Supplementary Information for

Thiophene-fused isoindigo based conjugated polymers for ambipolar organic field-effect transistors

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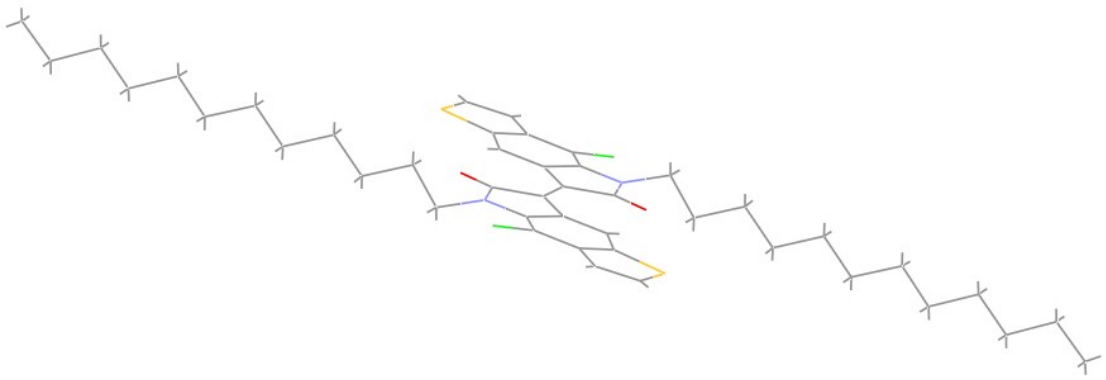


Figure S1. Single crystal structures of C12-TII.

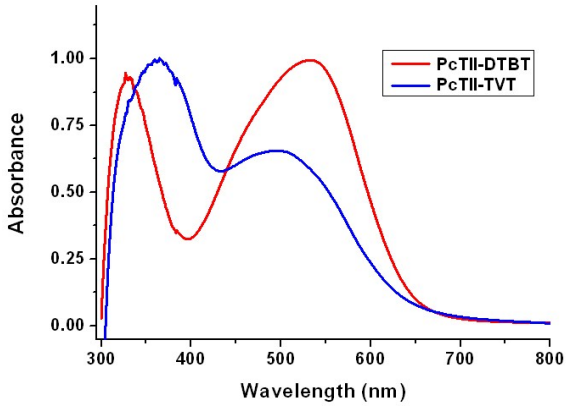


Figure S2. Normalized UV-vis absorption spectra of both TII-based cross-conjugated polymers in thin film.

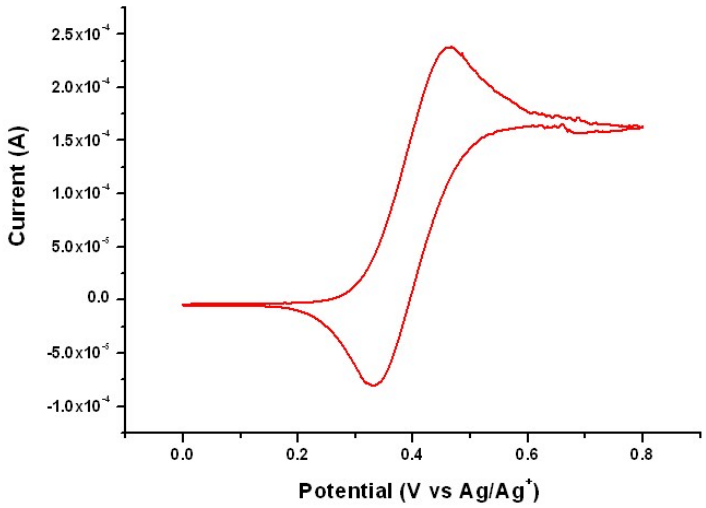


Figure S3. Cyclic voltammogram of ferrocene in 0.1M acetonitrile solution of *n*-Bu_4NPF_6.

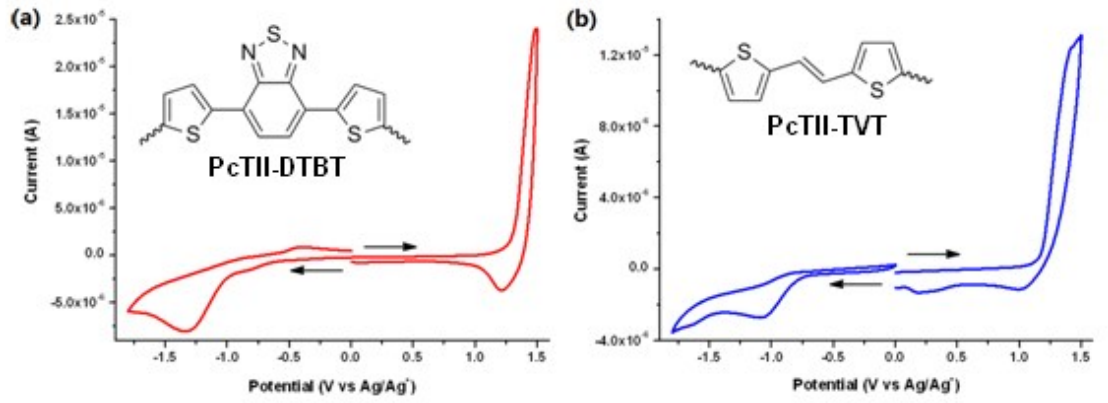


Figure S4. Cyclic voltammogram of (a) **P*c*TII-DTBT** and (b) **P*c*TII-TVT** in thin film drop-casting on a glassy carbon electrode and tested in *n*-Bu_4NPF_6/CH_3CN solution (scan rate: 0.1 V/s).

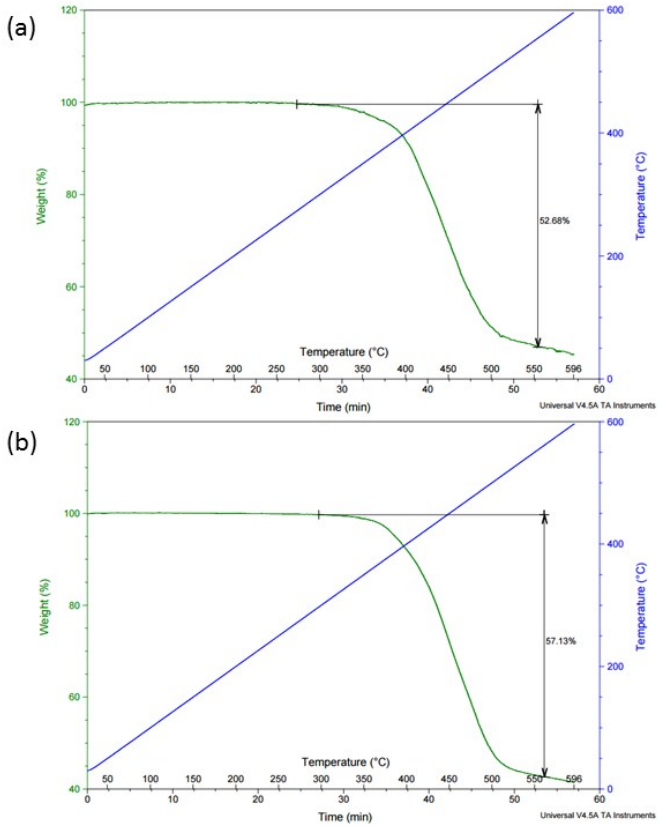


Figure S5. Thermal gravity analyses (TGA) of (a) **PTII-T** (5% loss, 380 °C) and (b) **PTII-TVT-8** (5% loss, 385 °C).

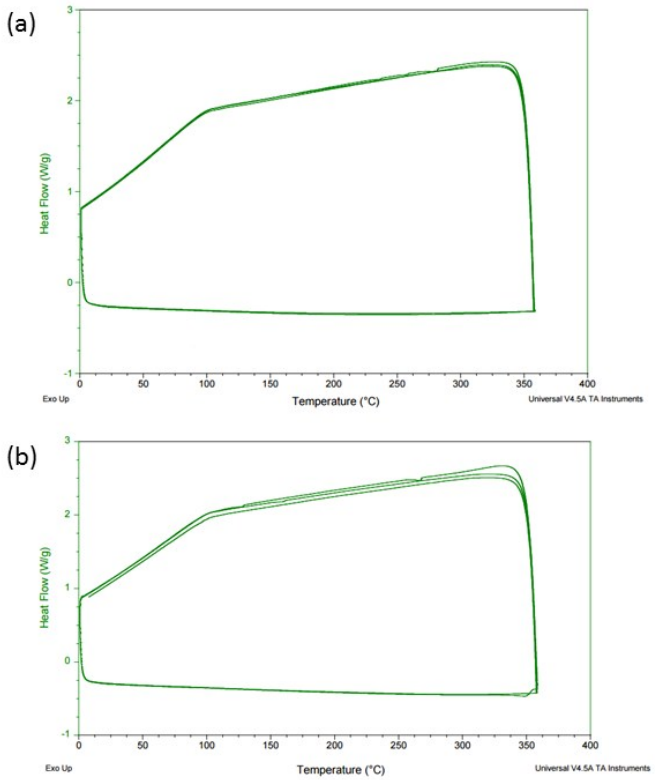


Figure S6. DSC traces of (a) **PTII-T** and (b) **PTII-TVT-8** (scan rate: 10 ^{o}C/min).

OFET properties of TII based polymers.

Table S1. Optical (UV-vis) properties and electrochemical data.

	λ_{max} (nm) solution	λ_{max} (nm) film	$E_g^{Optical}$ (eV)	LUMO (eV)	HOMO (eV)	E_g^{CV} (eV)	μ_e (cm^2/Vs)	μ_h (cm^2/Vs)
PcTII-DTBT	517	532	1.81	-3.85	-5.73	1.88	1.38×10^{-4}	1.53×10^{-5}
PcTII-TVT	492	497	1.81	-3.64	-5.61	1.97	1.15×10^{-4}	2.16×10^{-6}

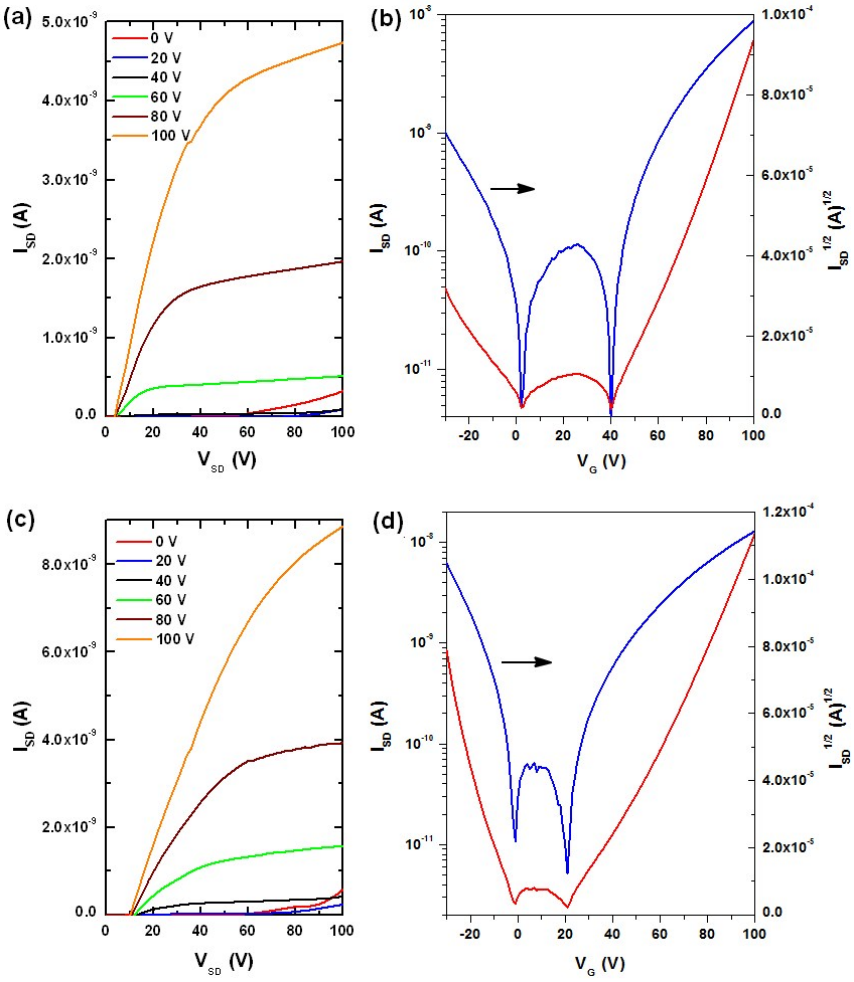


Figure S7. (a) Output and (b) transfer characteristics of **P*c*TII-TVT** devices fabricated in ambient; (c) output and (d) transfer characteristics of **P*c*TII-DTBT** devices fabricated in ambient. OFET devices (W/L = 20) were fabricated with CYTOP.

