Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
This journal is © The Royal Society of Chemistry 2017

Role of Phenothiazine/Phenoxazine Donor in Solid Ionic Conductors for Efficient Solid State Dye Sensitized Solar Cells

*Jayraj V. Vaghasiya,[a] Keval K. Sonigara,[a] Jyoti Prasad,[a] Thomas Beuvier,[b] Alain Gibaud,[b] Saurabh S. Soni[a,]**

[a]*Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar – 388 120, Gujarat, INDIA*

[b]*IMMM, Universite du Maine, Le Mans 72000, FRANCE*

Electronic supplementary information

Contents

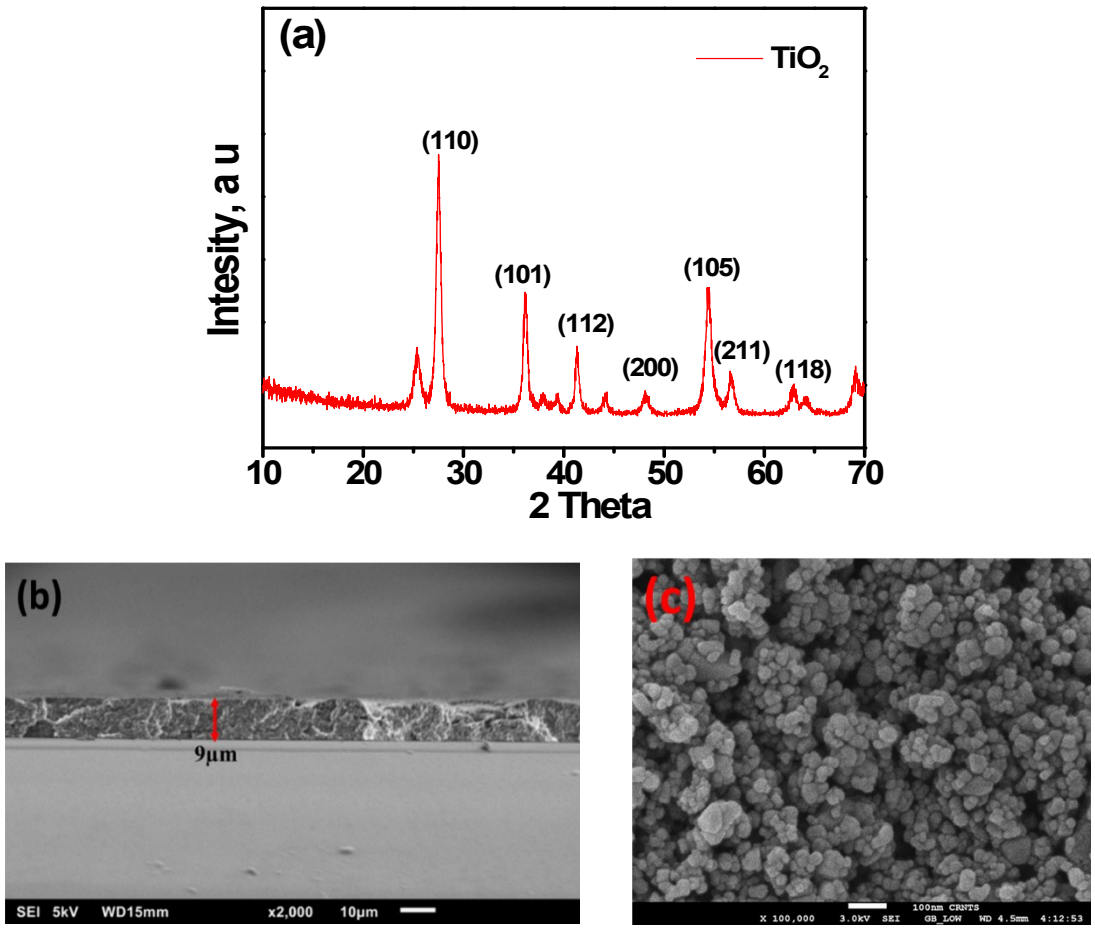
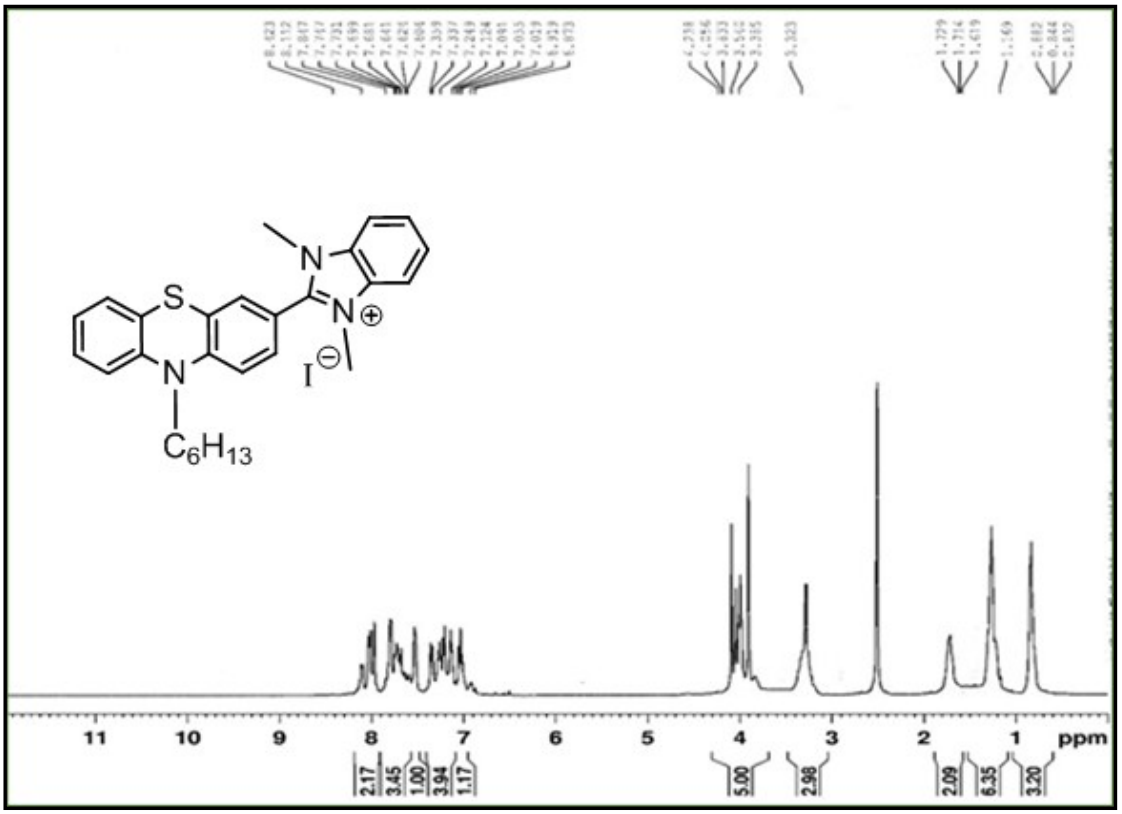
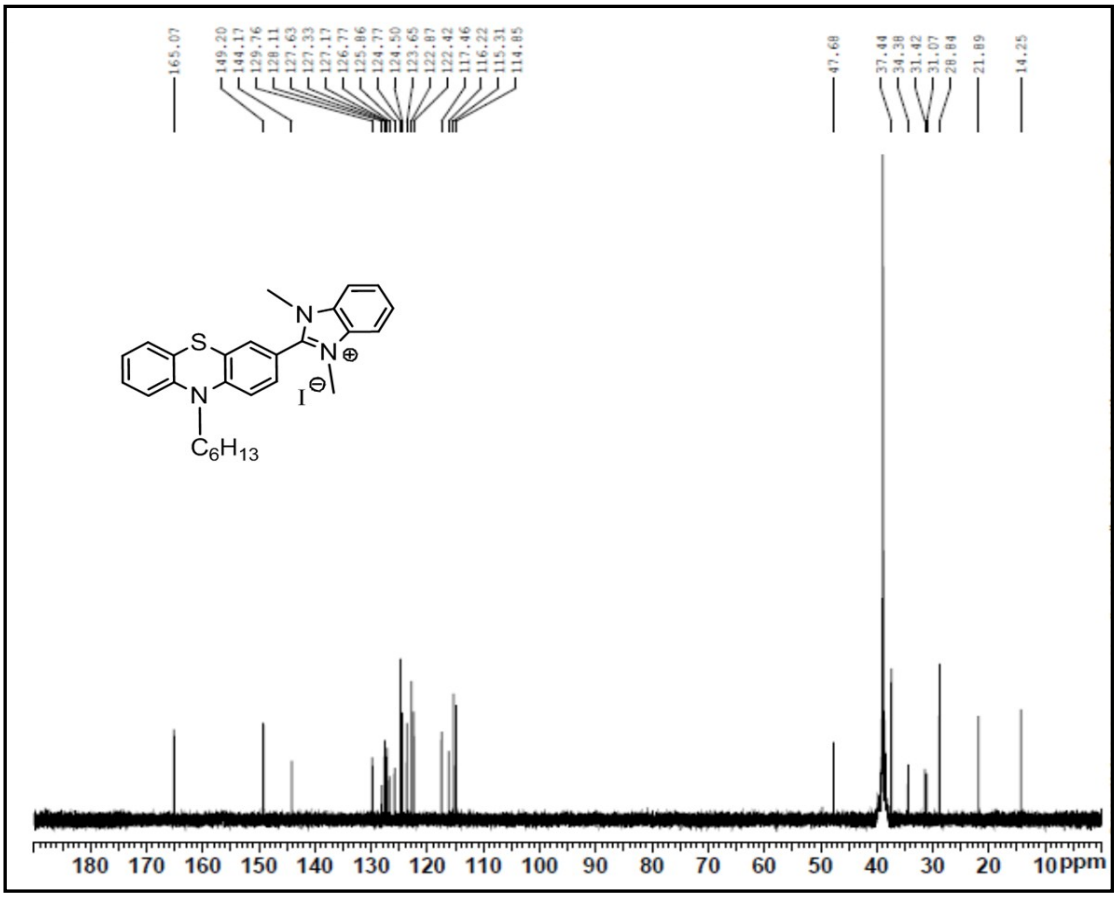
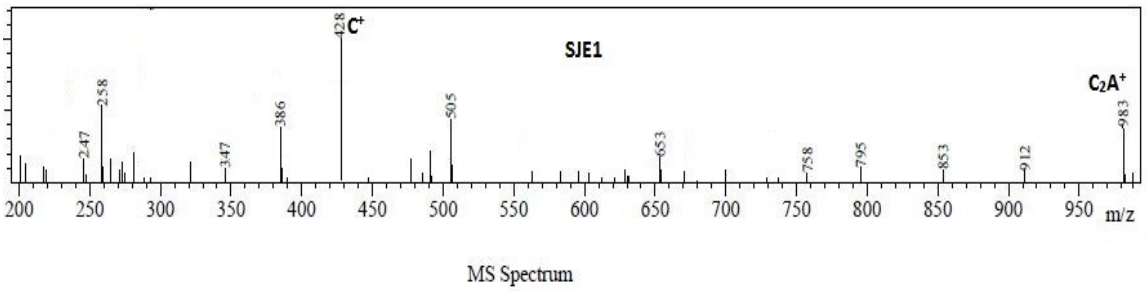


