CH), 126.6 (CH), 127.1 (CH), 129.0 (C_{quat}), 129.2 (CH), 130.3 (CH), 133.7 (CH), 135.9 (CH), 137.3 (C_{quat}), 137.4 (C_{quat}), 137.5 (C_{quat}), 139.9 (C_{quat}), 143.4 (C_{quat}), 146.1 (CH), 150.8 (C_{quat}), 151.5 (C_{quat}), 162.7 (C_{quat}). MS (MALDI-TOF) calcd for $\text{C}_{54}\text{H}_{71}\text{N}_3\text{OS-H}^+$ *m/z*: 810.54; Found: 810.5. IR: $\tilde{\nu}$ [cm⁻¹] = 3061 (w), 2920 (m), 2851 (m), 1678 (w), 1614 (w), 1597 (m), 1574 (m), 1557 (m), 1537 (w), 1497 (m), 1460 (s), 1418 (m), 1389 (w), 1356 (w), 1341 (w), 1317 (s), 1279 (w), 1250 (m), 1215 (s), 1190 (w), 1138 (m), 1109 (w), 1022 (w), 955 (m), 930 (w), 903 (w), 882 (w), 806 (m), 785 (w), 768 (m), 752 (m), 725 (w), 691 (m), 662 (w). Anal calcd for $\text{C}_{54}\text{H}_{71}\text{N}_3\text{OS}$ [810.2]: C 80.05, H 8.83, N 5.19, S 3.96; Found: C 80.29, H 8.82, N 5.27, S 3.95.

2.1.5.6. (*Z*)-3-[(10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl)-2-(4-nitrophenyl)acrylonitrile (12f)



$\text{C}_{52}\text{H}_{67}\text{N}_3\text{O}_2\text{S}$ [798.17]

⁴⁷ Two CH₃ signals coincide.

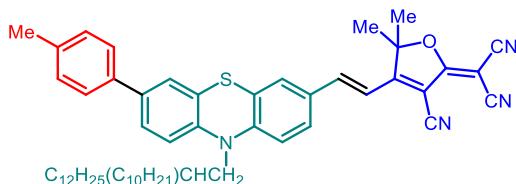
⁴⁸ Two CH₂ signals coincide.

⁴⁹ Four CH₂ signals coincide.

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/ethyl acetate 30:1) and drying under vacuo compound **12f** (490 mg, 87%) was obtained as a dark red resin. R_f (*n*-hexane/ethyl acetate 20:1) = 0.22.

^1H NMR (600 MHz, acetone-d₆): δ 0.84 (t, 3J = 7.0 Hz, 3 H), 0.85 (t, 3J = 7.0 Hz, 3 H), 1.16–1.48 (m, 40 H), 1.99–2.05 (m, 1 H), 2.35 (s, 3 H), 3.94 (d, 3J = 7.2 Hz, 2 H), 7.09–7.17 (m, 2 H), 7.24 (d, 3J = 7.9 Hz, 2 H), 7.41 (d, 4J = 2.1 Hz, 1 H), 7.49 (dd, 3J = 8.4 Hz, 4J = 2.2 Hz, 1 H), 7.51 (d, 3J = 8.0 Hz, 2 H), 7.84 (s, 1 H), 7.95 (dd, 3J = 8.6 Hz, 4J = 2.2 Hz, 1 H), 7.97–8.00 (m, 3 H), 8.32 (d, 3J = 8.5 Hz, 2 H). ^{13}C NMR (150 MHz, acetone-d₆): δ 14.4 (CH₃)⁵⁰, 21.1 (CH₃), 23.4 (CH₂),⁵¹ 26.7 (CH₂), 26.8 (CH₂), 30.1 (CH₂),⁵² 30.2 (CH₂), 30.35 (CH₂), 30.37 (CH₂), 30.39 (CH₂), 30.42 (CH₂), 30.43 (CH₂), 30.5 (CH₂), 30.60 (CH₂), 30.64 (CH₂), 31.9 (CH₂), 32.0 (CH₂), 32.66 (CH₂), 32.67 (CH₂), 35.5 (CH), 52.2 (CH₂), 106.49 (C_{quat}), 117.1 (CH), 118.0 (CH), 118.5 (C_{quat}), 125.1 (CH), 125.7 (C_{quat}), 126.09 (C_{quat}), 126.13 (CH), 126.7 (CH), 127.0 (CH), 127.4 (CH), 128.6 (C_{quat}), 129.5 (CH), 130.4 (2 CH), 130.9 (CH), 137.1 (C_{quat}), 137.4 (C_{quat}), 137.7 (C_{quat}), 142.0 (C_{quat}), 144.0 (C_{quat}), 145.1 (CH), 148.4 (C_{quat}), 149.5 (C_{quat}). MS (MALDI-TOF) calcd for C₅₂H₆₇N₃O₂S *m/z*: 797.50; Found: 797.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3024 (w), 2920 (m), 2851 (m), 2212 (w), 1603 (w), 1570 (m), 1520 (m), 1497 (w), 1462 (s), 1418 (w), 1402 (m), 1377 (w), 1337 (s), 1277 (m), 1206 (m), 1175 (m), 1047 (w), 1036 (w), 1003 (w), 918 (w), 881 (w), 872 (w), 851 (m), 806 (s), 781 (w), 752 (m), 719 (w), 688 (w), 663 (w), 623 (w). Anal calcd for C₅₂H₆₇N₃O₂S [798.2]: C 78.25, H 8.46, N 5.26; Found: C 77.96, H 8.23, N 5.18.

2.1.5.7. (*E*)-2-{3-Cyano-4-[2-(10-{2-decytetradecyl}-7-{*p*-tolyl}-10*H*-phenothiazin-3-yl)vinyl]-5,5-dimethylfuran-2[5*H*]-yliden}malonitrile (12g)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **12g** (358 mg, 81%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 3:1) = 0.24.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.90 (t, 3J = 6.7 Hz, 3 H), 0.91 (t, 3J = 6.7 Hz, 3 H), 1.21–1.52 (m, 40 H), 1.87 (s, 6 H), 2.01–2.07 (m, 1 H), 2.38 (s, 3 H), 3.96 (d, 3J = 7.1 Hz, 2 H), 7.10 (d, 3J = 8.8 Hz, 2 H), 7.15 (d, 3J = 16.3 Hz, 1 H), 7.20–7.26 (m, 2 H), 7.37 (d, 4J = 2.1 Hz,

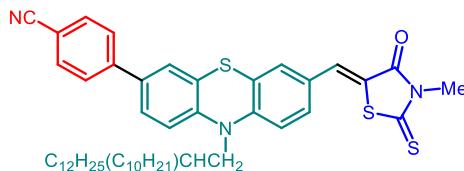
⁵⁰ Two CH₃ signals coincide.

⁵¹ Two CH₂ signals coincide.

⁵² Three CH₂ signals coincide.

1 H), 7.42–7.49 (m, 3 H), 7.66–7.73 (m, 2 H), 7.91 (d, $^3J = 16.3$ Hz, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃)⁵³ 21.4 (CH₃), 23.6 (CH₂)⁵⁴ 26.2 (CH₃), 27.1 (CH₂)⁵⁴ 30.30 (CH₂), 30.31 (CH₂), 30.4 (CH₂)⁵⁴ 30.58 (CH₂)⁵⁵ 30.60 (CH₂), 30.62 (CH₂), 30.64 (CH₂), 31.0 (CH₂)⁵⁴ 32.2 (CH₂)⁵⁴ 32.8 (CH₂)⁵⁴ 35.8 (CH), 52.5 (CH₂), 98.7 (C_{quat}), 98.9 (C_{quat})⁵⁶ 111.3 (C_{quat}), 112.0 (C_{quat}), 112.8 (C_{quat}), 113.7 (CH), 117.1 (CH), 118.0 (CH), 125.7 (C_{quat}), 126.2 (CH), 126.6 (C_{quat}), 126.7 (CH), 127.0 (CH), 128.7 (CH), 129.9 (C_{quat}), 130.4 (CH), 130.9 (CH), 137.3 (C_{quat})⁵⁶ 137.6 (C_{quat}), 143.5 (C_{quat}), 147.1 (CH), 150.5 (C_{quat}), 175.2 (C_{quat}), 177.0 (C_{quat}). MS (MALDI-TOF) calcd for C₅₅H₇₀N₄OS *m/z*: 834.53; Found: 834.6 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2955 (w), 2922 (m), 2853 (w), 2220 (w), 2210 (w), 1601 (w), 1568 (m), 1516 (s), 1495 (m), 1454 (s), 1420 (w), 1381 (w), 1339 (s), 1302 (s), 1279 (m), 1248 (m), 1209 (s), 1184 (m), 1155 (m), 1107 (m), 1057 (w), 1015 (w), 964 (m), 930 (w), 897 (w), 806 (m), 714 (w), 658 (w), 617 (w). Anal calcd for C₅₅H₇₀N₄OS [835.2]: C 79.09, H 8.45, N 6.71, S 3.84; Found: C 79.00, H 8.41, N 6.63, S 3.89.

2.1.5.8. (*Z*)-5-{{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12h)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 40:1) and drying under vacuo compound **12h** (375 mg, 95%) was obtained as a dark red solid, Mp 120–126 °C. R_f (*n*-hexane/acetone 10:1) = 0.51.

^1H NMR (300 MHz, CD₂Cl₂): δ 0.86 (t, $^3J = 6.7$ Hz, 3 H), 0.88 (t, $^3J = 6.7$ Hz, 3 H), 1.17–1.44 (m, 40 H), 1.94–2.04 (m, 1 H), 3.49 (s, 3 H), 3.82 (d, $^3J = 7.1$ Hz, 2 H), 6.98 (d, $^3J = 8.4$ Hz, 1 H), 7.01 (d, $^3J = 8.3$ Hz, 1 H), 7.28 (d, $^4J = 2.2$ Hz, 1 H), 7.35 (dd, $^3J = 8.4$ Hz, $^4J = 2.2$ Hz, 1 H), 7.41 (d, $^4J = 2.1$ Hz, 1 H), 7.45 (dd, $^3J = 8.4$ Hz, $^4J = 2.2$ Hz, 1 H), 7.61 (s, 1 H), 7.63–7.74 (m, 4 H). ^{13}C NMR (75 MHz, CD₂Cl₂): δ 14.5 (CH₃)⁵⁷ 23.3 (CH₂)⁵⁸ 26.7 (CH₂)⁵⁸ 29.9 (CH₂)⁵⁸ 30.0 (CH₂)⁵⁸ 30.18 (CH₂)⁵⁸ 30.20 (CH₂), 30.24 (CH₂)⁵⁸ 30.3 (CH₂), 30.45 (CH₂)⁵⁸ 31.7 (CH₃), 31.9 (CH₂)⁵⁸ 32.5 (CH₂)⁵⁸ 35.3 (CH), 52.4 (CH₂), 111.2 (C_{quat}), 117.0 (CH), 117.5 (CH), 119.4 (C_{quat}), 121.1 (C_{quat}), 126.1 (C_{quat}), 126.5 (CH), 126.6 (C_{quat}), 126.9 (CH), 127.4 (CH), 128.5

⁵³ Two CH₃ signals coincide.

⁵⁴ Two CH₂ signals coincide.

⁵⁵ Three CH₂ signals coincide.

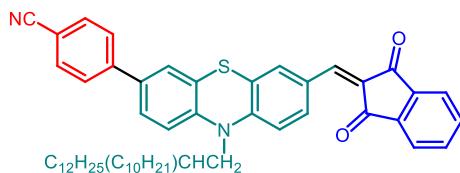
⁵⁶ Two quaternary signals coincide.

⁵⁷ Two CH₃ signals coincide.

⁵⁸ Two CH₂ signals coincide.

(C_{quat}), 129.9 (CH), 131.4 (CH), 132.5 (CH), 133.2 (CH), 134.7 (C_{quat}), 144.5 (C_{quat}), 145.3 (C_{quat}), 148.2 (C_{quat}), 168.2 (C_{quat}), 193.9 (C_{quat}). MS (MALDI-TOF) calcd for C₄₈H₆₃N₃OS₃ *m/z*: 793.41; Found: 793.4 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2920 (m), 2850 (w), 2225 (w), 1705 (m), 1565 (m), 1475 (m), 1398 (m), 1356 (w), 1279 (s), 1223 (m), 1126 (m), 1100 (s), 835 (m), 795 (m), 713 (w). Anal calcd for C₄₈H₆₃N₃OS₃ [794.2]: C 72.59, H 8.00, N 5.29; Found: C 72.38, H 7.78, N 5.27.

2.1.5.9. 4-{10-(2-Decyltetradecyl)-7-[(1,3-dioxo-1H-inden-2[3H]-yliden)methyl]-10H-phenothiazin-3-yl}benzonitrile (12i)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) and drying under vacuo compound **12i** (309 mg, 81%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.18.

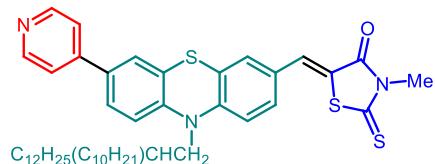
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.87 (t, ³J = 6.6 Hz, 3 H), 0.88 (t, ³J = 6.6 Hz, 3 H), 1.20–1.53 (m, 40 H), 2.07–2.13 (m, 1 H), 4.01 (d, ³J = 7.2 Hz, 2 H), 7.16 (t, ³J = 8.9 Hz, 2 H), 7.52 (d, ⁴J = 2.2 Hz, 1 H), 7.58 (dd, ³J = 8.5 Hz, ⁴J = 2.2 Hz, 1 H), 7.68 (s, 1 H), 7.75–8.00 (m, 8 H), 8.38 (dd, ³J = 8.7 Hz, ⁴J = 2.1 Hz, 1 H), 8.62 (d, ⁴J = 2.1 Hz, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃)⁵⁹ 23.6 (CH₂)⁶⁰ 27.0 (CH₂), 27.1 (CH₂), 30.3 (CH₂)⁶⁰ 30.4 (CH₂)⁶⁰ 30.6 (CH₂)⁶¹ 30.6 (CH₂), 30.7 (CH₂), 30.9 (CH₂)⁶⁰ 32.2 (CH₂)⁶⁰ 32.8 (CH₂)⁶⁰ 35.8 (CH), 52.5 (CH₂), 111.6 (C_{quat}), 116.8 (CH), 118.2 (CH), 119.1 (C_{quat}), 123.5 (CH), 123.7 (CH), 125.4 (C_{quat}), 126.5 (C_{quat}), 126.8 (CH), 127.3 (CH), 127.7 (C_{quat}), 127.9 (CH), 129.2 (C_{quat}), 133.4 (CH), 133.8 (CH), 135.1 (C_{quat}), 135.9 (CH), 136.0 (CH), 136.5 (CH), 140.8 (C_{quat}), 143.2 (C_{quat}), 144.5 (C_{quat}), 145.1 (C_{quat}), 145.3 (CH), 150.7 (C_{quat}), 189.5 (C_{quat}), 190.0 (C_{quat}). MS (MALDI-TOF) calcd for C₅₃H₆₄N₂O₂S *m/z*: 792.47; Found: 792.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3065 (w), 2920 (m), 2851 (w), 2224 (w), 1722 (w), 1678 (m), 1597 (m), 1560 (s), 1537 (m), 1493 (w), 1460 (s), 1412 (m), 1375 (w), 1337 (m), 1279 (m), 1250 (m), 1198 (s), 1175 (m), 1153 (m), 1107 (w), 1084 (m), 1045 (w), 1018 (w), 997 (m), 961 (w), 922 (w), 909 (w), 883 (w), 841 (w), 812 (m), 785 (w), 735 (m), 694 (w), 675 (w). Anal calcd for C₅₃H₆₄N₂O₂S [793.2]: C 80.26, H 8.13, N 3.53, S 4.04; Found: C 80.27, H 7.91, N 3.50, S 4.02.

⁵⁹ Two CH₃ signals coincide.

⁶⁰ Two CH₂ signals coincide.

⁶¹ Four CH₂ signals coincide.

2.1.5.10. (Z)-5-{{[10-(2-Decyltetradecyl)-7-(pyridin-4-yl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12j)}

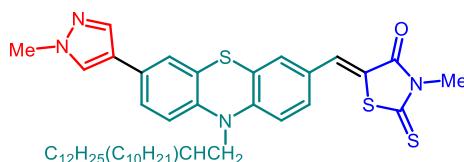


$\text{C}_{46}\text{H}_{63}\text{N}_3\text{OS}_3$ [770.21]

According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 20:1) and drying under vacuo compound **12j** (308 mg, 78%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 1:2) = 0.46.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.89 (t, 3J = 6.7 Hz, 3 H), 0.91 (t, 3J = 6.7 Hz, 3 H), 1.22–1.51 (m, 40 H), 2.02–2.08 (m, 1 H), 3.47 (s, 3 H), 3.96 (d, 3J = 7.2 Hz, 2 H), 7.16 (dd, 3J = 8.6 Hz, 4J = 1.6 Hz, 2 H), 7.36 (d, 4J = 2.1 Hz, 1 H), 7.46 (dd, 3J = 8.6 Hz, 4J = 2.2 Hz, 1 H), 7.55 (d, 4J = 2.2 Hz, 1 H), 7.55–7.58 (m, 2 H), 7.61 (dd, 3J = 8.5 Hz, 4J = 2.1, 1 H), 7.63 (s, 1 H), 8.55–8.61 (m, 2 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃),⁶² 23.6 (CH₂),⁶³ 27.06 (CH₂), 27.07 (CH₂), 30.3 (CH₂),⁶³ 30.4 (CH₂),⁶³ 30.59 (CH₂),⁶⁴ 30.62 (CH₂), 30.63 (CH₂), 30.7 (CH₂), 30.93 (2 CH₂),⁶³ 31.6 (CH), 32.2 (CH₂),⁶³ 32.9 (CH₂),⁶³ 35.7 (CH), 52.4 (CH₂), 117.6 (CH), 118.0 (CH), 121.3 (CH), 121.4 (C_{quat}), 126.2 (C_{quat}), 126.5 (CH), 126.7 (C_{quat}), 127.1 (CH), 129.0 (C_{quat}), 130.3 (CH), 131.6 (CH), 132.4 (CH), 133.9 (C_{quat}), 145.9 (C_{quat}), 146.8 (C_{quat}), 148.3 (C_{quat}), 151.1 (CH), 167.7 (C_{quat}), 193.5 (C_{quat}). MS (MALDI-TOF) calcd for $\text{C}_{46}\text{H}_{63}\text{N}_3\text{OS}_3\text{-H}^+$ *m/z*: 770.42; Found: 770.5. IR: $\tilde{\nu}$ [cm⁻¹] = 2920 (m), 2851 (w), 1715 (w), 1591 (w), 1568 (w), 1462 (m), 1422 (w), 1404 (w), 1348 (w), 1281 (s), 1252 (w), 1221 (w), 1192 (w), 1153 (w), 1125 (s), 1101 (s), 1057 (w), 991 (w), 959 (w), 899 (w), 870 (w), 804 (m), 731 (w), 720 (w), 692 (w), 673 (w), 610 (w). Anal calcd for $\text{C}_{46}\text{H}_{63}\text{N}_3\text{OS}_3$ [770.2]: C 71.73, H 8.24, N 5.46, S 12.49 gef.: C 71.58, H 8.05, N 5.32, S 12.59.

2.1.5.11. (Z)-5-{{[10-(2-Decyltetradecyl)-7-(1-methyl-1*H*-pyrazol-4-yl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12k)}



$\text{C}_{45}\text{H}_{64}\text{N}_4\text{OS}_3$ [773.21]

⁶² Two CH₃ signals coincide.

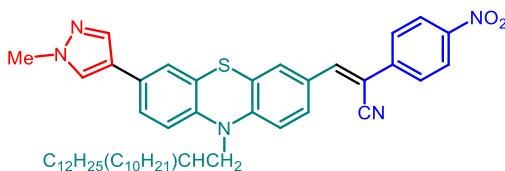
⁶³ Two CH₂ signals coincide.

⁶⁴ Three CH₃ signals coincide.

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 15:1) and drying under vacuo compound **12k** (333 mg, 80%) was obtained as a dark red viscous oil. R_f (*n*-hexane/acetone 4:1) = 0.25.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.90 (t, 3J = 6.7 Hz, 3 H), 0.91 (t, 3J = 6.7 Hz, 3 H), 1.23–1.49 (m, 40 H), 1.98–2.04 (m, 1 H), 3.47 (s, 3 H), 3.88–3.95 (m, 5 H), 6.99 (d, 3J = 8.4 Hz, 1 H), 7.08 (d, 3J = 8.6 Hz, 1 H), 7.29 (d, 4J = 2.1 Hz, 1 H), 7.31 (d, 4J = 2.2 Hz, 1 H), 7.34 (dd, 3J = 8.4 Hz, 4J = 2.1 Hz, 1 H), 7.42 (dd, 3J = 8.6 Hz, 4J = 2.2 Hz, 1 H), 7.61 (s, 1 H), 7.65 (s, 1 H), 7.82 (s, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃)⁶⁵, 23.7 (CH₂)⁶⁶, 27.1 (CH₂)⁶⁶, 30.3 (CH₂)⁶⁶, 30.4 (CH₂)⁶⁶, 30.60 (CH₂)⁶⁷, 30.63 (CH₂), 30.64 (CH₂), 30.7 (CH₂), 31.0 (CH₂)⁶⁶, 31.5 (CH₃), 32.2 (CH₂)⁶⁶, 32.9 (CH₂)⁶⁶, 35.7 (CH), 39.2 (CH₃), 52.3 (CH₂), 117.1 (CH), 117.8 (CH), 120.9 (C_{quat}), 122.4 (C_{quat}), 124.9 (CH), 125.3 (CH), 125.7 (C_{quat}), 126.9 (C_{quat}), 127.4 (CH), 128.4 (C_{quat}), 129.7 (C_{quat}), 130.2 (CH), 131.5 (CH), 132.7 (CH), 136.5 (CH), 142.7 (C_{quat}), 148.9 (C_{quat}), 167.7 (C_{quat}), 193.1 (C_{quat}). MS (MALDI-TOF) calcd for C₄₅H₆₄N₄OS₃ *m/z*: 772.42; Found: 772.4 ([M]⁺). ESI-HRMS calcd for C₄₅H₆₄N₄OS₃: 772.42422; Found: 772.42365 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2920 (m), 2851 (m), 1707 (m), 1600 (w), 1578 (m), 1561 (w), 1499 (w), 1474 (m), 1464 (m), 1424 (m), 1404 (m), 1350 (m), 1285 (s), 1254 (m), 1219 (m), 1169 (w), 1126 (s), 1099 (s), 1078 (w), 1057 (w), 1042 (w), 986 (w), 974 (m), 959 (w), 901 (w), 876 (w), 847 (w), 812 (m), 762 (w), 729 (w), 720 (w), 704 (w), 692 (w), 662 (w), 629 (w).

2.1.5.12. (Z)-3-[10-(2-Decyltetradecyl)-7-(1-methyl-1*H*-pyrazol-4-yl)-10*H*-phenothiazin-3-yl]-2-(4-nitrophenyl)acrylonitrile (12l)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/ethyl acetate 5:1) and drying under vacuo compound **12l** (288 mg, 71%) was obtained as a red brown amorphous solid, Mp 103–108 °C. R_f (*n*-hexane/ethyl acetate 5:1) = 0.13.

^1H NMR (300 MHz, acetone-d₆): δ 0.87 (t, 3J = 6.7 Hz, 3 H), 0.88 (t, 3J = 6.7 Hz, 3 H), 1.16–1.53 (m, 40 H), 1.98–2.03 (m, 1 H), 3.89 (s, 3 H), 3.92 (d, 3J = 7.5 Hz, 2 H), 7.03 (d, 3J = 8.4 Hz, 1 H), 7.12 (d, 3J = 8.7 Hz, 1 H), 7.33 (d, 4J = 2.0 Hz, 1 H), 7.38 (dd, 3J = 8.5 Hz, 4J = 2.0 Hz, 1 H), 7.71 (s, 1 H), 7.85 (d, 4J = 2.1 Hz, 1 H), 7.88 (s, 1 H), 7.92–8.02 (m, 4 H), 8.31 (d, 3J

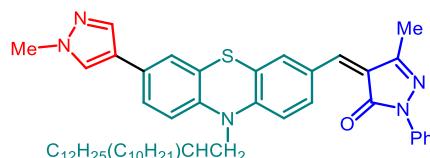
⁶⁵ Two CH₃ signals coincide.

⁶⁶ Two CH₂ signals coincide.

⁶⁷ Three CH₂ signals coincide.

= 8.7 Hz, 2 H). ^{13}C NMR (150 MHz, acetone-d₆): δ 14.6 (CH₃)⁶⁸, 23.5 (CH₂)⁶⁹, 26.95 (CH₂), 26.96 (CH₂), 30.2 (CH₂)⁶⁹, 30.3 (CH₂)⁶⁹, 30.49 (CH₂)⁷⁰, 30.52 (CH₂), 30.54 (CH₂), 30.6 (CH₂), 30.8 (CH₂)⁶⁹, 32.1 (CH₂)⁶⁹, 32.8 (CH₂)⁶⁹, 35.6 (CH), 39.2 (CH₃), 52.2 (CH₂), 106.3 (C_{quat}), 116.8 (CH), 117.9 (CH), 118.4 (C_{quat}), 122.4 (C_{quat}), 124.9 (CH), 125.0 (CH), 125.3 (CH), 125.7 (C_{quat}), 126.1 (C_{quat}), 127.3 (CH), 127.6 (CH), 128.4 (C_{quat}), 129.6 (CH), 129.7 (C_{quat}), 130.8 (CH), 136.6 (CH), 142.0 (C_{quat}), 142.8 (C_{quat}), 145.0 (CH), 148.2 (C_{quat}), 149.6 (C_{quat}). MS (MALDI-TOF) calcd for C₄₉H₆₅N₅O₂S *m/z*: 787.49; Found: 787.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2920 (m), 2851 (w), 2209 (w), 1603 (w), 1576 (m), 1560 (w), 1541 (w), 1516 (m), 1505 (m), 1475 (m), 1462 (m), 1402 (w), 1371 (w), 1335 (s), 1312 (m), 1254 (m), 1238 (m), 1209 (m), 1177 (w), 1109 (w), 1080 (w), 1038 (w), 1007 (w), 976 (w), 928 (w), 880 (w), 851 (m), 816 (m), 802 (m), 781 (w), 752 (w), 721 (w), 689 (w), 664 (w). Anal calcd for C₄₉H₆₅N₅O₂S [788.1]: C 74.67, H 8.31, N 8.89; Found: C 74.55, H 8.22, N 8.74.

2.1.5.13. (Z)-4-{{[10-(2-Decyltetradecyl)-7-(1-methyl-1H-pyrazol-4-yl)-10H-phenothiazin-3-yl]methylene}-3-methyl-1-phenyl-1H-pyrazol-5[4H]-one (12m)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 15:1) and drying under vacuo compound **12m** (288 mg, 69%) was obtained as a dark red viscous oil. R_f (*n*-hexane/acetone 10:1) = 0.10.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.89 (t, 3J = 6.7 Hz, 3 H), 0.90 (t, 3J = 6.7 Hz, 3 H), 1.23–1.49 (m, 40 H), 2.06–2.10 (m, 1 H), 2.34 (s, 3 H), 3.89 (s, 3 H), 3.94 (d, 3J = 7.2 Hz, 2 H), 7.01 (d, 3J = 8.4 Hz, 1 H), 7.07 (d, 3J = 8.8 Hz, 1 H), 7.09–7.18 (m, 1 H), 7.28–7.43 (m, 4 H), 7.48 (s, 1 H), 7.66 (s, 1 H), 7.83 (s, 1 H), 8.03 (d, 4J = 1.2 Hz, 1 H), 8.06 (d, 4J = 1.4 Hz, 1 H), 8.48 (dd, 3J = 8.7 Hz, 4J = 2.1 Hz, 1 H), 8.68 (d, 4J = 2.1 Hz, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.8 (CH₃), 14.9 (CH₃)⁶⁸, 23.8 (CH₂)⁷¹, 27.3 (CH₂)⁷², 30.5 (CH₂)⁷², 30.6 (CH₂)⁷², 30.77 (CH₂)⁷³, 30.82 (CH₂), 30.83 (CH₂), 31.1 (CH₂)⁷², 32.4 (CH₂)⁷², 33.0 (CH₂)⁷², 35.9 (CH), 39.3 (CH₃), 52.5 (CH₂), 116.2 (CH), 117.9 (CH), 119.0 (CH), 122.4 (C_{quat}), 124.8 (CH), 124.9 (CH), 125.2 (CH), 125.27 (C_{quat}), 125.31 (C_{quat}), 126.0 (C_{quat}), 127.5 (CH), 128.9 (C_{quat}), 129.3

⁶⁸ Two CH₃ signals coincide.

⁶⁹ Two CH₂ signals coincide.

⁷⁰ Three CH₂ signals coincide.

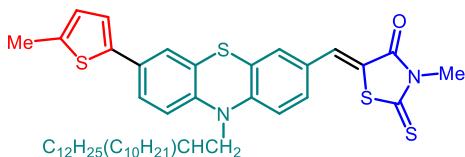
⁷¹ Two CH₃ signals coincide.

⁷² Two CH₂ signals coincide.

⁷³ Four CH₂ signals coincide.

(CH), 129.9 (C_{quat}), 133.7 (CH), 136.0 (CH), 136.5 (CH), 139.9 (C_{quat}), 142.3 (C_{quat}), 146.2 (CH), 151.0 (C_{quat}), 151.5 (C_{quat}), 162.8 (C_{quat}). MS (MALDI-TOF) calcd for C₅₁H₆₉N₅OS-H⁺ *m/z*: 800.53; Found: 800.5. ESI-HRMS calcd for C₅₁H₆₉N₅OS: 799.52228; Found: 799.52225 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2922 (s), 2851 (m), 1678 (w), 1597 (w), 1578 (m), 1555 (m), 1537 (w), 1499 (m), 1474 (s), 1464 (s), 1416 (m), 1358 (m), 1317 (s), 1254 (m), 1215 (s), 1138 (s), 1105 (w), 1078 (w), 1065 (w), 1022 (w), 955 (m), 974 (m), 932 (w), 903 (w), 878 (w), 845 (w), 816 (m), 793 (w), 768 (m), 752 (m), 723 (w), 714 (w), 691 (m), 664 (m), 652 (w), 640 (w).

2.1.5.14. (Z)-5-{{[10-(2-Decyltetradecyl)-7-(5-methylthiophen-2-yl)-10H-phenoxy]methylene}-3-methyl-2-thioxothiazolidin-4-one (12n)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **12n** (322 mg, 85%) was obtained as a red resin. R_f (*n*-hexane/acetone 10:1) = 0.47.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.91 (t, ³J = 6.7 Hz, 3 H), 0.92 (t, ³J = 6.7 Hz, 3 H), 1.20–1.50 (m, 40 H), 1.99–2.04 (m, 1 H), 2.51 (s, 3 H), 3.47 (s, 3 H), 3.91 (d, ³J = 7.2 Hz, 2 H), 6.73 (dd, ³J = 3.6 Hz, ⁵J = 1.2 Hz, 1 H), 7.01 (d, ³J = 8.5 Hz, 1 H), 7.08 (d, ³J = 3.5 Hz, 1 H), 7.11 (d, ³J = 8.6 Hz, 1 H), 7.31–7.35 (m, 2 H), 7.37 (dd, ³J = 8.4 Hz, ⁴J = 2.2 Hz, 1 H), 7.44 (dd, ³J = 8.6 Hz, ⁴J = 2.2 Hz, 1 H), 7.62 (s, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.8 (CH₃),⁷⁴ 15.7 (CH₃), 23.7 (CH₂),⁷⁵ 27.10 (CH₂), 27.12 (CH₂), 30.4 (CH₂),⁷⁵ 30.46 (CH₂), 30.48 (CH₂), 30.6 (CH₂),⁷⁶ 30.66 (CH₂), 30.68 (CH₂), 30.70 (CH₂), 30.97 (CH₂), 30.99 (CH₂), 31.5 (CH₃), 32.3 (CH₂),⁷⁵ 32.9 (CH₂),⁷⁵ 35.7 (CH), 52.4 (CH₂), 117.3 (CH), 117.8 (CH), 121.2 (C_{quat}), 123.5 (CH), 124.8 (CH), 125.4 (CH), 125.9 (C_{quat}), 126.7 (C_{quat}), 127.4 (CH), 128.6 (C_{quat}), 130.2 (CH), 131.2 (C_{quat}), 131.6 (CH), 132.5 (CH), 139.7 (C_{quat}), 141.3 (C_{quat}), 143.7 (C_{quat}), 148.6 (C_{quat}), 167.7 (C_{quat}), 193.2 (C_{quat}). MS (MALDI-TOF) calcd for C₄₆H₆₄N₂OS₄ *m/z*: 788.39; Found: 788.3 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2920 (m), 2851 (m), 1709 (m), 1591 (w), 1574 (m), 1505 (w), 1481 (m), 1458 (s), 1424 (m), 1402 (m), 1375 (w), 1348 (m), 1287 (s), 1265 (m), 1246 (m), 1221 (m), 1177 (w), 1165 (w), 1125 (s), 1101 (s), 1057 (w), 1040 (w), 991 (w), 959 (w), 937 (w), 897 (w), 864 (w), 814 (m), 795 (m), 758 (w), 729 (w), 720 (w), 691 (w), 662 (w), 646 (w),

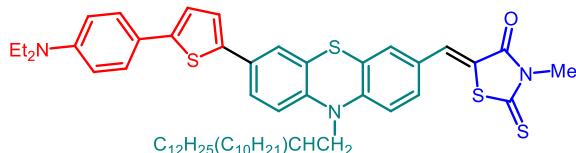
⁷⁴ Two CH₃ signals coincide.

⁷⁵ Two CH₂ signals coincide.

⁷⁶ Three CH₂ signals coincide.

606 (w). Anal calcd for $C_{46}H_{64}N_2OS_4$ [789.3]: C 70.00, H 8.17, N 3.55, S 16.25; Found: C 70.06, H 8.12, N 3.26, S 15.96.

2.1.5.15. (*Z*)-5-{{[10-(2-Decyltetradecyl)-7-(5-{4-[diethylamino]phenyl}thiophen-2-yl)-10*H*-phenothiazin-3-yl)methylene}-3-methyl-2-thioxothiazolidin-4-one (12o)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **12o** (355 mg, 67%) was obtained as a dark red amorphous solid, Mp 128–131 °C. R_f (*n*-hexane/acetone 10:1) = 0.43.

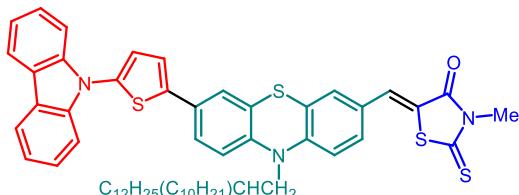
1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.91 (t, 3J = 6.3 Hz, 6 H), 1.21 (t, 3J = 7.0 Hz, 6 H), 1.23–1.55 (m, 40 H), 1.98–2.04 (m, 1 H), 3.44 (quart, 3J = 7.0 Hz, 4 H), 3.47 (s, 3 H), 3.91 (d, 3J = 7.0 Hz, 2 H), 6.68 (d, 3J = 8.6 Hz, 2 H), 7.02 (d, 3J = 8.4 Hz, 1 H), 7.08–7.14 (m, 2 H), 7.23 (d, 3J = 3.8 Hz, 1 H), 7.32–7.47 (m, 6 H), 7.62 (s, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.2 (CH₃), 14.8 (CH₃),⁷⁷ 23.7 (CH₂),⁷⁸ 27.10 (CH₂), 27.12 (CH₂), 30.4 (CH₂),⁷⁸ 30.5 (CH₂), 30.6 (CH₂),⁷⁹ 30.67 (CH₂),⁷⁸ 30.71 (CH₂), 30.97 (CH₂),⁷⁸ 31.5 (CH₃), 32.3 (CH₂),⁷⁸ 32.9 (CH₂),⁷⁸ 35.7 (CH), 45.1 (CH₂),⁷⁸ 52.4 (CH₂), 112.6 (CH), 117.3 (CH), 117.8 (CH), 121.1 (C_{quat}), 122.15 (CH), 122.19 (C_{quat}), 124.5 (CH), 124.7 (CH), 125.3 (CH), 125.9 (C_{quat}), 126.7 (C_{quat}), 127.5 (CH), 128.6 (C_{quat}), 130.3 (CH), 131.2 (C_{quat}), 131.6 (CH), 132.57 (CH), 139.9 (C_{quat}), 143.6 (C_{quat}), 145.4 (C_{quat}), 148.1 (C_{quat}), 148.6 (C_{quat}), 167.7 (C_{quat}), 193.3 (C_{quat}). MS (MALDI-TOF) calcd for $C_{55}H_{75}N_3OS_4$ *m/z*: 921.48; Found: 921.5 ([M]⁺). IR: IR: $\tilde{\nu}$ [cm⁻¹] = 2955 (w), 2918 (m), 2849 (w), 1707 (m), 1607 (w), 1589 (w), 1574 (m), 1555 (w), 1541 (w), 1518 (w), 1466 (s), 1425 (w), 1404 (m), 1375 (w), 1352 (m), 1339 (m), 1294 (m), 1287 (s), 1265 (m), 1250 (m), 1221 (m), 1198 (m), 1175 (w), 1155 (w), 1121 (m), 1109 (m), 1078 (m), 1039 (w), 1018 (w), 990 (w), 959 (w), 937 (w), 895 (w), 872 (w), 812 (w), 791 (m), 756 (w), 725 (w), 714 (w), 608 (w). Anal calcd for $C_{55}H_{75}N_3OS_4$ [922.5]: C 71.61, H 8.19, N 4.56, S 13.90; Found: C 71.82, H 8.13, N 4.47, S 13.60.

⁷⁷ Two CH₃ signals coincide.

⁷⁸ Two CH₂ signals coincide.

⁷⁹ Three CH₂ signals coincide.

2.1.5.16. (*Z*)-5-{{[7-(5-{9*H*-Carbazol-9-yl}thiophen-2-yl)-10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12p)}

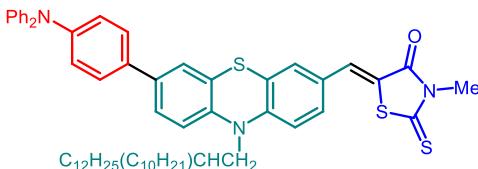


C₅₇H₆₉N₃OS₄ [940.44]

According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **12p** (391 mg, 74%) was obtained as an orange solid, Mp 95–98 °C. R_f (*n*-hexane/acetone 10:1) = 0.43.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86–0.94 (m, 6 H), 1.21–1.52 (m, 40 H), 2.06–2.09 (m, 1 H), 3.47 (s, 3 H), 3.94 (d, ³J = 7.1 Hz, 2 H), 7.09 (d, ³J = 8.3 Hz, 1 H), 7.14 (d, ³J = 8.6 Hz, 1 H), 7.26 (d, ³J = 4.0 Hz, 1 H), 7.27–7.33 (m, 2 H), 7.35 (d, ⁴J = 2.1 Hz, 1 H), 7.42–7.56 (m, 8 H), 7.62 (s, 1 H), 8.13 (dt, ³J = 7.8 Hz, ⁴J = 0.9 Hz, 2 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.76 (CH₃), 14.77 (CH₃), 23.7 (CH₂),⁸⁰ 27.1 (CH₂),⁸⁰ 30.4 (CH₂), 30.5 (CH₂),⁸⁰ 30.6 (CH₂),⁸¹ 30.65 (CH₂), 30.67 (CH₂), 30.69 (CH₂), 31.0 (CH₂),⁸⁰ 31.5 (CH₃), 32.3 (CH₂),⁸⁰ 32.9 (CH₂), 35.7 (CH), 52.4 (CH₂), 111.0 (CH), 117.4 (CH), 117.9 (CH), 121.1 (CH), 121.3 (C_{quat}), 121.7 (CH), 122.6 (CH), 124.4 (C_{quat}), 125.2 (CH), 125.9 (CH), 126.3 (C_{quat}), 126.6 (C_{quat}), 126.8 (CH), 127.2 (CH), 128.8 (C_{quat}), 130.29 (C_{quat}), 130.31 (C_{quat}), 131.6 (CH), 132.5 (CH), 137.9 (C_{quat}), 142.0 (C_{quat}), 142.4 (C_{quat}), 144.6 (C_{quat}), 148.4 (C_{quat}), 167.7 (C_{quat}), 193.4 (C_{quat}). MS (MALDI-TOF) calcd for C₅₇H₆₉N₃OS₄ m/z: 939.43; Found: 939.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3059 (w), 2953 (w), 2920 (m), 2851 (m), 1705 (m), 1595 (w), 1578 (m), 1557 (w), 1508 (w), 1481 (m), 1451 (m), 1443 (m), 1425 (w), 1404 (m), 1375 (w), 1335 (m), 1319 (m), 1281 (s), 1256 (m), 1223 (m), 1173 (w), 1161 (w), 1125 (m), 1105 (s), 1044 (w), 1018 (w), 990 (w), 959 (w), 926 (w), 891 (w), 870 (w), 851 (w), 804 (w), 797 (m), 748 (s), 740 (m), 719 (m), 714 (m), 692 (w), 667 (w), 652 (w), 637 (w), 617 (w). Anal calcd for C₅₇H₆₉N₃OS₄ [940.4]: C 72.80, H 7.40, N 4.47; Found: C 72.87, H 7.39, N 4.34.

2.1.5.17. (*Z*)-5-{{[10-(2-Decyltetradecyl)-7-(4-{diphenylamino}phenyl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12q)}



⁸⁰ Two CH₂ signals coincide.

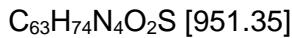
⁸¹ Three CH₂ signals coincide.



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **12q** (383 mg, 84%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 5:1) = 0.51.

^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86–0.92 (m, 6 H), 1.23–1.51 (m, 40 H), 2.06–2.09 (m, 1 H), 3.47 (s, 3 H), 3.94 (d, 3J = 7.0 Hz, 2 H), 7.01–7.16 (m, 10 H), 7.25–7.36 (m, 5 H), 7.40 (d, 4J = 2.1 Hz, 1 H), 7.46 (dt, 3J = 8.3 Hz, 4J = 2.2 Hz, 2 H), 7.49–7.55 (m, 2 H), 7.63 (s, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.6 (CH₃)⁸², 23.4 (CH₂)⁸³, 26.97 (CH₂), 26.99 (CH₂), 30.27 (CH₂)⁸³, 30.33 (CH₂), 30.4 (CH₂), 30.52 (CH₂), 30.54 (CH₂)⁸³, 30.57 (CH₂)⁸³, 30.61 (CH₂), 30.82 (CH₂), 30.84 (CH₂), 31.5 (CH₃), 32.2 (CH₂)⁸³, 32.8 (CH₂)⁸³, 35.6 (CH), 52.3 (CH₂), 117.4 (CH), 118.0 (CH), 121.1 (C_{quat}), 124.0 (CH), 124.5 (CH), 125.2 (CH), 125.8 (C_{quat}), 126.0 (CH), 126.5 (CH), 126.9 (C_{quat}), 128.0 (2 CH), 128.6 (C_{quat}), 130.2 (CH), 130.3 (CH), 131.6 (CH), 132.7 (CH), 134.3 (C_{quat}), 136.7 (C_{quat}), 143.8 (C_{quat}), 147.9 (C_{quat}), 148.4 (C_{quat}), 148.8 (C_{quat}), 167.9 (C_{quat}), 193.8 (C_{quat}). MS (MALDI-TOF) calcd for C₅₉H₇₃N₃OS₃ *m/z*: 935.49; Found: 935.5 ([M]⁺).

2.1.5.18. (Z)-3-{10-(2-Decyltetradecyl)-7-[4-(diphenylamino)phenyl]-10*H*-phenothiazin-3-yl}-2-(4-nitrophenyl)acrylonitrile (12r)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 15:1) and drying under vacuo compound **12r** (394 mg, 82%) was obtained as a black amorphous solid, Mp 38–42 °C. R_f (*n*-hexane/acetone 10:1) = 0.23.

^1H NMR (600 MHz, acetone-d₆): δ 0.83 (t, 3J = 7.0 Hz, 3 H), 0.84 (t, 3J = 7.0 Hz, 3 H), 1.14–1.50 (m, 40 H), 1.99–2.04 (m, 1 H), 3.91 (d, 3J = 7.1 Hz, 2 H), 7.02–7.10 (m, 9 H), 7.12 (d, 3J = 8.7 Hz, 1 H), 7.26–7.31 (m, 4 H), 7.38 (d, 4J = 2.1 Hz, 1 H), 7.47 (dd, 3J = 8.5 Hz, 4J = 2.2 Hz, 1 H), 7.50–7.54 (m, 2 H), 7.82 (d, 3J = 7.2 Hz, 1 H), 7.94 (dd, 3J = 8.8 Hz, 4J = 2.2 Hz, 1 H), 7.95–7.99 (m, 3 H), 8.29–8.33 (m, 2 H). ^{13}C NMR (150 MHz, acetone-d₆): δ 14.41 (CH₃), 14.42 (CH₃), 23.34 (CH₂), 23.35 (CH₂), 26.7 (CH₂), 26.8 (CH₂), 30.12 (CH₂)⁸⁴, 30.13 (CH₂), 30.2 (CH₂), 30.35 (CH₂), 30.37 (CH₂), 30.38 (CH₂), 30.41 (CH₂), 30.43 (CH₂), 30.5 (CH₂), 30.60 (CH₂), 30.63 (CH₂), 31.9 (CH₂), 32.0 (CH₂), 32.65 (CH₂), 32.66 (CH₂), 35.5 (CH), 52.2 (CH₂),

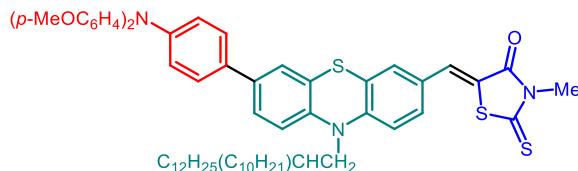
⁸² Two CH₃ signals coincide.

⁸³ Two CH₂ signals coincide.

⁸⁴ Two CH₂ signals coincide.

106.4 (C_{quat}), 177.0 (CH), 118.0 (CH), 118.5 (C_{quat}), 124.0 (CH), 124.5 (CH), 125.1 (CH), 125.2 (CH), 125.7 (C_{quat}), 125.8 (CH), 126.0 (C_{quat}), 126.4 (CH), 127.3 (CH), 127.9 (CH), 128.6 (C_{quat}), 129.5 (CH), 130.3 (CH), 130.9 (CH), 134.2 (C_{quat}), 136.5 (C_{quat}), 142.0 (C_{quat}), 143.8 (C_{quat}), 145.1 (CH), 148.0 (C_{quat}), 148.3 (C_{quat}), 148.5 (C_{quat}), 149.5 (C_{quat}). MS (MALDI-TOF) calcd for C₆₃H₇₄N₄O₂S m/z: 950.55; Found: 950.6 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2953 (w), 2922 (m), 2851 (w), 1591 (w), 1572 (m), 1518 (m), 1493 (m), 1462 (s), 1402 (w), 1337 (s), 1316 (m), 1277 (m), 1271 (m), 1252 (m), 1206 (m), 1175 (w), 1155 (w), 1109 (w), 1074 (w), 1028 (w), 1001 (w), 914 (w), 880 (m), 851 (m), 812 (m), 752 (m), 723 (w), 694 (s), 667 (w). Anal calcd for C₆₃H₇₄N₄O₂S [951.4]: C 79.54, H 7.84, N 5.89; Found: C 79.81, H 7.84, N 5.83.

2.1.5.19. (Z)-5-{{[7-(4-{Bis[4-methoxyphenyl]amino}phenyl)-10-(2-decytetradecyl)-10H-phenothiazin-3-yl)methylene}-3-methyl-2-thioxothiazolidin-4-one (12s)}



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 20:1) and drying under vacuo compound **12s** (417 mg, 83%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.14.

¹H NMR (300 MHz, acetone-d₆): δ 0.85 (t, ³J = 6.7 Hz, 3 H), 0.86 (t, ³J = 6.7 Hz, 3 H), 1.15–1.44 (m, 40 H), 1.95–2.04 (m, 1 H), 3.44 (s, 3 H), 3.78 (s, 6 H), 3.86 (d, ³J = 7.1 Hz, 2 H), 6.85–6.93 (m, 6 H), 7.00–7.09 (m, 6 H), 7.25 (d, ⁴J = 2.1 Hz, 1 H), 7.35 (d, ⁴J = 2.1 Hz, 1 H), 7.38 (dd, ³J = 8.7 Hz, ⁴J = 2.2 Hz, 1 H), 7.40–7.46 (m, 3 H), 7.58 (s, 1 H). ¹³C NMR (75 MHz, acetone-d₆): δ 14.5 (CH₃)⁸⁵ 23.4 (CH₂)⁸⁶ 26.7 (CH₂), 26.8 (CH₂), 30.2 (CH₂)⁸⁷ 30.37 (CH₂), 30.40 (CH₂), 30.42 (CH₂), 30.45 (CH₂)⁸⁶ 30.49 (CH₂), 31.5 (CH₃), 30.60 (CH₂), 30.64 (CH₂), 31.96 (CH₂), 31.98 (CH₂), 32.7 (CH₂)⁸⁶ 35.4 (CH), 52.2 (CH₂), 55.7 (CH₃), 115.6 (CH, C_{quat})⁸⁸ 117.4 (CH), 118.0 (CH), 120.9 (C_{quat}), 121.0 (CH), 125.57 (C_{quat}), 125.61 (CH), 126.1 (CH), 126.7 (C_{quat}), 127.6 (CH, C_{quat})⁸⁹ 128.4 (C_{quat}), 130.3 (CH), 131.5 (CH), 132.7 (CH), 136.9 (C_{quat}), 141.5 (C_{quat}), 143.4 (C_{quat}), 148.8 (C_{quat}), 157.2 (C_{quat}), 168.0 (C_{quat}), 194.0 (C_{quat}). MS (MALDI-TOF) calcd for C₆₁H₇₇N₃O₃S₃ m/z: 995.51; Found: 995.5 ([M]⁺). ESI-HRMS calcd for C₆₁H₇₇N₃O₃S₃: 995.51271; Found: 995.51226 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2920 (m), 2851 (w), 1732 (w), 1709 (w), 1595 (w), 1574 (m), 1503 (s), 1460 (s), 1439 (w), 1423 (w), 1404 (w), 1346 (w),

⁸⁵ Two CH₃ signals coincide.

⁸⁶ Two CH₂ signals coincide.

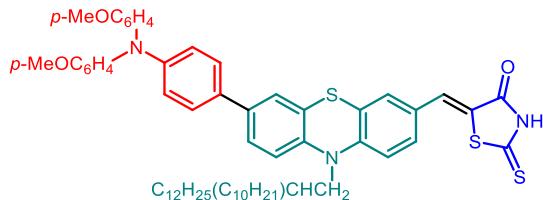
⁸⁷ Four CH₃ signals coincide.

⁸⁸ A CH and a quaternary signal coincide.

⁸⁹ Two CH and a quaternary signal coincide.

1317 (w), 1285 (s), 1238 (s), 1196 (w), 1179 (w), 1165 (w), 1126 (m), 1099 (m), 1036 (m), 990 (w), 959 (w), 901 (w), 883 (w), 826 (m), 812 (m), 766 (w), 718 (w), 694 (w), 660 (w), 638 (w). UV/VIS (CH_2Cl_2) λ_{max} ($\varepsilon \cdot 10^3 [\text{M}^{-1}\text{cm}^{-1}]$) [nm] = 303 (38), 345 (41), 489 (22).

2.1.5.20. (Z)-5-[[7-(4-{Bis[4-methoxyphenyl]amino}phenyl)phenyl]-10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl)methylene]-2-thioxothiazolidin-4-one (12t)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **12t** (400 mg, 79%) was obtained as a black amorphous solid, Mp softening >58 °C, melting >71 °C. R_f (*n*-hexane/ethyl acetate 5:1) = 0.26.

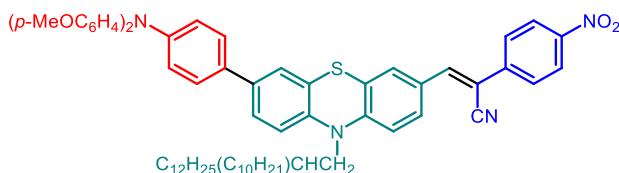
^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.90 (t, $^3J = 6.4$ Hz, 6 H), 1.15–1.54 (m, 40 H), 1.99–2.04 (m, 1 H), 3.79 (s, 6 H), 3.90 (d, $^3J = 6.7$ Hz, 2 H), 6.81–6.96 (m, 6 H), 6.98–7.15 (m, 6 H), 7.27–7.43 (m, 6 H), 7.46 (s, 1 H), 12.00 (br, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.8 (CH₃),⁹⁰ 23.7 (CH₂),⁹¹ 27.1 (CH₂),⁹¹ 30.39 (CH₂), 30.41 (CH₂), 30.49 (CH₂), 30.51 (CH₂), 30.7 (CH₂),⁹² 31.0 (CH₂),⁹¹ 32.25 (CH₂), 32.28 (CH₂), 32.9 (CH₂),⁹¹ 35.7 (CH), 52.3 (CH₂), 55.7 (CH₃), 115.5 (CH), 117.1 (CH), 117.7 (CH), 121.2 (CH), 123.7 (C_{quat}), 125.8 (C_{quat}), 125.8 (CH), 126.1 (CH), 126.9 (C_{quat}), 127.4 (CH), 127.6 (CH), 128.4 (C_{quat}), 130.1 (CH), 131.3 (CH), 131.7 (CH), 132.0 (C_{quat}), 136.9 (C_{quat}), 141.3 (C_{quat}), 143.3 (C_{quat}), 148.6 (C_{quat}), 148.8 (C_{quat}), 156.9 (C_{quat}), 169.1 (C_{quat}), 194.5 (C_{quat}). MS (MALDI-TOF) calcd for C₆₀H₇₅N₃O₃S₃ *m/z*: 981.50; Found: 981.5 ([M]⁺). ESI-HRMS calcd for C₆₀H₇₅N₃O₃S₃: 981.4971; Found: 981.4968 ([M]⁺). IR: IR: $\tilde{\nu}$ [cm⁻¹] = 2988 (w), 2970 (w), 2920 (m), 2851 (w), 1715 (w), 1697 (w), 1593 (w), 1572 (m), 1502 (m), 1460 (s), 1439 (m), 1404 (m), 1319 (w), 1275 (m), 1238 (s), 1175 (s), 1169 (s), 1105 (m), 1052 (m), 1038 (m), 903 (w), 872 (w), 824 (m), 808 (m), 781 (w), 718 (w), 692 (w), 669 (m), 645 (w), 631 (w).

⁹⁰ Two CH₃ signals coincide.

⁹¹ Two CH₂ signals coincide.

⁹² Six CH₂ signals coincide.

2.1.5.21. (*Z*)-3-[7-[4-(Bis{4-methoxyphenyl}amino)phenyl]phenyl]-10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl}-2-(4-nitrophenyl)acrylonitrile (12u)



$C_{65}H_{78}N_4O_4S$ [1011.40]

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/ethyl acetate 25:1) and drying under vacuo compound **12u** (412 mg, 81%) was obtained as a dark red amorphous solid, Mp softening >43 °C, melting >54 °C. R_f (*n*-hexane/ethyl acetate 5:1) = 0.49.

1H NMR (600 MHz, acetone-d₆): δ 0.83 (t, 3J = 6.8 Hz, 3 H), 0.84 (t, 3J = 6.8 Hz, 3 H), 1.13–1.49 (m, 40 H), 1.98–2.05 (m, 1 H), 3.77 (s, 6 H), 3.88 (d, 3J = 7.0 Hz, 2 H), 6.87–6.91 (m, 6 H), 7.02–7.09 (m, 6 H), 7.34 (d, 4J = 2.2 Hz, 1 H), 7.39–7.47 (m, 3 H), 7.80 (d, 4J = 2.1 Hz, 1 H), 7.90–8.00 (m, 4 H), 8.28–8.34 (m, 2 H). ^{13}C NMR (150 MHz, acetone-d₆): δ 14.43 (CH₃), 14.44 (CH₃), 23.4 (CH₂), ⁹³ 26.75 (CH₂), 26.79 (CH₂), 30.13 (CH₂), ⁹⁴ 30.2 (CH₂), 30.37 (CH₂), 30.39 (CH₂), 30.40 (CH₂), 30.43 (CH₂), 30.44 (CH₂), 30.5 (CH₂), 30.6 (CH₂), 30.7 (CH₂), 31.9 (CH₂), 32.0 (CH₂), 32.7 (CH₂), ⁹³ 35.5 (CH), 52.2 (CH₂), 55.7 (CH₃), 106.4 (C_{quat}), 115.6 (CH), 117.0 (CH), 118.0 (CH), 118.5 (C_{quat}), 121.0 (CH), 125.0 (CH), 125.6 (CH, C_{quat}), ⁹⁵ 126.0 (C_{quat}), 126.1 (CH), 127.3 (CH), 127.6 (CH), ⁹⁶ 128.5 (C_{quat}), 129.5 (CH), 130.8 (CH), 131.8 (C_{quat}), 136.9 (C_{quat}), 141.5 (C_{quat}), 142.0 (C_{quat}), 143.4 (C_{quat}), 145.0 (CH), 148.3 (C_{quat}), 149.1 (C_{quat}), 149.5 (C_{quat}), 157.2 (C_{quat}). MS (MALDI-TOF) calcd for $C_{65}H_{78}N_4O_4S$ *m/z*: 1010.57; Found: 1010.6 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2922 (m), 2851 (w), 2212 (w), 1601 (w), 1572 (m), 1505 (s), 1462 (s), 1439 (m), 1402 (w), 1339 (s), 1319 (m), 1285 (m), 1236 (s), 1206 (m), 1179 (m), 1109 (m), 1036 (m), 1009 (w), 955 (w), 912 (w), 880 (w), 851 (m), 820 (m), 814 (m), 781 (w), 752 (w), 729 (w), 692 (w), 637 (w), 623 (w). Anal calcd for $C_{65}H_{78}N_4O_4S$ [1011]: C 77.19, H 7.77, N 5.54, S 3.17; Found: C 77.07, H 7.67, N 5.50, S 2.99.

⁹³ Two CH₂ signals coincide.

⁹⁴ Three CH₂ signals coincide.

⁹⁵ A CH and a quaternary signal coincide.

⁹⁶ Two CH signals coincide.

2.1.5.22. (Z)-4-{{[7-(4-(Bis{4-methoxyphenyl}amino)phenyl]methylene}-3-methyl-1-phenyl-1H-pyrazol-5[4H]-one (12v)}



C₆₇H₈₂N₄O₃S [1023.46]

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 20:1) and drying under vacuo compound **12v** (376 mg, 72%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.20.

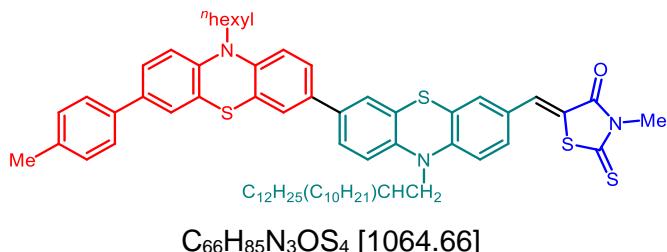
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.82–0.94 (m, 6 H), 1.23–1.51 (m, 40 H), 2.07–2.12 (m, 1 H), 2.32 (s, 3 H), 3.75 (s, 6 H), 3.96 (d, ³J = 7.2 Hz, 2 H), 6.85–6.95 (m, 6 H), 7.02–7.18 (m, 7 H), 7.34–7.46 (m, 6 H), 7.50 (s, 1 H), 8.03–8.08 (m, 2 H), 8.47 (dd, ³J = 8.8 Hz, ⁴J = 2.1 Hz, 1 H), 8.73 (d, ⁴J = 2.0 Hz, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.6 (CH₃), 14.6 (CH₃),⁹⁷ 23.6 (CH₂),⁹⁸ 27.00 (CH₂), 27.01 (CH₂), 30.3 (CH₂),⁹⁸ 30.36 (CH₂), 30.37 (CH₂), 30.55 (CH₂),⁹⁹ 30.57 (CH₂), 30.59 (CH₂), 30.62 (CH₂), 30.9 (CH₂),⁹⁸ 32.1 (CH₂),⁹⁸ 32.8 (CH₂),⁹⁸ 35.7 (CH), 52.4 (CH₂), 55.7 (CH₃), 115.6 (CH), 116.4 (CH), 118.1 (CH), 119.0 (CH), 121.2 (CH), 124.8 (CH), 125.3 (C_{quat}), 125.4 (C_{quat}), 125.7 (CH), 126.0 (C_{quat}), 126.1 (CH), 127.5 (CH), 127.7 (CH), 129.0 (C_{quat}), 129.3 (CH), 131.9 (C_{quat}), 133.7 (CH), 136.1 (CH), 137.2 (C_{quat}), 140.0 (C_{quat}), 141.4 (C_{quat}), 143.0 (C_{quat}), 146.4 (CH), 149.0 (C_{quat}), 151.0 (C_{quat}), 151.7 (C_{quat}), 157.1 (C_{quat}), 162.9 (C_{quat}). MS (MALDI-TOF) calcd for C₆₇H₈₂N₄O₃S m/z: 1022.61; Found: 1022.6 ([M]⁺). ESI-HRMS calcd for C₆₇H₈₂N₄O₃S: 1022.61076; Found: 1022.61107 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3059 (w), 2922 (m), 2851 (w), 2359 (w), 1676 (w), 1613 (w), 1595 (w), 1572 (w), 1559 (w), 1501 (s), 1458 (s), 1441 (w), 1420 (w), 1395 (w), 1317 (m), 1285 (w), 1238 (s), 1215 (s), 1177 (m), 1163 (m), 1138 (m), 1105 (w), 1036 (m), 995 (w), 930 (w), 878 (w), 826 (m), 814 (m), 779 (w), 768 (w), 752 (w), 721 (w), 664 (w), 635 (w).

⁹⁷ Two CH₃ signals coincide.

⁹⁸ Two CH₂ signals coincide.

⁹⁹ Three CH₂ signals coincide.

2.1.5.23. (*Z*)-5-{[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10*H*,10*H*'(3,3'-biphenothiazin)-7-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12w)



According to the GP and after purification by chromatography on silica gel (*n*-hexane/acetone 30:1) and drying under vacuo compound **12w** (446 mg, 80%) was obtained as a black resin. R_f (*n*-hexane/acetone 10:1) = 0.45.

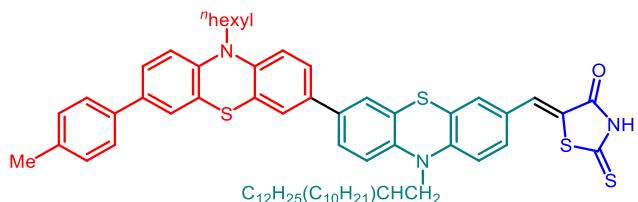
^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.85–0.97 (m, 9 H), 1.19–1.60 (m, 46 H), 1.87 (quin, 3J = 7.7 Hz, 2 H), 1.99–2.04 (m, 1 H), 2.37 (s, 3 H), 3.47 (s, 3 H), 3.92 (d, 3J = 7.4 Hz, 2 H), 3.96 (t, 3J = 7.1 Hz, 2 H), 6.98 (d, 4J = 2.1 Hz, 1 H), 7.01 (d, 3J = 2.0 Hz, 1 H), 7.06 (d, 3J = 8.5 Hz, 1 H), 7.11 (d, 3J = 8.6 Hz, 1 H), 7.21 (d, 3J = 7.9 Hz, 2 H), 7.30–7.48 (m, 10 H), 7.61 (s, 1 H). ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃), 14.8 (CH₃)¹⁰⁰ 21.4 (CH₃), 23.65 (CH₂), 23.67 (CH₂)¹⁰¹ 27.1 (CH₂)¹⁰¹ 27.5 (CH₂), 27.7 (CH₂), 30.4 (CH₂)¹⁰¹ 30.5 (CH₂)¹⁰¹ 30.6 (CH₂)¹⁰² 30.67 (CH₂), 30.69 (CH₂), 31.0 (CH₂)¹⁰¹ 31.5 (CH₃), 32.3 (CH₂)¹⁰¹ 32.5 (CH₂), 32.9 (CH₂)¹⁰¹ 35.7 (CH), 48.1 (CH₂), 52.4 (CH₂), 116.49 (CH), 116.51 (CH), 117.2 (CH), 117.8 (CH), 121.1 (C_{quat}), 125.4 (C_{quat}), 125.65 (CH), 125.66 (C_{quat}), 125.8 (C_{quat}), 125.9 (CH), 126.0 (CH), 126.1 (CH), 126.3 (CH), 126.5 (CH), 126.9 (C_{quat}), 127.0 (CH), 128.6 (C_{quat}), 130.2 (CH), 130.3 (CH), 131.6 (CH), 132.6 (CH), 134.5 (C_{quat}), 136.0 (C_{quat}), 136.1 (C_{quat}), 137.2 (C_{quat}), 137.7 (C_{quat}), 143.8 (C_{quat}), 144.6 (C_{quat}), 144.9 (C_{quat}), 148.7 (C_{quat}), 167.7 (C_{quat}), 193.3 (C_{quat}). MS (MALDI-TOF) calcd for C₆₆H₈₅N₃OS₄ *m/z*: 1063.56; Found: 1063.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2953 (w), 2920 (m), 2851 (m), 1711 (m), 1595 (w), 1574 (m), 1456 (s), 1418 (w), 1404 (w), 1377 (w), 1339 (m), 1287 (m), 1252 (m), 1221 (m), 1198 (w), 1126 (m), 1099 (m), 1063 (w), 1040 (w), 990 (w), 959 (w), 901 (w), 874 (w), 804 (m), 721 (w). Anal calcd for C₆₆H₈₅N₃OS₄ [1065]: C 74.46, H 8.05, N 3.95, S 12.05; Found: C 74.55, H 8.04, N 3.83, S 12.03.

¹⁰⁰ Two CH₃ signals coincide.

¹⁰¹ Two CH₂ signals coincide.

¹⁰² Four CH₂ signals coincide.

2.1.5.24. (*Z*)-5-{[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10*H*,10*H*'-*(3,3'*-biphenothiazin)-7-yl]methylene}-2-thioxothiazolidin-4-one (12x)



C₆₅H₈₃N₃OS₄ [1050.63]

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **12x** (520 mg, 89%) was obtained as a black amorphous solid, Mp 57–63 °C. R_f (*n*-hexane/acetone 1:1) = 0.76.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.86–0.95 (m, 9 H), 1.21–1.58 (m, 46 H), 1.87 (quin, ³J = 7.5 Hz, 2 H), 1.99–2.04 (m, 1 H), 2.37 (s, 3 H), 3.92 (d, ³J = 7.1 Hz, 2 H), 3.96 (t, ³J = 7.1 Hz, 2 H), 6.98 (d, ⁴J = 1.7 Hz, 1 H), 7.01 (d, ⁴J = 1.7 Hz, 1 H), 7.06 (d, ³J = 8.5 Hz, 1 H), 7.11 (d, ³J = 8.7 Hz, 1 H), 7.18–7.24 (m, 2 H), 7.30–7.47 (m, 10 H), 7.48 (s, 1 H), 12.11 (br, 1 H).

¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 14.7 (CH₃), 14.8 (CH₃),¹⁰³ 21.4 (CH₃), 23.66 (CH₂), 23.67 (CH₂),¹⁰⁴ 27.1 (CH₂),¹⁰⁴ 27.5 (CH₂), 27.7 (CH₂), 30.4 (CH₂),¹⁰⁴ 30.5 (CH₂),¹⁰⁴ 30.63 (CH₂), 30.64 (CH₂), 30.66 (CH₂),¹⁰⁵ 30.69 (CH₂), 31.0 (CH₂),¹⁰⁴ 32.3 (CH₂),¹⁰⁴ 32.5 (CH₂), 32.9 (CH₂),¹⁰⁴ 35.7 (CH), 48.1 (CH₂), 52.3 (CH₂), 116.5 (CH),¹⁰⁶ 117.2 (CH), 117.8 (CH), 123.8 (C_{quat}), 125.4 (C_{quat}), 125.7 (CH), 125.7 (C_{quat}), 125.9 (C_{quat}, CH),¹⁰⁷ 126.9 (CH), 126.1 (CH), 126.3 (CH), 126.5 (CH), 126.9 (C_{quat}), 127.0 (CH), 128.5 (C_{quat}), 130.1 (CH), 130.3 (CH), 131.4 (CH), 131.7 (CH), 134.5 (C_{quat}), 136.0 (C_{quat}), 136.1 (C_{quat}), 137.2 (C_{quat}), 137.7 (C_{quat}), 143.8 (C_{quat}), 144.6 (C_{quat}), 144.9 (C_{quat}), 148.6 (C_{quat}), 169.1 (C_{quat}), 194.6 (C_{quat}). MS (MALDI-TOF) calcd for C₆₅H₈₃N₃OS₄ m/z: 1049.54; Found: 1049.6 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2951 (w), 2920 (m), 2851 (w), 1690 (w), 1591 (w), 1570 (m) 1543 (w), 1458 (s), 1402 A(m), 1375 (w), 1335 (w), 1275 (w), 1250 (m), 1231 (m), 1182 (s), 1169 (s), 1105 (w), 1065 (w), 1038 (w), 1017 (w), 939 (w), 903 (w), 874 (w), 802 (m), 724 (w), 721 (w), 667 (m), 638 (w). Anal calcd for C₆₅H₈₃N₃OS₄ [1051]: C 74.31, H 7.96, N 4.00, S 12.21; Found: C 74.08, H 7.92, N 3.93, S 12.29.

¹⁰³ Two CH₃ signals coincide.

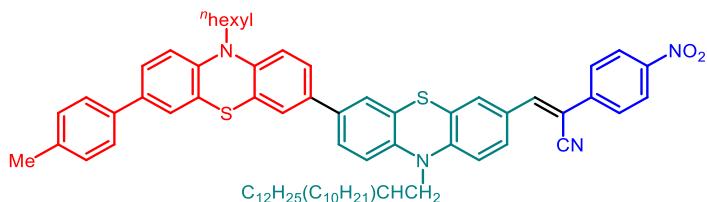
¹⁰⁴ Two CH₂ signals coincide.

¹⁰⁵ Three CH₂ signals coincide.

¹⁰⁶ Two CH signals coincide.

¹⁰⁷ A CH and quaternary signal coincide.

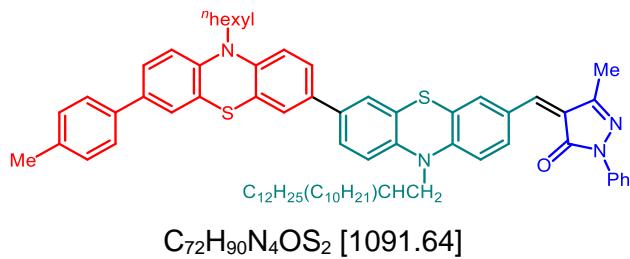
2.1.5.25. (*Z*)-3-[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10*H*,10*H*'(3,3'-biphenothiazin)-7-yl]-2-(4-nitrophenyl)acrylonitrile (12y)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **12y** (436 mg, 79%) was obtained as a dark red amorphous solid, Mp 62–64 °C. R_f (*n*-hexane/acetone 10:1) = 0.24.

1H NMR (600 MHz, acetone-d₆): δ 0.79–0.87 (m, 9 H), 1.13–1.47 (m, 46 H), 1.79 (quin, 3J = 7.8 Hz, 2 H), 1.99–2.04 (m, 1 H), 2.33 (s, 3 H), 3.86 (d, 3J = 7.2 Hz, 2 H), 3.89 (t, 3J = 7.1 Hz, 2 H), 6.95–7.01 (m, 2 H), 7.04 (d, 3J = 8.6 Hz, 1 H), 7.06 (d, 3J = 8.6 Hz, 1 H), 7.20 (d, 3J = 7.9 Hz, 2 H), 7.31–7.35 (m, 3 H), 7.36–7.43 (m, 3 H), 7.45–7.47 (m, 2 H), 7.77 (d, 4J = 2.1 Hz, 1 H), 7.87–7.96 (m, 4 H), 8.24–8.30 (m, 2 H). ^{13}C NMR (150 MHz, acetone-d₆): δ 14.35 (CH₃), 14.44 (CH₃), 14.45 (CH₃), 21.1 (CH₃), 23.35 (CH₂), 23.37 (CH₂), 23.38 (CH₂), 26.76 (CH₂), 26.81 (CH₂), 27.3 (CH₂), 27.5 (CH₂), 30.15 (CH₂), 30.16 (CH₂), 30.17 (CH₂), 30.20 (CH₂), 30.39 (CH₂), 30.41 (CH₂), 30.42 (CH₂), 30.45 (CH₂), 30.47 (CH₂), 30.51 (CH₂), 30.6 (CH₂), 30.7 (CH₂), 31.9 (CH₂), 32.0 (CH₂), 32.3 (CH₂), 32.68 (CH₂), 32.69 (CH₂), 35.5 (CH), 48.0 (CH₂), 52.2 (CH₂), 106.4 (C_{quat}), 116.6 (CH), 116.7 (CH), 117.0 (CH), 118.0 (CH), 118.5 (C_{quat}), 125.0 (CH), 125.3 (C_{quat}), 125.4 (C_{quat}), 125.6 (CH), 125.69 (C_{quat}), 125.72 (CH), 125.8 (CH), 126.0 (C_{quat}), 126.15 (CH), 126.22 (CH), 126.5 (CH), 126.9 (2 CH), 127.3 (2 CH), 128.5 (C_{quat}), 129.6 (CH), 130.3 (CH), 130.8 (CH), 131.2 (CH), 134.4 (C_{quat}), 135.9 (C_{quat}), 136.0 (C_{quat}), 137.4 (C_{quat}), 137.7 (C_{quat}), 142.0 (C_{quat}), 143.9 (C_{quat}), 144.8 (C_{quat}), 145.0 (C_{quat}), 148.3 (C_{quat}), 149.4 (C_{quat}). MS (MALDI-TOF) calcd for $C_{70}H_{86}N_4O_2S_2$ *m/z*: 1078.62; Found: 1078.6 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2980 (m), 2970 (w), 2959 (w), 2920 (m), 2851 (w), 1576 (m), 1562 (w), 1516 (m), 1505 (w), 1476 (m), 1462 (m), 1402 (w), 1373 (m), 1335 (s), 1312 (m), 1254 (m), 1238 (m), 1209 (m), 1163 (w), 1150 (w), 1109 (m), 1080 (w), 1007 (w), 990 (w), 974 (w), 930 (w), 893 (w), 879 (w), 851 (m), 815 (m), 801 (m), 750 (m), 720 (m), 687 (m), 665 (m), 635 (m). Anal calcd for $C_{70}H_{86}N_4O_2S_2$ [1080]: C 77.88, H 8.03, N 5.19; Found: C 77.62, H 8.05, N 5.02.

2.1.5.26. (*Z*)-4-{[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10H,10'H-(3,3'-biphenothiazin)-7-yl]methylene}-3-methyl-1-phenyl-1H-pyrazol-5[4H]-one (12z)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **12z** (371 mg, 68%) was obtained as a dark red amorphous solid, Mp 55–59 °C. R_f (*n*-hexane/acetone 10:1) = 0.27.

¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1): δ 0.84–0.96 (m, 9 H), 1.19–1.56 (m, 46 H), 1.85 (quin, ³J = 7.5 Hz, 2 H), 2.06–2.11 (m, 1 H), 2.33 (s, 3 H), 2.36 (s, 3 H), 3.90–3.99 (m, 4 H), 7.00 (dd, ³J = 8.5 Hz, ⁴J = 2.4 Hz, 2 H), 7.05 (s, 1 H), 7.08 (d, ⁴J = 1.3 Hz, 1 H), 7.10–7.18 (m, 1 H), 7.21 (d, ³J = 8.0 Hz, 2 H), 7.31–7.51 (m, 11 H), 8.04–8.10 (m, 2 H), 8.48 (dd, ³J = 8.7 Hz, ⁴J = 2.0 Hz, 1 H), 8.70 (d, ⁴J = 2.0 Hz, 1 H). ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1): δ 13.6 (CH₃), 14.6 (CH₃), 14.7 (CH₃),¹⁰⁸ 21.3 (CH₃), 23.6 (CH₂),¹⁰⁹ 27.0 (CH₂),¹¹⁰ 27.4 (CH₂), 27.7 (CH₂), 30.3 (CH₂),¹¹⁰ 30.4 (CH₂),¹¹⁰ 30.59 (CH₂),¹¹¹ 30.63 (CH₂), 30.7 (CH₂), 30.9 (CH₂),¹¹⁰ 32.2 (CH₂),¹¹⁰ 32.4 (CH₂), 32.8 (CH₂),¹¹⁰ 35.7 (CH), 48.1 (CH₂), 52.4 (CH₂), 116.4 (CH), 116.5 (CH), 116.6 (CH), 118.0 (CH), 119.0 (CH), 124.8 (CH), 125.3 (C_{quat}), 125.4 (C_{quat}),¹¹² 125.6 (CH, C_{quat}),¹¹³ 125.8 (CH), 125.9 (CH), 126.1 (C_{quat}), 126.2 (CH), 126.5 (CH), 127.0 (CH), 129.1 (C_{quat}), 129.3 (CH), 130.3 (CH), 133.7 (CH), 134.5 (C_{quat}), 136.0 (CH, C_{quat}),¹¹³ 136.2 (C_{quat}), 137.3 (C_{quat}), 137.7 (C_{quat}), 139.9 (C_{quat}), 143.4 (C_{quat}), 144.7 (C_{quat}), 145.0 (C_{quat}), 146.3 (CH), 150.8 (C_{quat}), 151.7 (C_{quat}), 162.9 (C_{quat}). MS (MALDI-TOF) calcd for C₇₂H₉₀N₄OS₂ m/z: 1090.66; Found: 1090.7 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2953 (w), 2920 (m), 2851 (w), 1678 (w), 1614 (w), 1595 (w), 1574 (w), 1559 (w), 1533 (w), 1497 (w), 1458 (s), 1416 (w), 1375 (w), 1356 (w), 1337 (w), 1317 (m), 1275 (w), 1250 (m), 1215 (w), 1138 (m), 1105 (w), 1057 (w), 1028 (w), 995 (w), 930 (w), 901 (w), 874 (w), 804 (m), 783 (w), 768 (w), 752 (w), 723 (w), 691 (w), 662 (w). Anal calcd for C₇₂H₉₀N₄OS₂ [1092]: C 79.22, H 8.31, N 5.13, S 5.87; Found: C 79.22, H 8.14, N 5.08, S 5.59.

¹⁰⁸ Two CH₃ signals coincide.

¹⁰⁹ Three CH₂ signals coincide.

¹¹⁰ Two CH₂ signals coincide.

¹¹¹ Four CH₂ signals coincide.

¹¹² Two quaternary signals coincide.

¹¹³ A CH and a quaternary signal coincide.

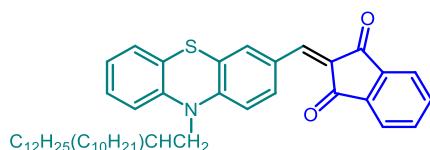
2.2. General Procedure (GP) for the Knoevenagel Condensation Synthesis of Reference Merocyanines 14-17

10-(2-Decyltetradecyl)-10H-phenothiazine-3-carbaldehyde (**13**), CH-acidic compound **7** (1.20 equivs), and a catalytic or equimolar amount of ammonium acetate or diethylamine in a screw-cap Schlenk vessel with a magnetic stir bar were dissolved in a mixture of 1,4-dioxane and acetic acid and heated at 95 °C (oil bath) for 3-8 h (for experimental details, see Table S6). Intensive red to dark violet solutions were formed. After cooling to room temp the reaction mixture was diluted with dichloromethane (25 mL/mmol) and the organic layer was washed with distilled water and saturated sodium sulfite solution until the aqueous phase did not smell like acetic acid. The combined aqueous phases were extracted with dichloromethane and the combined organic layers were dried (anhydrous magnesium sulfate) and the solvents were removed in vacuo. The dark red to violet residue was adsorbed on celite® and purified by flash chromatography on silica gel (*n*-hexane/acetone, toluene or ethyl acetate and gradients thereof) to furnish after drying under high vacuum for one day the chromophores **14-17**.

Table S6. Experimental details of the Knoevenagel condensation synthesis of phenothiazinyl-merocyanines **14-17**.

Entry	Phenothiazinyl aldehyde 13 [mg] (mmol)	methylene active compound 7 [mg] (mmol)	Organic catalyst [mg] (mmol)	1,4-dioxane/AcOH [mL]	Reaction time <i>t</i> [h]	Product [mg] (%) ^[a]
1	260 (0.461)	81 (0.55) of 7c	1 drop of Et ₂ NH 20 (0.25) of NH ₄ OAc 34 (0.44) of NH ₄ OAc	3.0/1.5	3	300 (94) of 14
2	141 (0.250)	44 (0.30) of 7a		2.0/1.0	5	166 (96) of 15
3	247 (0.438)	88 (0.53) of 7f		3.0/1.5	8	302 (97) of 16
4	563 (0.998)	210 (1.20) of 7e	1 drop of Et ₂ NH	4.0/2.0	3	621 (86) of 17

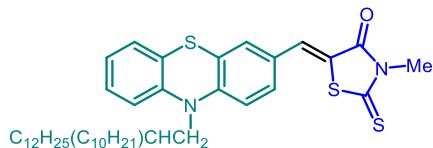
2.2.1. 2-{[10-(2-Decyltetradecyl)-10H-phenothiazin-3-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (**14**)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 40:1) and drying under vacuo compound **14** (300 mg, 94%) was obtained as a red amorphous solid, Mp 65–69 °C. R_f (*n*-hexane/acetone 10:1) = 0.29.

¹H NMR (300 MHz, CD₂Cl₂): δ 0.86 (t, ³J = 6.7 Hz, 3 H), 0.87 (t, ³J = 6.7 Hz, 3 H), 1.12–1.46 (m, 40 H), 1.99 (hep, ³J = 6.5 Hz, 1 H), 3.83 (d, ³J = 7.2 Hz, 2 H), 6.91–7.04 (m, 3 H), 7.14–7.24 (m, 2 H), 7.69 (s, 1 H), 7.75–7.81 (m, 2 H), 7.89–7.99 (m, 2 H), 8.30 (dd, ³J = 8.7 Hz, ⁴J = 2.1 Hz, 1 H), 8.45 (d, ⁴J = 2.0 Hz, 1 H). ¹³C NMR (75 MHz, CD₂Cl₂): δ 14.5 (CH₃),¹¹⁴ 23.3 (CH₂),¹¹⁵ 26.7 (CH₂),¹¹⁵ 29.95 (CH₂), 29.96 (CH₂), 30.0 (CH₂), 30.19 (CH₂),¹¹⁵ 30.20 (CH₂), 30.25 (CH₂),¹¹⁵ 30.29 (CH₂), 30.5 (CH₂),¹¹⁵ 31.9 (CH₂),¹¹⁵ 32.5 (CH₂),¹¹⁵ 35.4 (CH), 52.4 (CH₂), 116.1 (CH), 117.3 (CH), 123.3 (CH), 123.4 (CH), 124.2 (CH), 125.5 (C_{quat}), 125.8 (C_{quat}), 127.1 (C_{quat}), 128.0 (CH), 128.2 (CH), 128.5 (C_{quat}), 133.6 (CH), 135.4 (CH), 135.6 (CH), 135.9 (CH), 140.6 (C_{quat}), 143.0 (C_{quat}), 144.4 (C_{quat}), 145.7 (CH), 151.4 (C_{quat}), 189.9 (C_{quat}), 190.9 (C_{quat}). MS (MALDI-TOF) calcd. for C₄₆H₆₁NO₂S m/z: 691.44; Found: 691.5 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 3055 (w), 2951 (w), 2920 (m), 2849 (m), 1719 (w), 1676 (s), 1609 (w), 1584 (m), 1560 (s), 1535 (m), 1491 (m), 1456 (s), 1422 (w), 1375 (w), 1344 (m), 1328 (m), 1310 (w), 1285 (m), 1250 (w), 1202 (s), 1171 (w), 1155 (m), 1105 (w), 1084 (w), 1040 (w), 1017 (w), 995 (m), 966 (w), 945 (w), 924 (w), 878 (w), 845 (w), 827 (w), 783 (w), 739 (s), 720 (m), 706 (w), 671 (w). Anal. calcd. for C₄₆H₆₁NO₂S [692.1]: C 79.83, H 8.88, N 2.02, S 4.63; Found: C 79.61, H 8.68, N 2.01, S 4.34.

2.2.2. (Z)-5-{[10-(2-Decyltetradecyl)-10H-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (15)



C₄₁H₆₀N₂OS₃ [693.12]

According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/ethyl acetate 40:1) and drying under vacuo compound **15** (166 mg, 96%) was obtained as an orange amorphous solid, Mp 123–128 °C. R_f (*n*-hexane/acetone 10:1) = 0.49. ¹H NMR (300 MHz, acetone-d₆): δ 0.87 (t, ³J = 6.7 Hz, 3 H), 0.88 (t, ³J = 6.7 Hz, 3 H), 1.18–1.47 (m, 40 H), 1.94–2.05 (m, 1 H), 3.45 (s, 3 H), 3.91 (d, ³J = 7.2 Hz, 2 H), 7.01 (dt, ³J = 7.5 Hz, ⁴J = 1.2 Hz, 1 H), 7.07–7.28 (m, 4 H), 7.31 (d, ⁴J = 2.1 Hz, 1 H), 7.42 (dd, ³J = 8.6 Hz, ⁴J = 2.2 Hz, 1 H), 7.61 (s, 1 H). ¹³C NMR (75 MHz, acetone-d₆): δ 14.4 (CH₃),¹¹⁶ 23.4 (CH₂),¹¹⁷ 26.7 (CH₂), 26.8 (CH₂), 30.11 (CH₂), 30.14 (CH₂),¹¹⁷ 30.3 (CH₂), 30.35 (CH₂), 30.39 (CH₂), 30.42 (CH₂),¹¹⁷ 30.43 (CH₂), 30.5 (CH₂), 30.59 (CH₂), 30.62 (CH₂), 31.5 (CH₃), 31.98 (CH₂), 32.00 (CH₂), 32.7 (CH₂),¹¹⁷ 35.4 (CH), 52.2 (CH₂), 117.5 (CH), 117.8 (CH), 121.0 (C_{quat}), 124.4 (CH),

¹¹⁴ Two CH₃ signals coincide.

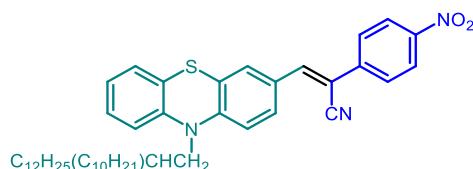
¹¹⁵ Two CH₂ signals coincide.

¹¹⁶ Two CH₃ signals coincide.

¹¹⁷ Two CH₂ signals coincide.

125.2 (C_{quat}), 127.1 (C_{quat}), 128.3 (CH), 128.5 (C_{quat}), 128.6 (CH), 130.2 (CH), 131.5 (CH), 132.6 (CH), 145.2 (C_{quat}), 149.1 (C_{quat}), 168.0 (C_{quat}), 194.1 (C_{quat}). MS (MALDI-TOF) calcd. for C₄₁H₆₀N₂OS₃ *m/z*: 692.39; Found: 692.4 ([M]⁺). IR (KBr): $\tilde{\nu}$ [cm⁻¹] = 3055 (w), 2951 (w), 2916 (m), 2849 (m), 1707 (s), 1587 (m), 1570 (m), 1495 (m), 1458 (s), 1442 (w), 1425 (m), 1402 (m), 1348 (w), 1335 (w), 1285 (s), 1250 (m), 1223 (m), 1169 (w), 1123 (s), 1103 (s), 1037 (w), 991 (w), 959 (w), 937 (w), 895 (w), 853 (w), 804 (w), 772 (w), 752 (m), 741 (m), 719 (w), 677 (w), 651 (w), 611 (w). Anal. calcd. for C₄₁H₆₀N₂OS₃ [693.1]: C 71.05, H 8.73; N 4.04, S 13.88; Found: C 70.91, H 8.72, N 4.01, S 13.73.

2.2.3. (*Z*)-3-(10-(2-Decyltetradecyl)-10*H*-phenothiazin-3-yl)-2-(4-nitrophenyl)acrylonitrile (16)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 30:1) and drying under vacuo compound **15** (302 mg, 97%) was obtained as a dark red resin. R_f (*n*-hexane/acetone 10:1) = 0.37.

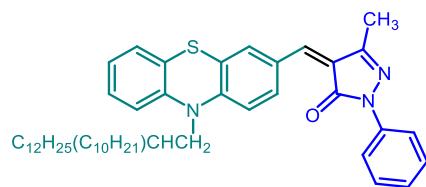
¹H NMR (300 MHz, acetone-d₆): δ 0.86 (t, ³J = 6.4 Hz, 6 H), 1.13–1.53 (m, 40 H), 1.96–2.04 (m, 1 H), 3.94 (d, ³J = 7.2 Hz, 2 H), 6.97–7.28 (m, 5 H), 7.85 (s, 1 H), 7.92–8.03 (m, 4 H), 8.33 (d, ³J = 8.8 Hz, 2 H). ¹³C NMR (75 MHz, acetone-d₆): δ 14.4 (CH₃), ¹¹⁸ 23.3 (CH₂), ¹¹⁹ 26.7 (CH₂), 26.8 (CH₂), 30.1 (CH₂), ¹²⁰ 30.3 (CH₂), ¹¹⁹ 30.36 (CH₂), 30.41 (CH₂), ¹¹⁹ 30.5 (CH₂), 30.60 (CH₂), 30.63 (CH₂), 31.96 (CH₂), 31.99 (CH₂), 32.7 (CH₂), ¹¹⁹ 35.4 (CH), 52.2 (CH₂), 106.5 (C_{quat}), 117.1 (CH), 117.8 (CH), 118.5 (C_{quat}), 124.3 (CH), 125.1 (CH), 125.2 (C_{quat}), 126.5 (C_{quat}), 127.4 (CH), 128.3 (CH), 128.59 (CH), 128.61 (C_{quat}), 129.5 (CH), 130.8 (CH), 142.0 (C_{quat}), 145.1 (CH), 145.2 (C_{quat}), 148.4 (C_{quat}), 149.7 (C_{quat}). MS (MALDI-TOF) calcd. for C₄₅H₆₁N₃O₂S *m/z*: 707.45; Found: 707.4 ([M]⁺). IR: $\tilde{\nu}$ [cm⁻¹] = 2957 (w), 2920 (s), 2851 (m), 2212 (w), 1587 (m), 1566 (s), 1514 (s), 1468 (s), 1456 (s), 1443 (m), 1422 (m), 1402 (s), 1375 (w), 1339 (s), 1285 (w), 1252 (m), 1211 (m), 1194 (w), 1175 (m), 1132 (w), 1109 (m), 1042 (w), 1003 (w), 934 (w), 878 (w), 847 (s), 810 (m), 746 (s), 721 (m), 687 (m), 625 (w). Anal. calcd. for C₄₅H₆₁N₃O₂S [708.1]: C 76.33, H 8.68, N 5.93, S 4.53; Found: C 76.36, H 8.70, N 5.83, S 4.41.

¹¹⁸ Two CH₃ signals coincide.

¹¹⁹ Two CH₂ signals coincide.

¹²⁰ Four CH₂ signals coincide.

2.2.4. (*Z*)-4-{[10-(2-Decyltetradecyl)-10*H*-phenothiazin-3-yl]methylene}-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (17)



According to the GP and after purification by chromatography on silica gel (*n*-hexane, *n*-hexane/acetone 20:1) and drying under vacuo compound **16** (621 mg, 86%) was obtained as a dark red viscous oil, Mp 65–69 °C. R_f (*n*-hexane/acetone 10:1) = 0.18.

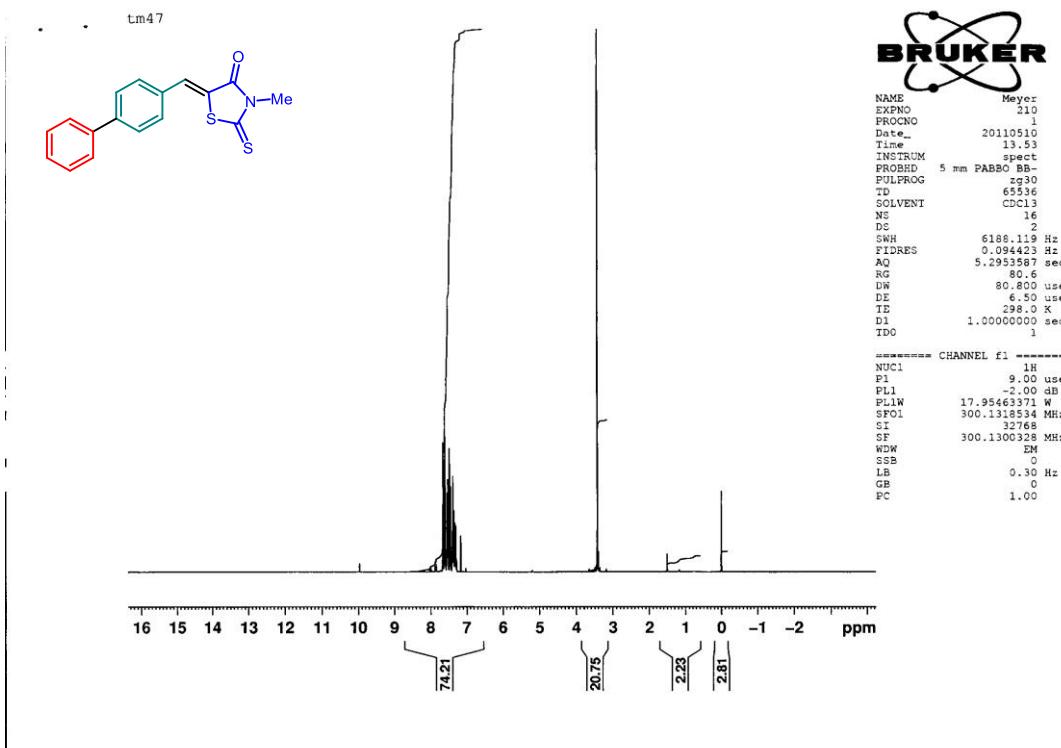
^1H NMR (300 MHz, CD_2Cl_2): δ 0.88 (m, 6 H), 1.16–1.46 (m, 40 H), 2.00 (hep, 3J = 6.4 Hz, 1 H), 2.30 (s, 3 H), 3.82 (d, 3J = 7.1 Hz, 2 H), 6.92–6.98 (m, 2 H), 7.00 (dd, 3J = 7.5 Hz, 4J = 1.1 Hz, 1 H), 7.13–7.21 (m, 3 H), 7.23 (s, 1 H), 7.37–7.45 (m, 2 H), 7.96–8.03 (m, 2 H), 8.38 (dd, 3J = 8.7 Hz, 4J = 2.1 Hz, 1 H), 8.51 (d, 4J = 2.1 Hz, 1 H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 13.7 (CH_3), 14.5 (CH_3),¹²¹ 23.3 (CH_2),¹²² 26.7 (CH_2),¹²² 29.95 (CH_2), 29.96 (CH_2), 30.03 (CH_2),¹²² 30.19 (CH_2),¹²² 30.21 (CH_2), 30.25 (CH_2),¹²² 30.29 (CH_2), 30.5 (CH_2),¹²² 32.0 (CH_2),¹²² 32.5 (CH_2),¹²² 35.4 (CH), 52.4 (CH_2), 116.0 (CH), 117.3 (CH), 119.3 (CH), 124.2 (CH), 124.9 (CH), 125.3 (C_{quat}), 125.5 (C_{quat}), 125.7 (C_{quat}), 128.0 (CH), 128.2 (CH), 128.4 (C_{quat}), 129.2 (CH), 133.3 (CH), 135.2 (CH), 139.4 (C_{quat}), 144.4 (C_{quat}), 145.8 (CH), 151.0 (C_{quat}), 151.5 (C_{quat}), 162.9 (C_{quat}). MS (MALDI-TOF) calcd. for $\text{C}_{47}\text{H}_{65}\text{N}_3\text{OS}-\text{H}^+$ m/z 720.49; Found: 720.5 ([MH] $^+$). IR: $\tilde{\nu}$ [cm^{-1}] = 3059 (w), 2920 (s), 2851 (m), 1721 (w), 1676 (s), 1614 (w), 1586 (m), 1559 (s), 1537 (m), 1495 (m), 1456 (s), 1445 (m), 1418 (w), 1373 (w), 1343 (m), 1317 (s), 1285 (m), 1250 (m), 1215 (s), 1202 (s), 1169 (m), 1138 (m), 1105 (w), 1084 (m), 1061 (w), 1038 (w), 1017 (w), 995 (m), 966 (w), 924 (w), 903 (w), 878 (w), 847 (w), 824 (w), 783 (w), 739 (s), 720 (m), 691 (m), 664 (m), 637 (w), 621 (w). Anal. calcd. for $\text{C}_{47}\text{H}_{65}\text{N}_3\text{OS}$ [720.1]: C 78.39, H 9.10, N 5.84, S 4.45; Found: C 78.63, H 9.29, N 5.82, S 4.52.

¹²¹ Two CH_3 signals coincide.

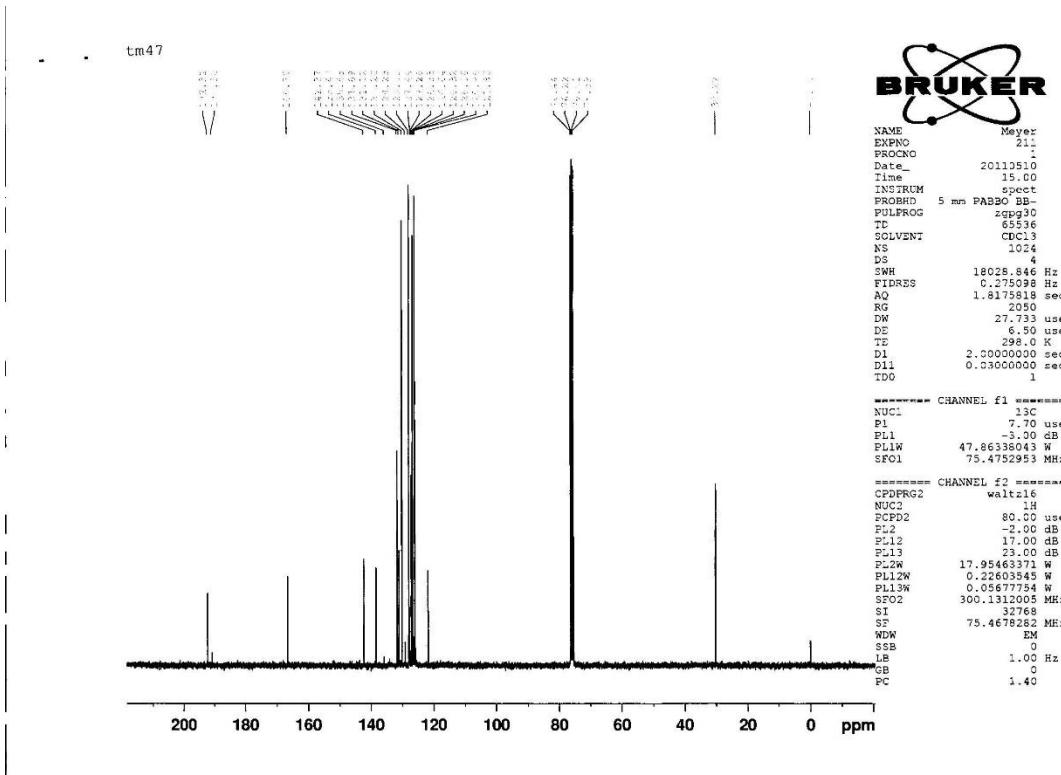
¹²² Two CH_2 signals coincide.

3. ^1H and ^{13}C NMR Spectra

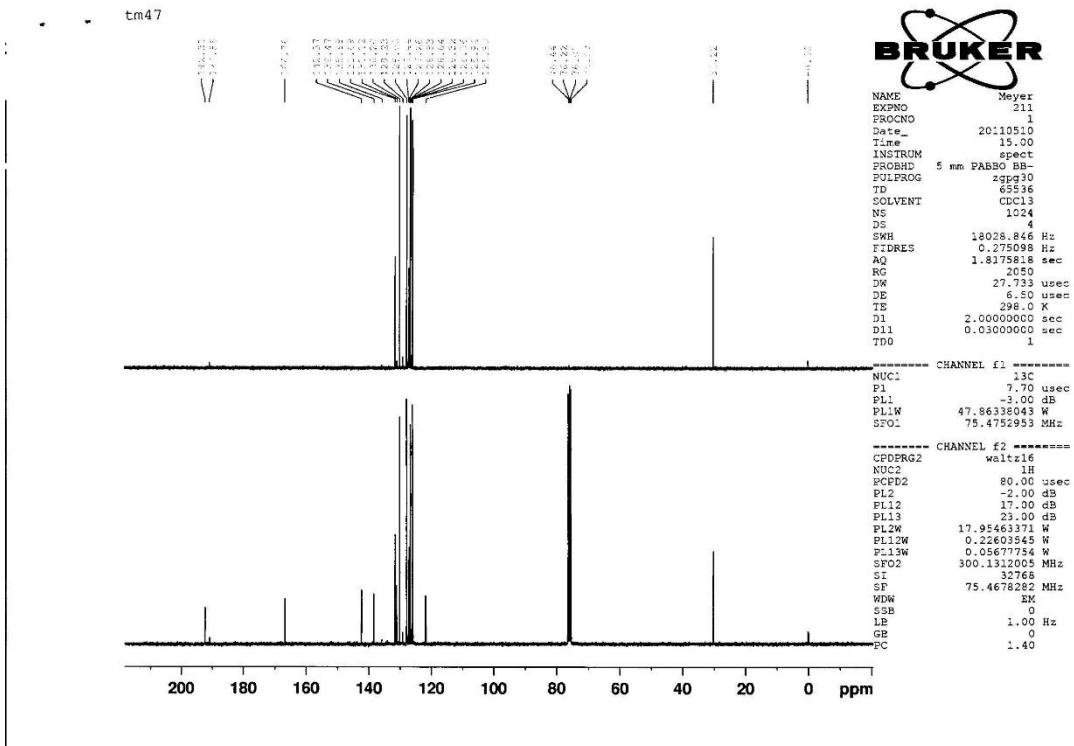
3.1. 5-(Biphenyl-4-ylmethylene)-3-methyl-2-thioxothiazolidin-4-one (8a)



^1H NMR (300 MHz, CDCl_3) of compound 8a.

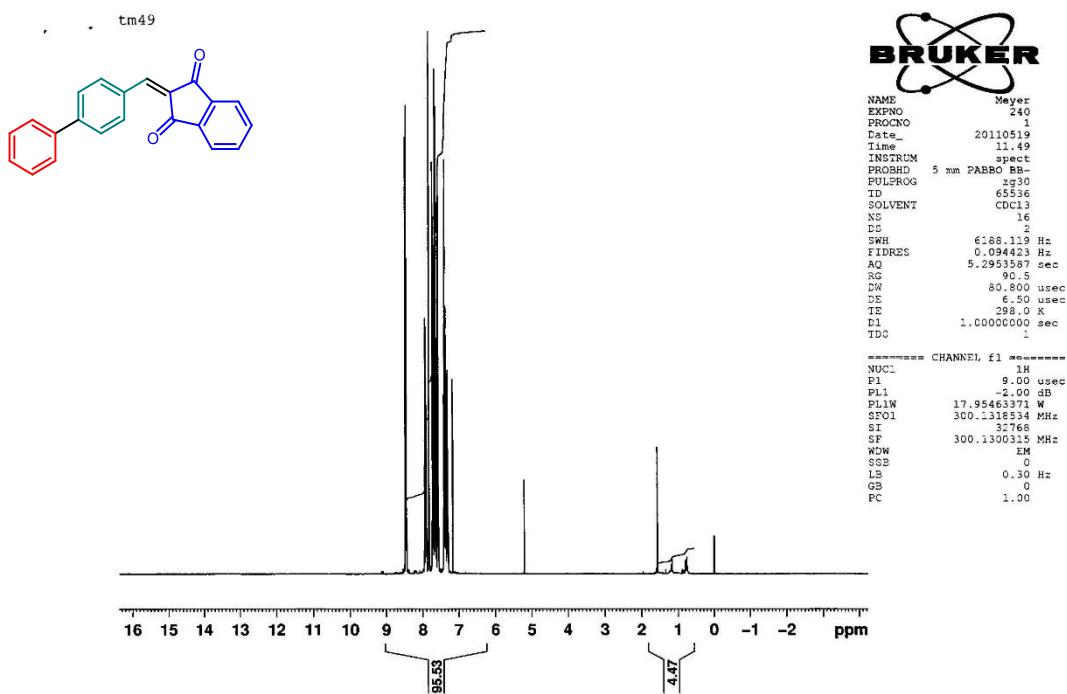


^{13}C NMR (75 MHz, CDCl_3) of compound 8a.

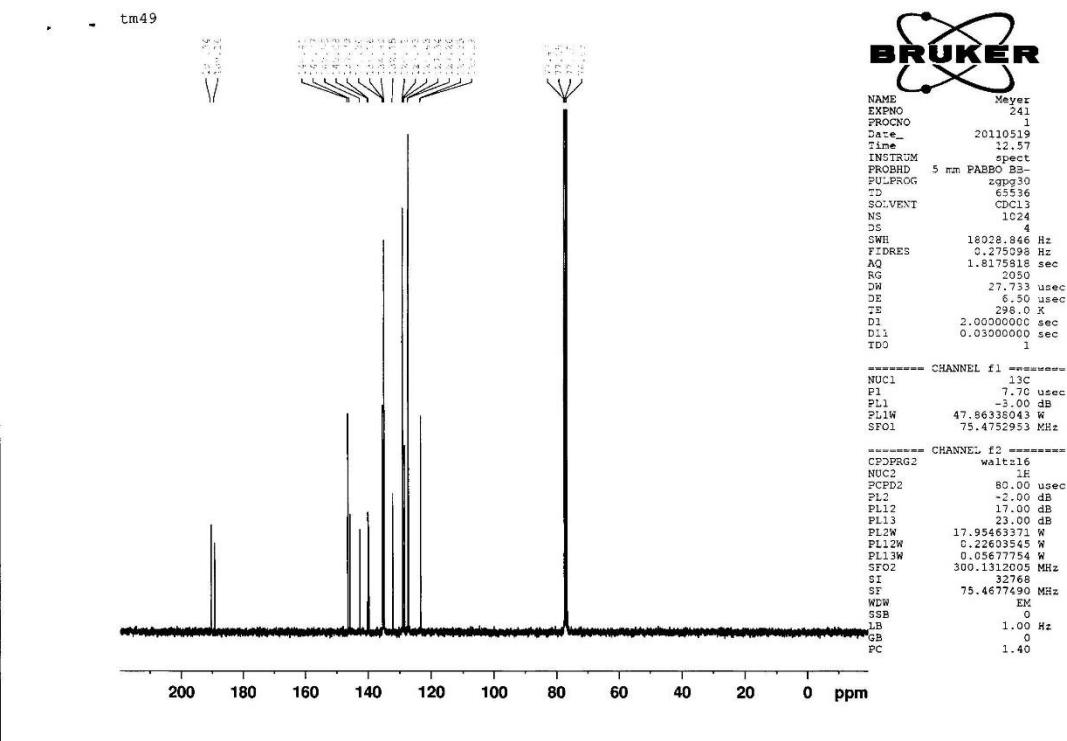


DEPT ^{13}C NMR (75 MHz, CDCl_3) of compound **8a**.

3.2. 2-(Biphenyl-4-ylmethylene)-1*H*-inden-1,3[2*H*]-dione (8b)

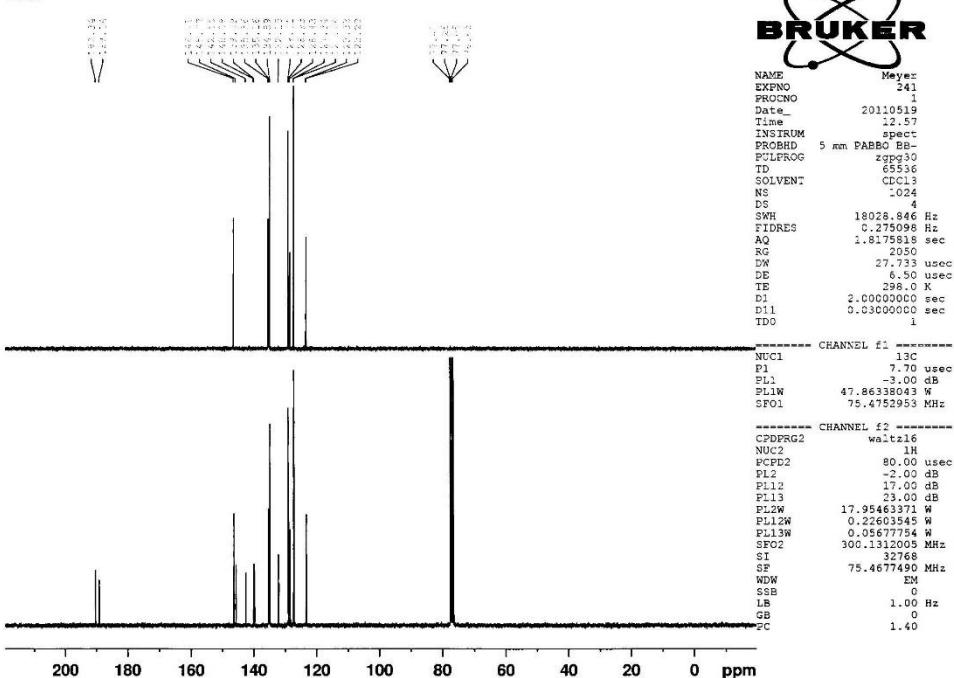


¹H NMR (300 MHz, CDCl₃) of compound 8b.



¹³C NMR (75 MHz, CDCl₃) of compound 8b.

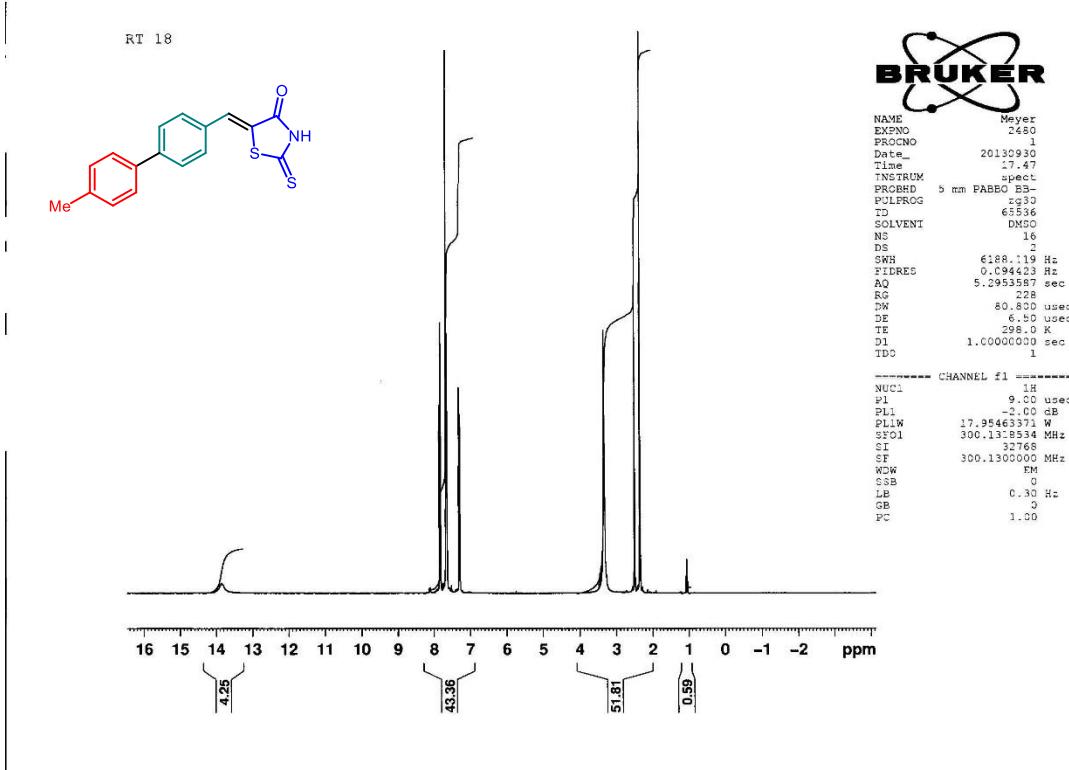
tm49



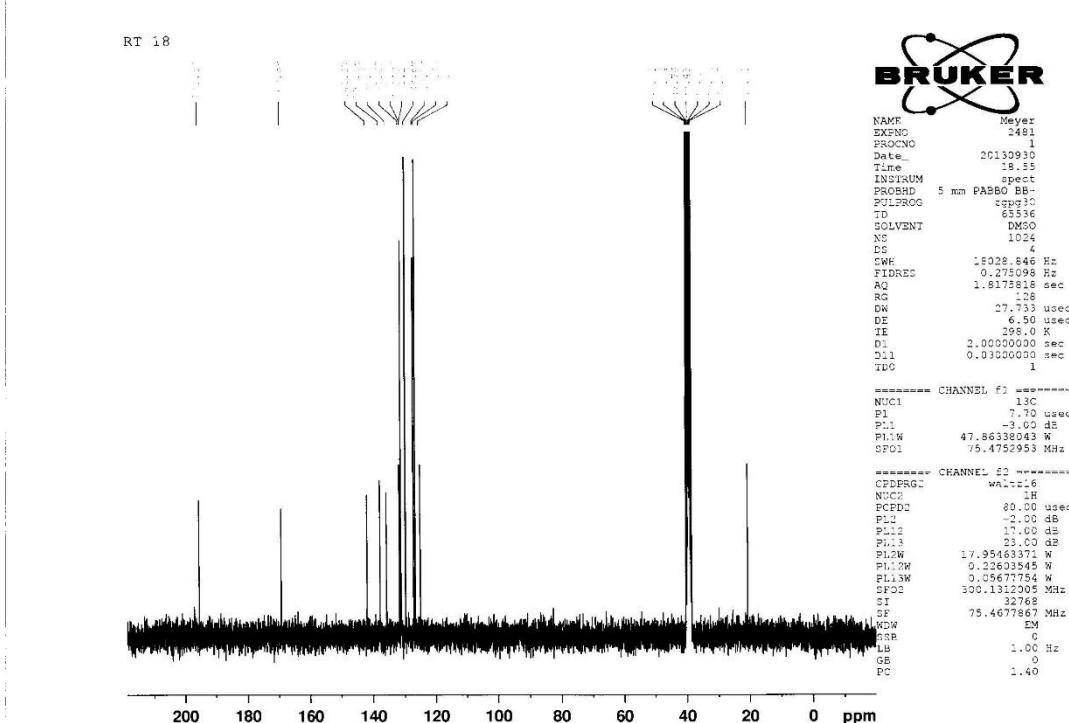
200 180 160 140 120 100 80 60 40 20 0 ppm

DEPT ^{13}C NMR (75 MHz, CDCl_3) of compound **8b**.

3.3. 5-{[4'-Methyl-(1,1'-biphenyl)-4-yl]methylene}-2-thioxothiazolidin-4-one (8c)



¹H NMR (300 MHz, DMSO-d₆) of compound 8c.



¹³C NMR (75 MHz, DMSO-d₆) of compound 8c.

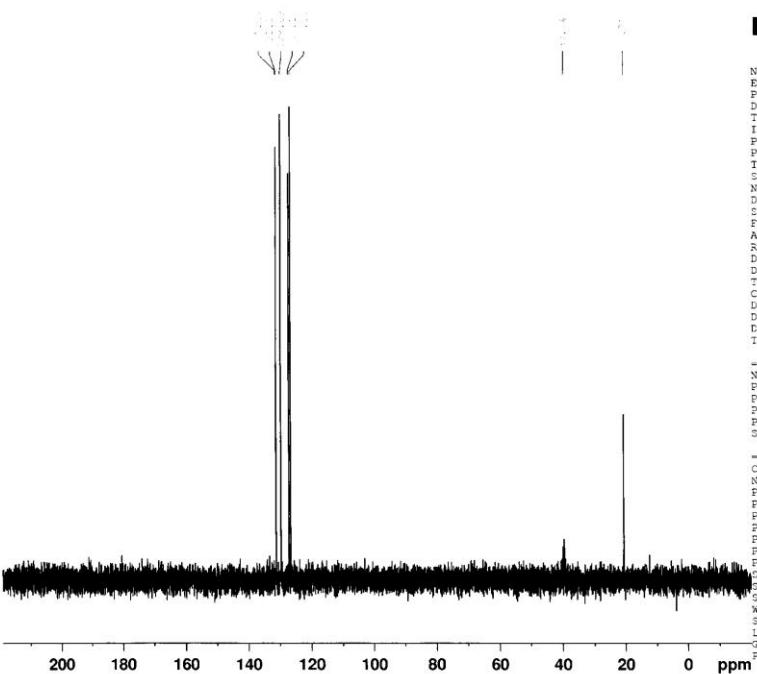
RT 18



NAME Meyer
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PROCNO 1
Date 20130910
Time 19.12
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TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 15028.846 Hz
FIDRES 0.279092 Hz
AQ 1.8173818 sec
RG 2050
DW 27.733 usec
DE 6.50 usec
TE 293.0 K
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D2 0.00344828 sec
D12 0.00032000 sec
TDD 1

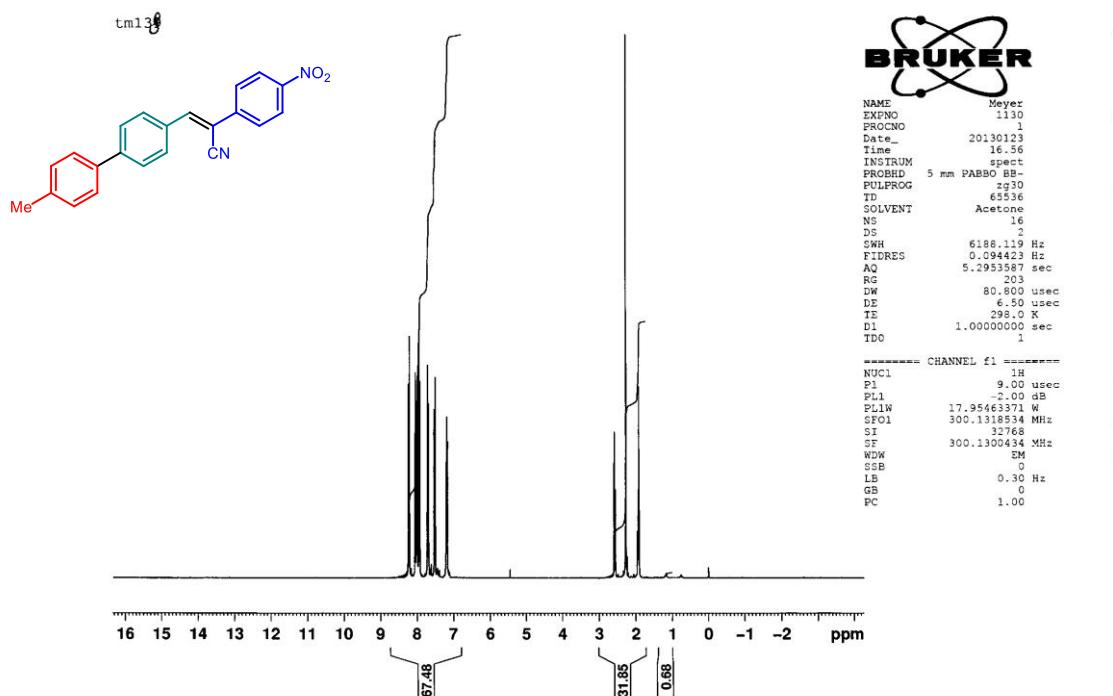
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P1 7.70 usec
P2 15.40 usec
P11 47.86338043 W
SF01 75.4751953 MHz

----- CHANNEL f2 -----
CPDPRG2 waitz16
NUC2 1H
P3 9.00 usec
P4 18.00 usec
PCPD2 80.00 usec
P12 -21.00 dB
P112 17.00 dB
PL2W 17.95463371 W
PL12W 0.22603545 W
CPFO2 300.170000 MHz
SF 32768
SF 75.4677867 MHz
WCW EM
SSB 0
LB 1.00 Hz
DS 1.40
PC

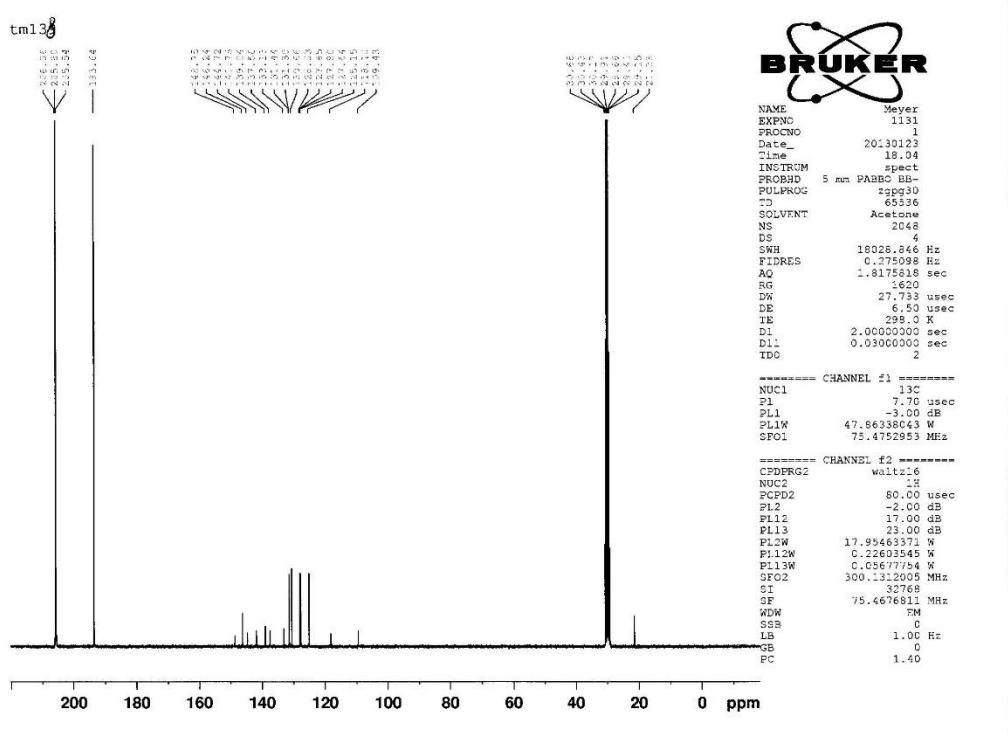


DEPT ^{13}C NMR (75 MHz, DMSO-d₆) of compound **8c**.

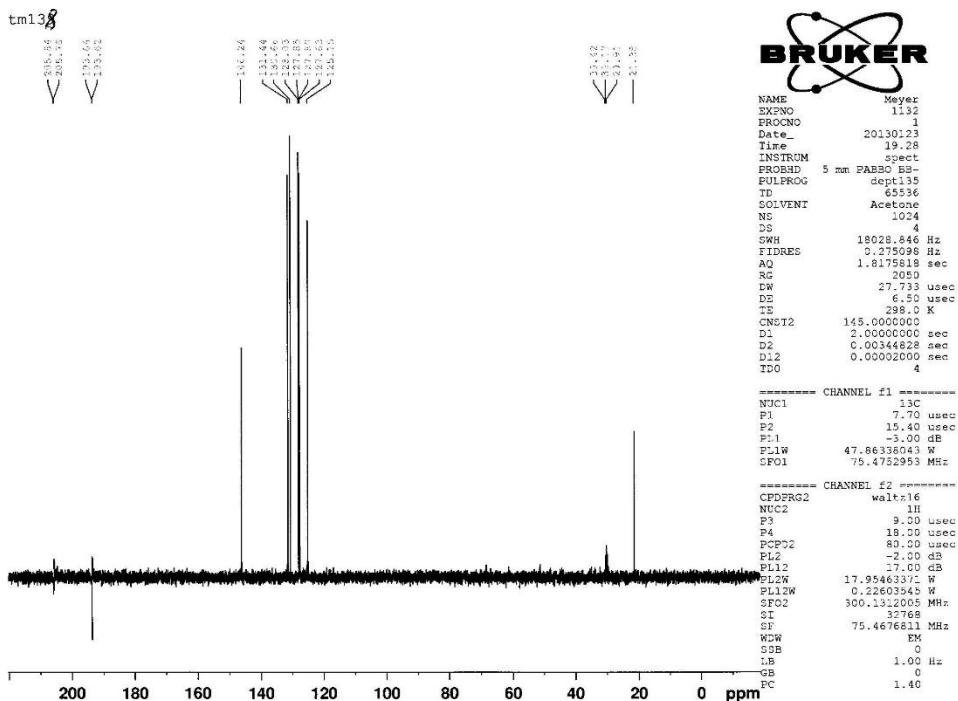
3.4. 3-(4'-Methyl-[1,1'-biphenyl]-4-yl)-2-(4-nitrophenyl)acrylnitrile (8d)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 8d.

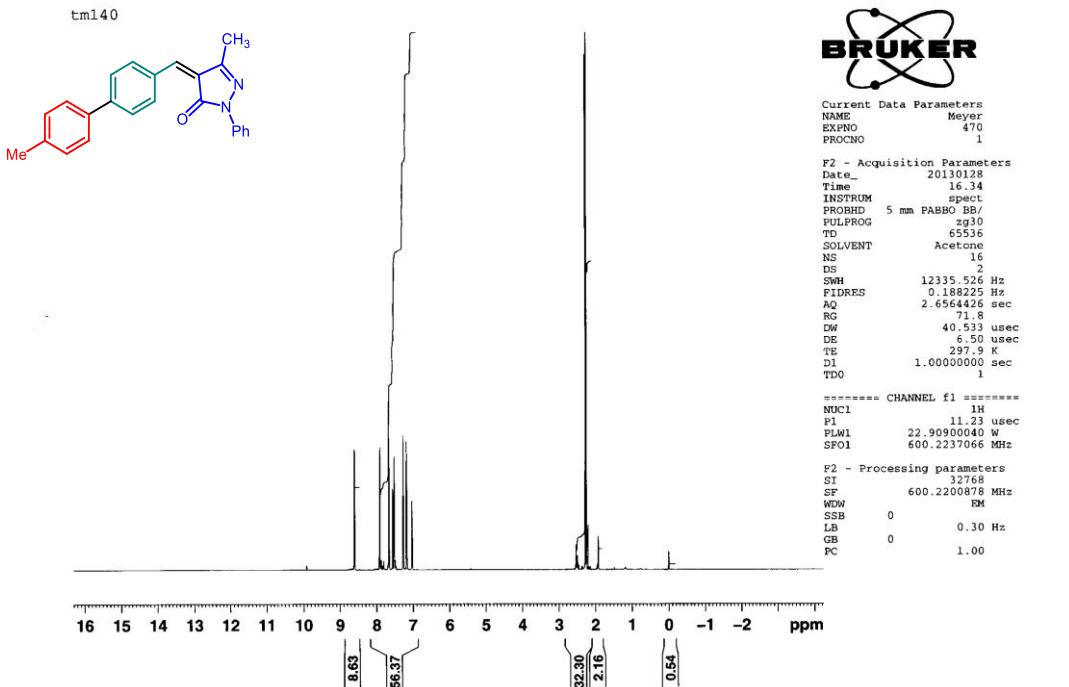


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 8d.

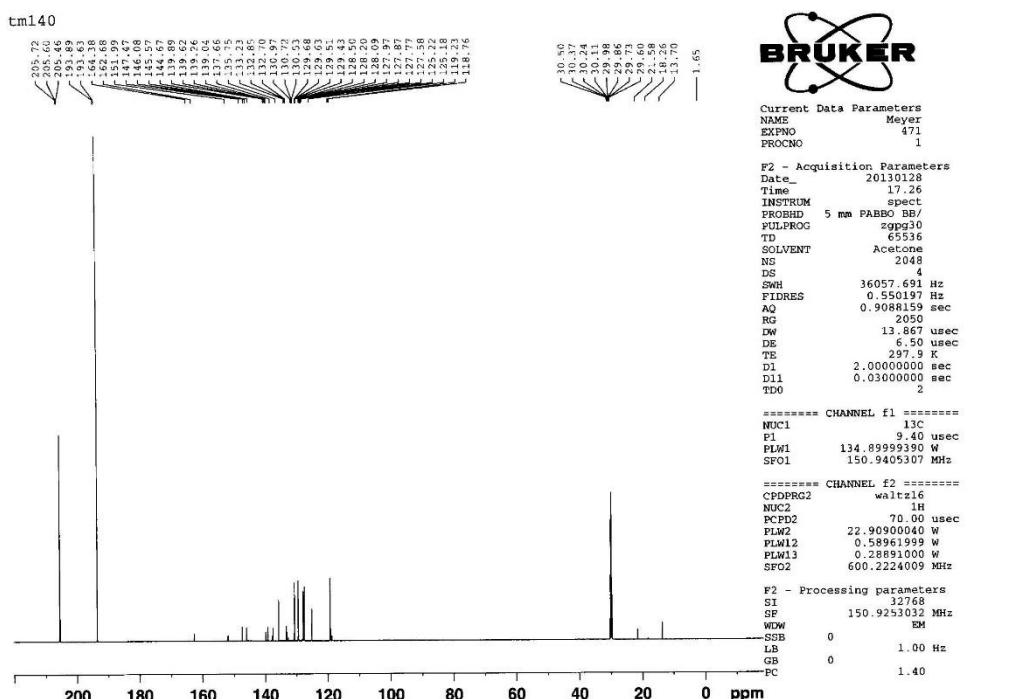


DEPT ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **8d**.

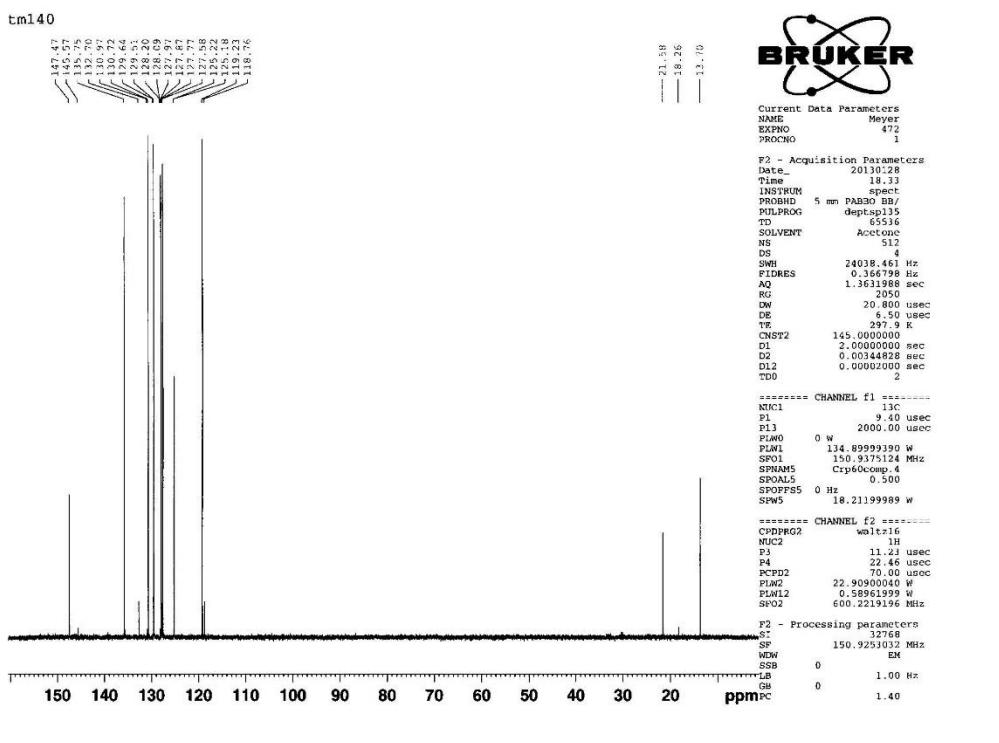
3.5. 3-Methyl-4-{[4'-methyl-(1,1'-biphenyl)-4-yl]methylen}-1-phenyl-1*H*-pyrazol-5[4*H*]-one (8e)



¹H NMR (600 MHz, acetone-d₆/CS₂ 4:1) of compound 8e.

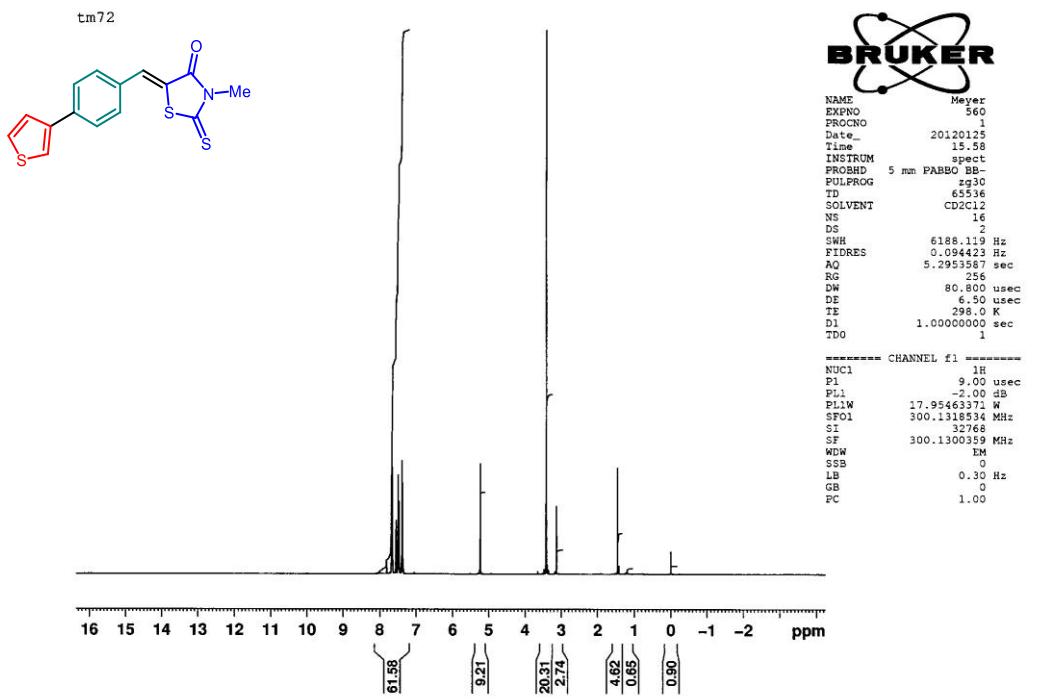


¹³C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound 8e.

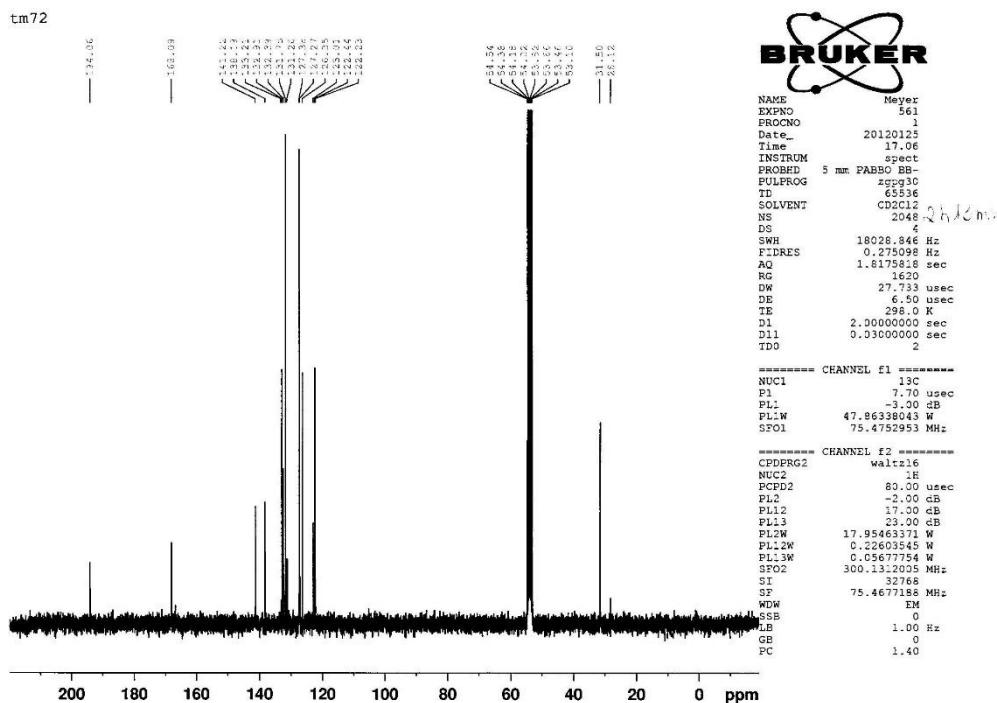


DEPT ^{13}C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound **8e**.

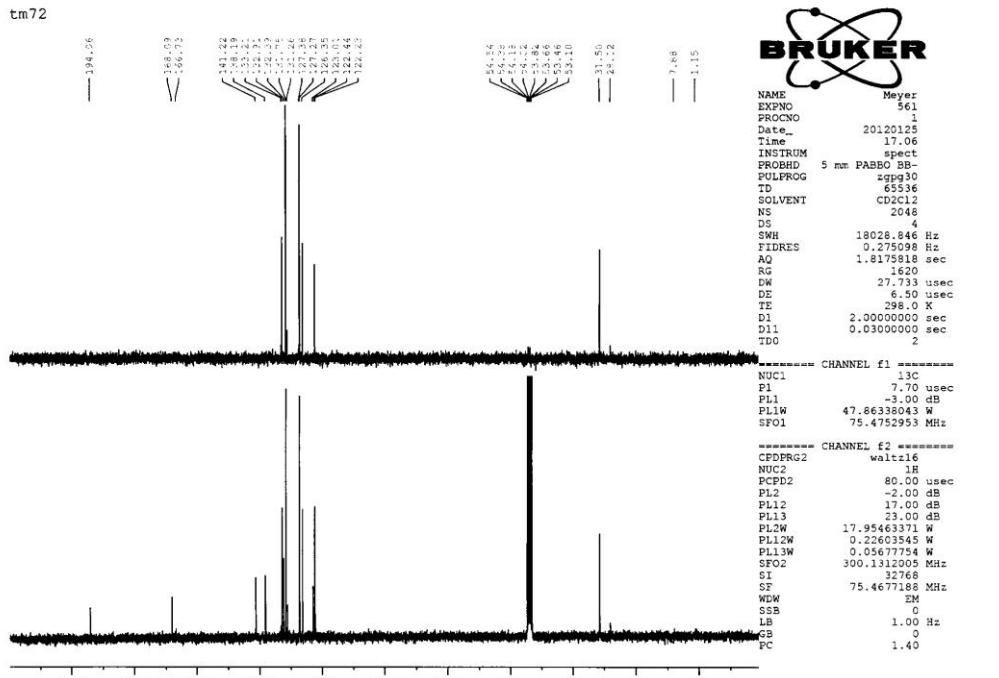
3.6. 3-Methyl-5-(4-(thiophen-3-yl)benzylidene)-2-thioxothiazolidin-4-one (8f)



¹H NMR (300 MHz, CD₂Cl₂) of compound 8f.

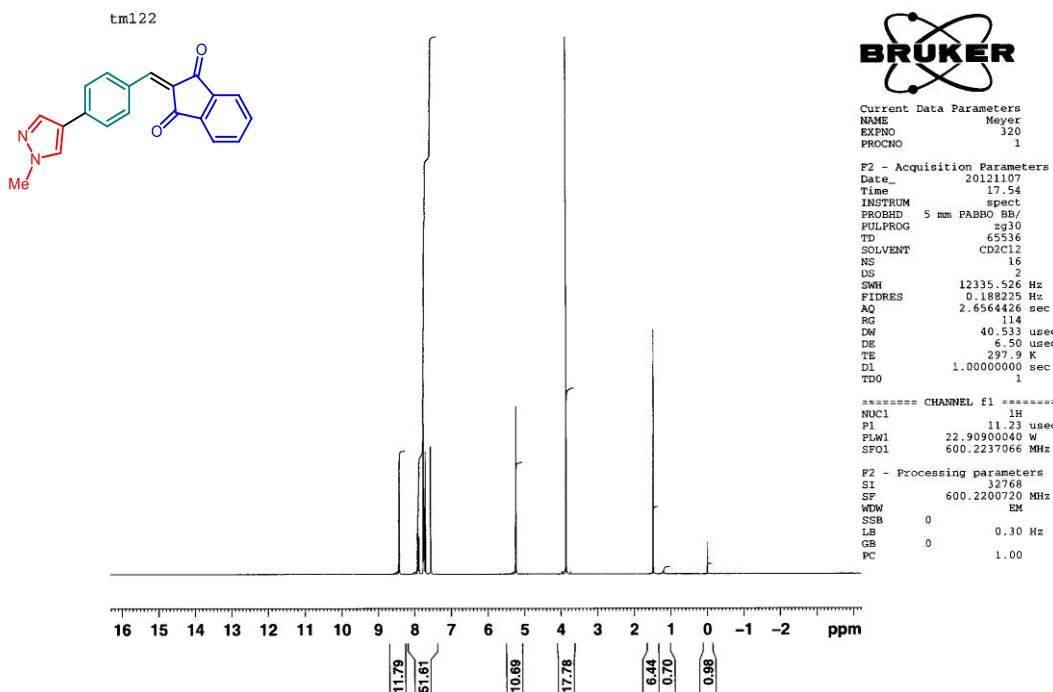


¹³C NMR (75 MHz, CD₂Cl₂) of compound 8f.

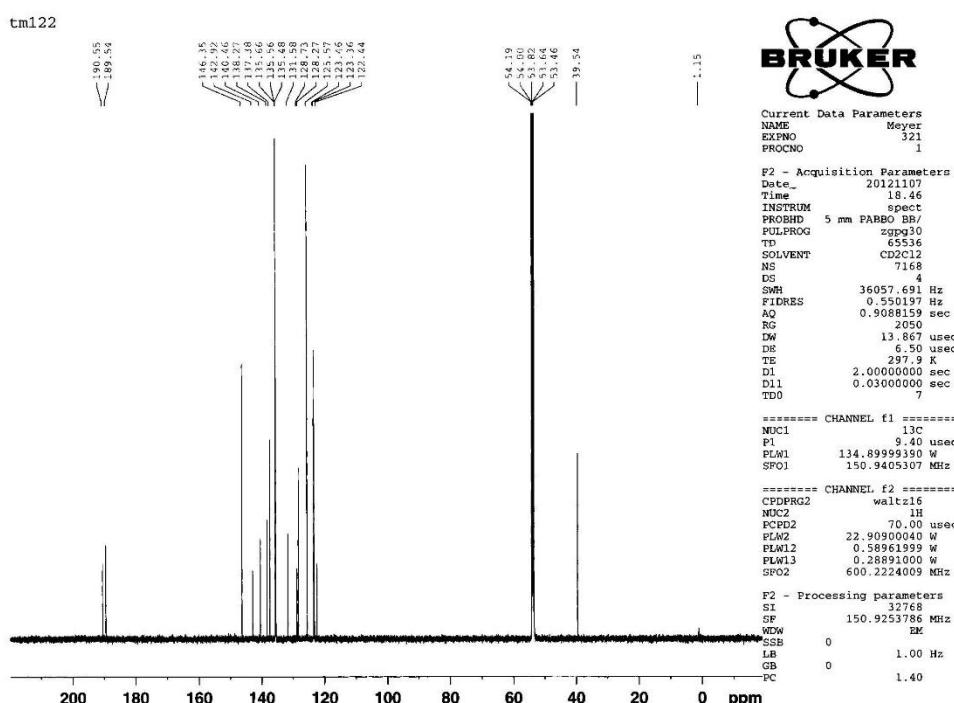


DEPT ¹³C NMR (75 MHz, CD₂Cl₂) of compound **8f**.

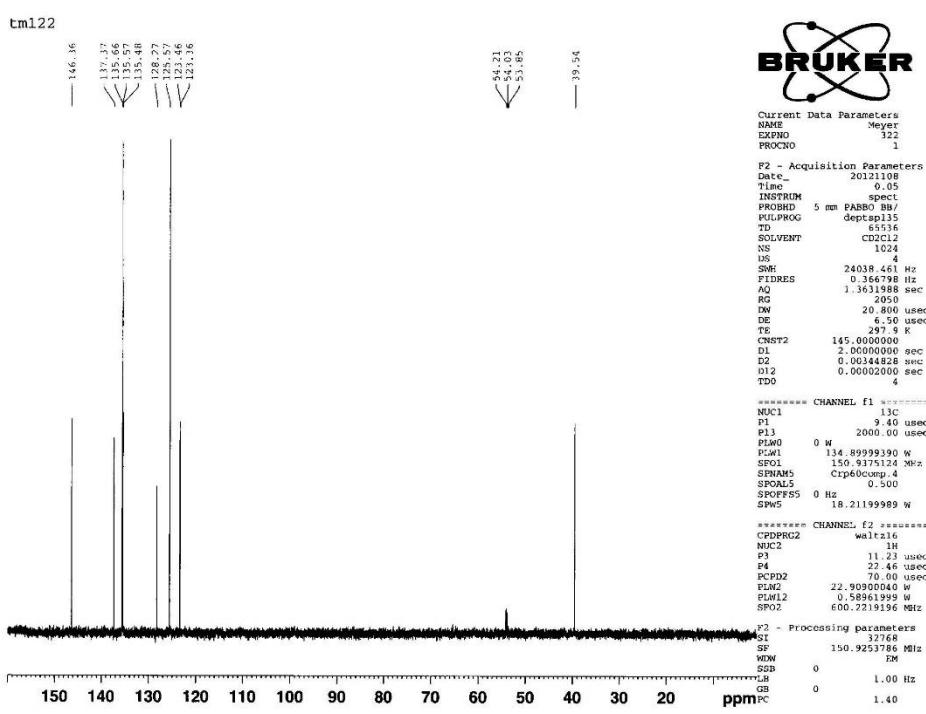
3.7. 2-[4-(1-Methyl-1*H*-pyrazol-4-yl)benzylidene]-1*H*-inden-1,3[2*H*]-dione (8g)



¹H NMR (600 MHz, CD₂Cl₂) of compound 8g.

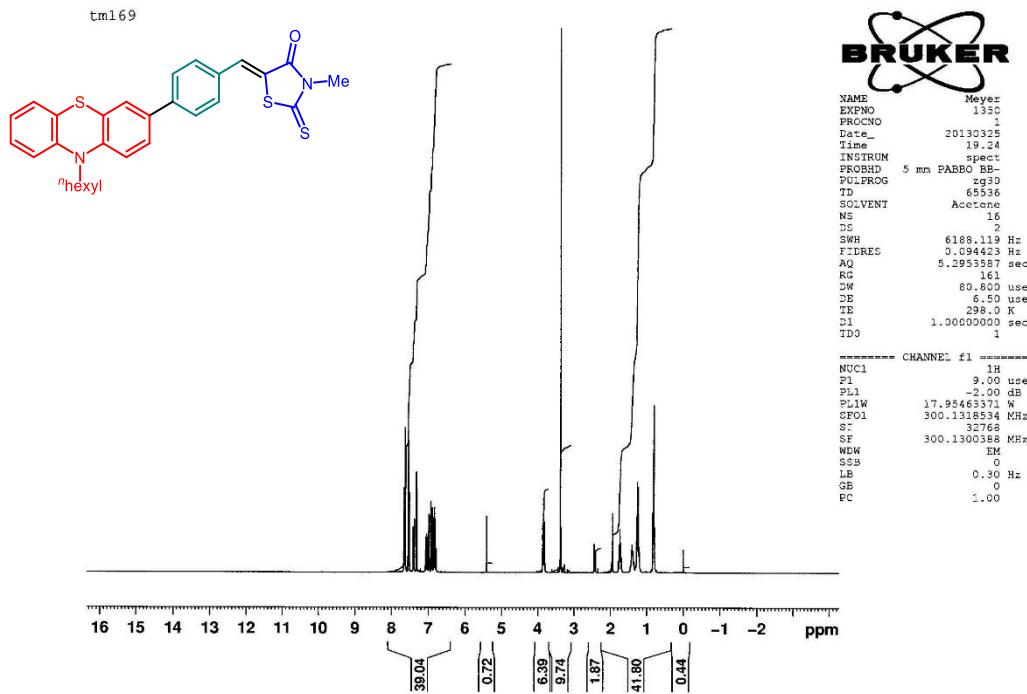


¹³C NMR (150 MHz, CD₂Cl₂) of compound 8g.

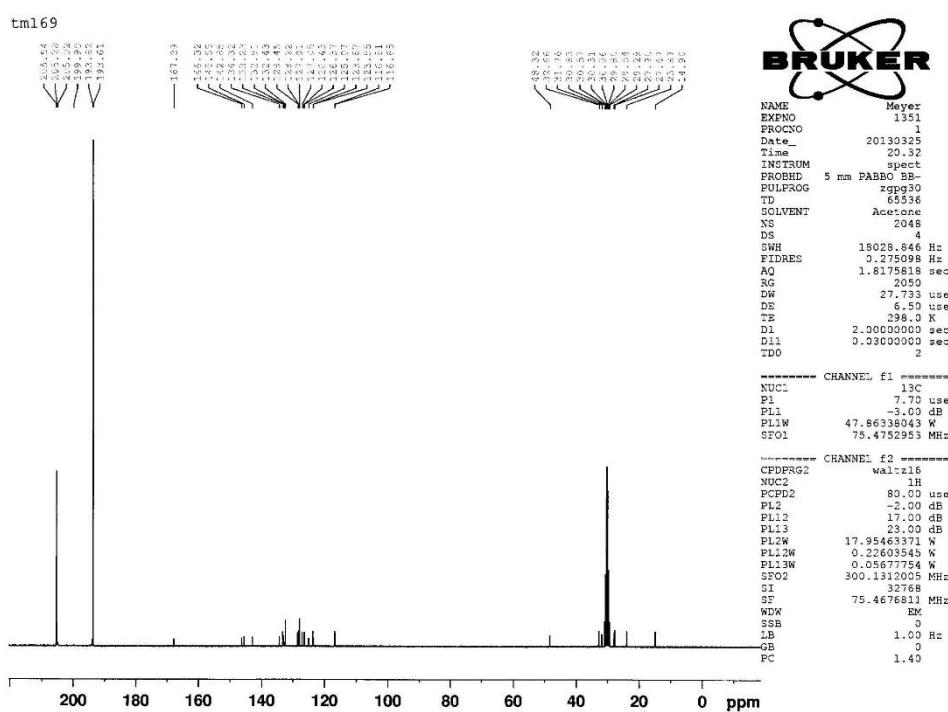


DEPT ¹³C NMR (150 MHz, CD₂Cl₂) of compound **8g**.

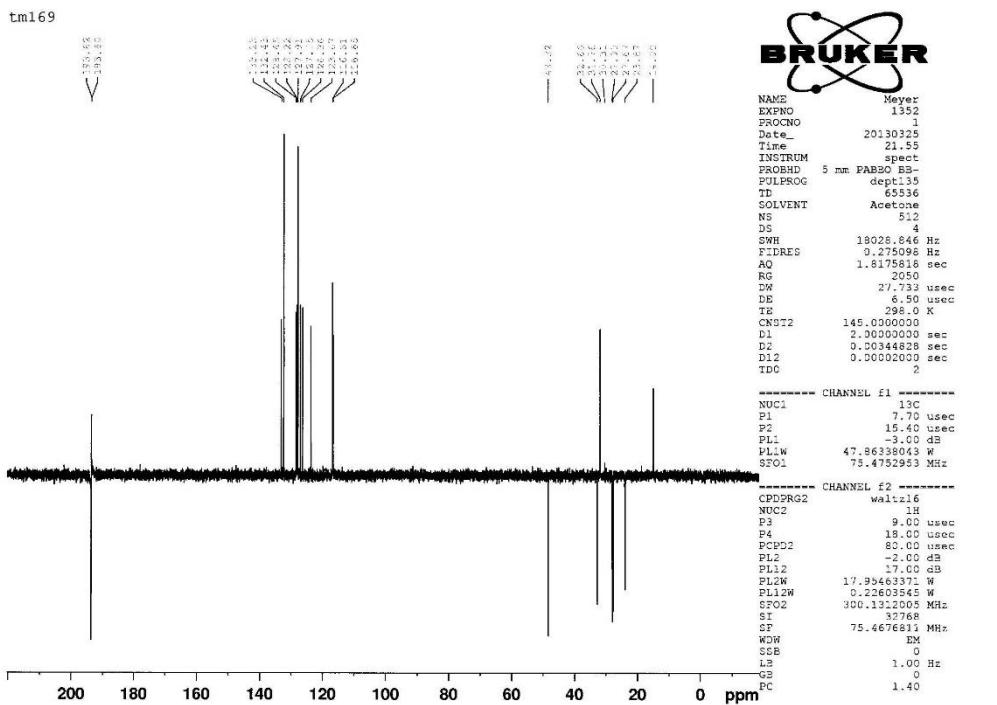
3.8. 5-[4-(10-Hexyl-10*H*-phenothiazin-3-yl)benzylidene]-3-methyl-2-thioxothiazolidin-4-one (8h)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **8h**.

