

*Electronic Supporting Information*

**Modulating Electrochromic Properties *via* Thiophene Donors in Thieno[3,4-*c*]pyrrole-4,6-dione-based Conjugated Polymers**

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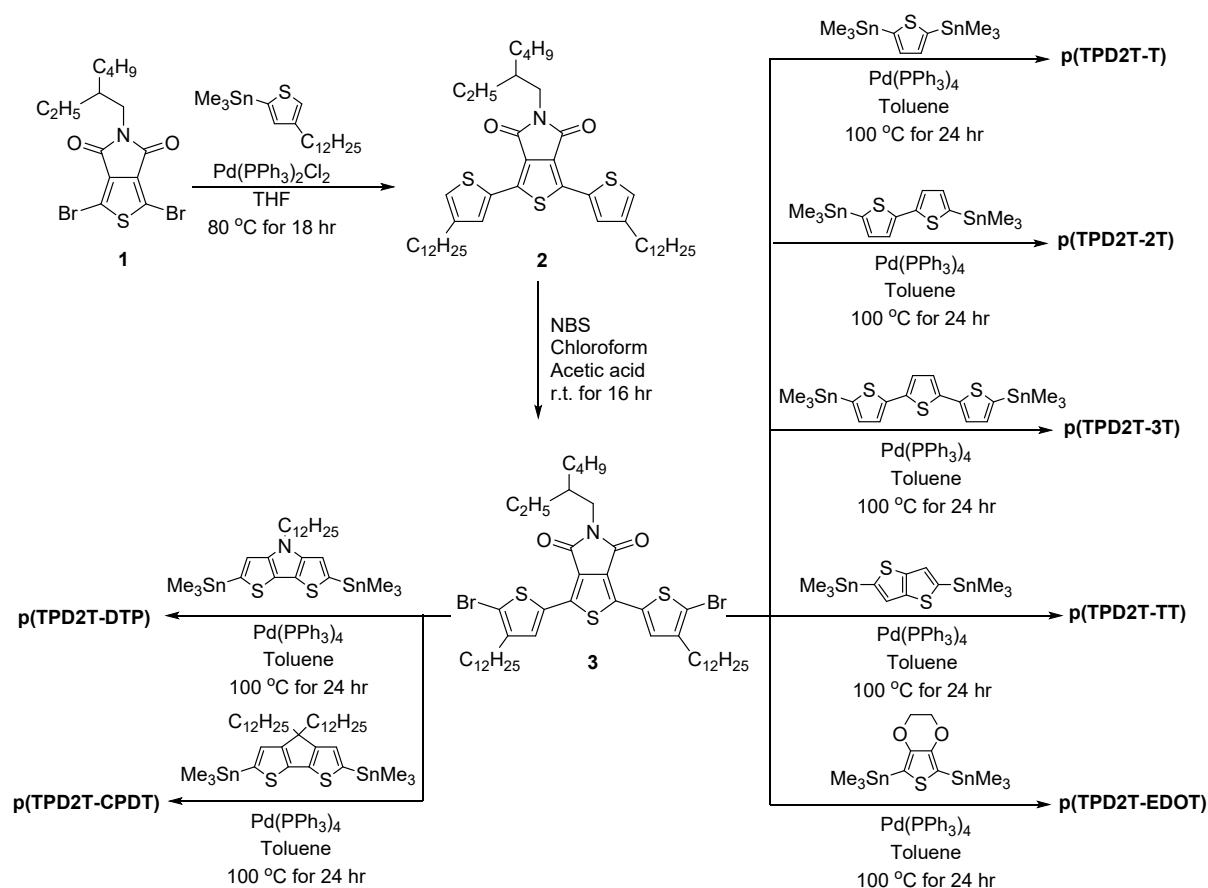
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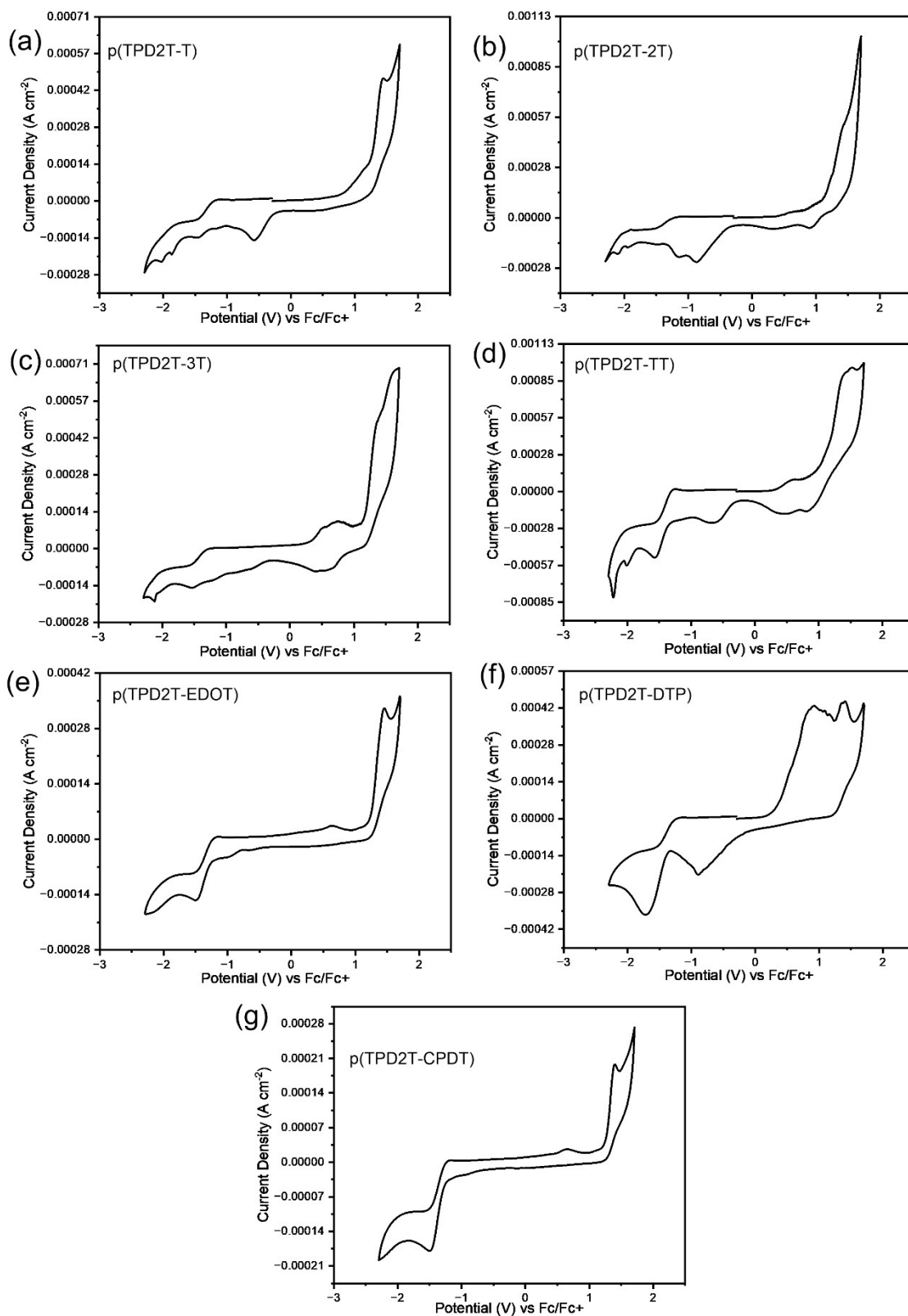


**Scheme S1.** Synthesis of TPD polymers p(TPD2T-T), p(TPD2T-2T), p(TPD2T-3T), p(TPD2T-TT), p(TPD2T-EDOT), p(TPD2T-DTP), and p(TPD2T-CPDT).

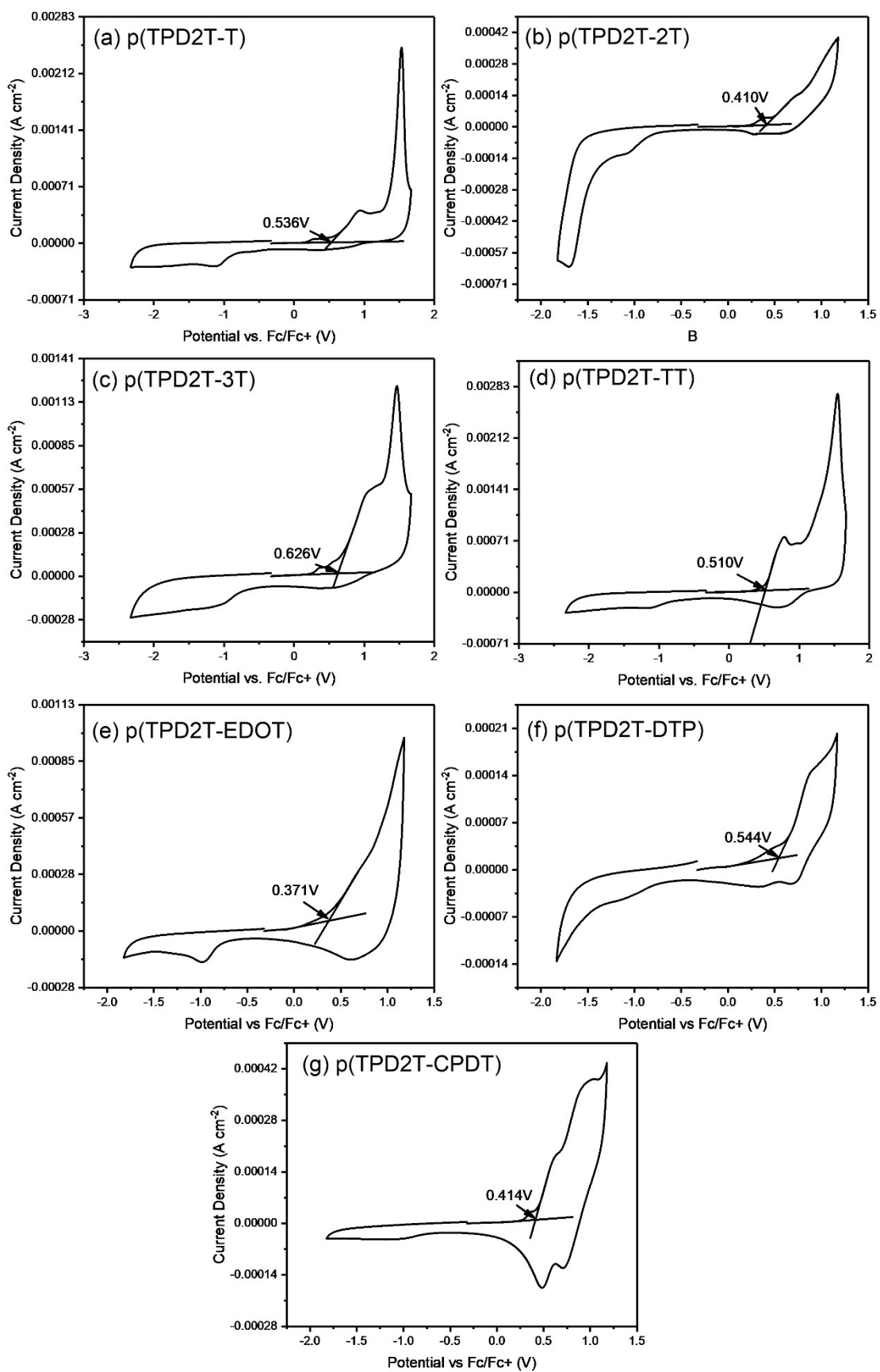
**Table S1.** Gel Permeation Chromatography (GPC) Characterization, Thermal Analysis, and Synthesis Yield of TPD polymers p(TPD2T-T), p(TPD2T-2T), p(TPD2T-3T), p(TPD2T-TT), p(TPD2T-EDOT), p(TPD2T-DTP), and p(TPD2T-CPDT).

| Polymer       | Gel Permeation Chromatography |                          |                  | Thermal Analysis                        | Synthesis |
|---------------|-------------------------------|--------------------------|------------------|---|-----------|
|               | $M_n$ (kDa) <sup>a</sup>      | $M_w$ (kDa) <sup>b</sup> | PDI <sup>c</sup> | $T_d$ ( $^\circ\text{C}$ ) <sup>d</sup> | Yield (%) |
| p(TPD2T-T)    | 9.017                         | 9.350                    | 1.037            | 415.13                                  | 98.0      |
| p(TPD2T-2T)   | 12.145                        | 17.822                   | 1.467            | 425.96                                  | 93.0      |
| p(TPD2T-3T)   | 54.295                        | 104.517                  | 1.925            | 230.68                                  | 14.0      |
| p(TPD2T-TT)   | 13.546                        | 21.500                   | 1.587            | 407.63                                  | 99.0      |
| p(TPD2T-EDOT) | 5.078                         | 9.650                    | 1.784            | 245.10                                  | 70.4      |
| p(TPD2T-DTP)  | 6.300                         | 10.632                   | 1.688            | 383.47                                  | 90.0      |
| p(TPD2T-CPDT) | 10.496                        | 19.442                   | 1.852            | 242.78                                  | 90.0      |

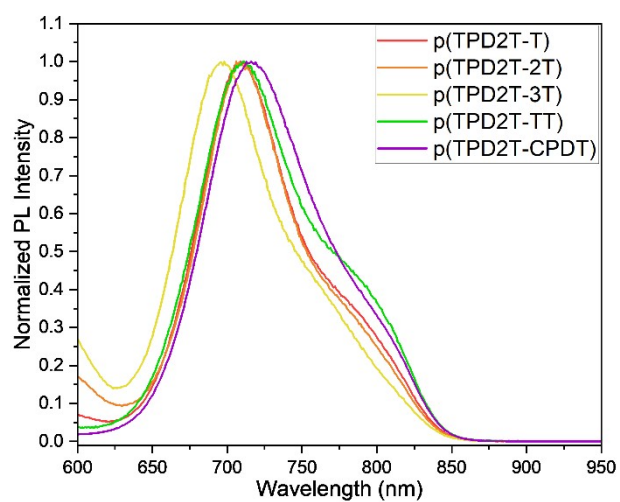
<sup>a</sup> number-average molecular weight; <sup>b</sup> weight-average molecular weight; <sup>c</sup> Polydispersity Index =  $M_w/M_n$ ; <sup>d</sup> Temperature at which 5% weight loss of the polymers were recorded from thermogravimetric analysis (TGA)



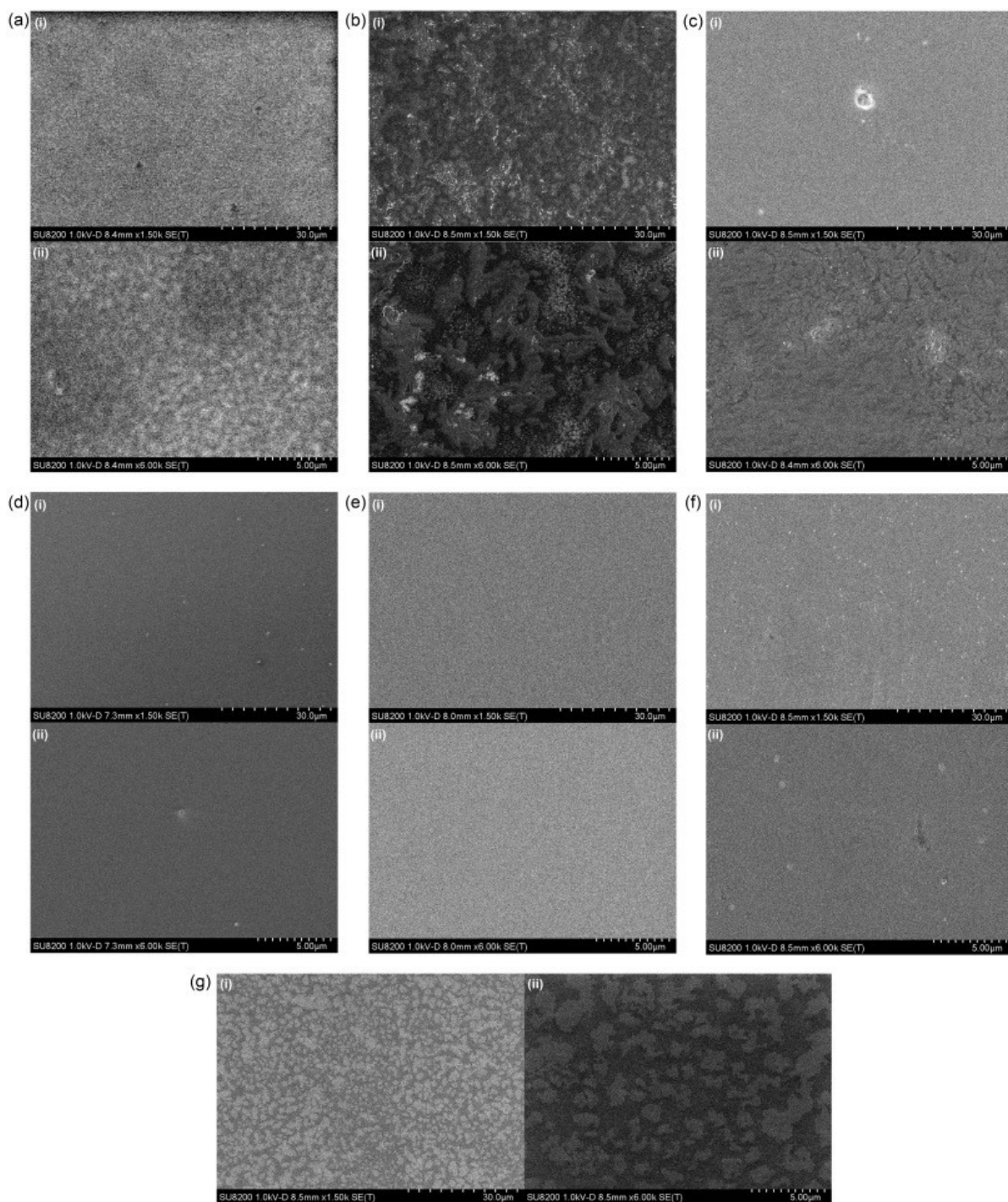
**Figure S1.** Cyclic voltammograms of polymers (a) p(TPD2T-T), (b) p(TPD2T-2T), (c) p(TPD2T-3T), (d) p(TPD2T-TT), (e) p(TPD2T-EDOT), (f) p(TPD2T-DTP), and (g) p(TPD2T-CPDT) in solution.



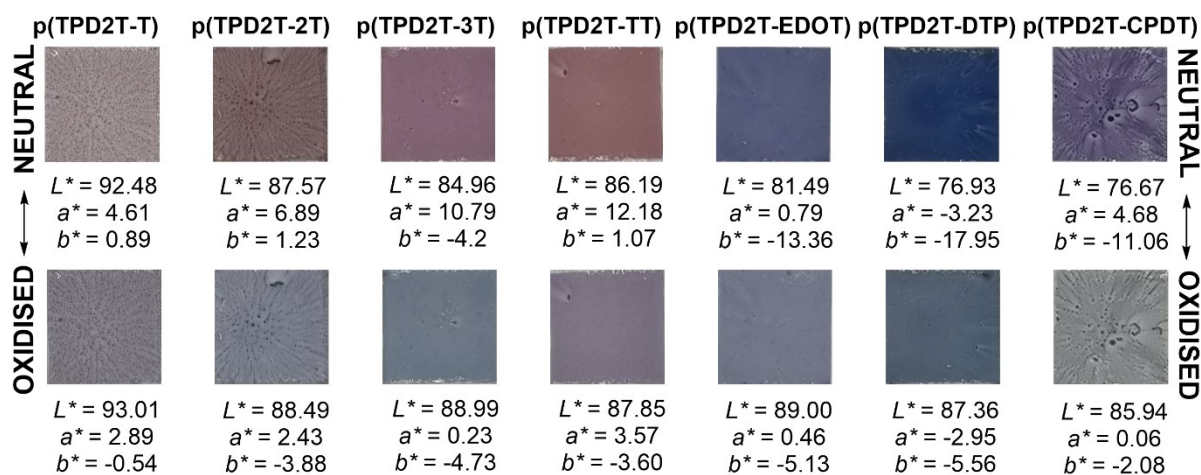
**Figure S2.** Cyclic voltammograms of polymers (a) p(TPD2T-T), (b) p(TPD2T-2T), (c) p(TPD2T-3T), (d) p(TPD2T-TT), (e) p(TPD2T-EDOT), (f) p(TPD2T-DTP), and (g) p(TPD2T-CPDT) in thin film.



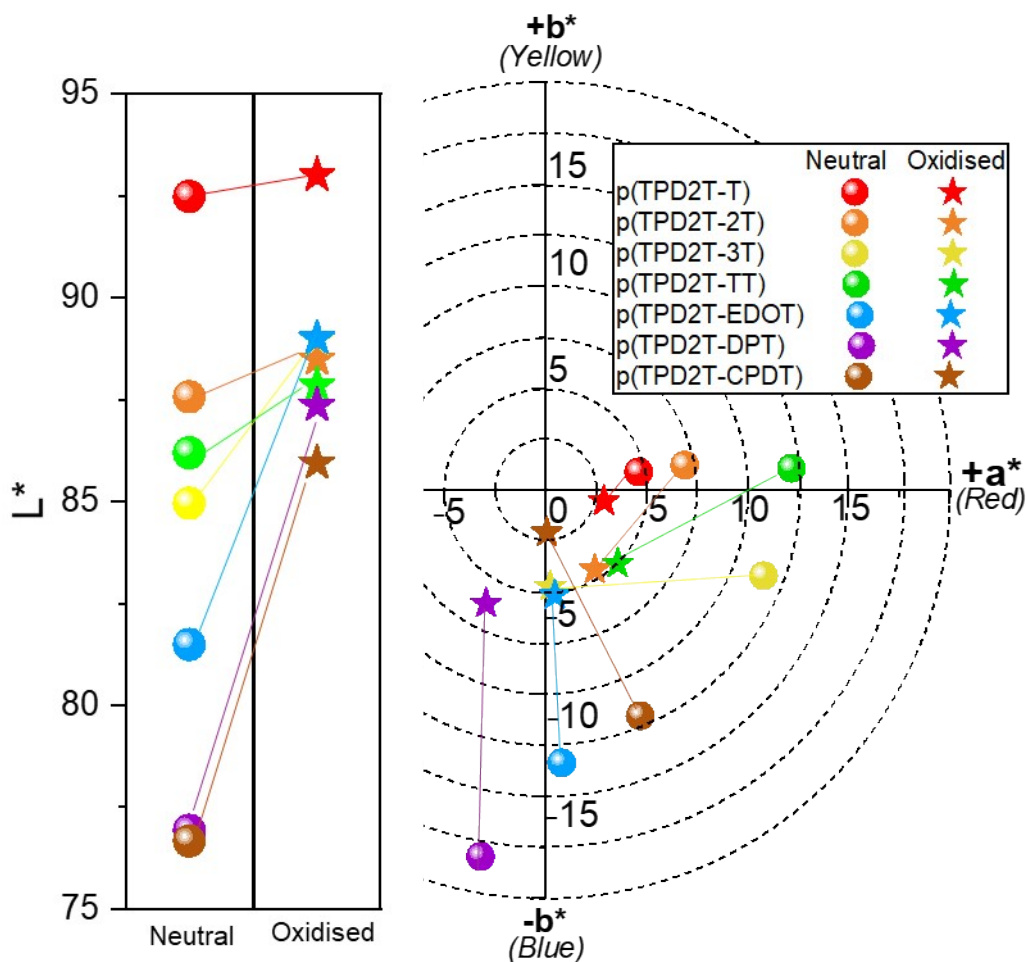
**Figure S3.** Normalized thin film photoluminescence spectra of polymers p(TPD2T-T), p(TPD2T-2T), p(TPD2T-3T), p(TPD2T-TT), and p(TPD2T-CPDT).



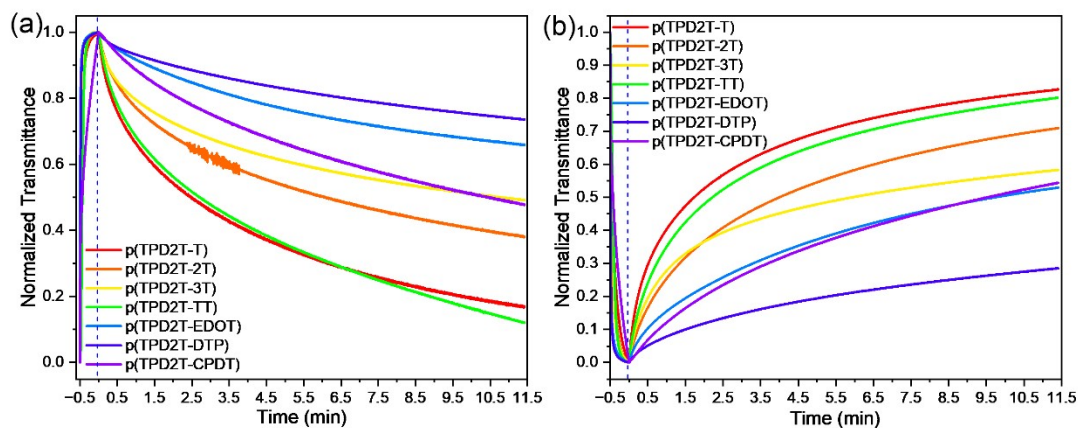
**Figure S4.** SEM images of polymers (a) p(TPD2T-T), (b) p(TPD2T-2T), (c) p(TPD2T-3T), (d) p(TPD2T-TT), (e) p(TPD2T-EDOT), (f) p(TPD2T-DTP), and (g) p(TPD2T-CPDT) under i) 1500x and ii) 6000x magnification.