Fig. S1. (a) XRD pattern, (b) SEM image of cross section and (c) SEM image tope view for TiO_2 Photoanode

We have used anatase nanoporous TiO_2 particles. Structural characterizations of TiO_2 particles were carried out by using XRD. Above **Fig. S1(a)** shows the X-Ray diffraction pattern of the TiO_2 nanoparticles showing the presence of pure crystalline anatase phase along with sign of little rutile domain. The peaks in the diffraction pattern can be attributed to the (110), (101), (112), (200), (105), (211) and (118) planes respectively.

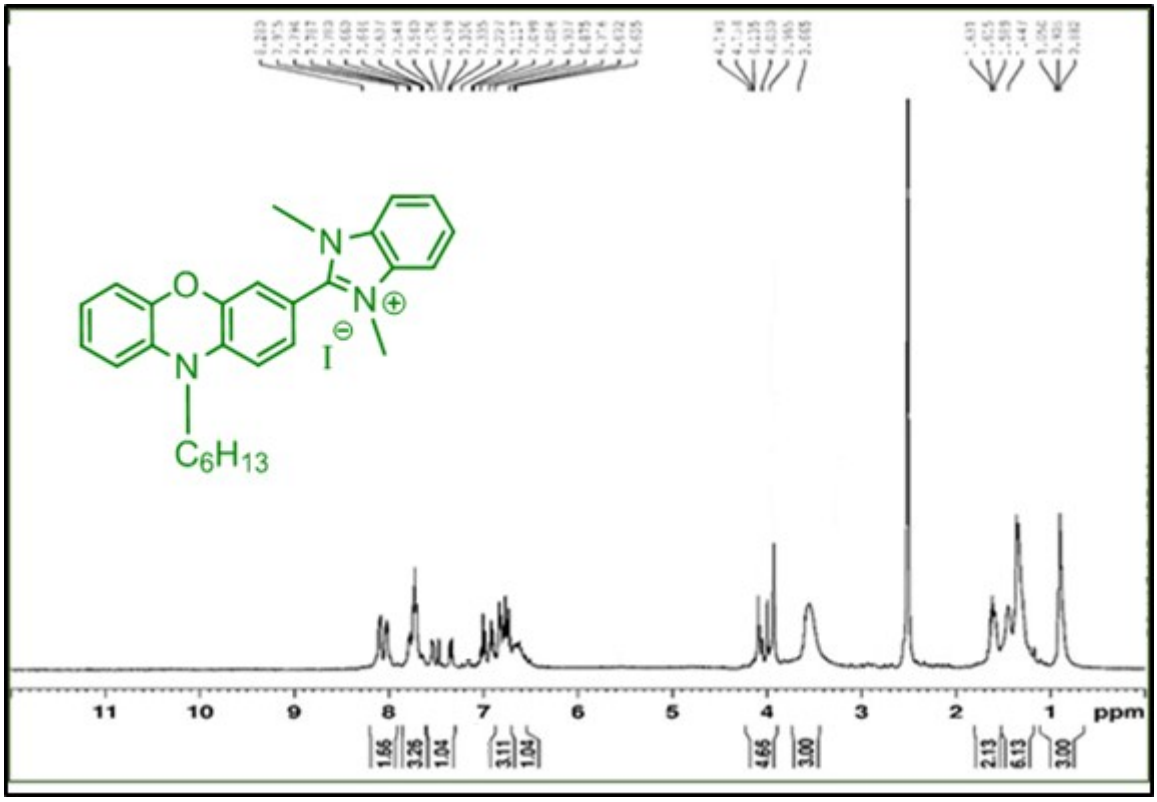

N
S
N
N⊕
I⊖
C6H13
11 10 9 8 7 6 5 4 3 2 1 ppm
2.17 3.45 1.00 3.94 1.17 5.00 2.98 2.09 6.35 3.20

