Supplementary Material (ESI) for *Journal of Materials Chemistry*

Supporting Information

for

π-Conjugated Oligothiophene-anthracene Co-oligomers: Synthesis, Physical Properties, and Self-assembly

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Figure S1. ^{1}H NMR spectrum of **T_1A**

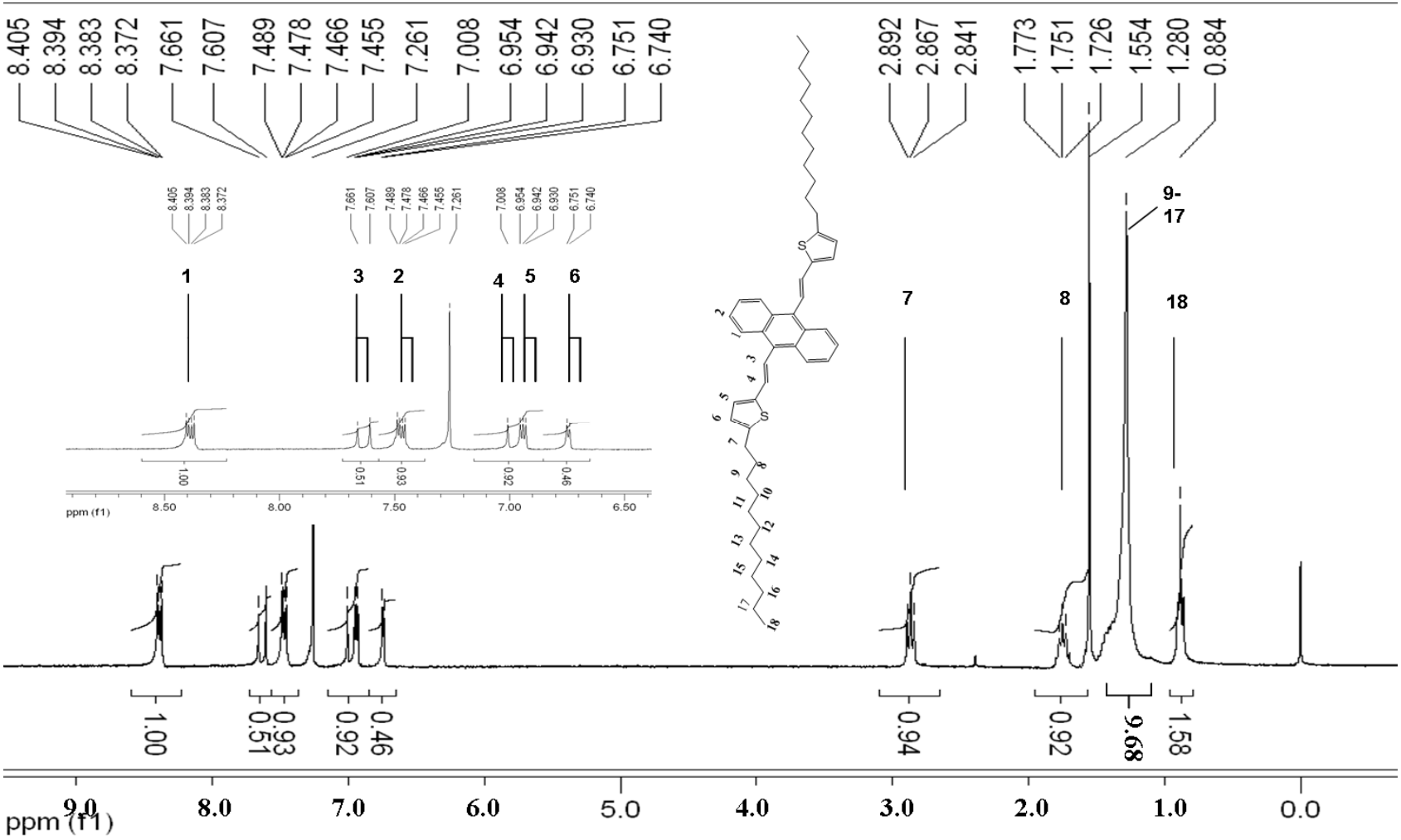


Figure S2. ^{13}C NMR spectrum of **T_1A**

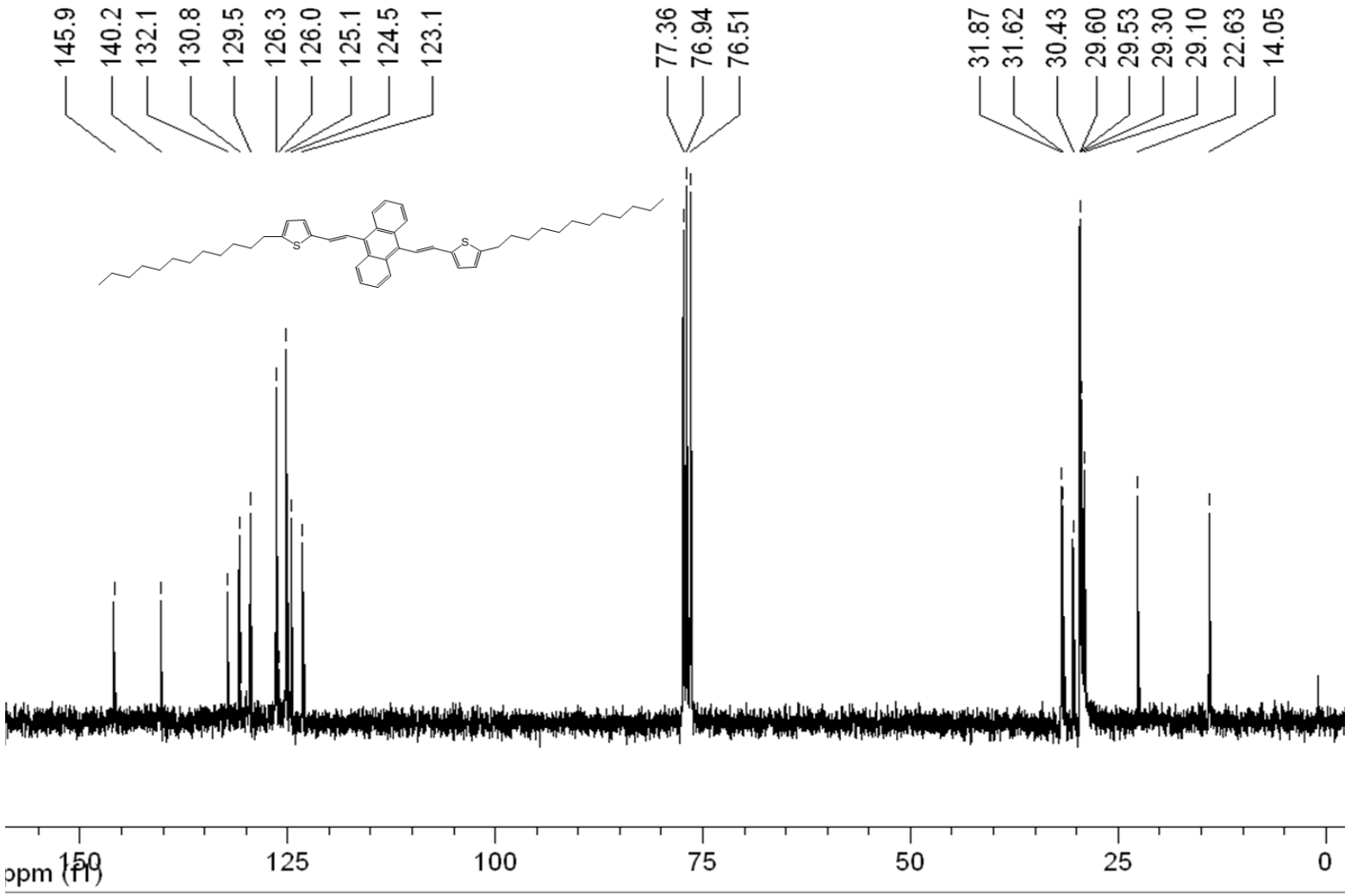


Figure S3. MALDI-TOF mass spectrum of **T_1A**

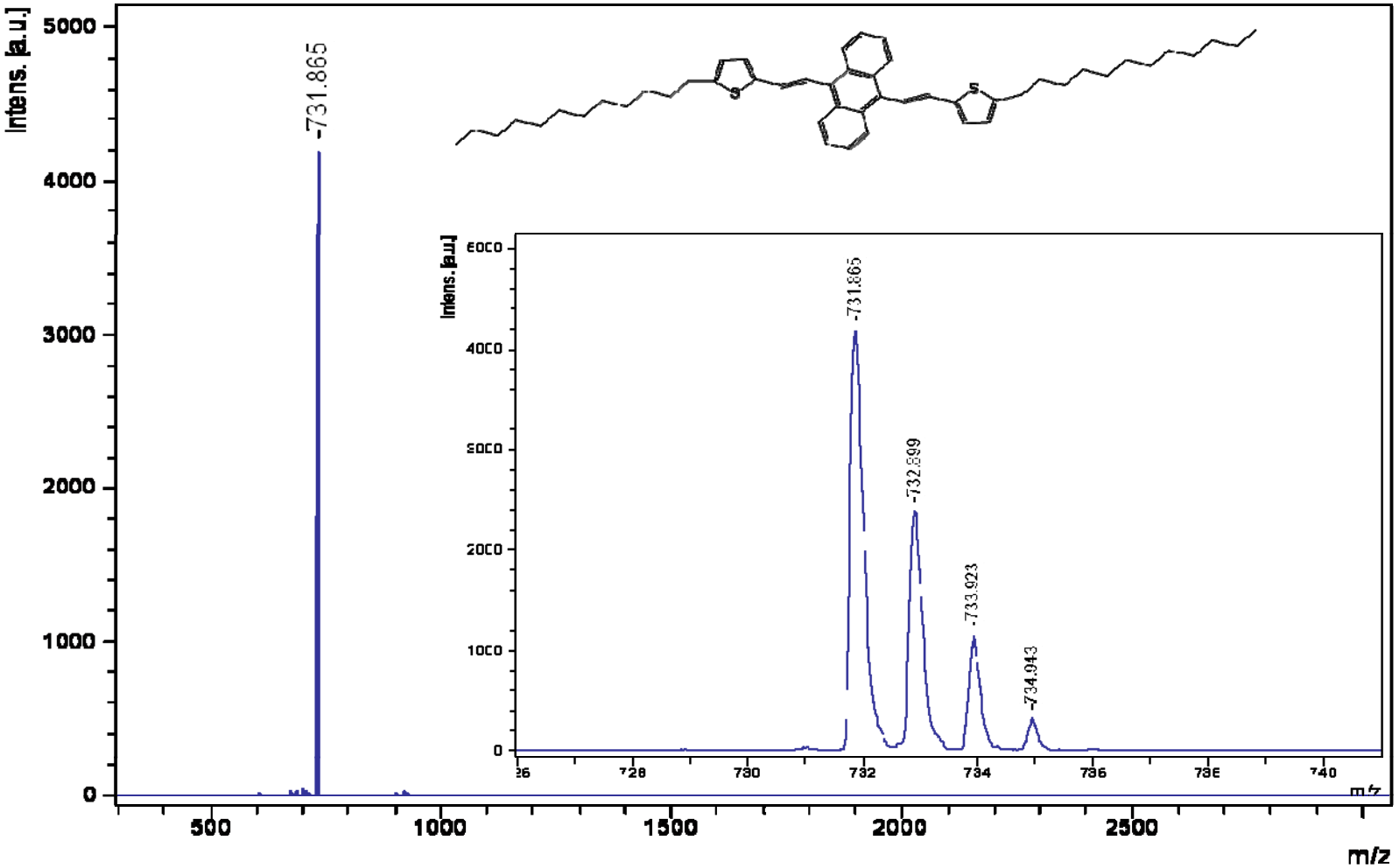


