SUPPORTING INFORMATION

Switching with orthogonal stimuli: Electrochemical ring-closure and photochemical ring-opening of bis(thiazolyl)maleimides

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1. Synthesis

General methods

Solvents and commercial starting materials were used as received. 3,4-Dibromo-1-*tert*-butyl-1*H*-pyrrole-2,5-dione (**8**),[1] 1,2-dibromocyclopentene (**12**),[2] morpholine-*N*-carbothioamide (**5**),[3] and 2-bromo-1,1-diethoxypropane[4] were prepared as described in the literature. All reactions requiring inert gas atmosphere were performed under argon atmosphere. Toluene and THF were distilled under argon atmosphere over sodium prior to use. Column chromatography was carried out with silica gel (0.035–0.070 mm, 60 Å) using eluents as specified. All experiments involving light-sensitive compounds, in particular the ring-closed diarylethenes, were carried out in the dark under red light. NMR spectra were recorded on a 500 MHz Bruker AV 500, a 400 MHz Bruker AV 400, or a 300 MHz Bruker DPX 300 spectrometer at 25 °C using residual protonated solvent signals as internal standards for ^{1}H- and ^{13}C-spectra (^{1}H: $\delta(CHCl_3) = 7.26$ ppm and ^{13}C: $\delta(CHCl_3) = 77.16$ ppm) or $CFCl_3$ as external standard for ^{19}F-spectra ($\delta(CFCl_3) = 0$ ppm). UPLC/MS was performed with a Waters UPLC Acquity equipped with a Waters LCT Premier XE Mass Detector for UPLC-HR-MS, with Waters Alliance systems (consisting of a Waters Separations Module 2695, a Waters Diode Array Detector 996 and a Waters Mass Detector ZQ 2000).

1-*tert*-Butyl-3,4-bis(5-methyl-2-morpholinothiazol-4-yl)-1*H*-pyrrole-2,5-dione (1a)

Thiazolylstannane **7** (10.02 g, 21.17 mmol) and 3,4-dibromo-1-*tert*-butyl-1*H*-pyrrole-2,5-dione (**8**) (1.65 g, 5.30 mmol) were dissolved in 200 mL of DMF and the mixture was degassed by bubbling argon through the solution for 10 min. After the addition of $Pd_2(dba)_3$ (450 mg, 0.50 mmol), $AsPh_3$ (974 mg, 3.18 mmol), and CuI (2.02 g, 10.60 mmol) the mixture was stirred for 6 h at room temperature. Then, the mixture was poured into 300 mL of water and extracted with 5 x 100 mL of ethyl acetate. The combined organic layers were washed with brine and dried over $MgSO_4$. Purification by column chromatography (hexane/ethyl acetate from 5:1 to 1:1) afforded compound **1a** (907 mg, 1.75 mmol, 33 %) as an orange solid. Crystals suitable for x-ray crystallography were obtained by recrystallization from acetonitrile.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.75 (t, $^{3}J_{H,H} = 4.8$ Hz, 8 H, CH_2), 3.34 (t, $^{3}J_{H,H} = 4.8$ Hz, 8 H, CH_2), 1.99 (s, 6 H, CH_3), 1.62 (s, 9 H, CH_3). **^{13}C-NMR (75.5 MHz, $CDCl_3$):** δ (ppm) = 170.8 (C_q), 168.2 (C_q), 137.3 (C_q), 133.9 (C_q), 125.7 (C_q), 66.2 (*C*H$_2$), 57.8 (C_q), 48.6 (*C*H$_2$), 29.1 (*C*H$_3$), 12.4 (*C*H$_3$). **HRMS (ESI+):** *m/z* = 518.183 (calcd. 518.190 for $[C_{24}H_{32}N_5O_4S_2]^+$).

[1] Dubernet, M.; Caubert, V.; Guillard, J.; Viaud-Massuard, M.-C. *Tetrahedron* **2005**, *61*, 4585–4593.

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[3] Hartmann, H.; Reuther, I. *J. Prakt. Chem.* **1973**, *315*, 144-148.

[4] Davis, H. A.; Brown, R. K. *Can. J. Chem.* **1971**, *49*, 2321-2335.

Isolation of ring-closed isomer 1b

A solution of **1a** (170 mg, 0.33 mmol) in 50 mL of acetonitrile was treated with ceric ammonium nitrate (330 mg, 0.60 mmol) and stirred at room temperature for 5 min. During this time the mixture initially turns dark before it gets an orange color. Then sodium ascorbate (200 mg, 1 mmol) was added and the mixture was stirred for 5 min. After filtration the solvent was removed *in vacuo* and the residue was partioned between 20 mL of chloroform and 20 mL of water. The organic layer was separated and dried over $MgSO_4$. Evaporation of the solvent yielded 170 mg of a red solid which was determined by UPLC to consist of **1a** (25 %), **1b** (47 %), and **1c** (35 %). An analytical sample of **1b** could be obtained by separation of the mixture via preparative HPLC (column: Luna Phenomenex, 10 µm, 20 x 250 mm, eluent: methanol/water from 50 % to 90 % methanol).

^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.05 - 3.40 (broad, 16 H, CH_2), 1.78 (s, 6 H, CH_3), 1.64 (s, 9 H, CH_3). **^{13}C-NMR (100.6 MHz, $CDCl_3$):** δ (ppm) = 172.3 (C_q), 166.8 (C_q), 157.7 (C_q), 103.9 (C_q), 72.2 (C_q), 66.4 (CH_2), 57.9 (C_q), 48.6 (CH_2), 29.3 (CH_3), 26.9 (CH_3). **HRMS (ESI+):** *m/z* = 518.194 (calcd. 518.190 for $[C_{24}H_{32}N_5O_4S_2]^+$).

Isolation of side-product 1c

A solution of **1a** (103 mg, 0.20 mmol) in 75 mL of acetonitrile containing 0.1 M Et_4NClO_4 was oxidized at a potential of 1 V using a divided H-cell with platinum nets as working and counter electrode and a standard calomel electrode (SCE) as reference. After a charge of 2 C/mol was transferred the mixture was stirred for 2 h at room temperature. The solvent was evaporated and to the residue were added 20 mL of water. After stirring for 30 min at room temperature the remaining solid was filtered off and dried *in vacuo* affording **1c** (49 mg, 0.08 mmol, 40 %) as a red solid. Crystals suitable for x-ray crystallography were obtained by recrystallization from chloroform.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 5.28 (broad, 2 H, CH_2), 3.97 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.79 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.64 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.54 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 2.49 (s, 3 H, CH_3), 1.65 (s, 9 H, CH_3). **^{13}C-NMR (75.5 MHz, $CDCl_3$):** δ (ppm) = 171.7 (C_q), 170.5 (C_q), 167.4 (C_q), 167.3 (C_q), 144.4 (C_q), 133.5 (C_q), 130.1 (C_q), 127.3 (C_q), 126.0 (C_q), 122.8 (C_q), 66.1 (CH_2), 65.3 (CH_2), 59.1 (C_q), 53.7 (CH_2), 48.6 (CH_2), 46.5 (CH_2), 29.0 (CH_3), 14.8 (CH_3). **HRMS (ESI+):** *m/z* = 516.155 ($[M\text{-}ClO_4^-]^+$, calcd. 516.174 for $[C_{24}H_{30}N_5O_4S_2]^+$).

1-*tert*-Butyl-3,4-bis(2-morpholino-5-trifluoromethylthiazol-4-yl)-1*H*-pyrrole-2,5-dione (2a)

Thiazolylstannane **11** (1.45 g, 2.75 mmol) and 3,4-dibromo-1-*tert*-butyl-1*H*-pyrrole-2,5-dione (**8**) (0.34 g, 1.1 mmol) were dissolved in 70 mL of toluene and the mixture was degassed by bubbling argon through the solution for 10 min. After the addition of $Pd(PPh_3)_4$ (165 mg, 0.14 mmol) the mixture was stirred at 110 °C for 20 h. After cooling to room temperature, the mixture was diluted with 100 mL of ethyl acetate and washed with 3 x 100 mL of water. The organic phase was dried over $MgSO_4$ and evaporated. Purification of the residue by column chromatography (dichloromethane/ethyl acetate 2:1, 1 % triethylamine) afforded compound **2a** (203 mg, 0.32 mmol, 29 %) as an orange solid.

^{1}H-NMR (500 MHz, $CDCl_3$): δ (ppm) = 3.75 (t, $^3J_{H,H}$ = 5.0 Hz, 8 H, CH_2), 3.42 (t, $^3J_{H,H}$ = 5.0 Hz, 8 H, CH_2), 1.63 (s, 9 H, CH_3). **^{13}C-NMR (125.77 MHz, $CDCl_3$):** δ (ppm) = 170.6 (C_q), 169.0 (C_q), 140.8, (C_q), 136.2 (C_q), 121.9 (q, $^1J_{C,F}$ = 267 Hz, CF_3), 114.1 (q, $^2J_{C,F}$ = 37 Hz, *C*-CF_3), 66.0 (CH_2), 58.5 (C_q), 48.4 (CH_2), 28.9 (CH_3).

^{19}F-NMR (470.6 MHz, $CDCl_3$): δ (ppm) = -52.65 (s, CF_3). **HRMS (ESI+):** *m/z* = 626.128 (calcd. 626.133 for $[C_{24}H_{26}F_6N_5O_4S_2]^+$).

Isolation of ring-closed isomer 2b

A solution of **2a** (120 mg, 0.19 mmol) in 40 mL of acetonitrile containing 0.1 M Et_4NPF_6 was oxidized at a potential of 1.8 V using a divided H-cell with platinum nets as working and counter electrode and a standard calomel electrode (SCE) as reference. After a charge of 2 C/mol was transferred the mixture was reduced at a potential of -0.2 V. The solvent was removed *in vacuo* and the residue was diluted with 50 mL of water. After extraction with 100 mL of chloroform the organic phase was washed 3 x with 30 mL of water and dried over $MgSO_4$. Evaporation of the solvent afforded compound **2b** (80 mg, 0.13 mmol, 67 %) as an orange solid.

^{1}H-NMR (500 MHz, $CDCl_3$): δ (ppm) = 4.10 – 3.40 (broad, 16 H, CH_2), 1.65 (s, 9 H, CH_3). **^{13}C-NMR (125.77 MHz, $CDCl_3$):** δ (ppm) = 169.4 (C_q), 165.7 (C_q), 146.3 (C_q), 124.6 (q, $^1J_{C,F}$ = 290 Hz, CF$_3$), 108.0 (C_q), 72.0 (q, $^2J_{C,F}$ = 26 Hz, *C*-CF$_3$), 66.4 (*C*H$_2$), 58.5 (C_q), 48.4 (*C*H$_2$), 29.1 (*C*H$_3$). **^{19}F-NMR (282.38 MHz, $CDCl_3$):** δ (ppm) = -52.68 (s, CF_3). **HRMS (ESI+):** *m/z* = 626.139 (calcd. 626.133 for $[C_{24}H_{26}F_6N_5O_4S_2]^+$).

1-*tert*-Butyl-3-(5-methyl-2-morpholinothiazol-4-yl)-4-(2-morpholino-5-(trifluoromethyl)-thiazol-4-yl)-1*H*-pyrrole-2,5-dione (3a)

5-Methyl-2-morpholino-4-(tributylstannyl)thiazole (**7**) (295 mg, 0.62 mmol), 2-morpholino-4-(tributylstannyl)-5-(trifluoromethyl)thiazole (**11**) (329 mg, 0.62 mmol), and 3,4-dibromo-1-*tert*-butyl-1*H*-pyrrole-2,5-dione (**8**) (162 mg, 0.52 mmol) were dissolved in 15 mL of dry toluene and degassed by bubbling argon through the solution for 5 min. Then, $Pd(PPh_3)_4$ (36 mg, 0.03 mmol) was added and the mixture was stirred at 100 °C for 48 h. After cooling to room temperature the mixture was filtered through a pad of Celite eluting with ethyl acetate. The filtrate was washed with brine and dried over $MgSO_4$. After evaporation of the solvents the crude mixture was separated by column chromatography (petrol ether/ethyl acetate from 10:1 to 1:1) affording compound **3a** (8 mg, 0.01 mmol, 3 %) as a yellow solid.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.77 (t, $^3J_{H,H}$ = 5.1 Hz, 4 H, CH_2), 3.72 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.44 (t, $^3J_{H,H}$ = 5.1 Hz, 4 H, CH_2), 3.26 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 2.29 (s, 3 H, CH_3), 1.63 (s, 9 H, CH_3). **^{13}C-NMR (75.47 MHz, $CDCl_3$):** δ (ppm) = 66.2 (*C*H$_2$), 66.0 (*C*H$_2$), 48.5 (*C*H$_2$), 48.4 (*C*H$_2$), 29.0 (*C*H$_3$), 13.3 (*C*H$_3$), quaternary carbons are not visible due to low concentration. **^{19}F-NMR (282.38 MHz, $CDCl_3$):** δ (ppm) = -53.09 (s, CF_3). **HRMS (ESI+):** *m/z* = 572.170 (calcd. 572.161 for $[C_{24}H_{29}F_3N_5O_4S_2]^+$).

1,2-Bis(5-methyl-2-morpholinothiazol-4-yl)cyclopentene (4a)

Thiazolylstannane **7** (5.92 g, 10.00 mmol) and 1,2-dibromocyclopentene (**12**) (0.90 g, 4.00 mmol) were dissolved in 40 mL of DMF and the mixture was degassed by bubbling argon through the solution for 10 min. After the addition of $PdCl_2(PPh_3)_2$ (84 mg, 0.12 mmol) the mixture was stirred for 20 h at 100 °C. Then, 100 mL of ethyl acetate were added and the mixture was filtered through a pad of celite. After evaporation of the solvents the residue was taken up in 150 mL of ethyl acetate and washed with 30 mL of water and 30 mL of brine. The organic layer was dried over anhydrous $MgSO_4$ and evaporated. Purification by column chromatography (petroleum ether/ethyl acetate 3:2) afforded compound **4a** (110 mg, 0.25 mmol, 6 %) as a viscous oil.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.78 (t, $^3J_{H,H}$ = 4.8 Hz, 8 H, CH_2), 3.36 (t, $^3J_{H,H}$ = 4.8 Hz, 8 H, CH_2), 2.84 (t, $^3J_{H,H}$ = 7.5 Hz, 4 H, CH_2), 2.02 (tt, $^3J_{H,H}$ = 7.5 Hz, 2 H, CH_2), 1.79 (s, 6 H, CH_3). **^{13}C-NMR (75.47 MHz,**

$CDCl_3$): δ (ppm) = 167.8 (C_q), 145.4 (C_q), 135.1 (C_q), 117.9 (C_q), 66.3 (CH_2), 48.7 (CH_2), 38.0 (CH_2), 22.5 (CH_2), 11.9 (CH_3). **HRMS (ESI+):** *m/z* = 433.166 (calcd. 433.173 for $[C_{21}H_{29}N_4O_2S_2]^+$).

