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Electronic Supplementary Information

Solution processable dithioalkylated methylidenyl cyclopentadithiophene based quinoidal small molecules for n-type organic field-effect transistors

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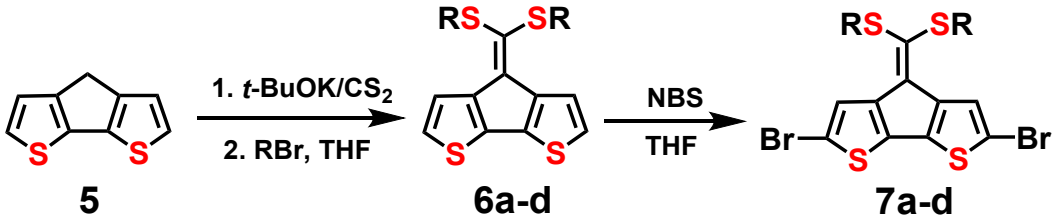
S.1 Materials

All the chemical reagents were purchased from Aldrich, Alfa and TCI Chemical Co. and used as received unless otherwise noted. Solvents for reactions (toluene and THF) were distilled under nitrogen from sodium/benzophenone ketyl, and halogenated solvents were distilled from CaH_2.

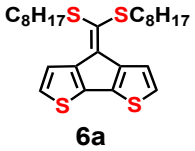
S.2 Synthesis



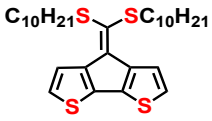
Scheme S1. Synthetic route to central core **7a–7d**.

General procedure for the synthesis of compounds 6a–6d

Under anhydrous condition solution of 4H-cyclopenta[2,1-b:3,4-b']dithiophene (1.5 mmol) in anhydrous THF (15 ml) was added to potassium *tert*-butoxide (3.6 mmol) containing flask using dropping funnel at 0°C and stirred the reaction for 1 hour. Carbon disulfide (1.9 mmol) was added via syringe to the reaction mixture and stirred for 10 min. Next, alkyl bromides (3.2 mmol) was added a via syringe over 5 min and the reaction mixture was stirred overnight under dark. After completion of reaction, it was quenched by aqueous ammonium chloride and THF was removed by rotary evaporator and extracted with water and ether, organic layer was dried over sodium sulphate. Organic layer was concentrated and crude product was purified by column chromatography using hexane as eluent to give desired products **6a–6d**.



Compound 6a. The title compound was obtained as a dark blue solid, 0.66 g (yield = 95%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (d, J = 5.0 Hz, 2H), 7.04 (d, J = 5.1 Hz, 2H), 2.97 (t, J = 7.4 Hz, 4H), 1.68-1.62 (m, 4H), 1.40 (m, 4H), 1.30 (m, 16H), 0.89 (t, J = 5 Hz, 6H).



6b

Compound 6b. The title compound was obtained as a dark blue solid, 1.3 g (yield = 87%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.86 (d, J = 5.0 Hz, 2H), 7.04 (d, J = 5.0 Hz, 2H), 2.97 (t, J = 7.3 Hz, 4H), 1.70-1.60 (m, 4H) 1.40 (m, 4H), 1.30 (m, 24H), 0.88 (t, J = 5 Hz, 6H).

6c

Compound 6c. The title compound was obtained as a dark blue solid, 0.58 g (yield = 88%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (d, J = 5.0 Hz, 2H), 7.04 (d, J = 5.0 Hz, 2H), 2.97 (t, J = 7.4 Hz, 4H), 1.68-1.62 (m, 4H) 1.40 (m, 4H), 1.30 (m, 32H), 0.89 (t, J = 5 Hz, 6H).

6d

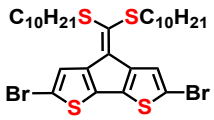
Compound 6d: The title compound was obtained as a dark blue solid, 0.52 g (yield = 84%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, J = 5.0 Hz, 2H), 7.2 (d, J = 5.0 Hz, 2H), 2.98 (t, J = 7.4 Hz, 4H), 1.68-1.62 (m, 4H) 1.40 (m, 4H), 1.30 (m, 40H), 0.88 (t, J = 5 Hz, 6H).

General procedure for the synthesis of compounds 7a–7d

To the stirred solution of compound **6a–6d** (0.4 mmol mmol) in THF (15 ml) was added NBS (0.9 mmol mmol) portion wise at 0°C and stirred the reaction for overnight. After completion of reaction, it was quenched by deionized water and THF was removed by rotary evaporator and extracted with ether, organic layer was dried over sodium sulphate. Organic layer was concentrated and crude product was purified by column chromatography using hexane as eluent to give desired products **7a–7d**.

7a

Compound 7a. The title compound was obtained as a dark blue solid, 0.24 g (yield = 91%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.88 (s, 2H), 2.97 (t, J = 7.3 Hz, 4H), 1.69-1.62 (m, 4H), 1.40 (m, 4H), 0.86 1.30 (m, 16H), 0.88 (t, J = 7 Hz, 6H).

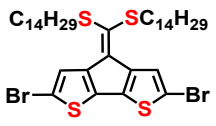


7b

Compound 7b. The title compound was obtained as a dark blue solid, 0.35 g (yield = 90%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.87 (s, 2H), 2.97 (t, J = 7.3 Hz, 4H), 1.69-1.59 (m, 4H), 1.40 (m, 4H), 1.30 (m, 24), 0.89 (t, J = 10 Hz, 6H).

7c

Compound 7c. The title compound was obtained as a dark blue solid, 0.25 g (yield = 89%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.88 (s, 2H), 2.97 (t, J = 7.4 Hz, 4H), 1.68-1.62 (m, 4H), 1.40 (m 4H), 1.30 (m, 32), 0.89 (t, J = 10 Hz, 6H).



7d

Compound 7d: The title compound was obtained as a dark blue solid, 0.22 g (yield = 85%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.88 (s, H), 2.98 (t, J = 7.4 Hz, 4H), 1.68-1.62 (m, 4H), 1.40 (m 4H), 1.30 (m, 40), 0.89 (t, J = 7 Hz, 6H).

S.3 Characterization

^{1}H and ^{13}C NMR were recorded using a Bruker 500 or 300 instrument for all materials, with reference to solvent signals. Elemental analyses were performed on a Heraeus CHN-O-Rapid elemental analyzer. Mass spectrometric data were obtained with a JMS-700 HRMS instrument. Differential scanning calorimetry (DSC) was carried out under a nitrogen atmosphere on a Mettler DSC 822 instrument (scanning rate of 10 °C min^{-1}). Thermogravimetric analysis (TGA) was carried out using a Perkin Elmer TGA-7 thermal analysis system using dry nitrogen as a carrier gas at a flow rate of 10 mL min^{-1} (heating rate of 10 °C min^{-1}), and the reported decomposition temperatures represent the temperature observed at 5 % mass loss. Differential pulse voltammetry experiments were performed with a conventional three-electrode configuration (a platinum disk working electrode, an auxiliary platinum wire electrode, and a non-aqueous Ag reference electrode, with a supporting electrolyte of 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) in the specified dry solvent using a CHI621C Electrochemical Analyzer (CH Instruments). All electrochemical potentials were referenced to an Fc^{+}/Fc internal standard (at 0.6 V). UV-Vis absorption spectra were recorded by using Hitachi U-4100 spectrophotometer. Polarized optical microscopy (POM) images were captured using a Leica 2700M microscope equipped with Nikon digital camera and polarizer. AFM imaging was performed by a Hitachi AFM5000 operating in air, in tapping mode, by using Hitachi SI-DF3PS tips (force-frequency = 70 kHz and force constant = 1.8 N m^{-1}). Grazing-incidence wide-angle X-ray scattering (GIWAXS) analyses were measured at the National Synchrotron Radiation Research Center (NSRRC) of Taiwan on the beamlines 13A1 and 17A1 of Taiwan Light Source (TLS).

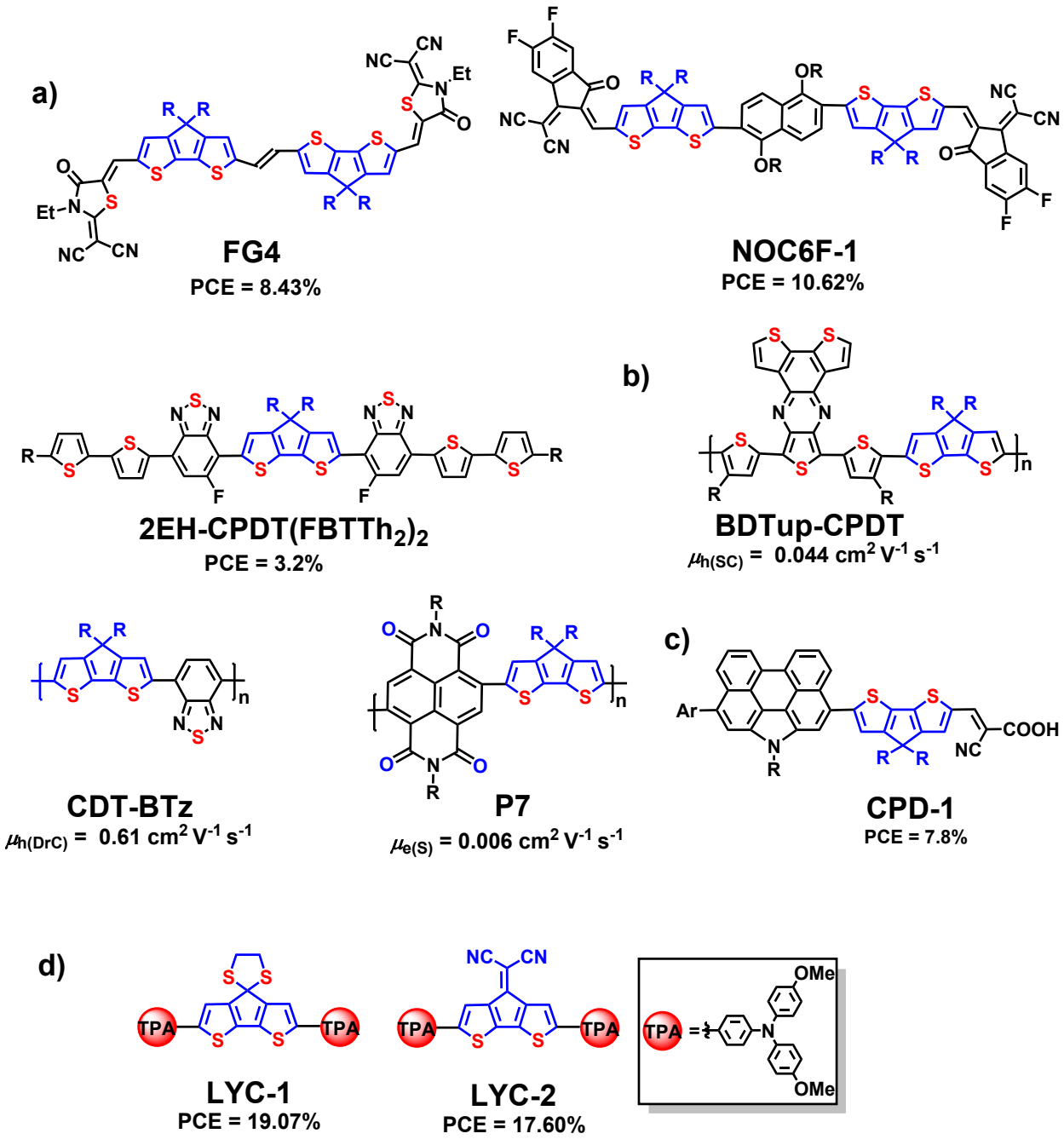


Figure S1. Chemical structures of the reported (a) cyclopentadithiophene (**CDT**)-based organic solar cells; (b) **CDT**-based polymeric organic semiconductors; (c) **CDT**-based dye sensitized solar cells; (d) **CDT**-based small molecular hole transporting materials (HTMs) for perovskite solar cells.

