Supplementary data

New advanced liquid crystalline materials bearing bis azomethine as central spacer

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1. Materials

Hexadecanoyl chloride, decanoyl chloride, hexanoyl chloride, 4-hydroxybenzaldehyde, and hydrazine hydrate were purchased from Sigma Aldrich (Germany). 4-dimethylaminopyridine (DMAP), Dichloromethane, and triethylamine were purchased from Aldrich (Wisconsin, USA).

2. Synthesis of 4,4'-((1E,1'E)-hydrazine-1,2 diylidenebis(methanylylidene))diphenol (**A**)

An ethanolic solution of p-hydroxy benzaldehyde (1.00 g, 8.20 mmol) was added dropwise to ethanolic solution of hydrazine monohydrate (0.200 g, 4.10 mmol) and resulting mixture was refluxed for 30 min. and then kept under stirring for 3-4 hours at room temperature till the starting materials are consumed, as indicated from TLC. A yellow precipitate formed, was washed with ethanol and diethyl ether and dried under vacuum.

3. Synthesis of ((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))bis(4,1-phenylene) dialkanoate, **I*n***

To a solution of the diphenol, 4,4'-((1E,1'E)-hydrazine-1,2 diylidenebis(methanylylidene))diphenol (**A**), 10 mmol in 30 mL of DCM, Triethylamine (Et3N) (20 mmol), dimethylaminopyridine (DMAP) (1 mmol) and the corresponding acyl chloride (12 mmol) were added at 0 °C and stirred. The reaction mixture was allowed to reach room temperature and was kept under stirring overnight at room temperature. The solvent was evaporated under reduced pressure, and the resultant oily residue dissolved in water and extracted with diethyl ether (3×30 mL). The combined organic phases were dried over anhydrous sodium sulfate (Na_2SO4) and filtered off and the solution evaporated till dryness under reduced pressure. Finally, purification by column chromatography afforded the desired liquid crystals, **I*n*.**

4,4'-((1E,1'E)-hydrazine-1,2 diylidenebis(methanylylidene))diphenol (**A**)

Yield: 93%; mp 107.0 °C, FTIR (ύ, cm^{-1}): 3400-3200 (OH), 2960, 2875 (CH_2 stretching), 1590 (C=N), 1610 (C=C). ^{1}H NMR (400 MHz, DMSO) δ 8.55 (s, 2H, CH=N), 7.70 (d, *J* = 8.3 Hz, 4H, Ar-H), 6.87 (d, *J* = 8.2 Hz, 4H, Ar-H). ^{13}C NMR (101 MHz, DMSO) δ 160.87 (CH), 160.75 (C), 130.58 (CH), 125.58 (C), 116.22 (CH). Elemental analyses: Found (Calc.): C, 69.99 (70.12); H, 5.03 (5.25); N, 11.66 (11.76).

2.2. ((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))bis(4,1-phenylene) dihexanoate, **I*5***

Yield: 94%; mp 95.0 °C, FTIR (ύ, cm^{-1}): 2950, 2885 (CH_2 stretching), 1763 (C=O), 1592 (C=N), 1600 (C=C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 2H, CH=N), 7.87 (d, *J* = 8.6 Hz, 4H, Ar-H), 7.20 (d, *J* = 8.5 Hz, 4H, Ar-H), 2.59 (t, *J* = 7.5 Hz, 4H, 2 CH_2CO), 1.90 – 1.64 (m, 4H, $2CH_2$), 1.41 (m, 8H, $4CH_2$), 0.95 (t, *J* = 7.0 Hz, 6H, $2CH_3$).^{13}C NMR (101 MHz, $CDCl_3$) δ 171.98 (CO), 161.12 (CH), 153.03 (C), 131.60 (C), 129.75 (CH), 122.10 (CH), 45.88 (CH_2), 34.38 (CH_2), 31.25 (CH_2), 24.57 (CH_2), 22.33 (CH_2), 13.93 (CH_3). Elemental analyses: Found (Calc.): C, 71.53 (71.36); H, 7.39 (7.18); N, 6.42 (6.53).

((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))bis(4,1-phenylene) didecanoate**, I*9***

Yield: 89 %; mp 104.0 °C, FTIR (ύ, cm^{-1}): 2970, 2870 (CH_2 stretching), 1765 (C=O), 1595 (C=N), 1610 (C=C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 2H, CH=N),

7.87 (d, *J* = 8.6 Hz, 4H, Ar-H), 7.20 (d, *J* = 8.5 Hz, 4H, Ar-H), 2.59 (t, *J* = 7.5 Hz, 4H, $2CH_2$), 2.40 (t, *J* = 7.5 Hz, 4H, $2CH_2$), 1.82 – 1.73 (m, 4H, $2CH_2$), 1.63 – 1.52 (m, 6H, $3CH_2$), 1.28 (s, 14H, $7CH_2$), 0.93 – 0.87 (m, 6H, $2CH_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.00 (CO), 161.13 (CH), 153.03 (C), 131.59 (C), 129.75 (CH), 122.10 (CH), 116.05 (CH), 42.83 (CH_2), 34.42 (CH_2), 31.87 (CH_2), 29.44 (CH_2), 29.43 (CH_2), 29.27 (CH_2), 29.26 (CH_2), 29.10 (CH_2), 24.89 (CH_2), 23.91 (CH_2), 22.67 (CH_2), 14.11(CH_3). Elemental analyses: Found (Calc.): C, 74.42 (74.38); H, 8.82 (9.10); N, 5.10 (5.25).

