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Supporting Information
For

Lithium Tetramethylpiperidine Promoted Cyclization towards Thiazoloisatin: a Novel Way towards Thiazoloisoindig o and its Derivatives

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Contents

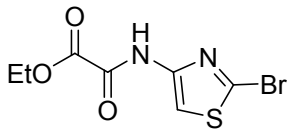
1. General Experimental Details

All glassware was completely dried before use. Reagents and solvents were purchased from commercial suppliers or purified by standard techniques. Reactions were monitored by thin-layer chromatography by exposing to UV-light irradiation at 254 and 365 nm and/or immersion in a phosphomolybdic acid staining solution followed by drying. Column chromatography was carried out by using silica gel 200-300 mesh. ^{1}H NMR and ^{13}C NMR spectra were obtained from a Bruker AVANCE-III 600 MHz with tetramethylsilane (TMS) as an internal standard at 298K and $CDCl_3$ was used as the solvent. The coupling constants *J* are given in Hz. Cyclic voltammetry curves were performed on an electrochemistry workstation (CHI660D, Chenhua Shanghai) at a scan rate of 0.1 V s^{-1}. A solution of 0.1 M Bu_4NPF_6 in DCM was used as the supporting electrolyte solution under a blanket of N_2 with Fc/Fc^+ as an internal reference. Dichloromethane (HPLC grade) was dried over calcium hydride under argon and degassed before using. Ag/AgCl, button glassy carbon and a platinum wire counter electrode were used as reference electrode, working electrode and auxiliary electrodes, respectively. The UV-Vis spectra were collected with a Hitachi U-4100 UV-Vis spectrophotometer in an anhydrous dichloromethane solution.

2. Experimental Procedures

2.1. Synthesis and characterization of key compounds

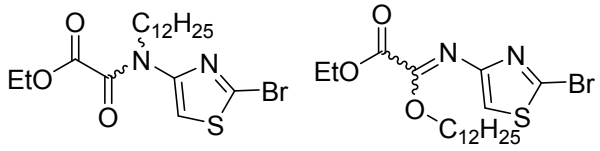
Synthesis of ethyl 2-(2-bromothiazol-4-ylamino)-2-oxoacetate (8).



8

A mixture of ethyl oxalyl monochloride (4.19 g, 30.7 mmol) and compound **5** (6.6 g, 25.6 mmol) in anhydrous THF(40 mL) was heated up to 100 °C and kept at this temperature for 4 h. The reaction mixture was then cooled to r.t. and the solvent was evaporated under reduced pressure. The residue was purified by column chromatography (eluent: petroleum ether / ethyl acetate = 30: 1) to afford a white solid **8** (5.38 g ,75.2%). M.P.: 102.2-104.8 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.63, 9.58 (s, s, 1H), 7.72, 7.67 (s, s, 1H), 4.43 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.6, 159.5, 153.6, 153.6, 151.2, 145.1, 143.7, 135.3, 107.7, 105.7, 63.9, 14.0; IR (solid) 3311, 3144, 2983, 1751, 1720, 1696, 1375, 1056, 535 cm^{-1}; HRMS(ESI, m/z) calcd. for $C_7H_7BrN_2O_3S$ $[M+H]^+$: 278.9434; found 278.9430.

Synthesis of ethyl 2-((2-bromothiazol-4-yl)(dodecyl)amino)-2-oxoacetate (9a) and ethyl 2-(2-bromothiazol-4-ylimino)-2-(dodecyloxy)acetate (9b)

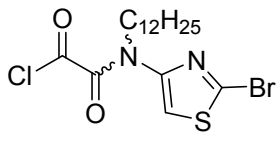


9a **9b**

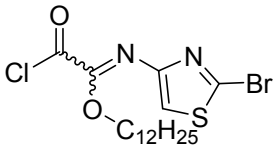
1-Bromododecane (2.617 g, 10.5 mmol) was added to a solution of compound **8** (1.953 g, 7 mmol) and K_2CO_3(1.45 g, 10.5 mmol) in anhydrous DMF(20 mL), and the reaction mixture was stirred at 100 °C for about 1 h. When the reaction was finished, the mixture was cooled down to r.t., extracted with EtOAc (3×50 mL), and the organic phase was collected and dried with $MgSO_4$. The solvent was removed under

reduced pressure, and the residue was purified by column chromatography on silica gel (eluent: petroleum ether / ethyl acetate = 50: 1) to afford a yellow oil composed of the inseparable mixture of **9a** and **9b** (2.51 g, 80.5%). The *N*-alkylated isomer: *O*-alkylated isomer = 3: 1; ^{1}H NMR (600 MHz, $CDCl_3$) for *N*-alkylated isomer: δ 6.88, 6.83 (s, s, 1H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.78 (t, *J* = 7.2 Hz, 2H), 1.58-1.56 (m, 2H), 1.26-1.18 (m, 21H), 0.85 (t, *J* = 7.1 Hz, 3H); ^{1}H NMR (600 MHz, $CDCl_3$) for *O*-alkylated isomers: δ 7.74, 7.70 (s, s, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.85 (t, *J* = 7.2 Hz, 2H), 1.67-1.65 (m, 2H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.26-1.18 (m, 18H), 0.85 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) for all the isomer: δ 162.1, 162.0, 161.0, 151.4, 149.2, 147.8, 145.4, 135.4, 113.0, 111.3, 109.8, 62.3, 62.0, 48.7, 47.0, 46.9, 31.8, 29.5, 29.44, 29.36, 29.2, 29.11, 29.08, 29.0, 27.2, 26.5, 26.4, 25.8, 22.6, 14.11, 13.9, 13.79, 13.75; IR (thin film) 3092, 2921, 2850, 1740, 1728, 1682, 1388, 1050, 720, 561 cm^{-1}; HRMS(ESI, m/z) calcd. for $C_{19}H_{31}BrN_2O_3S$ $[M+Na]^+$: 469.1131; found 469.1125.

Synthesis of 2-((2-bromothiazol-4-yl)(dodecyl)amino)-2-oxoacetyl chloride (10a) and dodecyl N-2-bromothiazol-4-yl-2-chloro-2-oxoacetimidate (10b)



10a



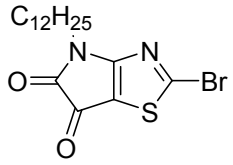
10b

LiOH aqueous solution (1.0 M solution, containing 172.5 mg LiOH, 7.2mmol) was added dropwise to a solution of 9 (1.066 g, 2.4 mmol) in a binary solvent system of MeOH (4 mL) and THF (12 mL), and the mixture was stirred at 0 °C for 10 minutes. Then the solution was acidified with HCl (1 M), and the solvent was evaporated under reduced pressure. The residue was extracted with EtOAc (3×50 mL) and the organic layer washed with brine, followed by drying over $MgSO_4$, and concentrated under reduced pressure to afford the corresponding acid. HRMS(ESI, m/z) calcd. for $C_{17}H_{28}BrN_2O_3S$ $[M+H]^+$: 419.0999, found 419.1000.

Then the acid was dissolved in dry THF (24 mL), to which $SOCl_2$ (309.53 mg, 2.4 mmol) was added dropwise under argon atmosphere at 0 °C. After 1h of stirring at r.t.,

the corresponding mixture of acid chlorides **10a** and **10b** was obtained and directly used for next step without further purification.

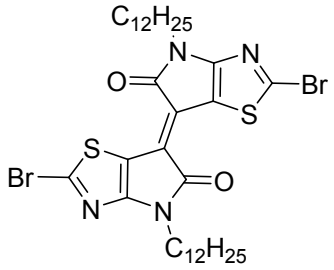
Synthesis of 2-bromo-4-dodecyl-4H-pyrrolo[2,3-d]thiazole-5,6-dione (7')



7'

n-BuLi (1.6 M, 2.99 mL) was added to a toluene solution containing TMP (678 mg, 4.8 mmol) and toluene (5 mL) under argon atmosphere at 0 °C. After 30 minutes of vigorous of stirring, the solution was added dropwise to the reaction mixture **10a** and **10b** (1.051 g, 2.4 mmol) under argon atmosphere at -30 °C. The mixture was stirred vigorously for 4 h at -30 °C. Then, the mixture was poured into NH_4Cl aqueous solution and extracted with EtOAc (3×50 mL). The combined organic layers were dried with $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by chromatography on a short column of silica gel (eluent: petroleum ether / ethyl acetate = 30: 1) to afford a red oil **7'** (348.5 mg , 37.5% overall yield for three steps). Decompose Temperature: 70-71 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.75 (t, *J* = 7.2 Hz, 2H), 1.74-1.71 (m, 2H), 1.33-1.25 (m, 18H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.3, 167.6, 166.9, 156.7, 99.0, 38.6, 28.8, 26.5, 26.44, 26.37, 26.25, 26.0, 25.1, 23.6, 19.6, 11.1; HRMS(ESI, m/z) calcd. for $C_{17}H_{27}BrN_2O_2S$ $[M+H]^+$: 401.0893, found 401.0892.