**Figure S5.** EC colour changes of polymers p(TPD2T-T), p(TPD2T-2T), p(TPD2T-3T), p(TPD2T-TT), and p(TPD2T-CPDT) upon undergoing electro-oxidation, and their corresponding  $L^*$   $a^*$   $b^*$  colour coordinates according to CIE 1976 colour space.



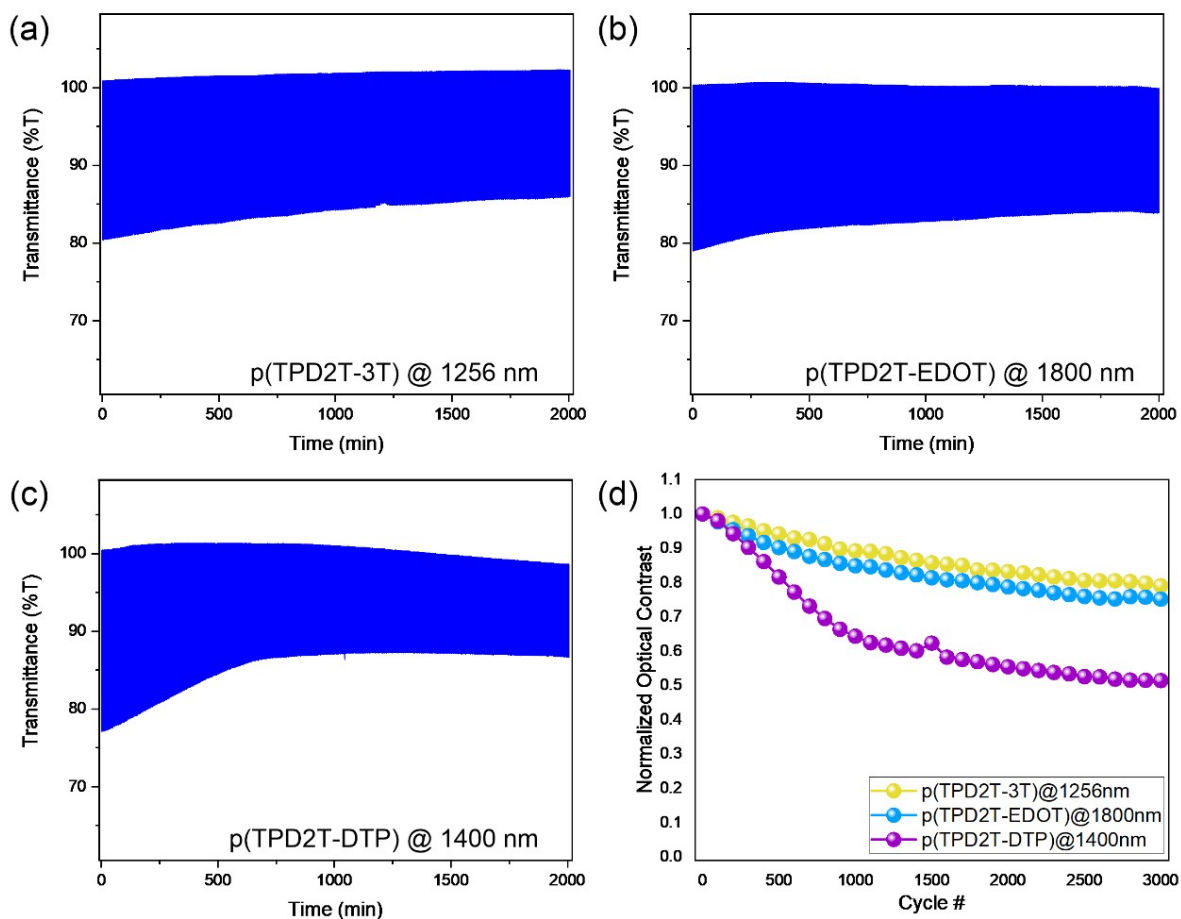
**Figure S6.** Plots of colour coordinates on a 1-dimensional  $L^*$  scale (left) and a 2-dimensional  $a^*$  vs  $b^*$  colour chart (right) for the seven TPD polymers in the neutral and oxidised states.



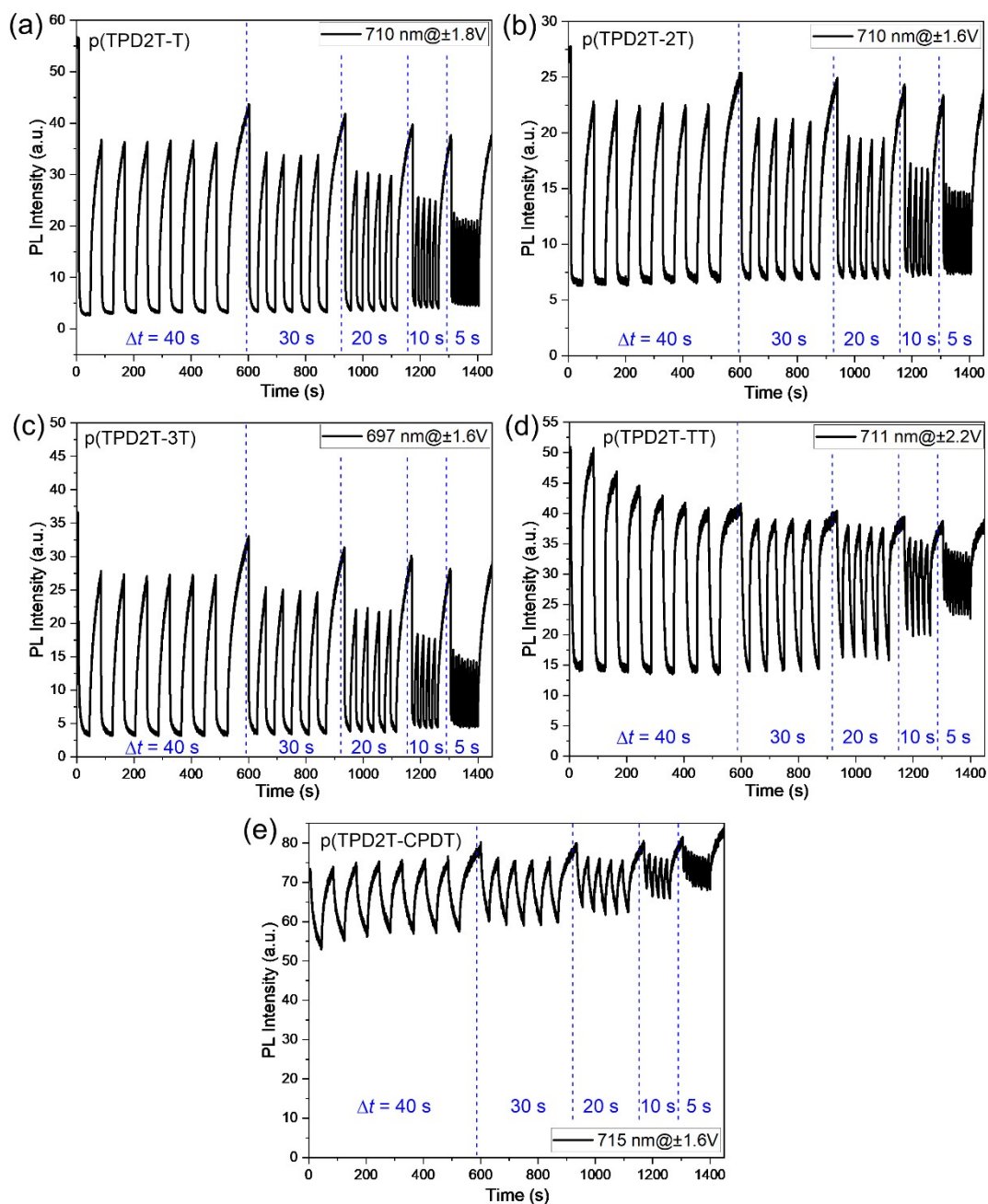
**Figure S7.** Open memory retention of the p(TPD2T-T), p(TPD2T-2T), p(TPD2T-3T), p(TPD2T-TT), and p(TPD2T-CPDT) at their respective (a) visible (492, 490, 520, 497, 595, 608, and 555 nm, respectively), and (b) NIR wavelengths of interest (1242, 1196, 1256, 1238, 1800, 1400, and 1380 nm, respectively), as reflected by the changes in normalized transmittance after oxidation, under open circuit conditions over 10 minutes.

**Table S2.** EC switching parameters of the seven TPD polymers from chronoabsorptometry studies.

| Polymer       | Film Thickness (nm) | Visible                     |                                 |                 |   |   |                                    | NIR                         |                               |                 |   |   |                                    |
|---------------|---------------------|-----------------------------|---------------------------------|-----------------|---|---|------------------------------------|-----------------------------|-------------------------------|-----------------|---|---|------------------------------------|
|               |                     | $\lambda_{\text{abs}}$ (nm) | Doping/ De-doping Potential (V) | $\Delta\%T$ (%) | $\tau_{\text{ox}}$ or $\tau_{\text{b}}$ (s) | $\tau_{\text{re}}$ or $\tau_{\text{c}}$ (s) | CE ( $\text{cm}^2 \text{C}^{-1}$ ) | $\lambda_{\text{abs}}$ (nm) | Doping/ De-doping Voltage (V) | $\Delta\%T$ (%) | $\tau_{\text{ox}}$ or $\tau_{\text{c}}$ (s) | $\tau_{\text{re}}$ or $\tau_{\text{b}}$ (s) | CE ( $\text{cm}^2 \text{C}^{-1}$ ) |
| p(TPD2T-T)    | 94.6±0.7            | 492                         | ±2.2                            | 19.8±2.0        | 11.5±1.6                                    | 3.7±1.7                                     | 349.6                              | 1242                        | ±2.2                          | 27.4±0.2        | 19.9±0.7                                    | 6.1±0.5                                     | 200.0                              |
| p(TPD2T-2T)   | 61.6±4.2            | 490                         | ±2.0                            | 12.4±1.1        | 27.3±1.6                                    | 10.4±0.6                                    | 207.5±3.5                          | 1196                        | ±2.0                          | 20.2±1.5        | 23.8±0.7                                    | 3.4±0.3                                     | 293.3±5.6                          |
| p(TPD2T-3T)   | 70.8±18.3           | 520                         | ±2.0                            | 17.5±2.5        | 16.7±4.3                                    | 3.0±0.3                                     | 377.3±64.7                         | 1256                        | ±2.0                          | 42.1±0.4        | 17.9±0.2                                    | 2.3±0.1                                     | 630.2±11.4                         |
| p(TPD2T-TT)   | 226.8±32.1          | 497                         | ±2.0                            | 17.7±0.3        | 24.4±6.4                                    | 3.1±1.4                                     | 275.1±23.4                         | 1238                        | ±2.0                          | 30.4±0.1        | 27.4±0.6                                    | 2.1±0.1                                     | 340.4±17.4                         |
| p(TPD2T-EDOT) | 95.1±2.6            | 595                         | ±2.0                            | 23.8±0.9        | 9.0±0.1                                     | 1.7±0.1                                     | 720.7±2.8                          | 1800                        | ±2.0                          | 46.7±3.3        | 11.9±0.4                                    | 1.3±0.0                                     | 1012.1±12.4                        |
| p(TPD2T-DTP)  | 46.4±19.0           | 608                         | ±2.0                            | 20.0±1.0        | 4.3±0.1                                     | 0.7±0.1                                     | 801.1±53.2                         | 1400                        | ±2.0                          | 44.8±3.7        | 6.8±0.3                                     | 1.2±0.1                                     | 1358.5±12.3                        |
| p(TPD2T-CPDT) | 59.2±7.7            | 555                         | ±2.0                            | 18.2±2.7        | 36.1±6.5                                    | 9.6±0.9                                     | 245.9±16.0                         | 1380                        | ±2.0                          | 23.7±2.6        | 46.4±6.7                                    | 3.6±0.4                                     | 247.6±29.2                         |

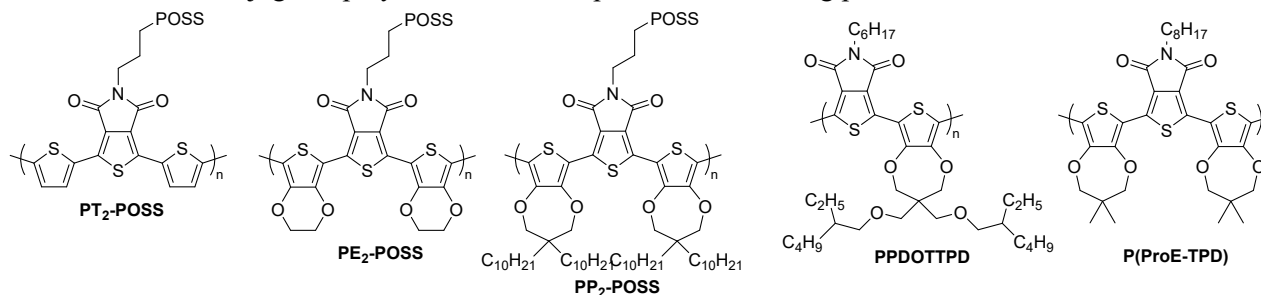


**Figure S8.** Long-term EC switching stability of (a) p(TPD2T-3T), (b) p(TPD2T-EDOT), and (c) p(TPD2T-DTP), switching at  $\pm 1.8$  V respectively, at 20 s time interval with transmittance at 1256, 1800, and 1400 nm, respectively, monitored over 3000 cycles. (d) Plot of normalized optical contrasts over number of cycles.



**Figure S9.** Chronofluorometry EFC switching studies for (a) p(TPD2T-T), (b) p(TPD2T-2T), (c) p(TPD2T-3T), (d) p(TPD2T-TT), and (e) p(TPD2T-CPDT), switching at 710, 710, 697, 711, and 715 nm by applying voltages of  $\pm 1.8$ ,  $\pm 1.6$ ,  $\pm 1.6$ ,  $\pm 2.2$ , and  $\pm 1.6$  V, respectively, at different time intervals ( $\Delta t$ ) of 40, 30, 20, 10, and 5 s.

**Table S3.** Prior studies of TPD-based EC conjugated polymers and their reported EC switching parameters.



| Polymer                 | Polymerization Approach           | Neutral State               |              |              |                            |              |  | Charged State               |                  |   | EC Switching                 |                          |  |                                    |  | Ref |
|-------------------------|-----------------------------------|-----------------------------|--------------|--------------|----------------------------|--------------|--|-----------------------------|------------------|---|------------------------------|--------------------------|--|------------------------------------|--|-----|
|                         |                                   | $\lambda_{\text{abs}}$ (nm) | HOMO (eV)    | LUMO (eV)    | $E_g$ (eV)                 | Colour       | $L^*, a^*, b^*$ values                           | $\lambda_{\text{abs}}$ (nm) | Colour           | $L^*, a^*, b^*$ values  | ECD                          | % $\Delta T$             | $\tau$ (s)                               | CE ( $\text{cm}^2 \text{C}^{-1}$ ) | Stability                                  |     |
| PT <sub>2</sub> -POSS   | Electro-polymerization            | 525                         | Not Reported | Not Reported | 1.79 (Opt.); 2.29 (Elec.)  | Reddish Pink | $L^* = 75.18$<br>$a^* = 8.23$<br>$b^* = -2.09$   | 740                         | Gray             | $L^* = 82.76$<br>$a^* = 5.36$<br>$b^* = 4.90$                               | Half-cell                    | 18 (525 nm)              | 0.6 (525 nm)                             | 204 (525 nm)                       | Not Studied, $\geq$ 5 cycles               | 1   |
| PE <sub>2</sub> -POSS   | Electro-polymerization            | 540, 600                    | Not Reported | Not Reported | 1.65 (Opt.); 1.55 (Elect.) | Dark Blue    | $L^* = 53.60$<br>$a^* = 8.07$<br>$b^* = -35.27$  | 846                         | Light Blue       | $L^* = 81.05$<br>$a^* = -7.54$<br>$b^* = -7.55$                             | Half-cell                    | 46 (545 nm); 33 (600 nm) | 0.6 (545 nm); 0.6 (600 nm)               | 472 (545 nm); 387 (600 nm)         | Not Studied, $\geq$ 5 cycles               | 1   |
| PP <sub>2</sub> -POSS   | Electro-polymerization            | 585, 640                    | Not Reported | Not Reported | 1.78 (Opt.); 2.06 (Elect.) | Blue         | $L^* = 71.71$<br>$a^* = -7.54$<br>$b^* = -24.28$ | 872                         | Colourless       | $L^* = 90.98$<br>$a^* = -0.18$<br>$b^* = 0.91$                              | Half-cell                    | 50 (585 nm); 52 (640 nm) | 0.4 (585 nm); 0.4 (640 nm)               | 522 (585 nm); 550 (640 nm)         | Not Studied, $\geq$ 5 cycles               | 1   |
| PE <sub>2</sub> -POSS-C | Oxidative chemical polymerization | 632                         | Not Reported | Not Reported | 1.52 (Opt.)                | Blue         | $L^* = 77.33$<br>$a^* = -3.41$<br>$b^* = -18.46$ | Ca. 900                     | Colourless       | $L^* = 87.51$<br>$a^* = 1.10$<br>$b^* = -5.98$                              | Half-cell                    | 30                       | 0.7                                      | 954 (632 nm)                       | Not Studied, $\geq$ 5 cycles               | 1   |
| PP <sub>2</sub> -POSS-C | Oxidative chemical polymerization | 585, 640                    | Not Reported | Not Reported | 1.80 (Opt.)                | Purple-Blue  | $L^* = 70.78$<br>$a^* = 3.15$<br>$b^* = -23.42$  | Ca. 825                     | Colourless       | $L^* = 84.91$<br>$a^* = 2.95$<br>$b^* = -5.10$                              | Half-cell                    | 23                       | 1.0                                      | 995 (585 nm); 720 (640 nm)         | Not Studied, $\geq$ 5 cycles               | 1   |
| PPDOTTPD                | Stille Polymerization             | 567                         | -5.22        | -3.37        | 1.85 (Opt.)                | Purple       | $L^* = 44.02$<br>$a^* = 22.95$<br>$b^* = 36.08$  | 460, 770                    | Transparent Gray | $L^* = 66.92$<br>$a^* = \text{Not Reported}$<br>$b^* = \text{Not Reported}$ | Liquid-based sandwich device | 52 (570 nm)              | $\tau_b = 0.5$ ; $\tau_c = 0.7$ (570 nm) | 427.1                              | 200 Cycles with ca. 20% drop in $\Delta T$ | 2   |
| P(ProE-                 | Electro-                          | 565                         | Not          | Not          | Not                        | Not          | Not  | 800,                        | Not              | Not   | Not                          | 27.1 (1000)              | Not reported                             | Not                                | Not Studied, $\geq$                        | 3   |

| TPD)          | polymerization        |     | Reported                                 | Reported                                 | Reported    | Reported      | Reported   | 1380      | Reported      | Reported  | Reported           | nm)                           |   | reported                         | 5 cycles  |           |
|---------------|-----------------------|-----|--|--|-------------|---------------|--|-----------|---------------|---|--------------------|-------------------------------|---|----------------------------------|---|-----------|
| p(TPD2T-T)    | Stille Polymerization | 510 | -5.77 <sup>a</sup><br>-5.34 <sup>b</sup> | -4.00 <sup>a</sup><br>-3.57 <sup>b</sup> | 1.77 (Opt.) | Light Grey    | $L^* = 92.48$<br>$a^* = 4.61$<br>$b^* = 0.89$    | 1242      | Dark Grey     | $L^* = 93.01$<br>$a^* = 2.89$<br>$b^* = -0.54$  | Sandwich Full Cell | 19.8 (492 nm); 27.4 (1242 nm) | $t_b = 3.7; t_c = 11.5$ (492 nm);<br>$t_b = 19.9; t_c = 6.1$ (1242 nm)              | 349.6 (492 nm); 200 (1242 nm)    | -   | This Work |
| p(TPD2T-2T)   | Stille Polymerization | 494 | -5.59 <sup>a</sup><br>-5.21 <sup>b</sup> | -3.80 <sup>a</sup><br>-3.42 <sup>b</sup> | 1.79 (Opt.) | Brown         | $L^* = 87.57$<br>$a^* = 6.89$<br>$b^* = 1.23$    | 1200      | Grey          | $L^* = 88.49$<br>$a^* = 2.43$<br>$b^* = -3.88$  | Sandwich Full Cell | 12.4 (490 nm); 20.2 (1196 nm) | $\tau_b = 10.4; \tau_c = 27.3$ (490 nm);<br>$\tau_b = 23.8; \tau_c = 3.4$ (1196 nm) | 207.5 (490 nm); 293.3 (1196 nm)  | -   | This Work |
| p(TPD2T-3T)   | Stille Polymerization | 498 | -5.35 <sup>a</sup><br>-5.43 <sup>b</sup> | -3.57 <sup>a</sup><br>-3.65 <sup>b</sup> | 1.78 (Opt.) | Magenta Brown | $L^* = 84.96$<br>$a^* = 10.79$<br>$b^* = -4.2$   | 1200      | Bluish Grey   | $L^* = 88.99$<br>$a^* = 0.23$<br>$b^* = -4.73$  | Sandwich Full Cell | 17.5 (520 nm); 42.1 (1256 nm) | $\tau_b = 3.0; \tau_c = 16.7$ (520 nm);<br>$\tau_b = 17.9; \tau_c = 2.3$ (1256 nm)  | 377.3 (520 nm); 630.2 (1256 nm)  | 3000 cycles with 15.1% loss at 1000th cycle and 24.8% loss at 3000th cycles | This Work |
| p(TPD2T-TT)   | Stille Polymerization | 520 | -5.65 <sup>a</sup><br>-5.31 <sup>b</sup> | -3.86 <sup>a</sup><br>-3.52 <sup>b</sup> | 1.79 (Opt.) | Reddish Brown | $L^* = 86.19$<br>$a^* = 12.18$<br>$b^* = 1.07$   | 1235      | Purplish Grey | $L^* = 87.85$<br>$a^* = 3.57$<br>$b^* = -3.60$  | Sandwich Full Cell | 17.7 (497 nm); 30.4 (1238 nm) | $\tau_b = 3.1; \tau_c = 24.4$ (497 nm);<br>$\tau_b = 27.4; \tau_c = 2.1$ (1238 nm)  | 275.1 (497 nm); 340.4 (1238 nm)  | -   | This Work |
| p(TPD2T-EDOT) | Stille Polymerization | 537 | -5.39 <sup>a</sup><br>-5.17 <sup>b</sup> | -3.73 <sup>a</sup><br>-3.51 <sup>b</sup> | 1.66 (Opt.) | Greyish Blue  | $L^* = 81.49$<br>$a^* = 0.79$<br>$b^* = -13.36$  | 830, 1825 | Grey          | $L^* = 89.00$<br>$a^* = 0.46$<br>$b^* = -5.13$  | Sandwich Full Cell | 23.8 (595 nm); 46.7 (1800 nm) | $\tau_b = 1.7; \tau_c = 9.0$ (595 nm);<br>$\tau_b = 11.9; \tau_c = 1.3$ (1800 nm)   | 720.7 (595 nm); 1012.1 (1800 nm) | 3000 cycles with 10.7% loss at 1000th cycle and 20.9% loss at 3000th cycles | This Work |
| p(TPD2T-DTP)  | Stille Polymerization | 565 | -5.22 <sup>a</sup><br>-5.34 <sup>b</sup> | -3.63 <sup>a</sup><br>-3.75 <sup>b</sup> | 1.59 (Opt.) | Dark Blue     | $L^* = 76.93$<br>$a^* = -3.23$<br>$b^* = -17.95$ | 755, 1400 | Bluish Grey   | $L^* = 87.36$<br>$a^* = -2.95$<br>$b^* = -5.56$ | Sandwich Full Cell | 20.0 (608 nm); 44.8 (1400 nm) | $\tau_b = 0.7; \tau_c = 4.3$ (608 nm);<br>$\tau_b = 6.8; \tau_c = 1.2$ (1400 nm)    | 801.1 (608 nm); 1358.5 (1400 nm) | 3000 cycles with 35.6% loss at 1000th cycle and 48.5% loss at 3000th cycles | This Work |
| p(TPD2T-CPDT) | Stille Polymerization | 558 | -5.32 <sup>a</sup><br>-5.21 <sup>b</sup> | -3.51 <sup>a</sup><br>-3.40 <sup>b</sup> | 1.81 (Opt.) | Purple        | $L^* = 76.67$<br>$a^* = 4.68$<br>$b^* = -11.06$  | 800, 1450 | Grey          | $L^* = 85.94$<br>$a^* = 0.06$<br>$b^* = -2.08$  | Sandwich Full Cell | 18.1 (555 nm); 23.7 (1380 nm) | $\tau_b = 9.6; \tau_c = 36.1$ (555 nm);<br>$\tau_b = 46.4; \tau_c = 3.6$ (1380 nm)  | 245.9 (555 nm); 247.6 (1380 nm)  | -   | This Work |

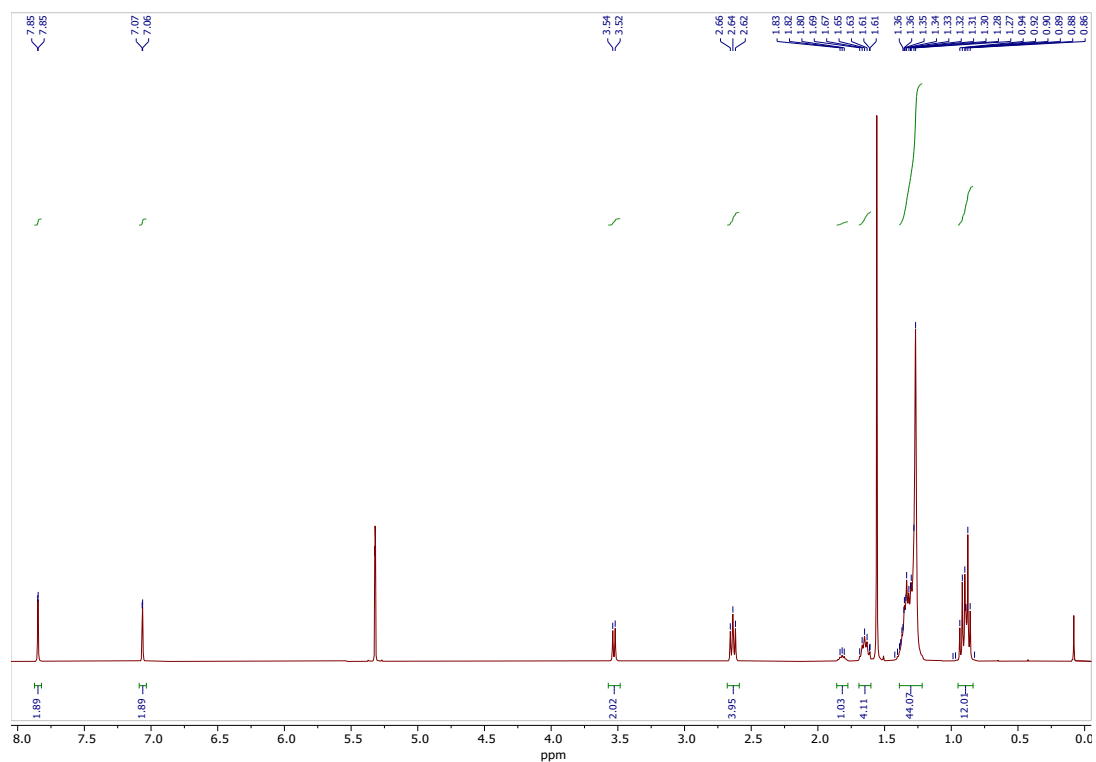
<sup>a</sup> Measured from solution-based CV; <sup>b</sup> measured from thin film-based CV.