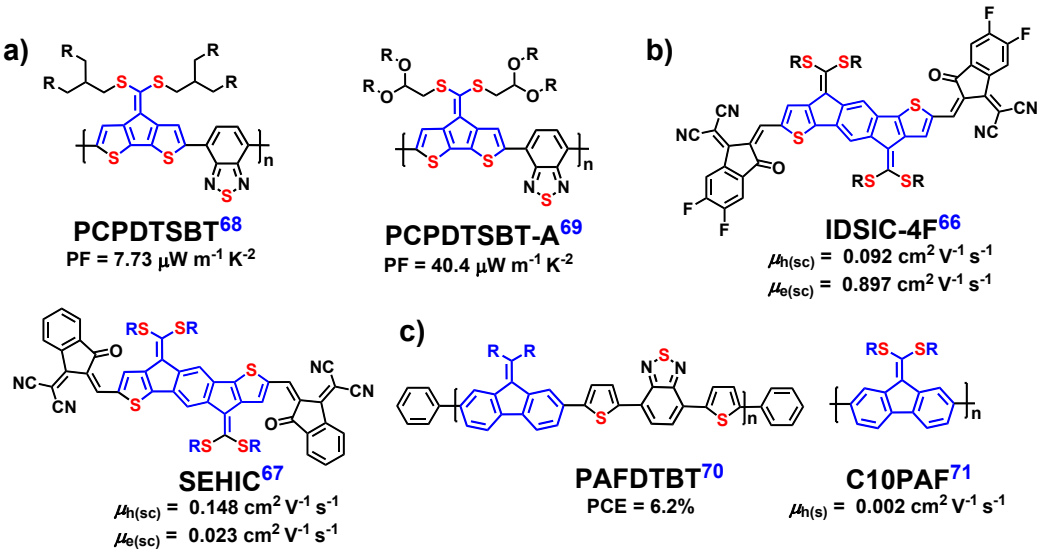


Figure S2. Chemical structures of the reported (a) dithioalkylated methylidenyl-CDT based p-type thermoelectric (TE) conjugated copolymers; (b) indacenodithiophene (IDT) based conjugated small molecular OFETs with dithioalkylated methylidenyl side chains; (c) dialkylated methylidenyl and dithioalkylated methylidenyl-fluorene based conjugated copolymer and OFETs. The symbols (sc) and (s) denote spin coating and solution processes semiconductor films. (Ref. 68; *Macromolecules*, 2018, **51**, 3360-3368), (Ref. 69; *Macromolecules*, 2020, **53**, 7063-7072), (66; *ACS Appl. Mater. Interfaces*, 2020, **12**, 41842-41851), (Ref. 67; *J. Mater. Chem. C*, 2018, **6**, 7604-7611), (Ref: 70; *Macromolecules*, 2011, **44**, 7617-7624.), (Ref. 71; *Macromolecules*, 2004, **37**, 5250-5256).

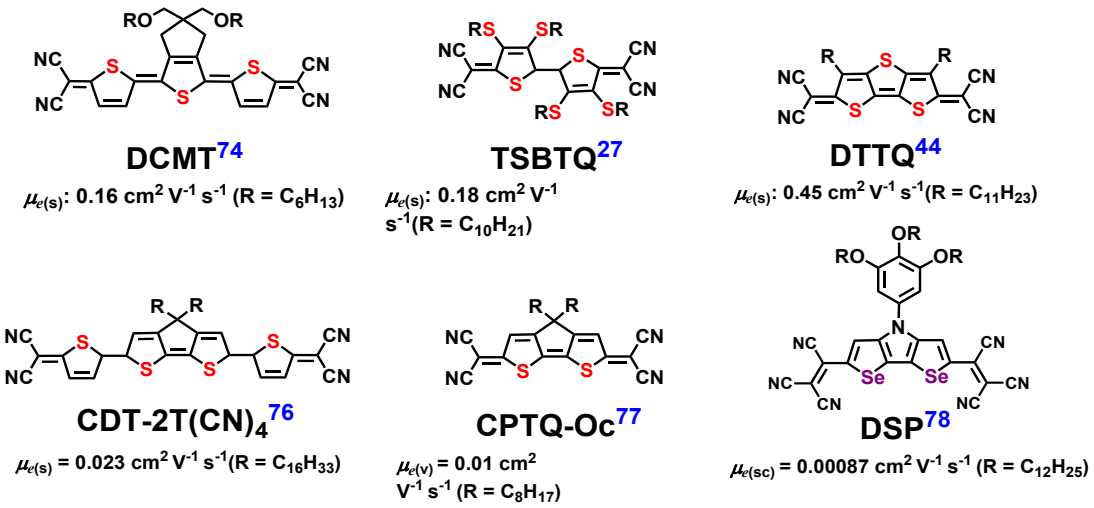


Figure S3. (a) Chemical structures of the reported dicyanomethylene-substituted n-type small molecules. The symbols (sc), (s) and (v) denote spin coating, solution, and vacuum processes semiconductor films. (Ref. 74; *Adv. Funct. Mater.*, 2009, **19**, 3427-3434), (Ref. 27; *J. Mater. Chem. C*, 2020, **8**, 15450-15458), (Ref. 44; *Adv. Funct. Mater.*, 2017, **27**, 1606761), (Ref. 76; *Mater. Chem. C*, 2013, **1**, 5128-5132), (Ref. 77; *J. Mater. Chem. C*, 2020, **8**, 15303-15311), (Ref, 78; *J. Org. Chem.*, 2012, **77**, 10931-10937

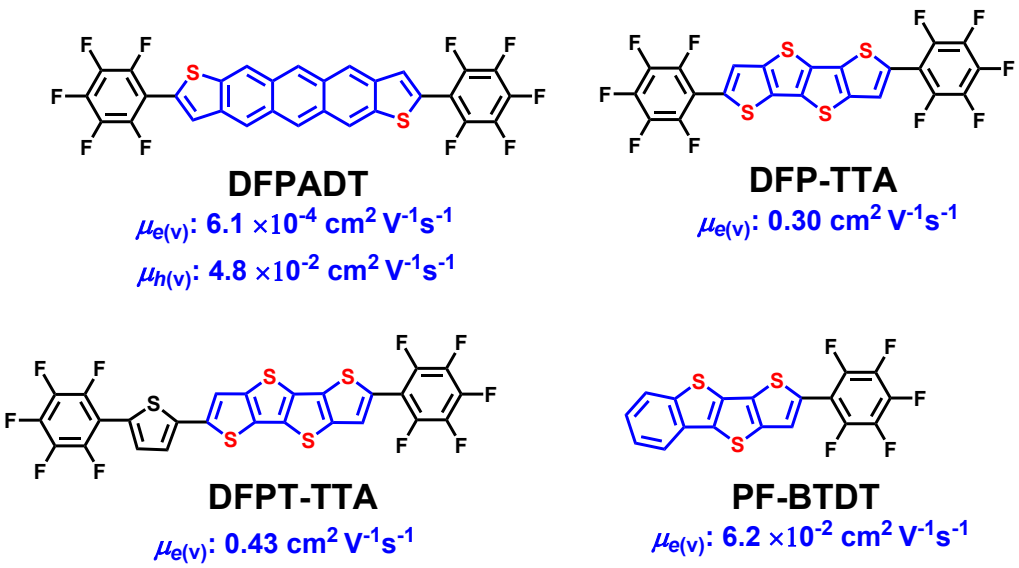


Figure S4. Examples of n-type fused oligothiophenes flanked by per fluorophenyls. The symbols (μ_e) and (μ_h) denote electron and hole mobility, respectively, while (v) denotes semiconductor films obtained from the vacuum process.

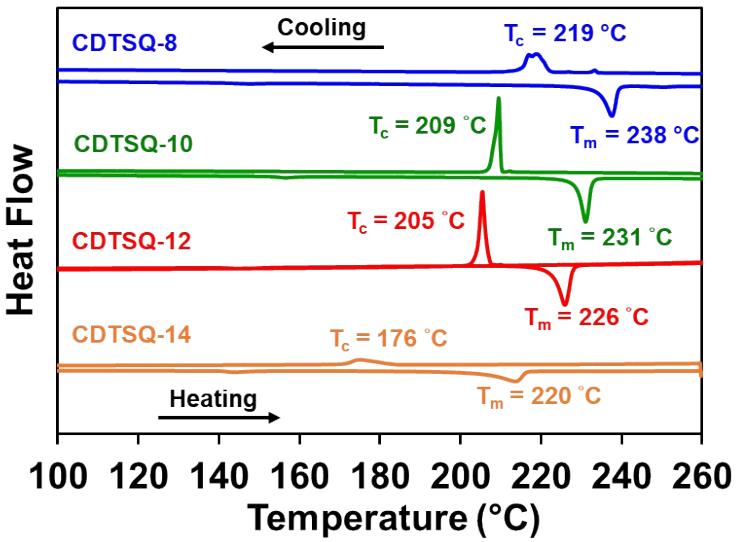


Figure S5. DSC curves of **CDTSQ**s (**1–4**)

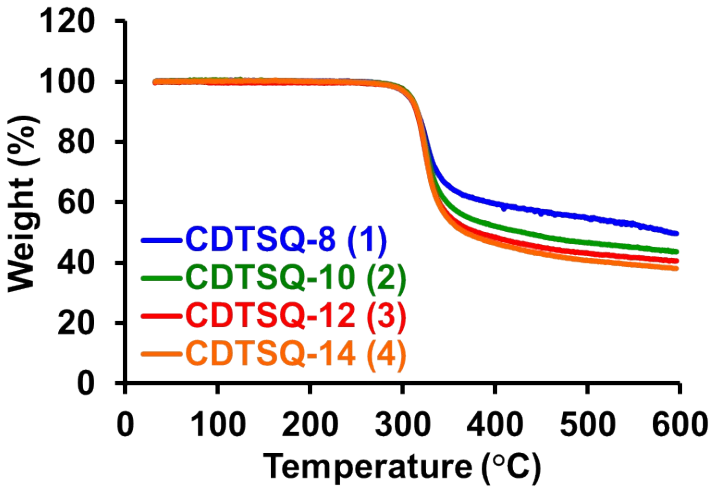


Figure S6. TGA curves of **CDTSQ**s (**1–4**).

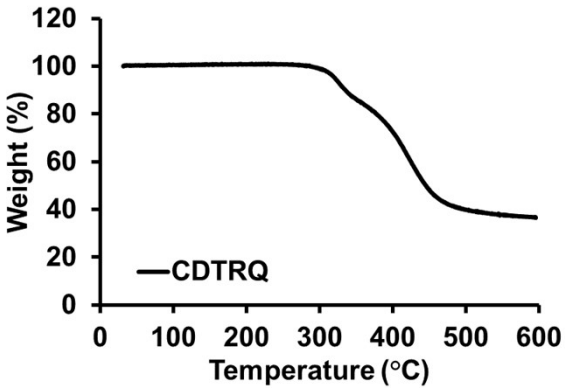


Figure S7. TGA curve of **CDTRQ**.

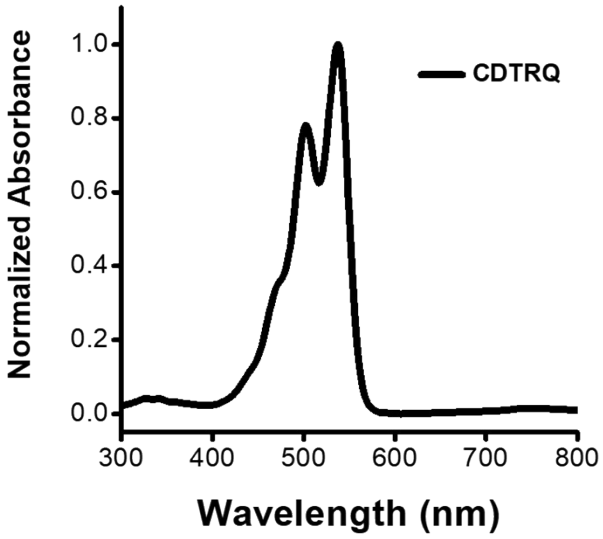


Figure S8. UV–vis absorption spectra of **CDTRQ** in diluted *o*-dichlorobenzene solution.