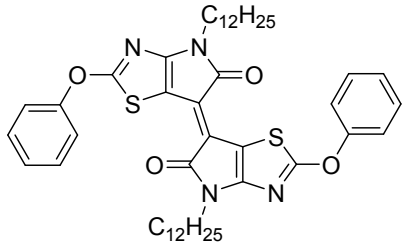
Synthesis of (*E*)-2,2'-dibromo-4,4'-didodecyl-[6,6'-bipyrrolo[2,3-d]thiazolylidene]- 5,5'(4H,4'H)-dione(4')



4'

Lawesson's reagent (101.1 mg, 0.25 mmol) was added to a dry toluene (15 mL) solution of compound **7'** (202.3 mg, 0.5 mmol) under argon atmosphere at r.t., and the mixture was stirred at 60 °C for 30 minutes. The reaction mixture concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: petroleum ether / ethyl acetate =150: 1) to afford a blue-colored soild **4'**(107.9 mg, 56%). M.P.: 126.7-127.0 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.84 (t, *J* = 7.2 Hz, 4H), 1.77-1.75 (m, 4H), 1.33-1.25 (m, 36H), 0.88 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.0, 160.9, 159.3, 119.3, 106.1, 41.3, 31.9, 29.53, 29.5, 29.47, 29.3, 29.1, 28.5, 26.7, 22.7, 14.1; IR (thin film) 1743, 1679, 1508, 1320, 721, 517 cm^{-1}. HRMS(APCI, m/z) calcd. for $C_{34}H_{50}Br_2N_4O_2S_2$ $[M+H]^+$: 769.1815, found 769.1803.

Synthesis of (*E*)-4,4'-didodecyl-2,2'-diphenoxy-[6,6'-bipyrrolo[2,3-d] thiazolylidene]-5,5'(4H,4'H)-dione(11)

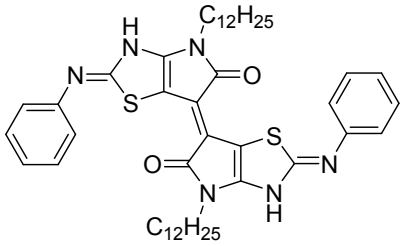


11

Compound **4'** (0.2 g, 0.26 mmol) was added to a solution of Phenol (0.061 g, 0.648 mmol) and NaOH(0.026 g, 0.648 mmol) in anhydrous THF (20 mL), and the reaction mixture was stirred at r.t. for about 3h. Then, the mixture was poured into NH_4Cl aqueous solution, extracted with EtOAc (3×20 mL). The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The crude

product was purified by column chromatography (eluent: petroleum ether / ethyl acetate =30: 1) to afford a blue-colored solid **11 (**51.6 mg, 25%**).** M.P.: 154 - 155 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (t, *J* = 8.0 Hz, 2H), 7.36-7.32 (m, 3H), 3.74 (t, *J* = 7.2 Hz, 2H), 1.73-1.70 (m, 2H), 1.29-1.23 (m, 18H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 180.7, 169.5, 158.3, 154.5, 130.4, 127.1, 120.6, 117.8, 98.2, 41.1, 31.9, 29.6, 29.54, 29.48, 29.3, 29.2, 28.7, 26.8, 22.7, 14.1; IR (thin film) 1659, 1632, 1518, 1472, 1164, 877, 738 cm^{-1}. HRMS(APCI, m/z) calcd. for $C_{46}H_{60}N_4O_4S_2$ $[M+H]^+$: 797.4129, found 797.4126.

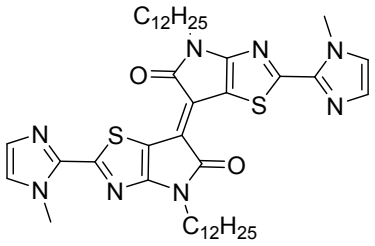
Synthesis of (*E*)-4,4'-didodecyl-2,2'-bis(phenylamino)-[6,6'-bipyrrolo[2,3-d]thiazolylidene]-5,5'(4H,4'H)-dione(12)



12

Aniline (1.09 g, 1.17 mmol) was added to a solution of compound **4'** (0.15g, 0.195 mmol) and DIPEA(0.194 g, 1.5 mmol) in anhydrous THF (15 mL), and the reaction mixture was stirred at 60 °C for about 5h. Then, the mixture was poured into NH_4Cl aqueous solution and extracted with EtOAc (3×20 mL). The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: petroleum ether / ethyl acetate =15: 1) to afford a red-colored solid **12**(46.7 mg, 31%). M.P.: 187-188 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (t, *J* = 7.8 Hz, 2H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.13 (d, *J* = 7.5 Hz, 2H), 3.80 (t, *J* = 7.2 Hz, 2H), 1.76-1.74 (m, 2H), 1.30-1.24 (m, 18H), 0.87 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.3, 170.1, 166.1, 148.3, 141.5, 129.4, 126.1, 121.1, 112.5, 41.8, 31.9, 29.6, 29.5, 29.4, 29.3, 29.1, 28.2, 26.7, 22.7, 14.1; IR (thin film) 3336, 1735, 1670, 1647, 1601, 1488, 1187, 721 cm^{-1}. HRMS(APCI, m/z) calcd. for $C_{46}H_{62}N_6O_2S_2$ $[M-H]^-$: 793.4303, found 793.4315.

Synthesis of (*E*)-4,4'-didodecyl-2,2'-bis(phenylamino)-[6,6'-bipyrrolo[2,3-d] thiazolylidene]-5,5'(4H,4'H)-dione(13)



13

1-Methylimidazole(0.5 mL) was added to a solution of CuI (3.9 mg, 0.02 mmol) and compound **4'** (77.1 mg, 0.1 mmol) in anhydrous Toluene (3 mL), and the reaction mixture was stirred at 100 °C for about 1h. Then, the mixture was poured into NH_4Cl aqueous solution, extracted with EtOAc and the organic layer washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: petroleum ether / $CHCl_3$ =1: 1) to afford a blue-colored solid **13** (34.8mg, 45%). M.P.: 190-191 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 2.5 Hz, 1H), 6.85 (d, *J* = 2.4 Hz, 1H), 3.89 (t, *J* = 7.2 Hz, 2H), 3.66 (s, 3H), 1.82-1.78 (m, 2H), 1.35-1.24 (m, 18H), 0.87 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.9, 161.7, 161.1, 159.4, 119.5, 119.0, 113.9, 103.6, 40.9, 34.9, 31.9, 29.64, 29.61, 29.5, 29.3, 29.2, 28.6, 26.8, 22.7, 14.1. Anal. Calcd. for $C_{42}H_{60}N_8O_2S_2$: C, 65.25; H, 7.82; N, 14.49; found: C, 65.38; H, 8.02; N, 14.48.

2.2. Tables of Optical and electrochemical data

Table S1. Optical and electrochemical data of C12-II, C12-ThII and C12-TzII

Compound	λ_{max} (nm)	λ_{onset} (nm)	ε_{max} (L mol^{-1} cm^{-1})	E^{opt}_g [a] (eV)	LUMO (eV)	HOMO (eV)	E^{CV}_g (eV)
C12-II	500	612	0.55×10^4	2.03	-3.60	-5.68	**2.08**
C12-Th-II	574	665	1.28×10^4	1.86	-3.54	-5.42	**1.87**
C12-Tz-II	567	660	1.24×10^4	1.88	-3.68	-5.64	**1.96**

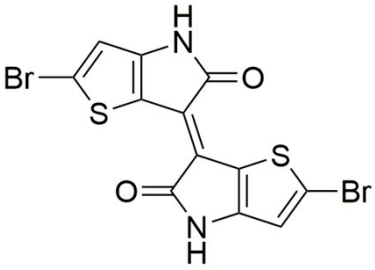
[a] Band gaps (*E*g) were estimated from the onset of UV-vis spectra of compounds, $E^{opt}_g=1240/\lambda_{onset}$. [b]Estimated from the LUMO and HOMO, $E^{CV}_g=E_{LUMO}- E_{HOMO}$.