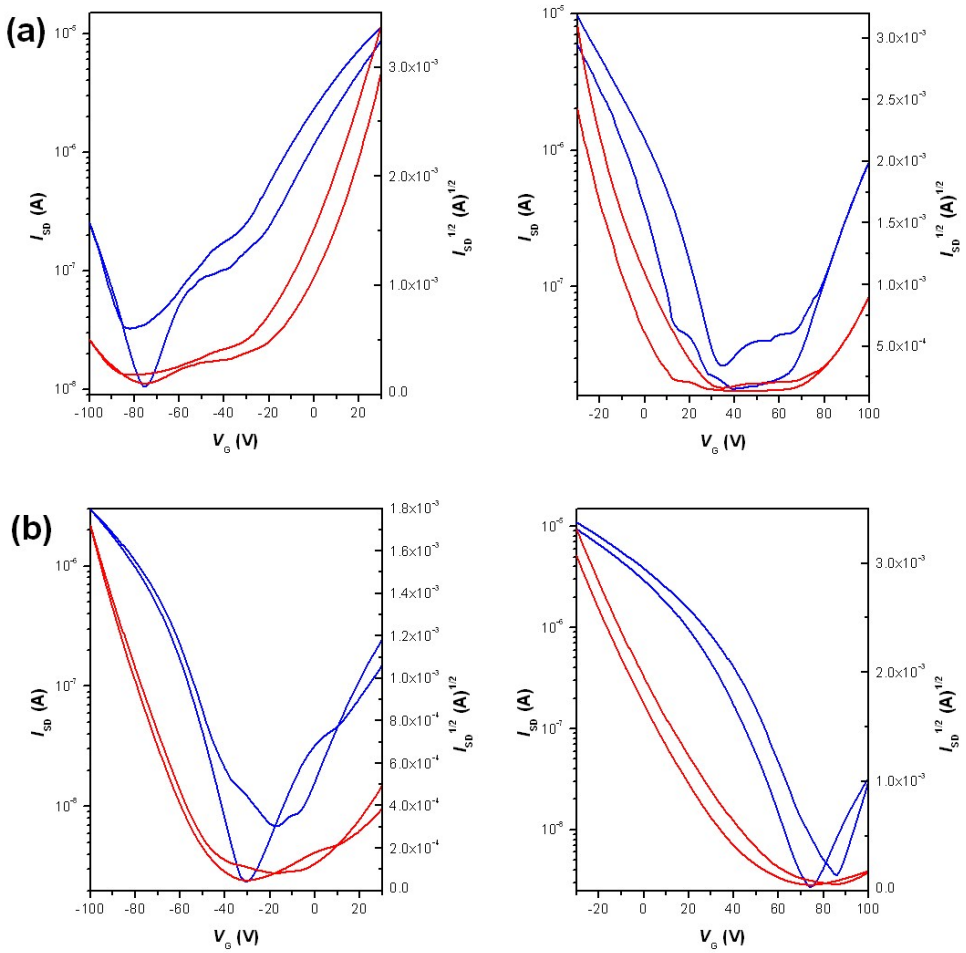
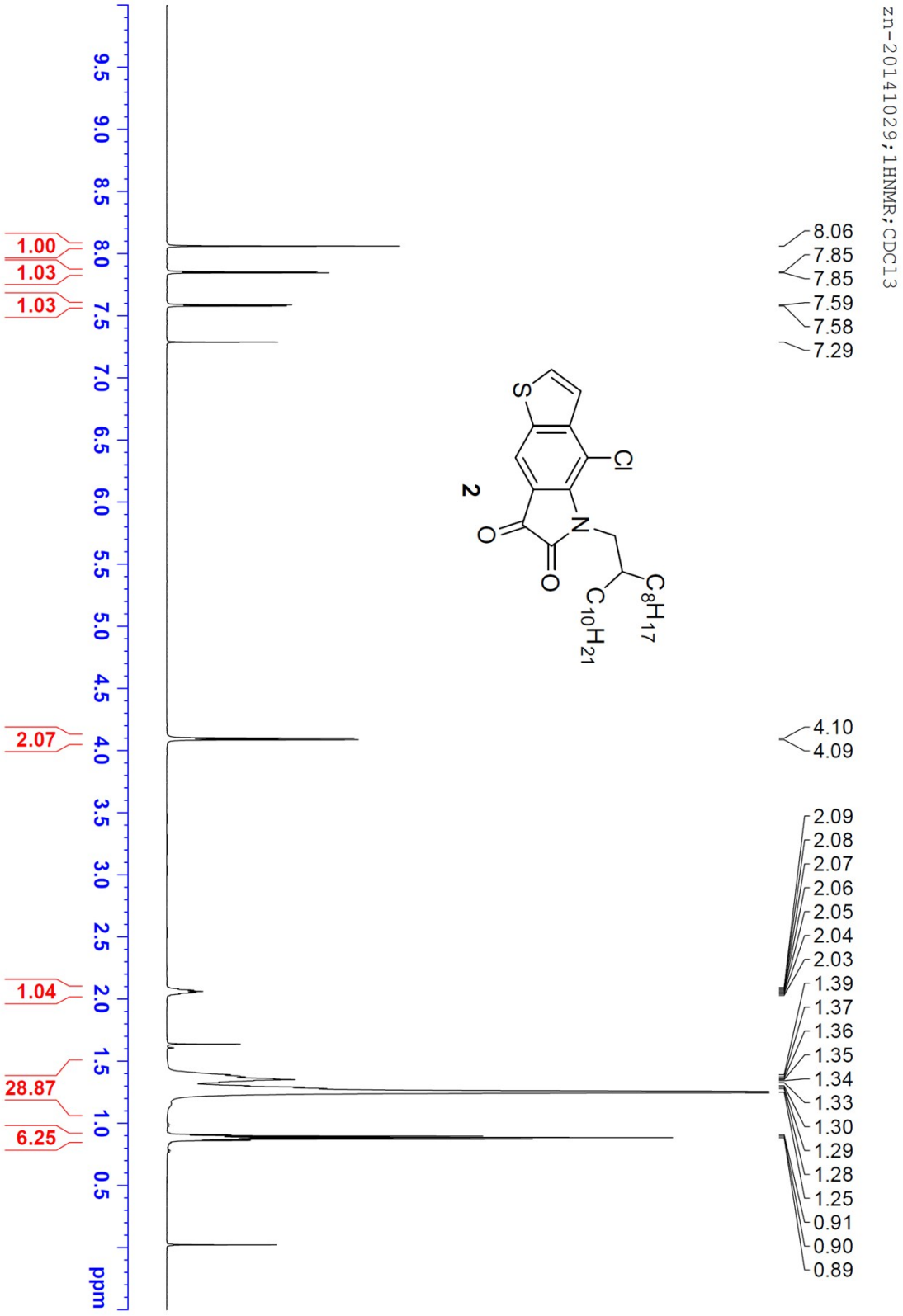
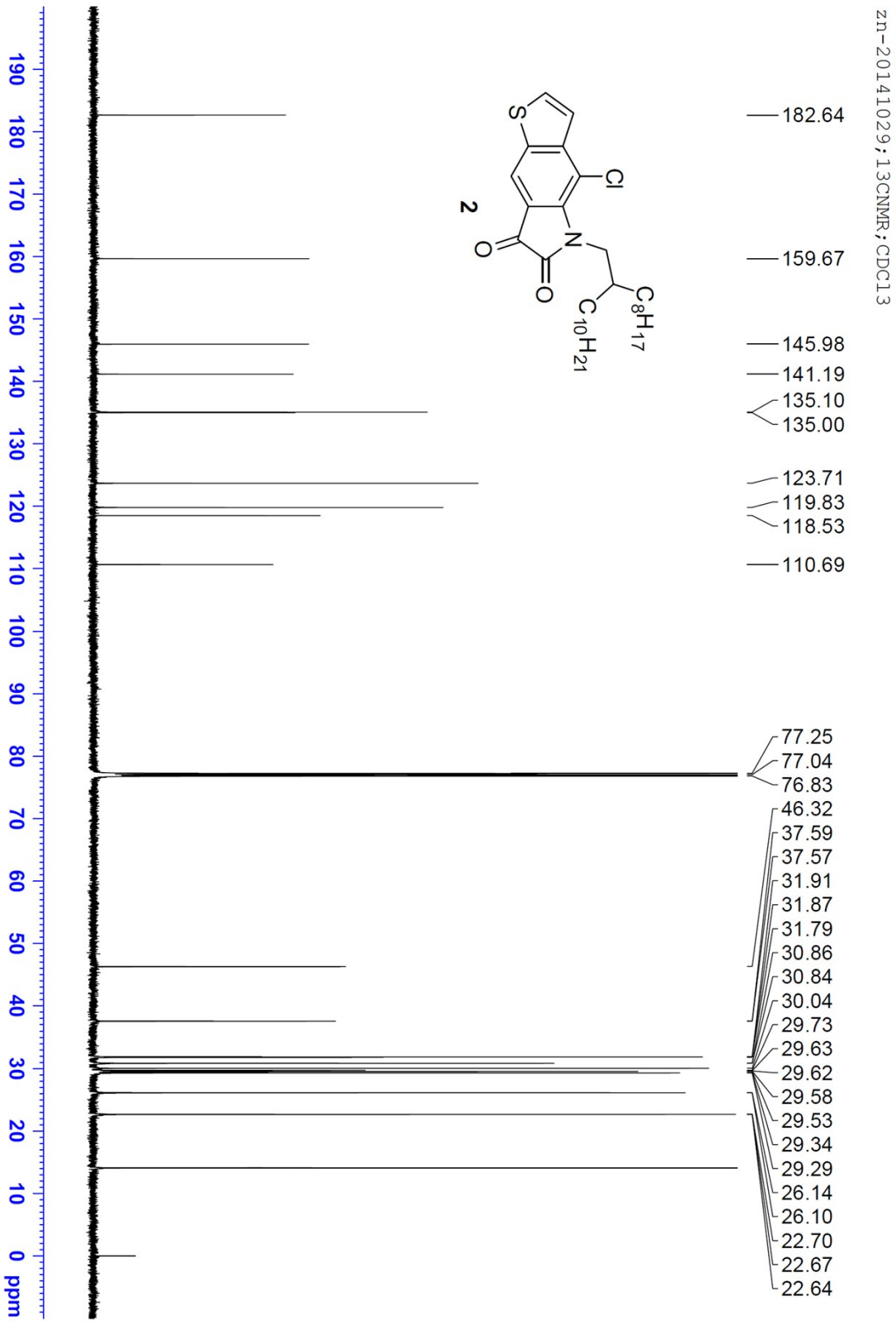


Figure S8. Transfer characteristics of (a) **PTII-T** and (b) **PTII-TVT-8** devices fabricated in ambient. OFET devices (W/L = 20) were fabricated with CYTOP.

^{1}H and ^{13}C NMR spectra of related compounds.