Isolation of ring-closed isomer 4b

A solution of **4a** (100 mg, 0.23 mmol) in 40 mL of acetonitrile containing 0.1 M Et_4NPF_6 was oxidized at a potential of 0.8 V using a divided H-cell with platinum nets as working and counter electrode and a standard calomel electrode (SCE) as reference. After a charge of 2 C/mol was transferred the mixture was reduced at a potential of -0.2 V. Then, the solvent was removed *in vacuo* and the residue was taken up with 200 mL of water. After extraction with 4 x 50 mL of chloroform the combined organic phases were dried over $MgSO_4$ and evaporated. Purification by column chromatography (petrol ether/ethyl acetate 2:1) afforded **4b** (50 mg, 0.12 mmol, 50 %) as a yellow solid.

^{1}H-NMR (500 MHz, $CDCl_3$): δ (ppm) = 3.74 (t, $^3J_{H,H}$ = 5.0 Hz, 8 H, CH_2), 3.54 (t, $^3J_{H,H}$ = 5.0 Hz, 8 H, CH_2), 2.55 – 2.42 (m, 4 H, CH_2), 1.79 (m, 2 H, CH_2), 1.72 (s, 6 H, CH_3). **^{13}C-NMR (125.77 MHz, $CDCl_3$):** δ (ppm) = 165.3 (C_q), 146.1 (C_q), 121.8 (C_q), 70.3 (C_q), 66.5 (CH_2), 48.5 (CH_2), 29.7 (CH_2), 27.2 (CH_2), 26.1 (CH_3). **HRMS (ESI+):** *m/z* = 433.163 (calcd. 433.173 for $[C_{21}H_{29}N_4O_2S_2]^+$).

5-Methyl-2-morpholinothiazole (6)

2-Bromo-1,1-diethoxypropane (11.00 g, 52.1 mmol), morpholine-*N*-carbothioamide (**5**) (6.93 g, 47.4 mmol), and *p*-toluenesulfonic acid (450 mg, 2.4 mmol) were dissolved in a mixture of 200 mL of ethanol and 20 mL of water. After stirring for 24 h at 90 °C consumption of the starting material was indicated by TLC. After cooling to room temperature an aqueous solution of $NaHCO_3$ was added until gas evolution ceased. The precipitate was filtered off and washed with ethanol. The filtrate was concentrated *in vacuo* and extracted with 3 x 100 mL of dichloromethane. The combined organic layers were washed with brine and dried over anhydrous $MgSO_4$. Purification by column chromatography (ethyl acetate) afforded 5-methyl-2-morpholinothiazole (**6**) (4.81 g, 26.1 mmol, 55 %) as a pale yellow solid.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 6.81 (q, $^4J_{H,H}$ = 1.2 Hz, 1 H, CH_{ar}), 3.78 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.38 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 2.28 (d, $^4J_{H,H}$ = 1.2 Hz, 3 H, CH_3). **^{13}C-NMR (75.5 MHz, $CDCl_3$):** δ (ppm) = 170.9 (C_q), 135.9 (CH), 122.4 (C_q), 66.2 (CH_2), 48.7 (CH_2), 12.1 (CH_3).). **HRMS (ESI+):** *m/z* = 185.063 (calcd. 185.075 for $[C_8H_{13}N_2OS]^+$).

5-Methyl-2-morpholino-4-(tributylstannyl)thiazole (7)

5-Methyl-2-morpholinothiazole (**6**) (4.09 g, 22.2 mmol) was dissolved in 120 mL of dry THF and the mixture was cooled to -78 °C. *tert*-Butyllithium (1.6 M in pentane, 14.92 mL, 24.4 mmol) was added dropwise and the mixture was stirred for 25 min. Tributyltinchloride (6.97 mL, 24.4 mmol) was added and the mixture was allowed to warm to room temperature over a period of 1 h. After the addition of 10 mL of an aqueous solution of NH_4Cl the mixture was extracted with 3 x 100 mL of diethylether. The combined organic layers were washed with brine and dried over $MgSO_4$. Evaporation of the solvent afforded compound **7** (13.08 g, quant.) as a yellow oil which was used without further purification.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.80 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.41 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 2.34 (s, 3 H, CH_3), 1.60 – 1.45 (m, 6 H, CH_2), 1.37 – 1.28 (m, 6 H, CH_2), 1.12 – 1.04 (m, 6 H, CH_2), 0.92 – 0.88 (m, 9 H, CH_3).

2-Morpholinothiazole

2-Bromo-1,1-diethoxyethane (17.60 mL, 117.0 mmol), morpholine-*N*-carbothioamide (**5**) (15.00 g, 103.0 mmol) and *p*-toluenesulfonic acid (0.98 g, 5.1 mmol) were dissolved in a mixture of 400 mL of ethanol and 40 mL of water. After stirring for 24 h at 90 °C consumption of the starting material was indicated by TLC. After cooling to room temperature an aqueous solution of Na_2CO_3 was added until gas evolution ceased. The precipitate was filtered off and washed with ethanol. The filtrate was concentrated *in vacuo* and extracted with 3 x 100 mL of ethyl acetate. The combined organic layers were washed with brine and dried over $MgSO_4$. Evaporation of the solvent afforded 2-morpholinothiazole (17.0 g, 99.9 mmol, 97 %) as a yellow oil.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.19 (d, $^3J_{H,H}$ = 3.6 Hz, 1 H, CH_{ar}), 6.58 (d, $^3J_{H,H}$ = 3.6 Hz, 1 H, CH_{ar}), 3.79 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.44 (t, $^3J_{H,H}$ = 4.8 Hz, 4 H, CH_2). **^{13}C-NMR (75.47 MHz, $CDCl_3$):** δ (ppm) = 172.5 (C_q), 139.7 (*C*H), 107.9 (*C*H), 66.3 (CH_2), 48.8 (CH_2).

5-Iodo-2-morpholinothiazole (9)

2-Morpholinothiazole (2.03 g, 11.9 mmol) was dissolved in 70 mL of dry THF and the mixture was cooled to -80 °C. *n*-Butyllithium (2.2 M in cyclohexane, 5.95 mL, 13.1 mmol) was added dropwise and the mixture was stirred at -80 °C for 20 min and warmed to -10 °C over 10 min. Then, a solution of iodine (3.62 g, 14.2 mmol) in 10 mL of THF was added and the resulting mixture was stirred at -10 °C for 30 min. After the addition of 20 mL of brine the mixture was extracted with 3 x 50 mL of diethylether, the combined organic phases were washed with an aqueous solution of $NaHCO_3$, an aqueous solution of $Na_2S_2O_3$, and brine, and were dried over $MgSO_4$. After evaporation of the solvent the crude product was filtered through a plug of silica using ethyl acetate as solvent to afford 5-iodo-2-morpholinothiazole (**9**) (2.95 g, 10.0 mmol, 84 %) as a yellow solid.

^{1}H-NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.20 (s, 1 H, CH_{ar}), 3.79 (t, $^3J_{H,H}$ = 5.0 Hz, 4 H, CH_2), 3.42 (t, $^3J_{H,H}$ = 5.0 Hz, 4 H, CH_2). **^{13}C-NMR (125.77 MHz, $CDCl_3$):** δ (ppm) = 175.5 (C_q), 147.3 (*C*H), 66.2 (CH_2), 55.0 (*C*-I), 48.6 (CH_2). **HRMS (ESI+):** *m/z* = 296.941 (calcd. 296.956 for $[C_7H_{10}IN_2OS]^+$).

2-Morpholino-5-trifluoromethylthiazole (10)

In analogy to a literature procedure,[5] KF (2.23 g, 38.4 mmol) and CuI (1.83 g, 9.6 mmol) were put into a Schlenk-tube equipped with a magnetic stirrer and a Teflon-coated screw-cap. The tube was evacuated and heated with the heatgun for 5 min until a pale greenish color evolved. Then, 2-morpholino-5-iodothiazole (**9**) (1.90 g, 6.4 mmol) was added and the tube was evacuated and refilled with argon twice. After the addition of 6 mL of dry DMF and 6 mL of dry NMP the mixture was stirred at room temperature for 5 min. $TMSCF_3$ (1.23 mL, 8.32 mmol) was added, the screw-cap was closed, and the tube was heated to 50 °C for 4.5 h. After cooling to room temperature, the mixture was poured into 50 mL of a diluted aqueous solution of ammonia and extracted with 3 x 30 mL of diethylether. The combined organic phases were washed with diluted ammonia solution until the aqueous phase remained colorless, washed with aqueous $NaHCO_3$ solution and brine, and dried over $MgSO_4$. After evaporation of the solvent the crude product was purified by column chromatography (dichloromethane/ethyl acetate 8:1) affording 2-morpholino-5-trifluoromethylthiazole (**10**) (0.55 g, 2.3 mmol, 36 %) as a white solid.

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[5] Cottet, F.; Schlosser, M. *Eur. J. Org. Chem.* **2002**, *2002*, 327-330.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.41 (s, 1 H, CH_{ar}), 3.80 (t, $^{3}J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.49 (t, $^{3}J_{H,H}$ = 4.8 Hz, 4 H, CH_2). **^{13}C-NMR (75.47 MHz, $CDCl_3$):** δ (ppm) = 173.6 (C_q), 141.8 (q, $^{3}J_{C,F}$ = 4 Hz, *C*H), 122.6 (q, $^{1}J_{C,F}$ = 267 Hz, *C*F_3), 114.0 (q, $^{2}J_{C,F}$ = 39 Hz, *C*-CF_3), 66.0 (CH_2), 48.4 (CH_2). **^{19}F-NMR (282.38 MHz, $CDCl_3$):** δ (ppm) = -54.89 (s, CF_3). **HRMS (ESI+):** *m/z* = 239.040 (calcd. 239.047 for $[C_8H_9F_3N_2OS]^+$).

2-Morpholino-4-(tributylstannyl)-5-trifluoromethylthiazole (11)

2-Morpholino-5-trifluoromethylthiazole (**10**) (0.47 g, 1.98 mmol) was dissolved in 15 mL of dry THF and cooled to -78 °C. *tert*-Butyllithium (1.7 M in pentane, 1.40 mL, 2.38 mmol) was added dropwise and the yellow solution was stirred for 25 min at that temperature. Then, Bu_3SnCl (0.64 mL, 2.38 mmol) dissolved in 2 mL of THF was added and the resulting colorless solution was stirred at -78 °C for 1 h. After warming to room temperature, the reaction was quenched by adding 10 mL of a saturated aqueous NH_4Cl-solution and the mixture was extracted with 3 x 20 mL of diethylether. The combined organic phases were washed with aqueous $NaHCO_3$-solution and brine, and were dried over $MgSO_4$. Evaporation of the solvent gave crude stannane **11** (1.27 g, quant.) as a pale yellow oil that was used without further purification.

^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.81 (t, $^{3}J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 3.51 (t, $^{3}J_{H,H}$ = 4.8 Hz, 4 H, CH_2), 1.57 – 1.49 (m, 6 H, CH_2), 1.35 – 1.28 (m, 6 H, CH_2), 1.14 – 1.10 (m, 6 H, CH_2), 0.88 (m, CH_3). **^{13}C-NMR (75.47 MHz, $CDCl_3$):** δ (ppm) = 173.0 (C_q), 66.2 (CH_2), 48.9 (CH_2), 29.0 (CH_2), 27.4 (CH_2), 13.8 (CH_3), 11.0 (CH_2); signals for quaternary carbons are not visible due to splitting by C-F couplings. **^{19}F-NMR (282.38 MHz, $CDCl_3$):** δ (ppm) = -51.87 (s, CF_3).

2. Photochemistry

UV/vis spectroscopy was performed on a Cary 50 spectrophotometer equipped with a Peltier thermostated cell holder at 25 ± 0.05 °C. Irradiation experiments were carried out in spectrophotometric grade acetonitrile or cyclohexane in quartz cuvettes using an Oriel 68810 500 W mercury-lamp in combination with an Oriel 77200 monochromator and an electronic shutter.

Determination of quantum yields

For the determination of quantum yields the "initial slope" method was used: The exact rate equation for the pure photochemical interconversion between species A and B denotes

$$\frac{da}{dt} = -\frac{db}{dt} = 1000 \cdot I_0 \cdot \frac{1-10^{-E'}}{E'} \cdot \left(-\Phi_{AB} \cdot \varepsilon'_A \cdot a + \Phi_{BA} \cdot \varepsilon'_B \cdot b\right) \qquad (1)$$

with I_0 as the light flux, E' as the total extinction at the irradiation wavelength, Φ_{AB} and Φ_{BA} as the quantum yields for the forward and back reaction, and ε'_A and ε'_B as the extinction coefficients of A and B at the irradiation wavelength. As this equation cannot be integrated in a closed form, a simplification is made by assuming that within the first 5 % of conversion the overall extinction at the irradiation wavelength E' stays constant and that the amount of the formed photoisomer is small letting the back reaction become negligible. Monitoring the process at a wavelength where only one isomer absorbs (typically the ring-closed isomer of diarylethenes) allows for the application of Beer's Law giving

$$\frac{dE^{obs}}{dt} = \pm\Phi_{AB} \cdot \varepsilon^{obs} \cdot 1000 \cdot I_0 \cdot \left(1-10^{-E'}\right) \qquad (2)$$

with E^{obs} the extinction at the observation wavelength and ε^{obs} the extinction coefficient of the observed isomer at the observation wavelength.

For ring-opening of diarylethenes **1b**, **2b**, and **4b** the maximum of the absorption band in the visible range was used as observation wavelength. In case of ring-closure reactions a wavelength in the visible range was used at which the absorbance of the ring-open isomer is minimal. From a plot of ΔE^{obs} against Δt containing at least 6 data points within the 5 % conversion limit the respective quantum yield was extracted by linear regression using equation 2.

I_0 values were obtained by measuring standard actinometers using the same procedure, i.e. azobenzene in methanol[6] for UV-irradiations (280 nm, 313nm) and Aberchrome 670 in toluene[7] for irradiations with visible light (436 nm, 546 nm). Thus obtained I_0-values did not alter significantly during the time needed for the determination of quantum yields.

The error for quantum yields determined with this procedure is assumed to be ±10 %.

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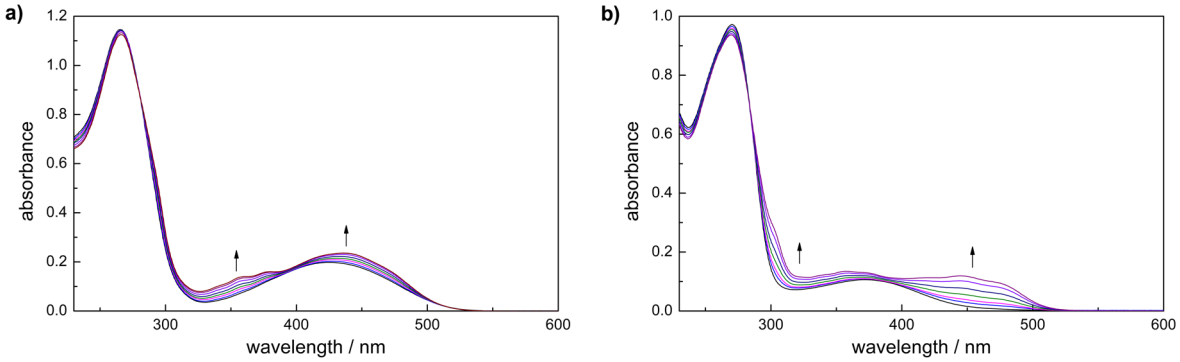

Figure S1. UV/vis spectra during the course of irradiation of solutions of a) **1a** and b) **2a** in cyclohexane ($c = 5 \cdot 10^{-5}$ M) with UV-light ($\lambda_{irr} = 280$ nm) until reaching the photostationary state.