4. Characterization

Perkin-Elmer B25 (Perkin-Elmer, Inc., Shelton, CT USA) spectrophotometer was used for infrared spectra measurements. Varian EM 350L 400 MHz spectrometer (Oxford, UK) was used for recording ^{1}HNMR spectra with tetramethyl silane as internal standard in $CDCl_3$; the chemical shift values recorded as δ (ppm units). Thermo Scientific Flash 2000 CHS/O Elemental Analyzer, Milan, Italy was used for Elemental analyses. TA Instruments Co. (Q20 Differential Scanning Calorimeter, DSC; USA) was used for recording phase transitions. DSC calibration was carried using lead and indium melting temperature and enthalpy. Samples of 2–3 mg were used in aluminum pans for DSC investigation. The heating rate was 10°C/min in nitrogen gas as an inert atmosphere (30 ml/min). All transitions measured for the second heating scan. Transition temperatures for the prepared compounds were checked and phases identified by Polarized optical microscope (POM, Wild, Germany) attached with Mettler FP82HT hot stage. Absorption spectra of prepared films were recorded through Agilent Cary 5000 UV-Vis-NIR spectrophotometer. The steady state emission and time resolved decay spectra were recorded through Horiba delta flex TCSPC lifetime fluorometer by exciting the sample from Delta-diode 320 nm with peak width ±10 nm.

5. Computational Method

Gaussian 09 software [1] was used for DFT calculations for the studied compounds. DFT/B3LYP methods using 6-31G (*d,p*) basis set was selected for the calculations. The geometries were optimized by minimizing the energies with respect to all geometrical parameters without imposing any molecular symmetry constraints. The

structures of the optimized geometries had been drawn with Gauss View [2]. Also, calculations frequencies were carried out by the same level of theory. The frequency calculations showed that all structures were stationary points in the geometry optimization method with non-imaginary frequencies.