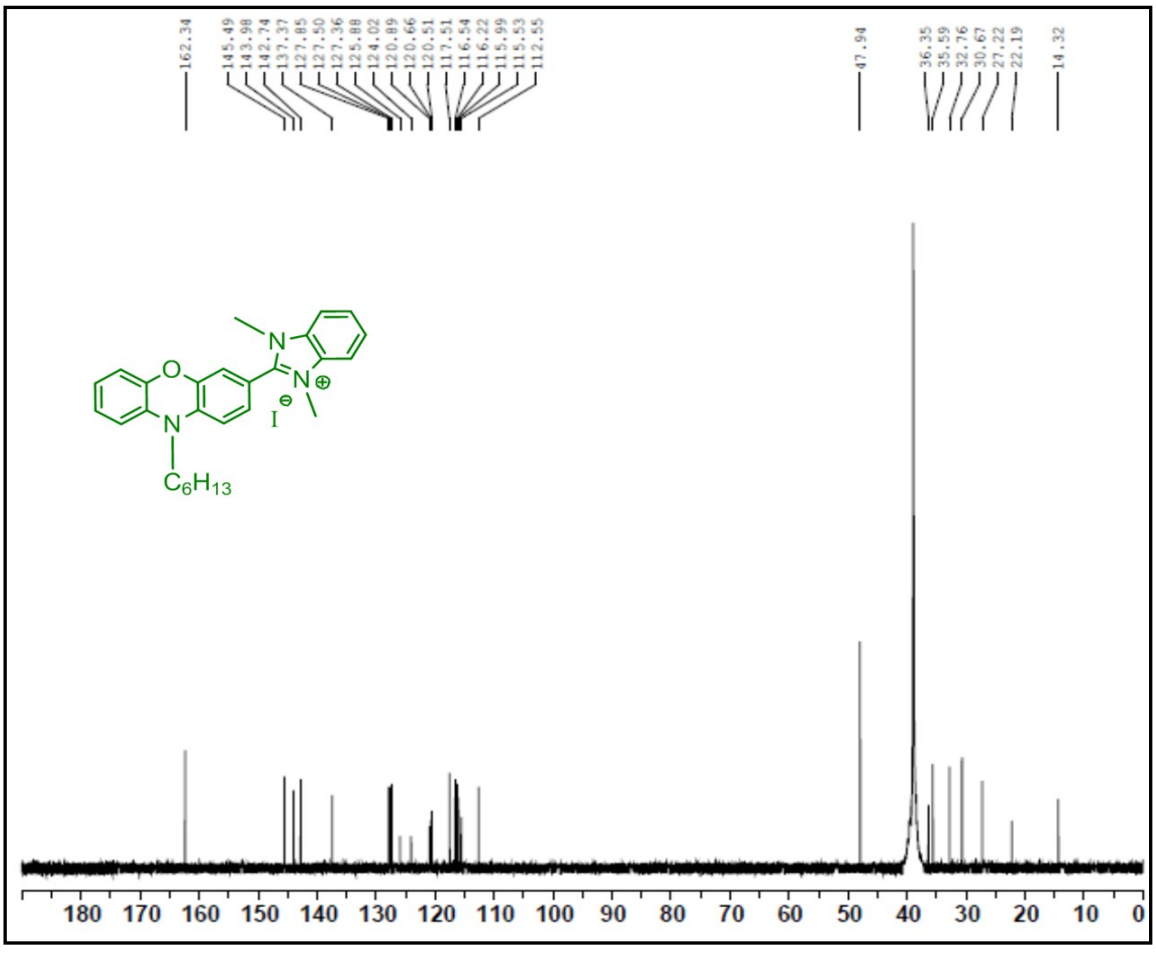

165.07
149.20
144.17
129.76
128.11
127.63
127.33
127.17
126.77
125.86
124.77
124.50
123.65
122.87
122.42
117.46
116.22
115.31
114.85
47.68
37.44
34.38
31.42
31.07
28.84
21.89
14.25
N
S
N
N⊕
I⊖
C6H13
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



MS Spectrum

Fig. S2. ^{1}H-NMR and ^{13}C-NMR and MS spectra of SJE 1


N
O
N
N⊕
I⊖
C6H13
11
10
9
8
7
6
5
4
3
2
1
ppm
1.66
2.25
1.04
3.11
1.04
4.65
3.00
2.13
6.13
3.00


162.34
145.49
143.98
142.74
137.37
127.85
127.50
127.36
125.88
124.02
120.89
120.66
120.51
117.51
116.54
116.22
115.99
115.53
112.55
47.94
36.35
35.59
32.76
30.67
27.22
22.19
14.32
N
O
N
N⊕
I⊖
C6H13
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

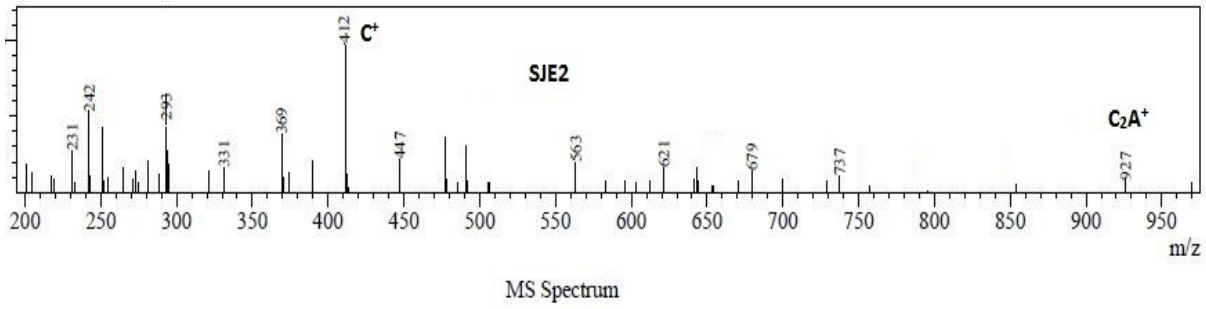
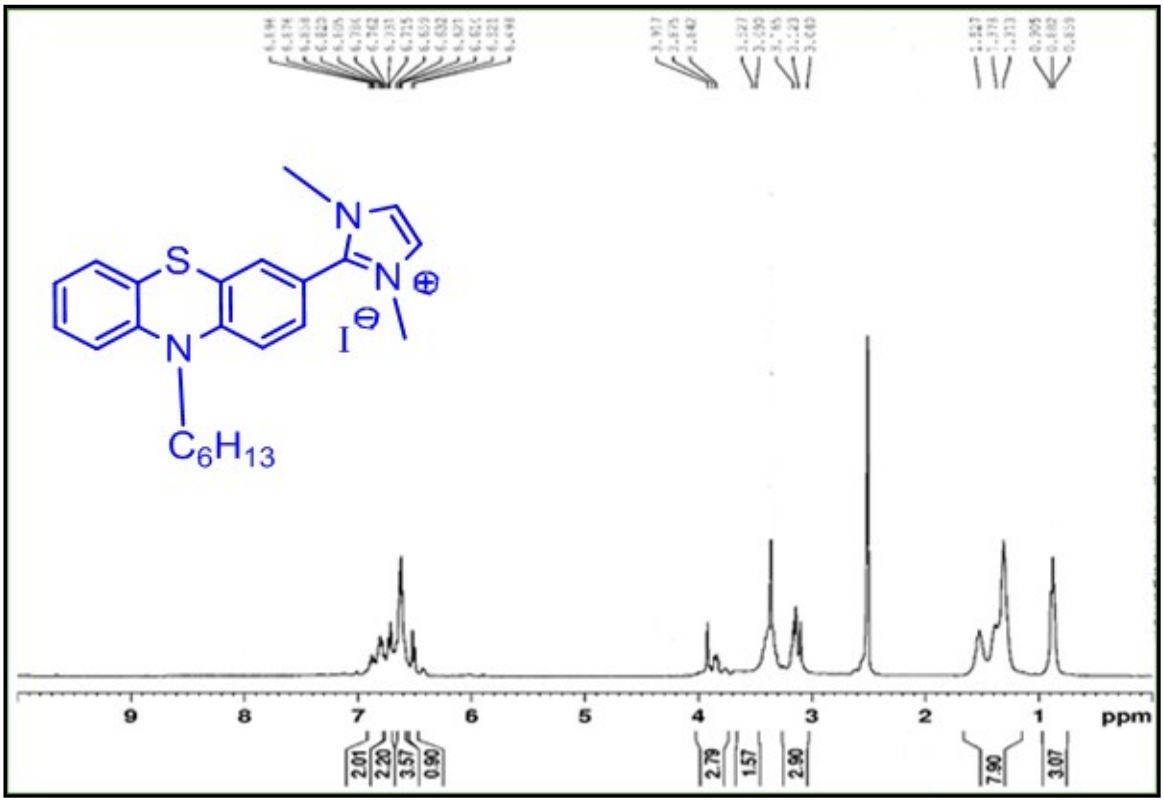
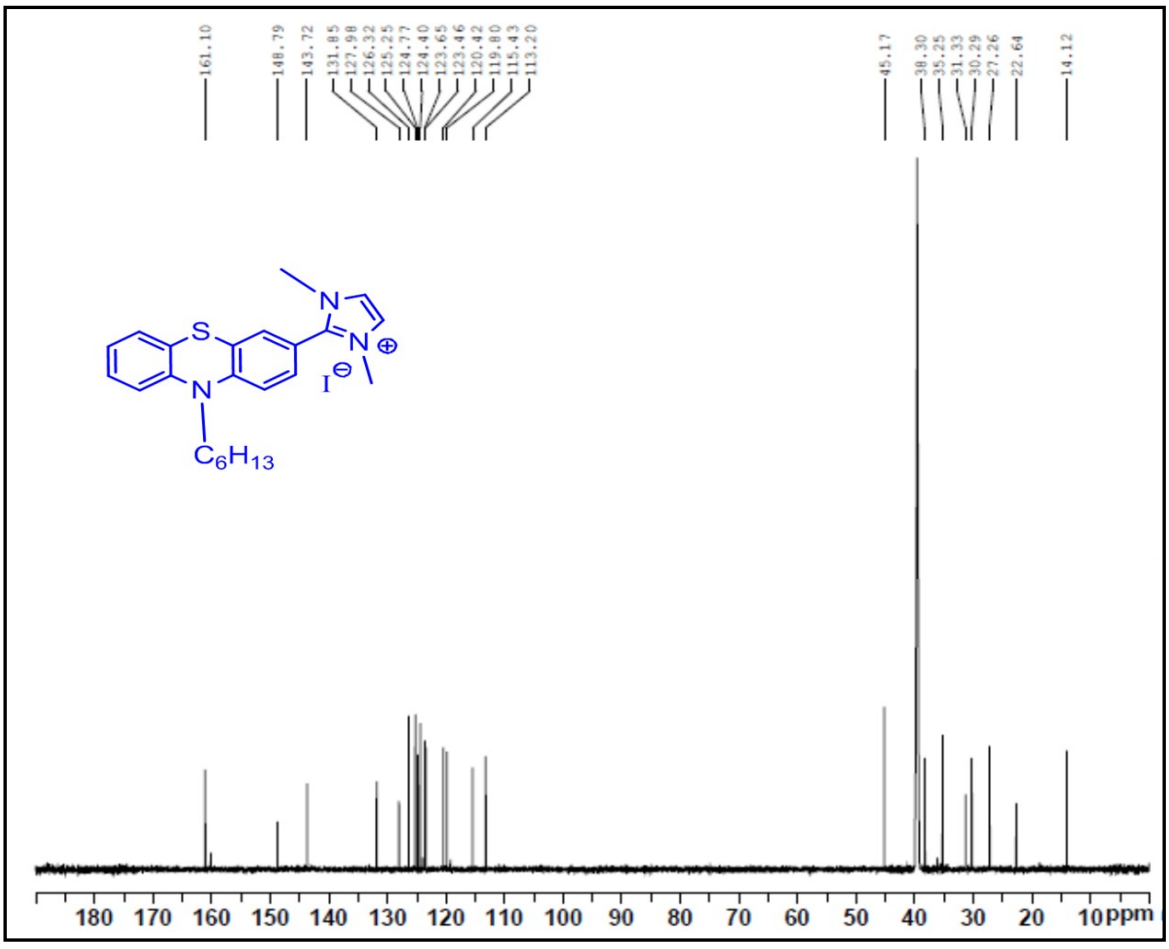