Table S1. Photophysical properties of **1a/b** and **2a/b** in cyclohexane.

comp.	λ_{max} [nm] (ε [10^3 L mol^{-1} cm^{-1}])		$\Phi_{o \rightarrow c}$ (280 nm)	conversion (280 nm)[a]
	open isomer	closed isomer		
1a/b	266 (24.4), 425 (4.2)	356 (10.4), 443 (10.2)	0.05	16 %
2a/b	270 (20.7), 373 (2.3)	449 (11.6)	0.05	16 %

a) Amount of ring-closed isomer in the photostationary state upon irradiation with UV-light determined by UPLC.

3. Cyclic Voltammetry

Cyclic voltammetry was performed using a PG310 USB (HEKA Elektronik) potentiostat interfaced to a PC with PotMaster v2x43 (HEKA Elektronik) software for data evaluation. A three-electrode configuration contained in a non-divided cell consisting of a platinum disc (d = 1 mm) as working electrode, a platinum plate as counter-electrode, and a saturated calomel electrode (SCE) with an agar-agar-plug in a Luggin capillary with a diaphragm as reference electrode was used. Measurements were carried out in acetonitrile (HPLC-grade, dried over calcium hydride and distilled) containing 0.1 M Bu_4NPF_6 using a scan rate of dE/dt = 1 V s^{-1}. The data is given in reference to the ferrocene redox couple (Fc/Fc^+), which was used as external standard. Peak potentials of all compounds are reported in Table 2 of the manuscript; cyclic voltammograms of compounds **1a/b**, **2a/b**, and **3a/b** are shown in Figure 4 and in Figure 6 of the manuscript. Cyclic voltammetry of compound **4a** is shown in Figure S2.

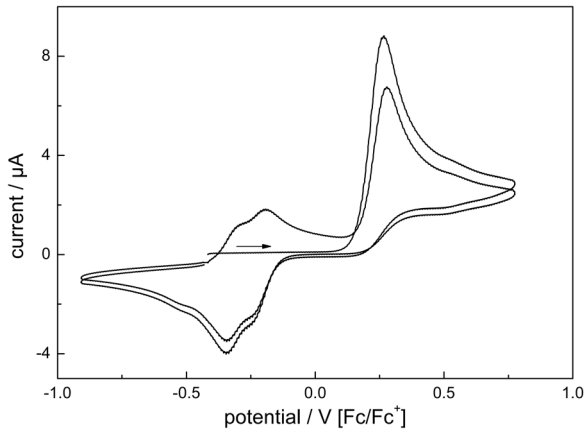

Figure S2. Cyclic voltammetry of **4a** in acetonitrile ($c = 1 \cdot 10^{-3}$ M). Two consecutive cycles are shown.

Additionally, CVs of compound **3a** were recorded using different scan rates between 100 mV/s and 1 V/s revealing the quasireversible nature of the first oxidation process at E_p = 0.70 V (Figure S3). While at higher scan rates the oxidation is fully reversible an irreversible reaction of the radical cation takes place at lower scan rates. However, the linear dependence of the peak current with the square root of the scan rate shows that the one-electronic nature of the oxidation is not altered (Figure S3, inset). Note that in contrast of the irreversible second oxidation step the quasireversible first oxidation does not yield the ring-closed isomer **3b** in any case.

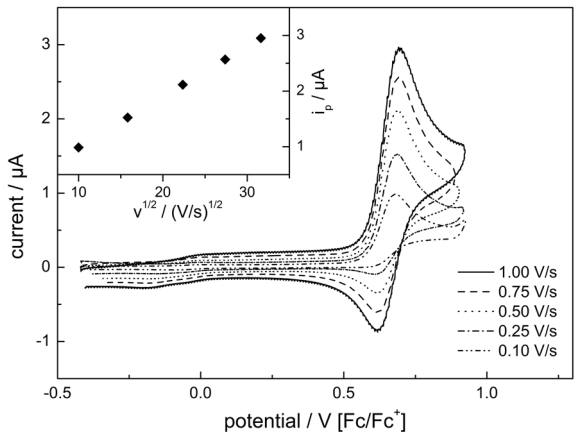

Figure S3. Cyclic voltammetry of **3a** in acetonitrile ($c = 1 \cdot 10^{-3}$ M) at varying scan rates.

4. Spectroelectrochemistry of 1a

Spectroelectrochemistry was performed using a quarz cuvette with 1 mm pathlength in an Avantes AvaSpec-2048x14 spectrometer combined with a AvaLight-DH-S-BAL light source. The cuvette was equipped with a platinum net as working electrode, a platinum wire as counter electrode, and an $Ag/AgNO_3$ reference electrode connected to an Autolab PGSTAT128N potentiostat from Metrohm GmbH, Germany. An acetonitrile solution of **1a** ($c = 5 \cdot 10^{-4}$ M) containing 0.1 M Bu_4NPF_6 was placed in the cuvette and a potential scan was performed using a scan rate of 10 mV/s while UV/vis-spectra were recorded every 10 mV. As reference the ferrocene/ferrocenium redox couple was determined to have an oxidation potential of 0.21 V in this configuration.

The initially observed UV/vis-spectrum shows absortpion bands typical for the ring-open isomer **1a** (Figure S4). Upon oxidation a new absorption band around 350 nm evolves, assigned to the dicationic ring-closed isomer $\mathbf{1b}^{2+}$. During the back sweep of the potential a broad, strongly blue-shifted absorption is observed, assigned to the monoradical cation $\mathbf{1b}^{\bullet+}$. Upon further reduction to the neutral ring-closed state **1b** this broad band diminishes again.

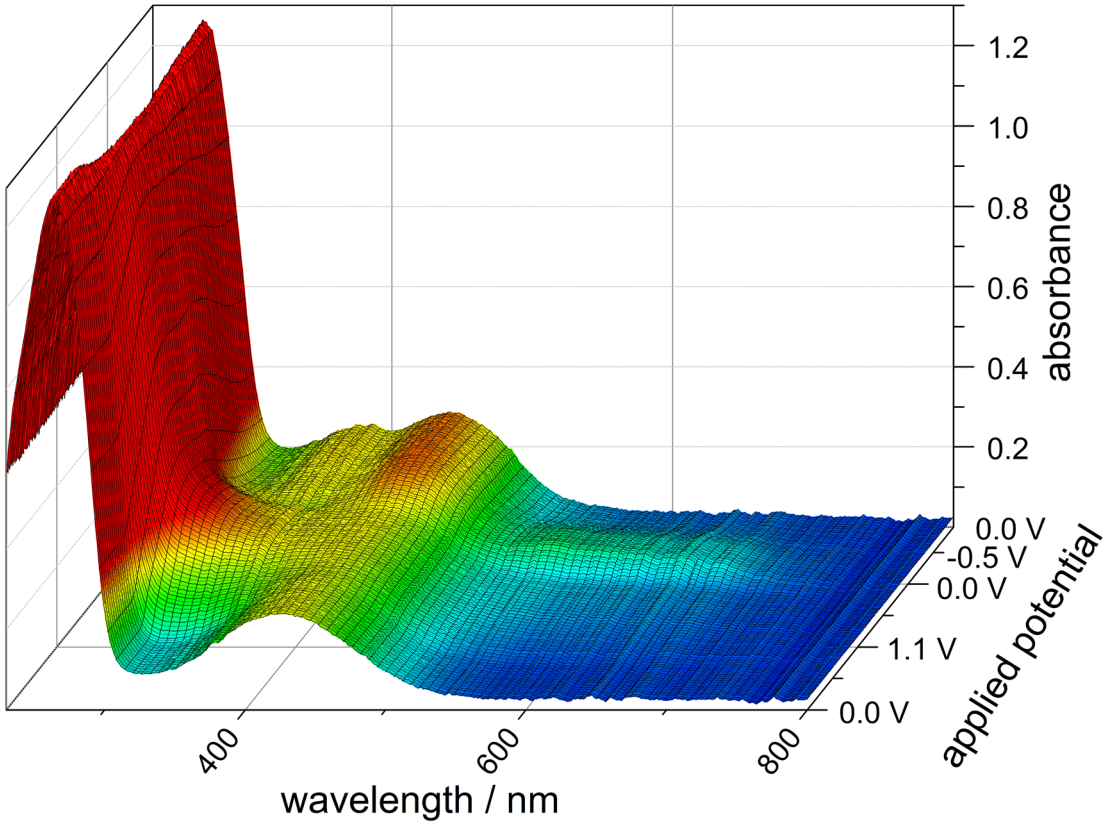

Figure S4. UV/vis spectral changes during cyclic voltammetry of compound **1a** in acetonitrile. The potential scan was performed starting from 0 V [Ag/Ag^+] with return points at 1.1 V [Ag/Ag^+] and -0.5 V [Ag/Ag^+].

5. Repetive electrochemical/photochemical switching of 1a and 2a

Repetive switching was performed with an argon saturated solution of the respective ring-open isomer ($c = 5 \cdot 10^{-4}$ M) in acetonitrile containing 0.1 M Bu_4NPF_6, which was placed into a divided H-cell equipped whith platinum nets as working and counter electrode, a standard calomel electrode (SCE) as reference, and a magnetic stir bar. Each switching cycle consisted of an oxidation step by applying a potential of 1.3 V in case of **1a** or a potential of 1.8 V in case of **2a** over a period of 5 min, immediately followed by a reduction at a potential of -0.3 V [SCE]. This procedure led to formation of the ring-closed isomer. Ring-opening was then accomplished by irradiating the cell with visible light using a 1000 W Xe lamp in combination with a cutoff-filter ($\lambda > 430$ nm) until no further changes could be observed by UV/vis spectroscopy. After each reduction step and irradiation step an analytical sample of the mixture was analyzed by UV/vis spectroscopy (see Figure 5b and 5e in the manusscript) and by UPLC (see Figure 5a and 5d in the manuscript).

6. Low temperature NMR of 1c

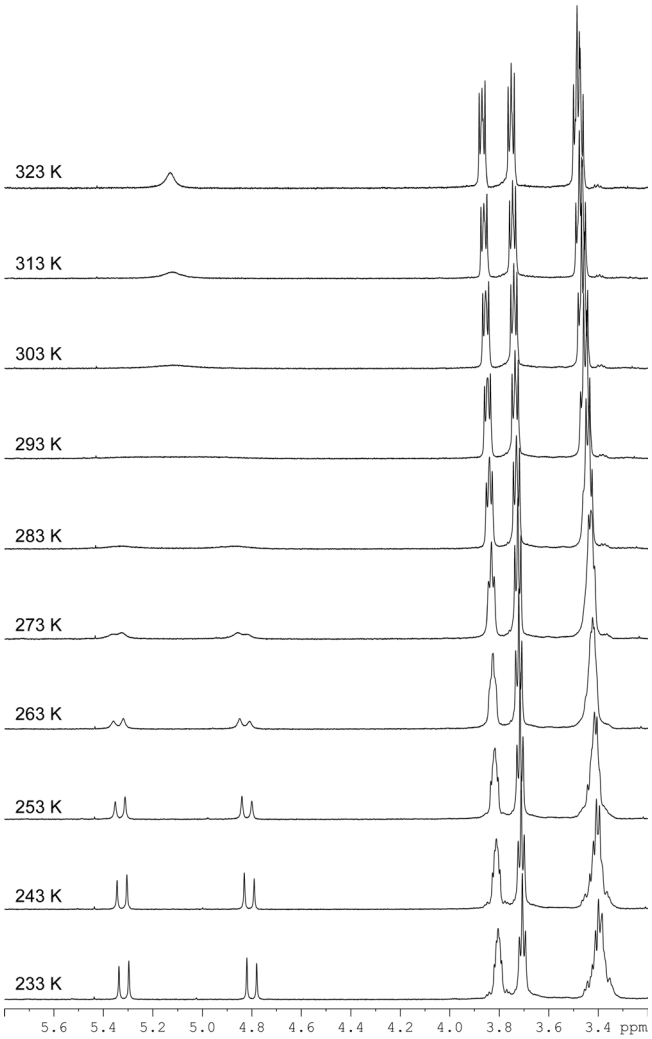

Figure S5. Detail of low temperature NMR spectra of **1c** in CD_3CN showing dynamic behavior of the bridging CH_2-group.

7. X-ray crystallography

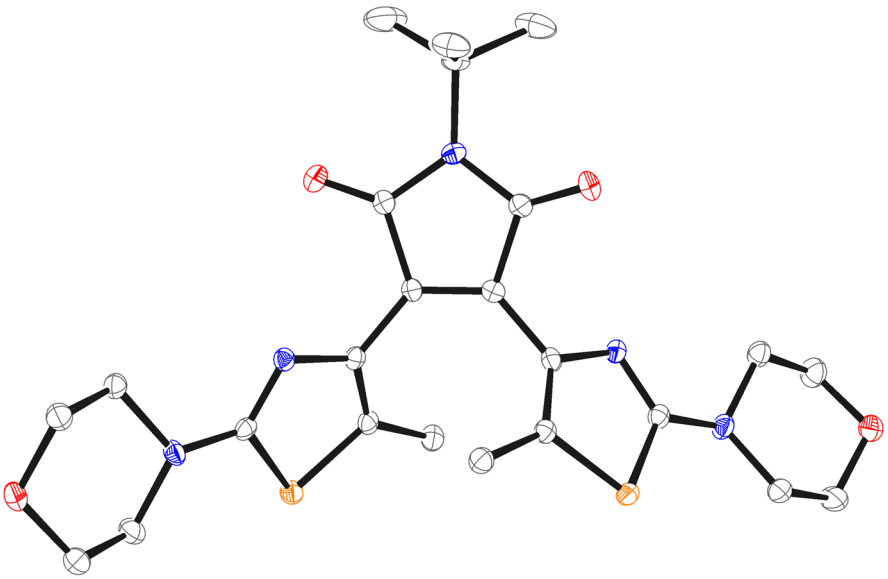

Figure S6. ORTEP-drawing (50 % probability thermal ellipsoids) of the molecular structure of **1a** in the crystal as determined by X-ray diffraction. Hydrogens are omitted for clarity. The unit cell consisted of a second molecule of **1a,** which only has minor differences in the conformation of one morpholino ring, and an additional solvent molecule (CH_3CN).