#### References:

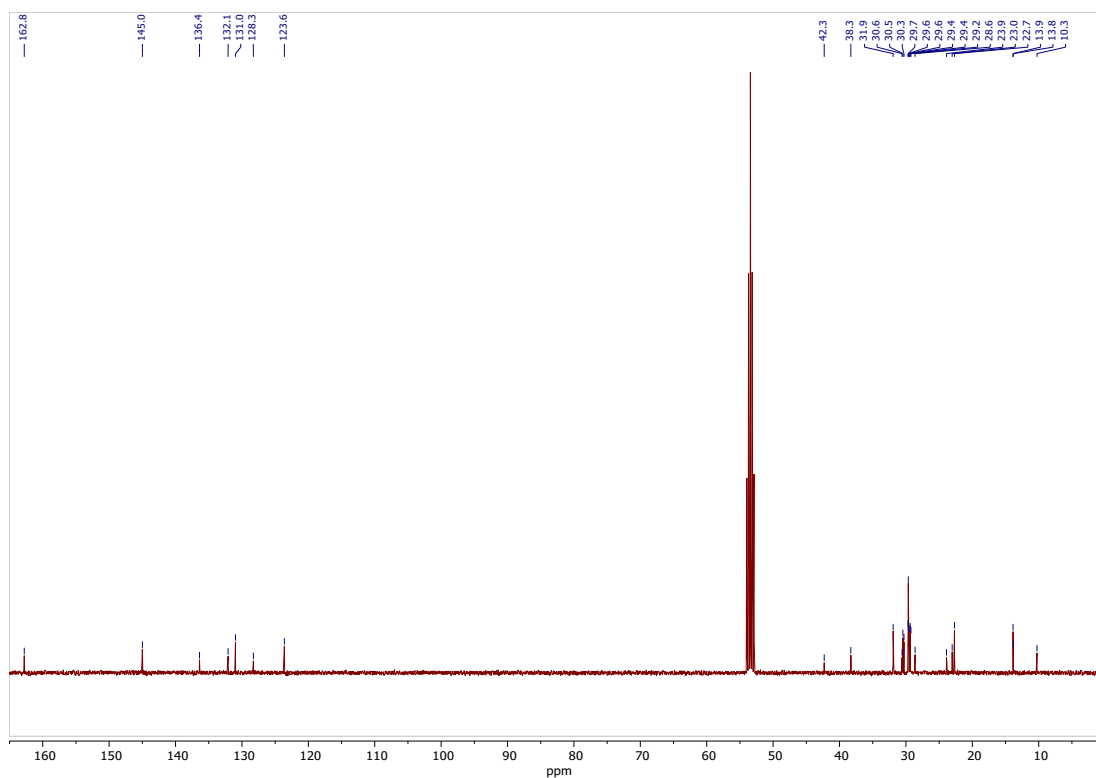
1. Deniz Çakal, Atilla Cihaner, Ahmet M. Önal, *Electrochimica Acta* (2021) 377, 138064 (DOI: 10.1016/j.electacta.2021.138064)
2. Peiyu Wu, Shengxiong Zhang, Wenjun Zhang, Weijie Song, *Dyes and Pigments* (2023) 219, 111566 (DOI: 10.1016/j.dyepig.2023.111566)
3. Zhe Xu, Shouyi Ming, Teng Zhang, Meijing Li, Shijie Zhen, *Luminescence* (2024), 39, e4843 (DOI: 10.1002/bio.4843)

## ANNEX

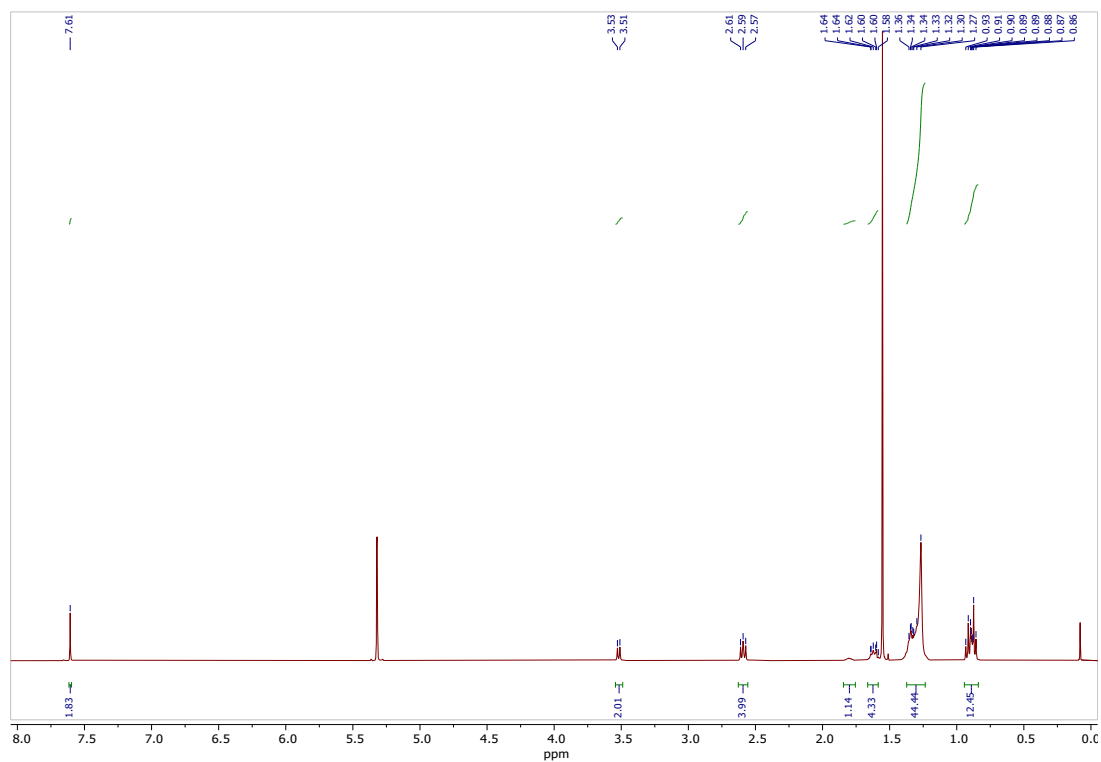
$^1\text{H}$  NMR of 1,3-bis(4-dodecylthiophen-2-yl)-5-(2-ethylhexyl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (2):



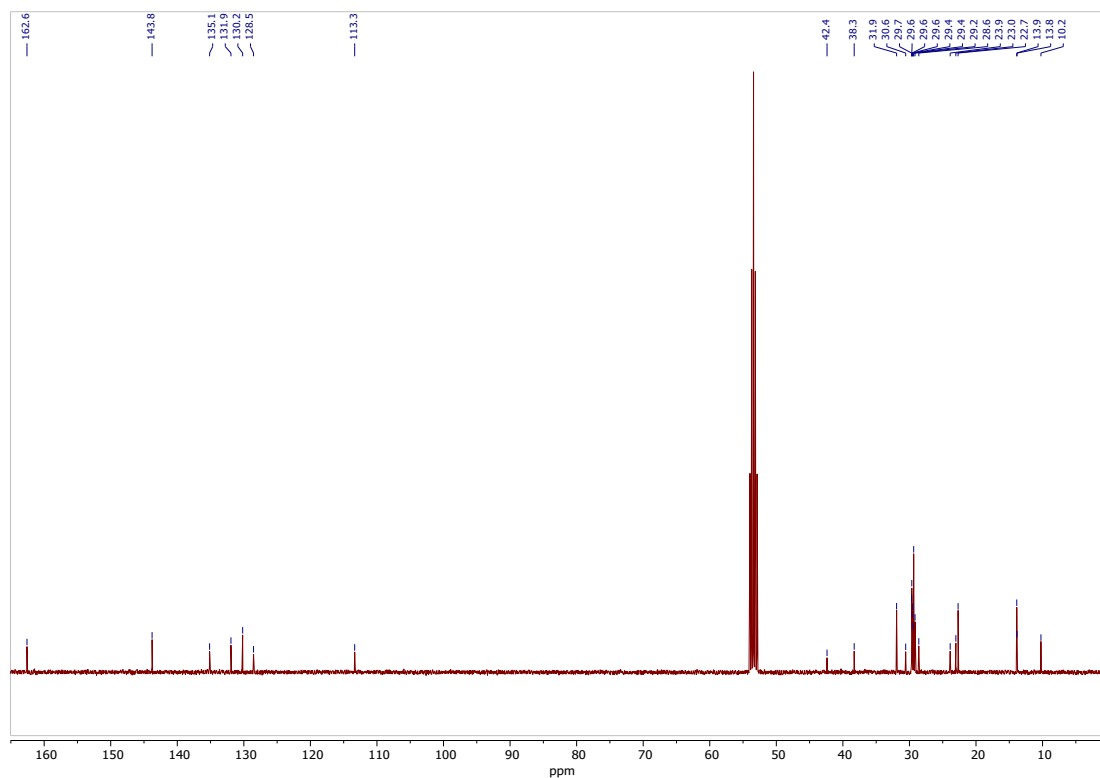
$^{13}\text{C}$  NMR of 1,3-bis(4-dodecylthiophen-2-yl)-5-(2-ethylhexyl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (2):



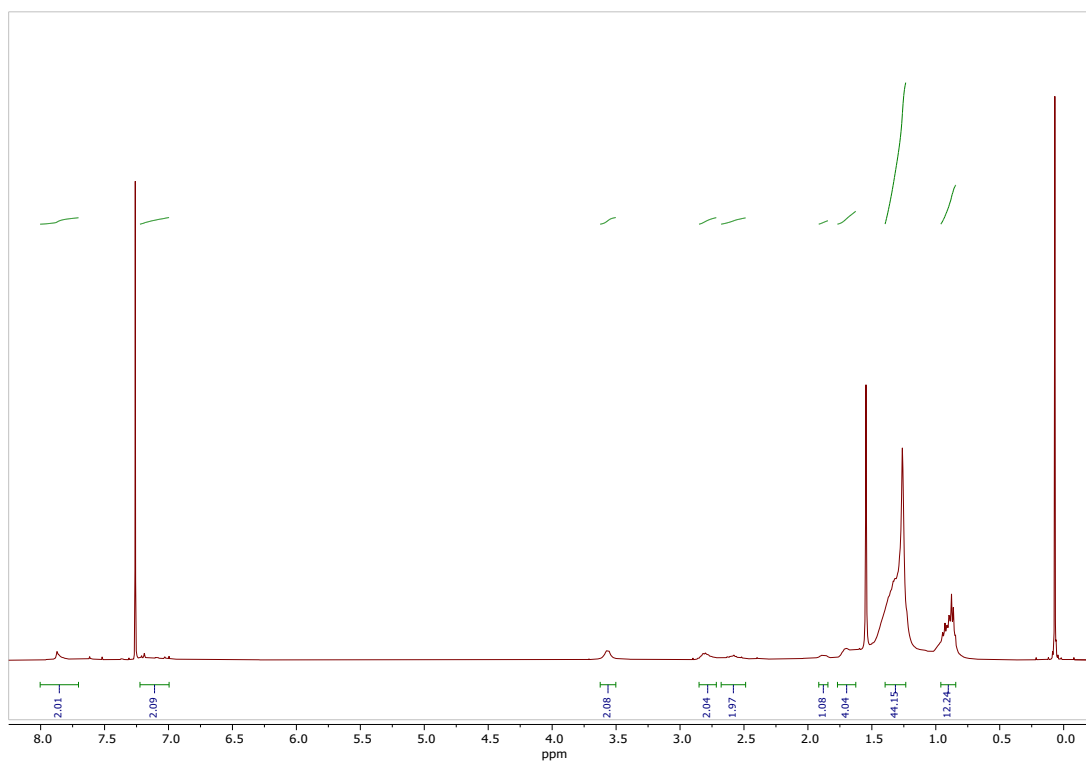
$^1\text{H}$  NMR of 1,3-bis(5-bromo-4-dodecylthiophen-2-yl)-5-(2-ethylhexyl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (**3**):



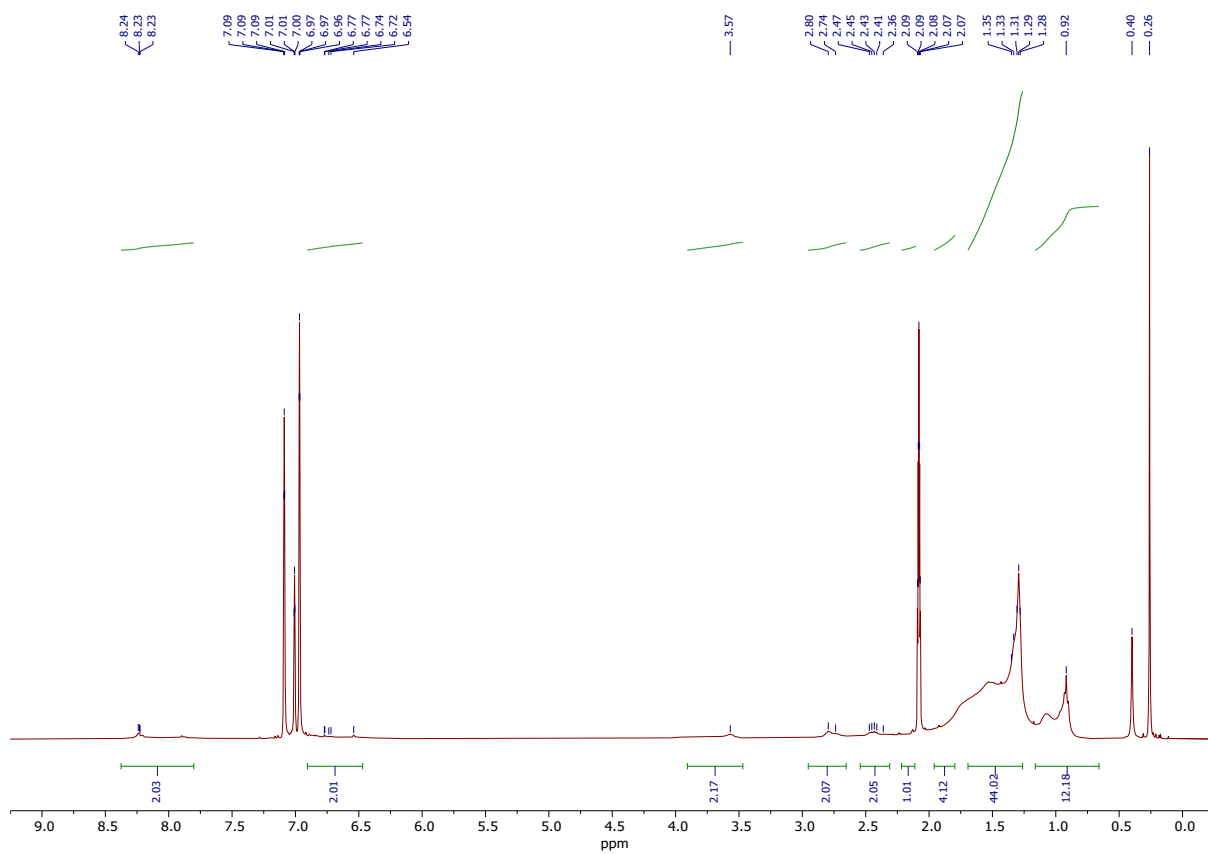
$^{13}\text{C}$  NMR of 1,3-bis(5-bromo-4-dodecylthiophen-2-yl)-5-(2-ethylhexyl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (**3**):



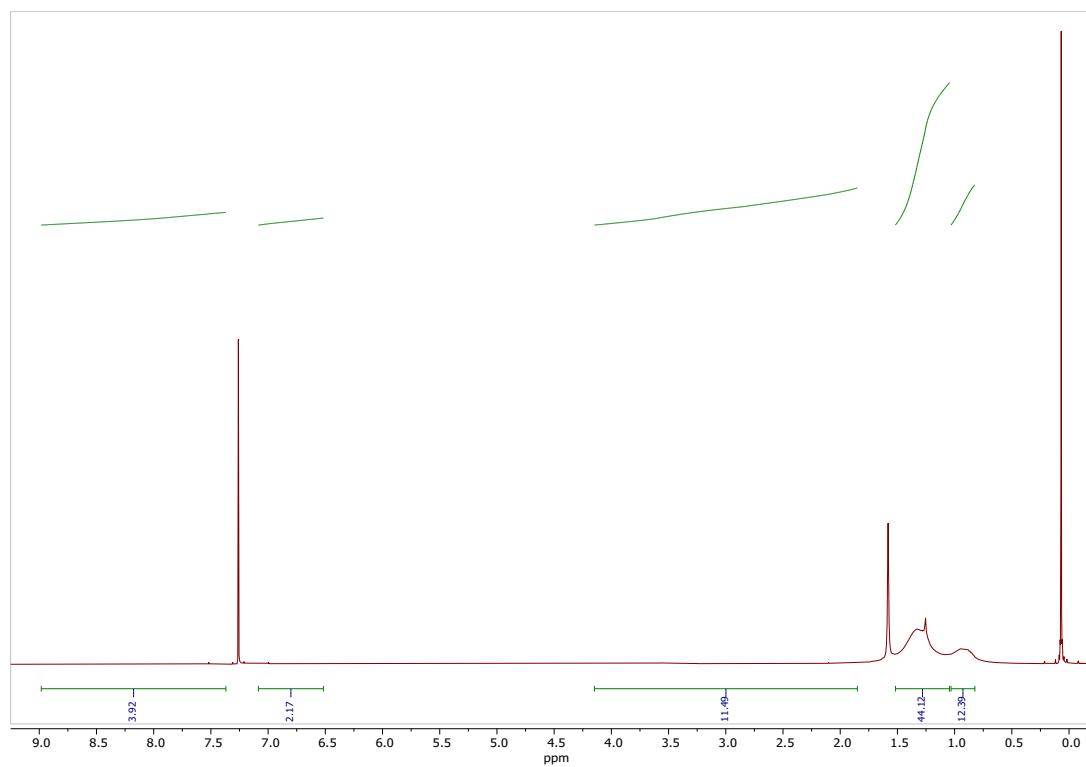
$^1\text{H}$  NMR of p(TPD2T-T) in  $\text{CDCl}_3$



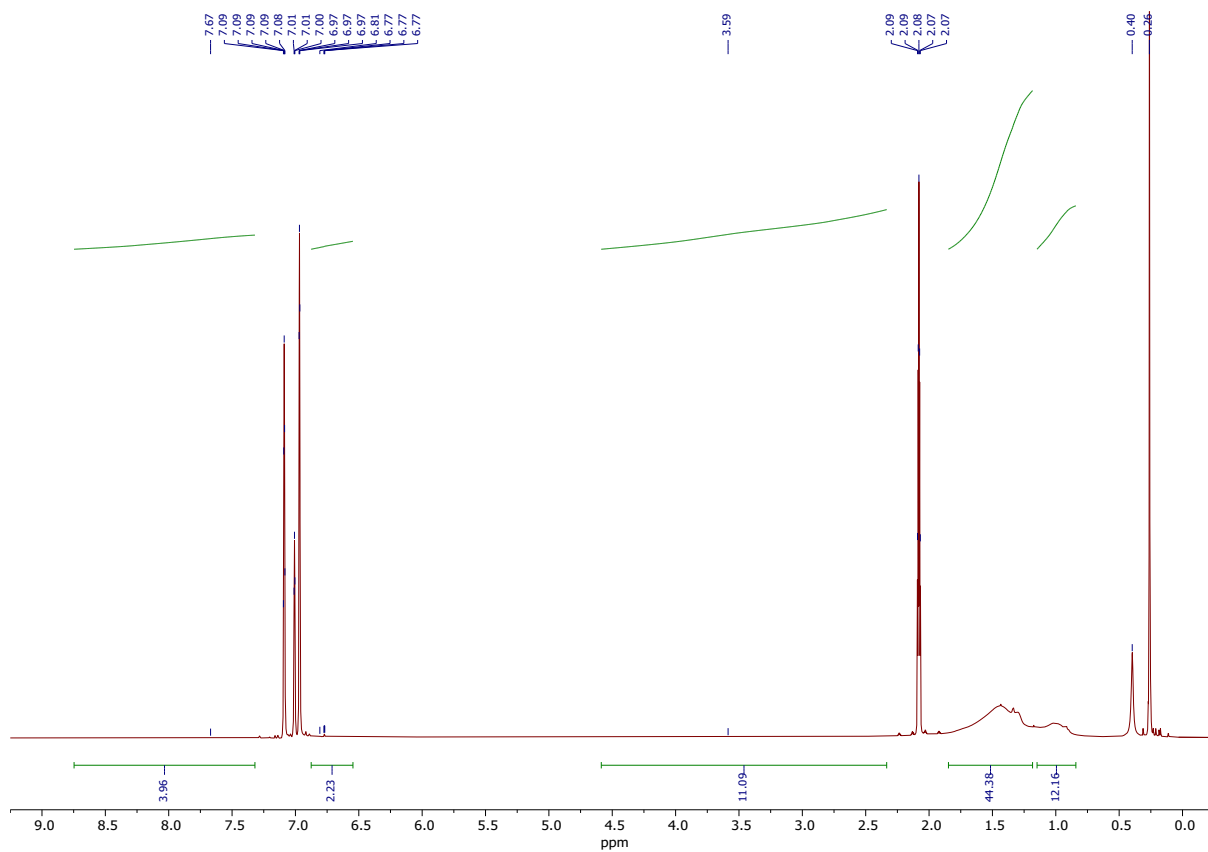
$^1\text{H}$  NMR of p(TPD2T-T) in Toluene- $\text{D}_8$