Figure S4. ^{1}H NMR spectrum of **T_2A**

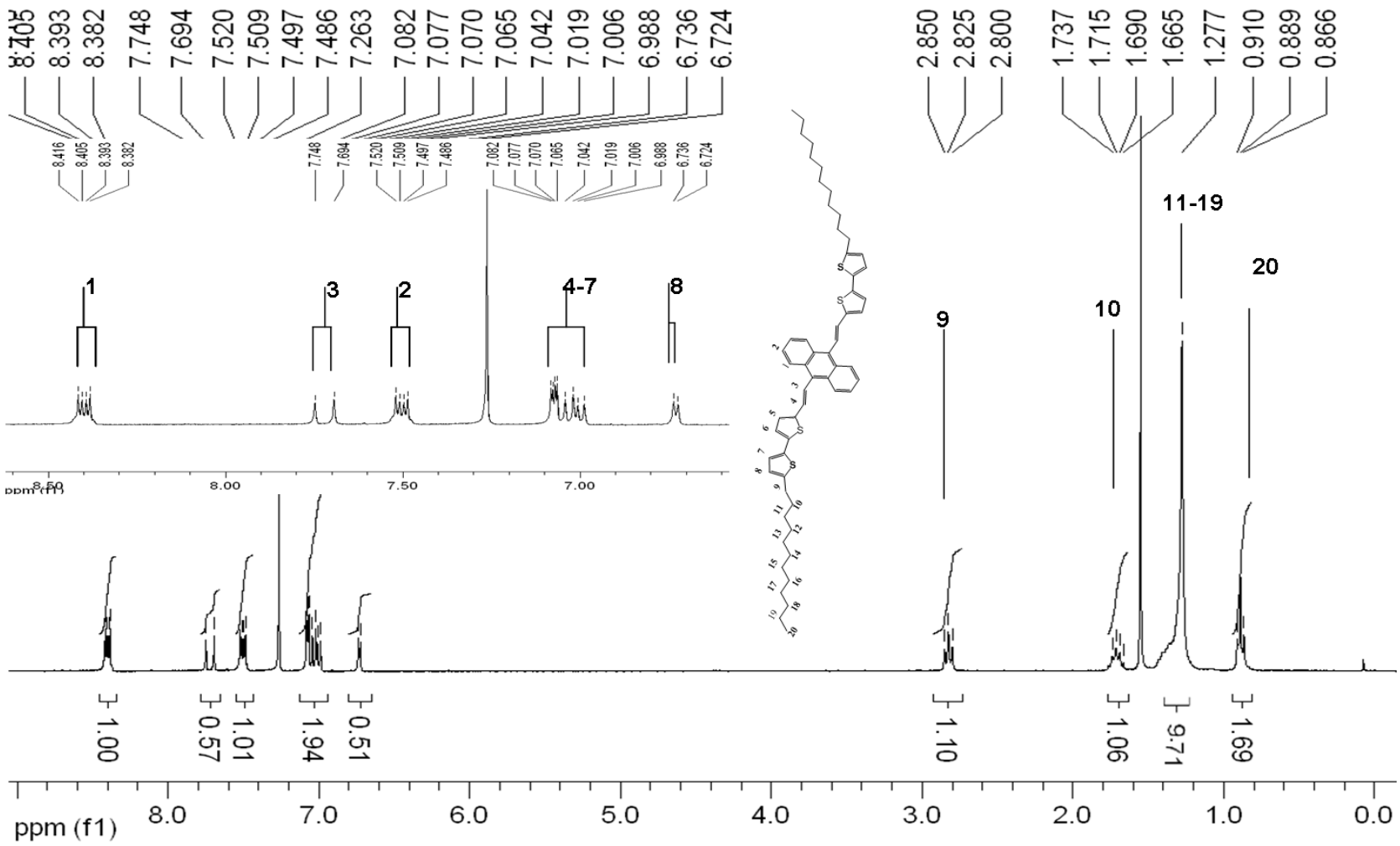


Figure S5. ^{13}C NMR spectrum of **T_2A**

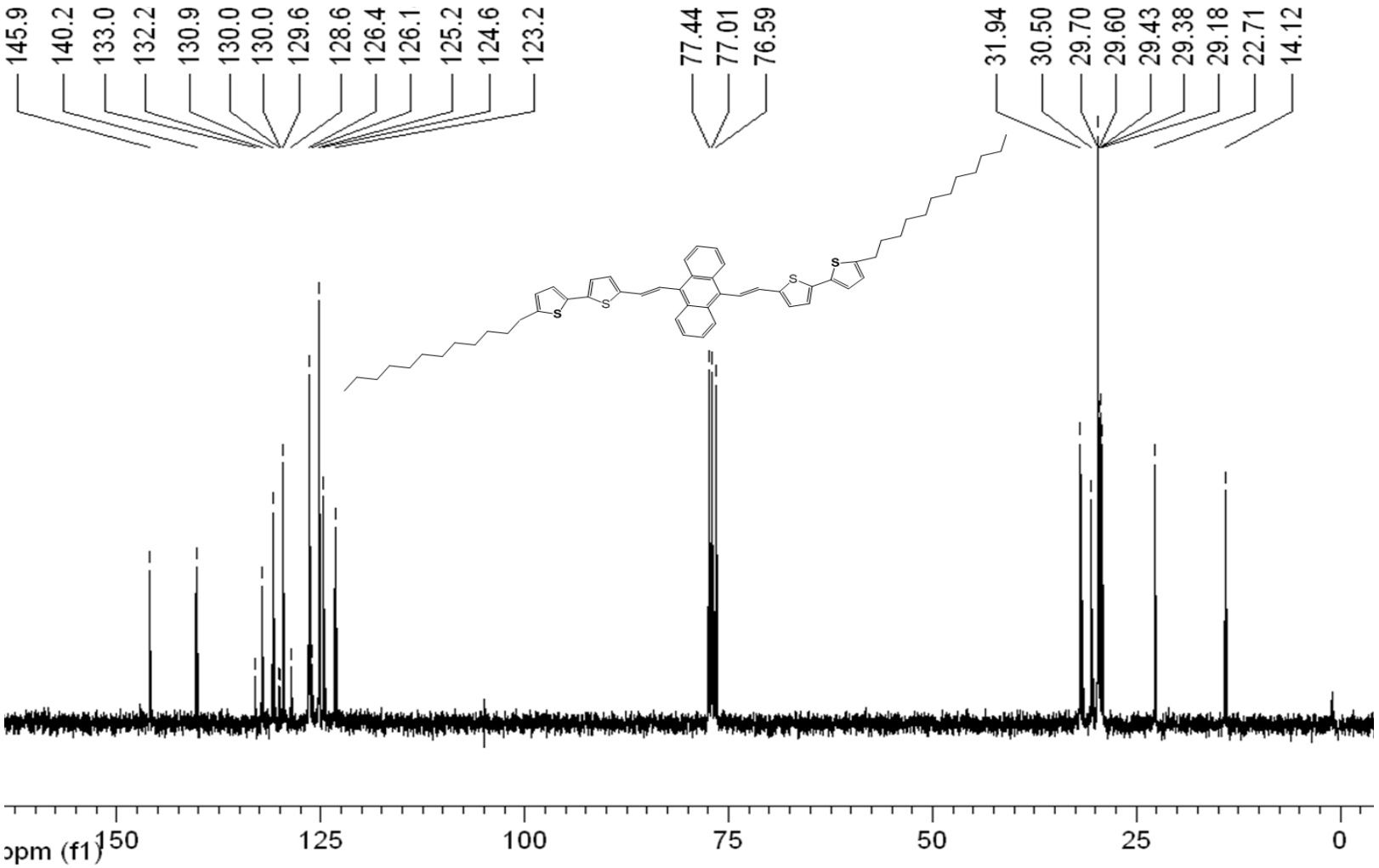


Figure S6. MALDI-TOF mass spectrum of **T_2A**

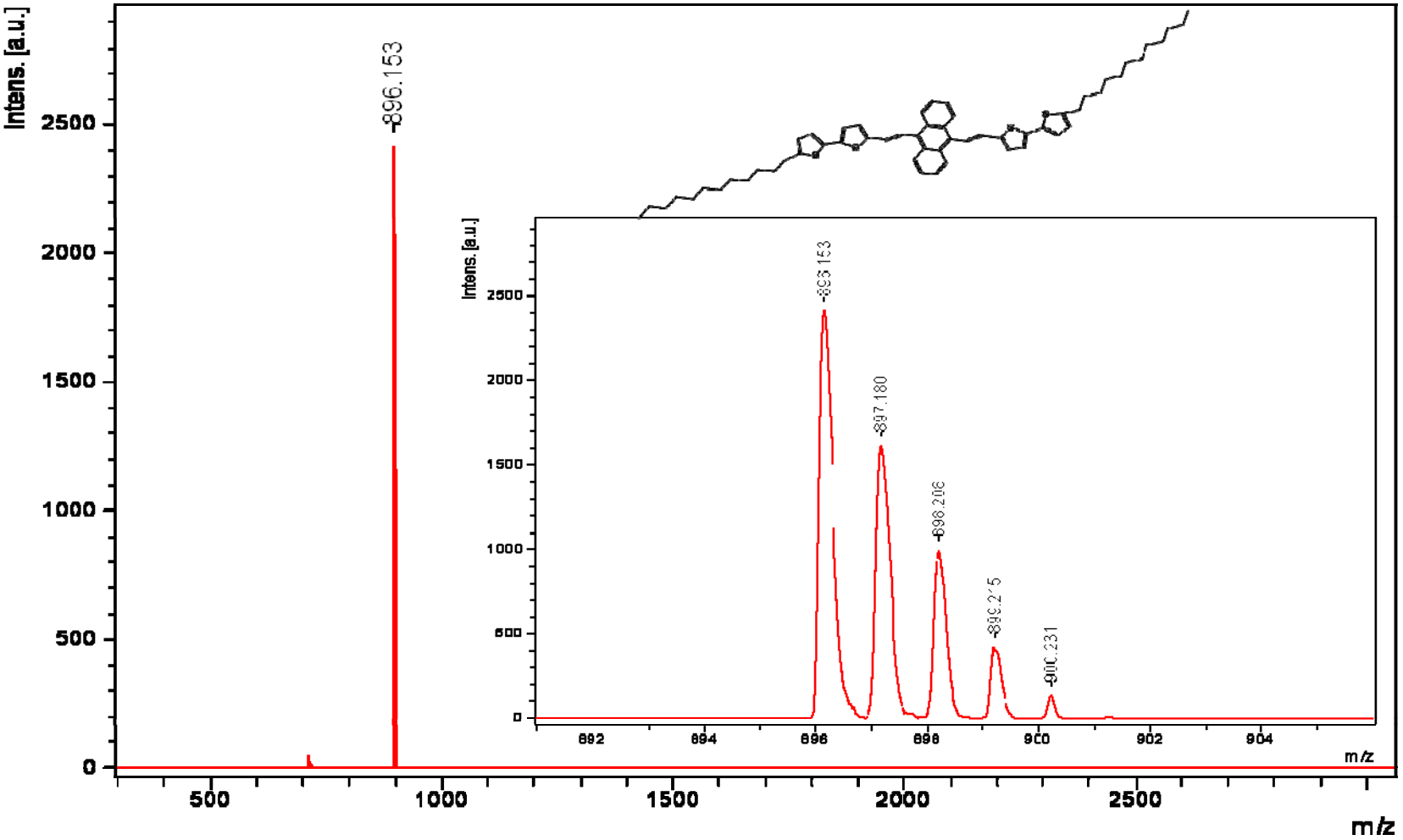