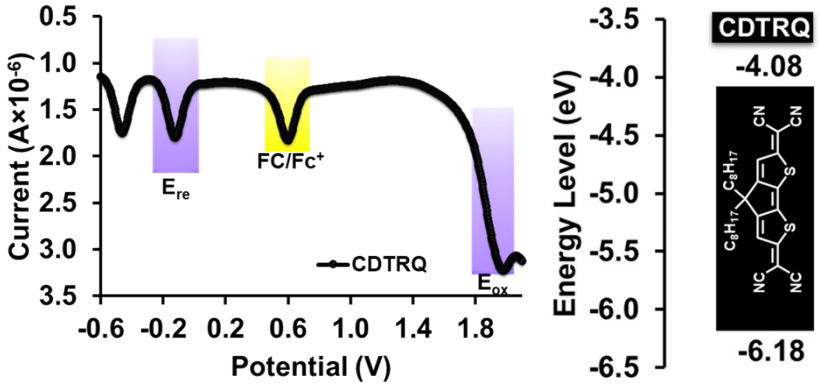


Figure S9. DPV response curve of **CDTRQ** in *o*-dichlorobenzene and DPV-derived HOMO/LUMO energy levels .

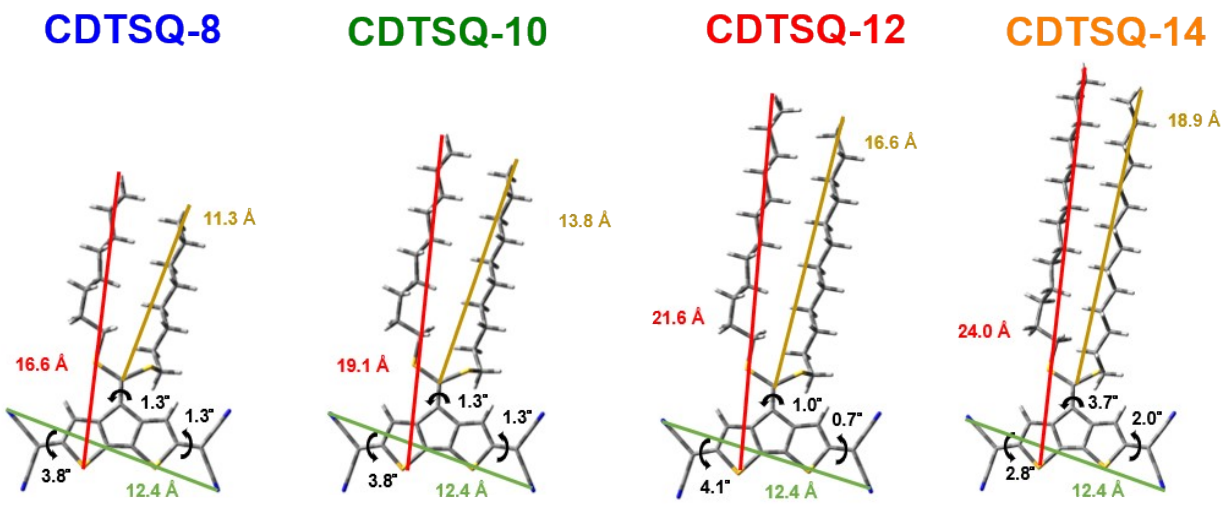


Figure S10. DFT optimized geometries of **CDTSQ**s (**1–4**).

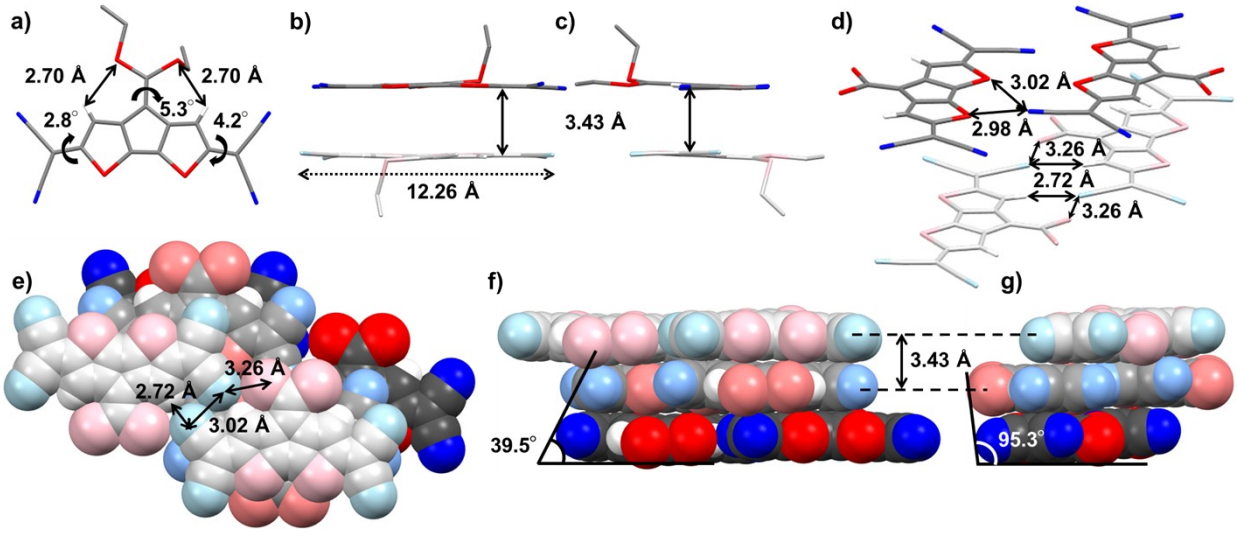


Figure S11. Single crystal structure of **CDTSQ-10** (**2**) in stick models (a-d) and space filling models (e-g). Sulphur and nitrogen atoms are specified in the red and blue color. Alkyl chains are omitted for clarity. (a) Top view of **CDTSQ-10** with intramolecular S···H distance of 2.70 Å and the shorter dihedral angles (2.8 Å and 4.2 Å) between the end capping unit and central core. The dihedral angles between dithioalkyl methylene and **CDT** core is 5.3°. (b-c) Front view and side view of **CDSTQ-10** molecules with π-π interplanar distances of 3.43 Å exhibiting brick type π-π stacking arrangement. The molecular length is 12.26 Å for **CDSTQ-10**. (d) Shortest intermolecular S (fused core)···N distances of 2.98, 3.02 Å, S (thioalkyl)···N distance of 3.26 Å and N···H interaction of 2.72 Å between **CDSTQ-10** layered molecules increases the order of π-π molecular stacking. (e-g) Molecular packing arrangement of **CDSTQ-10** molecules with a brick type stacking distance of 3.43 Å and exhibits the N···N intermolecular distance of 3.02 Å and slipping angles of 39.5° and 95.3° along the long and short molecular axes respectively.

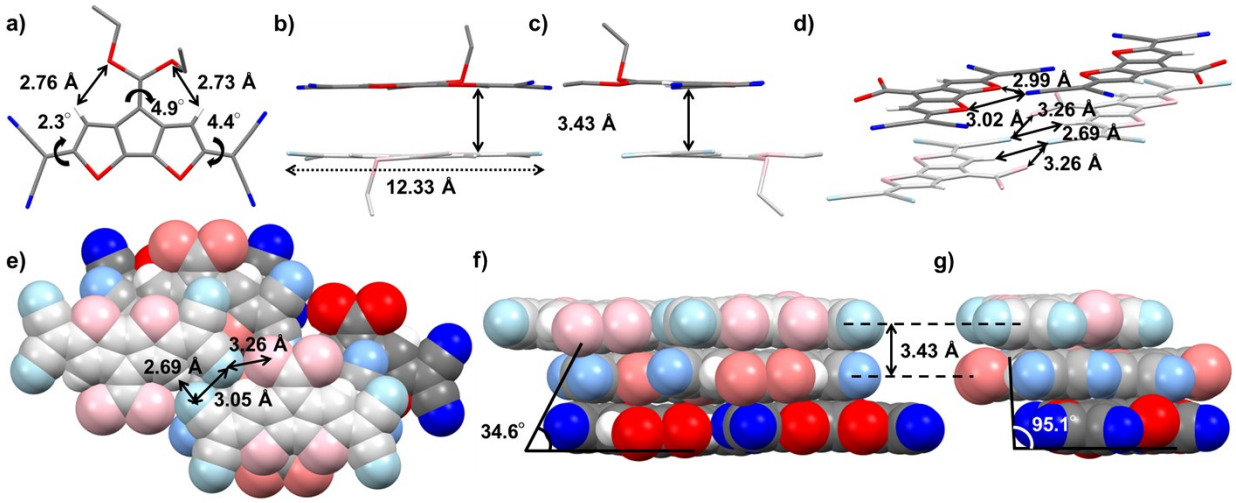


Figure S12. Single crystal structure of **CDTSQ-14** (**4**) in stick models (a-d) and space filling models (e-g). Sulphur and nitrogen atoms are specified in the red and blue color. Alkyl chains are omitted for clarity. (a) Top view of **CDTSQ-14** with intramolecular S···H distance of 2.76 Å, 2.73 Å, and the shorter dihedral angles (2.3 Å and 4.4 Å) between the end capping unit and central core. The dihedral angles between olefinic dithioalkyl methylene and central core is 4.9°. (b-c) Front view and sideview of **CDSTQ-14** molecules with π-π interplanar distances of 3.43 Å exhibiting brick type π-π stacking arrangement. The molecular length is 12.33 Å for **CDSTQ-14**. (d) Shortest intermolecular S (fused core)···N distances of 2.99 Å, 3.02 Å, S (thioalkyl)···N distance of 3.26 Å and N···H interaction of 2.69 Å between **CDSTQ-14** layered molecules increases the order of π-π molecular stacking. (e-g) Molecular packing arrangement of **CDSTQ-14** molecules with a brick type stacking distance of 3.43 Å and exhibits the N···N intermolecular distance of 3.05 Å and slipping angles of 34.6° and 95.1° along the long and short molecular axes respectively.

Table S1. Crystal data and structure refinement for **CDTSQ-10** (**2**).

Identification code	21FEB01	
Empirical formula	$C_{30}\ H_{27}\ N_4\ O_2\ S_3$	
Formula weight	571.73	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.600(6) Å	α= 90°.
	b = 30.500(12) Å	β= 105.890(19)°.
	c = 9.114(3) Å	λ = 90°.
Volume	3101(2) $Å^3$	
Z	4	
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	0.271 mm^{-1}	
F(000)	1196	
Crystal size	0.433 x 0.168 x 0.052 mm^3	
Theta range for data collection	1.944 to 28.281°.	
Index ranges	-15<=h<=15, -40<=k<=40, -12<=l<=10	
Reflections collected	73480	
Independent reflections	7673 [R(int) = 0.1089]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Numerical Mu Calculated	
Max. and min. transmission	0.7457 and 0.6971	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7673 / 0 / 353	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R_1 = 0.0610, wR_2 = 0.1471	
R indices (all data)	R_1 = 0.1575, wR_2 = 0.1968	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.393 and -0.229 $e.Å^{-3}$	

Crystallographic data (excluding structure factors) of **2** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. **CCDC 2178825.**

Table S2. Crystal data and structure refinement for **CDTSQ-12 (3)**.

Identification code	20MAR02	
Empirical formula	C_{34} H_{28} N_2 O_2 S	
Formula weight	528.64	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*P*2/*c*	
Unit cell dimensions	a = 18.352(5) Å	α= 90°.
	b = 5.7286(15) Å	β= 107.054(9)°.
	c = 29.160(8) Å	λ = 90°.
Volume	2930.8(14) Å^3	
Z	4	
Density (calculated)	1.198 Mg/m^3	
Absorption coefficient	0.143 mm^{-1}	
F(000)	1112	
Crystal size	0.406 x 0.036 x 0.028 mm^3	
Theta range for data collection	2.116 to 28.356°.	
Index ranges	-24<=h<=24, -7<=k<=7, -38<=l<=38	
Reflections collected	141263	
Independent reflections	7316 [R(int) = 0.2334]	
Completeness to theta = 25.242°	99.9 %	
Max. and min. transmission	0.7446 and 0.7051	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7316 / 0 / 355	
Goodness-of-fit on F^2	1.199	
Final R indices [I>2sigma(I)]	R_1 = 0.1530, wR_2 = 0.2640	
R indices (all data)	R_1 = 0.2194, wR_2 = 0.2942	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.345 and -0.449 e.Å^{-3}	

Crystallographic data (excluding structure factors) of **3** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. **CCDC 2178823**.