Fig. S3. ^{1}H-NMR and ^{13}C-NMR and MS spectra of SJE 2


N
S
N
N⊕
I⊖
C6H13
9
8
7
6
5
4
3
2
1
ppm
2.01
2.20
3.57
0.90
2.79
1.57
2.90
7.90
3.07


161.10
148.79
143.72
131.85
127.98
126.32
125.25
124.77
124.40
123.65
123.46
120.42
119.80
115.43
113.20
45.17
38.30
35.25
31.33
30.29
27.26
22.64
14.12
N
S
N
N⊕
I⊖
C6H13
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10ppm

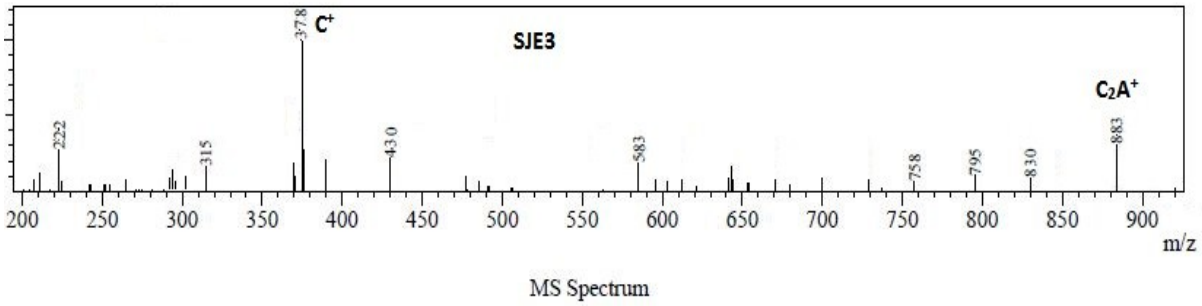
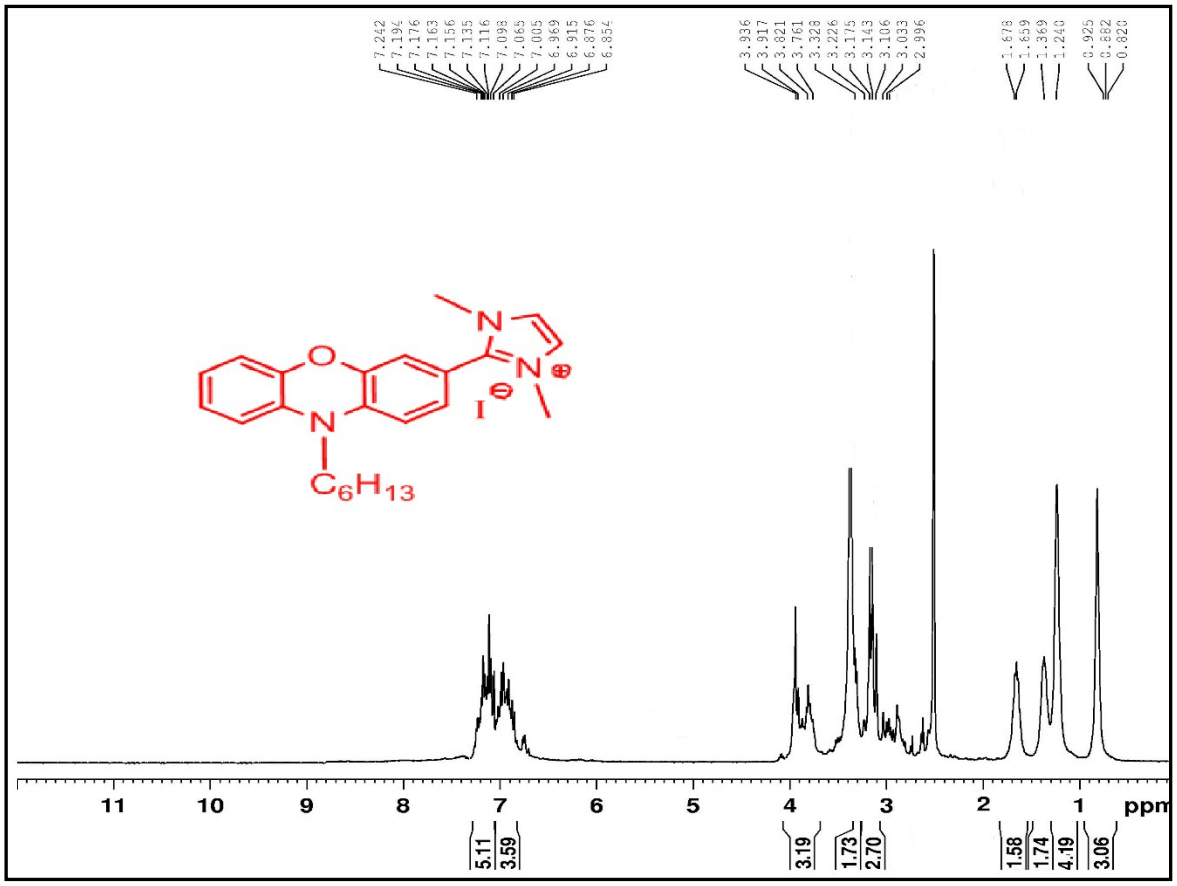
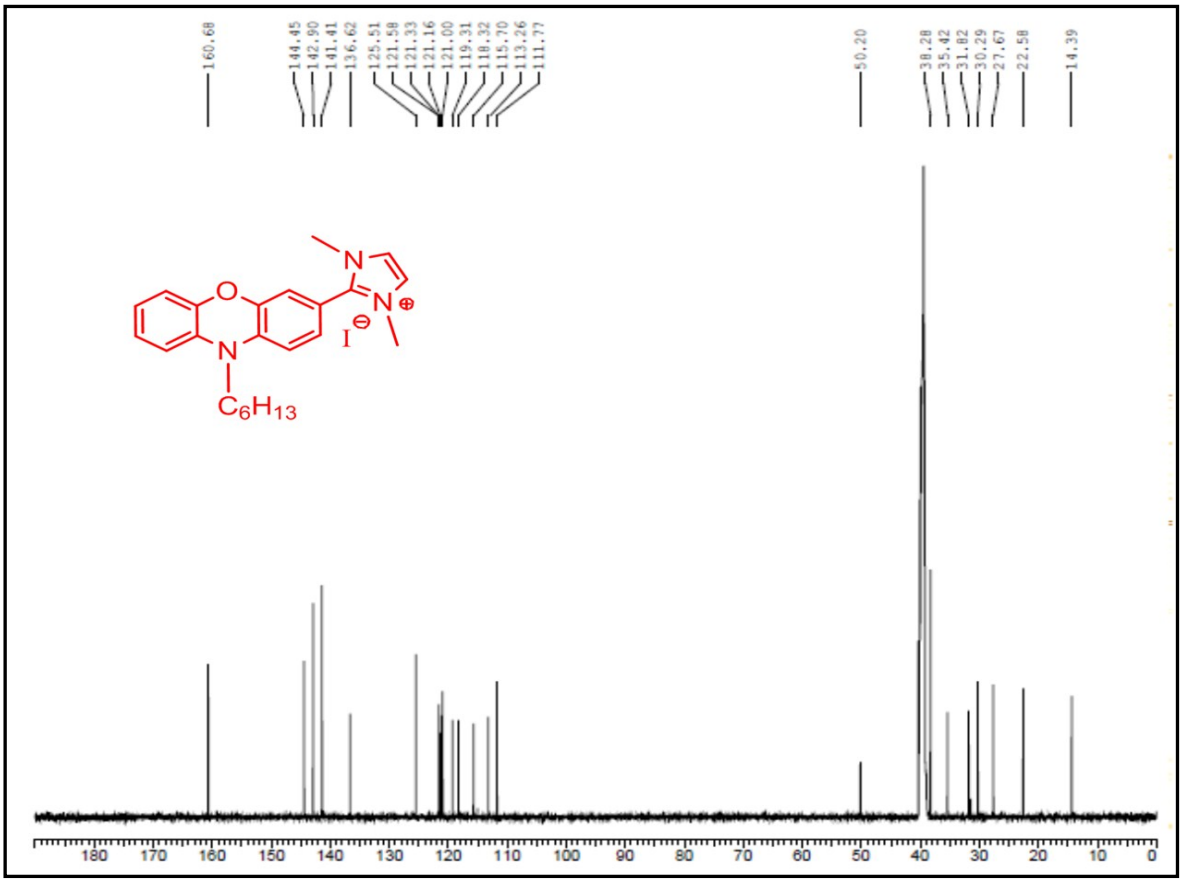