Figure S7. ^{1}H NMR spectrum of **T_3A**

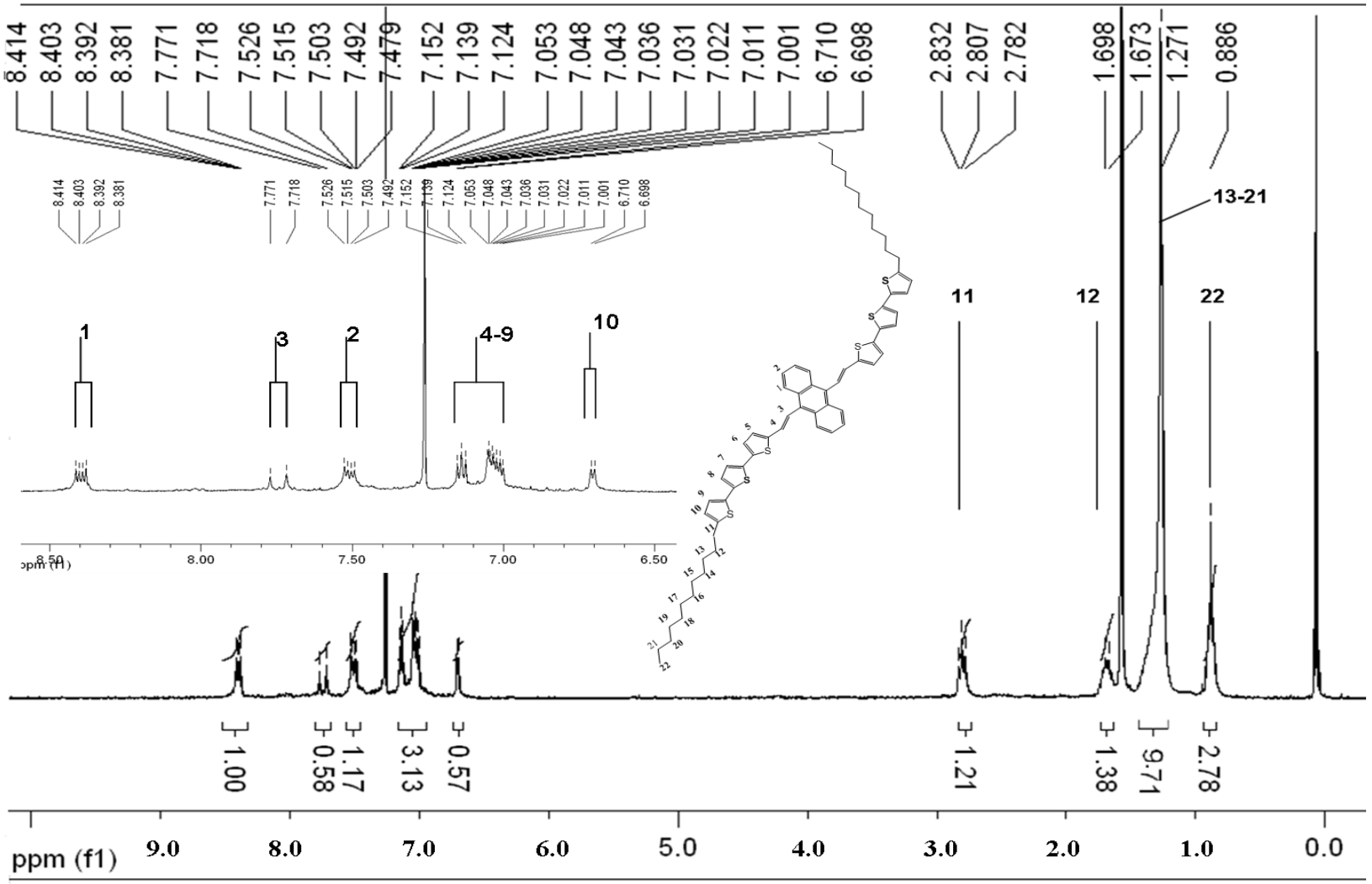


Figure S8. ^{13}C NMR spectrum of **T_3A**

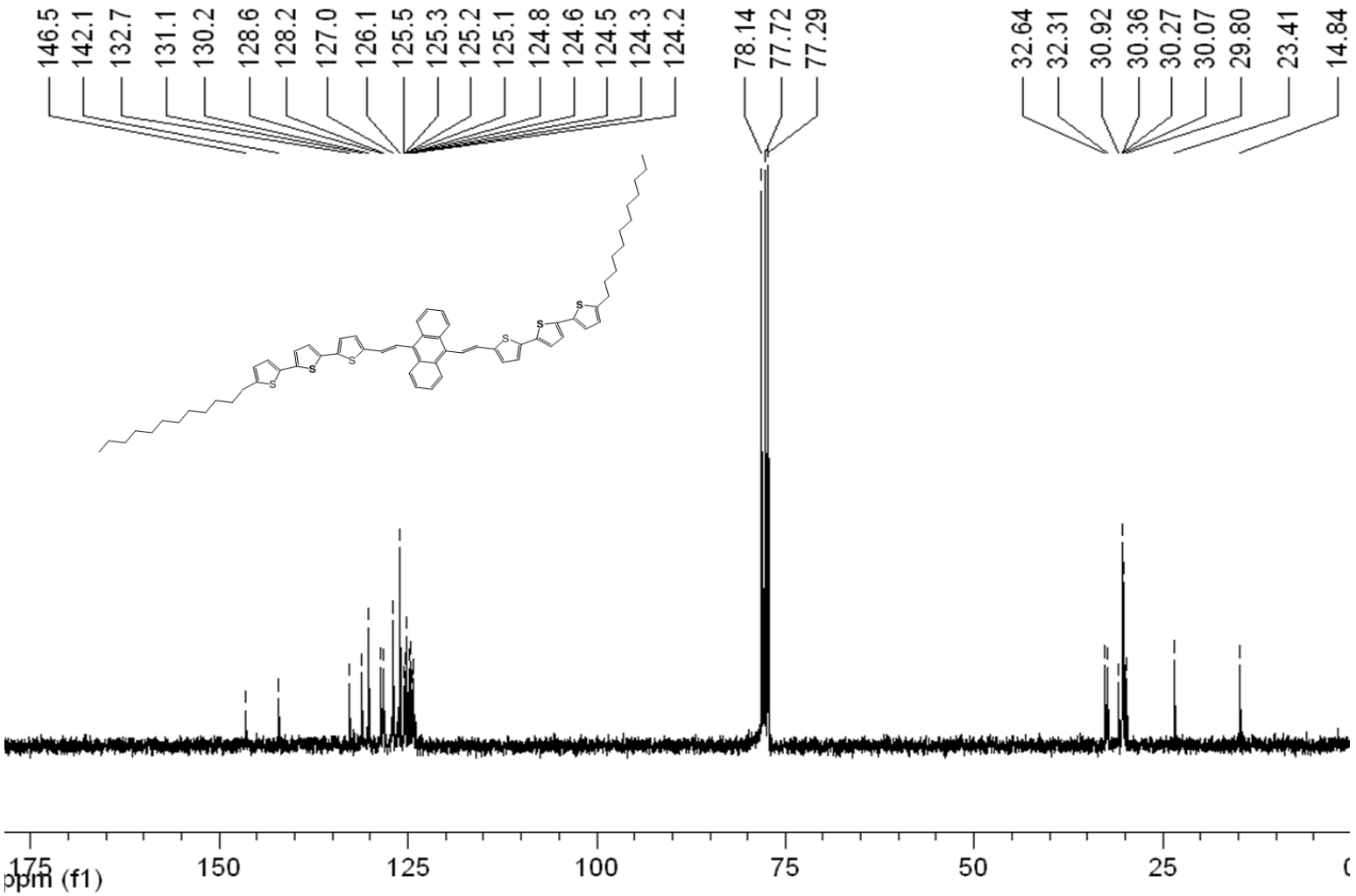
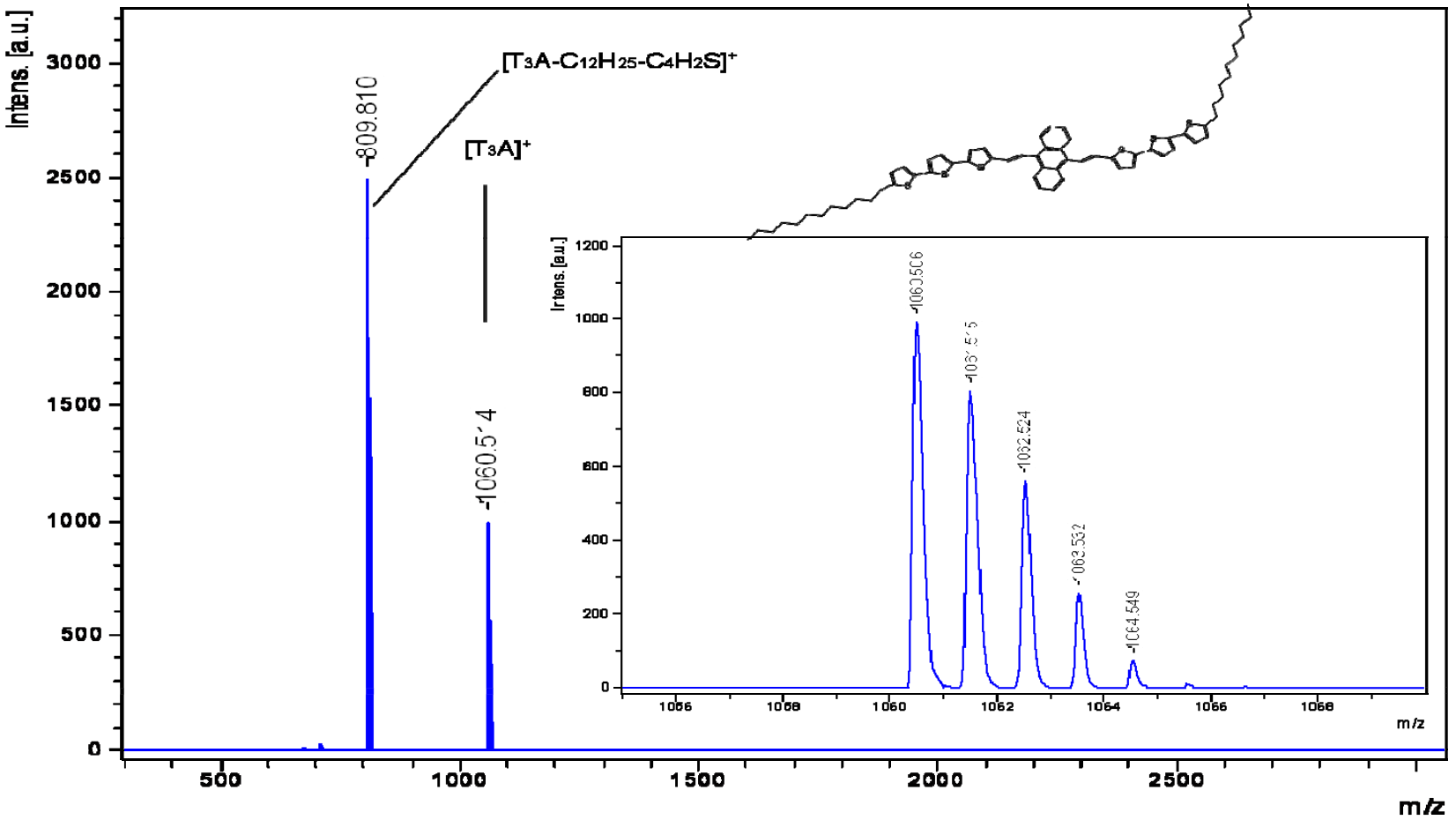
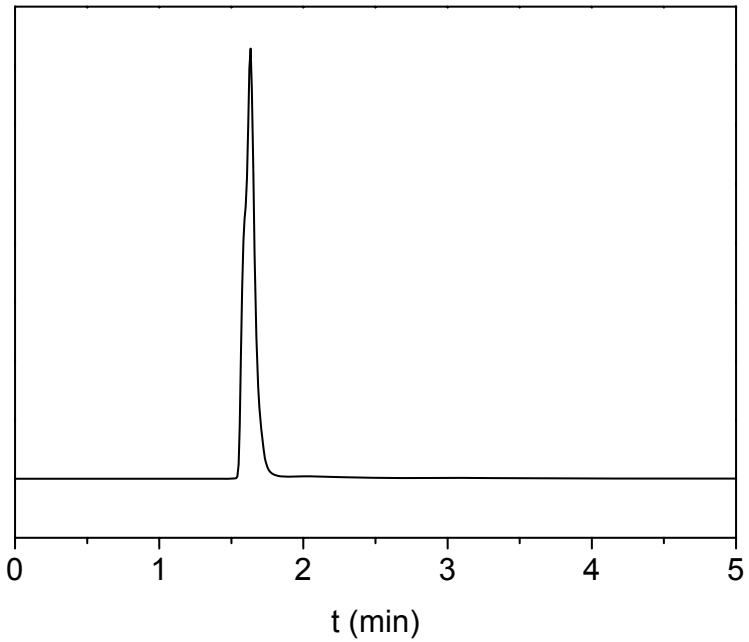