Crystal data for **1a** (CCDC: 904567):

Empirical formula	$C_{50}\ H_{65}\ N_{11}\ O_8\ S_4$
Formula weight	1076.41
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.5692(5) Å , α= 114.843(4) deg. b = 16.6697(9) Å, β = 100.625(4) deg. c = 18.3711(9) Å, γ = 90.647(4) deg.
Volume	2600.7(2) $Å^3$
Z, Calculated density	2, 1.375 Mg/m^3
Absorption coefficient	0.248 mm^{-1}
F(000)	1140
Crystal size	0.26 x 0.20 x 0.18 mm
Theta range for data collection	4.69 to 25.00 deg.
Limiting indices	-11<=h<=11, -19<=k<=17, -21<=l<=21
Reflections collected / unique	23457 / 8949 [R(int) = 0.0569]
Completeness to theta = 25.00	97.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9979 / 6 / 669
Goodness-of-fit on F^2	0.947
Final R indices [I>2σ(I)]	R_1 = 0.0426, wR^2 = 0.0757
R indices (all data)	R_1 = 0.0763, wR^2 = 0.0852
Largest diff. peak and hole	0.466 and -0.308 e $Å^{-3}$

Crystal data for **1c** (CCDC: 904568, see Figure 5c in the manusscript):

Empirical formula	$C_{24}H_{30}ClN_5O_8S_2$
Formula weight	616.10
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 10.7226(13) Å, α = 90 deg.
	b = 16.7313(14) Å, β = 90.781(11) deg.
	c = 14.7188(21) Å, γ = 90 deg.
Volume	2640.4(5) $Å^3$
Z, Calculated density	4, 1.550 Mg/m^3
Absorption coefficient	0.363 mm^{-1}
F(000)	1288
Crystal size	0.20 x 0.06 x 0.05 mm
Theta range for data collection	2.26 to 25.50 deg.
Limiting indices	-12<=h<=12, -19<=k<=20, -17<=l<=17
Reflections collected / unique	20441 / 4899 [R(int) = 0.1268]
Completeness to theta = 25.50	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4899 / 174 / 366
Goodness-of-fit on F^2	1.026
Final R indices [I>2σ(I)]	R_1 = 0.1099, wR^2 = 0.2809
R indices (all data)	R_1 = 0.1705, wR^2 = 0.3130
Largest diff. peak and hole	0.738 and -0.500 e A^{-3}

8. Quantum chemical methods

Density functional theory (DFT) calculations were performed using the B3LYP[8] and CAM-B3LYP[9] functionals with the 6-31G* basis set.[10] Minimum structures were obtained from ground state optimizations of the open and closed forms of the diarylethenes **1**-**4**. The minimum character was confirmed by normal mode analysis. All energies were calculated without zero-point correction.

In addition to neutral species, also singly and doubly charged cationic species were considered. All neutral species were treated as singlets, using restricted density functional theory (*e.g.*, (R)B3LYP). Singly charged cations were doublets, treated with unrestricted methods (*e.g.*, UB3LYP). For doubly charged cations closed-shell singlets (by (R)B3LYP, for example), triplets and singlet biradicals were considered. For triplets and biradical singlets, unrestricted DFT was used, in the latter case with an asymmetric guess (broken symmetry approach) in order to allow for unpaired spin density. Besides the equilibrium geometries, also transition states were determined, by the QST3 method.[11]

The solvent influence was modeled using the Polarizable Continuum Model (PCM).[12] Besides gas phase calculations, calculations were carried out for cyclohexane, tetrahydrofuran, and acetonitrile. The respective dielectric constants for the polarizable continuum are ε = 2.02, 7.43, and 35.69, respectively.

Excited states of neutral, singlet molecules (singlet excitation energies, oscillator strengths, and selected excited state geometries) were obtained from linear-response time-dependent DFT (TD-DFT) calculations.[13] The lowest 50 excited singlet states were computed. From the calculated oscillator strengths f_i and the corresponding vertical transition wavenumber $\tilde{\nu}_i = 1/\lambda_i$ extinction coefficients $\varepsilon(\tilde{\nu})$ were calculated by Gaussian broadening as follows:

$$\varepsilon(\tilde{\nu}) = \sum_i \frac{f_i}{\kappa} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{\tilde{\nu}-\tilde{\nu}_i}{\sigma}\right)^2} \qquad (1)$$

Here, $\kappa = 4.319 \cdot 10^{-10}$ mol m^{-1} and σ is an empirical broadening factor. σ was chosen as 1500 cm^{-1} in this work. All results were obtained using the GAUSSIAN 09 program package.[14]

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9. Theoretical UV/vis absorption spectra

Table S2 shows calculated wavelengths, oscillator strengths, and the character of selected intense transitions for compounds **1a**-**4b** in acetonitrile, obtained on the TD-CAM-B3LYP/PCM/6-31G* level of theory. UV/vis absorption spectra for neutral singlet species **1**-**4**, open (**a**) and closed forms (**b**), as obtained from (TD-)B3LYP/PCM/6-31G* for various solvents are summarized in Figure S7 and Table S3.

Table S2. Calculated wavelength λ in nm, oscillator strength *f*, and character of selected intense transitions for compounds **1a**-**4b** in acetonitrile on the TD-CAM-B3LYP/PCM/6-31G* level of theory.

molecule	λ	*f*	character	
1a	394	0.0765	HOMO	→ LUMO
	350	0.0487	HOMO-1	→ LUMO
	242	0.6068	HOMO-1	→ LUMO+2
1b	390	0.4330	HOMO	→ LUMO
	313	0.5544	HOMO	→ LUMO+1
	245	0.2733	HOMO-1	→ LUMO
2a	362	0.0333	HOMO	→ LUMO
	247	0.6963	HOMO-1	→ LUMO+2
	234	0.3888	HOMO-5	→ LUMO
2b	403	0.4552	HOMO	→ LUMO
	308	0.5119	HOMO	→ LUMO+1
	252	0.2907	HOMO-1	→ LUMO
3a	393	0.0706	HOMO	→ LUMO
	248	0.2105	HOMO-1	→ LUMO+1
	242	0.3851	HOMO	→ LUMO+2
3b	395	0.4464	HOMO	→ LUMO
	311	0.5312	HOMO	→ LUMO+1
	248	0.2984	HOMO-1	→ LUMO
4a	277	0.0946	HOMO	→ LUMO
	233	0.2597	HOMO	→ LUMO+1
	229	0.9179	HOMO-1	→ LUMO+1
4b	366	0.4816	HOMO	→ LUMO
	238	0.4444	HOMO	→ LUMO+2
	208	0.4307	HOMO-2	→ LUMO

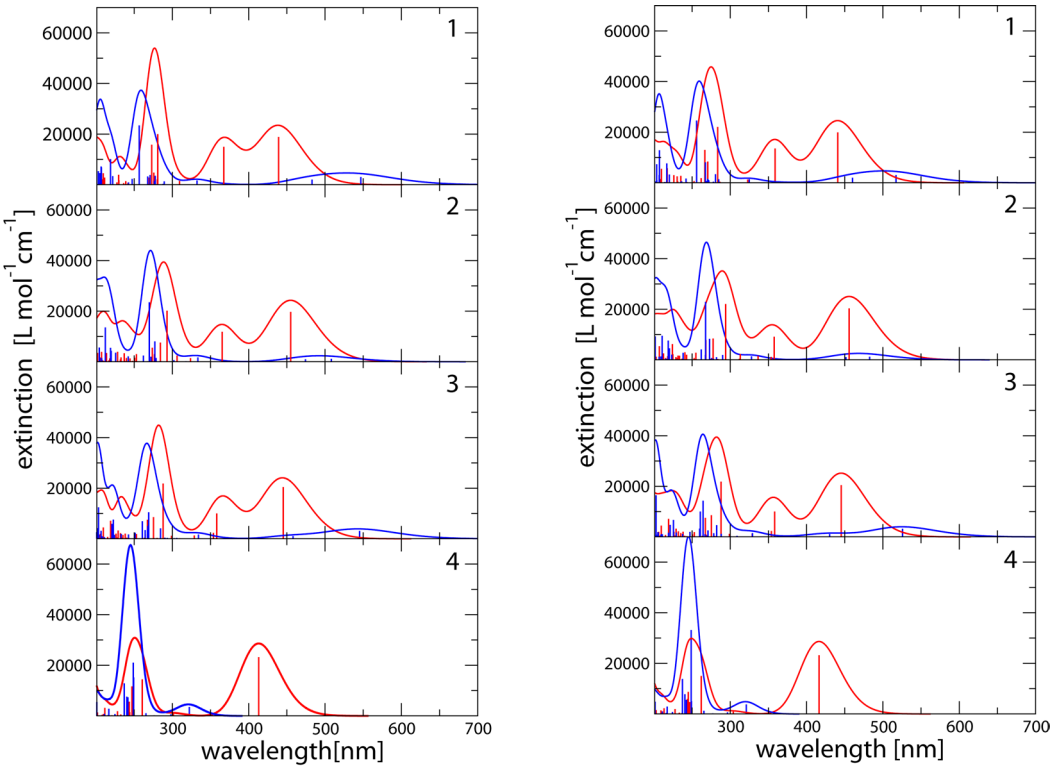


Figure S7. Calculated absorption spectra of **1-4** (**a** in blue, **b** in red) on TD-B3LYP/PCM/6-31G* level of theory. Left: acetonitrile, right: cyclohexane.

Table S3. Wavelength in nm and oscillator strengths (in brackets) of lowest transition, as well as two selected strong excitations with excitation wavelength above 250 nm, for optical absorption of compounds **1a-4b** in gasphase, cyclohexane, tetrahydrofurane, and acetonitrile, all on TD-B3LYP/(PCM)/6-31G* level of theory.

	gasphase	**cyclohexane**
1a	496.4 (0.05), 275.7 (0.08), 253.1 (0.45)	517.2 (0.06), 267.5 (0.16), 255.9 (0.49)
1b	433.0 (0.33), 283.8 (0.26), 262.8 (0.25)	440.9 (0.40), 358.7 (0.27), 283.6 (0.44)
2a	464.7 (0.02), 263.9 (0.23), 260.0 (0.24)	482.6 (0.03), 272.9 (0.17), 267.7 (0.46)
2b	446.9 (0.33), 292.7 (0.32), 264.1 (0.14)	455.7 (0.41), 357.6 (0.18), 293.9 (0.44)
3a	509.9 (0.05), 259.7 (0.21), 257.5 (0.19)	525.6 (0.06), 264.4 (0.29), 260.8 (0.20)
3b	436.9 (0.34), 348.8 (0.12), 287.4 (0.30)	445.4 (0.41), 287.9 (0.44), 275.3 (0.17)
4a	318.2 (0.06), 294.7 (0.01), 263.1 (0.02)	321.0 (0.08), 296.4 (0.01), 265.6 (0.03)
4b	409.6 (0.38), 304.8 (0.02), 260.3 (0.19)	416.3 (0.46), 304.0 (0.02), 262.0 (0.30)
	tetrahydrofuran	**acetonitrile**
1a	538.1 (0.06), 267.9 (0.10), 256.5 (0.48)	546.9 (0.06), 277.6 (0.07), 256.6 (0.47)
1b	440.1 (0.39), 365.1 (0.30), 281.6 (0.43)	439.2 (0.38), 280.9 (0.40), 272.9 (0.32)
2a	500.9 (0.02), 276.0 (0.17), 269.5 (0.48)	508.3 (0.02), 277.1 (0.16), 269.9 (0.47)
2b	455.8 (0.40), 363.0 (0.23), 293.2 (0.43)	455.0 (0.39), 365.2 (0.24), 293.0 (0.40)
3a	539.7 (0.06), 267.5 (0.17), 260.8 (0.16)	545.3 (0.06), 268.9 (0.21), 267.8 (0.10)
3b	445.2 (0.40), 363.6 (0.27), 286.7 (0.43)	444.5 (0.39), 286.3 (0.41), 280.6 (0.18)
4a	322.0 (0.07), 297.7 (0.01), 265.6 (0.02)	508.3 (0.02), 277.1 (0.16), 269.9 (0.47)
4b	414.7 (0.47), 302.3 (0.02), 261.2 (0.30)	455.0 (0.39), 365.2 (0.24), 293.0 (0.40)

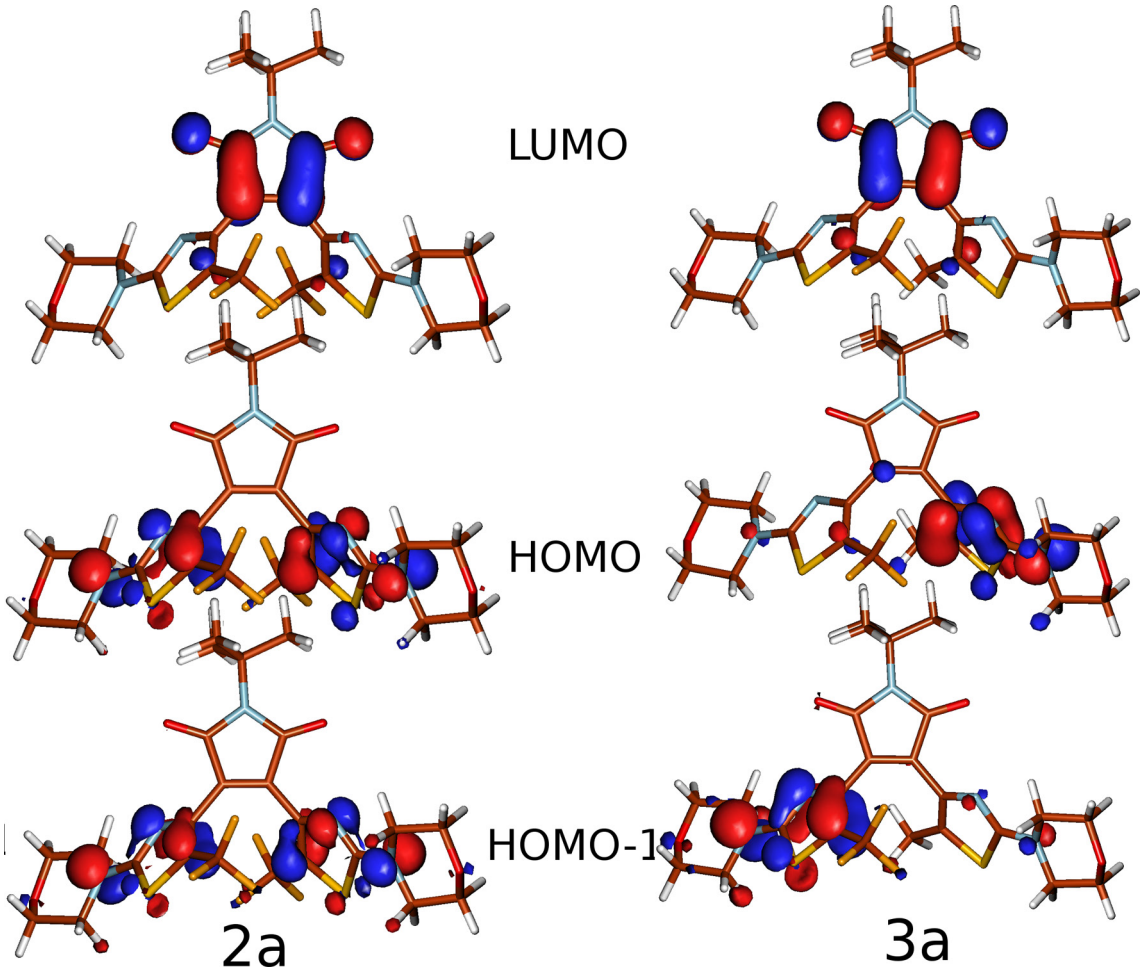


Figure S8. Isocontour plots of frontier orbitals for compounds **1a** and **4a** in acetonitrile, obtained on the CAM-B3LYP/PCM/6-31G* level of theory.