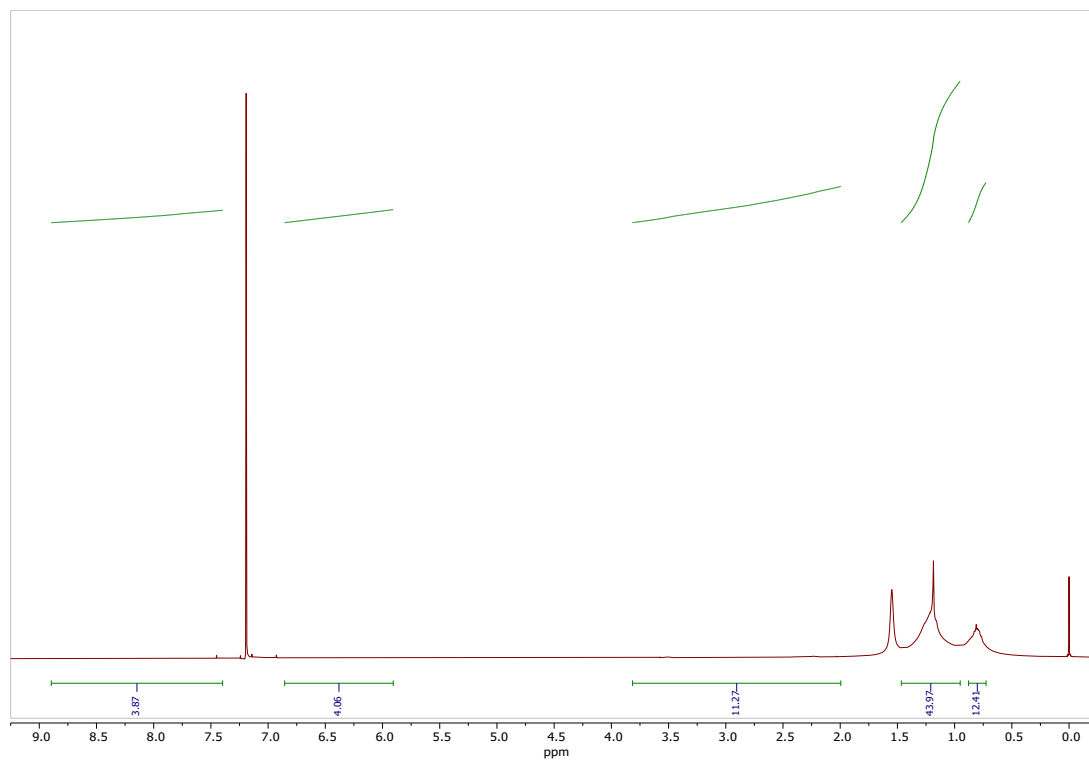
$^1\text{H}$  NMR of p(TPD2T-2T) in  $\text{CDCl}_3$



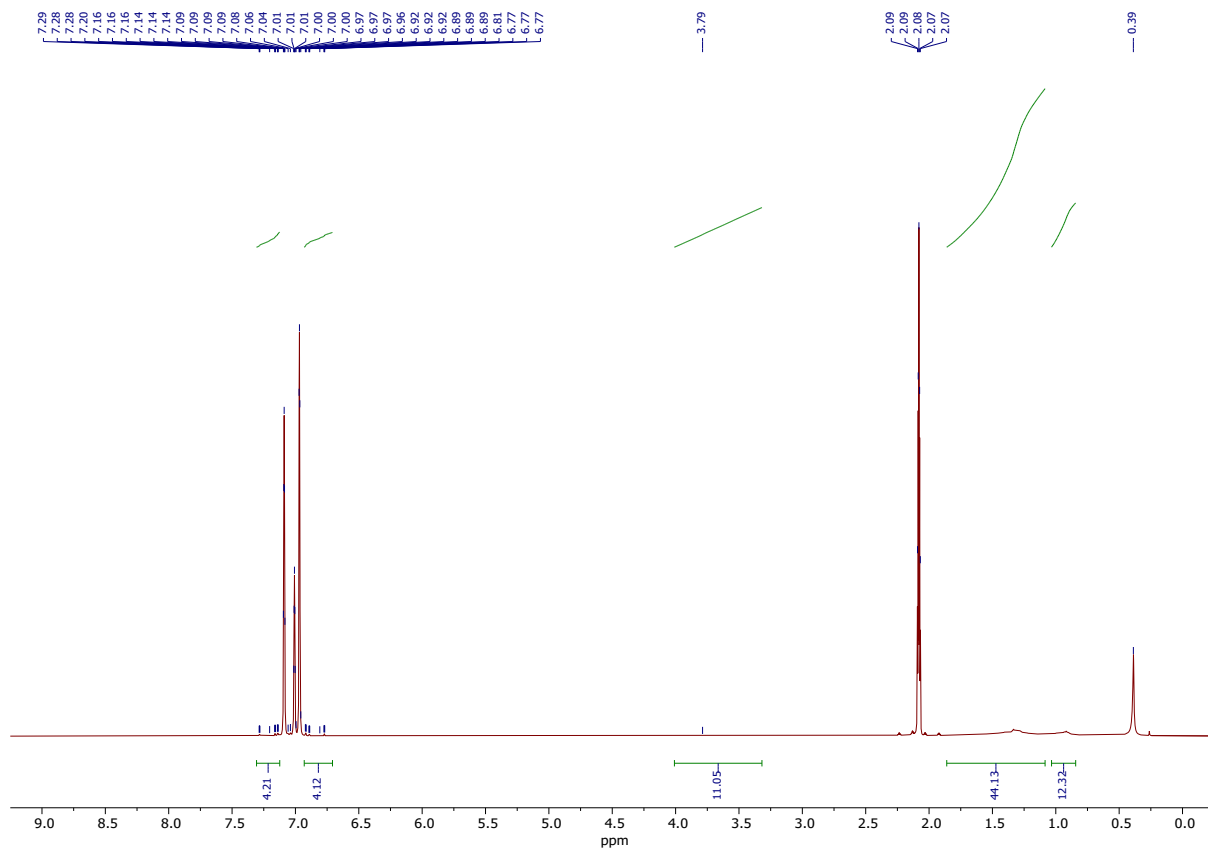
$^1\text{H}$  NMR of p(TPD2T-2T) in Toluene- $\text{D}_8$



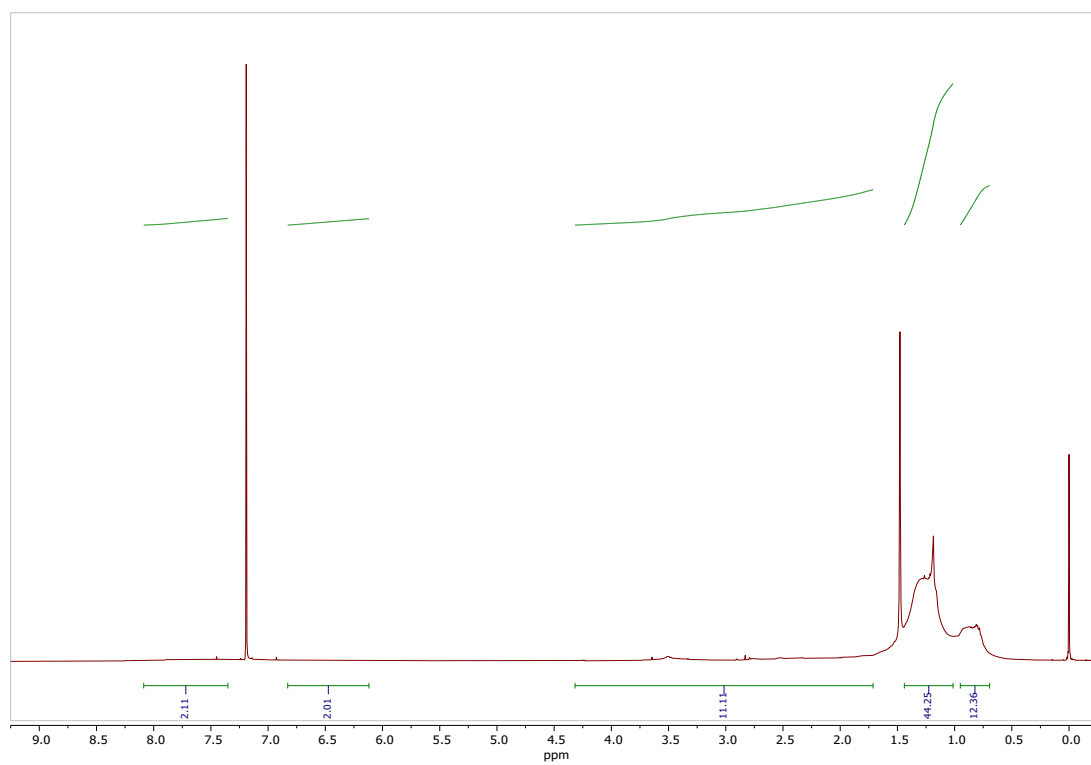
$^1\text{H}$  NMR of p(TPD2T-3T) in  $\text{CDCl}_3$



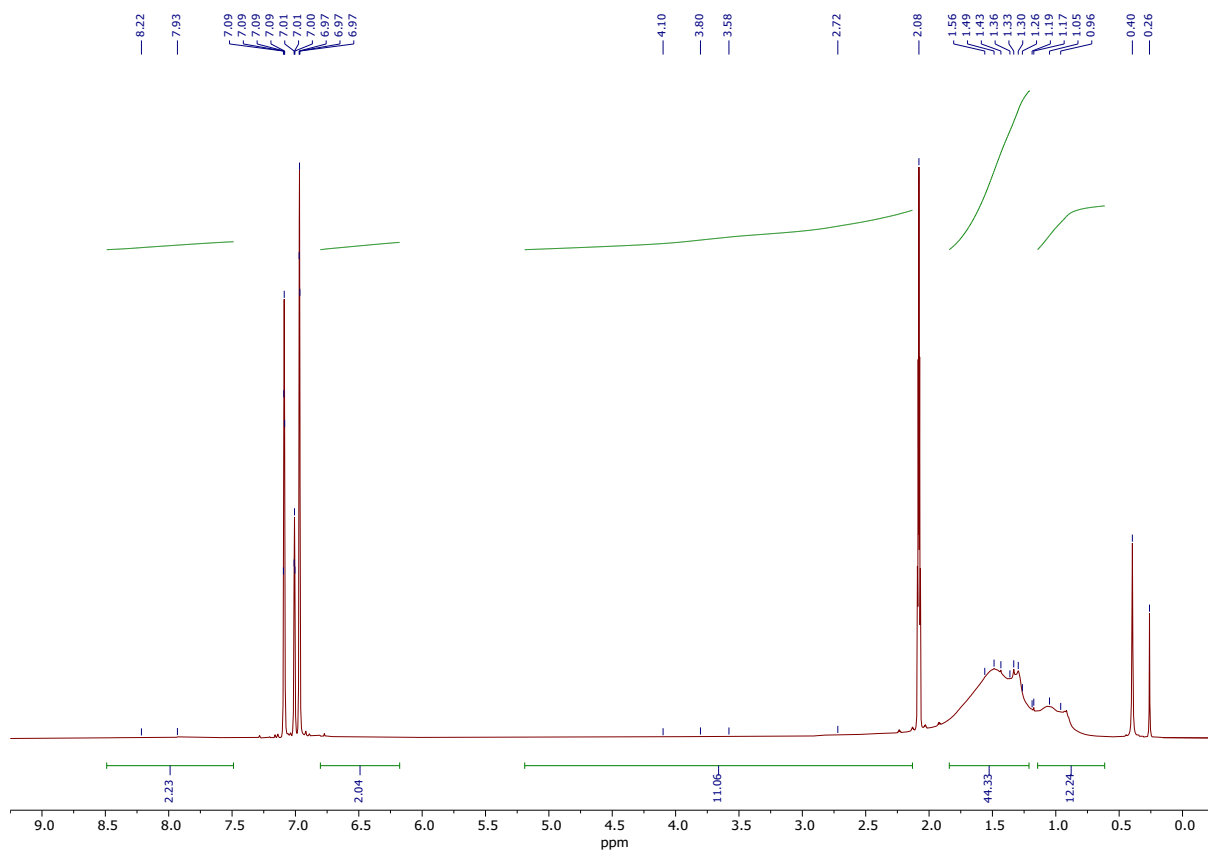
$^1\text{H}$  NMR of p(TPD2T-3T) in Toluene- $\text{D}_8$



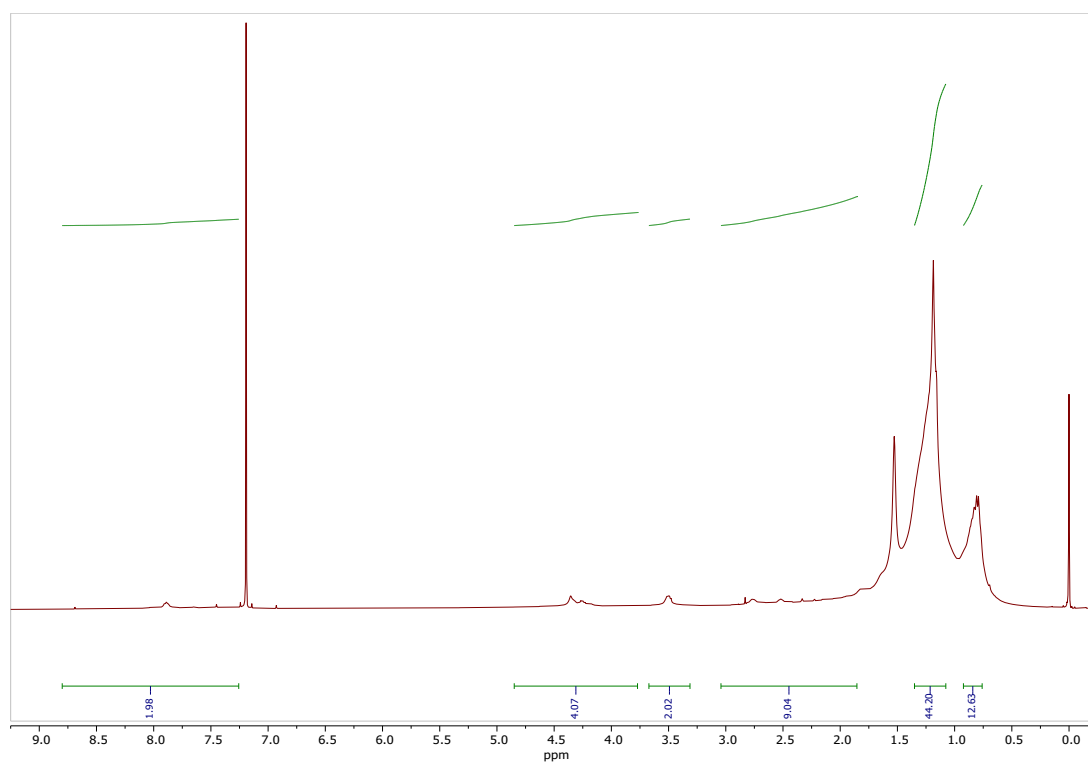
$^1\text{H}$  NMR of p(TPD2T-TT) in  $\text{CDCl}_3$



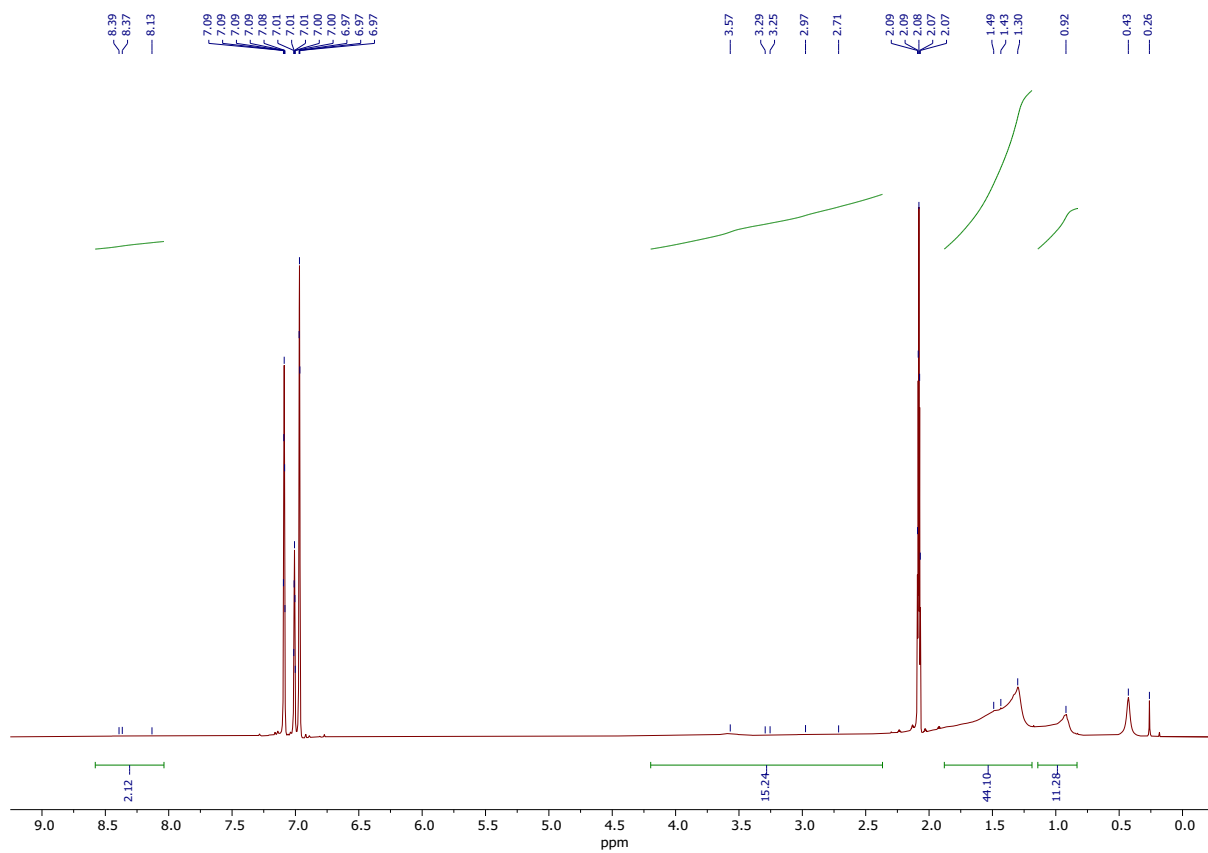
$^1\text{H}$  NMR of p(TPD2T-TT) in Toluene- $\text{D}_8$



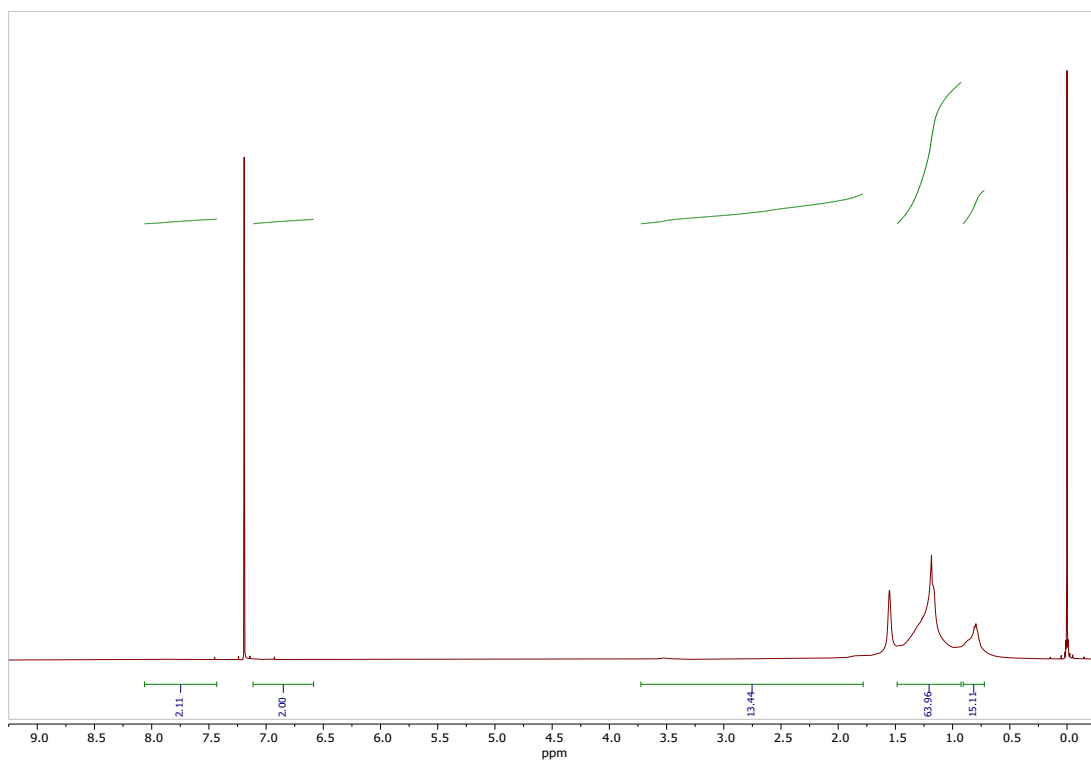
$^1\text{H}$  NMR of p(TPD2T-EDOT) in  $\text{CDCl}_3$



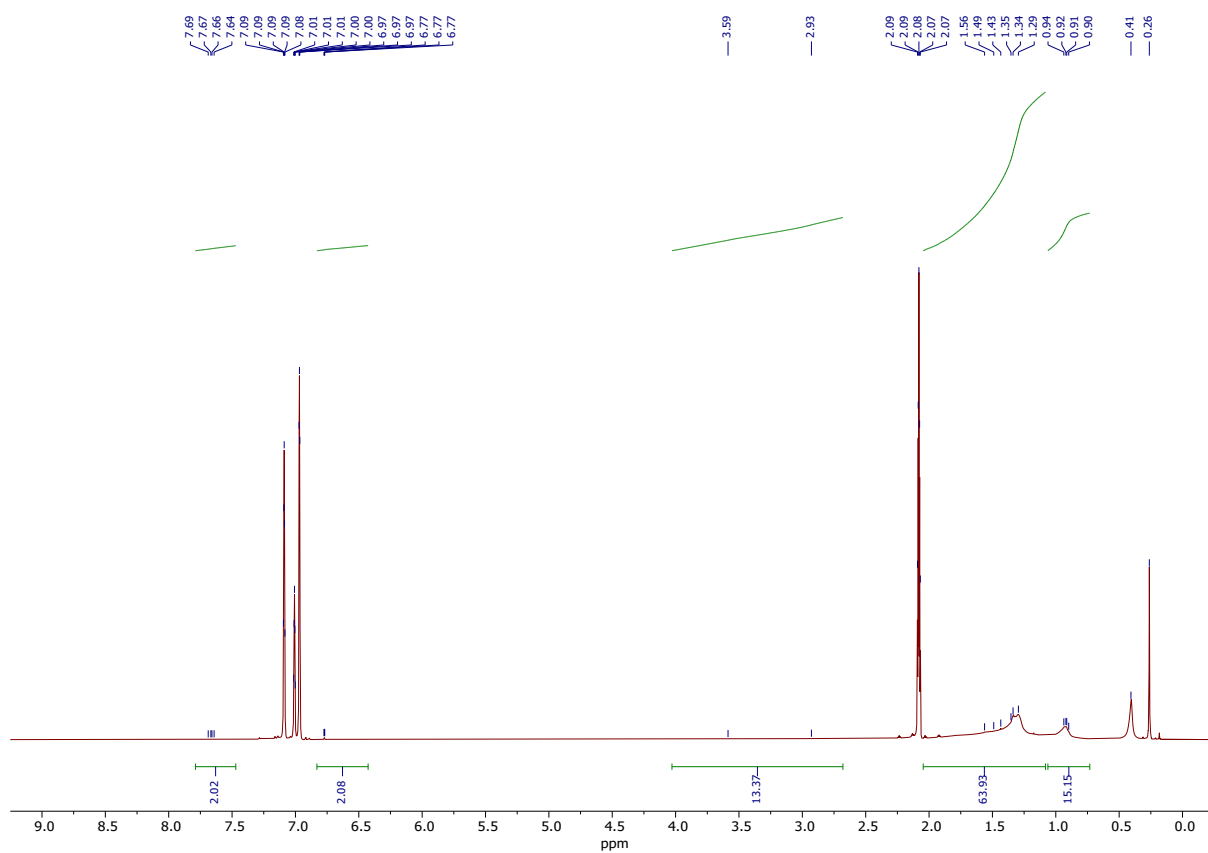
$^1\text{H}$  NMR of p(TPD2T-EDOT) in Toluene- $\text{D}_8$