Table S3. Crystal data and structure refinement for **CDTSQ-14 (4)**.

Identification code	22FEB07_1_0m	
Empirical formula	C_{44} H_{60} N_4 S_4	
Formula weight	773.20	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	*a* = 8.6648(2) Å	α= 89.1350(10)°.
	b = 10.4117(2) Å	β= 81.9180(10)°.
	c = 25.0237(5) Å	λ = 74.8170(10)°.
Volume	2156.52(8) Å^3	
Z	2	
Density (calculated)	1.191 Mg/m^3	
Absorption coefficient	0.255 mm^{-1}	
F(000)	832	
Crystal size	0.150 x 0.134 x 0.052 mm^3	
Theta range for data collection	2.027 to 28.356°.	
Index ranges	-11<=h<=11, -13<=k<=13, -33<=l<=33	
Reflections collected	74860	
Independent reflections	10604 [*R*(int) = 0.0884]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Numerical Mu Calculated	
Max. and min. transmission	0.7457 and 0.6540	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10604 / 0 / 477	
Goodness-of-fit on F^2	1.073	
Final R indices [I>2sigma(I)]	R_1 = 0.0532, wR_2 = 0.1496	
R indices (all data)	R_1 = 0.0850, wR_2 = 0.1710	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.554 and -0.358 e.Å^{-3}	

Crystallographic data (excluding structure factors) of **4** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. **CCDC 2178827**.

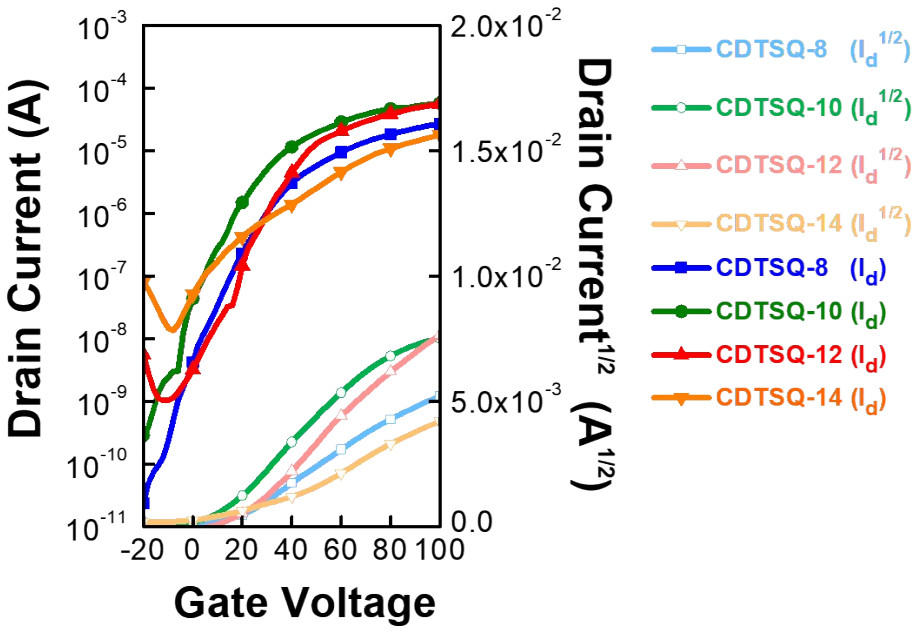


Figure S13. Transfer characteristics of spin-coated **CDTSQ**s OFETs.

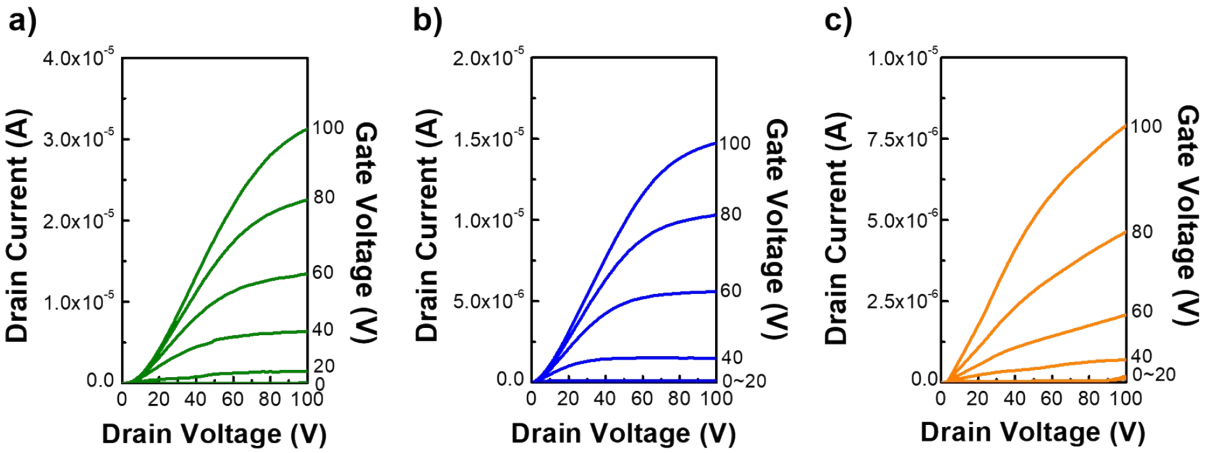


Figure S14. Output characteristics of solution-sheared (a) **CDTSQ-8**, (b) **CDTSQ-10**, (c) **CDTSQ-14** OFETs.

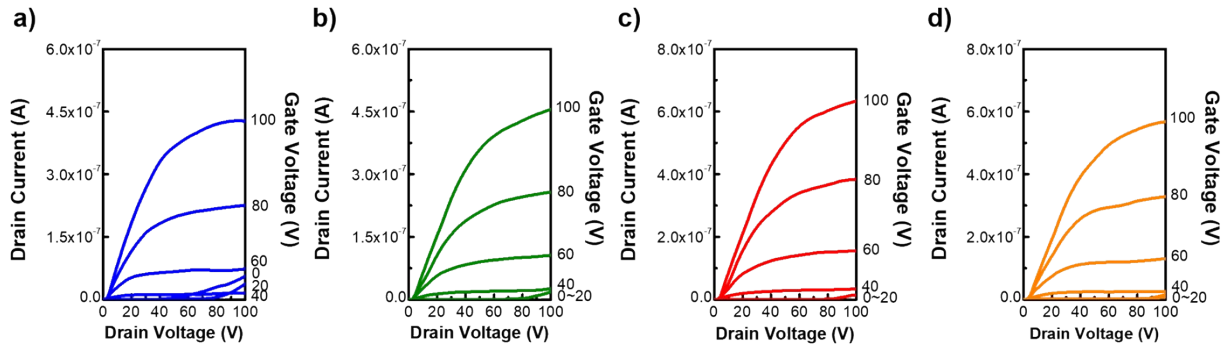


Figure S15. Output characteristics of spin-coated (a) **CDTSQ-8**, (b) **CDTSQ-10**, (c) **CDTSQ-12**, and (d) **CDTSQ-14** OFETs.

Table S4. Summary of OFETs electrical parameters for spin-coated **CDTSQ**s films.

Compound	μ_{max} [$cm^2 V^{-1} s^{-1}$]	I_{ON}/I_{OFF} [V]	V_{th} [V]
CDTSQ-8	5.25E-06	$10^2 \sim 10^3$	-4.35
CDTSQ-10	1.86E-05	$10^3 \sim 10^4$	9.75
CDTSQ-12	7.94E-05	$10^2 \sim 10^3$	26.86
CDTSQ-14	5.20E-05	$10^3 \sim 10^4$	3.72

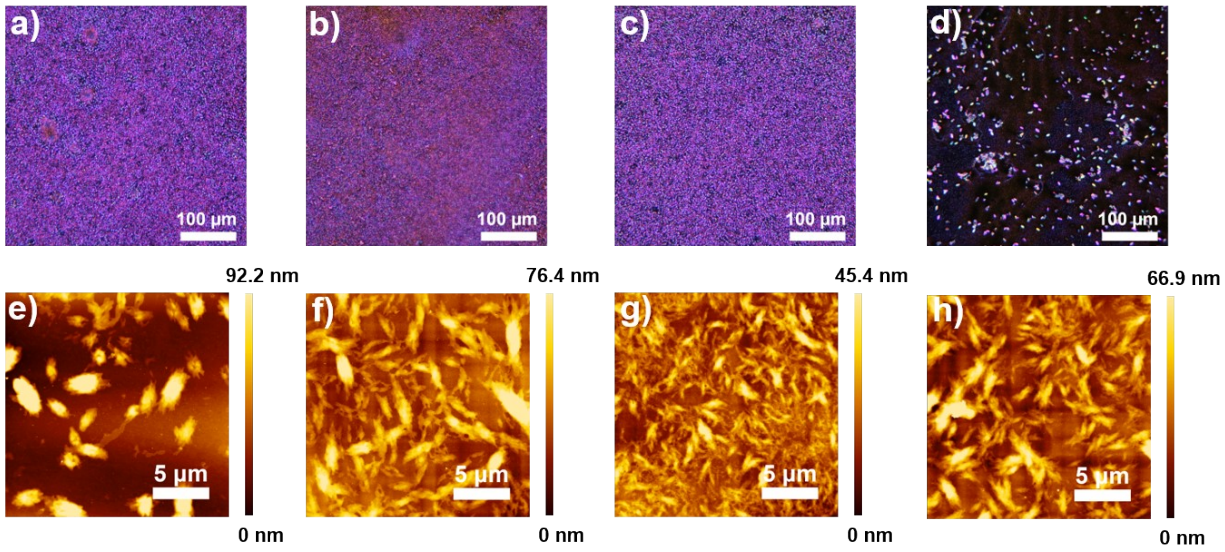


Figure S16. POM (upper) and AFM (lower) of spin-coated (a, e) **CDTSQ-8**, (b, f) **CDTSQ-10**, (c, g) **CDTSQ-12**, and (d, h) **CDTSQ-14**.

Table S5. Crystallographic information of **CDTSQ**s molecules obtained from GIWAXS.

Compound	*a* [Å]	*b* [Å]	*c* [Å]	FWHM [Å^{-1}]	L_c [Å]
CDTSQ-8	3.49	-	24.15	0.0208	302.1
CDTSQ-10	3.47	5.93	27.30	0.0154	408.0
CDTSQ-12	3.43	5.67	29.90	0.0151	416.1
CDTSQ-14	3.47	-	33.74	0.0155	405.4

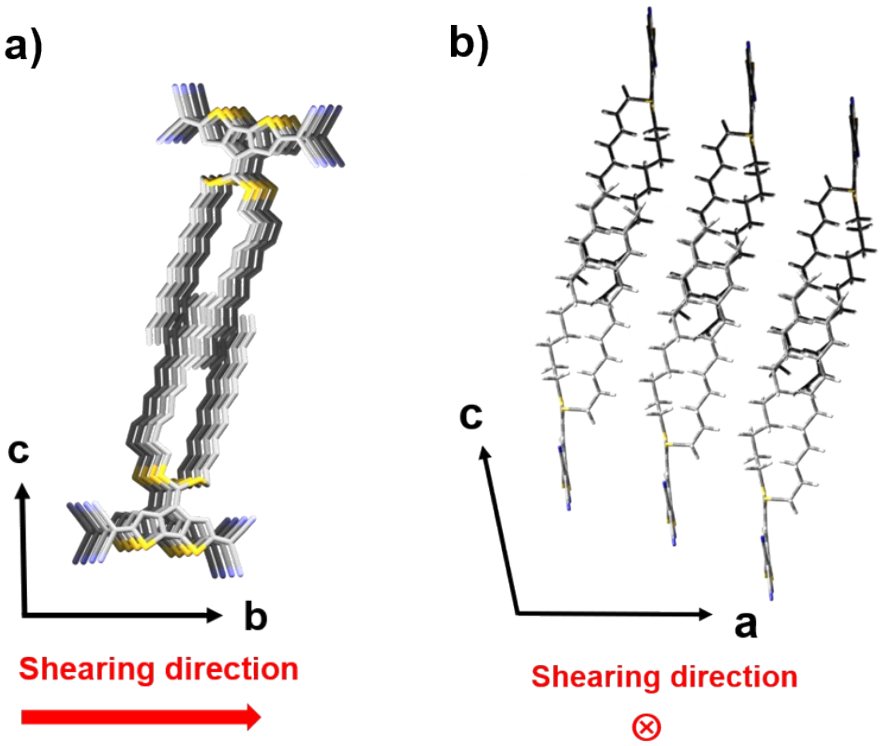


Figure S17. Schematic diagram of proposed molecular packing of solution-sheared **CDTSQ-12** film in the (a) a-axis and (b) b-axis projections.