10. Theoretical results on electrochemical switching

Figure S9 shows the largest, atom-projected Mulliken spin densities of the **1a** dication, for the triplet (^{T}**1a**$^{2+}$, only α-spins) and broken symmetry singlet (^{SU}**1a**$^{2+}$, α and β spins). Note that the unpaired electrons are localized at the two morpholino thiazole rings, where they are distributed over several atoms.

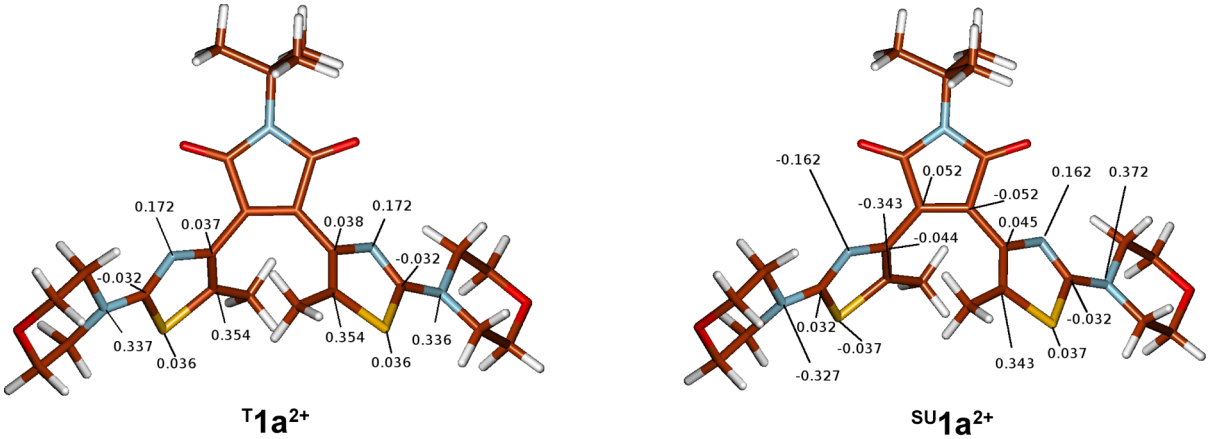


Figure S9. Mulliken spin densities of the ^{T}**1a**$^{2+}$ and ^{SU}**1a**$^{2+}$ species, all for UB3LYP/PCM(acetonitrile)/6-31G*, at optimized geometries. Positive numbers: Atomic α spin populations, negative numbers: β spin populations.

Tables S4, S5, and S6 give vertical and adiabatic ionization potentials for acetonitrile or the gasphase, for ions / configurations considered in this work. Table S7 shows for gasphase calculations B3LYP/6-31G* relative energies of reactants and products, activation energies, and maximal energy gains (reorganization energies). Finally Table S8 gives relative energies (B3LYP/PCM(acetonitrile)/6-31G*) for reactant, product, and transition state for the cyclization of compound **3** following a disrotatory pathway. The obtained energetic profile for the thermal cyclization of **3a** reported in Figure 7 of the manuscript is shown again including the energies for the disrotatory pathway in Figure S10.

Table S4. Vertical ionization potentials $IP^{v}(A^{n+} \rightarrow A^{m+})$ in eV calculated as energy differences between neutral (A^0) and not reoptimized ionized forms (A^+ and A^{2+}), obtained on the B3LYP/PCM(acetonitrile)/6-31G* level of theory. For the dication three different configurations were considered.

	$IP^{v}(A^0 \rightarrow A^+)$	$IP^{v}(A^0 \rightarrow A^{2+})$		
	$^{D}A^+$	$^{S}A^{2+}$	$^{SU}A^{2+}$	$^{T}A^{2+}$
1a	5.27	11.66	11.18	11.19
1b	4.91	11.08	11.08	11.90
2a	5.77	12.65	12.03	12.03
2b	5.16	11.62	11.62	12.29
3a	5.45	12.11	11.61	11.62
3b	5.03	11.35	11.35	12.08
4a	4.88	10.90	10.54	10.58
4b	4.32	10.01	10.01	11.00

Table S5. Adiabatic ionization potentials $IP(A^{n+} \rightarrow A^{m+})$ in eV for the gasphase calculated as energy differences between neutral (A^0) and not reoptimized ionized forms (A^+ and A^{2+}), obtained on the B3LYP/6-31G* level of theory. For the dication three different configurations were considered.

	$IP(A^0 \rightarrow A^+)$	$IP(A^0 \rightarrow A^{2+})$		
	$^{D}A^+$	$^{S}A^{2+}$	$^{SU}A^{2+}$	$^{T}A^{2+}$
1a	6.29	16.02	15.62	15.63
1b	5.82	15.06	15.06	16.36
2a	6.79	16.97	16.44	16.45
2b	6.07	15.57	15.57	16.75
3a	6.45	16.42	15.99	16.00
3b	5.95	15.34	15.34	16.56
4a	5.90	-	15.25	15.29
4b	5.21	13.98	13.98	15.67

Table S6. Vertical ionization potentials $IP^v(A^{n+} \rightarrow A^{m+})$ in eV for the gasphase calculated as energy differences between neutral (A^0) and not reoptimized ionized forms (A^+ and A^{2+}), obtained on the B3LYP/6-31G* level of theory. For the dication three different configurations were considered.

	$IP^v(A^0 \rightarrow A^+)$	$IP^v(A^0 \rightarrow A^{2+})$		
	$^DA^+$	$^SA^{2+}$	$^{SU}A^{2+}$	$^TA^{2+}$
1a	6.56	16.83	16.38	16.39
1b	6.15	16.26	16.26	16.79
2a	7.05	17.73	17.20	17.21
2b	6.37	16.68	16.68	17.12
3a	6.73	17.20	16.77	16.78
3b	6.26	16.47	16.47	16.94
4a	6.12	16.15	15.77	15.81
4b	5.56	15.32	15.32	16.13

Table S7. Energies (in eV) relative to open forms (**a**) for compounds **1-4** according to B3LYP/6-31G* gasphase calculations. The ΔE_g values are maximum energy gains of ionic ring-open species as defined in Eq. (2). Product and transition state energies refer to the conrotatory pathway for the cyclization reaction.

	neutral	$^DA^+$	$^SA^{2+}$	$^{SU}A^{2+}$	$^TA^{2+}$
1a	0.00	0.00	0.00	0.00	0.00
1b	-0.16	-0.63	-1.12	-0.72	0.57
1‡	2.32	0.90	0.02	0.48	1.93
ΔE_g		0.27	0.81	0.76	0.76
2a	0.00	0.00	0.00	0.00	0.00
2b	0.05	-0.68	-1.35	-0.83	0.35
2‡	2.26	0.82	0.17	0.65	1.78
ΔE_g		0.26	0.76	0.76	0.76
3a	0.00	0.00	0.00	0.00	0.00
3b	-0.09	-0.59	-1.17	-0.74	0.48
3‡	2.22	0.96	0.16	0.53	1.38
ΔE_g		0.28	0.78	0.78	0.78
4a	0.00	0.00	instable	0.00	0.00
4b	0.07	-0.62	-	-1.21	0.45
4‡	3.81	0.85	-	0.12	1.80
ΔE_g		0.22	-	0.52	0.51

Table S8. Energies (in eV) for a disrotatory cyclization reaction of compound **3** relative to the ring-open form (**a**) according to B3LYP/PCM(acetonitrile)/6-31G* calculations.

	neutral	$^{D}A^{+}$	$^{S}A^{2+}$	$^{SU}A^{2+}$	$^{T}A^{2+}$
3a	0.00	0.00	0.00	0.00	0.00
3b(dis)	0.41	0.06	-0.68	-0.34	1.10
3‡(dis)	1.67	1.18	0.60	0.95	2.08

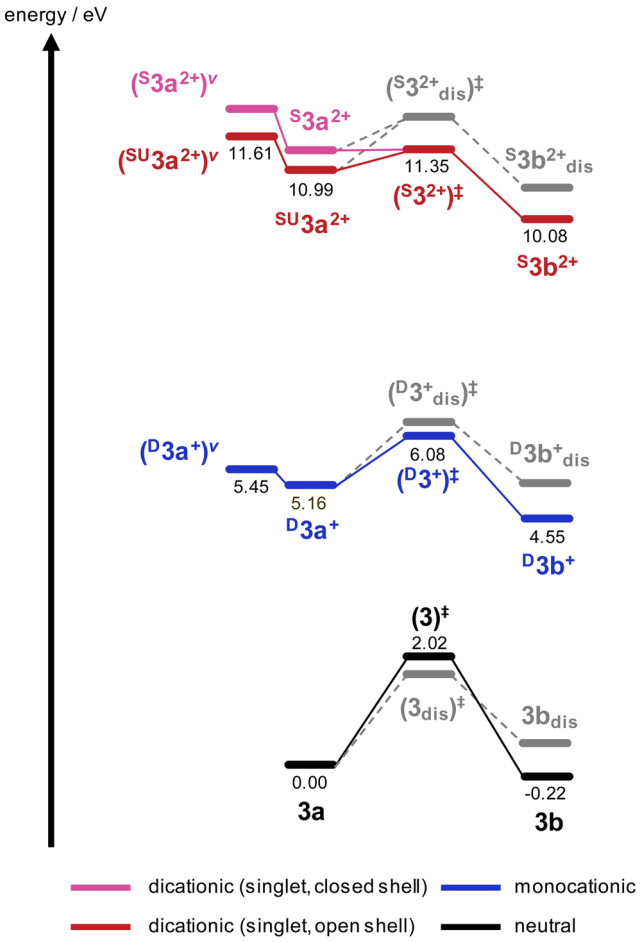
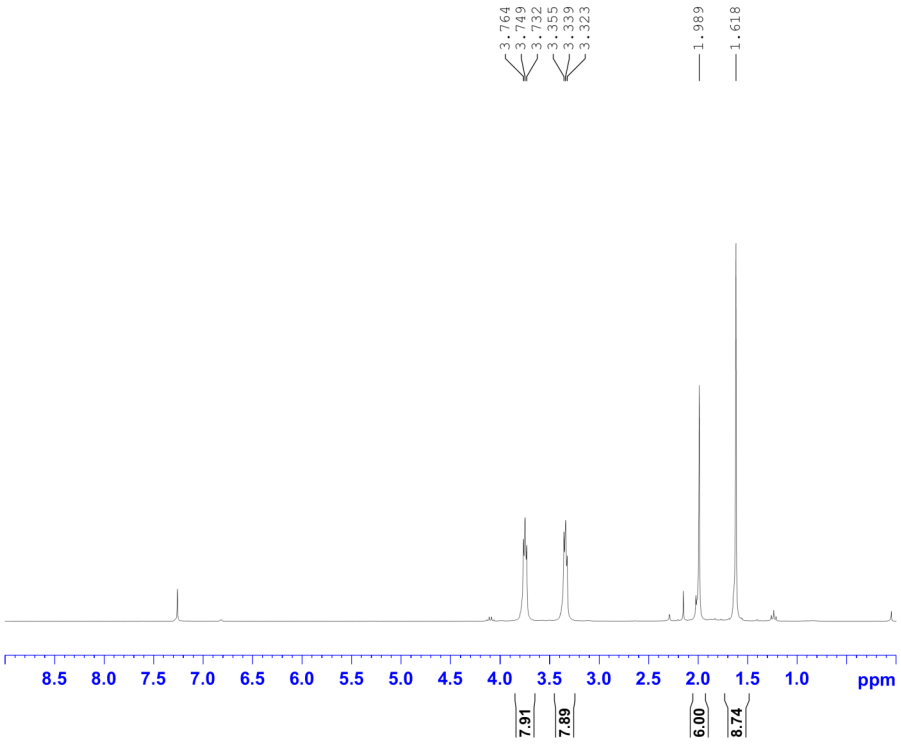


Figure S10. Energy profile for the thermal cyclization reaction of **3a** in its neutral, monocationic, and dicationic forms. Energies are in eV, relative to **3a**.

Appendix 1: ^{1}H- and ^{13}C-NMR spectra

1H, CDCl3, 300 MHz

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PROCNO                 1

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PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                  128
DW                80.800 usec
DE                 6.00 usec
TE                295.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                1H
P1                11.00 usec
PL1               -1.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
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WDW                   EM
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PC                 1.00
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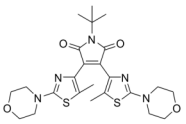
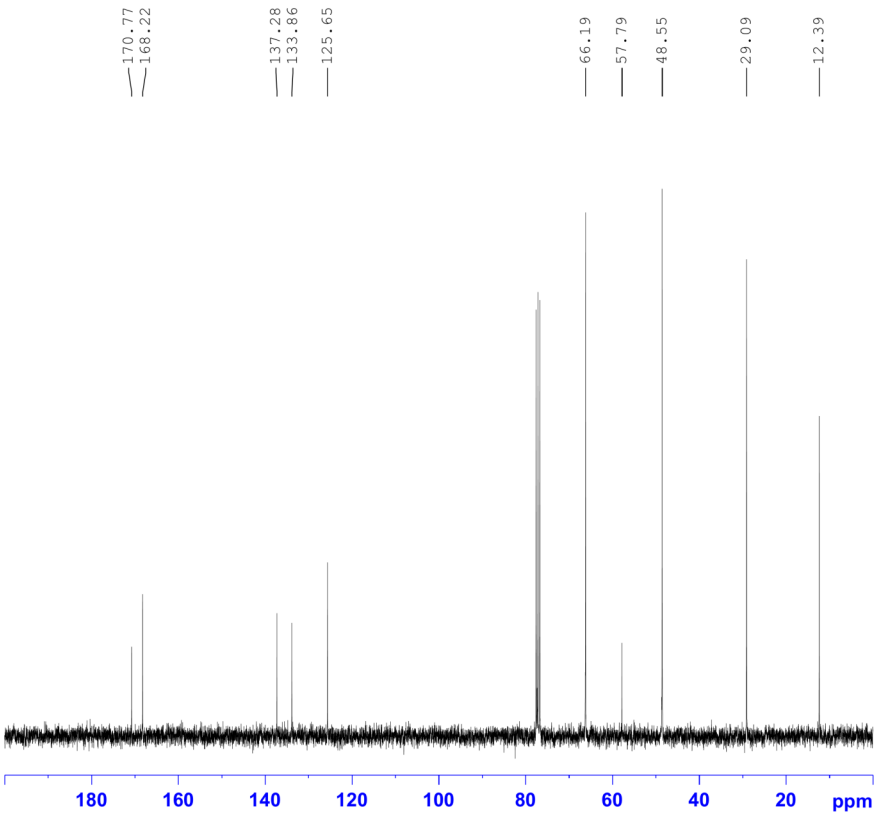