Figure S9. MALDI-TOF mass spectrum of **T_3A**



The peak at 809.810 should be assigned to $[T_3A\text{-}C_{12}H_{25}\text{-}C_4H_2S]^+$ fragment. The molecular structure and purity of **T_3A** can be confirmed by its ^1H NMR in Figure S7 and elemental analysis data in experimental section. In addition, as shown in Figure S10 below, HPLC elution curve for this compound exhibited a narrow peak, which further indicated its purity level above 99%.

Figure S10. High performance liquid chromatograms (HPLC) of **T_3A** (UV detection at 360 nm) using hexane



Calculated absorption spectra by TD-DFT simulations

Time-dependent DFT (TD-DFT) calculations have been performed at the B3LYP/6-31G** level of theory,[1-5] as implemented in the *Gaussian 03* (G03) program package.[6] The geometries of **T_1A**, **T_2A**, and **T_3A** were first fully optimized in gas phase using the default convergence criteria without any constraints and confirmed by frequency calculations. UV-Vis absorption spectra were generated assuming an average UV-vis width of 3000 cm^{-1} at half-height using the SWizard program.[7]

Table S1. Summary of Calculated Optical Transitions with Oscillator Strength $f > 0.02$

	calcd. (nm)	exp. (nm)	f	composition
T_1A	482.8	423	0.7464	HOMO->LUMO (82%)
	349.6	330	0.1982	HOMO-2->LUMO (62%)
				HOMO->LUMO+2 (23%)
	284.5		0.4821	HOMO-1->LUMO+1 (73%)
				HOMO-5->LUMO (14%)
T_2A	536.5	441	1.3946	HOMO->LUMO (85%)
	390.9	353	0.0980	HOMO-2->LUMO (48%)
				HOMO->LUMO+2 (32%)
	323.8		0.1476	HOMO-2->LUMO+2 (92%)
T_3A	573.3	440	2.0620	HOMO->LUMO (87%)
	424.5	400	0.0248	HOMO-1->LUMO+1 (34%)
				HOMO->LUMO+2 (30%)
				HOMO-2->LUMO (28%)
	407.7	384	1.1503	HOMO-1->LUMO+1 (53%)
				HOMO->LUMO+2 (12%)
				HOMO-2->LUMO (12%)
	357.3		0.1534	HOMO-2->LUMO+2 (80%)

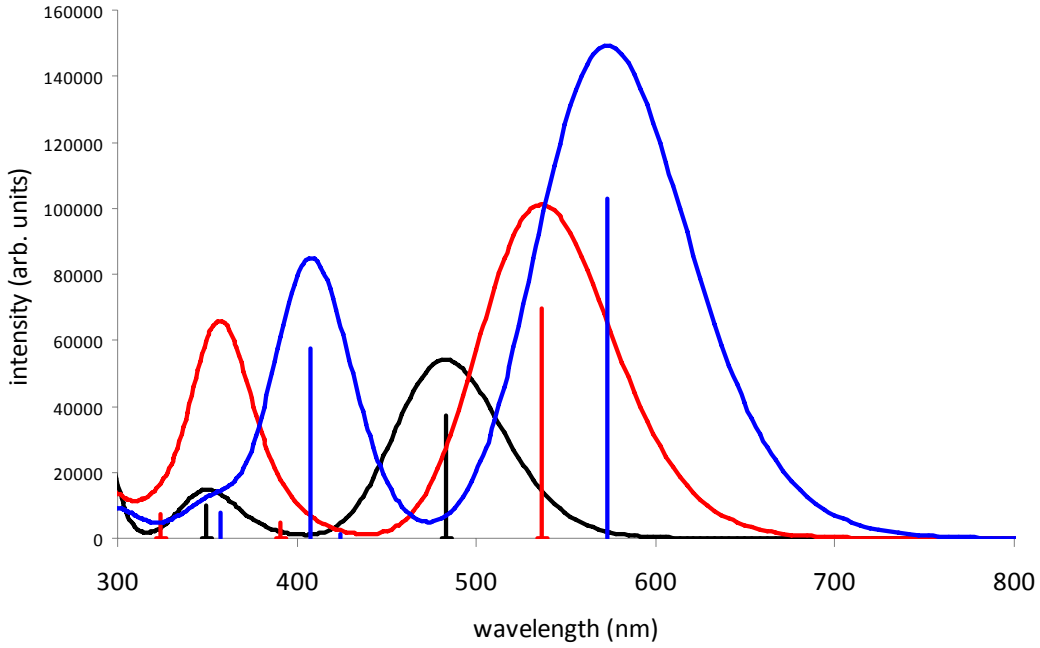


Figure S11. The UV-vis absorption spectra for **T_1A** (black curve), **T_2A** (red curve) and **T_3A** (blue curve) from TD-DFT calculations.

The TD-DFT calculations simulate the UV-vis spectra of **T_1A** and **T_2A** quite well with systematic red-shifted and slightly larger peak-peak separations. For **T_3A**, the experimental spectrum displays three closely overlapped bands, but its calculated spectrum shows two obvious absorption bands at 408 and 573 nm with a small band at 424 nm buried in that of the 408 nm one (see figure S11). We rationalize that this may be due to smaller experimental peak-peak separations and wider bandwidths. Nevertheless, no charge transfer band was obtained from the TD-DFT calculations. This is not surprised because both the anthrancene and oligothiophene groups are electron-donating. The calculated HOMO and LUMO profiles were shown in figure S12 and the absorption bands of **T_3A** can be correlated to the electronic state transitions (Table S1).

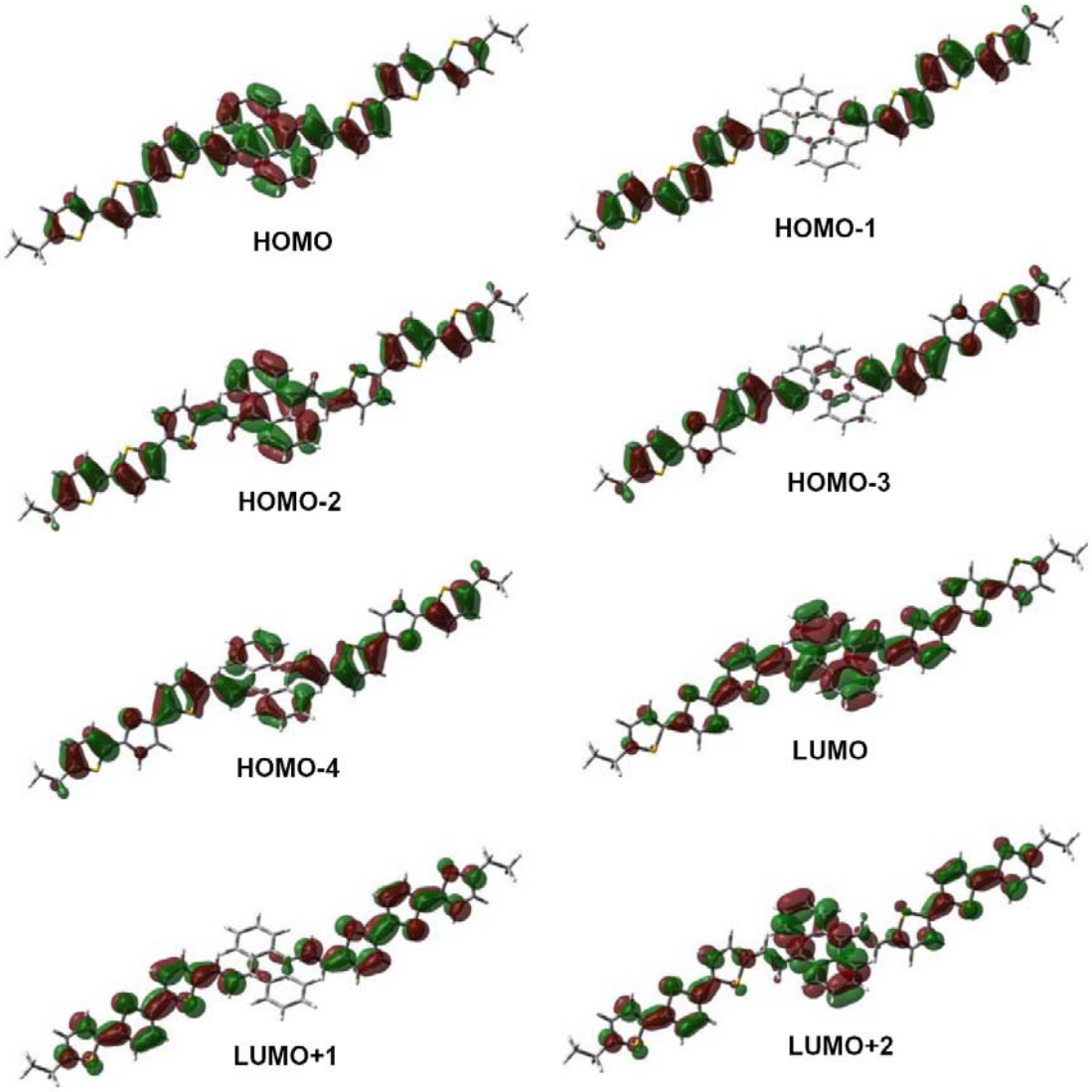


Figure S12. The HOMO and LUMO profiles for **T_3A** based on TD-DFT calculations.

