Electronic Supplementary Information

Tuning "Ligandless" Direct Arylation Polymerization toward Less-Branching EDOT Polymers

Xilin Pei [1,2,3], *Quan Yang* [3], *Yanlu Sun* [2], *Wei Wu* [3], *Jianyong Yu* [2], *Yong He* [1,2*],

1. State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University, Shanghai 201620, China

2. Innovation Center for Textile Science and Technology, Donghua University, Shanghai 201620, China

3. School of Materials Science and Engineering, Shanghai University, Shanghai 200444, China

** Corresponding author. Email: yhe@dhu.edu.cn*

Table of contents

1. General.....S3
2. Monomer Synthesis.....S4
3. General Polymerization Method S5
4. Polymerizations of P1 with Reduced Reaction Temperature S5
5. Evaluation of Molecular Weights by ^{1}H NMR and SEC.....S6
6. The UV-vis Spectra of P1-P5 and PEDOTF.....S8
7. NMR Spectra S9
8. GPC Traces.....S37
9. Calculation.....S46
10. References.....S75

1. General

All solvents and chemical reagents were purchased from commercial sources (Greagent-reagent, Adamas Chemical Co. and Macklin) and used without further purfications.

Nuclear magnetic resonance (NMR) spectra were recorded on a Avance III HD NMR spectrometer (Bruker Co. Switzerland). All ^{1}H NMR spectra were referenced to d-chloroform (7.26 ppm). Ultraviolet-visible (UV-Vis) absorption spectra were measured on a Shimadzu UV 3600 Plus spectrometer. All UV-Vis spectral data were subjected to normalization. After stirring at room temperature for more than 24 hours, the solutions of polymer samples were completely dissolved in chloroform-d prior to measurement. Number-average molecular weight (M_n by ^{1}H NMR), regioregularity (RR) and degree of branching (DB) were determined by ^{1}H NMR spectra in $CDCl_3$. The M_n by ^{1}H NMR of P1-P5 and PEDOTF was calculated according to the following equation (1):

$$M_n = \frac{I_{ethylenedioxide}}{3 * I_{end-groups}} * (M_{EDOT} + M_{Th})\ g/mol\#(1)$$

Where I represents the integration of ^{1}H NMR signals assigned to the ethylenedioxide of EDOT (δ 4.50 to 3.75 ppm) or H end-groups of EDOT (δ 6.35 to 6.15 ppm), and M_{EDOT} and M_{Th} are EDOT and thiophene derivates molar weight, respectively.

The number-average molecular weight (M_n by size exclusion chromatography, SEC), weight-average molecular weight (M_w) and polymer dispersity (PD) were determined by SEC using an Agilent 1260 Infinity II High Temperature gel permeation chromatography (GPC) and a Refractive Index (RI) detector. GPC was performed using PL gel 300 × 7.5 mm column and a PL gel Mixed C guard column, and the eluent was 1,2,4-trichlorobenzene (TCB) for HPLC grade. The flow rate of eluent was 0.5 mL/min and the column temperature was set to 140 °C. The instrument was calibrated vs. polystyrene standards purchased from Agilent. The polymer samples were dissolved in TCB (HPLC grade) at concentration of 1.0 mg/mL, stirred for 24h to facilitate solubilization, and then filtered through a 0.45 μL PTFE filter into a 2 mL

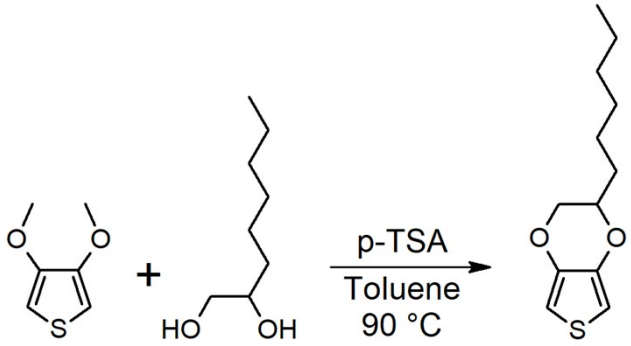
chromatography vial.

The degree of defects of **P1**-**P3** were verified by ^{1}H NMR spectra of these polymers. Specifically, peaks corresponding to the α-methylene groups on thiophene units in the range of δ 2.900-2.675 ppm were attributed to the main chain, while peaks in the range of δ 2.675-2.475 ppm associated with C-Br/C-Br homocoupling defects. Additionally, peaks in the range of δ 2.475-2.350 ppm indicated branching defects. The quantification of C-Br/C-Br homocoupling regiodefects was determined using equation (2), and the degree of branching (DB) was calculated according to the following equation (3):

$$Homocoupling\ (C-Br/C-Br) = \frac{I_{(\delta\ 2.675\ -\ 2.475\ ppm)}}{I_{(\delta\ 2.900\ -\ 2.350\ ppm)}} \#(2)$$

$$DB = \frac{I_{(\delta\ 2.475\ -\ 2.350\ ppm)}}{I_{\left(\delta\ 2.900\ -\ 2.350\ ppm\right)}} \#(3)$$

2. Monomer Synthesis



N-hexyl functionalized EDOT (**HE**) was synthesized following procedures previously reported[1]. 3,4-dimeyhoythiophene (0.60 g, 14.53 mmol) and 1,2-octanediol (1.85 g, 6.97 mmol) and p-toluenesulfonic acid (p-TSA) (1.04 g, 5.81 mmol) were added to a flask. Subsequently, the flask was sealed and inserted by three cycles of vacuum/nitrogen purging using a glass manifold. 100 mL anhydrous toluene was syringed into the flask. The reaction mixture was then stirred for 12 hours at 90 °C. The reaction is then cooled down to room temperature and extracted using ethyl ether and water. The organic phases were dried over $MgSO_4$, then filtered and concentrated under

reduced pressure. Purified using column chromatography (ethyl acetate/hexane = 1:10). 0.96 g, 70%. ^{1}H NMR (600 MHz, Chloroform-d) δ 6.22 (s, 2H), 4.13 – 3.95 (m, 2H), 3.78 (dd, J = 11.4, 8.1 Hz, 1H), 1.66 – 1.14 (m, 10H), 0.82 (t, J = 6.8 Hz, 3H).

3. General Polymerization Method

P1-**P5**, and **PEDOTF** were synthesized under general polymerization conditions. A Schlenk tube was charged with **HE** (1 eq.), dibromoarene (1 eq.), palladium acetate (10 mol%), potassium carbonate (2.5 eq.), pivalic acid (30 mol%), phosphine ligand (20 mol%) or not added ligand at a 0.25 mmol scale. Subsequently, the Schlenk tube was degassed by purging nitrogen for 30 minutes before selected amide solvent (0.125 M) was stringed into the tube. After completion the polymerization, the crude polymer precipitated into 150 mL methanol and filtered. In addition, crude product was purified by Soxhlet extraction with methanol and hexanes and followed by collection with chloroform. The final fraction was concentrated, followed by precipitated in methanol, and finally dried overnight under vacuum.

4. Polymerizations of P1 with Reduced Reaction Temperature

Table S1 Polymerization conditions and results[a].

Entry	Solvent	Temp. (°C)	Time (h)	Yield (%)	λ_{max}[b] (nm)	Homocoupling (C-Br/C-Br)[c] (%)	DB[d] (%)	M_n by ^{1}H NMR (kg/mol)
1	DMF	50	1	81	489	8	1.3	4.2
2	DMA	50	1	80	495	9	3.9	7.2
3	DIFP	50	12	66	495	13	0	12.9
4	DMF	40	1	70	489	13	1.3	3.8
5	DMA	40	1	80	492	9	3.1	5.7
6	DIFP	40	12	49	492	11	0.2	5.8
7	DMF	rt	12	82	493	10	1.9	4.7
8	DMA	rt	12	88	494	10	3.2	6.1
9	DIFP	rt	12	36	489	5	0.2	4.4

[a] Polymerization was performed on a 0.25 mmol scale in amide solvent (0.125 M) using

HE (1 eq.), M1 (1 eq.), $Pd(OAc)_2$ (10 mol%), K_2CO_3 (2.5 eq.) and PivOH (30 mol%). [b] The maximum absorption wavelength (λ_{max}) was recodrded by UV spectra in $CHCl_3$. [c] Homocoupling regiodefect (C-Br/C-Br) was calculated using eqn (2) in the ESI. [d] Degree of branching was determined using eqn (3) in the ESI.

5. Evaluation of Molecular Weights by ^{1}H NMR and SEC

Table S2 Molecular weights by ^{1}H NMR and SEC for polymerization results of Table 1.

Entry	Polymer	M_n by ^{1}H NMR (kg/mok)	M_n by SEC (kg/mol)	M_w by SEC (kg/mol)	PD
4	P1	9.5	11.4	23.5	2.057
5	P1	31.6	19.4	50.4	2.595
7	P1	15.2	7.0	11.0	1.561
8	P2	18.9	12.8	36.5	2.841
9	P2	49.1	3.8	5.4	1.422
10	P2	31.6	8.7	15.1	1.726
11	P3	3.7	8.8	12.8	1.529
12	P3	23.3	16.4	28.5	1.743
13	P3	43.4	8.7	15.1	1.726
14	P4	4.5	12.7	22.7	1.788
15	P4	28.1	37.7	98.0	2.601
16	P4	90.8	23.8	43.6	1.833
17	P5	4.2	8.4	21.7	2.597
18	P5	7.2	15.1	24.0	1.592
19	P5	23.3	17.6	31.5	1.790
20	PEDOTF	3.1	3.2	6.4	1.989
21	PEDOTF	8.0	9.7	17.3	1.789
22	PEDOTF	2.3	2.4	3.6	1.480

Table S3 Molecular weights by ^{1}H NMR and SEC for polymerization results of Table S1.

Entry	M_n by ^{1}H NMR (kg/mol)	M_n by SEC (kg/mol)	M_w by SEC (kg/mol)	PD
1	4.2	7.4	12.1	1.623
2	7.2	12.4	24.1	1.947
3	12.9	7.0	10.4	1.496
4	3.8	6.9	10.8	1.569
5	5.7	9.7	16.9	1.742
6	5.8	6.8	10.0	1.477
7	4.7	8.5	24.8	2.909
8	6.1	10.1	23.0	2.272
9	4.4	7.2	11.6	1.608

The oxygen atoms at the beta sites of EDOT contribute to the doping stability of poly[thiophene-derivates-alt-EDOT]s, which leads to aggregation under the negative pressure in the SEC column when using chloroform (a low-boiling solvent). Consequently, all poly[thiophene-derivates-alt-EDOT]s samples were blocked by the guard column, resulting in no RI signal detection. In contrast, the M_n by SEC of **P1**-**P5** were successfully determined when using TCB (a high-boiling solvent) as the eluent. However, significant variations were observed between measured M_n by ^{1}H NMR and SEC (**Tables S2**-**S3**). Specifically, the higher M_n by SEC compared to those by ^{1}H NMR suggests that TCB is a good solvent for these samples. Furthermore, as the polymer chains grow longer, the M_n by SEC becomes lower than the M_n by ^{1}H NMR, possibly indicating reduced solubility for high molecular weight polymers in TCB. Additionally, the M_n values of **PEDOTF** by both ^{1}H NMR and by SEC are highly consistent, likely due to the fused ring structure of 9,9-dioctyl-2,7-dibromofluorene.

6. The UV-vis Spectra of P1-P5 and PEDOTF

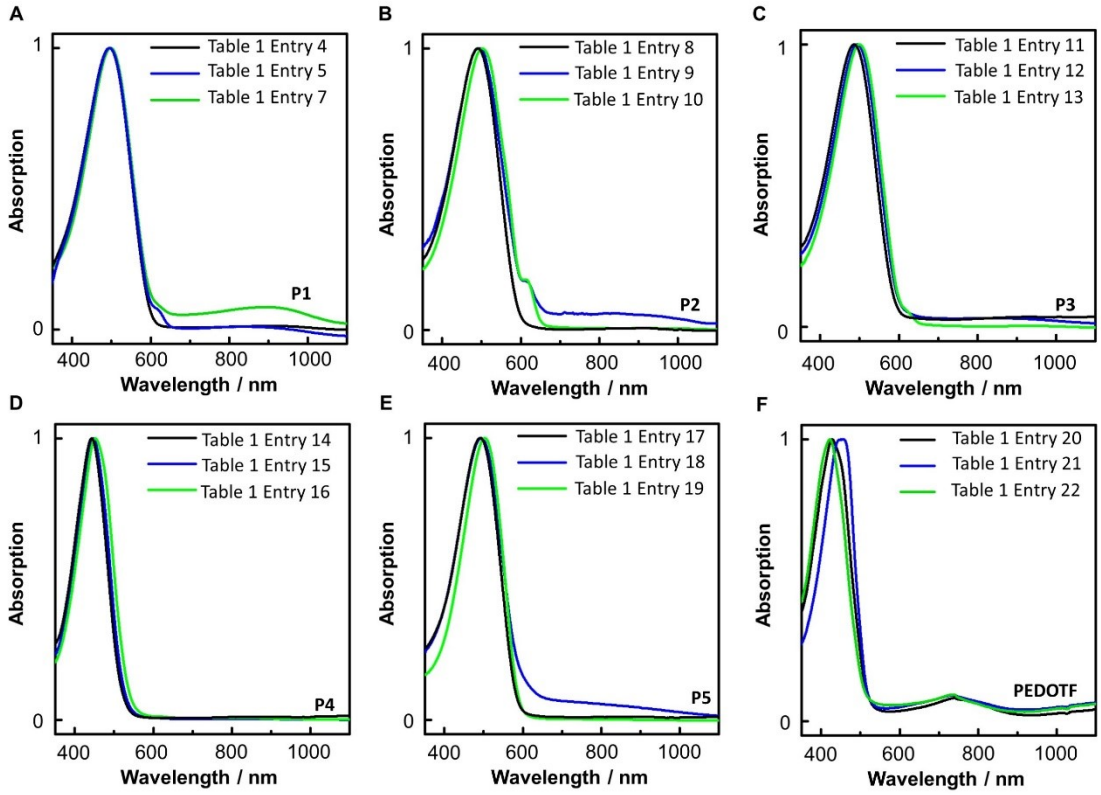


Figure S1 The UV-vis spectra of P1-P5 (**A**-**E**) and PEDOTF (**F**) in $CHCl_3$ solution.

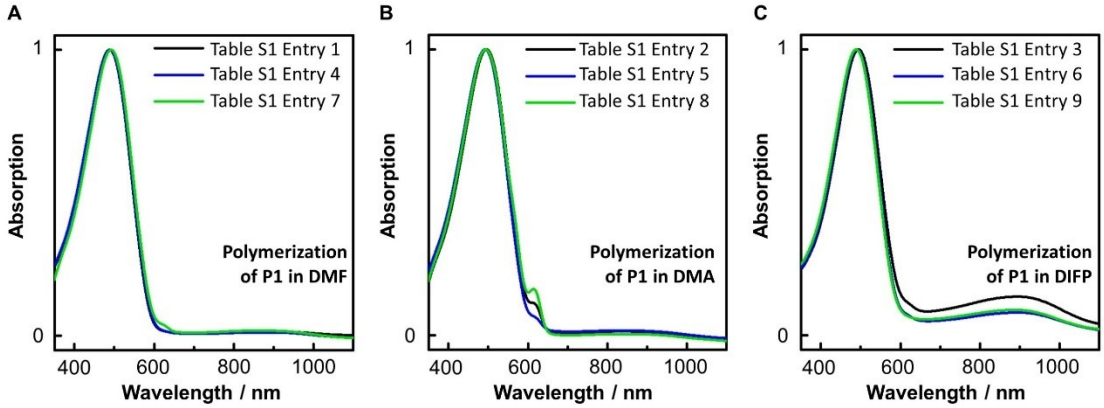
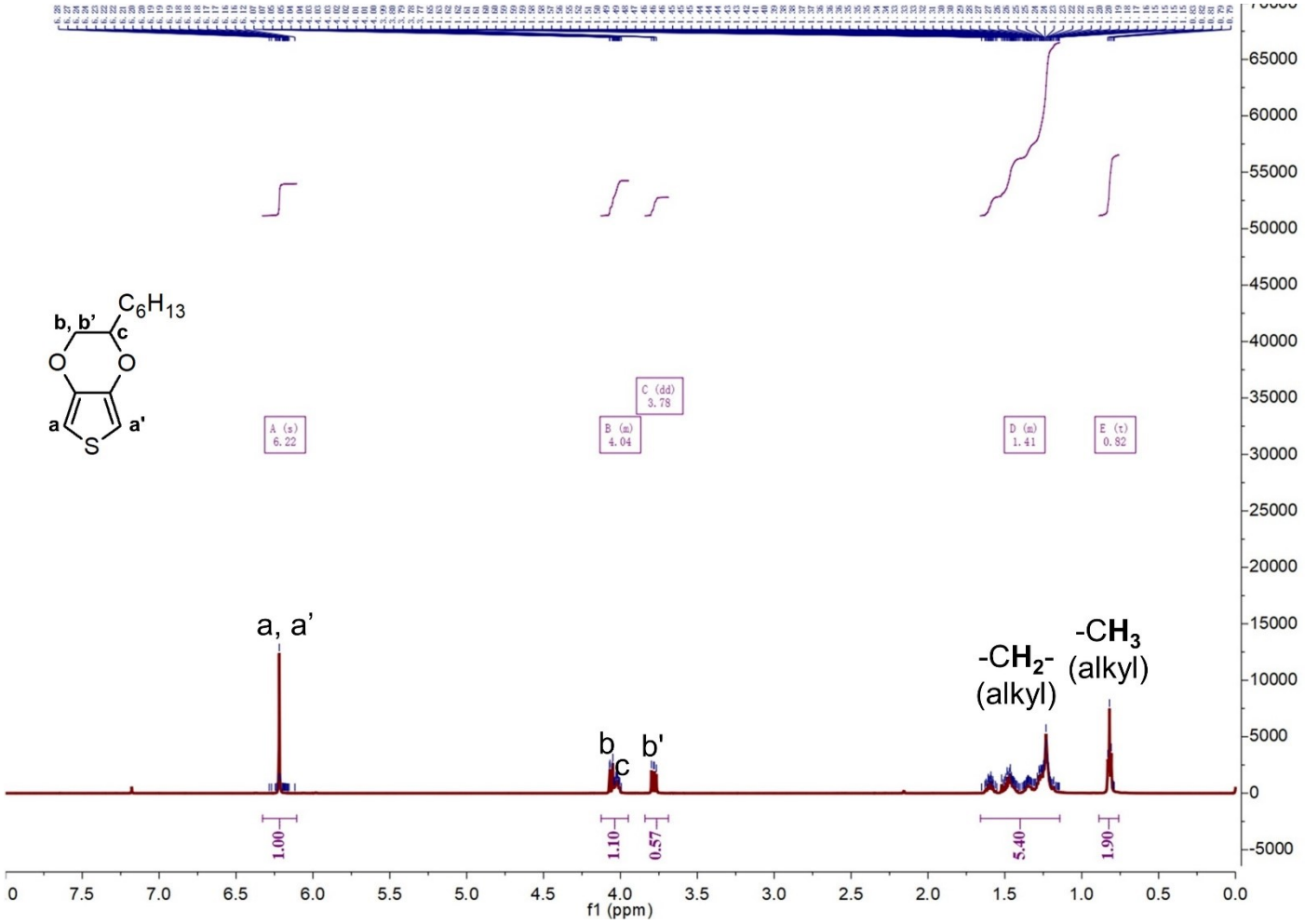


Figure S2 The UV-vis spectra of P1 in $CHCl_3$ solution for reducing the reaction temperature.

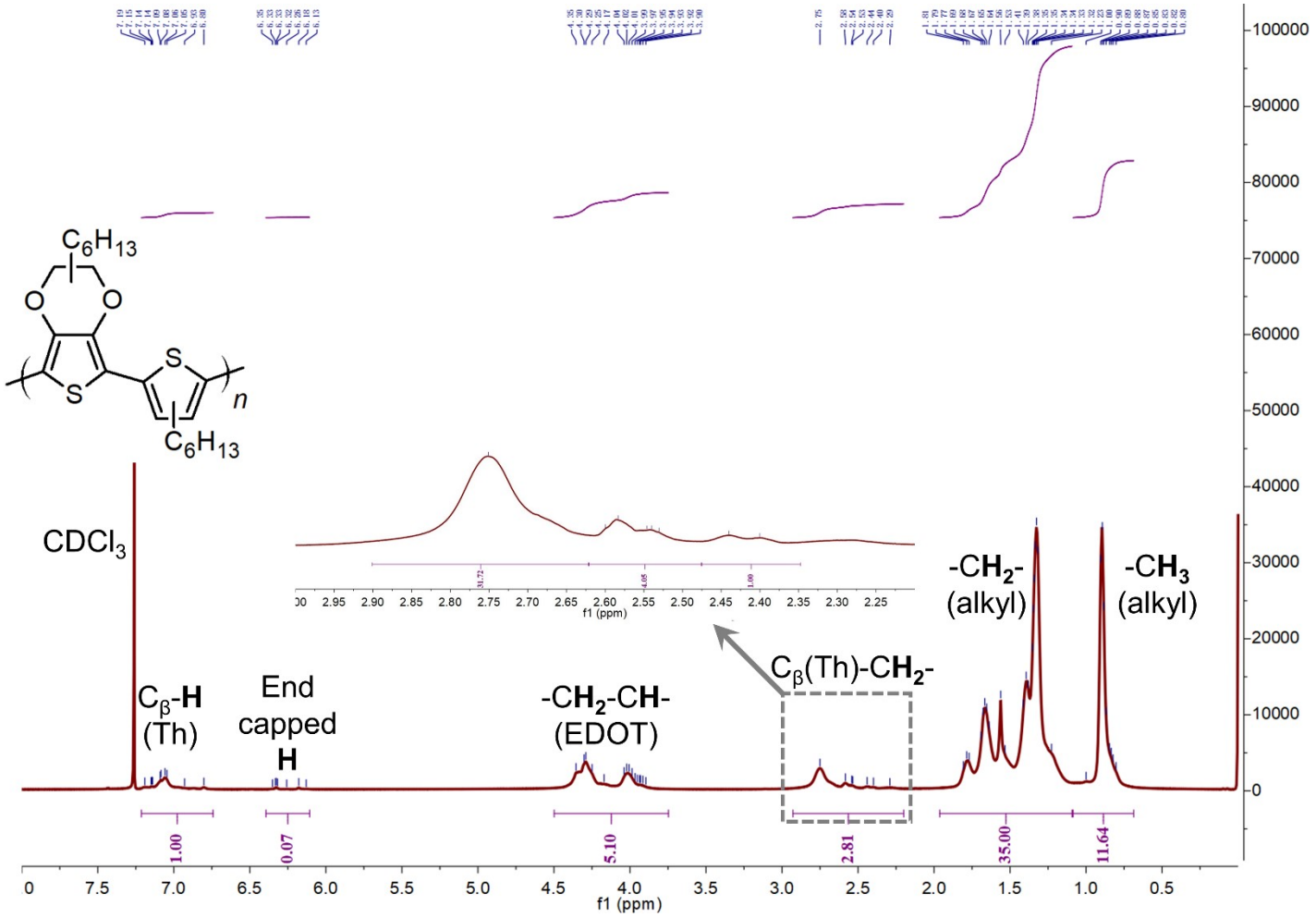
7. NMR Spectra

7.1 NMR spectrum of HE [600MHz, $CDCl_3$, 323K]

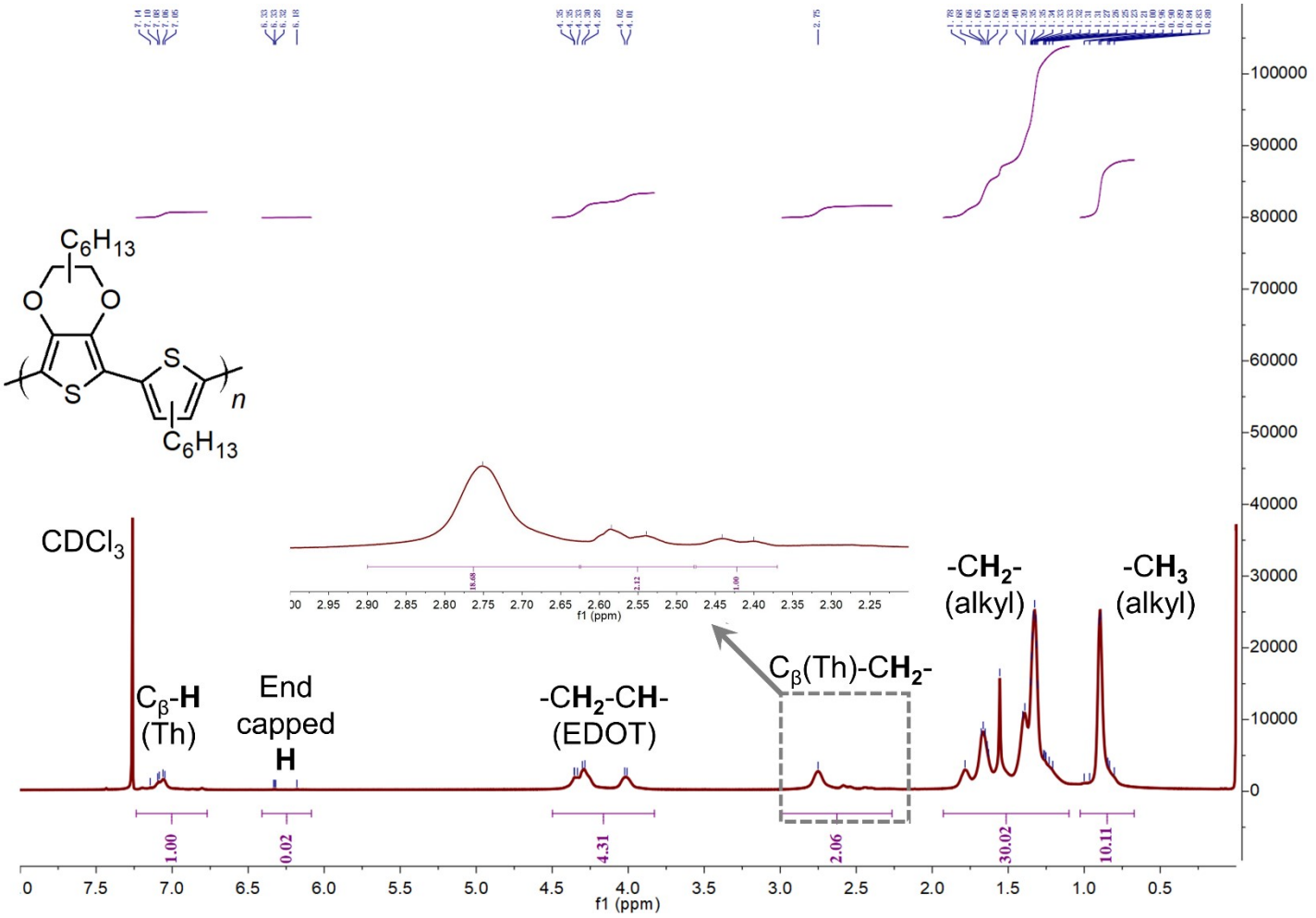


7.2 NMR spectra of P1-P5 and PEDOTF

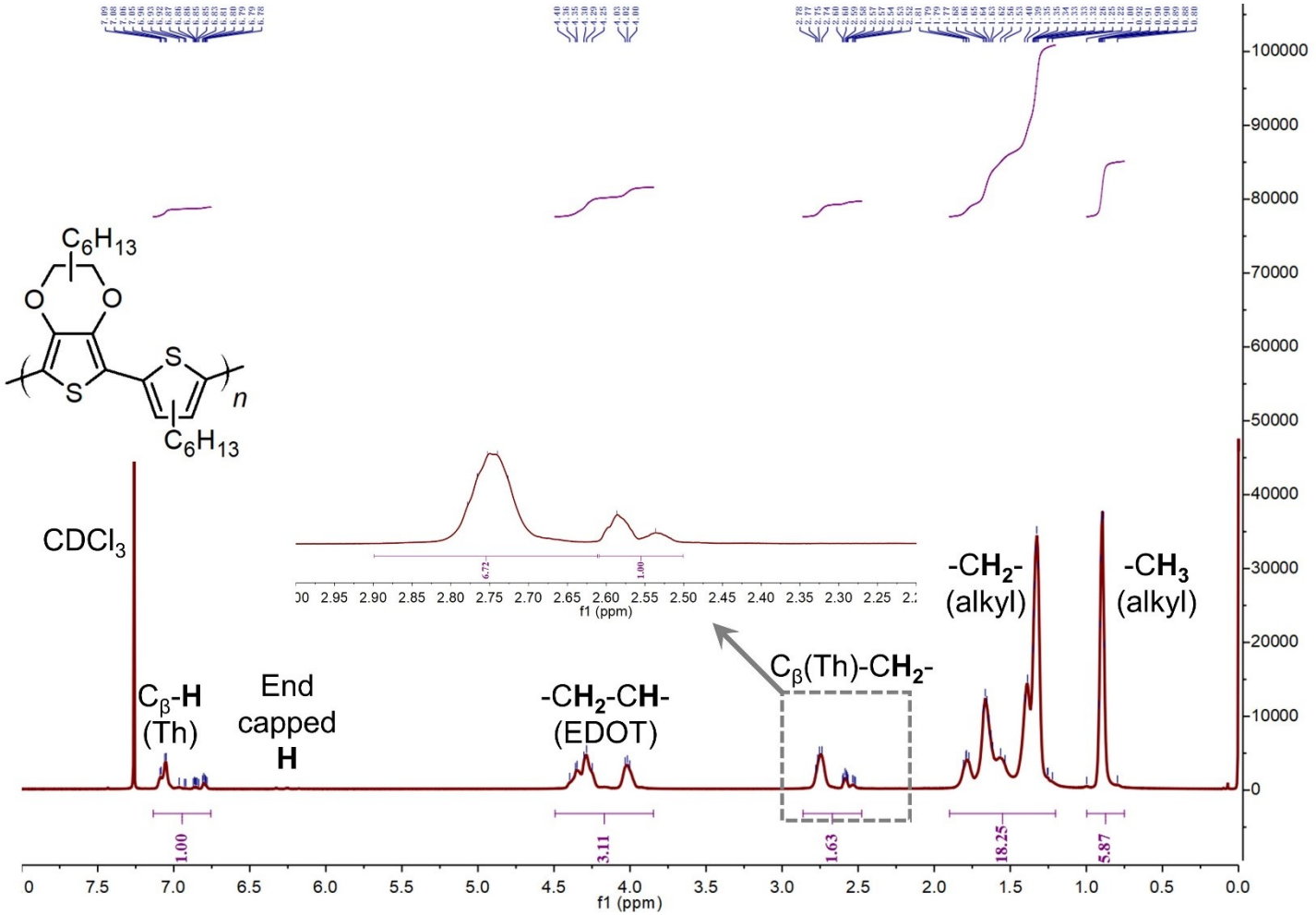
^{1}H NMR of P1 with entry 4 of Table 1 [600MHz, $CDCl_3$, 323K]