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135.10
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110.69
77.25
77.04
76.83
46.32
37.59
37.57
31.91
31.87
31.79
30.86
30.84
30.04
29.73
29.63
29.62
29.58
29.53
29.34
29.29
26.14
26.10
22.70
22.67
22.64
S
Cl
N
O
O
2
C8H17
C10H21
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60
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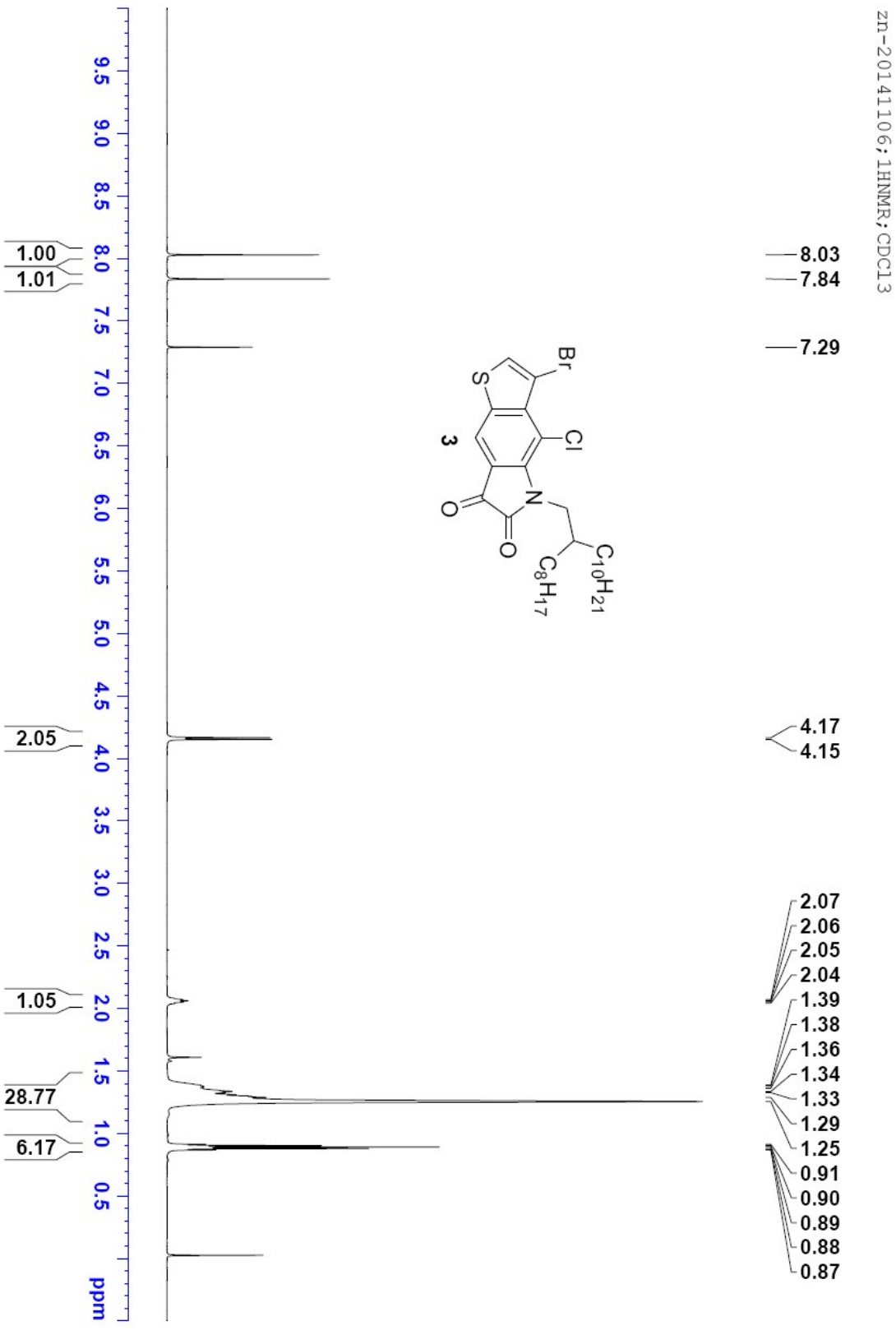
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1.36
1.34
1.33
1.29
1.25
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0.87
1.00
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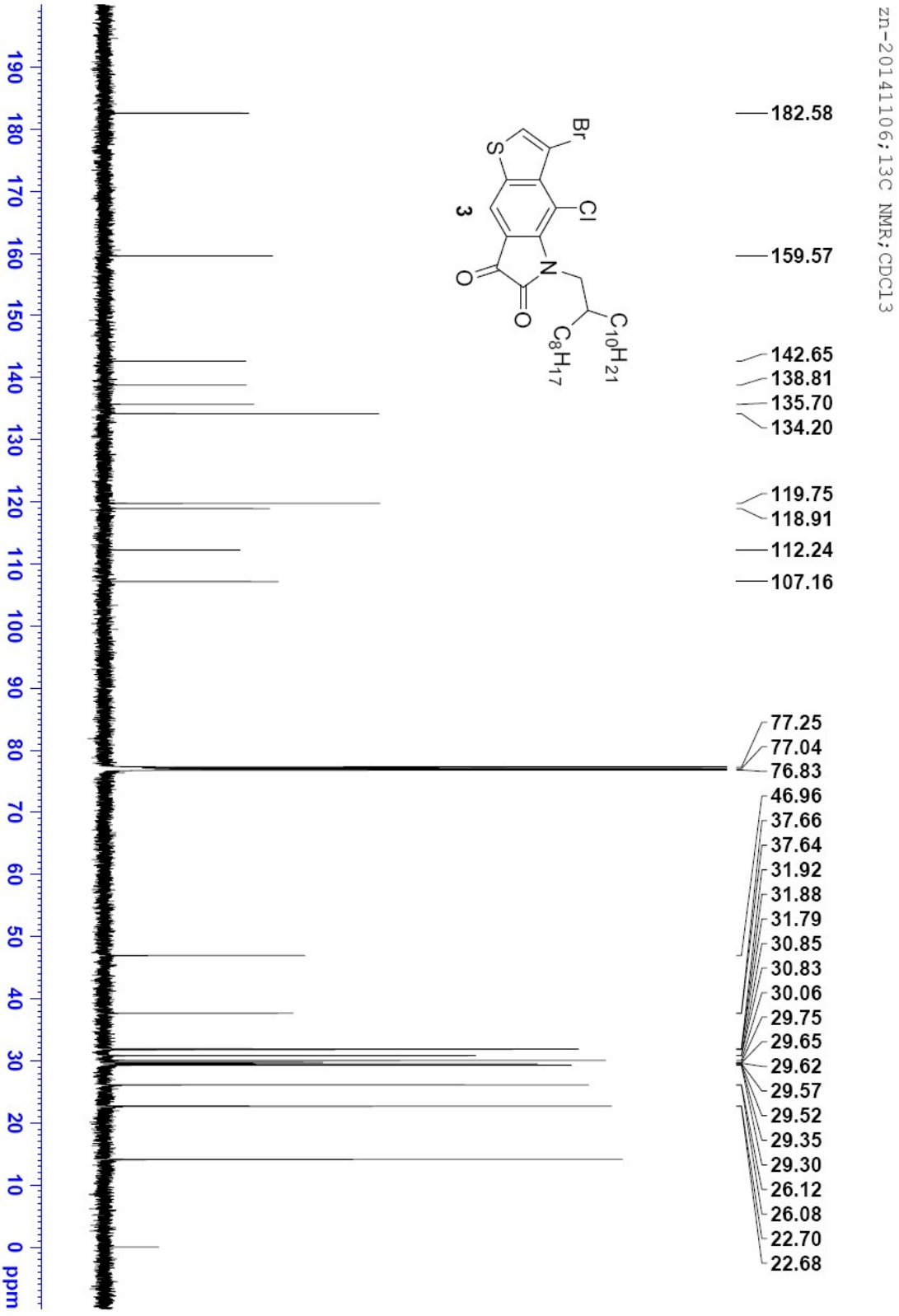
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37.66
37.64
31.92
31.88
31.79
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30.83
30.06
29.75
29.65
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29.57
29.52
29.35
29.30
26.12
26.08
22.70
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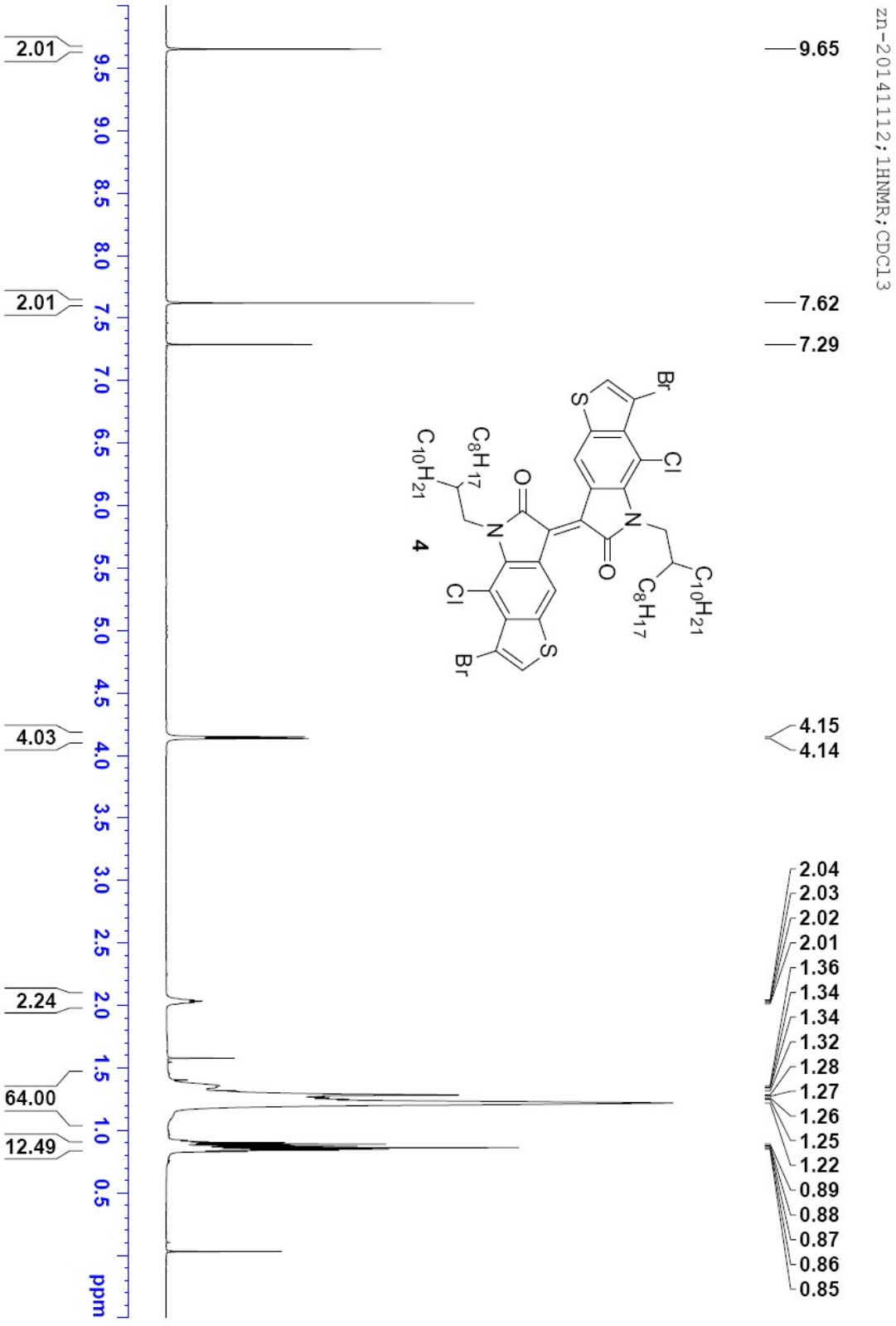
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1.34
1.34
1.32
1.28
1.27
1.26
1.25
1.22
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0.86
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2.01
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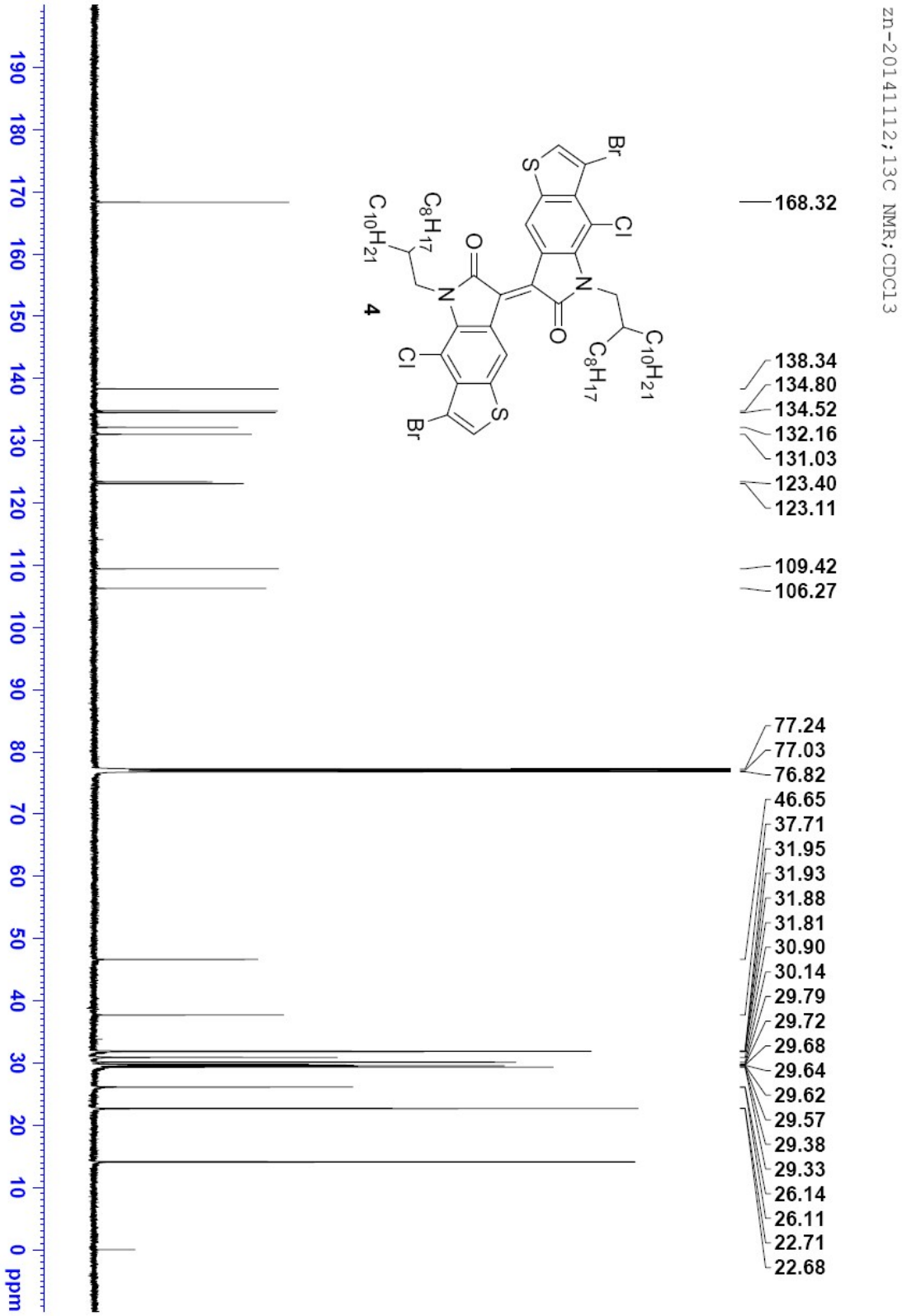
12.49
ppm
4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77.03
76.82
46.65
37.71
31.95
31.93
31.88
31.81
30.90
30.14
29.79
29.72
29.68
29.64
29.62
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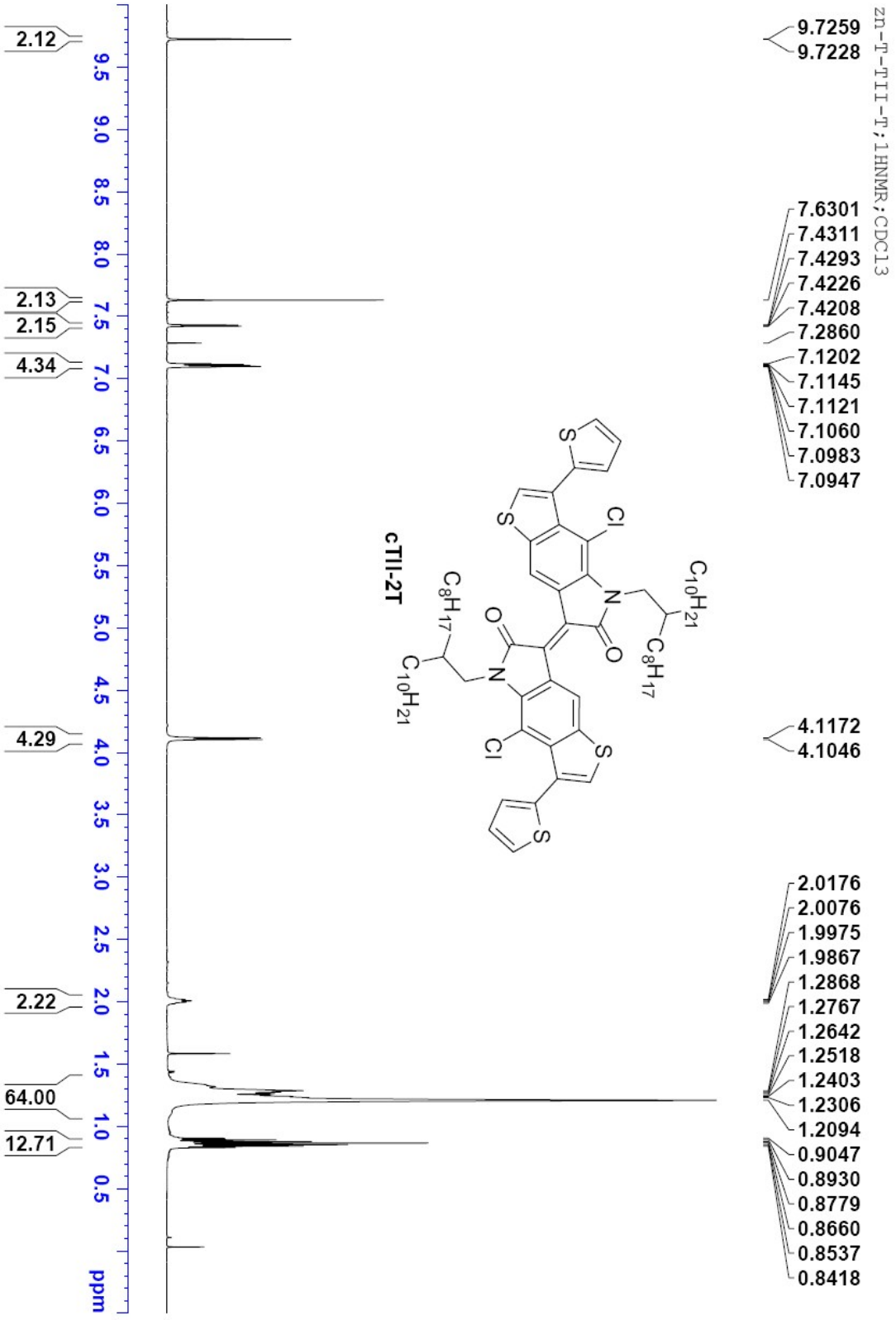
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7.4226
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7.1202
7.1145
7.1121
7.1060
7.0983
7.0947
4.1172
4.1046
2.0176
2.0076
1.9975
1.9867
1.2868
1.2767
1.2642
1.2518
1.2403
1.2306
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0.8930
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0.8660
0.8537
0.8418
2.12
2.13
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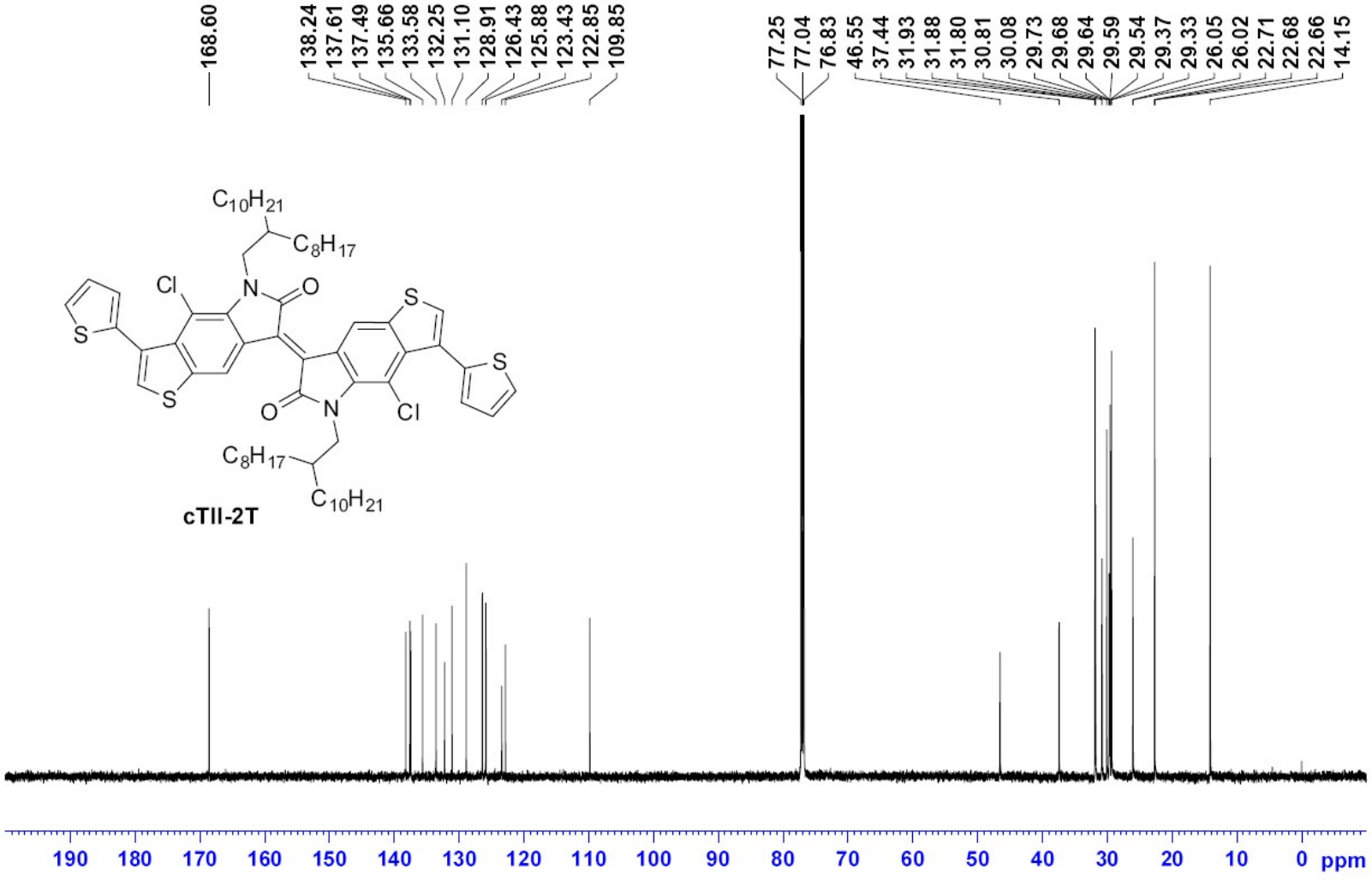
2.22
64.00
12.71
ppm
cTII-2T