References:

1. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
2. M. W. Wong, *Chem. Phys. Lett.*, 1996, **256**, 391-399.
3. R. Ditchfie, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724-728.
4. W. J. Hehre, R. Ditchfie and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.
5. P. C. Harihara and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213-222.
6. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. M. Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, N. Rega, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K.

Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle and J. A. Pople, Wallingford, CT, 2004.

7. S. I. Gorelsky, SWizard program, http://www.sg-chem.net/, 2009.

Morphology studies of thin films on substrates

The morphology of these materials was preliminarily studied by atomic force microscope (AFM) on octadecyltrichlorosilane (OTS) modified SiO_2 surface on silicon wafers. The AFM images were recorded in the tapping mode using digital instruments (Veeco metrocogy group). For experiments performed under silicon probes with resonance frequency of 300 kHz and force constant k of 40 N/m were typically used. Scan sizes of collected images corresponds to 5 μm. Images were processed and analyzed using NanoScope *5.30* software (Veeco). The thin films were prepared by spin coating techniques at 2000 rpm from 0.2 mg/ml chloroform solution by using Spin 150 instrument. The films formed by spin-coating from chloroform solutions disclosed homogeneous nanoparticles around 50 nm in diameter and 2 - 4 nm in height for all compounds (see Figure S13). Further studies on the morphology control by using other modified substrates and by choice of different solvents, temperatures and coating methods are undergoing in our lab.

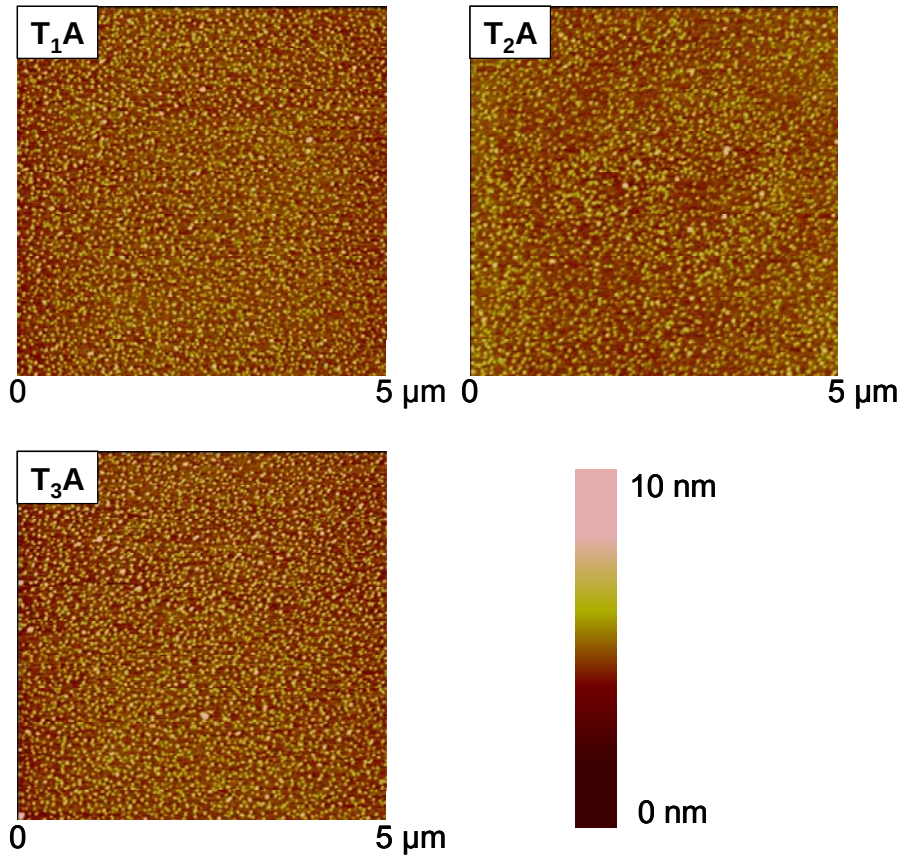


Figure S13. AFM images of **T_1A** to **T_3A** on OTS-modified silica substrate.

Crystal data of T_1A

.Table 1. Crystal data and structure refinement for T_1A.

Identification code	T_1A	
Empirical formula	C50 H66 S2	
Formula weight	731.15	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 19.6252(12) Å	α= 90°.
	b = 4.5677(3) Å	β= 101.2370(10)°.
	c = 23.5052(14) Å	γ = 90°.
Volume	2066.7(2) $Å^3$	
Z	2	
Density (calculated)	1.175 Mg/m^3	
Absorption coefficient	0.163 mm^{-1}	
F(000)	796	
Crystal size	0.80 x 0.20 x 0.16 mm^3	
Theta range for data collection	1.06 to 27.50°.	
Index ranges	-25<=h<=25, -5<=k<=5, -30<=l<=30	
Reflections collected	25113	
Independent reflections	4723 [R(int) = 0.0457]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Sadabs, (Sheldrick 2001)	
Max. and min. transmission	0.9745 and 0.8809	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4723 / 0 / 236	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0505, wR2 = 0.1278	
R indices (all data)	R1 = 0.0538, wR2 = 0.1305	
Largest diff. peak and hole	0.766 and -0.293 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for T_1A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1649(1)	-391(1)	2229(1)	18(1)
C(1)	355(1)	6869(3)	-330(1)	16(1)
C(2)	733(1)	8842(3)	-625(1)	19(1)
C(3)	1413(1)	9488(4)	-413(1)	21(1)
C(4)	1766(1)	8213(4)	113(1)	21(1)
C(5)	1421(1)	6392(3)	417(1)	19(1)
C(6)	707(1)	5645(3)	213(1)	16(1)
C(7)	351(1)	3815(3)	541(1)	16(1)
C(8)	734(1)	2588(3)	1098(1)	17(1)
C(9)	567(1)	3023(3)	1611(1)	18(1)
C(10)	925(1)	1852(3)	2163(1)	16(1)
C(11)	753(1)	2257(3)	2694(1)	17(1)
C(12)	1199(1)	761(3)	3150(1)	17(1)
C(13)	1713(1)	-766(3)	2968(1)	15(1)
C(14)	2284(1)	-2564(3)	3323(1)	17(1)
C(15)	2698(1)	-829(3)	3832(1)	17(1)
C(16)	3219(1)	-2684(3)	4245(1)	16(1)
C(17)	3620(1)	-921(3)	4752(1)	17(1)
C(18)	4111(1)	-2786(3)	5190(1)	16(1)
C(19)	4515(1)	-1021(3)	5697(1)	18(1)
C(20)	4985(1)	-2900(3)	6148(1)	17(1)
C(21)	5389(1)	-1147(3)	6654(1)	18(1)
C(22)	5843(1)	-3044(3)	7113(1)	19(1)
C(23)	6223(1)	-1327(4)	7635(1)	20(1)
C(24)	6652(1)	-3241(4)	8101(1)	22(1)
C(25)	6977(1)	-1537(4)	8644(1)	24(1)

Table 3. Bond lengths [Å] and angles [°] for T_1A.