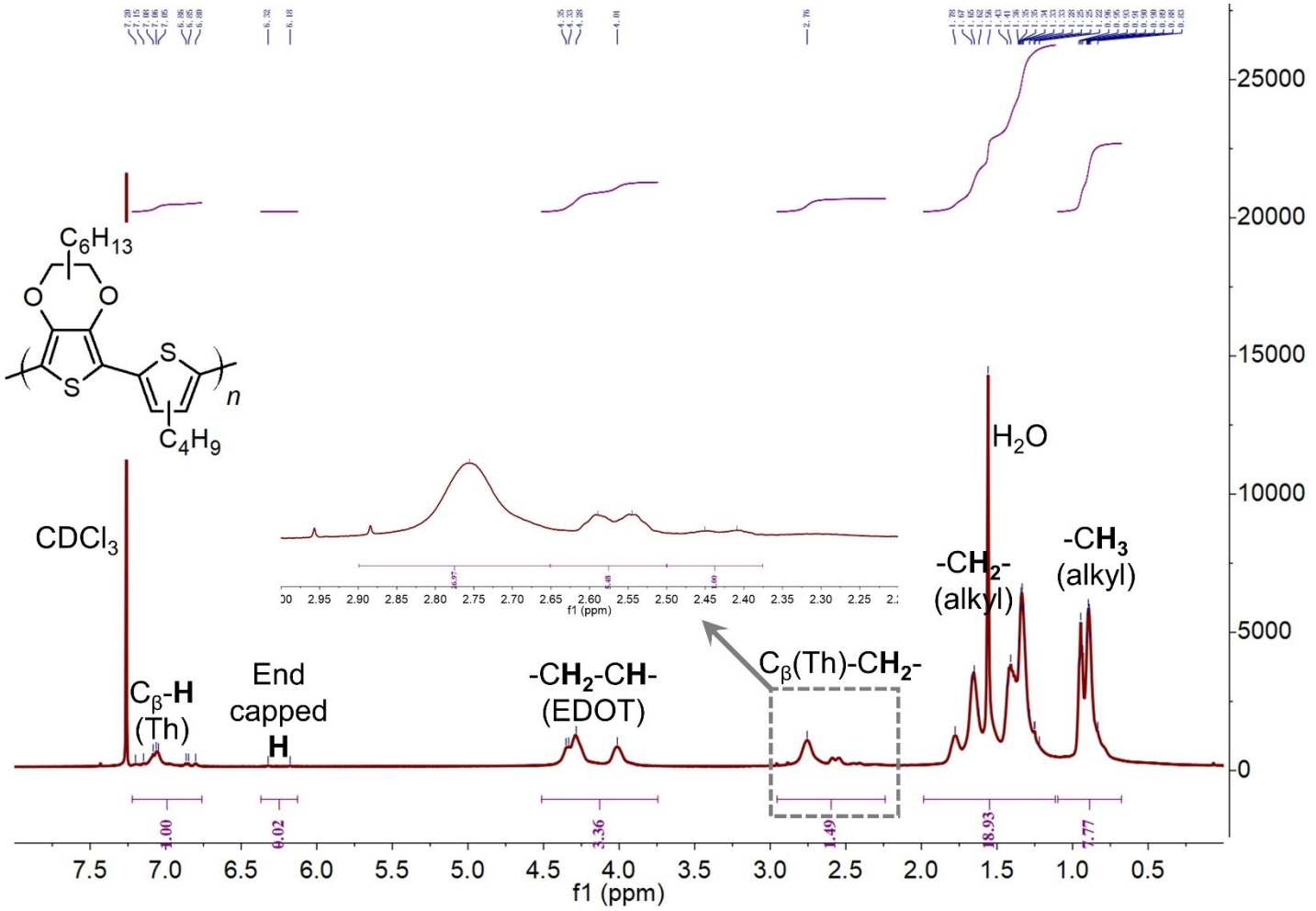
[1]H NMR of P1 with entry 5 of Table 1 [600MHz, $CDCl_3$, 323K]



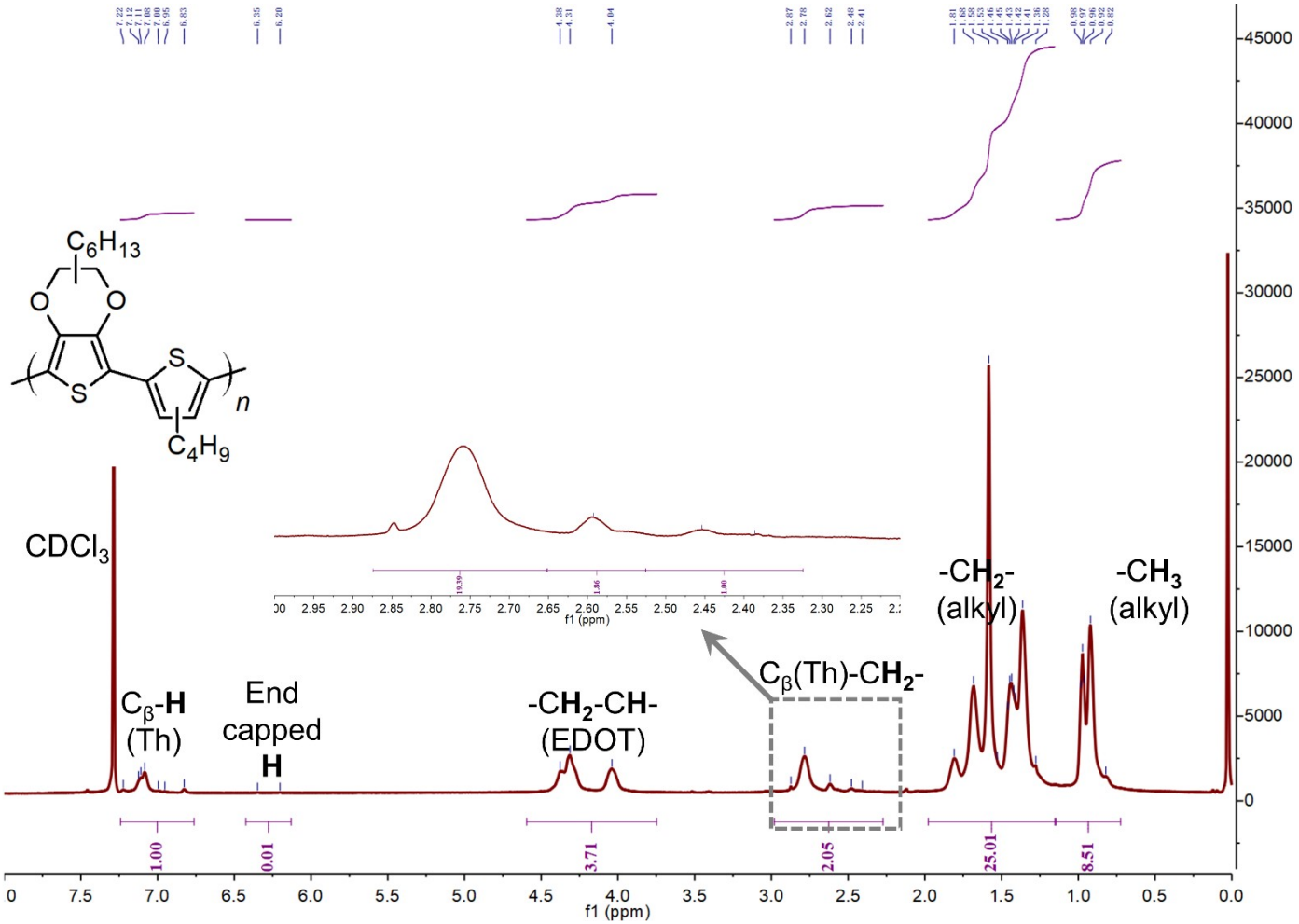
^{1}H NMR of P1 with entry 7 of Table 1 [600MHz, $CDCl_3$, 323K]



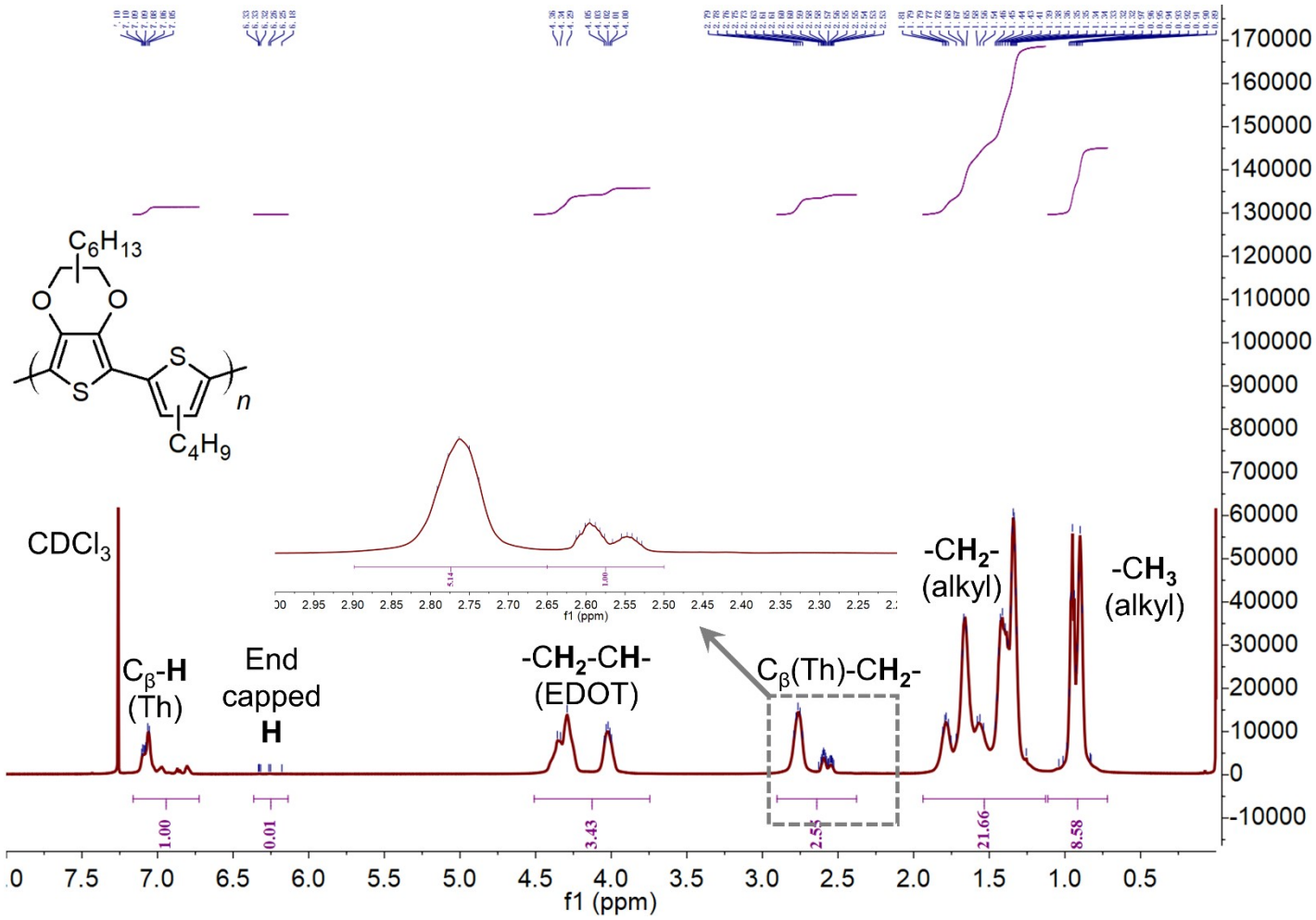
^{1}H NMR of P2 with entry 8 of Table 1 [600MHz, $CDCl_3$, 323K]



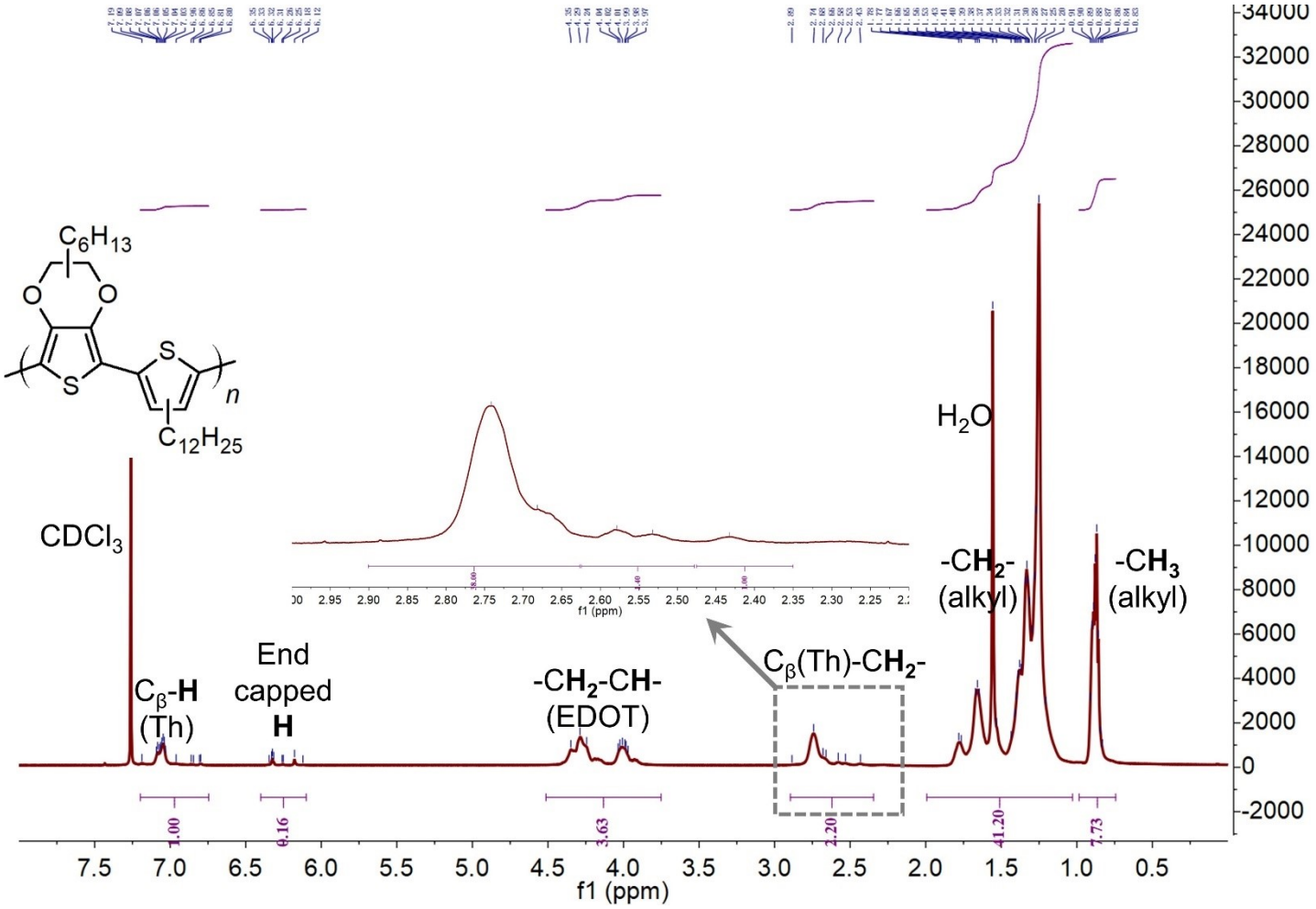
^{1}H NMR of P2 with entry 9 of Table 1 [600MHz, $CDCl_3$, 323K]



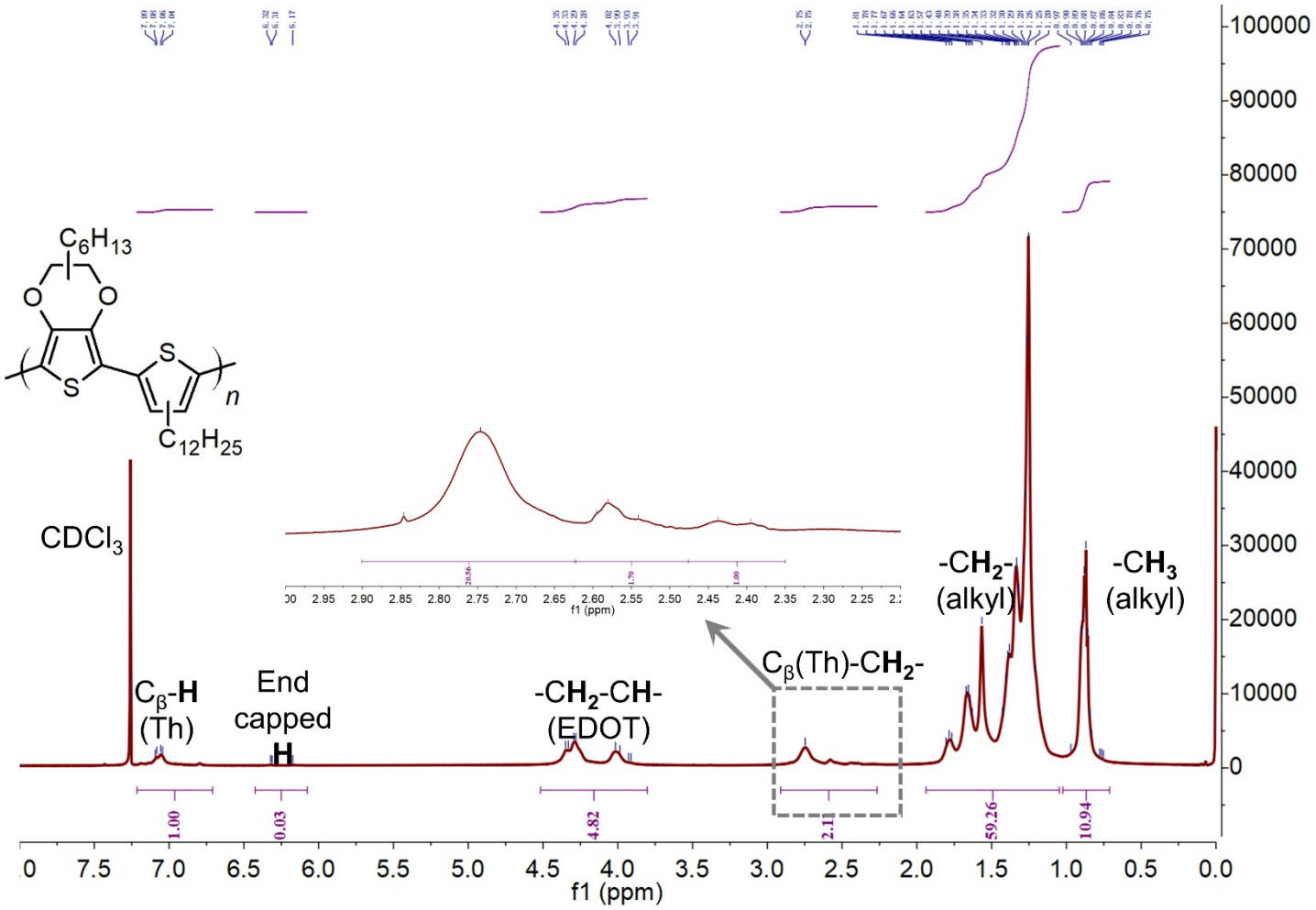
^{1}H NMR of P2 with entry 10 of Table 1 [600MHz, $CDCl_3$, 323 K



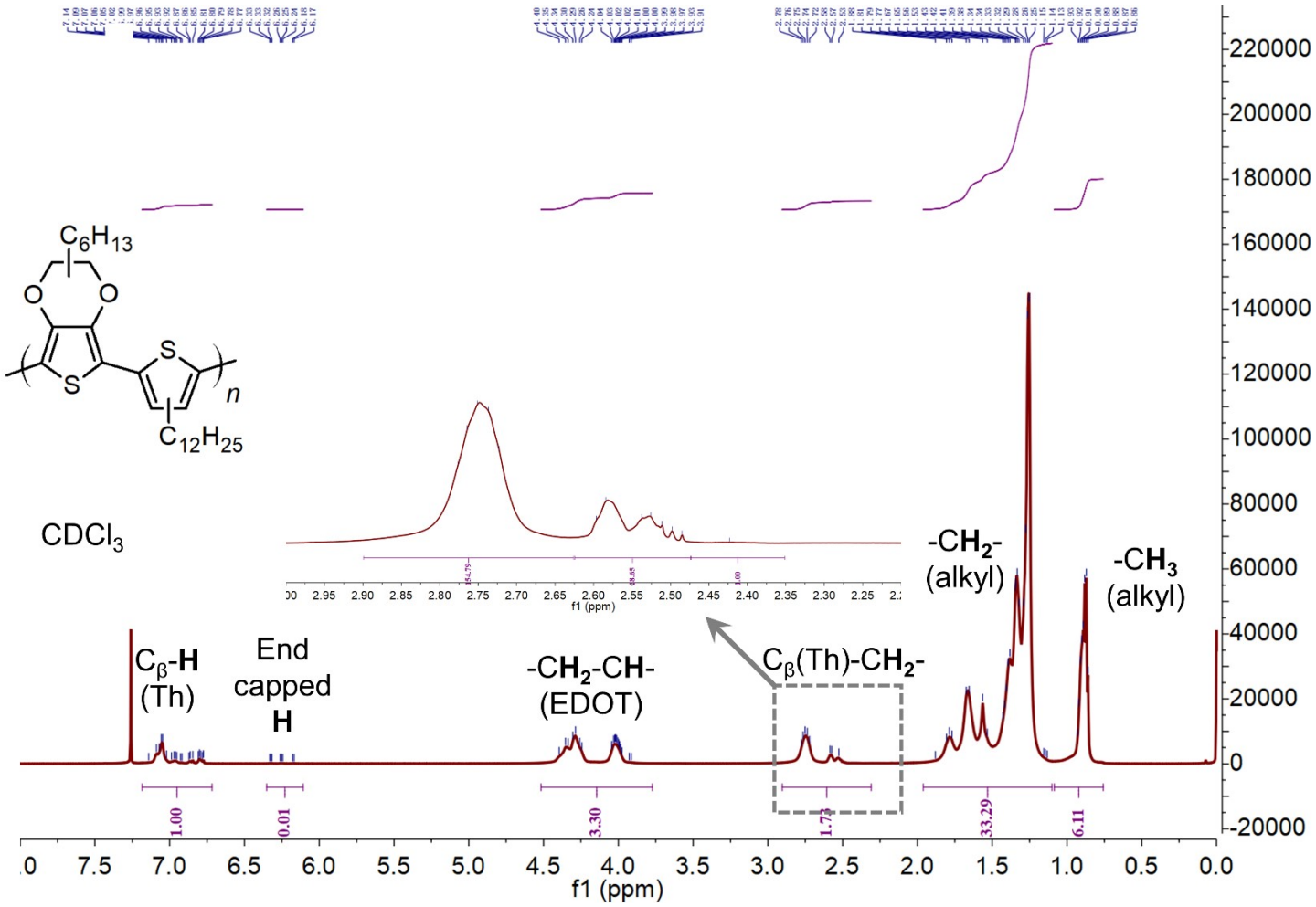
^{1}H NMR of P3 with entry 11 of Table 1 [600MH, $CDCl_3$, 323K]



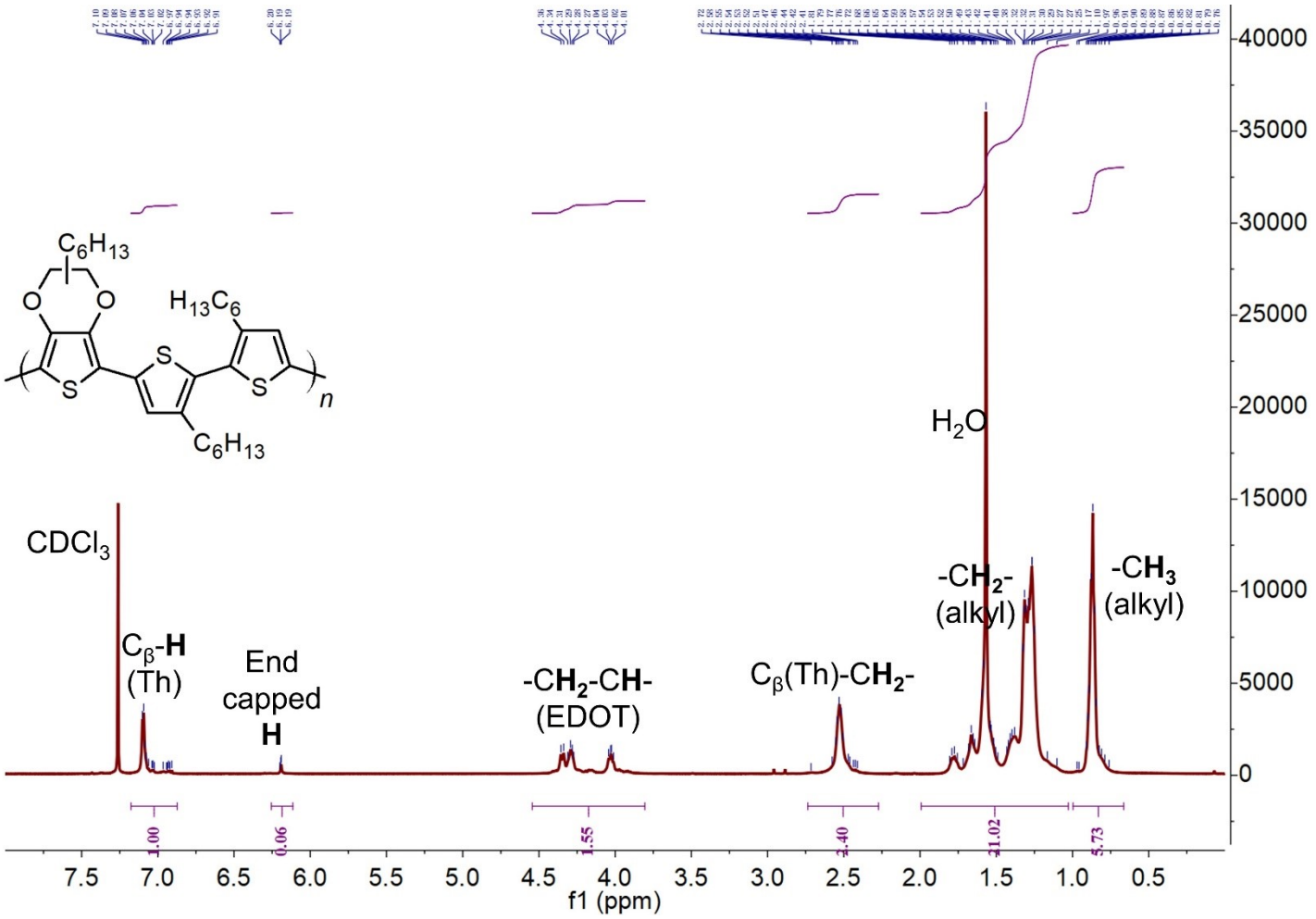
^{1}H NMR of P3 with entry 12 of Table 1 [600MHz, $CDCl_3$, 323K]