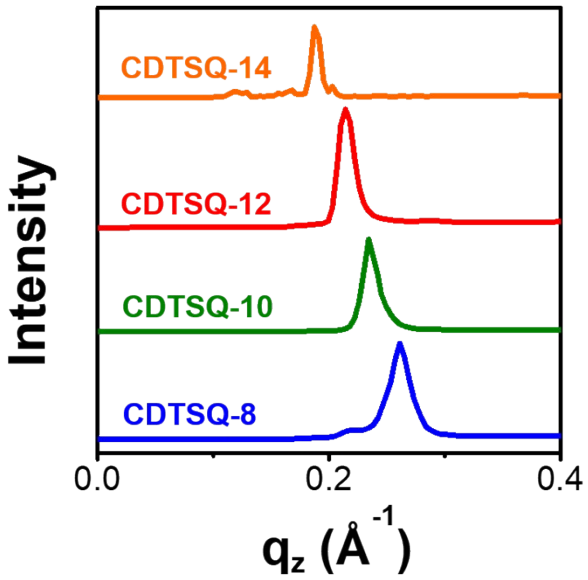


Figure S18. One-dimensional profile of (001) peak extracted from (a) **CDTSQ-8**, (b) **CDTSQ-10**, (c) **CDTSQ-12**, and (d) **CDTSQ-14** GIWAXS pattern.

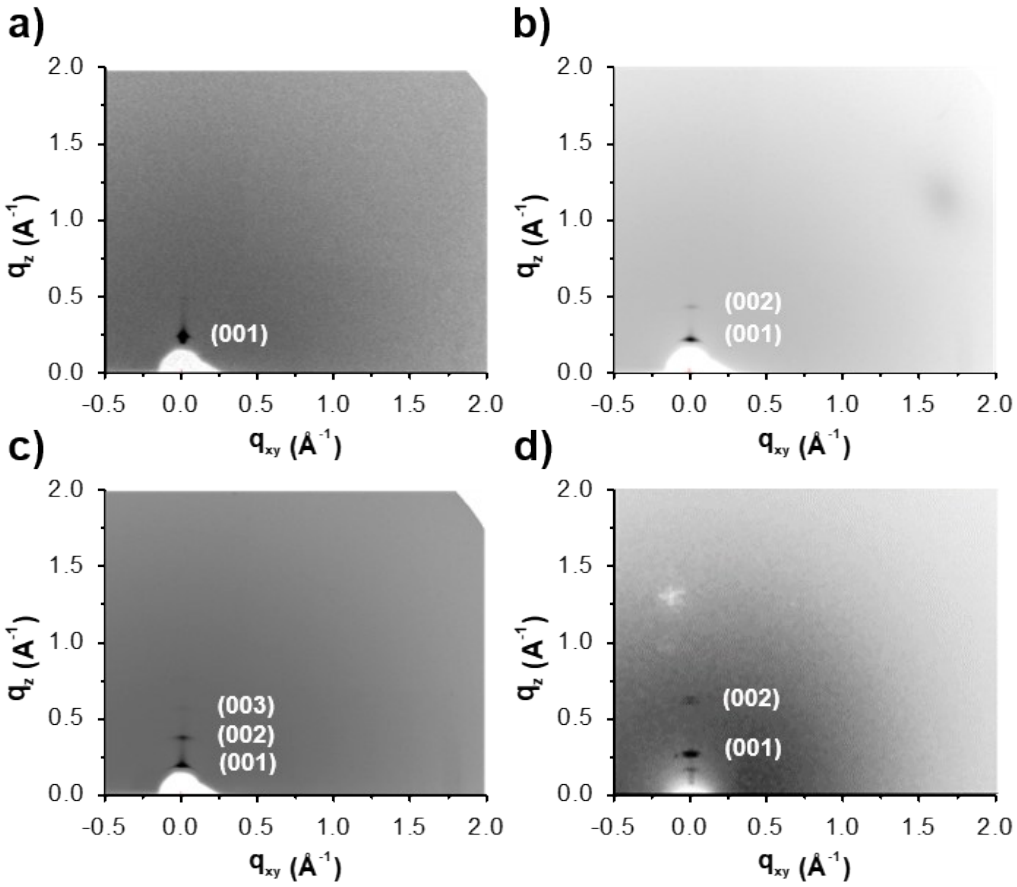


Figure S19. 2D GIWAXS patterns of spin-coated (a) **CDTSQ-8**, (b) **CDTSQ-10**, (c) **CDTSQ-12**, and (d) **CDTSQ-14** films.