Table S2. Optical and electrochemical data of compounds 11, 12 and 13

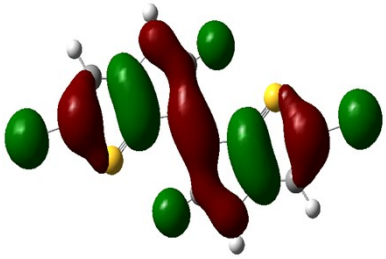
Compound	λ_{max} (nm)	λ_{onset} (nm)	ε_{max} (L mol^{-1} cm^{-1})	E^{opt}_g [a] (eV)	LUMO (eV)	HOMO (eV)	E^{CV}_g [b] (eV)
11	590	679	0.13×10^4	1.83	-3.48	-5.22	**1.74**
12	515	584	0.55×10^4	2.13	-3.82	-5.63	**1.81**
13	610	704	0.62×10^4	1.76	-3.55	-5.28	**1.73**

Band gaps (*E*g) were estimated from the onset of UV-vis spectra of compounds, $E^{opt}_g=1240/\lambda_{onset}$. [b]Estimated from the LUMO and HOMO, $E^{CV}_g=E_{LUMO}- E_{HOMO}$.

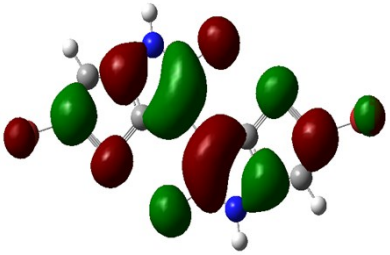
2.3. Theoretical calculations of C12-II, C12-ThII and C12-TzII



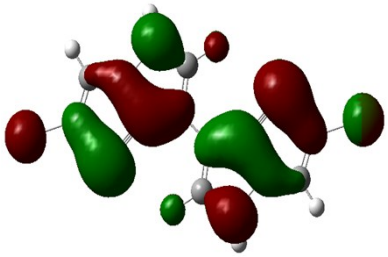
Homo (-5.27eV)



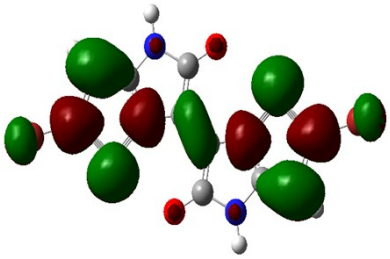
Lumo (-2.88eV)



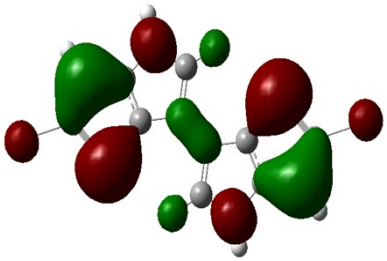
Homo-1 (-6.32eV)



Lumo+1 (-0.52eV)



Homo-2 (-6.80eV)



Lumo+2 (-0.38eV)

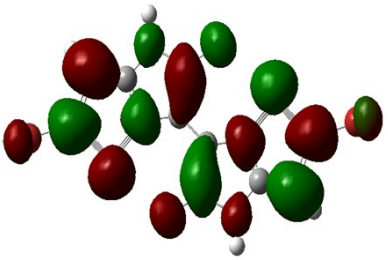
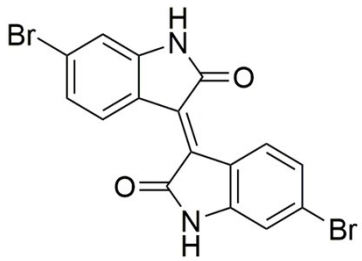
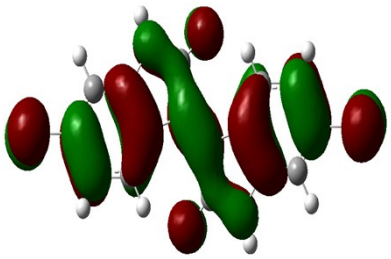


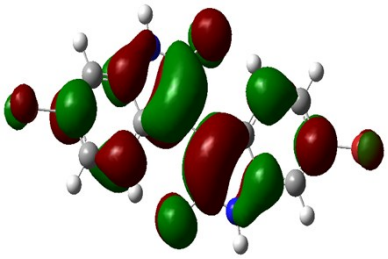
Figure S1. The molecular orbitals at the S0 minimum (optimized at the DFT/B3LYP/6-31G* level) for **C12-ThII**.



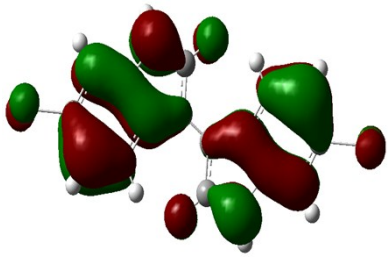
Homo (-5.93eV)



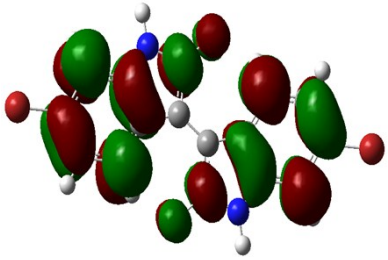
Lumo (-3.07eV)



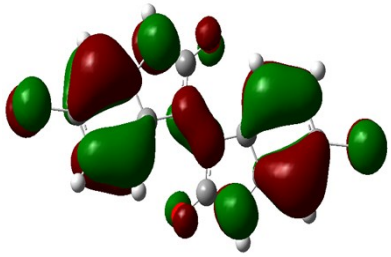
Homo-1 (-6.44eV)



Lumo+1 (-0.53eV)



Homo-2 (-6.73eV)



Lumo+2 (-0.45eV)

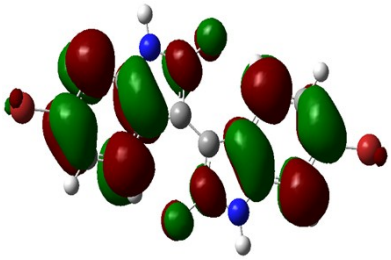
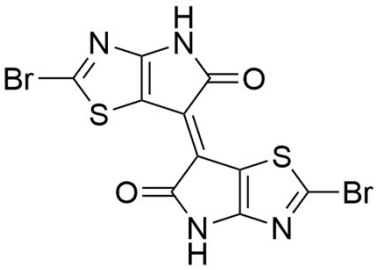
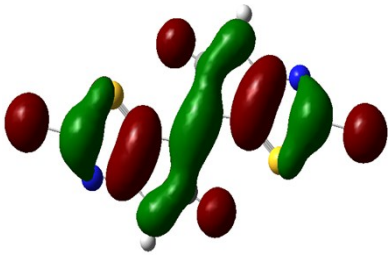


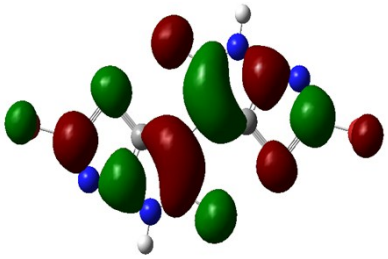
Figure S2. The molecular orbitals at the S0 minimum (optimized at the DFT/B3LYP/6-31G* level) for **C12-II**.



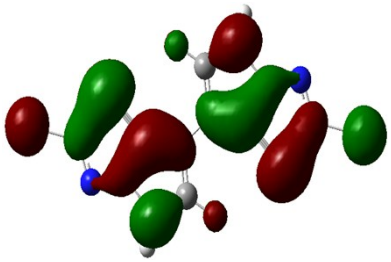
Homo (-5.64eV)



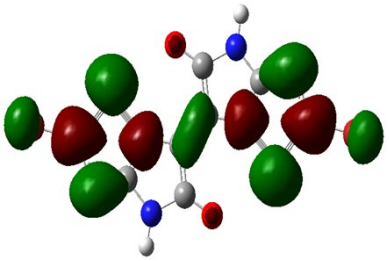
Lumo (-3.24eV)



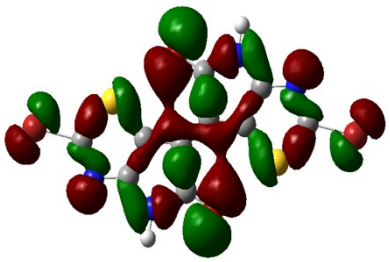
Homo-1 (-6.68eV)



Lumo+1 (-1.13eV)



Homo-2 (-7.70eV)



Lumo+2 (-0.96eV)

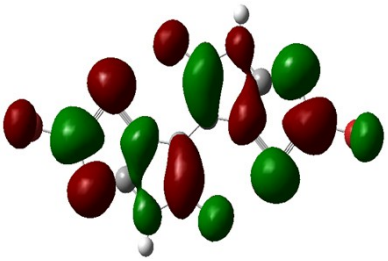


Figure S3. The molecular orbitals at the S0 minimum (optimized at the DFT/B3LYP/6-31G* level) for **C12-TzII**.