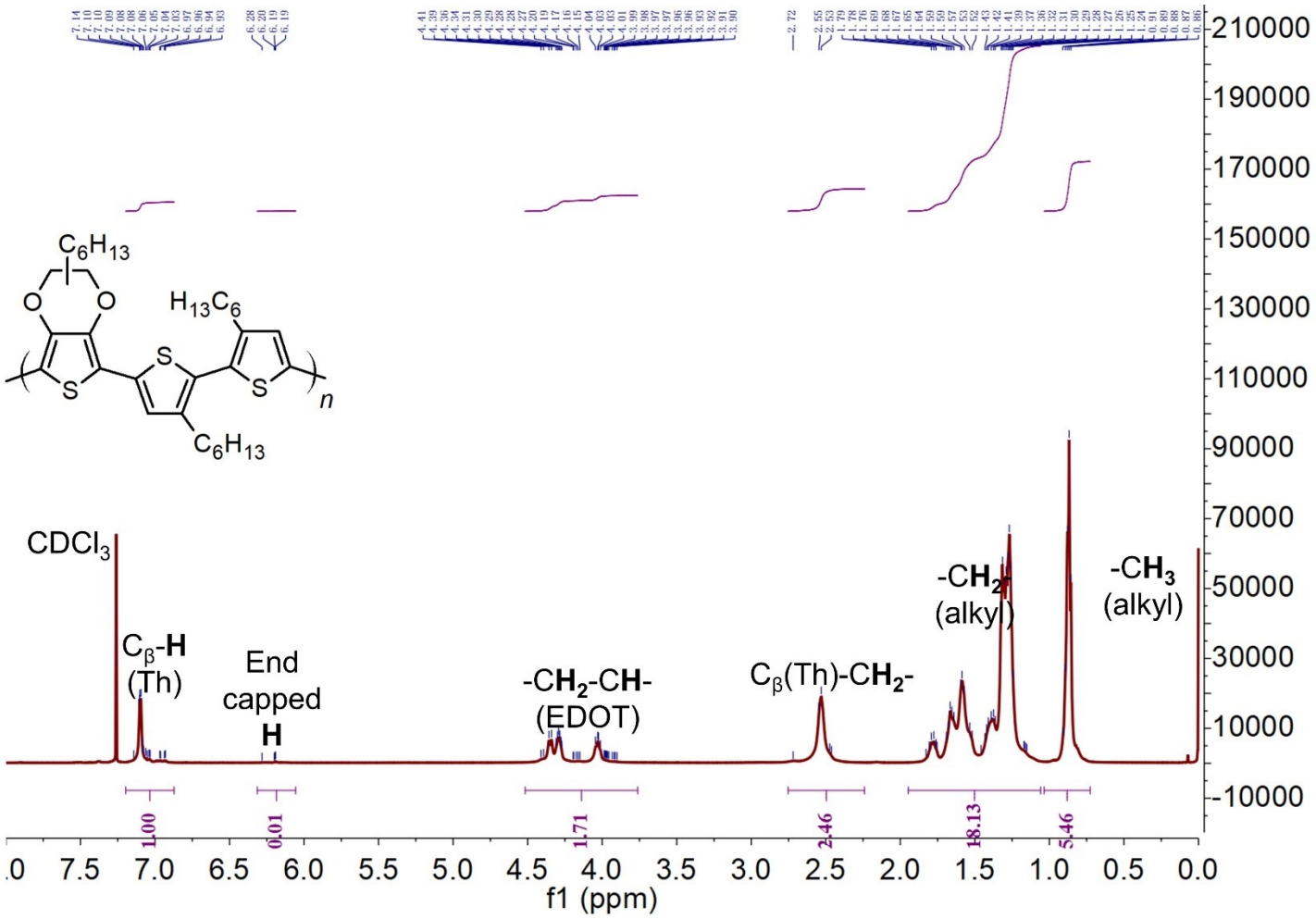
^{1}H NMR of P3 with entry 13 of Table 1 [600MHz, $CDCl_3$, 323K]



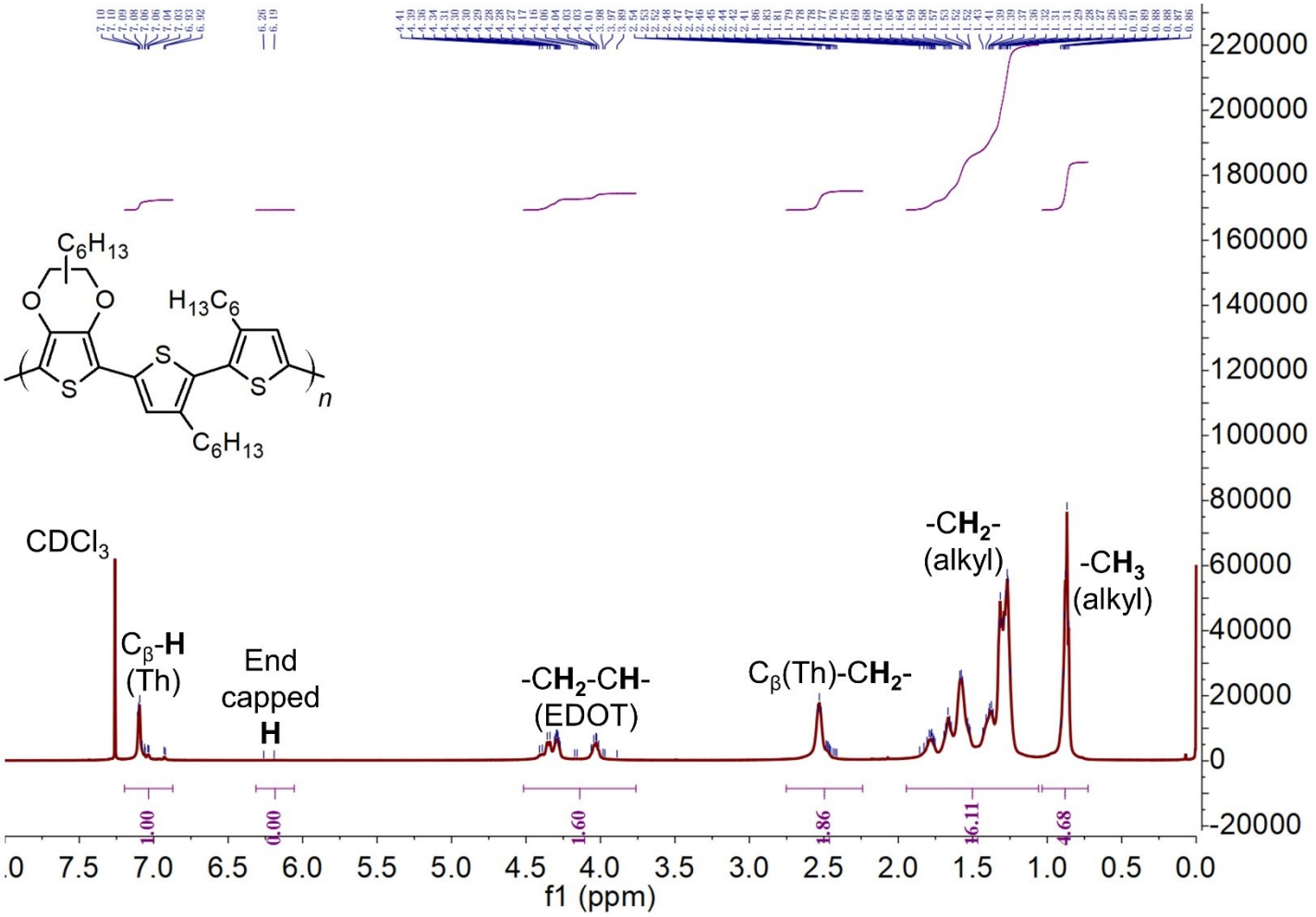
^{1}H NMR of P4 with entry 14 of Table 1 [600MHz, $CDCl_3$, 323K]



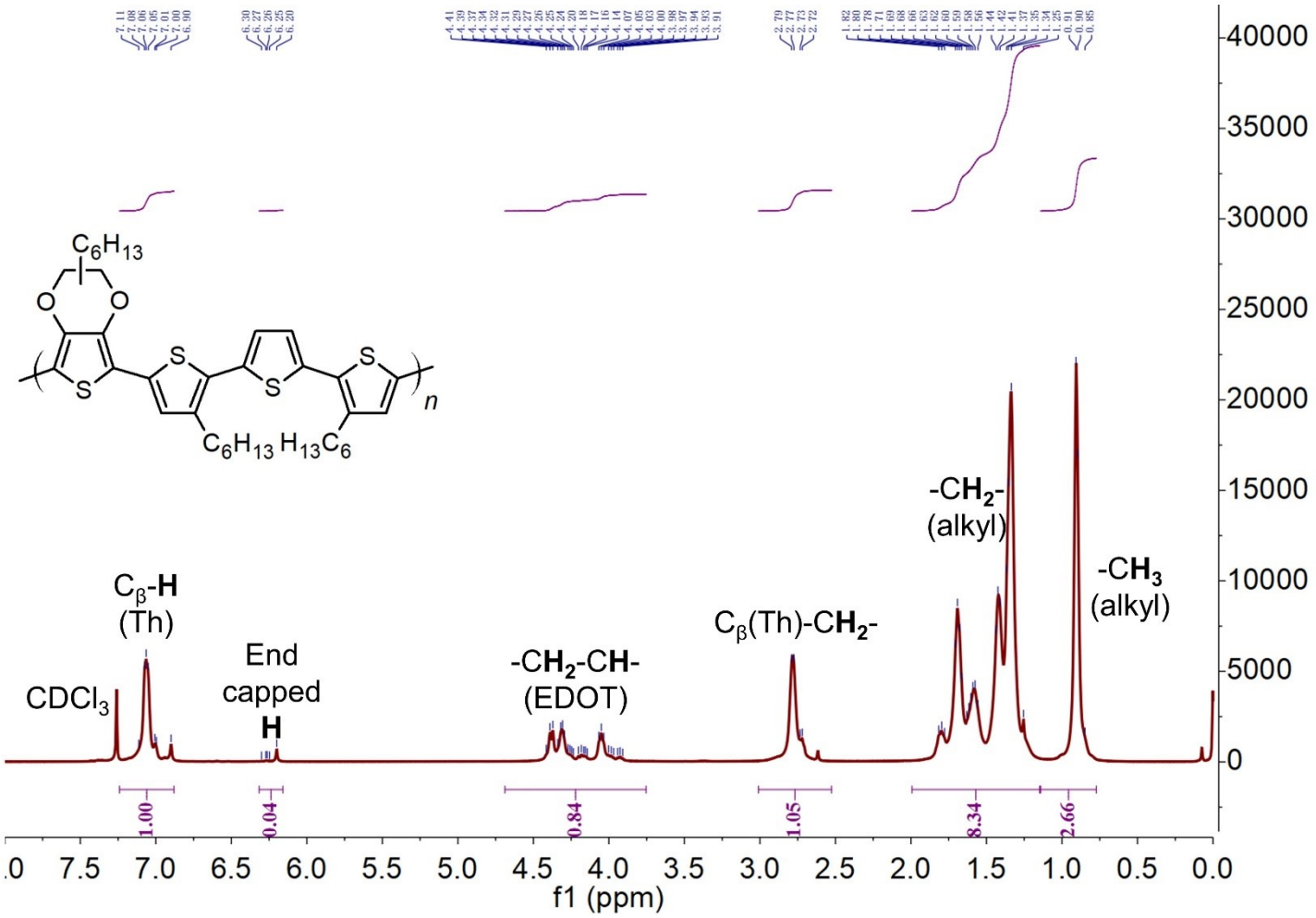
^{1}H NMR of P4 with entry 15 of Table 1 [600MHz, $CDCl_3$, 323K]



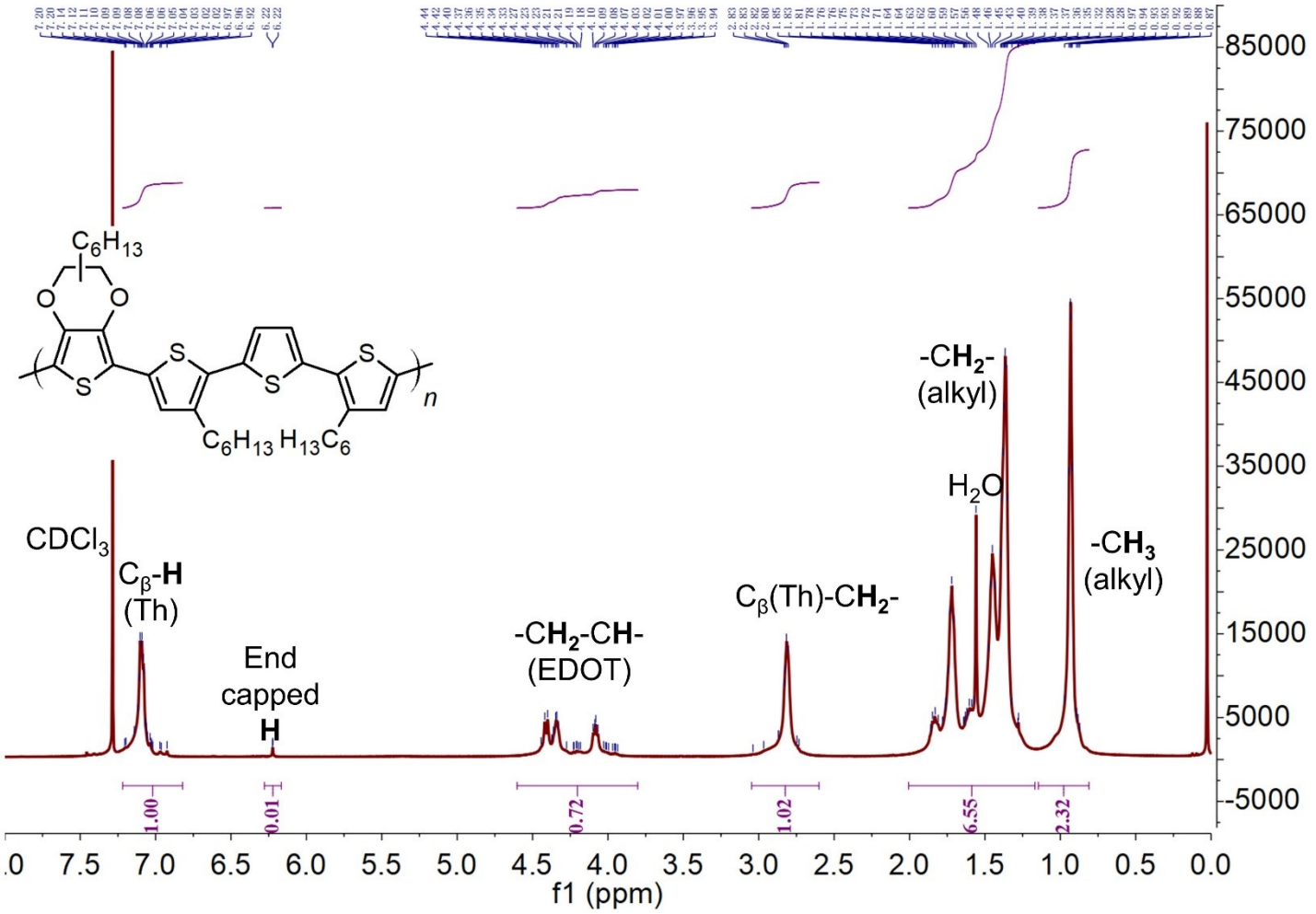
^{1}H NMR of P4 with entry 16 of Table 1 [600MHz, $CDCl_3$, 323K]



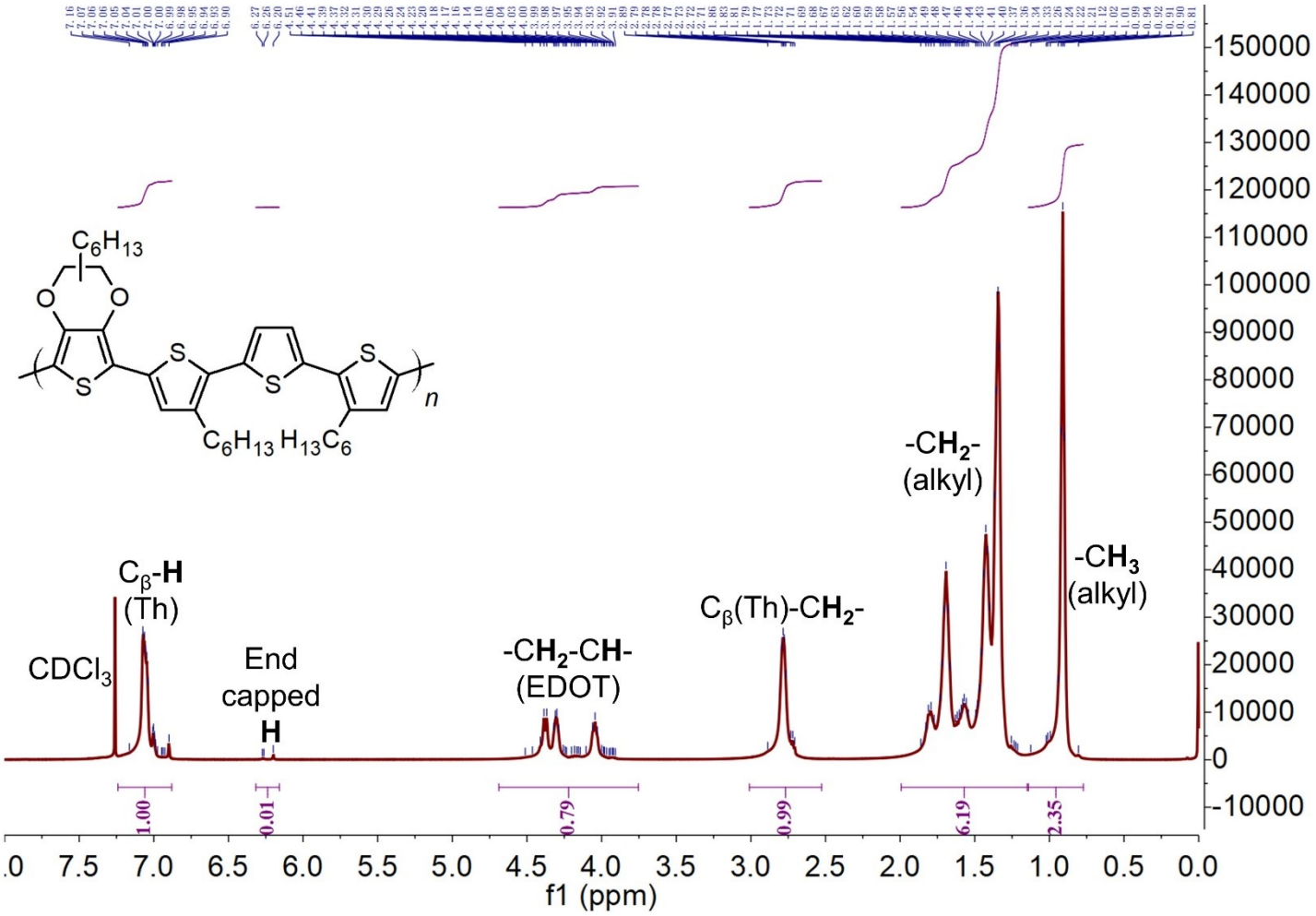
^{1}H NMR of P5 with entry 17 of Table 1 [600MHz, $CDCl_3$, 323K]



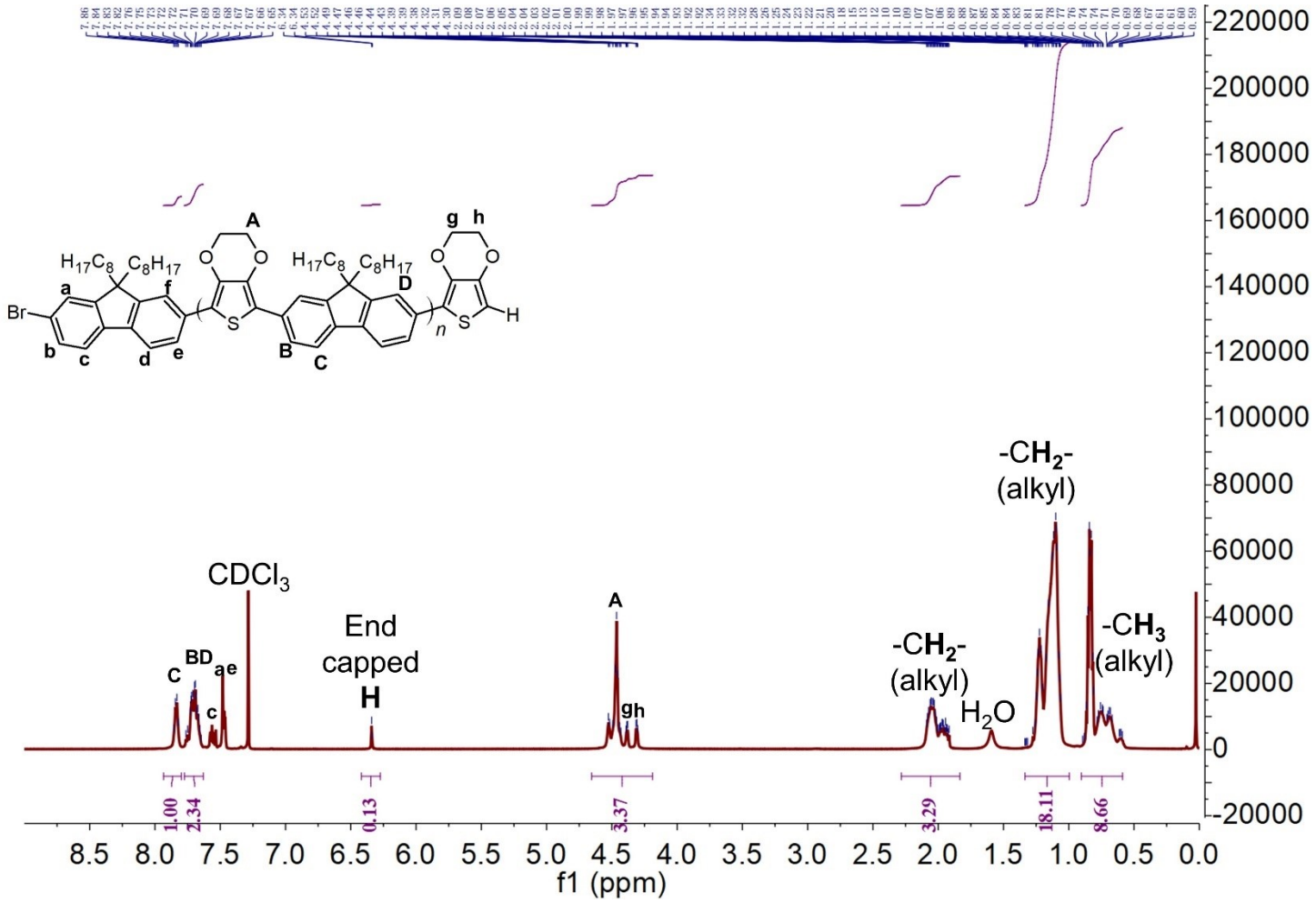
^{1}H NMR of P5 with entry 18 of Table 1 [600MHz, $CDCl_3$, 323K]



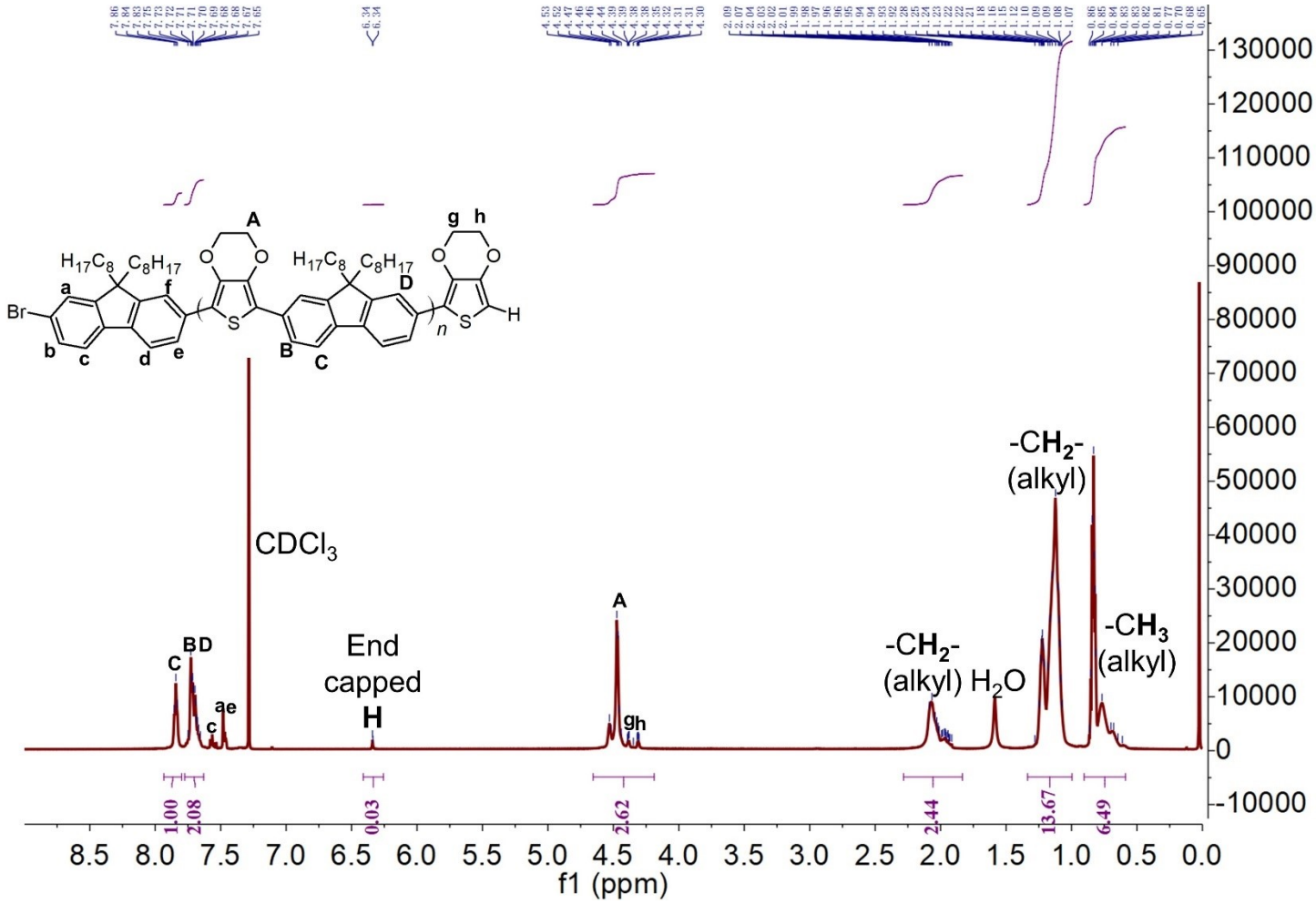
^{1}H NMR of P5 with entry 19 of Table 1 [600MHz, $CDCl_3$, 323K]



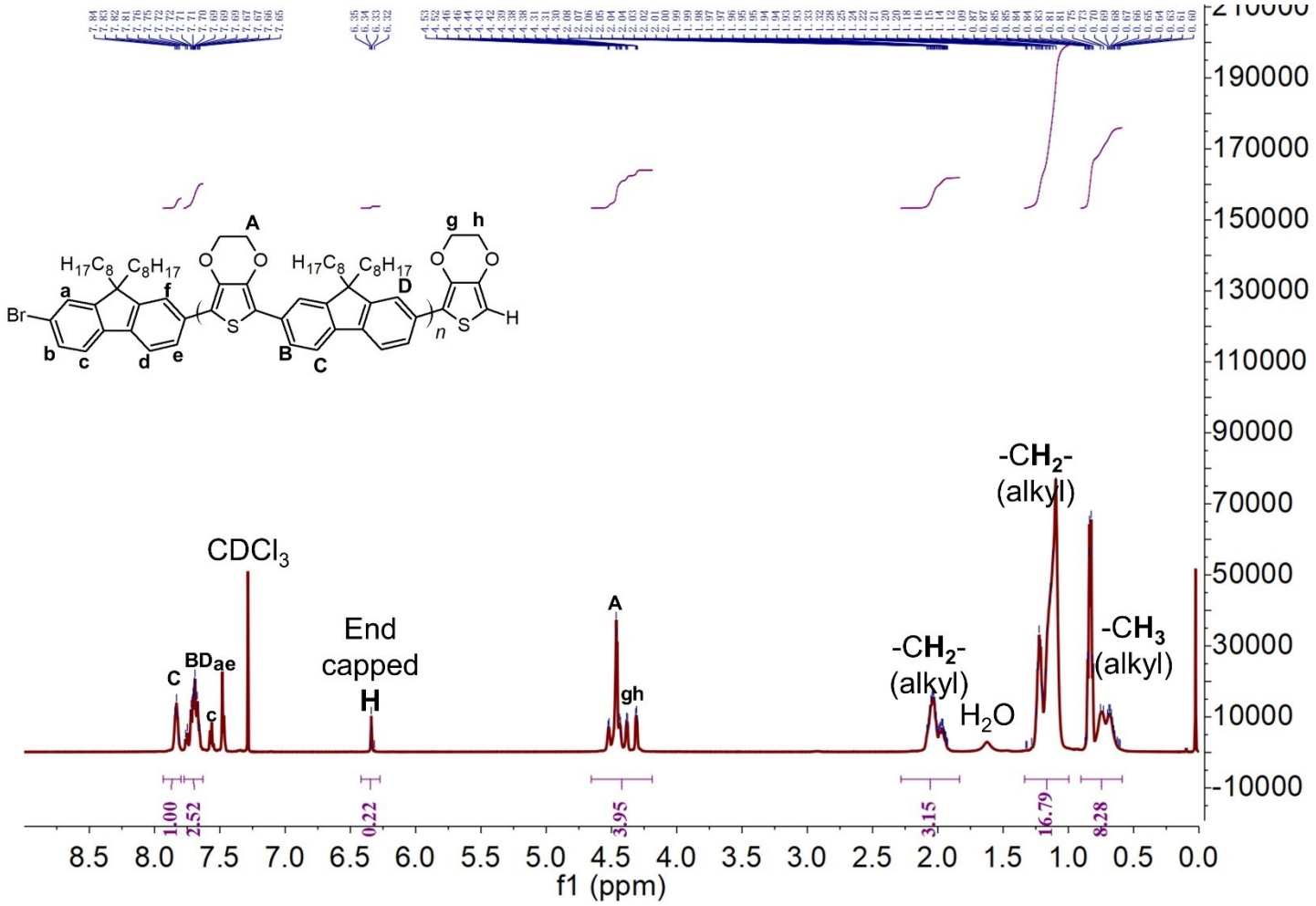
^{1}H NMR of PEDOTF with entry 20 of Table 1 [600MHz, $CDCl_3$, 323K]