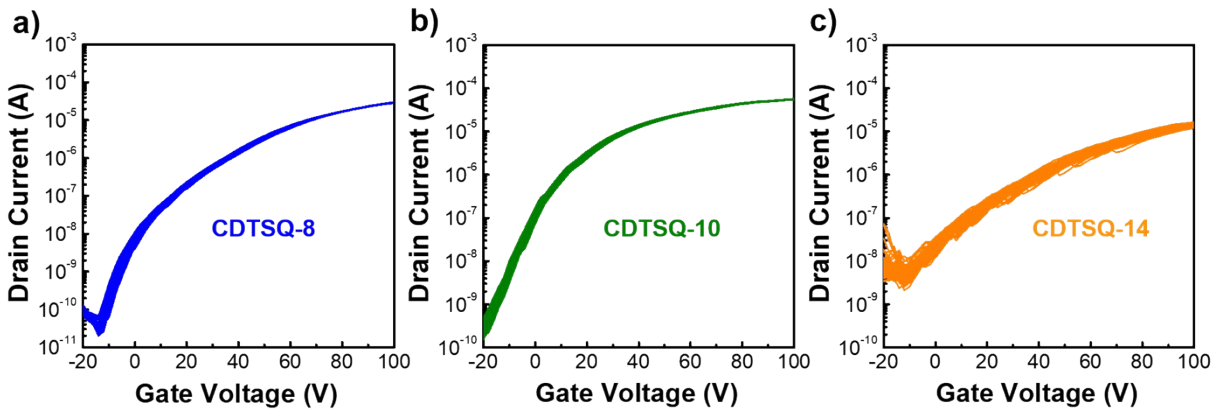
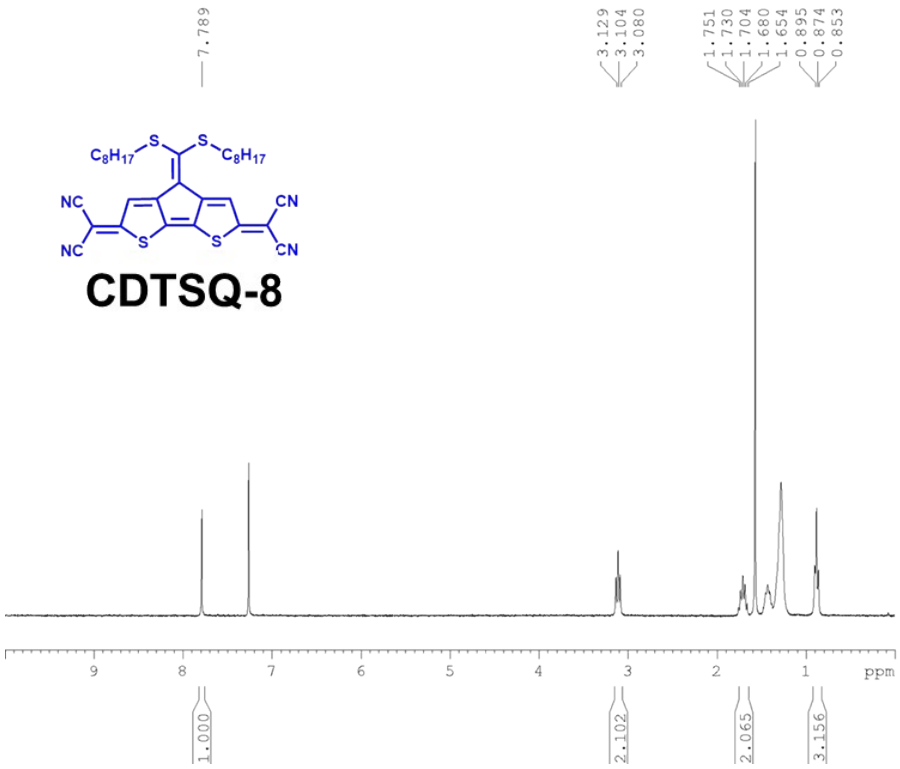
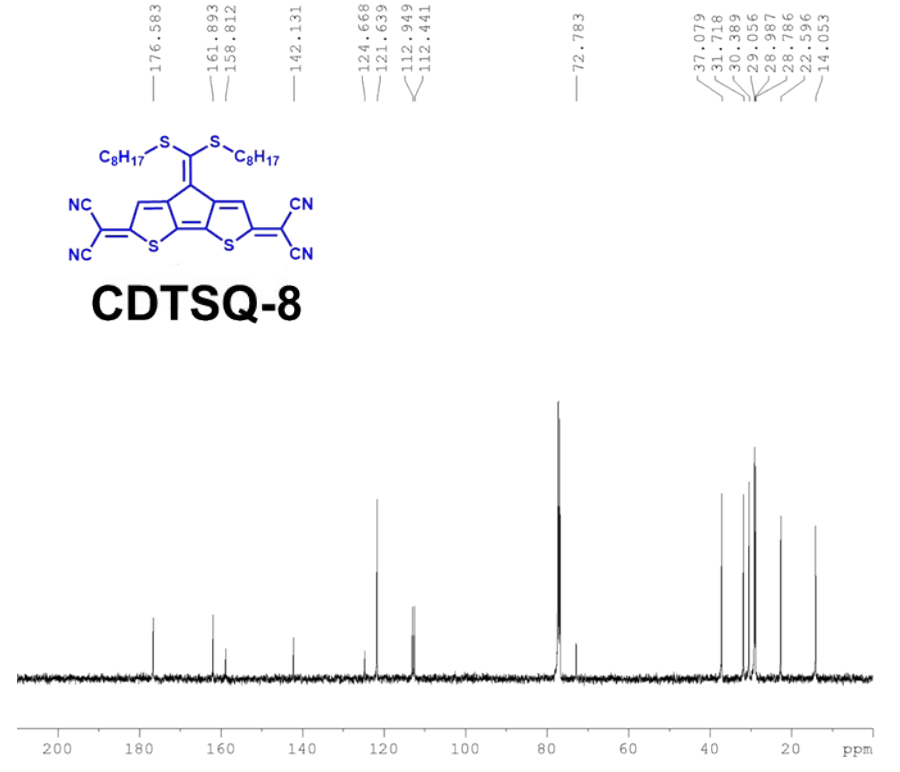
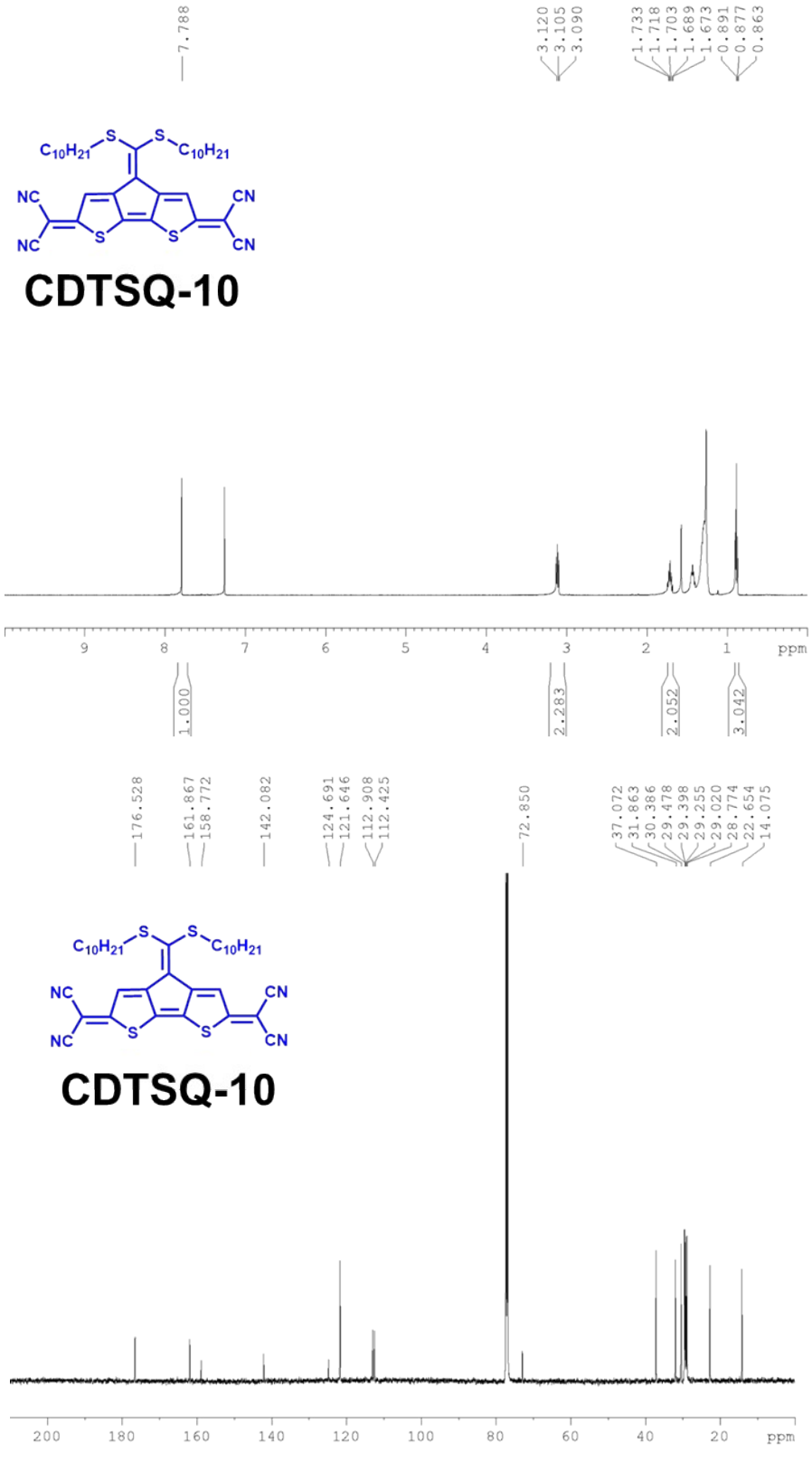
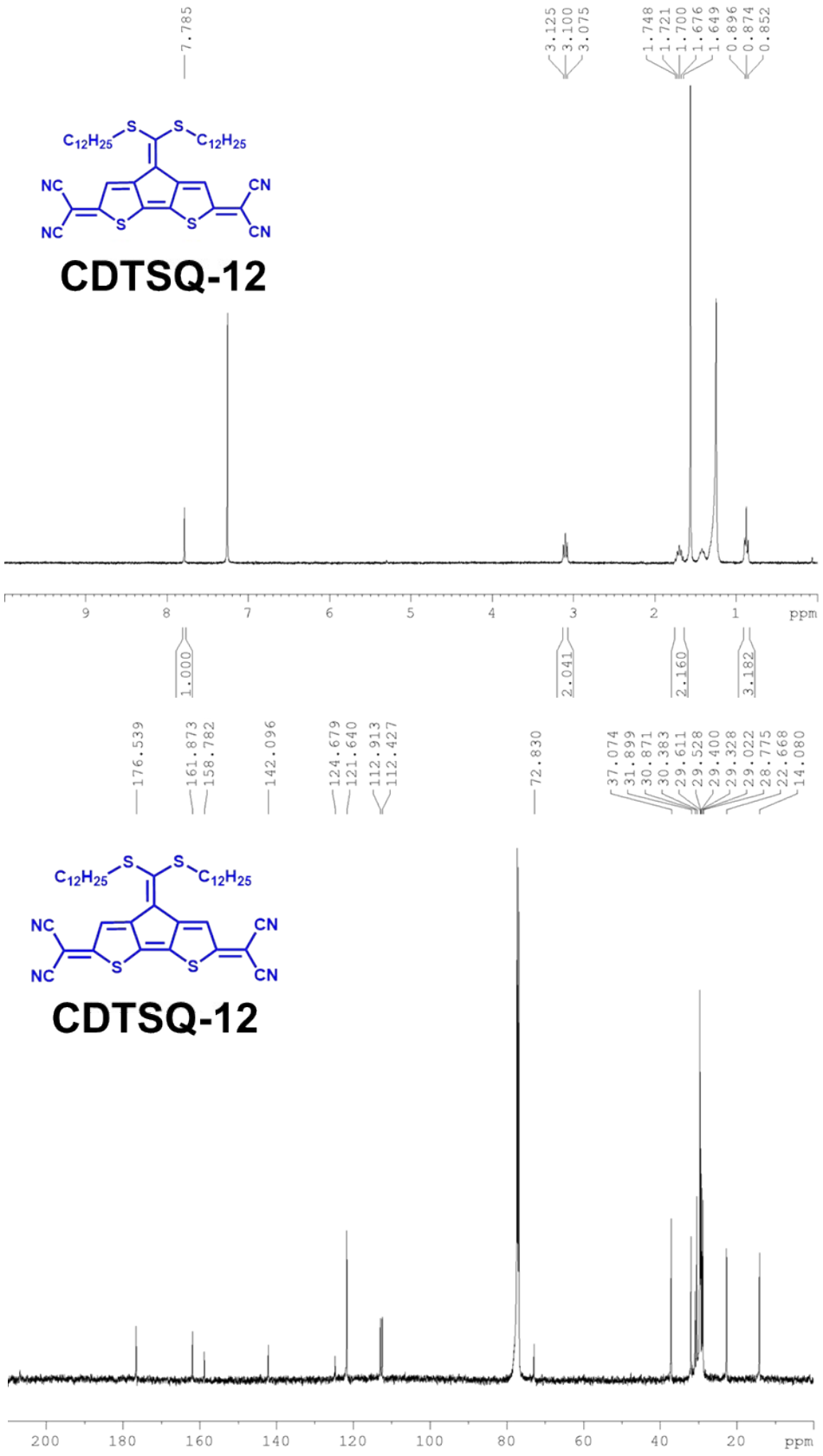


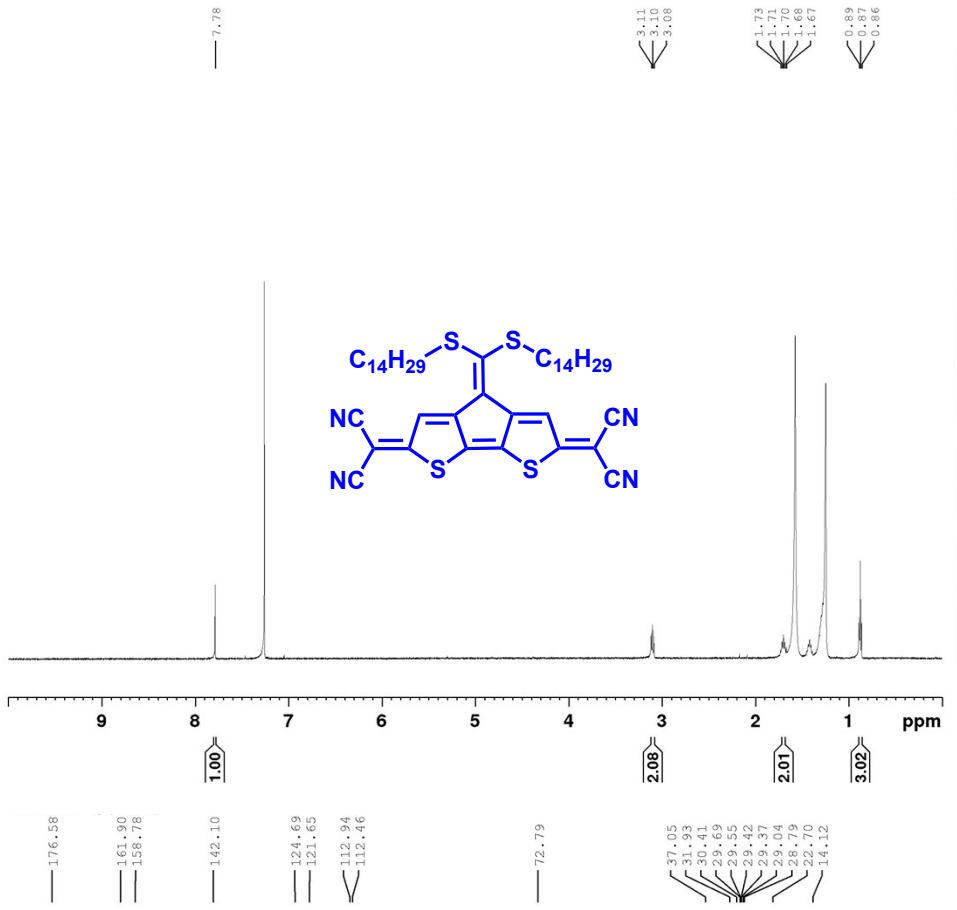
Figure S20. Multiple gate sweeps of (a) **CDTSQ-8**, (b) **CDTSQ-10**, and (c) **CDTSQ-14** OFETs for 100 cycles.


7.789
3.129
3.104
3.080
1.751
1.730
1.704
1.680
1.654
0.895
0.874
0.853
CDTSQ-8
ppm
1.000
2.102
2.065
3.156


176.583
161.893
158.812
142.131
124.668
121.639
112.949
112.441
72.783
37.079
31.718
30.389
29.056
28.987
28.786
22.596
14.053
CDTSQ-8
ppm


7.788
3.120
3.105
3.090
1.733
1.718
1.703
1.689
1.673
0.891
0.877
0.863
C10H21
S
S
C10H21
NC
NC
CN
CN
S
S
CDTSQ-10
9
8
7
6
5
4
3
2
1
ppm
1.000
2.283
2.052
3.042
176.528
161.867
158.772
142.082
124.691
121.646
112.908
112.425
72.850
37.072
31.863
30.386
29.478
29.398
29.255
29.020
28.774
22.654
14.075
C10H21
S
S
C10H21
NC
NC
CN
CN
S
S
CDTSQ-10
200
180
160
140
120
100
80
60
40
20
ppm


7.785
3.125
3.100
3.075
1.748
1.721
1.700
1.676
1.649
0.896
0.874
0.852
CDTSQ-12
9
8
7
6
5
4
3
2
1
ppm
1.000
2.041
2.160
3.182
176.539
161.873
158.782
142.096
124.679
121.640
112.913
112.427
72.830
37.074
31.899
30.871
30.383
29.611
29.528
29.400
29.328
29.022
28.775
22.668
14.080
CDTSQ-12
200
180
160
140
120
100
80
60
40
20
ppm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3.11
3.10
3.08
1.73
1.71
1.70
1.68
1.67
0.89
0.87
0.86
C14H29
S
S
C14H29
NC
CN
NC
CN
S
S
9
8
7
6
5
4
3
2
1
ppm
1.00
2.08
2.01
3.02