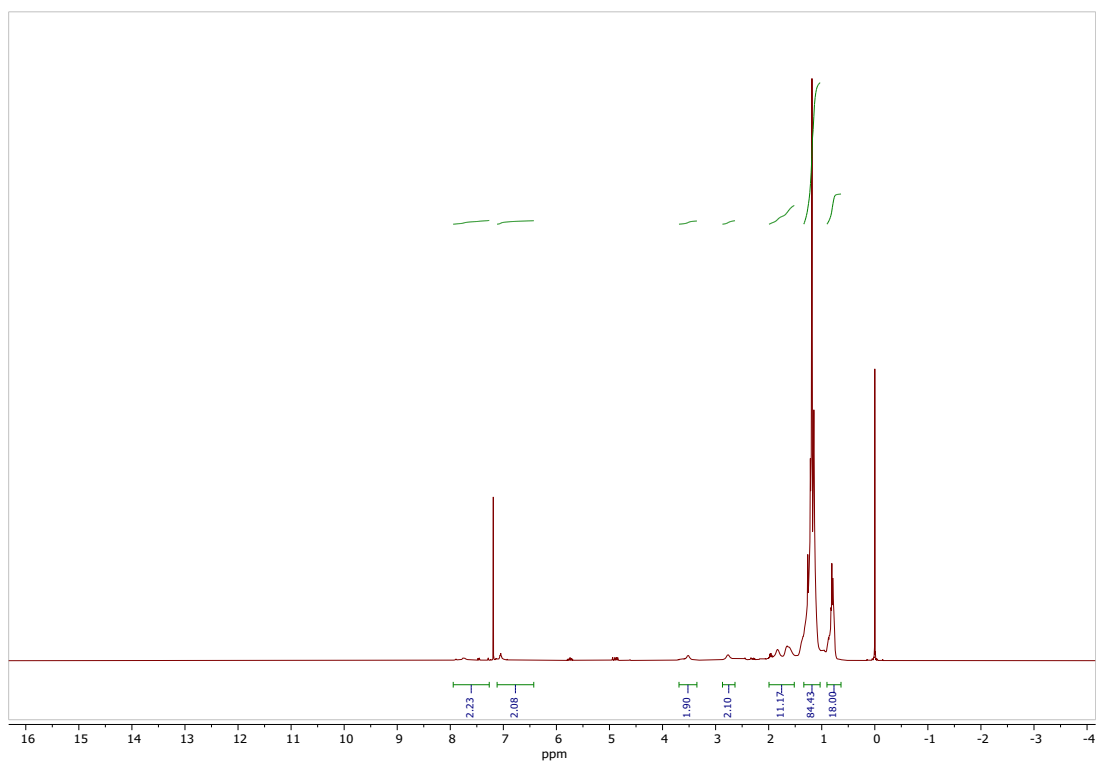
$^1\text{H}$  NMR of p(TPD2T-DTP) in  $\text{CDCl}_3$



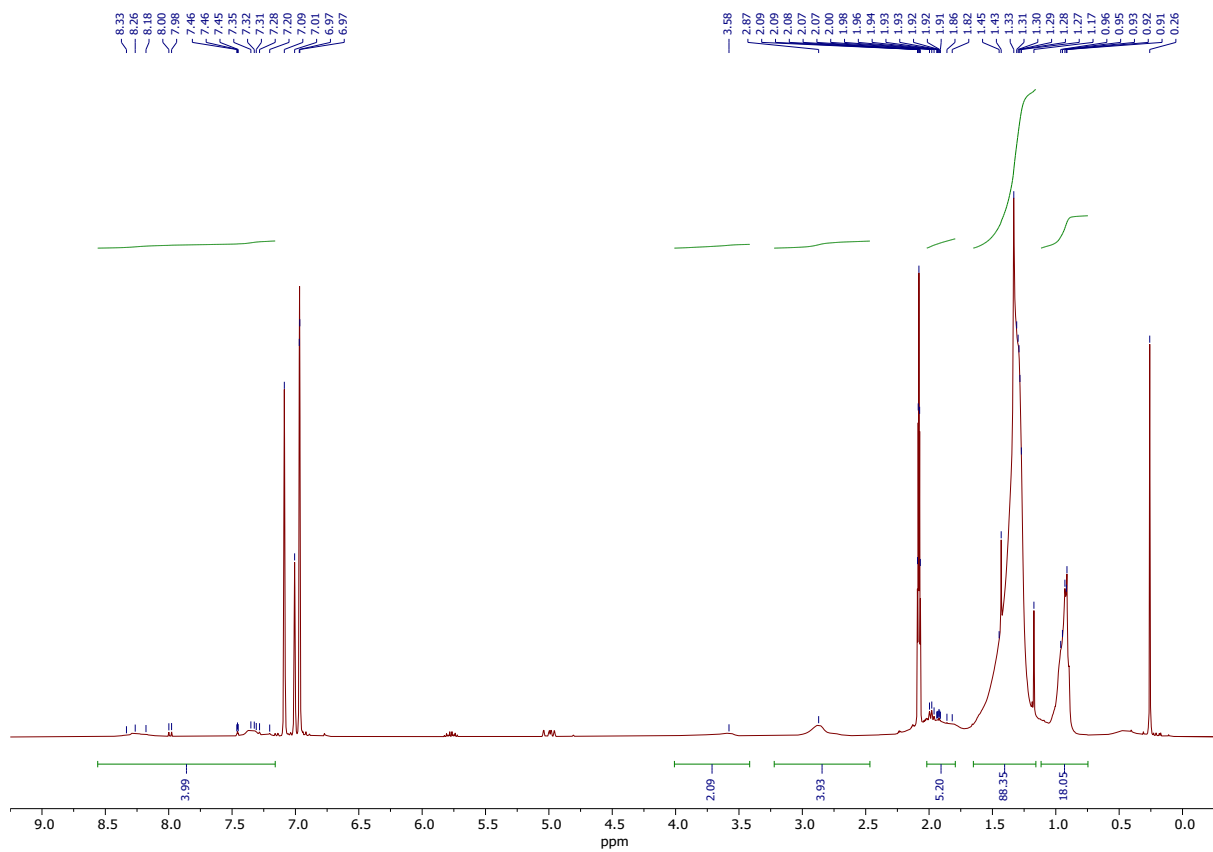
$^1\text{H}$  NMR of p(TPD2T-DTP) in Toluene- $\text{D}_8$



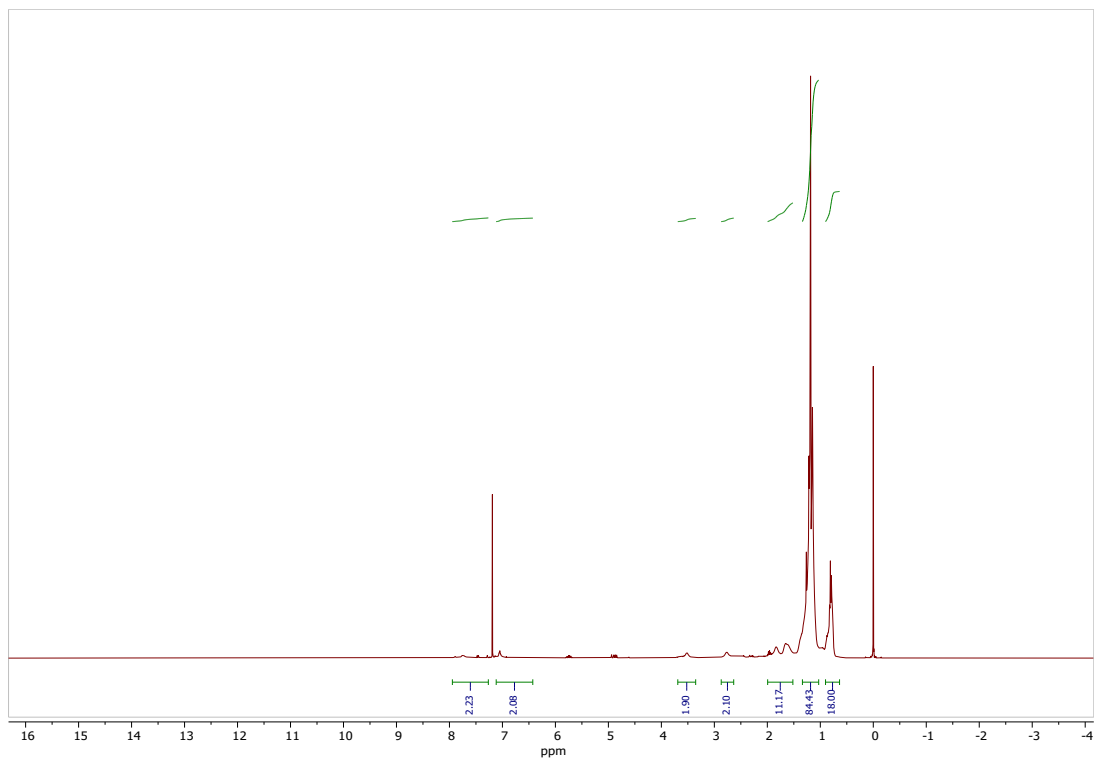
$^1\text{H}$  NMR of p(TPD2T-CPDT) in  $\text{CDCl}_3$



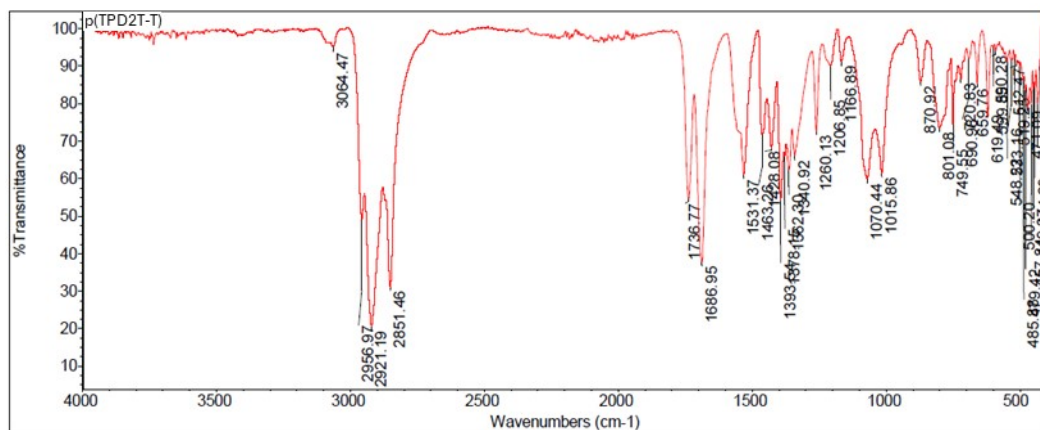
$^1\text{H}$  NMR of p(TPD2T-CPDT) in Toluene- $\text{D}_8$



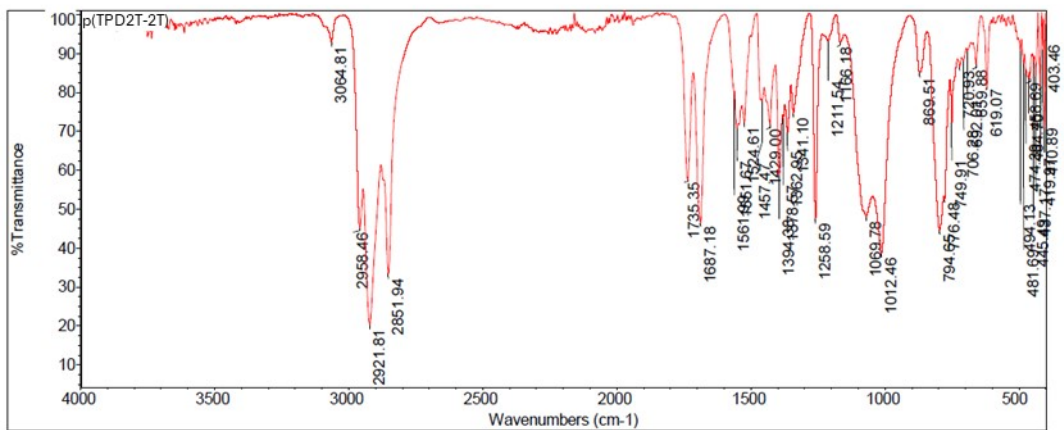
### <sup>1</sup>H NMR of p(TPD2T-CPDT)



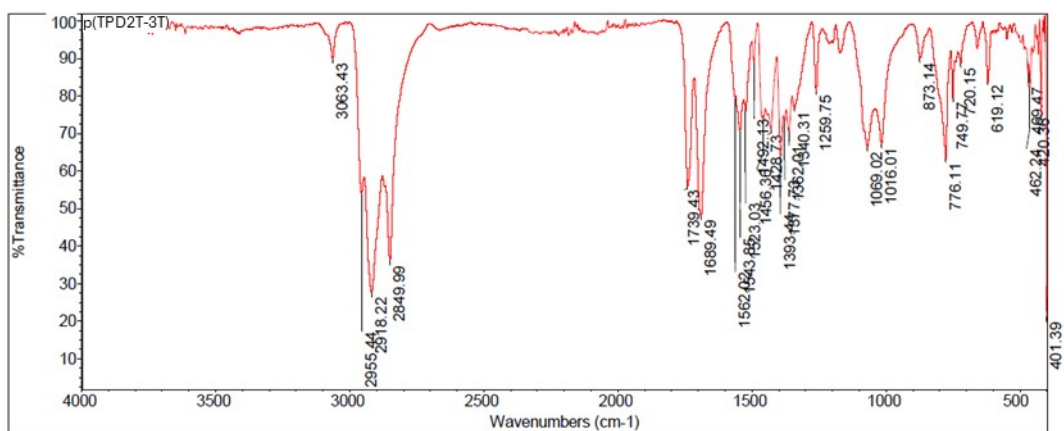
### FTIR Spectra of p(TPD2T-T)



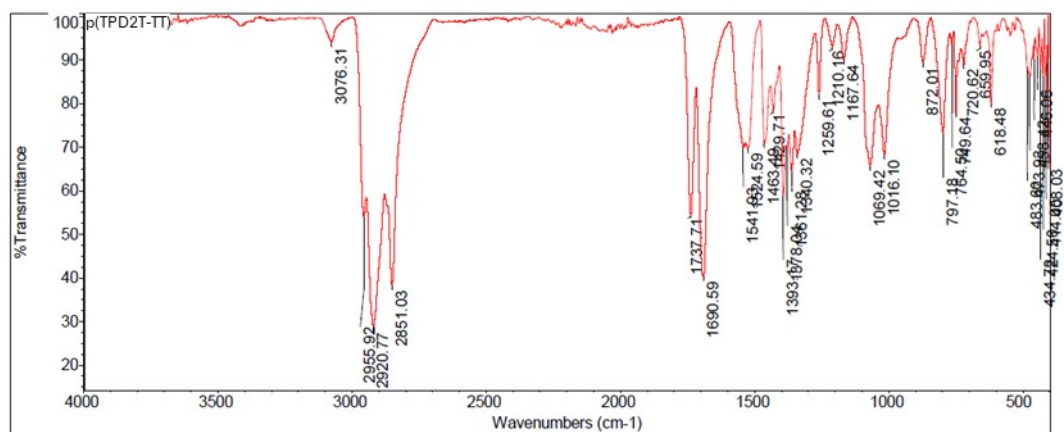
### FTIR Spectra of p(TPD2T-2T)



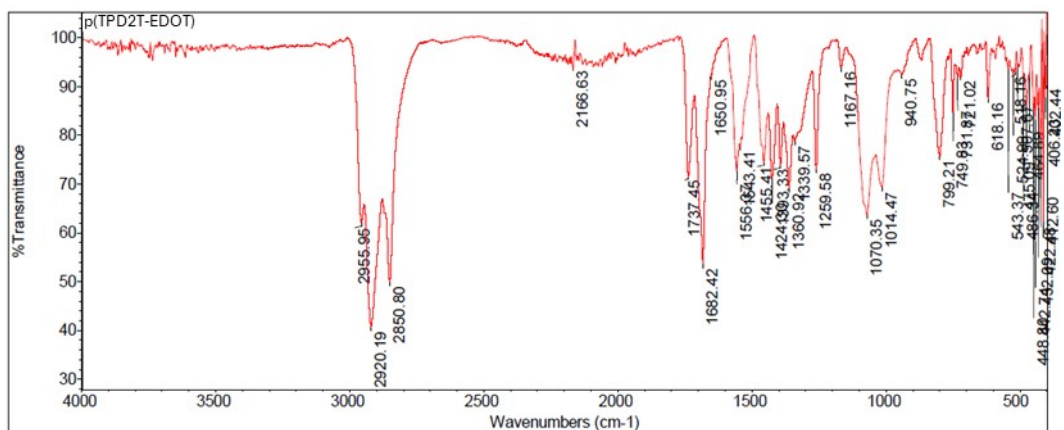
FTIR Spectra of p(TPD2T-3T)



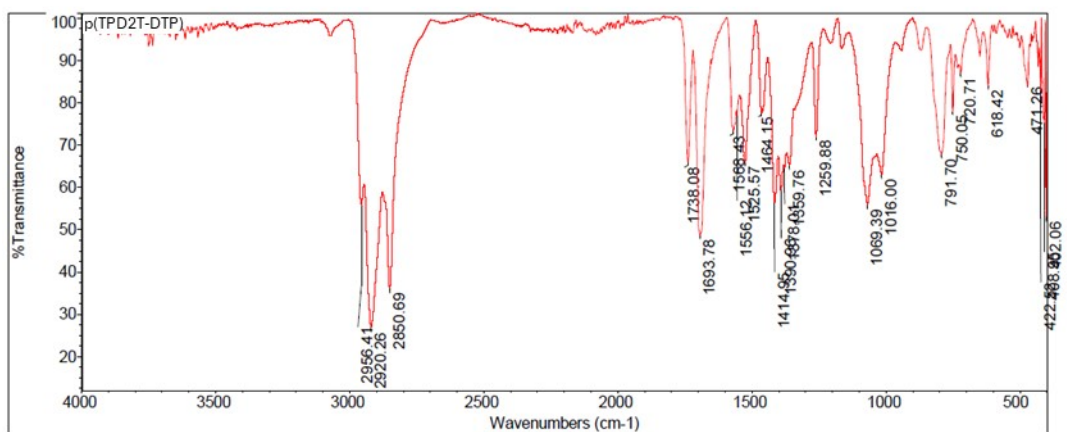
FTIR Spectra of p(TPD2T-TT)



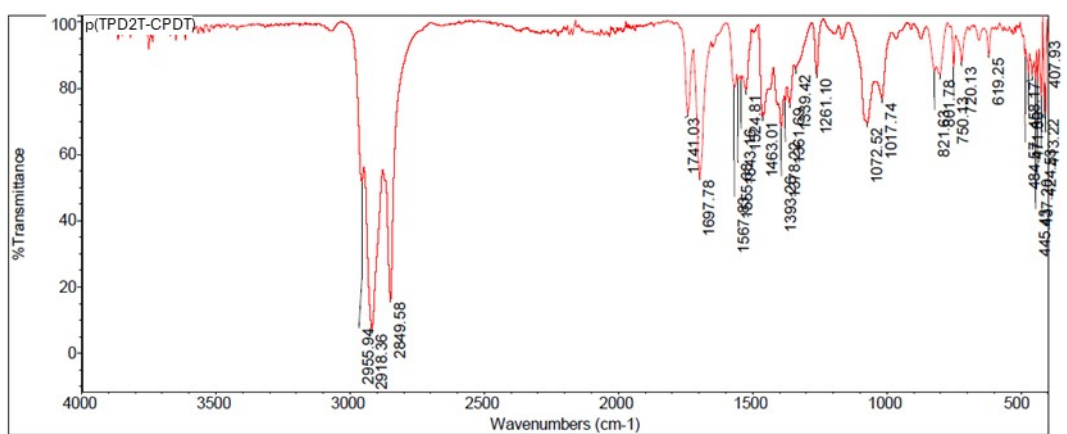
FTIR Spectra of p(TPD2T-EDOT)



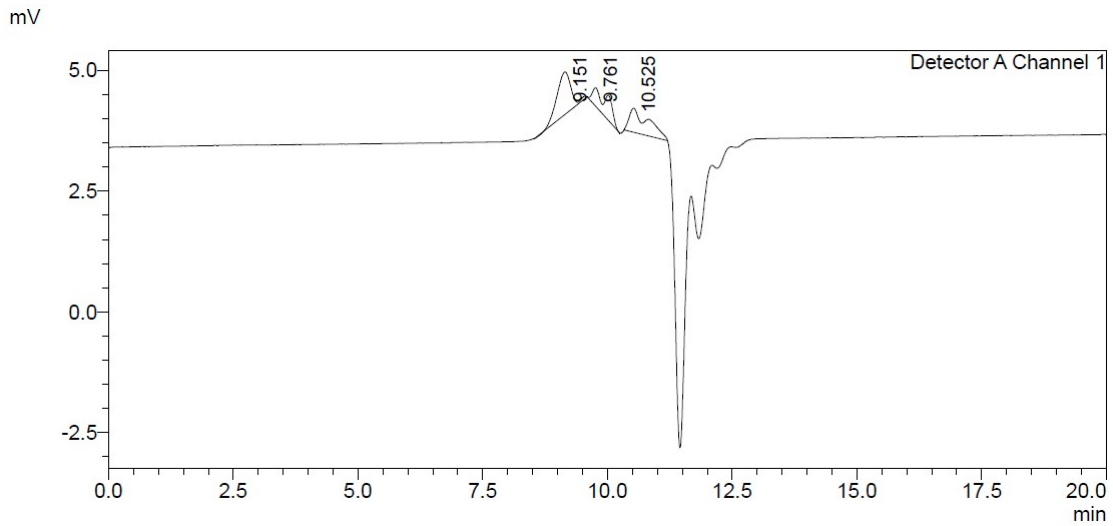
FTIR Spectra of p(TPD2T-DTP)



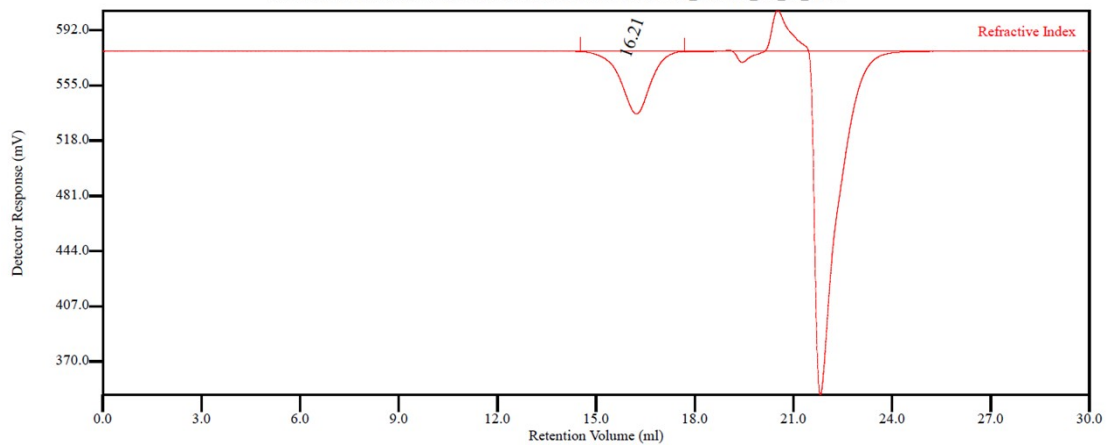
FTIR Spectra of p(TPD2T-CPDT)



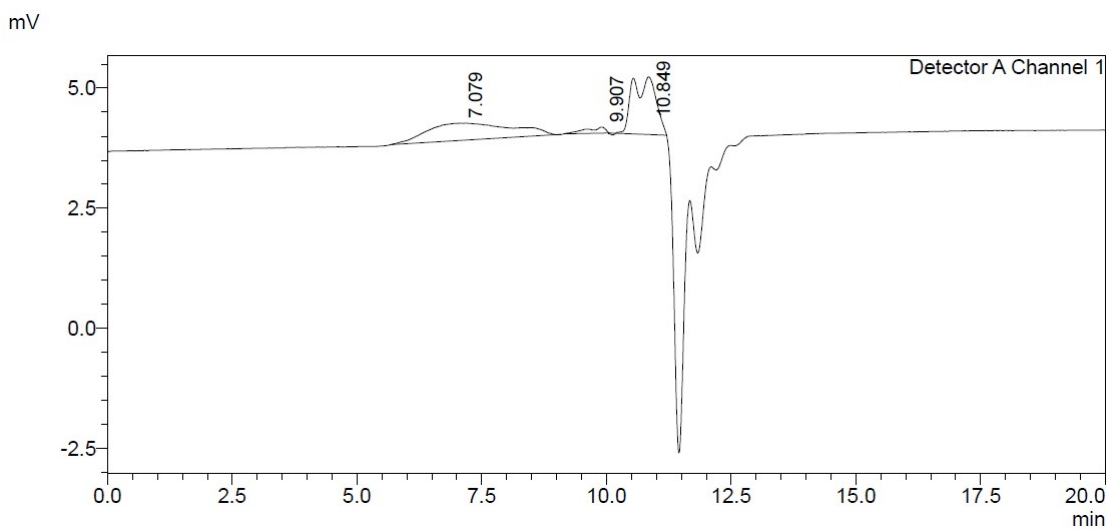
GPC Chromatogram of p(TPD2T-T)



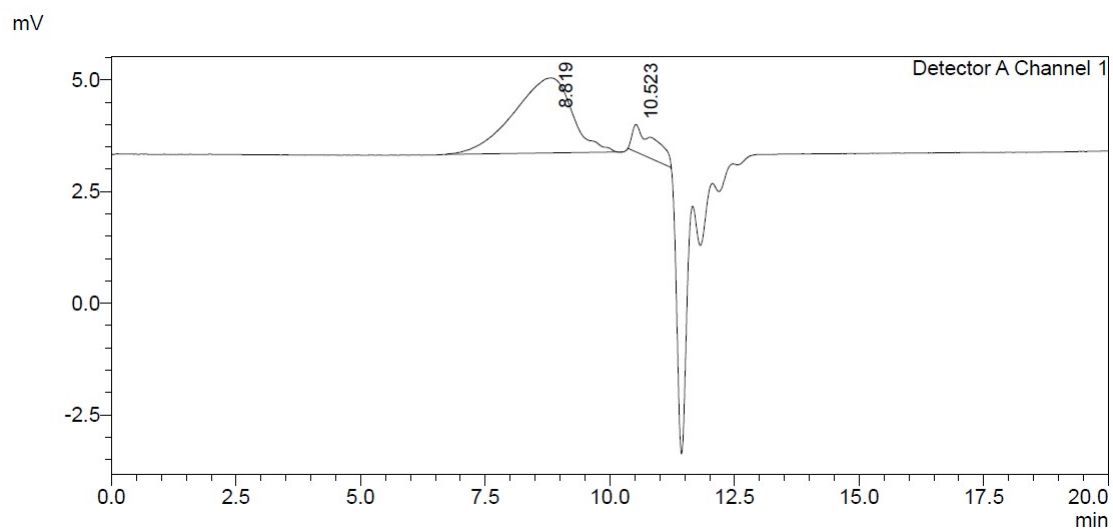
GPC Chromatogram of p(TPD2T-2T)