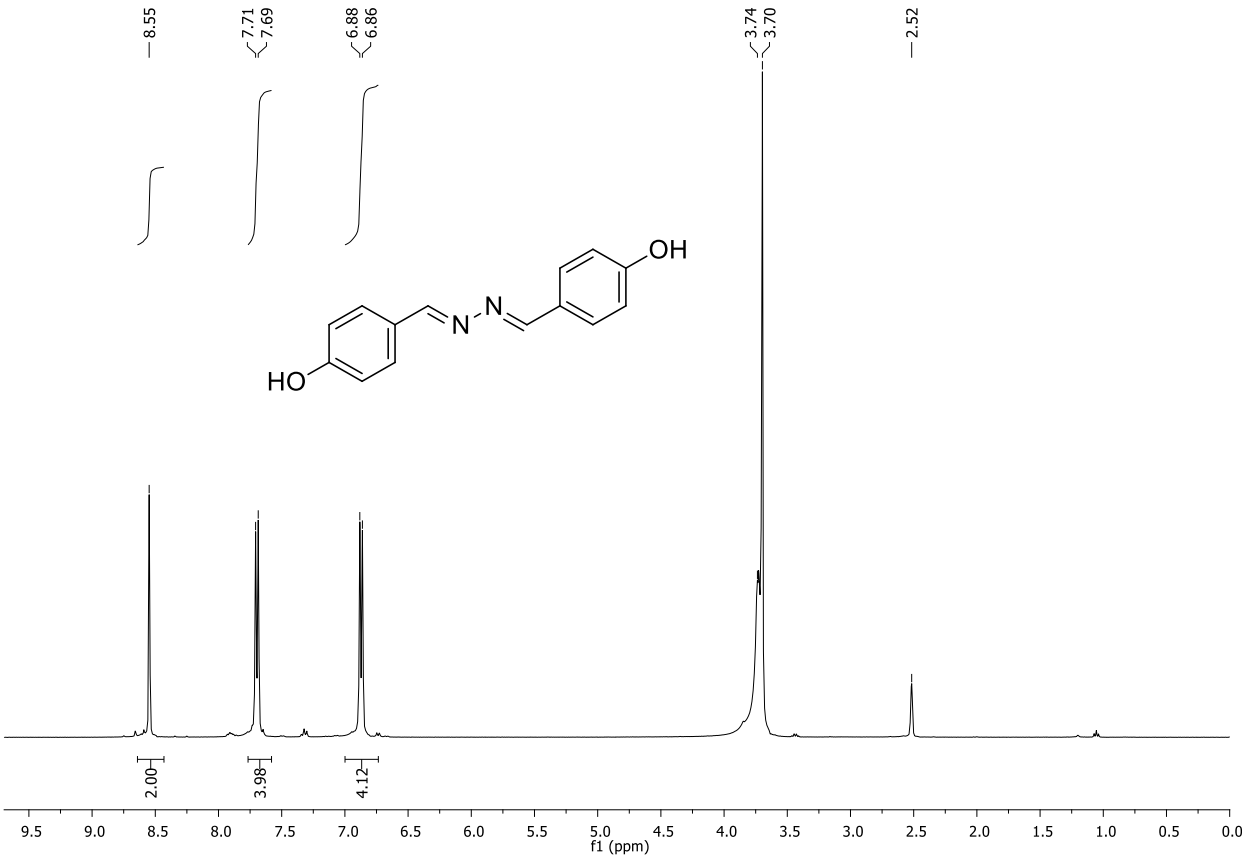


Figure S1. ^{1}H-NMR of 4,4'-((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))diphenol.

Figure S2. ^{13}C-NMR of 4,4'-((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))diphenol.

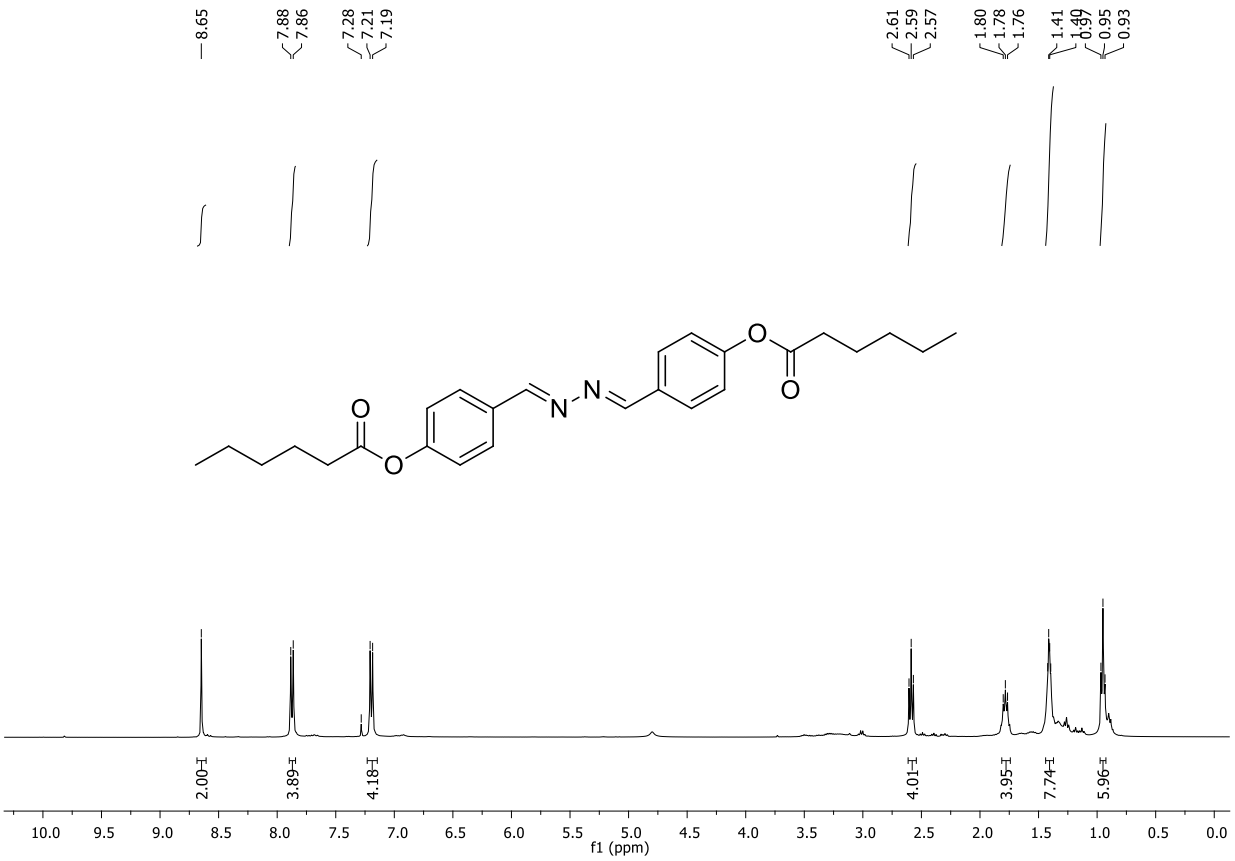


Figure S3. ^{1}H-NMR of ((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))bis(4,1-phenylene) dihexanoate.