13C, CDCl3, 75.47 MHz

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PROCNO                 1

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PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23809.523 Hz
FIDRES         0.363304 Hz
AQ            1.3763061 sec
RG                    5
DW                21.000 usec
DE                 6.00 usec
TE                295.6 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.00 usec
PL1               -3.00 dB
SFO1         75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             100.00 usec
PL2                -1.00 dB
PL12               18.17 dB
PL13               23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
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SF          75.4677424 MHz
WDW                   EM
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LB                 1.00 Hz
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PC                 1.40
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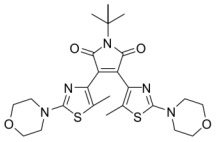
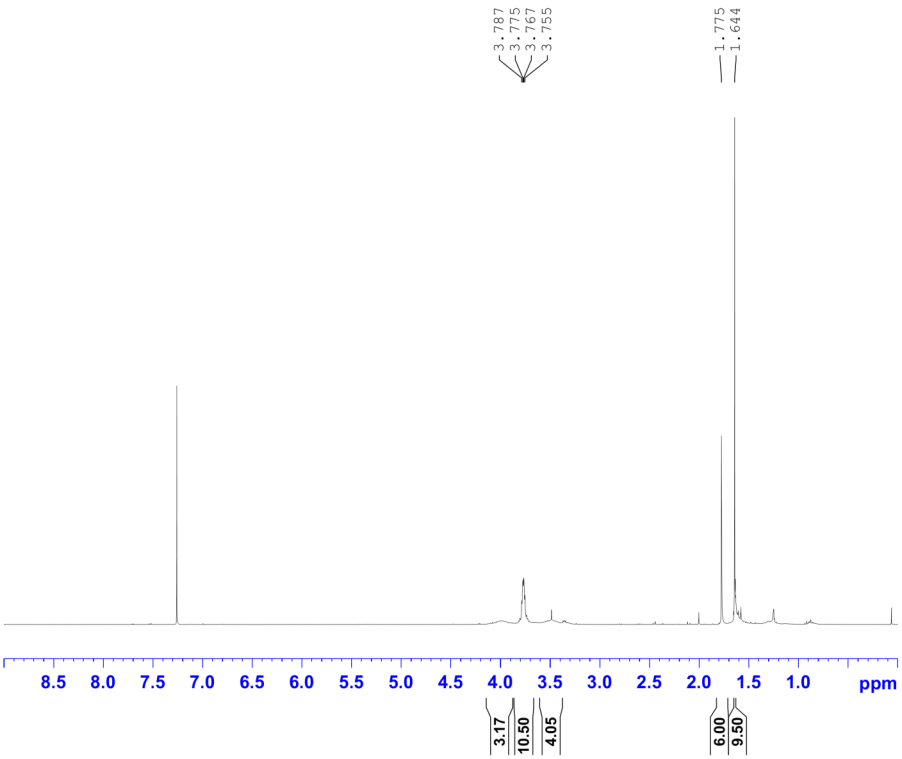


1H, CDCl3, 400 MHz

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PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ             3.9846387 sec
RG                406.4
DW               60.800 usec
DE                6.00 usec
TE               295.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.00 usec
PL1               -1.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
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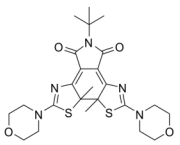
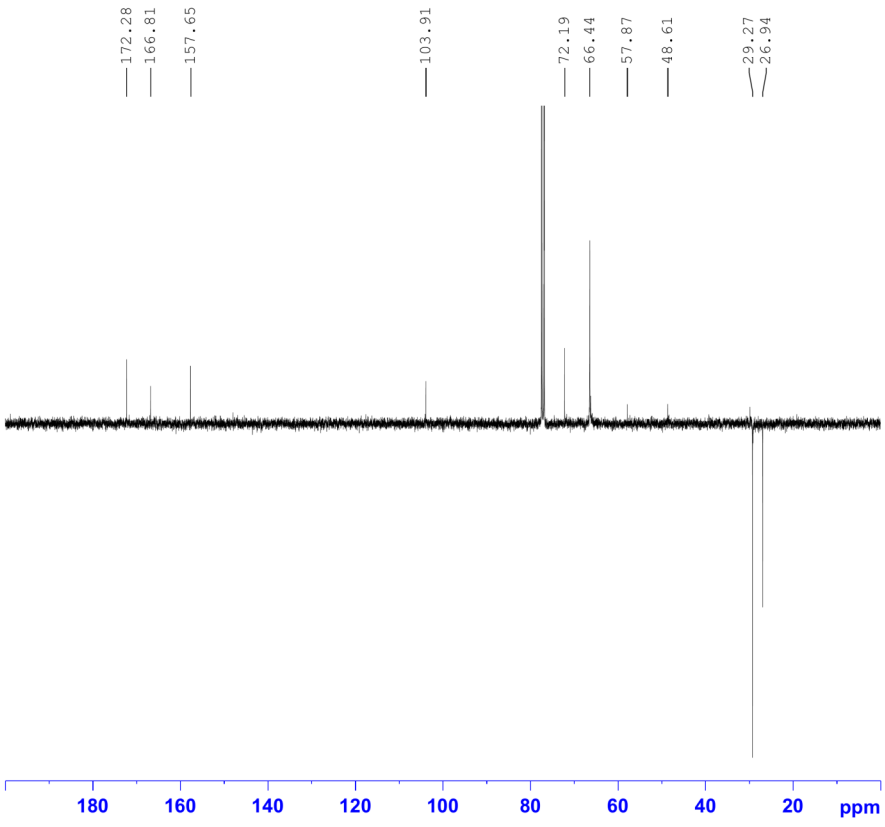


13C-APT, CDCl3, 100.62 MHz

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PULPROG            jmod
TD                65536
SOLVENT           CDCl3
NS                16000
DS                    4
SWH            22075.055 Hz
FIDRES          0.336839 Hz
AQ             1.4844404 sec
RG                23170.5
DW               22.650 usec
DE                6.00 usec
TE               295.8 K
CNST2         145.0000000
CNST11          1.0000000
D1            2.00000000 sec
d20           0.00689655 sec
DELTA         0.00001082 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                8.50 usec
p2               17.00 usec
PL1       0 dB
SFO1         100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2               -1.00 dB
PL12              16.08 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
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SF          100.6127556 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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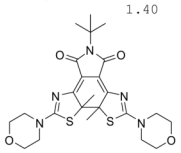
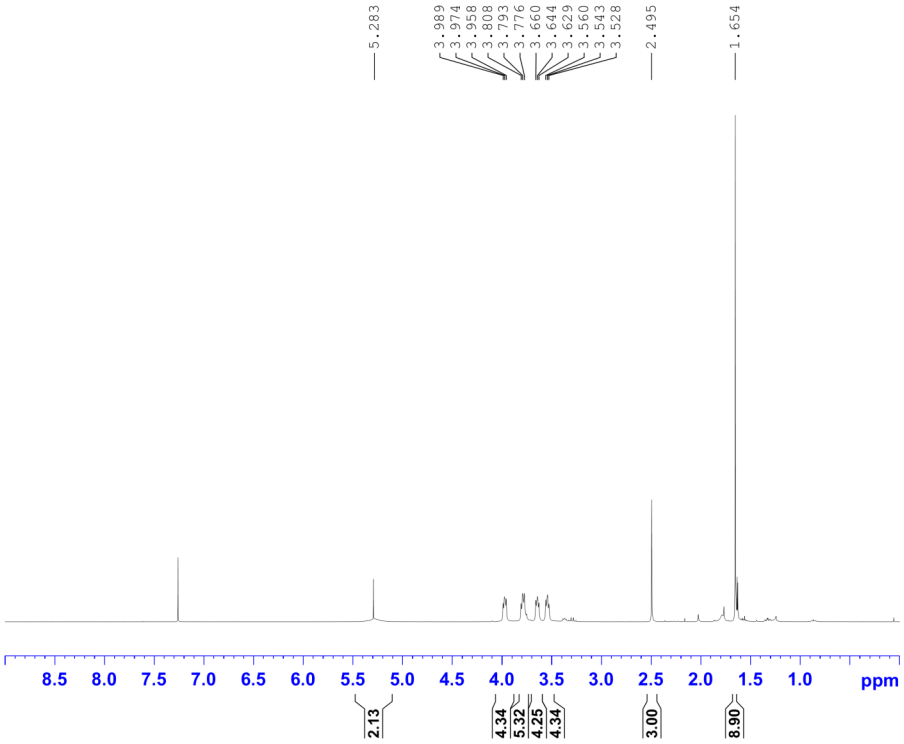


1H, CDCl3, 300 MHz

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PROCNO                       1

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PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 6188.119 Hz
FIDRES              0.094423 Hz
AQ                  5.2953587 sec
RG                       406
DW                    80.800 usec
DE                     6.00 usec
TE                    295.5 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                    -1.00 dB
SFO1             300.1318534 MHz

F2 - Processing parameters
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WDW                           EM
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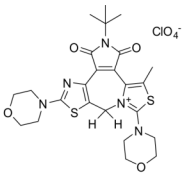
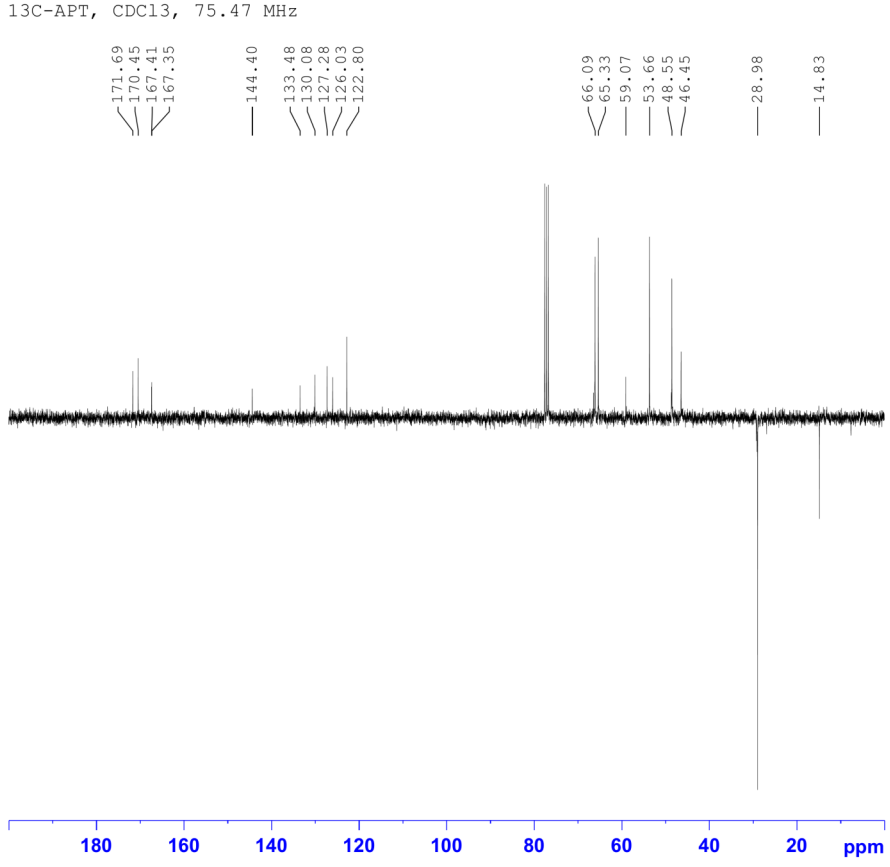


13C-APT, CDCl3, 75.47 MHz

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PROCNO                       1

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PULPROG                 jmod
TD                     65536
SOLVENT                CDCl3
NS                       512
DS                         4
SWH                23809.523 Hz
FIDRES              0.363304 Hz
AQ                  1.3763061 sec
RG                      2050
DW                    21.000 usec
DE                     6.00 usec
TE                    296.2 K
CNST2              145.0000000
CNST11               1.0000000
D1                  2.00000000 sec
d20                 0.00689655 sec
DELTA               0.00001019 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                      13C
P1                     8.00 usec
p2                    16.00 usec
PL1                    -3.00 dB
SFO1             75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 100.00 usec
PL2                    -1.00 dB
PL12                   18.17 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
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WDW                           EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
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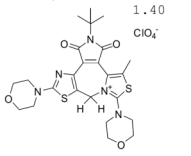
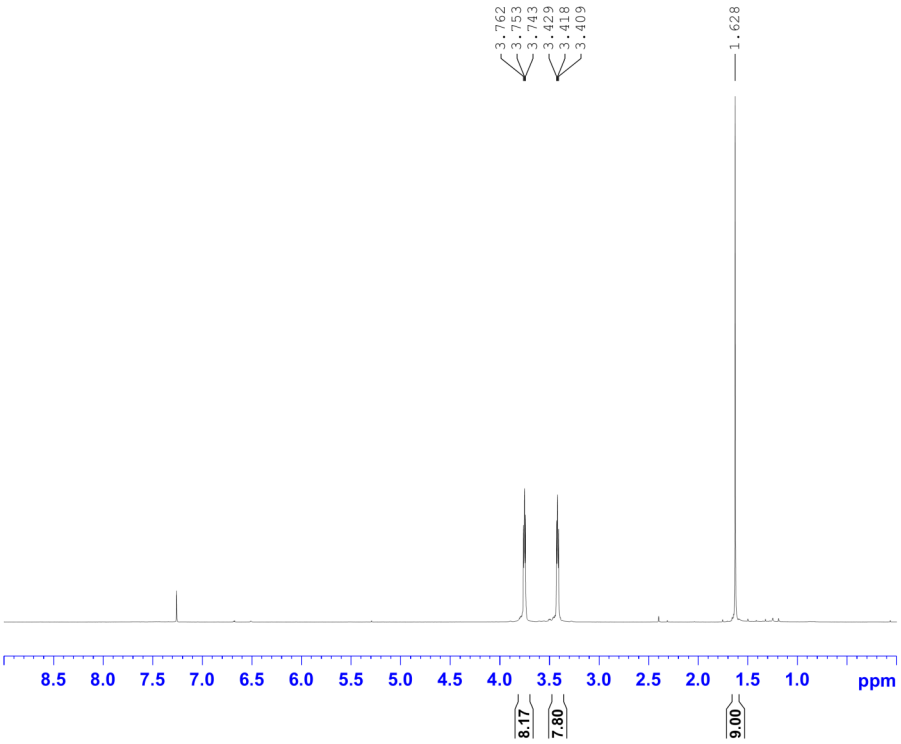


1H, CDCl3, 500 MHz

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PROCNO                       1

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PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10162.602 Hz
FIDRES             0.155069 Hz
AQ                 3.2244213 sec
RG                       161
DW                    49.200 usec
DE                     6.50 usec
TE                    295.0 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.50 usec
PLW1               12.91699982 W
SFO1               500.1330655 MHz