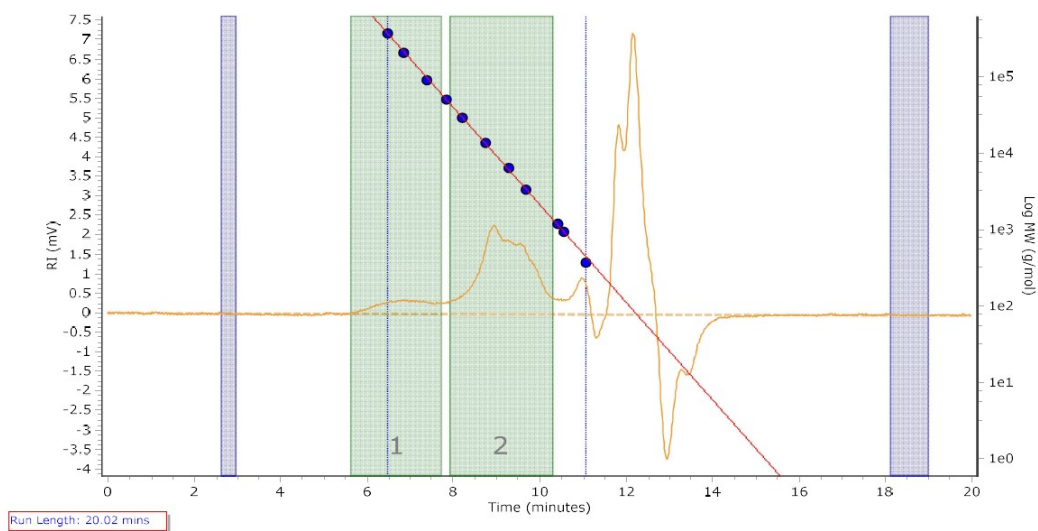
GPC Chromatogram of p(TPD2T-3T)



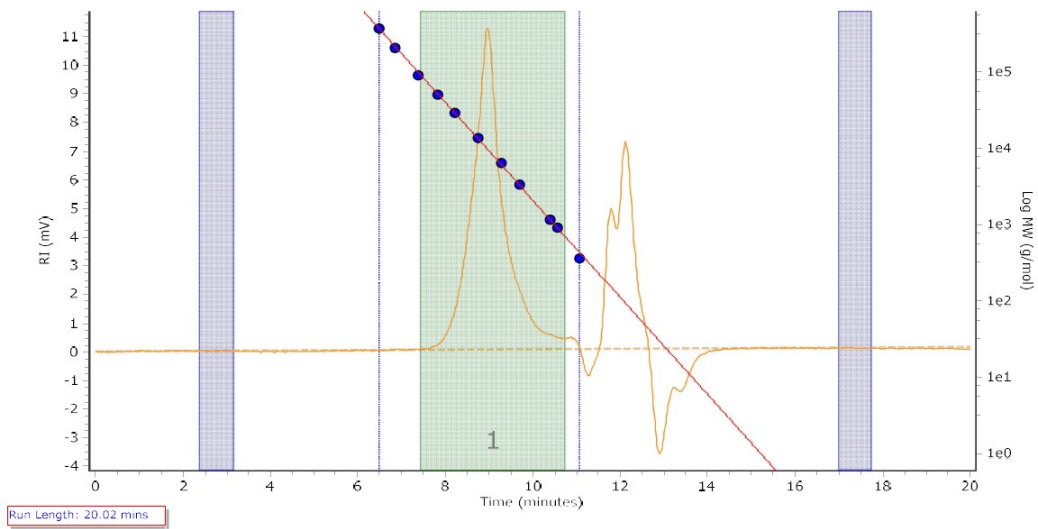
GPC Chromatogram of p(TPD2T-TT)



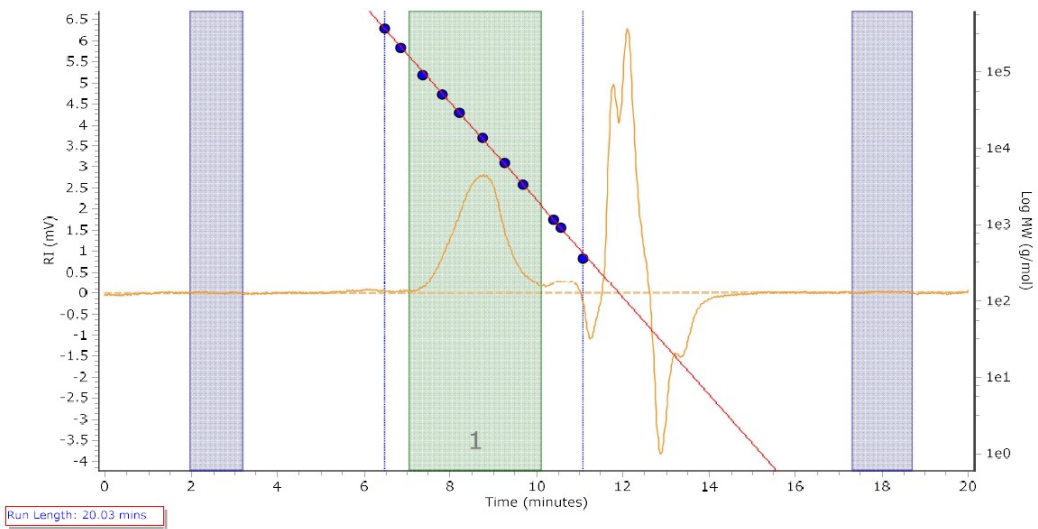
GPC Chromatogram of p(TPD2T-EDOT)



GPC Chromatogram of p(TPD2T-DTP)



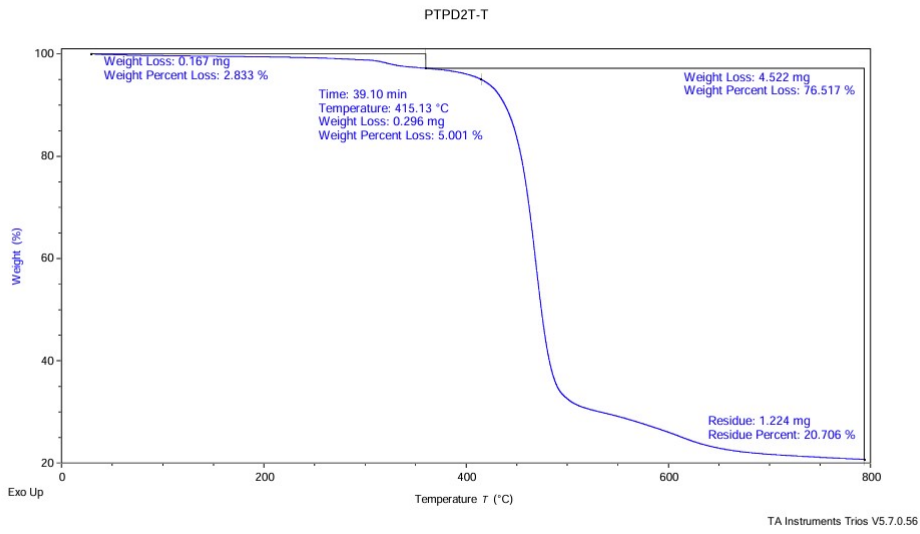
GPC Chromatogram of p(TPD2T-CPDT)



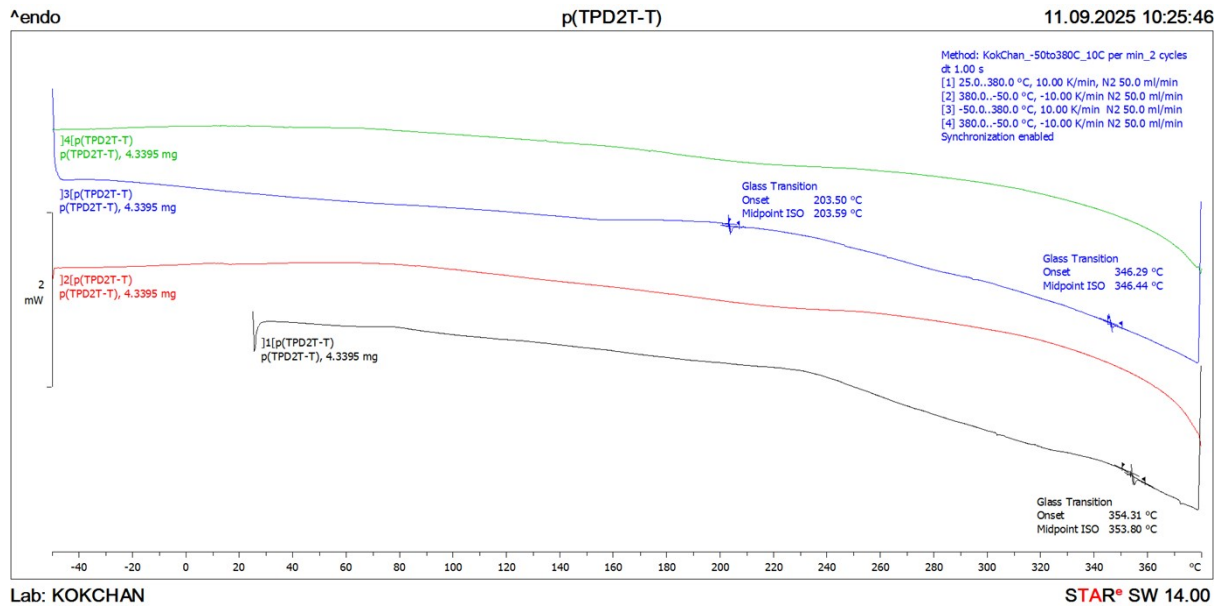
TGA Analysis of p(TPD2T-T)

PTPD2T-T  
 30-800C\_10C per min\_N2  
 Kok Chan  
 D:\TA Data\SDT 650\User Data\Kok Chan\AR25SDT20062\PTPD2T-T.tri

SDT650,6/6/2025 1:57:42 PM  
 5.909 mg  
 Alumina 90 ul



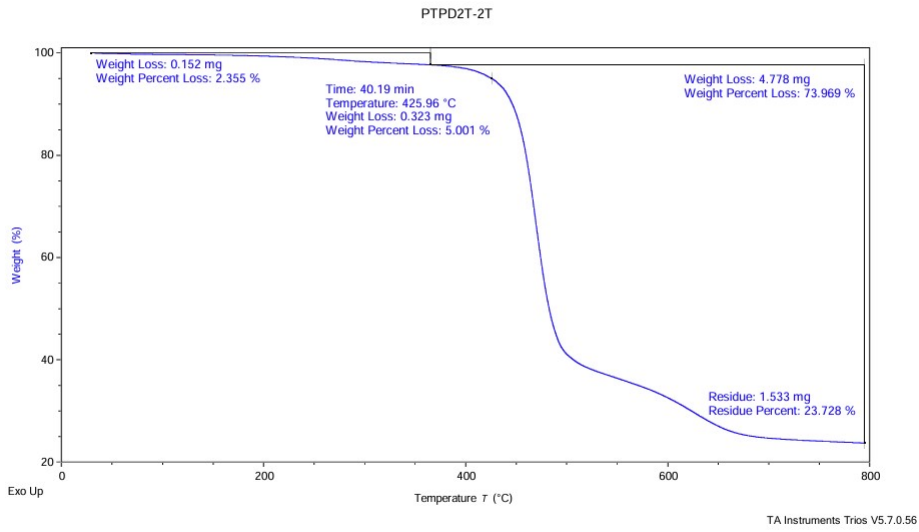
### DSC Analysis of p(TPA2T-T)



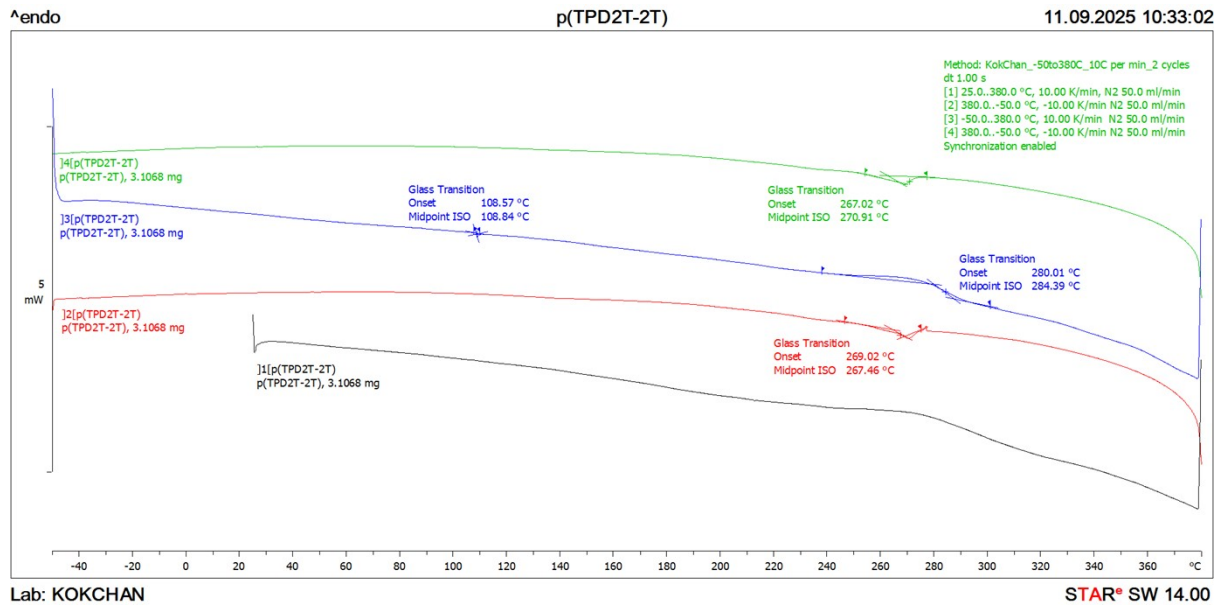
### TGA Analysis of p(TPD2T-2T)

PTPD2T-2T  
30-800C\_10C per min\_N2  
Kok Chan  
D:\TA Data\SDT 650\User Data\Kok Chan\AR25SDT20062\PTPD2T-2T.txi

SDT650.6/6/2025 7:28:09 PM  
6.460 mg  
Alumina 90 ul



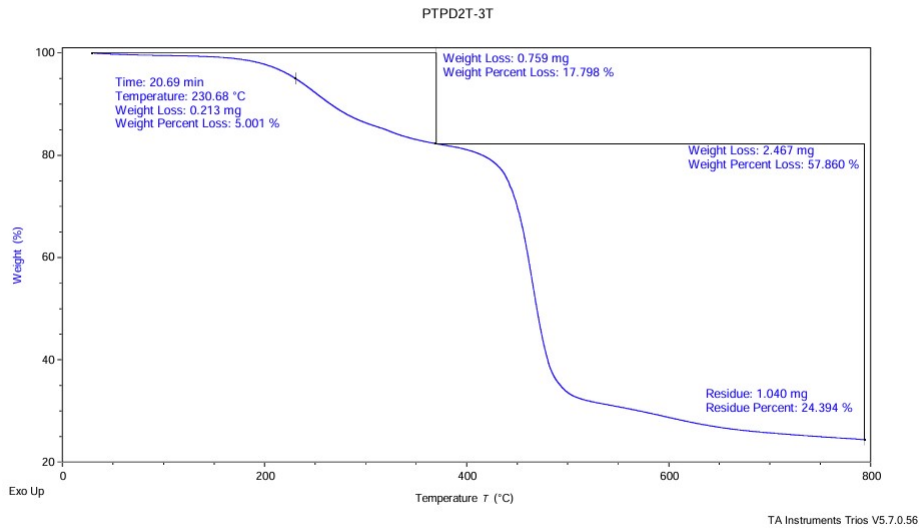
### DSC Analysis of p(TPD2T-2T)



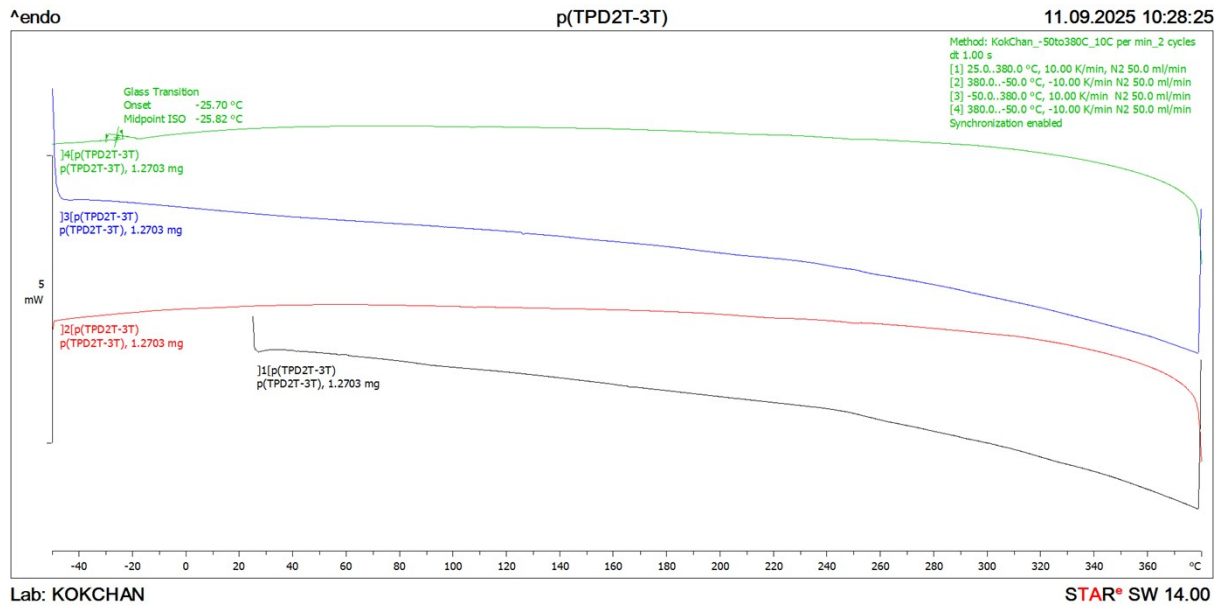
### TGA Analysis of p(TPD2T-3T)

PTPD2T-3T  
30-800C\_10C per min\_N2  
Kok Chan  
D:\TA Data\SDT 650\User Data\Kok Chan\AR25SDT20062\PTPD2T-3T.txi

SDT650.6/6/2025 4:45:22 PM  
4.263 mg  
Alumina 90 ul



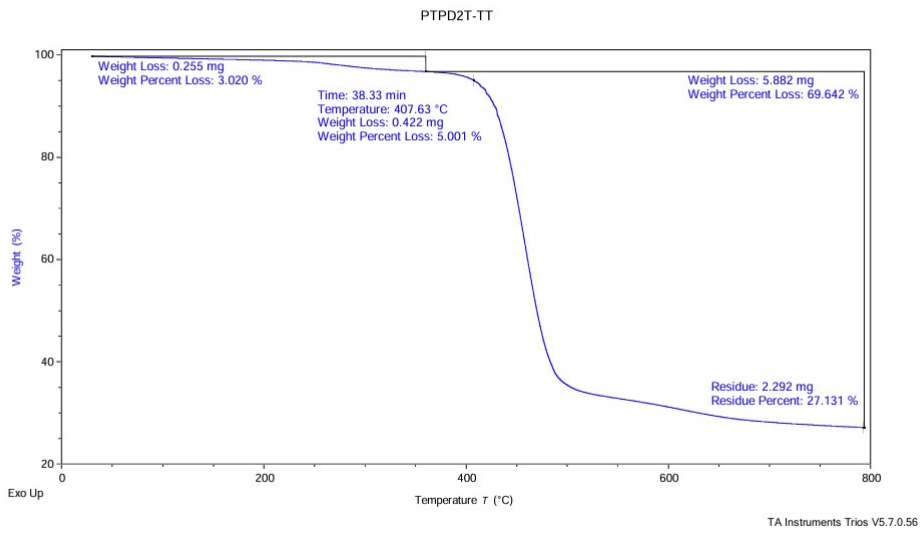
### DSC Analysis of p(TPD2T-3T)



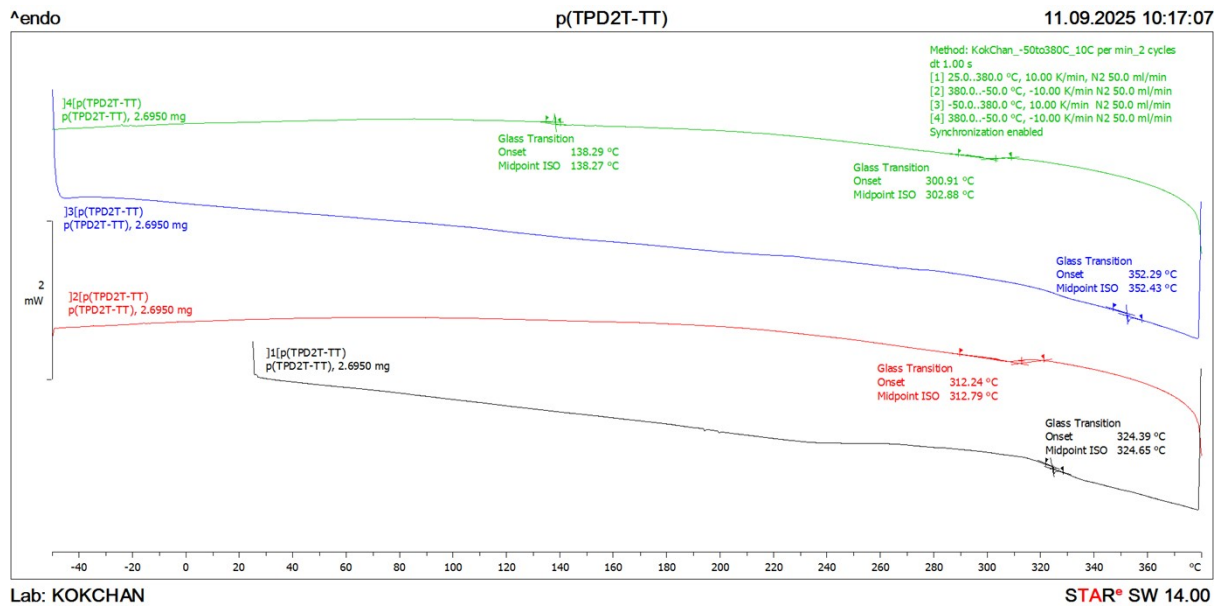
### TGA Analysis of p(TPD2T-TT)

PTPD2T-TT  
 30-800C\_10C per min\_N2  
 Kok Chan  
 D:\TA Data\SDT 650\User Data\Kok Chan\AR25SDT20062\PTPD2T-TT.tri

SDT650,6/6/2025 11:02:47 AM  
 8.447 mg  
 Alumina 90 ul



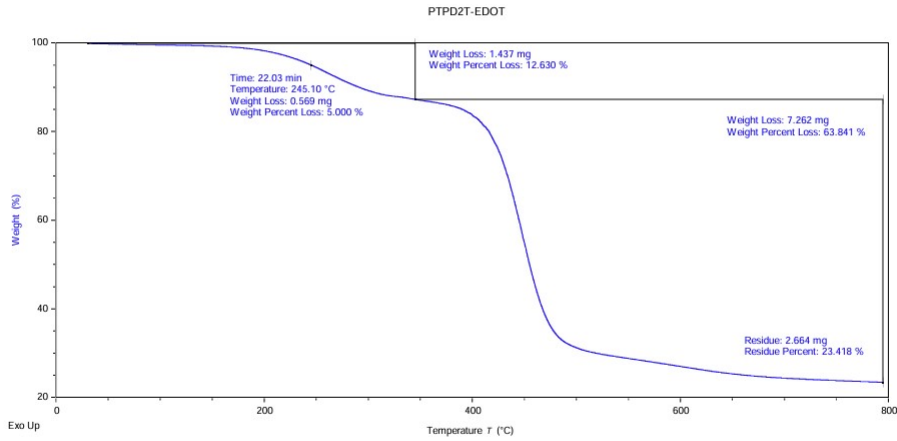
### DSC Analysis of p(TPD2T-TT)