zn-T-TII-T;13CNMR;CDCl3



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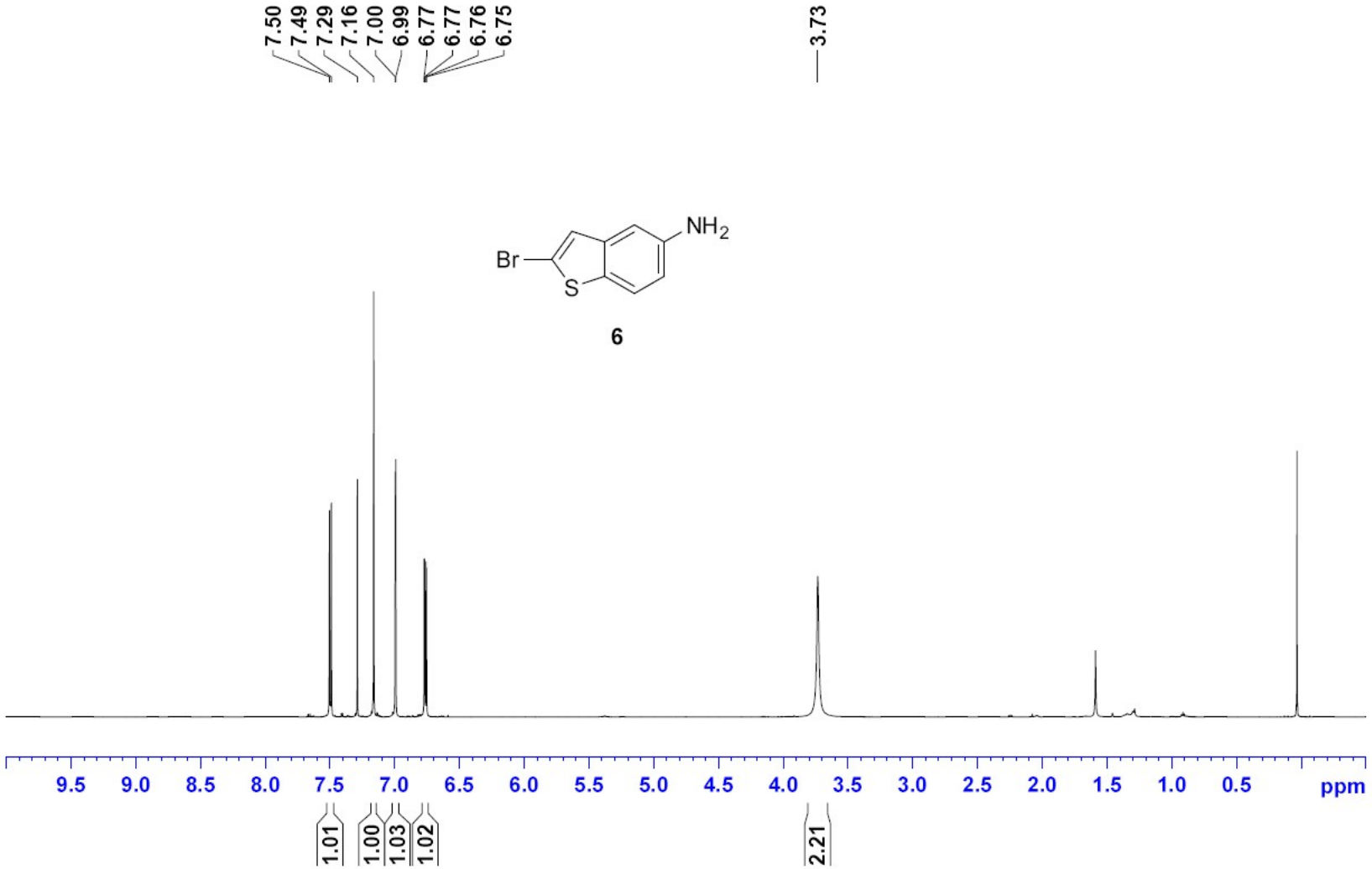

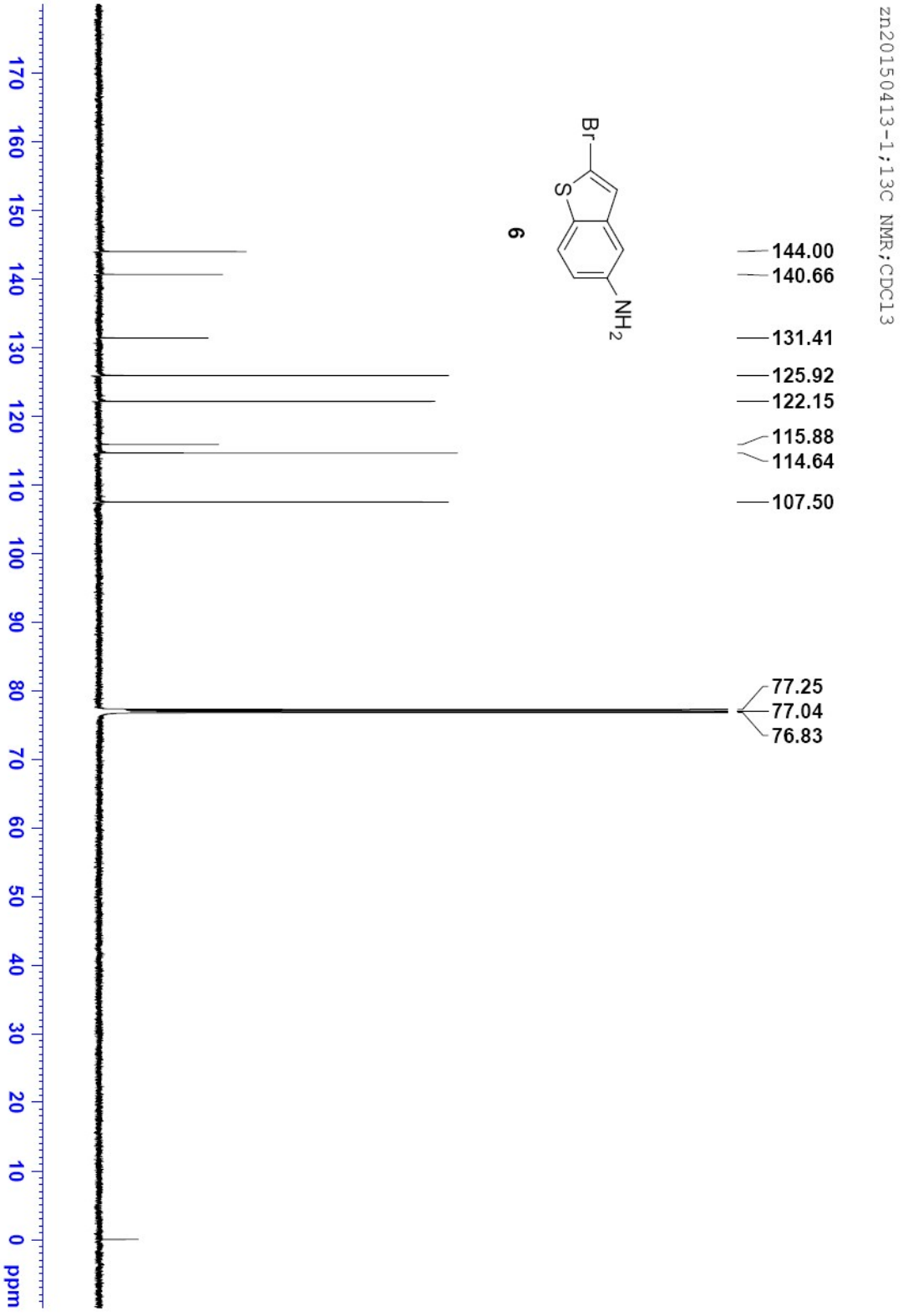
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Br
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NH2
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140.66
131.41
125.92
122.15
115.88
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107.50
77.25
77.04
76.83
170
160
150
140
130
120
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90
80
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50
40
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10
0
ppm