F2 - Processing parameters
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SF                 500.1300130 MHz
WDW                           EM
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LB                      0.20 Hz
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PC                      1.00
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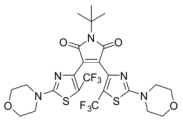
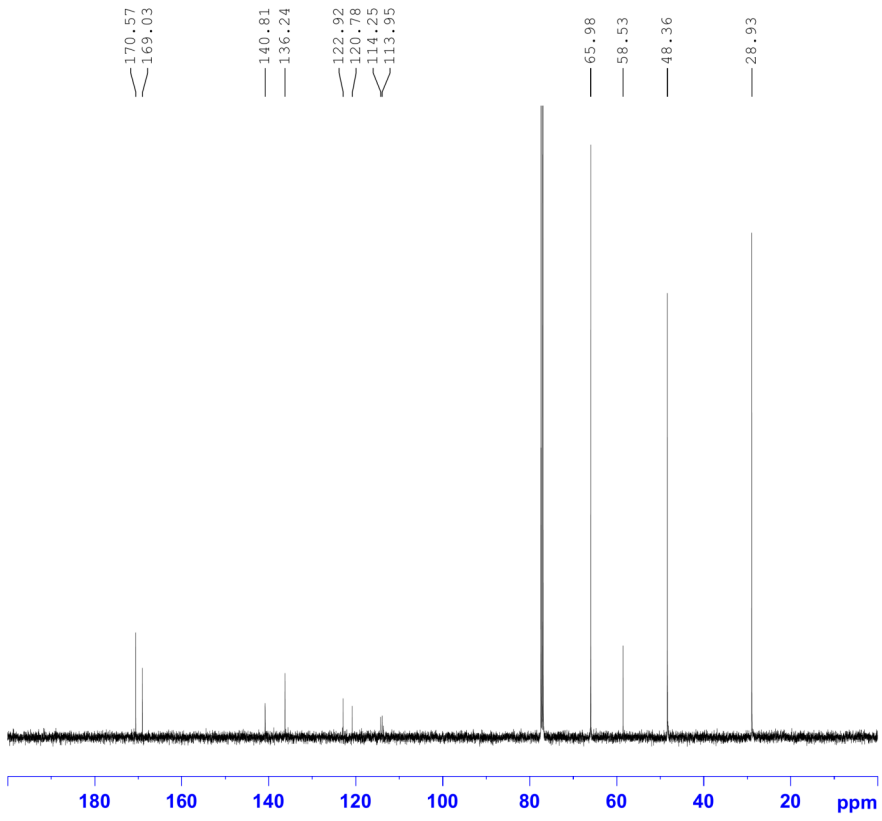


13C, CDCl3, 125.77 MHz

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PROCNO                       1

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Time                   12.11
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       256
DS                         4
SWH                39062.500 Hz
FIDRES             0.596046 Hz
AQ                 0.8389108 sec
RG                      2050
DW                    12.800 usec
DE                     6.50 usec
TE                    295.9 K
D1                 2.00000000 sec
D11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      8.50 usec
PLW1               92.94000244 W
SFO1               125.7716219 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PLW2               12.91699982 W
PLW12               0.31535000 W
PLW13               0.20183000 W
SFO2               500.1320005 MHz

F2 - Processing parameters
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SF                 125.7577738 MHz
WDW                           EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
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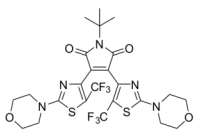
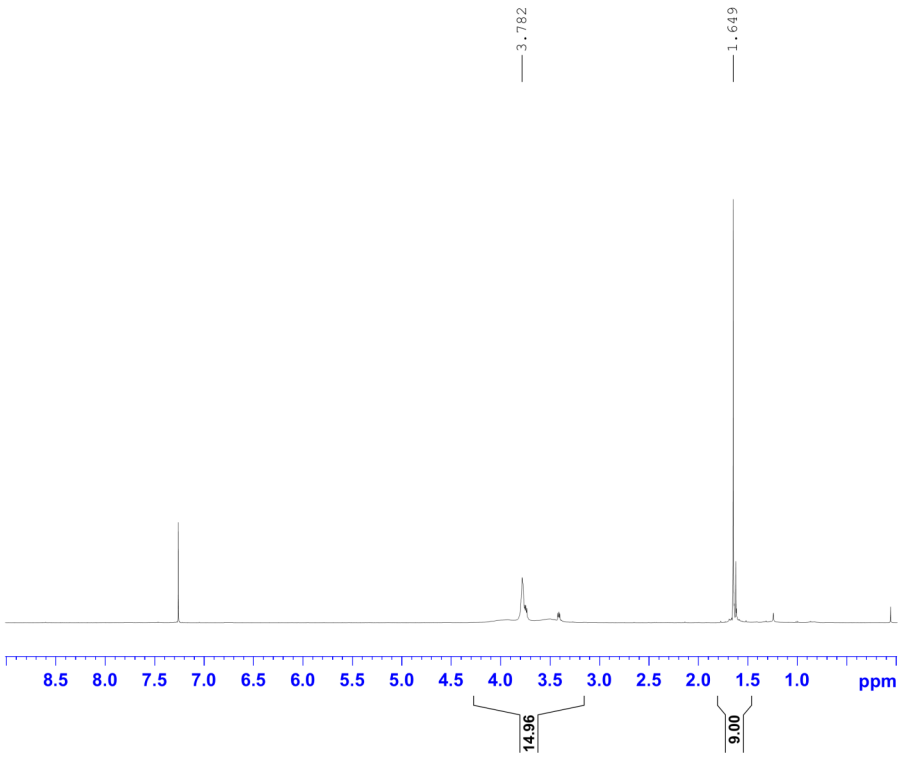


1H, CDCl3, 500 MHz

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PROCNO                 1

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INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10162.602 Hz
FIDRES         0.155069 Hz
AQ            3.2244213 sec
RG                 161
DW              49.200 usec
DE               6.50 usec
TE              296.2 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1              12.50 usec
PLW1        12.91699982 W
SFO1       500.1330655 MHz

F2 - Processing parameters
SI                 32768
SF          500.1300135 MHz
WDW                   EM
SSB       0
LB               0.20 Hz
GB        0
PC               1.00
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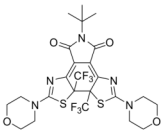
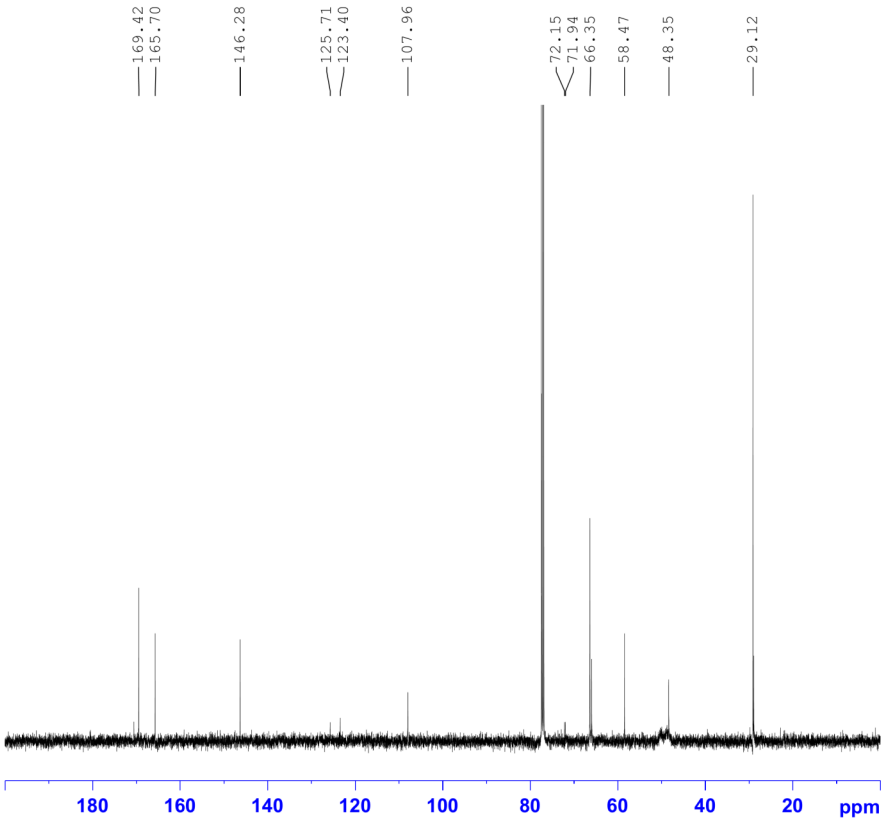


13C, CDCl3, 125.77 MHz

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PROCNO                 1

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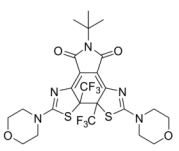
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH           39062.500 Hz
FIDRES         0.596046 Hz
AQ            0.8389108 sec
RG                2050
DW              12.800 usec
DE               6.50 usec
TE              297.2 K
D1           2.00000000 sec
D11          0.03000000 sec

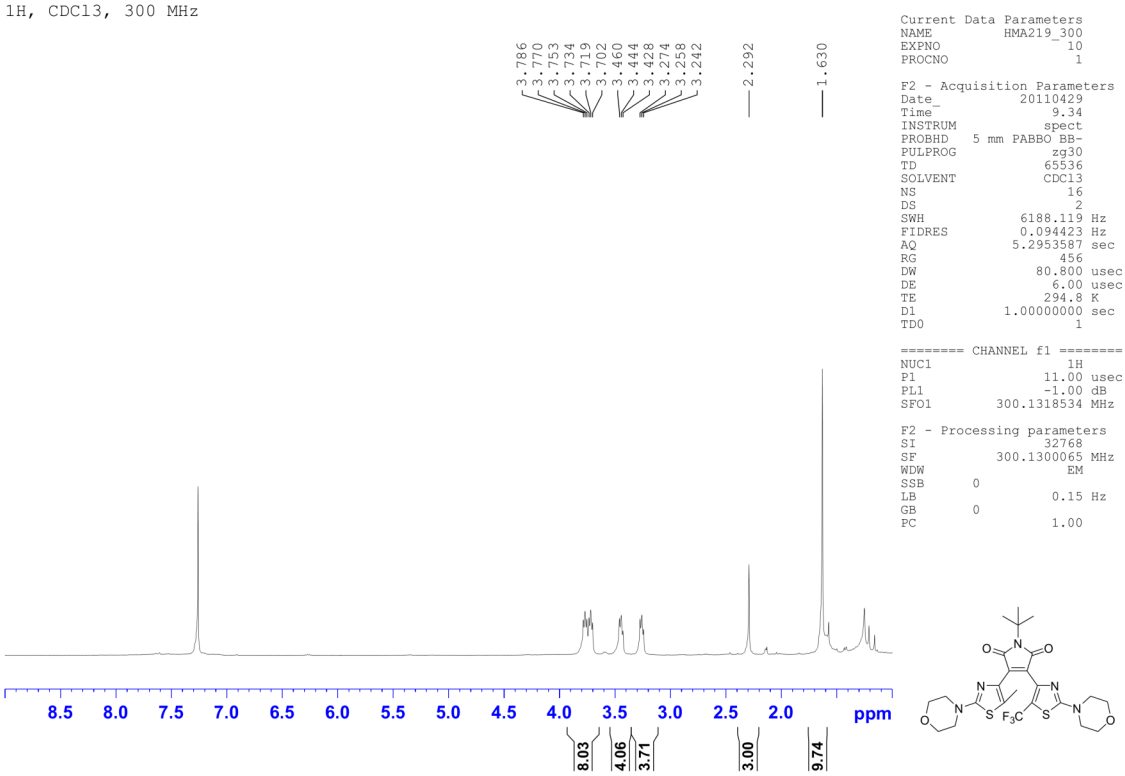
======== CHANNEL f1 ========
NUC1                13C
P1               8.50 usec
PLW1        92.94000244 W
SFO1       125.7716219 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           80.00 usec
PLW2        12.91699982 W
PLW12        0.31535000 W
PLW13        0.20183000 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577751 MHz
WDW                   EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```



1H, CDCl3, 300 MHz



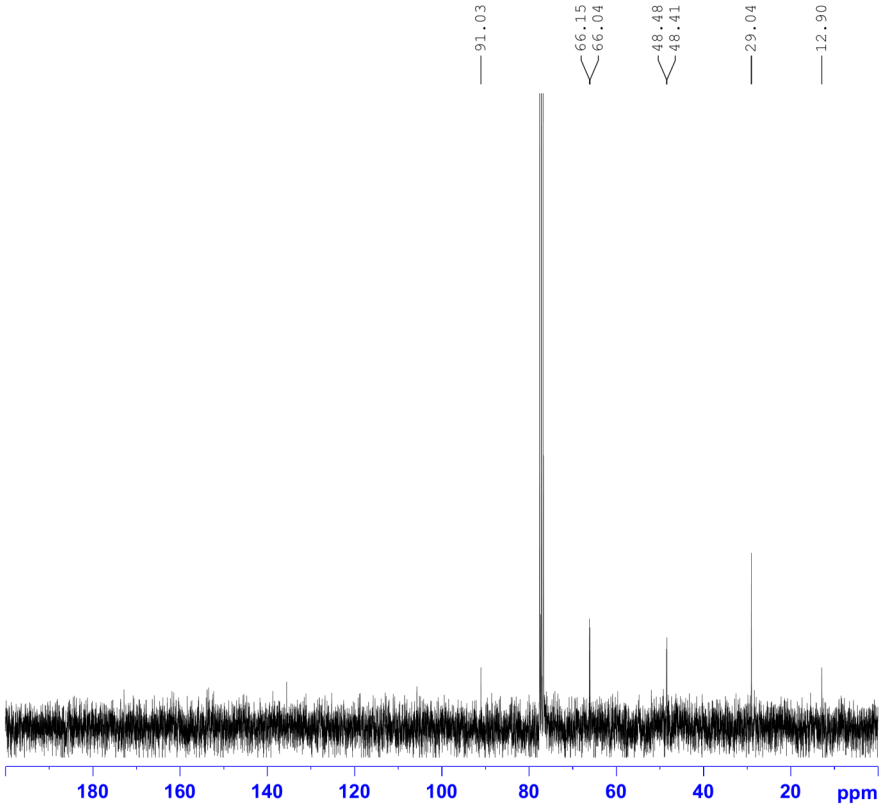

```
Current Data Parameters
NAME          HMA219_300
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110429
Time               9.34
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                  456
DW               80.800 usec
DE                6.00 usec
TE               294.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.00 usec
PL1               -1.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300065 MHz
WDW                   EM
SSB       0
LB                0.15 Hz
GB        0
PC                1.00
```