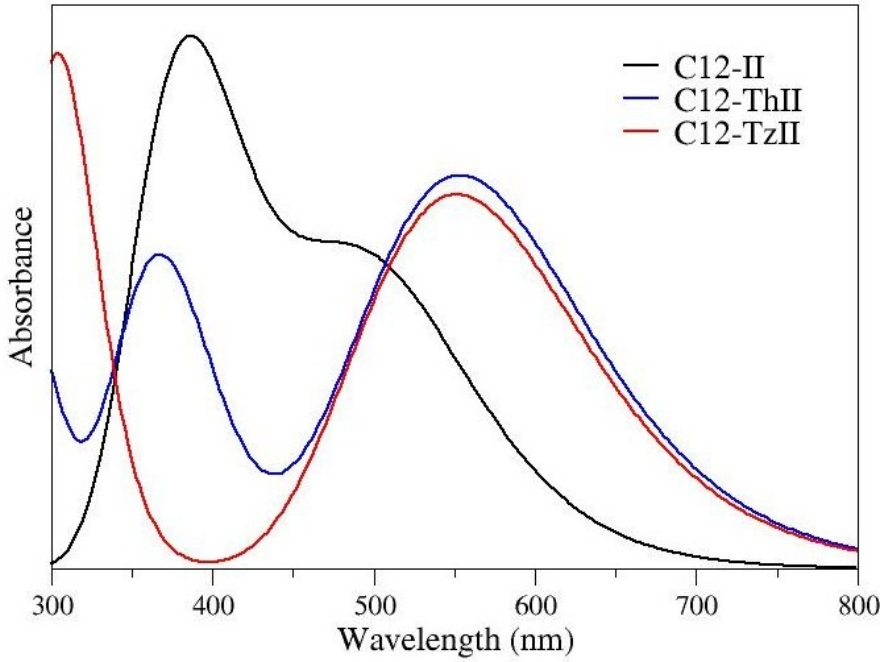


Figure S4. The absorption spectra (TD-B3LYP/6-31G* level) of **C12-II** (black), **C12-ThII** (blue) And **C12-TzII** (red).

The ground-state geometries of **C12-II**, **C12-ThII** and **C12-TzII** were optimized using the DFT method with B3LYP functional and 6-31G* basis set. The absorption spectra were computed at the TD-B3LYP/6-31G* level.

2.4. Stability test of C12-TzII and Compound 11, 12, 13.

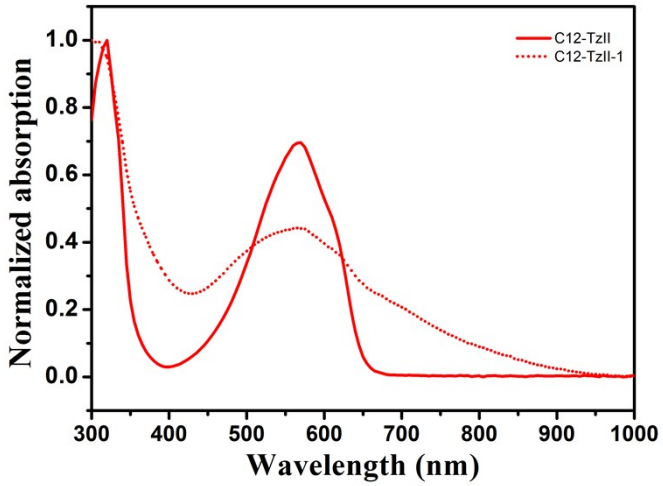


Figure S5. UV-vis spectrum evolution of **C12-TzII** (solid line: fresh prepared; dash line: detected after 3-days' storage.

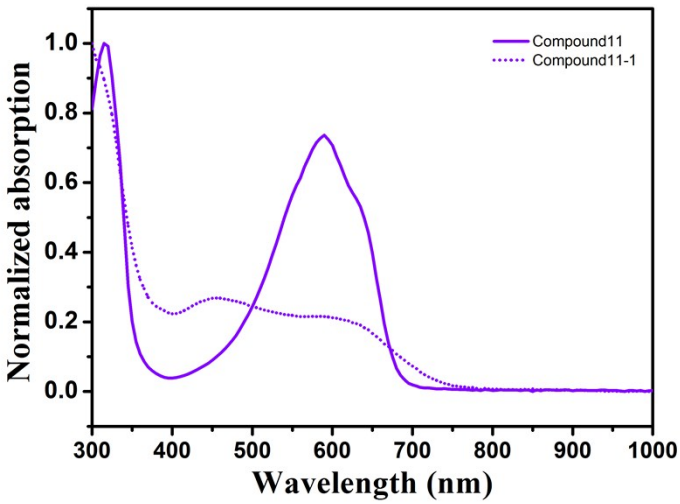


Figure S6. UV-vis spectrum evolution of Compound **11** (solid line: fresh prepared; dash line: detected after 3-days' storage.

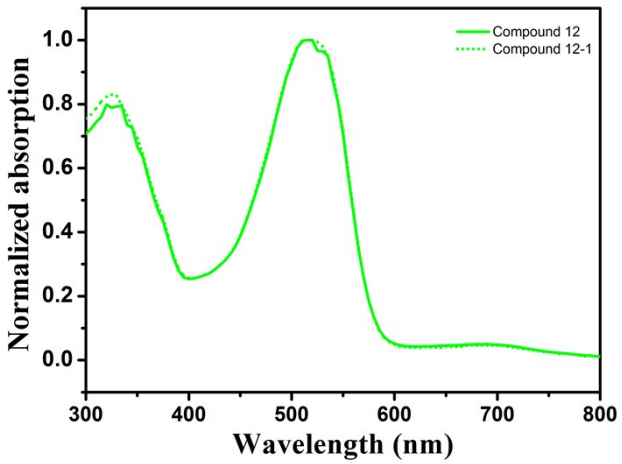


Figure S7. UV-vis spectrum evolution of Compound **12** (solid line: fresh prepared; dash line: detected after 3-days' storage.