### TGA Analysis of p(TPD2T-EDOT)

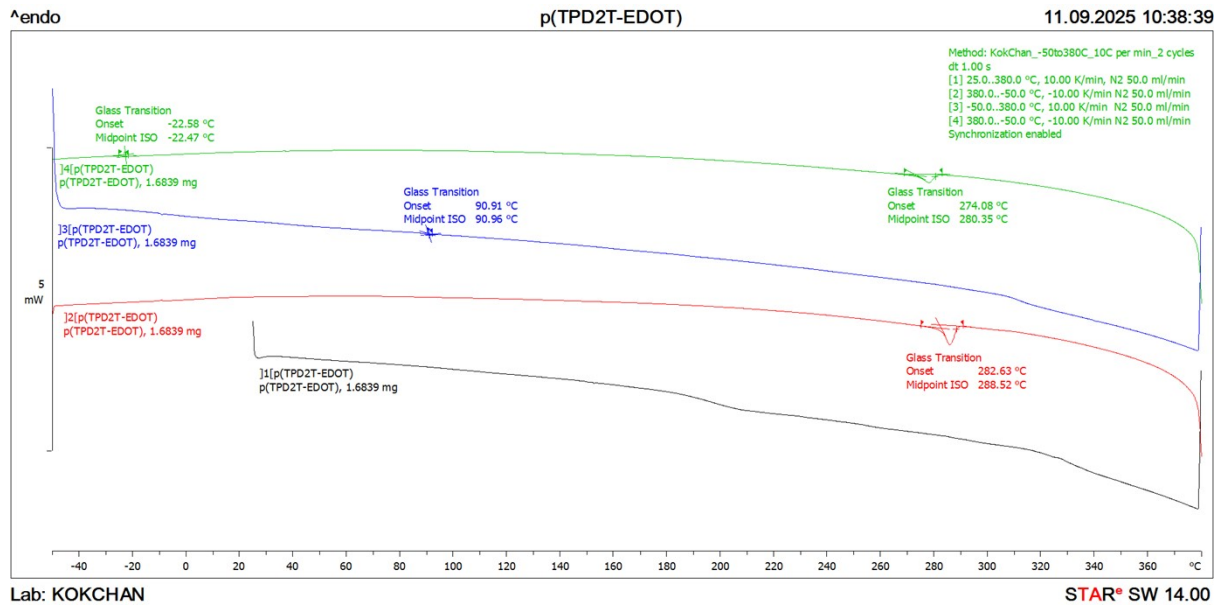
PTPD2T-EDOT  
30-800C\_10C per min\_N2  
Kok Chan  
D:\TA Data\SDT 650\User Data\Kok Chan\AR25SDT20053\PTPD2T-EDOT.txi

SDT650.5/5/2025 10:14:10 AM  
11.38 mg  
Alumina 90 ul



TA Instruments Trios V5.7.0.56

## DSC Analysis of p(TPD2T-EDOT)

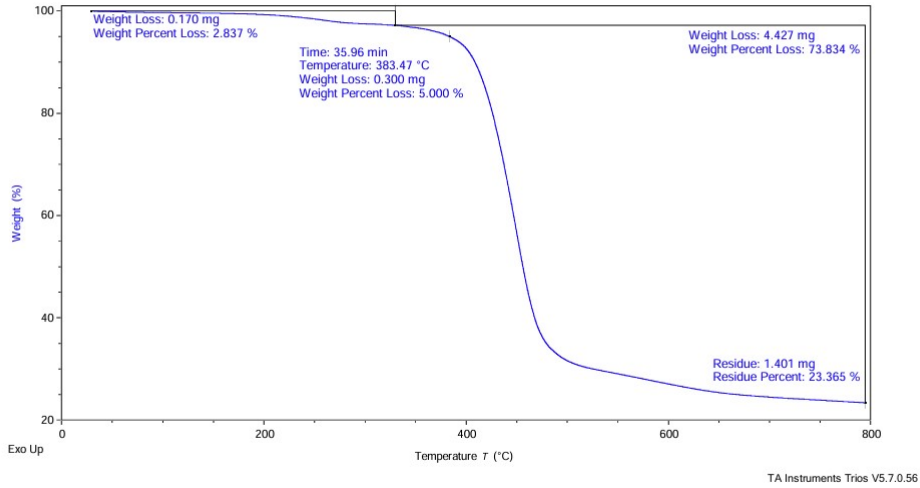


## TGA Analysis of p(TPD2T-DTP)

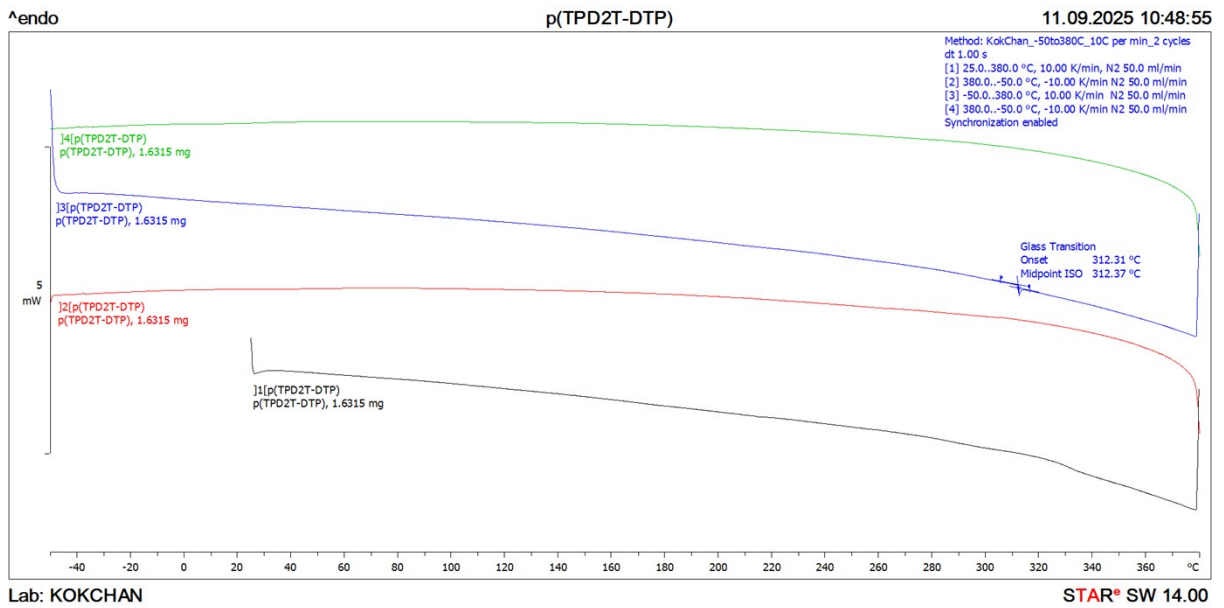
PTPD2T-DTP  
 30-800C\_10C per min\_N2  
 Kok Chan  
 D:\TA Data\SDT 650\User Data\Kok Chan\AR25SDT20062\PTPD2T-DTP.tri

SDT650.7/6/2025 12:53:39 AM  
 5.996 mg  
 Alumina 90 ul

PTPD2T-DTP



### DSC Analysis of p(TPD2T-DTP)

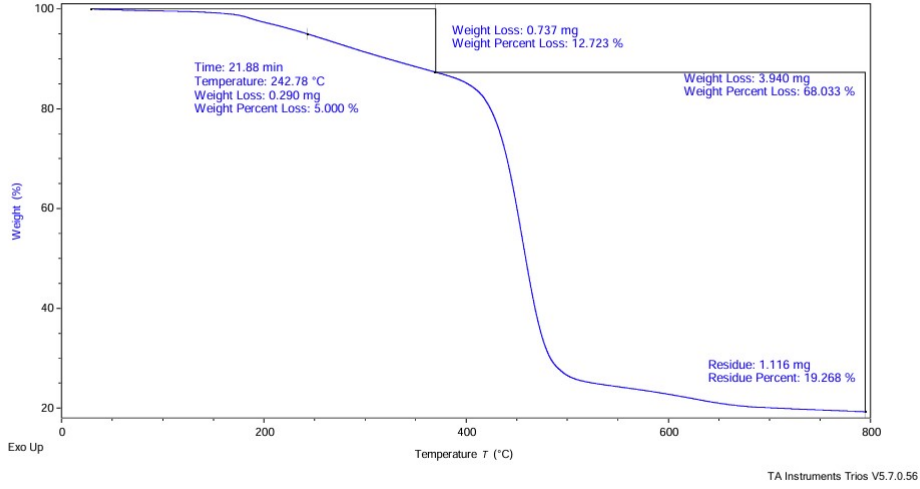


### TGA Analysis of p(TPD2T-CPDT)

PTPD2T-CPDT  
 30-800C\_10C per min\_N2  
 Kok Chan  
 D:\TA Data\SDT 650\User Data\Kok Chan\AR25SDT20062\PTPD2T-CPDT.tri

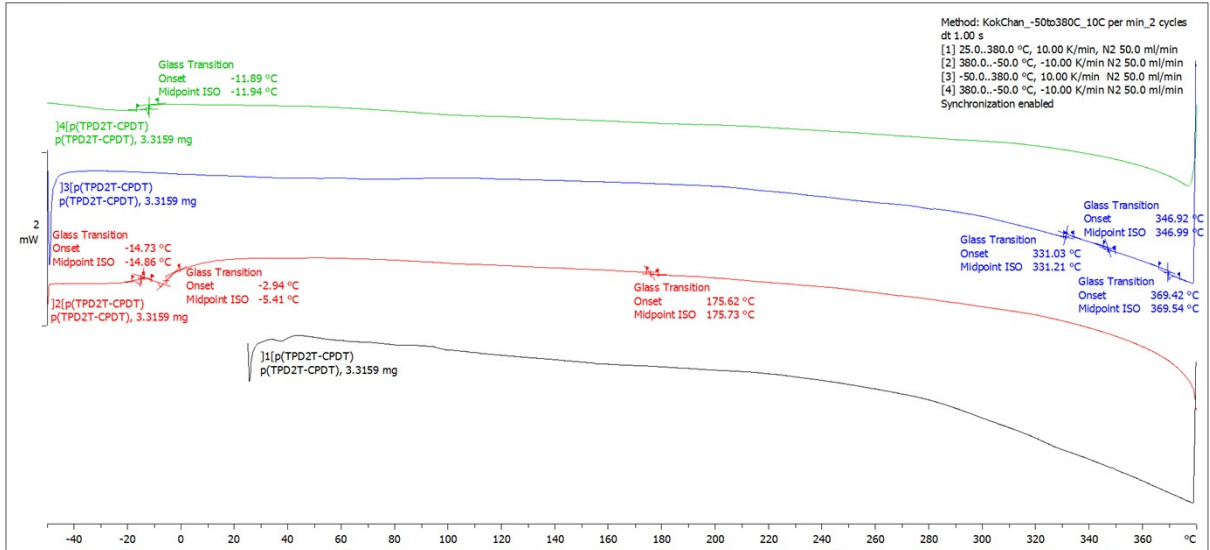
SDT650.6/6/2025 10:11:04 PM  
 5.791 mg  
 Alumina 90 ul

PTPD2T-CPDT



### DSC Analysis of p(TPD2T-CPDT)

^endo



Lab: KOKCHAN

STAR<sup>®</sup> SW 14.00

## GOAT(GFN2-xTB; ALPB(chloroform)) global minima

### TPD2T-T

130

O -3.64141735902328722574 0.43149486981083728931 -1.43163578802557056591  
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C -4.79135905513229420905 3.17945911235243938719 4.69823050716546752881  
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C 2.35709590008456215671 2.38226348905731644123 -1.26073513513909452044  
C 3.82080053849911349673 1.94991550182379969058 -1.31270107000866653735  
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C 4.51501989774560108515 -1.62557918591063743641 4.28517151606743684766  
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TPD2T-CPDT

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| H | 1.41777004556698  | -0.30606592359970 | 3.44255704761596  |
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| H | 0.35657808905502  | -2.25265641626513 | 5.53409548088433  |
| H | 1.95263260329370  | -1.49950447316673 | 5.54704640353015  |
| H | 0.37491830274489  | -0.26287283572742 | 7.03147874574790  |
| H | 0.88231418934491  | 0.75562146048887  | 5.68465501282321  |
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| H | -4.80190608068093 | -3.79778897134625 | 1.50967252948245  |
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#### TPD2T-DTP

173

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TPD2T-EDOT

136

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C -5.31009004461117850582 -2.21916437261281762616 -2.10057562161991295824  
S -3.82080212364618798659 -1.47435997975618704459 -2.51364295802883352948  
S -2.03587315567699533858 -0.20885753434468146139 1.30797040214874593644  
C -0.46896273727423437583 0.52694034844971504583 1.02164367019224999744  
C 0.31183088462173208510 0.99700641609971940582 2.10319435972772028620  
C 1.55548287831898268685 1.58760826347322003826 2.05215441063726355964  
C 2.03956134607256256430 2.01845916074424325259 3.29344507107060069373  
C 3.34582556431193856028 2.73646877968887203281 3.42555400314721891775  
C 3.50789778364843041203 3.92124941938644377970 2.46295077668227468948  
C 2.69256635239660901959 5.16049443928088269473 2.84197070002371132702  
C 1.17313410116327121457 5.01074923672337391167 2.74094735522376486969  
C 0.67275944026397060949 4.78955091969849089395 1.31454963053521645122  
C -0.81119421025954485671 4.43161958312629167267 1.27722844252104383855  
C -1.27879445084896037343 4.08770079663813223902 -0.13570849745254875973  
C -2.69904540170698714618 3.52773289928198252596 -0.15500939324300608280  
C -3.14580209693060730558 3.12966865228282697942 -1.55995229351106079463  
C -4.53486221157262914261 2.49602554043195157263 -1.56622996568322836453  
C -4.95424567633635248853 2.04442274608686114235 -2.96317932084591673103  
C -6.33763081736093614182 1.40468633420970978598 -2.96146009179046831861  
C 1.17178509426770505186 1.70355004088127182094 4.33238520011127015152  
C 1.27008249779577453431 1.90432197444546114085 5.74012593247719937750  
C 0.30267329500546613641 1.54186011710345227677 6.65733082606046178142  
C 0.64610112791950591316 1.83146610896280082059 8.00253665981306738786  
O -0.19149912467119351023 1.56122459568937910213 9.04897127609352125432  
C -1.52315484901021691577 1.30855144562719027945 8.61640723248232553999  
C -1.53732299757575008314 0.36041202191227128537 7.41873791358757284087  
O -0.87411881288408899149 0.94910502074480695978 6.30672640669944950531  
C 1.87833408666351653338 2.39862679277633450425 8.11962530133413551425  
S 2.62833287074897592461 2.59830752136772069605 6.58694220932119911538  
S -0.27005344886147653050 0.91659009382536738020 3.74437081795624848723  
C -0.22591025766869549107 0.55965396069275352708 -0.33573374134635625143  
N 0.34450936137620602473 0.71725227383769041278 -2.52567409879502413617  
C 1.10016691597778359935 0.97996094967234859130 -3.73037856928681055280  
C 2.29115951972691345162 0.02372228379748625784 -3.89099416130431841054  
C 1.85182932102854791445 -1.44842874473336680197 -3.91664602567948616496  
C 0.96349392213362317072 -1.83680176960227181659 -5.09436988991035377694  
C 3.10548782599434813889 0.39996283215499789376 -5.13528468963821982385  
C 4.01235868781777149650 1.61108347498178372526 -4.92018658181708978816

C 4.83975728278642058910 1.92672408112232163013 -6.16538134609225441096  
C 5.75369759926776414005 3.12812463207961721778 -5.95205873039861454998  
C 0.81280480479078021094 1.01260723461168544723 -1.25203509966742121406  
O 1.88663414182122934903 1.55027427542634876900 -1.03609458614621297023  
H -4.57823241128767666197 -1.39524008912153063555 1.02348016371957695192  
H -7.42997741313471138369 -3.24740064355412005881 -0.89718756333090010635  
H -7.36454195625347107779 -2.04670254738079826495 0.40127385427818845764  
H -7.25800073511975529783 -4.28887454109575827488 1.38123265711209386453  
H -5.73251742927461993560 -3.44388462154154817441 1.63067921988031661051  
H -6.34232633799424405652 -5.67101943541446296138 -0.34266356840035244735  
H -4.93728852682481367253 -4.63755971613966355704 -0.54921363867678663073  
H -4.45367138067020462699 -6.78830702863310353479 0.61580306876500179314  
H -5.52031206310690869543 -6.30528714022768710379 1.93397513970384338222  
H -4.02770823983316983430 -4.40732720261506560888 2.47834519546947706914  
H -3.19368896466041718440 -5.95197107773874201087 2.53401023353408438865  
H -3.03903920500671453908 -3.92909004139257289623 0.25604610431734742271  
H -2.25944665070926165029 -5.51225383092737075685 0.25302586423713485653  
H -1.75982599047440957385 -3.28062747686964328864 2.27554874509993121379  
H -0.96202344046049603765 -4.85392049565242800213 2.28170343939588393667  
H -0.80412953194686564995 -2.81856008008048597446 0.01345163420842262342  
H 0.01700061595950378909 -4.37492054265340701846 0.04958674272496010893  
H 0.45015477024170985620 -2.12627819838234799477 2.06757545323534230874  
H 1.29280819134542213078 -3.67406305466530547221 2.05987470077715828509  
H 2.23529568155630098403 -3.13941643435164330356 -0.19090096943500808879  
H 1.40456984548921637312 -1.58516094083434477824 -0.16200966279834241868  
H 2.67005341760066672308 -0.98550908332276854207 1.92372897903291018018  
H 3.56526767523564647178 -2.50087103134030064311 1.78212463416453248399  
H 4.87807637911952163279 -0.64837609236006710223 0.80466705669216564978  
H 4.39387153455286849635 -1.76051284438191824044 -0.47764084262541334214  
H 3.53995804648836376316 -0.23012225331632135683 -0.26522231387538114378  
H -5.91098312518298385498 -2.64806880259481447482 -2.87873901231441520210  
H 2.09410735992364793745 1.70135191712039479661 1.12975658185130622968  
H 4.14513009165331691719 2.01856664060403412364 3.22060894543144726754  
H 3.47754307064959711226 3.09594132827122425766 4.44462649813145560529  
H 3.26905123092645455429 3.61196065405444866059 1.44629099803691141268  
H 4.56234528544477324630 4.20716404320934334038 2.47361720104218063554  
H 2.94432827758932269546 5.43995086437981356653 3.86827663632121909743  
H 3.00352243946838193267 5.98226553588006293438 2.19147811621773458413  
H 0.70968998704575991798 5.91723513332552020216 3.13976006267437002251  
H 0.84787763297383356154 4.18037335302266477299 3.36777268761996229074  
H 0.85032604496172292663 5.68886057080174190048 0.71998168974874754422  
H 1.22756171577946560092 3.97362164148657459606 0.85024062613370543495  
H -1.40572034335059048438 5.25981667752191839327 1.66967167896115276093  
H -0.98143697417823838602 3.56765326654387804339 1.92500560400202247457  
H -0.59664872017333414611 3.34687460159041272334 -0.56320116971779621284  
H -1.22784333778883980592 4.97853060923868717680 -0.76609720236384770686  
H -3.38883822085987462813 4.27359835187744874219 0.24642911870634290339  
H -2.74618309102885671535 2.65225025595397712053 0.49762874660726841292  
H -2.42828316460525206466 2.41927103555710676375 -1.98133579819796734611  
H -3.14523273580076656586 4.01177212000847038809 -2.20486437003821711400  
H -4.53848867066708905327 1.63277991559657875698 -0.89573042957687665222  
H -5.26217405045756958515 3.21563678021822330066 -1.18265680905155767810  
H -4.22067870374398257383 1.32850373037246272112 -3.34308553950693898571  
H -4.95194877021101564907 2.90472155714463609044 -3.63690504150191751265  
H -6.35676753411241790559 0.54261980488882322060 -2.29803797786504082623

H -6.60591348511872933358 1.07404803385159164364 -3.96229450402725547065  
H -7.08664716621215884373 2.11664524445133217512 -2.62055270978505827628  
H -2.00349592633399442576 2.25612246671681226928 8.34030257932652574482  
H -2.03525014097668011104 0.86650462586746956895 9.47075752196286657636  
H -2.55605318271791448481 0.16111055384557074199 7.08752218207234907510  
H -1.03729773371161204665 -0.57930655838914257849 7.68508591249098138576  
H 2.37852769864404089972 2.70794915917792833326 9.01316319839668267377  
H 0.40563943402326357868 0.88262768392933221850 -4.56653265371894523383  
H 1.46509973377699820318 2.00866809392800993450 -3.67624042653098603850  
H 2.93165066210419267279 0.15397100531066437723 -3.01066292626474130145  
H 2.75324792399768503159 -2.06621869722700779448 -3.93069069042224272792  
H 1.32172018085205156268 -1.67632782559118242993 -2.98710747511164642631  
H 0.00566872497869106221 -1.32433070566984545380 -5.04795739580182889483  
H 0.76768257743324341824 -2.90690179301281048652 -5.06603235811572272240  
H 1.44362300258918696549 -1.60306051178393138557 -6.04044903111280451213  
H 2.42849496142593901382 0.60076437290655515522 -5.96761762200619383378  
H 3.73028412150507726608 -0.45234268895226903417 -5.41115507604205969727  
H 4.68418732891691291798 1.41347794967793594090 -4.08138455801392563416  
H 3.41395788032120250932 2.48664349169242848703 -4.66144111492123691676  
H 5.44358026121329707792 1.05461751297525552218 -6.42737473836212203082  
H 4.16726067615735740191 2.12709881535029277089 -7.00295534139977338128  
H 5.16960209738281051273 4.01358856018806076094 -5.70923548992785523382  
H 6.44485062325912139158 2.94036677465553397681 -5.13289664078893004273  
H 6.33217978199590714183 3.33370417254921891370 -6.85011099314352112088

**SMD(chloroform)-MN15/def2-SVP optimized geometries (truncated monomers)**

TPD2T-T

43

Coordinates from ORCA-job opt\_freq E -2597.010156405765

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | -3.63662123222927 | 0.41861247262620  | -1.44245730836093 |
| C | -2.51407742482335 | 0.12578147456445  | -1.19658126486973 |
| C | -1.73886453935406 | 0.27243403388984  | 0.06083001894344  |
| C | -1.93926129048362 | 0.75490044324782  | 1.31773544201646  |
| C | -3.11295007513210 | 1.41078375906797  | 1.90574878681314  |
| C | -3.24376034730685 | 1.89127417483467  | 3.19232944882593  |
| C | -4.46747500376415 | 2.54429304780096  | 3.42296610342600  |
| C | -4.85216118992899 | 3.20727847588538  | 4.71817420874641  |
| C | -5.25871148383494 | 2.51439688136330  | 2.31258846705063  |
| S | -4.53508232435992 | 1.72810964781020  | 0.96688697077395  |
| S | -0.47933038627721 | 0.53389703557714  | 2.24764151645089  |
| C | 0.38148575079107  | -0.19597092522804 | 0.92009691021615  |
| C | 1.78552438699895  | -0.60203157748188 | 1.05174836361023  |
| C | 2.59205034633055  | -0.44774415084463 | 2.12519394782714  |
| C | 3.92574850642018  | -0.90149159496799 | 1.93143924019685  |
| C | 4.93578974164813  | -0.80450934254958 | 3.04506282314964  |
| C | 4.11606025368666  | -1.39687727958157 | 0.66174513442281  |
| C | 5.31026017215704  | -1.93810563190611 | -0.01412463534383 |
| C | 5.33086141497268  | -2.50016704278269 | -1.27186575918996 |
| C | 6.60849675137056  | -2.91477008727352 | -1.68436170084764 |
| C | 7.56522239242212  | -2.67013975344042 | -0.75075610033325 |
| S | 6.91509973546652  | -1.92833168255875 | 0.65442596876655  |
| S | 2.65165567832792  | -1.34031466459014 | -0.28031378040198 |
| C | -0.44844987988413 | -0.26052836156020 | -0.16054128815669 |
| N | -1.64277376287225 | -0.47930200308272 | -2.10209377284846 |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | -2.00912644207168 | -0.79583946266271 | -3.46600601839064 |
| C | -0.38620451889896 | -0.75171285874901 | -1.55548697887789 |
| O | 0.49675121974863  | -1.28546321352178 | -2.13985276956511 |
| H | -2.46632995115830 | 1.76653255326540  | 3.93417117289532  |
| H | -5.83286509720584 | 3.67394448449683  | 4.62677538789289  |
| H | -4.94196083365478 | 2.47247547938405  | 5.52199276315794  |
| H | -6.24833137950643 | 2.93471343669254  | 2.20439995315264  |
| H | 2.24125540182366  | 0.00229071705404  | 3.04434022674214  |
| H | 5.03427881835979  | 0.22988149138780  | 3.38001228513453  |
| H | 5.93026972744613  | -1.10133096968321 | 2.73811321360426  |
| H | 4.45146402819941  | -2.61473811322522 | -1.88898259943738 |
| H | 6.80746702579428  | -3.37716799309078 | -2.64089317761293 |
| H | 8.62338621244644  | -2.88183472087128 | -0.79493596568704 |
| H | -1.29824418899965 | -1.51806967336505 | -3.85446768903698 |
| H | -2.99769903545647 | -1.24952732942159 | -3.47961159849283 |
| H | -4.12711554166742 | 3.96621058000473  | 5.01503051619060  |
| H | 4.65630234502341  | -1.44453156073292 | 3.88357038305408  |
| H | -2.01685930226378 | 0.09625760181847  | -4.09165179470739 |