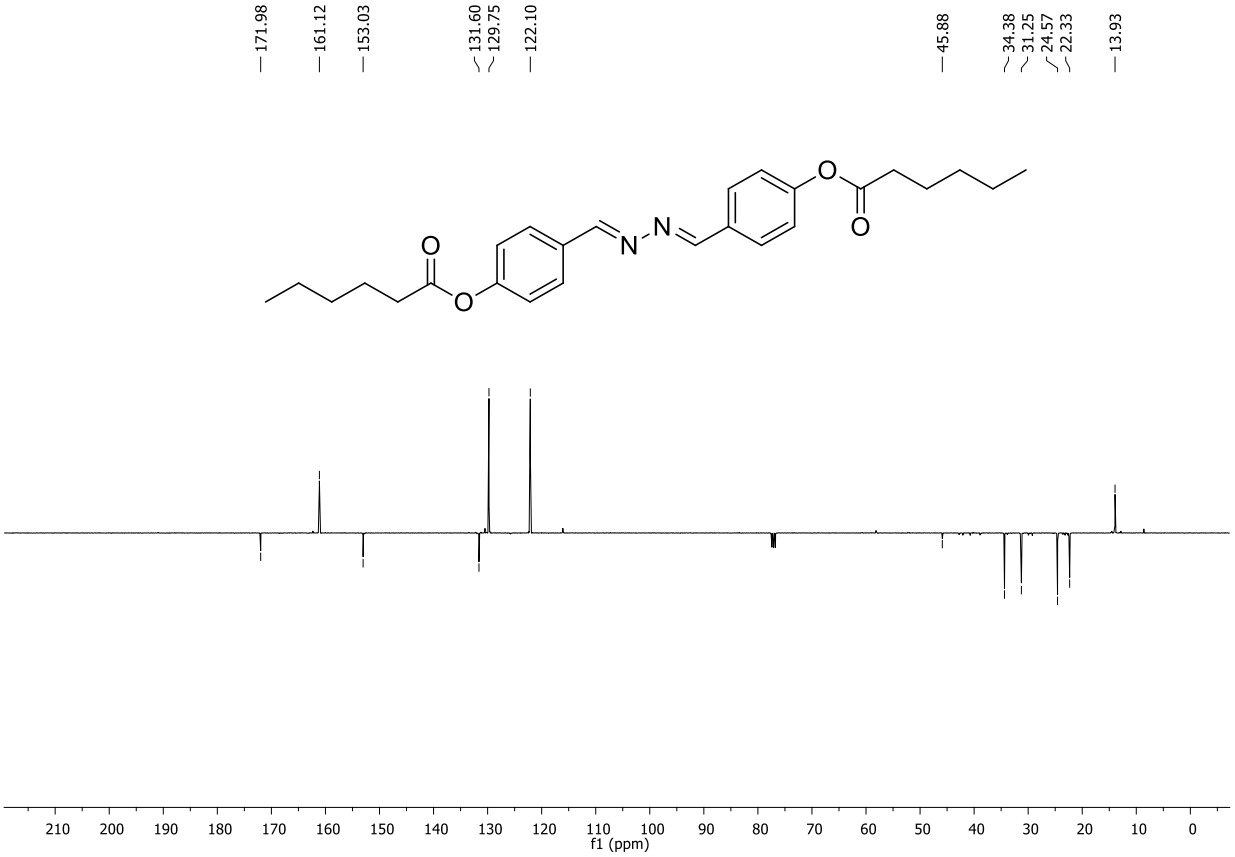


Figure S4. ^{13}C-NMR of ((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))bis(4,1-phenylene) dihexanoate.