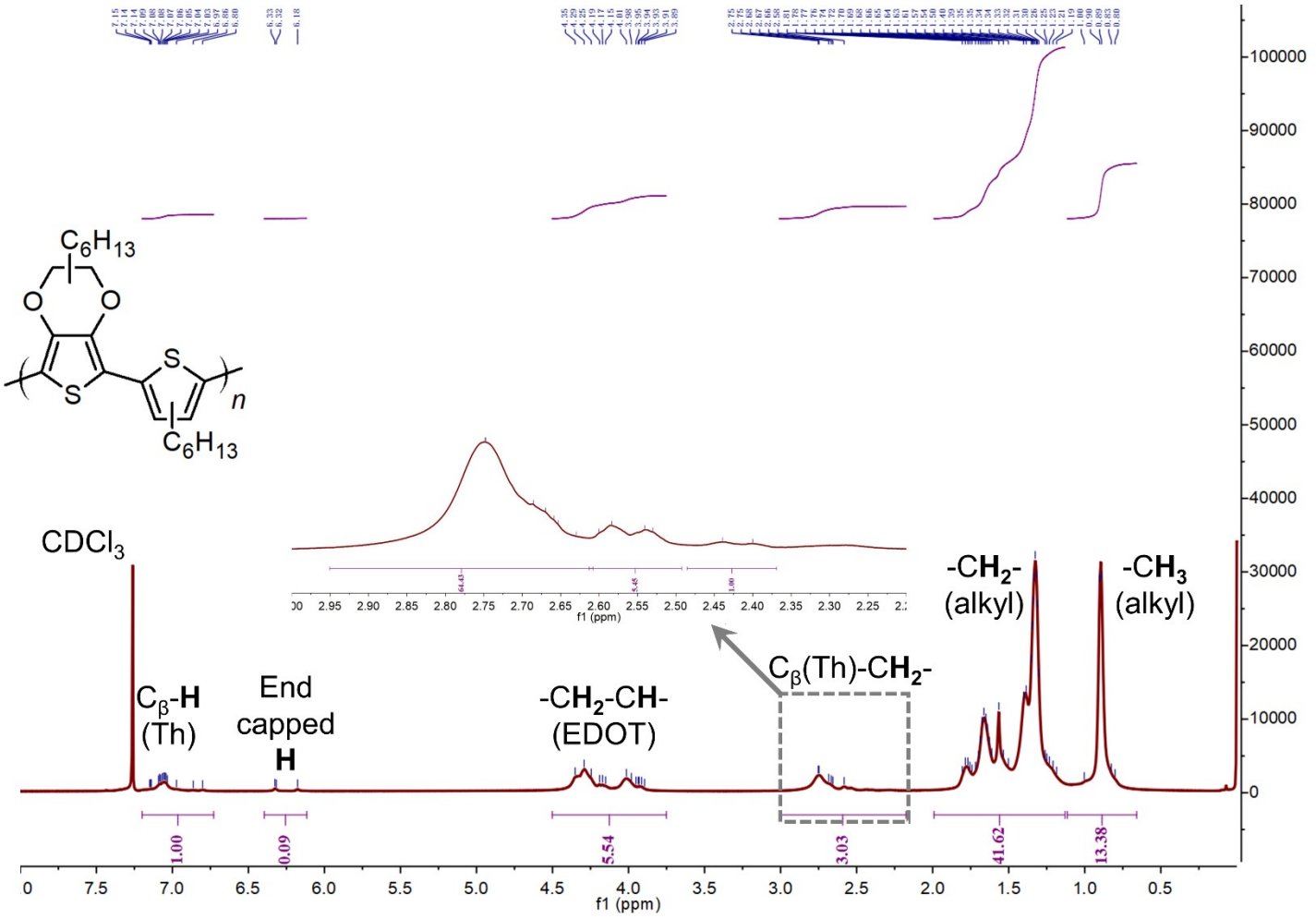
^{1}H NMR of PEDOTF with entry 21 of Table 1 [600MHz, $CDCl_3$, 323K]



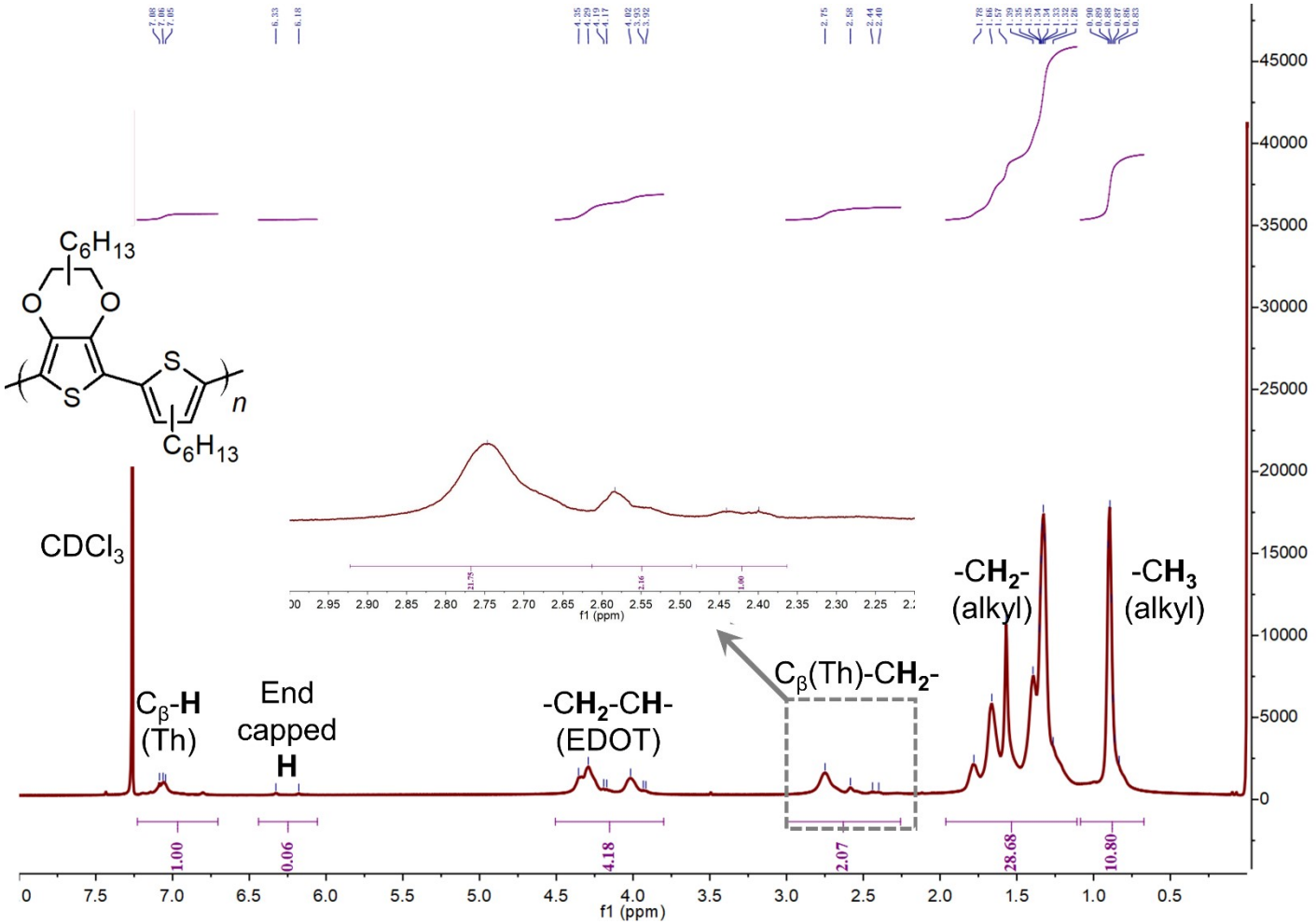
^{1}H NMR of PEDOTF with entry 22 of Table 1 [600MHz, $CDCl_3$, 323K]



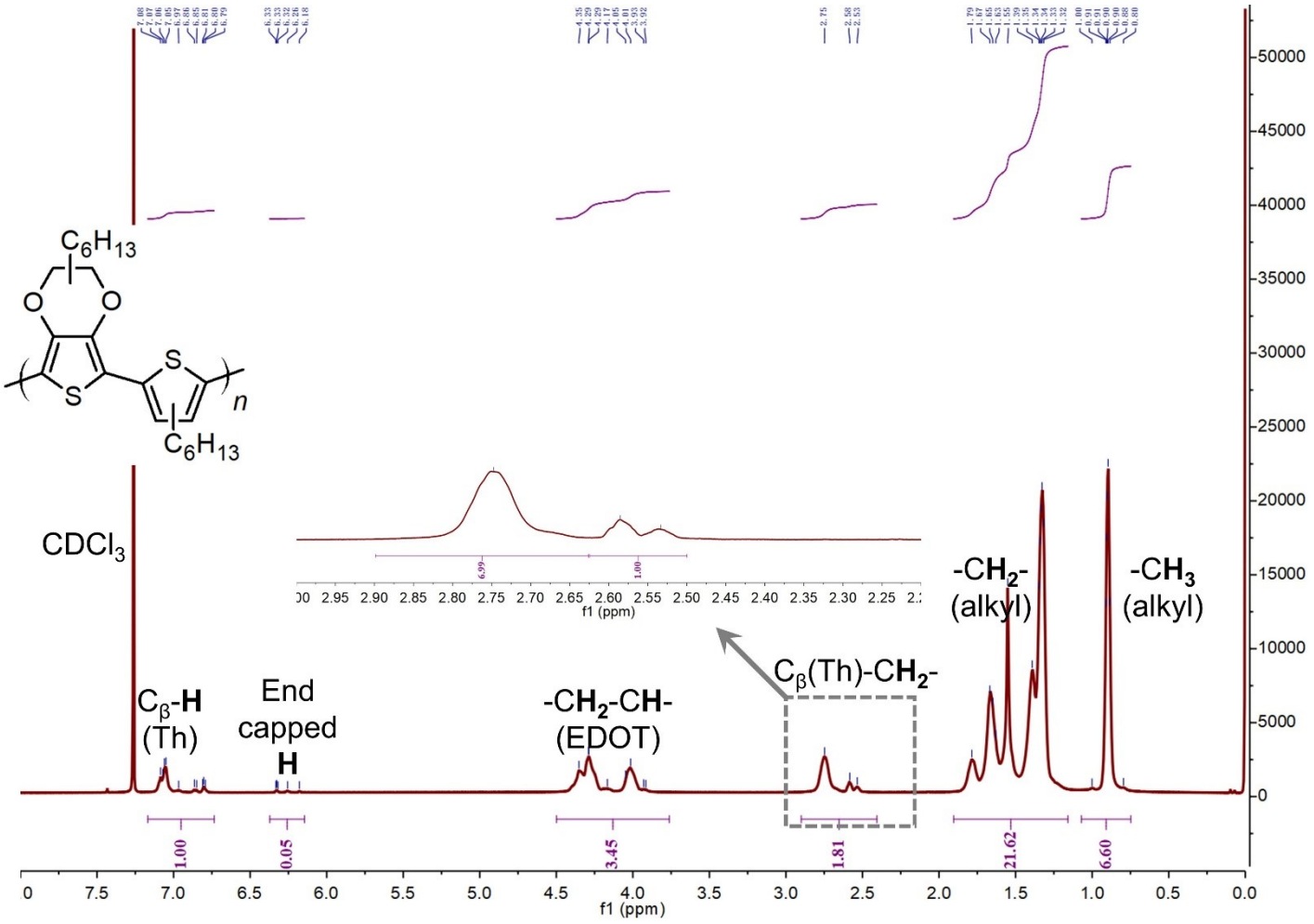
^{1}H NMR of P1 with entry 1 of Table S1 [600MHz, $CDCl_3$, 323K]



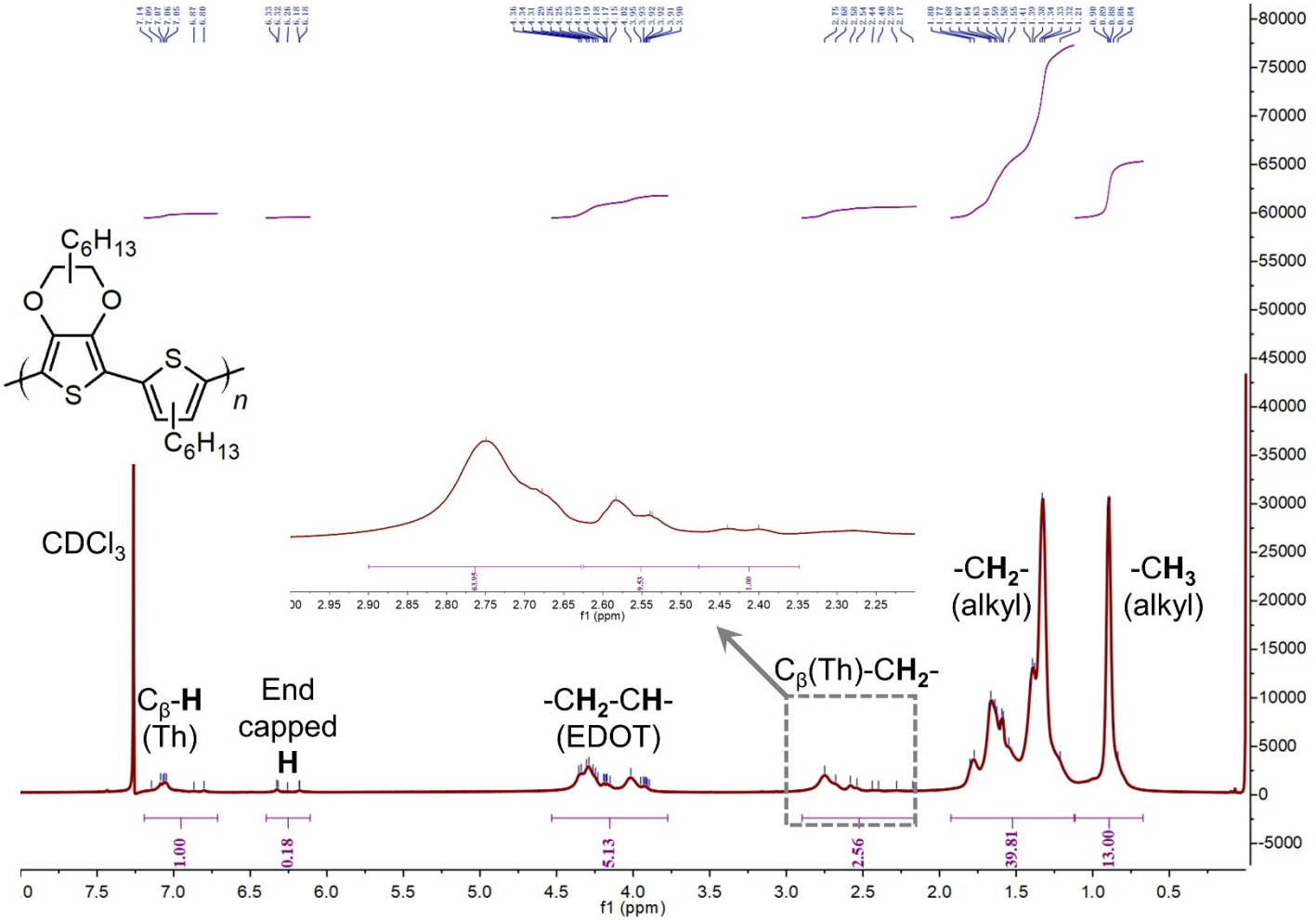
^{1}H NMR of P1 with entry 2 of Table S1 [600MHz, $CDCl_3$, 323K]



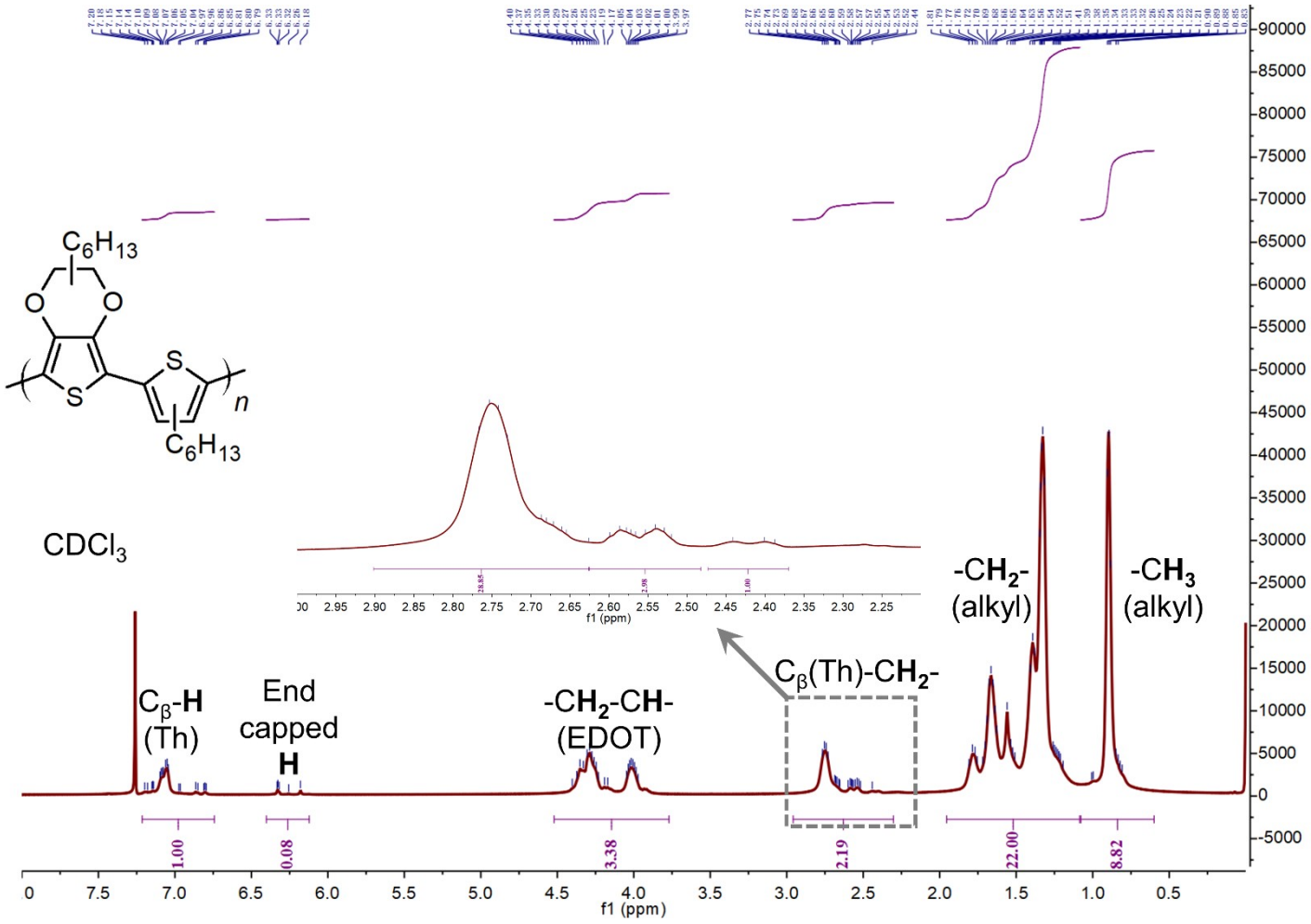
^{1}H NMR of P1 with entry 3 of Table S1 [600MHz, $CDCl_3$, 323K]



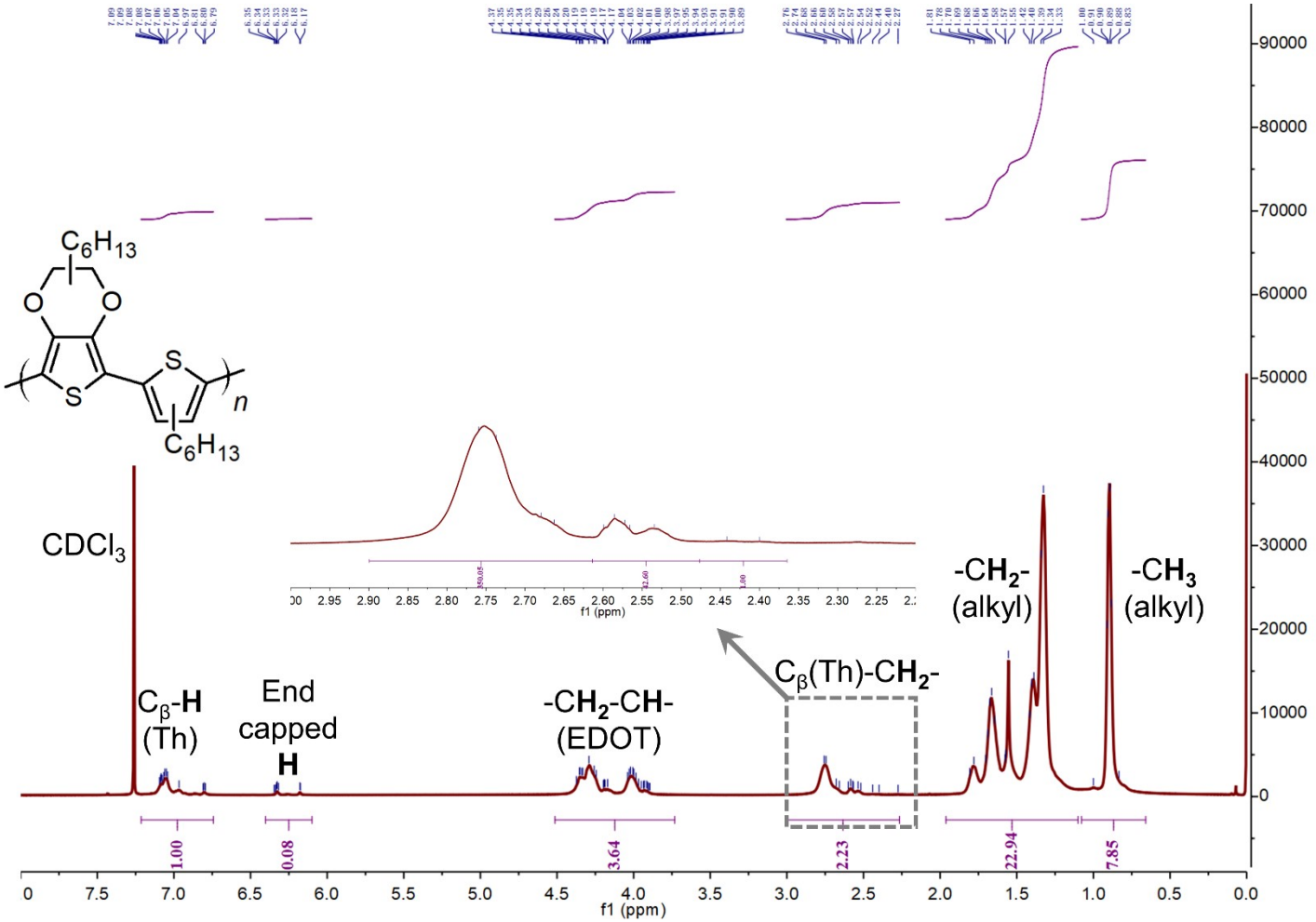
^{1}H NMR of P1 with entry 4 of Table S1 [600MHz, $CDCl_3$, 323K]



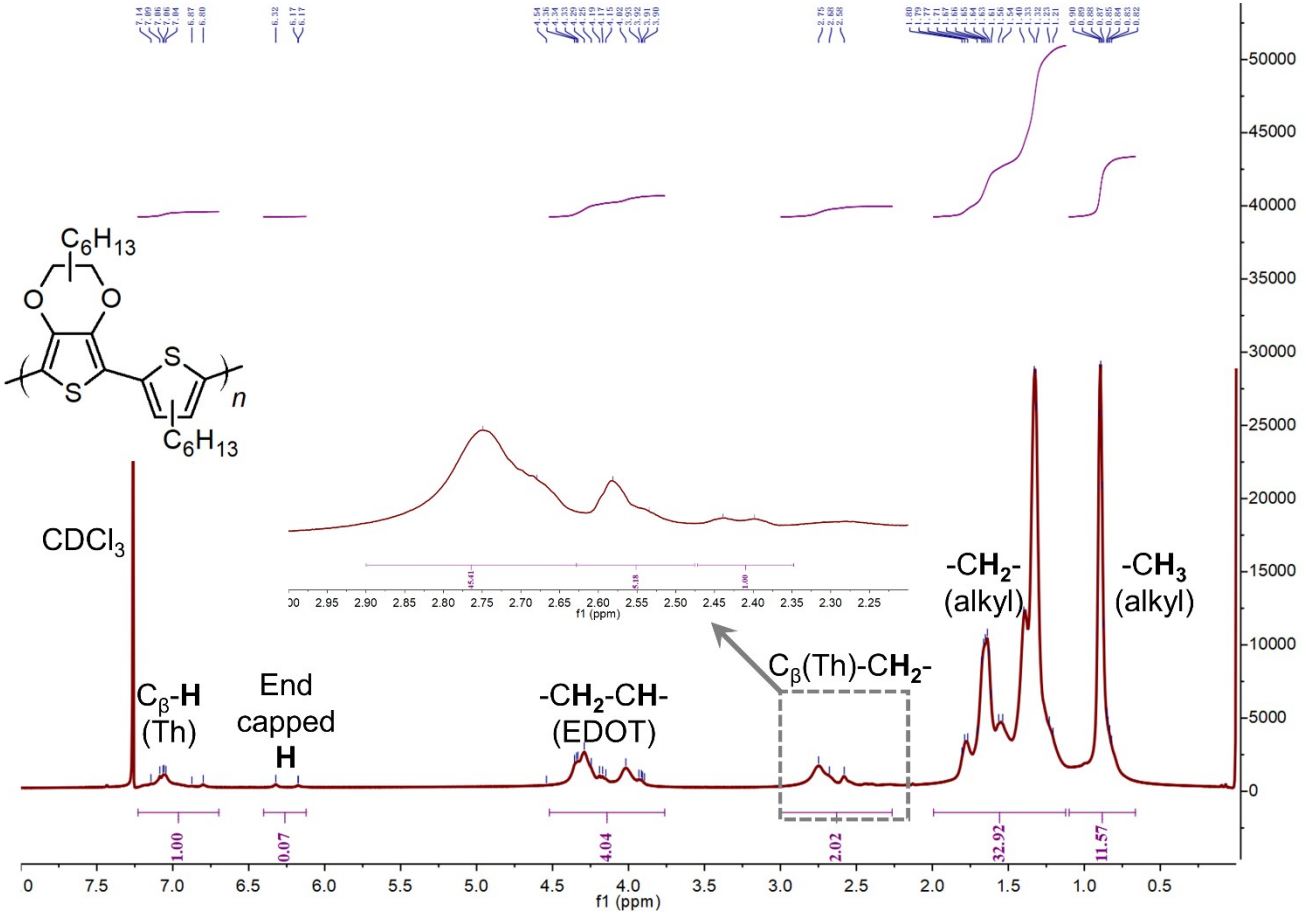
^{1}H NMR of P1 with entry 5 of Table S1 [600MHz, $CDCl_3$, 323K]