S(1)-C(13)	1.7246(14)
S(1)-C(10)	1.7333(14)
C(1)-C(7)#1	1.4121(19)
C(1)-C(2)	1.430(2)
C(1)-C(6)	1.4409(18)
C(2)-C(3)	1.362(2)
C(3)-C(4)	1.420(2)
C(4)-C(5)	1.360(2)
C(5)-C(6)	1.4309(19)
C(6)-C(7)	1.410(2)
C(7)-C(1)#1	1.4121(19)
C(7)-C(8)	1.4874(18)
C(8)-C(9)	1.324(2)
C(9)-C(10)	1.4525(18)
C(10)-C(11)	1.3674(19)
C(11)-C(12)	1.4201(18)
C(12)-C(13)	1.361(2)
C(13)-C(14)	1.5033(18)
C(14)-C(15)	1.5309(18)
C(15)-C(16)	1.5231(18)
C(16)-C(17)	1.5238(18)
C(17)-C(18)	1.5261(18)
C(18)-C(19)	1.5260(18)
C(19)-C(20)	1.5269(18)
C(20)-C(21)	1.5226(18)
C(21)-C(22)	1.5269(19)
C(22)-C(23)	1.5231(19)
C(23)-C(24)	1.5221(19)
C(24)-C(25)	1.525(2)
C(13)-S(1)-C(10)	92.72(7)
C(7)#1-C(1)-C(2)	122.41(13)
C(7)#1-C(1)-C(6)	119.56(13)
C(2)-C(1)-C(6)	117.99(13)

C(3)-C(2)-C(1)	121.60(13)
C(2)-C(3)-C(4)	120.35(14)
C(5)-C(4)-C(3)	120.09(13)
C(4)-C(5)-C(6)	121.68(13)
C(7)-C(6)-C(5)	121.06(13)
C(7)-C(6)-C(1)	120.68(13)
C(5)-C(6)-C(1)	118.24(13)
C(6)-C(7)-C(1)#1	119.75(12)
C(6)-C(7)-C(8)	118.98(12)
C(1)#1-C(7)-C(8)	121.25(13)
C(9)-C(8)-C(7)	124.92(13)
C(8)-C(9)-C(10)	126.56(13)
C(11)-C(10)-C(9)	127.09(13)
C(11)-C(10)-S(1)	109.99(10)
C(9)-C(10)-S(1)	122.91(11)
C(10)-C(11)-C(12)	113.41(13)
C(13)-C(12)-C(11)	113.32(12)
C(12)-C(13)-C(14)	128.59(13)
C(12)-C(13)-S(1)	110.56(10)
C(14)-C(13)-S(1)	120.84(11)
C(13)-C(14)-C(15)	112.03(12)
C(16)-C(15)-C(14)	113.45(12)
C(15)-C(16)-C(17)	112.59(12)
C(16)-C(17)-C(18)	113.27(12)
C(19)-C(18)-C(17)	113.31(12)
C(18)-C(19)-C(20)	113.37(12)
C(21)-C(20)-C(19)	113.53(12)
C(20)-C(21)-C(22)	113.36(12)
C(23)-C(22)-C(21)	113.77(13)
C(24)-C(23)-C(22)	113.58(13)
C(23)-C(24)-C(25)	113.10(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for T_1A. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	16(1)	23(1)	12(1)	2(1)	0(1)	5(1)
C(1)	18(1)	17(1)	12(1)	-1(1)	1(1)	4(1)
C(2)	21(1)	21(1)	13(1)	0(1)	1(1)	0(1)
C(3)	22(1)	24(1)	18(1)	0(1)	4(1)	-3(1)
C(4)	16(1)	28(1)	18(1)	-3(1)	0(1)	0(1)
C(5)	17(1)	25(1)	14(1)	-2(1)	-1(1)	3(1)
C(6)	16(1)	18(1)	12(1)	-1(1)	1(1)	4(1)
C(7)	18(1)	17(1)	12(1)	-1(1)	1(1)	4(1)
C(8)	14(1)	18(1)	18(1)	1(1)	-2(1)	4(1)
C(9)	13(1)	21(1)	17(1)	2(1)	-2(1)	2(1)
C(10)	13(1)	17(1)	16(1)	2(1)	-2(1)	1(1)
C(11)	13(1)	21(1)	16(1)	1(1)	-1(1)	1(1)
C(12)	16(1)	22(1)	12(1)	1(1)	-1(1)	-1(1)
C(13)	15(1)	17(1)	11(1)	1(1)	-3(1)	-2(1)
C(14)	18(1)	17(1)	14(1)	1(1)	-4(1)	2(1)
C(15)	16(1)	16(1)	17(1)	0(1)	-4(1)	1(1)
C(16)	14(1)	17(1)	14(1)	0(1)	-2(1)	2(1)
C(17)	16(1)	16(1)	16(1)	0(1)	-4(1)	1(1)
C(18)	15(1)	17(1)	14(1)	1(1)	-2(1)	1(1)
C(19)	16(1)	19(1)	15(1)	-1(1)	-3(1)	2(1)
C(20)	15(1)	20(1)	14(1)	-1(1)	-2(1)	1(1)
C(21)	18(1)	19(1)	15(1)	-1(1)	-3(1)	1(1)
C(22)	18(1)	22(1)	14(1)	-1(1)	-4(1)	1(1)
C(23)	18(1)	23(1)	16(1)	-2(1)	-4(1)	0(1)
C(24)	21(1)	26(1)	17(1)	-1(1)	-4(1)	3(1)
C(25)	19(1)	37(1)	15(1)	-2(1)	-3(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for T_1A.

	x	y	z	U(eq)
H(2)	505	9723	-977	22
H(3)	1653	10799	-619	26
H(4)	2243	8634	253	25
H(5)	1660	5594	774	23
H(8)	1129	1402	1085	21
H(9)	174	4223	1618	21
H(11)	372	3425	2752	20
H(12)	1145	821	3542	21
H(14A)	2602	-3242	3071	21
H(14B)	2080	-4315	3473	21
H(15A)	2948	777	3679	21
H(15B)	2369	69	4052	21
H(16A)	3552	-3565	4027	19
H(16B)	2970	-4300	4397	19
H(17A)	3285	70	4952	20
H(17B)	3893	612	4599	20
H(18A)	3838	-4315	5343	19
H(18B)	4445	-3783	4989	19
H(19A)	4181	37	5888	21
H(19B)	4802	458	5545	21
H(20A)	4698	-4380	6299	20
H(20B)	5319	-3958	5956	20
H(21A)	5056	-44	6839	22
H(21B)	5687	293	6504	22
H(22A)	5547	-4544	7249	22
H(22B)	6190	-4077	6931	22
H(23A)	6534	117	7501	24
H(23B)	5878	-228	7806	24
H(24A)	7025	-4198	7941	27
H(24B)	6350	-4800	8210	27

H(25A)	7305	-93	8546	36
H(25B)	7223	-2892	8937	36
H(25C)	6611	-529	8799	36

Crystal data of T_2A.

Table 6. Crystal data and structure refinement for T_2A.

Identification code	T_2A	
Empirical formula	C58 H70 S4	
Formula weight	895.38	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 5.5798(3) Å	α= 90°.
	b = 7.4484(4) Å	β= 92.5160(10)°.
	c = 58.222(3) Å	γ = 90°.
Volume	2417.4(2) $Å^3$	
Z	2	
Density (calculated)	1.230 Mg/m^3	
Absorption coefficient	0.235 mm^{-1}	
F(000)	964	
Crystal size	0.38 x 0.32 x 0.06 mm^3	
Theta range for data collection	1.40 to 27.50°.	
Index ranges	-7<=h<=7, -9<=k<=9, -75<=l<=75	
Reflections collected	30296	
Independent reflections	5551 [R(int) = 0.0425]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9860 and 0.9161	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5551 / 0 / 281	
Goodness-of-fit on F^2	1.210	
Final R indices [I>2sigma(I)]	R1 = 0.0607, wR2 = 0.1359	
R indices (all data)	R1 = 0.0660, wR2 = 0.1383	
Largest diff. peak and hole	0.641 and -0.401 $e.Å^{-3}$	

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for T_2A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	5581(1)	-3595(1)	674(1)	16(1)
S(2)	3198(1)	180(1)	1196(1)	19(1)
C(1)	3576(4)	-5373(3)	655(1)	17(1)
C(2)	1816(5)	-5160(3)	810(1)	23(1)
C(3)	2075(4)	-3585(3)	945(1)	20(1)
C(4)	4039(4)	-2588(3)	894(1)	15(1)
C(5)	4873(4)	-907(3)	993(1)	14(1)
C(6)	6921(4)	39(3)	956(1)	22(1)
C(7)	7118(4)	1636(3)	1089(1)	21(1)
C(8)	5253(4)	1913(3)	1227(1)	15(1)
C(9)	3734(4)	-6815(3)	489(1)	22(1)
C(10)	5128(4)	-6947(3)	314(1)	19(1)
C(11)	5054(4)	-8500(3)	152(1)	16(1)
C(12)	3303(4)	-8589(3)	-29(1)	16(1)
C(13)	3250(4)	-10112(3)	-182(1)	15(1)
C(14)	1423(4)	-10168(3)	-362(1)	19(1)
C(15)	-247(4)	-8851(3)	-389(1)	22(1)
C(16)	-190(4)	-7349(3)	-240(1)	21(1)
C(17)	1528(4)	-7226(3)	-66(1)	19(1)
C(18)	4836(4)	3409(3)	1393(1)	18(1)
C(19)	6742(4)	4885(3)	1391(1)	17(1)
C(20)	6304(4)	6350(3)	1567(1)	18(1)
C(21)	8161(4)	7851(3)	1567(1)	18(1)
C(22)	7786(4)	9263(3)	1752(1)	19(1)
C(23)	9633(4)	10776(3)	1755(1)	18(1)
C(24)	9262(4)	12167(3)	1943(1)	19(1)
C(25)	11101(4)	13685(3)	1946(1)	19(1)
C(26)	10725(4)	15074(3)	2134(1)	19(1)
C(27)	12531(4)	16608(3)	2138(1)	18(1)
C(28)	12107(4)	17990(3)	2324(1)	21(1)
C(29)	13924(5)	19511(4)	2332(1)	28(1)

Table 8. Bond lengths [Å] and angles [°] for T_2A.