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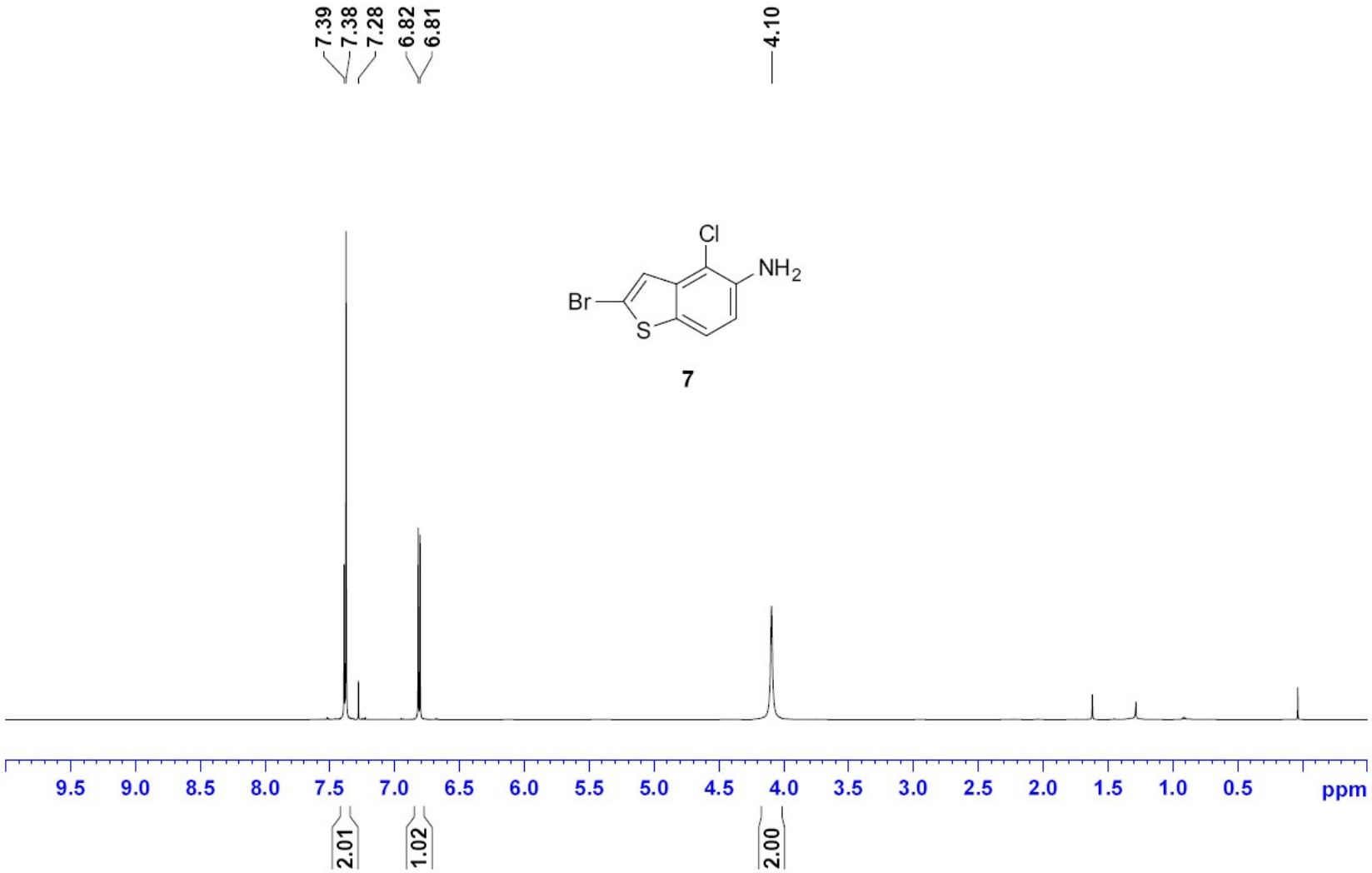

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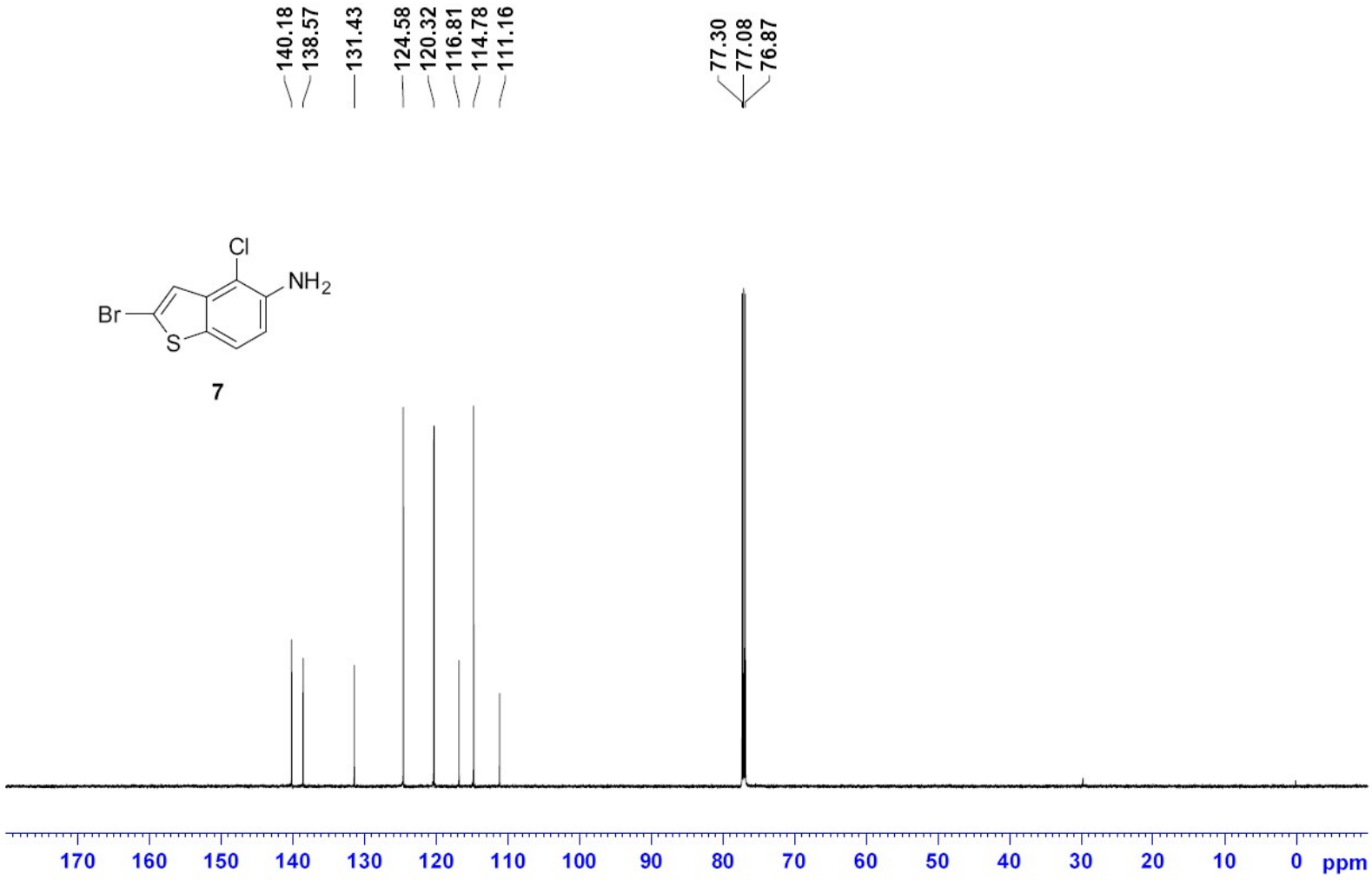
zn-20150415-1;13CNMR;CDCl3



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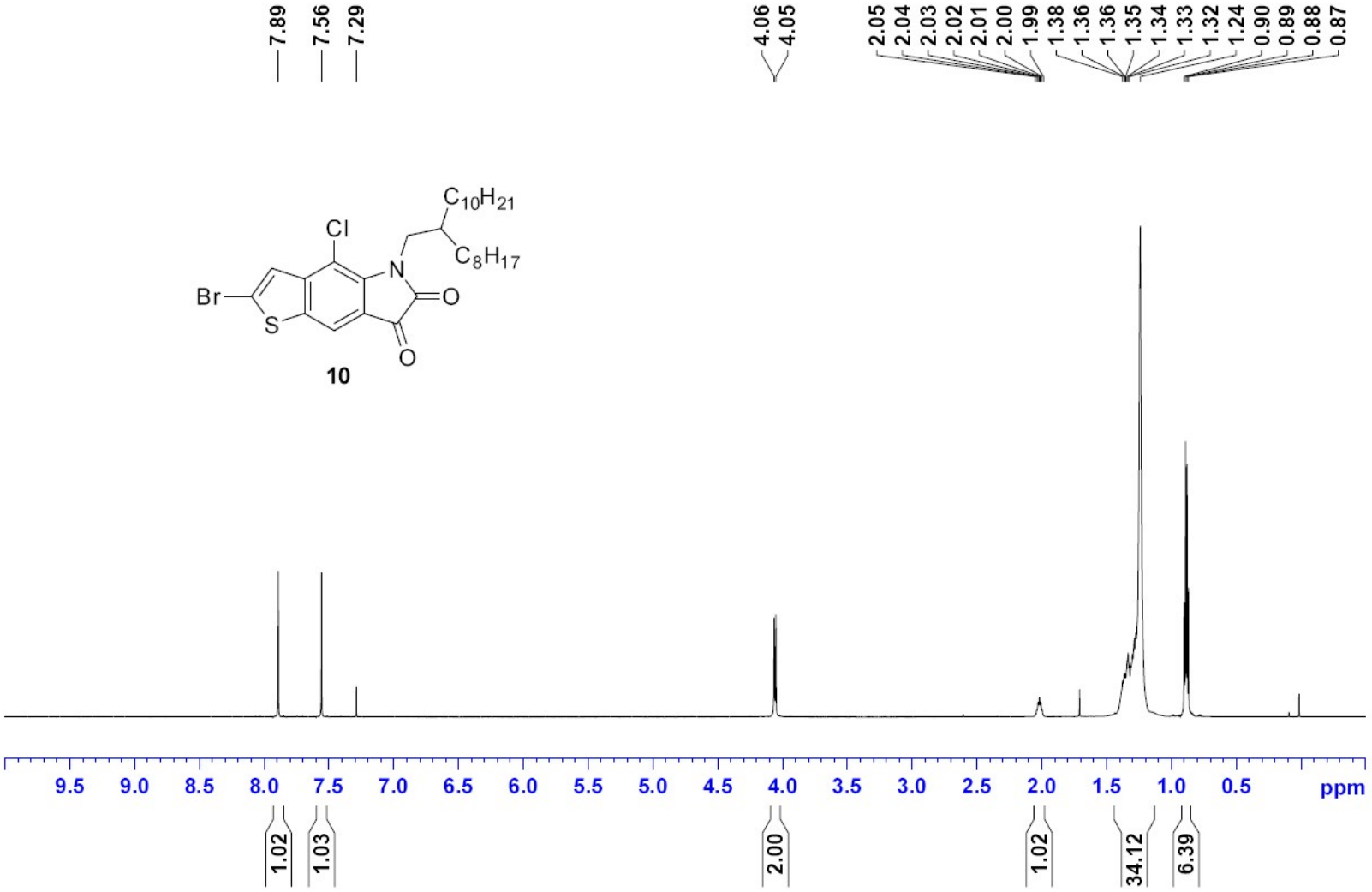