#### TPD2T-2T

50

Coordinates from ORCA-job opt\_freq E -3146.924411453214

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | 3.26664507899275  | 1.04760171741461  | -1.33374682915229 |
| C | 2.19709170098117  | 0.56073246392915  | -1.48920484825708 |
| C | 1.00127480242116  | 0.61393172680292  | -0.64173917848741 |
| C | 0.61694542002629  | 1.21383338120993  | 0.51613035790683  |
| C | 1.37098393419077  | 2.07418046086271  | 1.43064014265093  |
| C | 0.89581965285270  | 2.71242040542992  | 2.53988075995358  |
| C | 1.84245770621623  | 3.49977926410015  | 3.20564039229150  |
| C | 1.46357957606300  | 4.34371672956693  | 4.39530287812117  |
| C | 3.08651272659220  | 3.43605977764236  | 2.59426474675824  |
| C | 4.37851918731724  | 4.05351149445626  | 2.94179871108763  |
| C | 5.49789360854784  | 4.08351174195446  | 2.13751690598028  |
| C | 6.60875259836624  | 4.70156854463950  | 2.73903005611333  |
| C | 6.34779356378513  | 5.13367370319040  | 3.99843860566324  |
| S | 4.72817424893760  | 4.79776367801061  | 4.47109919656734  |
| S | 3.06117605770936  | 2.42613335785663  | 1.18211658324047  |
| S | -1.06579008690839 | 0.83588504272273  | 0.82218481681396  |
| C | -1.21658474496803 | -0.13477043972653 | -0.61874135953226 |
| C | -2.47348141705681 | -0.81280500815594 | -0.94638901445329 |
| C | -3.66278179358854 | -0.74247890036322 | -0.26295467221531 |
| C | -4.66961080937362 | -1.56502352811740 | -0.77136584406901 |
| C | -6.02875715820540 | -1.66296367919776 | -0.12831500198866 |
| C | -4.25085372647429 | -2.25189373059679 | -1.89895388578085 |
| C | -4.95273972547360 | -3.18828465135297 | -2.79563513458378 |
| C | -4.36900966504765 | -3.91000981863575 | -3.81421443332306 |
| C | -5.27893703373029 | -4.70564251301112 | -4.54122148861700 |
| C | -6.54752054943023 | -4.58995698837078 | -4.09129701108177 |
| S | -6.66003921342348 | -3.50094009993738 | -2.75598756541516 |
| S | -2.59118497589935 | -1.89718884186672 | -2.29443944738564 |
| C | -0.02283165190912 | -0.13825139792994 | -1.27856068415052 |
| N | 1.82783641683549  | -0.20766456008188 | -2.61190464976708 |
| C | 2.70354489733918  | -0.45071177502575 | -3.73829168372185 |
| C | 0.51999186089709  | -0.66295220606219 | -2.55228784332345 |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | -0.00286099388762 | -1.31335528185934 | -3.39690620581103 |
| H | -0.13328409044312 | 2.60991848588094  | 2.85654141350217  |
| H | 1.18748663704741  | 3.71436127896969  | 5.24469653864431  |
| H | 2.27607657466494  | 4.96872854771821  | 4.74322775674292  |
| H | 5.50784541319963  | 3.67212068131478  | 1.13840750244265  |
| H | 7.56629475312865  | 4.81749765245929  | 2.25112495169789  |
| H | 7.00565109823316  | 5.64045287118658  | 4.68892441939214  |
| H | -3.78429325285700 | -0.10010188513117 | 0.59882416398880  |
| H | -6.61234424558067 | -0.75887492135164 | -0.32122065226868 |
| H | -6.62329456523274 | -2.47016600208323 | -0.53654055723209 |
| H | -3.31080299766712 | -3.86390501967878 | -4.02690353768960 |
| H | -4.99170779396659 | -5.33827576551936 | -5.36934973260143 |
| H | -7.44050097018324 | -5.07904821567258 | -4.45131504282528 |
| H | 2.18616717500212  | -0.20130756651276 | -4.66294318877662 |
| H | 3.56254626553802  | 0.20665664424393  | -3.64993967748384 |
| H | 0.62821026208070  | 4.99986166955429  | 4.14739342145423  |
| H | -5.94198180205035 | -1.82214991628787 | 0.94653619120465  |
| H | 3.02464616069119  | -1.49072851048813 | -3.77638566622419 |

TPD2T-3T

57

Coordinates from ORCA-job opt\_freq E -3696.852062088439

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | 3.71762466129475  | -0.06981903013678 | -1.16929012284155 |
| C | 2.68020669025905  | -0.56039560628744 | -0.87127489505811 |
| C | 1.53399185168161  | 0.01604702483296  | -0.15199364950252 |
| C | 1.18656872238932  | 1.22302702547258  | 0.38695974887320  |
| C | 1.90536123779849  | 2.49851174182566  | 0.39414042993826  |
| C | 1.46168575100667  | 3.69715999447147  | 0.90681597515610  |
| C | 2.34367383351031  | 4.76897114855397  | 0.72422270345025  |
| C | 1.97818104804852  | 6.16954603520817  | 1.14665278800576  |
| C | 3.49050318080412  | 4.38225672161602  | 0.07534202545994  |
| C | 4.68739656789826  | 5.14643902414024  | -0.30710046215980 |
| C | 5.80129794623471  | 4.64179432293460  | -0.94190741063433 |
| C | 6.80615430253150  | 5.60578907447321  | -1.17418592770712 |
| C | 6.46430731268691  | 6.83216541681754  | -0.72548379798321 |
| S | 4.89615351839742  | 6.84313794886985  | -0.00125312506263 |
| S | 3.46944188064864  | 2.67336584090788  | -0.32092586121862 |
| S | -0.38922966362076 | 1.08402134076510  | 1.11176693442871  |
| C | -0.55947484735312 | -0.60064588583956 | 0.66790533544403  |
| C | -1.77455120022864 | -1.34209095511274 | 1.01333947466557  |
| C | -2.84489953302210 | -0.87242327804973 | 1.69731307513998  |
| C | -3.88453426300588 | -1.80802573269499 | 1.87409637266476  |
| C | -5.12570785599771 | -1.46630860456161 | 2.65805656129594  |
| C | -3.58345608268042 | -3.02604245933515 | 1.29075306803806  |
| C | -4.37093456906956 | -4.26272008074197 | 1.18647819764146  |
| C | -3.97674070759885 | -5.41202987727800 | 0.57549695521079  |
| C | -4.95050969566491 | -6.44521412527337 | 0.59881429223229  |
| C | -6.09587347501618 | -6.08577323163173 | 1.23089556102484  |
| C | -7.30790355379389 | -6.87996467504237 | 1.44240981216074  |
| C | -8.45606178906383 | -6.51422483404810 | 2.06768953227121  |
| C | -9.44663252878380 | -7.54609857501124 | 2.09492167540500  |
| C | -9.02249362443252 | -8.67400834027126 | 1.48688270270292  |
| S | -7.41613236792837 | -8.52011716852649 | 0.86563053656237  |
| S | -5.98923499286298 | -4.44400902660292 | 1.81693900283169  |
| S | -2.01405637027793 | -3.01290573598544 | 0.54259859658413  |

|   |                    |                   |                   |
|---|--------------------|-------------------|-------------------|
| C | 0.55865560063486   | -0.99660832264377 | 0.00155220585767  |
| N | 2.32248930390838   | -1.89259083919483 | -1.14141282500674 |
| C | 3.16445791119396   | -2.81194320067821 | -1.87676525961808 |
| C | 1.07568701518769   | -2.23189879817679 | -0.64083631651317 |
| O | 0.58487054869768   | -3.30874335449775 | -0.73323528313968 |
| H | 0.50191410142752   | 3.78742145183836  | 1.39656278560218  |
| H | 1.24358892275650   | 6.13813051610177  | 1.95073279238063  |
| H | 2.83261456624272   | 6.71732707341442  | 1.53535169266635  |
| H | 5.88607954899242   | 3.60330714768577  | -1.22799368900489 |
| H | 7.74646947451828   | 5.38602338058945  | -1.65999099413790 |
| H | 7.03448768761592   | 7.74845911104071  | -0.76666859805372 |
| H | -2.88092384213532  | 0.14082472125238  | 2.07296562037804  |
| H | -5.27812858835846  | -0.38755834413015 | 2.66474930953280  |
| H | -6.02083697561561  | -1.89609900401986 | 2.21550081914071  |
| H | -3.00501647649563  | -5.51440474540838 | 0.11454809888286  |
| H | -4.80710037793588  | -7.42323401750589 | 0.16174430126973  |
| H | -8.59399326964599  | -5.53211998707170 | 2.49877458076435  |
| H | -10.42091935594988 | -7.43567001336391 | 2.54927459138660  |
| H | -9.55567640307164  | -9.60449739783638 | 1.35876499306023  |
| H | 4.16175264287878   | -2.38809100826843 | -1.93606050714874 |
| H | 3.23239946428957   | -3.75551722831362 | -1.33898542537691 |
| H | 1.57508023533896   | 6.74491449381167  | 0.31059534476567  |
| H | -5.06369898072461  | -1.82962709951025 | 3.68608256551513  |
| H | 2.77192079386096   | -2.99536601137298 | -2.87622417172321 |

#### TPD2T-TT

46

Coordinates from ORCA-job opt\_freq E -3070.092376947178

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | 1.19256278578840  | 1.60941672403259  | -2.69995116699634 |
| C | 0.69168477665671  | 1.33842702412056  | -1.65485542828467 |
| C | 0.56180577127801  | 0.03569907257705  | -0.95597510799498 |
| C | 0.89919437127858  | -1.27603172652971 | -1.15139521552718 |
| C | 1.59642048968965  | -1.91925903709432 | -2.26498131176306 |
| C | 2.10298614206709  | -1.32996812529226 | -3.40385537447176 |
| C | 2.77375245463658  | -2.23487062621866 | -4.25328124068113 |
| C | 3.45593897203929  | -1.84185334851348 | -5.53555840687799 |
| C | 2.73199641625047  | -3.50552375236804 | -3.76597526859988 |
| S | 1.90929700097523  | -3.62476865655552 | -2.26128717612975 |
| S | 0.36775434064007  | -2.21329727314746 | 0.21329247964015  |
| C | -0.32481978534415 | -0.83035706276877 | 1.02944552316784  |
| C | -0.98453768430996 | -0.98068595709274 | 2.32917207178673  |
| C | -1.11613812797903 | -2.13035041428130 | 3.04847468684867  |
| C | -1.80821611306225 | -1.98512573174827 | 4.25704338808587  |
| C | -2.09243523897340 | -3.17020914604030 | 5.14444273206124  |
| C | -2.20804749228160 | -0.67176555922425 | 4.46644539003108  |
| C | -2.92056704586824 | -0.04582360983502 | 5.58965073141330  |
| C | -3.25383316077695 | 1.28244648055175  | 5.67663085126634  |
| C | -3.92365051591349 | 1.58857536121215  | 6.88660224864426  |
| C | -4.10249999682994 | 0.50073356734835  | 7.72438237029908  |
| C | -4.77868265178457 | 0.81406870510409  | 8.94229238542071  |
| C | -5.08611195696595 | 2.11775774958910  | 8.98043242157775  |
| S | -4.58882427277899 | 3.01563205154857  | 7.58318374368684  |
| S | -3.43454273734349 | -0.93842603863530 | 7.02338720936100  |
| S | -1.73290560722490 | 0.36295732620603  | 3.15636975258290  |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | -0.12863417380541 | 0.27435724462685  | 0.26208361253767  |
| N | 0.08032795353066  | 2.26720230291297  | -0.83161941137335 |
| C | -0.03748634580860 | 3.66913944269243  | -1.17207775869451 |
| C | -0.45217286051643 | 1.70119210515343  | 0.33964687387905  |
| O | -1.04209701992974 | 2.30635417675804  | 1.17115563297585  |
| H | 1.98486152670683  | -0.27773901223279 | -3.60888833587226 |
| H | 2.72798508701811  | -1.50033421058383 | -6.27513430494541 |
| H | 3.95391231648360  | -2.70441579009647 | -5.97857561108357 |
| H | 3.15447833270126  | -4.39629956383812 | -4.20725433009496 |
| H | -0.71200954223056 | -3.07046858032347 | 2.69957320548398  |
| H | -1.99833600116797 | -2.92423052853286 | 6.19932043865473  |
| H | -1.36946751415129 | -3.96199865358651 | 4.95177722074434  |
| H | -3.03047763954981 | 2.00953773948880  | 4.91024407601249  |
| H | -5.01064745758646 | 0.10350419316331  | 9.72191253267588  |
| H | -5.59828904100586 | 2.64935315373542  | 9.76949809654876  |
| H | -0.80199914656622 | 4.11120626346336  | -0.54102142274335 |
| H | -0.35657850217462 | 3.76596688140367  | -2.20753850809908 |
| H | 4.19433352925166  | -1.05577319329266 | -5.37421730834592 |
| H | -3.10243532137421 | -3.55505855156011 | 4.98868031011003  |
| H | 0.90869256471194  | 4.19189007990368  | -1.03693999521739 |

#### TPD2T-CPDT

57

Coordinates from ORCA-job opt\_freq E -3262.774621188197

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | -5.15548692189063 | -1.16442228715028 | 1.74290961619155  |
| C | -4.12146846204191 | -0.99826489772794 | 1.18525035497352  |
| C | -3.07494455149506 | 0.03681405724371  | 1.39461703472327  |
| C | -2.87755486592147 | 1.11725035378349  | 2.19369695617541  |
| C | -3.72516441550837 | 1.69178702715227  | 3.24487274369306  |
| C | -3.45562934962424 | 2.80751396590531  | 4.00447828163593  |
| C | -4.49997516597656 | 3.14904913953179  | 4.89575968783523  |
| C | -4.48133704908681 | 4.36481039455598  | 5.78248026751267  |
| C | -5.52818862947335 | 2.27583062426295  | 4.80253148544928  |
| S | -5.27799295737735 | 1.02163134411671  | 3.63861575157066  |
| S | -1.35936696970801 | 1.87087540596072  | 1.76665346894147  |
| C | -1.02211178271473 | 0.71437222919871  | 0.50635127590866  |
| C | 0.19584407635897  | 0.80789505089673  | -0.30355031936283 |
| C | 1.11250293481452  | 1.80522729448160  | -0.30946130749833 |
| C | 2.20468122091837  | 1.59714169267178  | -1.19803462071660 |
| C | 3.35115018135706  | 2.56950122616101  | -1.30036506349682 |
| C | 2.09741307464198  | 0.40578419052485  | -1.87058903831352 |
| C | 2.98463567747123  | -0.23960001062557 | -2.85509208098302 |
| C | 2.76172651251990  | -1.48284491528937 | -3.42881495634871 |
| C | 3.76779453197645  | -1.86144517680433 | -4.30032341868350 |
| C | 4.75969962466901  | -0.90947444155034 | -4.41762041574217 |
| C | 5.76567031275519  | -1.39579729585922 | -5.34119110732360 |
| S | 7.26123305823460  | -0.85486606231557 | -6.03552845806002 |
| C | 7.38387786273916  | -2.33839430725347 | -6.91659169380877 |
| C | 6.35441502103155  | -3.18604428225403 | -6.69259127845450 |
| C | 5.40921883115606  | -2.63843494916476 | -5.77461435321399 |
| C | 4.09605007105492  | -3.08366103929357 | -5.12803933357961 |
| S | 4.46906009708391  | 0.46765841955323  | -3.43461833053860 |
| S | 0.64172674095872  | -0.45562981411027 | -1.42716772384945 |
| C | -2.04118259697004 | -0.19236378151693 | 0.45416234511958  |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| N | -3.65780611746031 | -1.78494617118496 | 0.14020075313027  |
| C | -4.38438973503495 | -2.92191389647398 | -0.38296847992279 |
| C | -2.41500624721359 | -1.36093255881270 | -0.36053556703033 |
| O | -1.85277597250941 | -1.87212473583614 | -1.27032402094116 |
| H | -2.52928078720275 | 3.35787656050259  | 3.90819411770775  |
| H | -3.64689381157541 | 4.32516358587532  | 6.48631789733166  |
| H | -5.39277603278430 | 4.41787356927051  | 6.37760420878778  |
| H | -6.45379825197886 | 2.29411278472554  | 5.36005983267459  |
| H | 1.00931481554887  | 2.68026739306009  | 0.31804011109152  |
| H | 2.97641350359135  | 3.59406283768340  | -1.31892043164371 |
| H | 3.91212067557053  | 2.45938630567150  | -2.21872592607619 |
| H | 1.88358702076353  | -2.06844772987708 | -3.19915321291393 |
| H | 8.23878683178892  | -2.48623053613036 | -7.56020134897574 |
| H | 6.27263640206781  | -4.15694496667796 | -7.16093704950590 |
| H | -3.95052631473805 | -3.19293736876347 | -1.34013964072694 |
| H | -5.42180766585915 | -2.64245956663266 | -0.55611187266977 |
| H | -4.39498916345782 | 5.28161967982903  | 5.19697806403454  |
| H | 4.05526561090355  | 2.44685507252755  | -0.47460032807284 |
| C | 4.29192285242928  | -4.33916965464266 | -4.24138903504286 |
| C | 2.99634148188750  | -3.49762565446000 | -6.12650449944057 |
| H | -4.34875732914041 | -3.76733330696602 | 0.30304353143526  |
| H | 5.05623824374067  | -4.18349654240426 | -3.47703041131901 |
| H | 4.59880555520536  | -5.17973675674270 | -4.86440130188909 |
| H | 3.35778353089381  | -4.58378043987055 | -3.73470858666167 |
| H | 2.74976527780556  | -2.69661934617277 | -6.82700803273340 |
| H | 2.08937923590892  | -3.75981155614739 | -5.58045328547981 |
| H | 3.31501910219630  | -4.36729118093509 | -6.70186446870386 |

### TPD2T-DTP

53

Coordinates from ORCA-job opt\_freq E -3239.757638438616

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | 0.99026898991278  | -1.36967562670601 | 5.98273025628396  |
| C | 0.80129302174478  | -1.54006597181632 | 4.82122865961272  |
| C | 0.72705314568286  | -0.56524614209033 | 3.70407091360320  |
| C | 0.85827995343664  | 0.78313256271419  | 3.52109945913812  |
| C | 1.17808759451930  | 1.84515127895826  | 4.47718893312684  |
| C | 1.53083239328730  | 1.71891725376531  | 5.79636025249816  |
| C | 1.75702744880117  | 2.96730921109206  | 6.44583314931609  |
| C | 2.10668680924151  | 3.09423825285379  | 7.90352106351278  |
| C | 1.57451299706625  | 4.00669331866506  | 5.60681299174913  |
| S | 1.12481827810982  | 3.52086585569219  | 4.00897647143216  |
| S | 0.56325593819056  | 1.16084712186070  | 1.85543093362910  |
| C | 0.25551439455794  | -0.49818140100159 | 1.42097690075115  |
| C | -0.06981616575022 | -0.84729072894864 | 0.04042002429095  |
| C | -0.42321774755194 | -2.06084921053132 | -0.47805375644124 |
| C | -0.69122518245608 | -2.04974753302428 | -1.85264399057909 |
| C | -1.20850174676189 | -3.28403318723204 | -2.54691917741957 |
| C | -0.52487409196999 | -0.79153602975235 | -2.41586201203966 |
| C | -0.66273194122580 | -0.29080210043256 | -3.79270336407215 |
| C | -0.73943063565847 | 1.02709273536945  | -4.12575479202619 |
| C | -0.81496584827743 | 1.22523486276711  | -5.52898230167325 |
| C | -0.79899896880144 | 0.03311030989181  | -6.25839410712452 |
| C | -0.88888391382339 | 0.39417238632183  | -7.62001902950498 |
| S | -0.94067372791448 | -0.28345378320717 | -9.19847846779305 |

|   |                   |                   |                    |
|---|-------------------|-------------------|--------------------|
| C | -1.04302646821618 | 1.31040086593378  | -9.87624635419320  |
| C | -1.03913705629209 | 2.30829613092695  | -8.98377711217534  |
| C | -0.94892876560634 | 1.79186267797037  | -7.66034043311289  |
| N | -0.92021782027686 | 2.29890690519795  | -6.38721780659434  |
| C | -0.77121811345259 | 3.69247194318739  | -6.02711760084417  |
| S | -0.66715945027247 | -1.34348838924673 | -5.22158864740365  |
| S | -0.05259387501904 | 0.36636429298431  | -1.21306998686019  |
| C | 0.38391402913577  | -1.27886231891968 | 2.53178371660736   |
| N | 0.55254173746168  | -2.78156293377088 | 4.25125302639517   |
| C | 0.51753615614996  | -4.01484219316034 | 5.00936555867032   |
| C | 0.22414698172695  | -2.70236090774684 | 2.89656334957797   |
| O | -0.14701895728827 | -3.62792906546867 | 2.25001097050931   |
| H | 1.62074654696823  | 0.76007084238462  | 6.28102376318811   |
| H | 2.26297362590220  | 4.13940631547529  | 8.17015527592653   |
| H | 3.03470928140483  | 2.56526730062882  | 8.13020907438151   |
| H | 1.67414552751959  | 5.05914315247763  | 5.82871495390436   |
| H | -0.49244385911501 | -2.94779604676527 | 0.13130526470254   |
| H | -0.64957386910804 | -4.16309567057338 | -2.22443415795802  |
| H | -1.10160365630348 | -3.23940883891153 | -3.62426158816388  |
| H | -0.74802243091751 | 1.80863644244161  | -3.38117494434359  |
| H | -1.09989763163950 | 1.39473282725796  | -10.95184341640829 |
| H | -1.09592094118111 | 3.35443164170821  | -9.24664189475723  |
| H | -1.05632792771714 | 3.82638001731551  | -4.98689928163943  |
| H | -1.44386069463629 | 4.30044763763062  | -6.62970951328695  |
| H | 0.18161336069766  | -3.79845937817717 | 6.01962474025297   |
| H | -0.20674079502305 | -4.68444131273840 | 4.55464739201061   |
| H | 1.31470496753264  | 2.69094946041095  | 8.53662690238060   |
| H | -2.27021424765097 | -3.42711404219988 | -2.33596698137416  |
| H | 0.25293186827845  | 4.03807970511164  | -6.17446717322882  |
| H | 1.49618951677820  | -4.49264944127398 | 5.03967750046617   |

#### TPD2T-EDOT

49

Coordinates from ORCA-job opt\_freq E -2823.437557307014

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | -1.50920782470538 | -0.17332019596943 | -3.52622222431903 |
| C | -0.90913919283095 | 0.12645723365631  | -2.54875376485132 |
| C | -1.28165292857873 | 0.00640477653227  | -1.13338345232087 |
| C | -2.34683744133655 | -0.46483047245017 | -0.41865144511803 |
| C | -3.57773684779145 | -1.12445492249243 | -0.87184090346935 |
| C | -4.61285477854895 | -1.56505596963244 | -0.08355032097638 |
| C | -5.64232970476800 | -2.21755388672367 | -0.81389005418265 |
| C | -6.85075806033495 | -2.84802050273918 | -0.17660749492081 |
| C | -5.36254184885476 | -2.24541089552198 | -2.13328449261144 |
| S | -3.85965956323618 | -1.49355518167221 | -2.54633964341599 |
| S | -2.04285281192845 | -0.21345412452342 | 1.27413418456776  |
| C | -0.47827689277726 | 0.52149984003710  | 0.99220392530401  |
| C | 0.32562857689547  | 1.00538276610988  | 2.11085763556037  |
| C | 1.56800282981363  | 1.59550669696971  | 2.06296379773528  |
| C | 2.04862907333191  | 2.02382163159501  | 3.30290198529428  |
| C | 3.36375318318821  | 2.74678971718482  | 3.43933746609467  |
| C | 1.18196951169415  | 1.70862022941285  | 4.33617779178818  |
| C | 1.28111327447650  | 1.91487482479258  | 5.79594207692008  |
| C | 0.31212787018065  | 1.55120801181494  | 6.71075153992327  |
| C | 0.65259055313909  | 1.83875270875899  | 8.05532107476320  |

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| O | -0.17451212890782 | 1.57113051231526  | 9.08435769751238  |
| C | -1.49263385726872 | 1.32125058111296  | 8.65403068101547  |
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| O | -0.84486618905603 | 0.96843968580743  | 6.36291735294963  |
| C | 1.87917566909980  | 2.40337051172976  | 8.17492723171162  |
| S | 2.63251556636046  | 2.60520616783151  | 6.64293677219532  |
| S | -0.25726205846355 | 0.92310405593138  | 3.74503821284559  |
| C | -0.23574416817286 | 0.55554806845357  | -0.34774022019159 |
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| H | -4.64469635240323 | -1.43016958426076 | 0.98941727575399  |
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| H | 2.38192080985660  | 2.71420638658950  | 9.07743304833700  |
| H | 0.45077559079702  | 0.90071840657680  | -4.60283121732842 |
| H | 1.49819518700619  | 2.00998467495257  | -3.72915895038671 |
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| H | 3.41282789408695  | 3.59706361907977  | 2.75880808959140  |
| H | 1.95488657269816  | 0.29926723376288  | -3.85437086056080 |