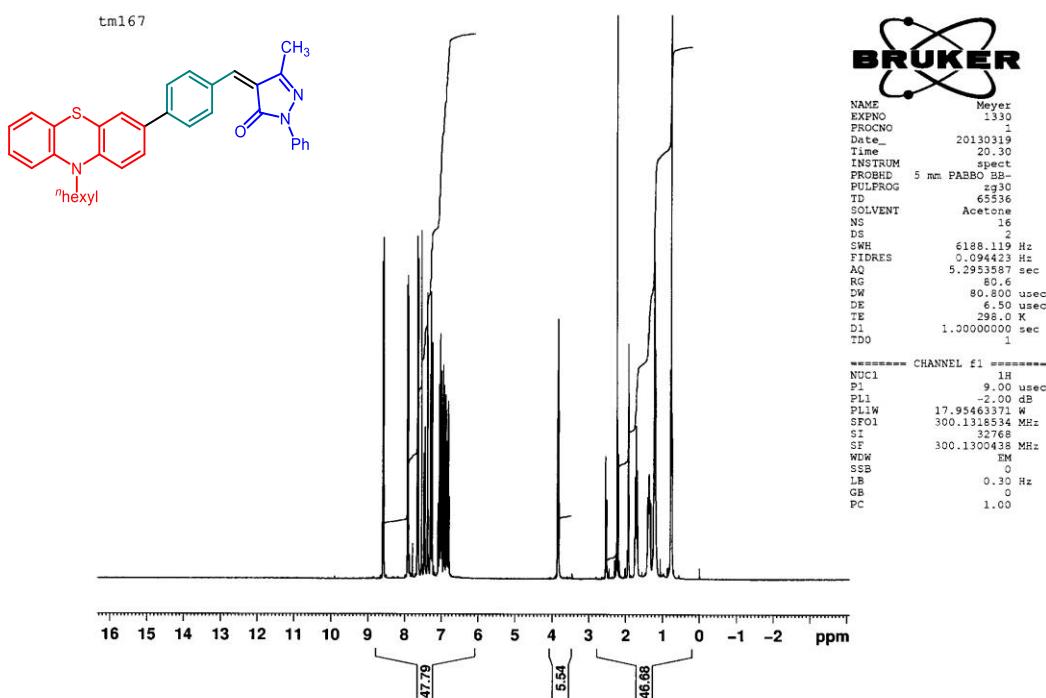


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **8h**.

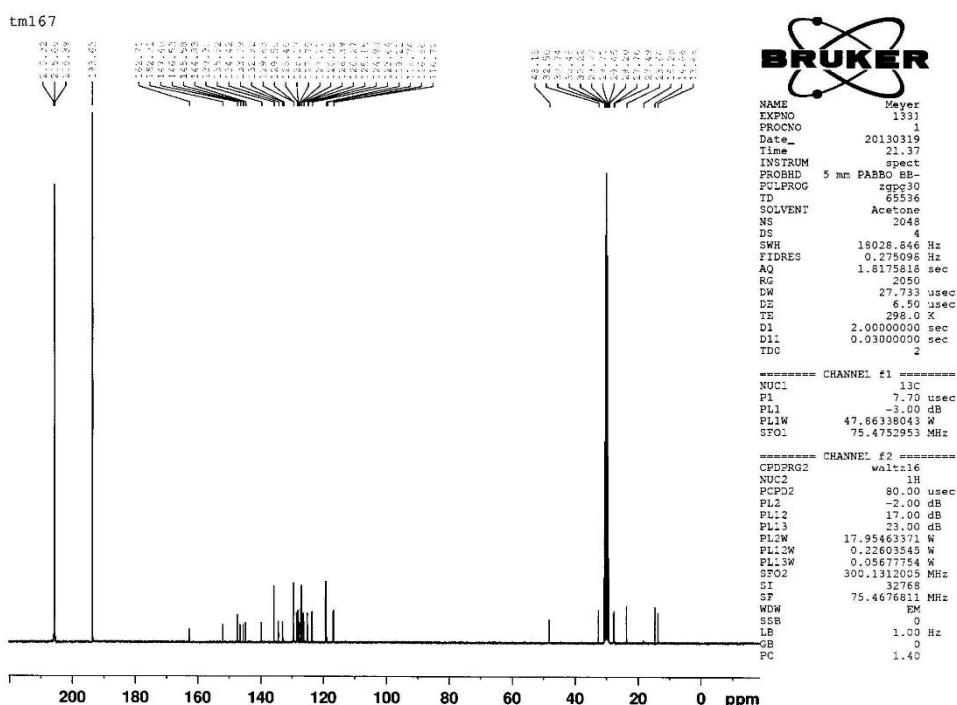


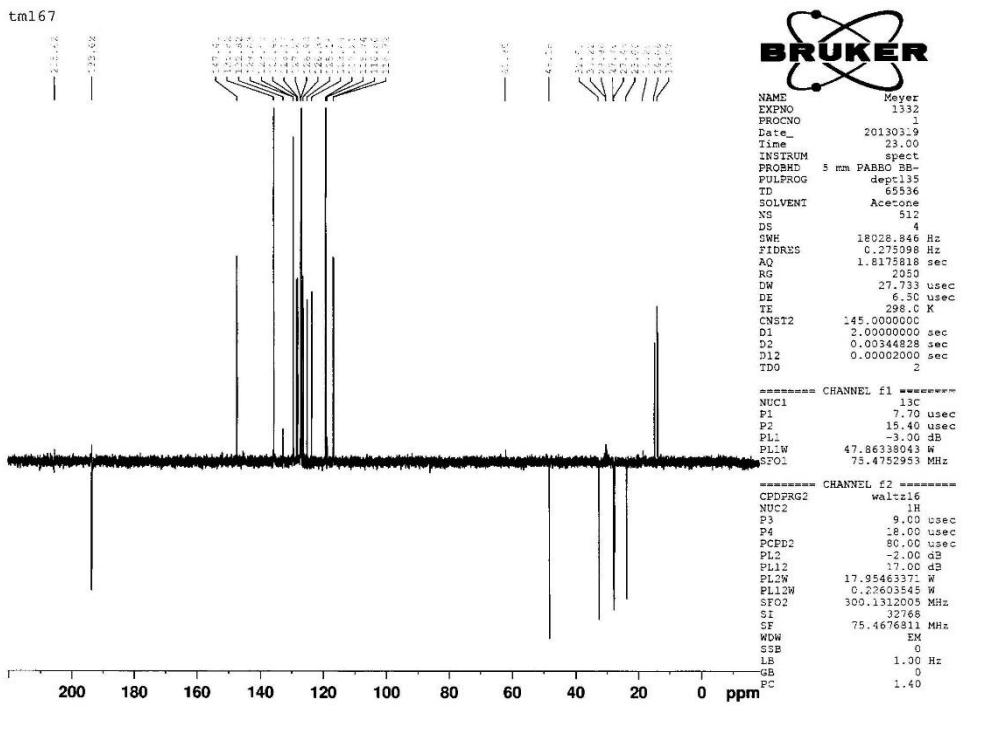
DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **8h**.

3.9. 4-[4-(10-Hexyl-10*H*-phenothiazin-3-yl)benzylidene]-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (8i)



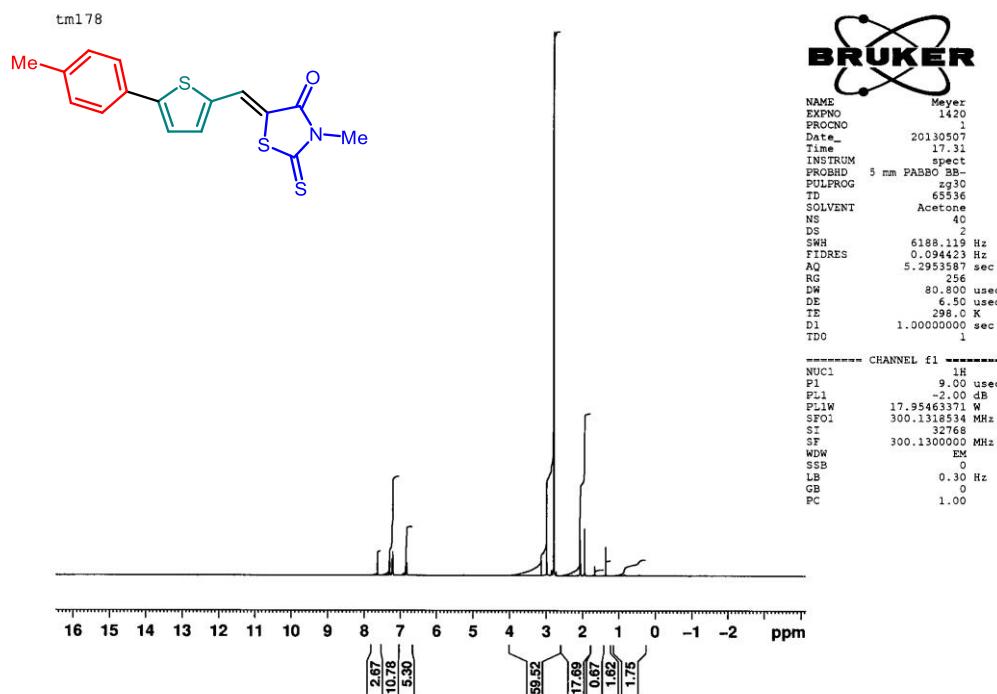
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 8i.



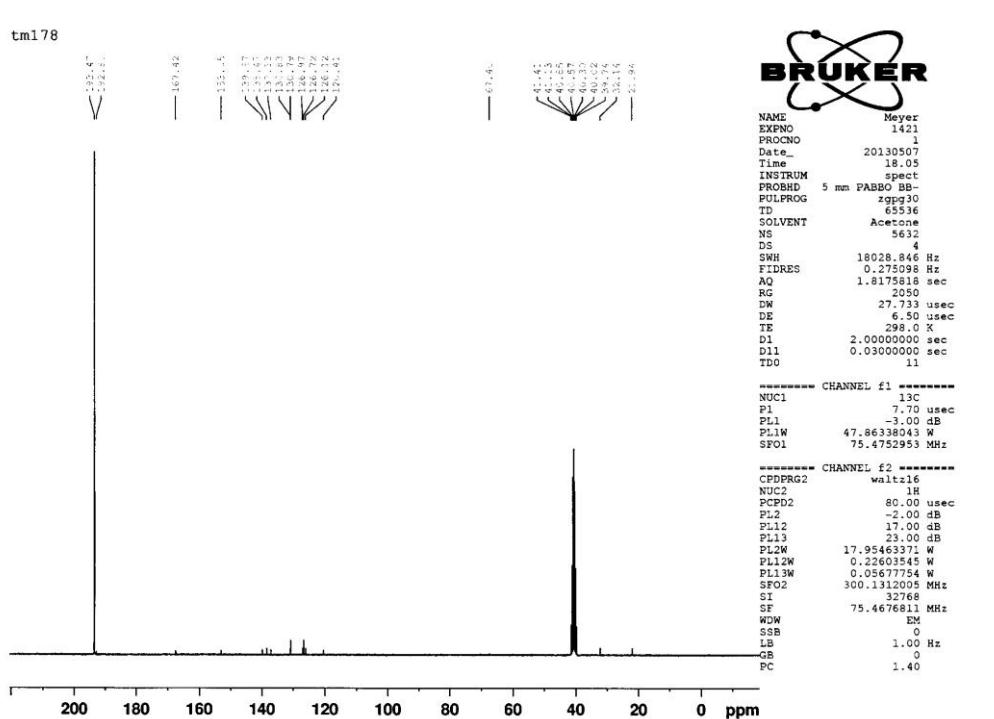


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **8i**.

3.10. 3-Methyl-2-thioxo-5-[(5-(*p*-tolyl)thiophen-2-yl)methylene]thiazolidin-4-one (9a)

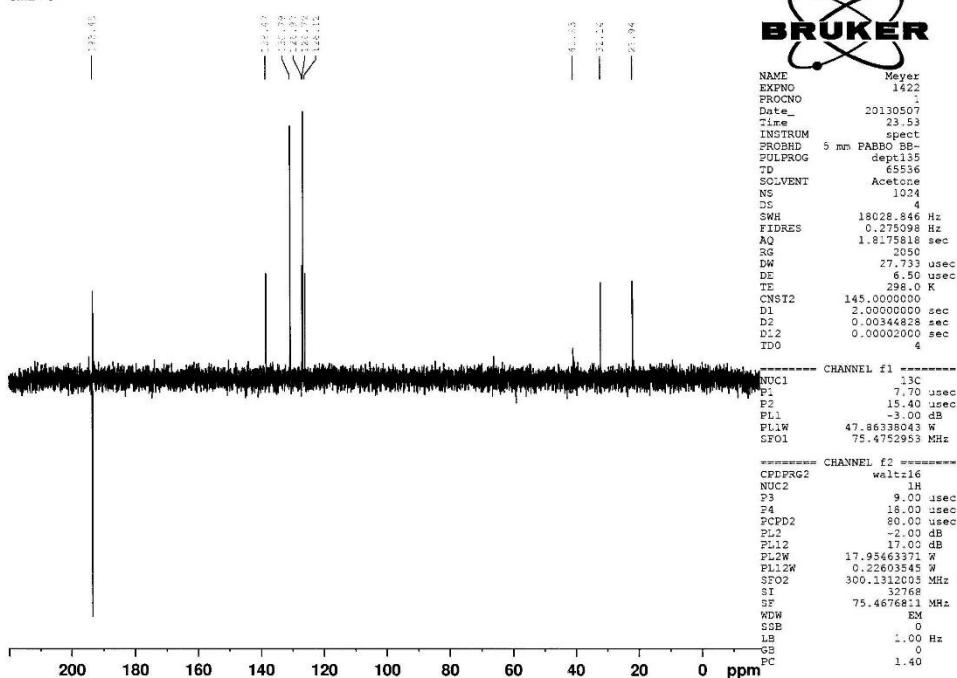


¹H NMR (300 MHz, DMSO-d₆/CS₂ 8:1) of compound 9a.



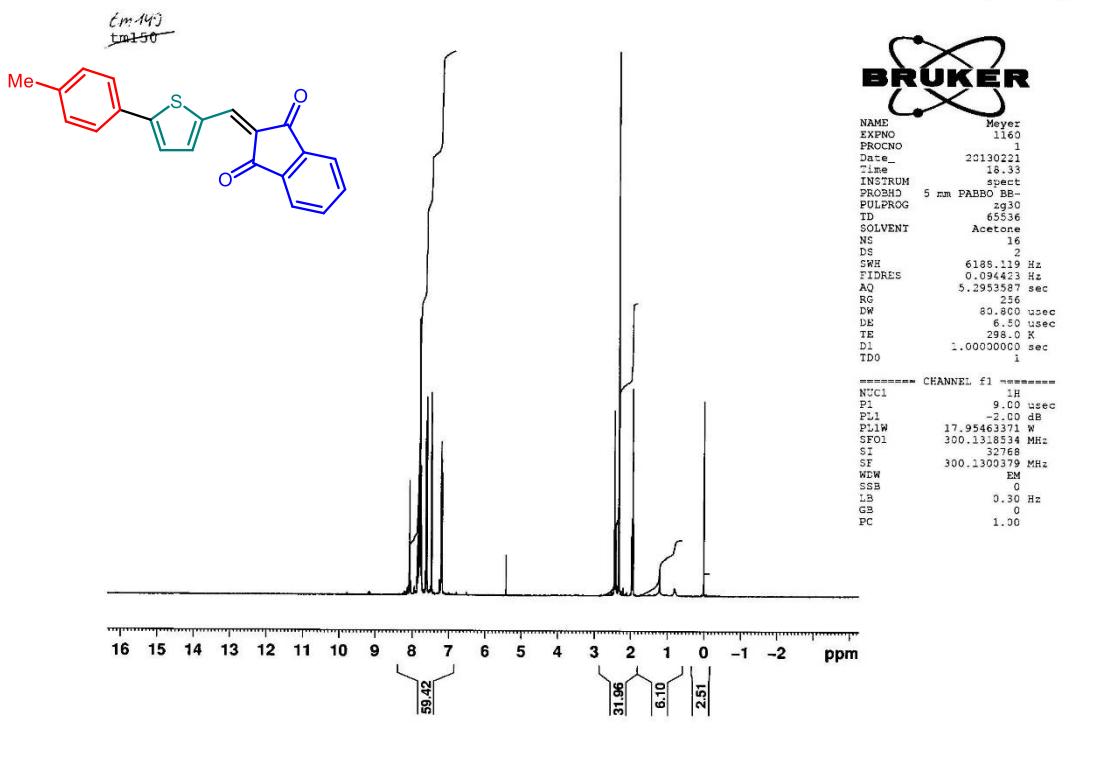
¹³C NMR (75 MHz, DMSO-d₆/CS₂ 8:1) of compound **9a**.

tm178

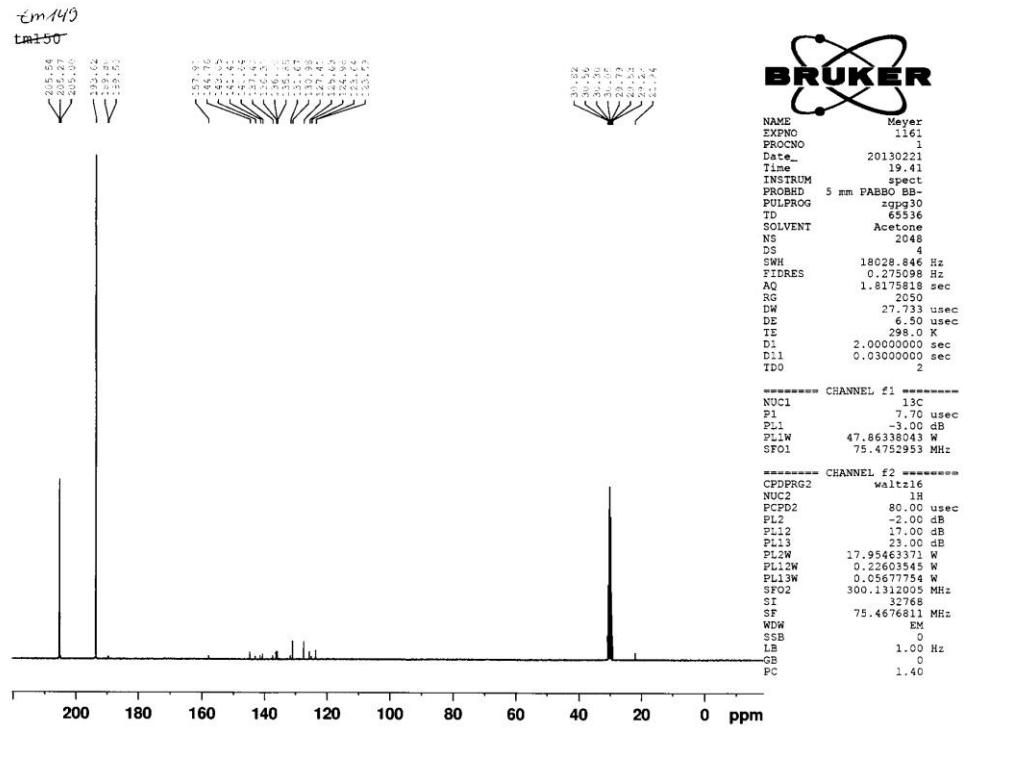


DEPT ¹³C NMR (75 MHz, DMSO-d₆/CS₂ 8:1) of compound 9a.

3.11. 2-{[5-(*p*-Tolyl)thiophen-2-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (9b)

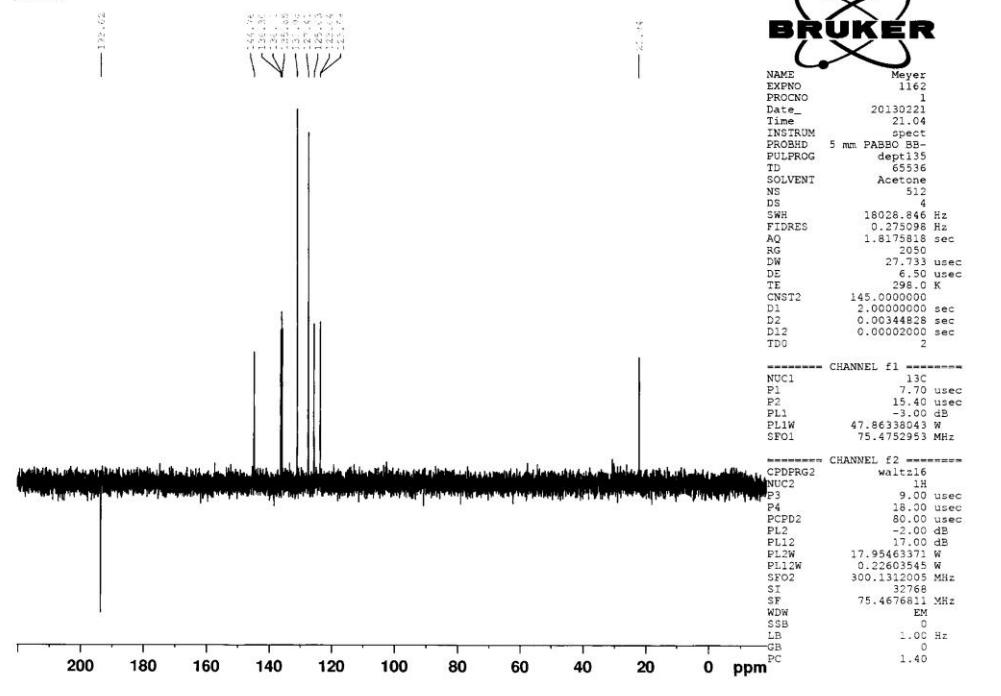


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 9b.



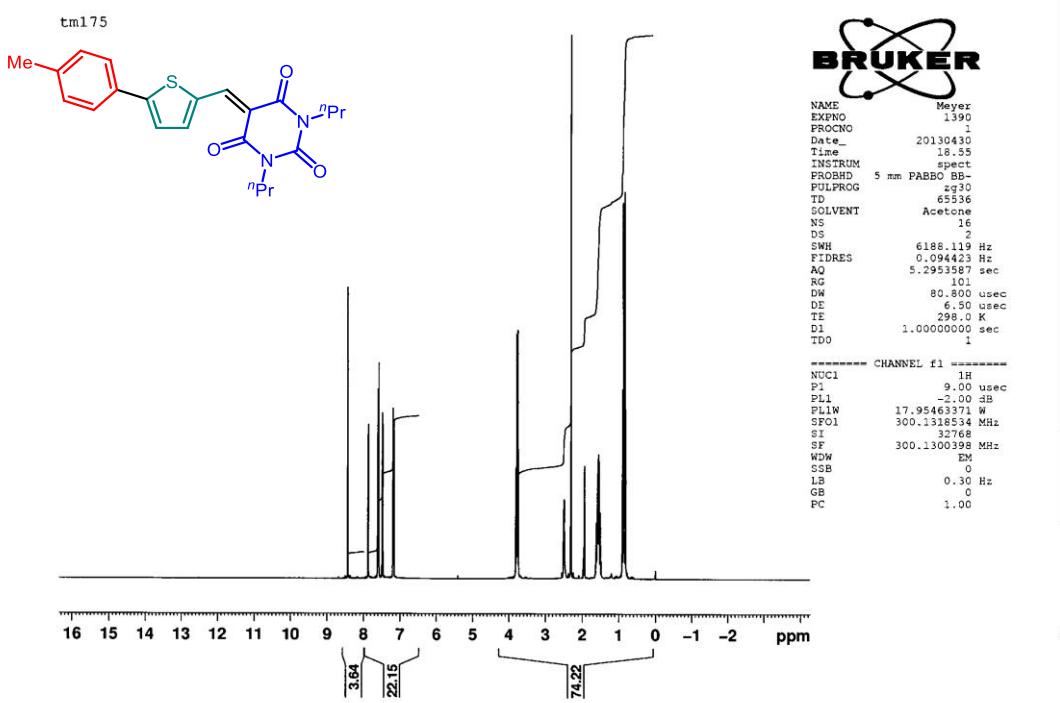
¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **9b**.

2020415
1m450

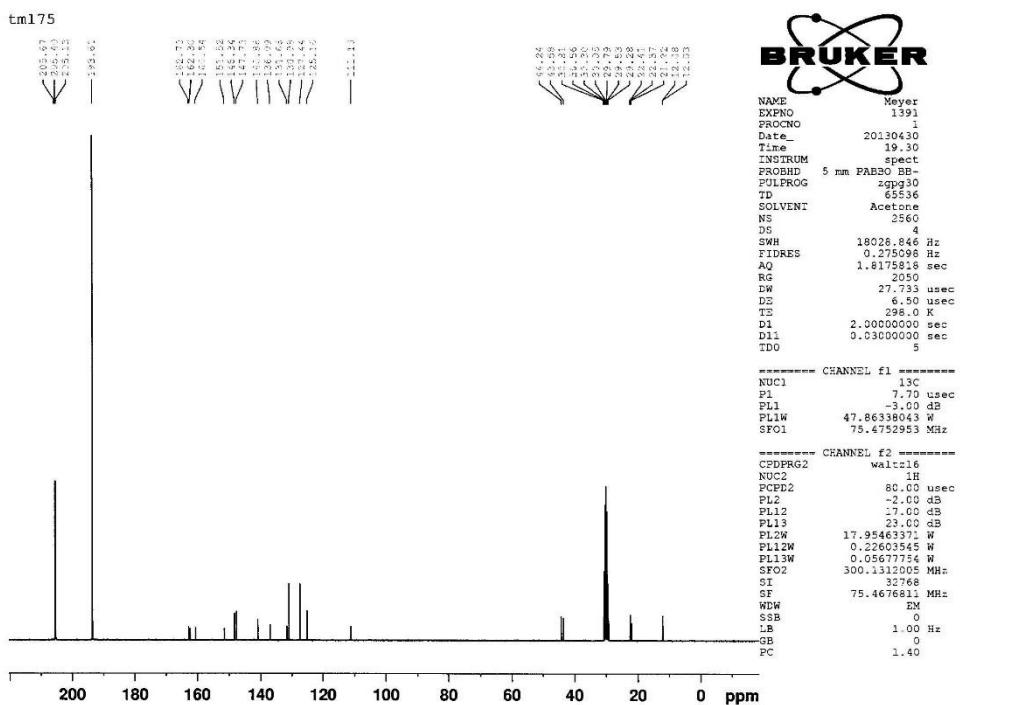


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **9b**.

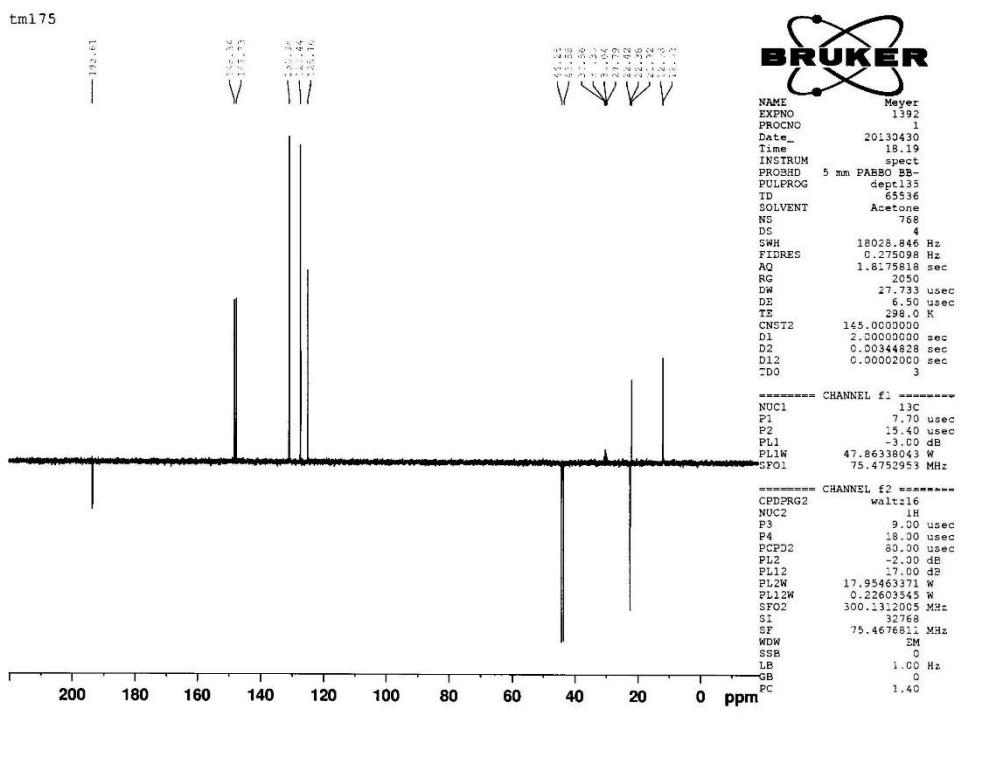
3.12. 1,3-Dipropyl-5-{{[5-(*p*-tolyl)thiophen-2-yl]methylene}pyrimidin-2,4,6[1*H*,3*H*,5*H*]-trione (9c)}



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **9c**.

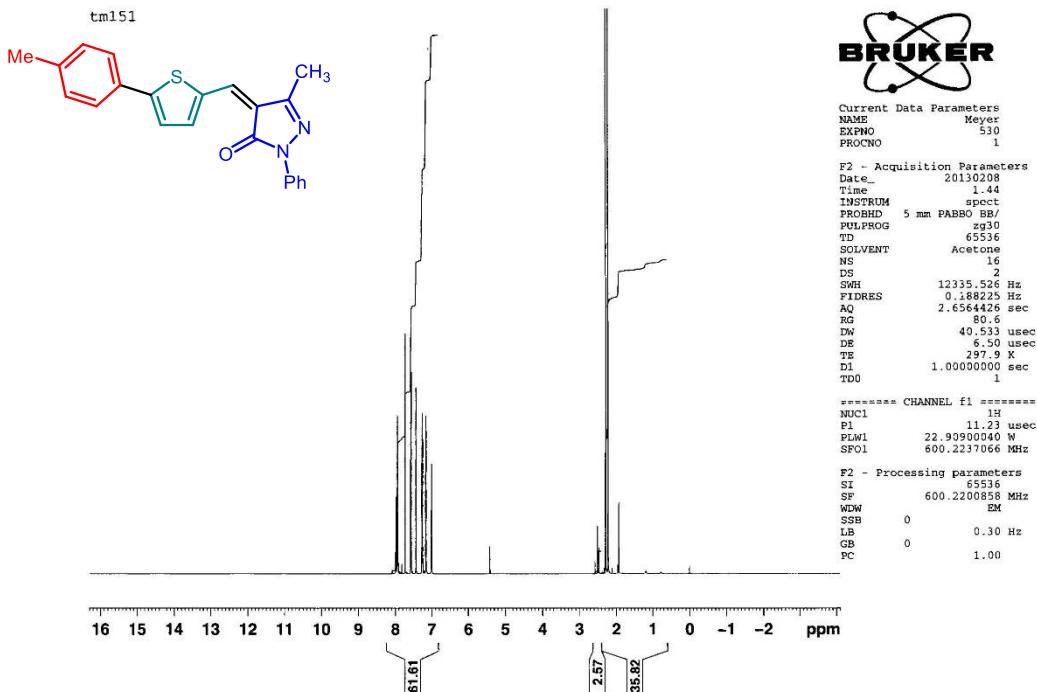


¹³C NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 9c.

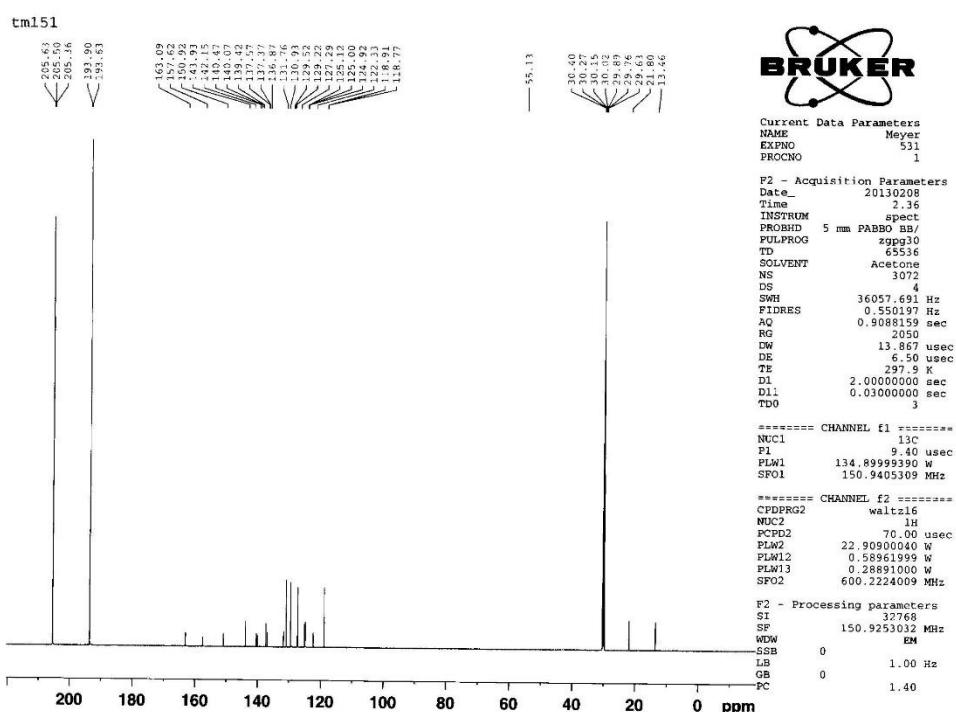


DEPT ^{13}C NMR (300 MHz, acetone- d_6 /CS₂ 4:1) of compound **9c**.

3.13. 3-Methyl-1-phenyl-4-{{[5-(*p*-tolyl)thiophen-2-yl]methylene}-1*H*-pyrazol-5[4*H*]-one (9d)}

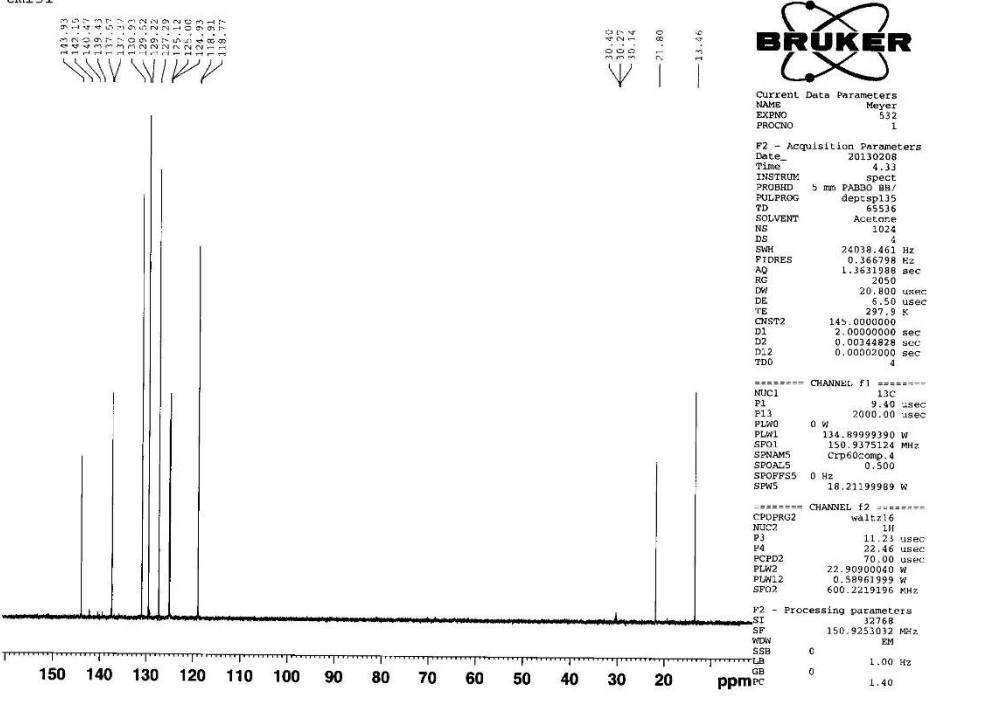


¹H NMR (600 MHz, acetone-d₆/CS₂) of compound 9d.

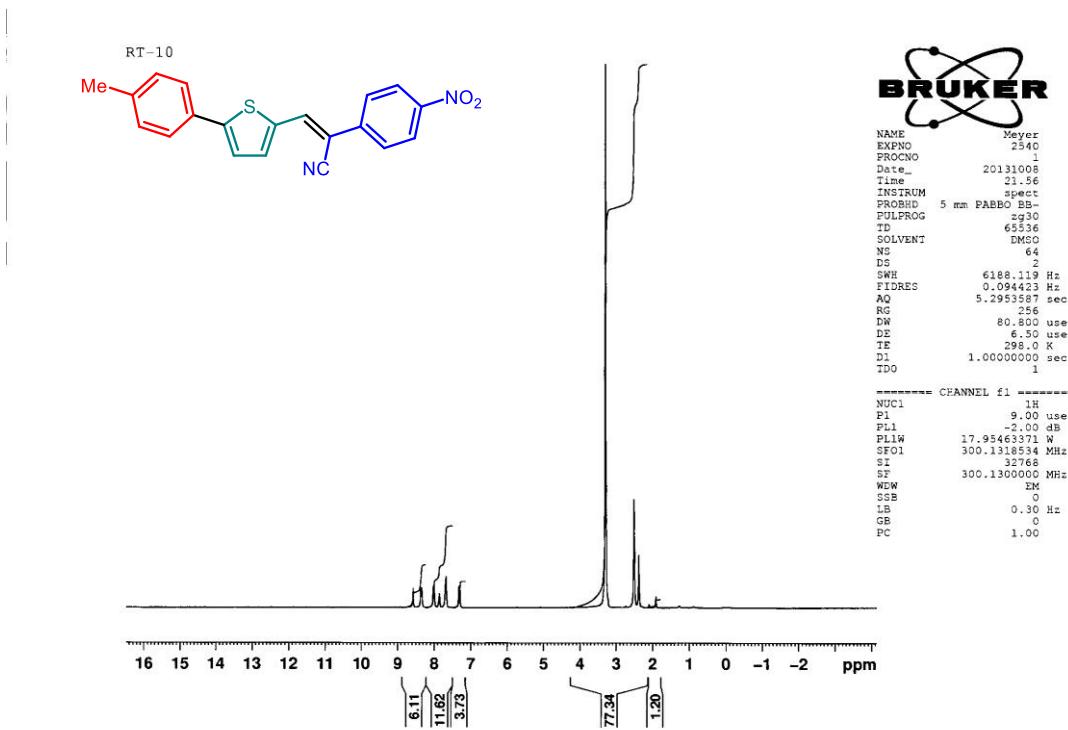


¹³C NMR (150 MHz, acetone-d₆/CS₂) of compound 9d.

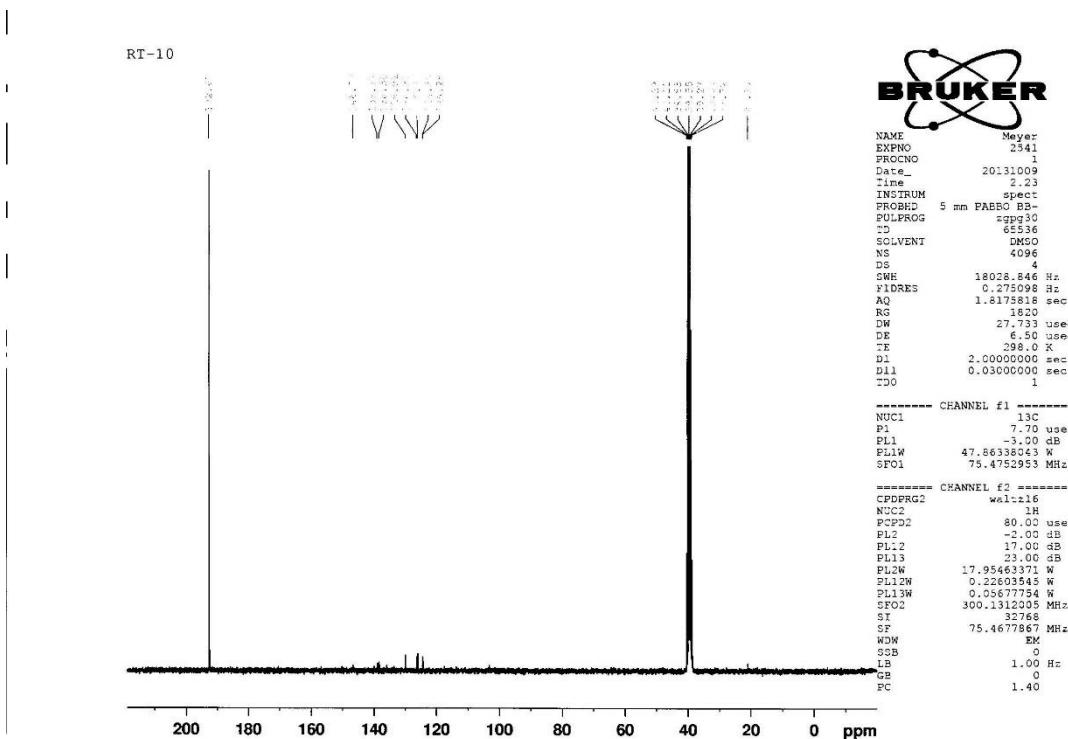
tm151

DEPT ^{13}C NMR (150 MHz, acetone-d₆/CS₂) of compound **9d**.

3.14. 2-(4-Nitrophenyl)-3-[5-(*p*-tolyl)thiophen-2-yl]acrylonitrile (9e)



¹H NMR (300 MHz, DMSO-d₆) of compound **9e**.



¹³C NMR (75 MHz, DMSO-d₆) of compound **9e**.

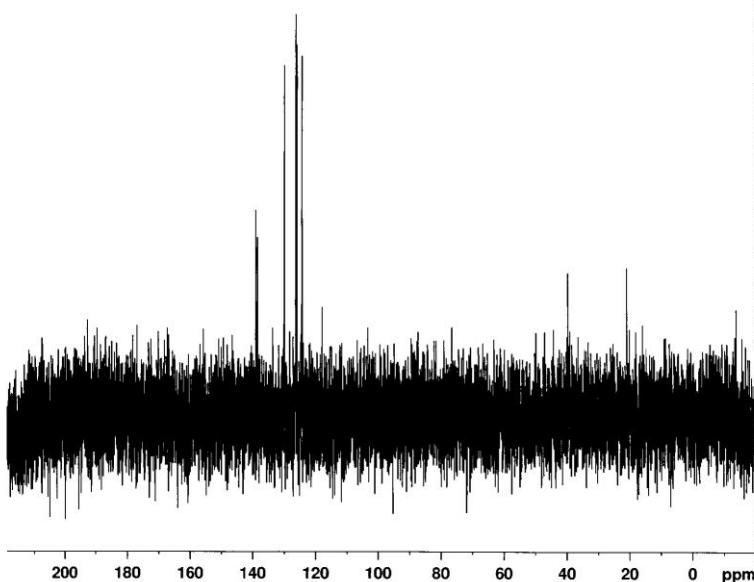
RT-10



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Date 20131009
Time 3.29
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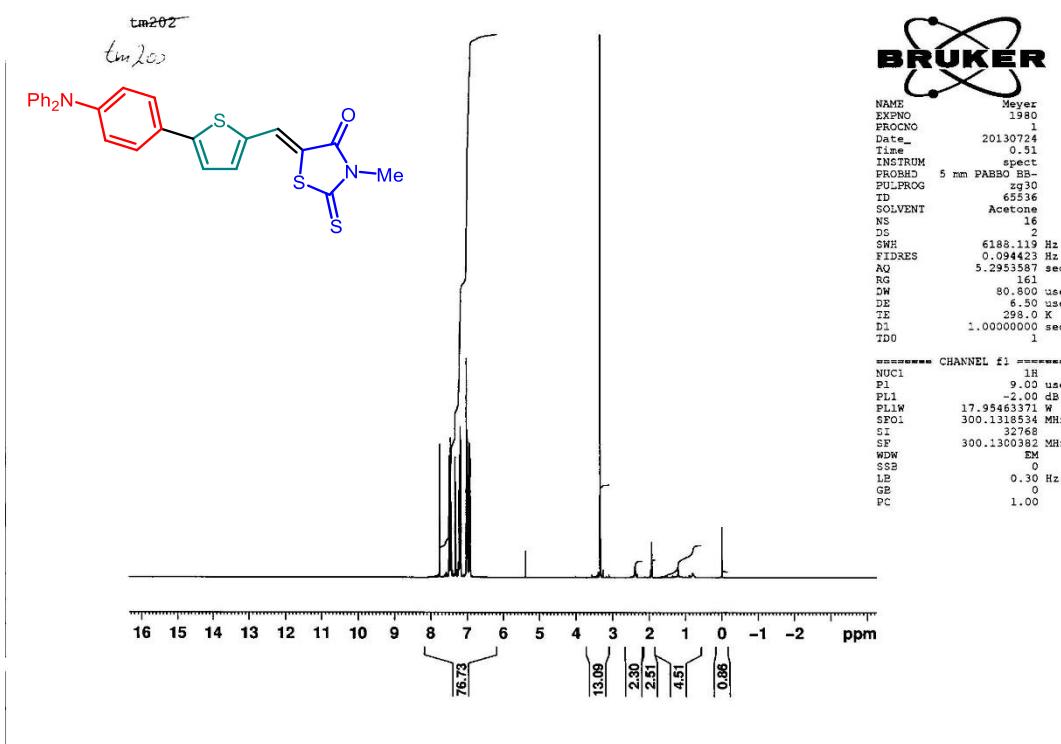
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----- CHANNEL f2 -----
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NUC2 1H
P3 9.00 usec
P4 18.00 usec
PCPD2 80.00 usec
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PL12 17.00 dB
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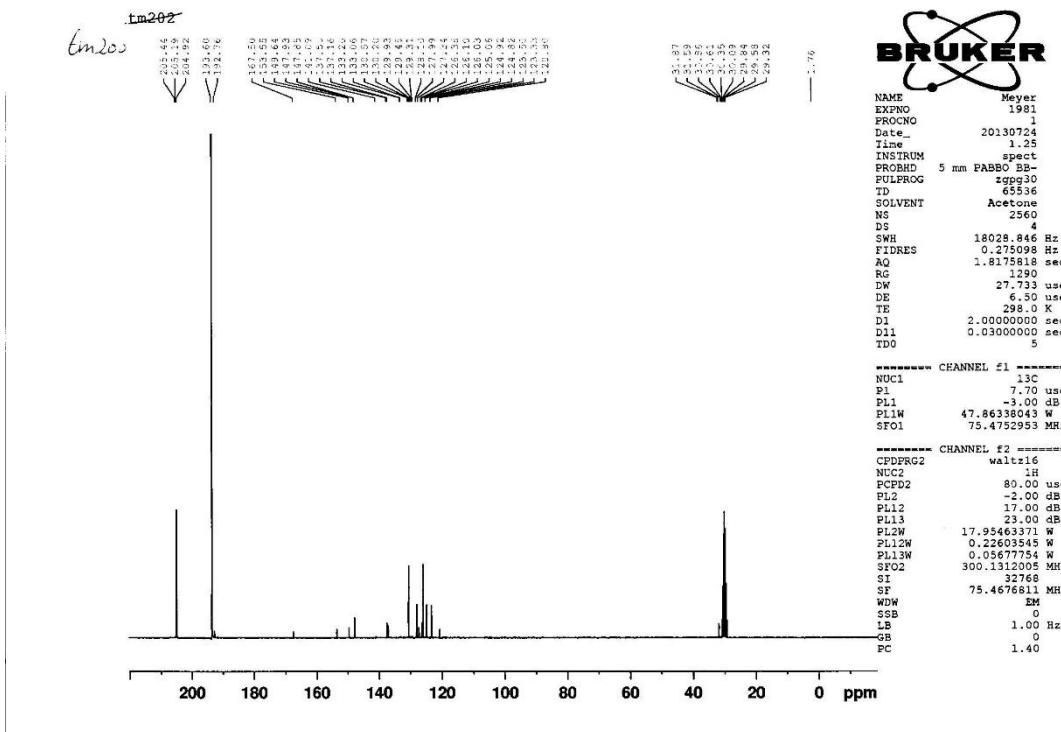


DEPT ^{13}C NMR (75 MHz, DMSO-d₆) of compound **9e**.

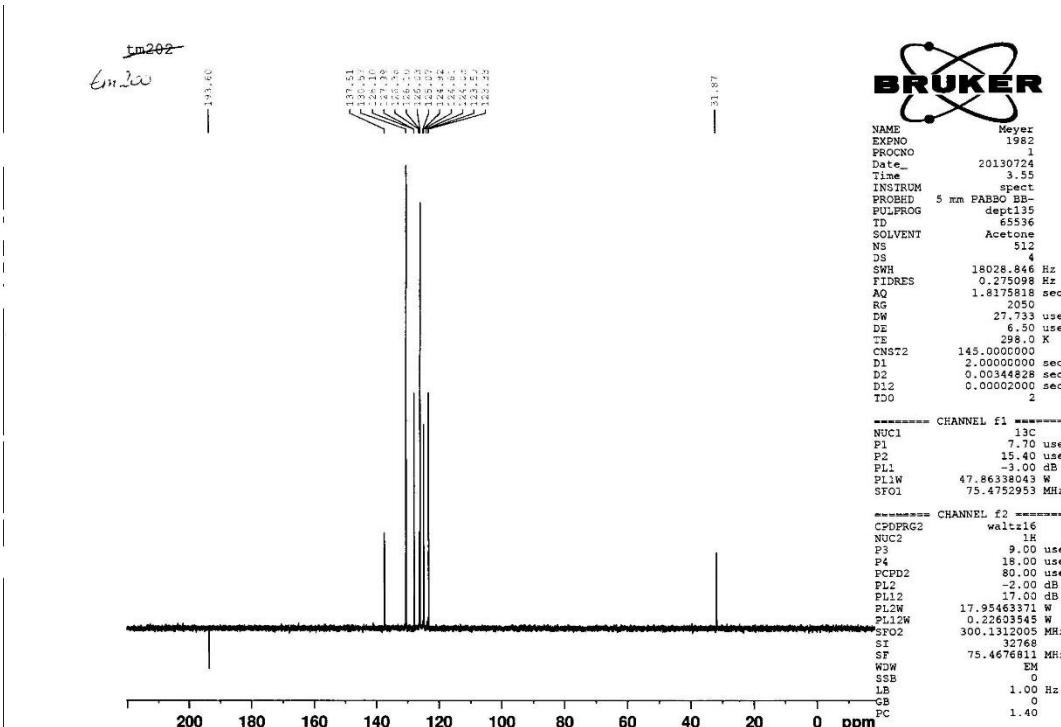
3.15. 5-{[5-(4-{Diphenylamino}phenyl)thiophen-2-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (9f)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 9f.

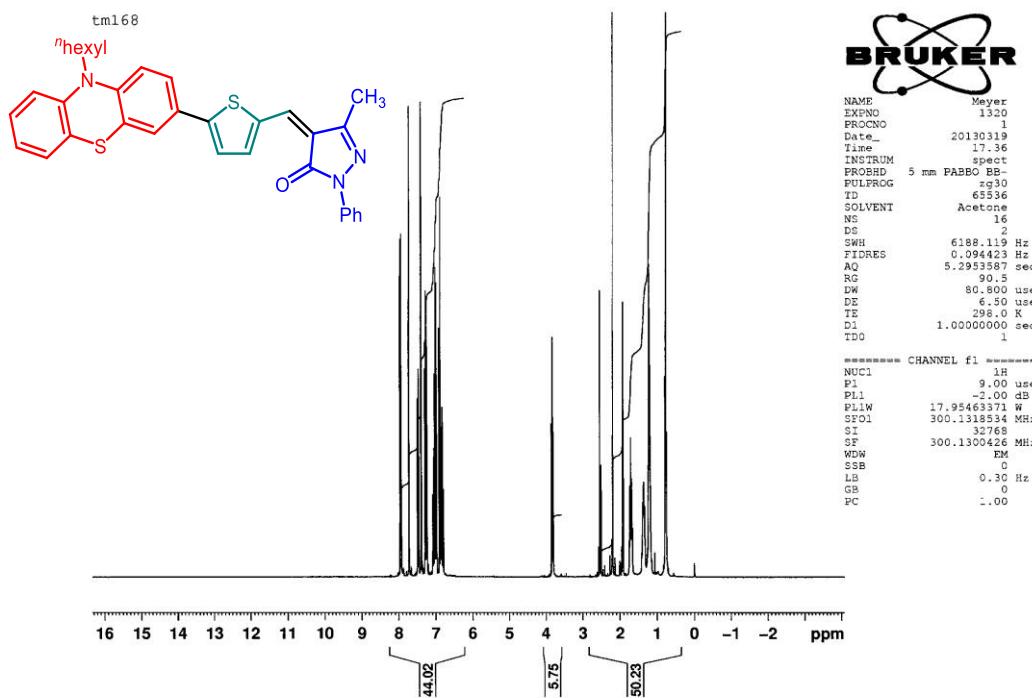


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 9f.

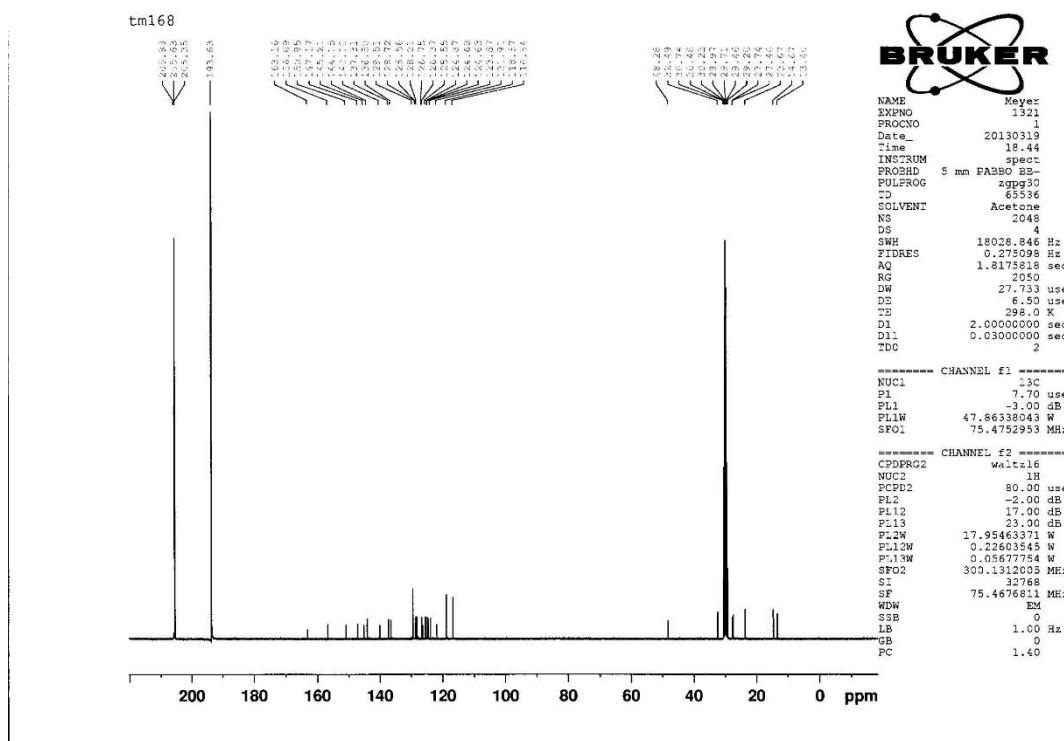


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **9f**.

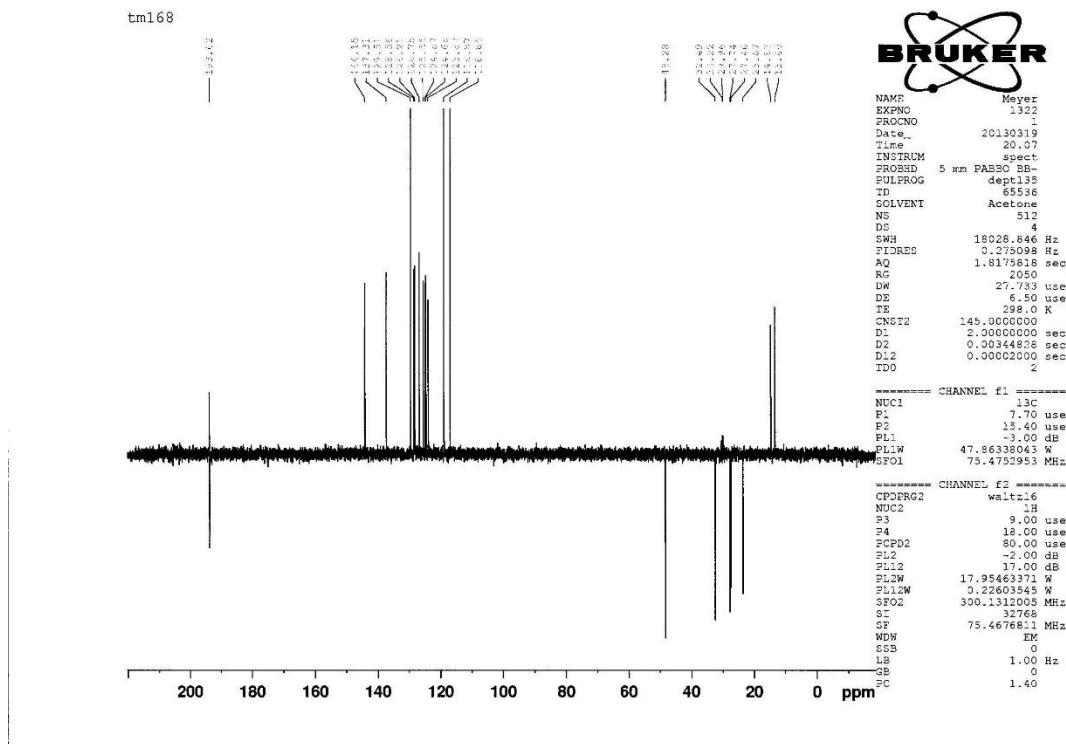
3.16. 4-[{5-(10-Hexyl-10*H*-phenothiazin-3-yl)thiophen-2-yl]methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (9g)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 9g.

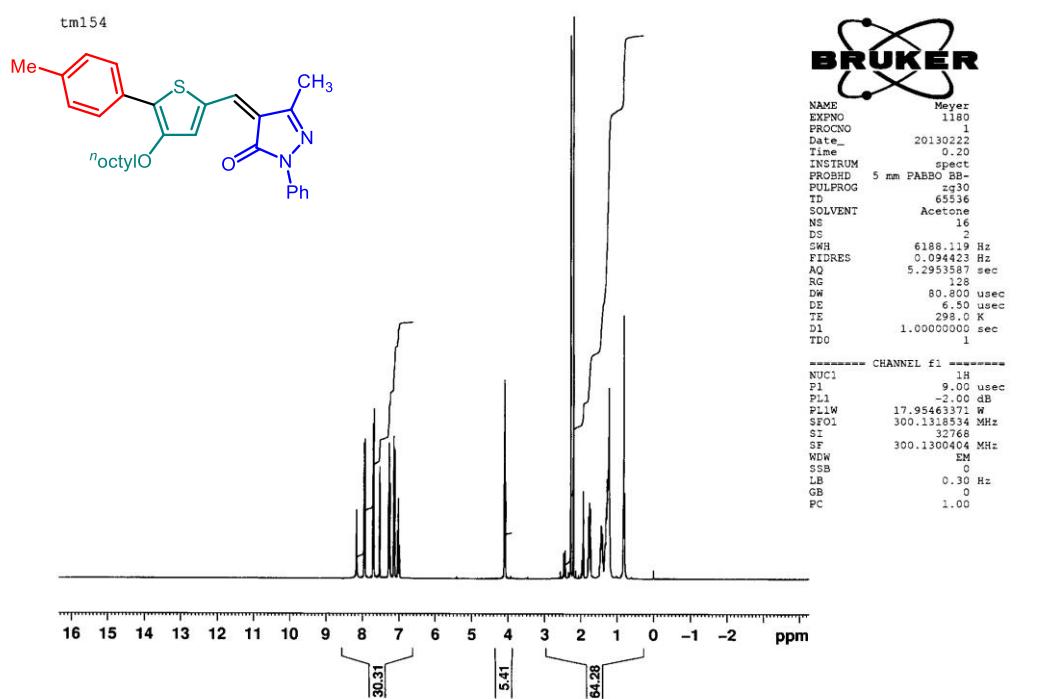


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 9g.

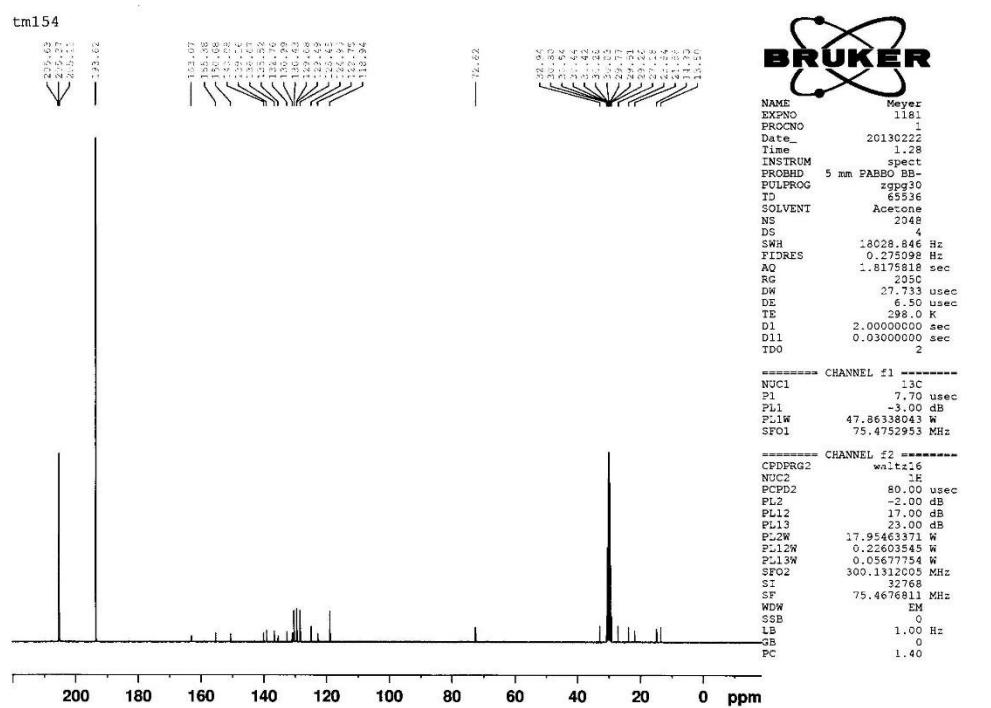


DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **9g**.

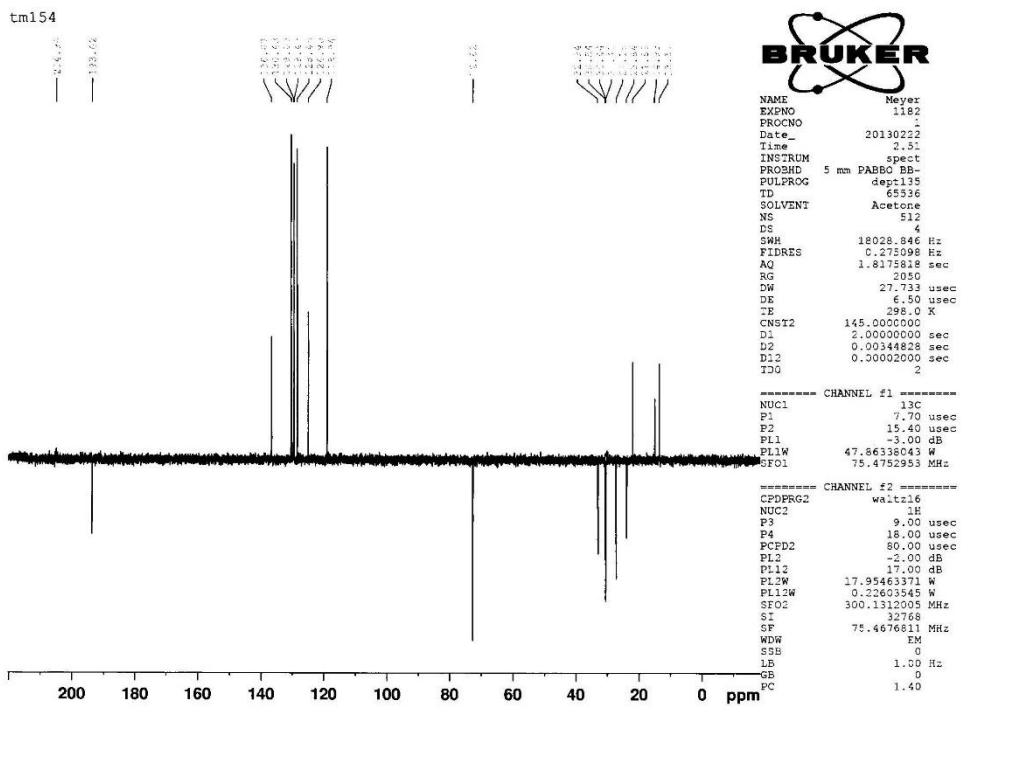
3.17. (*Z*)-5-methyl-4-((4-(octyloxy)-5-(*p*-tolyl)thiophen-2-yl)methylene)-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (10a)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **10a**.

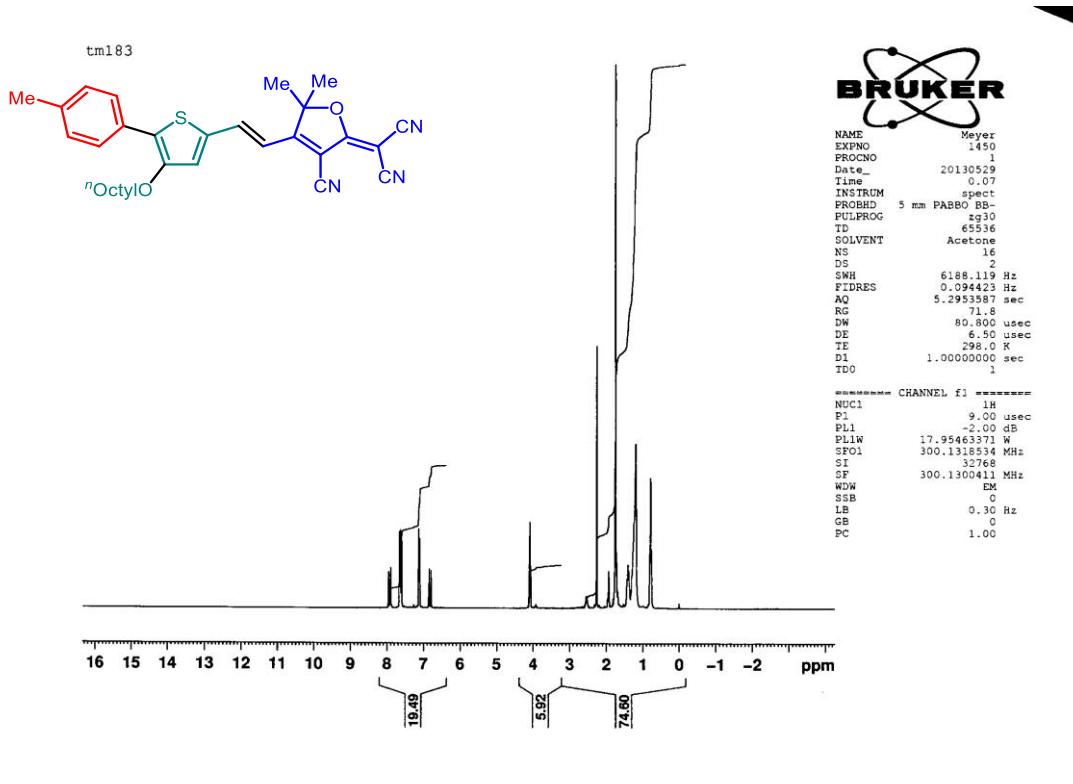


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 10a.

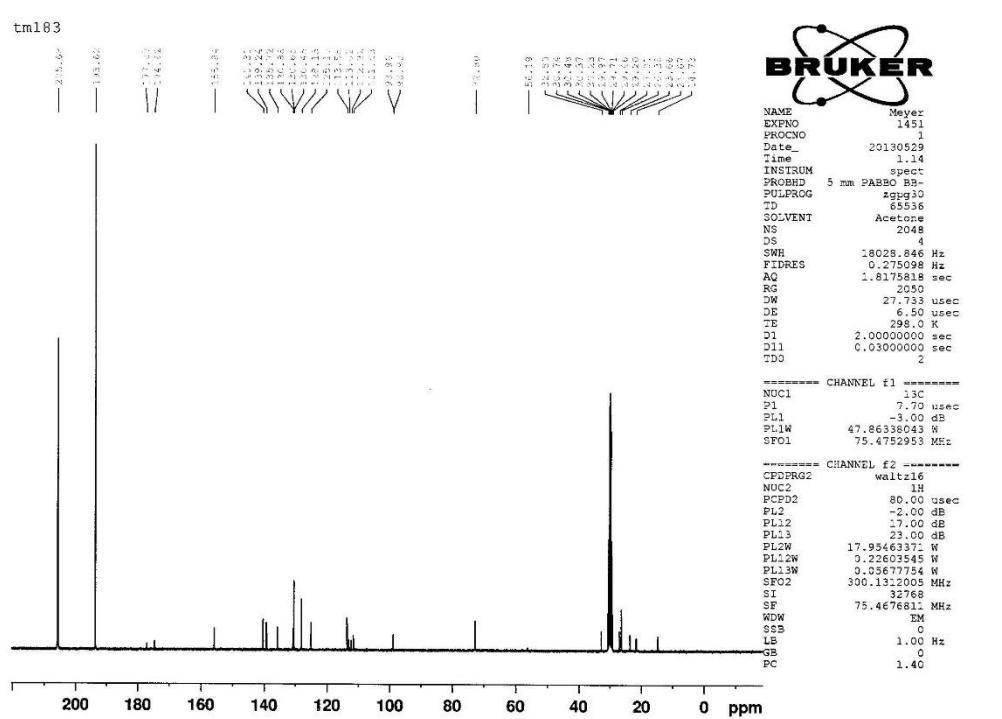


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10a**.

3.18. (*E*)-2-(3-cyano-5,5-dimethyl-4-(2-(4-(octyloxy)-5-(*p*-tolyl)thiophen-2-yl)vinyl)furan-2(5*H*)-ylidene)malononitrile (10b)

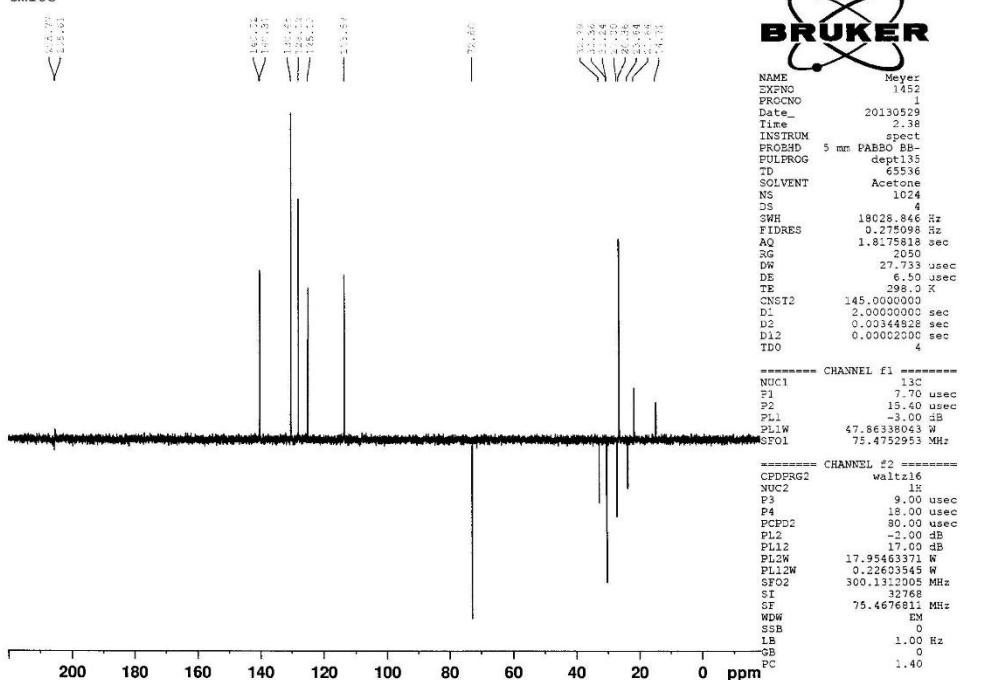


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **10b**.

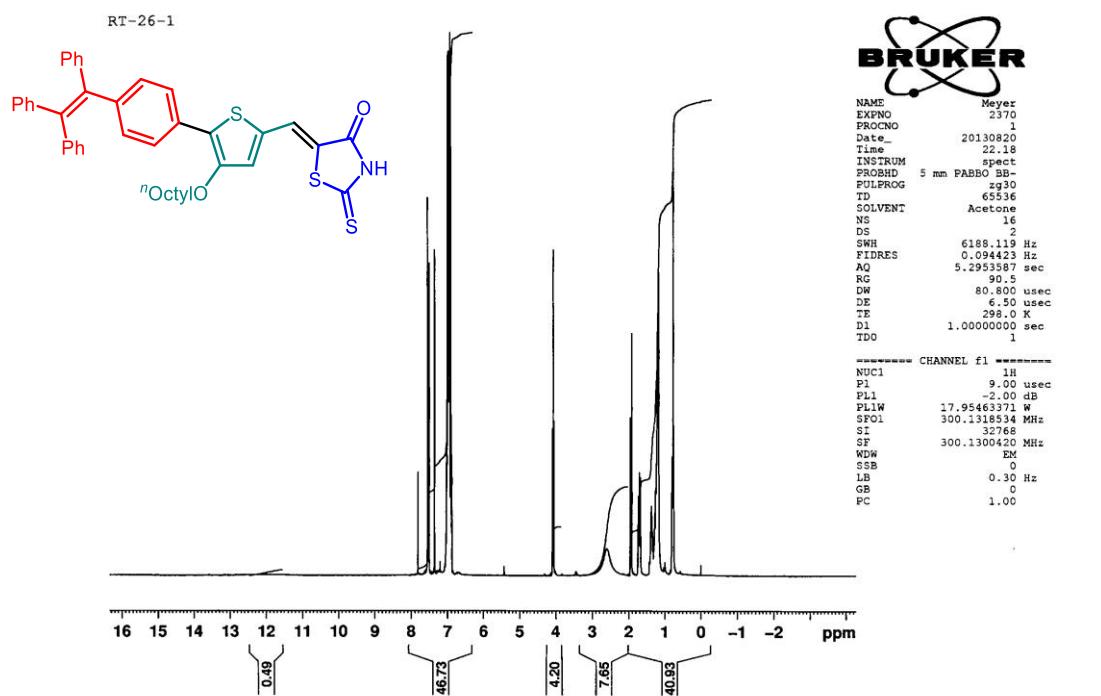


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10b**.