176.58
161.90
158.78
142.10
124.69
121.65
112.94
112.46
72.79
37.05
31.93
30.41
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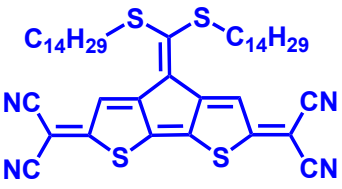
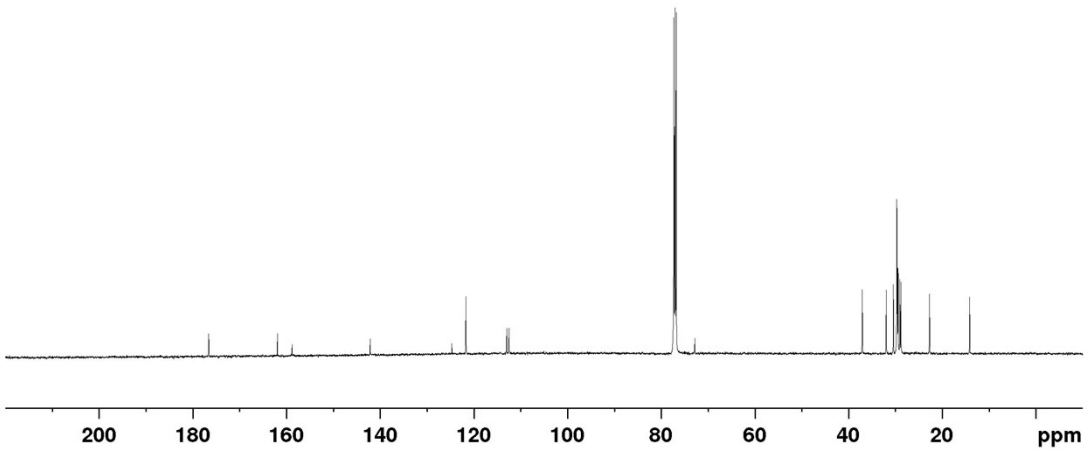
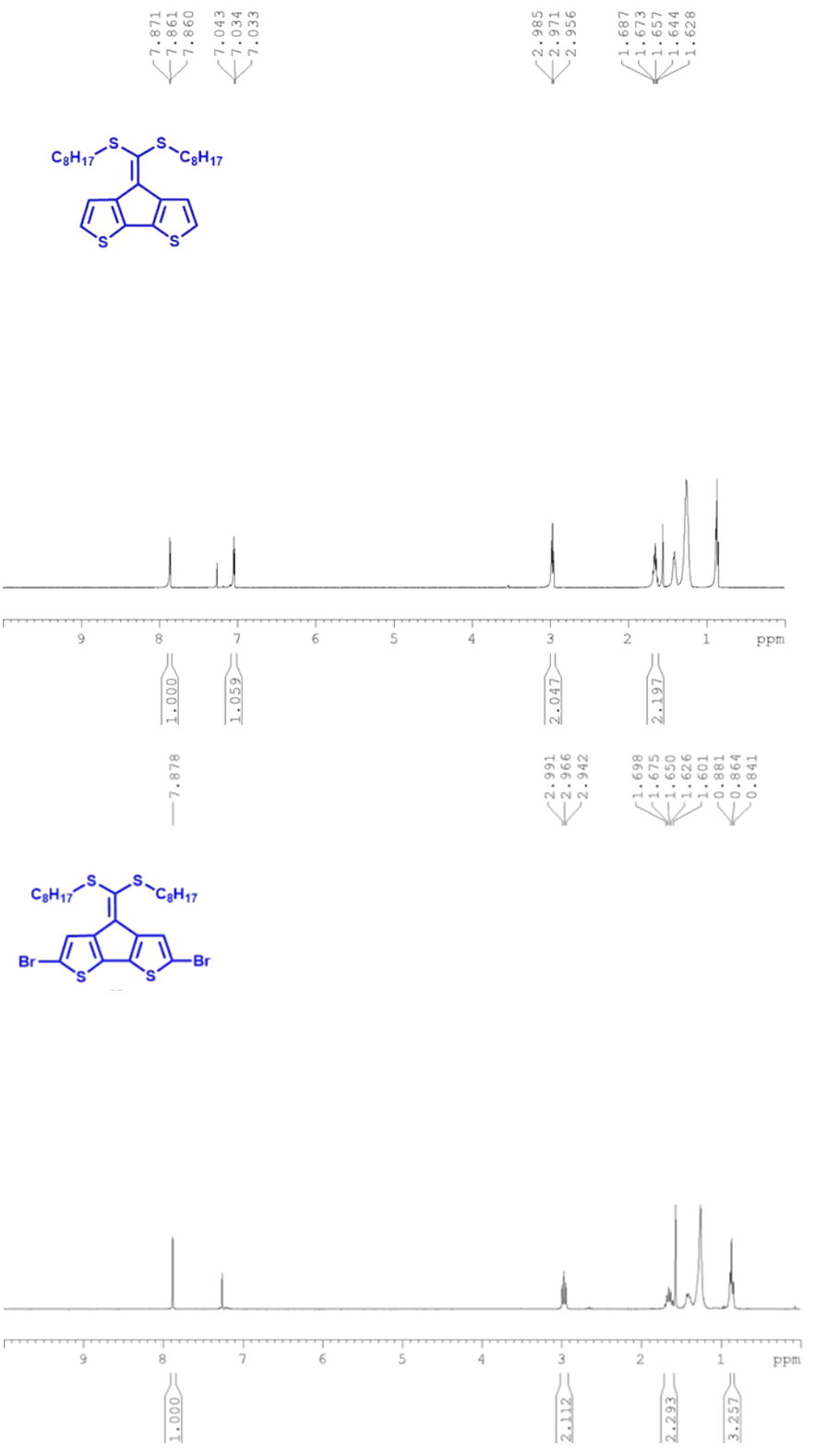
29.55
29.42
29.37
29.04
28.79
22.70
14.12


C14H29
S
S
C14H29
NC
CN
NC
CN
S
S


200
180
160
140
120
100
80
60
40
20
ppm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7.861
7.860
7.043
7.034
7.033
2.985
2.971
2.956
1.687
1.673
1.657
1.644
1.628
C8H17
S
S
C8H17
S
S
9
8
7
6
5
4
3
2
1
ppm
1.000
1.059
2.047
2.197
7.878
2.991
2.966
2.942
1.698
1.675
1.650
1.626
1.601
0.881
0.864
0.841
C8H17
S
S
C8H17
Br
S
S
Br
9
8
7
6
5
4
3
2
1
ppm
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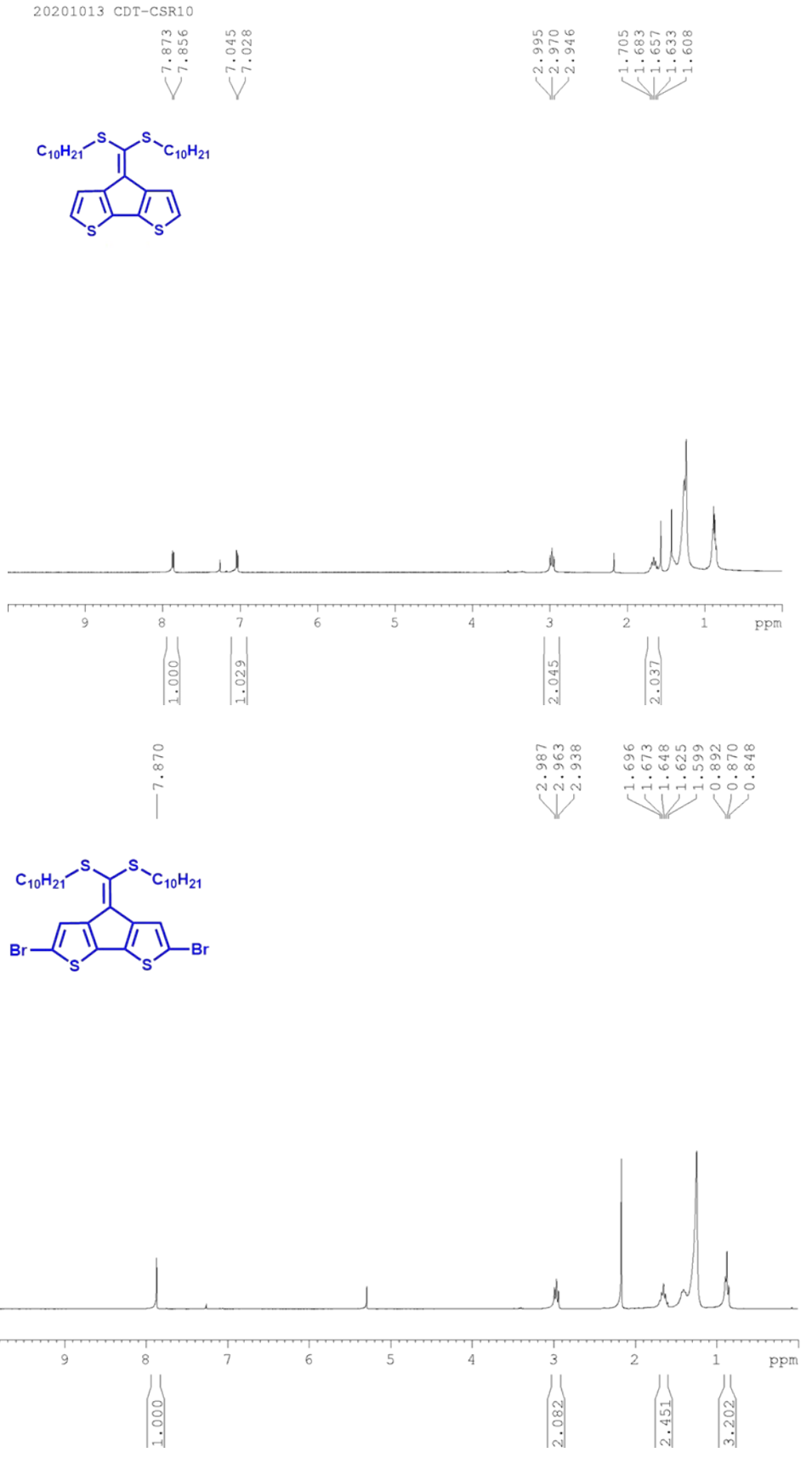
3.257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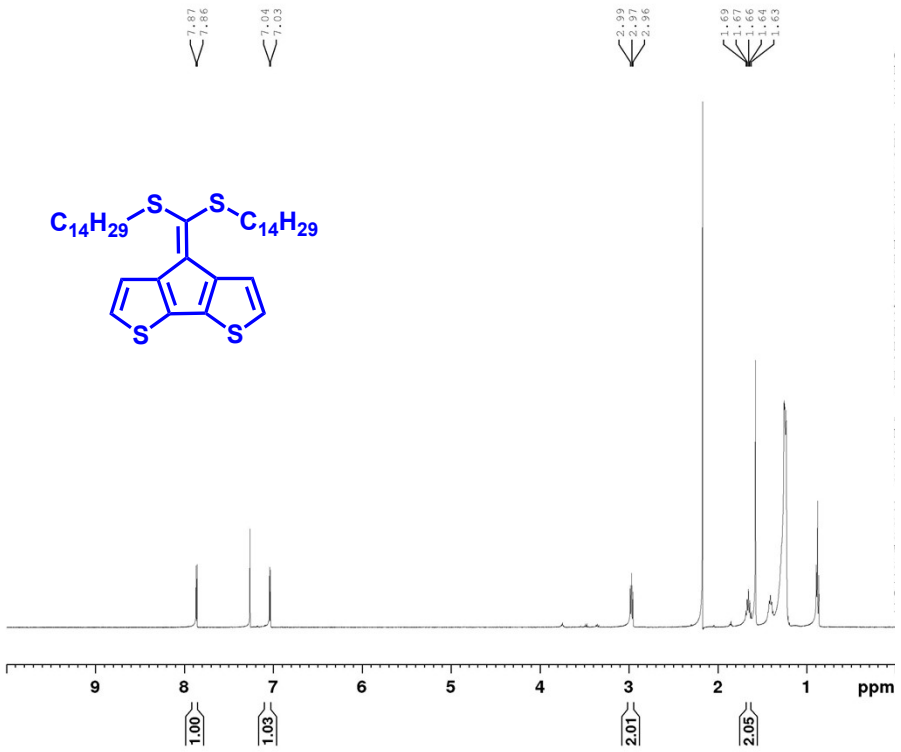
1.683
1.657
1.633
1.608
C10H21
S
S
C10H21
S
S
9
8
7
6
5
4
3
2
1
ppm
1.000
1.029
2.045
2.037
7.870
2.987
2.963
2.938
1.696
1.673
1.648
1.625
1.599
0.892
0.870
0.848
C10H21
S
S
C10H21
Br
Br
S
S
9
8
7
6
5
4
3
2
1
ppm
1.000
2.082
2.451
3.202