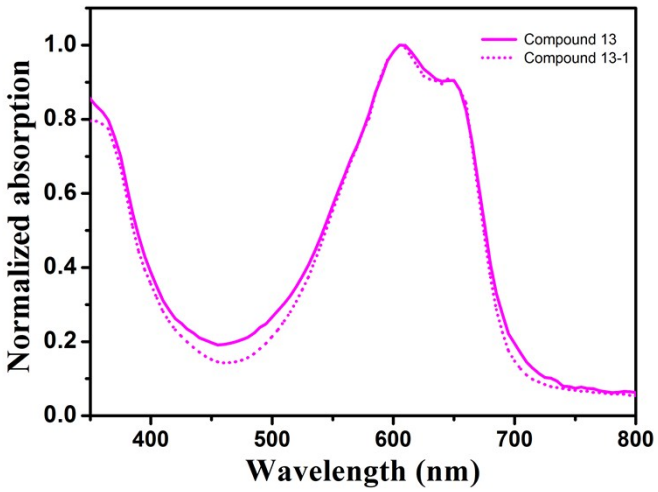
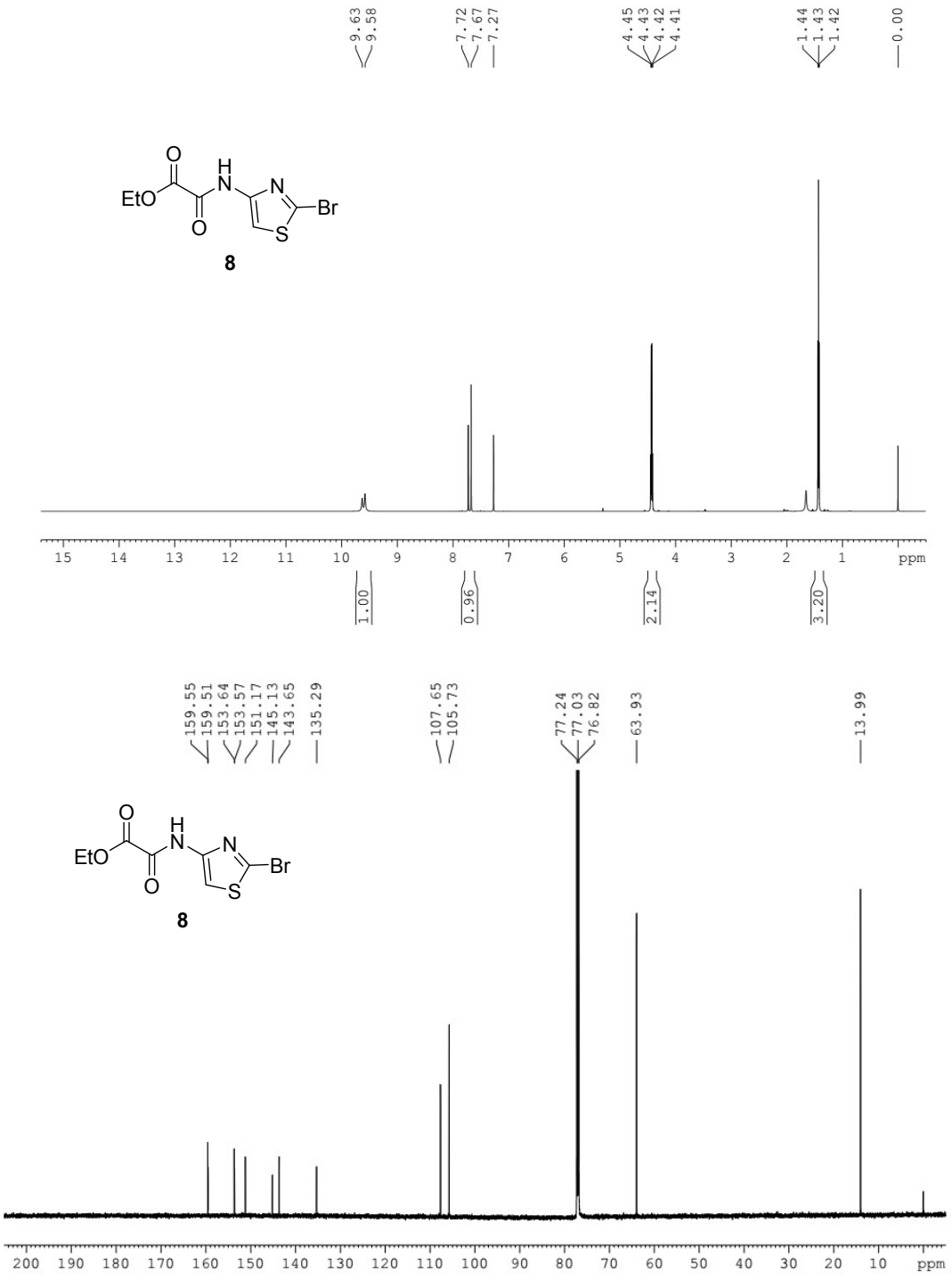
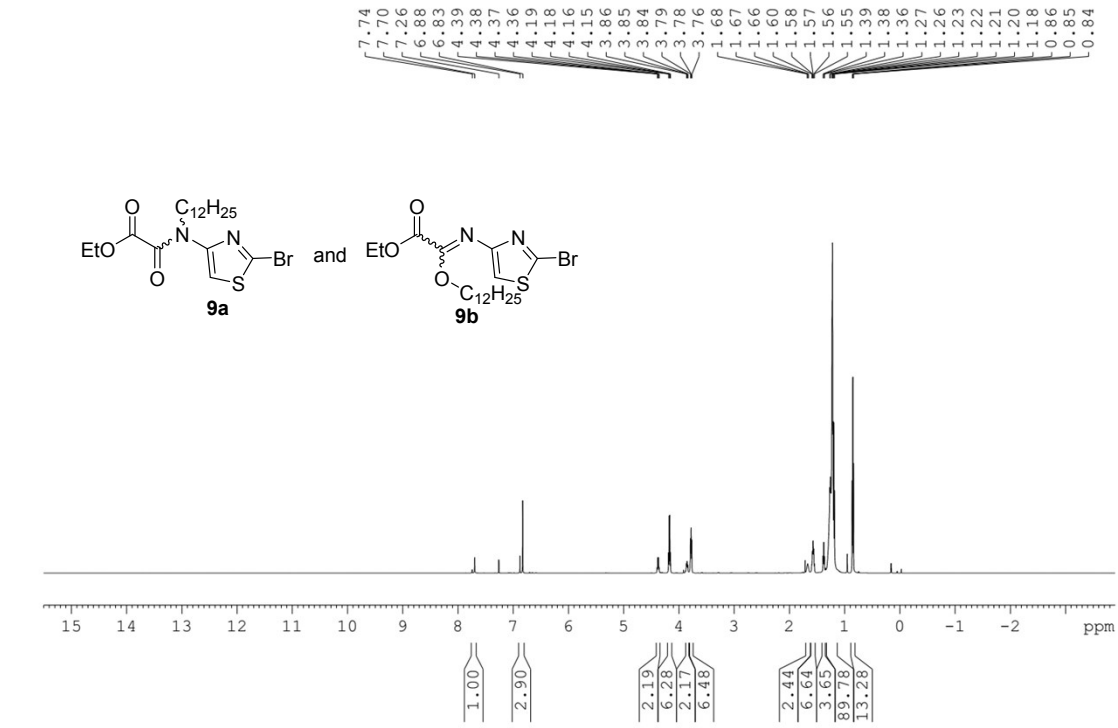
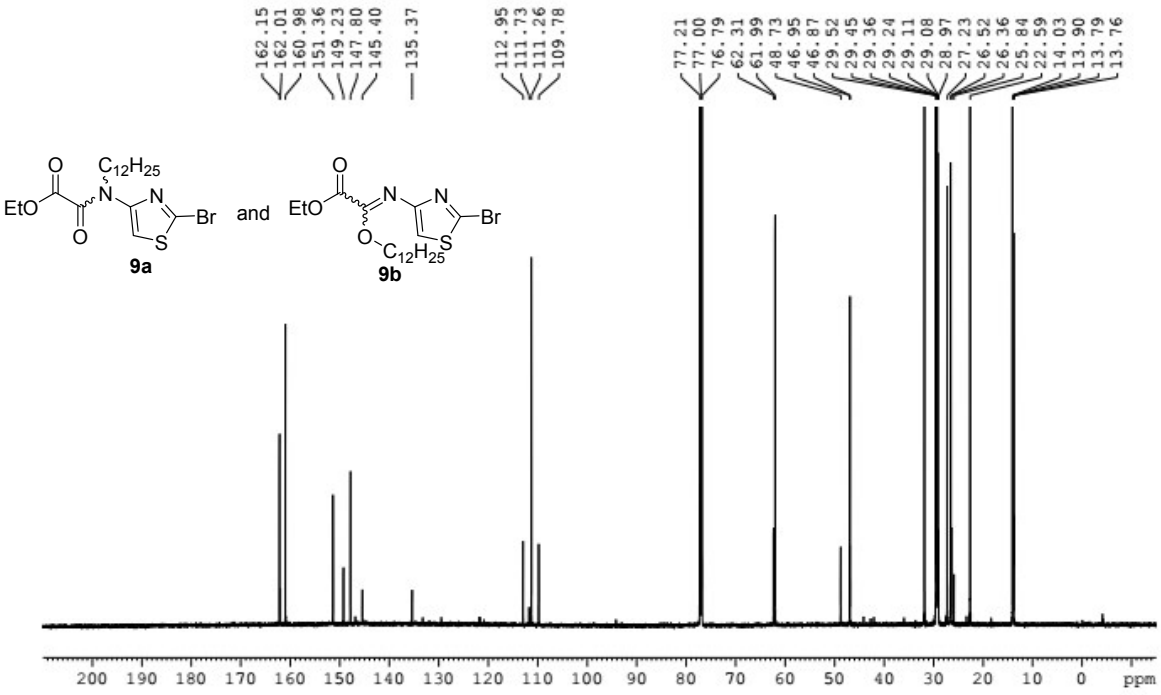