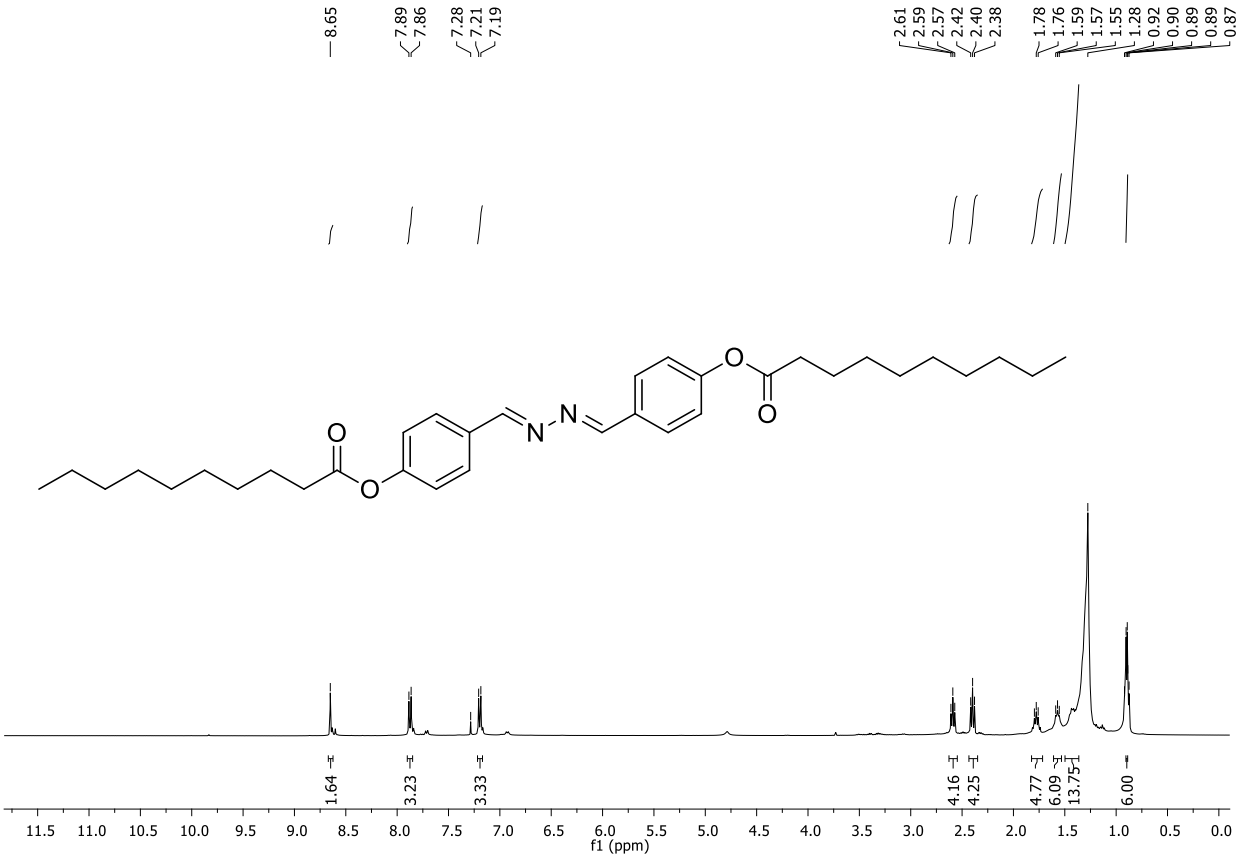


Figure S5. ^{1}H-NMR of ((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))bis(4,1-phenylene) bis(decanoate).