7.868
7.858
7.041
7.031
2.984
2.969
2.954
1.684
1.670
1.655
1.640
1.625
C12H25
S
S
C12H25
S
S
9
8
7
6
5
4
3
2
1
ppm
1.000
1.010
2.065
2.275


7.878
2.983
2.969
2.954
1.681
1.667
1.651
1.637
1.622
0.890
0.879
0.862
C12H25
S
S
C12H25
Br
S
S
Br
9
8
7
6
5
4
3
2
1
ppm
1.000
2.170
2.477
3.904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7.86
7.04
7.03
2.99
2.97
2.96
1.69
1.67
1.66
1.64
1.63
C14H29
S
S
C14H29
S
S
9
8
7
6
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4
3
2
1
ppm
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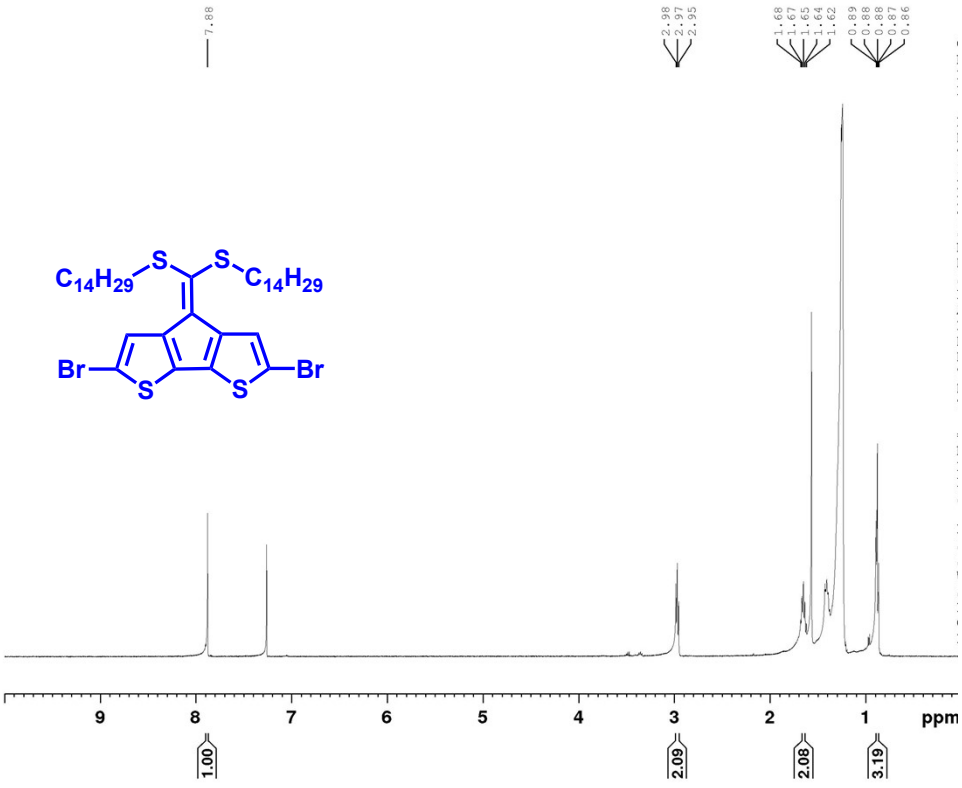
2.05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1.64
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0.89
0.88
0.88
0.87
0.86
C14H29
S
S
C14H29
Br
S
S
Br
9
8
7
6
5
4
3
2
1
ppm
1.00
2.09
2.08
3.19

SmartFormula

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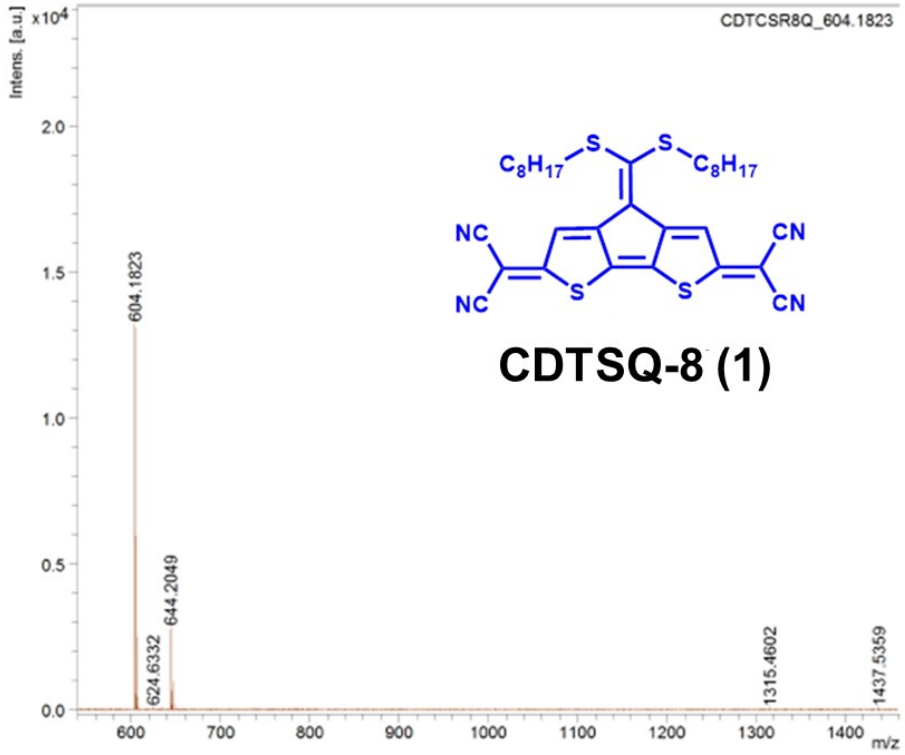

CDTSQ-8 (1)

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Voltage polarity	POS
Number of shots	1000
Name of spectrum used for calibration	
Calibration reference list used	PEG-Na -Calibration Mono-T

Instrument Info

User	NCU
Instrument	ATS-00670
Instrument type	autoflex

Bruker Daltonics flexAnalysis printed: 2021-05-06 2:30:18 PM

SmartFormula

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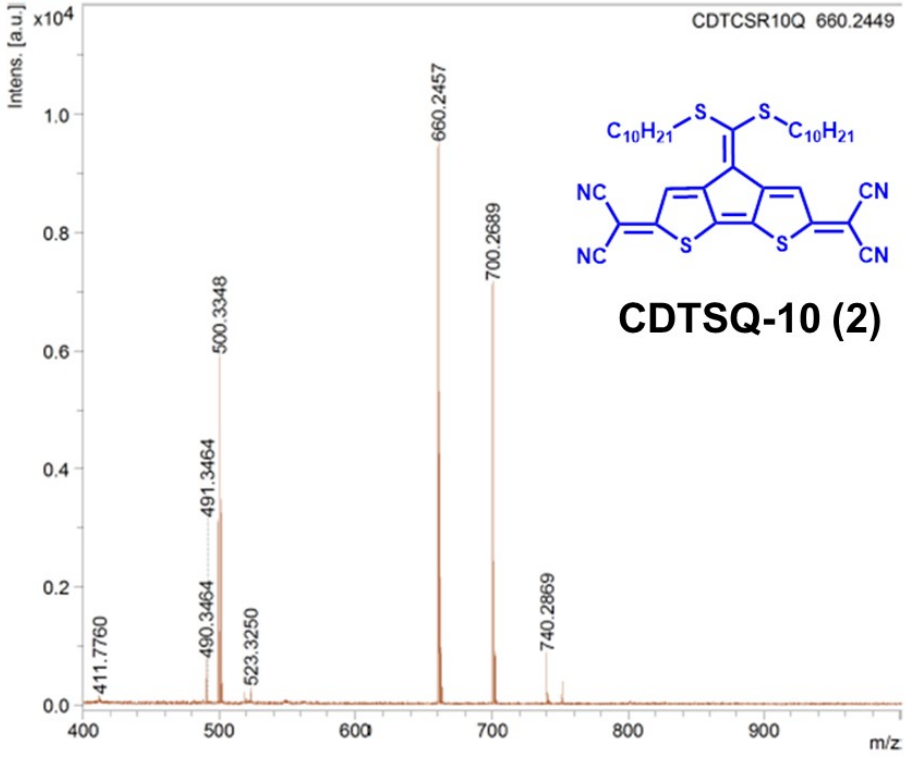
Comment 2



CDTSQ-10 (2)

Acquisition Parameter

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Name of spectrum used for calibration	
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Instrument Info

User	NCU
Instrument	ATS-00670
Instrument type	autoflex

Bruker Daltonics flexAnalysis printed: 2020-10-29 2:17:59 PM

SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
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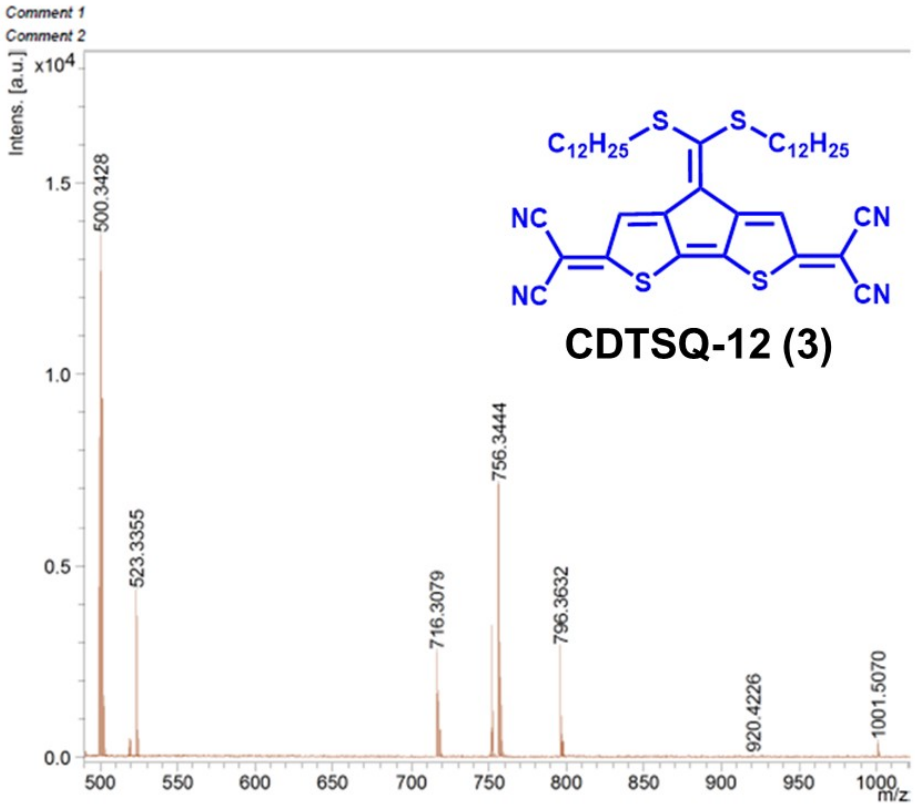

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Name of spectrum used for calibration	
Calibration reference list used	PEG-Na -Calibration Mono-T

Instrument Info

User	NCU
Instrument	ATS-00670
Instrument type	autoflex

Bruker Daltonics flexAnalysis printed: 2020-10-29 2:23:42 PM

SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
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