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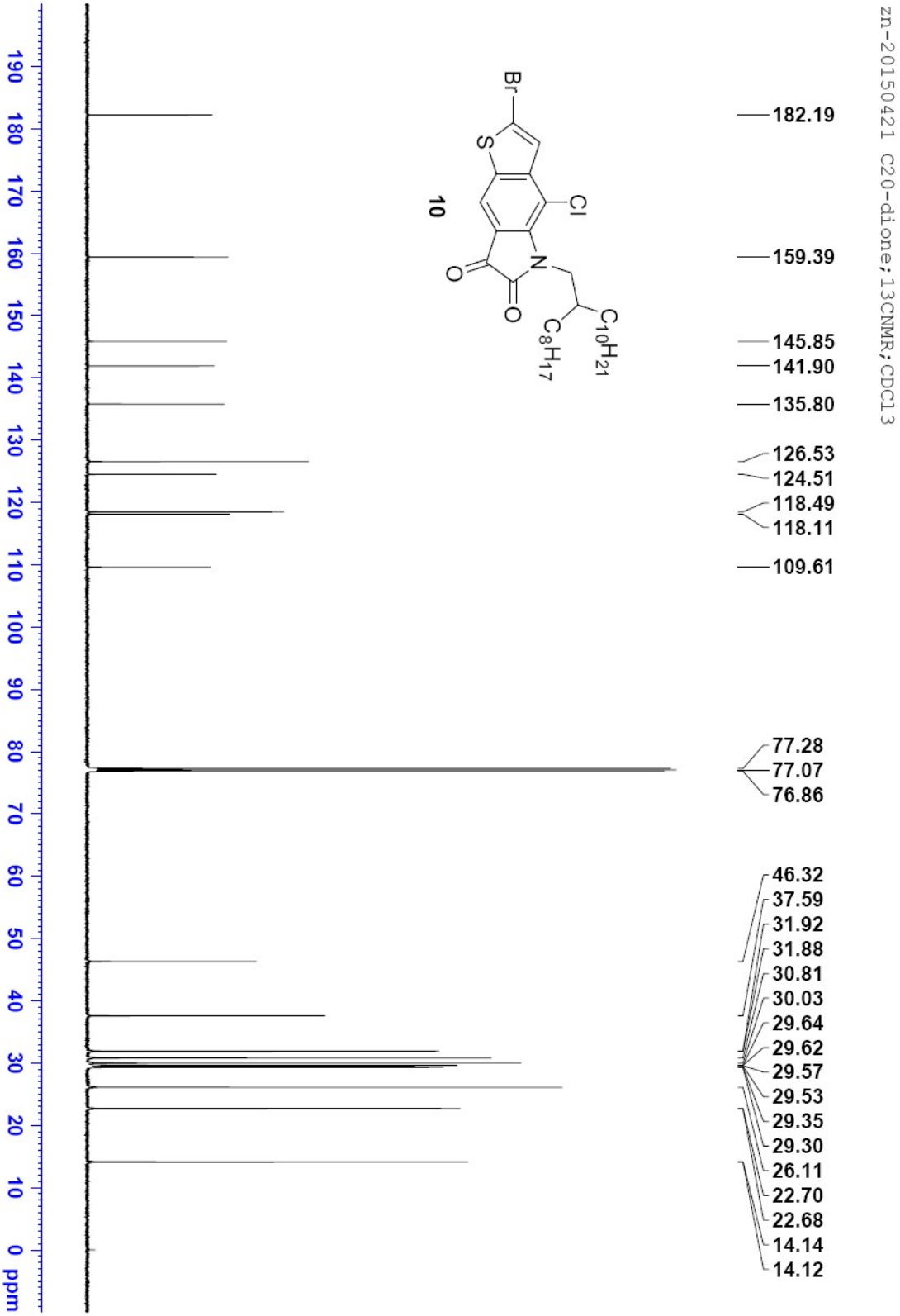
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182.19
159.39
145.85
141.90
135.80
126.53
124.51
118.49
118.11
109.61
77.28
77.07
76.86
46.32
37.59
31.92
31.88
30.81
30.03
29.64
29.62
29.57
29.53
29.35
29.30
26.11
22.70
22.68
14.14
14.12
10
Br
S
Cl
N
O
O
C10H21
C8H17
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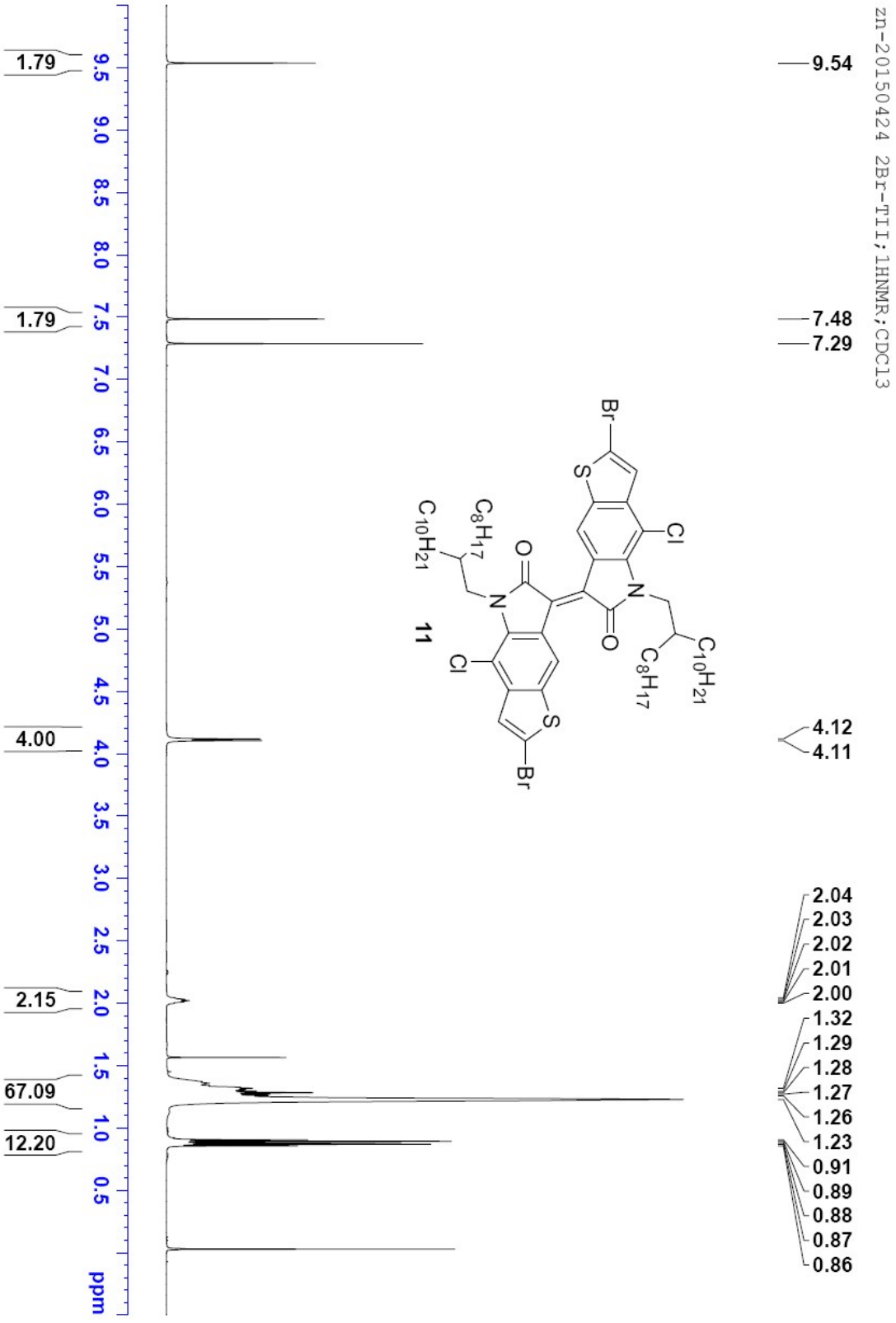
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2.04
2.03
2.02
2.01
2.00
1.32
1.29
1.28
1.27
1.26
1.23
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1.79
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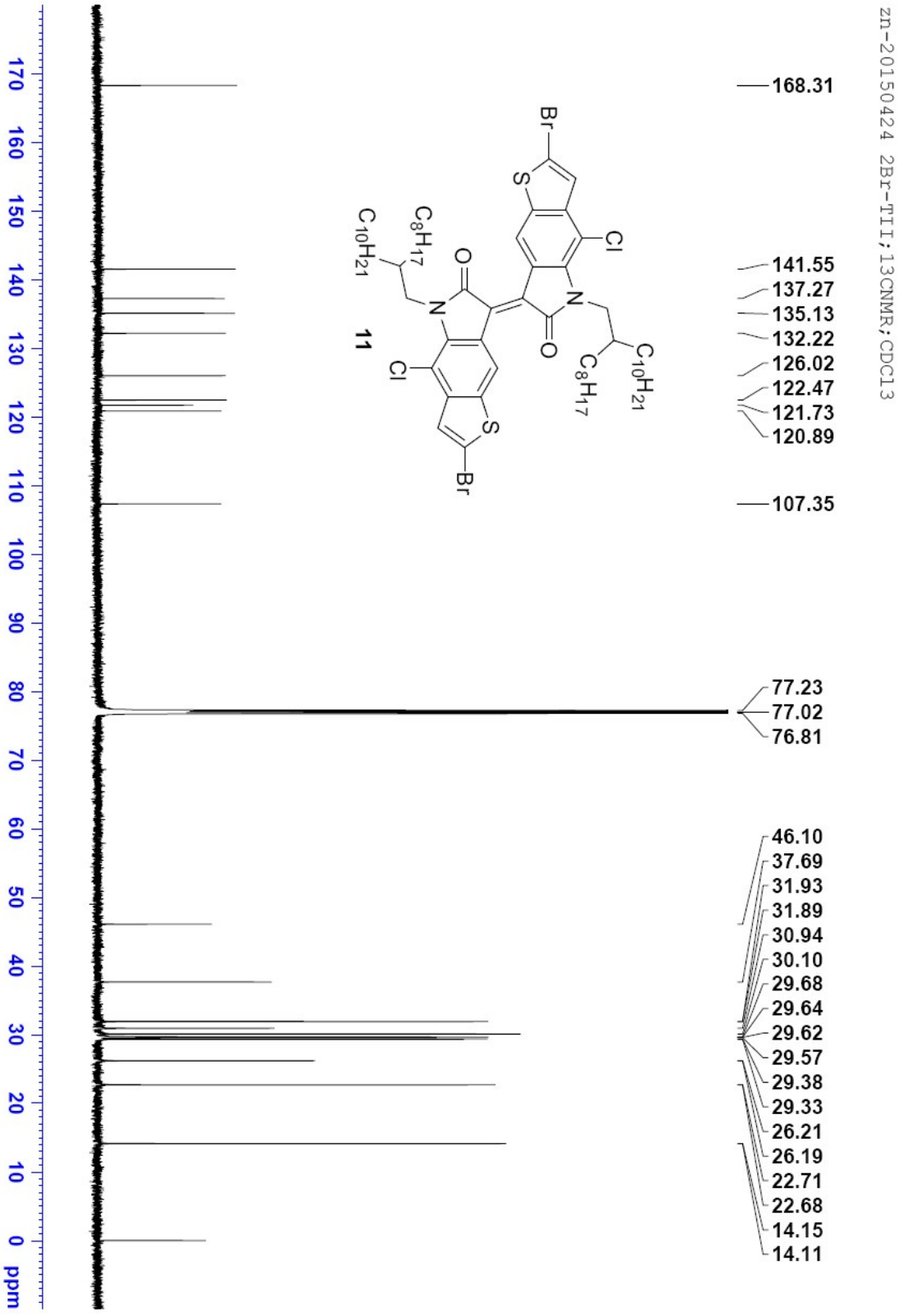
ppm
11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141.55
137.27
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132.22
126.02
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121.73
120.89
107.35
77.23
77.02
76.81
46.10
37.69
31.93
31.89
30.94
30.10
29.68
29.64
29.62
29.57
29.38
29.33
26.21
26.19
22.71
22.68
14.15
14.11
11
ppm

Determination of absolute configuration

(a) Absolute configuration of dodecane substituted compound **3**.

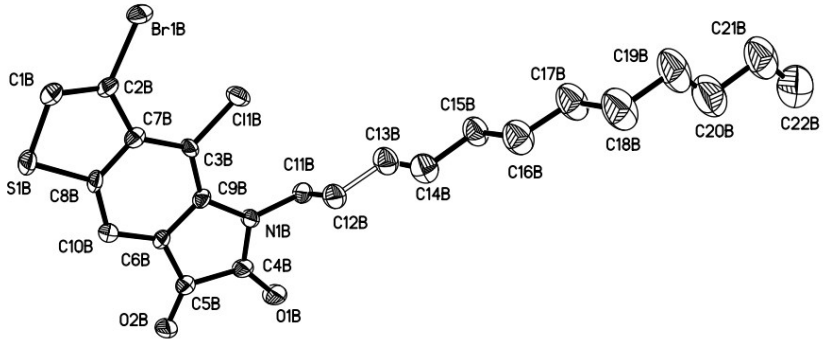

Table S2. Crystal data and structure refinement for dodecane substituted compound **3**.

Empirical formula	C22 H27 Br Cl N O2 S
Formula weight	484.87
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 15.2293(8) Å alpha = 110.314 (1) deg b = 17.6141(9) Å beta = 90.518 (1) deg c = 19.9261(10) Å gamma = 114.615 (1) deg
Volume	4482.6(4)
Z	8
Density (calculated)	1.437 Mg/m^3
Absorption coefficient	2.064
F(000)	2000.0
Crystal size	0.25 x 0.23 x 0.20 mm
Theta range for data collection	1.11 to 26.30 deg.
Limiting indices	-18<=h<=18; -21<=k<=21; -24<=l<=24
Reflections collected	36121
Independent reflections	17885 [R(int) = 0.0420]
Completeness to theta = 26.30	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6742
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17885 / 1588 / 1373
Goodness-of-fit on F^2	1.047
Final R indices [I >2sigma (I)]	R1 = 0.0453, wR2 = 0.0829
R indices (all data)	R1 = 0.0954, wR2 = 0.0956
Largest diff. peak and hole	0.412 and -0.629 e. $Å^{-3}$

Table S3. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for dodecane substituted compound **3**. U(eq) is defined as one third of the trace of the orthogonalized U ij tensor.