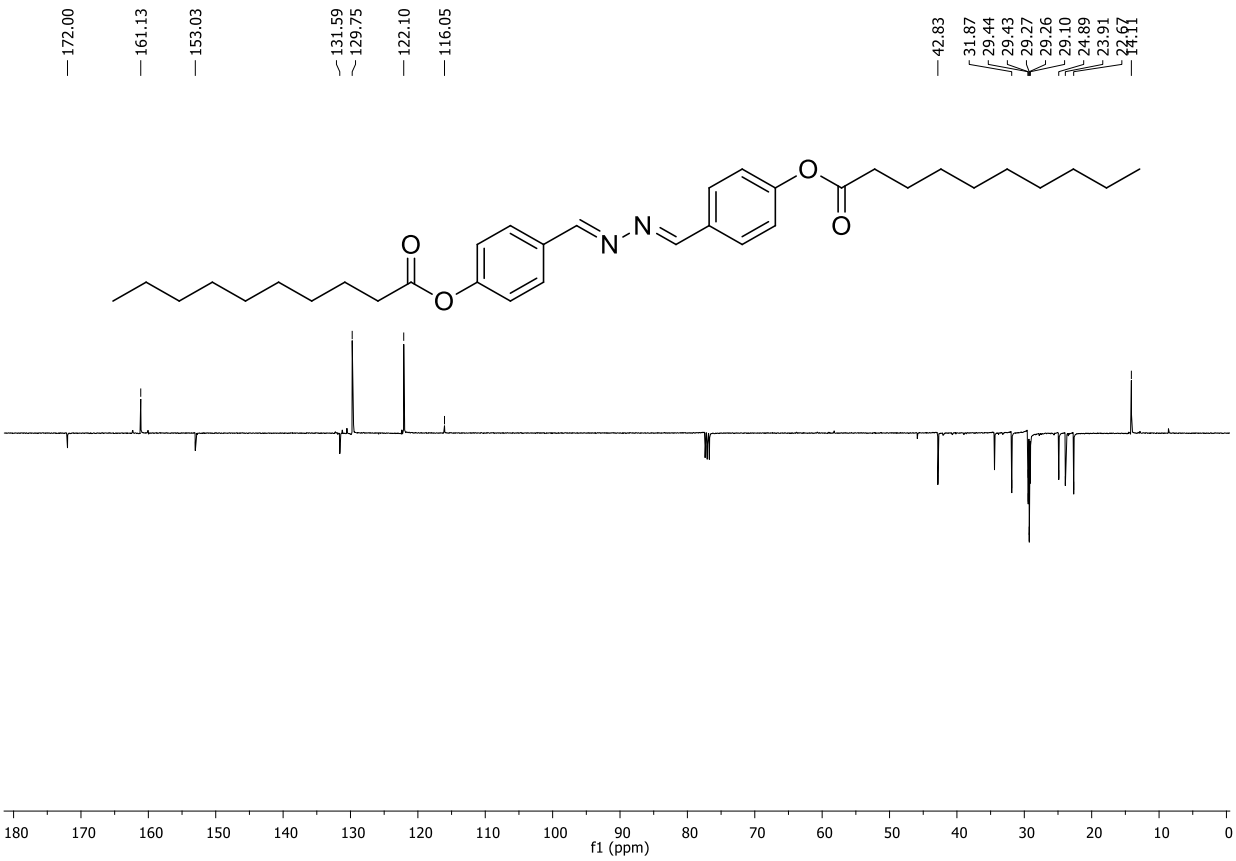


Figure S6. ^{13}C-NMR of ((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene))bis(4,1-phenylene) bis(decanoate).

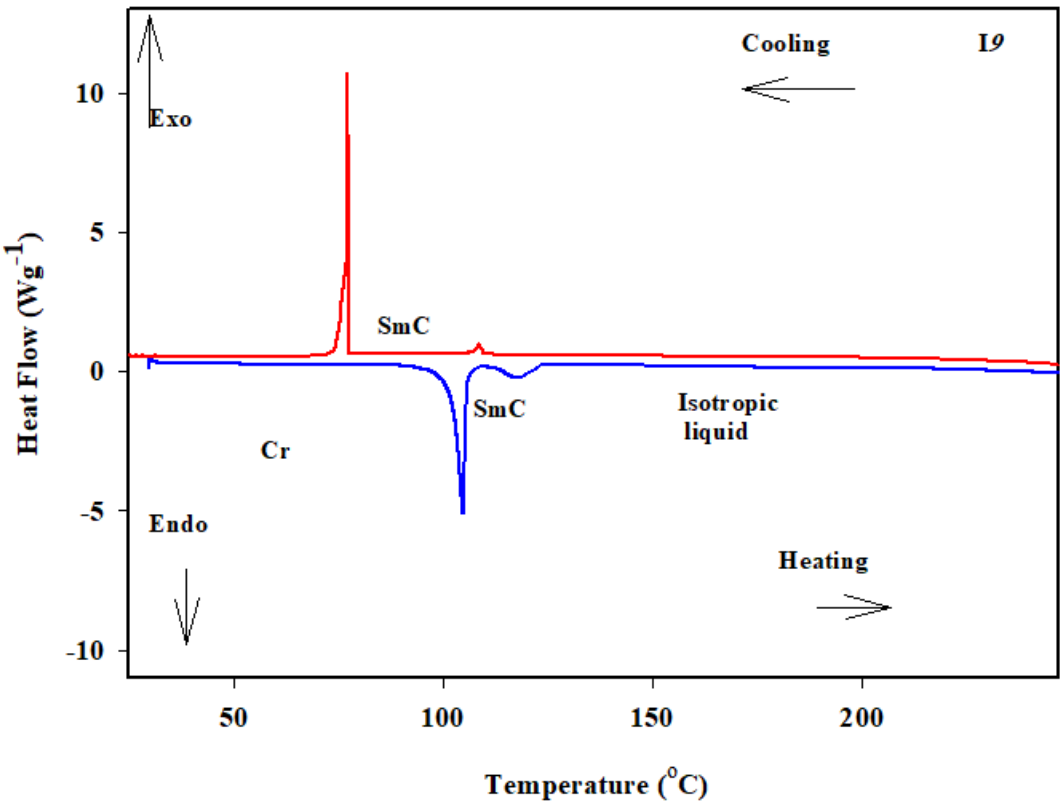


Figure S7. DSC cycles recorded from the second heating and cooling scan with heating rate 10°C/min of compound **I*9***.