13C, CDCl3, 75.47 MHz



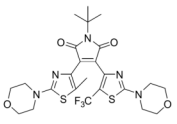

```
Current Data Parameters
NAME          HMA219_300
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110429
Time               9.50
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23809.523 Hz
FIDRES         0.363304 Hz
AQ            1.3763061 sec
RG                    5
DW               21.000 usec
DE                6.00 usec
TE               295.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

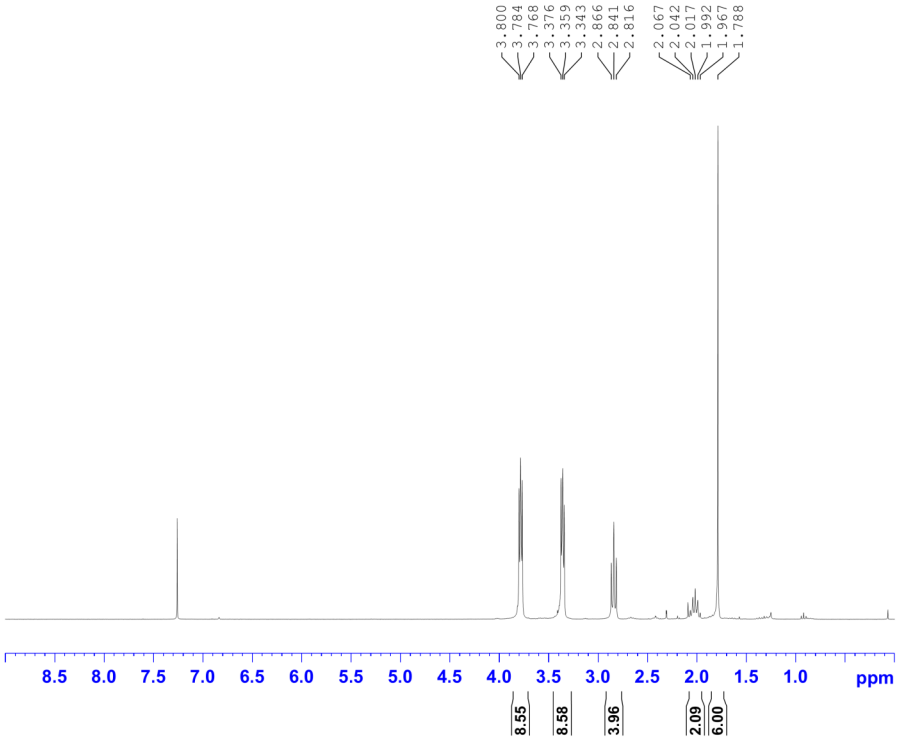
======== CHANNEL f1 ========
NUC1                 13C
P1                8.00 usec
PL1              -3.00 dB
SFO1         75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2               -1.00 dB
PL12              18.17 dB
PL13              23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677403 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



1H, CDCl3, 300 MHz

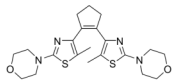



```
Current Data Parameters
NAME      HMA185-4a.dpx
EXPNO                10
PROCNO                1

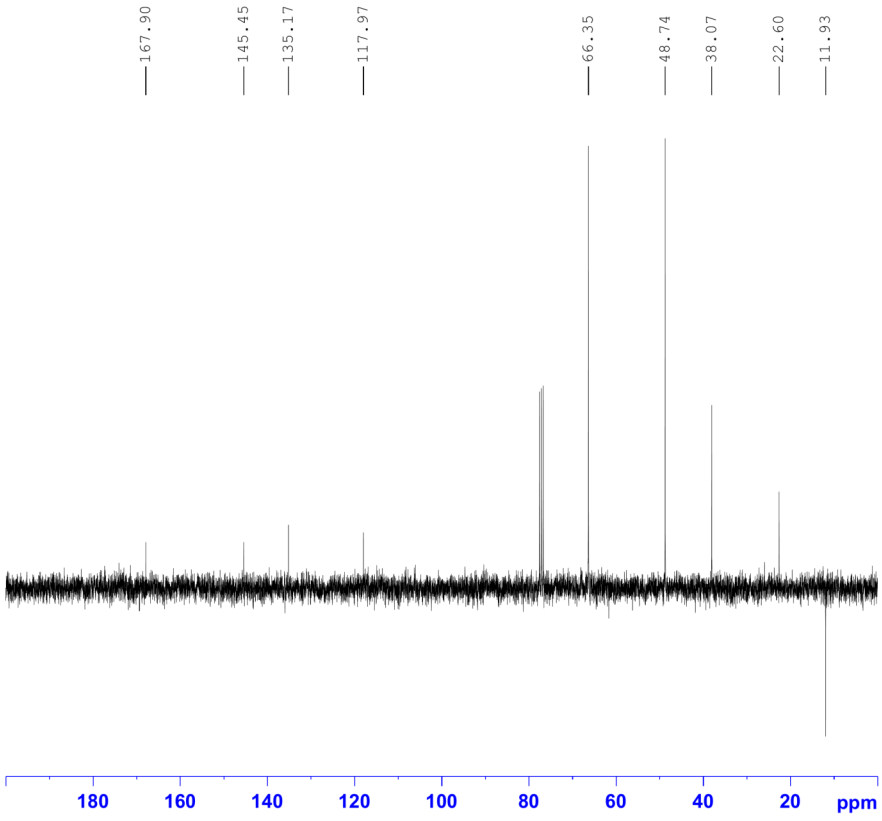
F2 - Acquisition Parameters
Date_          20101109
Time               9.40
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           6172.839 Hz
FIDRES        0.094190 Hz
AQ            5.3084660 sec
RG                 512
DW              81.000 usec
DE               6.00 usec
TE              295.2 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1              12.00 usec
PL1             -5.00 dB
SFO1       300.1318530 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300065 MHz
WDW                   EM
SSB       0
LB               0.20 Hz
GB        0
PC               1.00
```



13C-APT, CDCl3, 75.47 MHz



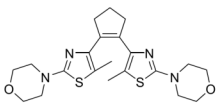

```
Current Data Parameters
NAME      HMA185-4a.dpx
EXPNO               11
PROCNO               1

F2 - Acquisition Parameters
Date_          20101109
Time               9.50
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG           jmod
TD               65536
SOLVENT          CDCl3
NS                 128
DS                   4
SWH           17985.611 Hz
FIDRES          0.274439 Hz
AQ            1.8219508 sec
RG               7298.2
DW              27.800 usec
DE               6.00 usec
TE              296.2 K
CNST2       145.0000000
CNST11        1.0000000
D1            2.00000000 sec
d20           0.00689655 sec
DELTA         0.00001210 sec
TD0                  1

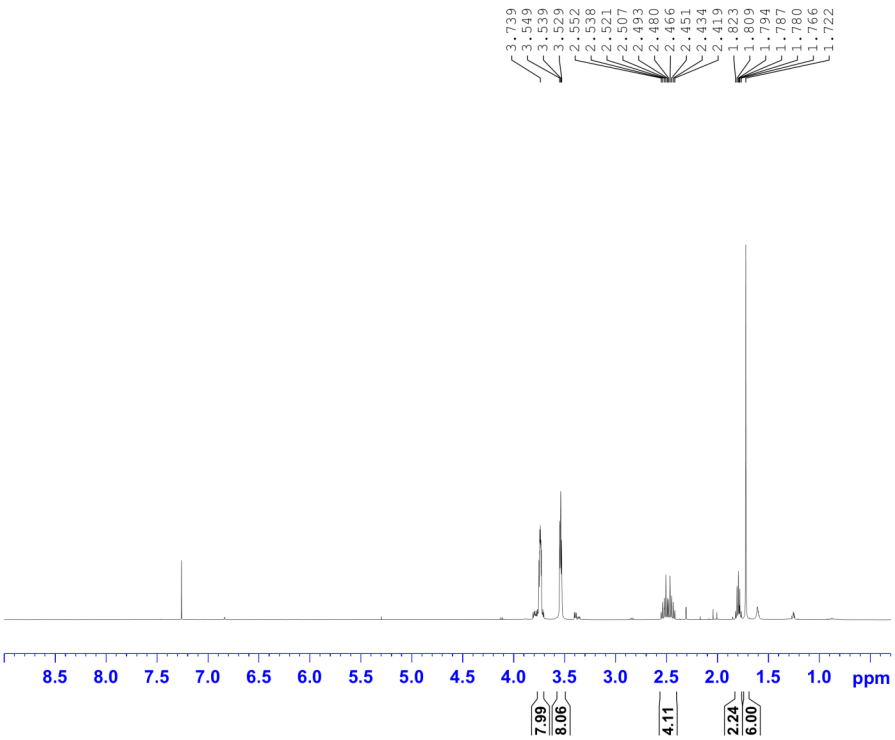
======== CHANNEL f1 ========
NUC1                13C
P1               9.50 usec
p2              19.00 usec
PL1             -1.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2           100.00 usec
PL2              -5.00 dB
PL12             13.42 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677387 MHz
WDW                   EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```



1H, CDCl3, 500 MHz

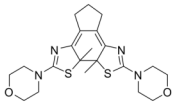



```
Current Data Parameters
NAME        HMA199a_500
EXPNO                10
PROCNO                1

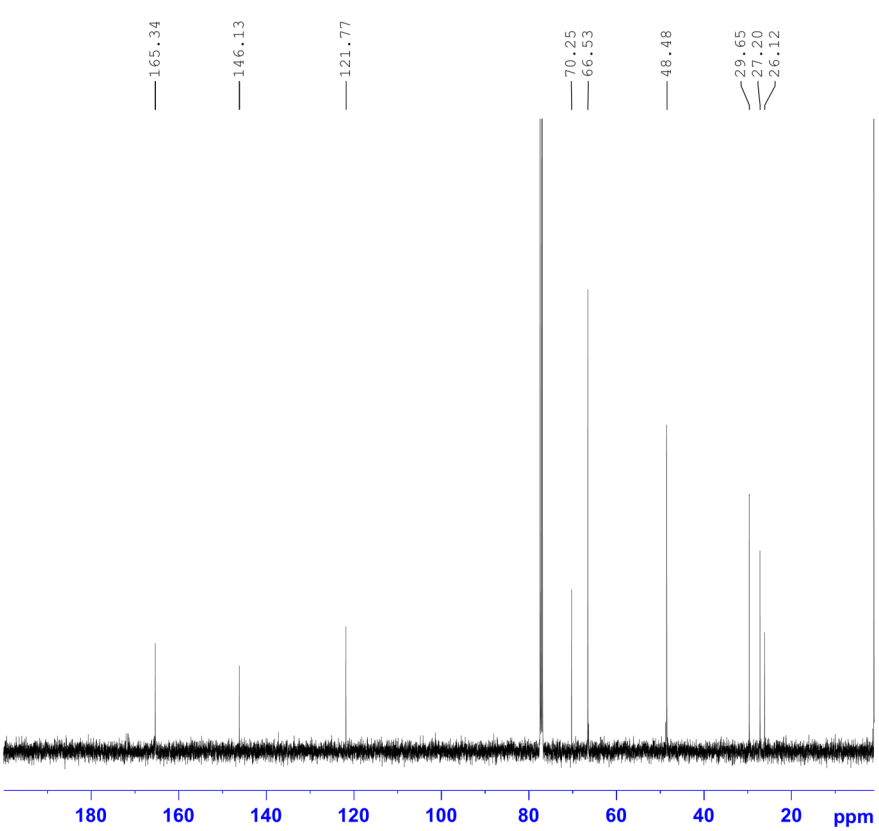
F2 - Acquisition Parameters
Date_          20110103
Time              13.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10162.602 Hz
FIDRES         0.155069 Hz
AQ            3.2244213 sec
RG                  161
DW               49.200 usec
DE                6.50 usec
TE               295.1 K
D1            1.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                12.50 usec
PLW1         12.91699982 W
SFO1         500.1330655 MHz

F2 - Processing parameters
SI                32768
SF          500.1300132 MHz
WDW                  EM
SSB       0
LB                0.20 Hz
GB        0
PC                1.00
```



13C, CDCl3, 125.77 MHz



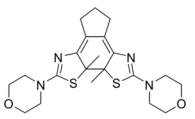

```
Current Data Parameters
NAME        HMA199a_500
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20110103
Time              13.46
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           39062.500 Hz
FIDRES         0.596046 Hz
AQ            0.8389108 sec
RG                 2050
DW               12.800 usec
DE                6.50 usec
TE               296.7 K
D1            2.00000000 sec
D11           0.03000000 sec

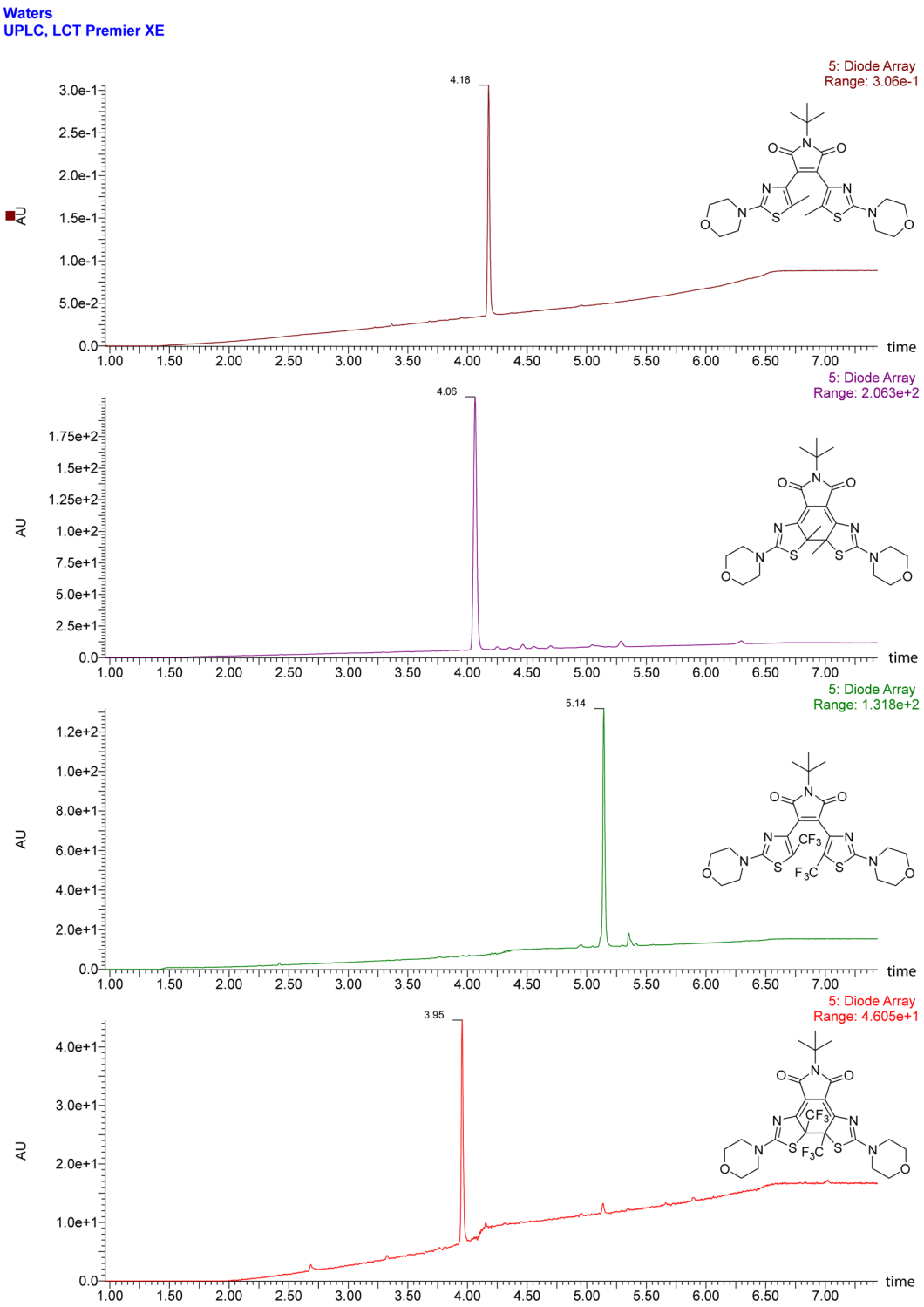
======== CHANNEL f1 ========
NUC1                13C
P1                8.50 usec
PLW1         92.94000244 W
SFO1         125.7716219 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.91699982 W
PLW12         0.31535000 W
PLW13         0.20183000 W
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577697 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



Appendix 2: UPLC traces



Waters
UPLC, LCT Premier XE