Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Benzodi(pyridothiophene)：A novel acceptor unit for application in the A_1-A-A_1 type photovoltaic small molecules

Jianhua Chen,[a] Manjun Xiao,[a,b] Linrui Duan,[a] Qiong Wang,[a] Hua Tan, Ning Su,[a] Yu Liu, Renqiang Yang,*[,b] Weiguo Zhu*[,a]

Contents

1. Thermal properties of SMs

Table S1. Thermal properties of the A_1-A-A_1 SMs

SMs	T_d (°C)	T_m (°C)	T_c (°C)
BDPT-2BT	447	274	258
BDPT-2FBT	451	331	323
BDPT-2DPP	423	295	266

2. The calculated frontier orbital distribution of SMs

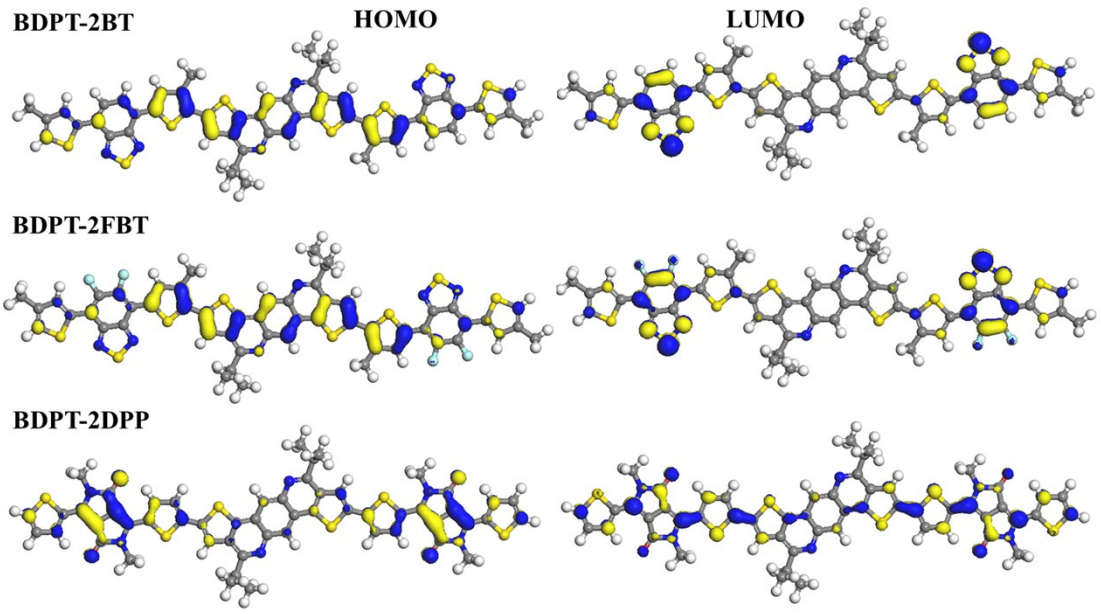

Fig. S1. Frontier molecular orbital distributions: HOMO (left) and LUMO (right) levels.

3. **Photovoltaic properties of the SMs/$PC_{71}BM$-based solar cells**

Table S2. Photovoltaic properties of SMs/$PC_{71}BM$ based device under different ratios.

SMs	D/A ratio	DIO ratio	V_{oc} (V)	J_{sc} (mA/cm^2)	*FF* (%)	PCE (%)
BDPT-2BT	1:2	No	0.84	4.17	45.57	1.57
	1:1	No	0.84	5.08	51.25	2.18
	2:1	No	0.75	5.28	50.60	2.01
	1:1	1%	0.58	2.20	30.29	0.38
BDPT-2FBT	1:2	No	0.70	4.04	53.38	1.50
	1:1	No	0.80	6.83	48.07	2.63
	2:1	No	0.70	7.44	45.26	2.35
	1:1	1%	0.77	6.0	37.58	1.74
BDPT-2DPP	1:2	No	0.70	1.19	52.85	0.44
	1:2	1%	0.82	5.69	42.82	1.99
	1:1	No	0.73	1.55	47.00	0.53
	1:1	1%	0.84	8.00	46.12	3.09
	2:1	No	0.81	1.47	45.86	0.54
	2:1	1%	0.89	6.82	49.12	2.98
	1.5:1	1%	0.84	9.0	52.37	3.97

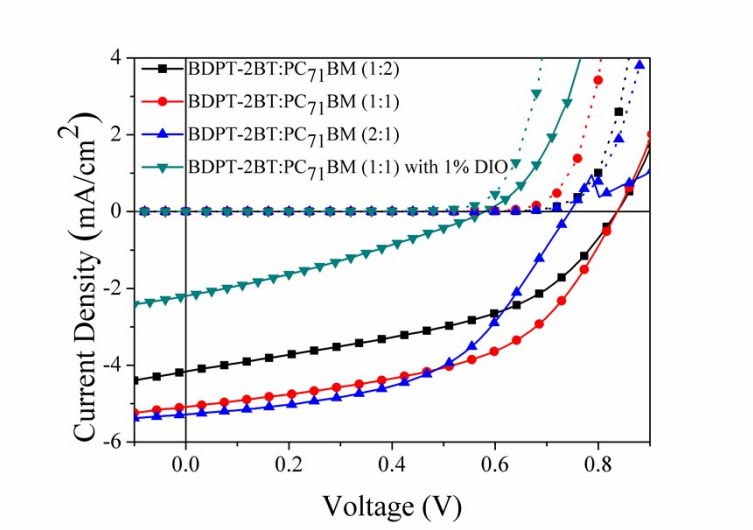

Fig. S2. *J*−*V* characteristics of BDPT-2BT/$PC_{71}BM$ based device (The dashed lines plus symbols represent the corresponding dark currents).

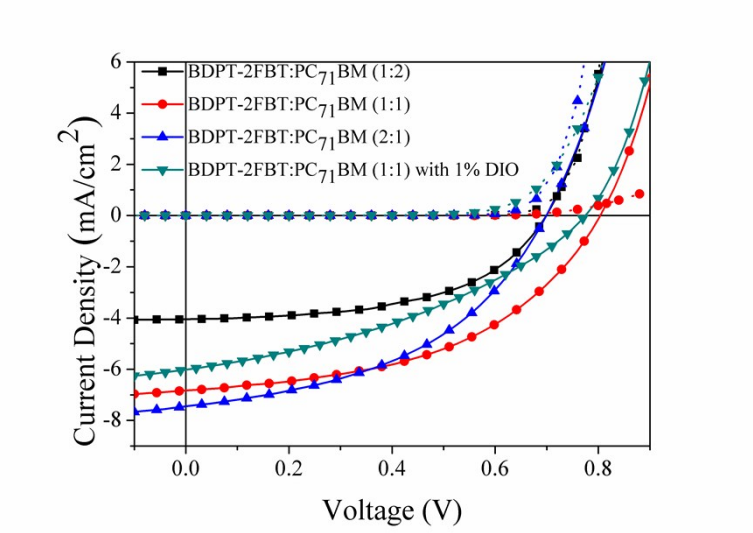

Fig. S3. *J*−*V* characteristics of BDPT-2FBT/ $PC_{71}BM$ based device (The dashed lines plus symbols represent the corresponding dark currents).

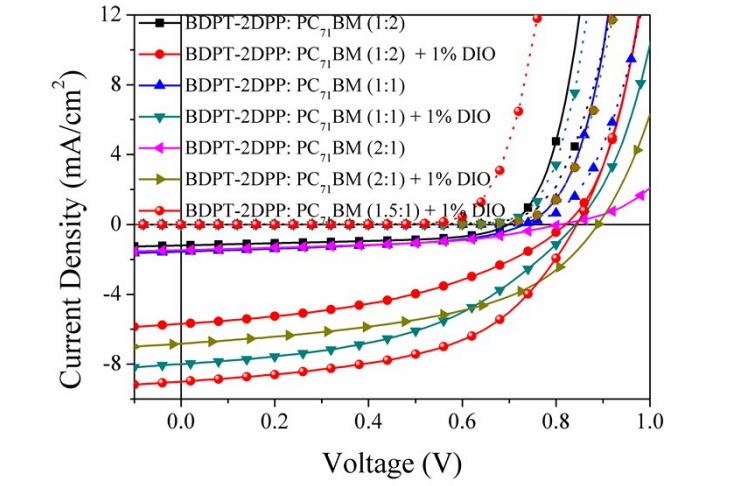

Fig. S4. *J*−*V* characteristics of BDPT-2DPP/$PC_{71}BM$ based device (The dashed lines plus symbols represent the corresponding dark currents).

4. NMR spectra

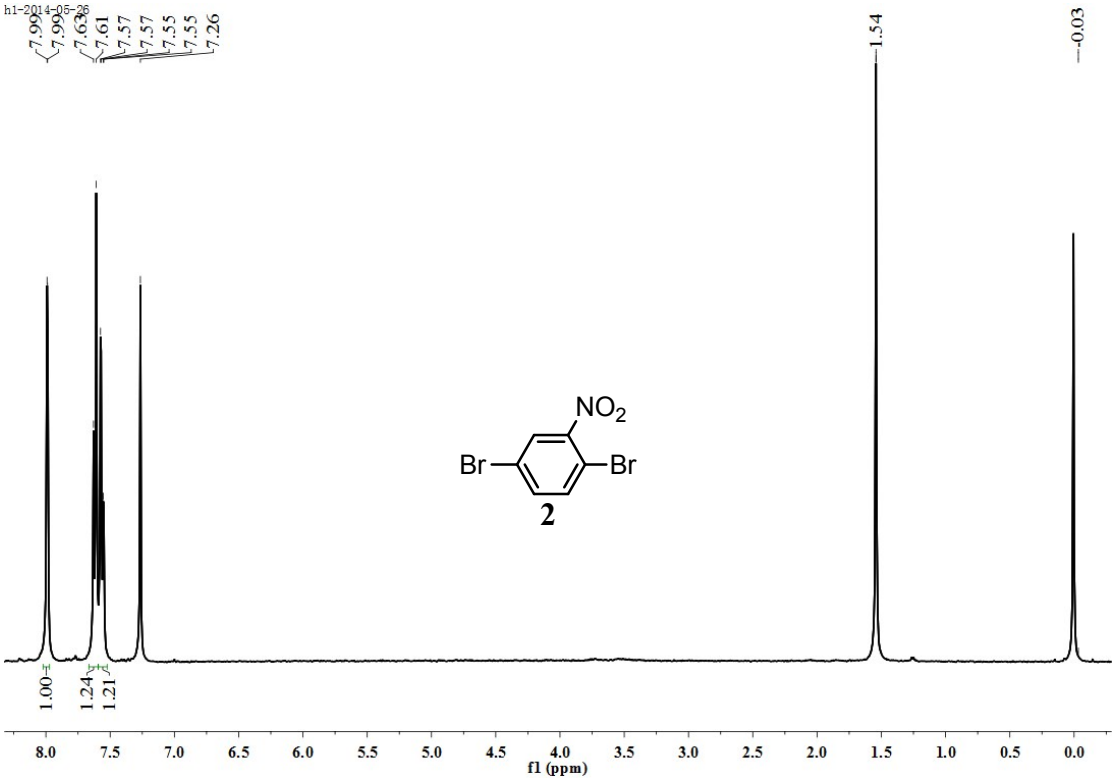

Fig. S5. ^{1}H-NMR of compound **2**.