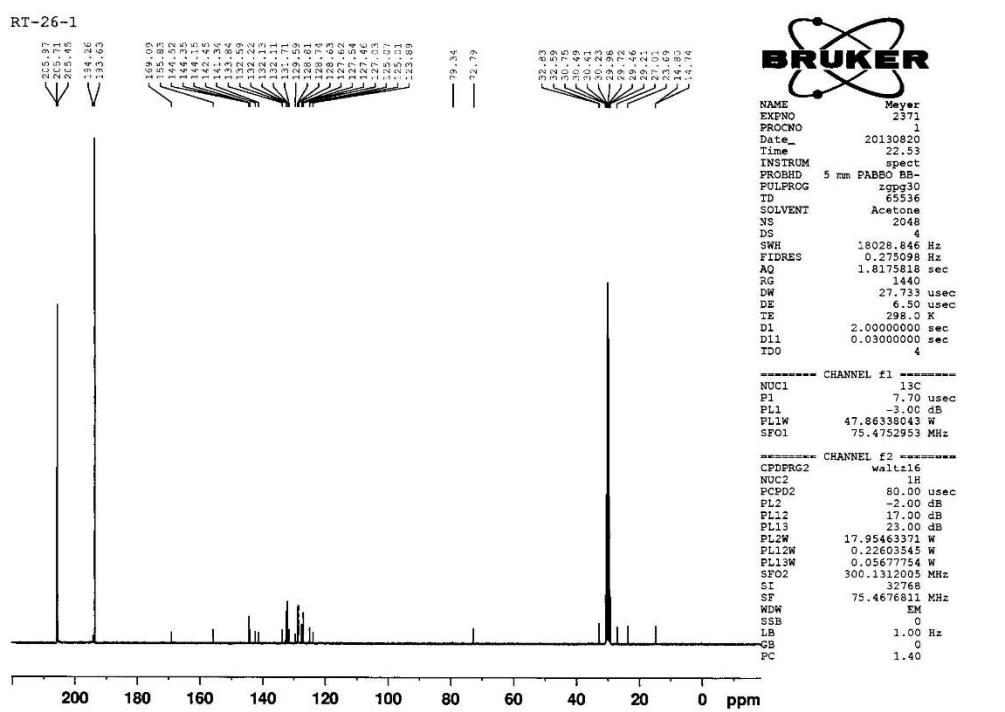
tm183

DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10b**.

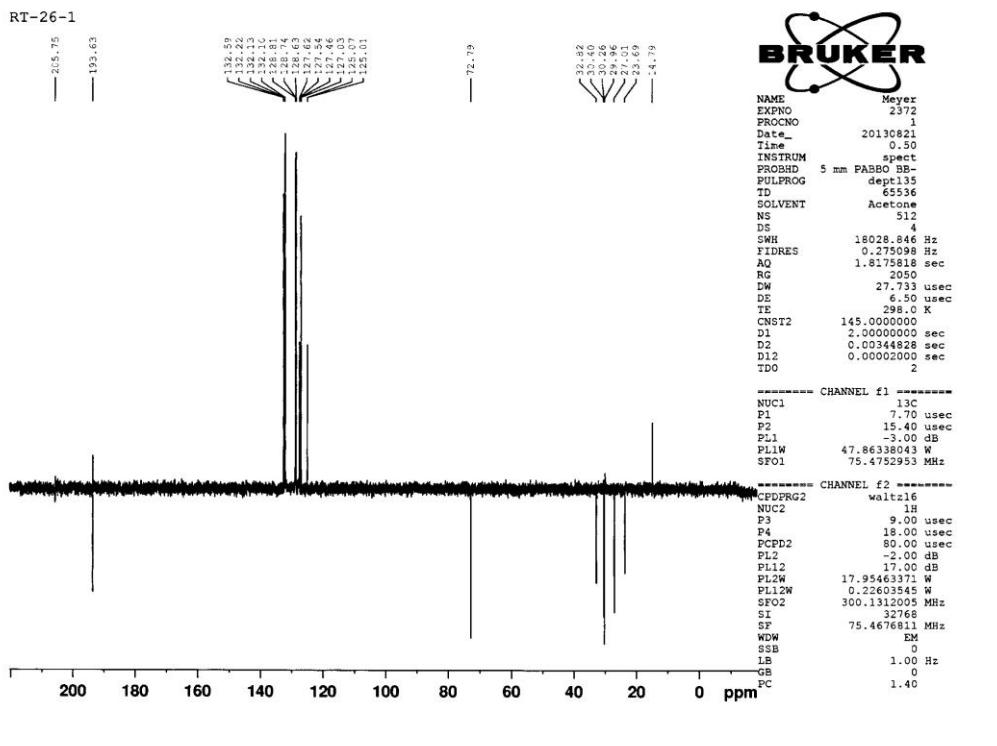
3.19. (Z)-5-((4-(octyloxy)-5-(4-(1,2,2-triphenylvinyl)phenyl)thiophen-2-yl)methylene)-2-thioxothiazolidin-4-one (10c)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **10c**.

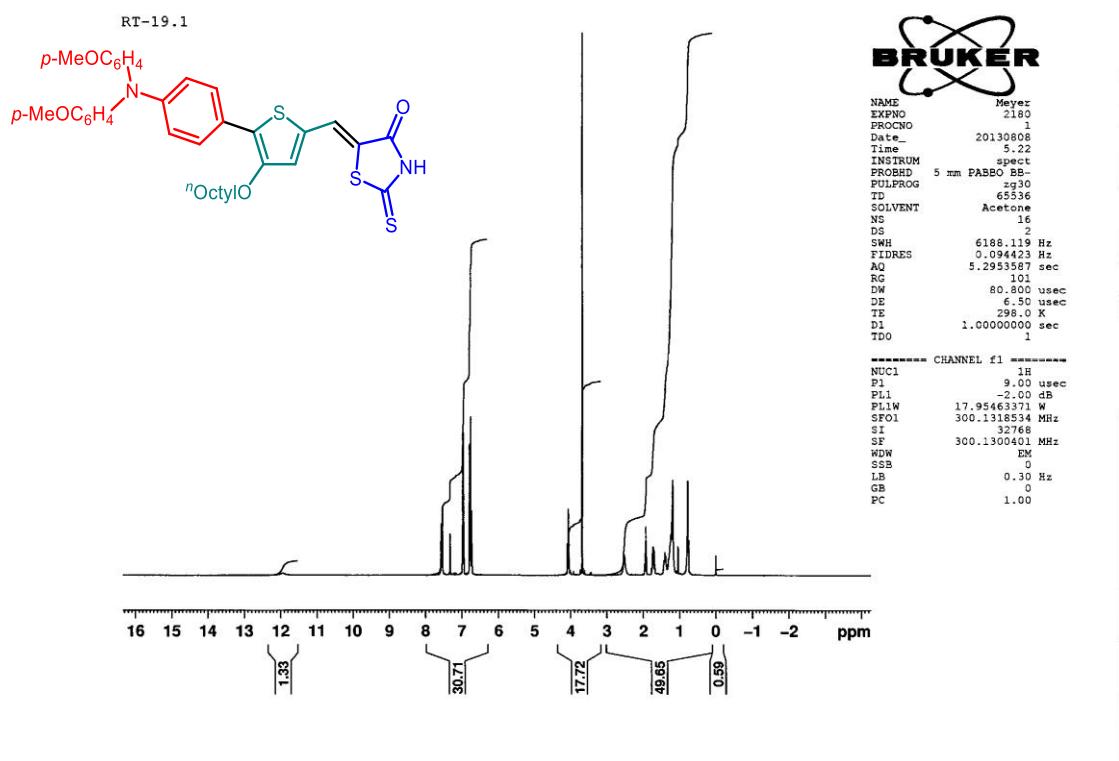


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10c**.

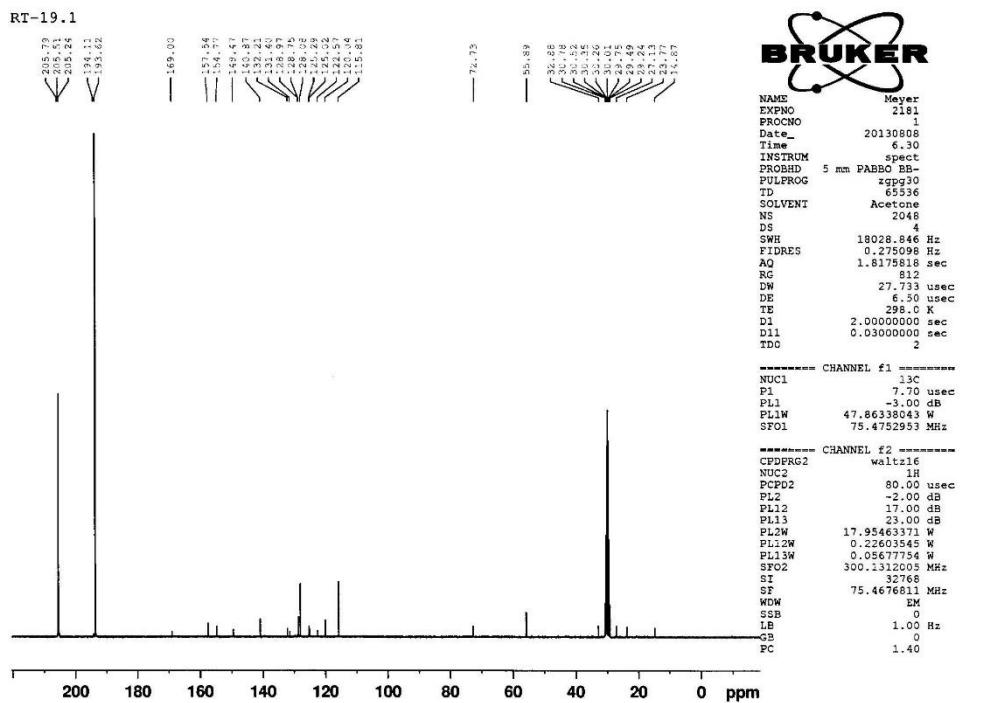


DEPT ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10c**.

3.20. 5-{{[5-(4-{Bis[4-methoxyphenyl]amino}phenyl)-3-(octyloxy)thiophen-2-yl]methylene}-2-thioxothiazolidin-4-one (10d)}

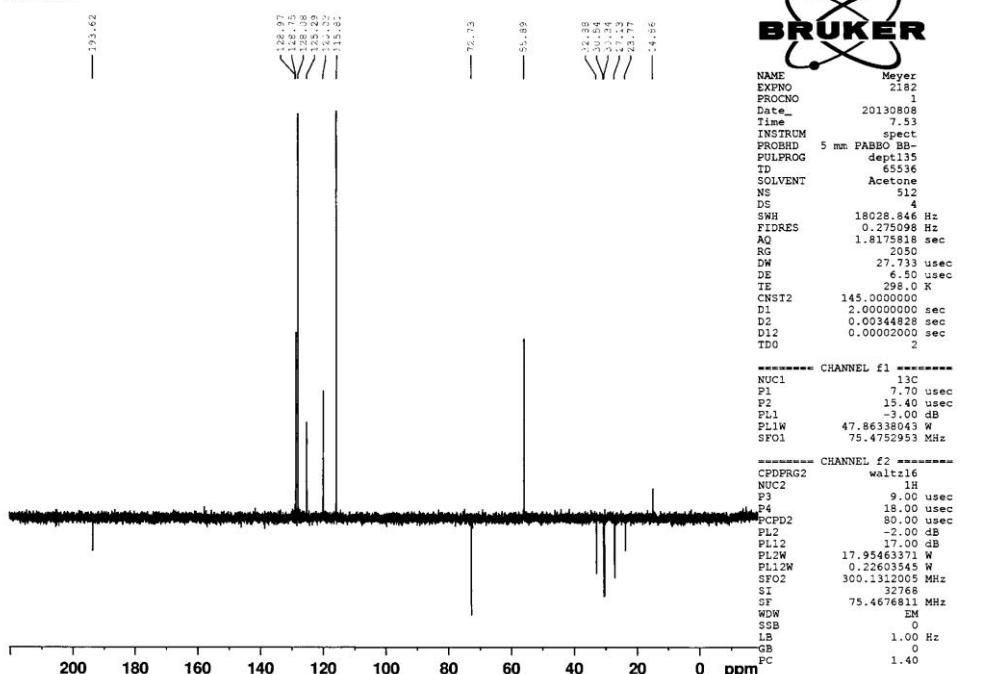


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **10d**.



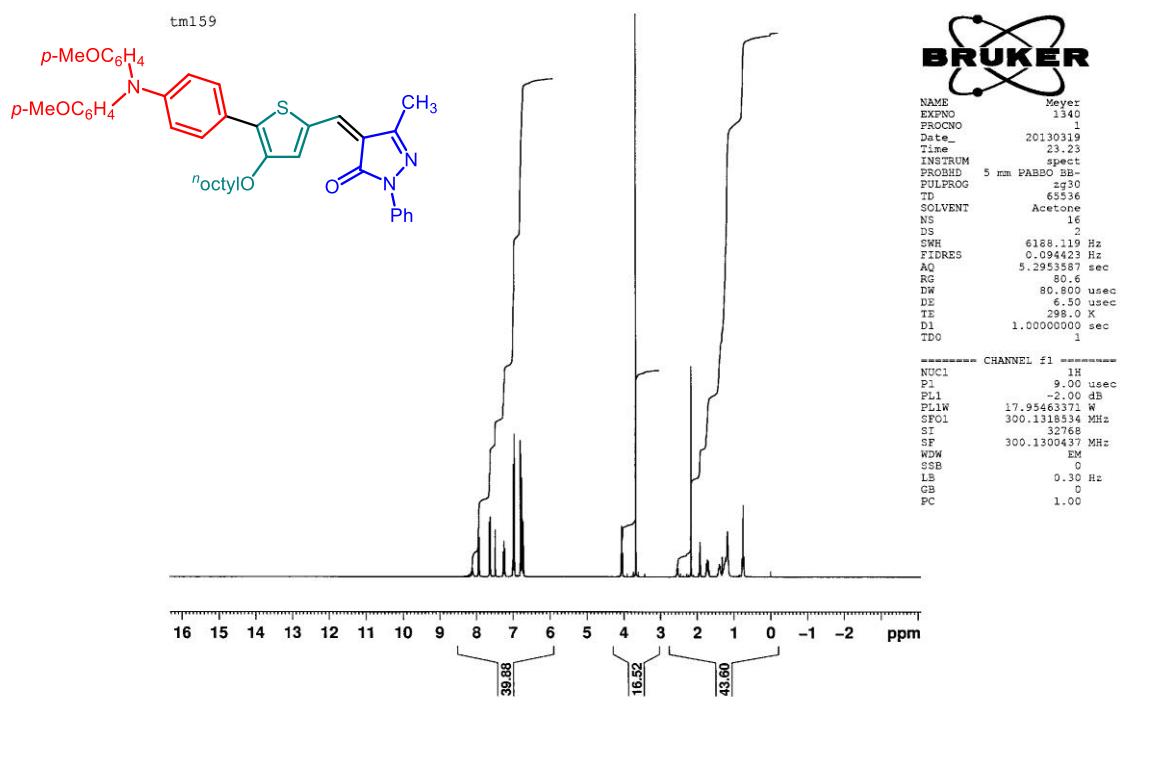
¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10d**.

RT-19.1

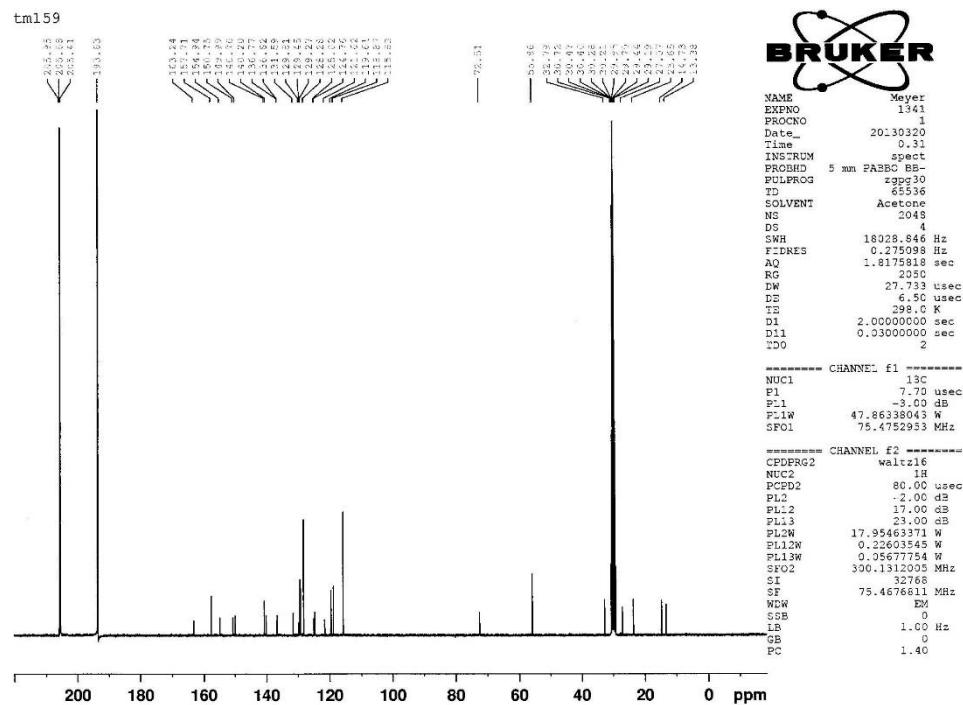


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10d**.

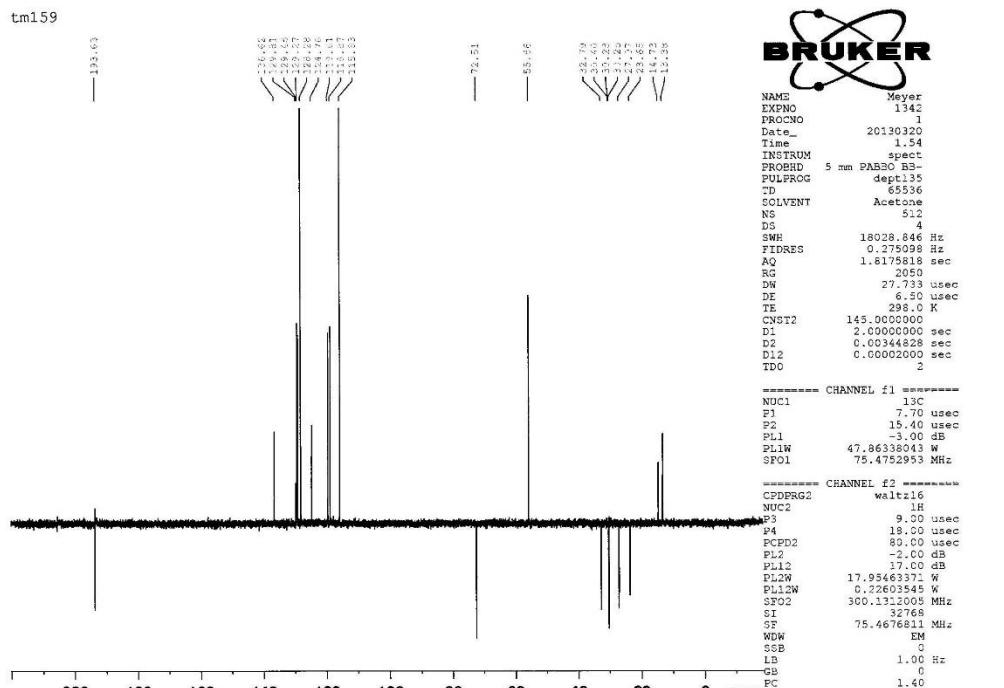
3.21. (*Z*)-4-((5-(4-(bis(4-methoxyphenyl)amino)phenyl)-4-(octyloxy)thiophen-2-yl)methylene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (10e)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **10e**.

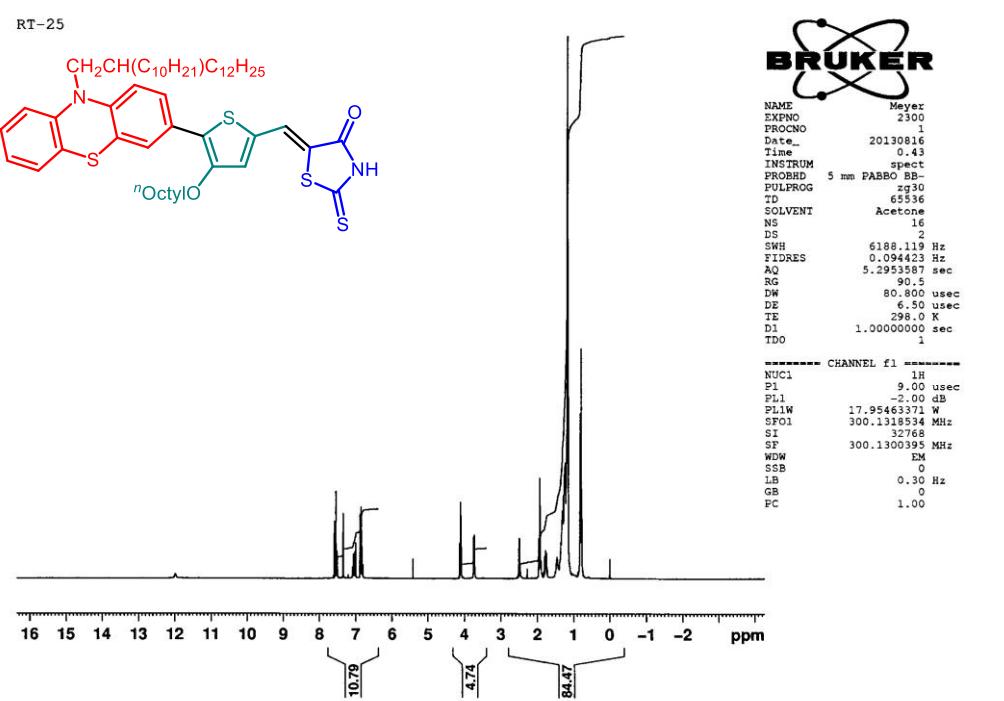


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10e**.

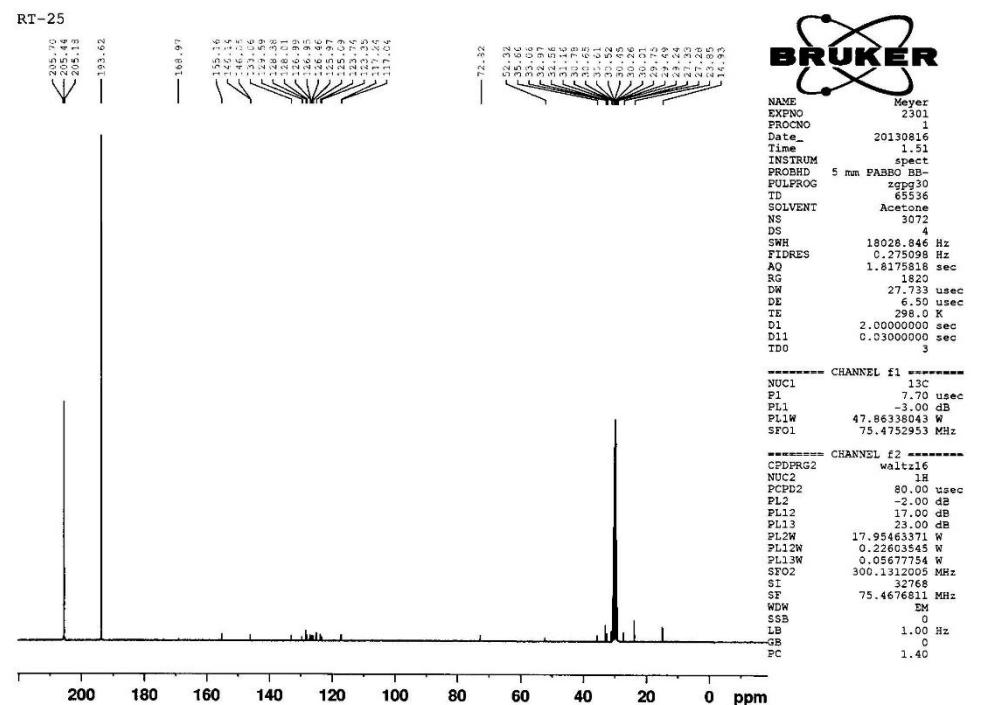


DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **10e**.

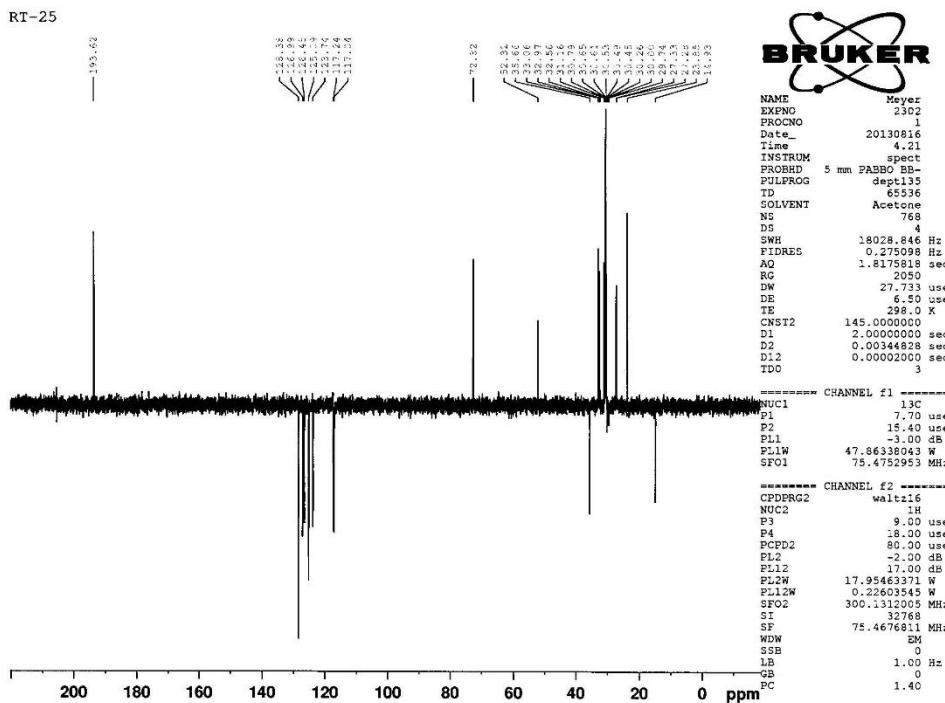
3.22. (Z)-5-((5-(10-(2-decyldodecyl)-10*H*-phenothiazin-3-yl)-4-(octyloxy)thiophen-2-yl)methylene)-2-thioxothiazolidin-4-one (10f)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **10f**.

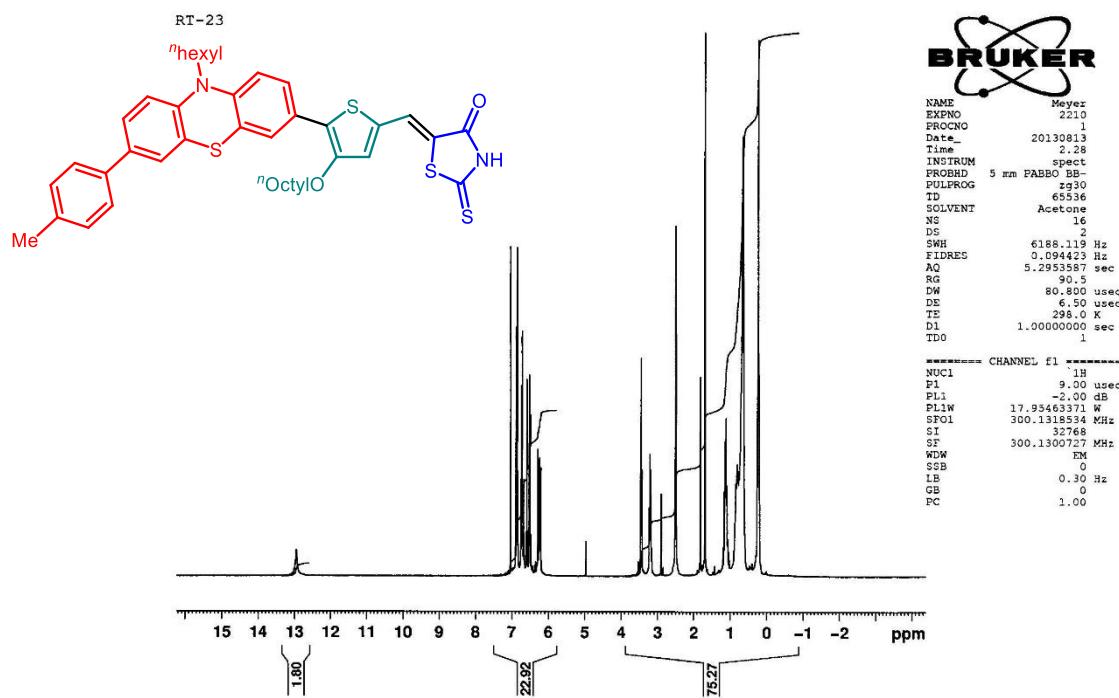


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10f**.

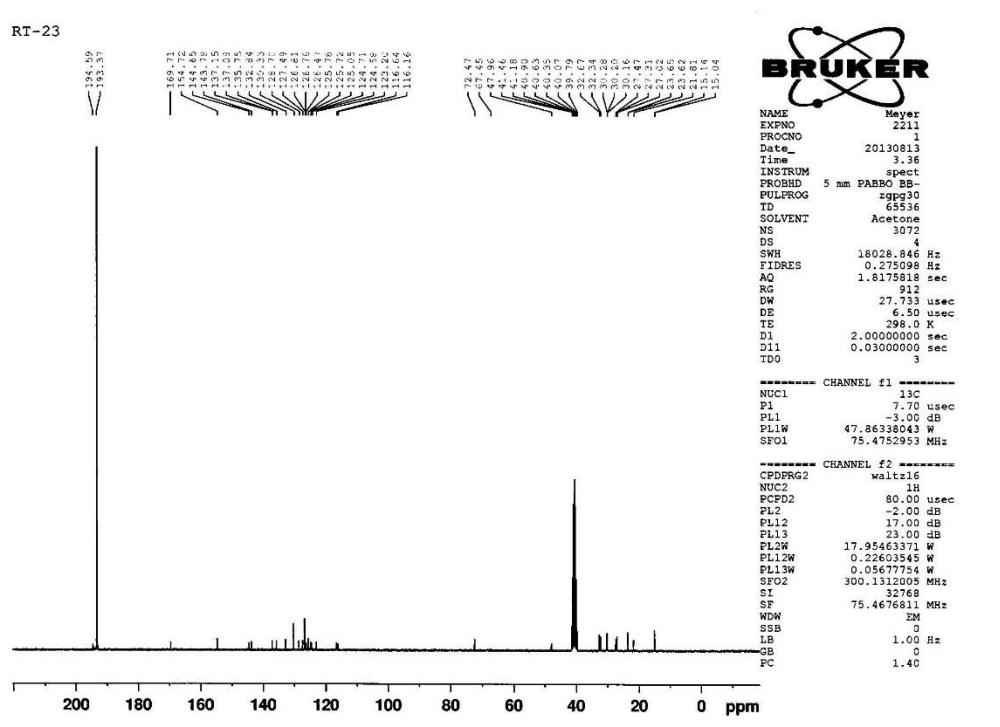


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10f**.

3.23. **(Z)-5-((5-(10-hexyl-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl)-4-(octyloxy)thiophen-2-yl)methylene)-2-thioxothiazolidin-4-one (10g)**

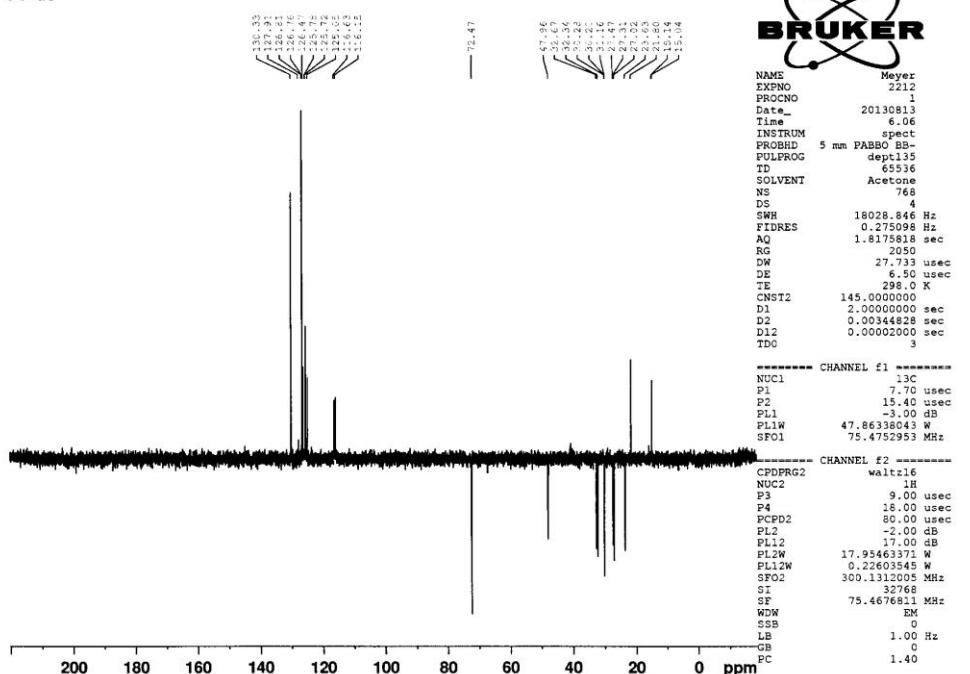


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **10g**.



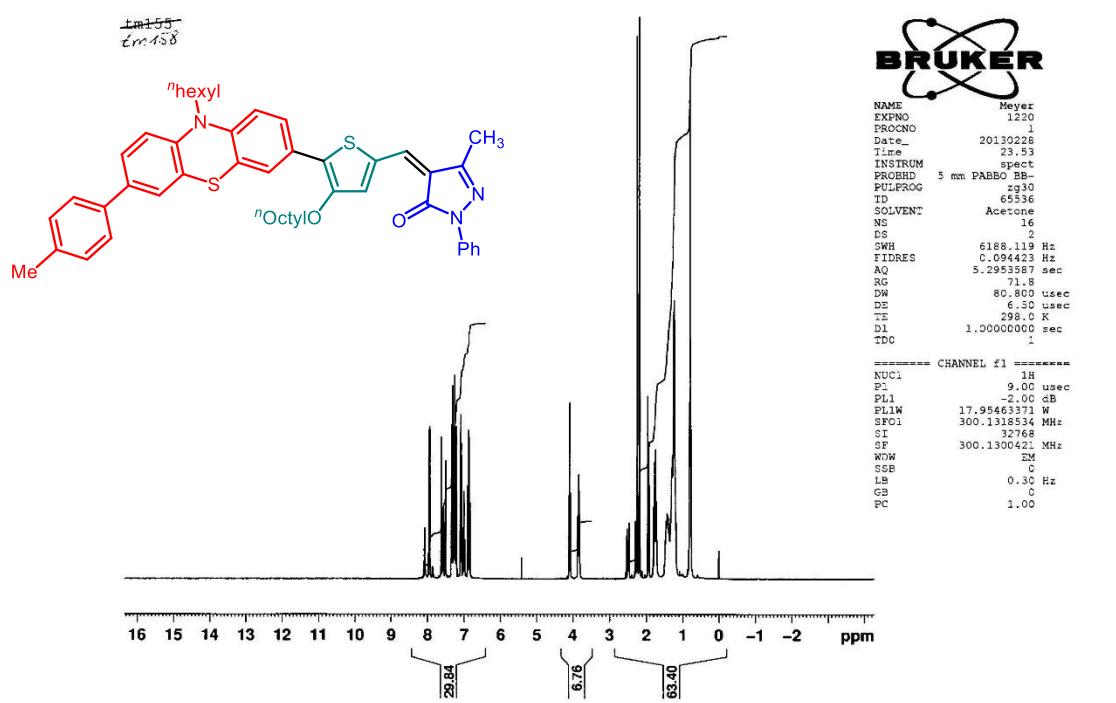
¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10g**.

RT-23

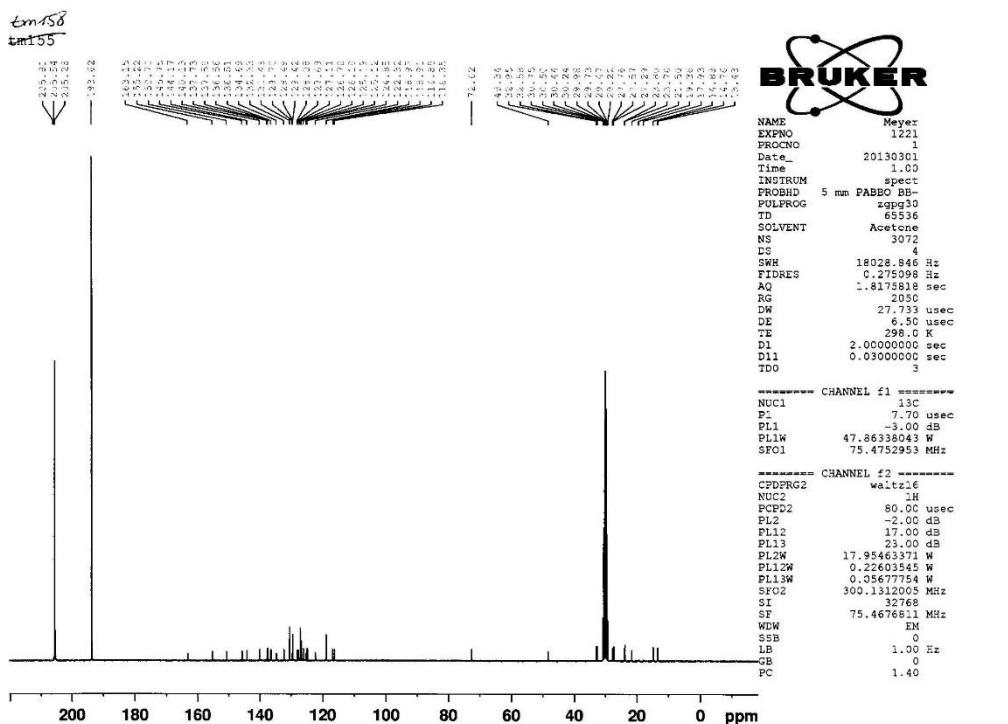


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10g**.

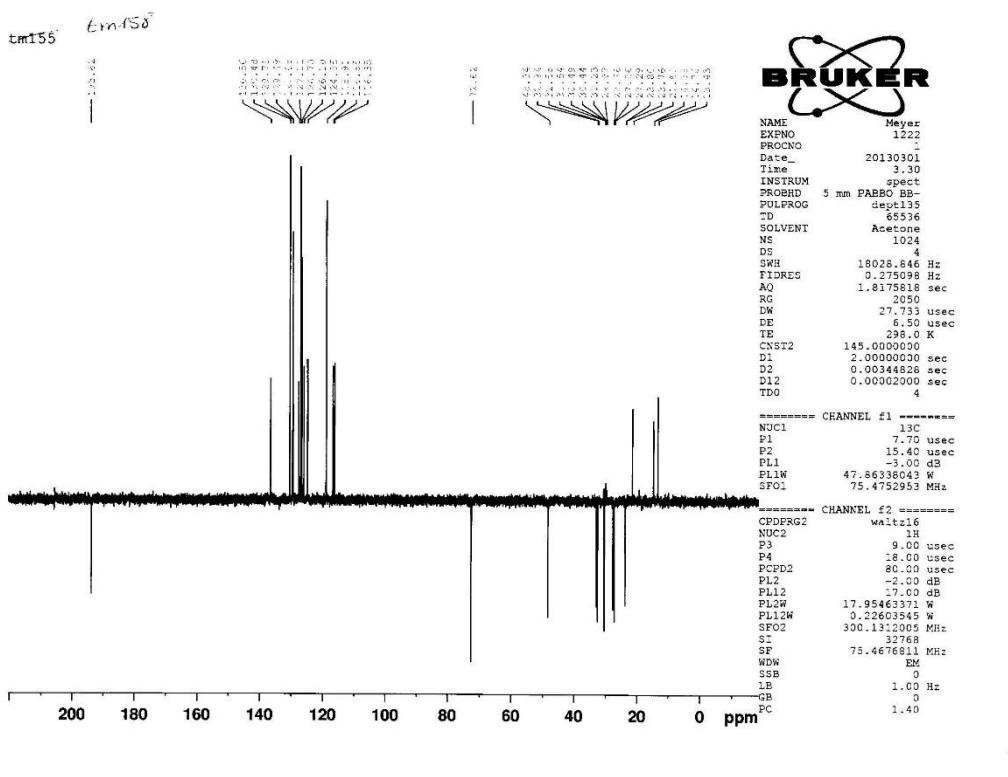
3.24. (*Z*)-4-((5-(10-hexyl-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl)-4-(octyloxy)thiophen-2-yl)methylene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (10h)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 10h.

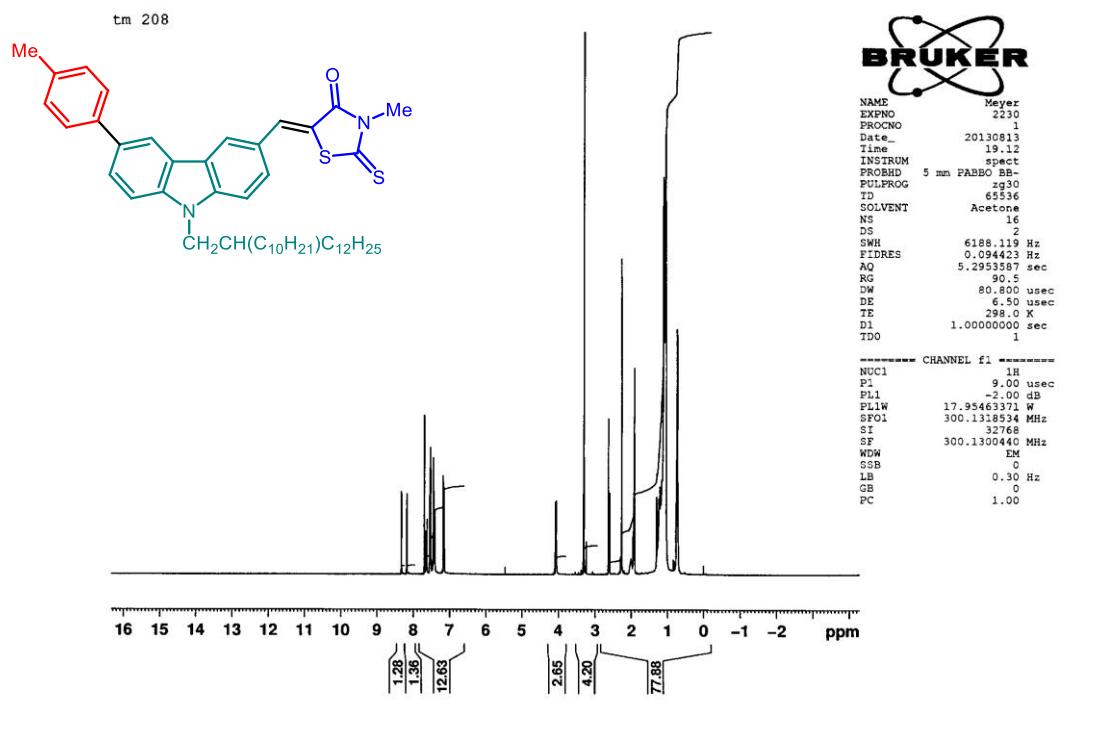


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 10h.

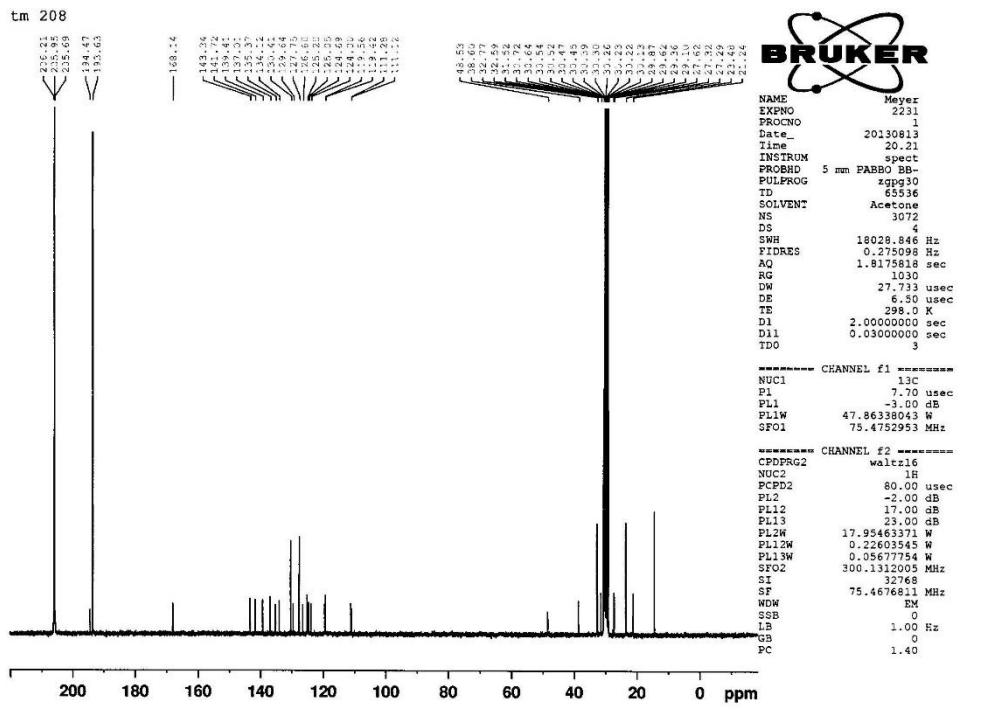


DEPT ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **10h**.

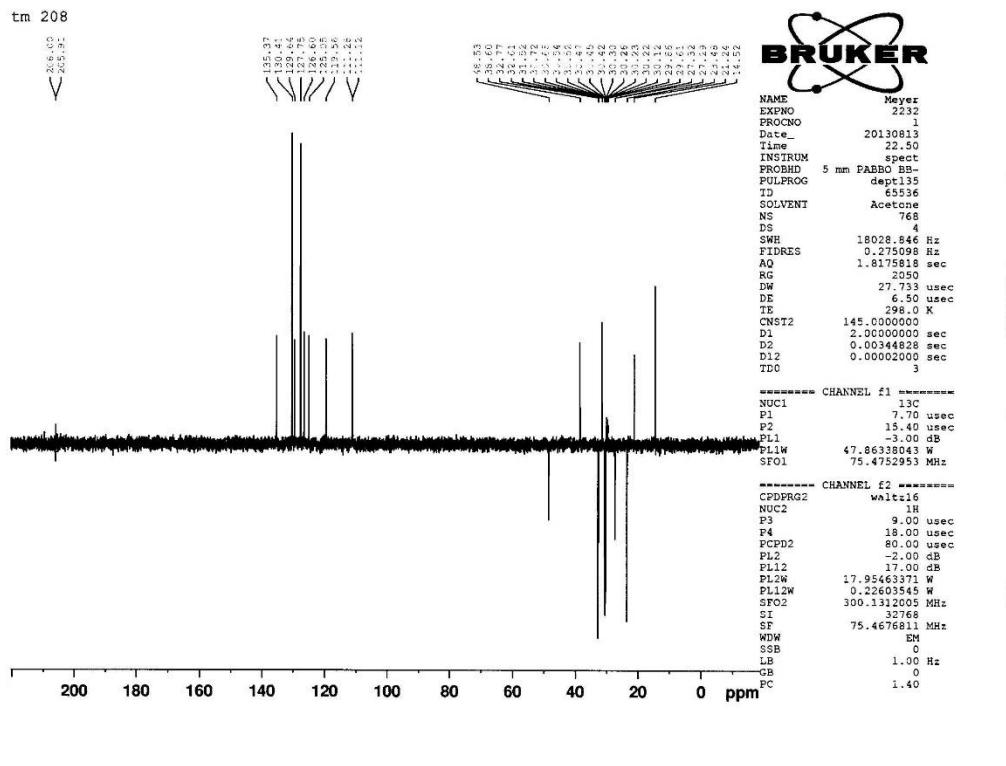
3.25. 5-[{[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (11a)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 11a.

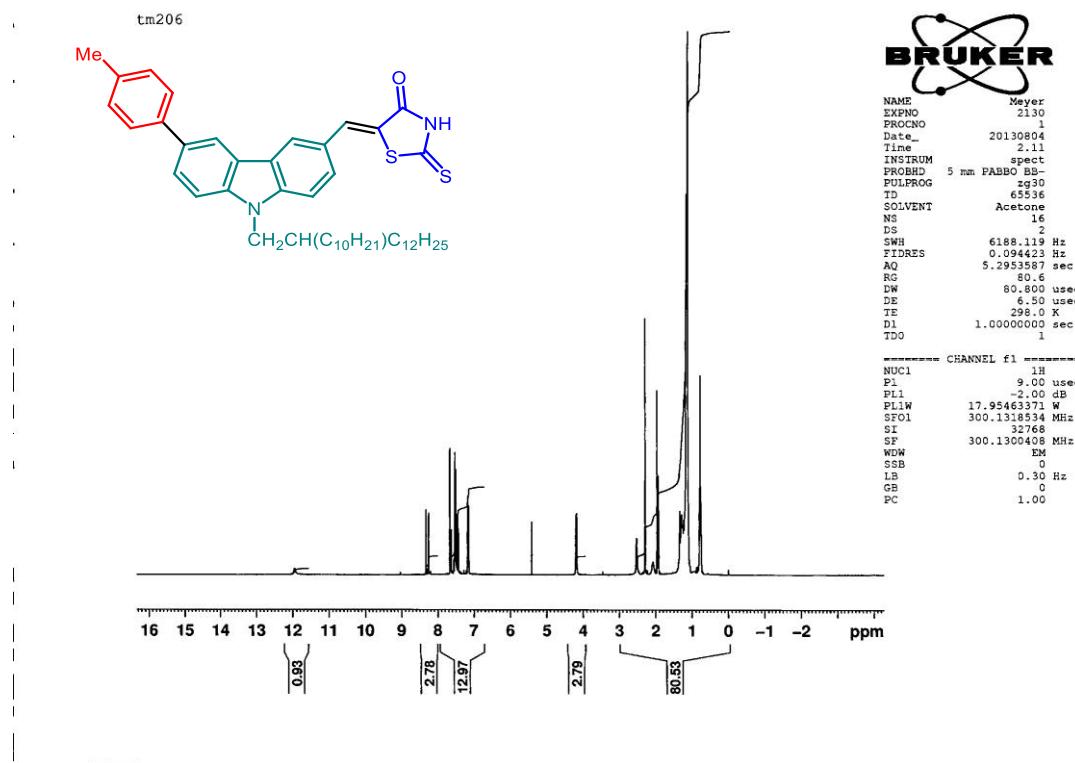


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 11a.

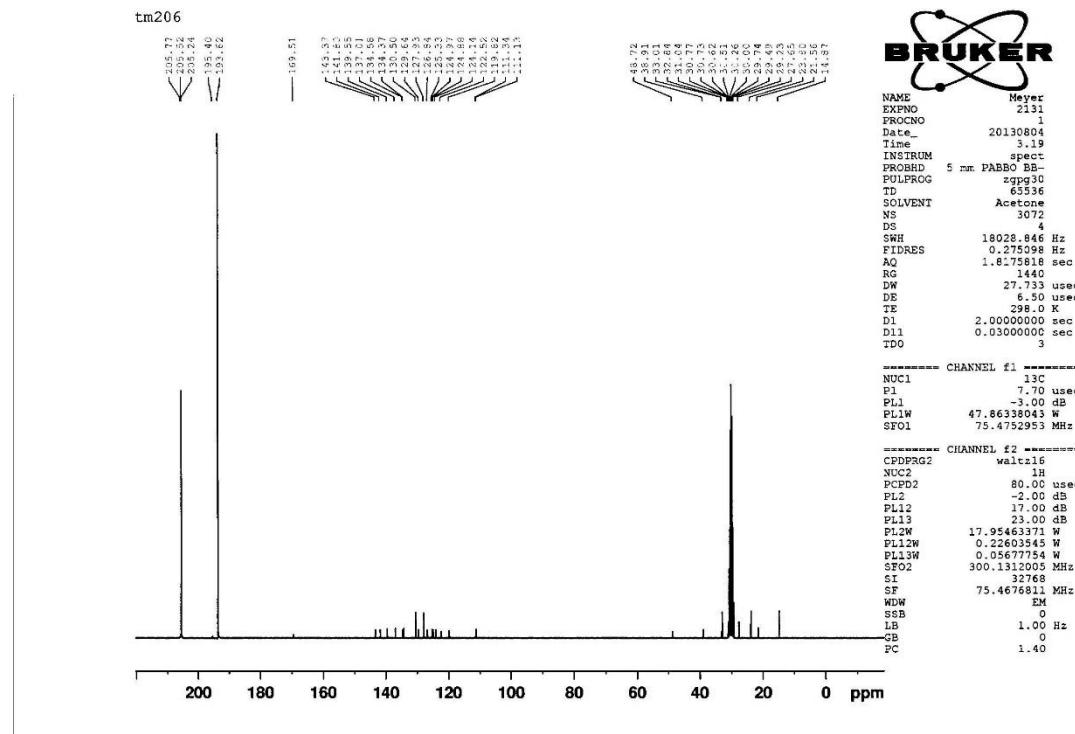


DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound 11a.

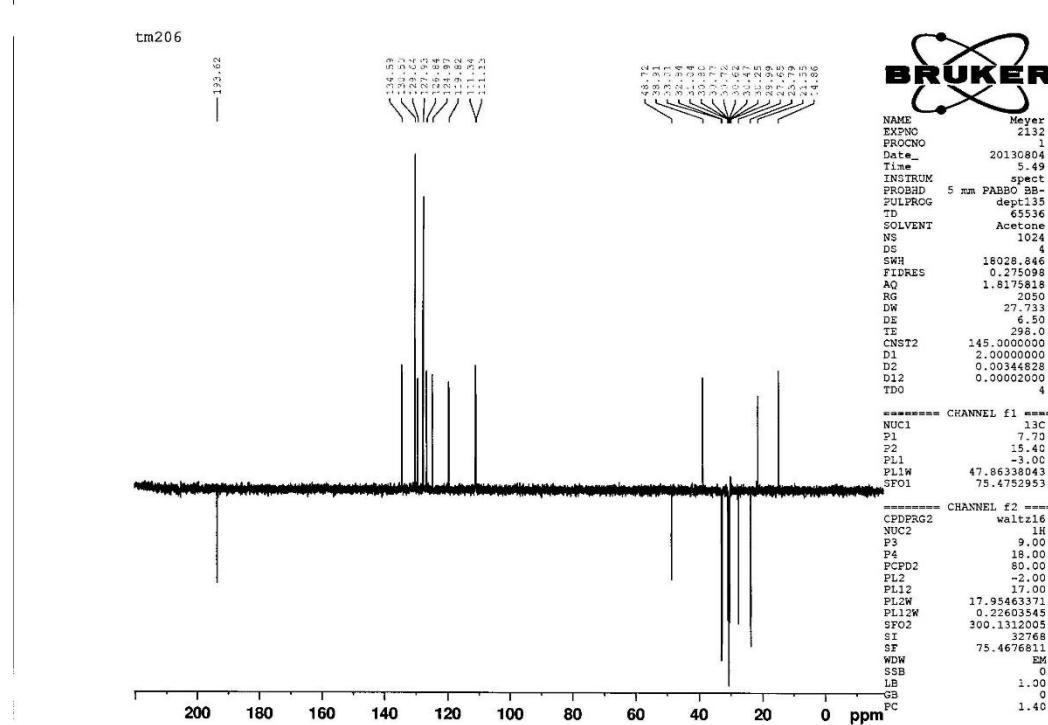
3.26. 5-{[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9H-carbazol-3-yl]methylene}-2-thioxothiazolidin-4-one (11b)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 11b.

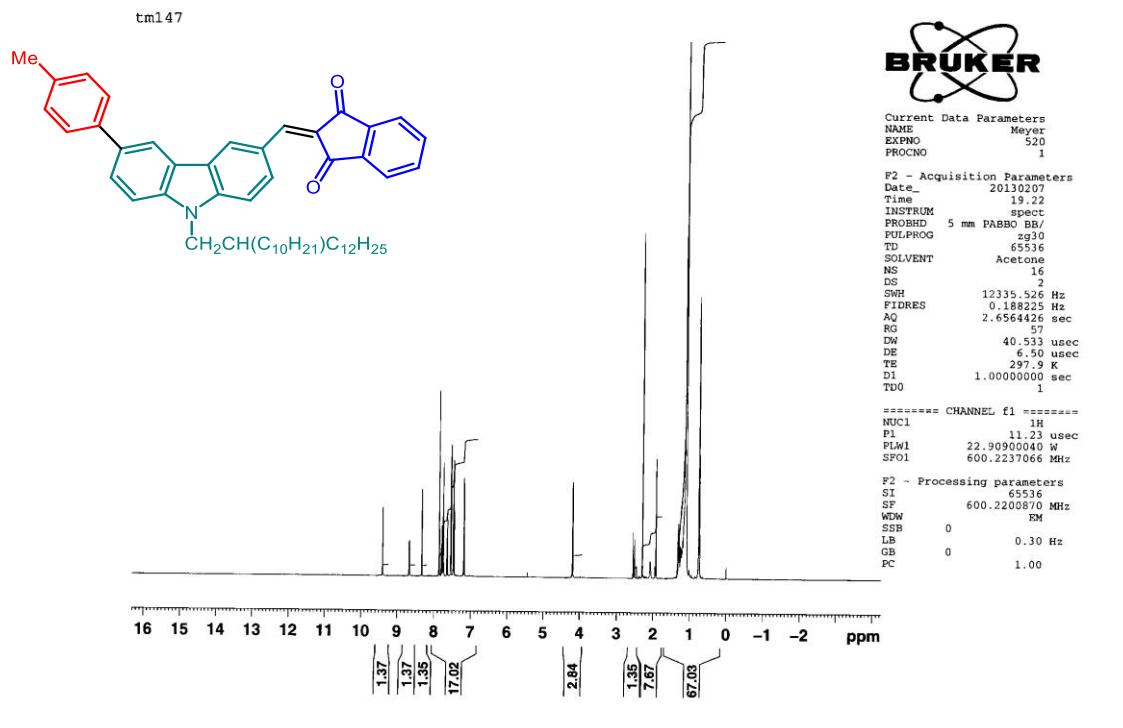


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 11b.

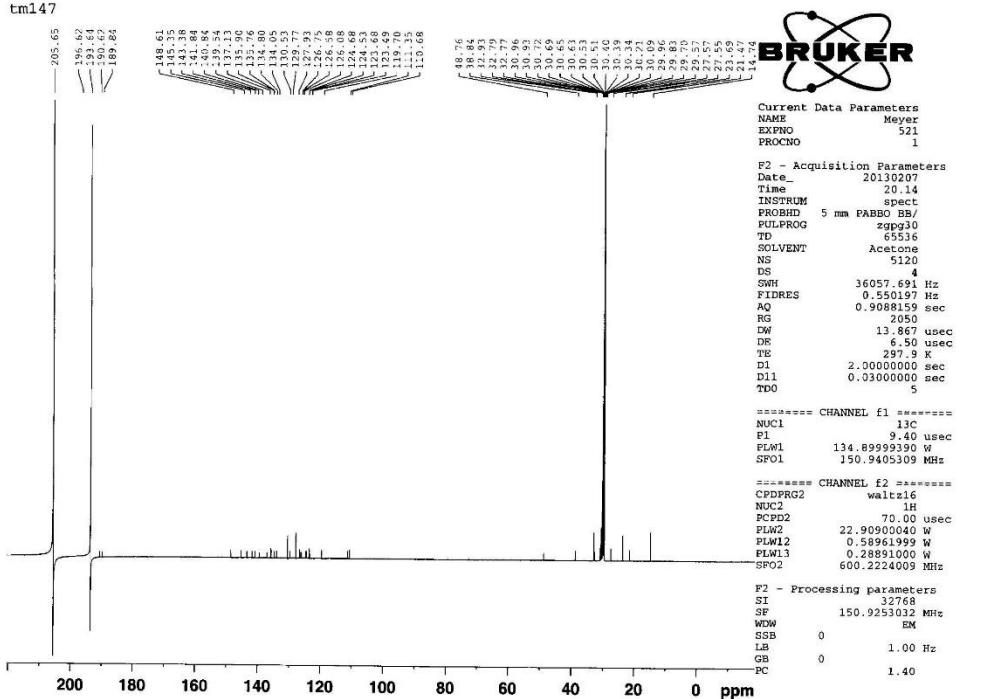


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 11b.

3.27. 2-{[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (11c)

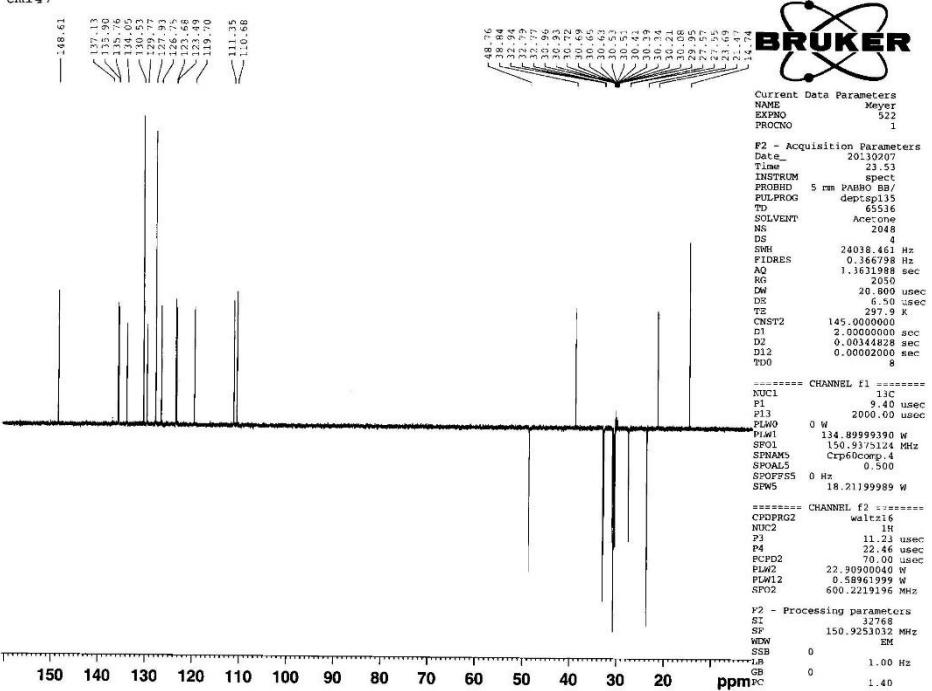


¹H NMR (600 MHz, acetone-d₆/CS₂ 4:1) of compound 11c.



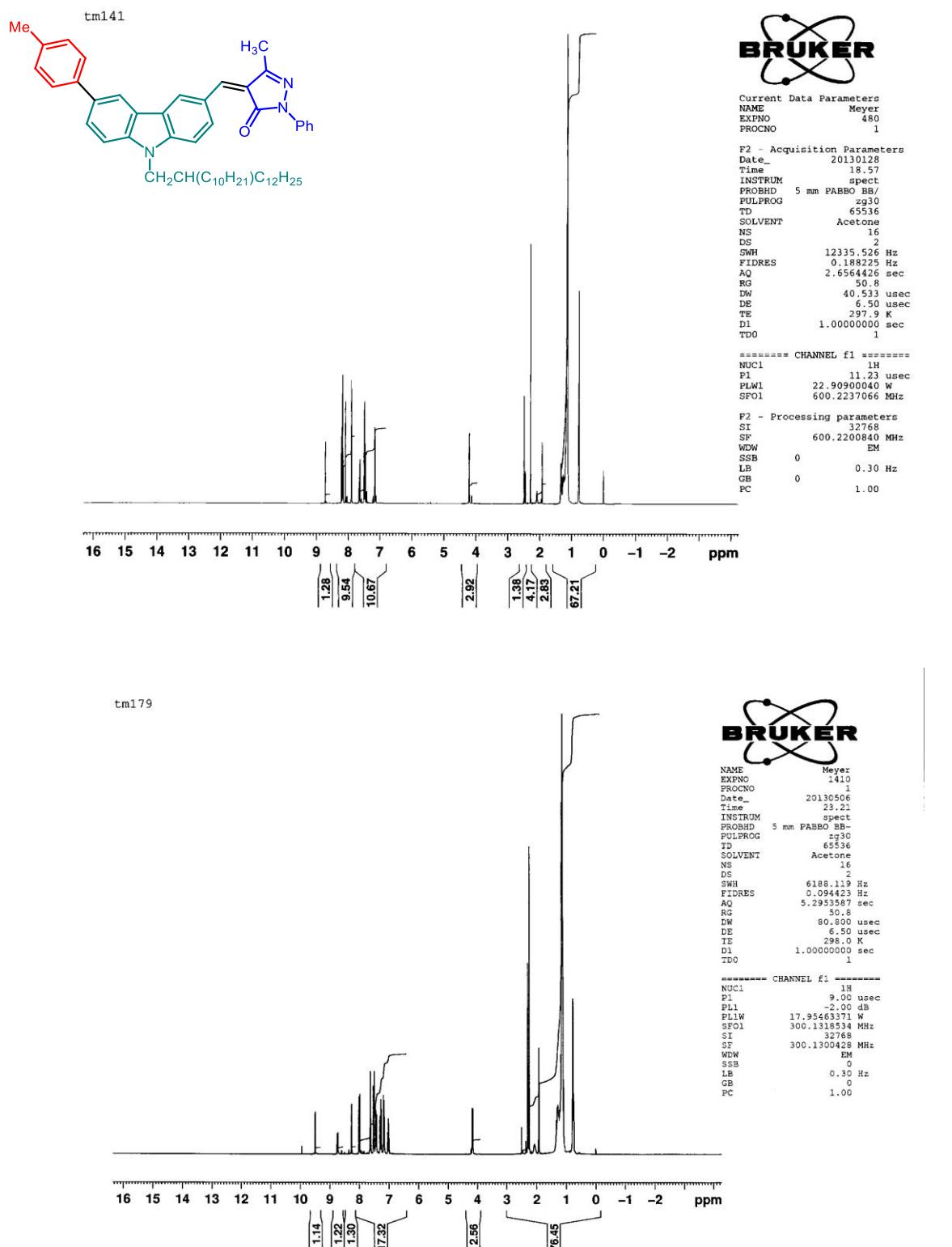
¹³C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound 11c.

tm147

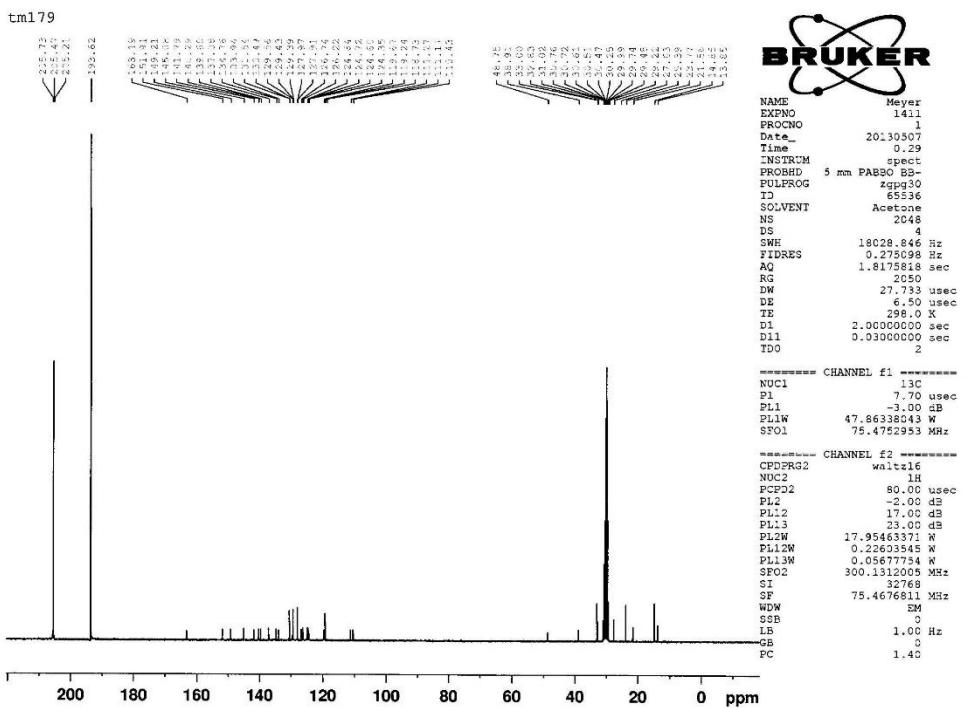


DEPT ^{13}C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound 11c.

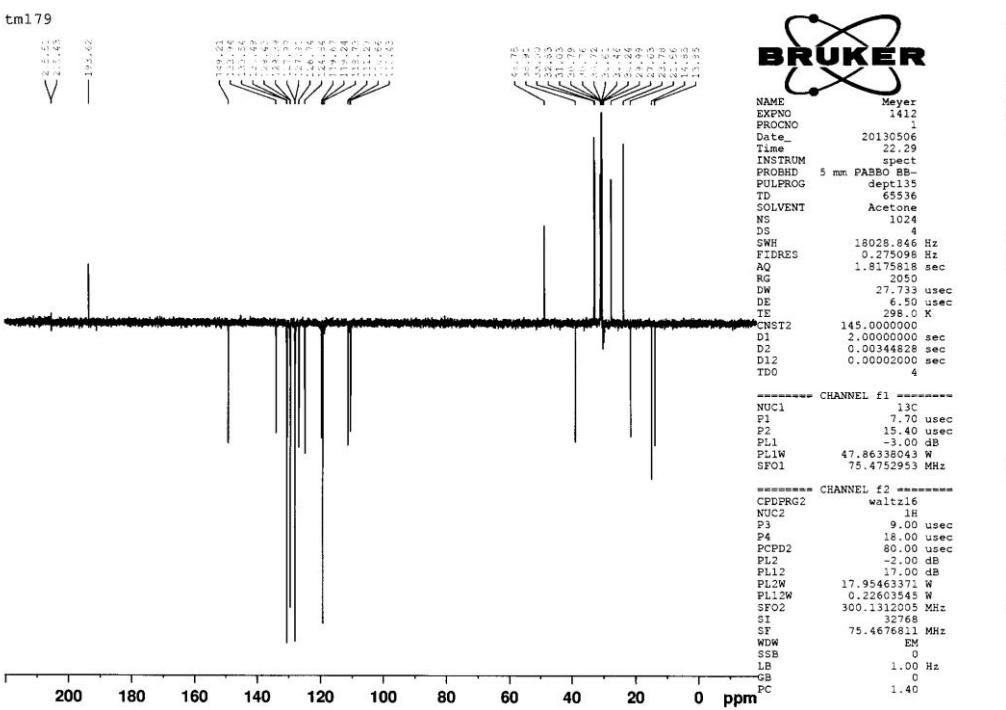
3.28. 4-{[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (11d)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 11d.

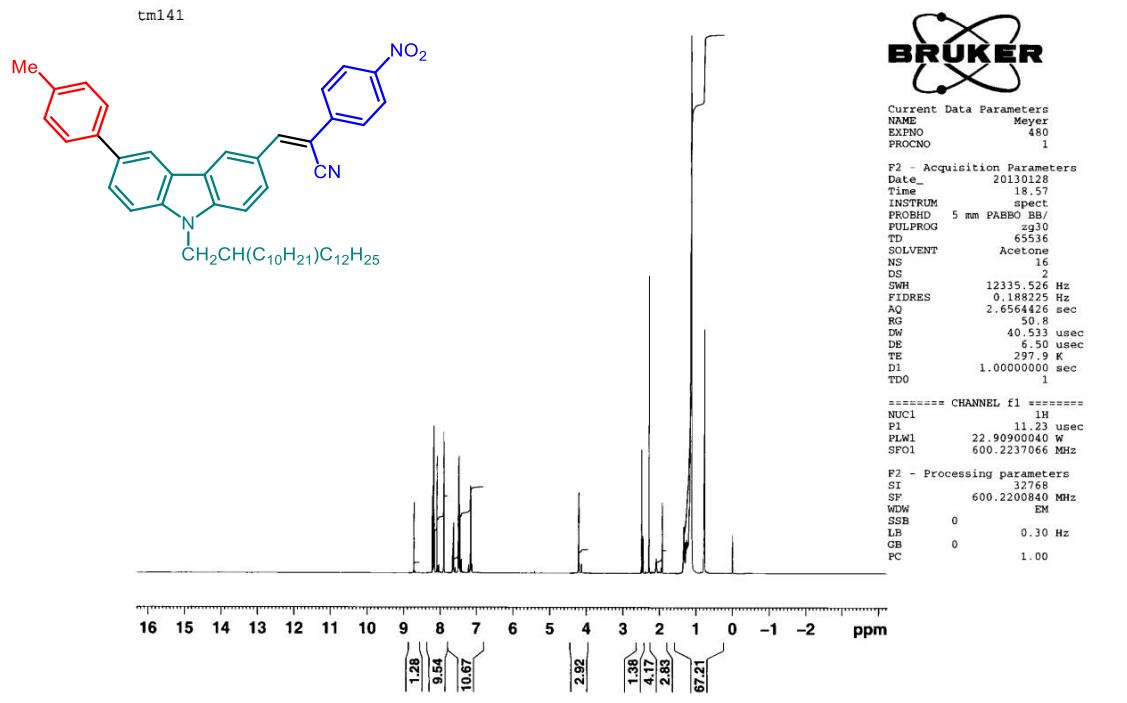


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **11d**.

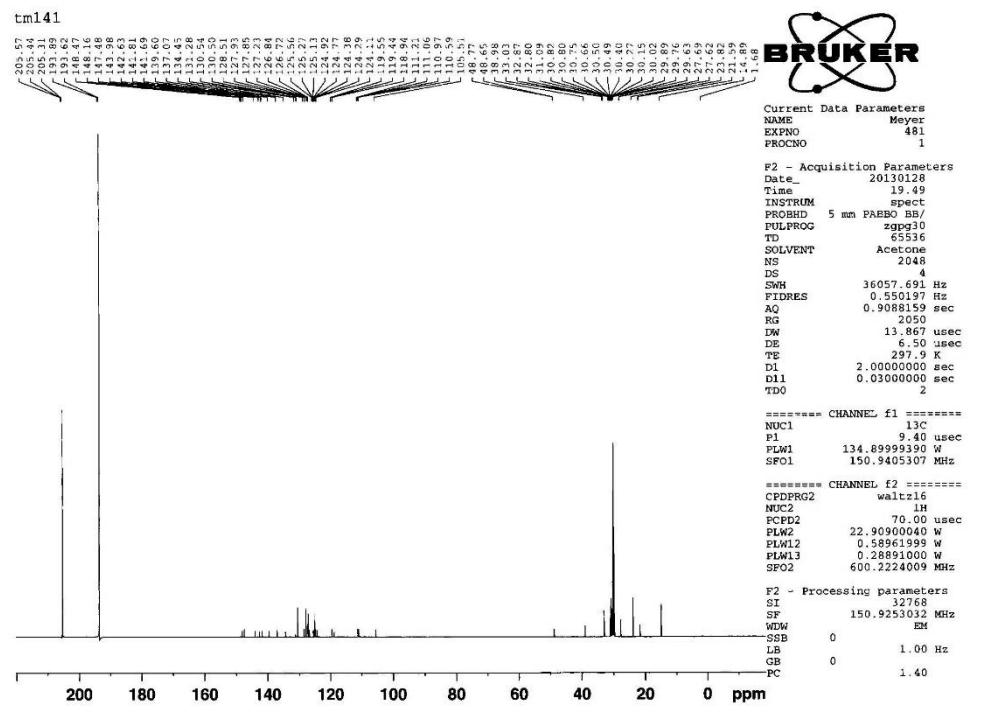


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **11d**.

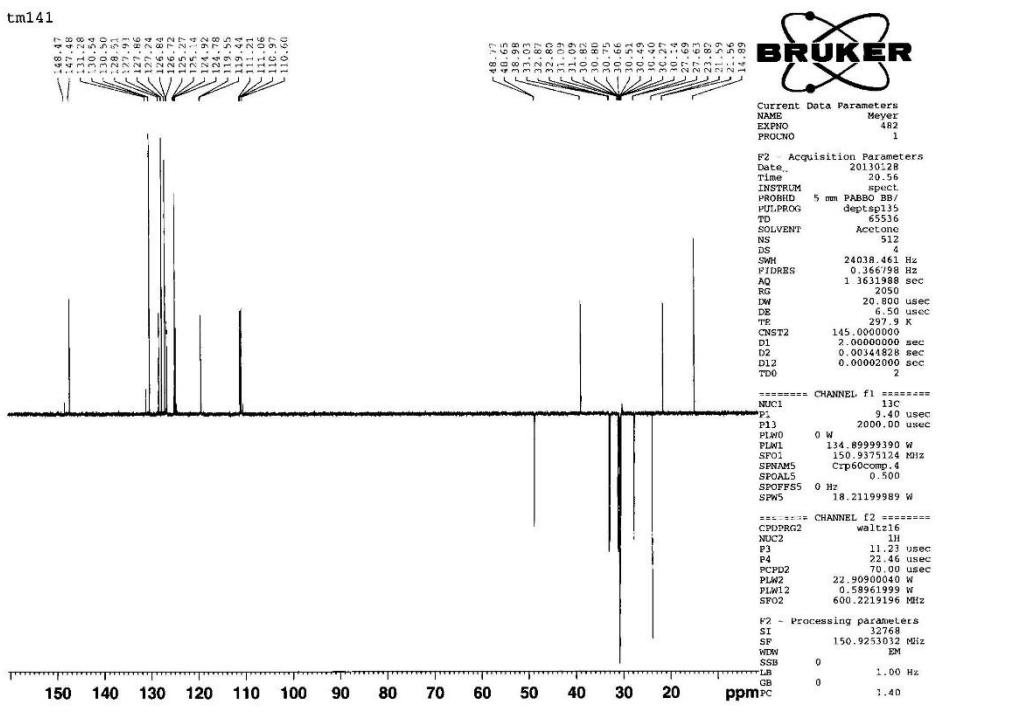
3.29. 3-[9-(2-Decyltetradecyl)-6-(*p*-tolyl)-9*H*-carbazol-3-yl]-2-(4-nitrophenyl)acrylonitrile (11e)



¹H NMR (600 MHz, acetone-d₆/CS₂ 4:1) of compound 11e.