Fig. S4. ^{1}H-NMR and ^{13}C-NMR and MS spectra of SJE 3


7.242
7.194
7.176
7.163
7.156
7.135
7.116
7.098
7.065
7.005
6.969
6.915
6.876
6.854
3.936
3.917
3.821
3.761
3.328
3.226
3.175
3.143
3.106
3.033
2.996
1.678
1.659
1.369
1.240
0.925
0.862
0.823
N
O
N
N⊕
I⊖
C6H13
11
10
9
8
7
6
5
4
3
2
1
ppm
5.11
3.59
3.19
1.73
2.70
1.58
1.74
4.19
3.06


160.68
144.45
142.90
141.41
136.62
125.51
121.58
121.33
121.16
121.00
119.31
118.32
115.70
113.26
111.77
60.20
38.28
35.42
31.82
30.29
27.67
22.58
14.39
N
O
N
N⊕
I⊖
C6H13
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

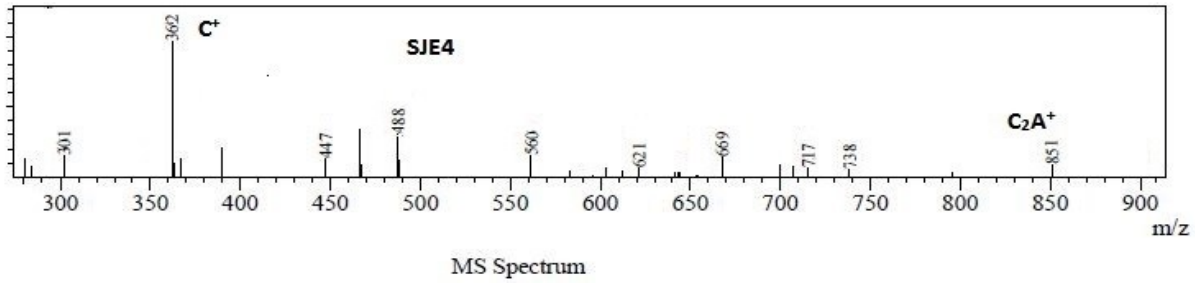
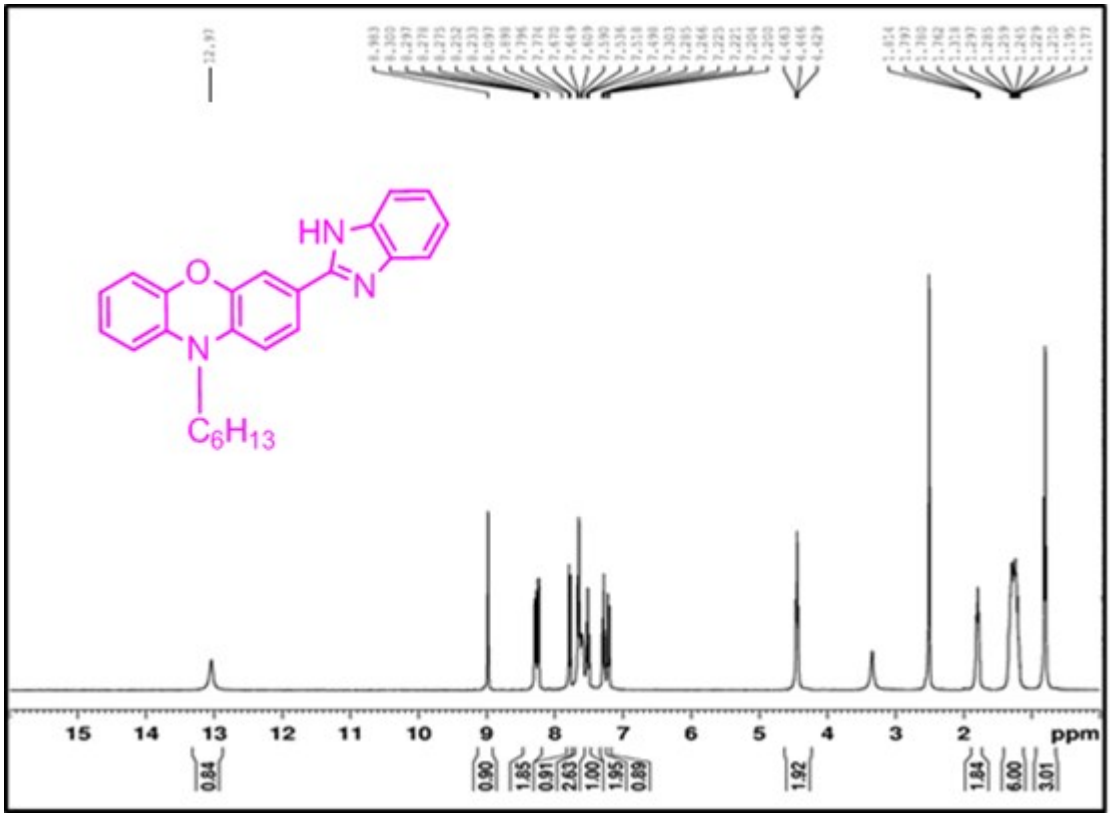


Fig. S5. ^{1}H-NMR and ^{13}C-NMR and MS spectra of SJE 4



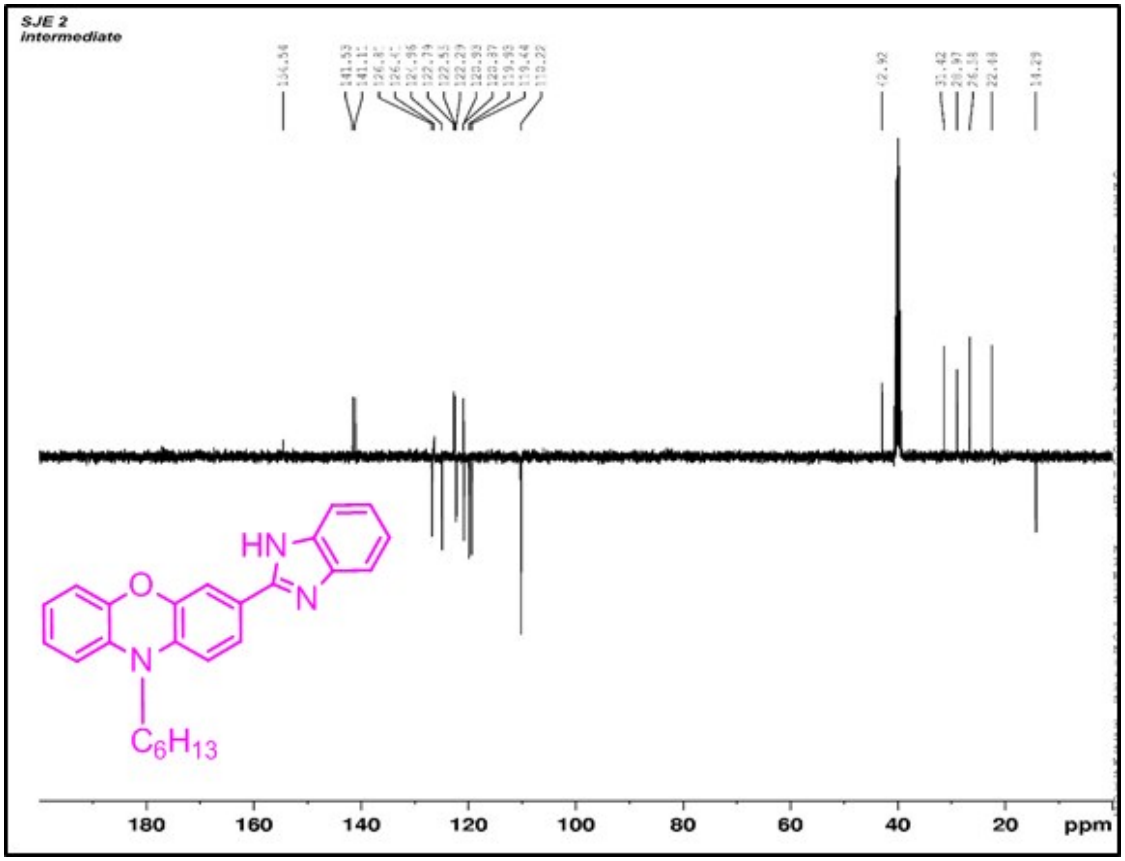


Fig. S6. [1]H-NMR and [13]C-NMR and MS spectra of SJE 2 intermediate

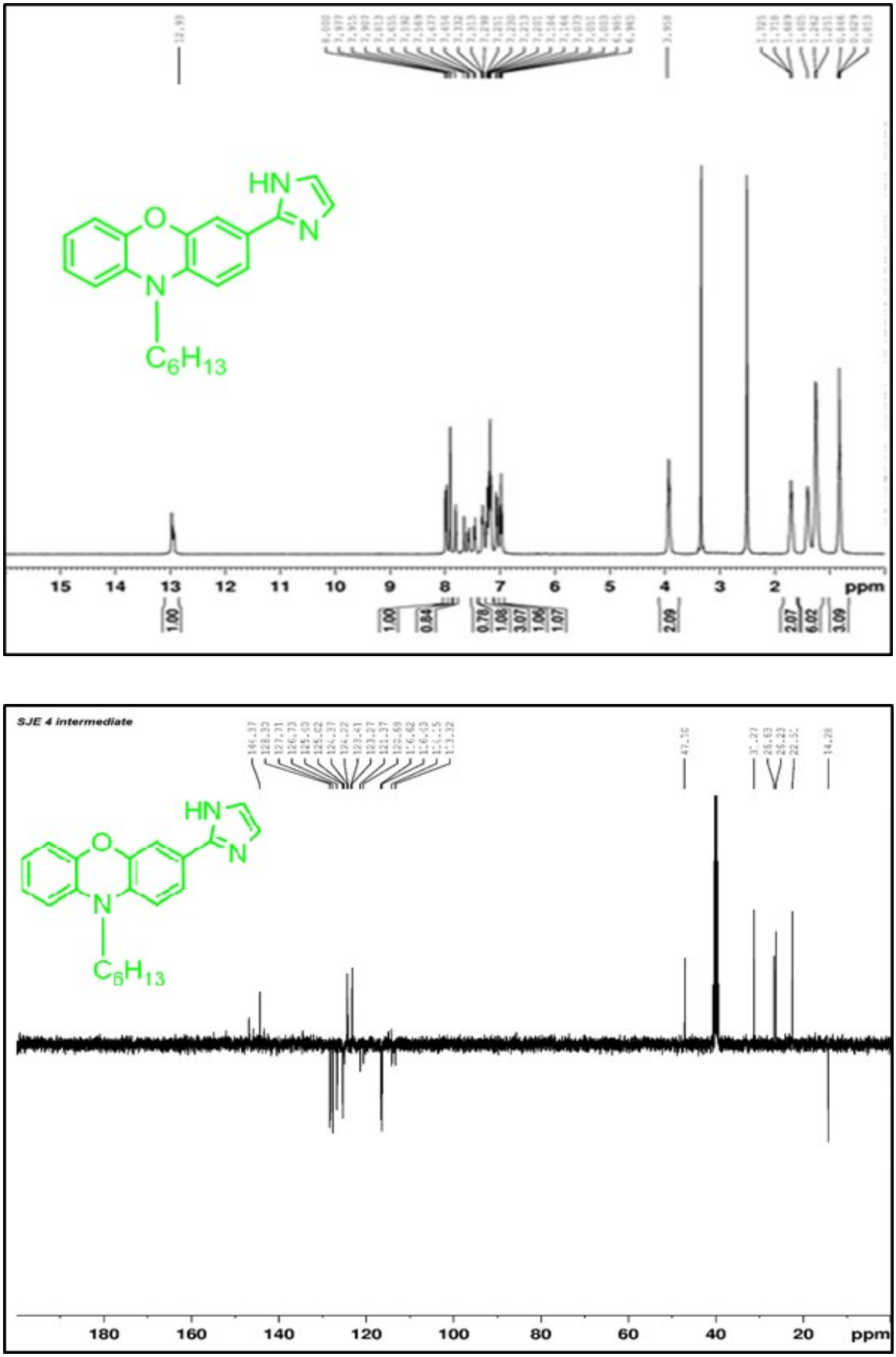


Fig. S7. ^{1}H-NMR and ^{13}C-NMR and MS spectra of SJE 4 intermediate

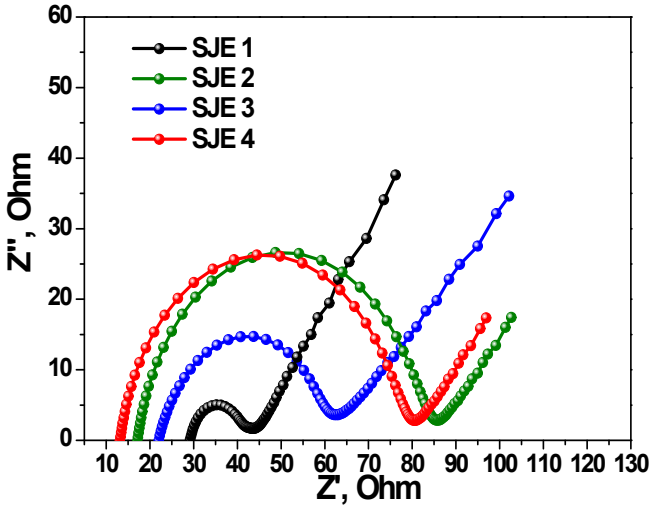


Fig. S8. EIS spectra of SJE 1- 4 between two platinum electrodes. The analysis were under frequency range 100MHz to 0.1Hz and an AC amplitude of 10mV. Conductivity was calculated from the R_b (Bulk resistance). The thickness of SOICs in between two symmetrical conducting plate, L = 60µm and area, A = 1.27cm^2

Electrolytes	R_b (Ω)	Conductivity σ (mS/cm)
SJE 1	29	1.62
SJE 2	17	2.94
SJE 3	22	2.13
SJE 4	13	3.61

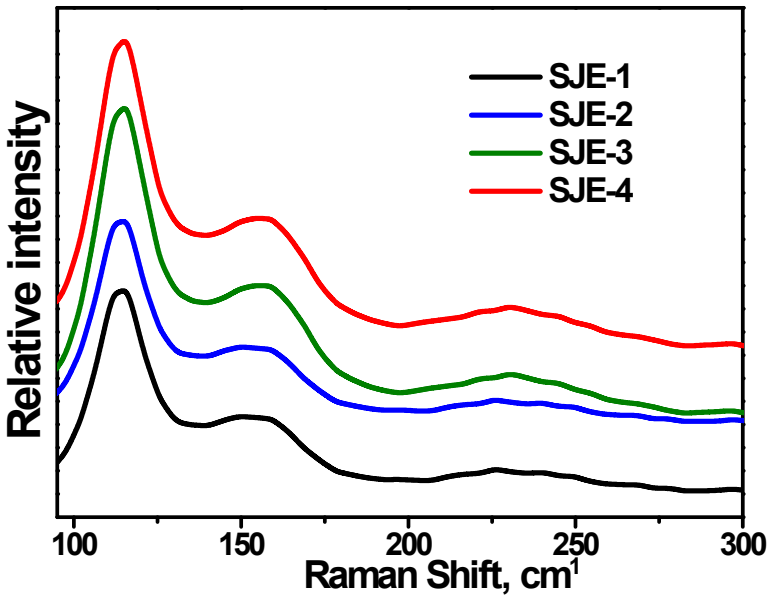


Fig. S9. Raman spectra of SJE 1- 4

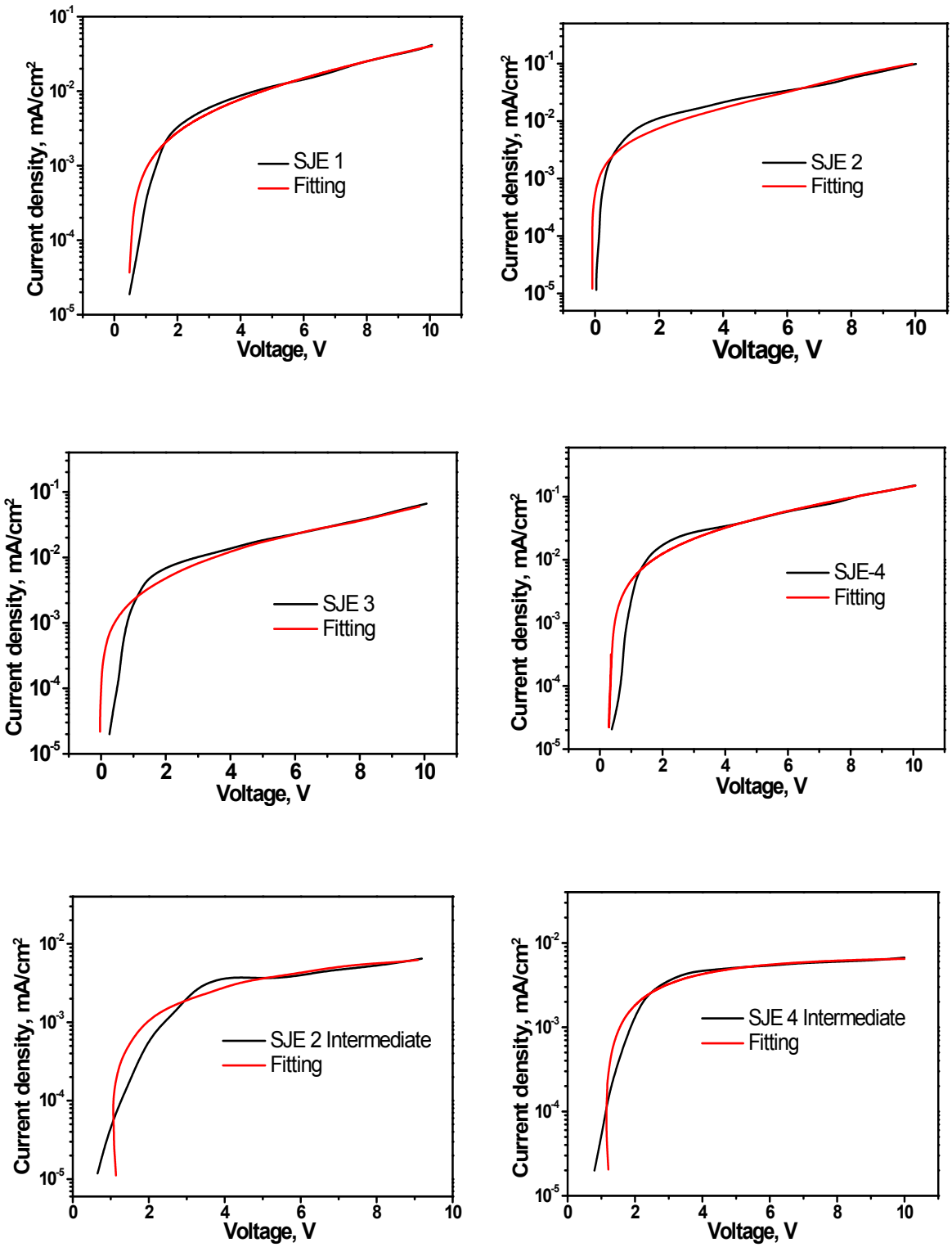


Fig. S10. *J-V* curve of hole only devices fabricated for determination of hole mobility

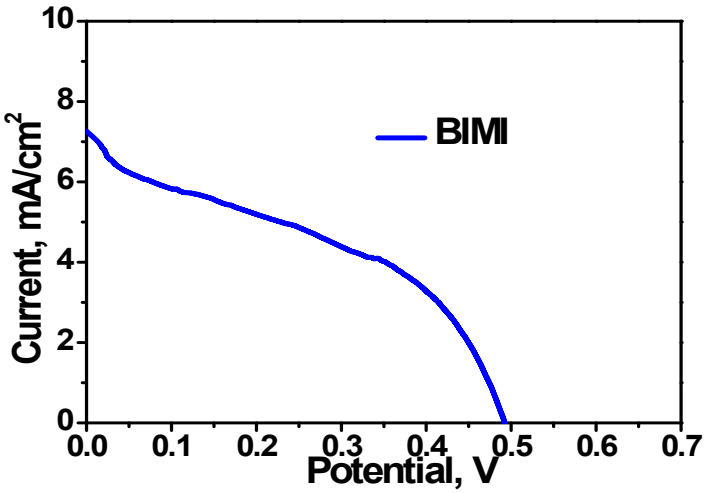


Fig. S11. *J-V* curve of BIMI electrolyte based device under simulated solar light AM1.5, 100mW/cm^2

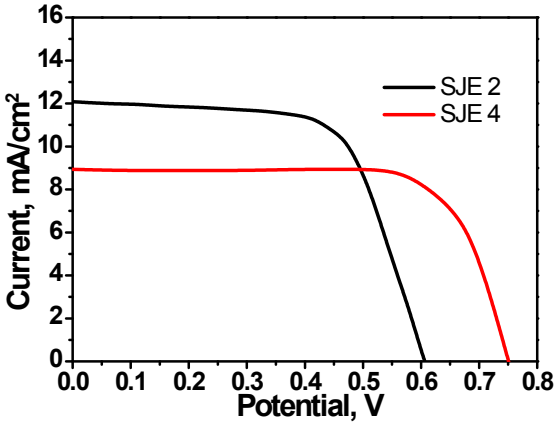


Fig. S12. *J-V* curve for ss-DSSC with 60µm spacer for SJE 2 and SJE 4

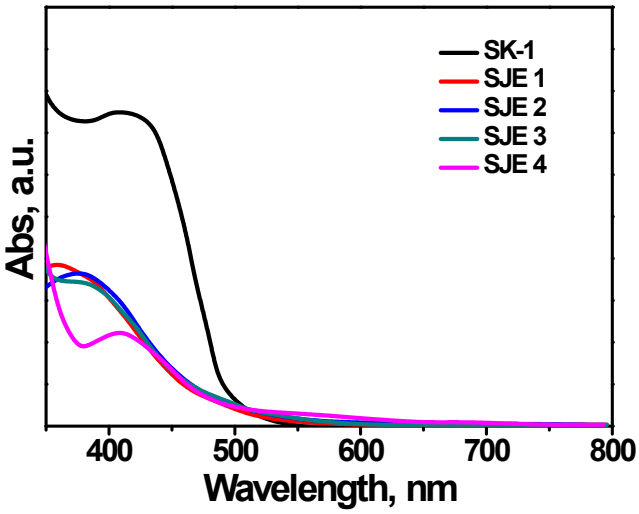


Fig. S13. UV-Vis spectra of pure SK 1 sensitizer and SJE 1-4

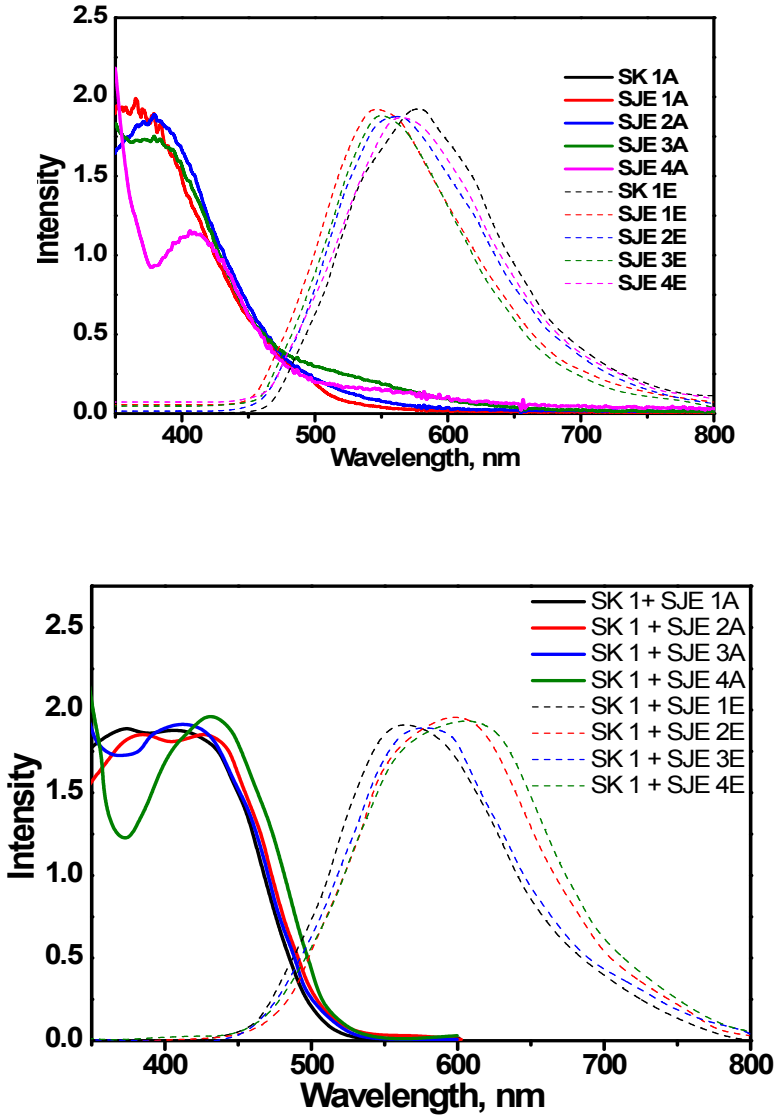


Fig. S14. UV-Vis and fluorescence spectra of SK 1 sensitizer and SJE 1-4

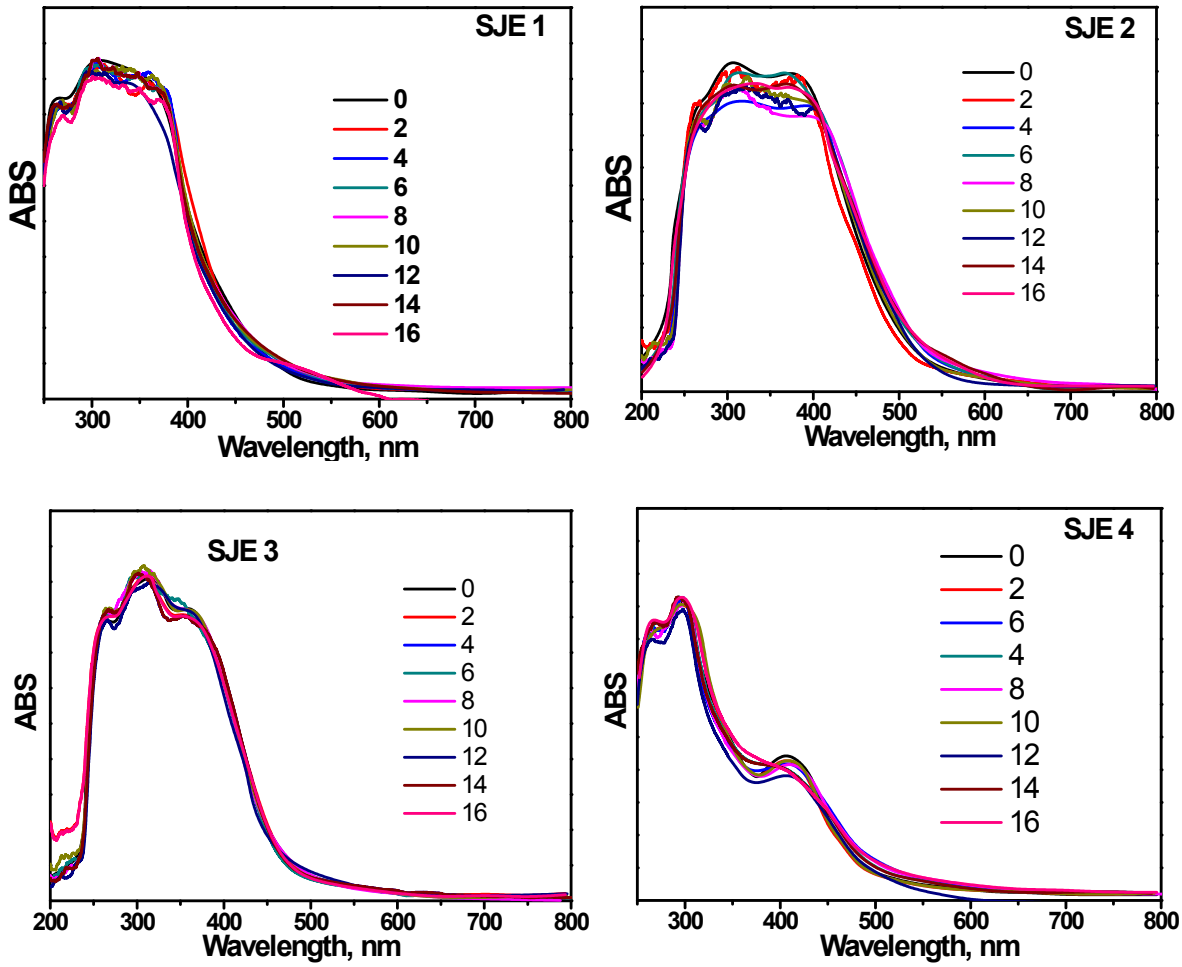
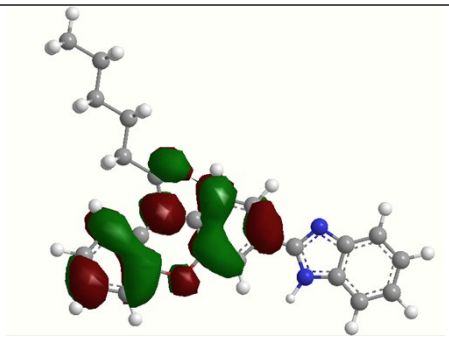
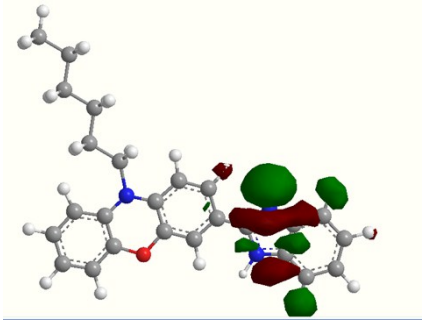
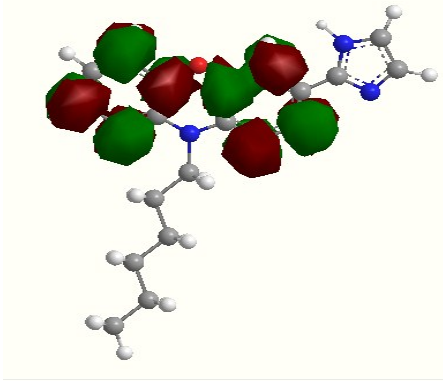
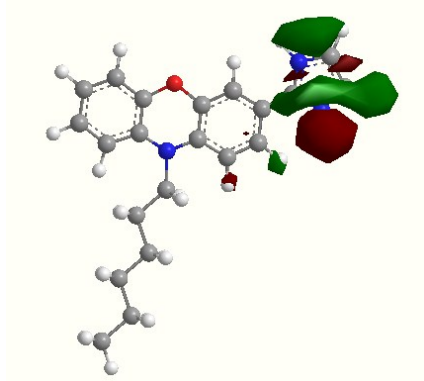


Fig. S15. Photostability study of SJE 1-4

We have carried out the UV-vis absorbance of all electrolytes in acetonitrile with different interval of sun light illumination from 0 to 16 days. There is no degradation observed in this compounds during this illumination. So, we can conclude that, these materials are highly stable and same is reflects in the device stability performance.

Table S1. HOMO-LUMO (DFT) calculation of SJE 2 and 4 intermediates

Intermediate	HOMO	LUMO
SJE 2	 **1.18V**	 **-1.31V**
SJE 4	 **1.22V**	 **-1.28V**

SJE intermediate HOMO-LUMO level shows by computational method. Gaussian, DFT calculations were carried out for optimization using the B3LYP functional with 6-31G(d p) basis set.