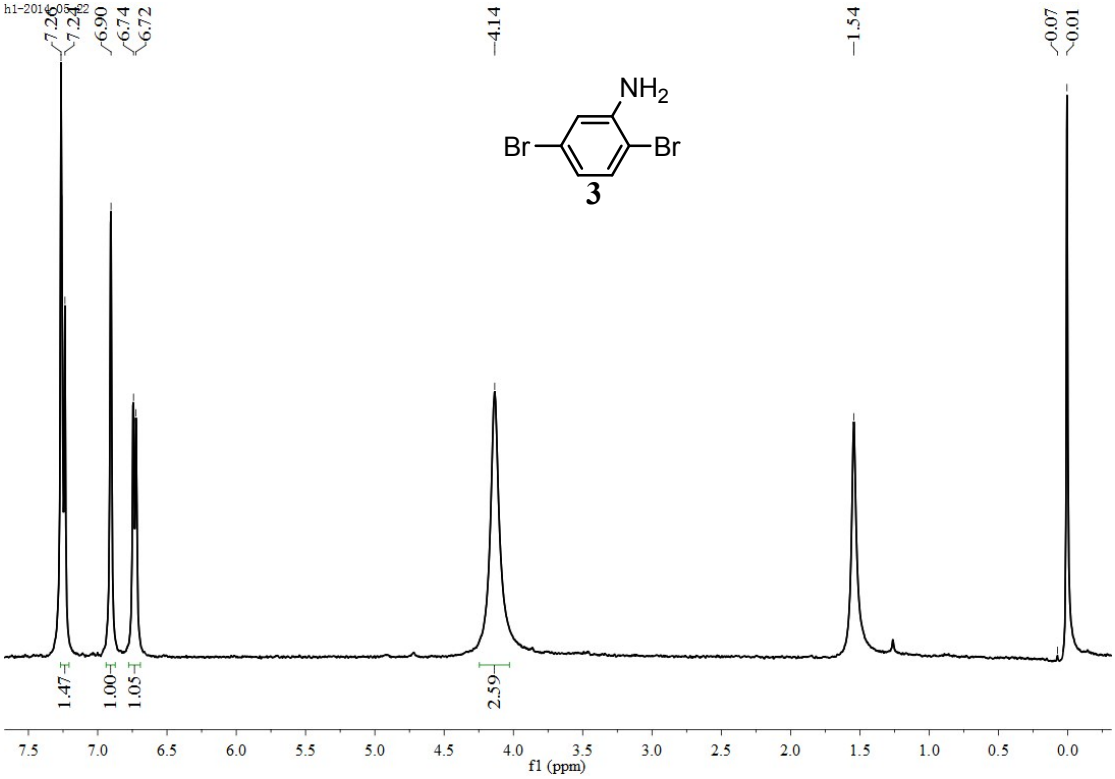

Fig. S6. ^{1}H-NMR of compound **3**.

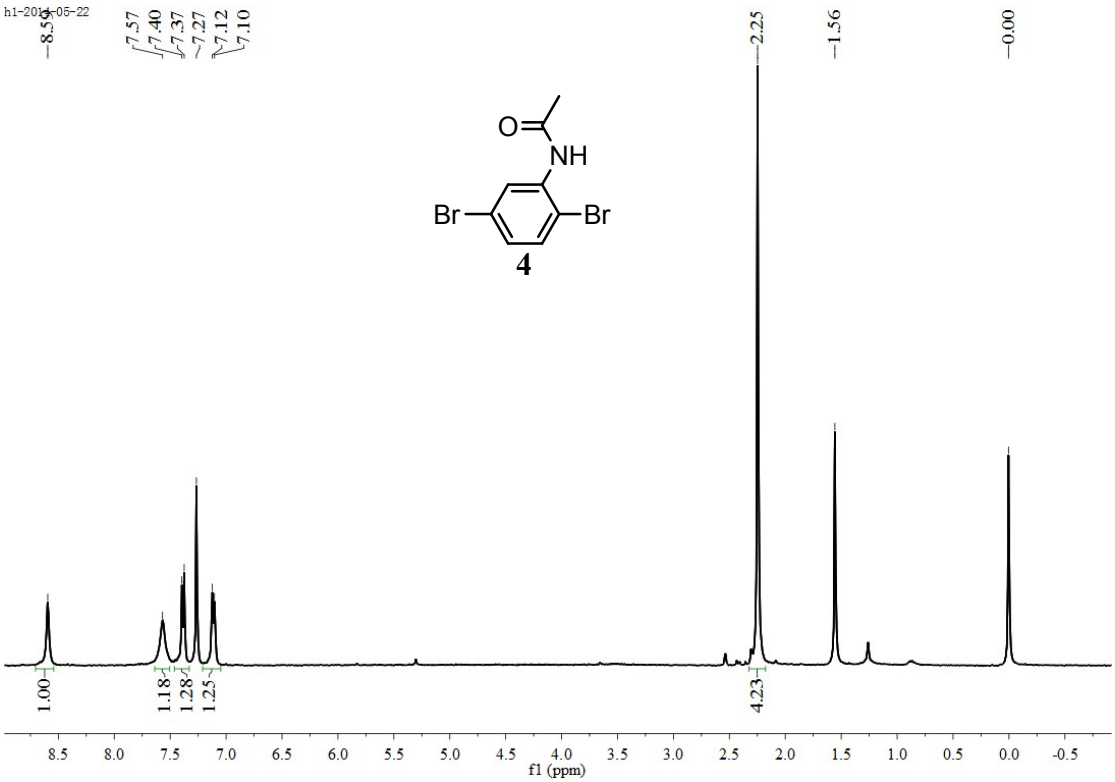

Fig. S7. ^{1}H-NMR of compound **4**.

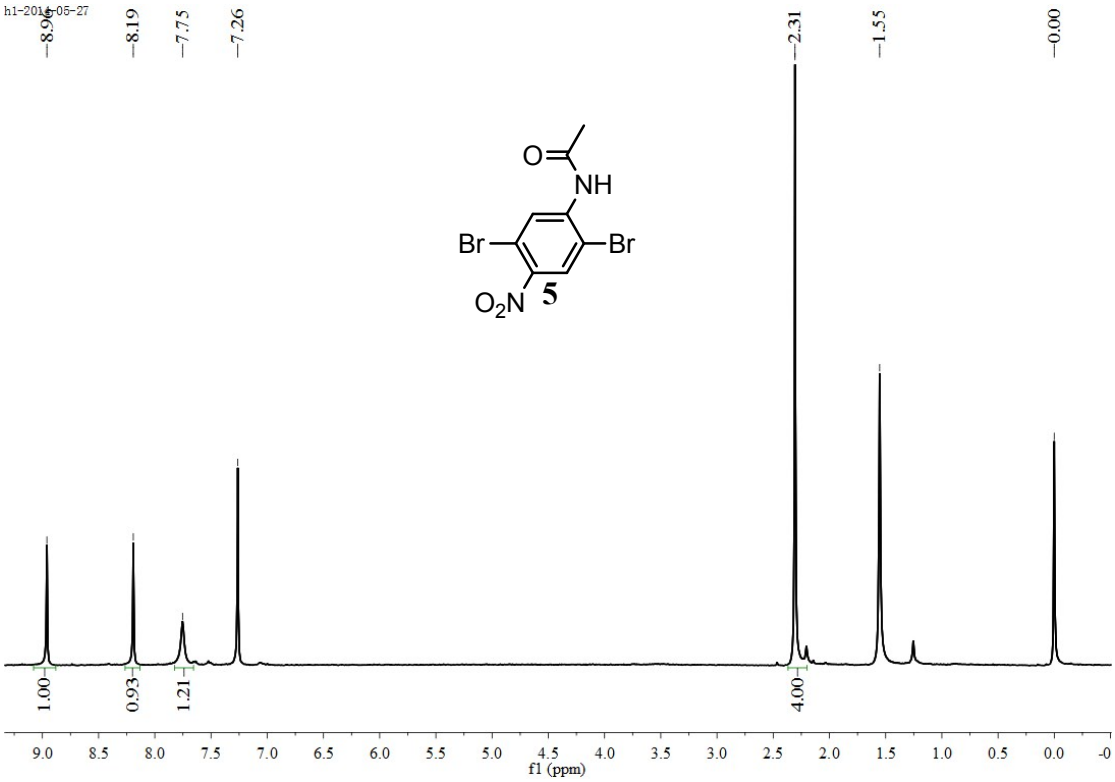

Fig. S8. ^{1}H-NMR of compound **5**.