Atom	x	y	z	U(eq)
Br(1B)	877(1)	4839(1)	11194(1)	41(1)
C(1B)	-925(2)	4882(2)	11121(2)	35(1)
C(2B)	-402(2)	4481(2)	10748(2)	27(1)
C(3B)	-634(2)	3253(2)	9464(2)	25(1)
C(4B)	-1994(2)	1690(2)	7642(2)	33(1)
C(5B)	-2684(2)	2093(2)	7965(2)	29(1)
C(6B)	-2478(2)	3257(2)	9233(2)	30(1)
C(7B)	-909(2)	3826(2)	10024(2)	26(1)
C(8B)	-1833(2)	3804(2)	9901(2)	27(1)
C(9B)	-1280(2)	2700(2)	8817(2)	24(1)
C(10B)	-2181(2)	2720(2)	8705(2)	25(1)
Cl(1B)	485(1)	3258(1)	9621(1)	54(1)
N(1B)	-1197(2)	2061(2)	8175(1)	30(1)
O(1B)	-2151(2)	1125(2)	7032(1)	48(1)
O(2B)	-3482(2)	1889(2)	7642(1)	38(1)
S(1B)	-2063(1)	4520(1)	10646(1)	40(1)
C(11B)	-436(2)	1749(2)	8065(2)	32(1)
C(12B)	-570(3)	1076(2)	8412(2)	40(1)
C(13B)	311(3)	869(2)	8422(2)	43(1)
C(14B)	131(9)	117(8)	8698(9)	46(3)
C(15B)	1009(9)	-74(8)	8733(9)	47(3)
C(16B)	845(10)	-818(8)	9009(8)	60(3)
C(17B)	1700(9)	-1048(8)	9013(9)	66(3)
C(18B)	1511(9)	-1817(9)	9263(9)	82(4)
C(19B)	2402(9)	-2015(9)	9275(8)	81(4)
C(20B)	2504(11)	-2533(11)	8526(9)	94(4)
C(21B)	3409(11)	-2709(11)	8530(8)	85(4)
C(22B)	3439(12)	-3298(11)	7785(9)	126(5)

Table S4. Bond lengths [Å] and angles [deg] for dodecane substituted compound **3**.

Br(1B)-C(2B)	1.881(3)
C(1B)-C(2B)	1.342(4)
C(1B)-S(1B)	1.713(3)
C(1B)-H(1B)	0.9500
C(2B)-C(7B)	1.446(4)
C(3B)-C(9B)	1.373(4)
C(3B)-C(7B)	1.421(4)
C(3B)-Cl(1B)	1.725(3)
C(4B)-O(1B)	1.218(3)
C(4B)-N(1B)	1.364(4)
C(4B)-C(5B)	1.529(4)
C(5B)-O(2B)	1.218(4)
C(5B)-C(10B)	1.458(4)
C(6B)-C(10B)	1.371(4)
C(6B)-C(8B)	1.400(4)
C(6B)-H(6B)	0.9500
C(7B)-C(8B)	1.408(4)
C(8B)-S(1B)	1.731(3)
C(9B)-C(10B)	1.405(4)
C(9B)-N(1B)	1.429(4)
N(1B)-C(11B)	1.465(4)
C(11B)-C(12B)	1.516(4)
C(11B)-H(11B)	0.9900
C(12B)-C(13B)	1.531(4)
C(12B)-H(12B)	0.9900
C(13B)-C(14B)	1.529(9)
C(13B)-H(13B)	0.9900
C(14B)-C(15B)	1.517(9)
C(14B)-H(14B)	0.9900
C(15B)-C(16B)	1.519(10)
C(15B)-H(15B)	0.9900
C(16B)-C(17B)	1.516(10)
C(16B)-H(16B)	0.9900
C(17B)-C(18B)	1.521(10)
C(17B)-H(17B)	0.9900
C(18B)-C(19B)	1.537(10)
C(18B)-H(18B)	0.9900
C(19B)-C(20B)	1.503(11)
C(19B)-H(19B)	0.9900
C(20B)-C(21B)	1.535(11)
C(20B)-H(20B)	0.9900
C(21B)-C(22B)	1.500(12)

C(21B)-H(21B)	0.9900
C(22B)-H(22B)	0.9800
C(2B)-C(1B)-S(1B)	113.8(2)
C(2B)-C(1B)-H(1B)	123.1
S(1B)-C(1B)-H(1B)	123.1
C(1B)-C(2B)-C(7B)	113.7(3)
C(1B)-C(2B)-Br(1B)	118.3(2)
C(7B)-C(2B)-Br(1B)	127.9(2)
C(9B)-C(3B)-C(7B)	118.6(3)
C(9B)-C(3B)-Cl(1B)	122.2(2)
C(7B)-C(3B)-Cl(1B)	119.3(2)
O(1B)-C(4B)-N(1B)	127.2(3)
O(1B)-C(4B)-C(5B)	125.9(3)
N(1B)-C(4B)-C(5B)	106.9(3)
O(2B)-C(5B)-C(10B)	130.4(3)
O(2B)-C(5B)-C(4B)	124.4(3)
C(10B)-C(5B)-C(4B)	105.2(3)
C(10B)-C(6B)-C(8B)	116.9(3)
C(10B)-C(6B)-H(6B)	121.6
C(8B)-C(6B)-H(6B)	121.6
C(8B)-C(7B)-C(3B)	119.1(3)
C(8B)-C(7B)-C(2B)	108.9(3)
C(3B)-C(7B)-C(2B)	131.9(3)
C(6B)-C(8B)-C(7B)	122.1(3)
C(6B)-C(8B)-S(1B)	124.7(3)
C(7B)-C(8B)-S(1B)	113.1(2)
C(3B)-C(9B)-C(10B)	120.6(3)
C(3B)-C(9B)-N(1B)	130.2(3)
C(10B)-C(9B)-N(1B)	109.2(3)
C(6B)-C(10B)-C(9B)	122.7(3)
C(6B)-C(10B)-C(5B)	129.4(3)
C(9B)-C(10B)-C(5B)	108.0(3)
C(4B)-N(1B)-C(9B)	110.7(3)
C(4B)-N(1B)-C(11B)	120.7(3)
C(9B)-N(1B)-C(11B)	128.4(3)
C(1B)-S(1B)-C(8B)	90.40(16)
N(1B)-C(11B)-C(12B)	111.7(3)
N(1B)-C(11B)-H(11B)	109.3
C(12B)-C(11B)-H(11B)	109.3
C(11B)-C(12B)-C(13B)	112.6(3)
C(11B)-C(12B)-H(12B)	109.1
C(13B)-C(12B)-H(12B)	109.1
C(14B)-C(13B)-C(12B)	112.5(5)

C(14B)-C(13B)-H(13B)	109.1
C(12B)-C(13B)-H(13B)	109.1
C(15B)-C(14B)-C(13B)	113.1(8)
C(15B)-C(14B)-H(14B)	109.0
C(13B)-C(14B)-H(14B)	109.0
C(14B)-C(15B)-C(16B)	113.8(8)
C(14B)-C(15B)-H(15B)	108.8
C(16B)-C(15B)-H(15B)	108.8
C(17B)-C(16B)-C(15B)	114.4(8)
C(17B)-C(16B)-H(16B)	108.7
C(15B)-C(16B)-H(16B)	108.7
C(16B)-C(17B)-C(18B)	113.8(8)
C(16B)-C(17B)-H(17B)	108.8
C(18B)-C(17B)-H(17B)	108.8
C(17B)-C(18B)-C(19B)	112.2(7)
C(17B)-C(18B)-H(18B)	109.2
C(19B)-C(18B)-H(18B)	109.2
C(20B)-C(19B)-C(18B)	112.3(8)
C(20B)-C(19B)-H(19B)	109.1
C(18B)-C(19B)-H(19B)	109.1
C(19B)-C(20B)-C(21B)	112.7(9)
C(19B)-C(20B)-H(20B)	109.1
C(21B)-C(20B)-H(20B)	109.1
C(22B)-C(21B)-C(20B)	111.2(9)
C(22B)-C(21B)-H(21B)	109.4
C(20B)-C(21B)-H(21B)	109.4
C(21B)-C(22B)-H(22B)	109.5

Table S5. Anisotropic displacement parameters [$Å^2$ x 10^3] for dodecane substituted compound **3**. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ (h\ a^*)^2\ U\ 11 + ... + 2\ h\ k\ a^*\ b^*\ U\ 12\ ]$.

	U11	U22	U33	U23	U13	U12
Br(1B)	33(1)	46(1)	26(1)	-5(1)	-7(1)	16(1)
C(1B)	37(2)	35(2)	24(2)	-1(2)	-1(2)	18(2)
C(2B)	30(2)	24(2)	21(2)	1(2)	-1(2)	11(2)
C(3B)	18(2)	33(2)	23(2)	3(2)	4(2)	15(2)
C(4B)	27(2)	35(2)	23(2)	-3(2)	-1(2)	13(2)
C(5B)	26(2)	27(2)	26(2)	3(2)	3(2)	11(2)
C(6B)	24(2)	28(2)	32(2)	3(2)	-2(2)	13(2)
C(7B)	29(2)	24(2)	22(2)	6(2)	2(2)	11(2)
C(8B)	32(2)	26(2)	21(2)	1(2)	5(2)	19(2)
C(9B)	25(2)	23(2)	19(2)	1(2)	6(2)	10(2)
C(10B)	27(2)	24(2)	20(2)	-1(2)	-1(2)	14(2)
Cl(1B)	32(1)	70(1)	38(1)	-17(1)	-10(1)	32(1)
N(1B)	22(2)	36(2)	21(2)	-4(1)	1(1)	16(1)
O(1B)	34(2)	54(2)	28(1)	-14(1)	-4(1)	20(1)
O(2B)	28(1)	42(2)	30(1)	-1(1)	-6(1)	17(1)
S(1B)	43(1)	44(1)	28(1)	-6(1)	-1(1)	30(1)
C(11B)	27(2)	34(2)	25(2)	-1(2)	6(2)	15(2)
C(12B)	32(2)	45(2)	39(2)	8(2)	11(2)	20(2)
C(13B)	38(2)	49(2)	48(2)	21(2)	17(2)	23(2)
C(14B)	42(5)	49(5)	56(6)	29(5)	18(4)	20(4)
C(15B)	38(5)	48(6)	64(6)	28(5)	16(4)	23(5)
C(16B)	58(6)	64(6)	74(7)	40(6)	17(5)	31(5)
C(17B)	59(6)	74(7)	93(8)	57(6)	20(5)	35(5)
C(18B)	72(6)	85(7)	124(9)	77(7)	23(6)	38(6)
C(19B)	79(7)	93(8)	117(10)	77(7)	28(6)	51(6)
C(20B)	87(7)	98(8)	125(11)	61(7)	13(7)	53(6)
C(21B)	84(8)	92(9)	118(12)	72(8)	23(7)	47(7)
C(22B)	138(12)	98(12)	133(13)	14(9)	-16(10)	70(9)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for dodecane substituted compound **3**.

	x	y	z	U(eq)
H(1A)	4512	5525	11499	38
H(6A)	2368	3686	8929	33
H(1B)	-686	5326	11603	42
H(6B)	-3093	3258	9151	36
H(11A)	217	2277	8277	39
H(11B)	-457	1463	7537	39
H(12A)	-1167	506	8141	48
H(12B)	-671	1321	8918	48
H(13A)	456	687	7924	52
H(13B)	893	1426	8738	52
H(14A)	-37	291	9189	55
H(14B)	-439	-444	8373	55
H(15A)	1579	488	9056	56
H(15B)	1175	-249	8241	56
H(16A)	711	-629	9510	72
H(16B)	255	-1371	8701	72
H(17A)	2285	-501	9336	79
H(17B)	1851	-1215	8515	79
H(18A)	938	-2370	8933	98
H(18B)	1350	-1657	9758	98
H(19A)	3006	-1436	9498	97
H(19B)	2335	-2368	9580	97
H(20A)	2551	-2188	8216	112
H(20B)	1908	-3119	8309	112
H(21A)	4011	-2125	8703	102
H(21B)	3395	-3007	8872	102
H(22A)	4018	-3405	7805	189
H(22B)	3473	-2995	7449	189
H(22C)	2844	-3877	7615	189

(b) Absolute configuration of dodecane substituted TII.

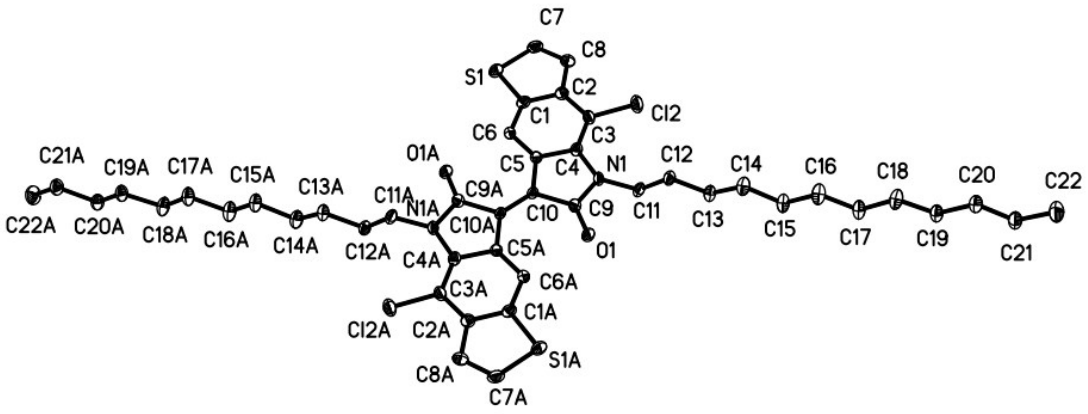

Table S7. Crystal data and structure refinement for dodecane substituted TII.