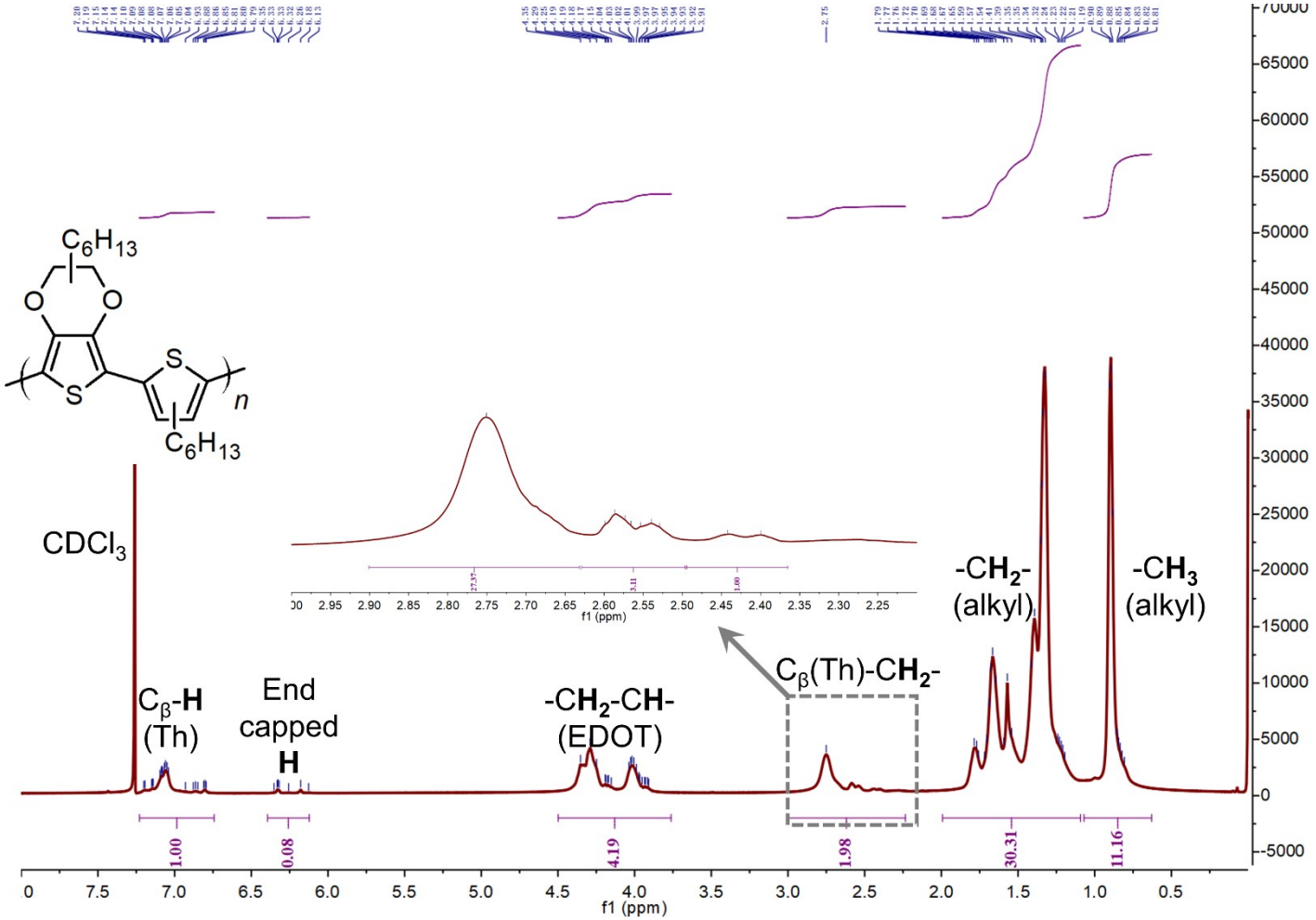
^{1}H NMR of P1 with entry 6 of Table S1 [600MHz, $CDCl_3$, 323K]



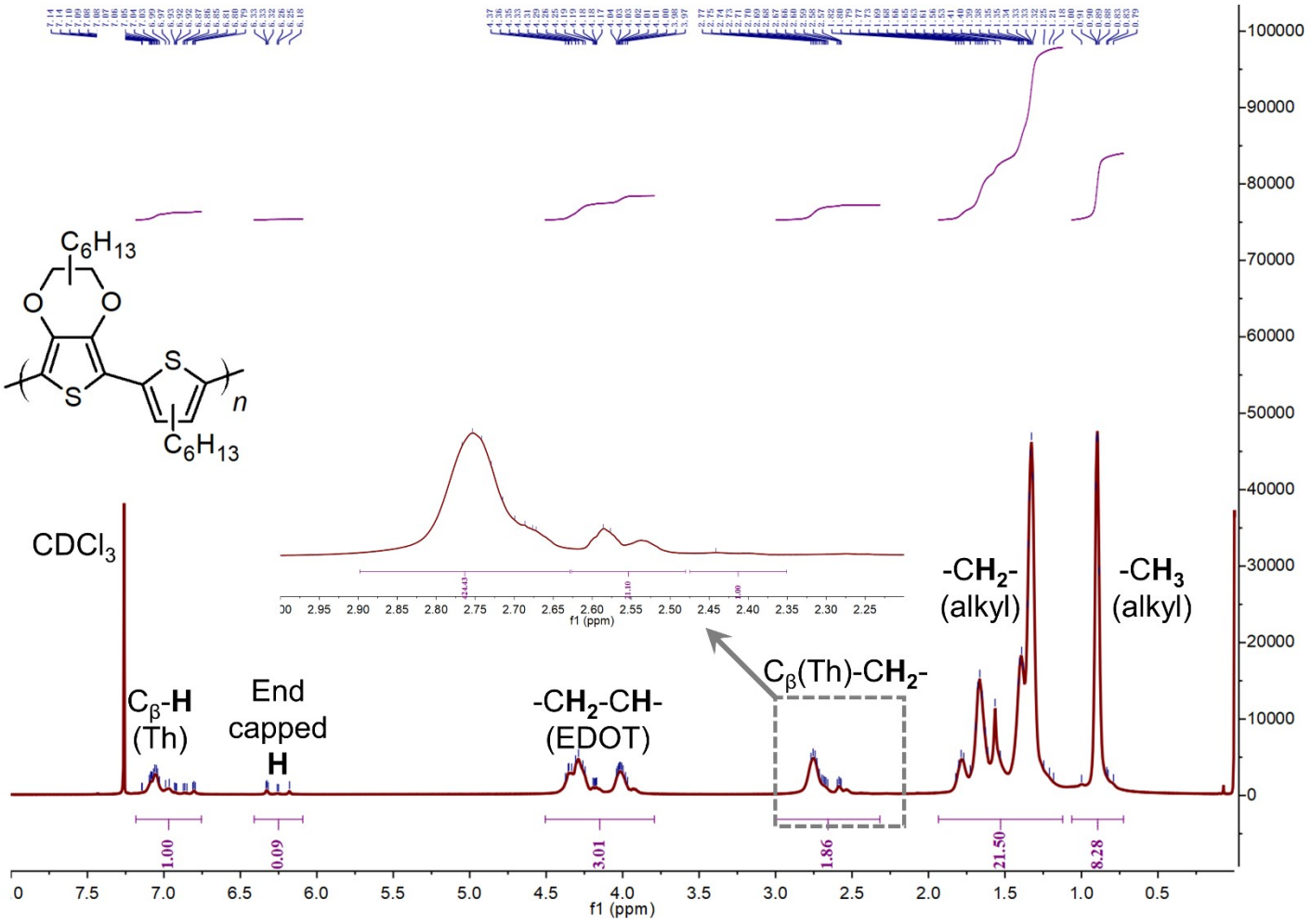
^{1}H NMR of P1 with entry 7 of Table S1 [600MHz, $CDCl_3$, 323K]



^{1}H NMR of P1 with entry 8 of Table S1 [600MHz, $CDCl_3$, 323K]



^{1}H NMR of P1 with entry 9 of Table S1 [600MHz, $CDCl_3$, 323K]



8. GPC traces

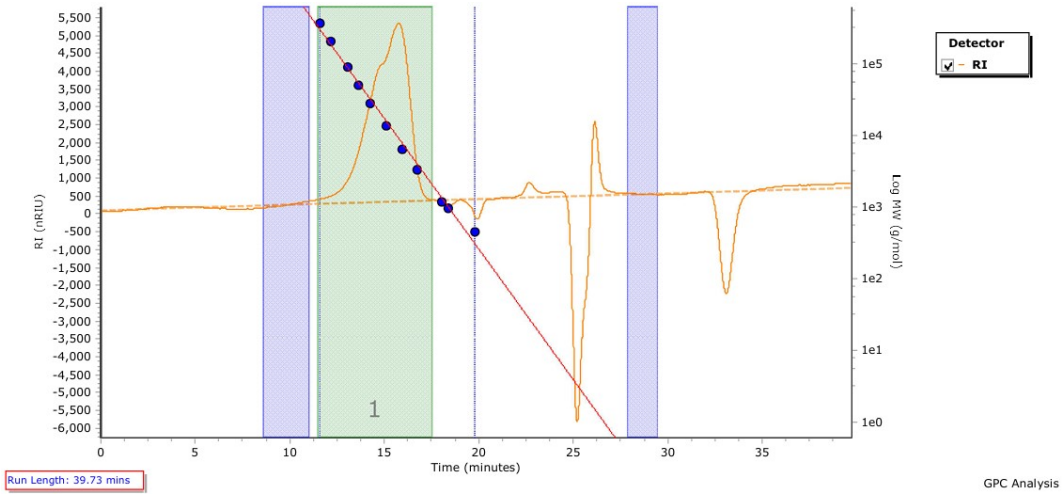


Figure S3 GPC trace of P1 (Table 1, entry 4). M_n= 11426 g/mol, M_w=23507 g/mol and PD=2.057.

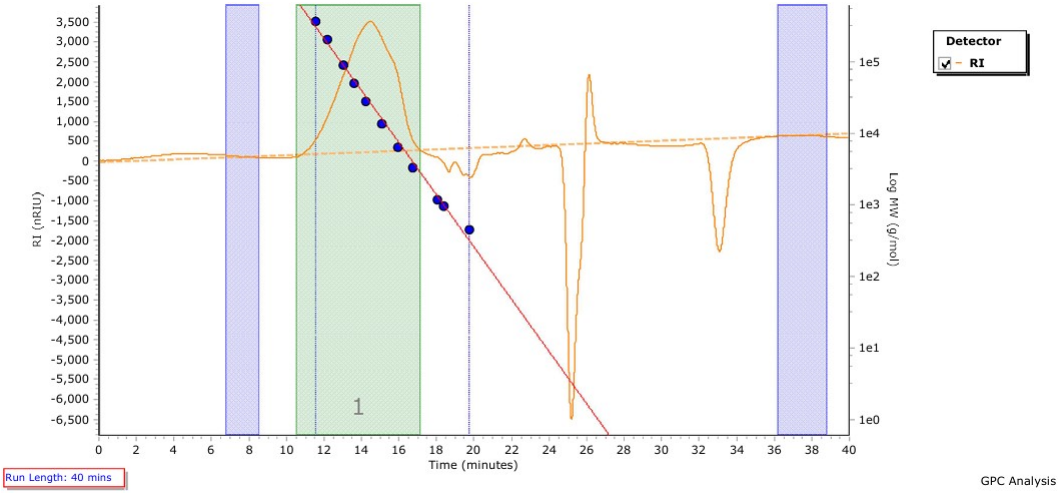


Figure S4 GPC trace of P1 (Table 1, entry 5). M_n= 19436 g/mol, M_w=50434 g/mol and PD=2.595.

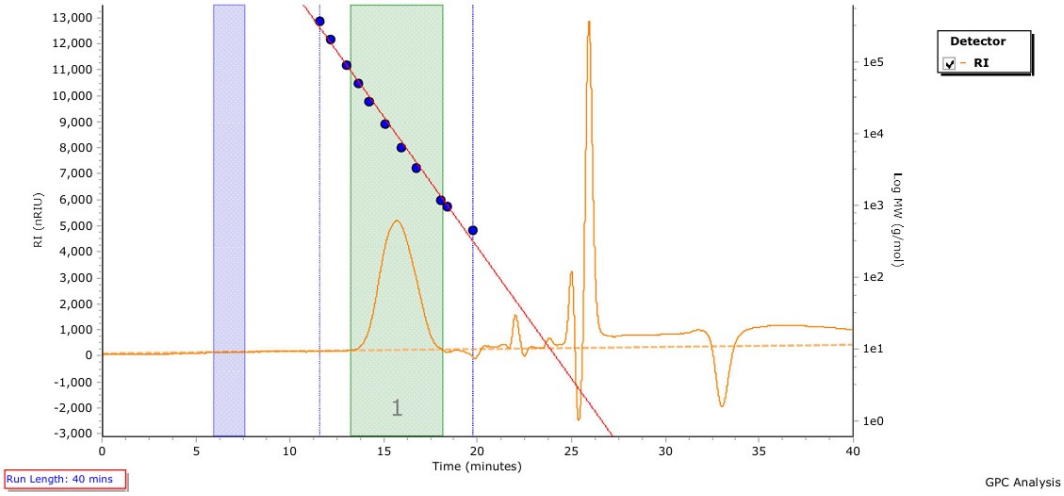


Figure S5 GPC trace of P1 (Table 1, entry 7). M_n= 7039 g/mol, M_w=10990 g/mol and PD=1.561.

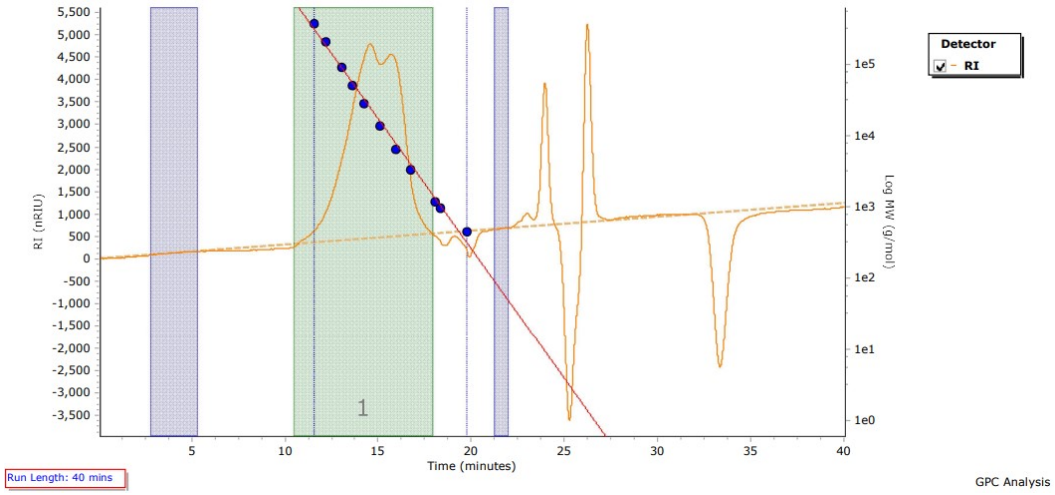


Figure S6 GPC trace of P2 (Table 1, entry 8). M_n= 12842 g/mol, M_w=36488 g/mol and PD=2.841.

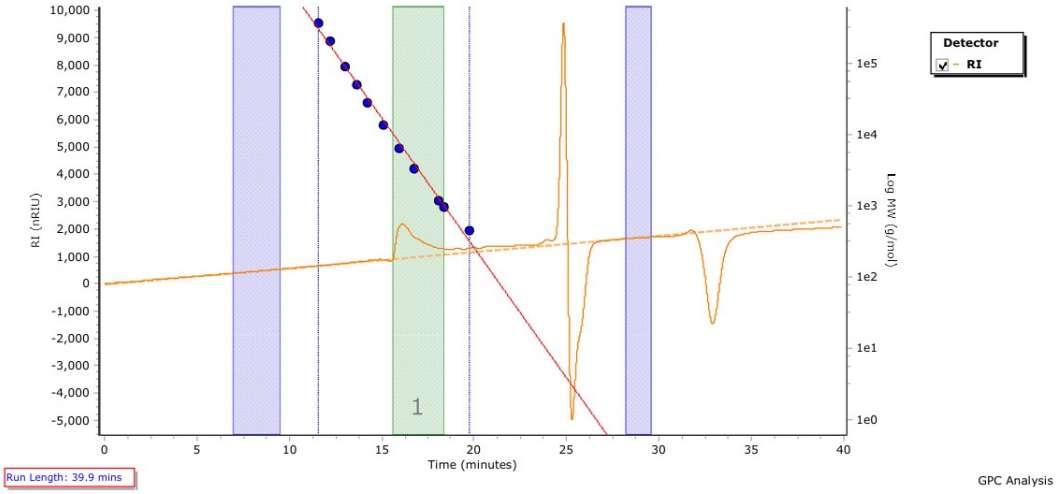


Figure S7 GPC trace of P2 (Table 1, entry 9). M_n= 3782 g/mol, M_w=5377 g/mol and PD=1.422.

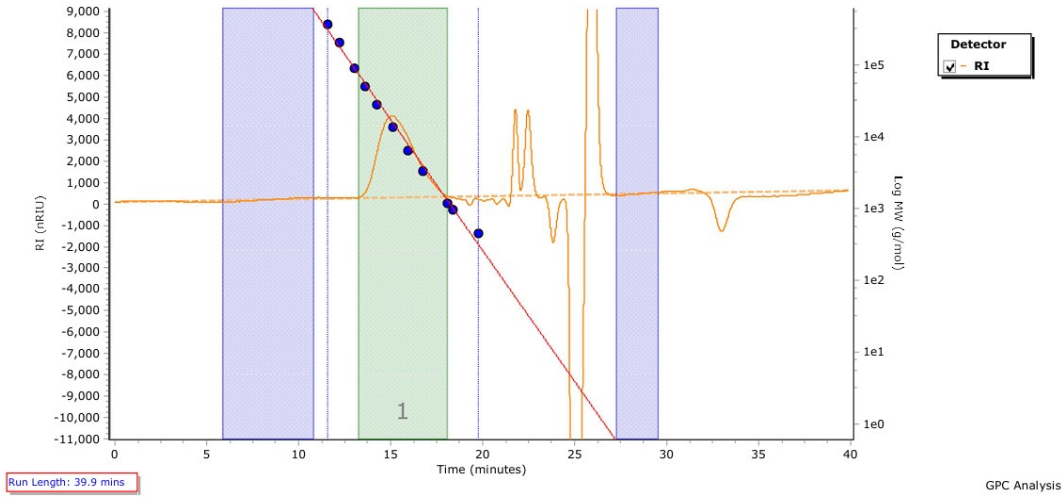


Figure S8 GPC trace of P2 (Table 1, entry 10). M_n= 8729 g/mol, M_w=15064 g/mol and PD=1.726.

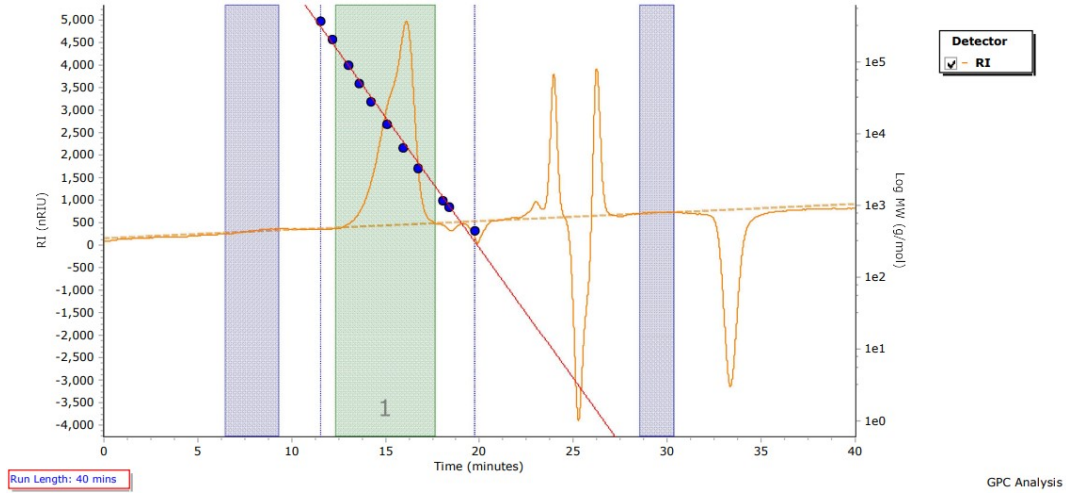


Figure S9 GPC trace of P3 (Table 1, entry 11). M_n= 8773 g/mol, M_w=12799 g/mol and PD=1.529.

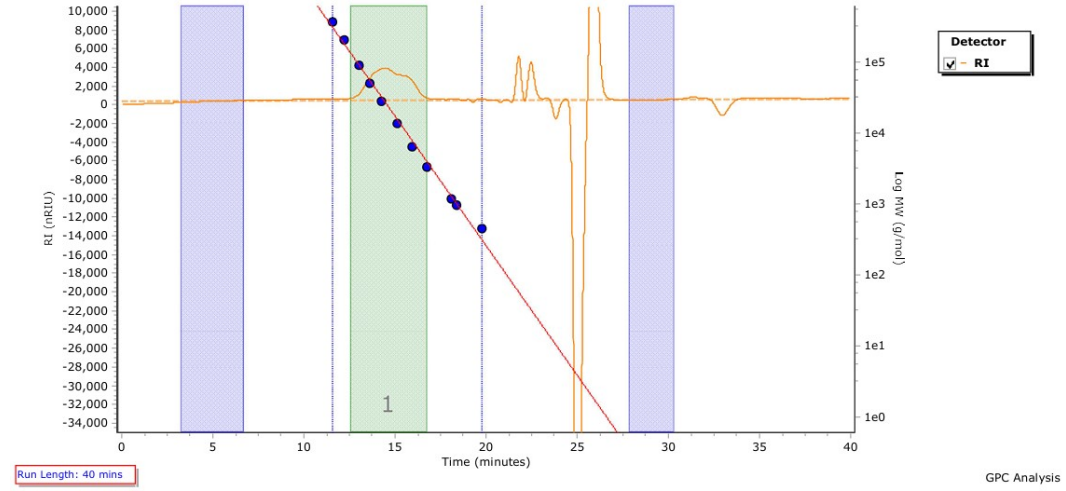


Figure S10 GPC trace of P3 (Table 1, entry 12). M_n= 16370 g/mol, M_w=28534 g/mol and PD=1.743.

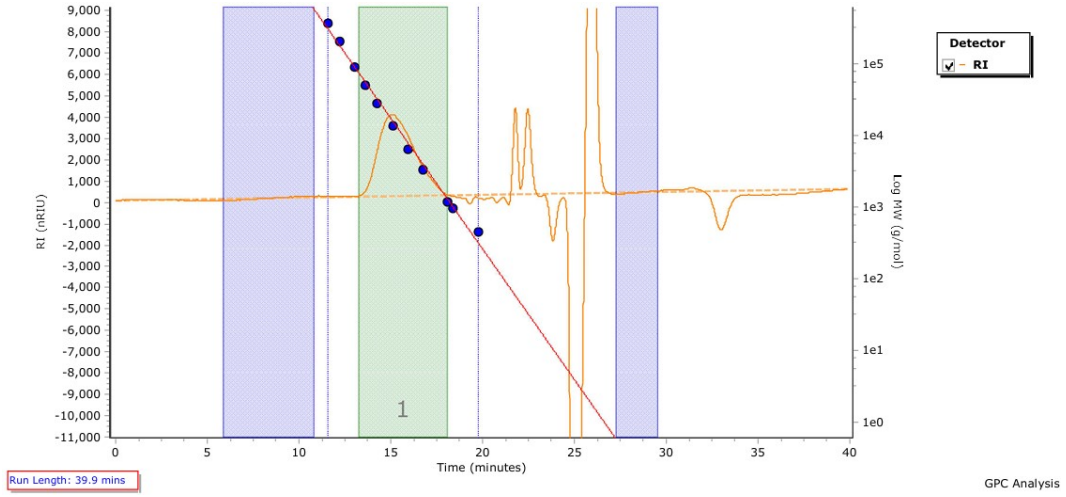


Figure S11 GPC trace of P3 (Table 1, entry 13). M_n= 8729 g/mol, M_w=15064 g/mol and PD=1.726.

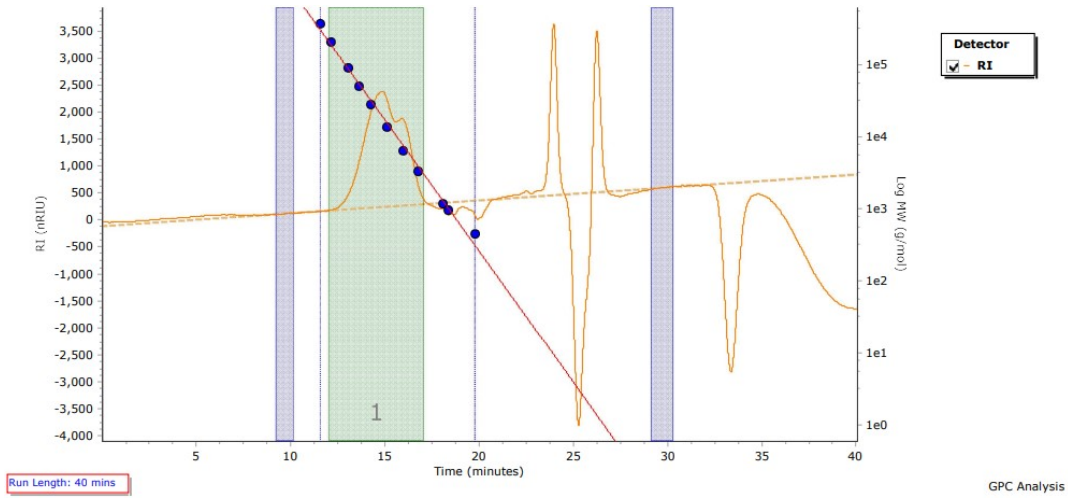


Figure S12 GPC trace of P4 (Table 1, entry 14). M_n= 12708 g/mol, M_w=22719 g/mol and PD=1.788.

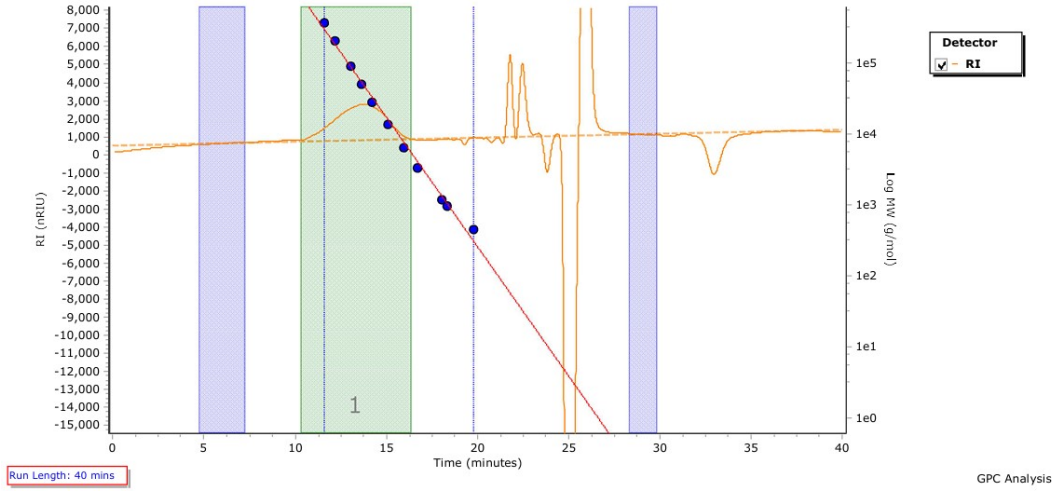


Figure S13 GPC trace of P4 (Table 1, entry 15). M_n= 37682 g/mol, M_w=98003 g/mol and PD=2.601.

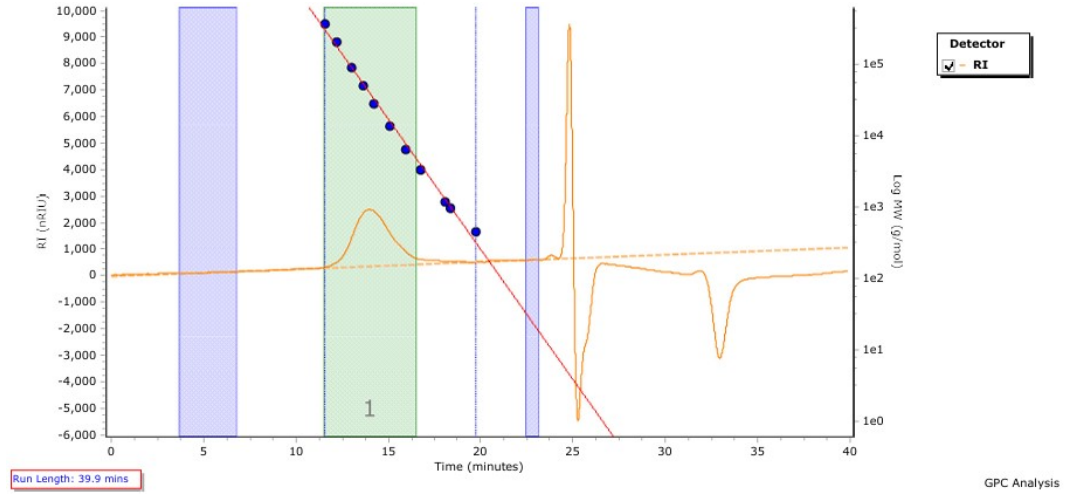


Figure S14 GPC trace of P4 (Table 1, entry 16). M_n= 23812 g/mol, M_w=43649 g/mol and PD=1.833.

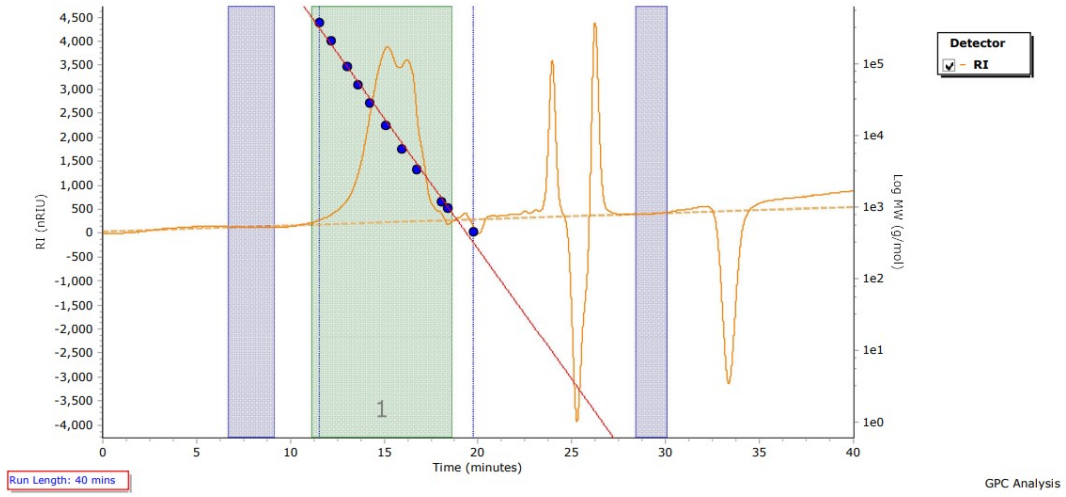


Figure S15 GPC trace of P5 (Table 1, entry 17). M_n= 8360 g/mol, M_w=21709 g/mol and PD=2.597.