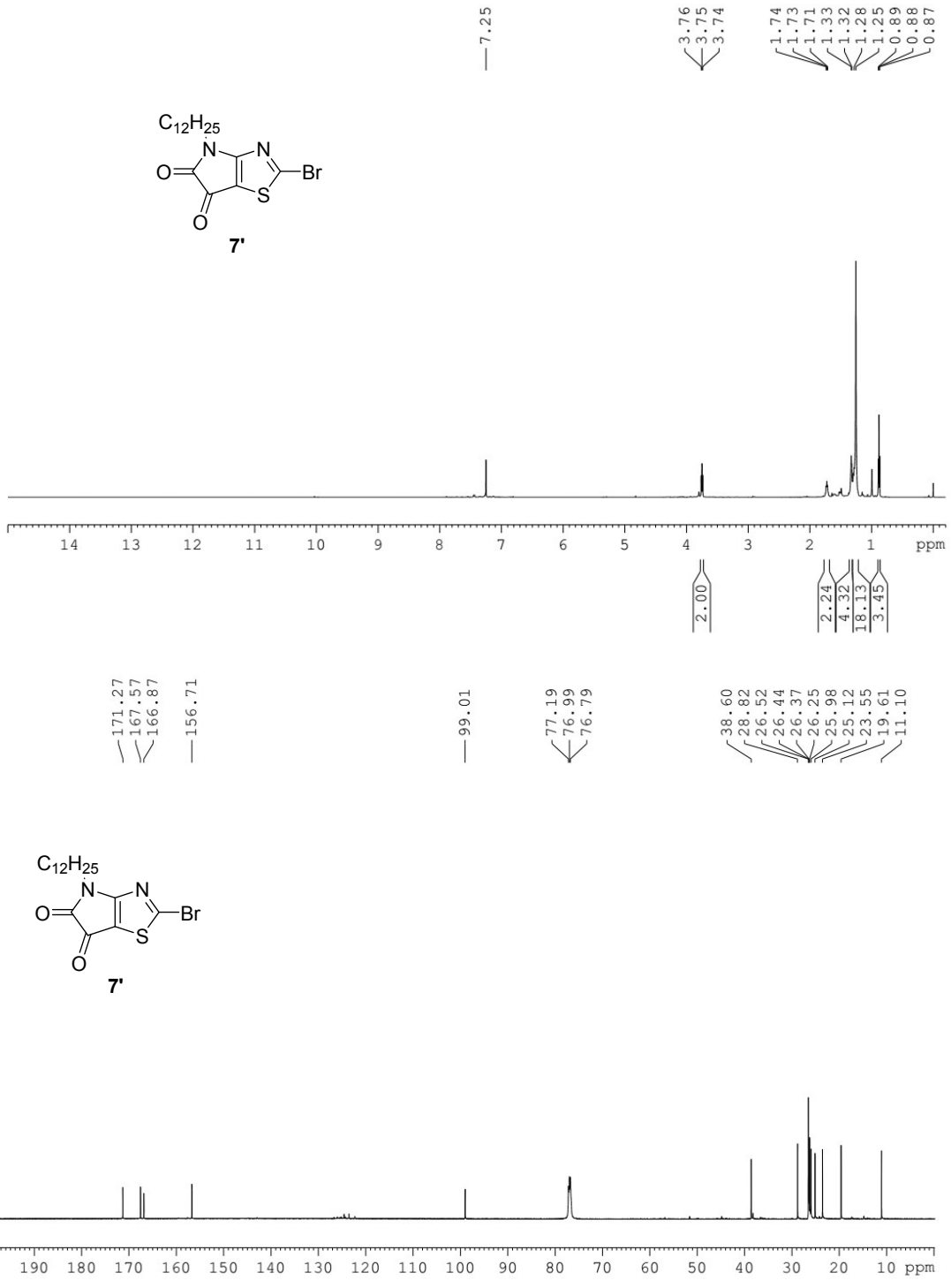
Figure S8. UV-vis spectrum evolution of Compound **13** (solid line: fresh prepared; dash line: detected after 3-days' storage.