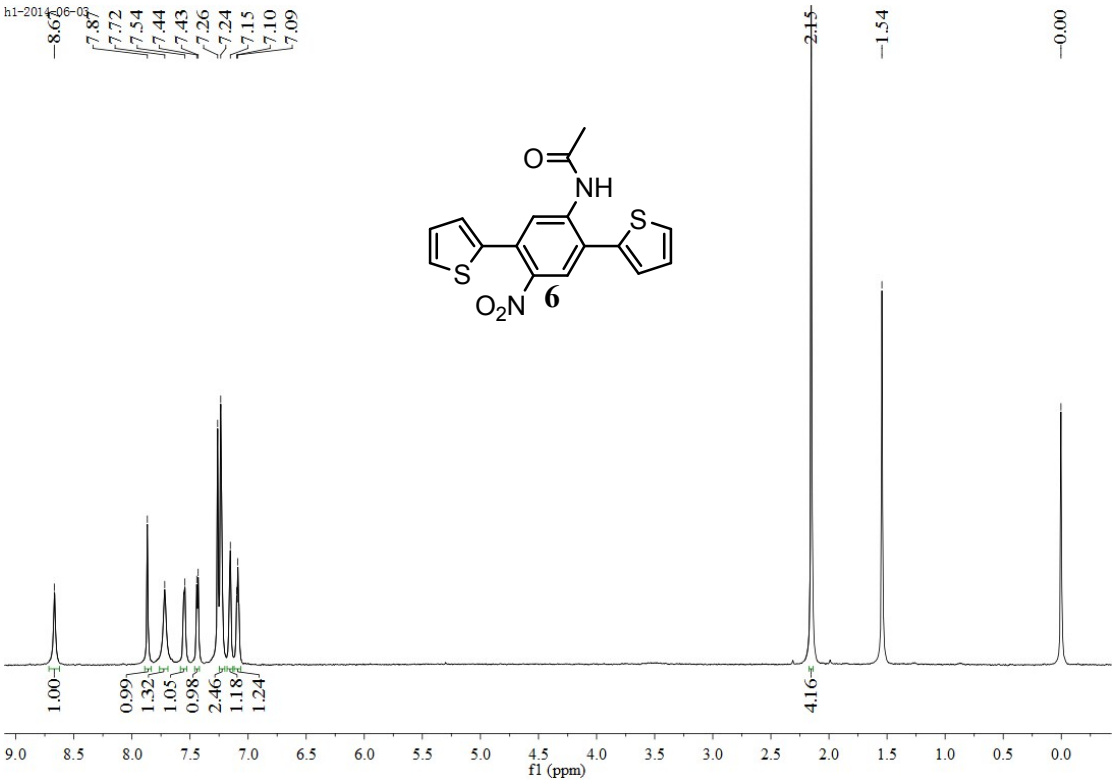

Fig. S9. [1]H-NMR of compound **6**.

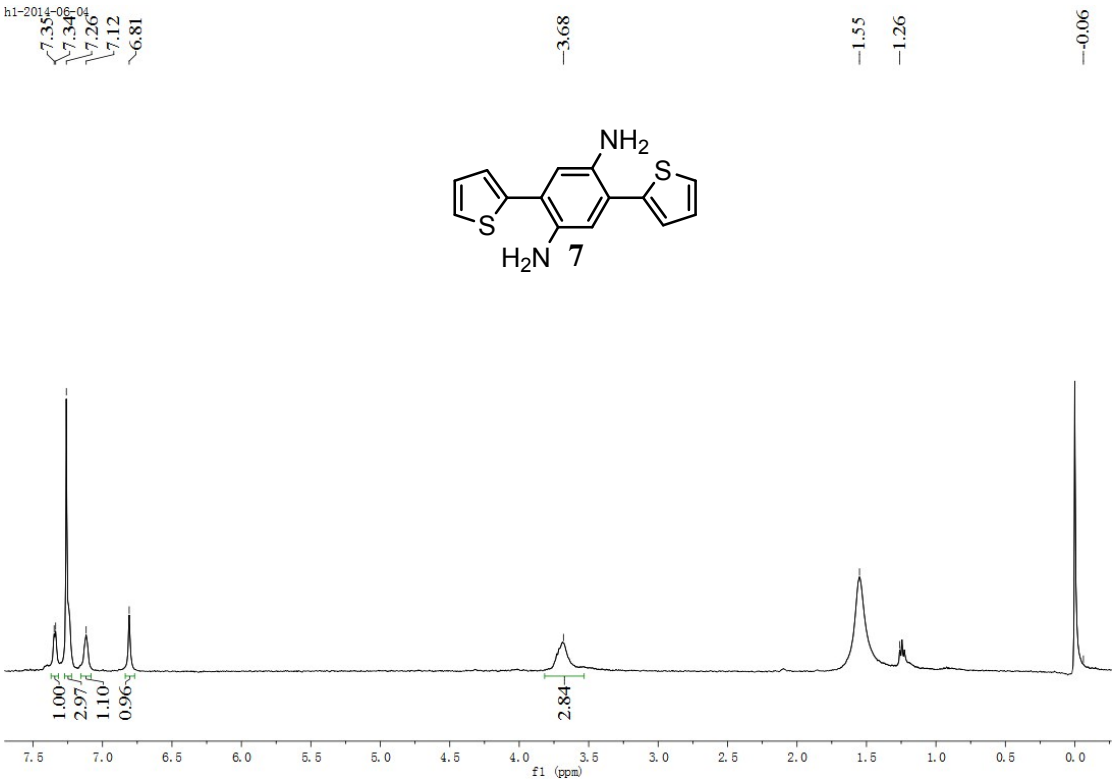

Fig. S10. [1]H-NMR of compound **7**.

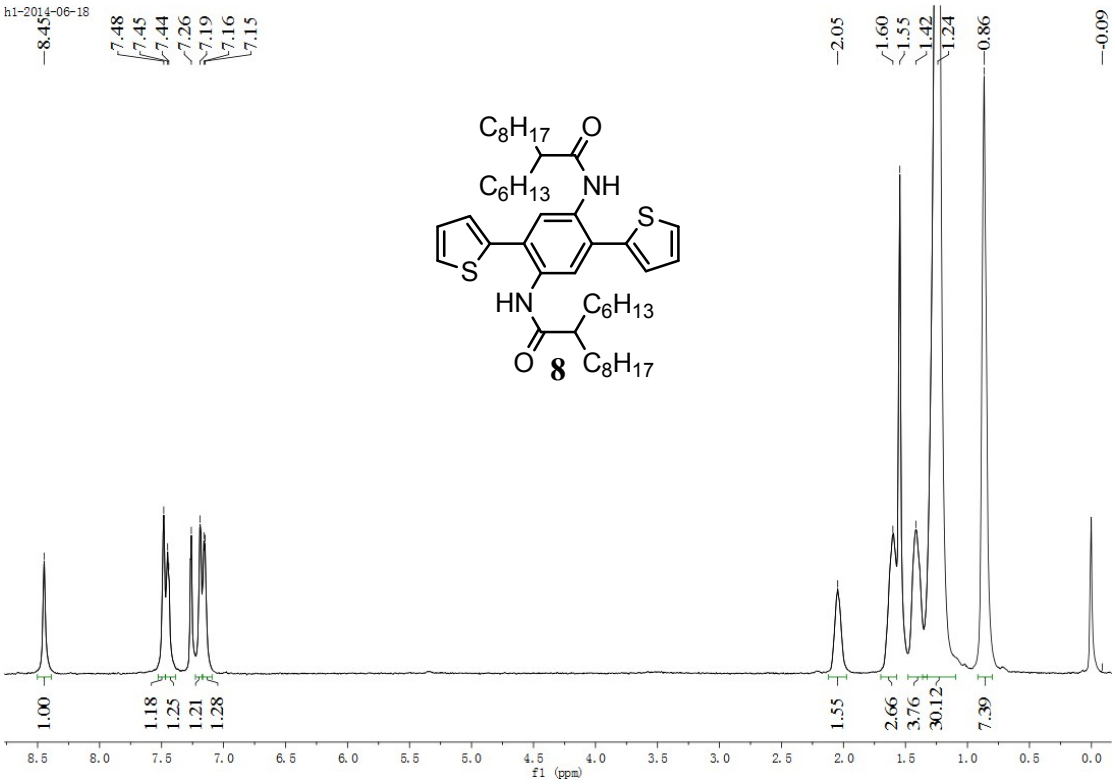

Fig. S11. ^{1}H-NMR of compound **8**.

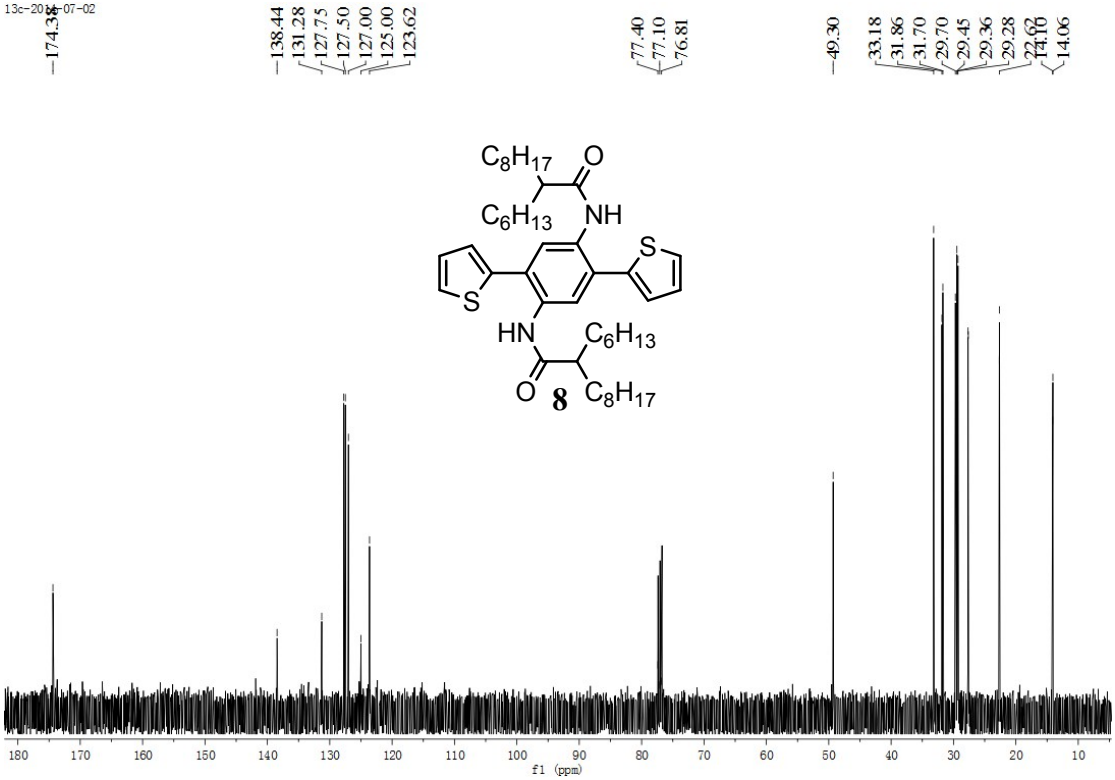

Fig. S12. ^{13}C-NMR of compound **8**.

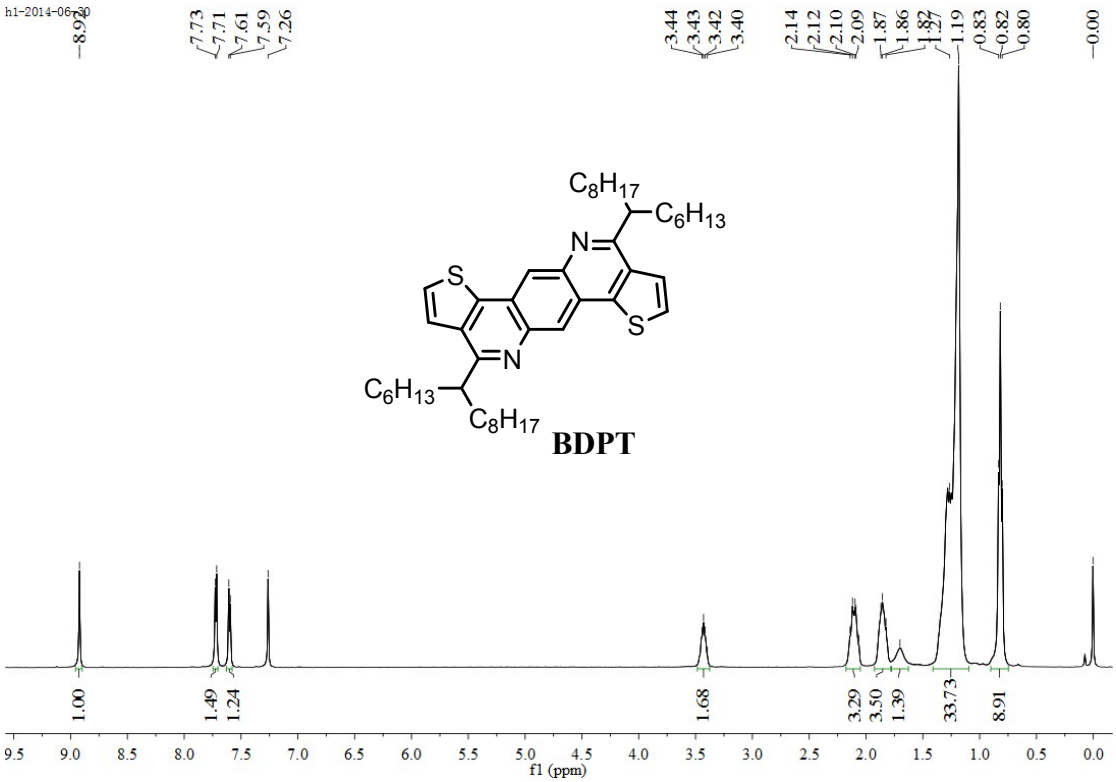

Fig. S13. ^{1}H-NMR of compound **BDPT**.

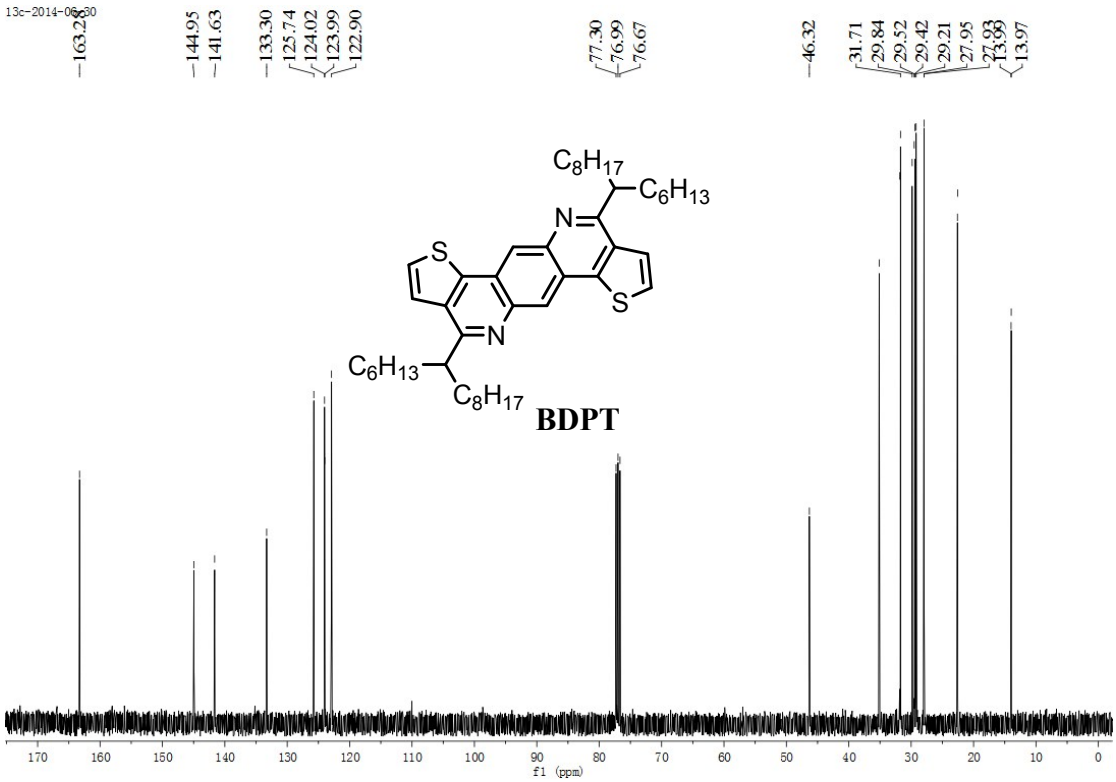

Fig. S14. ^{13}C-NMR of compound **BDPT**.

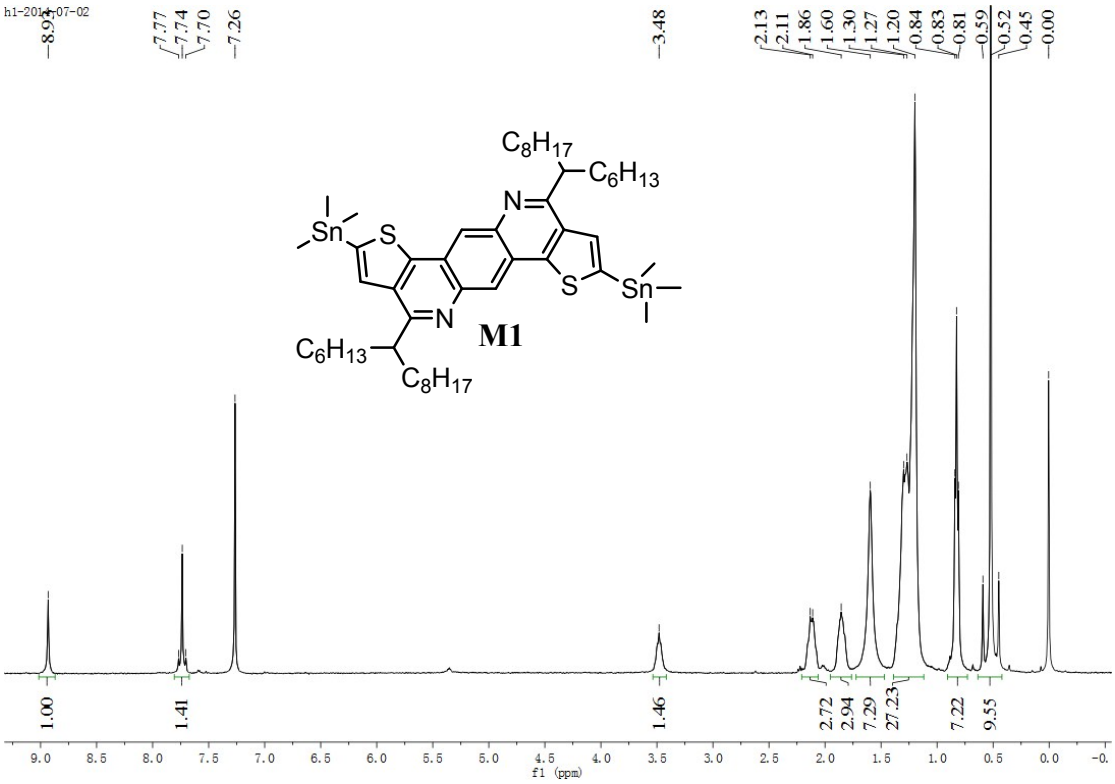

Fig. S15. ^{1}H-NMR of compound **M1**.

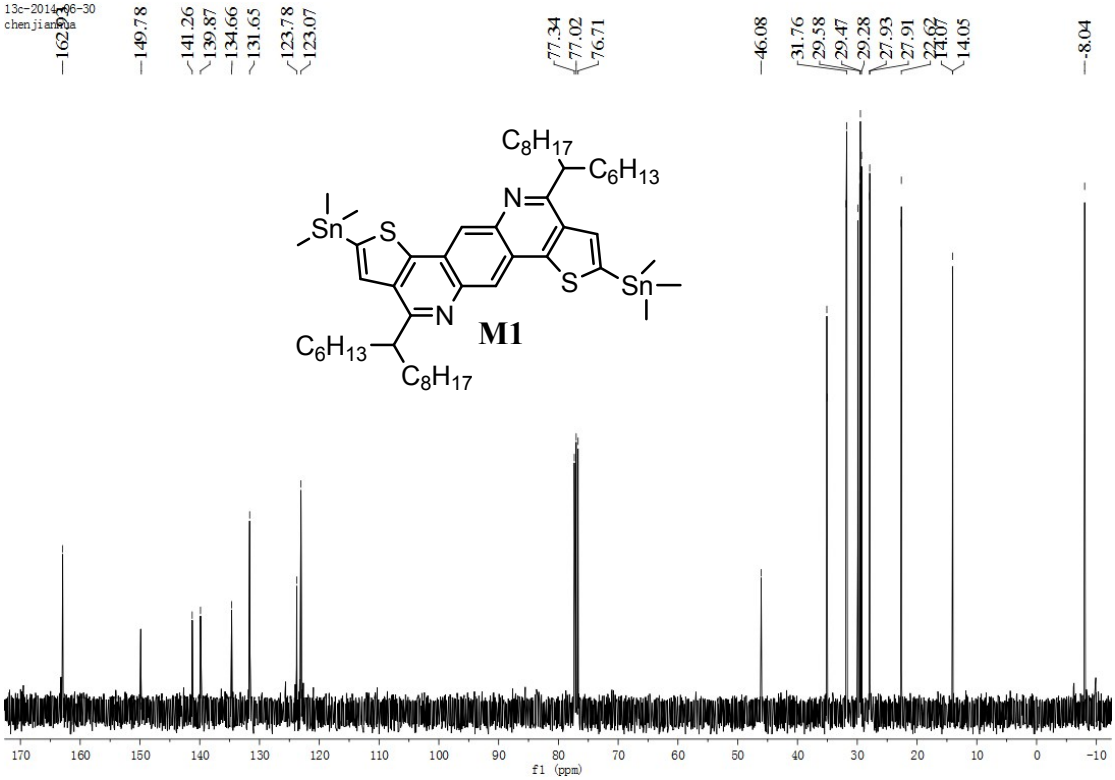

Fig. S16. ^{13}C-NMR of compound **M1**.

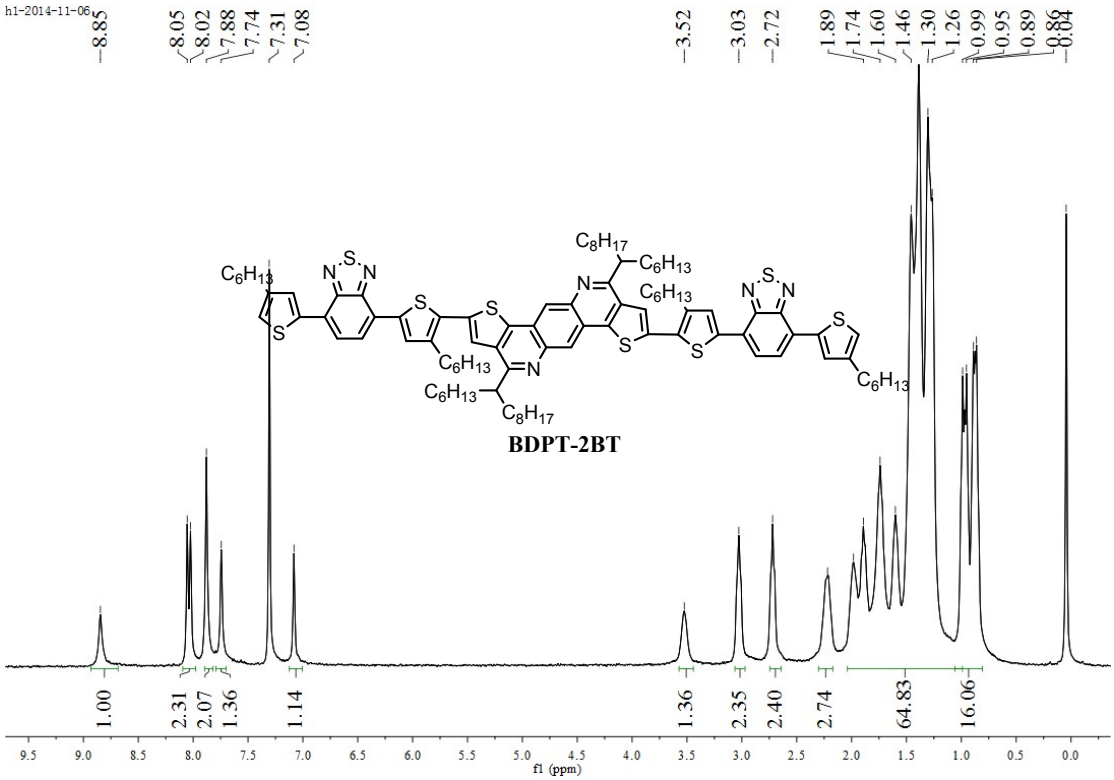

Fig. S17. [1]H-NMR of compound **BDPT-2BT**.

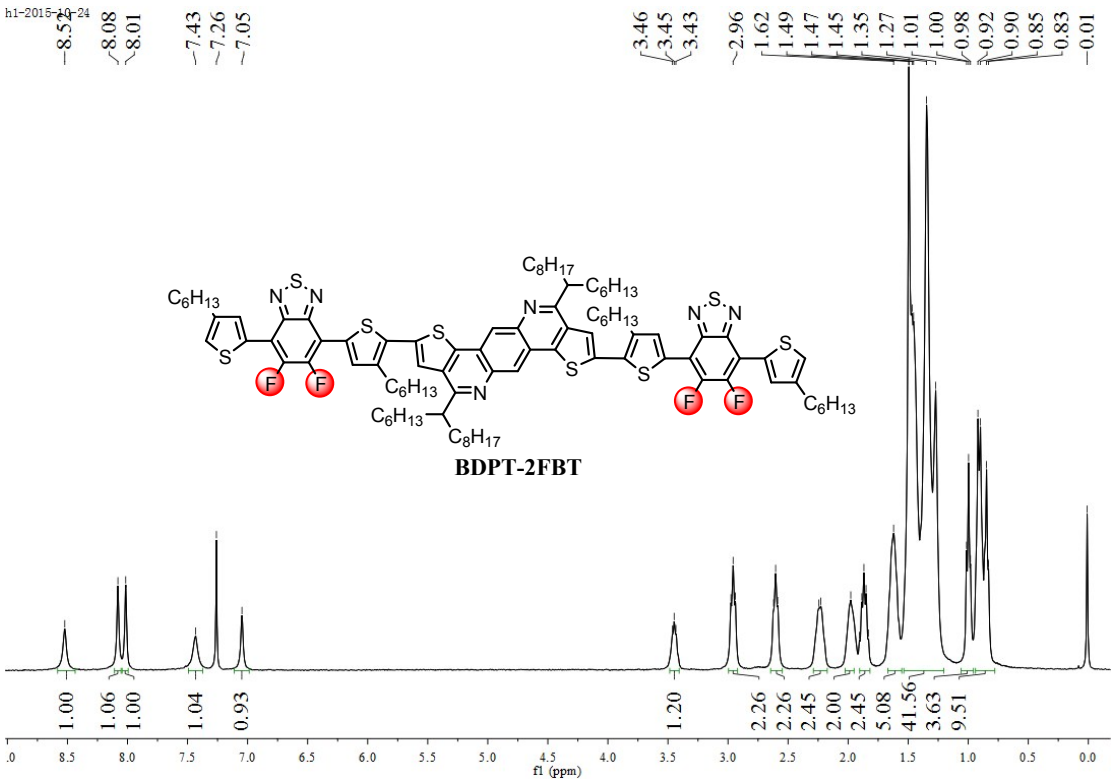

Fig. S18. [1]H-NMR of compound **BDPT-2FBT**.

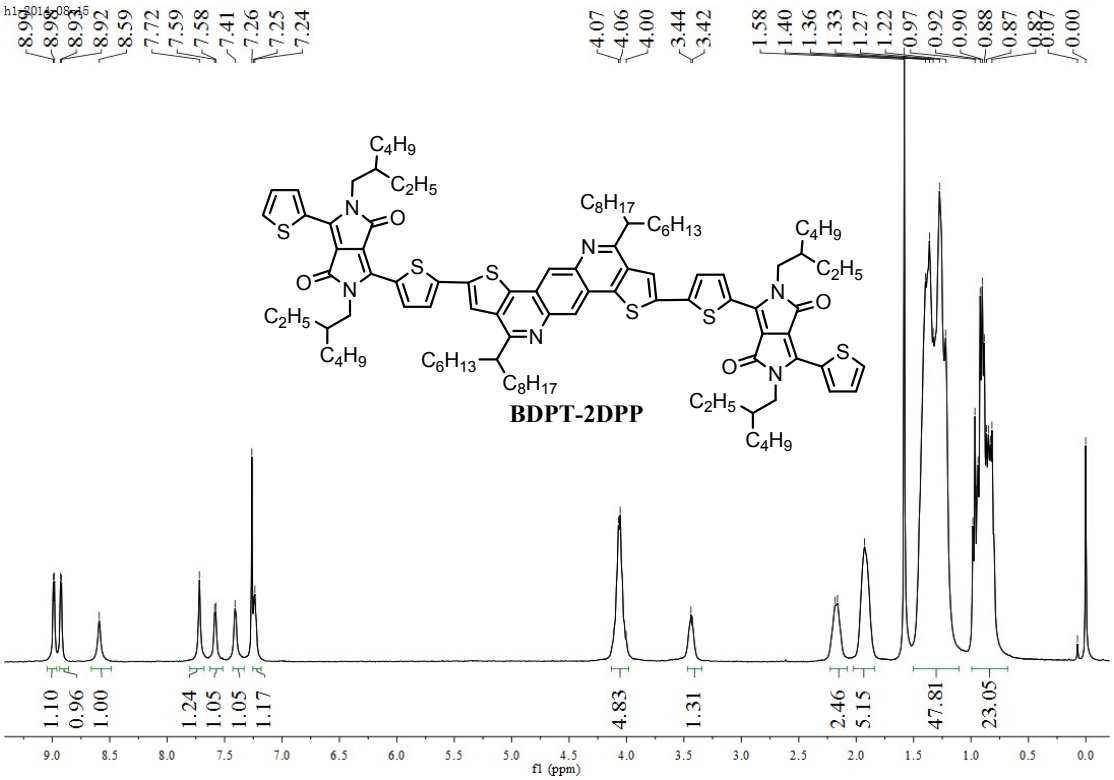

Fig. S19. [1]H-NMR of compound **TPTQ-2DPP**.

5. MALDI-MS data

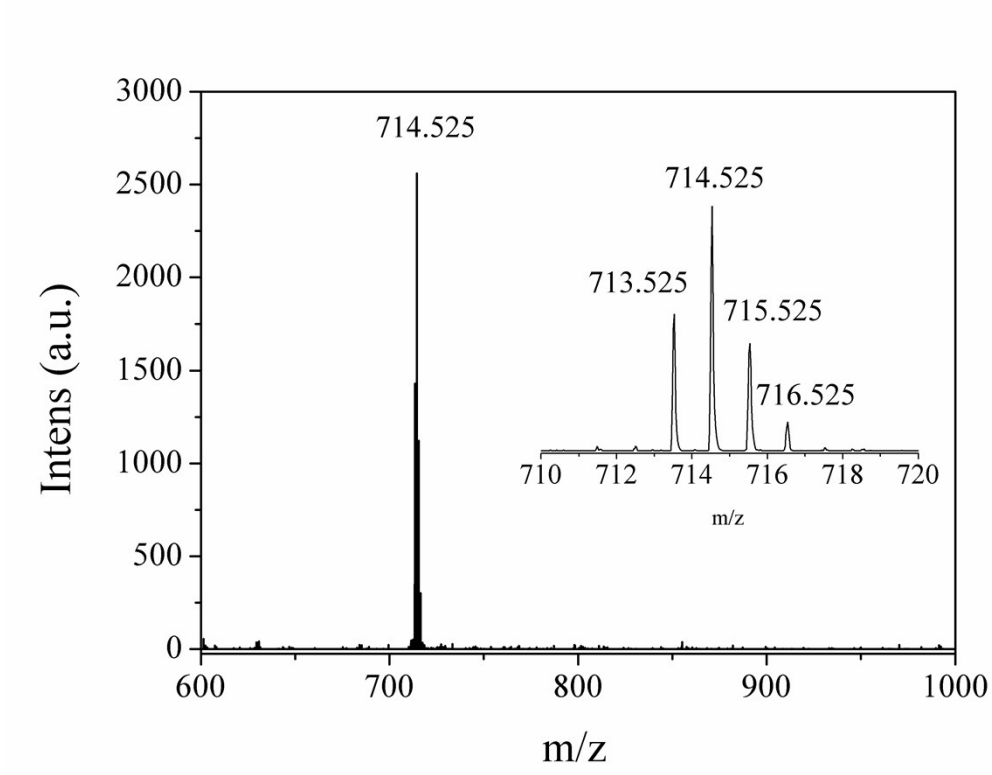

Fig. S20. MS of compound **BDPT**.

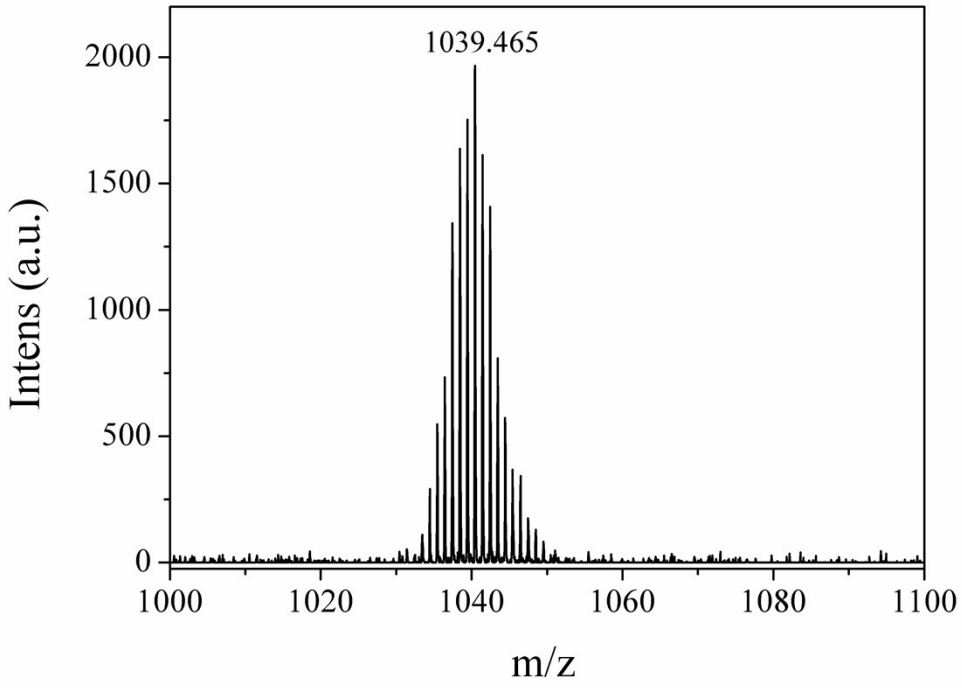

Fig. S21. MS of compound **M1**.

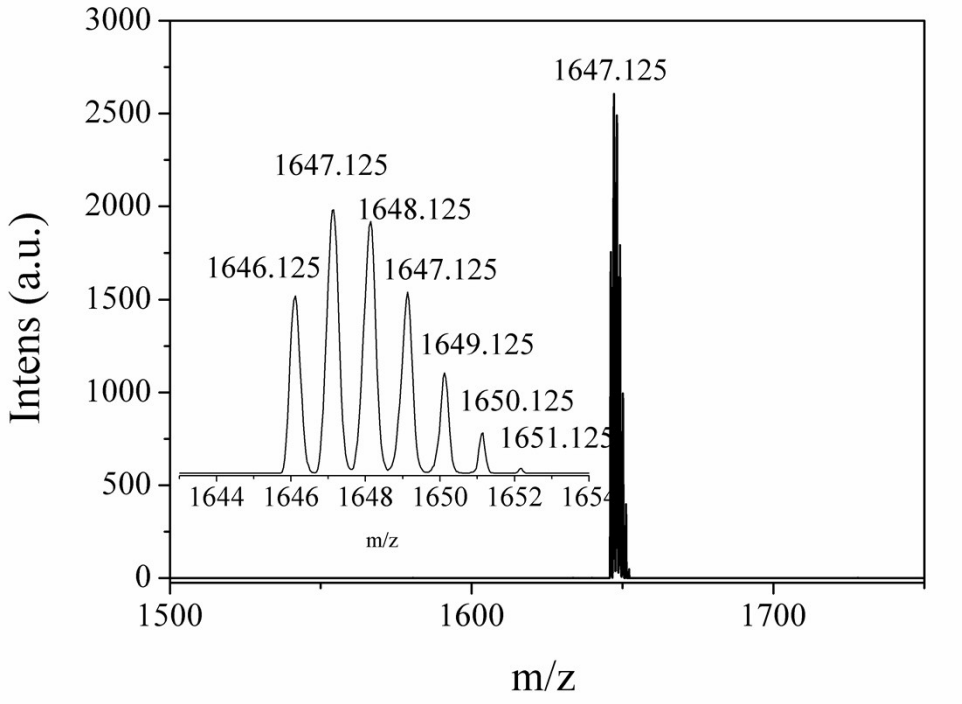

Fig. S22. MS of compound **BDPT-2BT**.

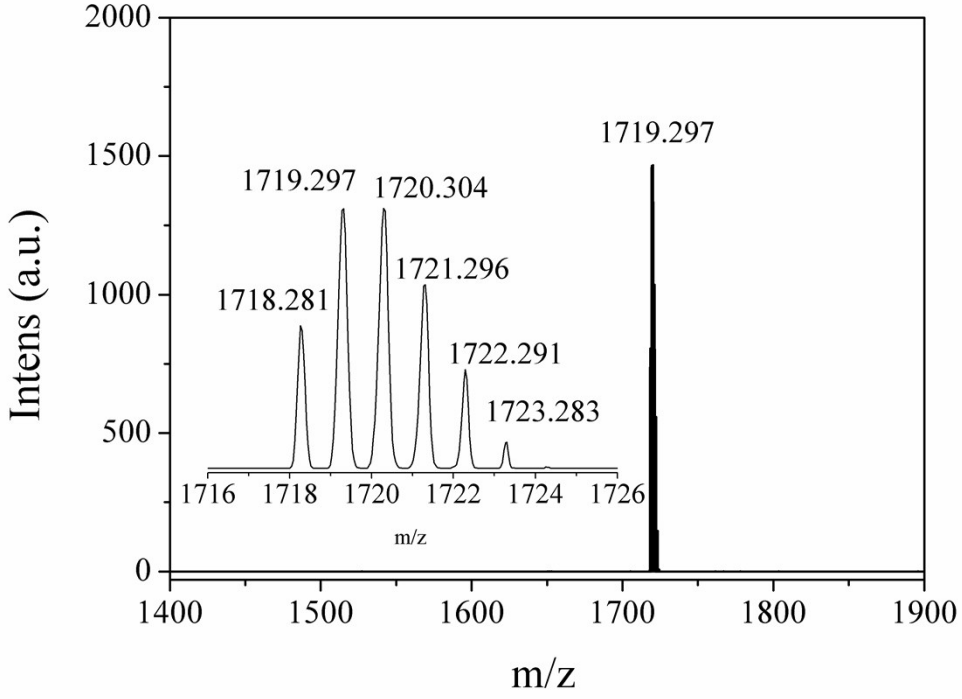

Fig. S23. MS of compound **BDPT-2FBT**.

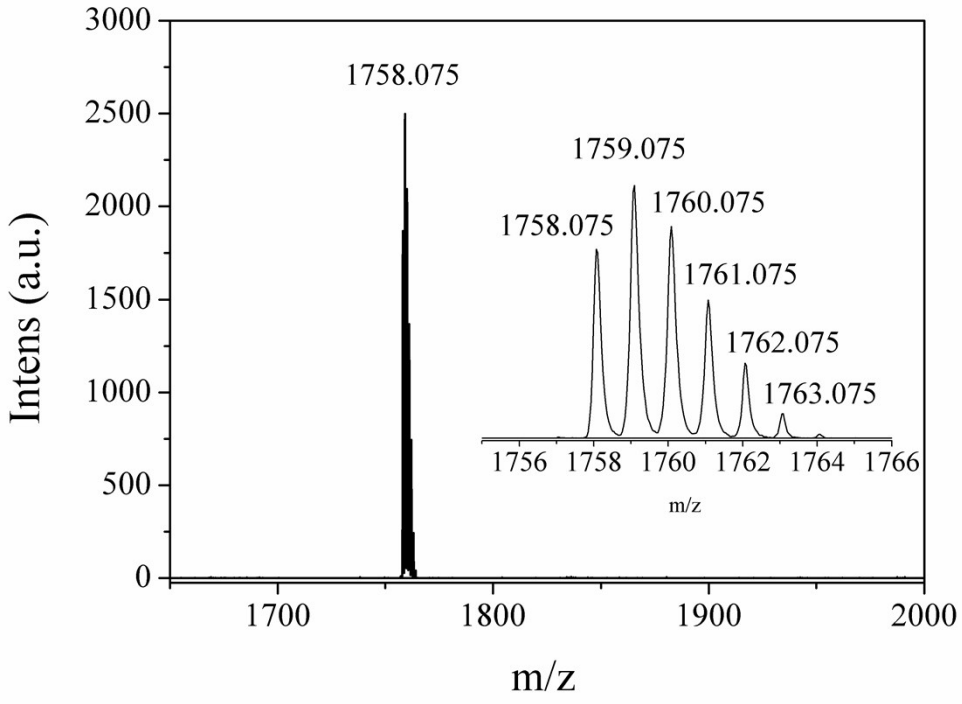

Fig. S24. MS of compound **BDPT-2DPP**.

6. Crystal data of BDPT

Computing details

Data collection: *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.21 (release 20-01-2012 CrysAlis171 .NET) (compiled Jan 23 2012,18:06:46); cell refinement: *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.21 (release 20-01-2012 CrysAlis171 .NET) (compiled Jan 23 2012,18:06:46); data reduction: *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.21 (release 20-01-2012 CrysAlis171 .NET) (compiled Jan 23 2012,18:06:46); program(s) used to solve structure: XS, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122; program(s) used to refine structure: XL, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122; molecular graphics: O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.; software used to prepare material for publication: O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.

Crystal data

$C_{46}H_{68}N_2S_2$	$Z = 1$
$M_r = 713.14$	$F(000) = 390$
Triclinic, $P\bar{1}$	$D_x = 1.120$ Mg m^{-3}
$a = 5.51930$ (13) Å	Mo Ka radiation, l = 0.7107 Å
$b = 8.7116$ (2) Å	Cell parameters from 3998 reflections
$c = 23.1468$ (6) Å	q = 3.9–28.4°
a = 84.894 (2)°	m = 0.16 mm^{-1}
b = 88.701 (2)°	$T = 293$ K
g = 72.509 (2)°	0.20 × 0.08 × 0.05 mm
$V = 1057.26$ (5) Å^3	

Data collection

SuperNova, Single source at offset, Eos diffractometer	4291 independent reflections
Radiation source: SuperNova (Mo) X-ray Source	3654 reflections with $I > 2s(I)$
mirror	$R_{int} = 0.018$
Detector resolution: 15.9784 pixels mm^{-}	$q_{max} = 26.4°$, $q_{min} = 3.5°$

1	
w scans	h = -6®6
Absorption correction: multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.36.32 (release 02-08-2013 CrysAlis171 .NET) (compiled Aug 2 2013,16:46:58) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	k = -10®10
T_{min} = 0.799, T_{max} = 1.000	l = -28®28
8615 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2s(F^2)]$ = 0.061	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.194	H atoms treated by a mixture of independent and constrained refinement
S = 1.09	$w = 1/[s^2(F_o^2) + (0.1018P)^2 + 0.5124P]$ where $P = (F_o^2 + 2F_c^2)/3$
4291 reflections	$(D/s)_{max} < 0.001$
228 parameters	$D\rho_{max}$ = 0.41 e Å^{-3}
25 restraints	$D\rho_{min}$ = -0.42 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR

and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.78841 (12)	0.87107 (7)	0.03308 (3)	0.0417 (2)
N1	0.8595 (4)	0.3484 (2)	0.08695 (8)	0.0341 (4)
C1	0.4593 (4)	0.6612 (3)	-0.02103 (9)	0.0324 (5)
H1	0.4330	0.7685	-0.0348	0.039*
C2	0.6400 (4)	0.5915 (3)	0.02232 (9)	0.0309 (5)
C3	0.6822 (4)	0.4269 (3)	0.04403 (9)	0.0317 (5)
C4	0.9990 (4)	0.4274 (3)	0.10880 (9)	0.0332 (5)
C5	0.9721 (4)	0.5938 (3)	0.09055 (9)	0.0333 (5)
C6	1.1086 (5)	0.6979 (3)	0.10930 (10)	0.0396 (5)
H6	1.2384	0.6652	0.1368	0.048*
C7	1.0268 (5)	0.8482 (3)	0.08251 (11)	0.0445 (6)
H7	1.0927	0.9310	0.0900	0.053*
C8	0.7924 (4)	0.6734 (3)	0.04845 (9)	0.0321 (5)
C9	1.1951 (4)	0.3402 (3)	0.15501 (10)	0.0365 (5)
H9	1.3502	0.3690	0.1448	0.044*
C10	1.2643 (5)	0.1562 (3)	0.15526 (11)	0.0393 (5)
H10A	1.1205	0.1223	0.1697	0.047*
H10B	1.2950	0.1272	0.1157	0.047*
C11	1.4980 (5)	0.0639 (3)	0.19212 (13)	0.0497 (7)
H11A	1.6480	0.0804	0.1732	0.060*
H11B	1.4829	0.1085	0.2295	0.060*
C12	1.5339 (6)	-0.1166 (3)	0.20197 (13)	0.0535 (7)
H12A	1.5336	-0.1587	0.1646	0.064*

H12B	1.6996	-0.1687	0.2195	0.064*
C13	1.3343 (6)	-0.1628 (4)	0.24011 (13)	0.0614 (8)
H13A	1.1683	-0.1082	0.2232	0.074*
H13B	1.3620	-0.2781	0.2398	0.074*
C14	1.3318 (8)	-0.1231 (6)	0.30218 (17)	0.0828 (11)
H14A	1.3080	-0.0083	0.3028	0.099*
H14B	1.4954	-0.1806	0.3198	0.099*
C15	1.1250 (11)	-0.1670 (8)	0.3378 (2)	0.1180 (18)
H15A	0.9619	-0.1122	0.3195	0.142*
H15B	1.1519	-0.2823	0.3382	0.142*
C16	1.118 (2)	-0.1233 (16)	0.3981 (5)	0.234 (4)
H16A	1.0931	-0.0081	0.3979	0.281*
H16B	1.2796	-0.1797	0.4169	0.281*
C17	0.871 (3)	-0.174 (2)	0.4376 (6)	0.354 (8)
H17A	0.7798	-0.2200	0.4127	0.532*
H17B	0.7567	-0.0782	0.4517	0.532*
H17C	0.9416	-0.2506	0.4697	0.532*
C18	0.4326 (15)	0.3219 (13)	0.4342 (3)	0.199 (4)
H18A	0.2674	0.3892	0.4214	0.299*
H18B	0.4512	0.3286	0.4749	0.299*
H18C	0.4511	0.2120	0.4271	0.299*
C19	0.6347 (12)	0.3784 (9)	0.4011 (2)	0.128 (2)
H19A	0.6013	0.4930	0.4048	0.153*
H19B	0.7984	0.3228	0.4190	0.153*
C20	0.6506 (9)	0.3515 (7)	0.33830 (17)	0.1047 (16)
H20A	0.6801	0.2372	0.3348	0.126*
H20B	0.4874	0.4087	0.3205	0.126*
C21	0.8498 (8)	0.4030 (6)	0.30517 (15)	0.0792 (11)
H21A	1.0100	0.3552	0.3256	0.095*
H21B	0.8094	0.5193	0.3052	0.095*
C22	0.8869 (6)	0.3602 (5)	0.24259 (13)	0.0622 (8)
H22A	0.9119	0.2454	0.2415	0.075*

H22B	0.7347	0.4179	0.2204	0.075*
C23	1.1117 (5)	0.4022 (3)	0.21493 (11)	0.0448 (6)
H23A	1.2552	0.3600	0.2413	0.054*
H23B	1.0724	0.5189	0.2111	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0513 (4)	0.0284 (3)	0.0495 (4)	-0.0186 (3)	-0.0068 (3)	0.0001 (2)
N1	0.0383 (10)	0.0314 (10)	0.0340 (9)	-0.0131 (8)	-0.0023 (8)	-0.0001 (8)
C1	0.0374 (12)	0.0246 (11)	0.0362 (11)	-0.0113 (9)	0.0015 (9)	-0.0002 (8)
C2	0.0347 (11)	0.0272 (11)	0.0329 (11)	-0.0121 (9)	0.0028 (9)	-0.0040 (8)
C3	0.0349 (11)	0.0287 (11)	0.0322 (11)	-0.0112 (9)	0.0017 (9)	-0.0011 (8)
C4	0.0359 (12)	0.0349 (12)	0.0315 (11)	-0.0147 (9)	0.0011 (9)	-0.0023 (9)
C5	0.0364 (12)	0.0340 (12)	0.0333 (11)	-0.0157 (10)	0.0012 (9)	-0.0044 (9)
C6	0.0438 (13)	0.0423 (14)	0.0385 (12)	-0.0215 (11)	-0.0018 (10)	-0.0037 (10)
C7	0.0528 (15)	0.0405 (14)	0.0491 (14)	-0.0270 (12)	-0.0031 (11)	-0.0053 (11)
C8	0.0369 (12)	0.0278 (11)	0.0343 (11)	-0.0137 (9)	0.0033 (9)	-0.0033 (9)
C9	0.0387 (12)	0.0362 (13)	0.0376 (12)	-0.0162 (10)	-0.0054 (9)	0.0004 (9)
C10	0.0412 (13)	0.0379 (13)	0.0406 (12)	-0.0152 (10)	-0.0056 (10)	-0.0003 (10)
C11	0.0433 (14)	0.0472 (16)	0.0584 (16)	-0.0154 (12)	-0.0130 (12)	0.0056 (12)
C12	0.0527 (16)	0.0431 (15)	0.0599 (17)	-0.0082 (12)	-0.0113 (13)	0.0024 (12)
C13	0.072 (2)	0.0502 (18)	0.0634 (18)	-0.0238 (15)	-0.0131 (15)	0.0093 (14)

C14	0.087 (3)	0.093 (3)	0.073 (2)	-0.037 (2)	0.001 (2)	-0.001 (2)
C15	0.130 (4)	0.149 (5)	0.083 (3)	-0.058 (4)	0.010 (3)	0.009 (3)
C16	0.232 (8)	0.266 (9)	0.210 (7)	-0.083 (7)	0.006 (7)	-0.015 (7)
C17	0.341 (15)	0.428 (18)	0.317 (14)	-0.163 (13)	0.024 (13)	0.010 (13)
C18	0.156 (6)	0.355 (12)	0.112 (5)	-0.124 (7)	0.037 (5)	0.002 (6)
C19	0.125 (4)	0.196 (6)	0.068 (3)	-0.060 (4)	0.016 (3)	-0.004 (3)
C20	0.099 (3)	0.169 (5)	0.062 (2)	-0.064 (3)	0.013 (2)	-0.018 (3)
C21	0.084 (3)	0.106 (3)	0.0532 (18)	-0.036 (2)	0.0112 (17)	-0.0163 (19)
C22	0.0632 (19)	0.083 (2)	0.0488 (16)	-0.0336 (17)	0.0062 (14)	-0.0123 (15)
C23	0.0529 (15)	0.0446 (15)	0.0396 (13)	-0.0185 (12)	-0.0081 (11)	-0.0030 (11)

Geometric parameters (Å, º)

S1—C7	1.718 (3)	C13—C14	1.506 (5)
S1—C8	1.720 (2)	C14—H14A	0.9700
N1—C3	1.390 (3)	C14—H14B	0.9700
N1—C4	1.311 (3)	C14—C15	1.514 (6)
C1—H1	0.9300	C15—H15A	0.9700
C1—C2	1.394 (3)	C15—H15B	0.9700
C1—C3^{i}	1.391 (3)	C15—C16	1.475 (11)
C2—C3	1.428 (3)	C16—H16A	0.9700
C2—C8	1.430 (3)	C16—H16B	0.9700
C3—C1^{i}	1.391 (3)	C16—C17	1.768 (15)
C4—C5	1.438 (3)	C17—H17A	0.9600
C4—C9	1.519 (3)	C17—H17B	0.9600
C5—C6	1.440 (3)	C17—H17C	0.9600
C5—C8	1.387 (3)	C18—H18A	0.9600
C6—H6	0.9300	C18—H18B	0.9600
C6—C7	1.347 (4)	C18—H18C	0.9600
C7—H7	0.9300	C18—C19	1.516 (8)
C9—H9	0.9800	C19—H19A	0.9700

C9—C10	1.531 (3)	C19—H19B	0.9700
C9—C23	1.543 (3)	C19—C20	1.489 (6)
C10—H10A	0.9700	C20—H20A	0.9700
C10—H10B	0.9700	C20—H20B	0.9700
C10—C11	1.530 (3)	C20—C21	1.481 (5)
C11—H11A	0.9700	C21—H21A	0.9700
C11—H11B	0.9700	C21—H21B	0.9700
C11—C12	1.522 (4)	C21—C22	1.522 (4)
C12—H12A	0.9700	C22—H22A	0.9700
C12—H12B	0.9700	C22—H22B	0.9700
C12—C13	1.522 (4)	C22—C23	1.510 (4)
C13—H13A	0.9700	C23—H23A	0.9700
C13—H13B	0.9700	C23—H23B	0.9700
C7—S1—C8	91.43 (11)	C13—C14—C15	113.0 (4)
C4—N1—C3	119.2 (2)	H14A—C14—H14B	107.8
C2—C1—H1	119.4	C15—C14—H14A	109.0
C3^{i}—C1—H1	119.4	C15—C14—H14B	109.0
C3^{i}—C1—C2	121.2 (2)	C14—C15—H15A	109.0
C1—C2—C3	120.0 (2)	C14—C15—H15B	109.0
C1—C2—C8	124.8 (2)	H15A—C15—H15B	107.8
C3—C2—C8	115.2 (2)	C16—C15—C14	112.8 (6)
N1—C3—C1^{i}	117.7 (2)	C16—C15—H15A	109.0
N1—C3—C2	123.6 (2)	C16—C15—H15B	109.0
C1^{i}—C3—C2	118.8 (2)	C15—C16—H16A	109.4
N1—C4—C5	122.2 (2)	C15—C16—H16B	109.4
N1—C4—C9	118.9 (2)	C15—C16—C17	111.1 (9)
C5—C4—C9	118.90 (19)	H16A—C16—H16B	108.0
C4—C5—C6	129.7 (2)	C17—C16—H16A	109.4
C8—C5—C4	118.9 (2)	C17—C16—H16B	109.4

C8—C5—C6	111.5 (2)	C16—C17—H17A	109.5
C5—C6—H6	123.8	C16—C17—H17B	109.5
C7—C6—C5	112.4 (2)	C16—C17—H17C	109.5
C7—C6—H6	123.8	H17A—C17—H17B	109.5
S1—C7—H7	123.5	H17A—C17—H17C	109.5
C6—C7—S1	113.01 (19)	H17B—C17—H17C	109.5
C6—C7—H7	123.5	H18A—C18—H18B	109.5
C2—C8—S1	127.25 (18)	H18A—C18—H18C	109.5
C5—C8—S1	111.72 (16)	H18B—C18—H18C	109.5
C5—C8—C2	121.0 (2)	C19—C18—H18A	109.5
C4—C9—H9	106.6	C19—C18—H18B	109.5
C4—C9—C10	112.35 (18)	C19—C18—H18C	109.5
C4—C9—C23	110.9 (2)	C18—C19—H19A	108.6
C10—C9—H9	106.6	C18—C19—H19B	108.6
C10—C9—C23	113.3 (2)	H19A—C19—H19B	107.6
C23—C9—H9	106.6	C20—C19—C18	114.7 (5)
C9—C10—H10A	108.7	C20—C19—H19A	108.6
C9—C10—H10B	108.7	C20—C19—H19B	108.6
H10A—C10—H10B	107.6	C19—C20—H20A	108.3
C11—C10—C9	114.1 (2)	C19—C20—H20B	108.3
C11—C10—H10A	108.7	H20A—C20—H20B	107.4
C11—C10—H10B	108.7	C21—C20—C19	115.8 (4)
C10—C11—H11A	108.8	C21—C20—H20A	108.3
C10—C11—H11B	108.8	C21—C20—H20B	108.3
H11A—C11—H11B	107.7	C20—C21—H21A	108.2

C12—C11—C10	113.6 (2)	C20—C21—H21B	108.2
C12—C11—H11A	108.8	C20—C21—C22	116.4 (3)
C12—C11—H11B	108.8	H21A—C21—H21B	107.4
C11—C12—H12A	108.5	C22—C21—H21A	108.2
C11—C12—H12B	108.5	C22—C21—H21B	108.2
H12A—C12—H12B	107.5	C21—C22—H22A	109.2
C13—C12—C11	115.0 (2)	C21—C22—H22B	109.2
C13—C12—H12A	108.5	H22A—C22—H22B	107.9
C13—C12—H12B	108.5	C23—C22—C21	112.0 (3)
C12—C13—H13A	108.5	C23—C22—H22A	109.2
C12—C13—H13B	108.5	C23—C22—H22B	109.2
H13A—C13—H13B	107.5	C9—C23—H23A	108.1
C14—C13—C12	115.1 (3)	C9—C23—H23B	108.1
C14—C13—H13A	108.5	C22—C23—C9	116.8 (2)
C14—C13—H13B	108.5	C22—C23—H23A	108.1
C13—C14—H14A	109.0	C22—C23—H23B	108.1
C13—C14—H14B	109.0	H23A—C23—H23B	107.3
N1—C4—C5—C6	-179.5 (2)	C5—C6—C7—S1	-1.0 (3)
N1—C4—C5—C8	0.0 (3)	C6—C5—C8—S1	-0.8 (3)
N1—C4—C9—C10	19.4 (3)	C6—C5—C8—C2	178.10 (19)
N1—C4—C9—C23	-108.6 (2)	C7—S1—C8—C2	-178.6 (2)
C1—C2—C3—N1	179.7 (2)	C7—S1—C8—C5	0.19 (18)
C1—C2—C3—C1^{i}	0.1 (4)	C8—S1—C7—C6	0.5 (2)
C1—C2—C8—S1	0.1 (3)	C8—C2—C3—N1	-0.7 (3)
C1—C2—C8—C5	-178.6 (2)	C8—C2—C3—C1^{i}	179.74 (19)
C3—N1—C4—C5	1.1 (3)	C8—C5—C6—C7	1.2 (3)

C3—N1—C4—C9	-179.08 (19)	C9—C4—C5—C6	0.6 (4)
C3^{i}—C1—C2—C3	-0.1 (4)	C9—C4—C5—C8	-179.8 (2)
C3^{i}—C1—C2—C8	-179.7 (2)	C9—C10—C11—C12	168.4 (2)
C3—C2—C8—S1	-179.49 (16)	C10—C9—C23—C22	-58.2 (3)
C3—C2—C8—C5	1.8 (3)	C10—C11—C12—C13	-68.2 (3)
C4—N1—C3—C1^{i}	178.8 (2)	C11—C12—C13—C14	-65.1 (4)
C4—N1—C3—C2	-0.7 (3)	C12—C13—C14—C15	178.3 (4)
C4—C5—C6—C7	-179.2 (2)	C13—C14—C15—C16	-178.2 (6)
C4—C5—C8—S1	179.58 (16)	C14—C15—C16—C17	179.1 (8)
C4—C5—C8—C2	-1.5 (3)	C18—C19—C20—C21	-178.9 (6)
C4—C9—C10—C11	168.1 (2)	C19—C20—C21—C22	173.7 (5)
C4—C9—C23—C22	69.2 (3)	C20—C21—C22—C23	-173.9 (4)
C5—C4—C9—C10	-160.7 (2)	C21—C22—C23—C9	170.5 (3)
C5—C4—C9—C23	71.3 (3)	C23—C9—C10—C11	-65.2 (3)

Symmetry code: (i) -*x*+1, -*y*+1, -*z*.