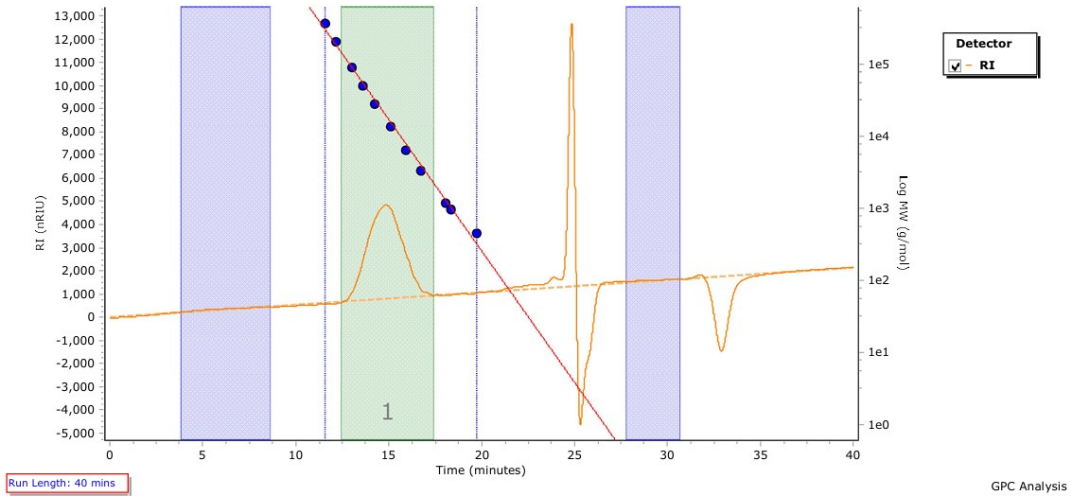


Figure S16 GPC trace of P5 (Table 1, entry 18). M_n= 15096 g/mol, M_w=24029 g/mol and PD=1.592.

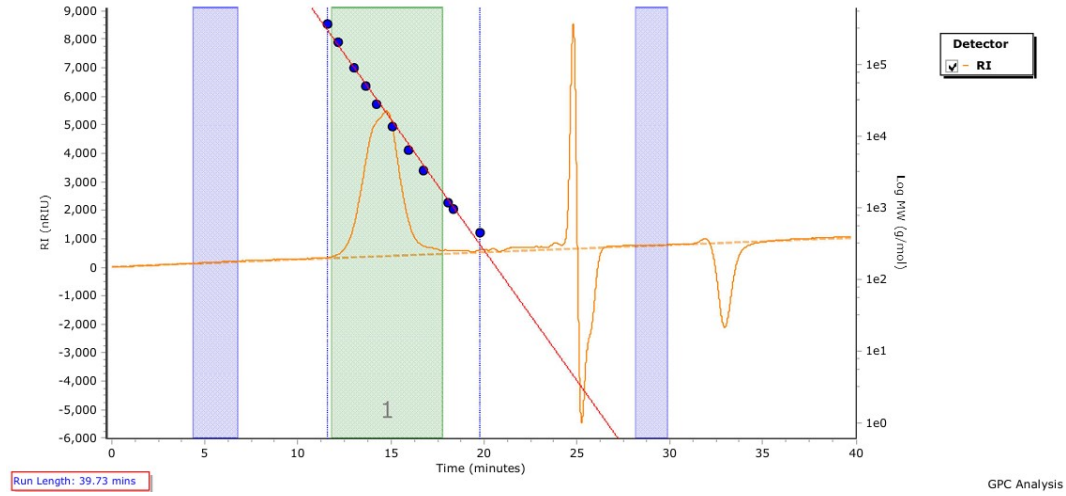


Figure S17 GPC trace of P5 (Table 1, entry 19). M_n= 17636 g/mol, M_w=31571 g/mol and PD=1.790.

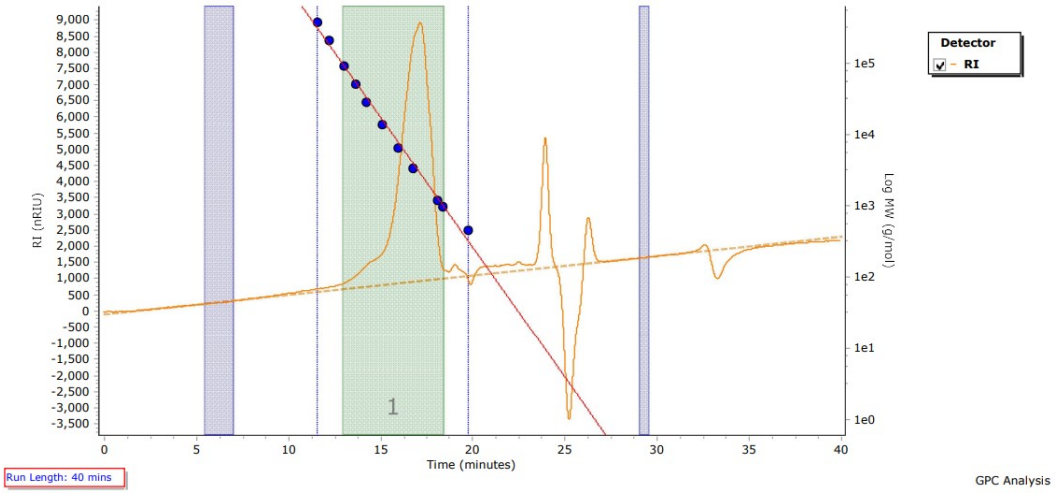


Figure S18 GPC trace of PEDOTF (Table 1, entry 20). M_n= 3238 g/mol, M_w=6440 g/mol and PD=1.989.

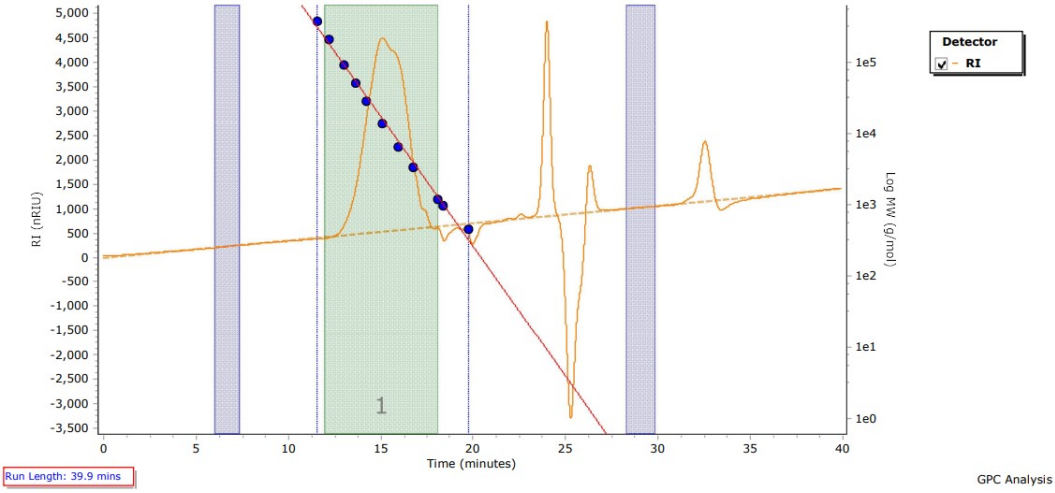


Figure S19 GPC trace of PEDOTF (Table 1, entry 21). M_n= 9666 g/mol, M_w=17292 g/mol and PD=1.789.

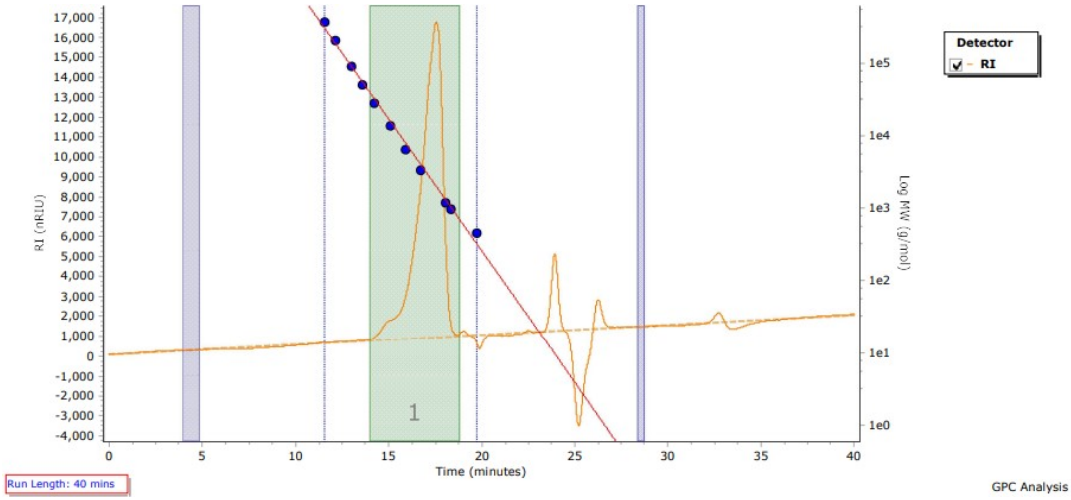


Figure S20 GPC trace of PEDOTF (Table 1, entry 22). M_n= 2408 g/mol, M_w=3565 g/mol and PD=1.480.

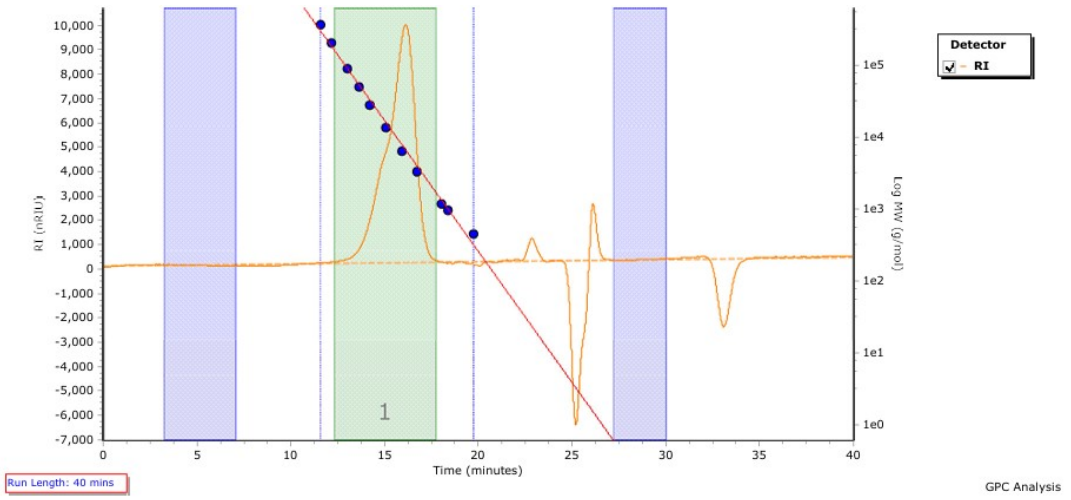


Figure S21 GPC trace of P1 (Table S1, entry 1). M_n= 7442 g/mol, M_w=12078 g/mol and PD=1.623.

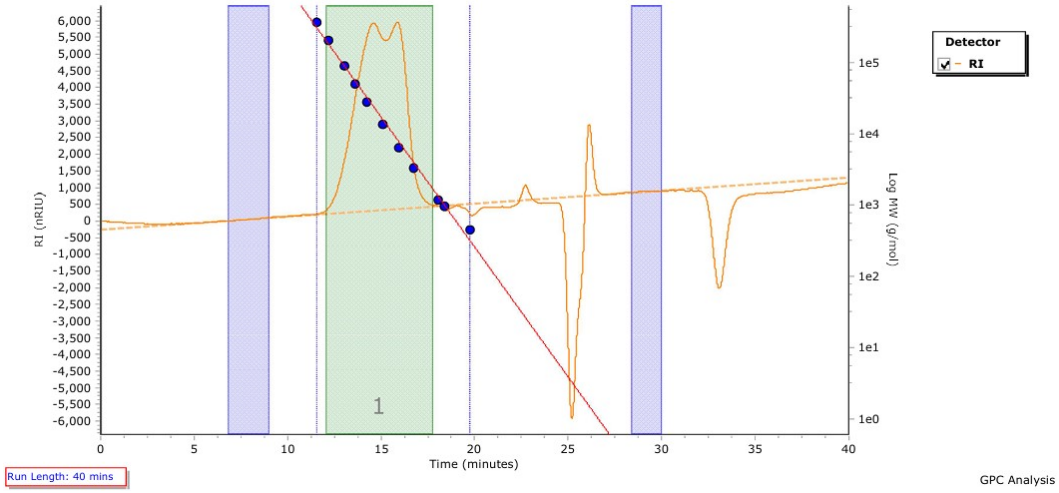


Figure S22 GPC trace of P1 (Table S1, entry 2). M_n= 12369 g/mol, M_w=24086 g/mol and PD=1.947.

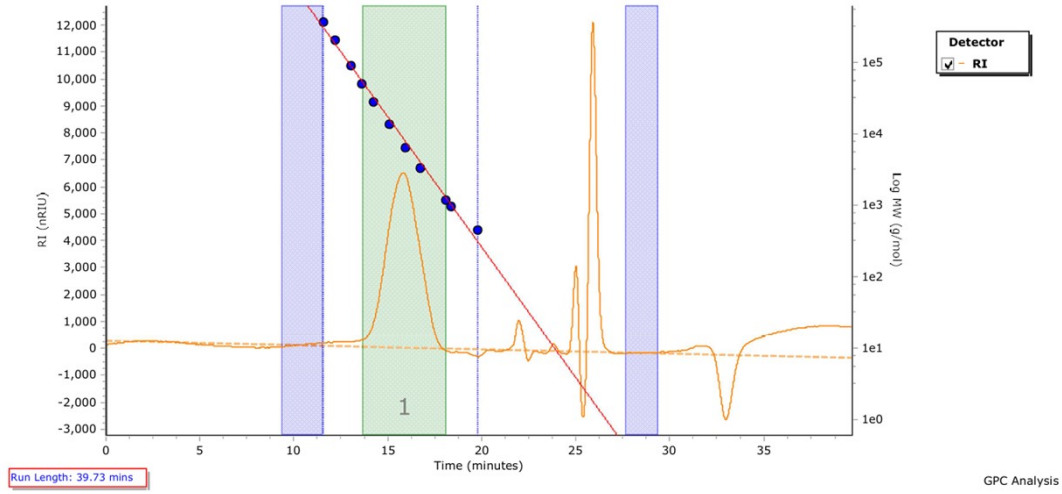


Figure S23 GPC trace of P1 (Table S1, entry 3). M_n= 6970 g/mol, M_w=10428 g/mol and PD=1.496.

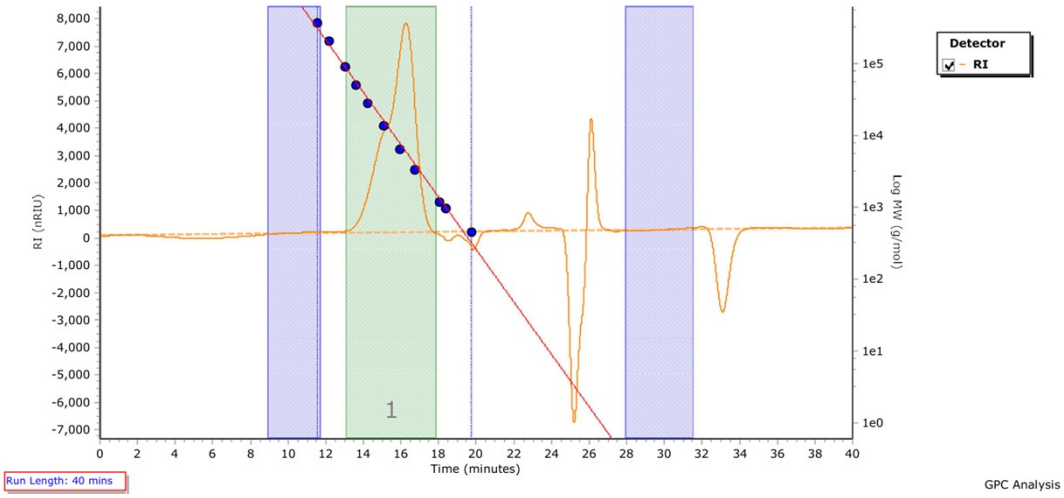


Figure S24 GPC trace of P1 (Table S1, entry 4). M_n= 6882 g/mol, M_w=10801 g/mol and PD=1.569.

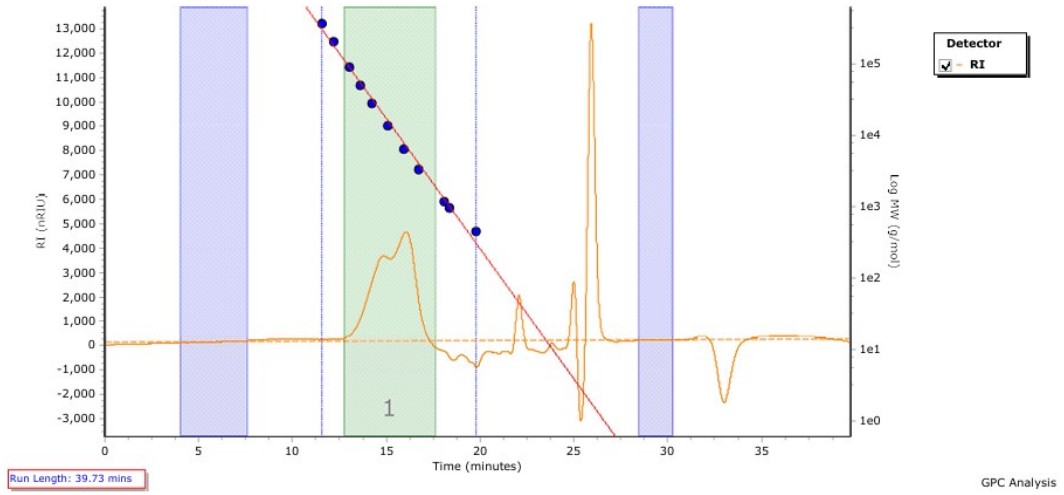


Figure S25 GPC trace of P1 (Table S1, entry 5). M_n= 9689 g/mol, M_w=16875 g/mol and PD=1.742.

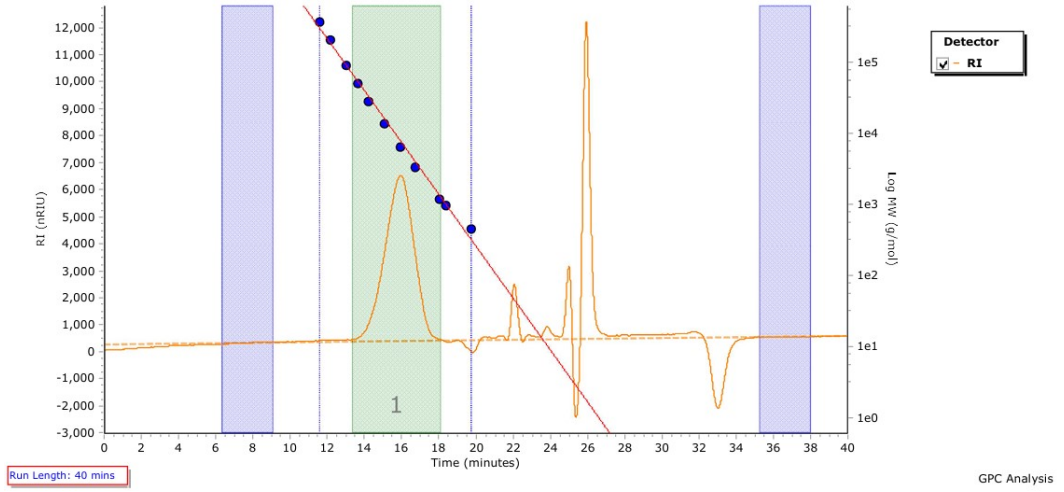


Figure S26 GPC trace of P1 (Table S1, entry 6). M_n= 6786 g/mol, M_w=10024 g/mol and PD=1.477.

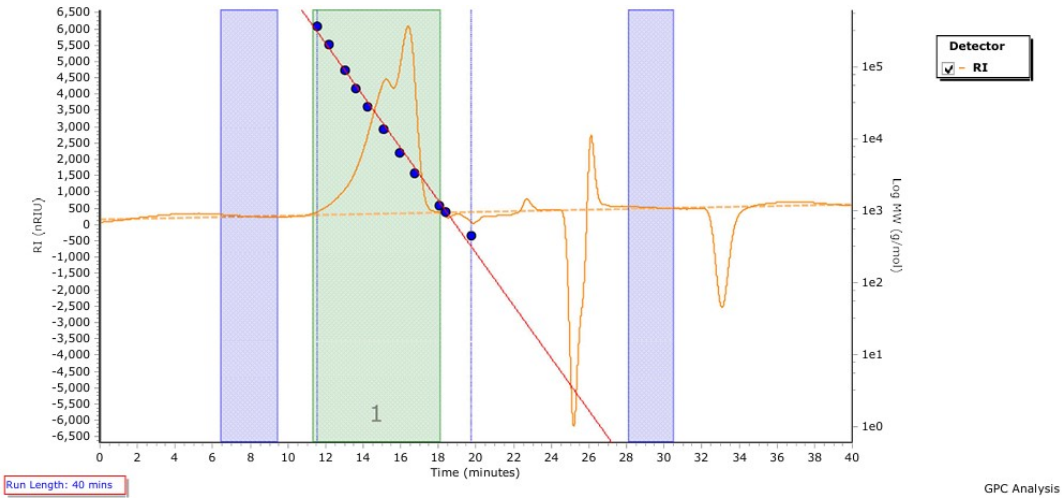


Figure S27 GPC trace of P1 (Table S1, entry 7). M_n= 8529 g/mol, M_w=24809 g/mol and PD=2.909.

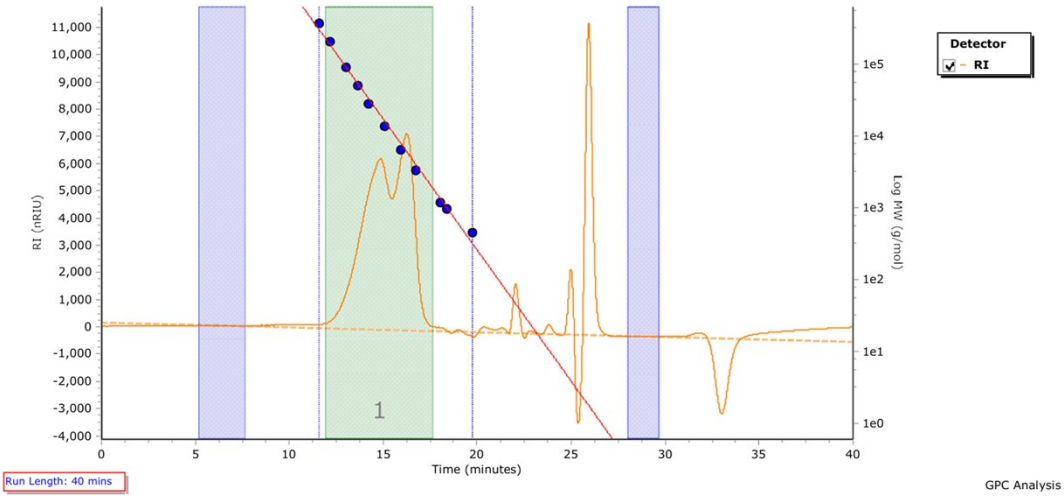


Figure S28 GPC trace of P1 (Table S1, entry 8). M_n= 10104 g/mol, M_w=22953 g/mol and PD=2.272.

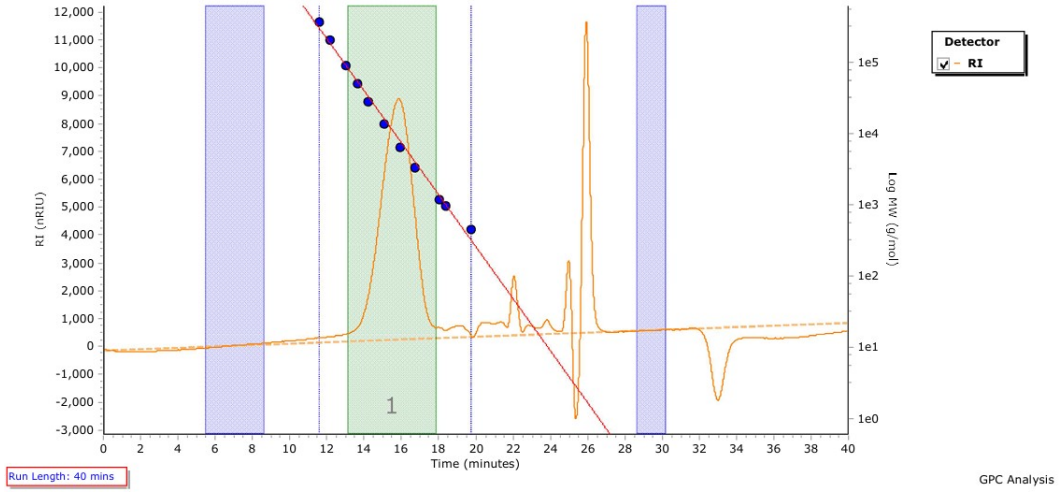


Figure S29 GPC trace of P1 (Table S1, entry 9). M_n= 7233 g/mol, M_w=11634 g/mol and PD=1.608.

9. Calculation

9.1 Calculation methods

All DFT calculations were performed with the Gaussian 09 package[2]. Geometry optimizations and frequency calculations were performed with M06-L functional, employing the Stuttgart/Dresden ECP(SDD) basis set for Pd atom and the 6-31G(d) basis set for other atoms[3, 4]. Thermal energy corrections were obtained at same level of theory. Single point energies were computed using M06-L/ (SDD basis-set for Pd and 6-31G++(d,p) for all other atoms). PCM solvent compensation (DMAc, ε=37.781) was assessed throughout the reaction when DMA as reaction solvent. When DMF as reaction solvent, PCM solvent compensation was assessed using (DMF, ε=37.219). Additionally, when DIFP as reaction solvent, PCM solvent compensation was assessed using (solvent=generic, eps=24.2, epsinf=2.06). All transition were verified to connect reactants and products by intrinsic reaction coordinate (IRC).

The optimized transition states were assessed for Wiberg bond index (WBI) and NPA charge on EDOT using natural bond order (NBO) analysis[5]. These calculations involved a single point task with keyword (pop=NBORead) in the route section, along with keyword ($NBO DMNAO $END) after the molecular geometry section. The geometries of transition state in Table 2 were visualized with CYLview20[6].