S(1)-C(1)	1.733(2)
S(1)-C(4)	1.742(2)
S(2)-C(8)	1.731(2)
S(2)-C(5)	1.739(2)
C(1)-C(2)	1.371(3)
C(1)-C(9)	1.453(3)
C(2)-C(3)	1.417(3)
C(3)-C(4)	1.368(3)
C(4)-C(5)	1.447(3)
C(5)-C(6)	1.367(3)
C(6)-C(7)	1.421(3)
C(7)-C(8)	1.356(3)
C(8)-C(18)	1.500(3)
C(9)-C(10)	1.313(3)
C(10)-C(11)	1.490(3)
C(11)-C(13)#1	1.407(3)
C(11)-C(12)	1.407(3)
C(12)-C(17)	1.428(3)
C(12)-C(13)	1.441(3)
C(13)-C(11)#1	1.407(3)
C(13)-C(14)	1.433(3)
C(14)-C(15)	1.357(3)
C(15)-C(16)	1.414(3)
C(16)-C(17)	1.366(3)
C(18)-C(19)	1.530(3)
C(19)-C(20)	1.525(3)
C(20)-C(21)	1.524(3)
C(21)-C(22)	1.527(3)
C(22)-C(23)	1.527(3)

C(23)-C(24)	1.527(3)
C(24)-C(25)	1.526(3)
C(25)-C(26)	1.526(3)
C(26)-C(27)	1.523(3)
C(27)-C(28)	1.523(3)
C(28)-C(29)	1.520(3)

C(1)-S(1)-C(4)	92.15(11)
C(8)-S(2)-C(5)	92.55(11)
C(2)-C(1)-C(9)	126.2(2)
C(2)-C(1)-S(1)	110.41(18)
C(9)-C(1)-S(1)	123.34(18)
C(1)-C(2)-C(3)	113.8(2)
C(4)-C(3)-C(2)	113.0(2)
C(3)-C(4)-C(5)	129.0(2)
C(3)-C(4)-S(1)	110.70(17)
C(5)-C(4)-S(1)	120.30(17)
C(6)-C(5)-C(4)	129.8(2)
C(6)-C(5)-S(2)	110.10(17)
C(4)-C(5)-S(2)	120.04(17)
C(5)-C(6)-C(7)	113.1(2)
C(8)-C(7)-C(6)	114.0(2)
C(7)-C(8)-C(18)	129.7(2)
C(7)-C(8)-S(2)	110.32(18)
C(18)-C(8)-S(2)	120.00(17)
C(10)-C(9)-C(1)	129.0(2)
C(9)-C(10)-C(11)	123.2(2)
C(13)#1-C(11)-C(12)	119.9(2)
C(13)#1-C(11)-C(10)	119.5(2)
C(12)-C(11)-C(10)	120.6(2)
C(11)-C(12)-C(17)	122.3(2)
C(11)-C(12)-C(13)	119.6(2)
C(17)-C(12)-C(13)	118.1(2)
C(11)#1-C(13)-C(14)	121.5(2)
C(11)#1-C(13)-C(12)	120.5(2)
C(14)-C(13)-C(12)	118.1(2)

C(15)-C(14)-C(13)	121.6(2)
C(14)-C(15)-C(16)	120.4(2)
C(17)-C(16)-C(15)	120.2(2)
C(16)-C(17)-C(12)	121.6(2)
C(8)-C(18)-C(19)	113.62(19)
C(20)-C(19)-C(18)	112.14(19)
C(21)-C(20)-C(19)	113.40(19)
C(20)-C(21)-C(22)	113.08(19)
C(23)-C(22)-C(21)	113.69(19)
C(22)-C(23)-C(24)	113.27(19)
C(25)-C(24)-C(23)	113.6(2)
C(26)-C(25)-C(24)	113.5(2)
C(27)-C(26)-C(25)	114.0(2)
C(28)-C(27)-C(26)	113.2(2)
C(29)-C(28)-C(27)	113.6(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y-2,-z

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for T_2A. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	15(1)	16(1)	18(1)	-7(1)	2(1)	-2(1)
S(2)	15(1)	17(1)	24(1)	-9(1)	4(1)	-3(1)
C(1)	21(1)	14(1)	17(1)	-3(1)	1(1)	-2(1)
C(2)	27(1)	20(1)	23(1)	-6(1)	7(1)	-8(1)
C(3)	23(1)	20(1)	18(1)	-4(1)	5(1)	-1(1)
C(4)	16(1)	16(1)	13(1)	-4(1)	1(1)	5(1)
C(5)	17(1)	15(1)	12(1)	-4(1)	0(1)	3(1)
C(6)	23(1)	22(1)	21(1)	-4(1)	7(1)	0(1)
C(7)	23(1)	19(1)	21(1)	-3(1)	5(1)	-6(1)
C(8)	17(1)	12(1)	17(1)	-1(1)	-1(1)	-1(1)
C(9)	24(1)	15(1)	25(1)	-7(1)	3(1)	-5(1)
C(10)	22(1)	13(1)	21(1)	-5(1)	1(1)	-2(1)
C(11)	21(1)	13(1)	14(1)	-1(1)	5(1)	-3(1)
C(12)	20(1)	14(1)	14(1)	-1(1)	4(1)	-2(1)
C(13)	19(1)	14(1)	14(1)	-1(1)	2(1)	-2(1)
C(14)	24(1)	15(1)	18(1)	-3(1)	0(1)	-2(1)
C(15)	23(1)	20(1)	21(1)	1(1)	-5(1)	-2(1)
C(16)	23(1)	16(1)	25(1)	1(1)	1(1)	5(1)
C(17)	24(1)	13(1)	19(1)	-4(1)	2(1)	2(1)
C(18)	20(1)	17(1)	17(1)	-5(1)	3(1)	-1(1)
C(19)	19(1)	14(1)	19(1)	-2(1)	1(1)	1(1)
C(20)	20(1)	13(1)	20(1)	-3(1)	2(1)	-1(1)
C(21)	19(1)	13(1)	21(1)	-3(1)	0(1)	-1(1)
C(22)	21(1)	14(1)	20(1)	-3(1)	1(1)	-1(1)
C(23)	20(1)	14(1)	20(1)	-3(1)	1(1)	-1(1)
C(24)	22(1)	15(1)	20(1)	-3(1)	2(1)	-1(1)
C(25)	21(1)	16(1)	20(1)	-3(1)	1(1)	-1(1)
C(26)	23(1)	15(1)	19(1)	-3(1)	1(1)	-2(1)
C(27)	22(1)	15(1)	17(1)	-2(1)	0(1)	-3(1)
C(28)	24(1)	19(1)	20(1)	-5(1)	0(1)	-2(1)
C(29)	34(1)	21(1)	29(1)	-9(1)	-1(1)	-7(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for T_2A.

	x	y	z	U(eq)
H(2)	541	-5990	825	28
H(3)	997	-3257	1060	24
H(6)	8092	-333	853	26
H(7)	8438	2437	1083	25
H(9)	2683	-7800	509	26
H(10)	6238	-6007	289	22
H(14A)	1380	-11151	-466	23
H(15A)	-1463	-8939	-508	26
H(16A)	-1350	-6423	-261	26
H(17A)	1543	-6208	32	23
H(18A)	4800	2903	1550	21
H(18B)	3245	3949	1355	21
H(19A)	8342	4346	1424	21
H(19B)	6743	5426	1235	21
H(20A)	4693	6872	1534	21
H(20B)	6313	5804	1722	21
H(21A)	8091	8443	1415	22
H(21B)	9780	7323	1591	22
H(22A)	6164	9788	1728	22
H(22B)	7852	8668	1904	22
H(23A)	9551	11384	1604	22
H(23B)	11257	10252	1777	22
H(24A)	7637	12688	1920	23
H(24B)	9344	11557	2094	23
H(25A)	12727	13165	1969	23

H(25B)	11020	14296	1795	23
H(26A)	9090	15580	2112	23
H(26B)	10824	14464	2285	23
H(27A)	14166	16108	2162	21
H(27B)	12448	17214	1986	21
H(28A)	10480	18503	2298	25
H(28B)	12159	17378	2475	25
H(29A)	15528	19026	2369	42
H(29B)	13506	20379	2450	42
H(29C)	13912	20109	2182	42