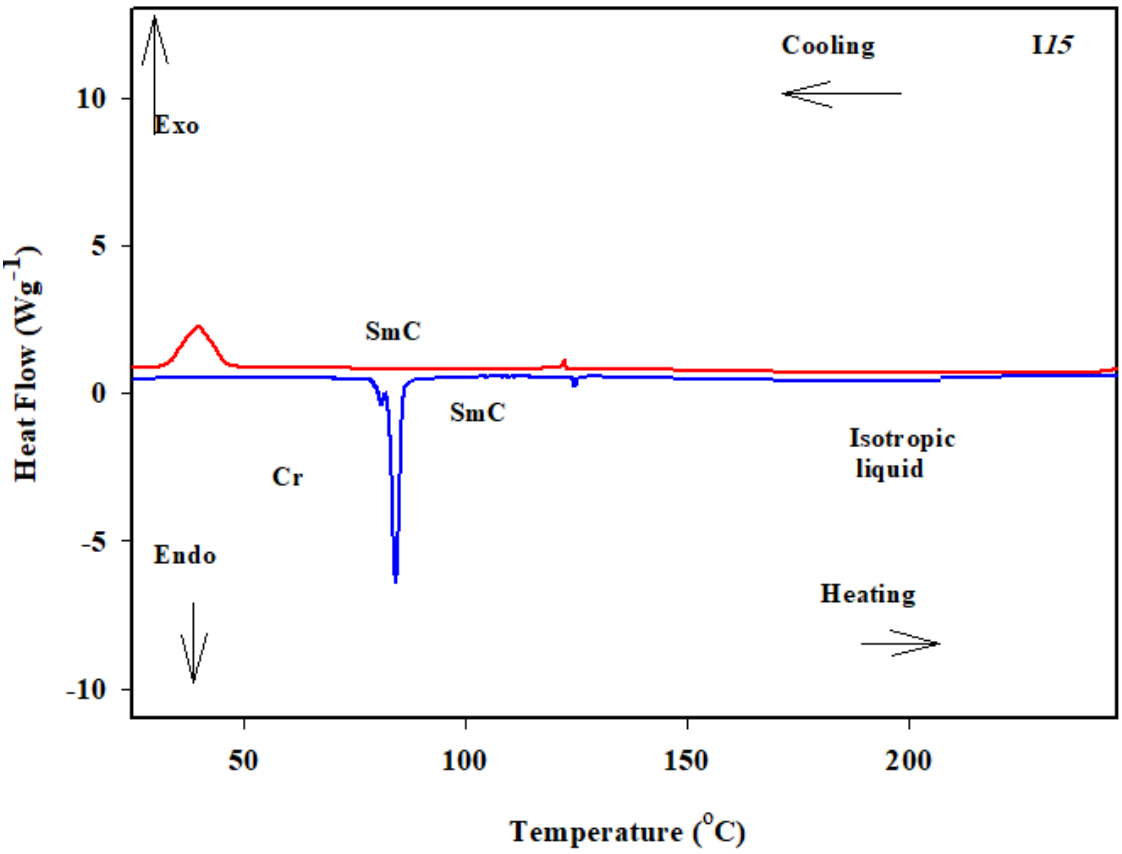
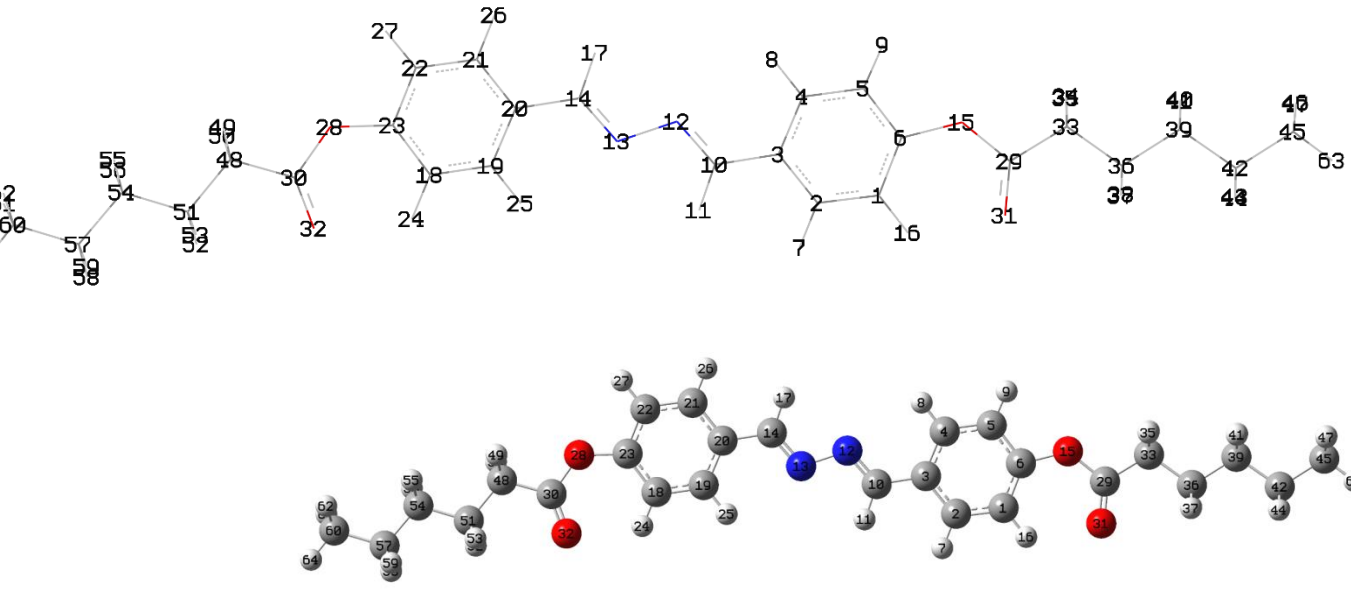


Figure S8. DSC cycles recorded from the second heating and cooling scan with heating rate 10°C/min of compound **I*15***.