9.2 Cartesian coordinates

EDOT (DMF)

M06-L electronic energy (Hartree): -780.905414
M06-L thermal correction to free energy (Hartree): 0.080635
Three lowest frequencies (cm^{-1}): 123.49, 205.89, 312.42

C	-0.01065600	0.71422000	0.04292900
C	-0.01065600	-0.71421900	-0.04293600
C	1.24948800	1.24431900	0.07797700
C	1.24948800	-1.24431600	-0.07801100
S	2.44348300	-0.00000100	0.00001200
O	-1.15857000	1.44692100	0.09562700
C	-2.29709000	0.68103400	-0.32350700
O	-1.15856800	-1.44692100	-0.09562000

C	-2.29709200	-0.68103400	0.32351200
H	1.53271100	2.28709400	0.13514500
H	-3.17478800	1.25911100	-0.02528400
H	-2.28768300	0.58403900	-1.41862300
H	-3.17478700	-1.25911200	0.02528500
H	1.53270800	-2.28709100	-0.13519200
H	-2.28768800	-0.58404000	1.41862700

EDOT (DMA)

M06-L electronic energy (Hartree): -780.905491
M06-L thermal correction to free energy (Hartree): 0.079796
Three lowest frequencies (cm^{-1}): 116.61, 202.45, 311.65

C	0.00896600	0.71275100	-0.04215700
C	0.00896100	-0.71275000	0.04210900
C	-1.25025100	1.24181100	-0.07593800
C	-1.25026200	-1.24179200	0.07599900
S	-2.44153100	-0.00000200	0.00000900
O	1.15660300	1.44440600	-0.09698700
C	2.29874400	0.68170400	0.32061000
O	1.15658300	-1.44440800	0.09696500
C	2.29876300	-0.68170700	-0.32058500
H	-1.53452900	2.28111300	-0.13349700
H	3.17501200	1.25413500	0.01740000
H	2.29420700	0.59264600	1.41376400
H	3.17501200	-1.25413300	-0.01731700
H	-1.53448700	-2.28113500	0.13318100
H	2.29427300	-0.59266400	-1.41373700

EDOT (DIFP)

M06-L electronic energy (Hartree): -780.905260
M06-L thermal correction to free energy (Hartree): 0.080640
Three lowest frequencies (cm^{-1}): 123.57, 205.90, 312.49

C	0.01065400	0.71419400	-0.04292500
C	0.01065400	-0.71419300	0.04293200
C	-1.24946500	1.24428600	-0.07796700
C	-1.24946500	-1.24428300	0.07800100
S	-2.44340800	-0.00000100	-0.00001200
O	1.15862800	1.44691700	-0.09565300
C	2.29692000	0.68106400	0.32353000
O	1.15862600	-1.44691800	0.09564500

C	2.29692100	-0.68106400	-0.32353400
H	-1.53256800	2.28708100	-0.13516400
H	3.17468600	1.25918700	0.02547100
H	2.28746800	0.58390100	1.41866500
H	3.17468600	-1.25918800	-0.02547200
H	-1.53256500	-2.28707800	0.13521100
H	2.28747300	-0.58390200	-1.41866900

$(PCy_3)Pd(Th)(OAc)$

M06-L electronic energy (Hartree): -1956.277882
M06-L thermal correction to free energy (Hartree): 0.530964
Three lowest frequencies (cm^{-1}): 3.23, 26.23, 40.09

Pd	-0.12209600	-1.51866500	-0.49599400
O	-0.55222100	-3.64643000	-0.92354200
O	-2.21802300	-2.23428400	-0.57898600
C	-1.80222700	-3.41200900	-0.82811600
C	-2.78155700	-4.53495000	-0.97861700
C	1.85801800	-1.52106800	-0.52518500
C	2.69450600	-1.60505600	-1.61626600
S	2.79365000	-1.72152900	0.93618200
C	4.06074000	-1.83793900	-1.28221500
C	4.27783200	-1.92249100	0.06477600
H	5.20808600	-2.09851800	0.59289400
H	-2.93862300	-5.01080900	-0.00345200
H	-3.74934700	-4.16901400	-1.33090000
H	-2.39935100	-5.29896000	-1.66072100
C	-1.40743900	-0.21082500	4.46079200
H	-1.25549600	-1.29628100	4.34886400
H	-1.73350400	-0.04779300	5.49629200
C	-2.48581500	0.24343100	3.48403000
H	-3.41812000	-0.31132200	3.65205900
H	-2.71833100	1.30571800	3.66311500
C	-0.08808500	0.50512900	4.19910300
H	-0.20411500	1.57965300	4.41377400
H	0.69329500	0.13564600	4.87574500
C	0.35790100	0.33494100	2.75070800
H	1.31232600	0.85340100	2.58103400
H	0.54447800	-0.73293500	2.54547400
C	-2.03138800	0.07072900	2.03929200
H	-2.82007200	0.39633100	1.34641400
H	-1.86196800	-0.99656000	1.82232400
C	-0.72414600	0.83176900	1.78688000

H	-0.89734200	1.90499400	1.97666500
P	-0.18669900	0.68784300	0.02679200
C	-4.02223100	2.70547800	-1.87664100
H	-4.70986600	2.30351900	-1.11516700
H	-4.63684000	3.29379900	-2.57043500
C	-3.35128100	1.54859200	-2.60599600
H	-4.10187600	0.89375300	-3.06755700
H	-2.73712300	1.94721800	-3.42960500
C	-2.98833800	3.59425300	-1.19663500
H	-2.35533000	4.07055800	-1.96215600
H	-3.47668200	4.40824400	-0.64527800
C	-2.10364700	2.79020700	-0.24849700
H	-1.36423400	3.44683900	0.22823000
H	-2.72710100	2.38575300	0.56368500
C	-2.46172400	0.73720400	-1.67132300
H	-1.96035500	-0.07382600	-2.21695400
H	-3.07706000	0.24393800	-0.90381600
C	-1.42085100	1.63560500	-0.99594300
H	-0.80668300	2.07715700	-1.79876700
C	3.39579200	3.65291400	-0.84390300
H	2.82208800	4.41455500	-1.39594200
H	4.43668500	4.00144300	-0.82849400
C	3.28758500	2.32188500	-1.58063800
H	3.62677900	2.42803400	-2.61945500
H	3.95167100	1.57993400	-1.10799100
C	2.85124000	3.55453700	0.57716000
H	3.49504600	2.88683700	1.17212900
H	2.88270400	4.53536600	1.06934900
C	1.42531600	3.00596700	0.60237300
H	1.06236900	2.94311800	1.63796100
H	0.75790700	3.70505000	0.07451800
C	1.85831500	1.79332100	-1.54573900
H	1.78440700	0.83732000	-2.07980700
H	1.20147100	2.50713500	-2.06768300
C	1.39128900	1.64068200	-0.09477200
H	2.11962800	0.98659800	0.41136900
H	4.85306100	-1.93766900	-2.02069000
H	2.33904700	-1.50092700	-2.63964600

CMD-TS(PCy_3)

M06-L electronic energy (Hartree): -2737.167246
M06-L thermal correction to free energy (Hartree): 0.632168
Three lowest frequencies (cm^{-1}): -437.86, 8.01, 21.12

Pd	0.49464000	-0.50589300	-0.55080300
O	1.81128800	-3.53333600	-0.32327400
O	-0.21243400	-2.59756500	-0.61604200
C	0.51905500	-3.58345600	-0.38893300
C	-0.10220700	-4.92124200	-0.13299600
C	1.23460300	1.35128300	-0.50632100
C	1.63690900	2.14170500	-1.56066900
S	1.64696600	2.15671100	0.98851700
C	2.25149900	3.36881600	-1.17739200
C	2.33320200	3.52654700	0.17887400
H	2.74042200	4.35776400	0.74366400
C	4.74230100	-0.18686300	-0.59631300
C	3.53460400	-0.63557300	0.00603700
C	4.70730400	-0.28011100	-1.96458000
C	2.54018300	-1.06345200	-0.86561300
S	3.18841500	-0.89962600	-2.48744000
O	5.80224900	0.28412300	0.12422300
C	5.38440400	0.68493100	1.43579400
O	3.35671600	-0.64731900	1.35460500
C	4.56599200	-0.40164100	2.08604500
H	5.50696300	-0.04503100	-2.65799300
H	6.29940900	0.87898500	2.00036200
H	4.79809700	1.61464900	1.36415900
H	4.25450200	-0.11344300	3.09323800
H	2.12496700	-2.47098900	-0.54574000
H	-0.27031500	-5.02722100	0.94601200
H	-1.07251500	-4.99441000	-0.62972800
H	0.55247800	-5.73648000	-0.44946500
H	5.14693500	-1.33299200	2.14426600
C	-1.28179700	-1.31210600	4.43762000
H	-0.22874200	-1.61257600	4.31458900
H	-1.55188800	-1.54574000	5.47582900
C	-2.14109000	-2.11331200	3.46586200
H	-2.00428300	-3.19086200	3.62854700
H	-3.20622600	-1.90193400	3.65510700
C	-1.40352500	0.18498300	4.17852800
H	-2.43000700	0.51355900	4.40894100
H	-0.74044700	0.74805400	4.84848600
C	-1.09192400	0.53023500	2.72636900
H	-1.18853200	1.61355700	2.56719200
H	-0.04187600	0.27724500	2.49758300
C	-1.80799300	-1.75811100	2.02168600
H	-2.40596600	-2.35976600	1.32158500

H	-0.75660400	-2.01267400	1.81429900
C	-1.99832500	-0.25698900	1.77498700
H	-3.04486700	0.00254900	2.00630600
P	-1.69824900	0.20962600	0.00542000
C	-5.34362500	-2.21783400	-1.85376800
H	-5.24068600	-3.08741800	-1.18462500
H	-6.19294700	-2.43425200	-2.51516600
C	-4.06189700	-2.05534200	-2.66191600
H	-3.84693500	-2.96875300	-3.23249000
H	-4.20063600	-1.25169400	-3.40362800
C	-5.62297600	-0.97683600	-1.01553400
H	-5.82575900	-0.12307900	-1.68231700
H	-6.52549900	-1.11553500	-0.40567500
C	-4.43894100	-0.63291000	-0.11743300
H	-4.66379100	0.26269200	0.47530700
H	-4.28363300	-1.45028800	0.60472200
C	-2.87824100	-1.71007600	-1.76511600
H	-1.96189000	-1.57955000	-2.35632000
H	-2.67389100	-2.54561600	-1.07957500
C	-3.16466800	-0.44486000	-0.95254400
H	-3.36562800	0.36163100	-1.67903000
C	-2.97763300	4.72191500	-0.65843800
H	-3.89967200	4.52316900	-1.22828200
H	-2.88504900	5.81401500	-0.59157700
C	-1.79191200	4.12966500	-1.41273200
H	-1.74182000	4.53683500	-2.43151800
H	-0.85241700	4.41867900	-0.91369400
C	-3.11705900	4.11537600	0.73350800
H	-2.24861000	4.40392800	1.34814900
H	-4.00468700	4.51637100	1.24062100
C	-3.18849400	2.59119200	0.67421900
H	-3.29361200	2.17718300	1.68728200
H	-4.09016900	2.29250800	0.11547700
C	-1.87151600	2.60703500	-1.45655200
H	-1.00797100	2.18942200	-1.99071500
H	-2.77318700	2.31221800	-2.01789200
C	-1.94525800	2.04378200	-0.03290500
H	-1.06046200	2.42373200	0.50210000
H	2.61999900	4.10733400	-1.88651700
H	1.50324600	1.83984400	-2.59820300

Post-TS(PCy_3)

M06-L electronic energy (Hartree): -2737.171753

M06-L thermal correction to free energy (Hartree): 0.636221
Three lowest frequencies (cm^{-1}): 21.47, 26.09, 30.29

Pd	0.56228100	-0.11406100	-0.72723300
O	2.34470300	-2.98291000	-0.25067700
O	0.33843100	-2.33875000	-1.04102100
C	1.10635900	-3.22046800	-0.64469900
C	0.69280900	-4.64598800	-0.52349200
C	0.79824100	1.85700700	-0.59074300
C	0.71829100	2.79146400	-1.59975800
S	1.19999800	2.66729900	0.90164000
C	0.93906900	4.13417200	-1.17459900
C	1.21020200	4.23544000	0.16124700
H	1.41565600	5.12334200	0.74818100
C	4.93150800	-0.00694800	-0.56727000
C	3.59690800	-0.07864000	-0.05600100
C	4.97219800	0.01144500	-1.93502500
C	2.60135100	-0.14234500	-1.00734100
S	3.36275700	-0.06580600	-2.57157500
O	6.03591700	0.01571400	0.23556200
C	5.70177400	0.28860600	1.60182300
O	3.34017000	-0.12720500	1.29566900
C	4.50158700	-0.51529800	2.03466700
H	5.84639300	0.03565000	-2.57416200
H	6.58701100	0.02679400	2.18660200
H	5.49958100	1.36335200	1.72142100
H	4.26765500	-0.33802600	3.08737400
H	2.52518100	-2.01067300	-0.40197400
H	0.40437100	-4.83627100	0.51805900
H	-0.17048000	-4.84931200	-1.15886100
H	1.51590100	-5.32268700	-0.76426600
H	4.69102900	-1.59017000	1.88724500
C	-0.38397900	-1.59555700	4.22485500
H	0.68620900	-1.57517700	3.96023400
H	-0.44121300	-1.96184800	5.25833500
C	-1.10899200	-2.54437800	3.27754000
H	-0.66354800	-3.54750300	3.31843100
H	-2.15818200	-2.65400300	3.59691800
C	-0.94662600	-0.18212100	4.12776600
H	-1.98498900	-0.17639400	4.49719500
H	-0.38341500	0.50169000	4.77649300
C	-0.92968200	0.33222800	2.69160400
H	-1.33815100	1.35166500	2.64953500
H	0.11231400	0.40384700	2.33604500

C	-1.07447300	-2.01376200	1.85017100
H	-1.56591700	-2.71390500	1.15811200
H	-0.02568600	-1.93686800	1.51531000
C	-1.69890800	-0.61578100	1.76635400
H	-2.73952900	-0.67619800	2.12524400
P	-1.74101600	-0.00930300	0.01237300
C	-4.85031800	-3.21272300	-1.64044000
H	-4.40604400	-4.06236900	-1.09729900
H	-5.69875000	-3.61661300	-2.20847600
C	-3.80695400	-2.62171500	-2.58018200
H	-3.44129400	-3.38408000	-3.28110600
H	-4.27567400	-1.83461800	-3.19293800
C	-5.32966100	-2.17384500	-0.63477800
H	-5.85981900	-1.36795100	-1.16766100
H	-6.05455300	-2.61345300	0.06309400
C	-4.16410100	-1.56867900	0.14321100
H	-4.53580000	-0.81779000	0.85252500
H	-3.68686400	-2.35651800	0.74767700
C	-2.63998000	-2.02401600	-1.80216600
H	-1.89248800	-1.59375900	-2.48250100
H	-2.11941200	-2.82148100	-1.25196200
C	-3.12940600	-0.96294900	-0.81330900
H	-3.64942400	-0.18976500	-1.40455800
C	-4.18090300	4.04503200	-0.16903300
H	-5.08393700	3.63618700	-0.65047200
H	-4.36340400	5.11911500	-0.03113000
C	-2.98449900	3.81942900	-1.08774200
H	-3.16615900	4.26941600	-2.07310200
H	-2.09549400	4.32231100	-0.67330600
C	-3.98878800	3.36095700	1.18060200
H	-3.15618700	3.84200300	1.71972600
H	-4.88113700	3.48982600	1.80739200
C	-3.67075100	1.87756000	1.01426500
H	-3.54053300	1.40687800	1.99907600
H	-4.52693100	1.37497400	0.53478800
C	-2.67596700	2.33325900	-1.23688000
H	-1.80858800	2.18070800	-1.89192000
H	-3.53402800	1.83707900	-1.71896800
C	-2.42626500	1.70546600	0.13931400
H	-1.60231100	2.27420600	0.60146400
H	0.89648500	4.99306300	-1.84122500
H	0.49433500	2.52187300	-2.63053400

$(PPh_3)Pd(Th)(OAc)$

M06-L electronic energy (Hartree): -1945.384368

M06-L thermal correction to free energy (Hartree): 0.319088

Three lowest frequencies (cm^{-1}): 16.48, 24.24, 25.35

Pd	-0.76370700	-1.40674700	-0.10399400
O	-1.84036200	-3.33177300	-0.16681200
O	-2.96707600	-1.44368700	0.05131900
C	-2.94891100	-2.71452500	-0.03452100
C	-4.22373600	-3.49493400	0.04339300
C	1.13727100	-1.93120100	-0.31482300
C	1.77919400	-2.29320900	-1.47810100
S	2.23052600	-2.09185300	1.03313700
C	3.12537800	-2.71423300	-1.28261400
C	3.51954800	-2.66054500	0.02637500
H	4.47498300	-2.93507700	0.45840600
H	-5.09272800	-2.85353100	-0.12022500
H	-4.22110200	-4.31149700	-0.68433900
H	-4.31222200	-3.94874900	1.03720900
C	1.09117400	1.29578900	-1.29424500
C	2.44137400	0.91909800	-1.23206600
C	0.64273700	2.05899700	-2.37831000
C	3.32278100	1.30520600	-2.23512600
H	2.80300600	0.32247300	-0.39448300
C	1.52973300	2.43841500	-3.38350600
H	-0.40018700	2.36537000	-2.43842700
C	2.86865000	2.06286500	-3.31448000
H	4.36806400	1.00843800	-2.17416400
H	1.17005900	3.03431000	-4.21970300
H	3.55994500	2.36132600	-4.09998900
C	0.74846700	1.12508200	1.58132200
C	1.68273600	2.16154800	1.69813800
C	0.37604800	0.40168100	2.72177600
C	2.23977400	2.46209100	2.93848600
H	1.97652100	2.73337600	0.81897800
C	0.93163800	0.70803100	3.95955300
H	-0.34371200	-0.41350000	2.62951600
C	1.86666300	1.73633300	4.06793100
H	2.96796700	3.26613800	3.02090100
H	0.64089000	0.13736100	4.83887100
H	2.30747800	1.97095900	5.03462300
C	-1.49957200	1.82752500	-0.11244100
C	-2.50011700	1.52947200	-1.04826100
C	-1.62309400	2.96949900	0.68821400

C	-3.59866500	2.37094000	-1.19129700
H	-2.41816400	0.62936800	-1.65765600
C	-2.72941100	3.80315700	0.54702700
H	-0.85545900	3.20887800	1.42249100
C	-3.71518100	3.50719500	-0.39208900
H	-4.36889600	2.13400300	-1.92211600
H	-2.81947900	4.68762500	1.17416100
H	-4.57864000	4.16066600	-0.49836100
P	-0.05492600	0.72435000	0.00076500
H	1.30189700	-2.24062300	-2.45452600
H	3.77840800	-3.04453700	-2.08717300

CMD-TS(PPh_3)

M06-L electronic energy (Hartree): -2726.276673

M06-L thermal correction to free energy (Hartree): 0.422378

Three lowest frequencies (cm^{-1}): -492.71, 19.89, 22.70

Pd	-0.41050200	0.58296600	-0.44811600
O	-1.87649200	3.54496700	-0.38134300
O	0.18229000	2.67614400	-0.11945800
C	-0.61363500	3.64324300	-0.13793700
C	-0.11094900	5.02545200	0.14795500
C	-0.93863000	-1.32851900	-0.65415300
C	-1.02445300	-2.11656700	-1.77833500
S	-1.38791500	-2.27176800	0.74365700
C	-1.42800700	-3.45942800	-1.51979100
C	-1.66142800	-3.70412800	-0.19471100
H	-1.98056400	-4.62501300	0.28035500
C	-4.61978200	0.04851500	-0.38518000
C	-3.41202000	0.56855200	0.15462700
C	-4.64145600	0.10433600	-1.75617700
C	-2.48014700	1.03065200	-0.77035600
S	-3.17886800	0.77878500	-2.36050100
O	-5.63417300	-0.43896500	0.38637600
C	-5.17306700	-0.75417700	1.70666100
O	-3.17588500	0.60810300	1.49357000
C	-4.35940200	0.38014500	2.27491800
H	-5.45579000	-0.18967700	-2.40871300
H	-6.06860900	-0.93300800	2.30613400
H	-4.57281900	-1.67523800	1.67214900
H	-4.01193200	0.15005600	3.28473300
H	-2.13296600	2.42401400	-0.55869900
H	0.98019400	5.04714500	0.17412400

H	-0.48165000	5.72837300	-0.60368700
H	-0.49676700	5.36088000	1.11701500
H	-4.95453400	1.30348100	2.30206500
C	2.48324400	-1.49382700	-0.90753100
C	2.00929400	-2.79418000	-0.67888600
C	3.42906800	-1.28406100	-1.91846900
C	2.47603900	-3.85801500	-1.44253400
H	1.26872200	-2.97452100	0.10010400
C	3.89013400	-2.35250500	-2.68458500
H	3.81524000	-0.28356200	-2.10783300
C	3.41553800	-3.64038600	-2.44938600
H	2.09626300	-4.86067600	-1.25308700
H	4.62868100	-2.17521200	-3.46395600
H	3.77693600	-4.47390600	-3.04867500
C	1.85074800	-0.64544300	1.78513400
C	2.80565700	-1.55481600	2.25693400
C	0.92455300	-0.09885400	2.68361600
C	2.83052900	-1.90959000	3.60337000
H	3.52943600	-1.98883100	1.56762500
C	0.95378100	-0.45228200	4.02921000
H	0.16929800	0.59904100	2.31534900
C	1.90558600	-1.36022000	4.48970300
H	3.57479000	-2.61841700	3.96077700
H	0.22639800	-0.02552300	4.71675600
H	1.92476300	-1.64328500	5.54013400
C	3.02499000	1.21805200	-0.09984400
C	2.96535000	2.07317900	-1.20860900
C	4.04237700	1.39283500	0.84430000
C	3.91712200	3.07370100	-1.37787800
H	2.16127700	1.95452500	-1.93538700
C	4.98782200	2.40228600	0.67775000
H	4.09728100	0.74153100	1.71540100
C	4.92818600	3.24142300	-0.43227900
H	3.86338300	3.73019500	-2.24411400
H	5.77335400	2.53184300	1.41961700
H	5.66756600	4.02961300	-0.56003100
P	1.77673400	-0.10635800	0.04552900
H	-0.78757600	-1.74435500	-2.77367200
H	-1.53796100	-4.21706000	-2.29297200

Post-TS (PPh_3)

M06-L electronic energy (Hartree): -2726.284213

M06-L thermal correction to free energy (Hartree): 0.419511

Three lowest frequencies (cm^{-1}): 2.81, 16.94, 21.30

Pd	0.53250100	0.24247700	-0.02965100
O	2.28191800	-1.96945300	-1.62287900
O	0.90583600	-1.95334500	0.15844800
C	1.57383900	-2.56728000	-0.67826300
C	1.65987700	-4.05164500	-0.70522400
C	0.06375400	2.16261000	-0.17631400
C	-0.29592500	2.90947200	-1.27421600
S	0.04791700	3.16950900	1.24288200
C	-0.58121800	4.27369700	-0.97452600
C	-0.44235700	4.57433100	0.35208000
H	-0.60196300	5.52155200	0.85429700
C	4.90653300	0.71457500	-0.02120300
C	3.65264600	0.09523800	0.27499600
C	4.76529900	1.87378400	-0.73409300
C	2.53460200	0.74685100	-0.21046000
S	3.09136400	2.19132500	-1.02012100
O	6.11145800	0.18820900	0.35279900
C	5.97349200	-0.86039600	1.31748200
O	3.59166900	-1.08122400	0.98812600
C	4.83740600	-1.78146400	0.95225800
H	5.54877700	2.53131700	-1.09086000
H	6.92927800	-1.39067300	1.32591800
H	5.79997800	-0.42373600	2.31214200
H	4.74730200	-2.60182600	1.66887300
H	2.26299400	-0.99038700	-1.44198400
H	0.79739300	-4.48943000	-0.19978200
H	1.72954100	-4.42132700	-1.73116100
H	2.56855400	-4.36651200	-0.17839500
H	4.99406200	-2.20213900	-0.05390900
C	-2.98949600	0.81357000	-0.56716000
C	-3.32763100	1.91692900	0.22886900
C	-3.51420100	0.71798300	-1.85994500
C	-4.17995400	2.90082000	-0.25911900
H	-2.91514600	2.00877900	1.23366600
C	-4.36313700	1.70962200	-2.34776600
H	-3.26327800	-0.13398900	-2.49046400
C	-4.69619800	2.80204100	-1.55084700
H	-4.43396800	3.75286000	0.36883000
H	-4.76846600	1.62274600	-3.35401600
H	-5.35915300	3.57518500	-1.93417800
C	-2.32376800	-0.76287500	1.74599900
C	-3.68429300	-0.84785400	2.07336700

C	-1.36366700	-0.99919600	2.73804700
C	-4.07360900	-1.17167800	3.36943100
H	-4.43894000	-0.65419400	1.31115800
C	-1.75670500	-1.32416900	4.03409400
H	-0.30440900	-0.92056700	2.48792500
C	-3.11082000	-1.41070800	4.34975500
H	-5.13155000	-1.23551900	3.61559100
H	-1.00394100	-1.50263100	4.79911300
H	-3.41836000	-1.65971600	5.36342200
C	-1.99139800	-1.88873400	-0.92233600
C	-1.33388300	-1.96559300	-2.15949900
C	-2.73778800	-2.98432700	-0.47847500
C	-1.43409100	-3.11003700	-2.94378900
H	-0.72682300	-1.12270100	-2.49843900
C	-2.82978900	-4.13342300	-1.26237800
H	-3.24294500	-2.94674500	0.48565200
C	-2.18099600	-4.19843300	-2.49311500
H	-0.91812300	-3.15695600	-3.90079900
H	-3.40962800	-4.98234100	-0.90559300
H	-2.25126200	-5.09918900	-3.09946000
P	-1.75563100	-0.36854700	0.06212200
H	-0.36121300	2.48837200	-2.27638600
H	-0.88395500	5.00493700	-1.72104800

(P(*o*- anysil)$_3$)Pd(Th)(OAc)

M06-L electronic energy (Hartree): -2289.016748

M06-L thermal correction to free energy (Hartree): 0.416196

Three lowest frequencies (cm^{-1}): 31.05, 36.53, 45.33

C	0.84958400	0.60021000	1.83802100
C	0.49673400	-0.48833100	2.66632100
C	1.91480100	1.41760400	2.22170900
C	1.22154400	-0.75734100	3.82790400
C	2.63754700	1.15556400	3.38262000
H	2.18832000	2.26421900	1.59452300
C	2.29129600	0.06382500	4.17425500
H	0.95607000	-1.59875900	4.46179100
H	3.46754500	1.79942400	3.66335000
H	2.85408200	-0.15436700	5.07987800
C	-1.70646400	1.37398400	0.72614400
C	-2.06497800	1.64195500	2.04937600
C	-2.69400500	1.46261800	-0.27803300
C	-3.37248200	1.98406900	2.38289000

H	-1.30862300	1.57263600	2.82972800
C	-4.00896900	1.79187000	0.05443300
C	-4.33840200	2.05144100	1.38228200
H	-3.63342600	2.19232800	3.41766300
H	-4.77232400	1.85350800	-0.71628700
H	-5.36563200	2.31072000	1.63134600
C	0.70924100	2.21625800	-0.59921100
C	2.04237000	2.14909000	-1.06177000
C	-0.03097200	3.37216400	-0.87043000
C	2.59166800	3.20513900	-1.79433700
C	0.51563700	4.42798400	-1.59368100
H	-1.05249800	3.44840700	-0.50585200
C	1.82355500	4.33475500	-2.05933400
H	3.61629300	3.15153400	-2.15061100
H	-0.08027700	5.31550100	-1.79184300
H	2.26159400	5.15128500	-2.63026400
P	-0.04051400	0.79892700	0.26646100
O	-2.26769800	1.23638700	-1.54502100
O	2.72014600	1.03254200	-0.72548300
O	-0.57052200	-1.21669200	2.25622600
C	-0.87216900	-2.41790000	2.95039000
H	-1.19177600	-2.21172700	3.97921600
H	-1.69234800	-2.87790800	2.39625500
H	-0.00801900	-3.09404500	2.96235300
C	-3.25461900	0.98736700	-2.53627400
H	-2.70746000	0.66410700	-3.42323000
H	-3.93370300	0.19124100	-2.20833400
H	-3.82331200	1.89641800	-2.76914700
C	4.04072500	0.87605900	-1.22054400
H	4.05671800	0.90761000	-2.31744800
H	4.70576200	1.65285700	-0.82120100
H	4.36488000	-0.10934800	-0.88162000
Pd	-0.45026500	-1.19447300	-0.74365500
O	-1.41557400	-3.03641900	-1.49956400
O	-2.65537900	-1.47574500	-0.54548900
C	-2.55131600	-2.61784900	-1.09395900
C	-3.76108400	-3.48999100	-1.23550700
C	1.44468700	-1.64113000	-1.07601900
C	2.07116100	-1.87196800	-2.28035400
S	2.47351500	-2.17062700	0.22879000
C	3.35088300	-2.48817500	-2.15355000
C	3.71178300	-2.71998100	-0.85475800
H	4.62004500	-3.17225500	-0.47258200
H	-4.63895800	-2.89375400	-1.50135100

H	-3.60435600	-4.27414600	-1.98020500
H	-3.97450100	-3.97050000	-0.27314600
H	3.98190700	-2.74670000	-3.00137100
H	1.62333000	-1.61271400	-3.23790100

CMD-TS(P(*o*- anysil)$_3$)

M06-L electronic energy (Hartree): -3069.909243
M06-L thermal correction to free energy (Hartree): 0.517651
Three lowest frequencies (cm^{-1}): -623.25, 26.56, 32.92

C	1.95564100	-1.23572200	1.51989700
C	1.23409400	-0.85065000	2.66962800
C	2.73499900	-2.39229600	1.57790200
C	1.27674300	-1.62750200	3.82840200
C	2.78809100	-3.16819600	2.73323900
H	3.30086000	-2.69550000	0.69860200
C	2.05228300	-2.78434400	3.85091000
H	0.71085500	-1.33512500	4.70872200
H	3.39803100	-4.06819100	2.75655700
H	2.07995000	-3.38600100	4.75744900
C	2.77372900	1.22442400	0.28585000
C	3.44837400	1.46372700	1.48315100
C	2.79231500	2.22170000	-0.71064800
C	4.12525900	2.66301200	1.70104700
H	3.44117800	0.70125200	2.26081800
C	3.46460000	3.42507200	-0.49872200
C	4.12648100	3.63821700	0.70893000
H	4.64586200	2.83049100	2.64125900
H	3.47092400	4.19606200	-1.26477700
H	4.64709500	4.58098900	0.86851900
C	2.68649600	-1.17167200	-1.27675600
C	2.21311000	-2.41951300	-1.73579600
C	3.85951400	-0.66398100	-1.84187400
C	2.88135900	-3.10545700	-2.75371500
C	4.53521100	-1.34649500	-2.85051300
H	4.25556800	0.28425700	-1.48688700
C	4.03656400	-2.56152300	-3.30869400
H	2.50804800	-4.06255900	-3.10699800
H	5.44574300	-0.92746600	-3.27253900
H	4.55058600	-3.10230100	-4.10116600
P	1.74245900	-0.25444200	-0.00163000
O	2.13812000	1.90880300	-1.85753900
O	1.11318000	-2.88516200	-1.10571200