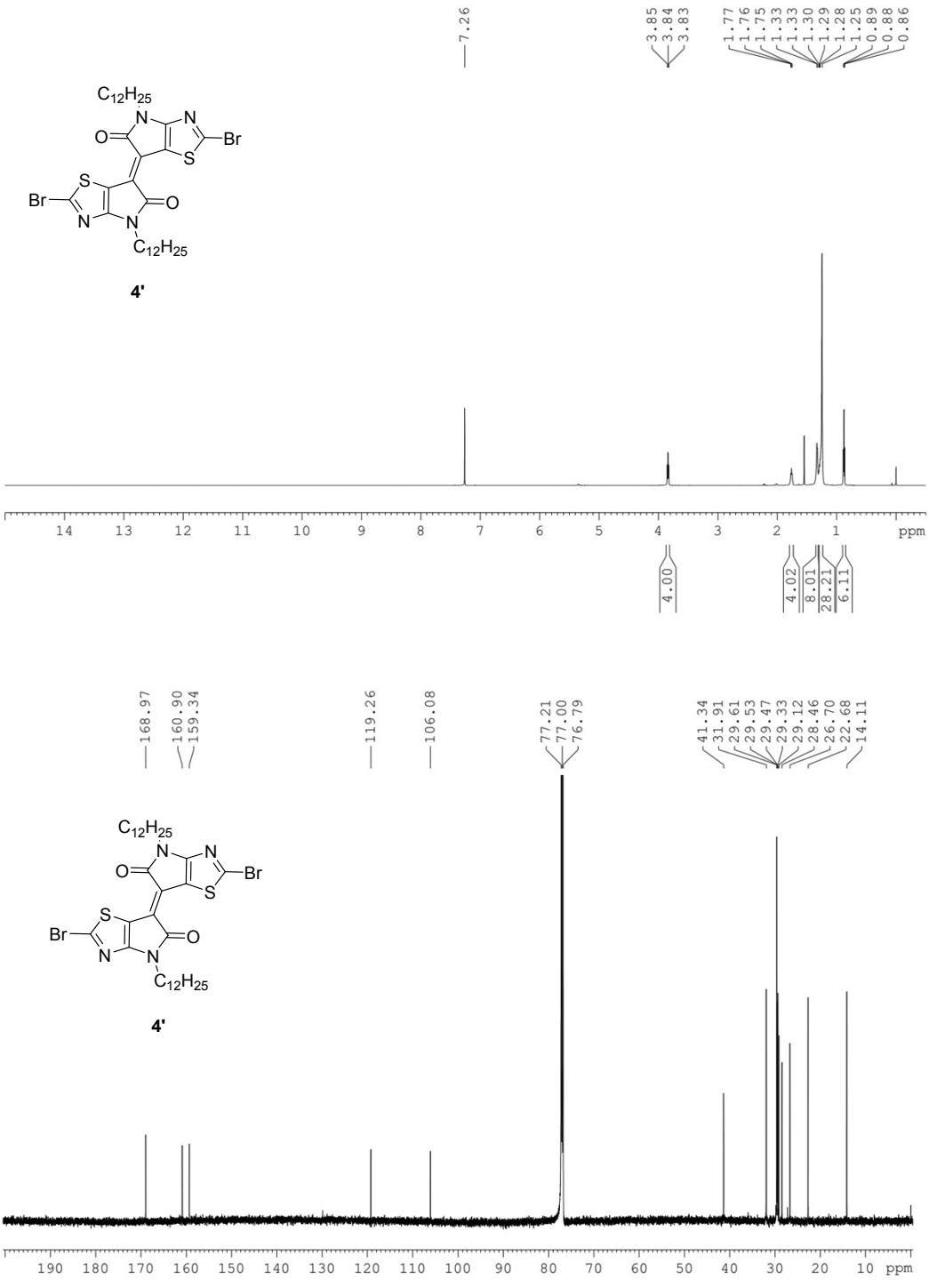
3. NMR Spectra of Key Compounds

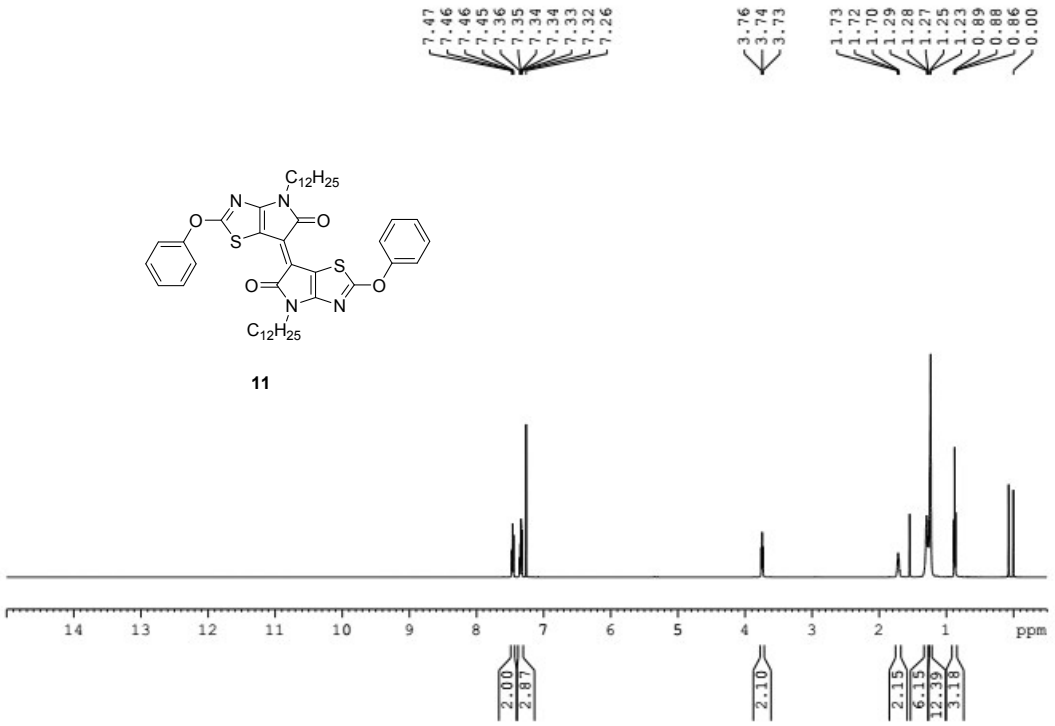


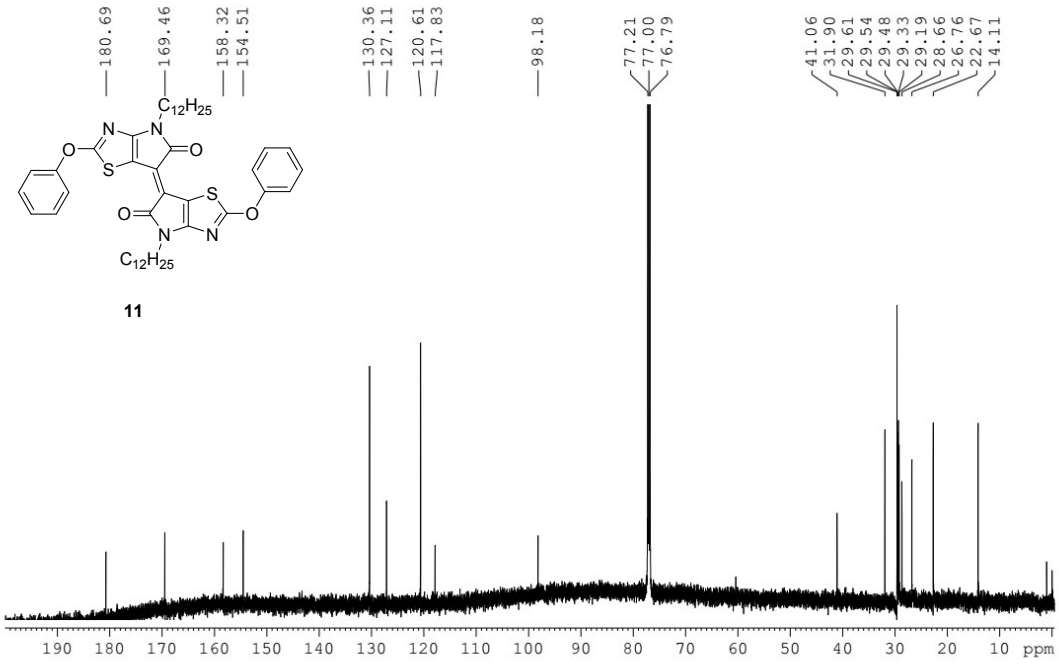

7.74
7.70
7.26
6.88
6.83
4.39
4.38
4.37
4.36
4.19
4.18
4.16
4.15
3.86
3.85
3.84
3.79
3.78
3.76
1.68
1.67
1.66
1.60
1.58
1.57
1.56
1.55
1.39
1.38
1.36
1.27
1.26
1.23
1.22
1.21
1.20
1.18
0.86
0.85
0.84
EtO
Br
and
9a
9b
ppm
1.00
2.90
2.19
6.28
2.17
6.48
2.44
6.64
3.65
89.78
13.28

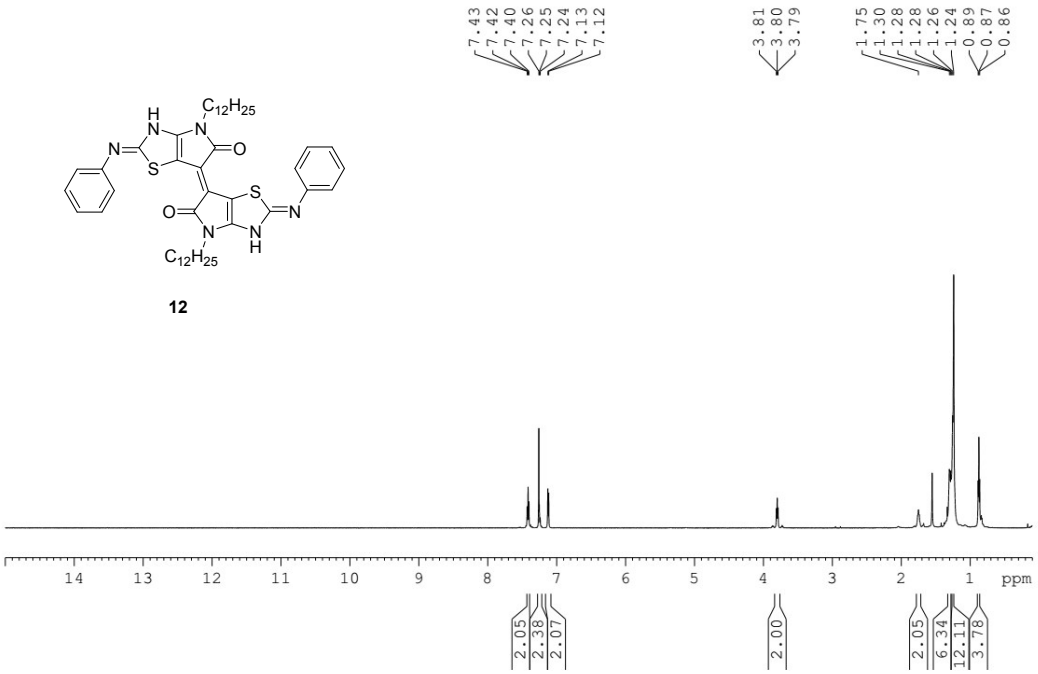

162.15
162.01
160.98
151.36
149.23
147.80
145.40
135.37
112.95
111.73
111.26
109.78
77.21
77.00
76.79
62.31
61.99
48.73
46.95
46.87
29.52
29.45
29.36
29.24
29.11
29.08
28.97
27.23
26.52
26.36
25.84
22.59
14.03
13.90
13.79
13.76
EtO
Br
and
9a
9b
ppm


7.25
3.76
3.75
3.74
1.74
1.73
1.71
1.33
1.32
1.28
1.25
0.89
0.88
0.87
C12H25
N
N
O
Br
S
O
7'
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
2.00
2.24
4.32
18.13
3.45
171.27
167.57
166.87
156.71
99.01
77.19
76.99
76.79
38.60
28.82
26.52
26.44
26.37
26.25
25.98
25.12
23.55
19.61
11.10
C12H25
N
N
O
Br
S
O
7'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