Empirical formula	C44 H56 Cl2 N2 O2 S2
Formula weight	779.93
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 9.6299(10) Å alpha = 90 deg
	b = 4.8972(5) Å beta = 95.129(3) deg
	c = 42.482(5) Å gamma = 90 deg
Volume	1995.4(4)
Z	2
Density (calculated)	1.298 Mg/m^3
Absorption coefficient	0.307
F(000)	832
Crystal size	0.31 x 0.15 x 0.11 mm
Theta range for data collection	0.96 to 25.38 deg.
Limiting indices	-11<=h<=9; -5<=k<=5; -44<=l<=51
Reflections collected	10417
Independent reflections	3601 [R(int) = 0.0472]
Completeness to theta = 25.38	98.6 %
Max. and min. transmission	0.9670 and 0.9108
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3601 / 0 / 236
Goodness-of-fit on F^2	1.086
Final R indices [I >2sigma (I)]	R1 = 0.0490, wR2 = 0.1255
R indices (all data)	R1 = 0.1060, wR2 = 0.1816
Largest diff. peak and hole	0.497 and -0.802 e. $Å^{-3}$

Table S8. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for dodecane substituted TII. U(eq) is defined as one third of the trace of the orthogonalized U ij tensor.

	x	y	z	U(eq)
C(1)	2284(3)	10875(7)	354(1)	21(1)
C(2)	3001(3)	12018(7)	620(1)	20(1)
C(3)	4377(4)	11126(7)	706(1)	21(1)
C(4)	4969(3)	9235(7)	519(1)	19(1)
C(5)	4198(3)	7975(7)	254(1)	17(1)
C(6)	2845(3)	8846(7)	172(1)	20(1)
C(7)	921(4)	14331(8)	610(1)	27(1)
C(8)	2192(4)	14008(8)	767(1)	26(1)
C(9)	6476(3)	6195(7)	327(1)	18(1)
C(10)	5112(3)	5921(7)	123(1)	16(1)
C(11)	7583(3)	9342(7)	716(1)	22(1)
C(12)	8084(3)	7976(7)	1026(1)	22(1)
C(13)	9443(4)	9277(7)	1164(1)	24(1)
C(14)	10096(4)	7916(8)	1460(1)	29(1)
C(15)	11472(4)	9187(8)	1587(1)	29(1)
C(16)	12090(4)	7910(8)	1893(1)	33(1)
C(17)	13444(4)	9195(8)	2030(1)	30(1)
C(18)	14026(4)	7970(8)	2343(1)	30(1)
C(19)	15339(4)	9366(8)	2486(1)	26(1)
C(20)	15960(4)	8126(8)	2795(1)	26(1)
C(21)	17300(4)	9498(8)	2923(1)	29(1)
C(22)	17954(4)	8294(9)	3230(1)	39(1)
Cl(2)	5217(1)	12424(2)	1053(1)	39(1)
N(1)	6326(3)	8153(6)	551(1)	19(1)
O(1)	7586(2)	5021(5)	308(1)	25(1)
S(1)	637(1)	12275(2)	285(1)	27(1)

Table S9. Bond lengths [Å] and angles [deg] for dodecane substituted TII.

C(1)-C(2)	1.389(5)
C(1)-C(6)	1.397(5)
C(1)-S(1)	1.729(3)
C(2)-C(3)	1.412(5)
C(2)-C(8)	1.426(5)
C(3)-C(4)	1.377(5)
C(3)-Cl(2)	1.735(4)
C(4)-N(1)	1.406(4)
C(4)-C(5)	1.431(5)
C(5)-C(6)	1.386(4)
C(5)-C(10)	1.477(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.351(5)
C(7)-S(1)	1.712(4)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-O(1)	1.222(4)
C(9)-N(1)	1.369(4)
C(9)-C(10)	1.512(5)
C(10)-C(10)#1	1.386(6)
C(11)-N(1)	1.465(4)
C(11)-C(12)	1.514(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.525(5)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.509(5)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.520(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.516(5)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.516(5)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.519(5)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900

C(18)-C(19)	1.516(5)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.521(5)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.511(5)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.519(5)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800

C(2)-C(1)-C(6)	123.2(3)
C(2)-C(1)-S(1)	111.1(3)
C(6)-C(1)-S(1)	125.6(3)
C(1)-C(2)-C(3)	118.3(3)
C(1)-C(2)-C(8)	112.4(3)
C(3)-C(2)-C(8)	129.3(3)
C(4)-C(3)-C(2)	119.0(3)
C(4)-C(3)-Cl(2)	123.4(3)
C(2)-C(3)-Cl(2)	117.5(3)
C(3)-C(4)-N(1)	128.9(3)
C(3)-C(4)-C(5)	122.1(3)
N(1)-C(4)-C(5)	109.0(3)
C(6)-C(5)-C(4)	118.4(3)
C(6)-C(5)-C(10)	133.8(3)
C(4)-C(5)-C(10)	107.8(3)
C(5)-C(6)-C(1)	118.7(3)
C(5)-C(6)-H(6)	120.6
C(1)-C(6)-H(6)	120.6
C(8)-C(7)-S(1)	113.7(3)
C(8)-C(7)-H(7)	123.1
S(1)-C(7)-H(7)	123.1
C(7)-C(8)-C(2)	111.7(3)
C(7)-C(8)-H(8)	124.1
C(2)-C(8)-H(8)	124.1
O(1)-C(9)-N(1)	121.5(3)
O(1)-C(9)-C(10)	129.8(3)
N(1)-C(9)-C(10)	108.6(3)
C(10)#1-C(10)-C(5)	132.2(4)

C(10)#1-C(10)-C(9)	123.9(4)
C(5)-C(10)-C(9)	103.9(3)
N(1)-C(11)-C(12)	115.2(3)
N(1)-C(11)-H(11A)	108.5
C(12)-C(11)-H(11A)	108.5
N(1)-C(11)-H(11B)	108.5
C(12)-C(11)-H(11B)	108.5
H(11A)-C(11)-H(11B)	107.5
C(11)-C(12)-C(13)	110.2(3)
C(11)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12B)	109.6
C(13)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
C(14)-C(13)-C(12)	114.5(3)
C(14)-C(13)-H(13A)	108.6
C(12)-C(13)-H(13A)	108.6
C(14)-C(13)-H(13B)	108.6
C(12)-C(13)-H(13B)	108.6
H(13A)-C(13)-H(13B)	107.6
C(13)-C(14)-C(15)	113.6(3)
C(13)-C(14)-H(14A)	108.8
C(15)-C(14)-H(14A)	108.8
C(13)-C(14)-H(14B)	108.8
C(15)-C(14)-H(14B)	108.8
H(14A)-C(14)-H(14B)	107.7
C(16)-C(15)-C(14)	113.6(3)
C(16)-C(15)-H(15A)	108.9
C(14)-C(15)-H(15A)	108.9
C(16)-C(15)-H(15B)	108.9
C(14)-C(15)-H(15B)	108.9
H(15A)-C(15)-H(15B)	107.7
C(17)-C(16)-C(15)	114.6(3)
C(17)-C(16)-H(16A)	108.6
C(15)-C(16)-H(16A)	108.6
C(17)-C(16)-H(16B)	108.6
C(15)-C(16)-H(16B)	108.6
H(16A)-C(16)-H(16B)	107.6
C(16)-C(17)-C(18)	114.2(3)
C(16)-C(17)-H(17A)	108.7
C(18)-C(17)-H(17A)	108.7
C(16)-C(17)-H(17B)	108.7
C(18)-C(17)-H(17B)	108.7
H(17A)-C(17)-H(17B)	107.6

C(19)-C(18)-C(17)	113.7(3)
C(19)-C(18)-H(18A)	108.8
C(17)-C(18)-H(18A)	108.8
C(19)-C(18)-H(18B)	108.8
C(17)-C(18)-H(18B)	108.8
H(18A)-C(18)-H(18B)	107.7
C(18)-C(19)-C(20)	114.6(3)
C(18)-C(19)-H(19A)	108.6
C(20)-C(19)-H(19A)	108.6
C(18)-C(19)-H(19B)	108.6
C(20)-C(19)-H(19B)	108.6
H(19A)-C(19)-H(19B)	107.6
C(21)-C(20)-C(19)	112.9(3)
C(21)-C(20)-H(20A)	109.0
C(19)-C(20)-H(20A)	109.0
C(21)-C(20)-H(20B)	109.0
C(19)-C(20)-H(20B)	109.0
H(20A)-C(20)-H(20B)	107.8
C(20)-C(21)-C(22)	114.3(3)
C(20)-C(21)-H(21A)	108.7
C(22)-C(21)-H(21A)	108.7
C(20)-C(21)-H(21B)	108.7
C(22)-C(21)-H(21B)	108.7
H(21A)-C(21)-H(21B)	107.6
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(9)-N(1)-C(4)	110.6(3)
C(9)-N(1)-C(11)	118.6(3)
C(4)-N(1)-C(11)	128.1(3)
C(7)-S(1)-C(1)	91.04(17)

Symmetry transformations used to generate equivalent atoms: -x+1,-y+1,-z

Table S10. Anisotropic displacement parameters [$Å^2$ x 10^3] for dodecane substituted TII. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ (h\ a^*)^2\ U\ 11 + ... + 2\ h\ k\ a^*\ b^*\ U\ 12\ ]$.

	U11	U22	U33	U23	U13	U12
C(1)	16(2)	19(2)	26(2)	0(2)	3(2)	4(2)
C(2)	20(2)	19(2)	22(2)	0(2)	2(2)	2(2)
C(3)	23(2)	21(2)	19(2)	-5(2)	-2(2)	3(2)
C(4)	17(2)	18(2)	21(2)	0(2)	-2(2)	2(2)
C(5)	16(2)	19(2)	15(2)	1(2)	1(1)	1(2)
C(6)	17(2)	25(2)	17(2)	-3(2)	0(2)	1(2)
C(7)	20(2)	28(2)	34(2)	-5(2)	8(2)	5(2)
C(8)	24(2)	28(2)	28(2)	-8(2)	6(2)	5(2)
C(9)	19(2)	19(2)	16(2)	4(2)	-1(2)	3(2)
C(10)	12(2)	19(2)	16(2)	2(2)	-1(2)	2(2)
C(11)	14(2)	22(2)	29(2)	-4(2)	-3(2)	-1(2)
C(12)	17(2)	27(2)	22(2)	-1(2)	-4(2)	2(2)
C(13)	22(2)	23(2)	25(2)	-2(2)	-6(2)	-2(2)
C(14)	27(2)	27(2)	30(2)	3(2)	-7(2)	-2(2)
C(15)	27(2)	31(2)	28(2)	0(2)	-9(2)	-3(2)
C(16)	32(2)	31(2)	34(2)	1(2)	-11(2)	-4(2)
C(17)	29(2)	31(2)	28(2)	-1(2)	-10(2)	-1(2)
C(18)	26(2)	28(2)	34(2)	3(2)	-11(2)	-2(2)
C(19)	25(2)	26(2)	25(2)	-1(2)	-7(2)	2(2)
C(20)	25(2)	28(2)	25(2)	1(2)	-5(2)	1(2)
C(21)	27(2)	32(2)	27(2)	-1(2)	-5(2)	0(2)
C(22)	36(2)	49(3)	31(2)	1(2)	-10(2)	3(2)
Cl(2)	30(1)	51(1)	33(1)	-23(1)	-9(1)	11(1)
N(1)	17(2)	21(2)	17(2)	-4(1)	-4(1)	3(1)
O(1)	16(1)	31(2)	28(2)	-8(1)	-3(1)	10(1)
S(1)	17(1)	31(1)	33(1)	-5(1)	0(1)	9(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for dodecane substituted TII.

	x	y	z	U(eq)
H(6)	2310	8078	-5	24
H(7)	247	15583	674	32
H(8)	2509	14987	953	32
H(11A)	7399	11291	759	26
H(11B)	8343	9267	574	26
H(12A)	8233	6004	990	27
H(12B)	7366	8165	1177	27
H(13A)	10119	9236	1002	28
H(13B)	9262	11215	1212	28
H(14A)	10251	5963	1414	34
H(14B)	9435	8015	1625	34
H(15A)	12148	9002	1426	35
H(15B)	11327	11161	1622	35
H(16A)	11399	8044	2051	40
H(16B)	12257	5947	1855	40
H(17A)	13288	11172	2060	36
H(17B)	14148	8998	1875	36
H(18A)	13305	8080	2494	36
H(18B)	14231	6014	2310	36
H(19A)	15125	11311	2522	31
H(19B)	16048	9299	2331	31
H(20A)	15273	8270	2954	32
H(20B)	16144	6163	2762	32
H(21A)	17111	11459	2956	35
H(21B)	17980	9369	2762	35
H(22A)	17302	8463	3393	59
H(22B)	18816	9281	3297	59
H(22C)	18167	6362	3199	59