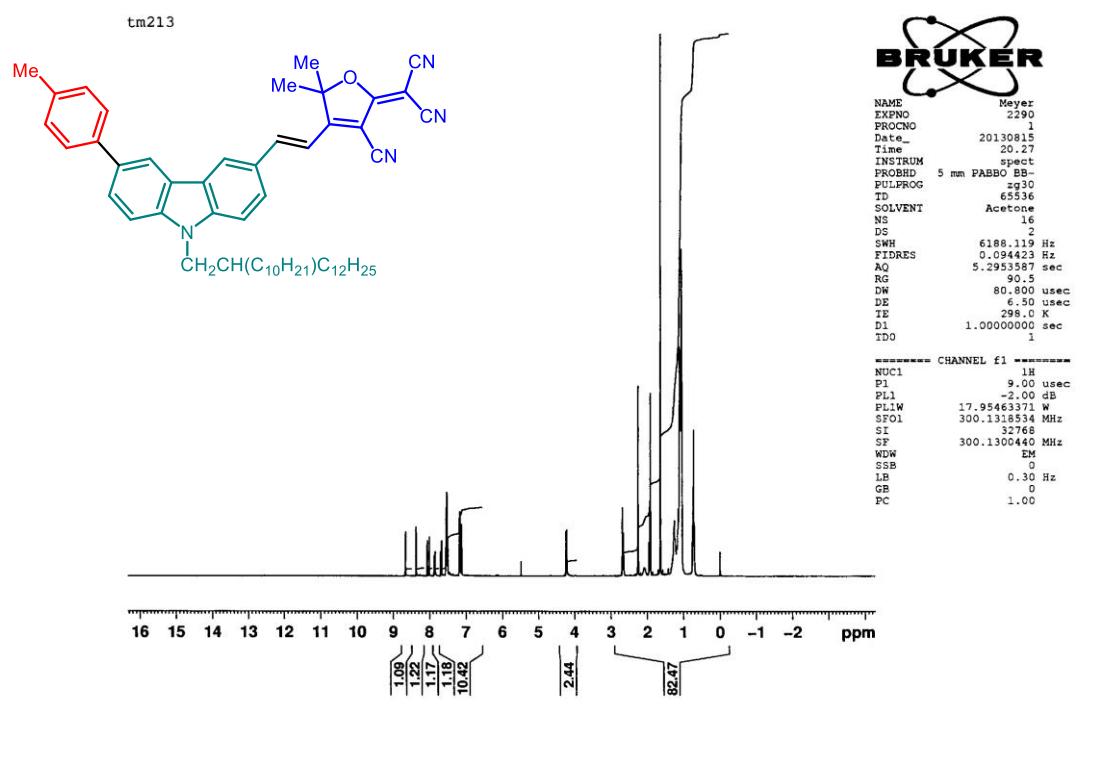


¹³C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound **11e**.

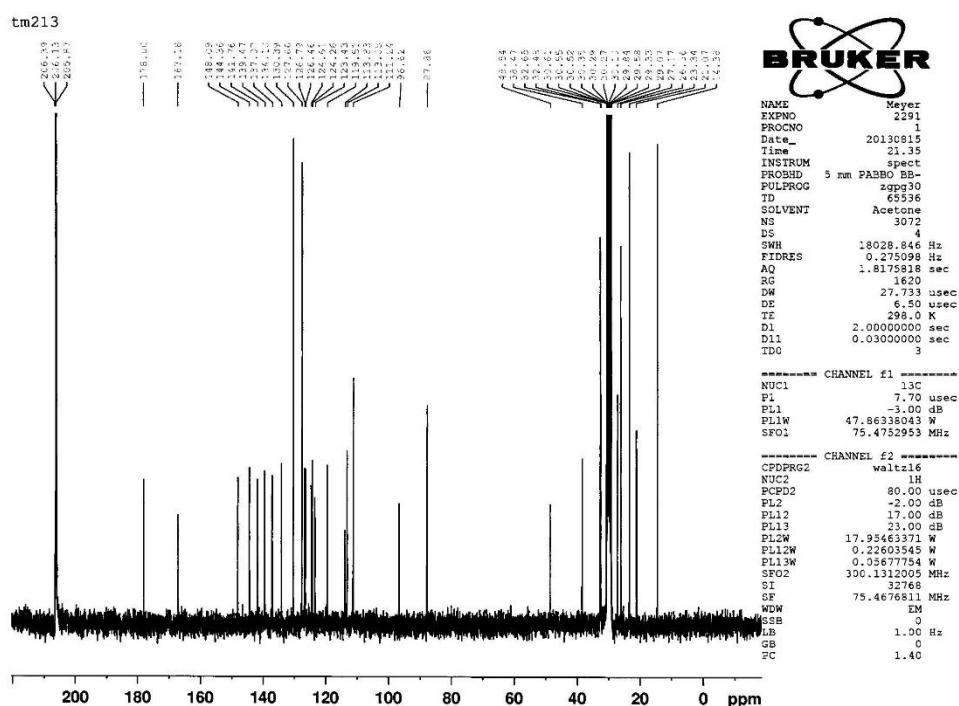


DEPT ^{13}C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound **11e**.

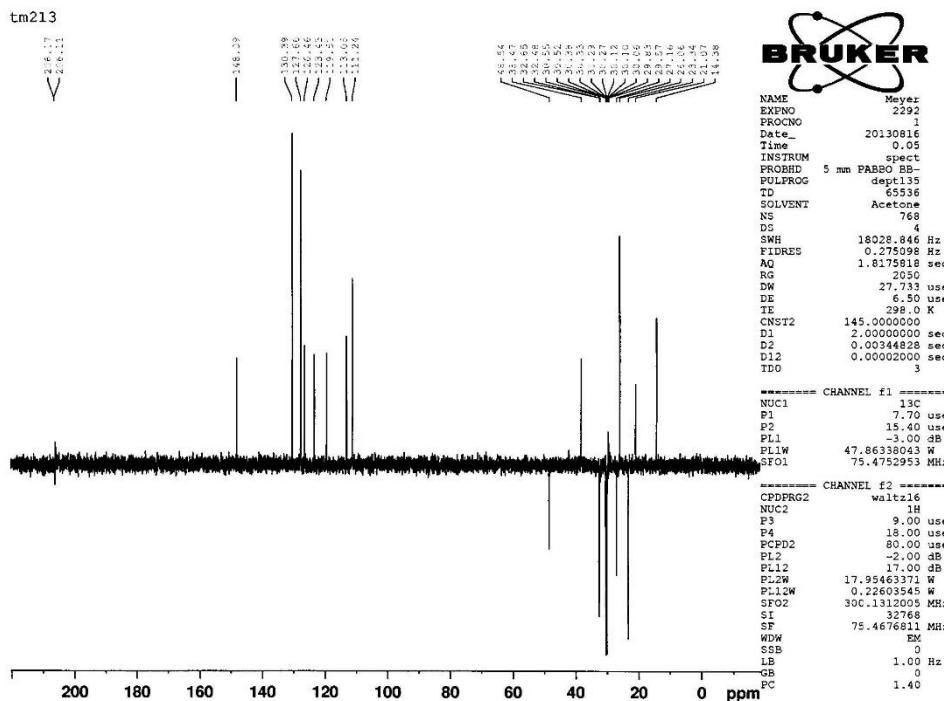
3.30. (*E*)-2-{3-Cyano-4-[2-(9-{2-decyltetradecyl}-6-{*p*-tolyl}-9*H*-carbazol-3-yl)vinyl]-5,5-dimethylfuran-2[5*H*]-yliden}malonitrile (11f)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 11f.

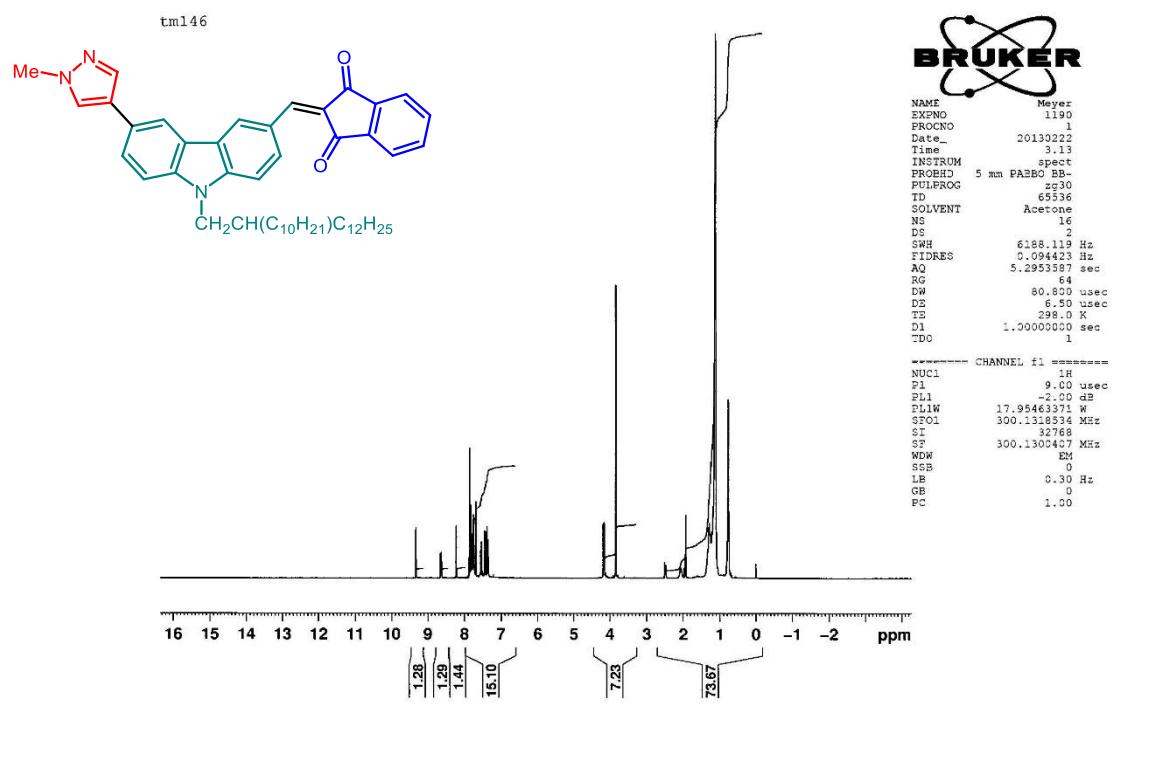


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 11f.

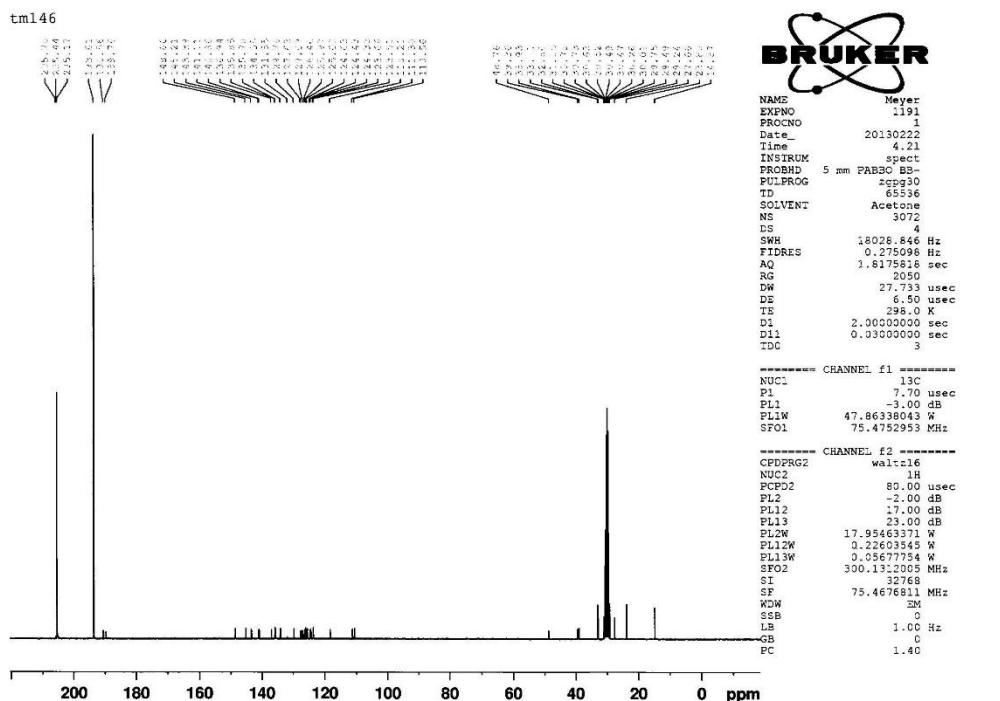


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **11f**.

3.31. 2-{[9-(2-Decyltetradecyl)-6-(1-methyl-1H-pyrazol-4-yl)-9H-carbazol-3-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (11g)

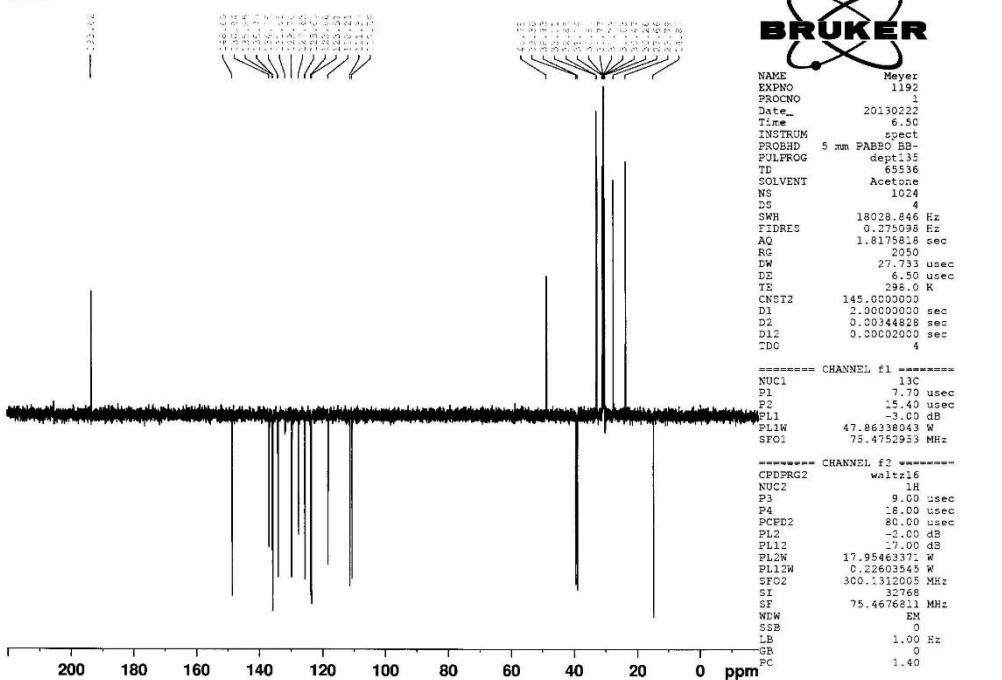


¹H NMR (600 MHz, acetone-d₆/CS₂ 4:1) of compound 11g.



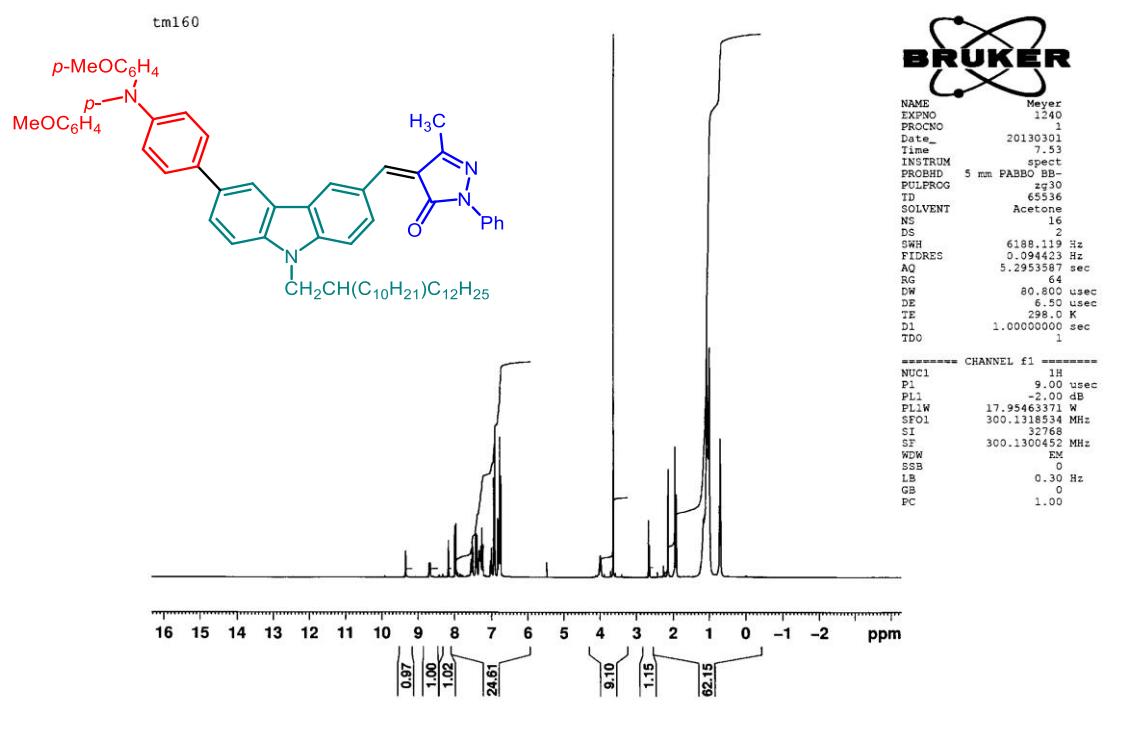
¹³C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound 11g.

tm146

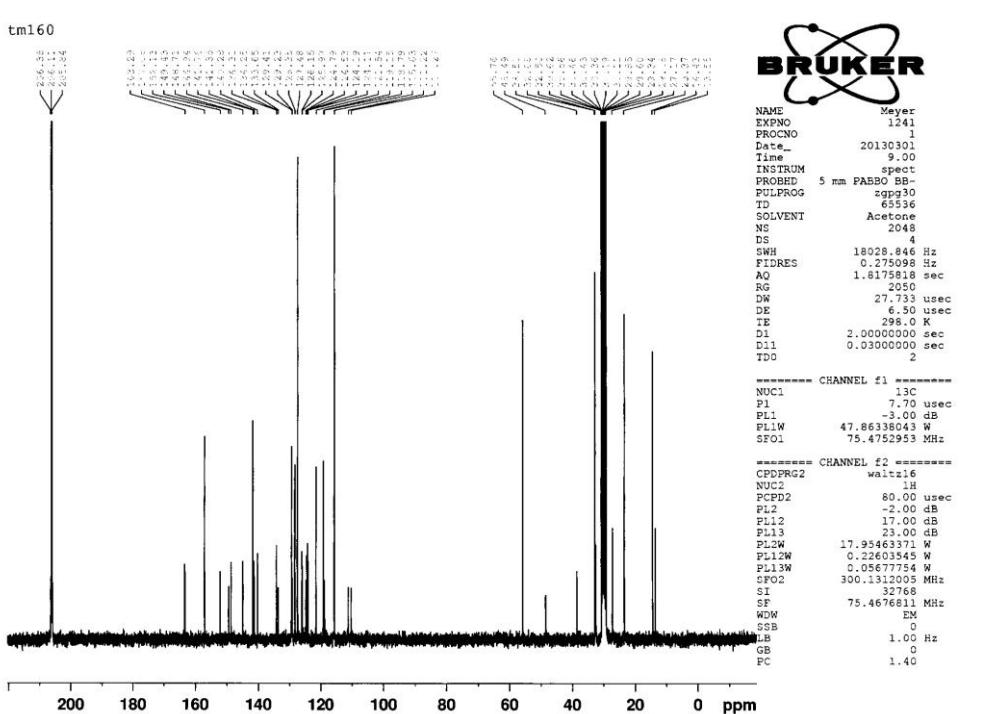


DEPT ^{13}C NMR (150 MHz, acetone-d₆/CS₂ 4:1) of compound **11g**.

3.32. 4-{[6-(4-{Bis[4-methoxyphenyl]amino}phenyl)-9-(2-decytetradecyl)-9*H*-carbazol-3-yl]methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (11h)

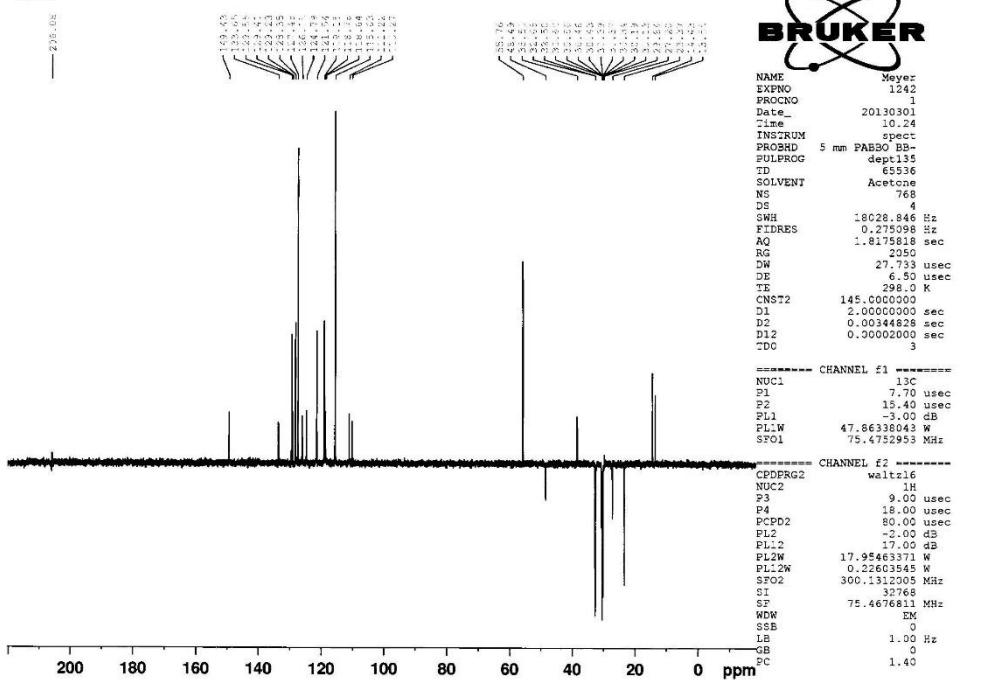


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 11h.

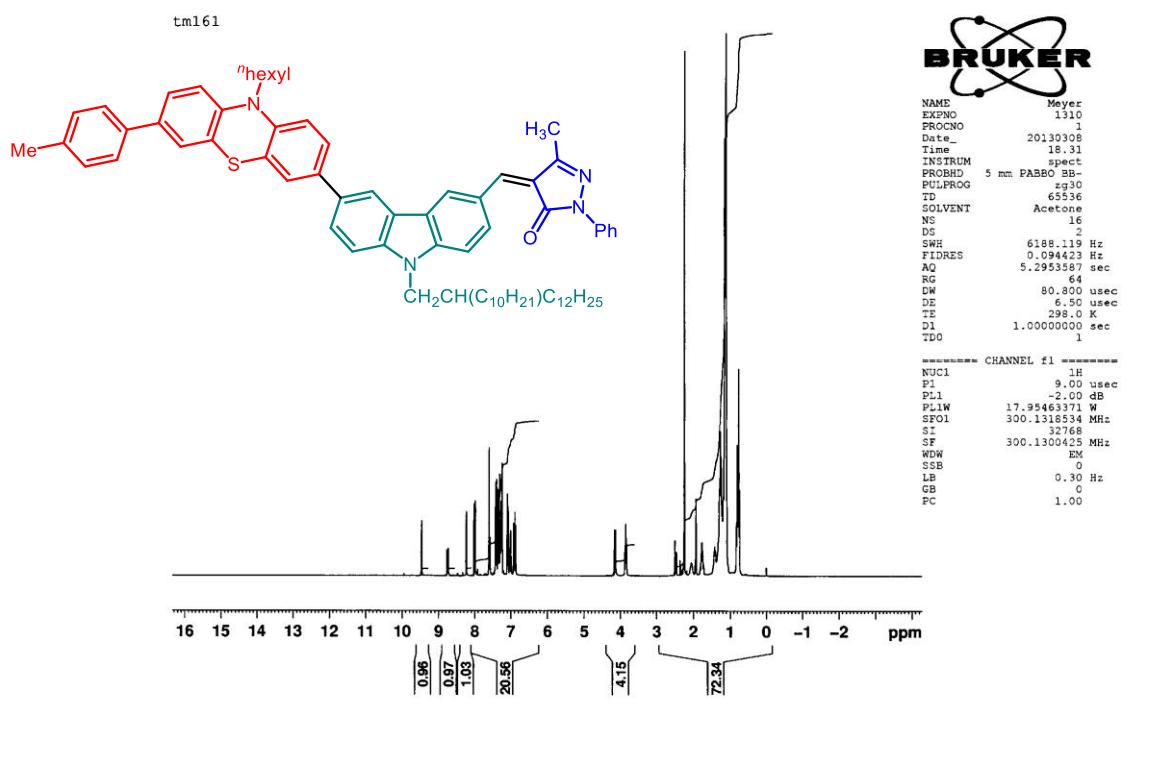


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 11h.

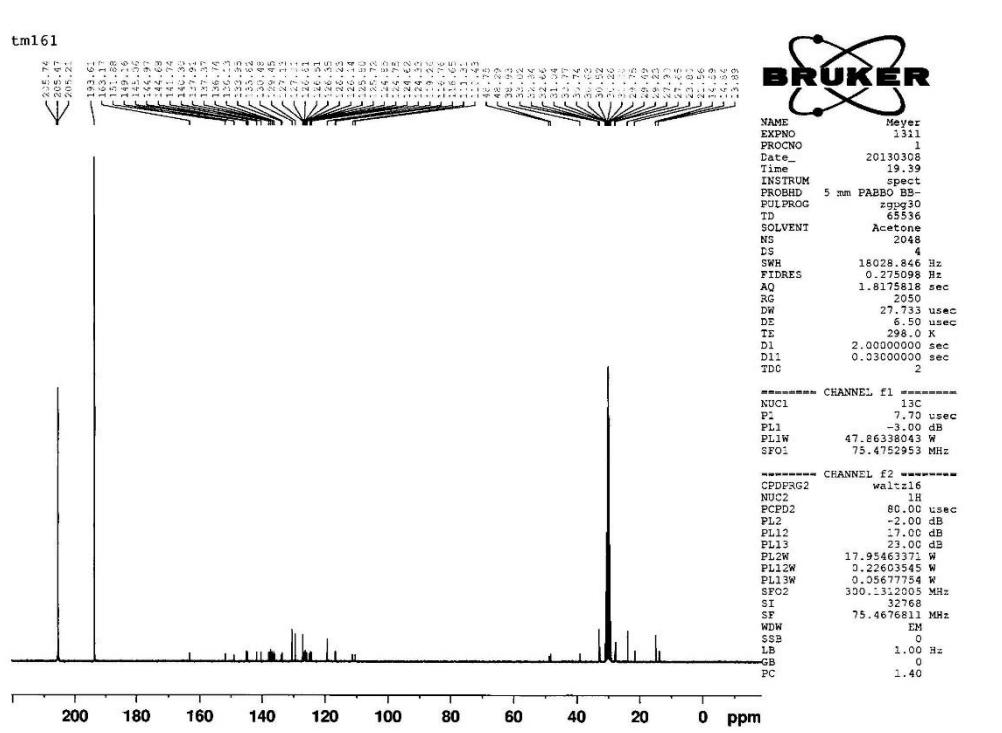
tm160

DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 11h.

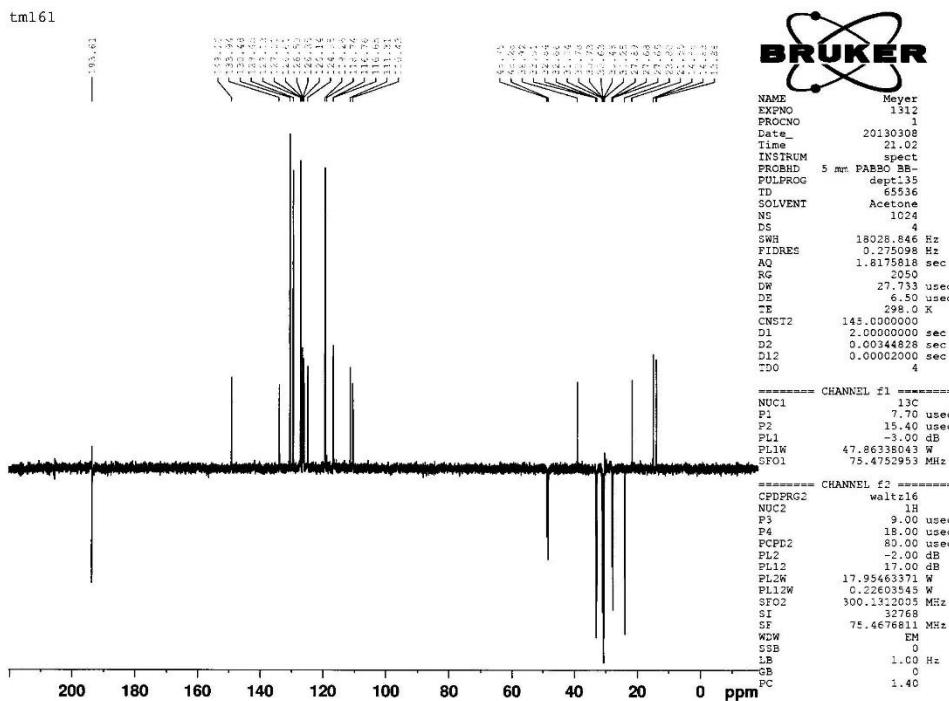
3.33. 4-{{[9-(2-Decyltetradecyl)-6-(10-hexyl-7-{*p*-tolyl}-10*H*-phenothiazin-3-yl)-9*H*-carbazol-3-yl]methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (11i)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 11i.

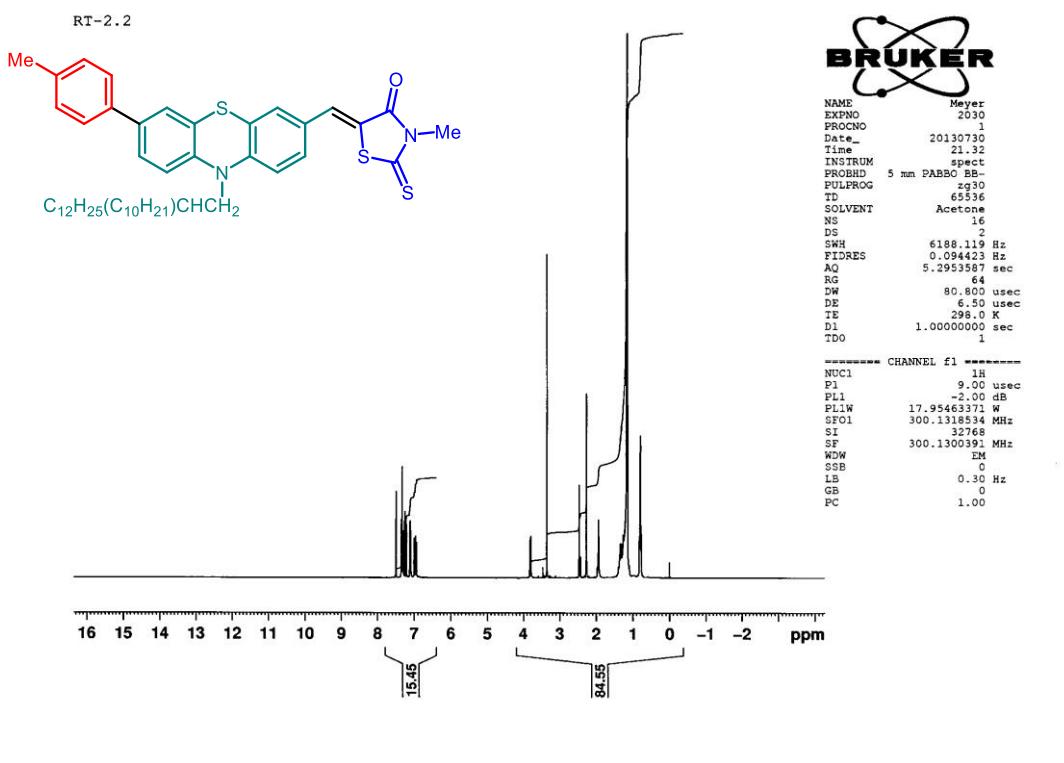


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 11i.

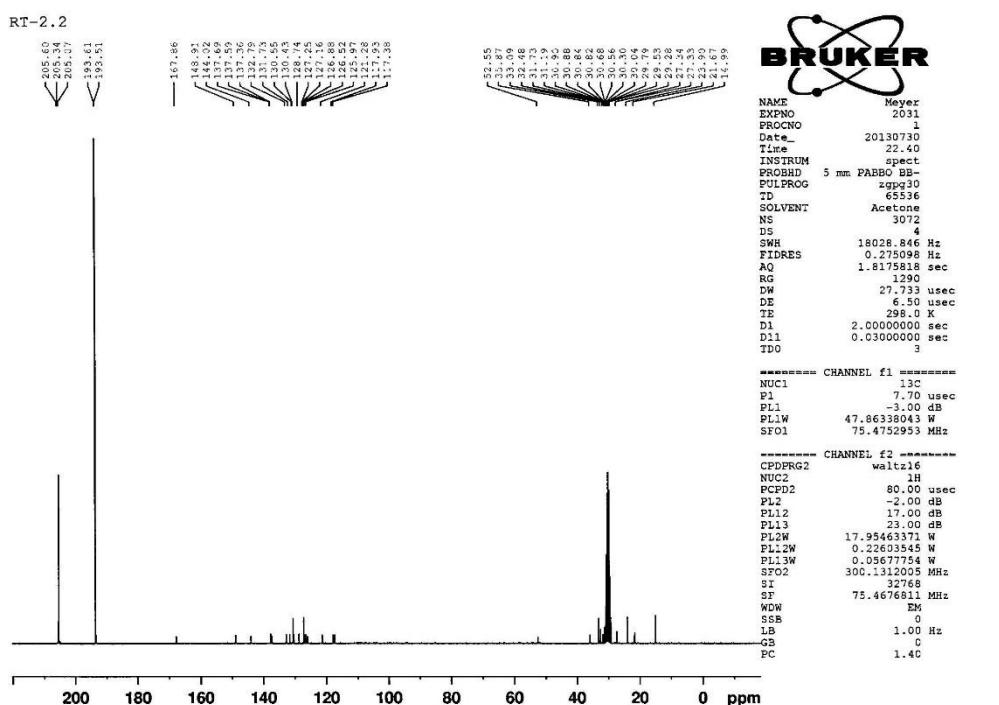


DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **11i**.

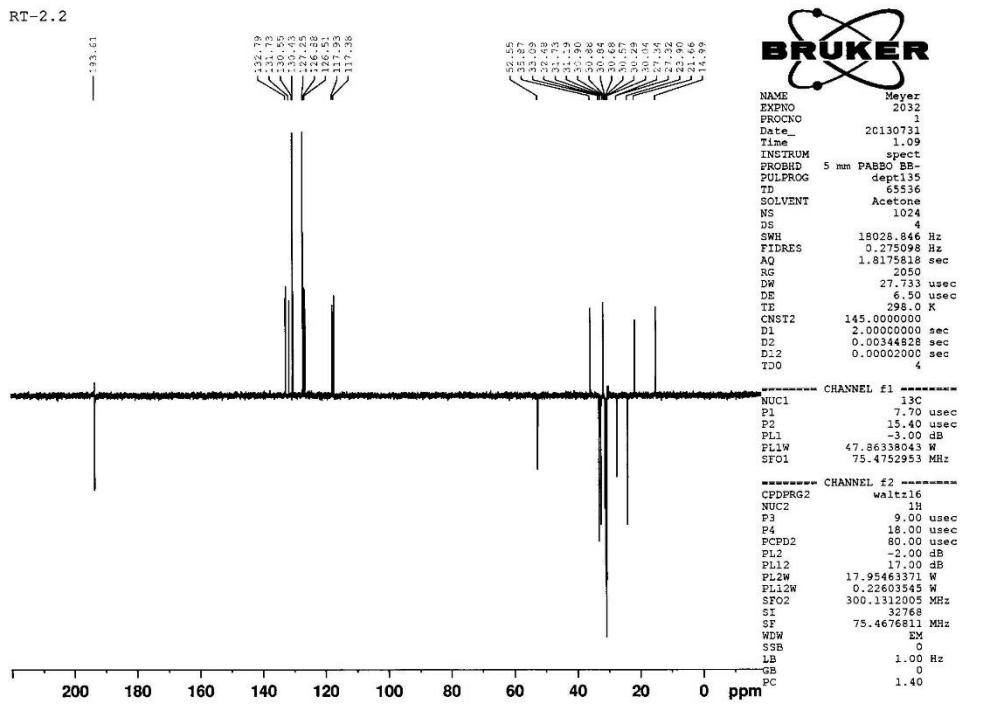
3.34. (*Z*)-5-{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12a)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12a.

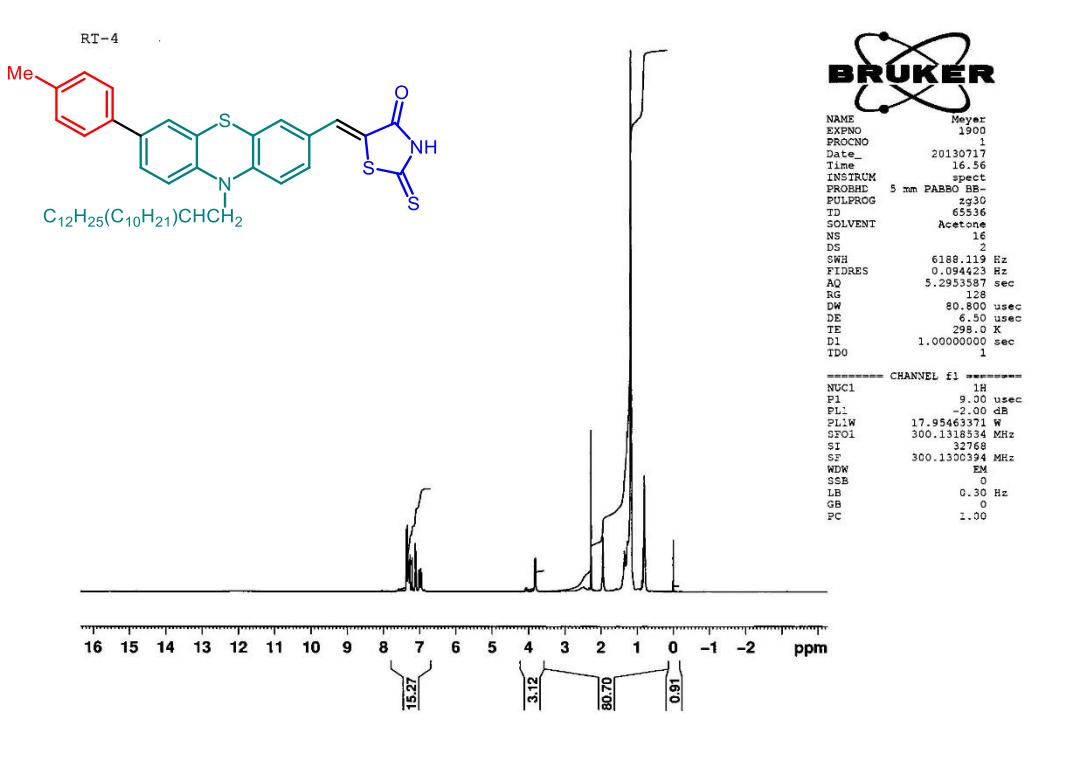


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12a.

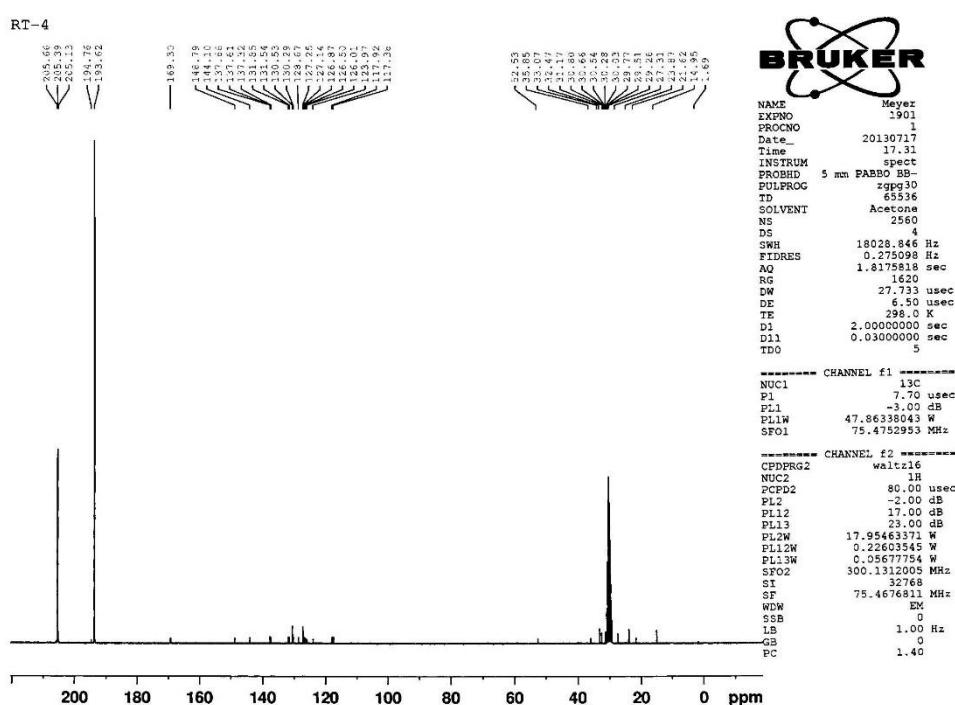


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12a**.

3.35. (Z)-5-{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-2-thioxothiazolidin-4-one (12b)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **12b**.



¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12b**.

RT-4

— 5.93, t, 2J

131.85
129.56
120.55
115.29
73.74
23.68
13.67
11.54
11.52
11.72
11.73

67.34

52.53
39.99
35.15
32.87
32.17
30.92
30.66
30.55
29.75
28.51
22.93
22.39
22.31
22.62
14.95



NMR
EXPNO
PRGRQD
Date_
Time_
INSTRUM
PROBHD
PULPROG
TITL
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
CQST2
D1
D2
D12
TDO

Meyer
1902
1
20130717
20.01
spect
5 mm PABBO BB
dec35
65536
Acetone
768
4
18028.846 Hz
0.2000000 Hz
1.6172818 sec
2050
27.733 usec
6.50 usec
293.0 K
145.0000000
2.30000000 sec
0.003446828 sec
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3

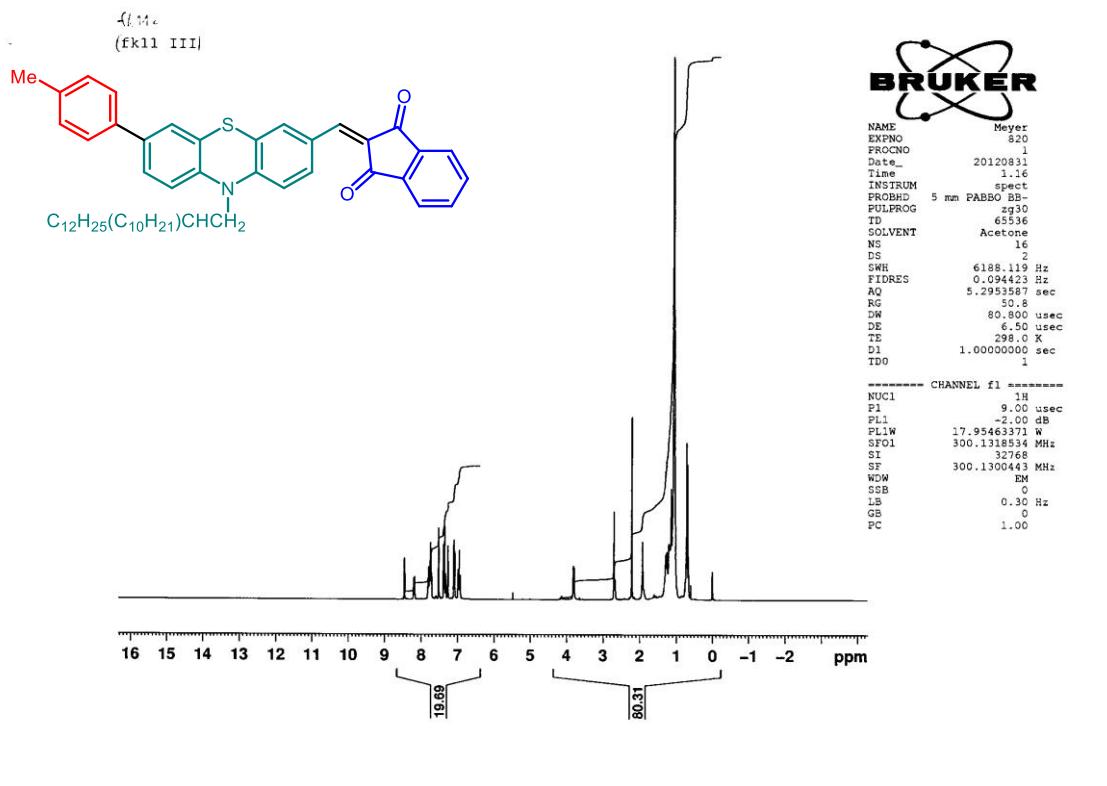
----- CHANNEL f1 -----
NUC1 13C
P1 7.70 usec
P2 15.40 usec
P11 -3.00 dB
P11W 47.8838043 W
SF01 75.4752953 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P3 8.00 usec
P4 18.00 usec
PCPD2 60.00 usec
P52 -2.00 dB
P112 17.00 dB
P12W 17.95463371 W
P112W 0.22603545 W
SF02 300.113255 MHz
SI 32768
SF 75.4676811 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

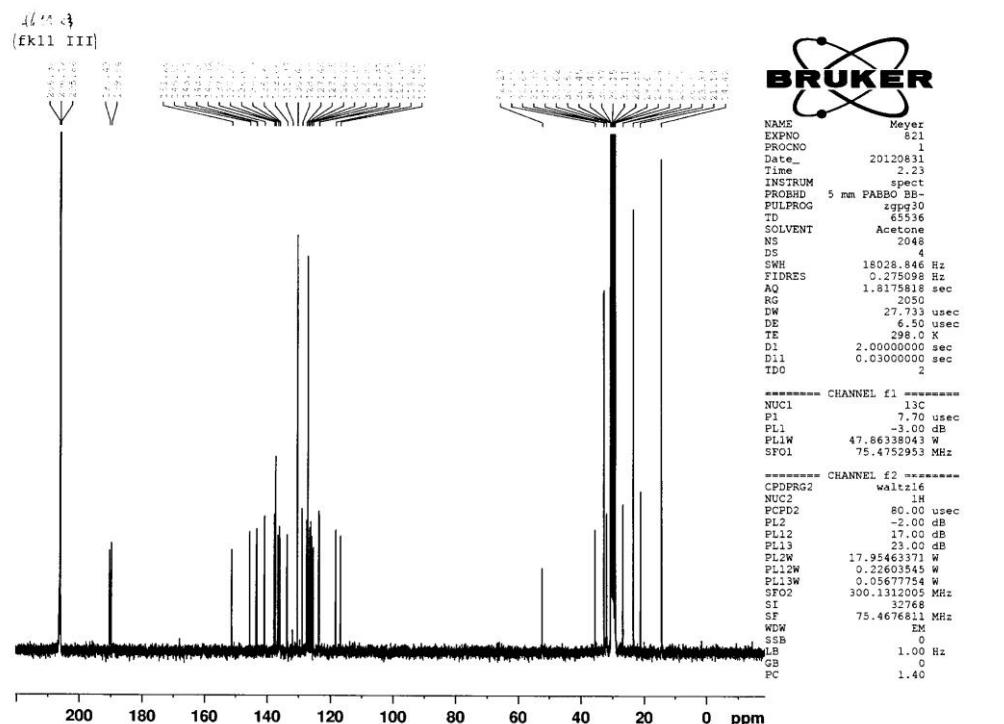
200 180 160 140 120 100 80 60 40 20 0 ppm

DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12b**.

3.36. 2-{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (12c)

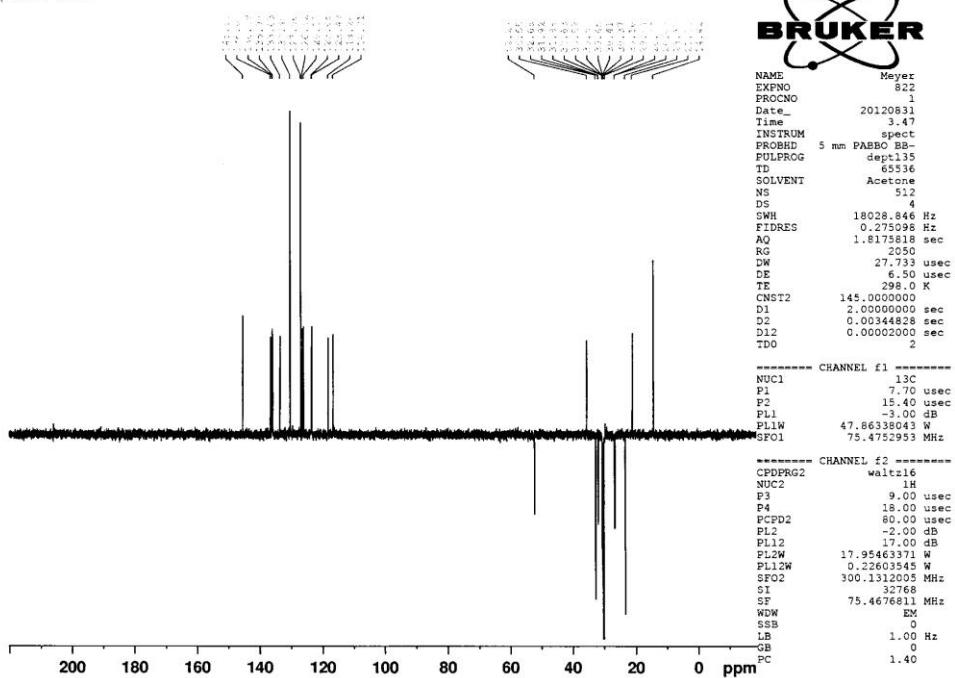


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12c.



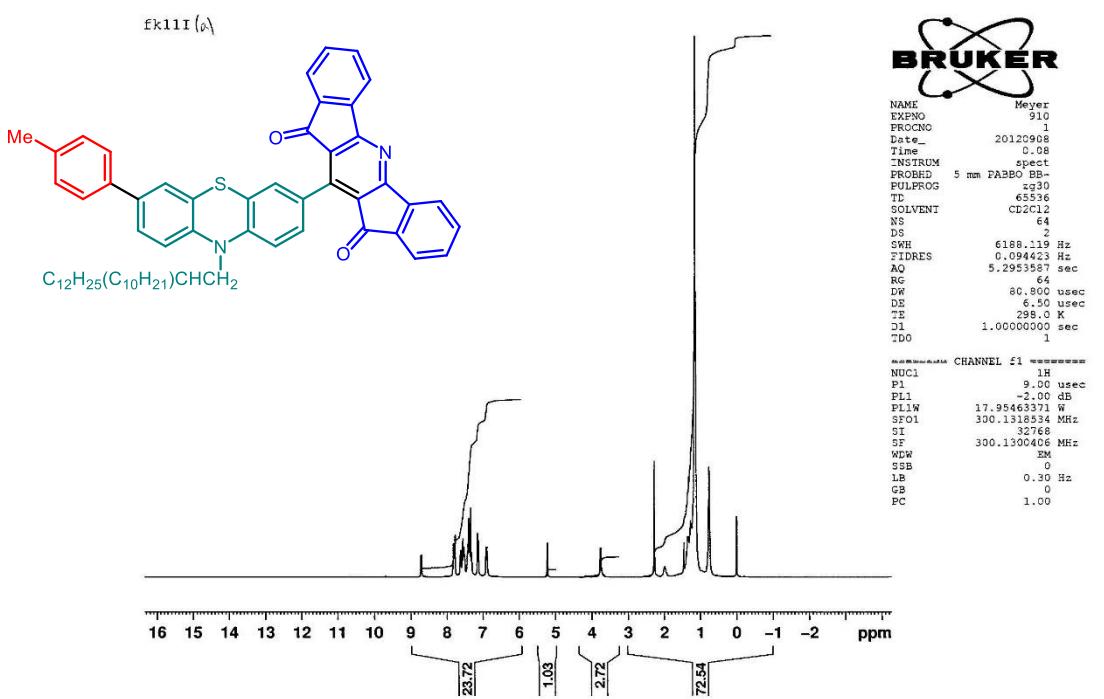
¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12c.

file
(fk11 III)

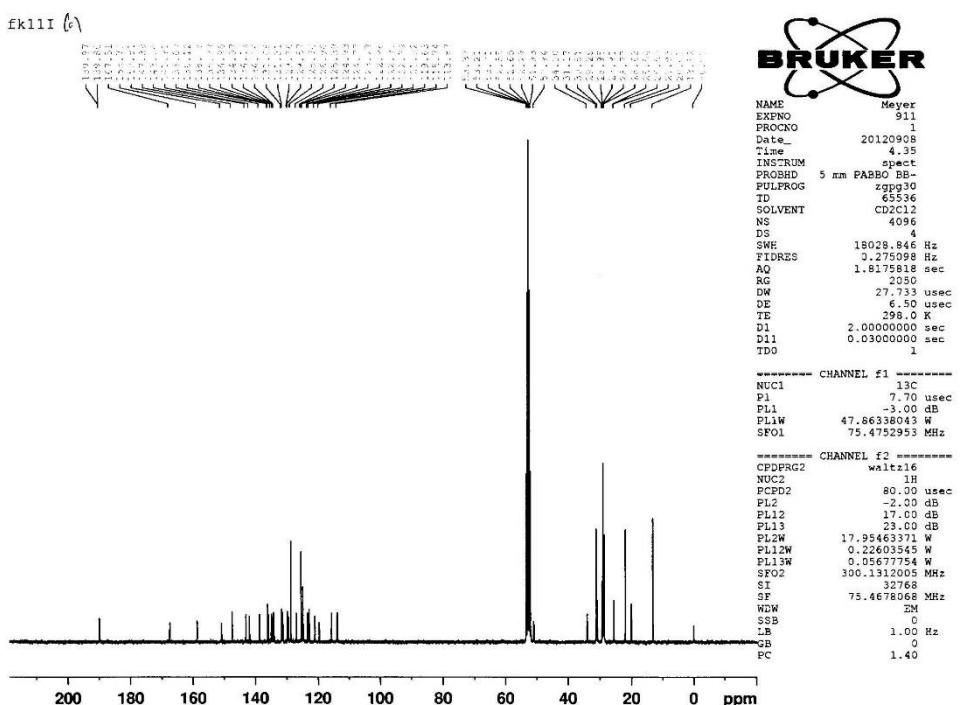


DEPT ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12c.

3.37. 11-[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]diindeno[1,2-*b*:2',1'-*e*]pyridin-10,12-dione (12d)

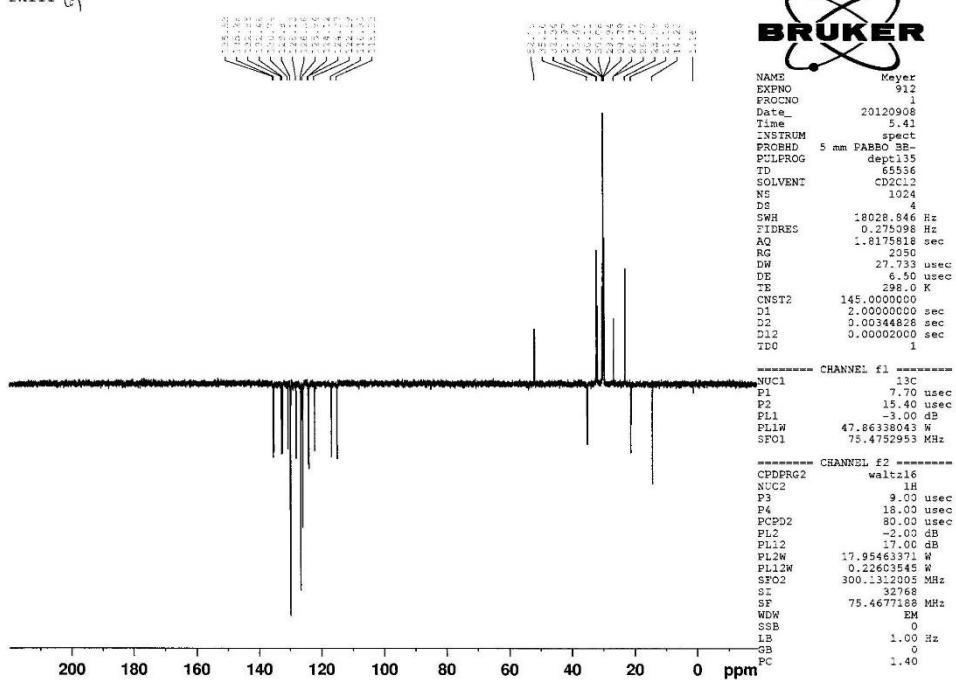


¹H NMR (300 MHz, CD₂Cl₂) of compound **12d**.



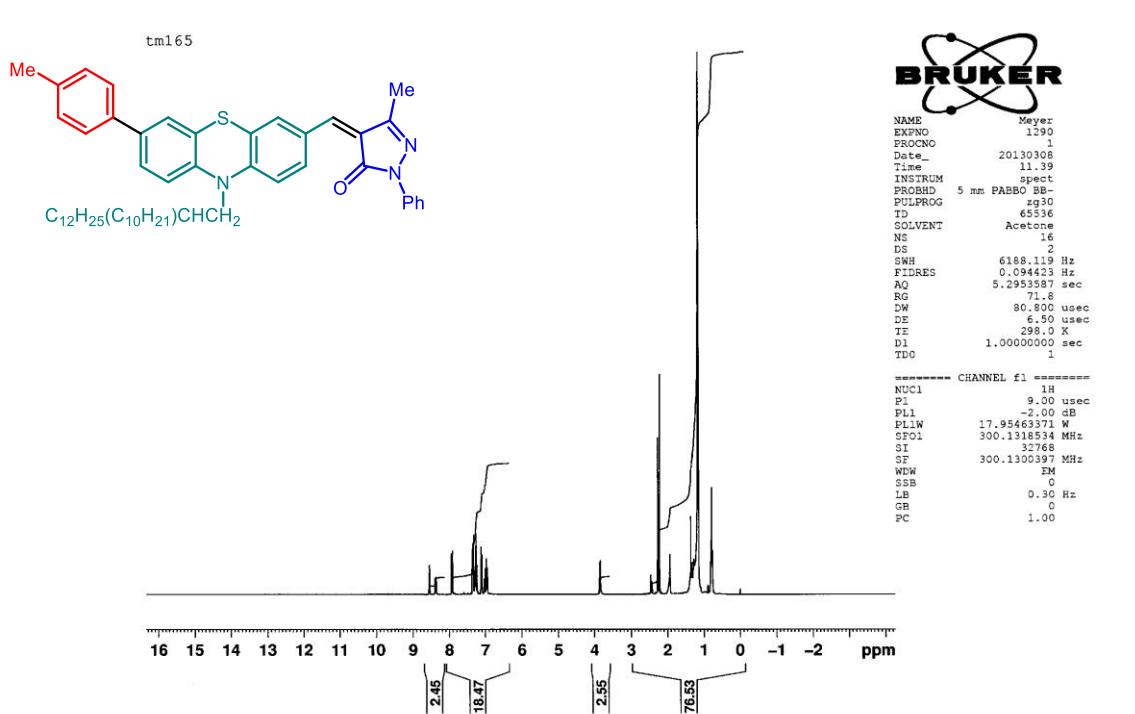
¹³C NMR (75 MHz, CD₂Cl₂) of compound **12d**.

fklli (1)

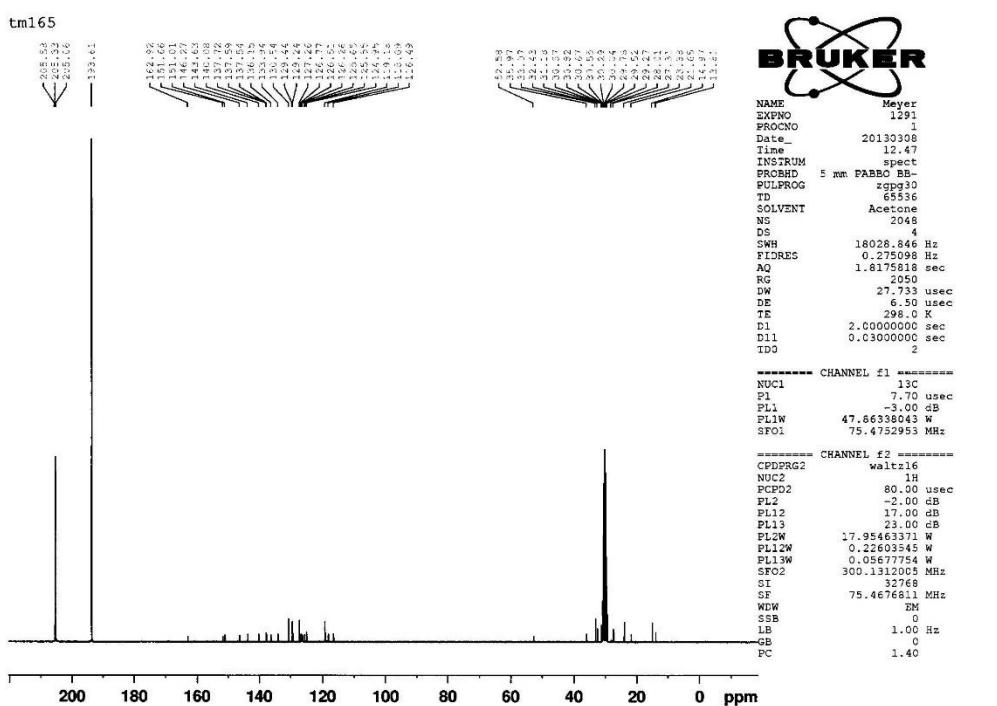


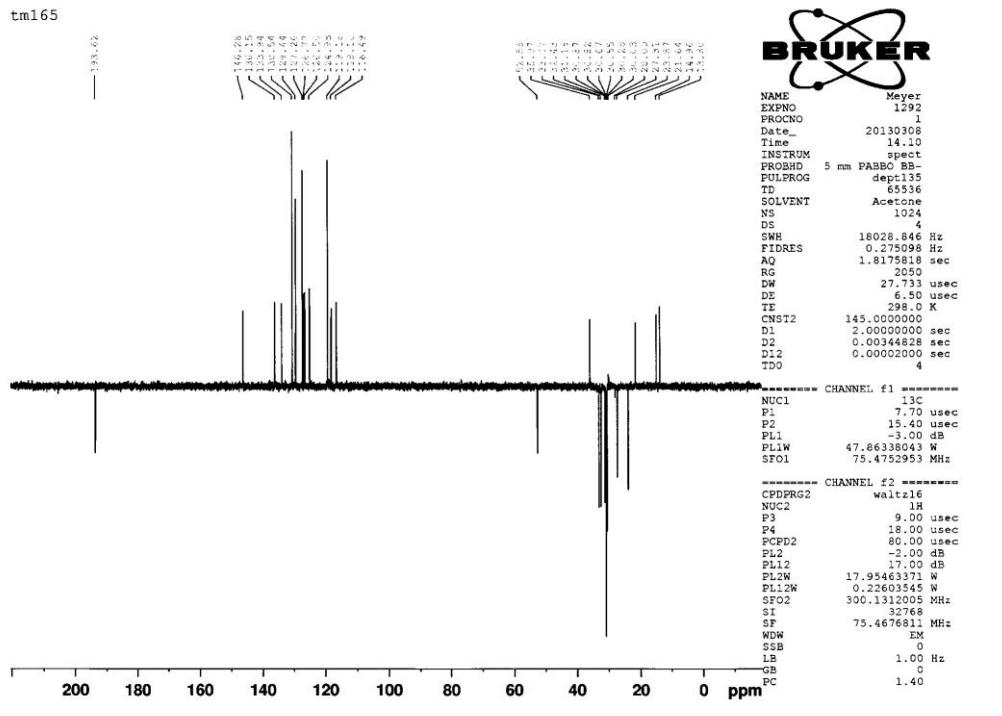
DEPT ¹³C NMR (75 MHz, CD₂Cl₂) of compound 12d.

3.38. (*Z*)-4-[(10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl)methylene]-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (12e)



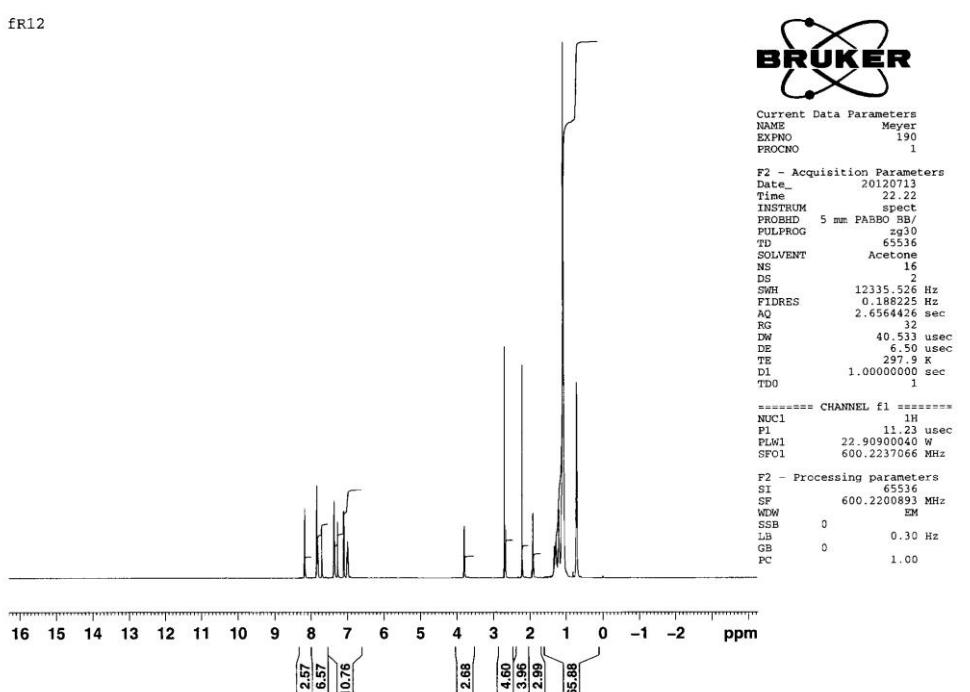
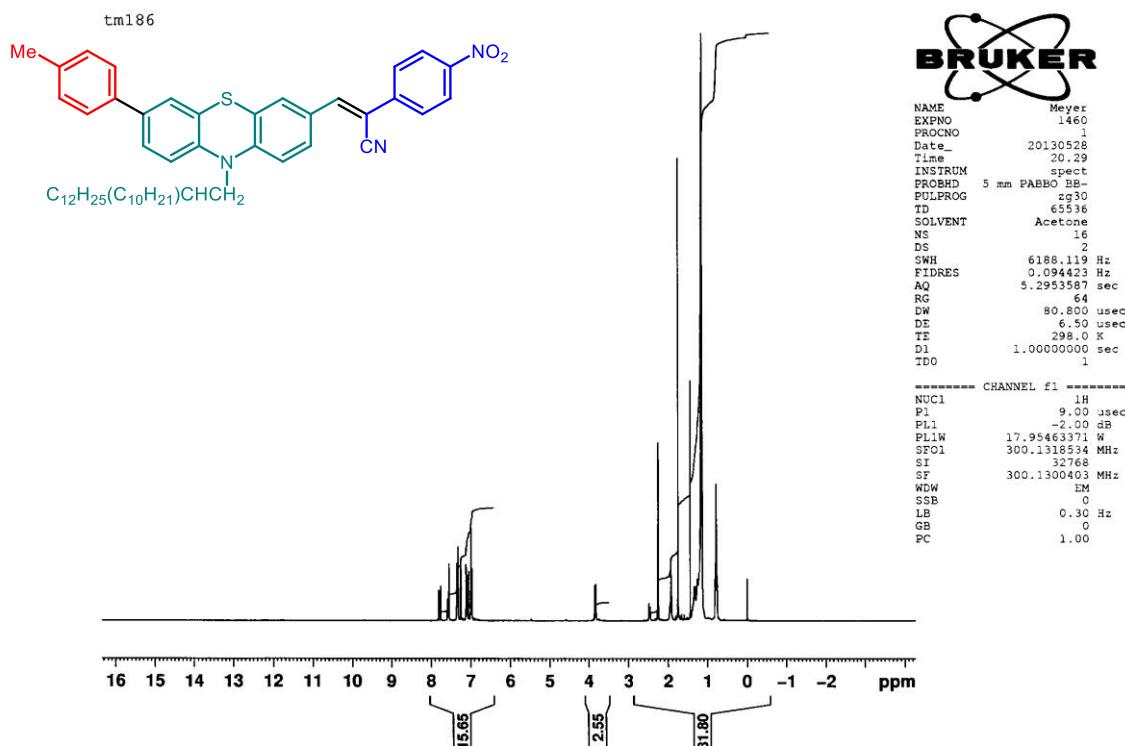
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12e.



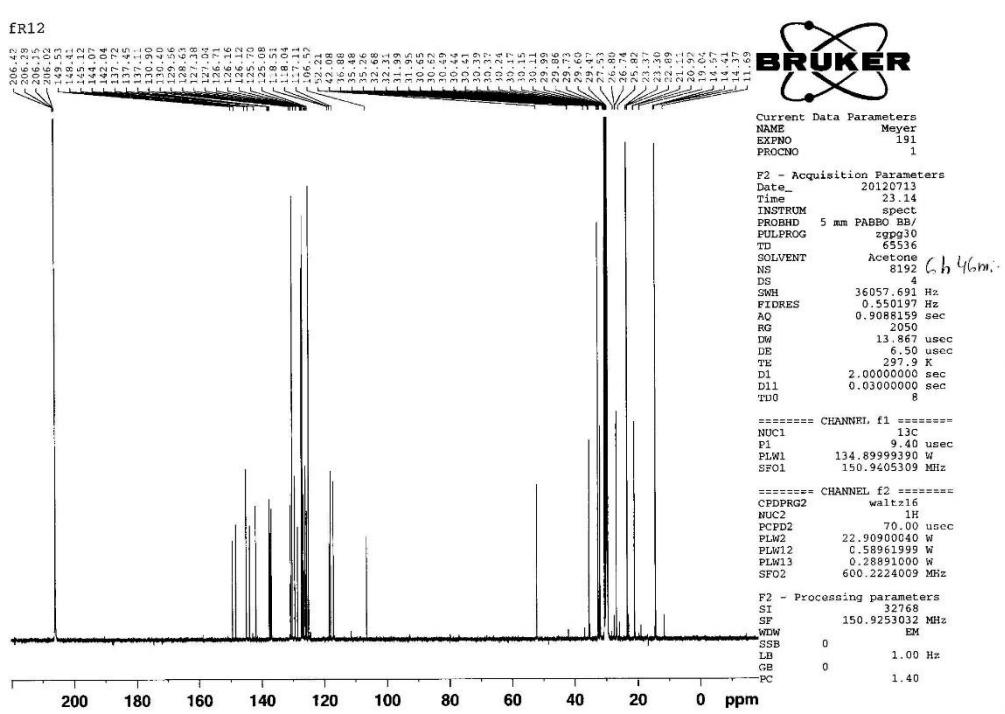


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12e**.

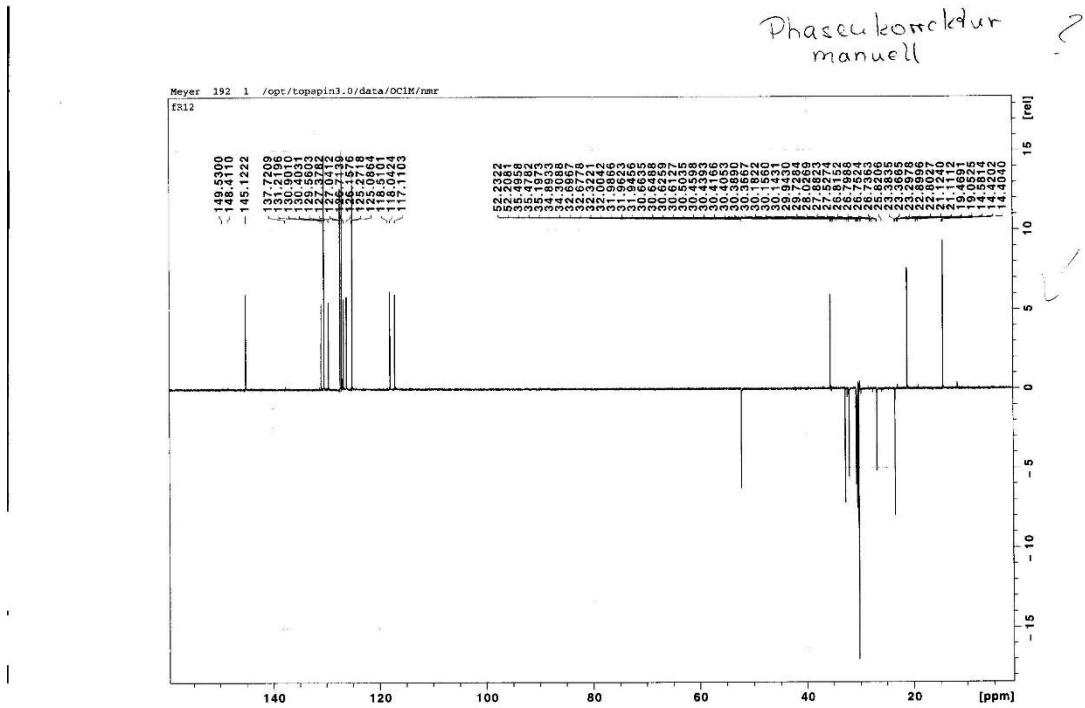
3.39. (*Z*)-3-[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10H-phenothiazin-3-yl]-2-(4-nitrophenyl)acrylonitrile (12f)



¹H NMR (600 MHz, acetone-d₆) of compound 12f.

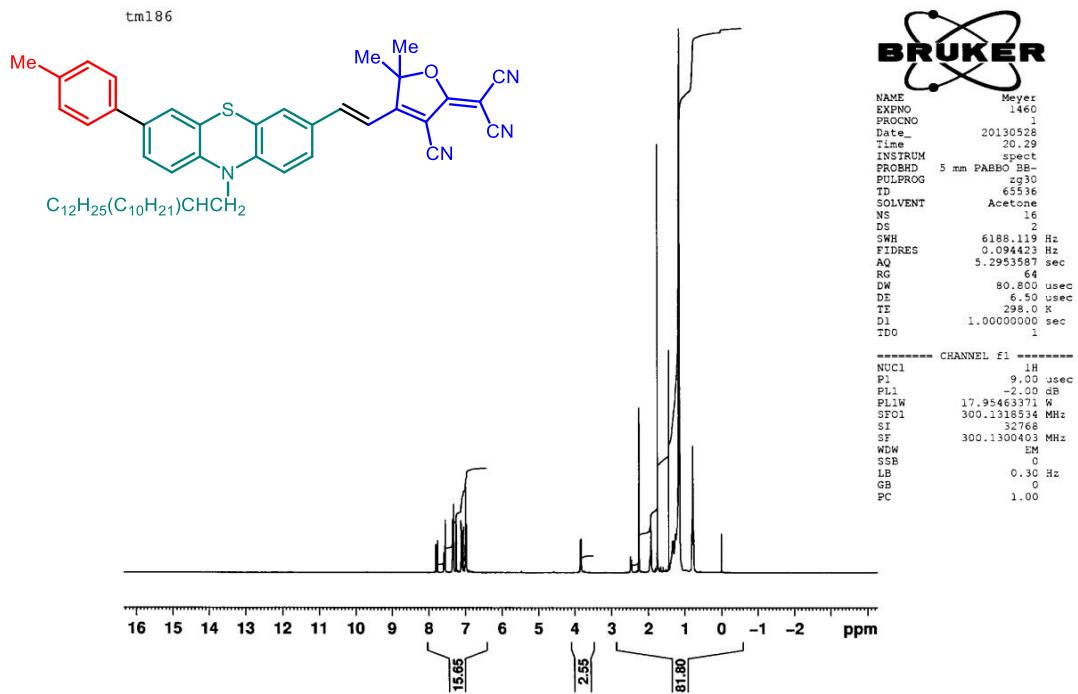


¹³C NMR (150 MHz, acetone-d₆) of compound **12f**.

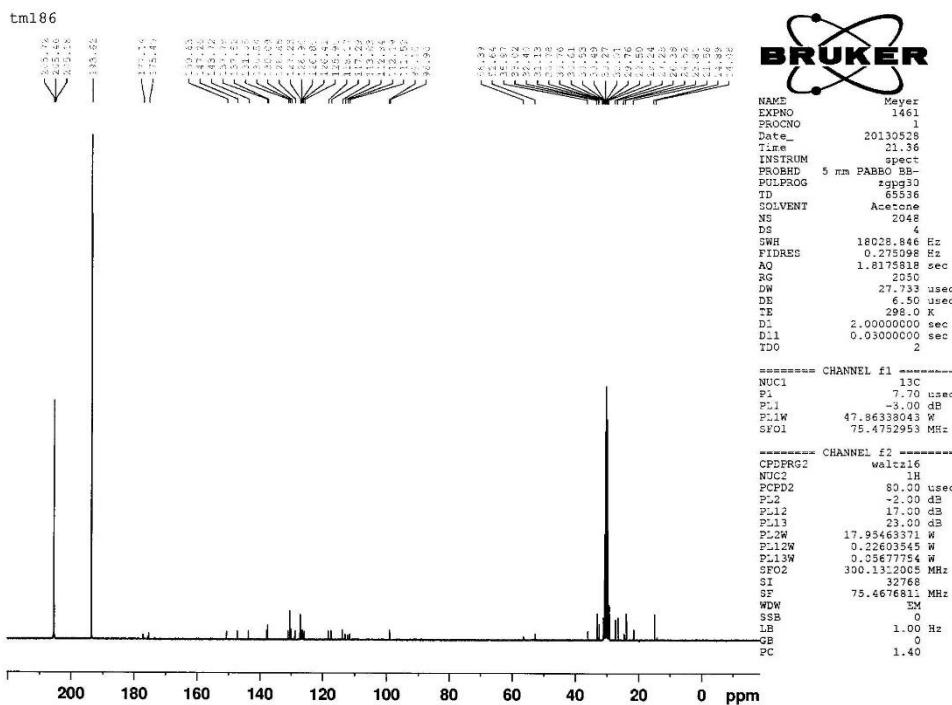


DEPT ^{13}C NMR (150 MHz, acetone- d_6) of compound **12f**.

3.40. (*E*)-2-{3-Cyano-4-[2-(10-{2-decytetradecyl}-7-{*p*-tolyl}-10*H*-phenothiazin-3-yl)vinyl]-5,5-dimethylfuran-2[5*H*]-yliden}malonitrile (12g)

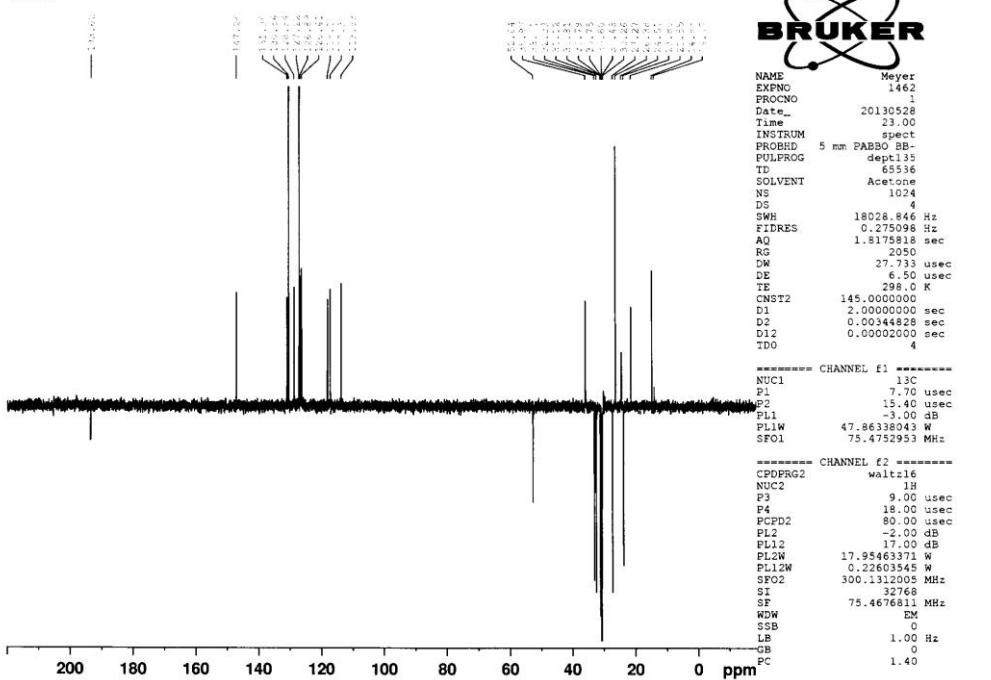


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12g.



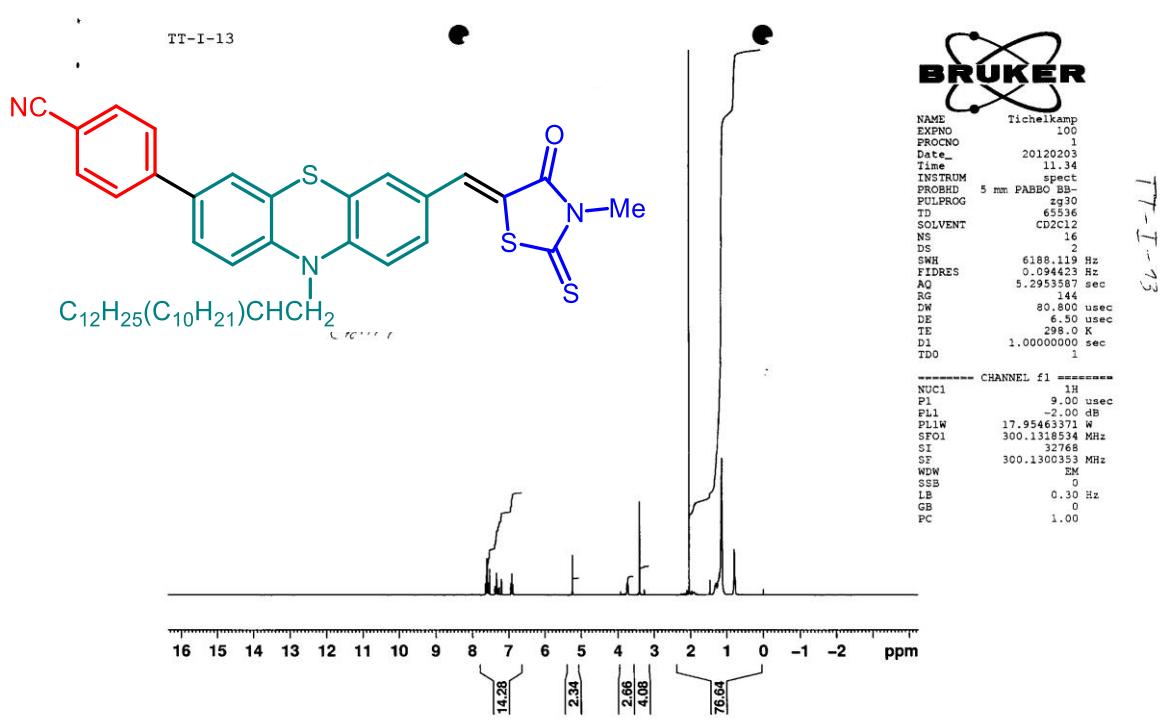
¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12g**.

tm186

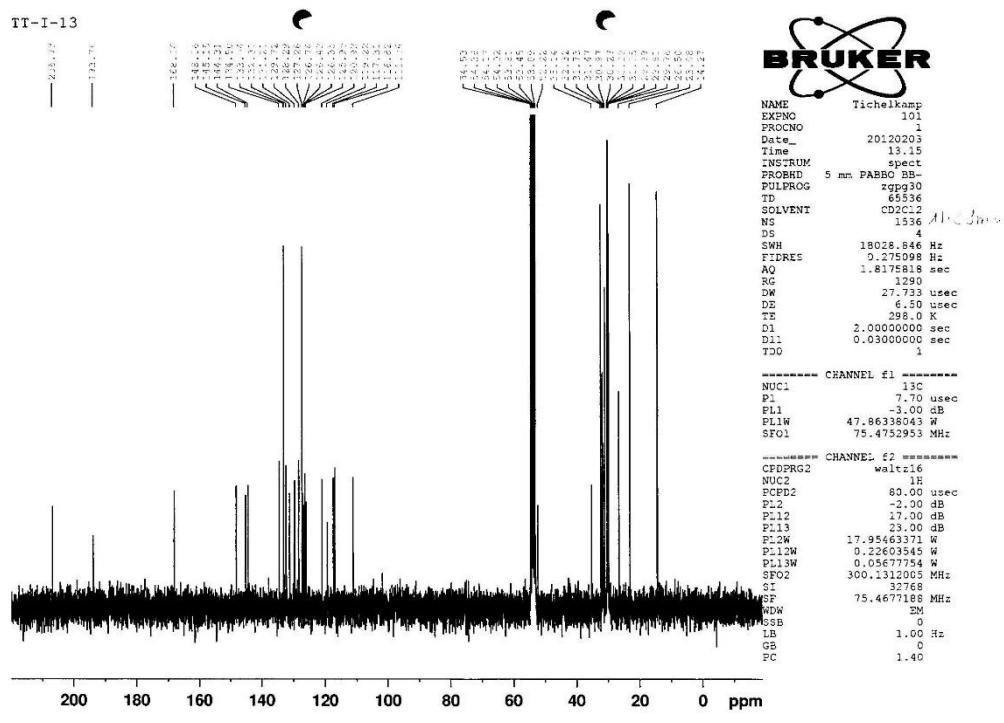


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12g**.

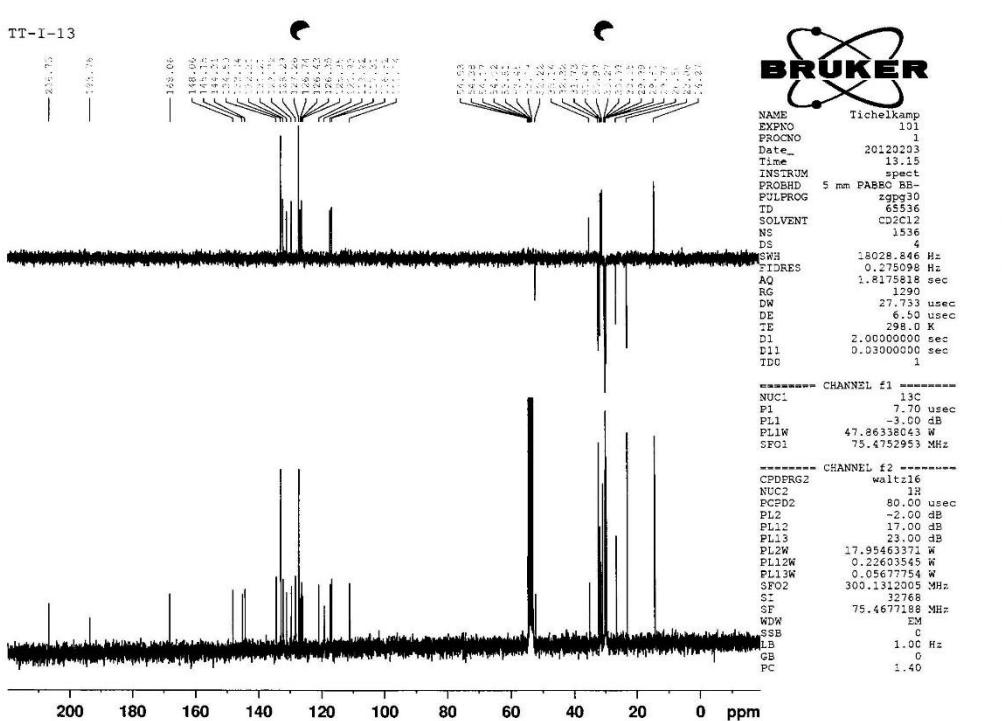
3.41. (*Z*)-5-{[10-(2-Decyltetradecyl)-7-(*p*-tolyl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12h)



¹H NMR (300 MHz, CD₂Cl₂) of compound 12h.

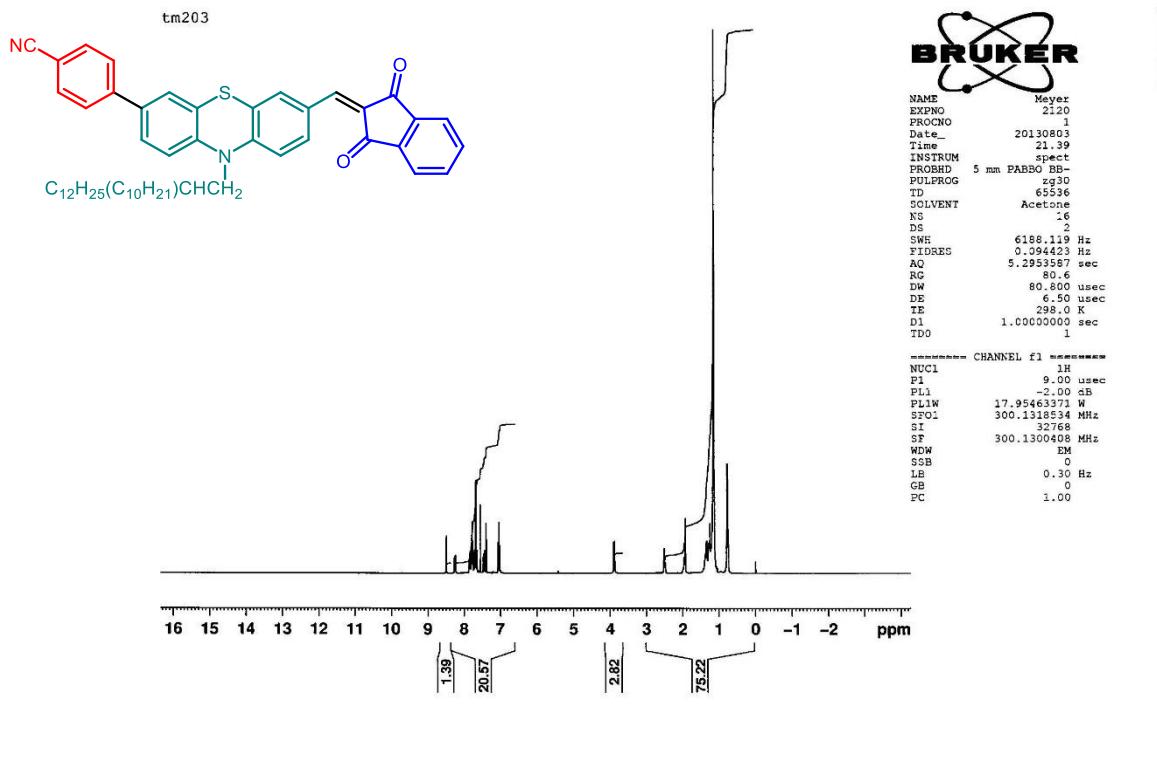


¹³C NMR (75 MHz, CD₂Cl₂) of compound 12h.

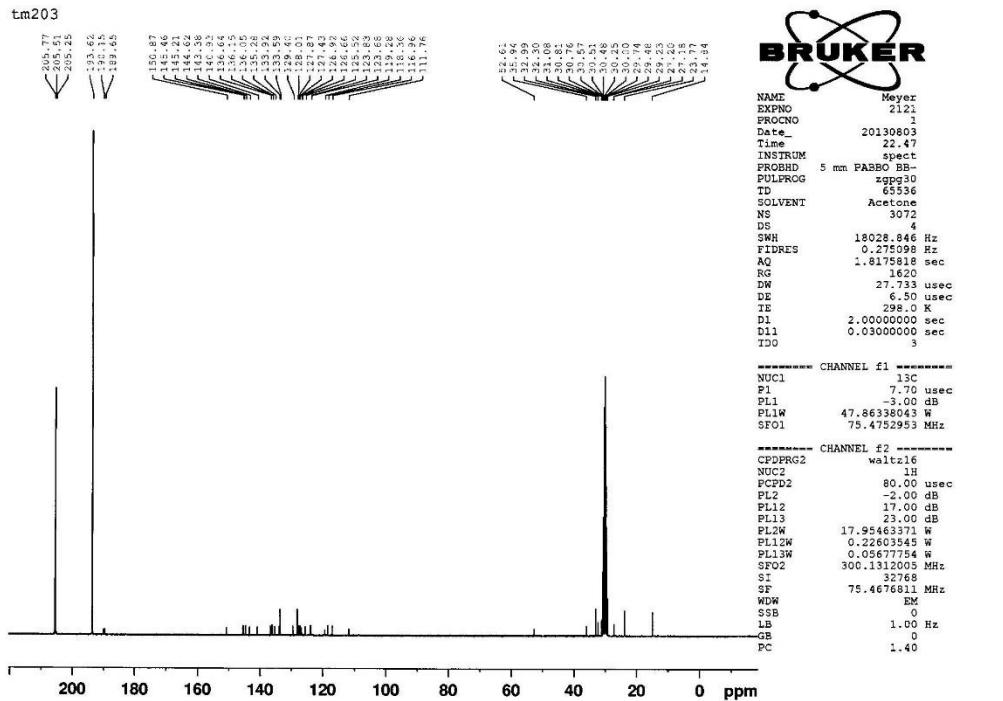


DEPT ¹³C NMR (75 MHz, CD₂Cl₂) of compound 12h.

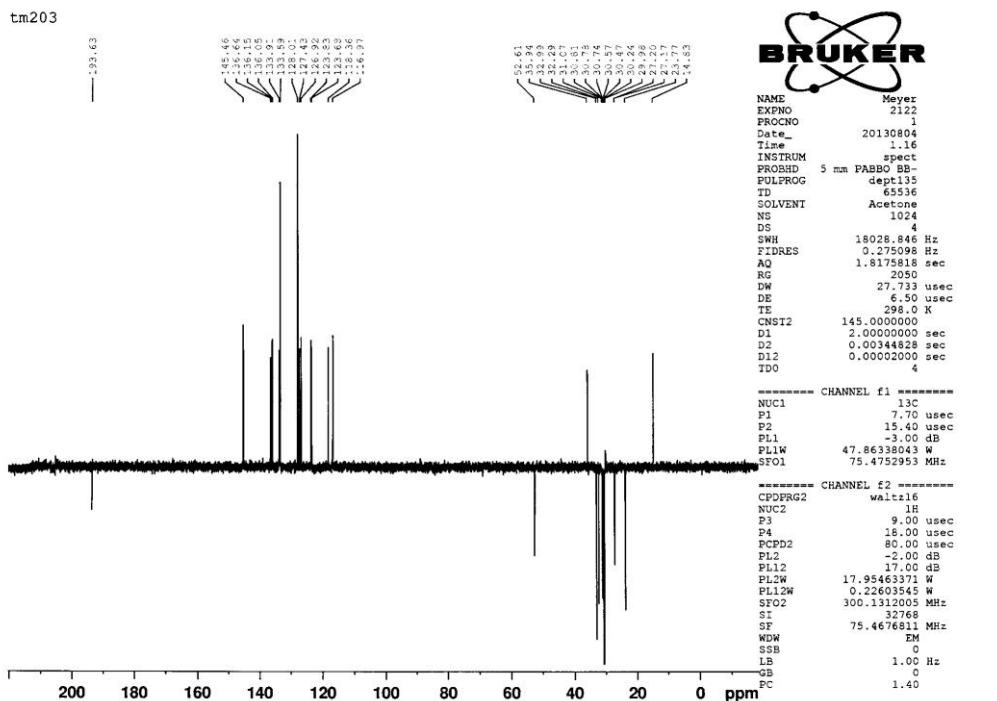
3.42. 4-{10-(2-Decyltetradecyl)-7-[(1,3-dioxo-1H-inden-2[3H]-yliden)methyl]-10H-phenothiazin-3-yl}benzonitrile (12i)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **12i**.

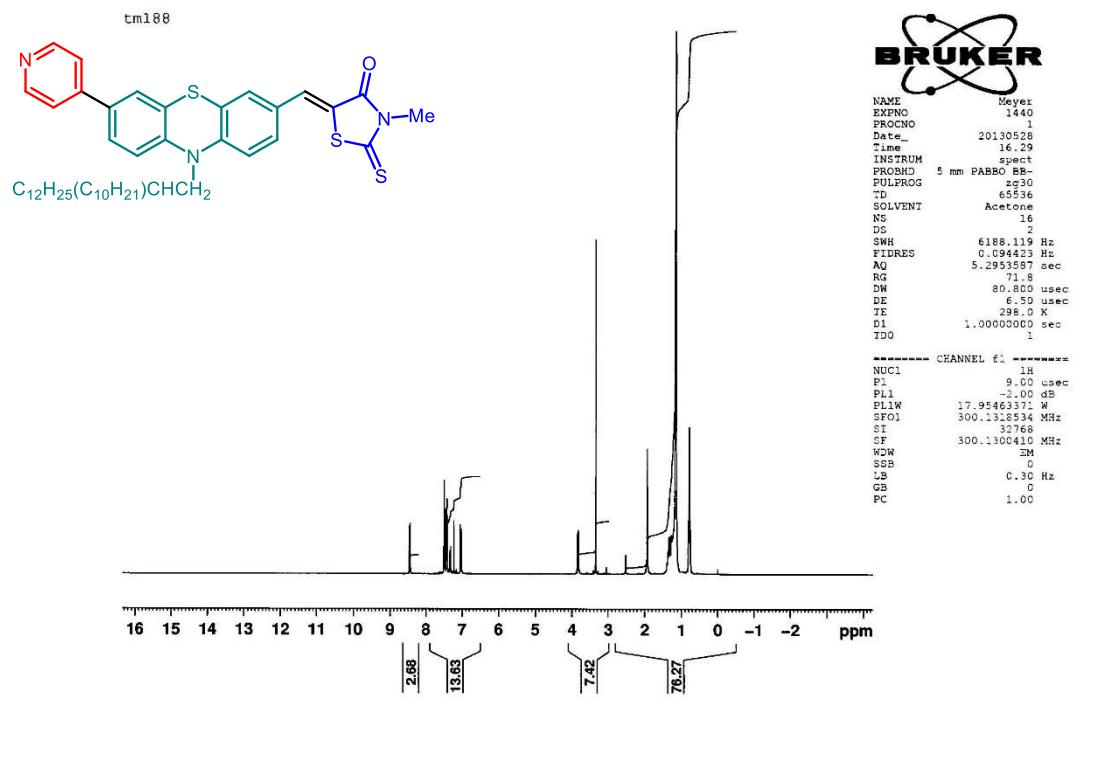


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12i.

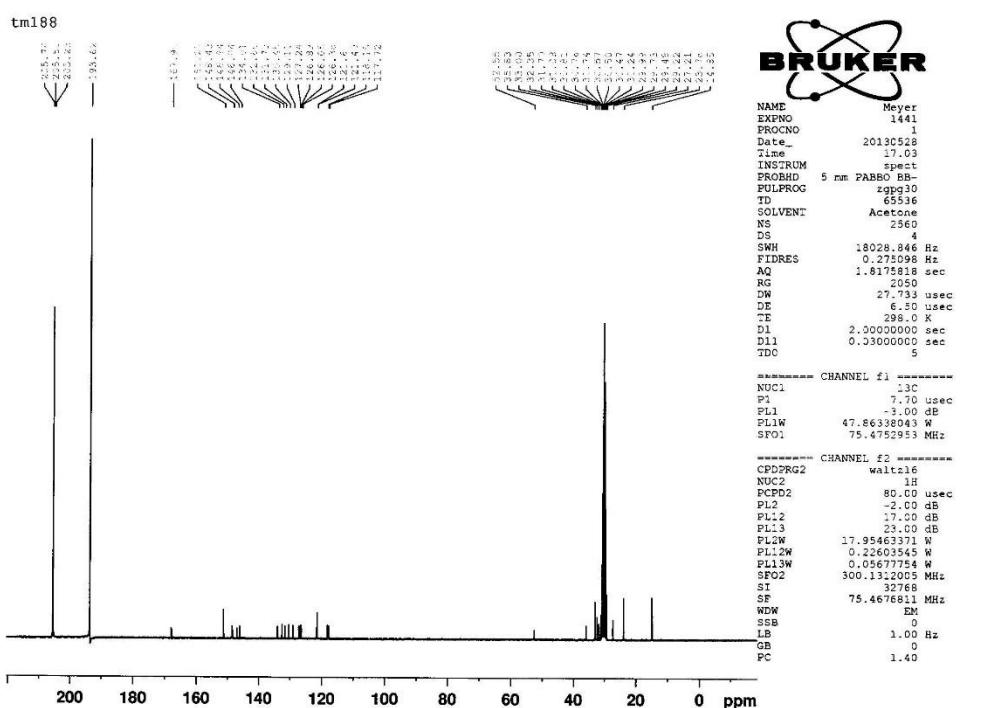


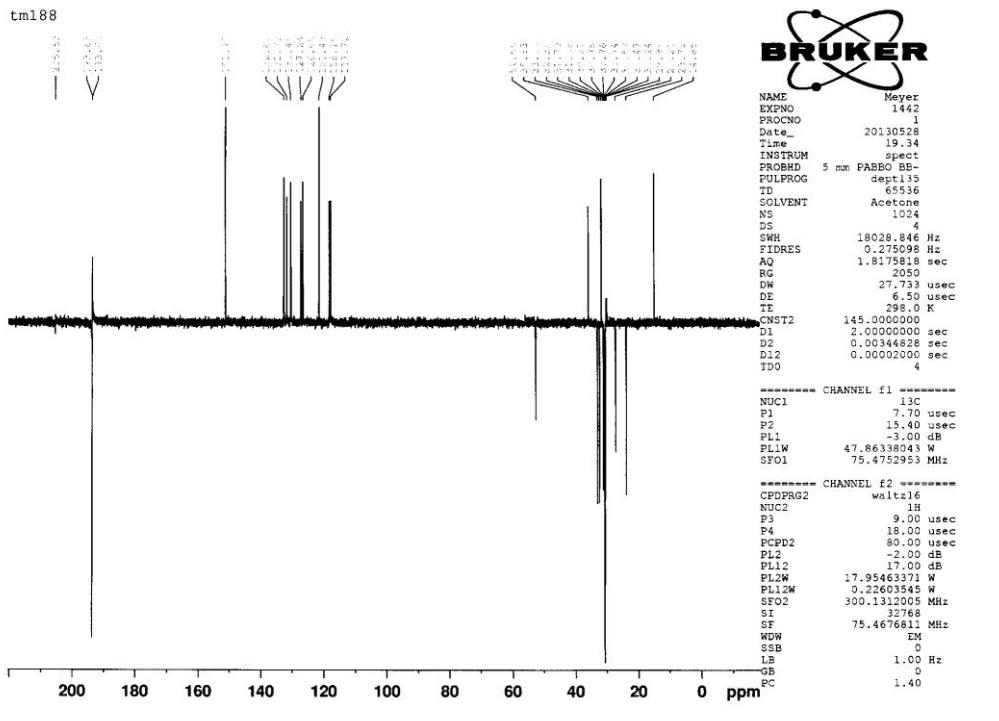
DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **12i**.

3.43. (Z)-5-{[10-(2-Decyltetradecyl)-7-(pyridin-4-yl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12j)



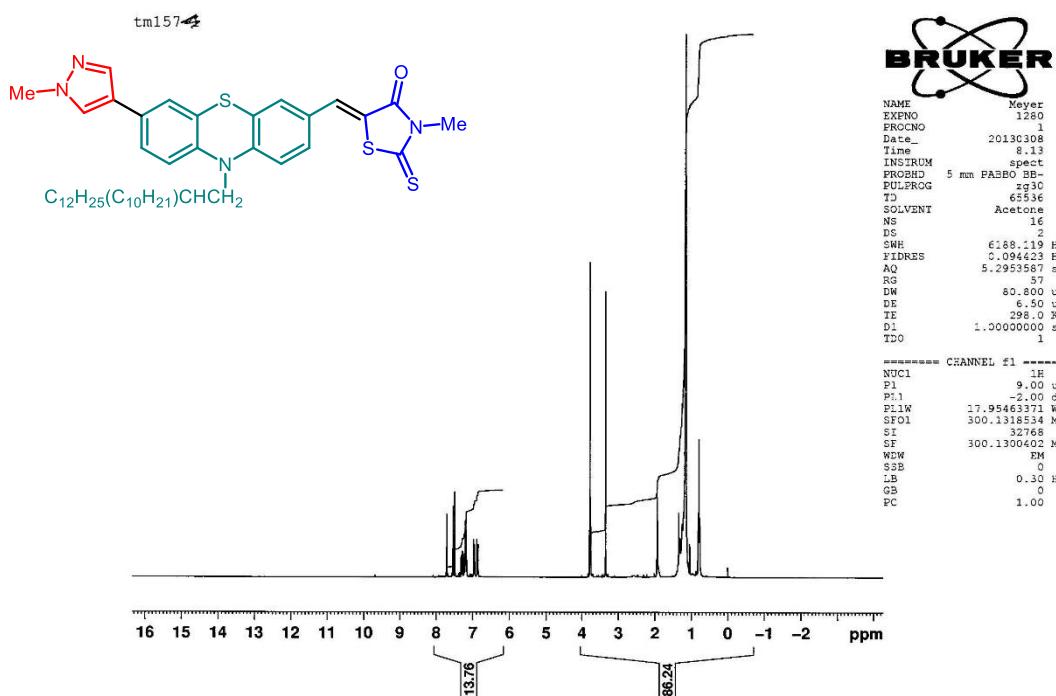
^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12j.



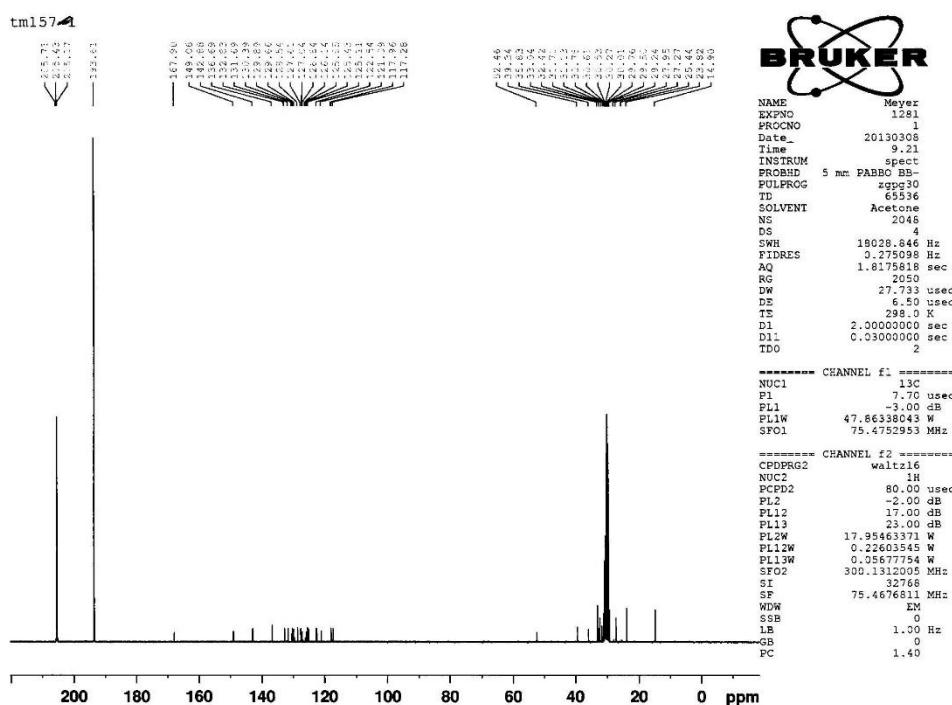


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12j**.

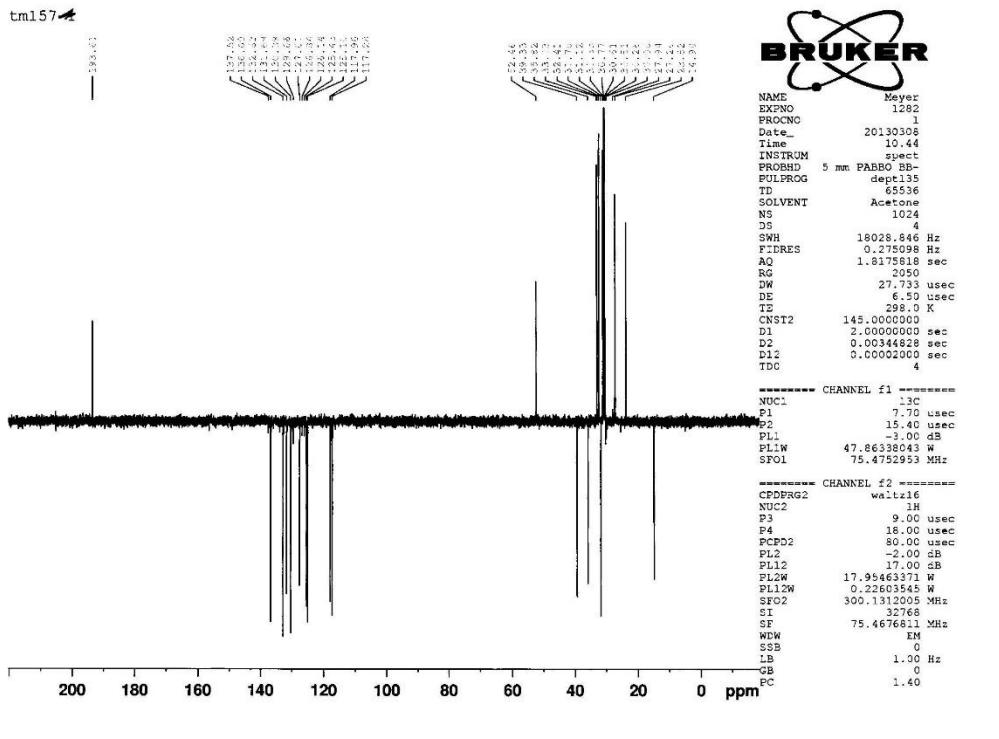
3.44. (*Z*)-5-{[10-(2-Decyltetradecyl)-7-(1-methyl-1*H*-pyrazol-4-yl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12k)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12k.

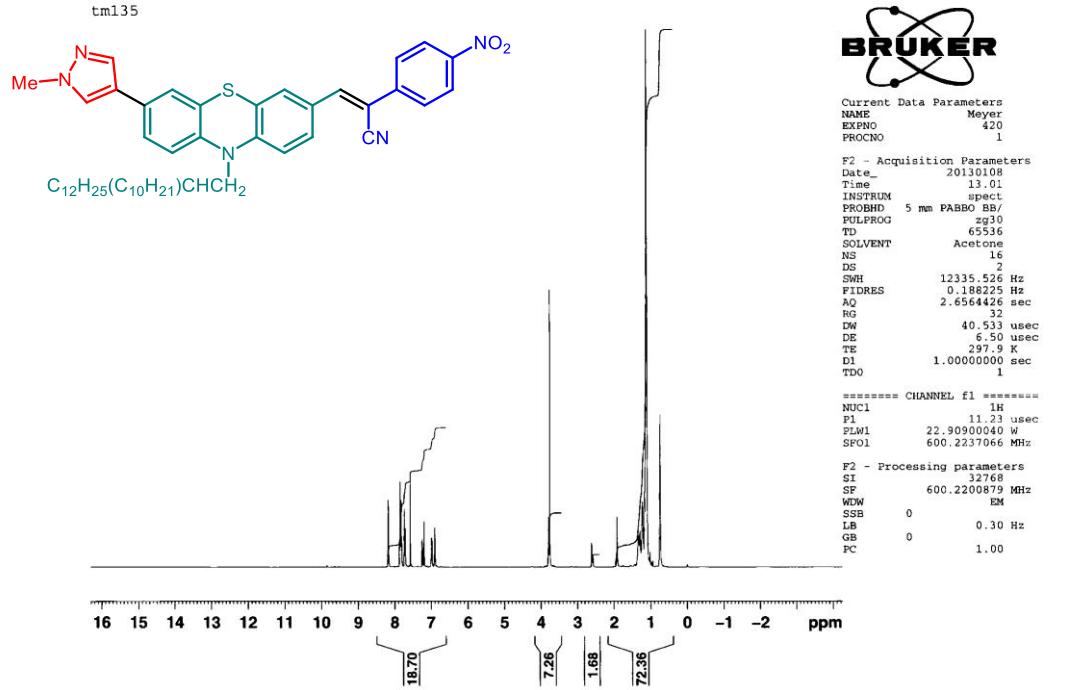


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12k.

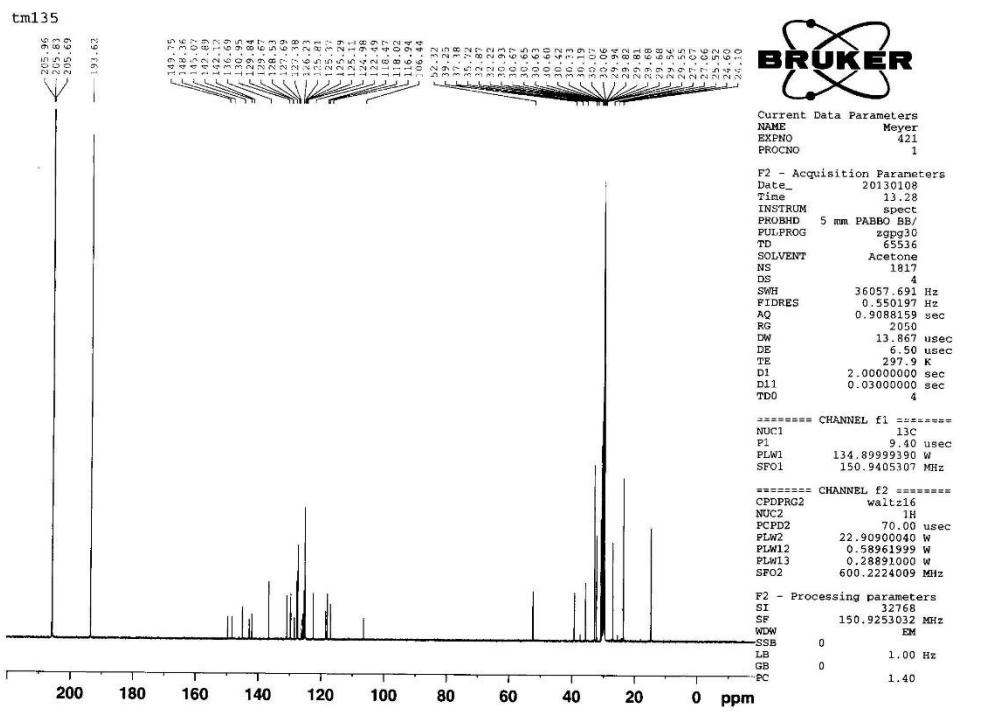


DEPT ¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12k**.

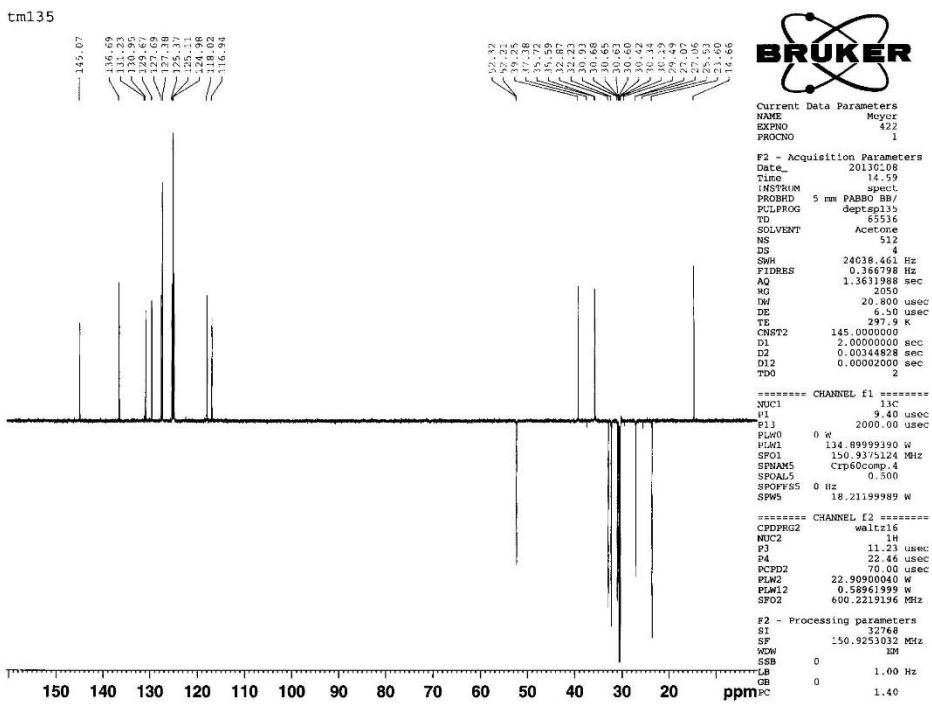
3.45. (Z)-3-[10-(2-Decyltetradecyl)-7-(1-methyl-1*H*-pyrazol-4-yl)-10*H*-phenothiazin-3-yl]-2-(4-nitrophenyl)acrylonitrile (12l)



¹H NMR (300 MHz, acetone-d₆) of compound **12I**.

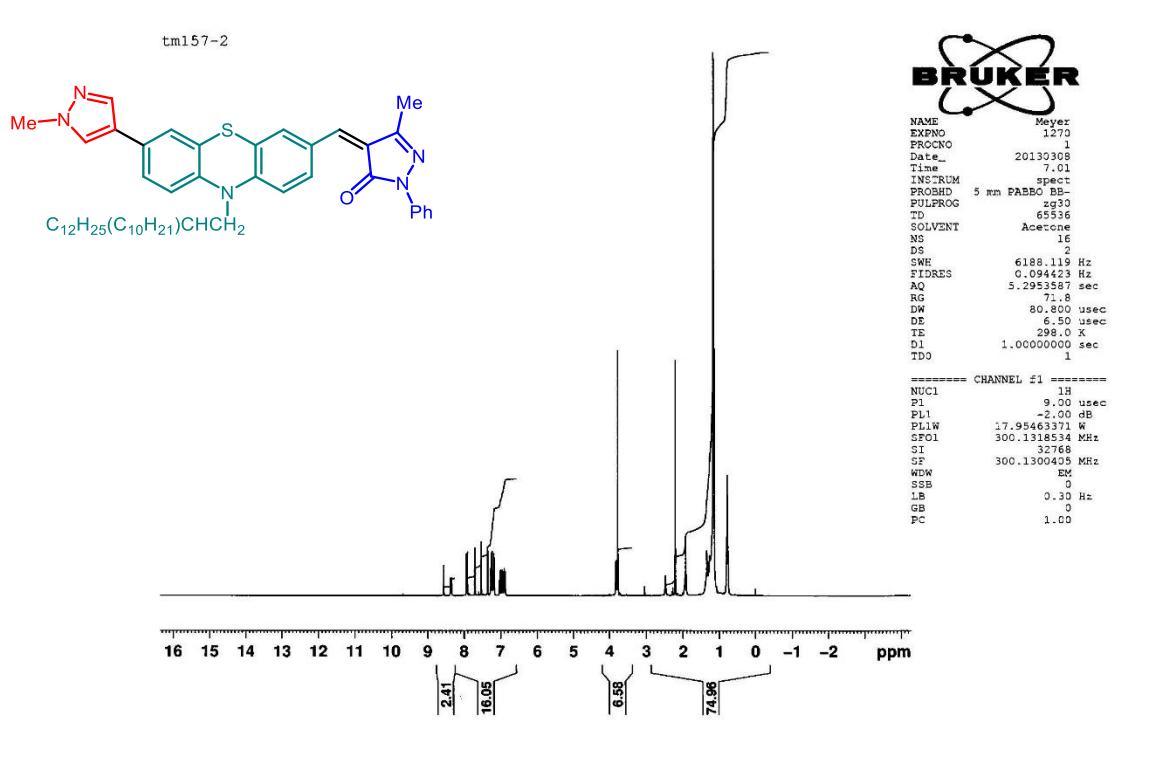


¹³C NMR (150 MHz, acetone-d₆) of compound **12I**.

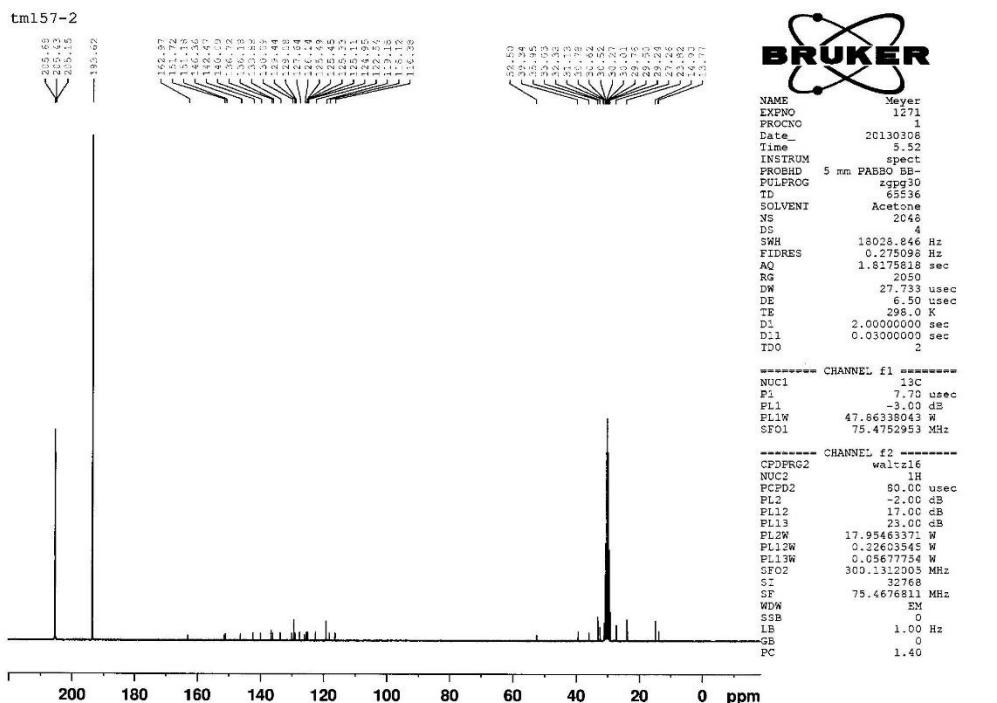


DEPT ^{13}C NMR (150 MHz, acetone-d₆) of compound **12I**.

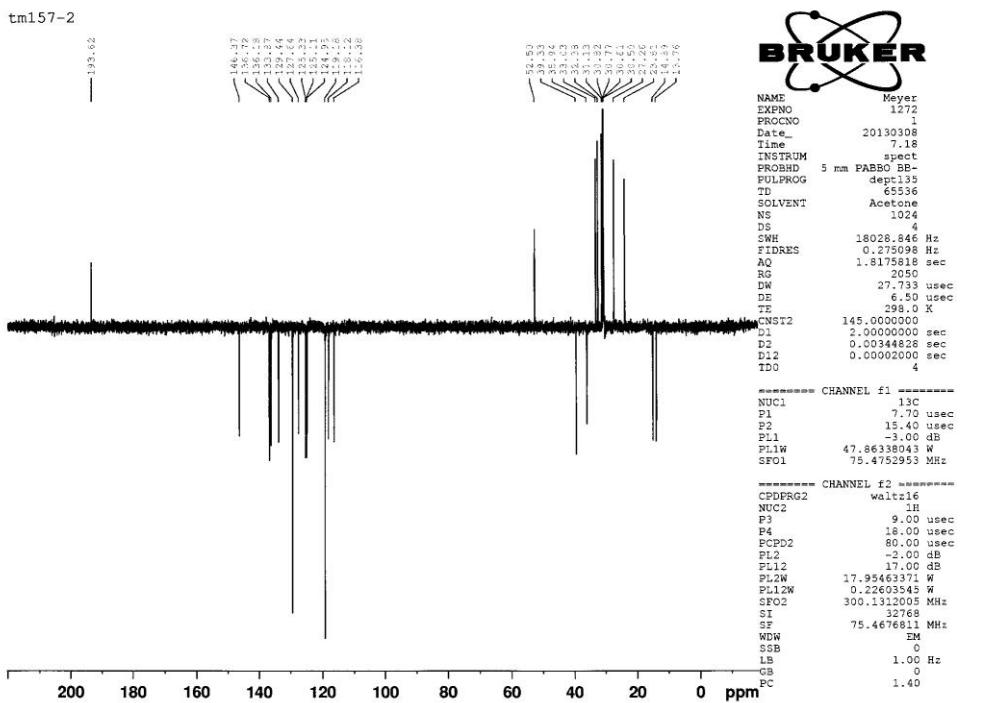
3.46. (Z)-4-{[10-(2-Decyltetradecyl)-7-(1-methyl-1H-pyrazol-4-yl)-10H-phenothiazin-3-yl]methylene}-3-methyl-1-phenyl-1H-pyrazol-5[4H]-one (12m)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12m.

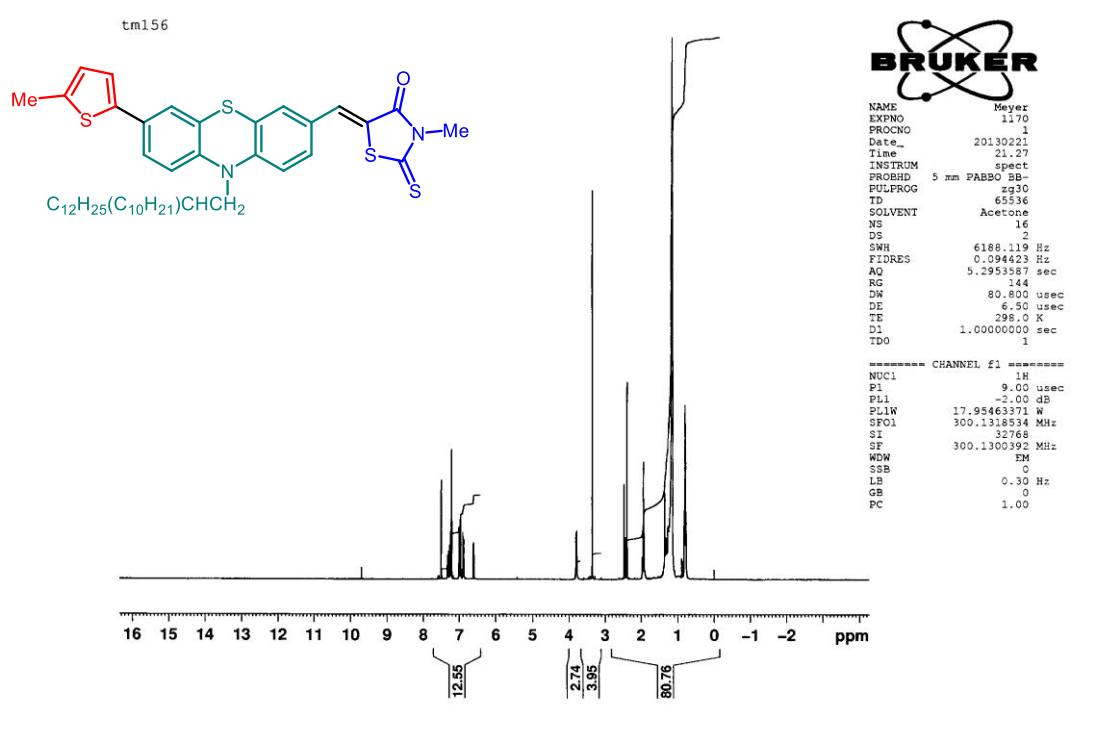


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12m**.

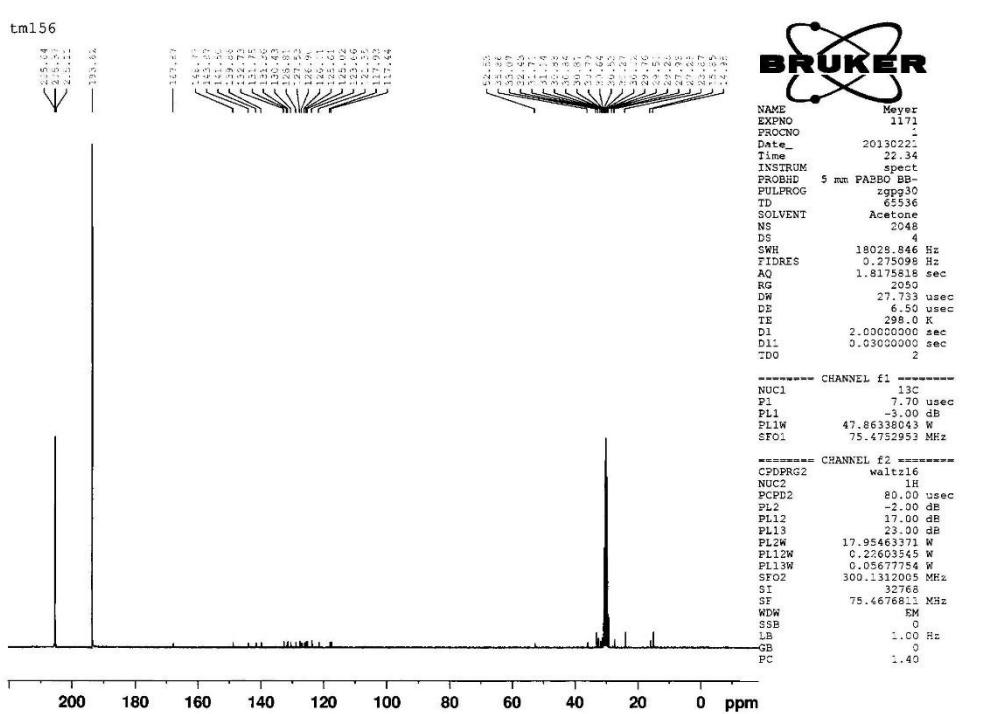


DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **12m**.

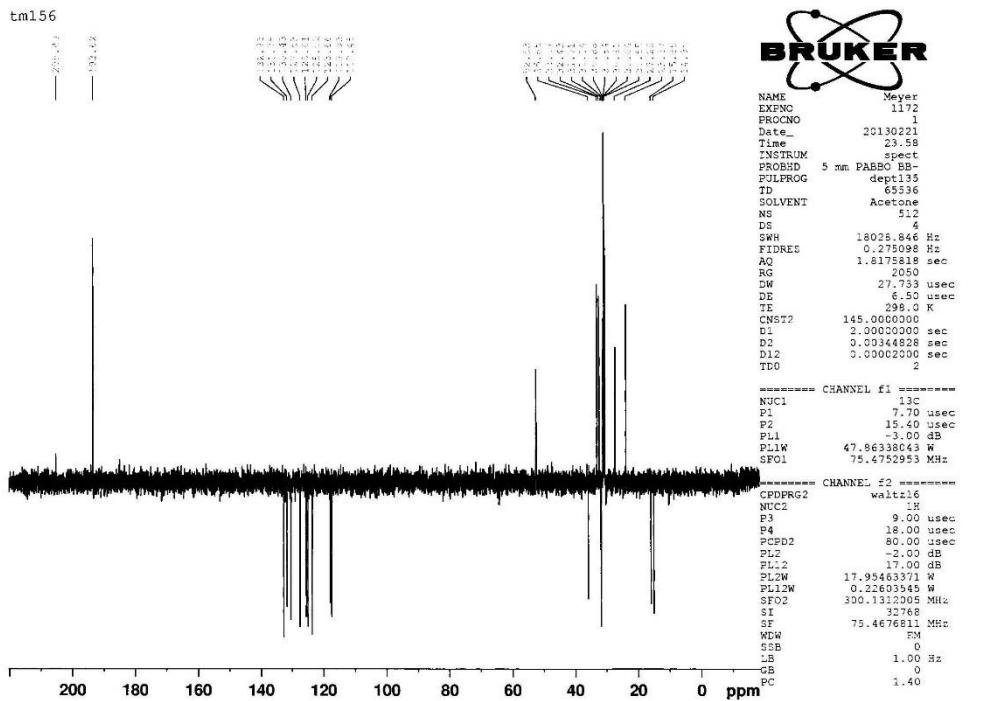
3.47. (*Z*)-5-{[10-(2-Decyltetradecyl)-7-(5-methylthiophen-2-yl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12n)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12n.

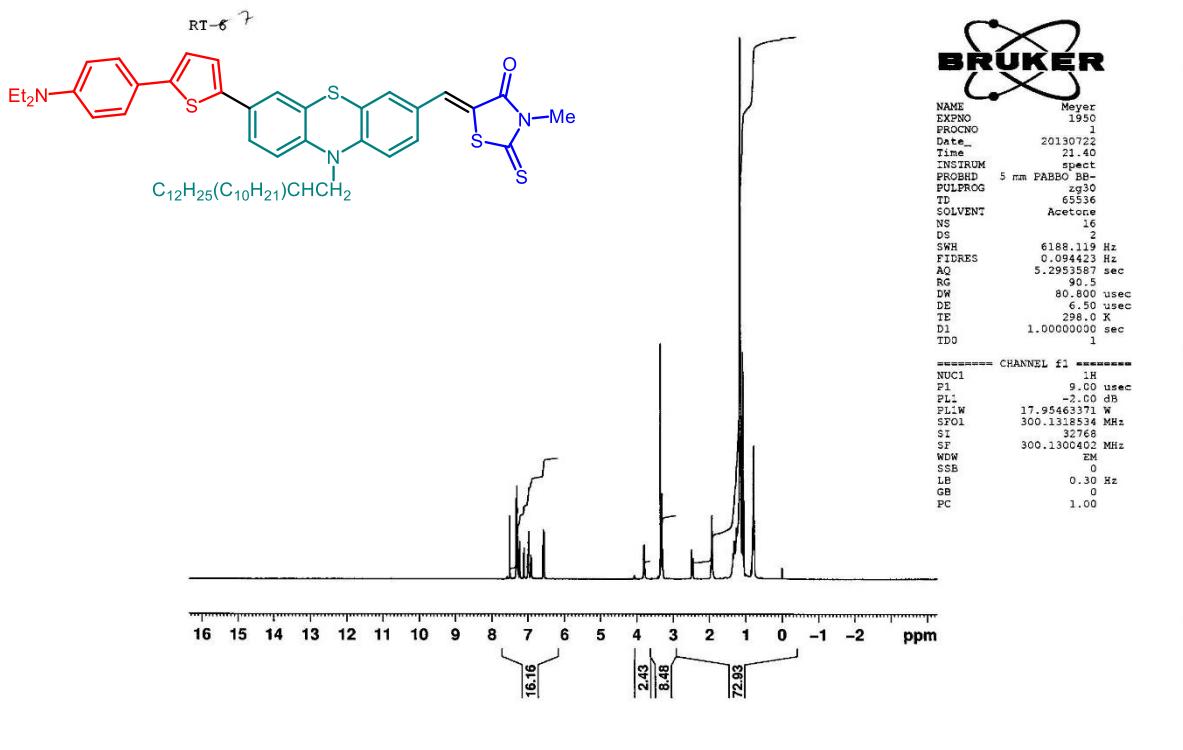


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12n.

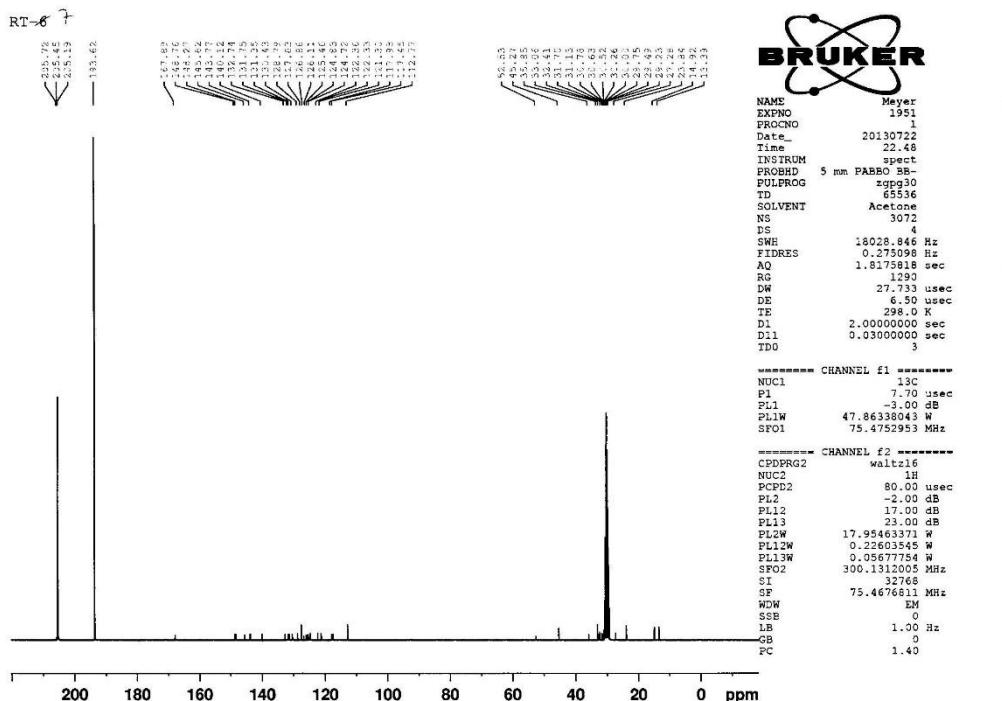


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12n**.

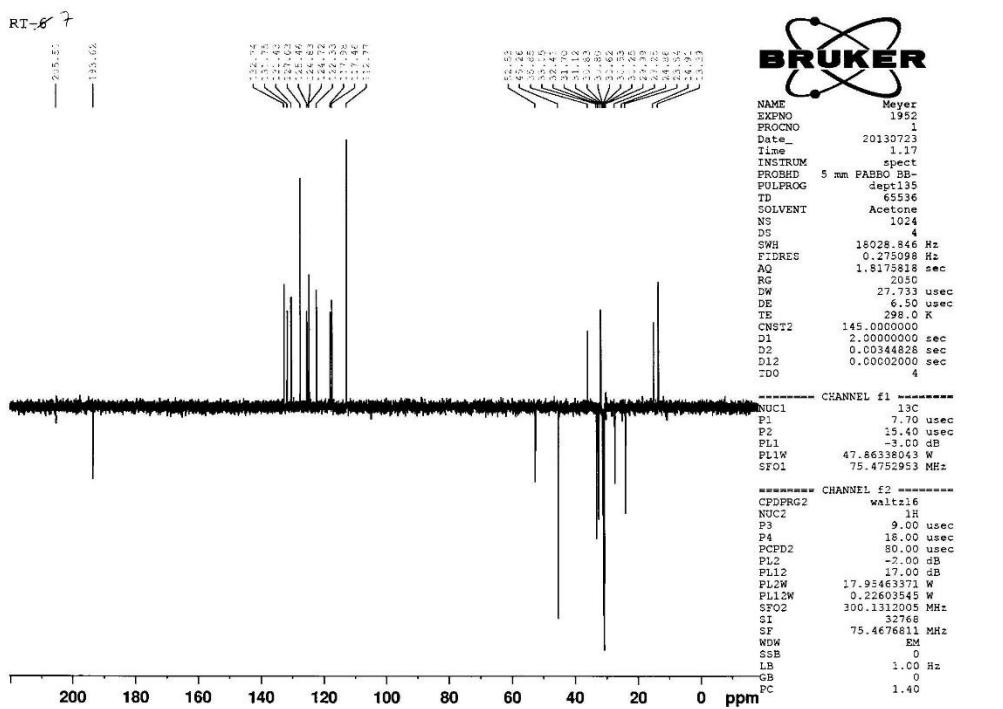
3.48. (Z)-5-{[10-(2-Decyltetradecyl)-7-(5-{4-[diethylamino]phenyl}thiophen-2-yl)-10H-phenothiazin-3-yl)methylene}-3-methyl-2-thioxothiazolidin-4-one (12o)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **12o**.

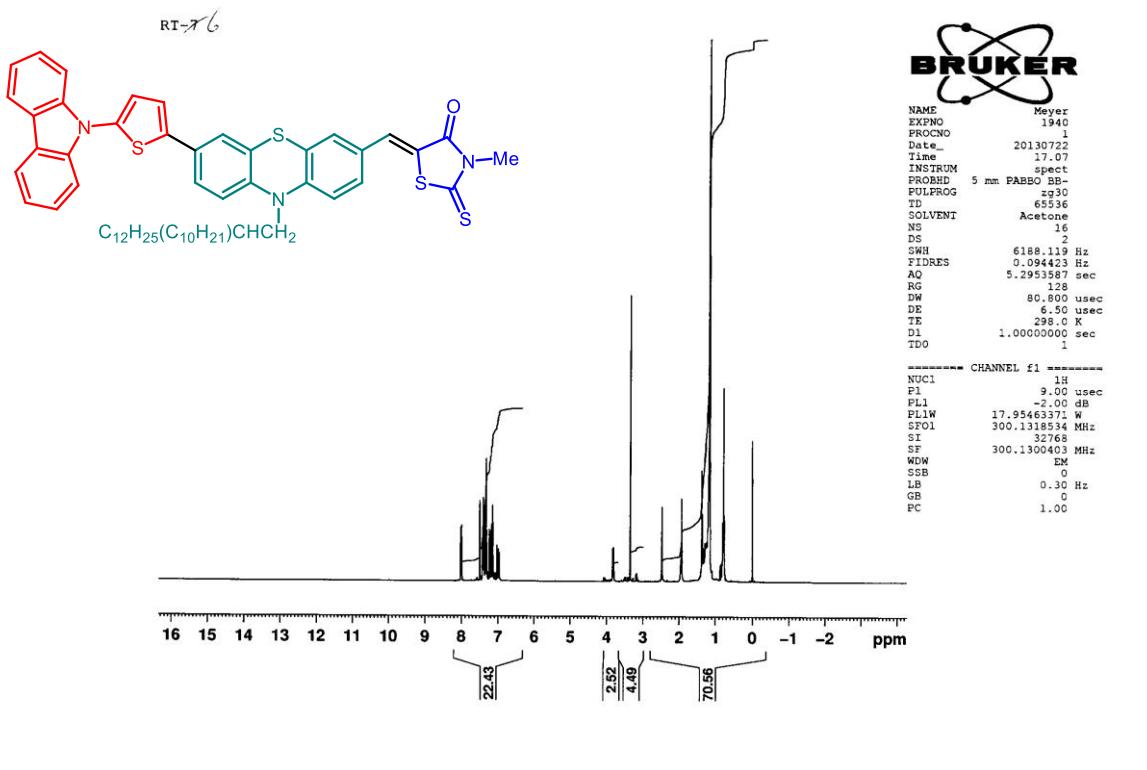


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12o**.

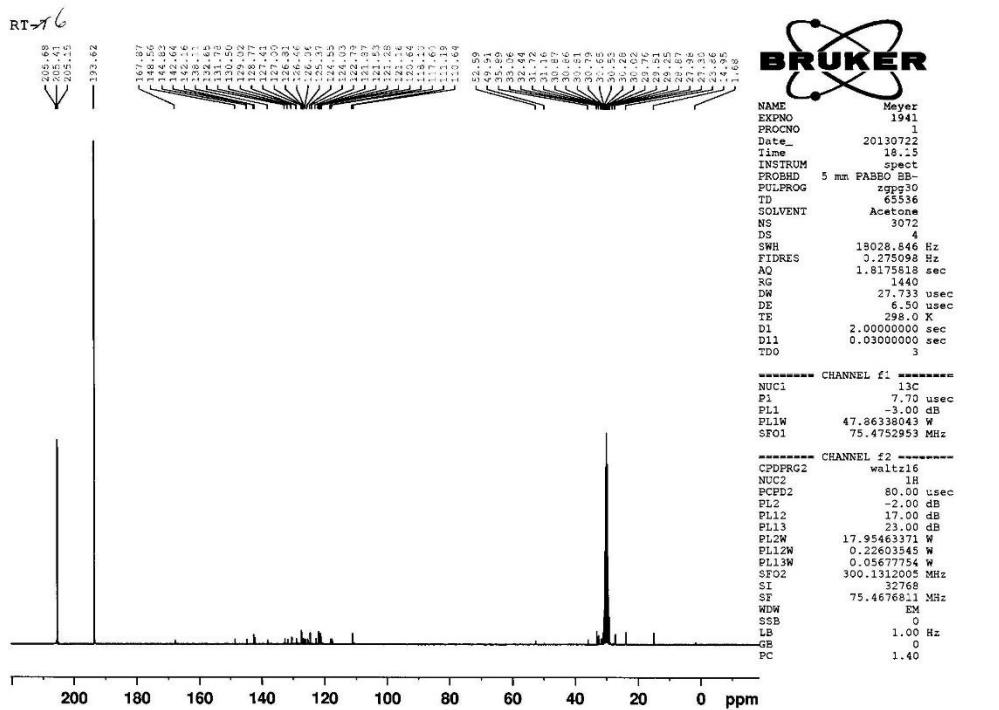


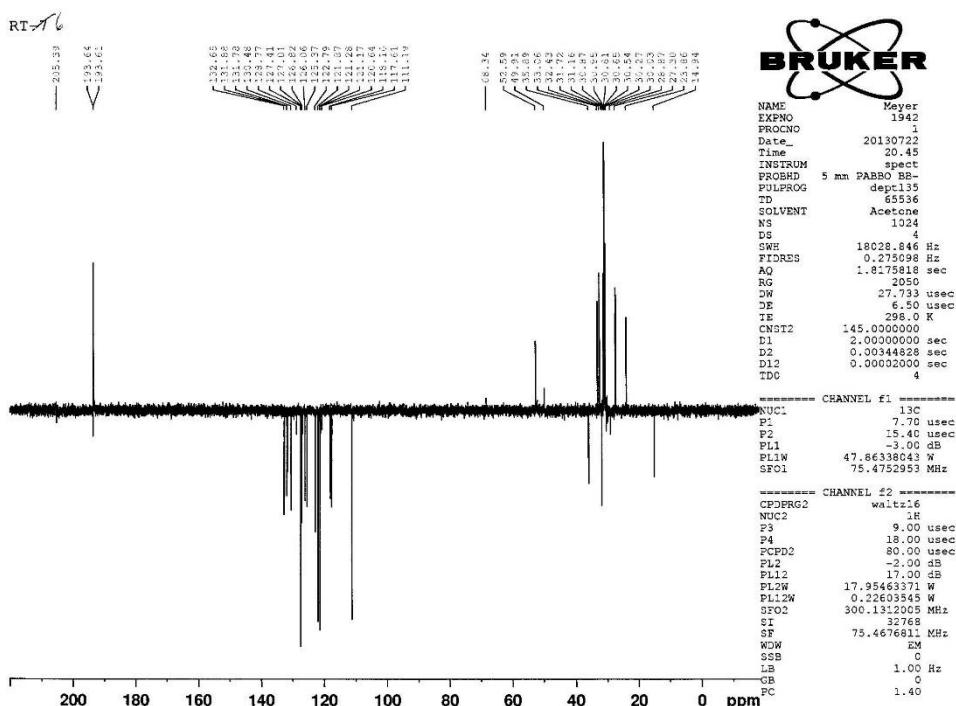
DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12o**.

3.49. (*Z*)-5-{[7-(5-{9*H*-Carbazol-9-yl}thiophen-2-yl)-10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl)methylene}-3-methyl-2-thioxothiazolidin-4-one (12p)



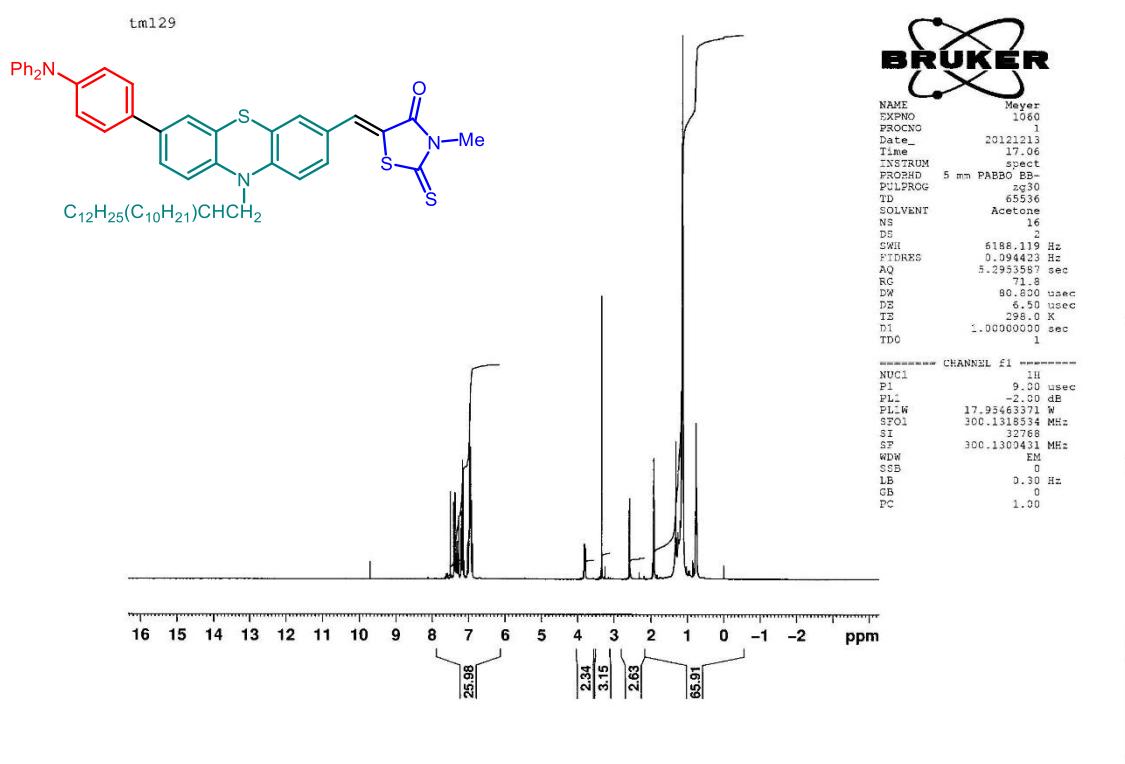
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12p.



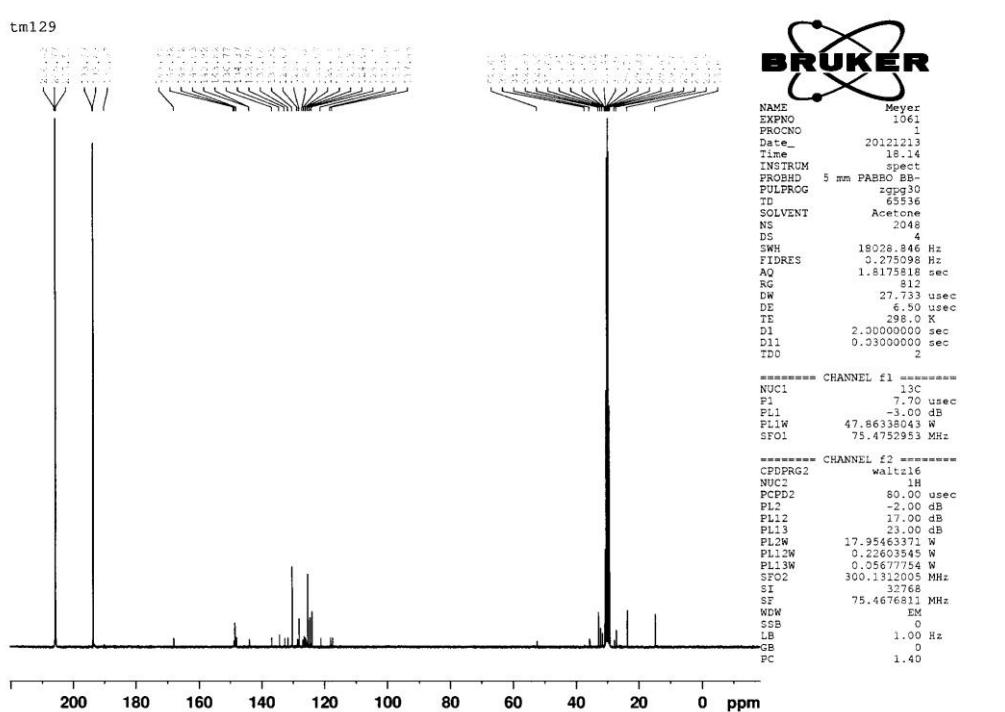


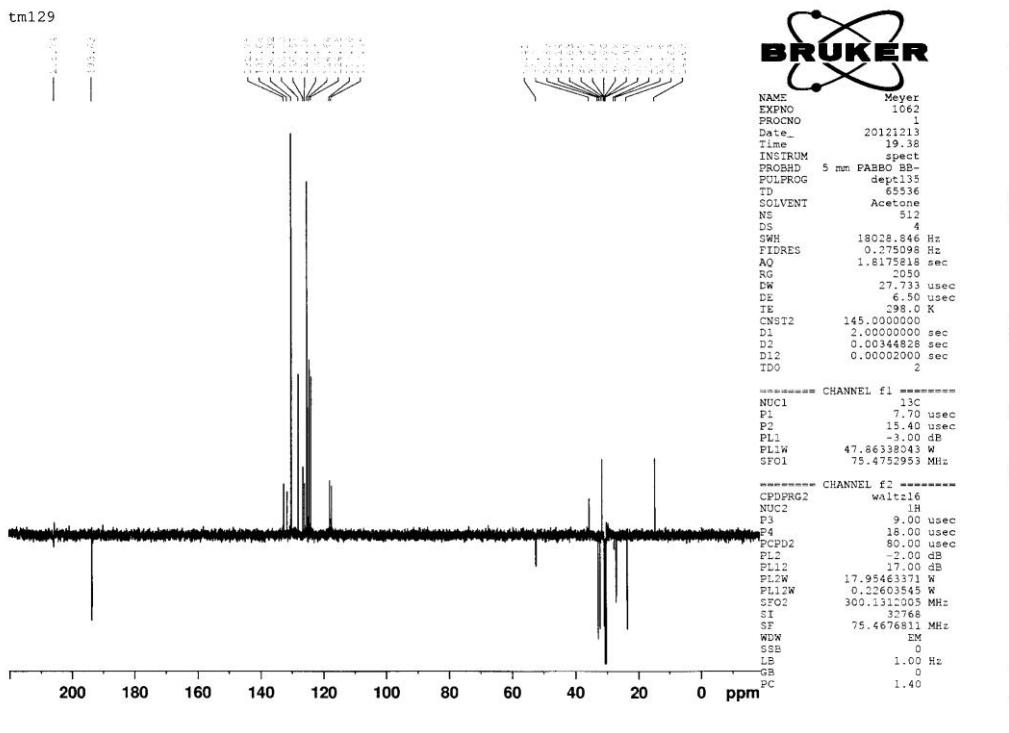
DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **12p**.

3.50. (*Z*)-5-{[10-(2-Decyltetradecyl)-7-(4-{diphenylamino}phenyl)-10*H*-phenothiazin-3-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12q)



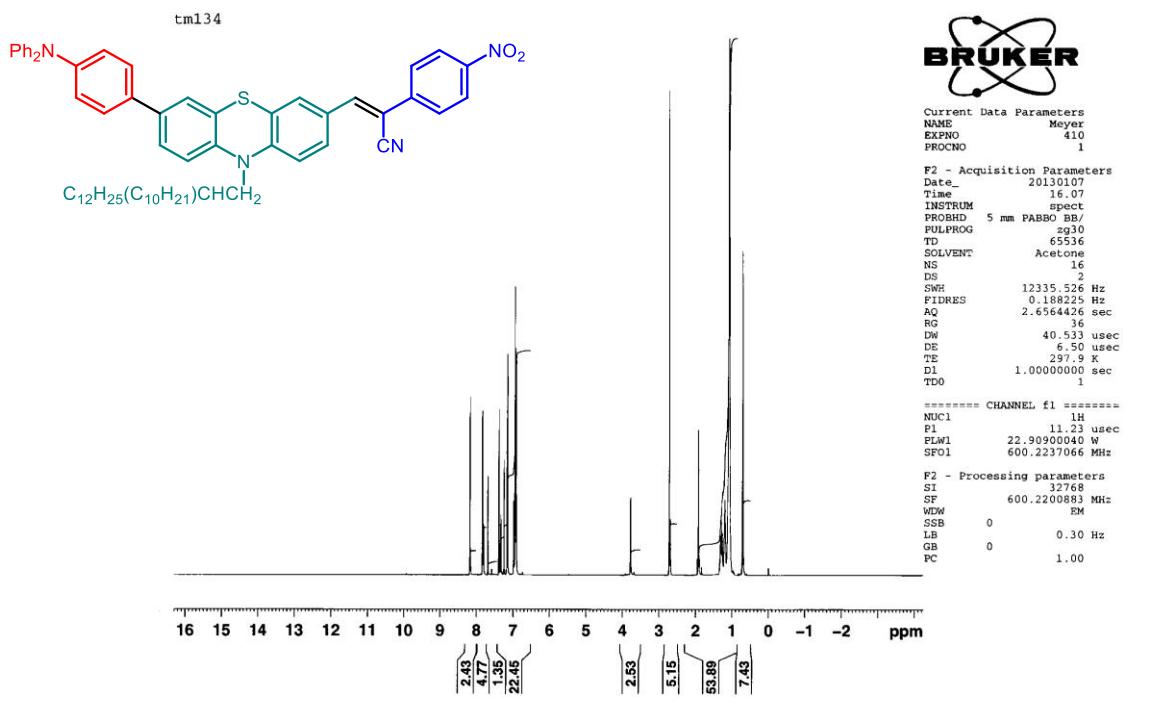
^1H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12q.



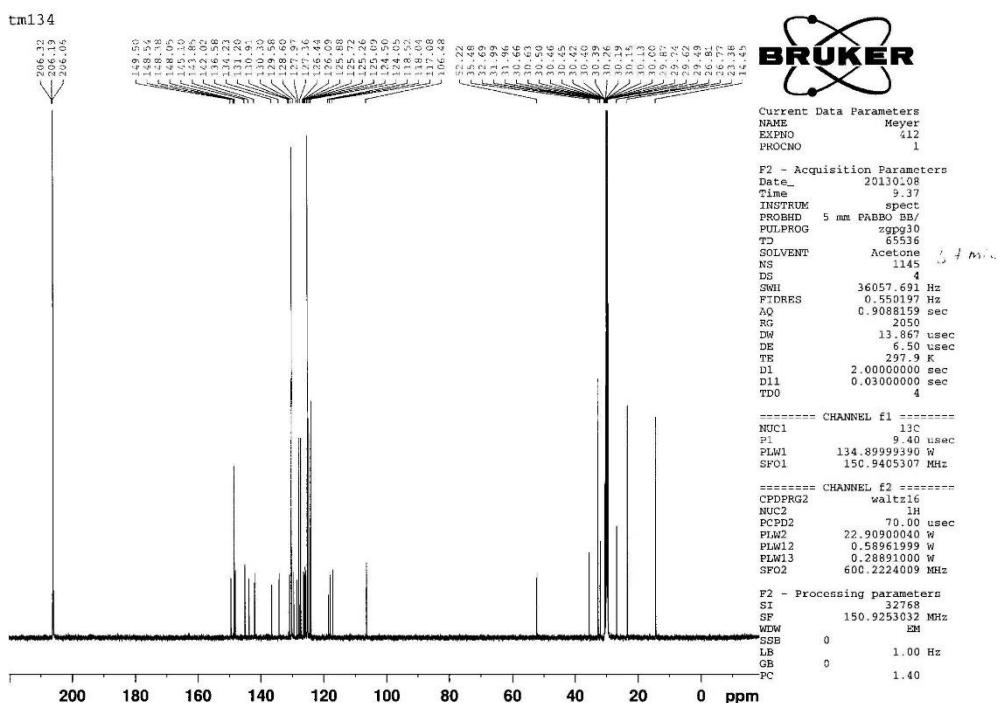


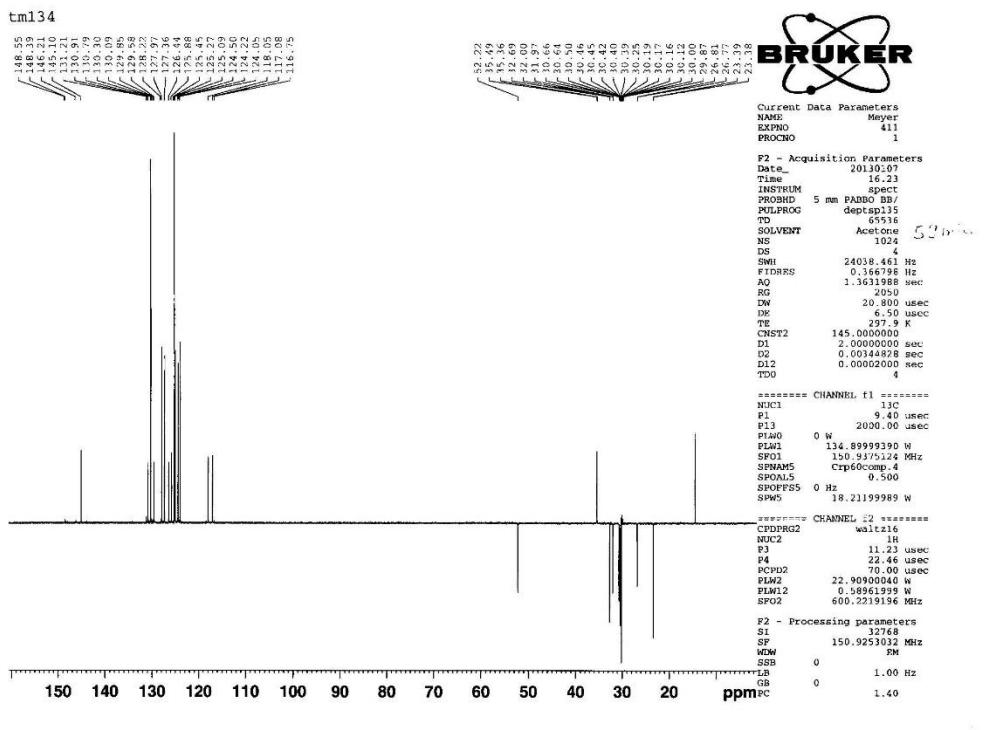
DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12q**.

3.51. (*Z*)-3-{10-(2-Decyltetradecyl)-7-[4-(diphenylamino)phenyl]-10*H*-phenothiazin-3-yl}-2-(4-nitrophenyl)acrylonitrile (12r)



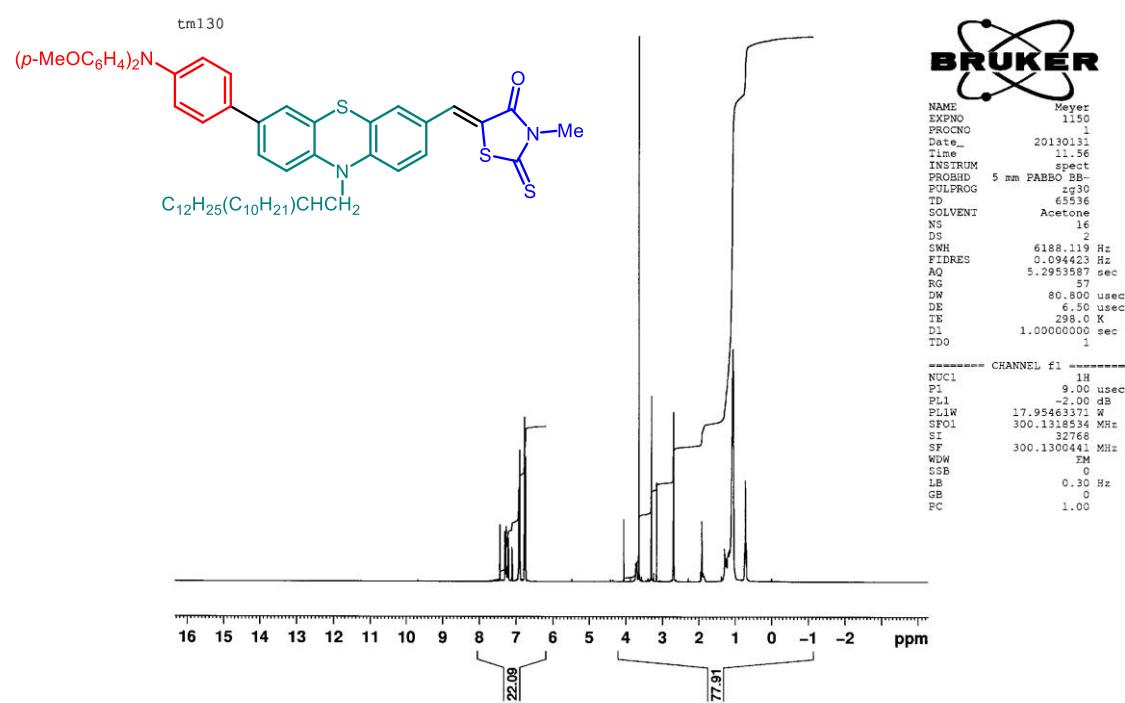
¹H NMR (600 MHz, acetone-d₆) of compound 12r.



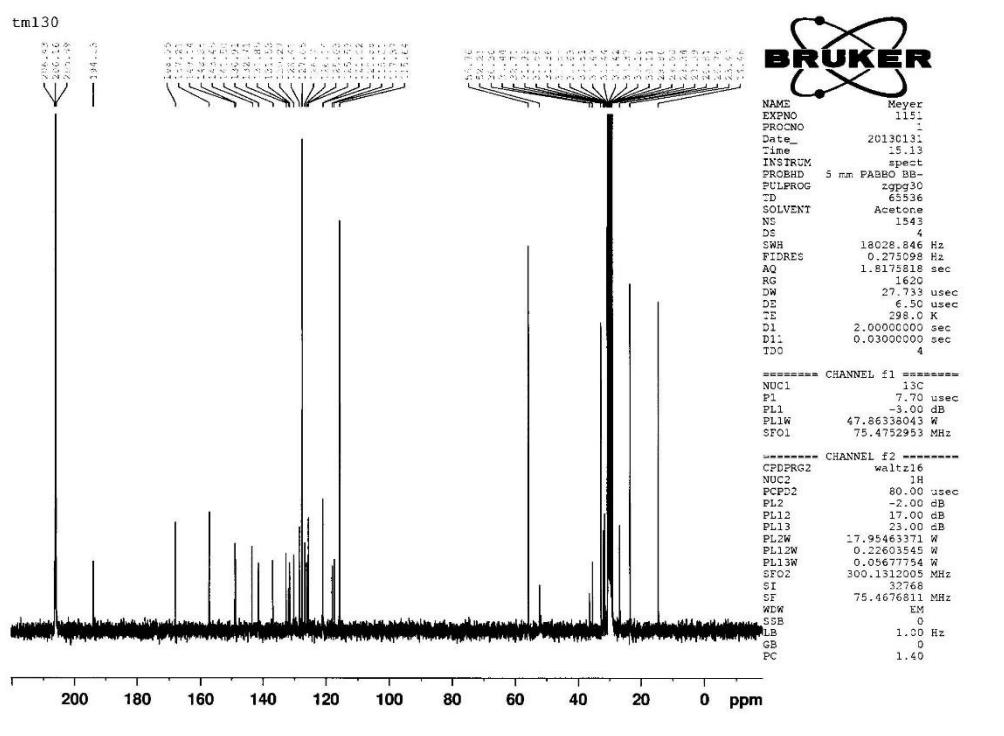


DEPT ^{13}C NMR (150 MHz, acetone-d₆) of compound **12r**.

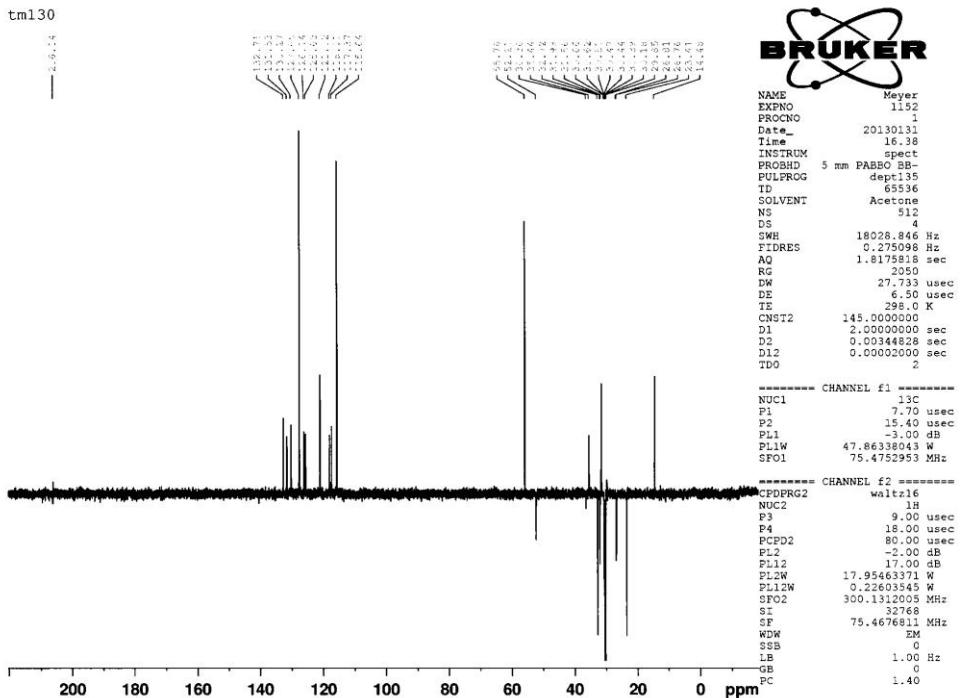
3.52. (*Z*)-5-{[7-(4-{Bis[4-methoxyphenyl]amino}phenyl)phenyl]-10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl)methylene}-3-methyl-2-thioxothiazolidin-4-one (12s)



¹H NMR (300 MHz, acetone-d₆) of compound 12s.

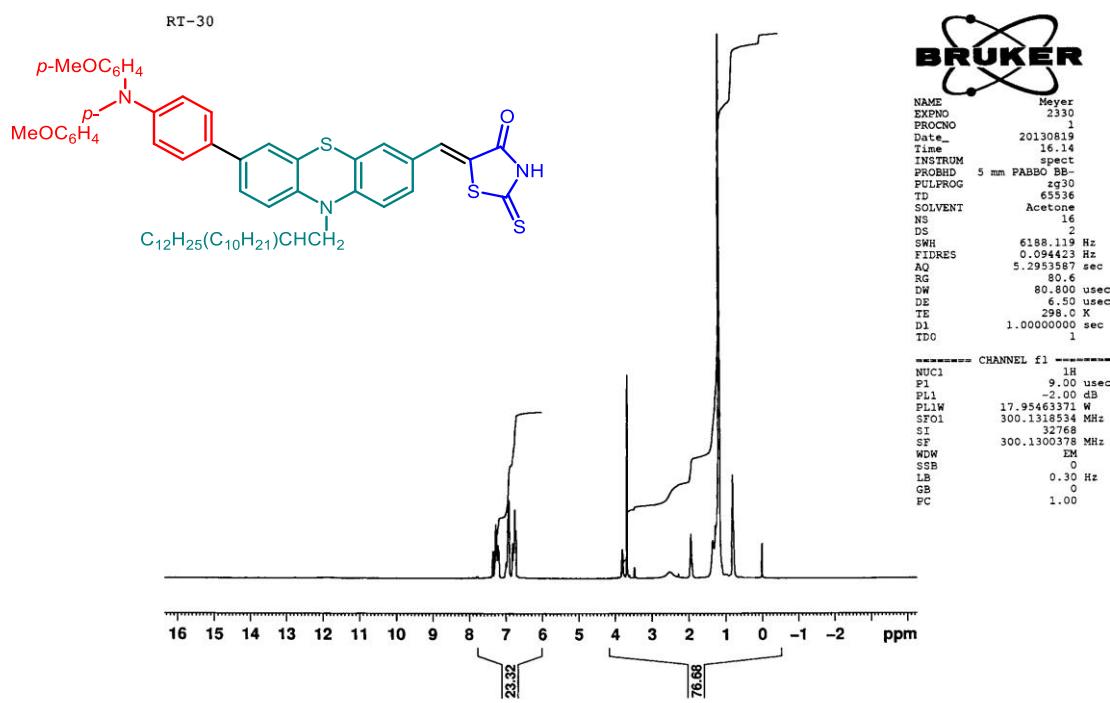


¹³C NMR (75 MHz, acetone-d₆) of compound 12s.

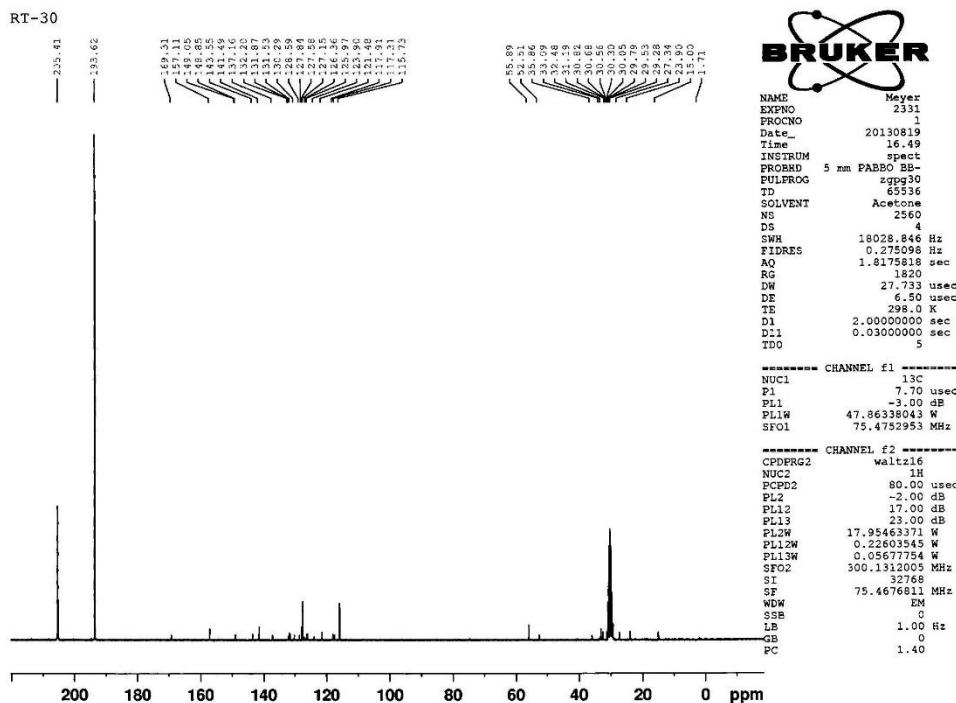


DEPT ^{13}C NMR (75 MHz, acetone-d₆) of compound **12s**.

3.53. (*Z*)-5-{[7-(4-{Bis[4-methoxyphenyl]amino}phenyl)-10-(2-decyldodecyl)-10*H*-phenothiazin-3-yl)methylene}-2-thioxothiazolidin-4-one (12t)

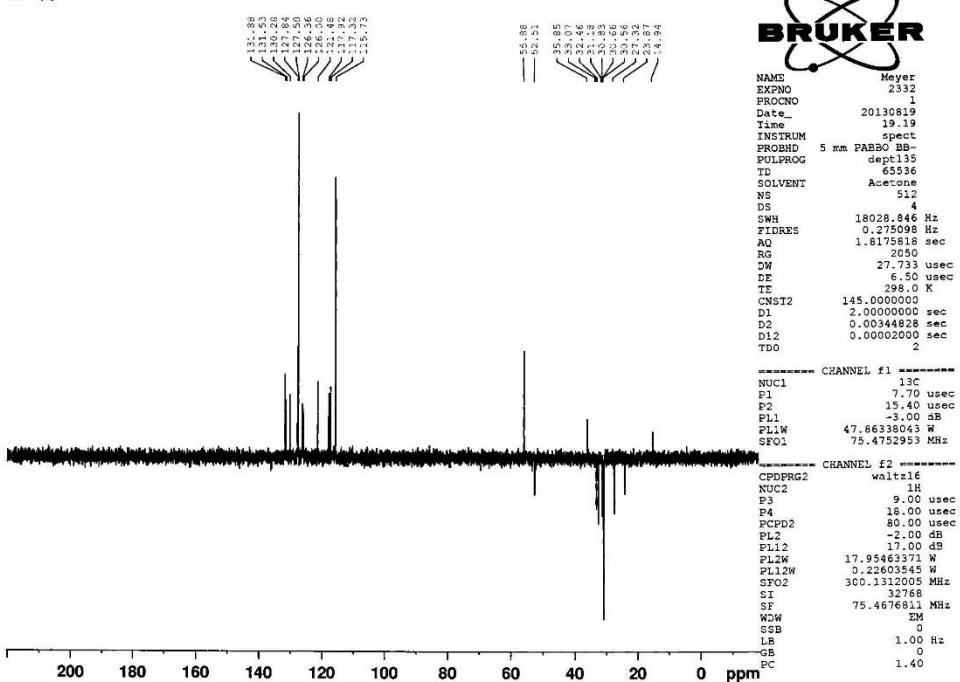


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **12t**.



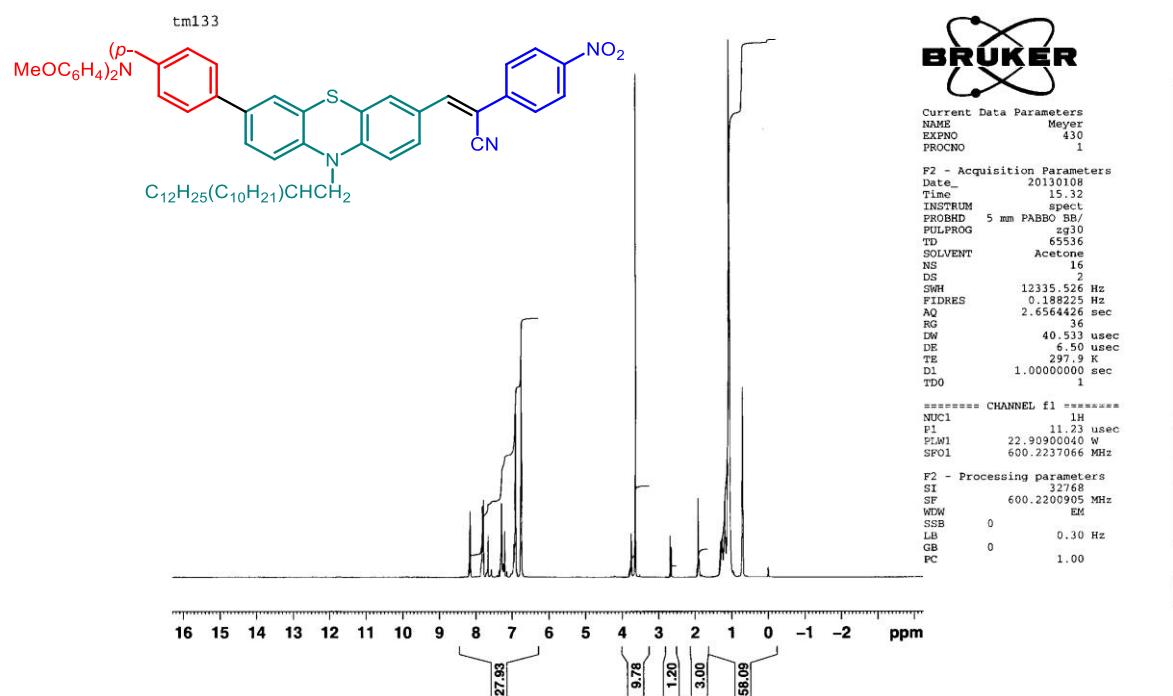
¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12t.

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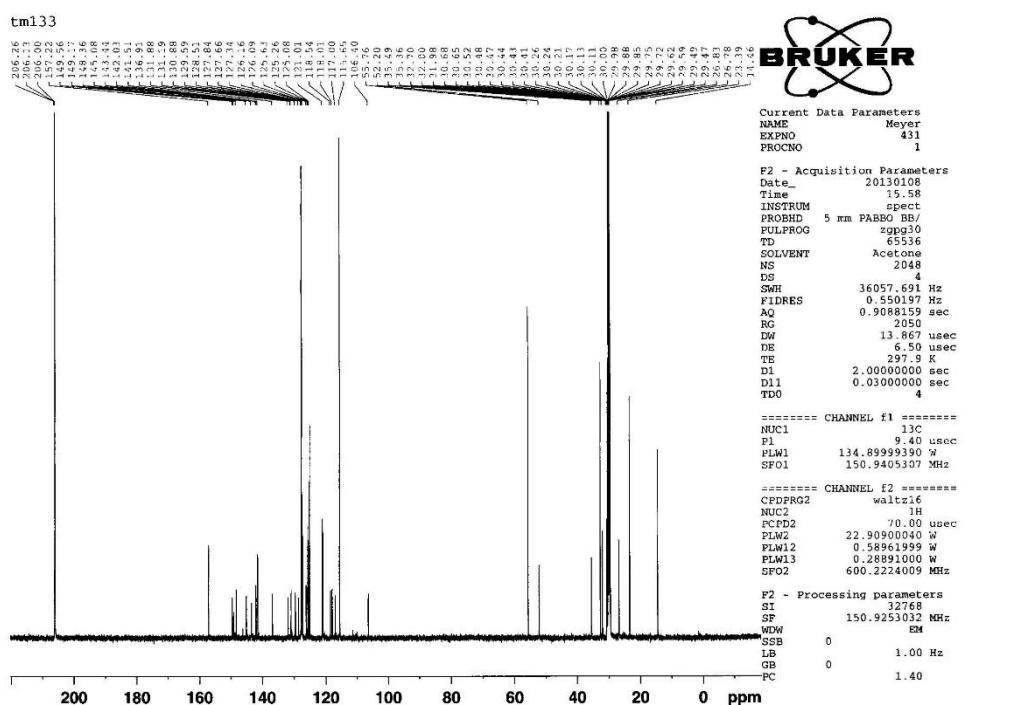


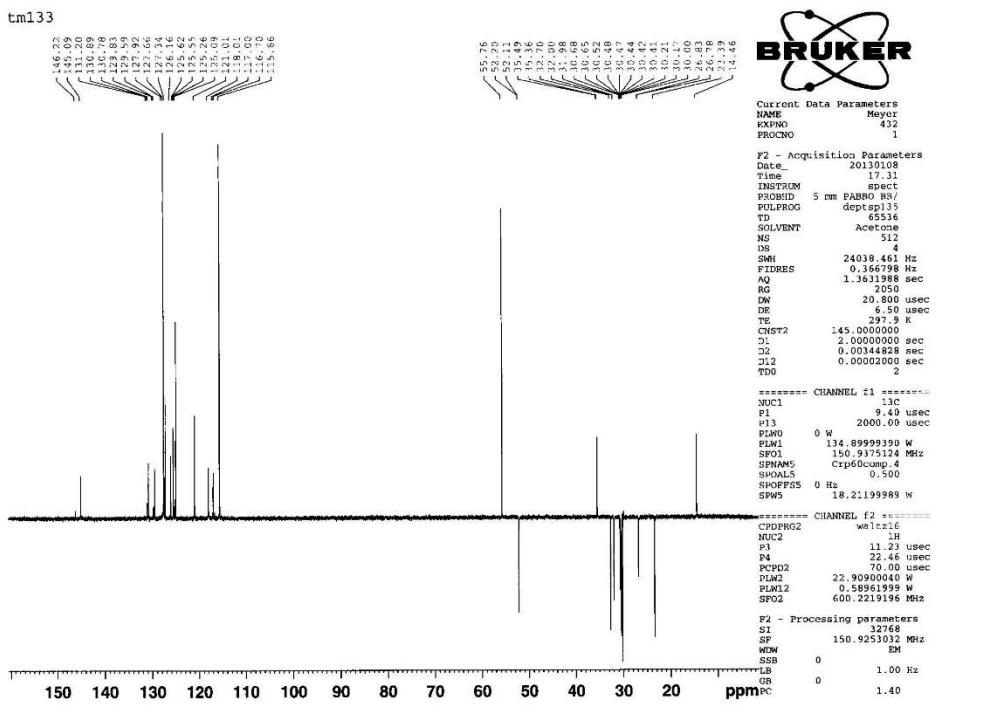
DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12t**.

3.54. (*Z*)-3-{7-[4-(Bis{4-methoxyphenyl}amino)phenyl]phenyl}-10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl}-2-(4-nitrophenyl)acrylonitrile (12u)



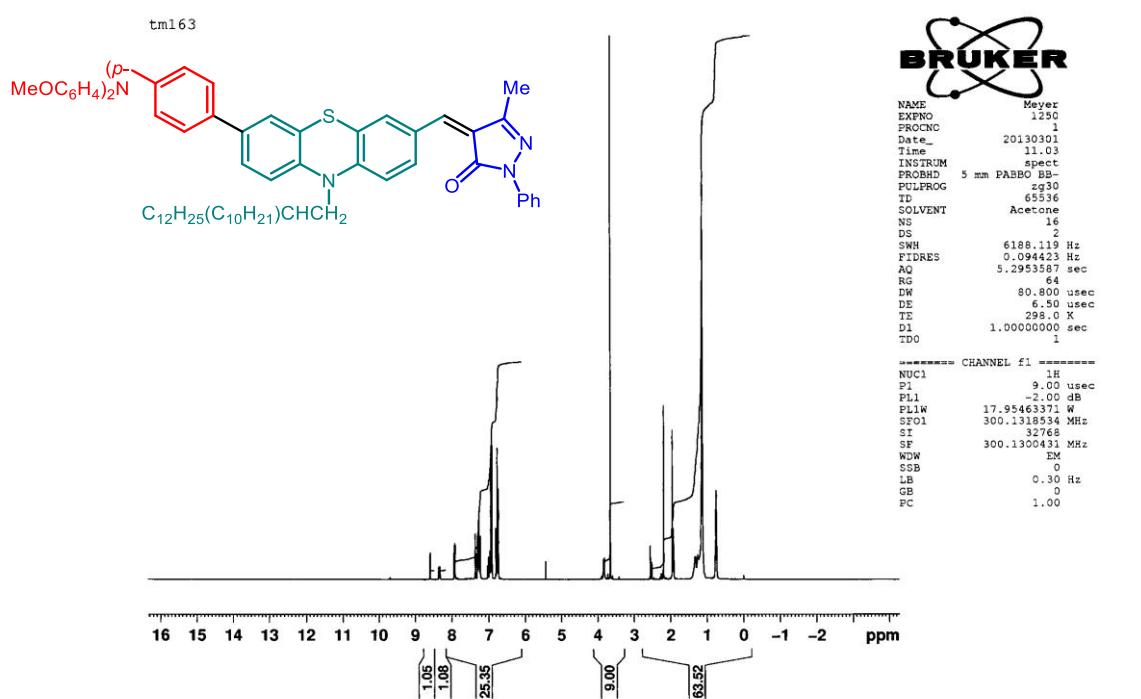
¹H NMR (600 MHz, acetone-d₆) of compound 12u.



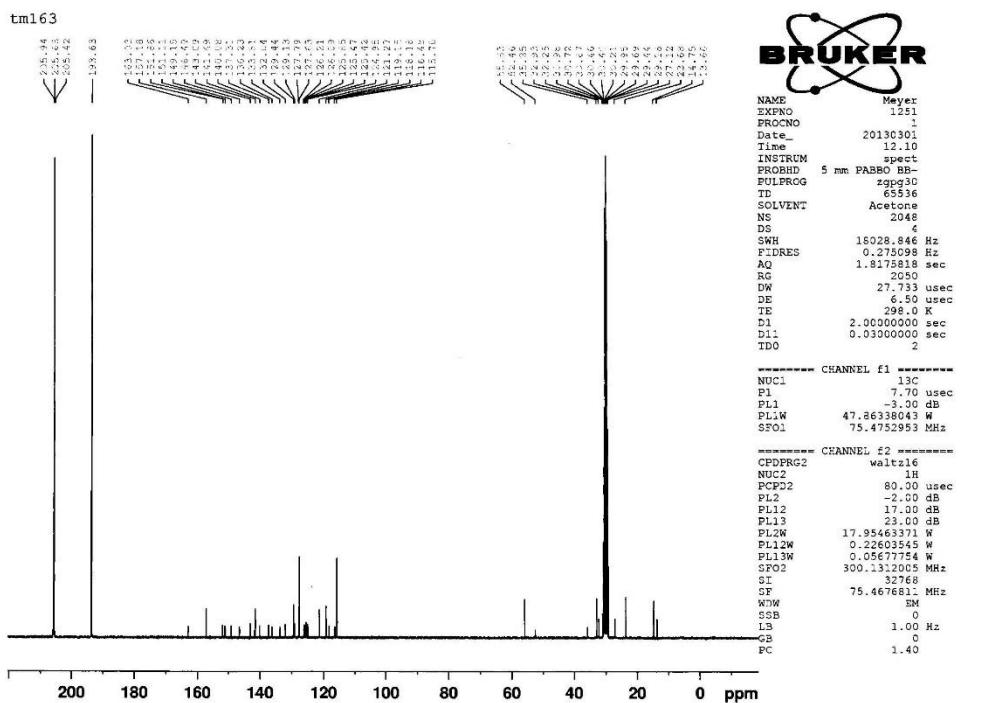


DEPT ^{13}C NMR (150 MHz, acetone-d₆) of compound **12u**.

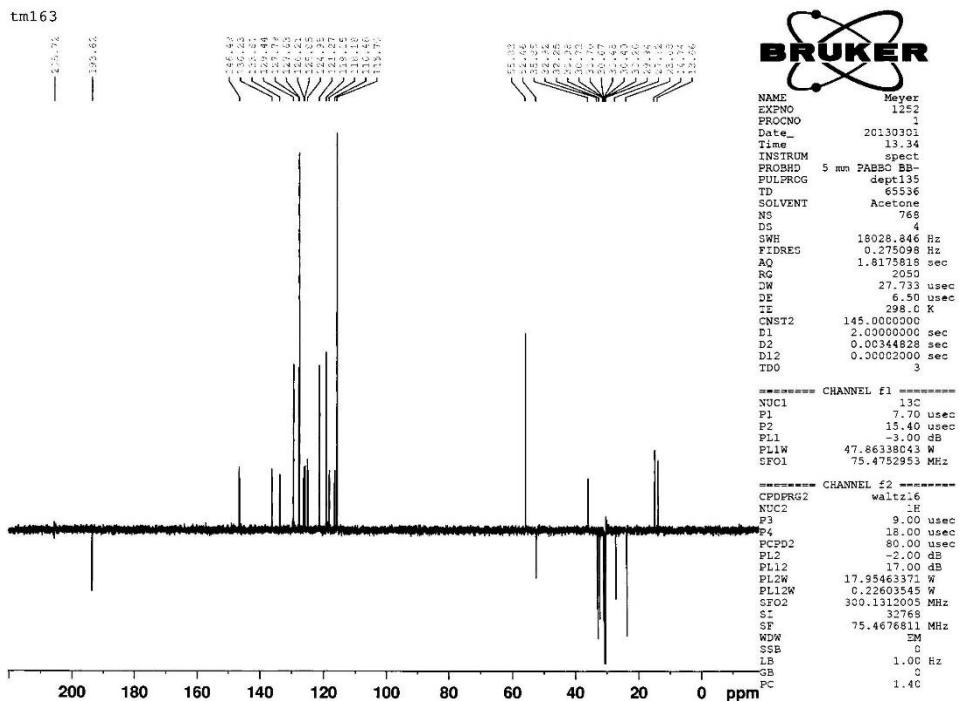
3.55. (*Z*)-4-{[7-(4-(Bis{4-methoxyphenyl}amino)phenyl]phenyl]-10-(2-decytetradecyl)-10*H*-phenothiazin-3-yl)methylene}-3-methyl-1-phenyl-1*H*-pyrazol-5[4*H*]-one (12v)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12v.

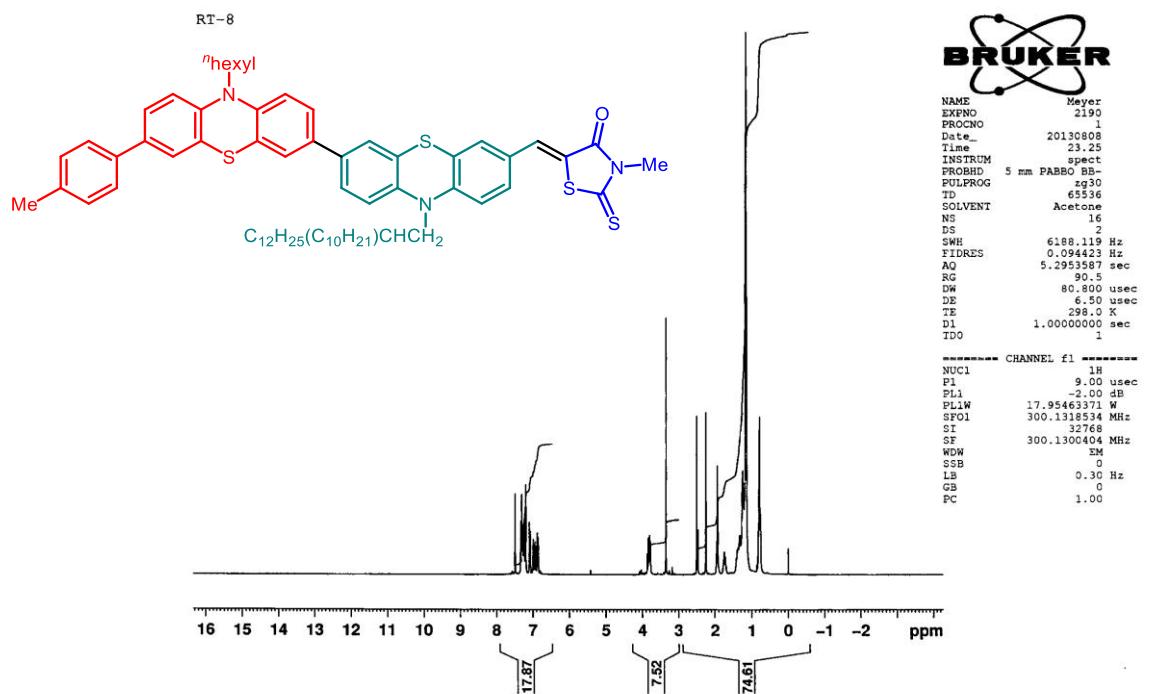


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12v.

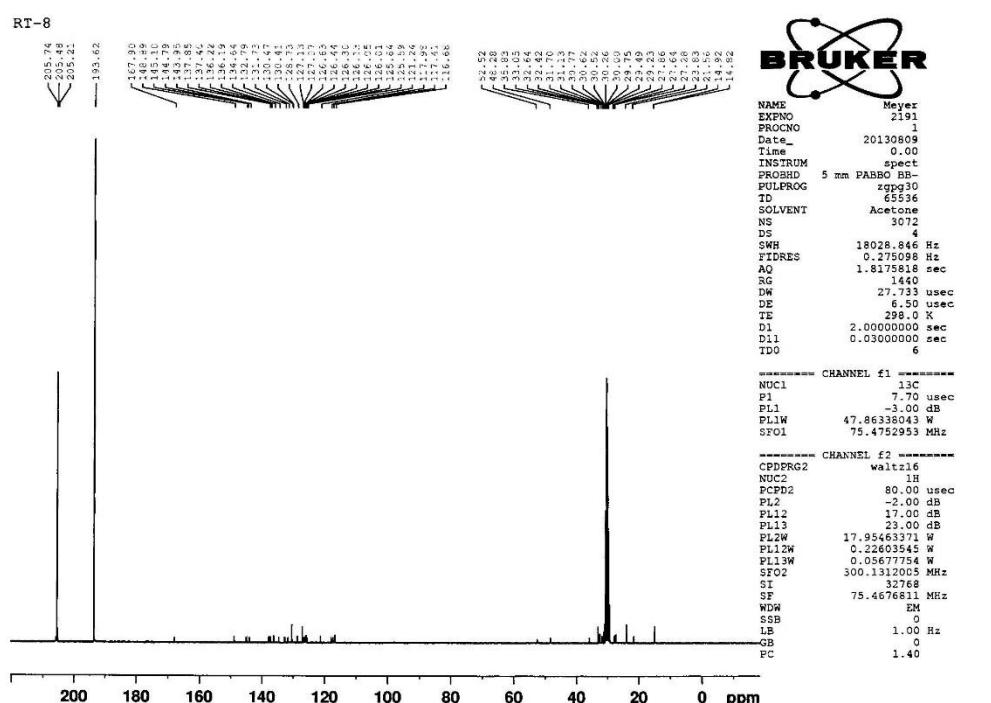


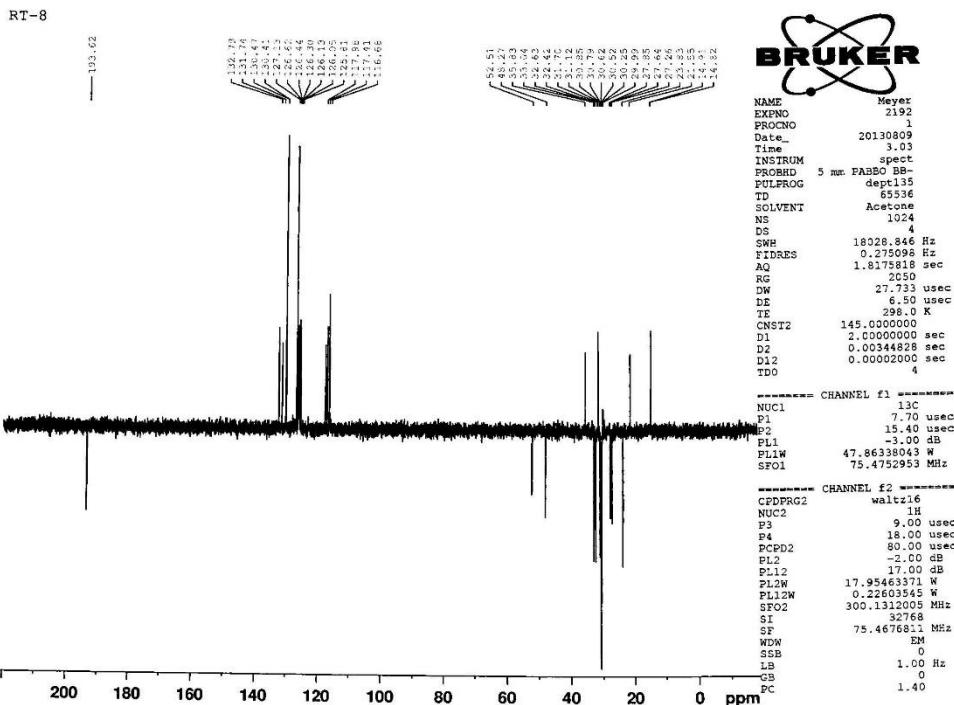
DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound 12v.

3.56. (*Z*)-5-{[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10*H*,10'*H*-(3,3'-biphenothiazin)-7-yl]methylene}-3-methyl-2-thioxothiazolidin-4-one (12w)



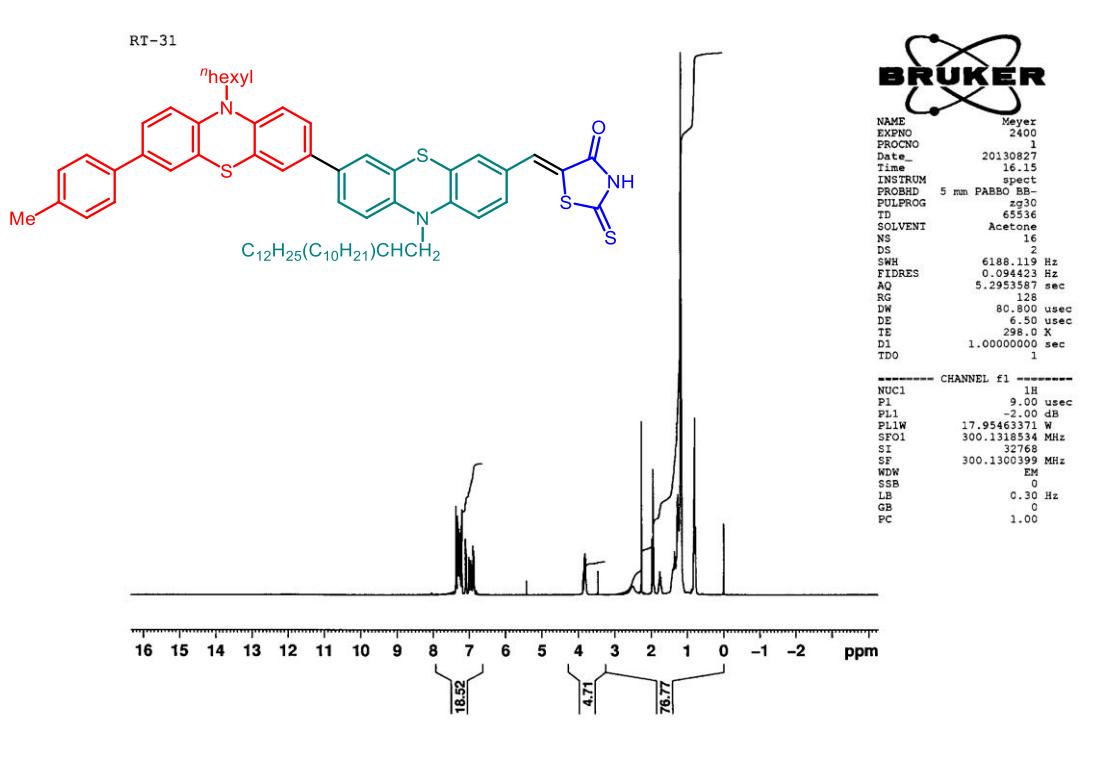
¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound 12w.



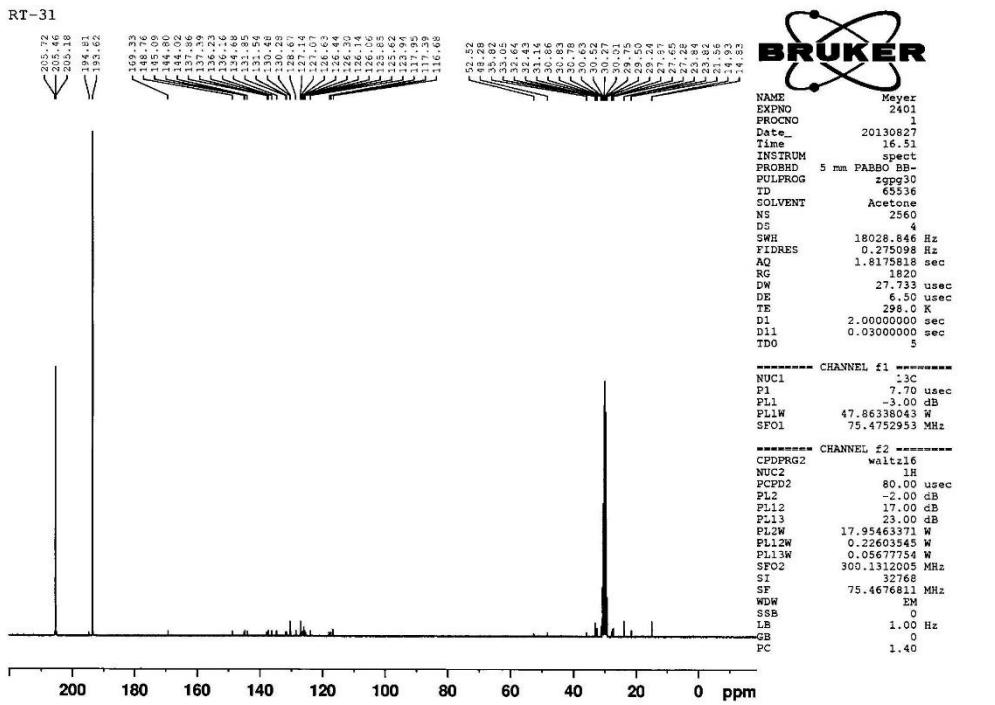


DEPT ^{13}C NMR (75 MHz, acetone- d_6 /CS₂ 4:1) of compound **12w**.

3.57. (*Z*)-5-{[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10*H*,10*H*'-3,3'-biphenothiazin)-7-yl]methylene}-2-thioxothiazolidin-4-one (12x)

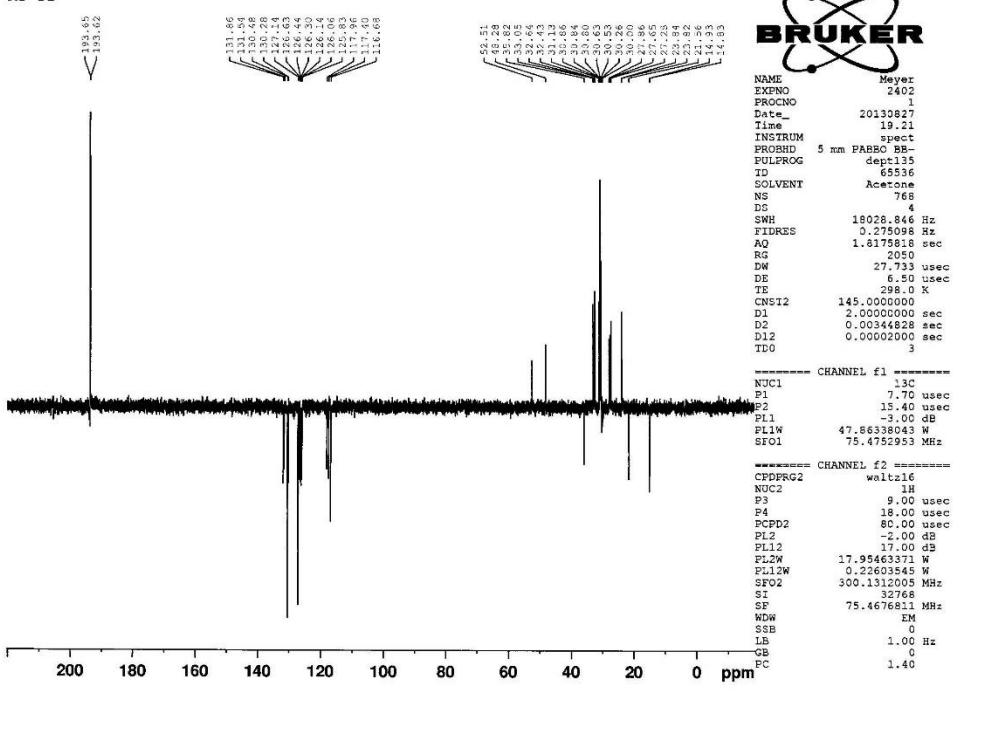


¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **12x**.

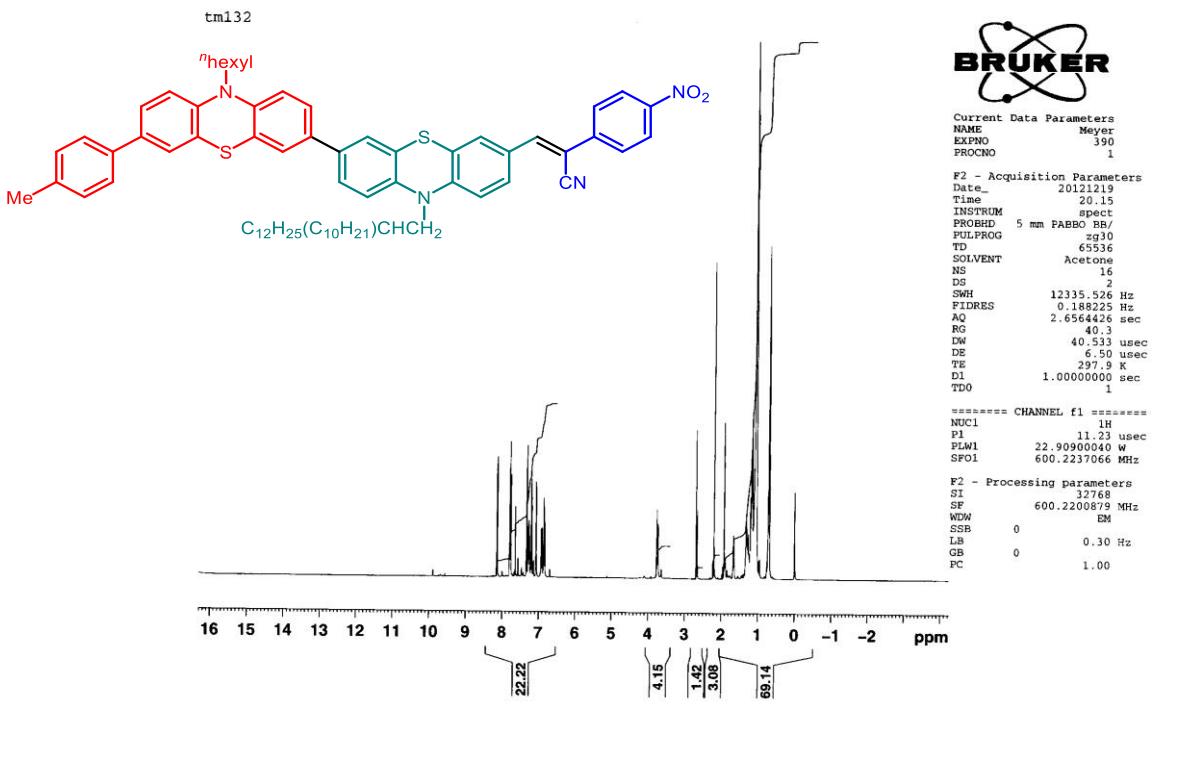


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12x**.

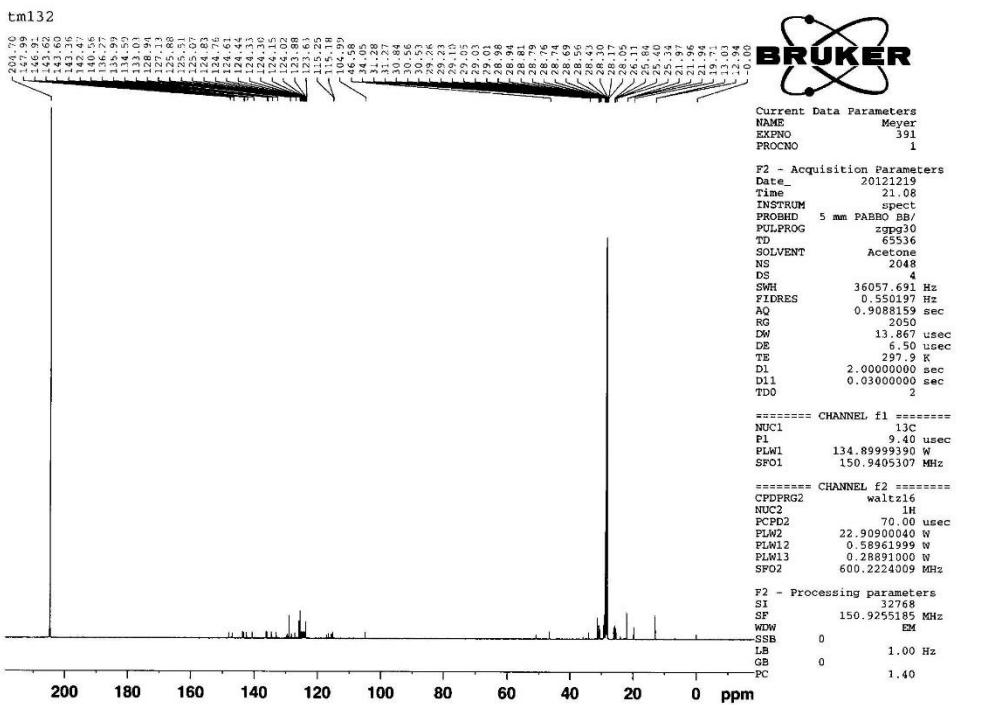
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DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12x**.

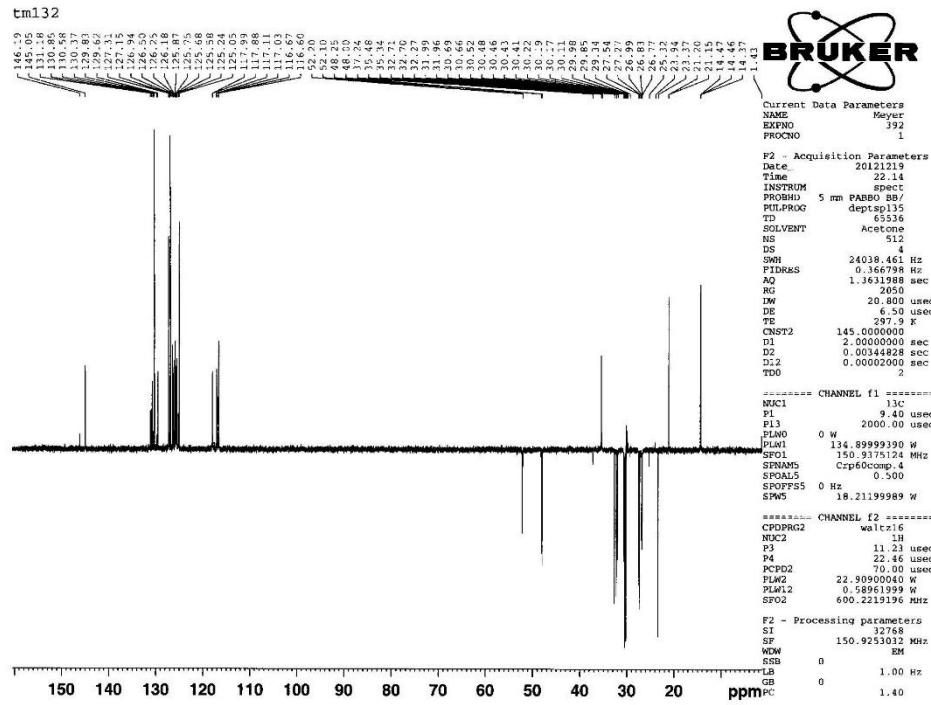
3.58. (Z)-3-[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10*H*,10'*H*'-(3,3'-biphenothiazin)-7-yl]-2-(4-nitrophenyl)acrylonitrile (12y)



¹H NMR (600 MHz, acetone-d₆) of compound 12y.

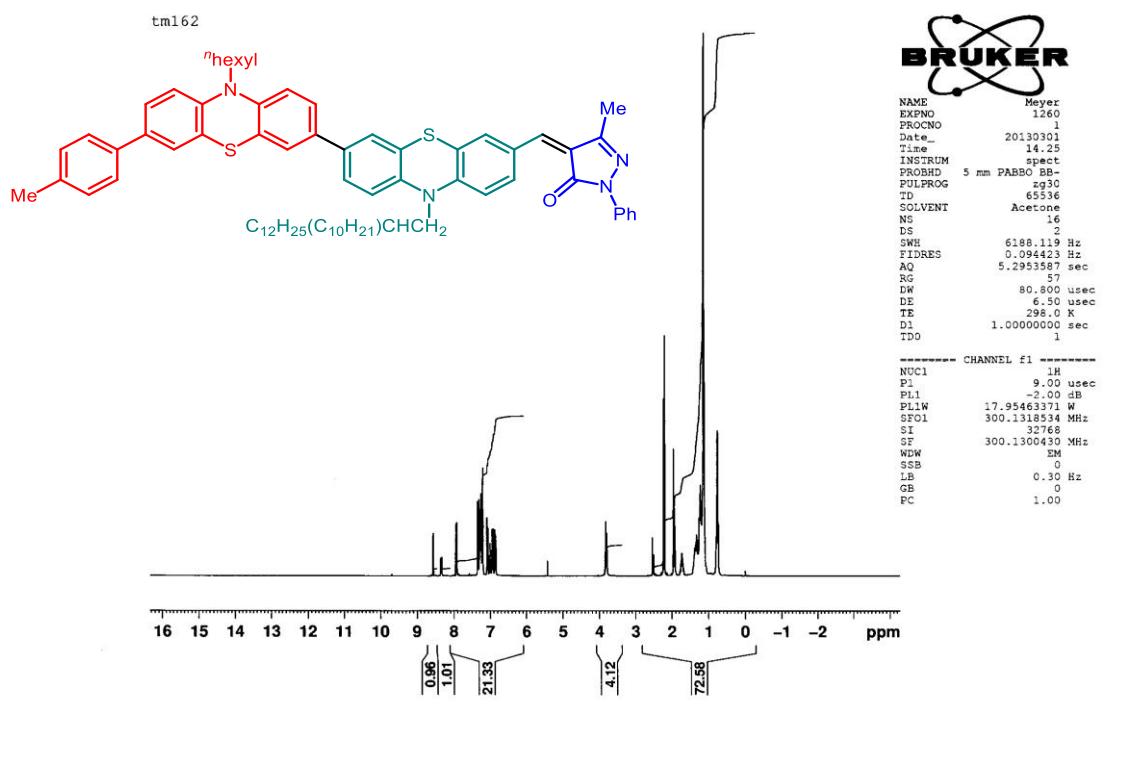


¹³C NMR (150 MHz, acetone-d₆) of compound **12y**.

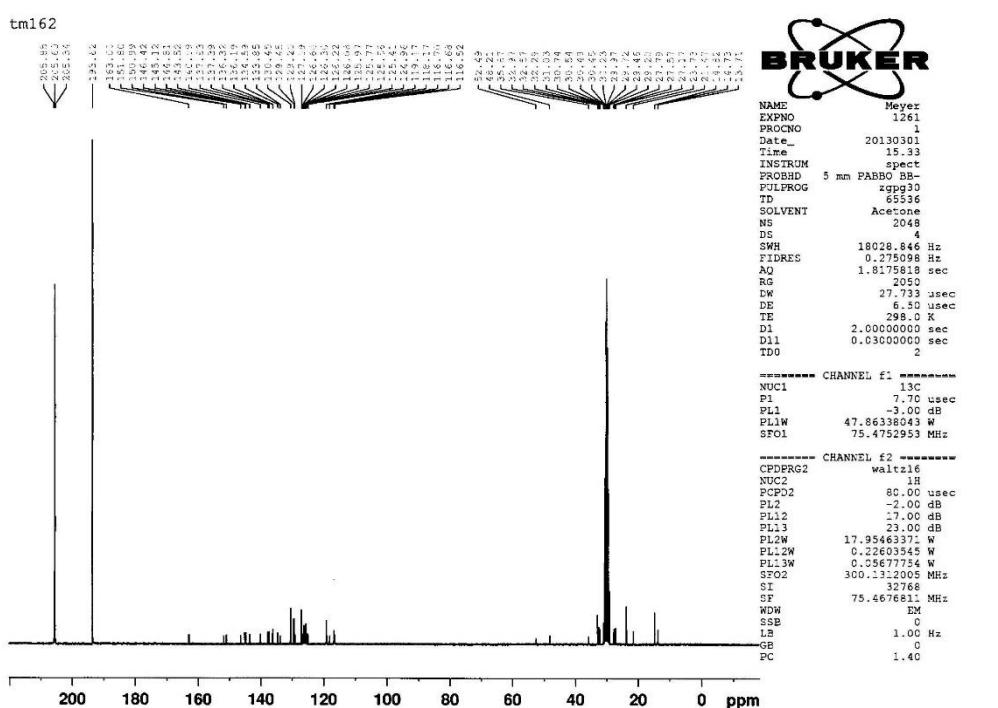


DEPT ^{13}C NMR (150 MHz, acetone- d_6) of compound **12y**.

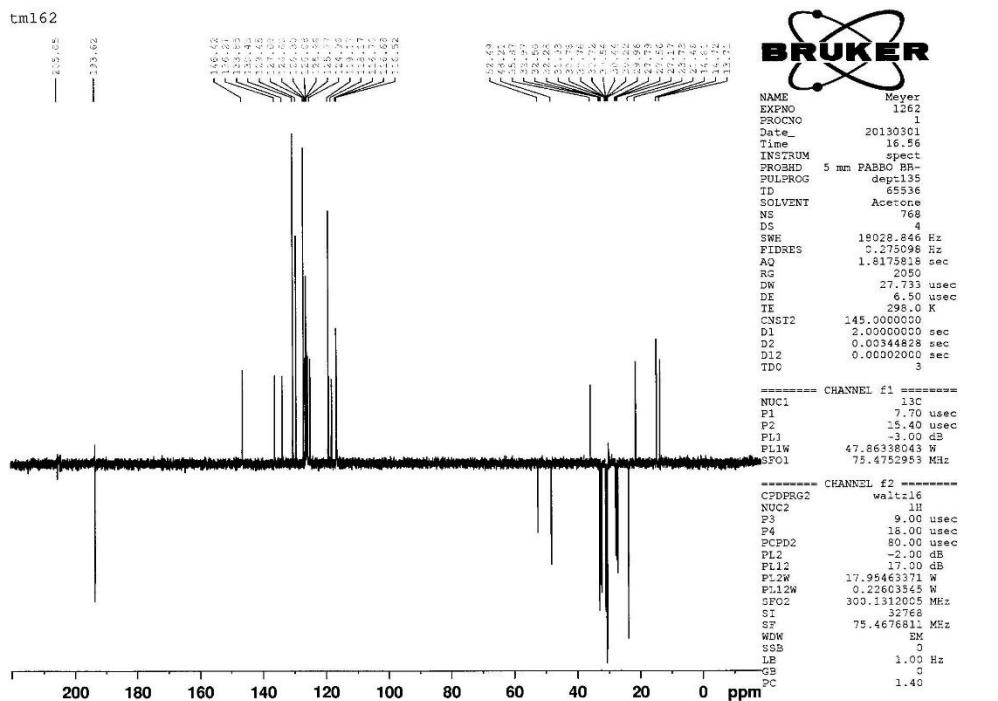
3.59. (*Z*)-4-{{[10-(2-Decyltetradecyl)-10'-hexyl-7'-(*p*-tolyl)-10H,10'H-(3,3'-biphenothiazin)-7-yl]methylene}-3-methyl-1-phenyl-1H-pyrazol-5[4H]-one (12z)



¹H NMR (300 MHz, acetone-d₆/CS₂ 4:1) of compound **12z**.

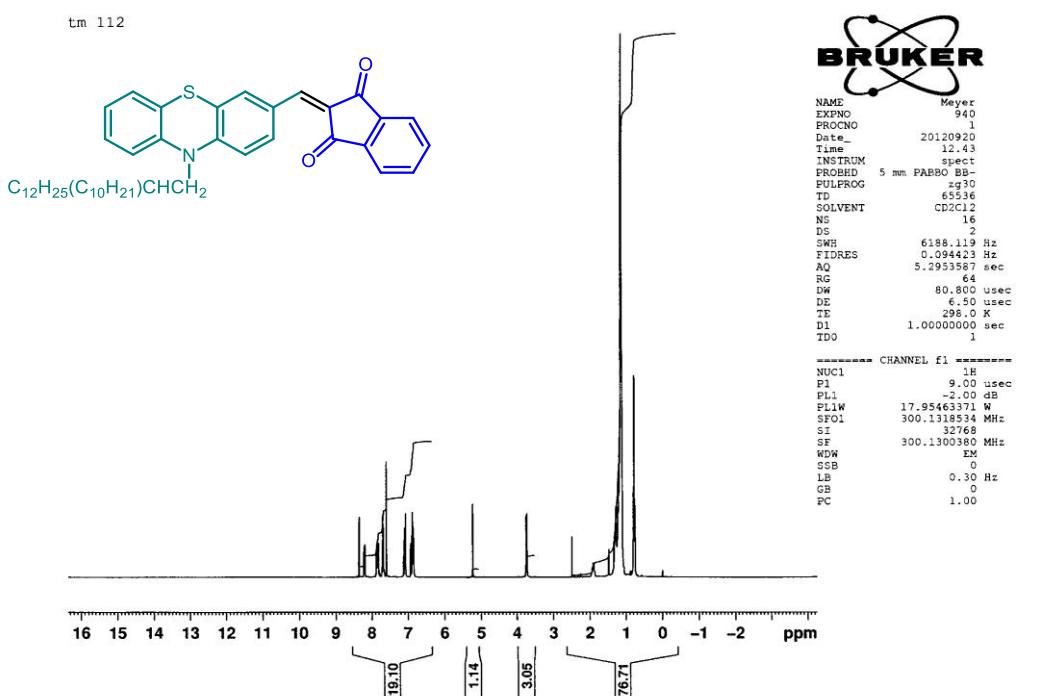


¹³C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12z**.

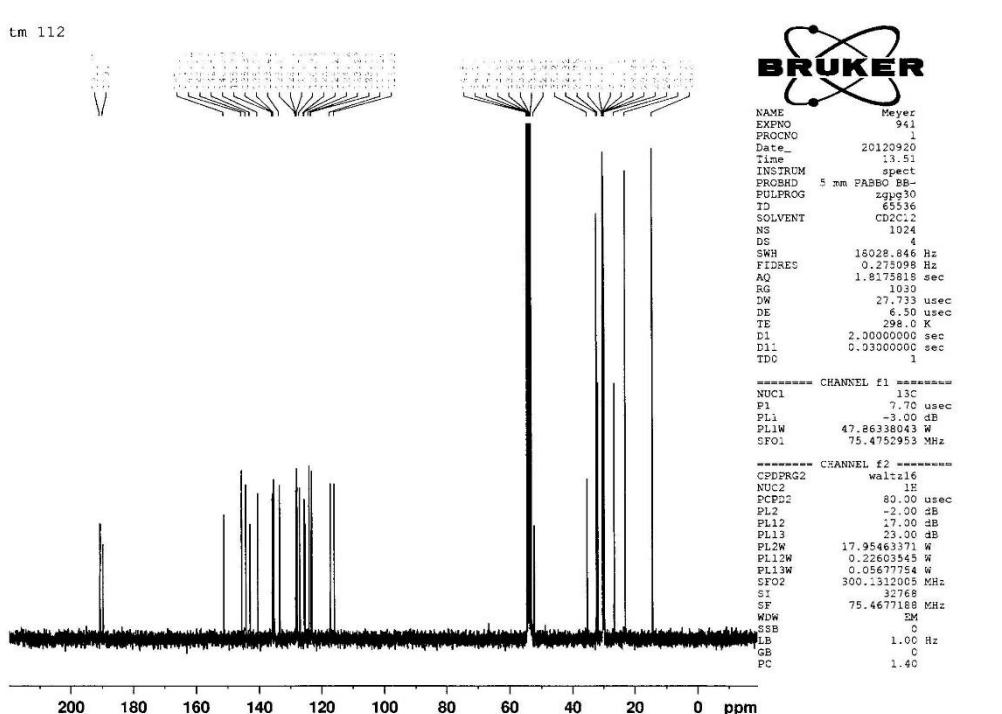


DEPT ^{13}C NMR (75 MHz, acetone-d₆/CS₂ 4:1) of compound **12z**.

3.60. 2-{[10-(2-Decyltetradecyl)-10*H*-phenothiazin-3-yl]methylene}-1*H*-inden-1,3[2*H*]-dione (14)

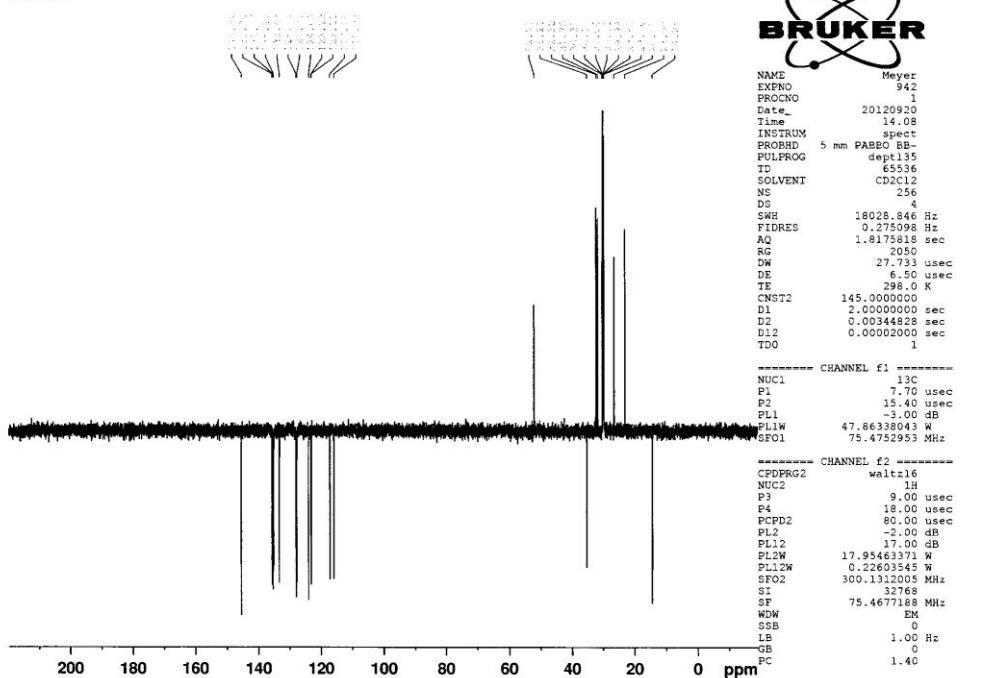


¹H NMR (300 MHz, CD₂Cl₂) of compound 14.



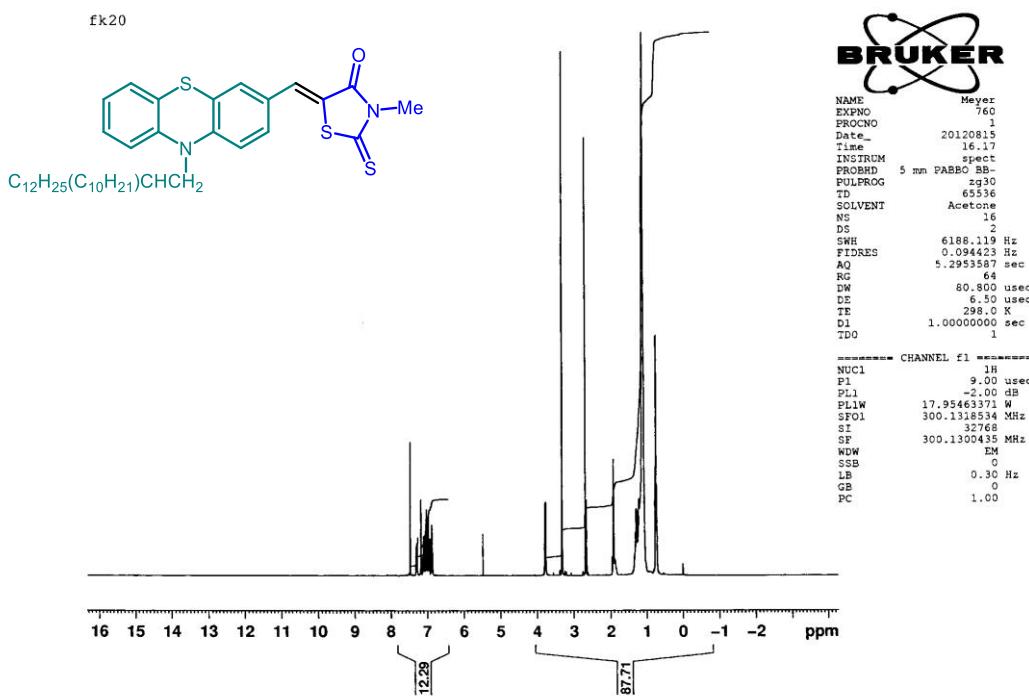
¹³C NMR (75 MHz, CD₂Cl₂) of compound 14.

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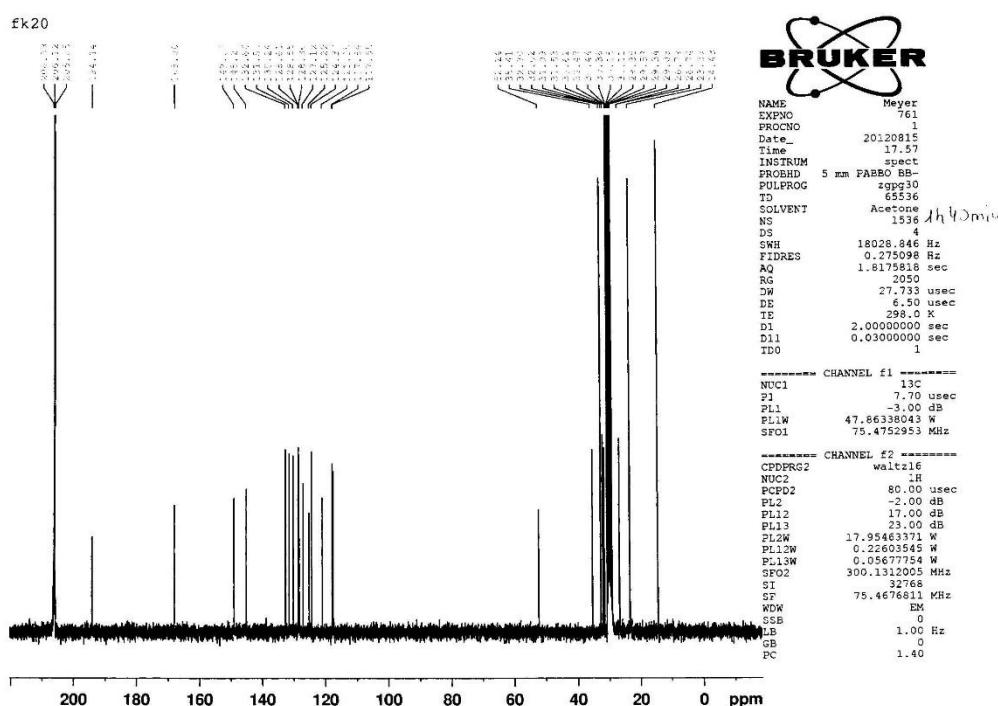


DEPT ¹³C NMR (75 MHz, CD₂Cl₂) of compound 14.

3.61. (*Z*)-5-([10-(2-Decyltetradecyl)-10H-phenothiazin-3-yl]methylene)-3-methyl-2-thioxothiazolidin-4-one (15)

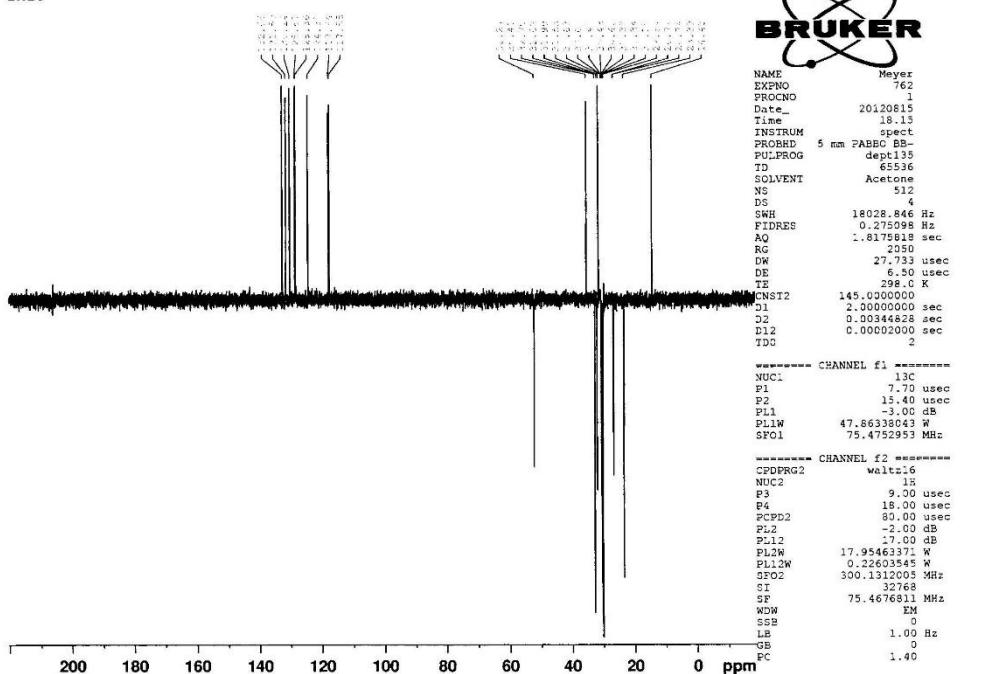


¹H NMR (300 MHz, acetone-d₆) of compound 15.



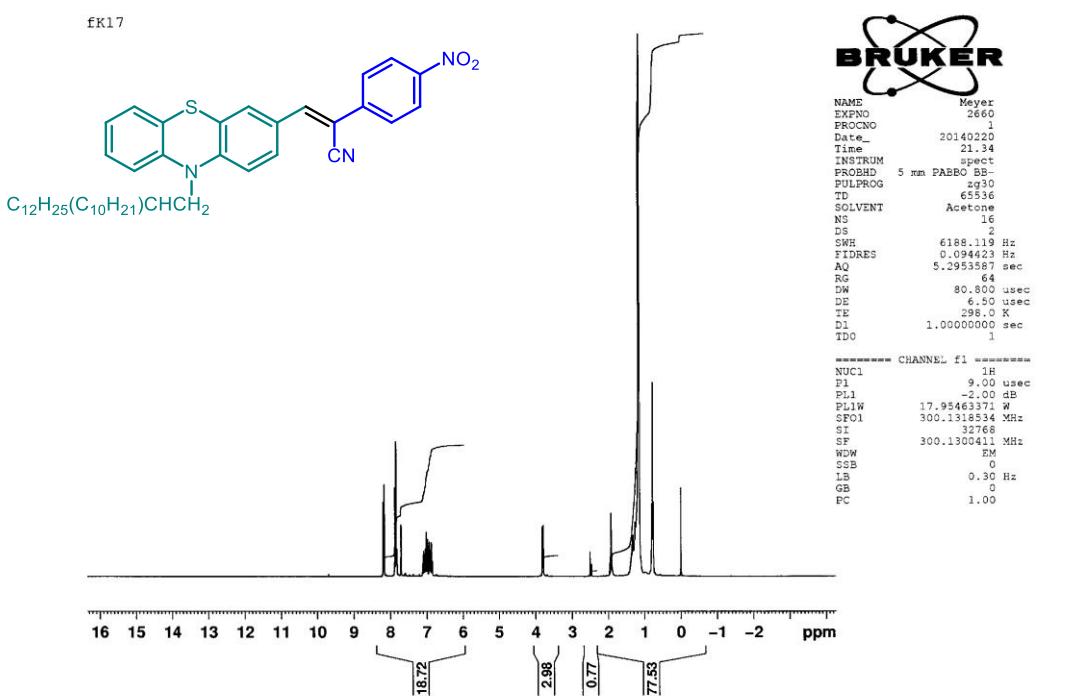
¹³C NMR (75 MHz, acetone-d₆) of compound 15.

fk20

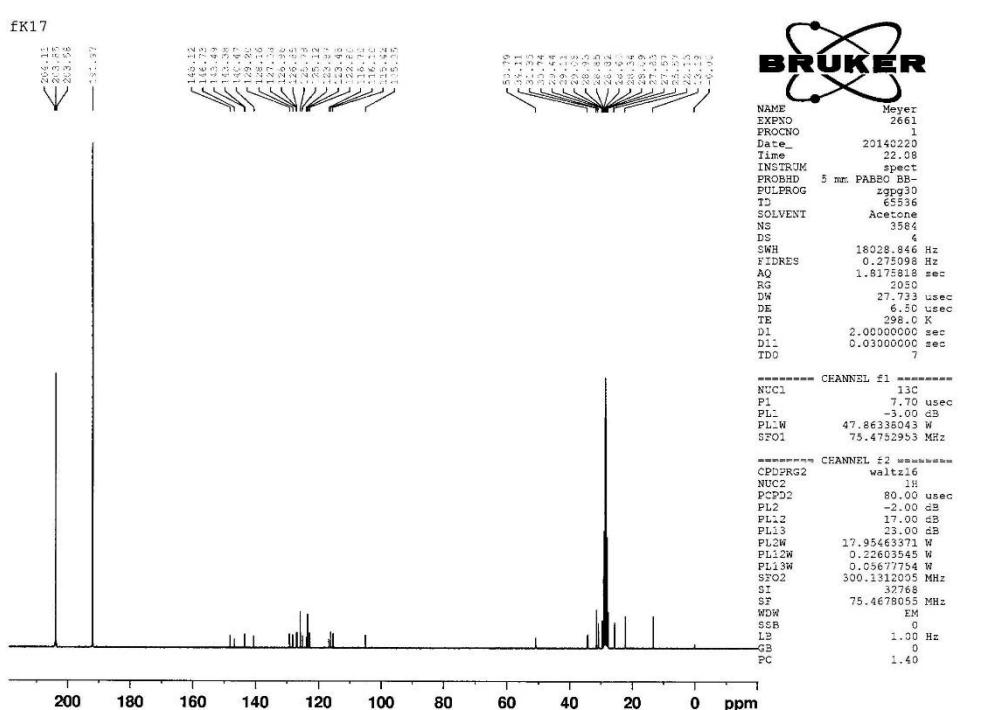


DEPT ^{13}C NMR (75 MHz, acetone-d₆) of compound 15.

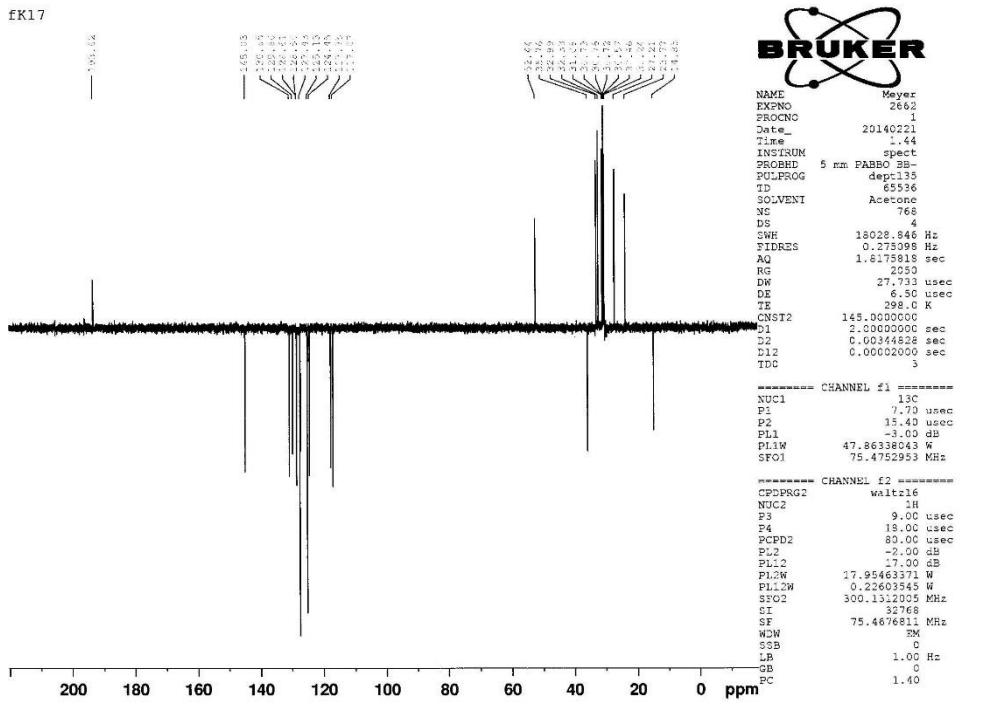
3.62. (*Z*)-3-(10-(2-Decyltetradecyl)-10*H*-phenothiazin-3-yl)-2-(4-nitrophenyl)acrylonitrile (16)



¹H NMR (300 MHz, acetone-d₆) of compound 16.

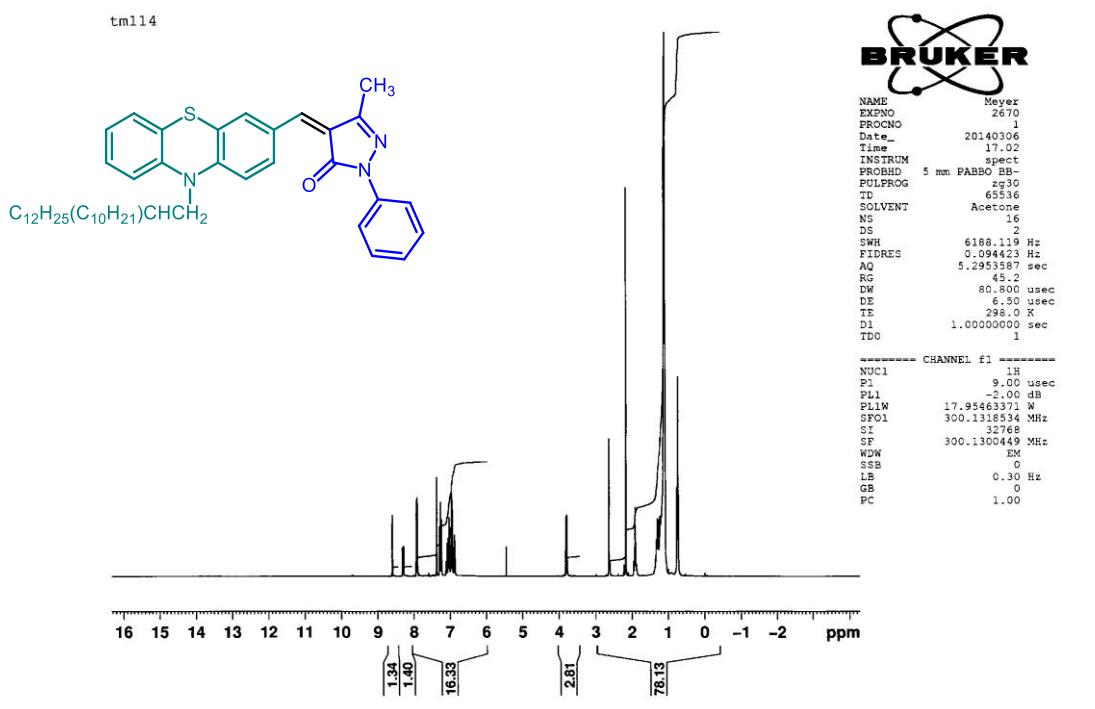


¹³C NMR (75 MHz, acetone-d₆) of compound 16.

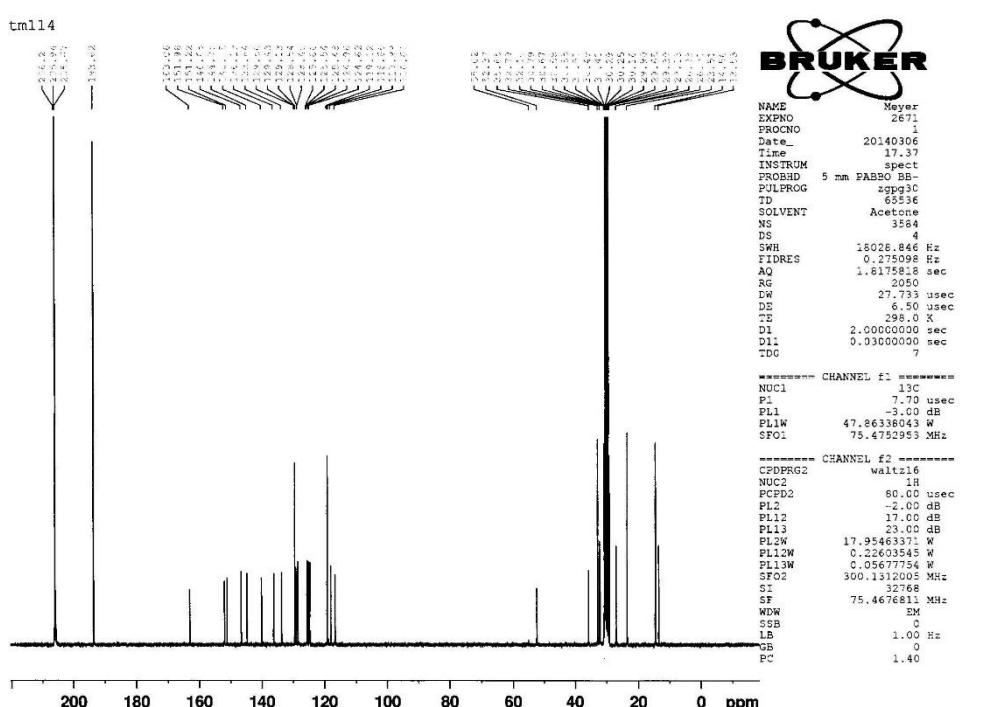


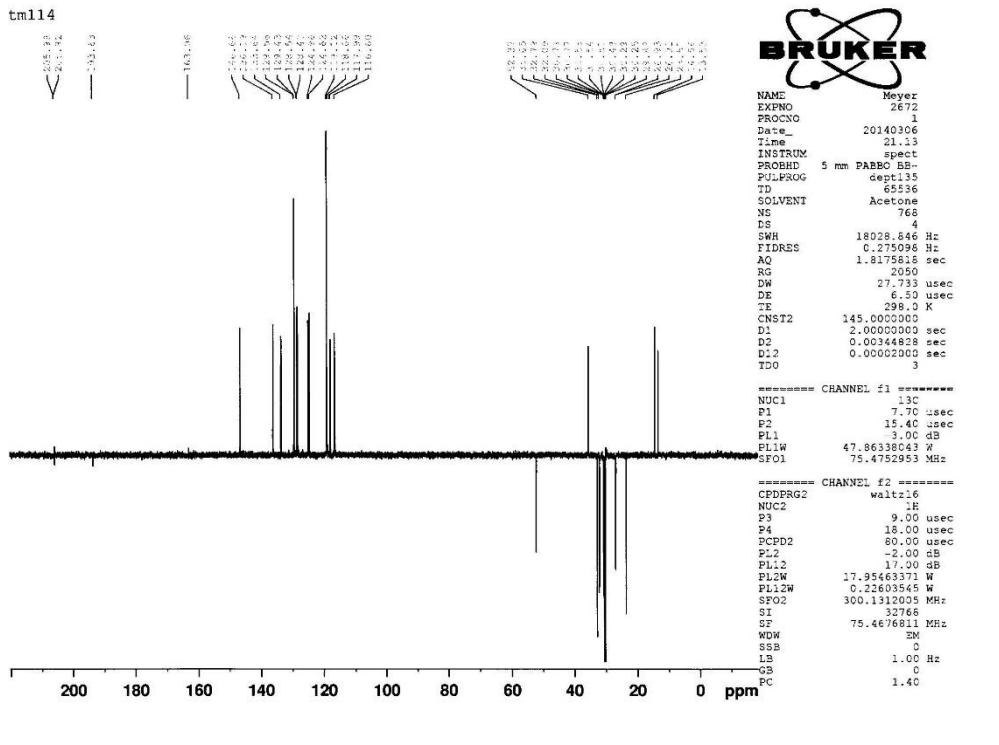
DEPT ^{13}C NMR (75 MHz, acetone-d₆) of compound **16**.

3.63. (*Z*)-4-[(10-(2-Decyltetradecyl)-10*H*-phenothiazin-3-yl)methylene]-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (17)



¹H NMR (300 MHz, CD₂Cl₂) of compound 17.



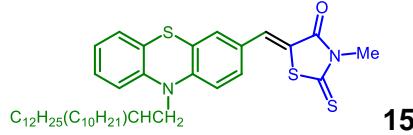
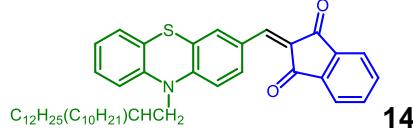
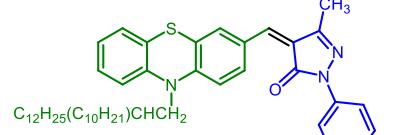
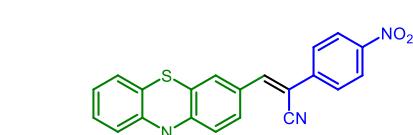


DEPT ^{13}C NMR (75 MHz, CD_2Cl_2) of compound 17.

4. Correlation Analyses

4.1. Correlations of the Model Chromophores 14-17

Table S6. Selected electronic data of chromophores 14-17

Compound	$E_{1/2}$ [V]	$\lambda_{\max,\text{abs}}$ [eV]	$\lambda_{\max,\text{em}}$ [eV]	$\Delta\tilde{\nu}$ [eV]	E_{0-0} [eV]
	1.09	2.629	1.933	0.696	2.281
	1.10	2.467	1.841	0.626	2.154
	1.09	2.607	1.939	0.668	2.273
	1.08	2.686	2.196	0.489	2.441

For linear correlation analyses the corresponding optical parameters (in eV) were plotted against the first oxidation potential $E_{1/2}$ (in V). The goodness of fit is expressed by the quadratic linear correlation coefficient r^2 (see Figures S1-S4).

$\lambda_{\max,\text{abs}}$ vs $E_{1/2}$: $\lambda_{\max,\text{abs}} = 14.53275 - 10.95 \cdot E_{1/2}$ [eV]; $r^2 = 0.92429$.

$\lambda_{\max,\text{em}}$ vs $E_{1/2}$: $\lambda_{\max,\text{em}} = 21.32475 - 17.75 \cdot E_{1/2}$ [eV]; $r^2 = 0.90228$.

$\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = -6.84675 - 6.85 \cdot E_{1/2}$ [eV]; $r^2 = 0.37127$.

E_{00} vs $E_{1/2}$: $E_{00} = 17.92875 - 14.35 \cdot E_{1/2}$ [eV]; $r^2 = 0.98914$.

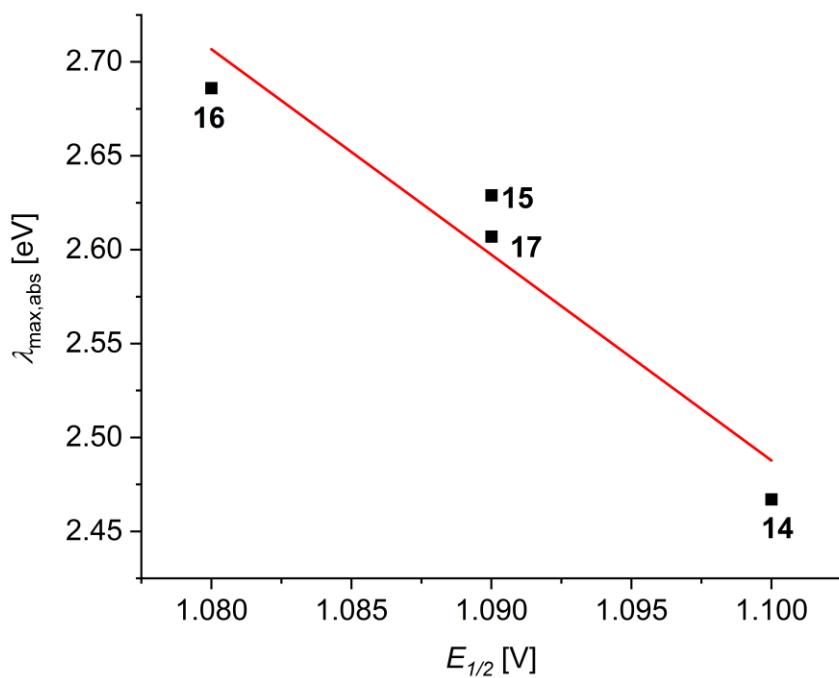


Figure S1. Correlation $\lambda_{\text{max,abs}}$ vs $E_{1/2}$: $\lambda_{\text{max,abs}} = 14.53275 - 10.95 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.92429$.

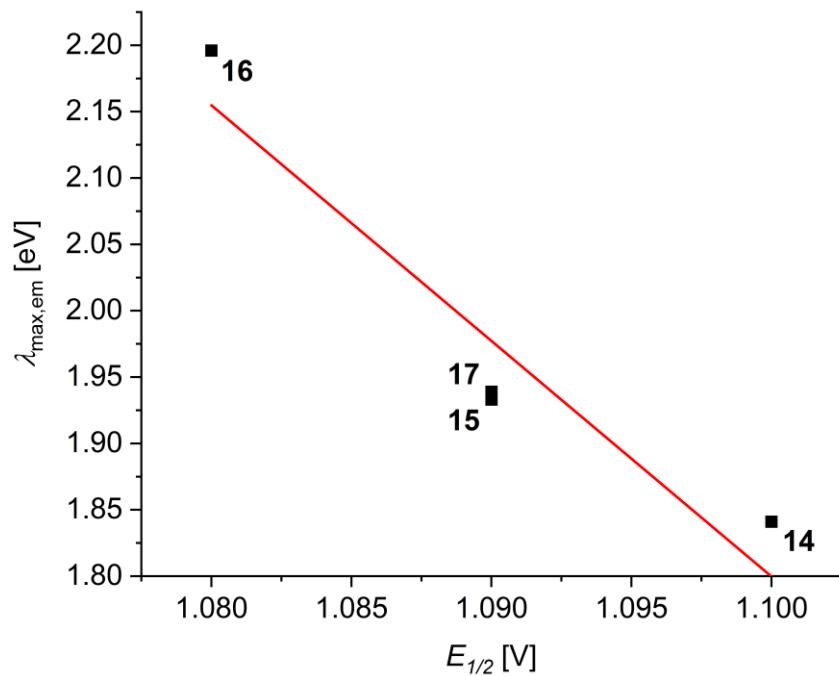


Figure S2. Correlation $\lambda_{\text{max,em}}$ vs $E_{1/2}$: $\lambda_{\text{max,em}} = 21.32475 - 17.75 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.90228$.

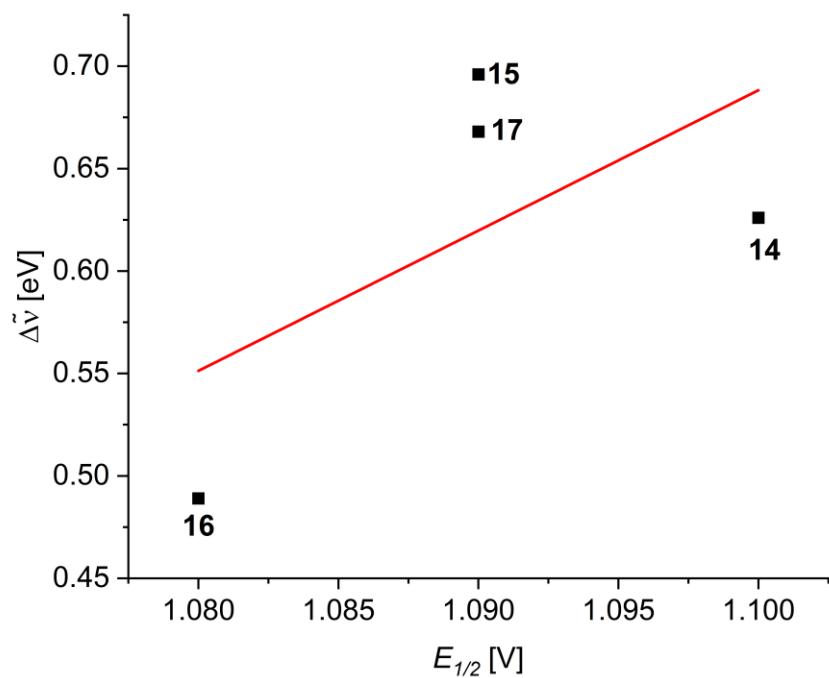


Figure S3. Correlation $\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = -6.84675 - 6.85 \cdot E_{1/2}$ [eV]; $r^2 = 0.37127$.

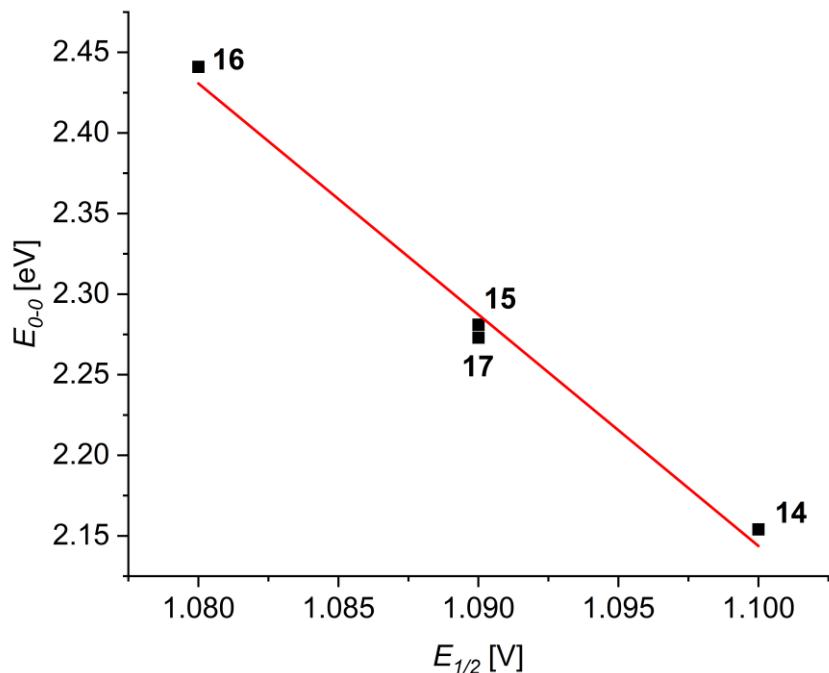
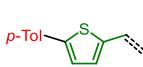
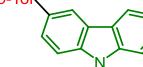
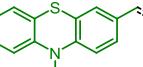
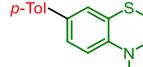
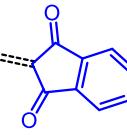
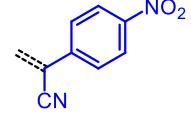


Figure S4. Correlation E_{00} vs $E_{1/2}$: $E_{00} = 17.92875 - 14.35 \cdot E_{1/2}$ [eV]; $r^2 = 0.98914$.

4.2. Correlations of Consanguineous Acceptor Series

Table S7. Selected electronic properties of merocyanine series **9**, **11**, **12**, and **14-17** employed in the correlation analyses.

Donor					
Acceptor	9a, 9b, 9d, 9e	11a, 11c, 11d, 11e	14-17	12a, 12c, 12e, 12f	
	$E_{1/2}$ [V]	$\lambda_{\text{max,abs}}$ [eV]	$\lambda_{\text{max,em}}$ [eV]	$\Delta \tilde{\nu}$ [eV]	E_{0-0} [eV]
	9a 1.66	2.752	2.414	0.337	2.583
	11a 1.44	2.740	2.359	0.380	2.549
	12a 1.05	2.575	1.895	0.680	2.235
	15 1.09	2.629	1.933	0.696	2.281
	9b 1.76	2.758	2.419	0.339	2.588
	11c 1.46	2.675	2.212	0.462	2.443
	12c 1.05	2.424	1.812	0.612	2.118
	14 1.10	2.467	1.841	0.626	2.154
	9d 1.61	2.948	2.580	0.368	2.764
	11d 1.45	2.899	2.359	0.540	2.629
	12e 1.05	2.548	1.945	0.603	2.246
	17 1.09	2.607	1.939	0.668	2.273
	9e 1.71	3.207	2.364	0.843	2.785
	11e 1.44	2.879	2.224	0.655	2.552
	12f 1.03	2.629	2.140	0.490	2.384
	16 1.08	2.686	2.196	0.489	2.441

For linear correlation analyses of consanguineous acceptor series the corresponding optical parameters (in eV) were plotted against the first oxidation potential $E_{1/2}$ (in V). The goodness of fit is expressed by the quadratic linear correlation coefficient r^2 (see Figures S5-S20).

4.2.1. Correlations of 3-Methyl-4-oxo-2-thioxothiazolidin-5-ylidene Merocyanines

$\lambda_{\text{max,abs}}$ vs $E_{1/2}$: $\lambda_{\text{max,abs}} = 2.30772 + 0.27943 \cdot E_{1/2}$ [eV]; $r^2 = 0.89872$.

$\lambda_{\text{max,em}}$ vs $E_{1/2}$: $\lambda_{\text{max,em}} = 0.95076 + 0.91572 \cdot E_{1/2}$ [eV]; $r^2 = 0.95763$.

$\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = 1.35696 - 0.63628 \cdot E_{1/2}$ [eV]; $r^2 = 0.94385$.

E_{00} vs $E_{1/2}$: $E_{00} = 1.62924 + 0.59758 \cdot E_{1/2}$ [eV]; $r^2 = 0.94309$.

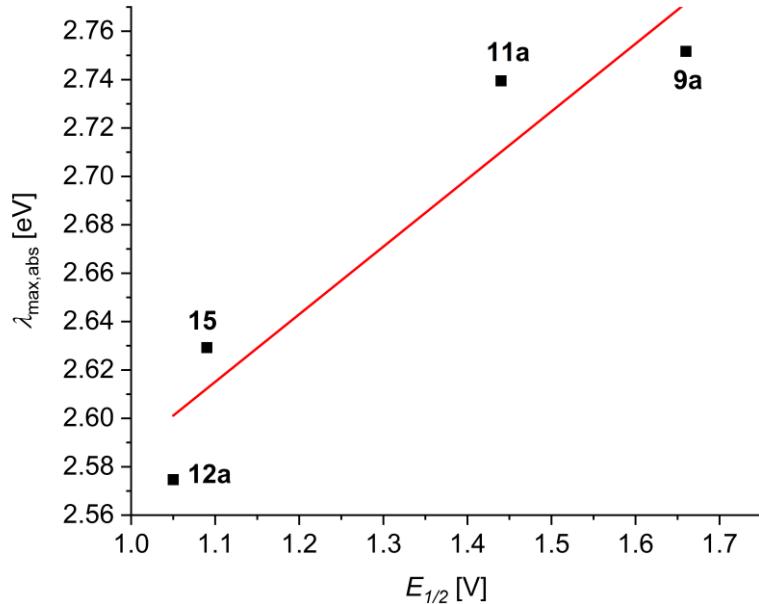


Figure S5. Correlation $\lambda_{\text{max,abs}}$ vs $E_{1/2}$: $\lambda_{\text{max,abs}} = 2.30772 + 0.27943 \cdot E_{1/2}$ [eV]; $r^2 = 0.89872$.

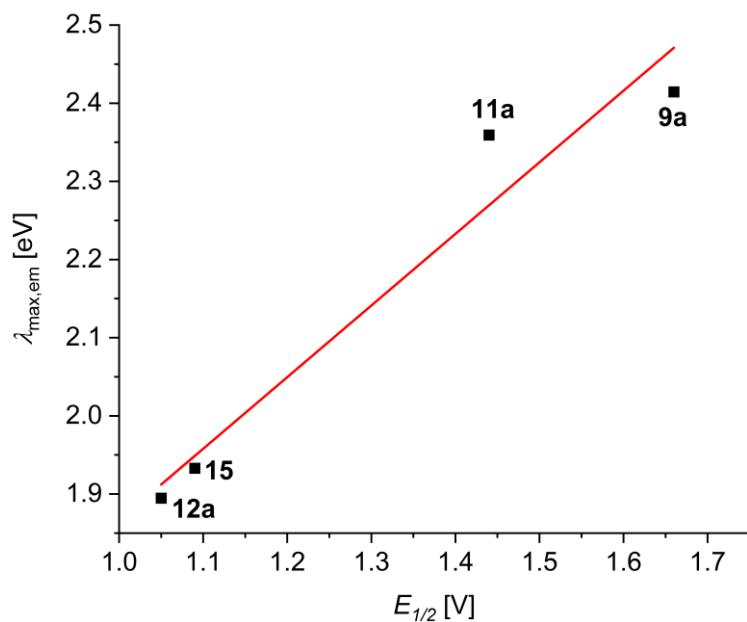


Figure S6. Correlation $\lambda_{\text{max,em}}$ vs $E_{1/2}$: $\lambda_{\text{max,em}} = 0.95076 + 0.91572 \cdot E_{1/2}$ [eV]; $r^2 = 0.95763$.

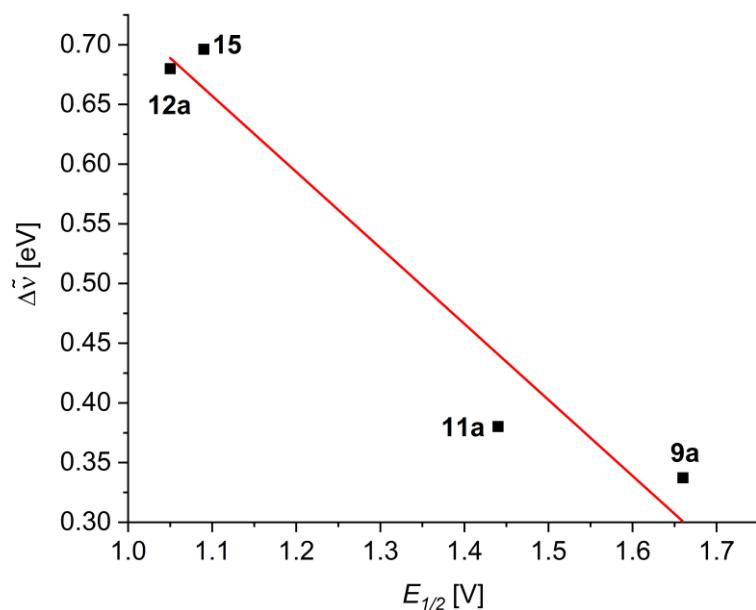


Figure S7. Correlation $\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = 1.35696 - 0.63628 \cdot E_{1/2}$ [eV]; $r^2 = 0.94385$.

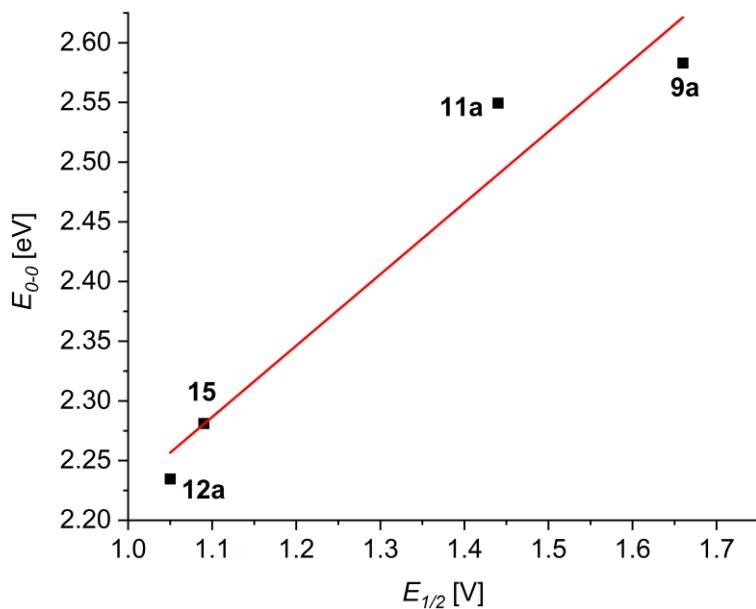


Figure S8. Correlation E_{00} vs $E_{1/2}$: $E_{00} = 1.62924 + 0.59758 \cdot E_{1/2}$ [eV]; $r^2 = 0.94309$.

4.2.2. Correlations of 1,3-Dioxo-1,3-dihydro-2*H*-inden-2-ylidene Merocyanines

$\lambda_{\max,\text{abs}}$ vs $E_{1/2}$: $\lambda_{\max,\text{abs}} = 1.94136 + 0.47633 \cdot E_{1/2}$ [eV]; $r^2 = 0.97137$.

$\lambda_{\max,\text{em}}$ vs $E_{1/2}$: $\lambda_{\max,\text{em}} = 0.88599 + 0.88272 \cdot E_{1/2}$ [eV]; $r^2 = 0.9921$.

$\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = 1.05538 - 0.40638 \cdot E_{1/2}$ [eV]; $r^2 = 0.98946$.

E_{00} vs $E_{1/2}$: $E_{00} = 1.41368 + 0.67953 \cdot E_{1/2}$ [eV]; $r^2 = 0.98716$.

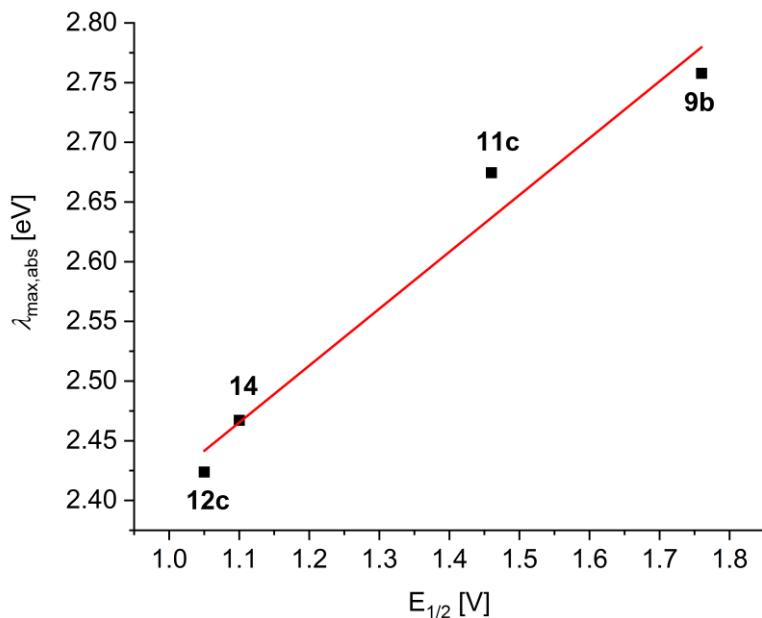


Figure S9. Correlation $\lambda_{\max,\text{abs}}$ vs $E_{1/2}$: $\lambda_{\max,\text{abs}} = 1.94136 + 0.47633 \cdot E_{1/2}$ [eV]; $r^2 = 0.97137$.

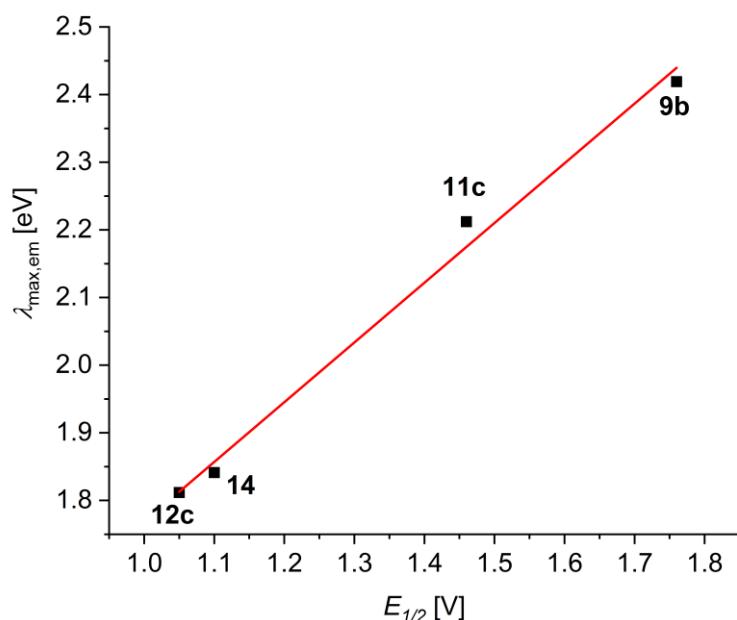


Figure S10. Correlation $\lambda_{\max,\text{em}}$ vs $E_{1/2}$: $\lambda_{\max,\text{em}} = 0.88599 + 0.88272 \cdot E_{1/2}$ [eV]; $r^2 = 0.9921$.

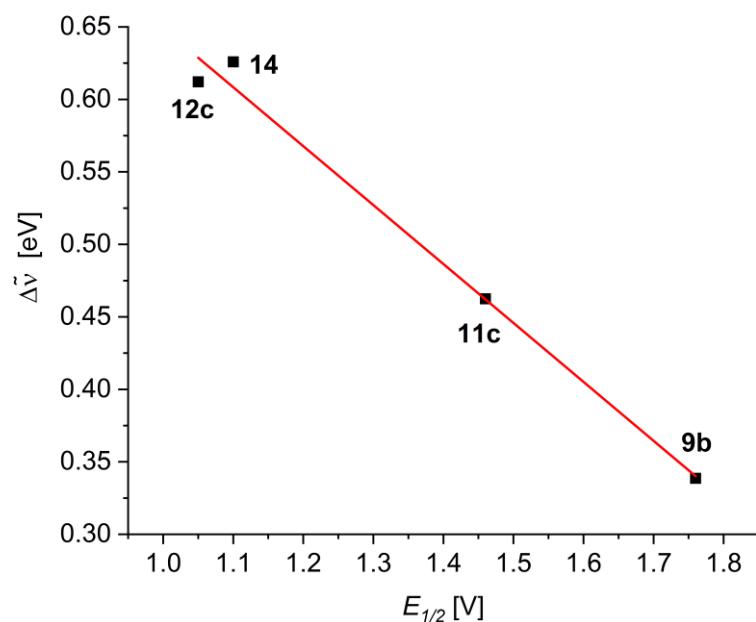


Figure S11. Correlation $\tilde{\Delta\nu}$ vs $E_{1/2}$: $\tilde{\Delta\nu} = 1.05538 - 0.40638 \cdot E_{1/2}$ [eV]; $r^2 = 0.98946$.

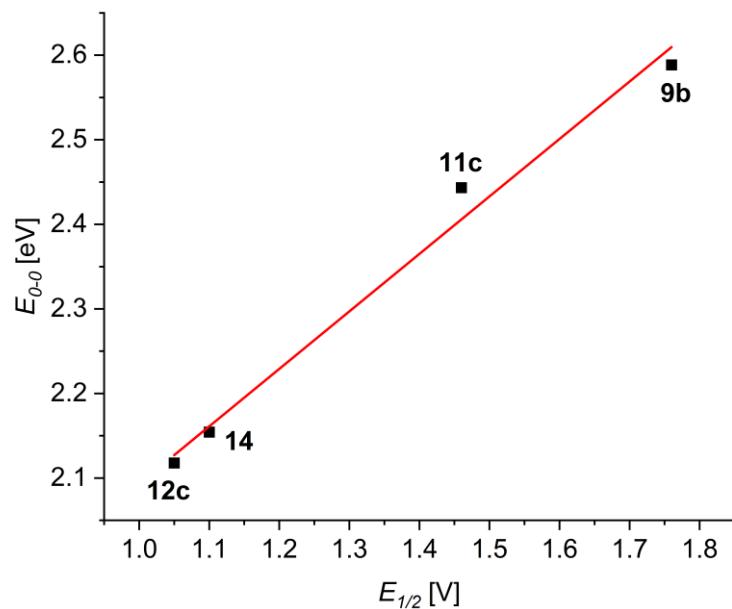


Figure S12. Correlation E_{00} vs $E_{1/2}$: $E_{00} = 1.41368 + 0.67953 \cdot E_{1/2}$ [eV]; $r^2 = 0.98716$.

4.2.3. Correlations of 3-Methyl-5-oxo-1-phenyl-1,5-dihydro-4*H*-pyrazol-4-ylidene Merocyanines

$\lambda_{\max,\text{abs}}$ vs $E_{1/2}$: $\lambda_{\max,\text{abs}} = 1.80299 + 0.72898 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.97638$.

$\lambda_{\max,\text{em}}$ vs $E_{1/2}$: $\lambda_{\max,\text{em}} = 0.70372 + 1.15551 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.99331$.

$\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = 1.09927 - 0.42653 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.81969$.

E_{00} vs $E_{1/2}$: $E_{00} = 1.25336 + 0.94225 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.99896$.

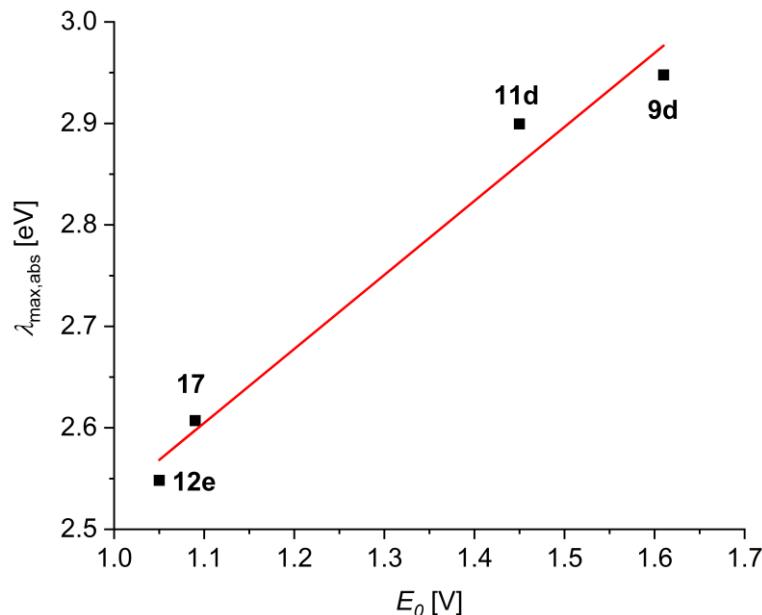


Figure S13. Correlation $\lambda_{\max,\text{abs}}$ vs $E_{1/2}$: $\lambda_{\max,\text{abs}} = 1.80299 + 0.72898 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.97638$.

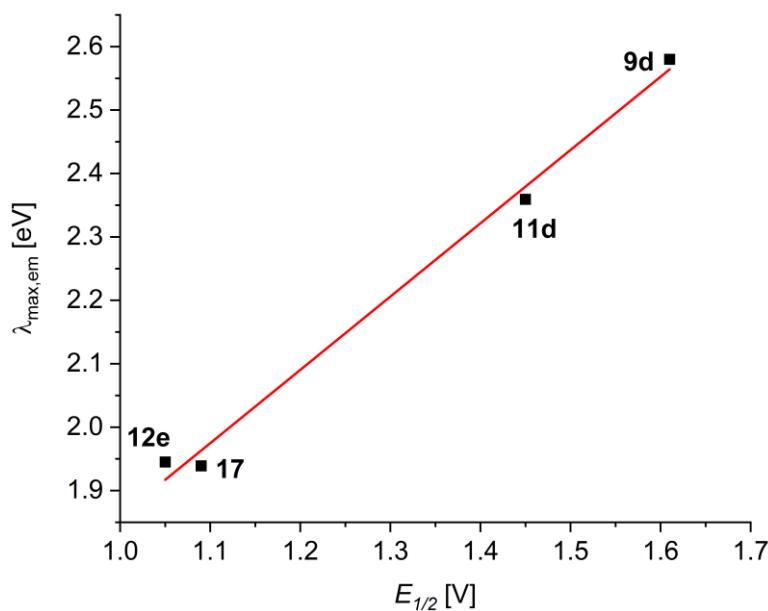


Figure S14. Correlation $\lambda_{\max,\text{em}}$ vs $E_{1/2}$: $\lambda_{\max,\text{em}} = 0.70372 + 1.15551 \cdot E_{1/2} [\text{eV}]$; $r^2 = 0.99331$.

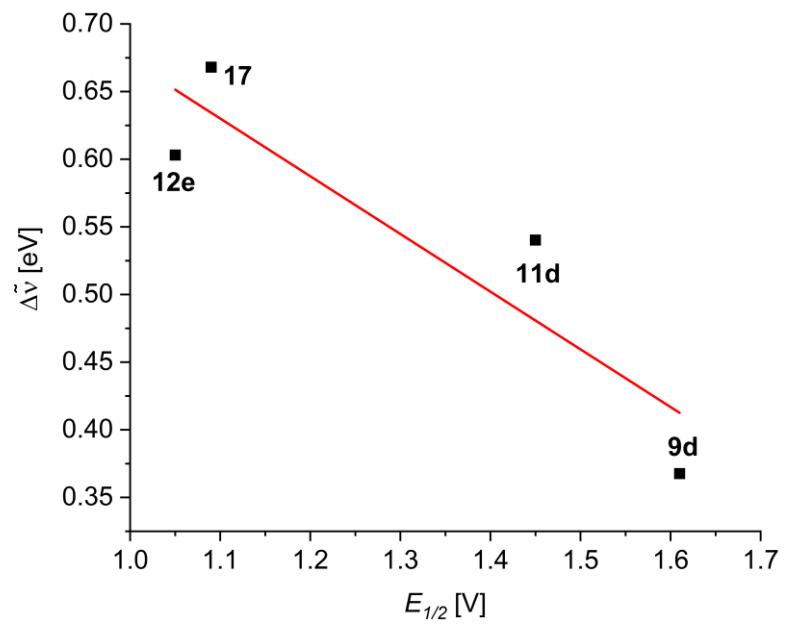


Figure S15. Correlation $\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = 1.09927 - 0.42653 \cdot E_{1/2}$ [eV]; $r^2 = 0.81969$.

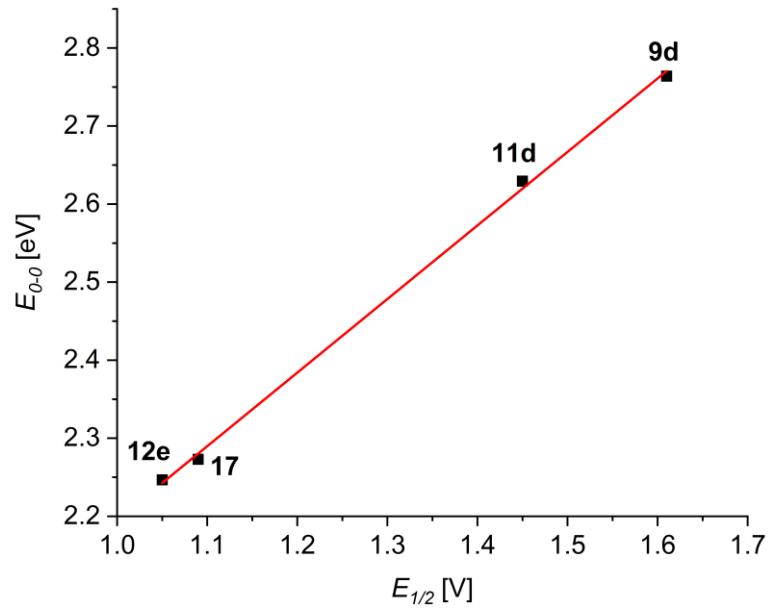


Figure S16. Correlation E_{00} vs $E_{1/2}$: $E_{00} = 1.25336 + 0.94225 \cdot E_{1/2}$ [eV]; $r^2 = 0.99896$.

4.2.4. Correlations of Cyano(4-nitrophenyl)-methylene Merocyanines

$\lambda_{\text{max,abs}}$ vs $E_{1/2}$: $\lambda_{\text{max,abs}} = 1.80299 + 0.79843 \cdot E_{1/2}$ [eV]; $r^2 = 0.96424$.

$\lambda_{\text{max,em}}$ vs $E_{1/2}$: $\lambda_{\text{max,em}} = 1.86505 + 0.27828 \cdot E_{1/2}$ [eV]; $r^2 = 0.87637$.

$\Delta\tilde{\nu}$ vs $E_{1/2}$: $\Delta\tilde{\nu} = -0.06462 + 0.52015 \cdot E_{1/2}$ [eV]; $r^2 = 0.98155$.

E_{00} vs $E_{1/2}$: $E_{00} = 1.83274 + 0.53835 \cdot E_{1/2}$ [eV]; $r^2 = 0.94765$.

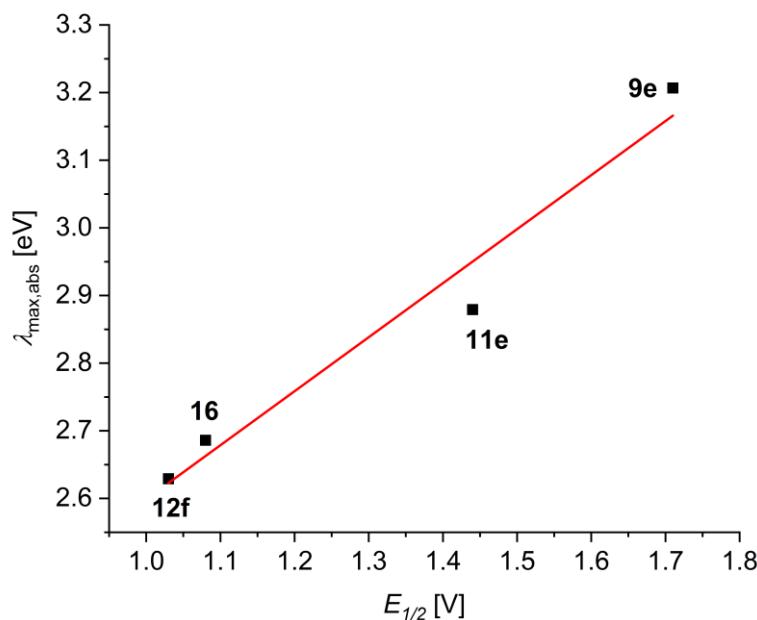


Figure S17. Correlation $\lambda_{\text{max,abs}}$ vs $E_{1/2}$: $\lambda_{\text{max,abs}} = 1.80299 + 0.79843 \cdot E_{1/2}$ [eV]; $r^2 = 0.96424$.

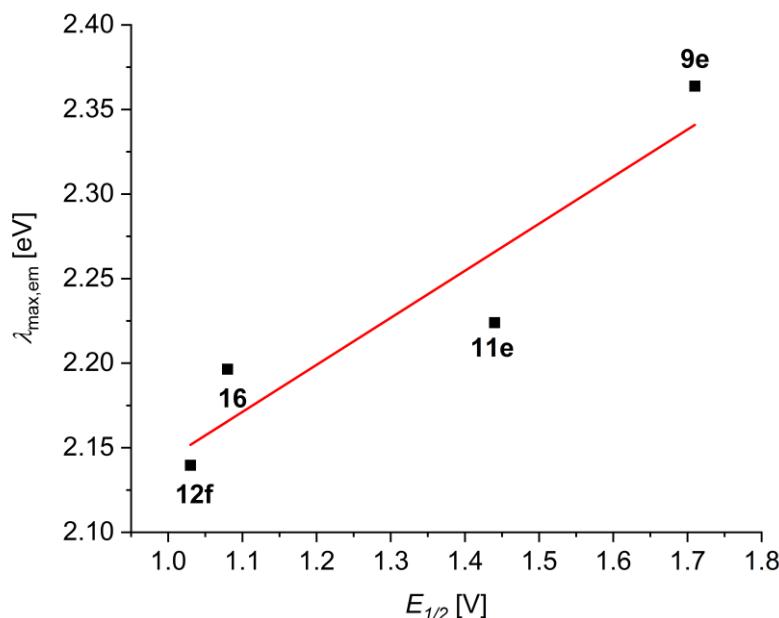


Figure S18. Correlation $\lambda_{\text{max,em}}$ vs $E_{1/2}$: $\lambda_{\text{max,em}} = 1.86505 + 0.27828 \cdot E_{1/2}$ [eV]; $r^2 = 0.87637$.

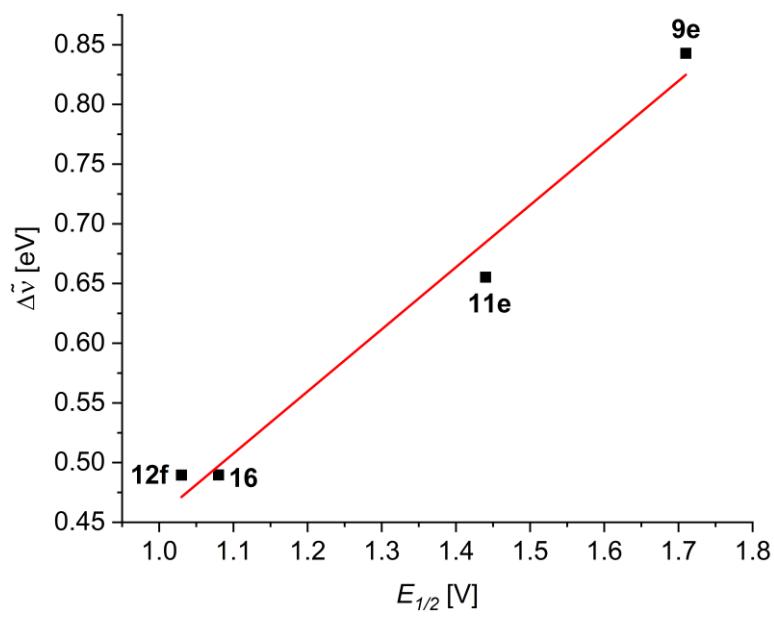


Figure S19. Correlation $\tilde{\Delta\nu}$ vs $E_{1/2}$: $\tilde{\Delta\nu} = -0.06462 + 0.52015 \cdot E_{1/2}$ [eV]; $r^2 = 0.98155$.

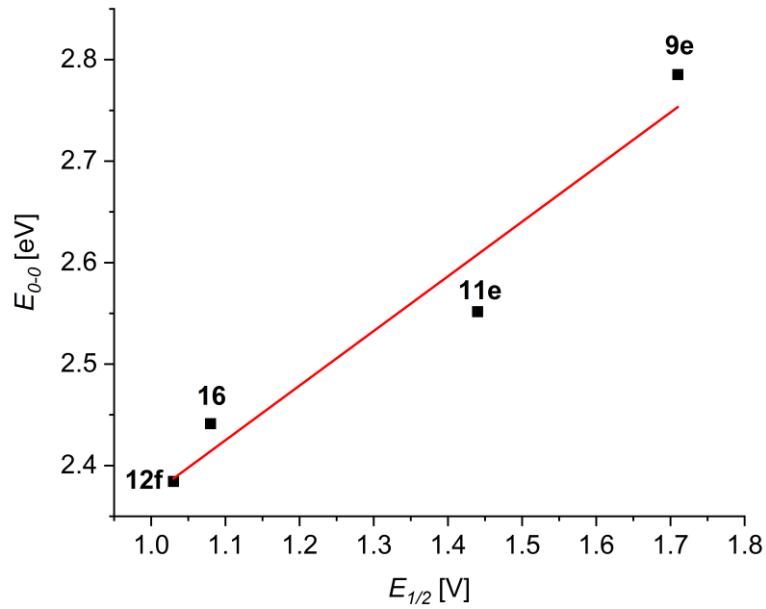
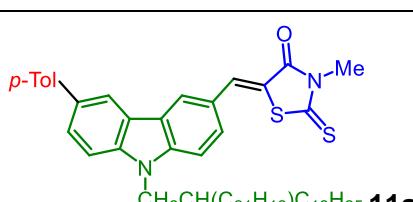
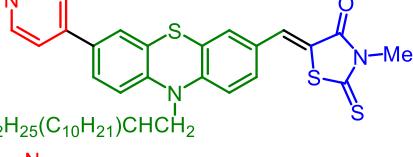
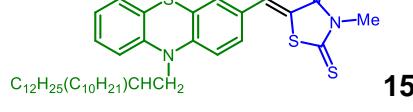
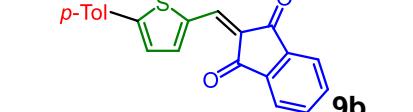


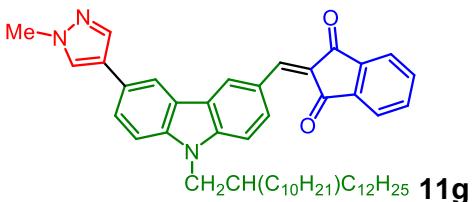
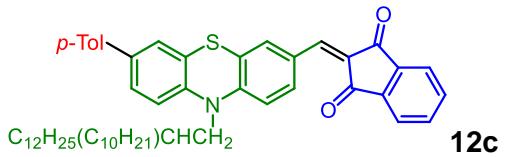
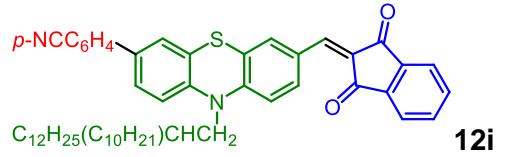
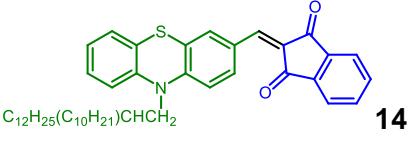
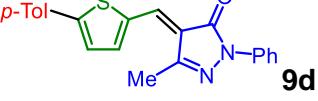
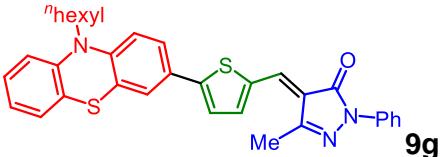
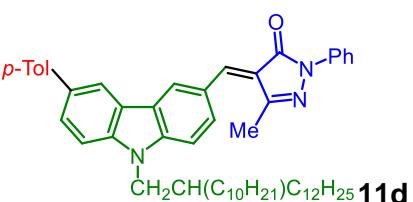
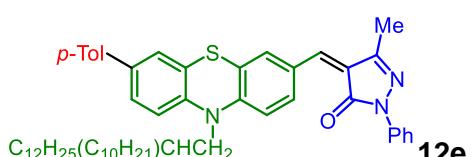
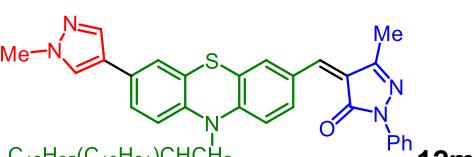
Figure S20. Correlation E_{00} vs $E_{1/2}$: $E_{00} = 1.83274 + 0.53835 \cdot E_{1/2}$ [eV]; $r^2 = 0.94765$.

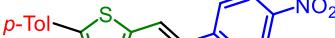
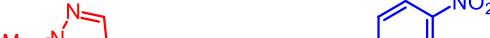
4.3. Linear and Planar Correlations with 24 Compounds

For linear correlation analysis the optical band gaps E_{0-0} (in eV) were plotted against the first oxidation potential $E_{1/2}$ (in V). The goodness of fit is expressed by the quadratic linear correlation coefficient r^2 (see Figure S21). For a two parameter planar correlation analysis the optical band gaps E_{0-0} (in eV) were plotted against the first oxidation potential $E_{1/2}$ (in V) and the emission maxima $\lambda_{\text{max,em}}$ [in eV]. The goodness of fit is expressed by the quadratic linear correlation coefficient r^2 (see Figure S22).

Table S8. Selected electronic properties of 24 merocyanines the series **9**, **11**, **12**, and **14-17** employed in the correlation analysis.

Compound	$E_{1/2}$ [V]	$\lambda_{\text{max,em}}$ [eV]	E_{0-0} [eV]
 11a	1.44	2.419	2.549
 12a	1.05	2.212	2.235
 12n	1.03	2.129	2.254
 12j	1.17	1.812	2.290
 12k	1.01	1.858	2.222
 15	1.09	1.841	2.281
 9b	1.76	2.359	2.588

	1.46	1.895	2.443
	1.34	1.939	2.393
	1.05	1.951	2.118
	1.13	1.880	2.160
	1.10	1.933	2.154
	1.61	2.364	2.764
	0.93	2.224	2.294
	1.45	2.140	2.629
	1.05	2.140	2.246
	1.00	1.889	2.279

	1.09	2.196	2.273	
	1.71	2.580	2.785	
	1.44	2.055	2.552	
	1.03	2.359	2.384	
	1.03	1.945	2.379	
	0.85	2.021	2.195	
	1.08	1.939	2.441	

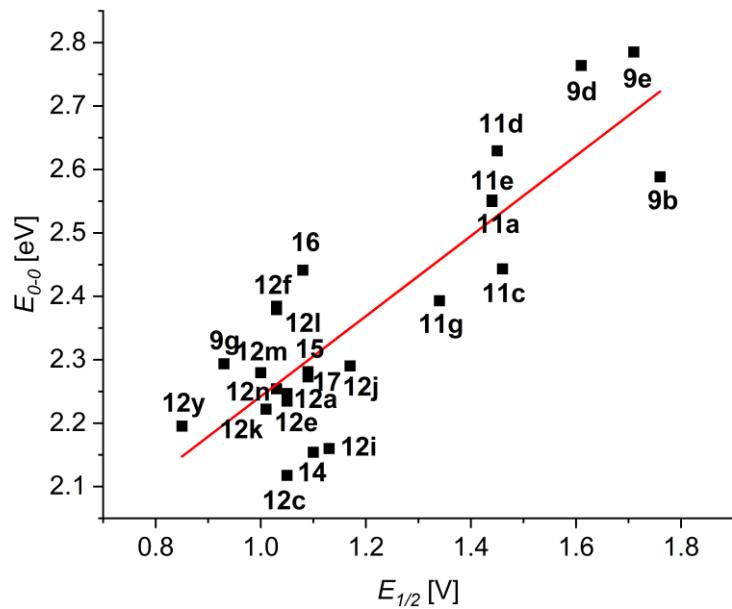


Figure S21. Correlation E_{0-0} vs $E_{1/2}$: $E_{0-0} = 1.60975 + 0.63246 \cdot E_{1/2}$ [eV]; $r^2 = 0.73381$.

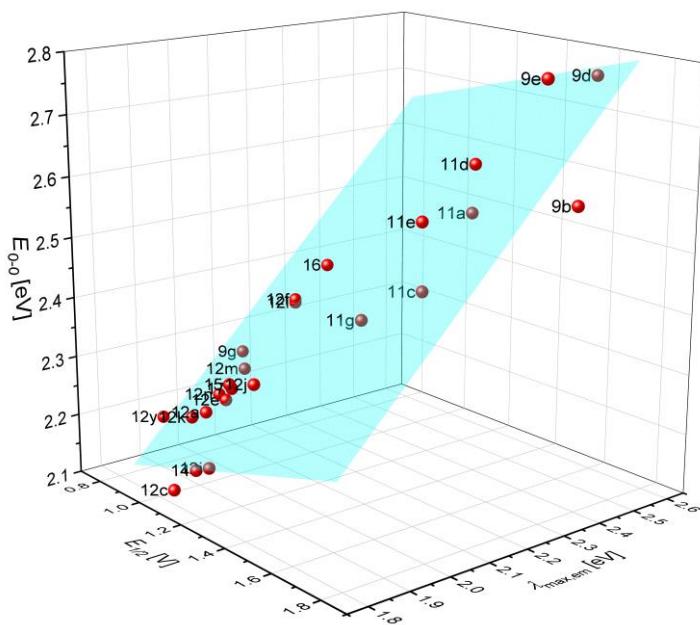


Figure S22. Correlation E_{0-0} vs $E_{1/2}$ and $\lambda_{\text{max,em}}$: $E_{0-0} = 0.147 \cdot E_{1/2} + 0.7019 \cdot \lambda_{\text{max,em}} + 0.7296$; $r^2 = 0.93504$.

5. References

- ¹ a) Krämer, C. S.; Zimmermann, T. J.; Sailer, M.; Müller, T. J. J. Syntheses of Phenothiazinyl Boronic Acid Derivatives - Suitable Starting Points for the Construction of Redox Active Materials. *Synthesis* **2002**, 1163-1170. DOI: 10.1055/s-2002-32527 b) Franz, A. W.; Müller, S205

- T. J. J. Facile Synthesis of Functionalized (Oligo)Phenothiazines via One-Pot Bromine-Lithium Exchange-Borylation-Suzuki-Coupling (BLEBS). *Synthesis* **2008**, 1121-1125. DOI: 10.1055/s-2008-1032118
- ² a) Muschelknautz, C.; Sailer, M.; Müller, T. J. J. Sequential Electrophilic Trapping Reactions for the Desymmetrization of Dilithio(hetero)arenes. *Synlett* **2008**, 845-848. DOI: 10.1055/s-2008-1042911 b) Dostert, C.; Czajkowski, D.; Müller, T. J. J. 2,6-Difunctionalization of N-Substituted Dithienothiazines via Dilithiation. *Synlett* **2014**, 25, 371-374. DOI: 10.1055/s-0033-1340307 c) Dostert, C.; Müller, T. J. J. A one-pot dilithiation–lithium–zinc exchange–Negishi coupling approach to 2,6-di(hetero)aryl substituted dithienothiazines – a novel class of electronically fine-tunable redox systems. *Org. Chem. Front.* **2015**, 2, 481-491. DOI: 10.1039/C5QO00046G
- ³ Meyer, T.; Ogermann, D.; Pankrath, A.; Kleinermanns, K.; Müller, T. J. J. Phenothiazinyl Rhodanylidene Merocyanines for Dye-Sensitized Solar Cells. *J. Org. Chem.* **2012**, 77, 3704-3715. DOI: 10.1021/jo202608w
- ⁴ Kofler, L. Identifizierung organischer Substanzen. *Sci. Pharm.* **1966**, 2, 147-166.