O	0.52169700	0.30181300	2.55806500
C	-0.45517800	0.57743300	3.55229200
H	0.01103400	0.80623800	4.51880500
H	-1.00218100	1.45206400	3.19372600
H	-1.14633700	-0.26891200	3.66490500
C	1.83162500	2.97116700	-2.74587800
H	1.19086700	2.54069200	-3.51738100
H	1.29359700	3.76971000	-2.21884900
H	2.73768700	3.37774400	-3.21318700
C	0.55542200	-4.11242700	-1.54492400
H	0.26567800	-4.06036700	-2.60264000
H	1.26236000	-4.94051300	-1.40143200
H	-0.33432700	-4.26536500	-0.93008600
Pd	-0.53506600	0.49601800	-0.25807200
O	-1.72081900	3.22080300	1.05632500
O	0.16030700	2.58672500	0.00588700
C	-0.47274700	3.36598700	0.75221600
C	0.24411300	4.52303800	1.37716400
C	-1.37667900	-1.30884000	-0.34309200
C	-2.23063600	-1.84016700	-1.28433800
S	-1.35936800	-2.34690700	1.05772900
C	-2.85409900	-3.05904200	-0.88851900
C	-2.49662400	-3.46060300	0.37087700
H	-2.79606300	-4.35217500	0.91055900
C	-4.74432800	0.64608600	-1.05212300
C	-3.69481700	0.65226700	-0.09157400
C	-4.38344700	1.25634500	-2.22629000
C	-2.50846800	1.25876900	-0.49199500
S	-2.75873000	1.81929200	-2.14350300
O	-5.96017800	0.07324700	-0.81718900
C	-5.87611500	-0.87094600	0.25957900
O	-3.83872200	0.10758400	1.14054700
C	-5.19341600	-0.25243400	1.45152800
H	-5.00149200	1.40109000	-3.10535100
H	-6.90394000	-1.15340500	0.49725900
H	-5.32125600	-1.76008300	-0.07713200
H	-5.13043000	-0.95942000	2.28268500
H	-2.10132400	2.31792000	0.41074900
H	1.03824500	4.88017700	0.71574800
H	-0.43804800	5.33569300	1.63634500
H	0.72405000	4.17193200	2.30011700
H	-5.73591800	0.64380400	1.78275500
H	-3.54457800	-3.61833800	-1.51770600
H	-2.44212800	-1.33588100	-2.22731200

Post-TS(P(*o*- anysil)$_3$)

M06-L electronic energy (Hartree): -3069.915179

M06-L thermal correction to free energy (Hartree): 0.521207

Three lowest frequencies (cm^{-1}): 20.58, 26.66, 28.96

C	2.16780000	-1.04834700	1.51426100
C	1.44931500	-0.73169900	2.68712600
C	3.06429100	-2.11800800	1.55176000
C	1.61671000	-1.48801700	3.84813600
C	3.23884000	-2.87440200	2.70807900
H	3.62838500	-2.36902100	0.65465800
C	2.50885100	-2.55785300	3.84959500
H	1.06016400	-1.24769900	4.74952700
H	3.93840700	-3.70720600	2.71342800
H	2.63197900	-3.14349700	4.75877900
C	2.62467200	1.48965000	0.23768700
C	3.34428600	1.81493400	1.38719800
C	2.45472000	2.47621500	-0.75477500
C	3.88493000	3.08875400	1.56157700
H	3.47910500	1.06071900	2.16144200
C	2.98763200	3.75386500	-0.58562200
C	3.70026300	4.05182600	0.57460500
H	4.44449100	3.32380300	2.46410500
H	2.84905700	4.51461300	-1.34917600
H	4.11434500	5.05066400	0.70058100
C	2.81004800	-0.90014300	-1.30998500
C	2.49515200	-2.20263100	-1.75369700
C	3.87457500	-0.23678100	-1.92833200
C	3.21106100	-2.79595200	-2.79666200
C	4.59448100	-0.82366300	-2.96645900
H	4.14800600	0.76025100	-1.59052200
C	4.25398900	-2.09990300	-3.40124400
H	2.96070100	-3.79781300	-3.13365300
H	5.41575400	-0.28214200	-3.43012100
H	4.80462000	-2.56902000	-4.21453400
P	1.78650200	-0.11525800	-0.00579800
O	1.76815300	2.07908000	-1.85637800
O	1.49245800	-2.81590900	-1.08789100
O	0.61626000	0.34012000	2.59874300
C	-0.29554100	0.55867100	3.66547100
H	0.22821100	0.85243300	4.58381200
H	-0.94668000	1.37246900	3.34047000

H	-0.89830900	-0.33838500	3.85644200
C	1.29780400	3.08742100	-2.73542100
H	0.65352500	2.57881500	-3.45483900
H	0.71690500	3.84041500	-2.18699600
H	2.12558900	3.57427800	-3.26687900
C	1.09465500	-4.10480800	-1.52371700
H	0.76811500	-4.08482800	-2.57180300
H	1.91218000	-4.82933400	-1.41098400
H	0.25333900	-4.38236700	-0.88654300
Pd	-0.61120000	0.31933400	-0.27877800
O	-2.01362200	2.83037400	1.35036500
O	-0.17040200	2.50613100	0.09815000
C	-0.80558600	3.16327700	0.92798400
C	-0.24086100	4.38483800	1.56612300
C	-1.21734000	-1.57203600	-0.38079600
C	-1.97730100	-2.22217300	-1.32764100
S	-1.04956600	-2.60406400	1.01866500
C	-2.40663700	-3.52458700	-0.94332100
C	-1.99705900	-3.87536700	0.31500400
H	-2.16215800	-4.80510400	0.84845800
C	-4.92592700	0.61997200	-0.94983600
C	-3.78204600	0.26879800	-0.16767700
C	-4.61783500	1.41009600	-2.02412900
C	-2.58223800	0.77722500	-0.61953700
S	-2.91455100	1.71044000	-2.06227800
O	-6.19071300	0.20246000	-0.64195300
C	-6.16455300	-0.92053000	0.24624500
O	-3.88480700	-0.51797000	0.94831600
C	-5.23300700	-0.65929000	1.40165400
H	-5.29889800	1.83842300	-2.74958400
H	-7.19279200	-1.06220900	0.58765800
H	-5.84201300	-1.81718500	-0.30550200
H	-5.22905500	-1.49827600	2.10269800
H	-2.29663900	2.02394600	0.81701300
H	0.40849800	4.90833100	0.86079500
H	-1.02195200	5.04951600	1.94007900
H	0.38080300	4.07418000	2.41563500
H	-5.54194500	0.25092400	1.93766400
H	-2.99976600	-4.17876600	-1.57961300
H	-2.25590900	-1.75385200	-2.27064900

(DMF)Pd(Th)(OAc)

M06-L electronic energy (Hartree): -1157.520727

M06-L thermal correction to free energy (Hartree): 0.164327
Three lowest frequencies (cm^{-1}): 18.65, 40.83, 46.28

Pd	-0.81655700	-0.21661800	-0.29379700
O	0.67907800	-1.43461700	-1.14339600
O	-2.53568700	0.73373800	0.38494300
O	-2.75470600	-1.36866000	-0.23706100
C	1.75833400	-1.93309200	-0.75182300
C	-3.27735500	-0.30469200	0.20240300
C	-4.73917600	-0.20534500	0.48612500
N	2.28619700	-1.94755600	0.46857900
C	0.41543200	1.29257400	-0.07907100
C	0.16798100	2.42876900	0.65776500
S	2.01428200	1.37810700	-0.78145900
C	1.25007300	3.35408300	0.65859200
C	2.32262500	2.92742600	-0.07507100
H	3.26676900	3.43039000	-0.25099100
H	-5.27048800	0.04903500	-0.43843200
H	-5.12906000	-1.16389100	0.83835600
H	-4.94795800	0.57745100	1.21939200
H	-0.77071000	2.59106600	1.18236800
H	1.23103400	4.30522400	1.18593300
C	3.61939400	-2.48987700	0.67339600
H	4.29845900	-1.69382200	0.99954100
H	3.58978400	-3.26760800	1.44303200
H	3.99599300	-2.91899200	-0.25744200
C	1.66122800	-1.35751900	1.63794700
H	2.10904200	-0.38087600	1.86004200
H	0.58952400	-1.22142100	1.46919800
H	1.81361100	-2.02661500	2.49009700
H	2.37306200	-2.44997300	-1.50058900

CMD-TS(DMF)

M06-L electronic energy (Hartree): -1938.425698
M06-L thermal correction to free energy (Hartree): 0.261918
Three lowest frequencies (cm^{-1}): -1321.46, 11.77, 24.83

Pd	0.71955100	-0.00496300	-0.21334100
O	2.47537400	1.09800200	-0.93224700
O	0.15223400	-3.15332300	-0.75768900
O	1.93631900	-1.79625900	-0.56014000
C	3.67225400	1.13440800	-0.59554000
C	1.40852800	-2.91110800	-0.81577300

C	2.28725400	-4.05416500	-1.23819900
N	4.22529100	0.74533300	0.55659200
C	-0.31441800	1.66065000	0.07501600
C	-1.29822500	2.01738200	0.97253300
S	-0.04441100	2.99635200	-1.02578500
C	-1.80860000	3.33426200	0.79403800
C	-1.23451300	3.99218700	-0.25949400
H	-1.42092900	5.00113200	-0.61036400
C	-3.28262100	-0.88986400	0.82817100
C	-2.24443700	-0.76040700	-0.13081800
C	-2.80983100	-1.25784200	2.06355500
C	-0.95210300	-1.04752600	0.33494300
S	-1.10160600	-1.42802900	2.06014500
O	-4.59237200	-0.65777200	0.54072400
C	-4.72236500	0.12485200	-0.65546300
O	-2.48248100	-0.41657400	-1.41105400
C	-3.88114700	-0.45686900	-1.76028900
H	-3.40104000	-1.45122500	2.95172800
H	-5.78220900	0.10767100	-0.91648000
H	-4.41718800	1.16034700	-0.44483100
H	-3.97228100	0.12194000	-2.68115000
H	-0.42713900	-2.12115500	-0.27789100
H	2.13553600	-4.25111000	-2.30537100
H	3.34141900	-3.82549000	-1.07051300
H	2.01203300	-4.96679400	-0.70190900
H	-4.16386600	-1.49867300	-1.95788400
H	-1.65726300	1.33808900	1.74517400
H	-2.57443700	3.77769400	1.42713200
C	5.66149500	0.83397800	0.74592700
H	5.88969900	1.46844600	1.60947400
H	6.07968000	-0.16329500	0.92321700
H	6.12886000	1.26163500	-0.14428300
C	3.47286800	0.21226500	1.67459200
H	3.68662600	0.80355200	2.57171700
H	2.39894500	0.25470900	1.46061900
H	3.75872000	-0.82958900	1.85865400
H	4.40732200	1.54411800	-1.30518600

Post-TS(DMF)

M06-L electronic energy (Hartree): -1938.437703

M06-L thermal correction to free energy (Hartree): 0.264748

Three lowest frequencies (cm^{-1}): 14.84, 22.29, 26.01

Pd	0.57228700	-0.14623900	-0.19783500
O	2.51719800	-0.16350900	-1.24564700
O	-1.25022600	-3.05442600	-0.10876600
O	0.88611800	-2.35639400	-0.25087500
C	3.69931600	-0.43198900	-0.97038600
C	0.04669300	-3.26304900	-0.24842200
C	0.40773900	-4.69913800	-0.40342800
N	4.25980000	-0.55101800	0.23656300
C	0.48634600	1.83453300	-0.10438500
C	-0.47020600	2.75143500	0.28280100
S	1.95146800	2.70690200	-0.53494900
C	-0.04412900	4.10801700	0.23093800
C	1.24928000	4.24806300	-0.19041700
H	1.82206500	5.15898700	-0.32577300
C	-3.61829900	0.05131700	0.71859400
C	-2.46428700	-0.00919100	-0.12478000
C	-3.31019500	-0.03567500	2.04885300
C	-1.26833800	-0.17176100	0.54221700
S	-1.59868600	-0.19719700	2.25560300
O	-4.88719000	0.15991000	0.22949100
C	-4.90082200	0.57993800	-1.14103800
O	-2.55787200	0.08990900	-1.48859900
C	-3.88616900	-0.18840600	-1.94862000
H	-3.99302900	-0.05947000	2.88922600
H	-5.91596600	0.39761700	-1.50132300
H	-4.69101700	1.65820000	-1.19363700
H	-3.91151800	0.10744200	-2.99963600
H	-1.39294800	-2.07769200	0.03797200
H	0.10228300	-5.25732900	0.48744100
H	-0.13444100	-5.13094500	-1.25050100
H	1.48117400	-4.81103800	-0.55592400
H	-4.07870200	-1.26938400	-1.87550900
H	-1.46558900	2.45397800	0.60552400
H	-0.67783600	4.95085100	0.49866000
C	5.66987500	-0.86932800	0.36397000
H	6.19046500	-0.06823700	0.90047900
H	5.79521900	-1.80425500	0.92145600
H	6.11686200	-0.98332500	-0.62636500
C	3.53930300	-0.35877200	1.47886500
H	3.97375700	0.48130000	2.03282500
H	2.48471900	-0.14404400	1.27349700
H	3.61050100	-1.26288200	2.09391000
H	4.41481400	-0.59076800	-1.79177200

(DMA)Pd(Th)(OAc)

M06-L electronic energy (Hartree): -1196.844559
M06-L thermal correction to free energy (Hartree): 0.190973
Three lowest frequencies (cm^{-1}): 21.33, 229.61, 46.42

Pd	-0.61560200	-0.37803900	-0.25059700
O	1.36448400	-0.19427700	-0.97068000
O	-2.58098900	-0.88622000	0.22555200
O	-1.22236600	-2.54799900	-0.27811800
C	2.46379400	-0.64013000	-0.53677500
C	-2.37655200	-2.14599200	0.04789300
C	-3.52193800	-3.09094700	0.20127400
C	3.52485200	-0.95160000	-1.54953400
N	2.72917400	-0.82550200	0.76199000
H	4.49672900	-0.53009300	-1.27620300
H	3.21390600	-0.54718200	-2.51341800
H	3.64986200	-2.03485100	-1.66109500
C	-0.74712600	1.56070300	-0.01991100
C	-1.83679200	2.25829800	0.45061800
S	0.55492400	2.66749900	-0.38873900
C	-1.62708500	3.66549600	0.51296800
C	-0.38082600	4.04168500	0.09260800
H	0.03975300	5.03931200	0.03275300
H	-4.28232400	-2.68624300	0.87365500
H	-3.98972800	-3.25379700	-0.77665700
H	-3.17423400	-4.06032400	0.56753900
H	-2.76268200	1.76774900	0.74251100
H	-2.37736300	4.37312800	0.85867200
C	3.95024400	-1.45664700	1.24069500
H	4.63643700	-0.70875500	1.65563400
H	3.69152500	-2.16949900	2.02936100
H	4.45199300	-2.00098400	0.44223100
C	1.80490100	-0.38515200	1.79634700
H	1.32297100	0.55026200	1.50169000
H	1.03259100	-1.14016400	1.99234200
H	2.37538700	-0.21655700	2.71319800

CMD-TS(DMA)

M06-L electronic energy (Hartree): -1977.750601
M06-L thermal correction to free energy (Hartree): 0.289243
Three lowest frequencies (cm^{-1}): -1367.41, 22.60, 30.78

Pd	0.52735300	0.08896100	-0.11846200
O	2.37383800	0.95774700	-0.95180800
O	0.00055000	-3.14138500	-0.00027200
O	1.72709000	-1.73012000	-0.27435400
C	3.49441400	0.46132700	-0.67069900
C	1.23442100	-2.88871100	-0.21911100
C	2.14098400	-4.06353100	-0.45362400
C	4.39775100	0.02969600	-1.78680900
N	3.91684500	0.32785200	0.59901000
H	5.42022600	0.40462800	-1.67997200
H	3.98167600	0.38907200	-2.72890900
H	4.44574100	-1.06533700	-1.83080300
C	-0.38959300	1.84088100	0.03019200
C	-1.60829600	2.26395900	0.52141000
S	0.49709700	3.25014700	-0.53767100
C	-1.82455100	3.66858700	0.44680400
C	-0.77122100	4.34287800	-0.10632600
H	-0.66668000	5.40812700	-0.28129700
C	-3.57751500	-0.82514200	0.58083800
C	-2.40728500	-0.80347000	-0.22107600
C	-3.28713800	-0.85498800	1.92381900
C	-1.19195900	-0.85467000	0.48022800
S	-1.59513300	-0.84819700	2.20455900
O	-4.83555200	-0.81647400	0.06351900
C	-4.83078800	-0.36900500	-1.30014800
O	-2.45512500	-0.78112600	-1.56748100
C	-3.76590200	-1.08292500	-2.08989000
H	-4.00151400	-0.90363300	2.73807500
H	-5.82525900	-0.58669100	-1.69431900
H	-4.66387100	0.71747600	-1.32316000
H	-3.75231900	-0.75578800	-3.13093800
H	-0.60510600	-2.01865200	0.21246900
H	1.83747200	-4.92243900	0.14990800
H	2.07435900	-4.36137900	-1.50647700
H	3.18038700	-3.80064500	-0.24217200
H	-3.91540800	-2.16937800	-2.05352100
H	-2.34240600	1.57801700	0.94039300
H	-2.73185300	4.15910400	0.79383000
C	5.05133000	-0.49405600	0.97955300
H	5.63042100	0.01626500	1.75560700
H	4.70208600	-1.45561700	1.38063600
H	5.70362900	-0.68813200	0.12931500
C	3.06541500	0.75250400	1.69511700
H	2.46873400	1.61511300	1.39057700

H	2.38650200	-0.05569800	2.00488900
H	3.69879600	1.02809500	2.54334200

Post-TS(DMA)

M06-L electronic energy (Hartree): -1977.762781

M06-L thermal correction to free energy (Hartree): 0.292242

Three lowest frequencies (cm^{-1}): 21.18, 22.83, 30.20

Pd	0.49283300	0.17085100	-0.11248800
O	2.47511100	0.64125700	-0.99796000
O	-0.49255200	-3.12782100	-0.03710300
O	1.37690600	-1.88270800	-0.17348500
C	3.49506000	-0.03473400	-0.71242800
C	0.81340600	-2.98237200	-0.16447300
C	1.55301000	-4.26696600	-0.30223000
C	4.26498400	-0.69704400	-1.81589000
N	3.92536300	-0.16979000	0.55543800
H	5.34321700	-0.52149800	-1.75287200
H	3.89610500	-0.31956500	-2.77054200
H	4.10126700	-1.78165400	-1.79204100
C	-0.10235000	2.05694700	-0.03640700
C	-1.27490000	2.69638900	0.31201500
S	1.09477200	3.27695100	-0.45456800
C	-1.21772500	4.11646300	0.24249300
C	0.00422400	4.58438900	-0.15527200
H	0.32174900	5.61173300	-0.29656200
C	-3.65062700	-0.71895300	0.61587500
C	-2.49172200	-0.47113900	-0.18613000
C	-3.37456700	-0.75517800	1.95585700
C	-1.31565800	-0.34351400	0.52190200
S	-1.68534200	-0.48563700	2.22321700
O	-4.89061500	-0.91910900	0.08326300
C	-4.96706800	-0.48368900	-1.28013900
O	-2.56565200	-0.36332600	-1.55040500
C	-3.76709400	-0.95177000	-2.06306100
H	-4.05755000	-0.96961100	2.76871100
H	-5.89116500	-0.90789700	-1.68021500
H	-5.03596000	0.61356300	-1.30892800
H	-3.83389600	-0.64311900	-3.10875800
H	-0.89470000	-2.22090200	0.07909200
H	1.34245600	-4.91523700	0.55385600
H	1.20987200	-4.79793900	-1.19607900
H	2.62585100	-4.08512600	-0.37438700

H	-3.68545800	-2.04809000	-2.01799600
H	-2.16601500	2.15201600	0.61706700
H	-2.05675200	4.76663200	0.48144100
C	4.89358600	-1.16999400	0.96627000
H	5.56960200	-0.74223000	1.71310100
H	4.37941200	-2.03221000	1.41315400
H	5.48566200	-1.51736400	0.12074700
C	3.19908100	0.47442300	1.63505200
H	2.77922100	1.42052300	1.28602200
H	2.37955800	-0.16271700	1.99919600
H	3.89336300	0.66316500	2.45894400

(DIFP)Pd(Th)(OAc)

M06-L electronic energy (Hartree): -1314.801774

M06-L thermal correction to free energy (Hartree): 0.274317

Three lowest frequencies (cm^{-1}): 32.69, 36.78, 45.80

Pd	-1.29355100	-0.37502700	-0.48793600
O	0.44275900	-1.14987000	-1.38022400
O	-3.18785100	0.09647600	0.23834400
O	-2.83148800	-2.01266100	-0.29729100
C	1.66631800	-1.11324900	-1.10416900
C	-3.60850000	-1.11806500	0.14418200
C	-4.99723300	-1.43788400	0.58878800
N	2.27773400	-0.88119700	0.05075000
C	-0.46270000	1.40149400	-0.44127800
C	0.56922400	1.94233400	-1.17640500
S	-1.00000400	2.54518900	0.76137000
C	0.92004200	3.26314100	-0.77439800
C	0.16364200	3.72682100	0.26764300
H	0.20926000	4.69205800	0.75923900
H	-4.96806600	-1.83545300	1.60994200
H	-5.63004200	-0.54733500	0.58914700
H	-5.43503000	-2.20885400	-0.05092200
H	1.06401700	1.41175300	-1.98652100
H	1.70551100	3.84831700	-1.24768700
C	3.76836700	-0.84662600	0.06454800
H	4.03014300	-0.76421600	1.12509400
C	1.56448300	-0.66789500	1.32713700
H	0.49874400	-0.63503400	1.06248600
H	2.35637000	-1.32016700	-1.93363200
C	4.27732400	0.38940700	-0.65905400
H	5.36701600	0.45803800	-0.57284200

H	4.02847800	0.35248500	-1.72743600
H	3.83950000	1.30332600	-0.24156100
C	4.37442400	-2.13816400	-0.46073700
H	5.45616400	-2.12874600	-0.29086800
H	3.95504600	-3.01105600	0.05132400
H	4.21783400	-2.26332500	-1.53857900
C	1.79959000	-1.84885400	2.25604600
H	2.85462100	-1.93805700	2.54516500
H	1.21870500	-1.71568700	3.17508100
H	1.49140800	-2.79011800	1.78782000
C	1.93859200	0.66478200	1.95491900
H	1.76647700	1.49445100	1.25927900
H	1.31813500	0.83099500	2.84231200
H	2.98615600	0.68819600	2.28111400

CMD-TS(DIFP)

M06-L electronic energy (Hartree): -2095.706451

M06-L thermal correction to free energy (Hartree): 0.372886

Three lowest frequencies (cm^{-1}): -1398.21, 21.94, 28.87

Pd	0.11873600	0.04356100	-0.53756700
O	1.91905100	0.72284500	-1.62148700
O	-0.39397400	-3.07582300	0.34482500
O	1.17199900	-1.86651000	-0.72172900
C	3.06576500	0.36001700	-1.28023300
C	0.73112200	-2.94795600	-0.24716800
C	1.59172000	-4.17685400	-0.33744100
N	3.58951700	0.34631500	-0.05548900
C	-0.62863200	1.87489500	-0.44760900
C	0.11868900	3.03389800	-0.54229900
S	-2.31227700	2.30729300	-0.26117900
C	-0.64608700	4.23248500	-0.47975900
C	-1.98677200	4.00429700	-0.33080400
H	-2.79224900	4.72700100	-0.26379400
C	-3.84183300	-0.66918800	0.92677600
C	-2.80213200	-0.81702500	-0.02693100
C	-3.36091200	-0.38801600	2.18186700
C	-1.49590500	-0.69912300	0.47921800
S	-1.64976500	-0.28417100	2.19497100
O	-5.16015200	-0.79826400	0.61739100
C	-5.37533100	-0.69151100	-0.79763000
O	-3.04220400	-1.11125800	-1.31955100
C	-4.39687200	-1.55166200	-1.55319100

H	-3.94881100	-0.24875300	3.08237000
H	-6.40173100	-1.01955300	-0.97340000
H	-5.27703100	0.36057300	-1.09995500
H	-4.54955900	-1.47871900	-2.63130400
H	-0.95184900	-1.89959500	0.41031100
H	2.17431400	-4.26770400	0.58750400
H	0.98148000	-5.07845600	-0.43106300
H	2.29343000	-4.10596400	-1.17186000
H	-4.48010800	-2.60152300	-1.24547500
H	1.19940300	3.01773300	-0.67062100
H	-0.21393200	5.22874000	-0.54777600
C	4.94611100	-0.22616000	0.14623100
H	5.14777600	-0.08983100	1.21514900
C	2.85625600	0.86095500	1.11857300
H	1.89212900	1.20923400	0.72676100
H	3.76573600	0.02442800	-2.06140700
C	6.00368200	0.54159600	-0.63099400
H	6.99992500	0.17147100	-0.36602700
H	5.88663800	0.41663100	-1.71399500
H	5.96320600	1.61232600	-0.40408600
C	4.95290900	-1.71683100	-0.15441300
H	5.93179600	-2.14728800	0.08354300
H	4.19123200	-2.24191100	0.43272500
H	4.75204400	-1.90989100	-1.21584200
C	2.58963900	-0.24167200	2.13043800
H	3.51790300	-0.64150600	2.55837200
H	1.99119600	0.15573600	2.95805700
H	2.03321700	-1.06757700	1.67050100
C	3.58586000	2.05409500	1.71562000
H	3.74946500	2.83429200	0.96377600
H	2.98753400	2.48133000	2.52768700
H	4.55962200	1.77547200	2.13858700

Post-TS(DIFP)

M06-L electronic energy (Hartree): -2095.718674

M06-L thermal correction to free energy (Hartree): 0.374986

Three lowest frequencies (cm^{-1}): 13.07, 26.50, 27.25

Pd	0.08680600	0.14212400	-0.51118700
O	1.96305000	0.58698200	-1.61387900
O	-0.71309200	-3.14881000	0.12216700
O	0.99680700	-1.90085100	-0.64328200
C	3.08223100	0.15840100	-1.26296000

C	0.51153900	-2.99798500	-0.34683100
C	1.27877900	-4.26925800	-0.46047600
N	3.60730300	0.15376400	-0.03791500
C	-0.47906300	2.03624900	-0.44710900
C	0.36928800	3.11251800	-0.62867700
S	-2.09460800	2.63191500	-0.14889300
C	-0.27114800	4.38080400	-0.54250900
C	-1.61242200	4.28619000	-0.29090800
H	-2.33647600	5.08592400	-0.18230000
C	-3.85666800	-0.77887700	0.94905600
C	-2.84626400	-0.62051700	-0.05118100
C	-3.37995800	-0.61236200	2.22070300
C	-1.58468600	-0.35394700	0.43992900
S	-1.68782000	-0.25441000	2.18138200
O	-5.15278500	-1.08115600	0.64847400
C	-5.45187500	-0.83214200	-0.73082700
O	-3.12523700	-0.72718500	-1.38765100
C	-4.37271400	-1.39157100	-1.62204000
H	-3.92279700	-0.71993800	3.15205000
H	-6.41352600	-1.31415200	-0.92234800
H	-5.55569700	0.25112200	-0.89215800
H	-4.60774900	-1.23038400	-2.67662300
H	-1.12344600	-2.24145400	0.21236400
H	1.71176500	-4.50974700	0.51779900
H	0.62744100	-5.09904200	-0.74416500
H	2.09354200	-4.15918500	-1.17752000
H	-4.25133700	-2.47030200	-1.44309200
H	1.43167800	2.98912300	-0.83043000
H	0.24806600	5.32904800	-0.66585700
C	4.91645800	-0.51108700	0.18698400
H	5.11983900	-0.36745100	1.25478100
C	2.91957400	0.77441400	1.11075800
H	1.99488500	1.19645800	0.69724600
H	3.75505800	-0.25842400	-2.02945200
C	6.03120100	0.16122100	-0.59848200
H	6.99631000	-0.28067000	-0.32844500
H	5.90288200	0.03162800	-1.67972300
H	6.07321100	1.23486500	-0.38597500
C	4.81400100	-2.00435100	-0.08186100
H	5.75320300	-2.50365800	0.18022600
H	4.00553400	-2.45411500	0.50539000
H	4.61320800	-2.20628300	-1.14173800
C	2.54710400	-0.26354600	2.15806600
H	3.43280400	-0.72808800	2.61064500

H	1.97793500	0.21336700	2.96405700
H	1.92445300	-1.05519100	1.72300100
C	3.75139600	1.91591600	1.67439700
H	3.98109600	2.65669500	0.90028500
H	3.19440300	2.41768800	2.47307900
H	4.69779700	1.56578000	2.10624300

10. References

(1) Bhardwaj, D.; Shahjad; Gupta, S.; Yadav, P.; Bhargav, R.; Patra, A. All Conjugated Poly(3-hexylthiophene)-block-poly(hexyl-3,4-ethylenedioxythiophene) Copolymers. *ChemistrySelect* **2017**, *2* (29), 9557-9562.

(2) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. S211 Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision E.01, Gaussian, Inc., Wallingford CT, 2013.

(3) Zhao, Y.; Truhlar, D. G. A New Local Density Functional for Main-Group Thermochemistry, Transition Metal Bonding, Thermochemical Kinetics, and Noncovalent Interactions. *J. Chem. Phys.* **2006**, *125* (19), 194101.

(4) Feller, D. The Role df Databases in Support of Computational Chemistry Calculations. *J. Comput. Chem.* **1996**, *17* (13), 1571-1586.

(5) NBO Version 3.1, E. D. Glendening, A. E. Reed, J. E. Carpenter, and F. Weinhold.

(6) CYLview20; Legault, C. Y., Université de Sherbrooke, 2020 (http://www.cylview.org).