6. *Optimized geometrical structure of In derivatives with atom numbering*



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0.0314301	119.4970471	1.3965712	20	21	22	C	23
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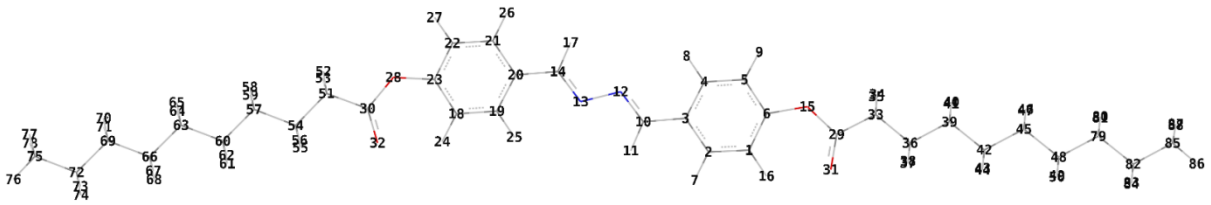

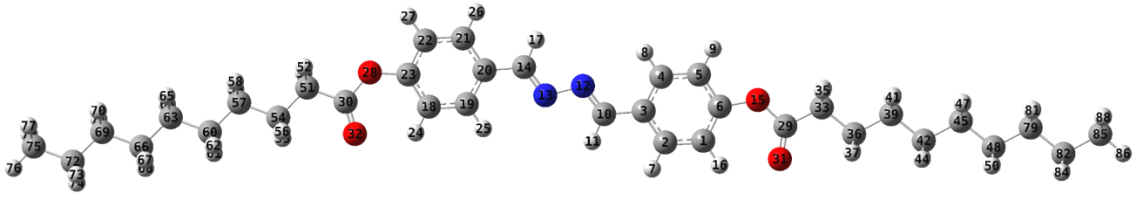

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		179.9823258		113.2416636	
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		179.9262345		111.3983990	
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		-59.9604498		111.1128350	
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		59.8239900		111.1028055	
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		179.8403987		113.5397546	
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		57.8091837		109.2666192	
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		179.9311206		113.5869899	
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		57.7572761		109.1372026	
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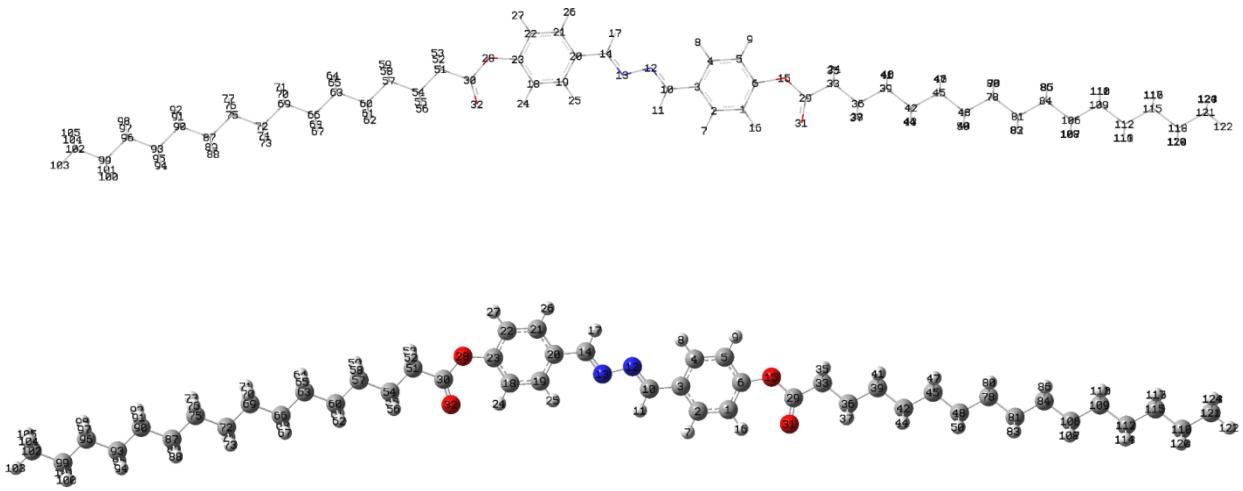

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118.7946901	1.0798794	2	3	4	H -179.9958881	8
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111.1081905	1.0930629	115	118	121	H -59.9367957	123
111.1047498	1.0930616	115	118	121	H 59.8430866	124

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1. Frisch, M.; Trucks, G.; Schlegel, H.B.; Scuseria, G.; Robb, M.; Cheeseman, J.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. Gaussian 09, revision a. 02, gaussian. *Inc., Wallingford, CT* **2009**, *200*.
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