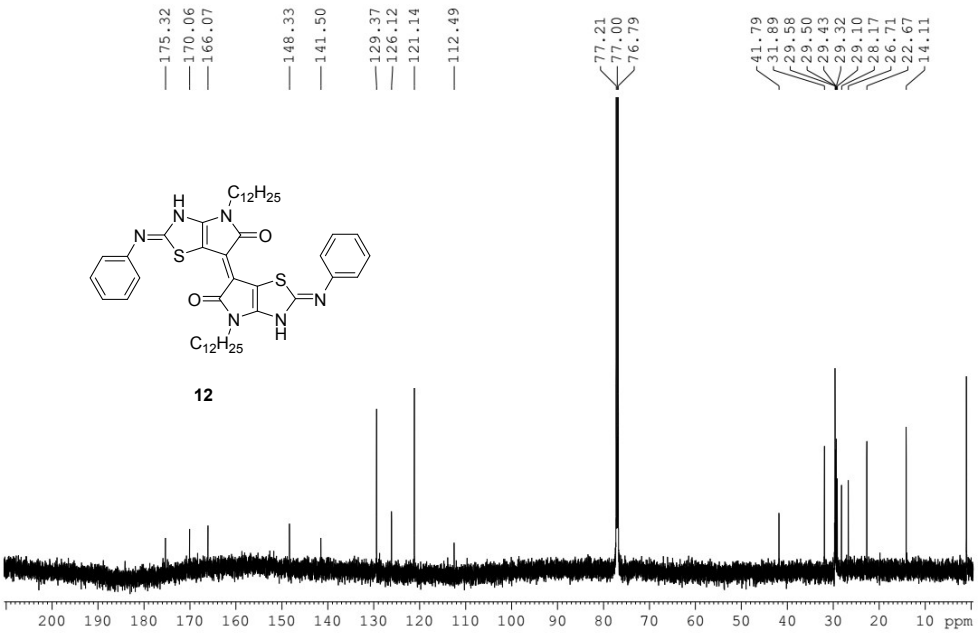

7.26
3.85
3.84
3.83
1.77
1.76
1.75
1.33
1.30
1.29
1.28
1.25
0.89
0.88
0.86
C12H25
Br
O
N
S
4'
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
4.00
4.02
8.01
28.21
6.11
168.97
160.90
159.34
119.26
106.08
77.21
77.00
76.79
41.34
31.91
29.61
29.53
29.47
29.33
29.12
28.46
26.70
22.68
14.11
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.47
7.46
7.46
7.45
7.36
7.35
7.34
7.34
7.33
7.32
7.26
3.76
3.74
3.73
1.73
1.72
1.70
1.29
1.28
1.27
1.25
1.23
0.89
0.88
0.86
0.00
C12H25
O
N
S
O
O
S
O
N
C12H25
11
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.87
2.10
2.15
6.15
12.39
3.18

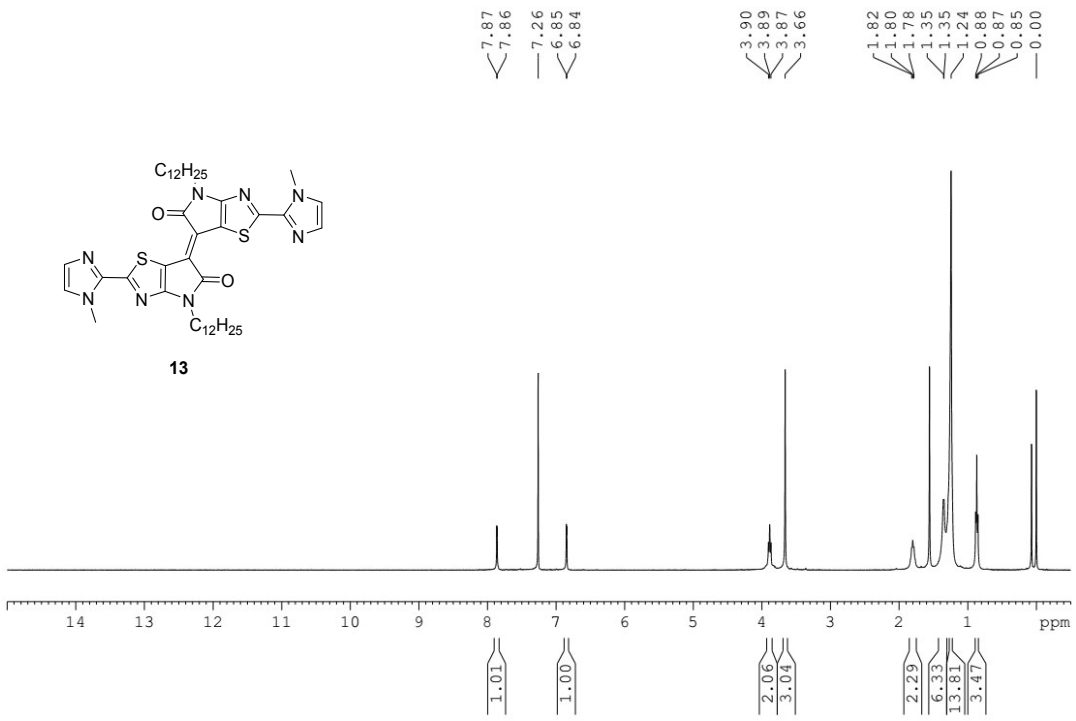

180.69
169.46
158.32
154.51
130.36
127.11
120.61
117.83
98.18
77.21
77.00
76.79
41.06
31.90
29.61
29.54
29.48
29.33
29.19
28.66
26.76
22.67
14.11
C12H25
O
N
S
O
O
S
O
N
C12H25
11
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

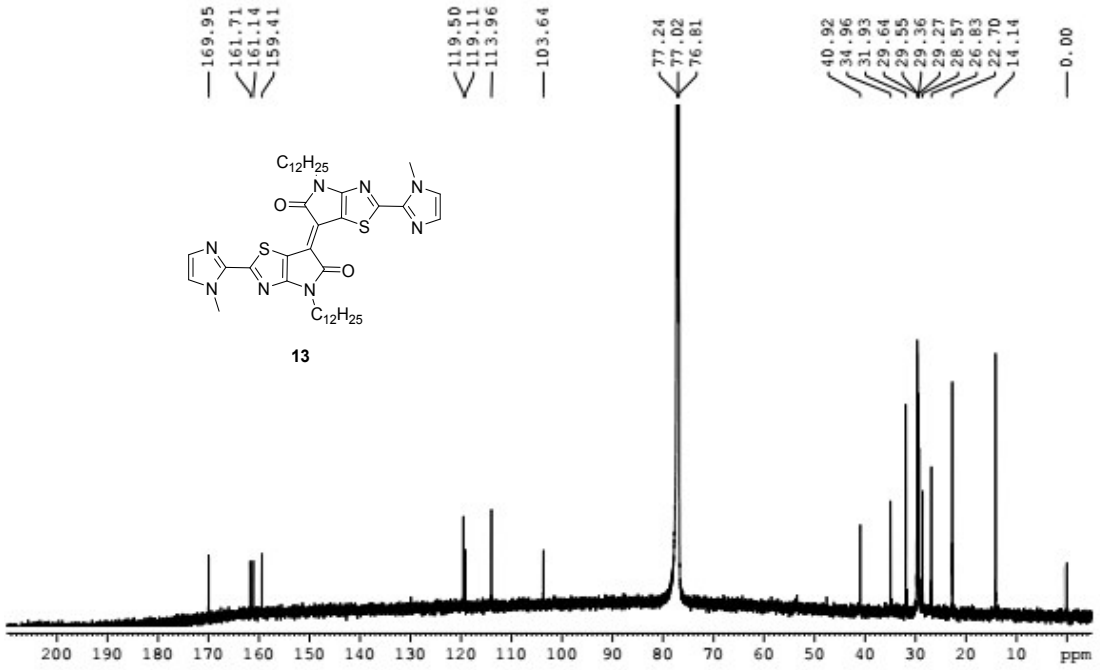

7.43
7.42
7.40
7.26
7.25
7.24
7.13
7.12
3.81
3.80
3.79
1.75
1.30
1.28
1.28
1.26
1.24
0.89
0.87
0.86
C12H25
H
N
N
O
N
S
S
O
S
N
N
N
H
H
C12H25
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
2.05
2.38
2.07
2.00
2.05
6.34
12.11
3.78

12


175.32
170.06
166.07
148.33
141.50
129.37
126.12
121.14
112.49
77.21
77.00
76.79
41.79
31.89
29.58
29.50
29.43
29.32
29.10
28.17
26.71
22.67
14.11
C12H25
H
N
N
O
N
S
S
O
S
N
N
N
H
H
C12H25
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

12


7.87
7.86
7.26
6.85
6.84
3.90
3.89
3.87
3.66
1.82
1.80
1.78
1.35
1.35
1.24
0.88
0.87
0.85
0.00
C12H25
C12H25
13
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.01
1.00
2.06
3.04
2.29
6.33
13.81
3.47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161.71
161.14
159.41
119.50
119.11
113.96
103.64
77.24
77.02
76.81
40.92
34.96
31.93
29.64
29.55
29.36
29.27
28.57
26.83
22.70
14.14
0.00
C12H25
C12H25
13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm