Diazaisoindigo Based Polymers with High Performance Charge Transport Properties: From Computational Screening to Experimental Characterization

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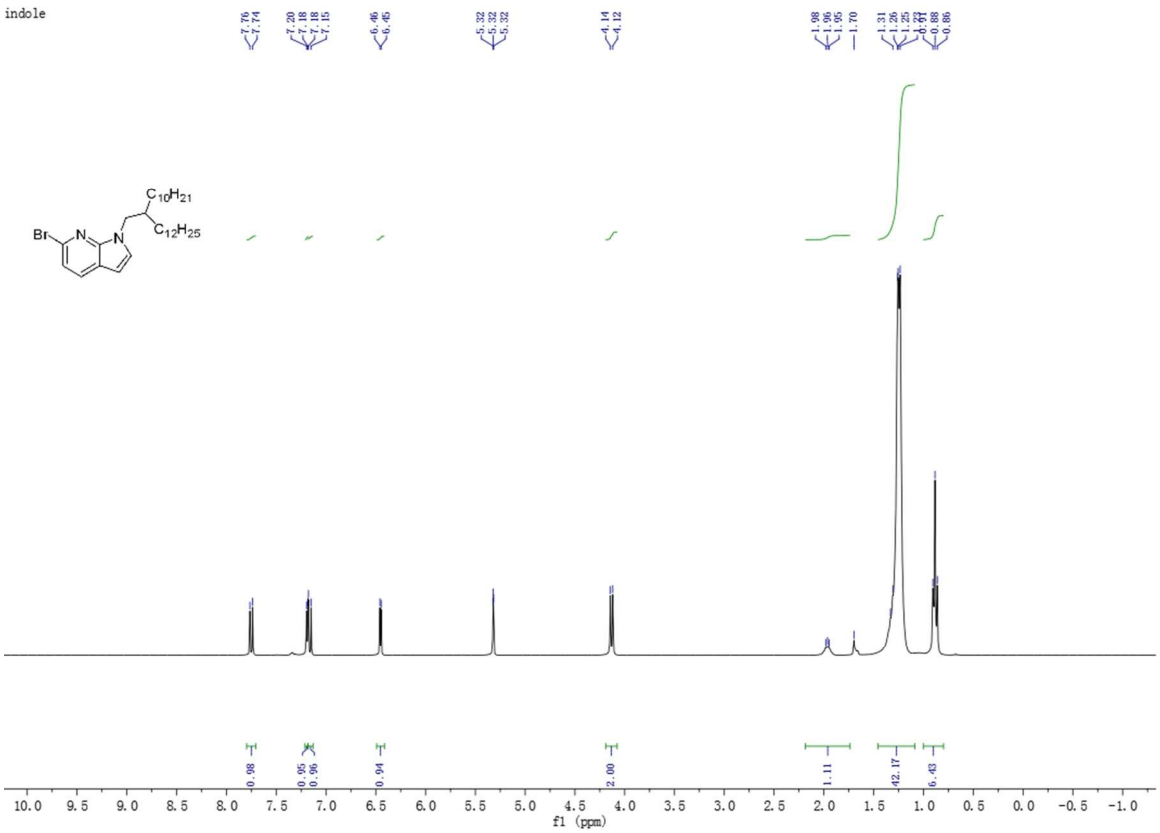
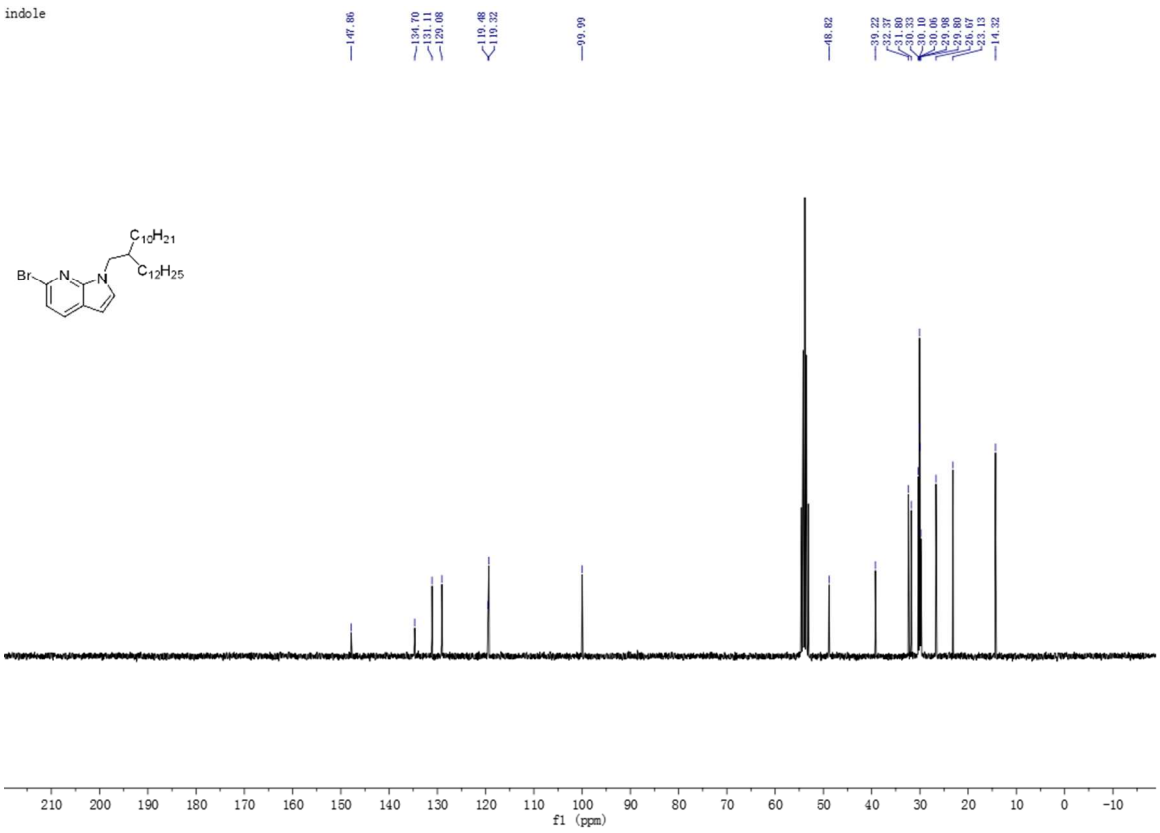
Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China

1. ^{1}H NMR and ^{13}C NMR spectra of new compounds
2. HR-MS profiles of new compounds
3. Theoretical calculations
4. Cyclic voltammetry of the polymer
5. Annealing temperature dependence of the mobilities
6. 1D-GIXRD profiles
7. Absorption coefficients of monomers and polymers


indole
7.76
7.74
7.20
7.18
7.18
7.15
6.46
6.45
5.32
5.32
5.32
4.14
4.12
1.98
1.96
1.95
1.70
1.31
1.26
1.25
0.88
0.86
Br
N
N
$C_{10}H_{21}$
$C_{12}H_{25}$
0.98
0.95
0.96
0.94
2.00
1.11
42.17
6.43
f1 (ppm)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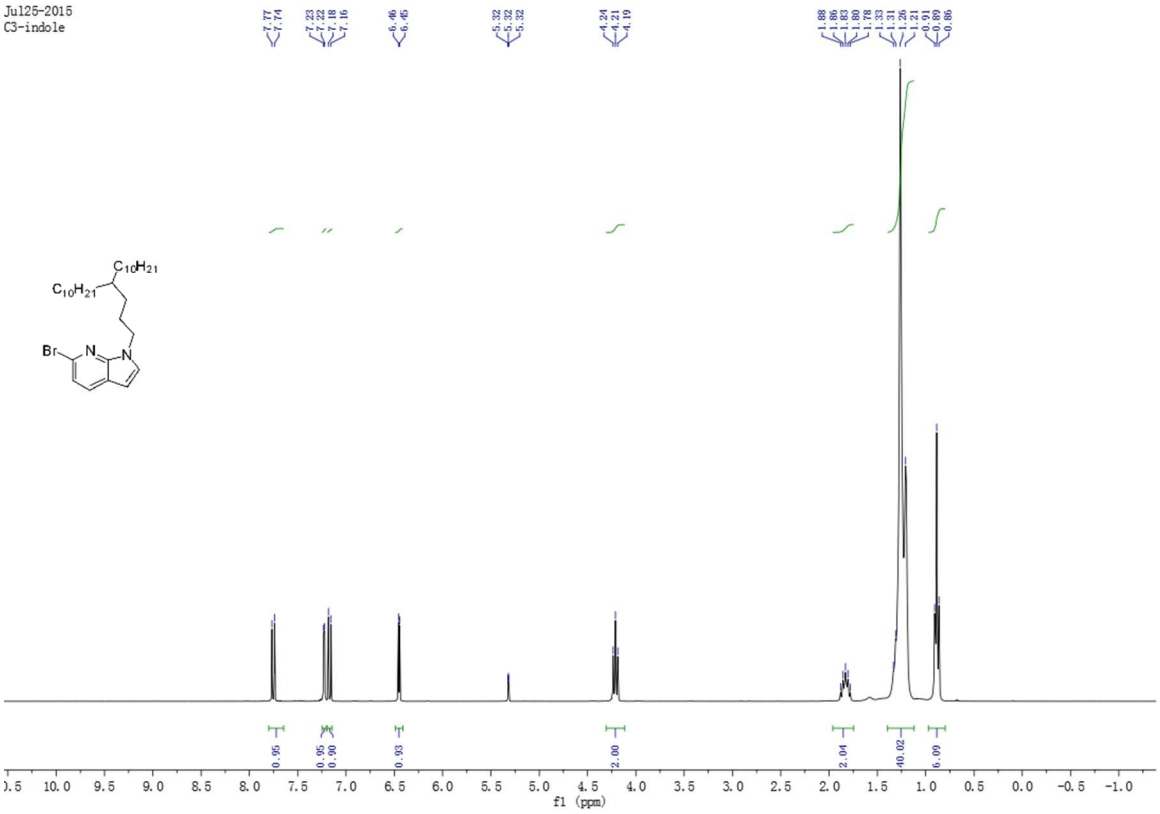
134.70
131.11
129.08
119.48
119.32
99.99
48.82
39.22
32.37
31.89
30.33
30.10
30.06
29.98
29.80
29.67
26.13
14.32
Br
N
N
$C_{10}H_{21}$
$C_{12}H_{25}$
f1 (ppm)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7.74
7.23
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7.18
7.16
6.46
6.45
5.32
5.32
5.32
4.24
4.21
4.19
1.88
1.86
1.83
1.80
1.78
1.33
1.31
1.26
1.21
0.91
0.89
0.86
C10H21
C10H21
Br
N
N
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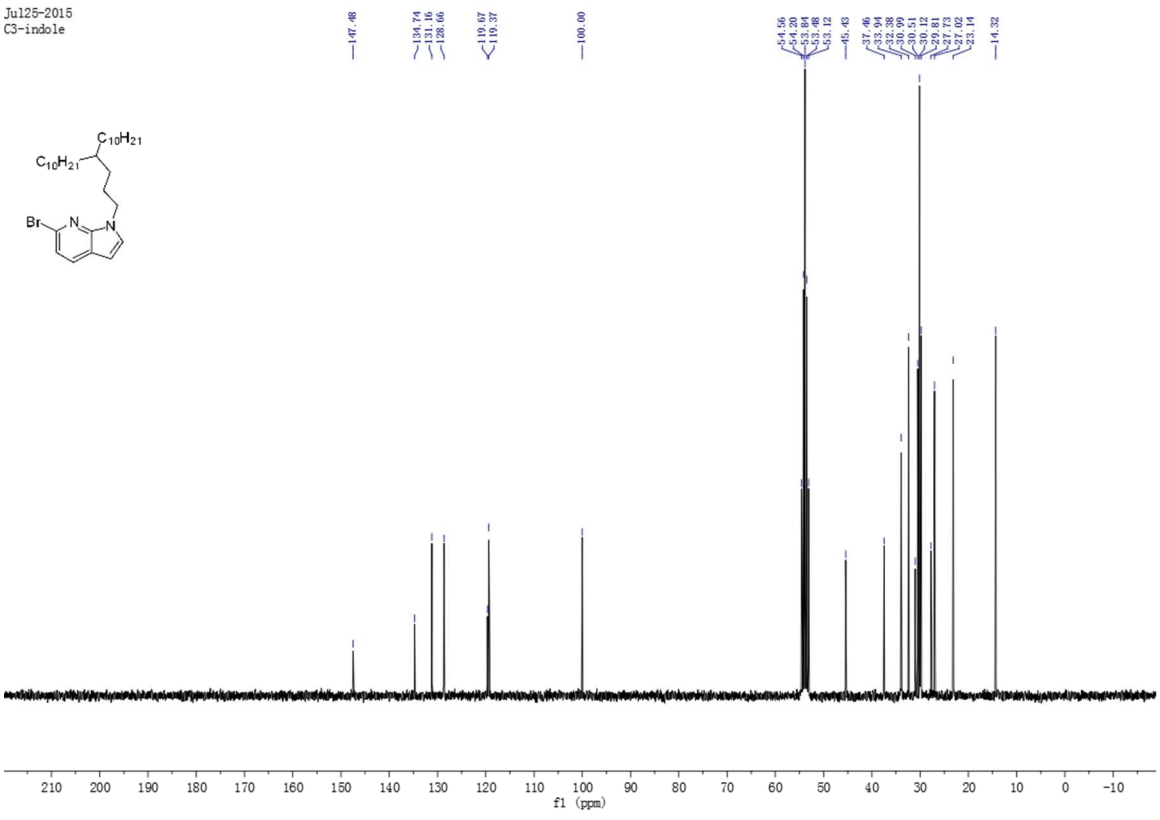
0.95
0.90
0.93
2.00
2.04
40.02
6.09
f1 (ppm)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53.84
53.48
53.12
45.43
37.46
33.94
32.38
30.99
30.51
30.12
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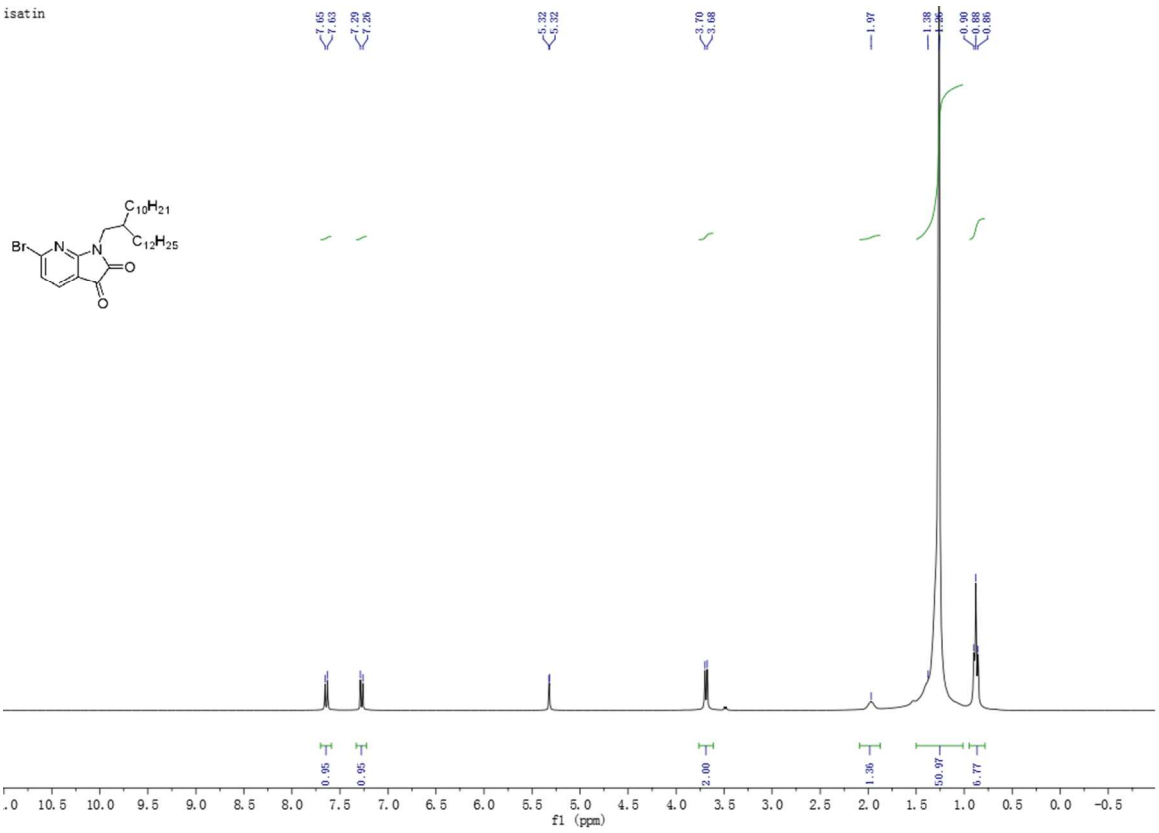
23.14
14.32
C10H21
C10H21
Br
N
N
f1 (ppm)

isatin



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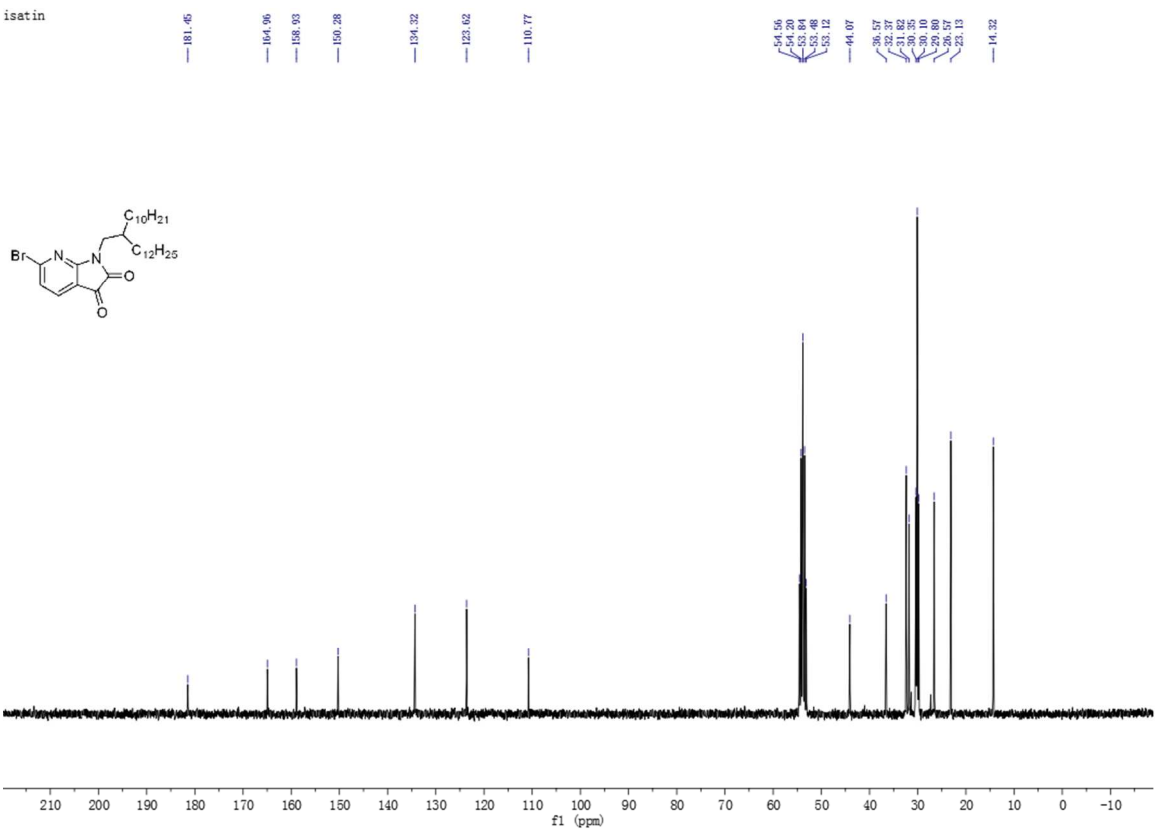

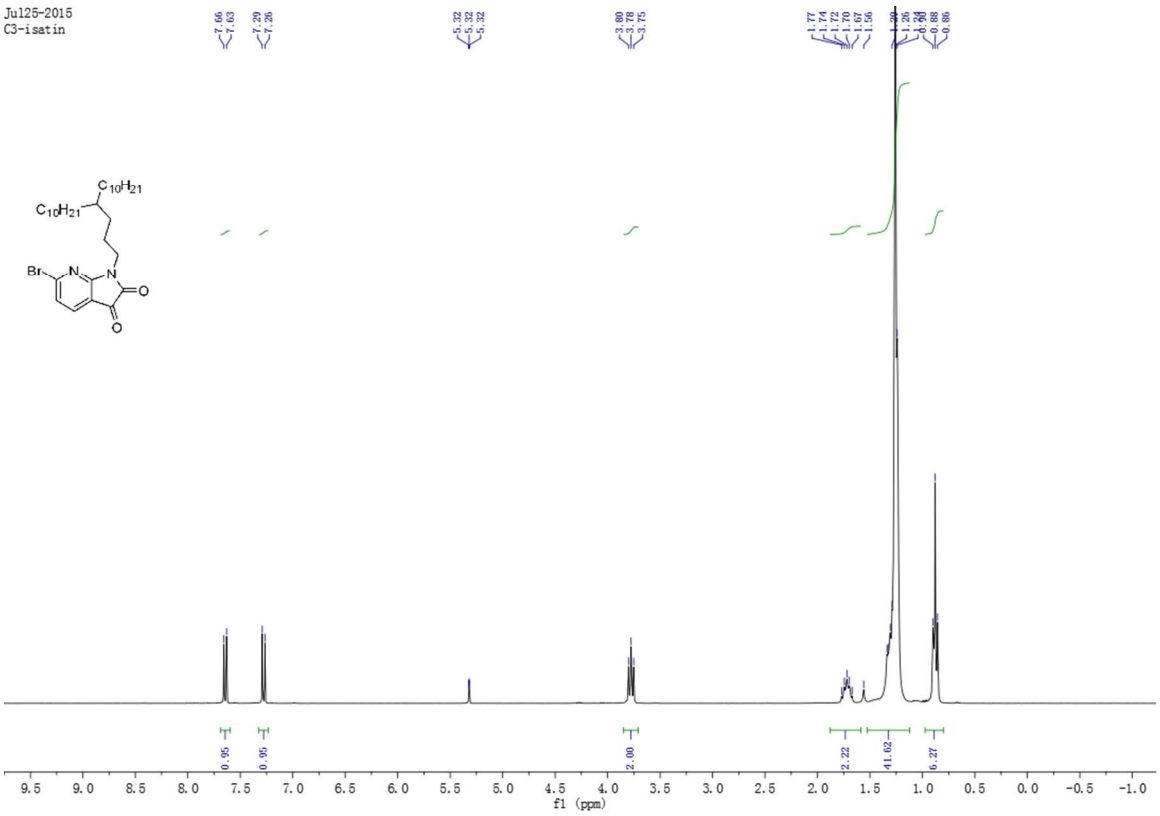
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7.63
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5.32
5.32
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1.77
1.74
1.72
1.70
1.67
1.56
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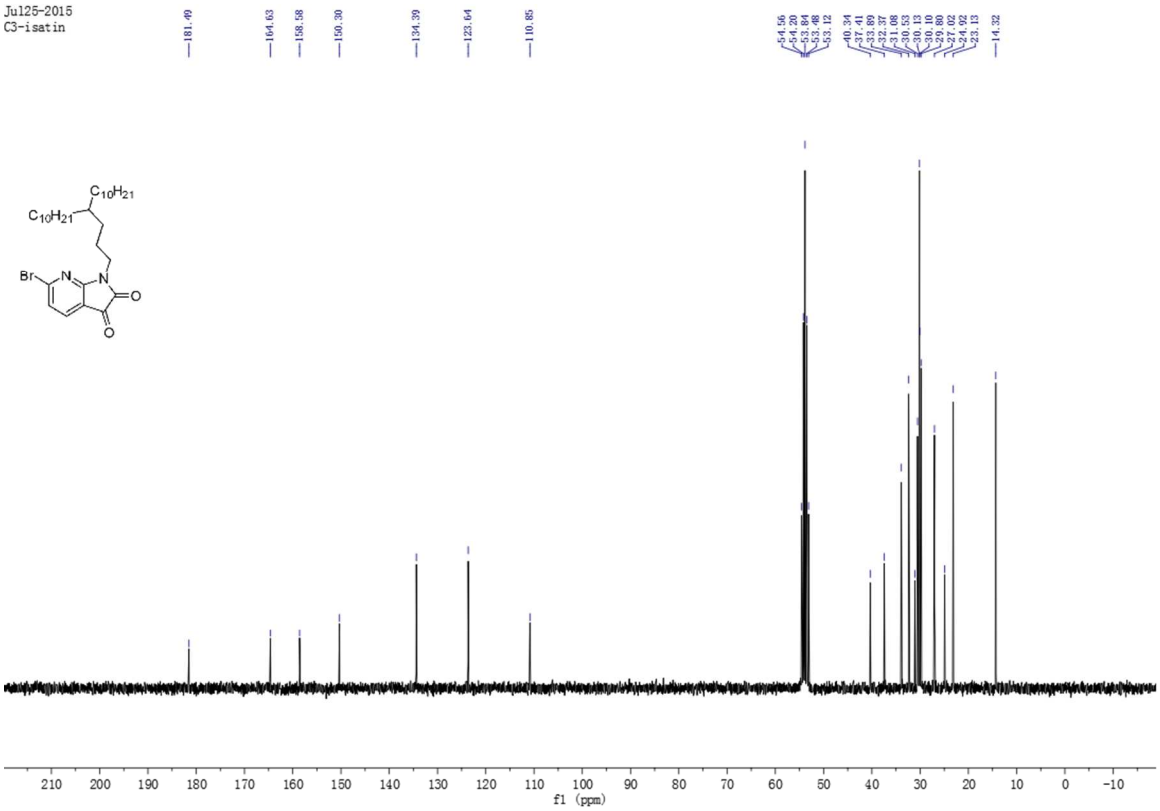
0.88
0.86
0.95
0.95
2.00
2.22
41.62
6.27
f1 (ppm)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164.63
158.58
150.30
134.39
123.64
110.85
54.56
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53.84
53.48
53.12
40.34
37.41
33.89
32.37
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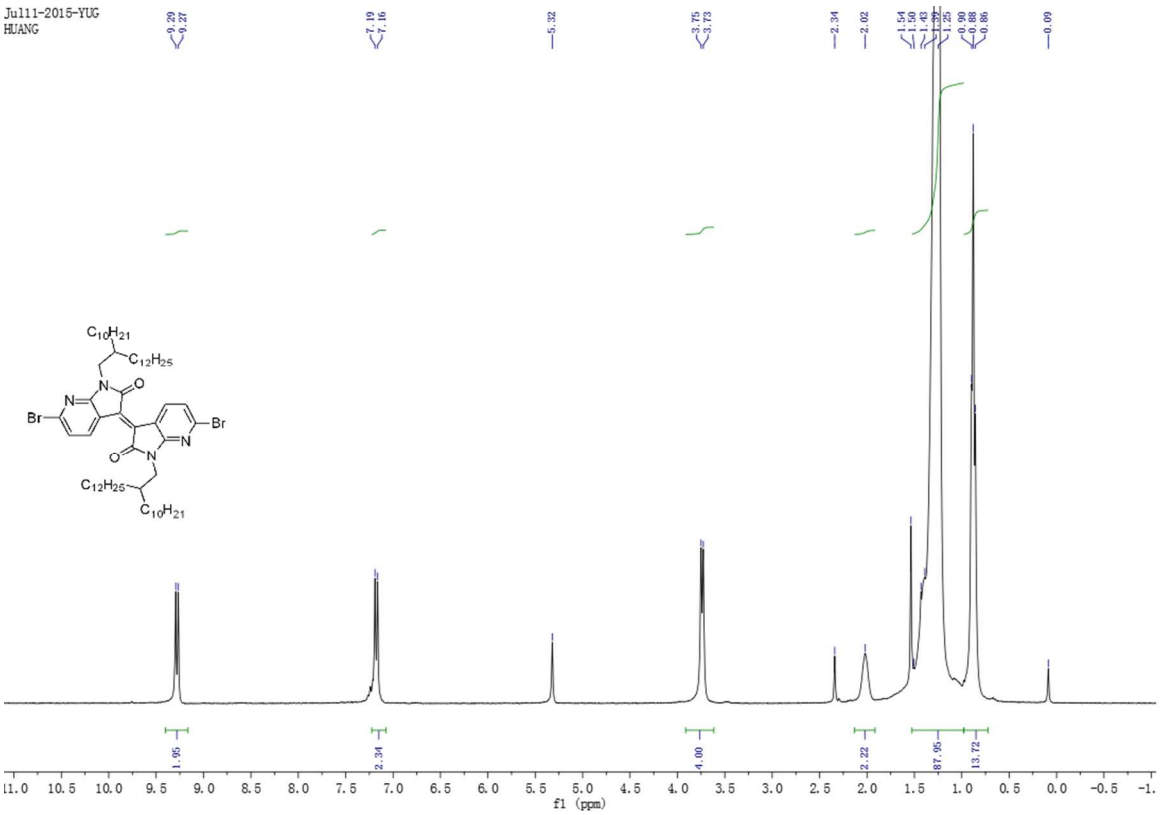
30.53
30.13
30.10
29.89
27.02
24.92
23.13
14.32
f1 (ppm)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HUANG
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9.27
7.19
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2.34
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1.50
1.43
1.32
1.25
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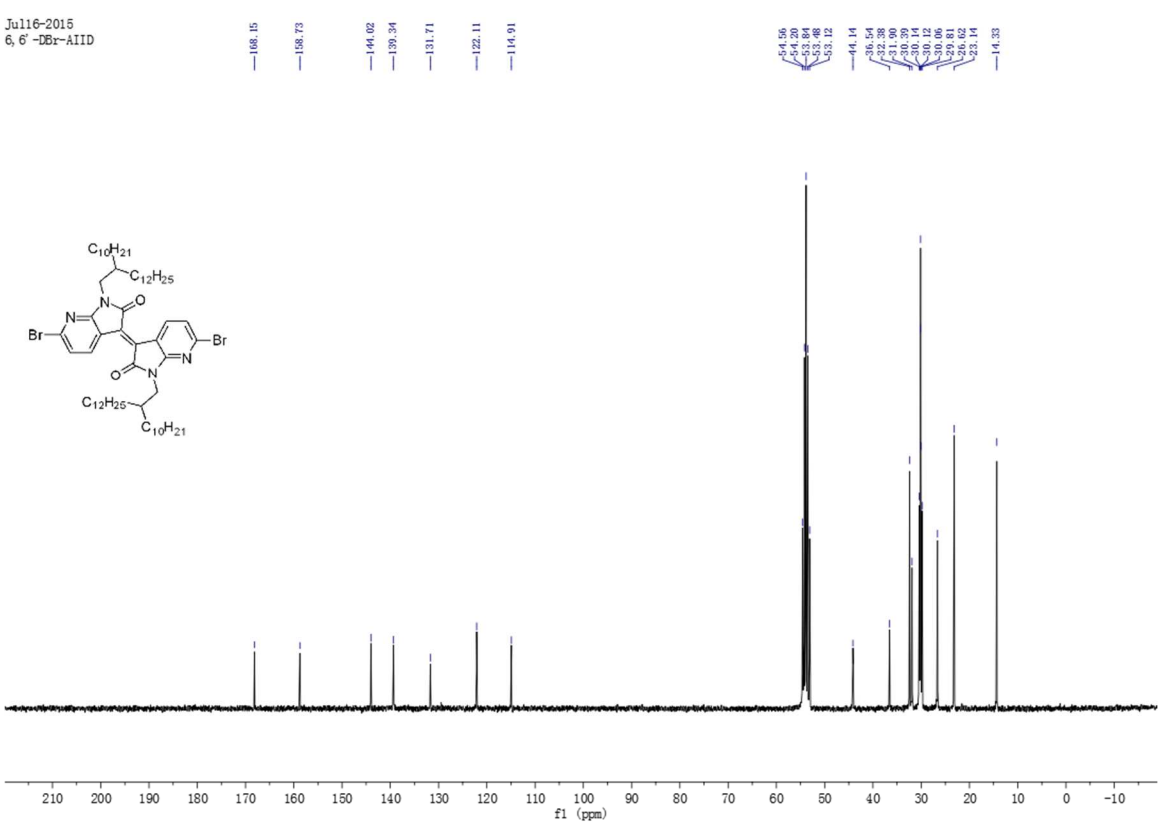
0.86
0.09
1.95
2.34
4.00
2.22
87.95
13.72
f1 (ppm)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139.34
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114.91
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53.84
53.48
53.12
44.14
36.54
32.38
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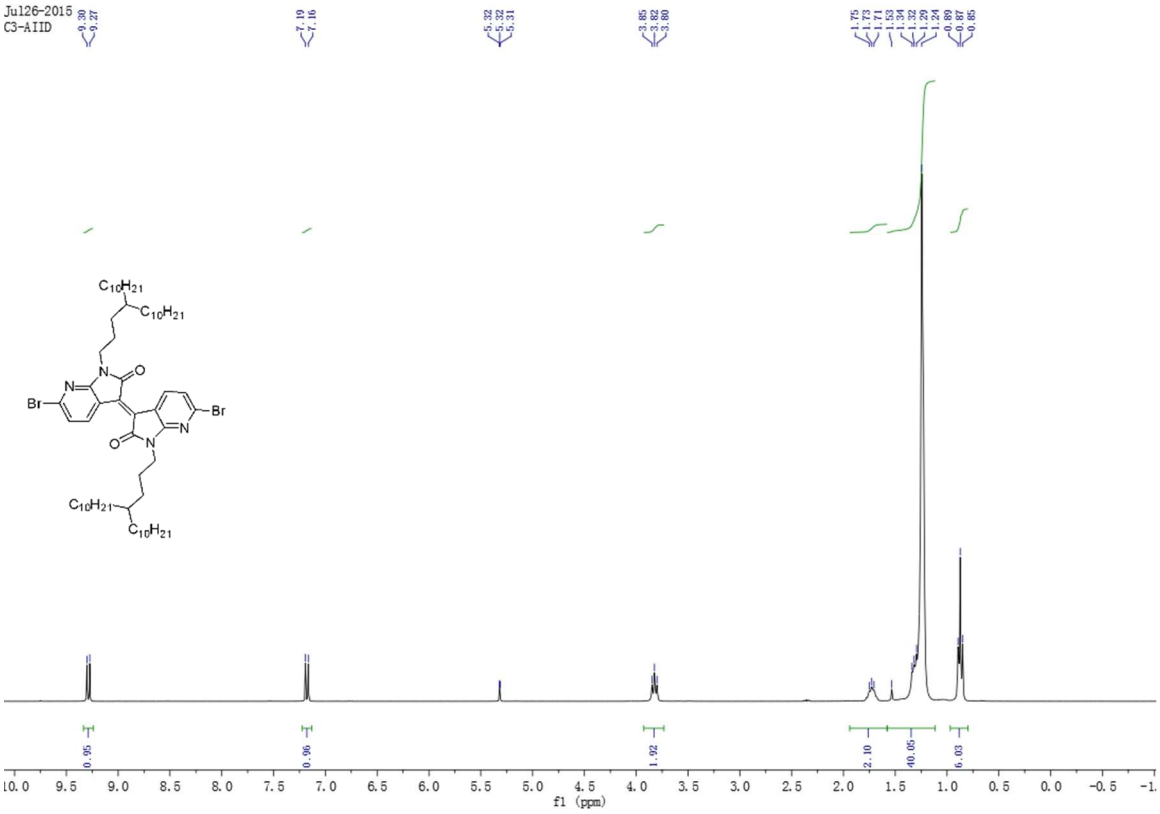
30.39
30.14
30.12
30.06
29.81
26.62
23.14
14.33
f1 (ppm)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3.82
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1.75
1.73
1.71
1.53
1.34
1.32
1.29
1.24
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0.87
0.85
0.95
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1.92
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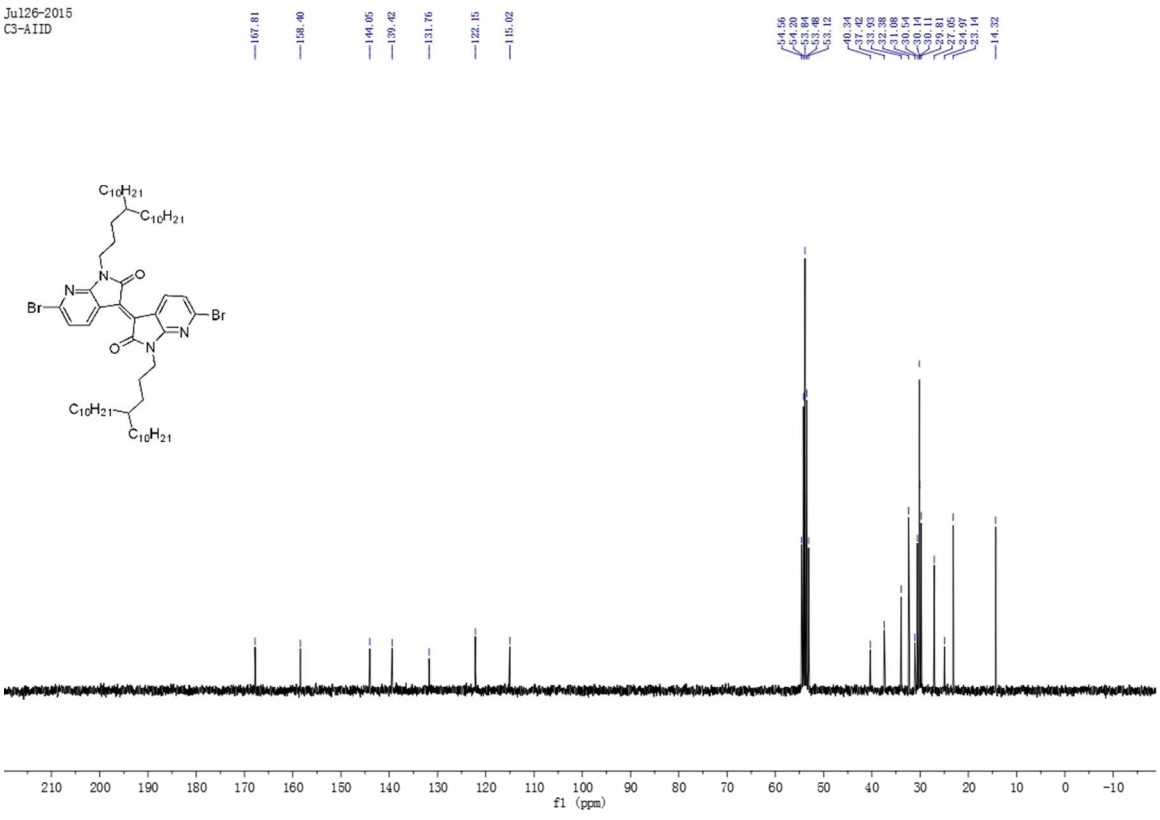
40.05
6.03
f1 (ppm)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C3-AIID
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158.40
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139.42
131.76
122.15
115.02
54.56
54.20
53.84
53.48
53.12
40.34
37.92
33.55
32.38
31.08
30.54
30.14
30.11
29.81
27.05
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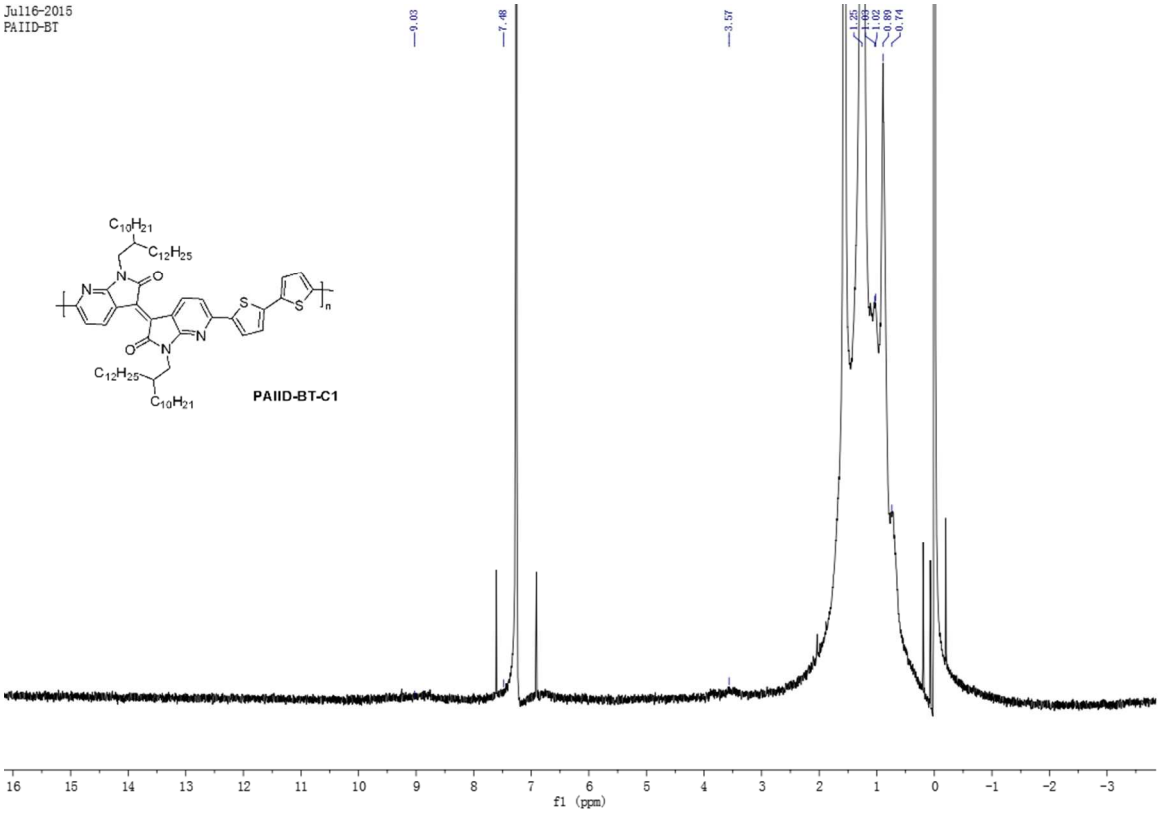
14.32
f1 (ppm)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PAIID-BT
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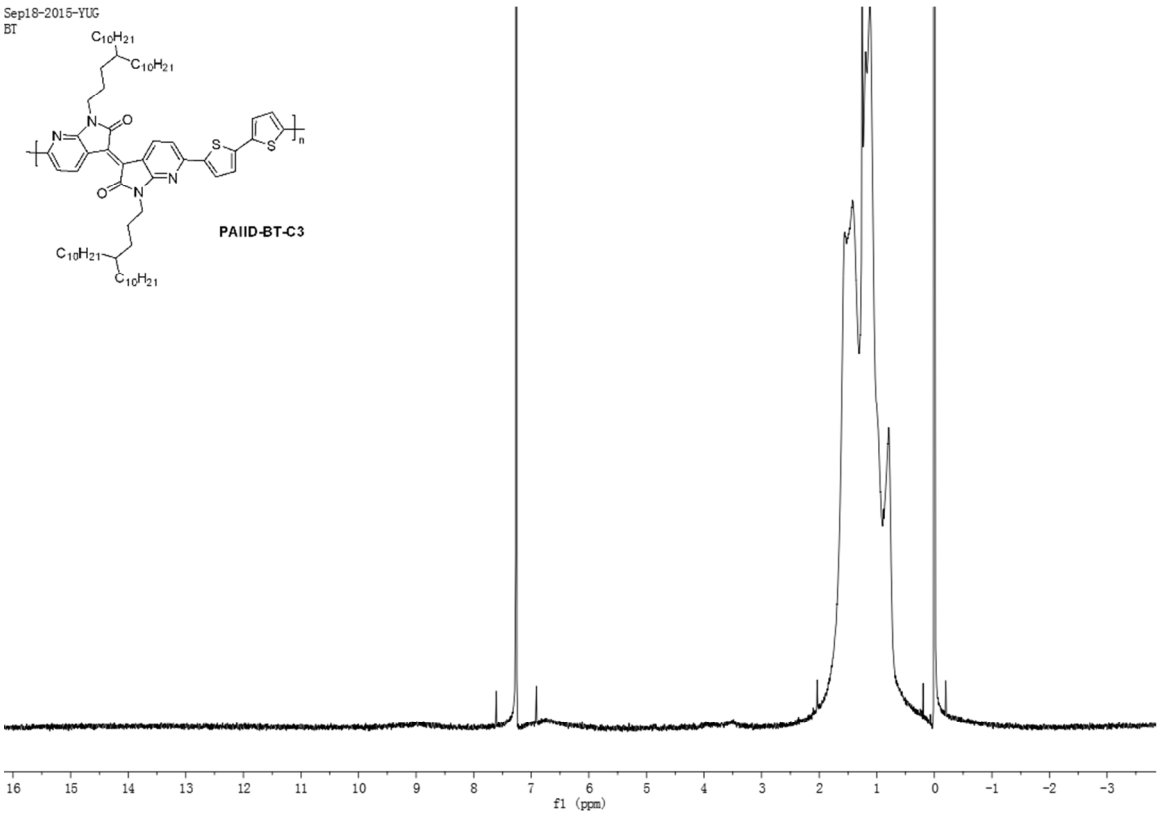
1.03
1.02
0.89
0.74
PAIID-BT-C1
f1 (ppm)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BT
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MALDI(p),c1-indole,20150813

Analysis Info

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Method	MALDI_N_100-900	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

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Broadband High Mass	1000.0 m/z	Laser Power	33.4 lp	Apodization	Sine-Bell Multiplication
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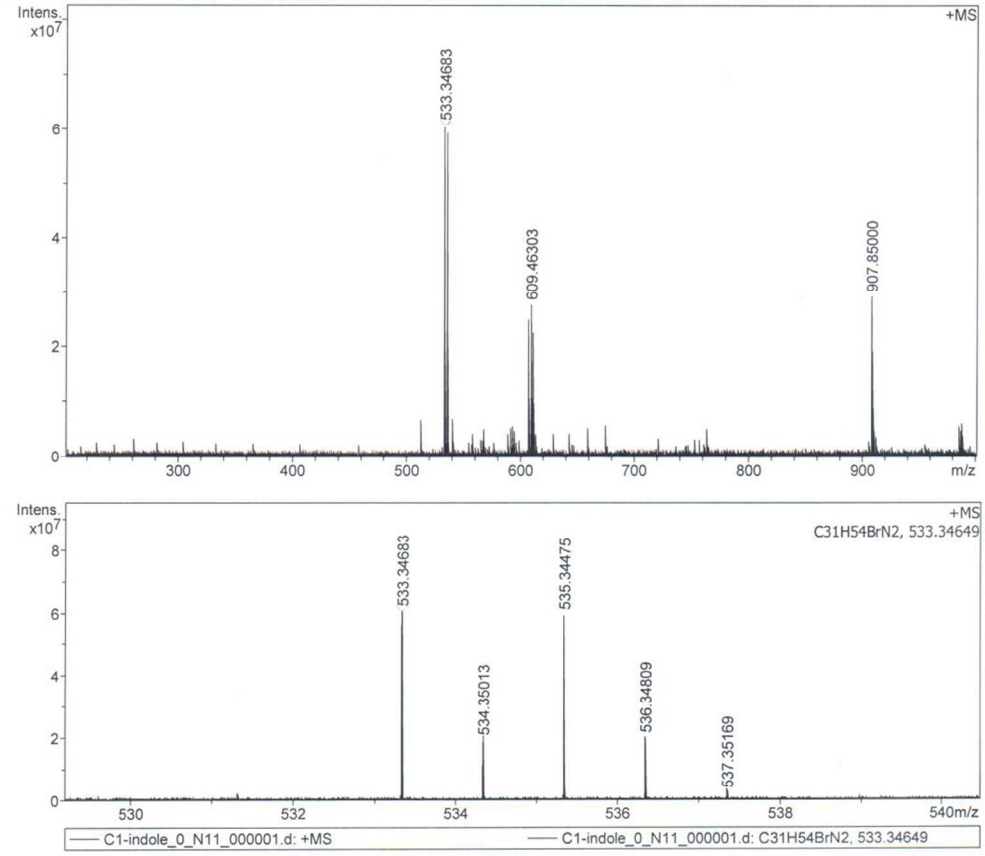
Ion Accumulation Time	0.300 sec				



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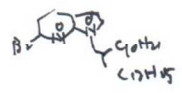

MALDI,azaisatin,20150303

Analysis Info

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Method	MALDI_P_100-3000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	3	Calibration Date	Tue Mar 3 05:12:11 2015
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Broadband High Mass	1000.0 m/z	Laser Power	20.6 lp	Apodization	Sine-Bell Multiplication
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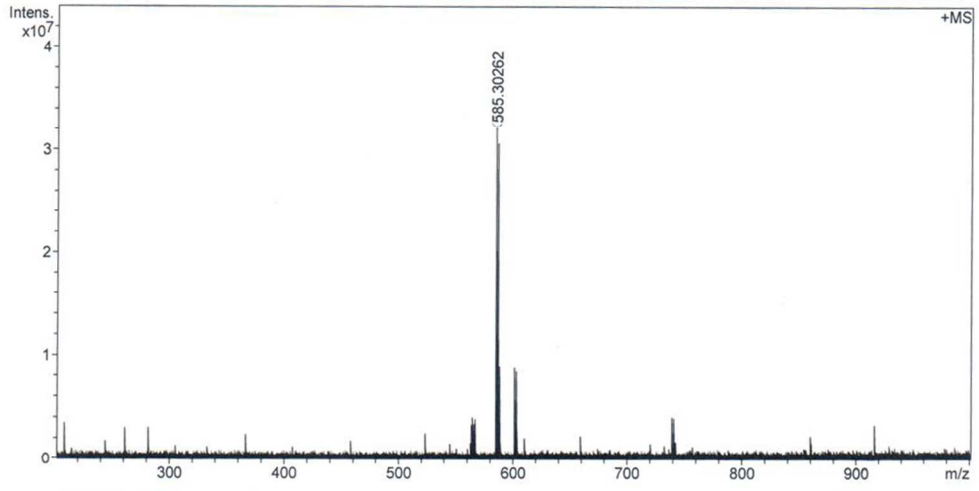
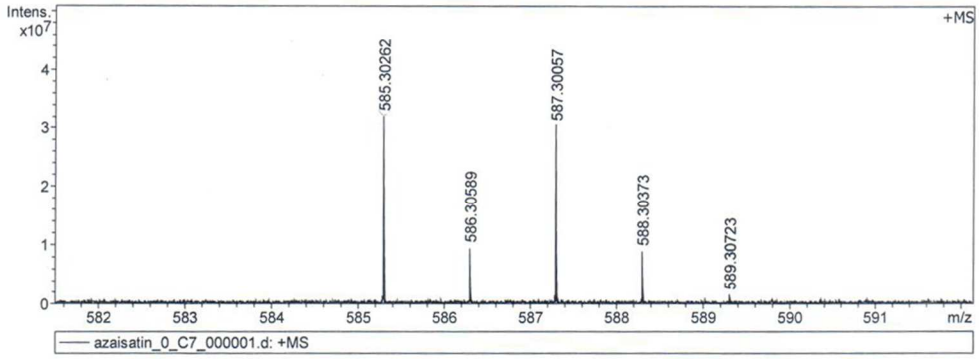
Ion Accumulation Time	0.300 sec				





Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
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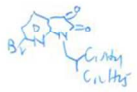

MALDI(p),c1-AIID,20150813

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Method	MALDI_N_100-900	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	5	Calibration Date	Wed Aug 12 10:32:19
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Broadband High Mass	2000.0 m/z	Laser Power	27.8 lp	Apodization	Sine-Bell Multiplication
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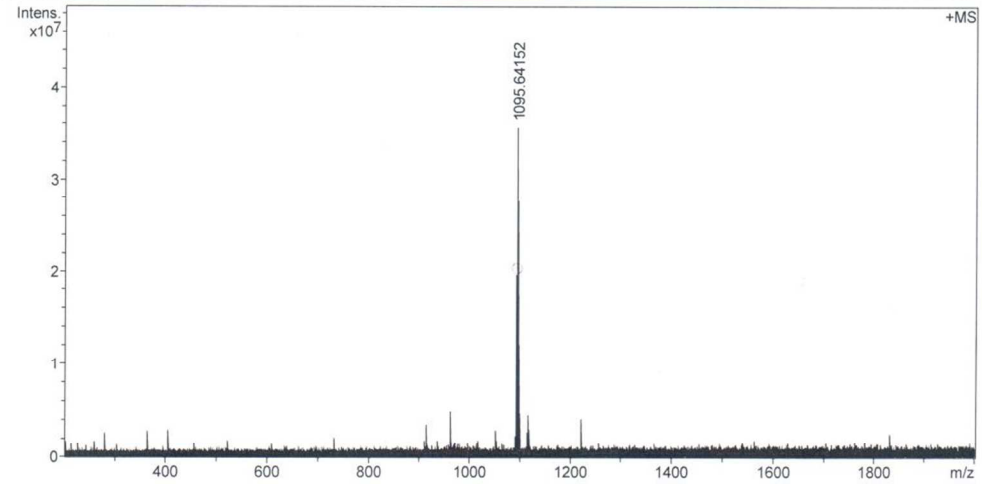
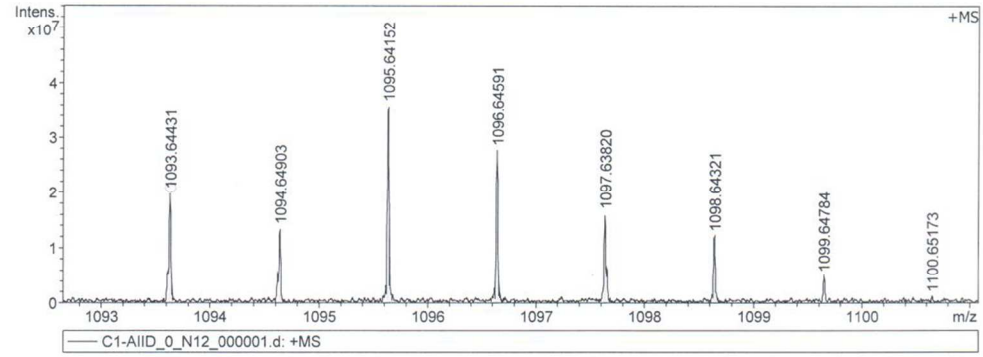
Ion Accumulation Time	0.300 sec				





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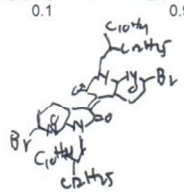

MALDI(p),C3-indole,20150818

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Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	5	Calibration Date	Wed Aug 12 10:32:19
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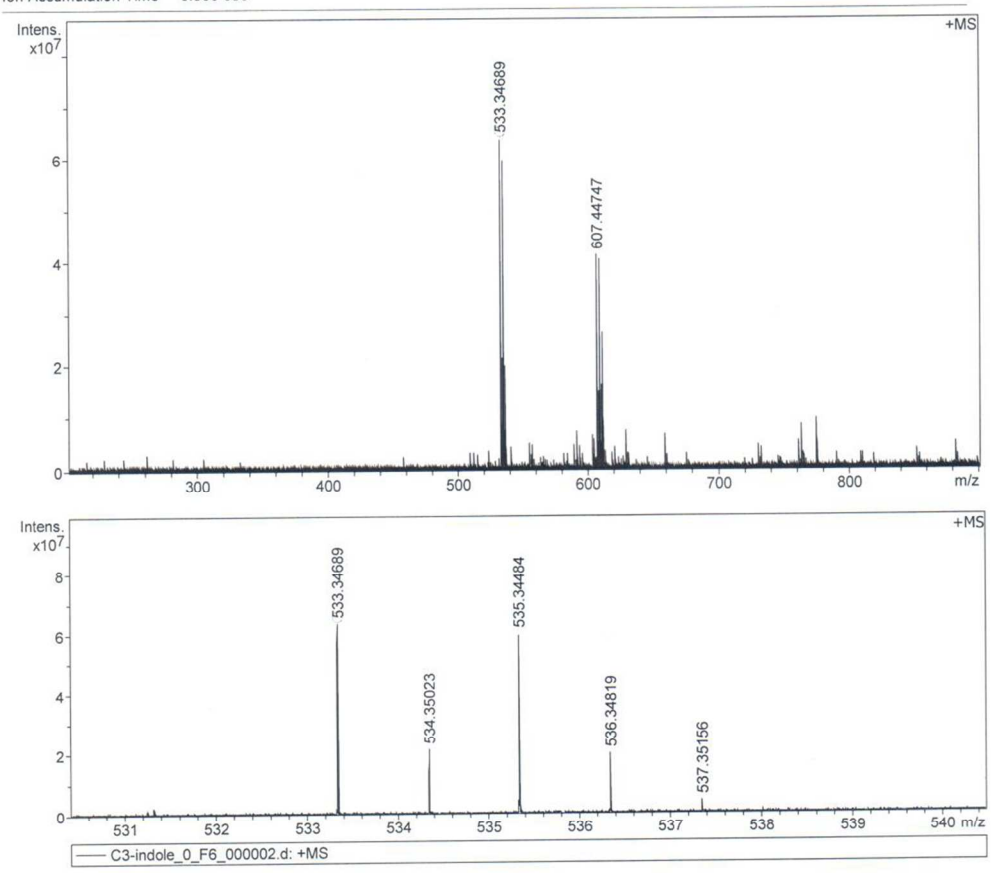
Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	2097152
Broadband High Mass	900.0 m/z	Laser Power	29.6 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.300 sec				



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
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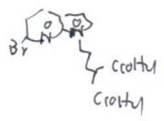

MALDI(p),C3-isatin,20150814

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Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

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Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	2097152
Broadband High Mass	1300.0 m/z	Laser Power	30.6 lp	Apodization	Sine-Bell Multiplication
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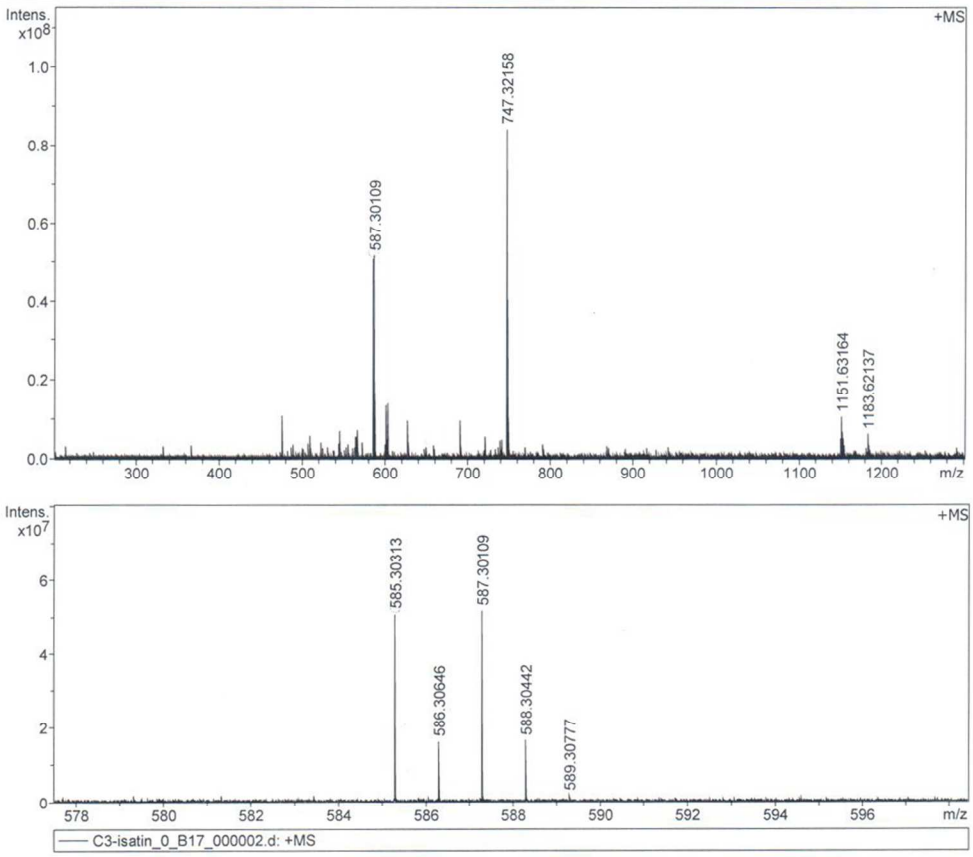
Ion Accumulation Time	0.300 sec				



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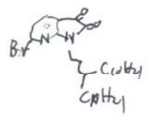

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Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

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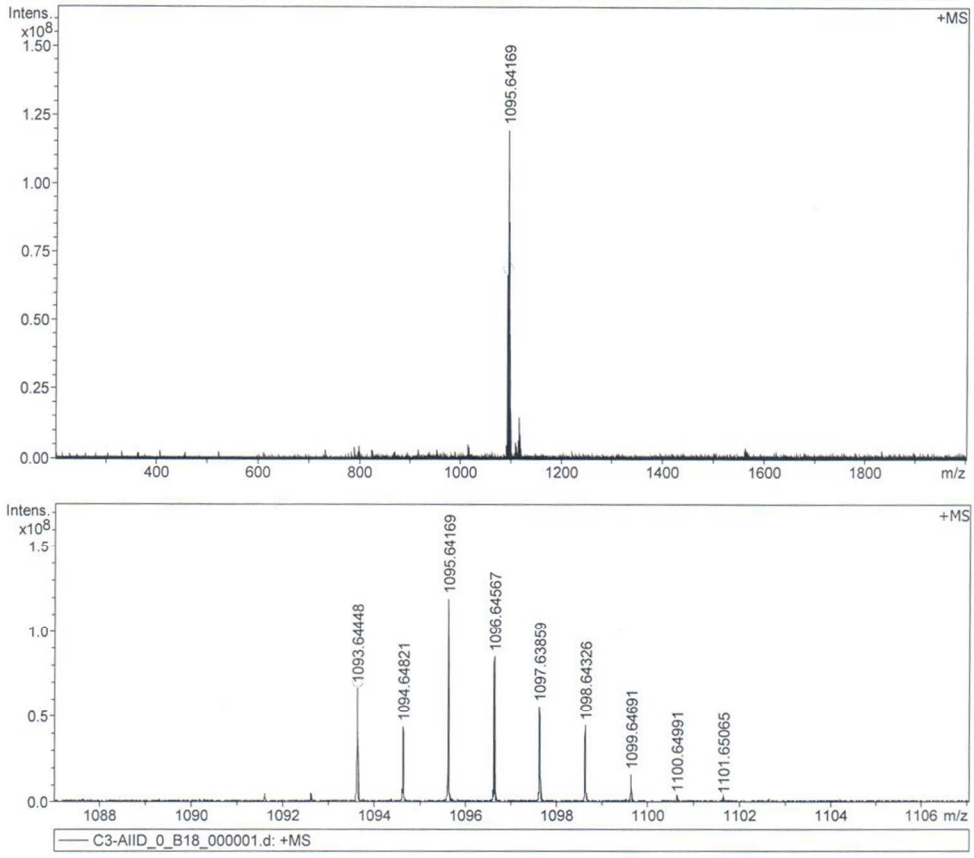
Broadband High Mass	2000.0 m/z	Laser Power	30.6 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.300 sec				



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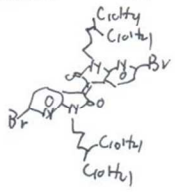

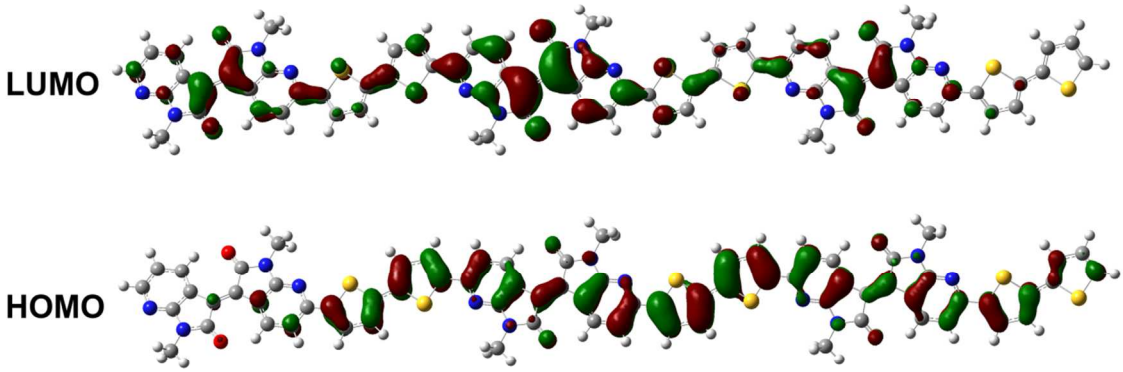

Figure S1. Frontier molecular orbitals of PAIID-BT trimmer according to DFT calculations at B3LYP/6-31G* level.

Optimized molecular coordinates:

Isoindigo:

C	4.60735500	1.38080600	-0.27752500
C	3.57684700	2.31324600	-0.40157500
C	2.23685800	1.92539400	-0.30610800
C	1.91405200	0.57962000	-0.08113900
C	2.98616700	-0.34583200	0.01647200
C	4.32013400	0.02709600	-0.07002500
C	1.10674200	-1.63873100	0.16767400
N	2.48939700	-1.63576500	0.18359900
O	0.44046500	-2.65519700	0.30824700
C	3.28393800	-2.83466100	0.34054100
C	-4.60730900	-1.38088200	-0.27755400
C	-3.57677100	-2.31327500	-0.40170400
C	-2.23680200	-1.92537300	-0.30619300
C	-1.91405700	-0.57960700	-0.08109000
C	-2.98619400	0.34580600	0.01661300
C	-4.32014300	-0.02718100	-0.06990700
C	-0.66140400	0.19037400	0.01044500

C	-1.10678600	1.63874700	0.16772600
N	-2.48945100	1.63573200	0.18385200
C	0.66139000	-0.19034100	0.01043200
O	-0.44052200	2.65524900	0.30809900
C	-3.28392900	2.83474200	0.34037400
H	5.64345900	1.70146700	-0.34589000
H	3.81245500	3.36006300	-0.56935100
H	1.45117100	2.65964100	-0.38782300
H	5.11448200	-0.70760400	0.01459400
H	3.92224000	-2.76464700	1.22905400
H	3.91718900	-3.00205000	-0.53888900
H	2.59283900	-3.67073400	0.45501600
H	-5.64340400	-1.70156700	-0.34593900
H	-3.81234700	-3.36008300	-0.56958000
H	-1.45104900	-2.65955100	-0.38793400
H	-5.11453800	0.70746000	0.01479100
H	-2.59277400	3.67078100	0.45473900
H	-3.91700900	3.00195900	-0.53921400
H	-3.92240700	2.76498200	1.22877000

4,4’-Diazaisoindigo:

C	-0.05047900	4.27586000	-0.20214900
C	-1.39598200	4.44189600	-0.54051000
C	-2.22000100	3.31920000	-0.69123400
N	-1.80819500	2.06076900	-0.50175600
C	-0.53790300	1.89352600	-0.13278900
C	0.37835800	2.96860800	-0.00654300
C	1.64472400	1.08518200	0.33594900
N	1.64472400	2.48614900	0.28319400
O	2.61241200	0.42446500	0.65413300
C	0.05047900	-4.27586000	-0.20214900

C	1.39598200	-4.44189600	-0.54051000
C	2.22000100	-3.31920000	-0.69123400
N	1.80819500	-2.06076900	-0.50175600
C	0.53790300	-1.89352600	-0.13278900
C	-0.37835800	-2.96860800	-0.00654300
C	-0.21200500	-0.64945700	0.05809600
C	-1.64472400	-1.08518200	0.33594900
N	-1.64472400	-2.48614900	0.28319400
O	-2.61241200	-0.42446500	0.65413300
C	0.21200500	0.64945700	0.05809600
H	-1.80203900	5.43602100	-0.70296100
H	-3.26097700	3.44112300	-0.98264400
C	2.82072500	3.28640800	0.55012900
H	1.80203900	-5.43602100	-0.70296100
H	3.26097700	-3.44112300	-0.98264400
C	-2.82072500	-3.28640800	0.55012900
H	3.63497200	2.59682900	0.77809200
H	3.09070800	3.89252900	-0.32302800
H	2.65676100	3.94993900	1.40762000
H	-3.09070800	-3.89252900	-0.32302800
H	-2.65676100	-3.94993900	1.40762000
H	-3.63497200	-2.59682900	0.77809200
H	0.62212400	5.12255500	-0.10590700
H	-0.62212400	-5.12255500	-0.10590700

5,5’-Diazaisoindigo:

C	-4.51661700	1.44757400	-0.20914400
N	-3.54155000	2.35533700	-0.32325900
C	-2.26736600	1.93511300	-0.25436400
C	-1.91224400	0.58980500	-0.06906500
C	-2.98405400	-0.33600900	0.02074300

C	-4.30682800	0.07643900	-0.03935800
C	-1.11127600	-1.63167900	0.12251900
N	-2.49997900	-1.62511100	0.15101800
O	-0.44833200	-2.65102900	0.22340500
C	4.51655000	-1.44766600	-0.20906200
N	3.54144700	-2.35535900	-0.32345300
C	2.26728600	-1.93507500	-0.25463000
C	1.91222200	-0.58978400	-0.06909400
C	2.98406000	0.33597800	0.02083600
C	4.30682300	-0.07653300	-0.03918000
C	0.66213000	0.18424900	-0.00467000
C	1.11131500	1.63172400	0.12243100
N	2.50001900	1.62510300	0.15104100
O	0.44842700	2.65112600	0.22313100
C	-0.66212900	-0.18418700	-0.00462500
C	3.29900500	2.82756900	0.27696500
C	-3.29893500	-2.82757600	0.27699100
H	-5.53407500	1.83264900	-0.26159900
H	-1.50771300	2.69680800	-0.34247100
H	-5.13671300	-0.61836700	0.03316400
H	5.53399500	-1.83278200	-0.26148200
H	1.50758600	-2.69671000	-0.34287700
H	5.13674100	0.61821800	0.03346300
H	2.60948500	3.66868900	0.35849600
H	3.92769200	2.78289900	1.17318000
H	3.93838700	2.96369700	-0.60258900
H	-2.60939300	-3.66857000	0.35963000
H	-3.92837800	-2.78238700	1.17262200
H	-3.93757100	-2.96436600	-0.60302200

7,7’-Diazaisoindigo:

N	0.08918700	-4.28061000	0.00000200
C	-1.22039900	-4.60027400	0.00010700
C	-2.24312800	-3.65809800	0.00015900
C	-1.93453800	-2.29097600	0.00010800
C	-0.58857900	-1.91351500	0.00000400
C	0.34676200	-2.98500200	-0.00003300
C	1.64483700	-1.11438900	-0.00003400
N	1.64483700	-2.49532100	-0.00007200
O	2.66729000	-0.44456000	-0.00005300
N	-0.08918700	4.28061000	0.00000200
C	1.22039900	4.60027400	0.00010700
C	2.24312800	3.65809800	0.00015900
C	1.93453800	2.29097600	0.00010800
C	0.58857900	1.91351500	0.00000400
C	-0.34676200	2.98500200	-0.00003300
C	-0.18654200	0.66152900	-0.00000100
C	-1.64483700	1.11438900	-0.00003400
N	-1.64483700	2.49532100	-0.00007200
O	-2.66729000	0.44456000	-0.00005300
C	0.18654200	-0.66152900	-0.00000100
H	-1.44486400	-5.66494400	0.00010600
H	-3.27920100	-3.98128200	0.00024700
H	-2.71264700	-1.54394700	0.00013600
C	2.84191600	-3.31429800	-0.00015200
H	1.44486400	5.66494400	0.00010600
H	3.27920100	3.98128200	0.00024700
H	2.71264700	1.54394700	0.00013600
C	-2.84191600	3.31429800	-0.00015200
H	3.69839000	-2.63949800	-0.00104800
H	2.86474200	-3.95356800	-0.88770900
H	2.86577900	-3.95239500	0.88823600

H	-3.69839000	2.63949800	-0.00104800
H	-2.86474200	3.95356800	-0.88770900
H	-2.86577900	3.95239500	0.88823600

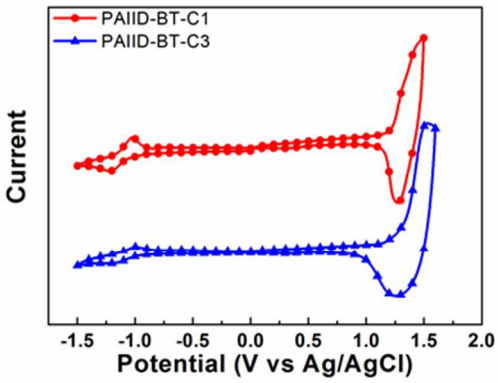

Figure S2. Cyclic voltammetry of PAIID-BT-C1 and PAIID-BT-C3.

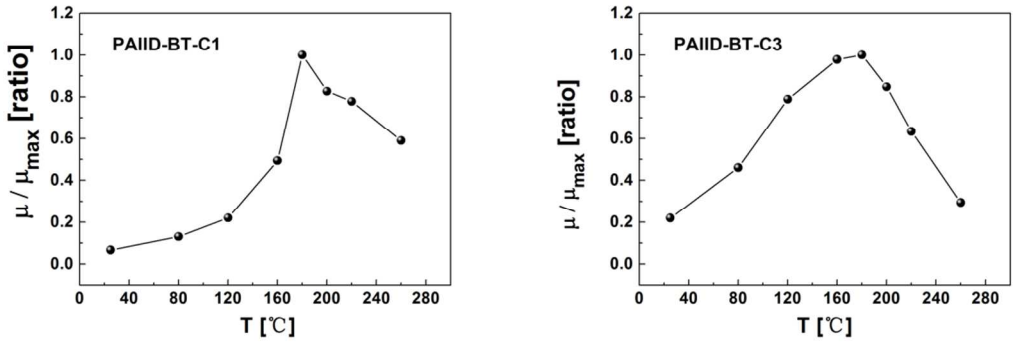

Figure S3. Annealing temperature-dependence of mobilities for PAIID-BT-C1 and PAIID-BT-C3. Both polymers showed highest mobilities after annealing at 180 °C.

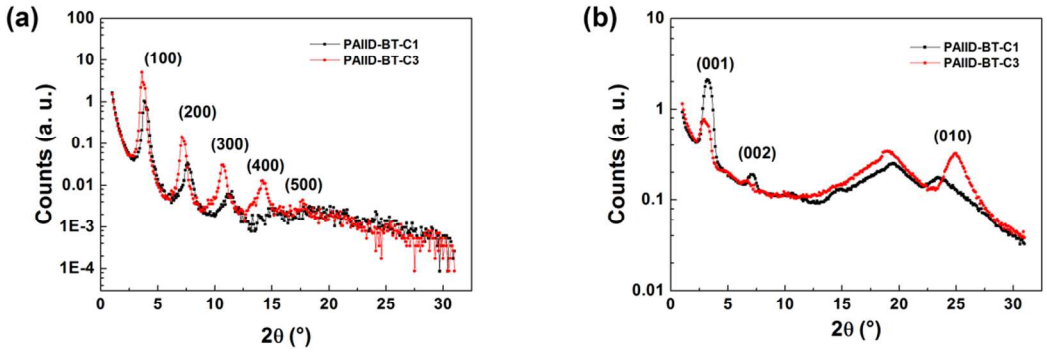

Figure S4. 1D-GIXRD profiles of PAIID-BT: (a) out-of-plane, (b) in-plane.

Table S1. Summary of Coherence Length Results According to GIXRD Peak Fitting

Polymer	d-d (Å)	π-π (Å)
PAIID-BT-C1	202±2	37±4
PAIID-BT-C3	221±3	48±1

Figure S5 shows the UV-vis absorption spectra of AIID monomers and polymers. For both polymers in chloroform solutions, the absorption spectra are identical in the range of 300~600 nm. The vibronic absorption peaks are slightly different due to the introduction of different alkyl chains providing varying degrees of aggregating properties.

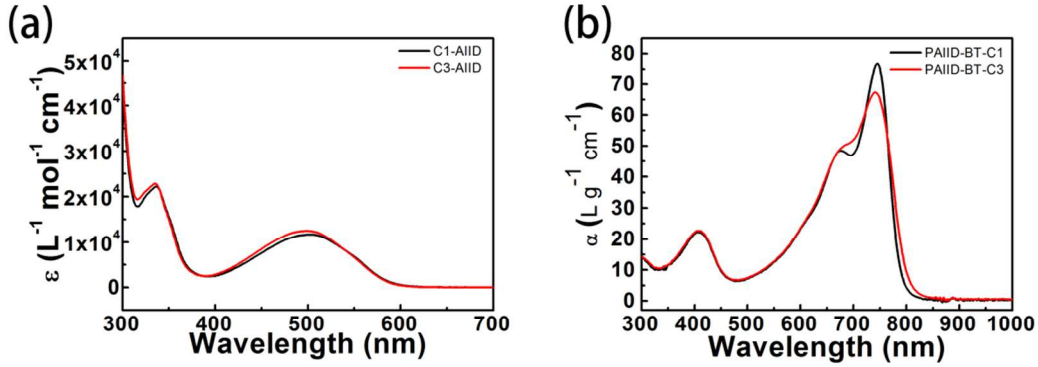

Figure S5. UV-vis absorption spectra of monomers and polymers: (a) molar absorptivity of brominated azaisoindigo monomers C1-AIID and C3-AIID, (b) polymers in chloroform solution at concentrations of 0.003 mg/mL.