Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Novel efficient hole-transporting materials based on a 1,1'-bi-2-naphthol core for perovskite solar cells

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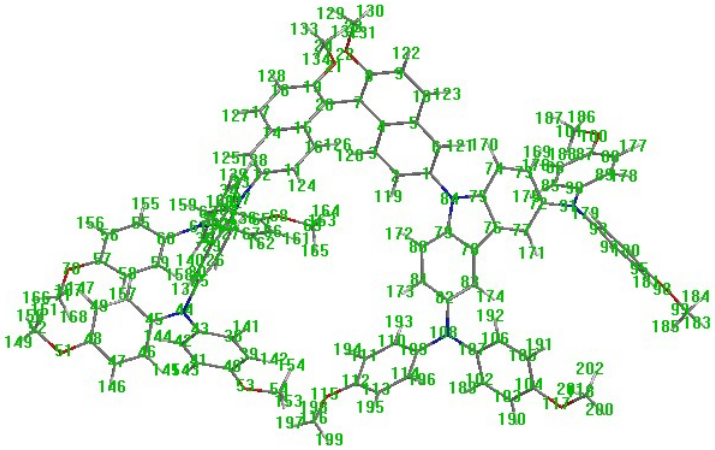
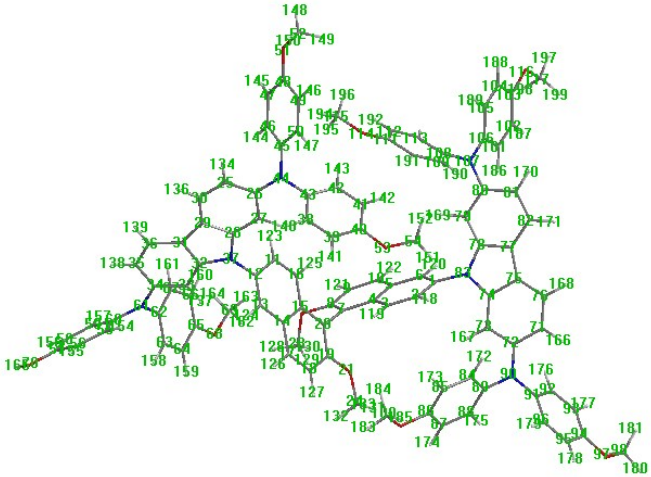
Numbered molecular

Q205



Q197



Q198

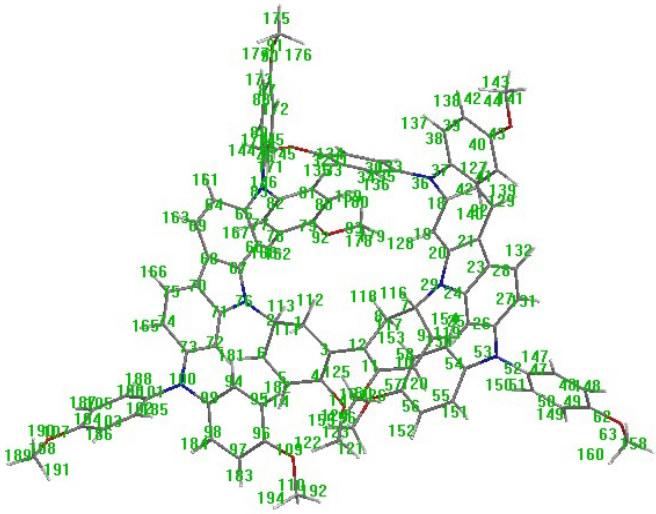
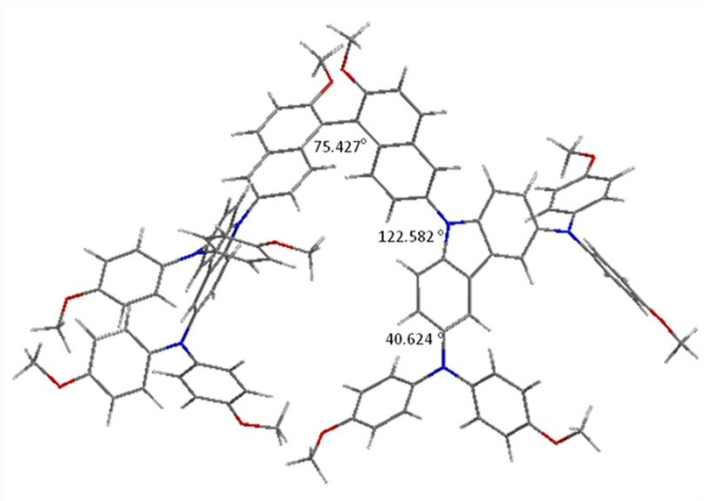


Fig. S1. Frontier molecular orbitals of **Q205, Q197 and Q198**.

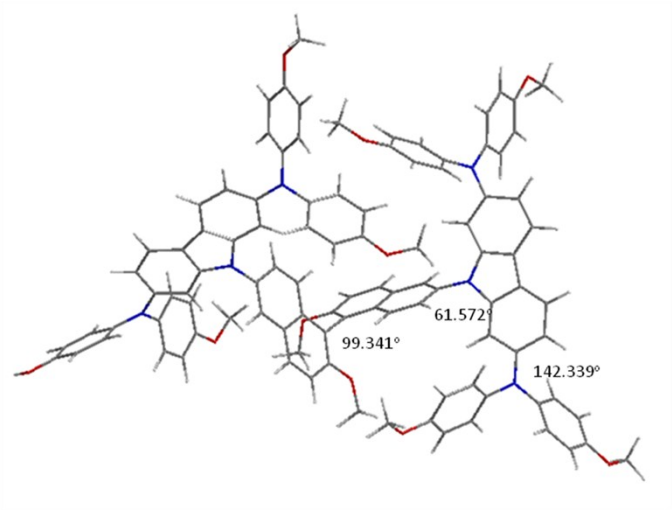
Table S1. Bond angles (dihedral) and bond lengths of **Q205, Q197 and Q198**

HTMs	Bond (dihedral) angle(°)		Bond length(Å)	
Q205	C(4)-C(7)-C(20)-C(15)	75.427	C(7)-C(20)	1.494
	C(1)-N(84)-C(75)	127.001	C(75)-N(84)	1.408
	C(1)-N(84)-C(79)	124.736	C(79)-N(84)	1.408
	C(2)-C(1)-N(84)-C(75)	122.582	C(1)-N(84)	1.425
	C(26)-C(25)-N(44)-C(43)	40.624	C(25)-N(44)	1.430
	C(25)-N(44)-C(43)	119.988	C(43)-N(44)	1.431
	C(25)-N(44)-C(45)	120.279	N(44)-C(45)	1.428
Q197	C(4)-C(7)-C(20)-C(15)	99.341	C(7)-C(20)	1.492
	C(1)-N(83)-C(74)	124.586	C(78)-N(83)	1.407
	C(1)-N(83)-C(78)	126.967	C(74)-N(83)	1.407
	C(2)-C(1)-N(83)-C(74)	61.572	C(1)-N(83)	1.428
	C(26)-N(44)-C(43)	119.476	C(43)-N(44)	1.436
	C(26)-N(44)-C(45)	121.142	N(44)-C(45)	1.426
	C(27)-C(26)-N(44)-C(45)	142.339	C(26)-N(44)	1.426
Q198	C(1)-C(3)-C(12)-C(11)	114.004	C(3)-C(12)	1.482
	C(7)-N(29)-C(20)	124.820	C(20)-N(29)	1.408
	C(7)-N(29)-C(24)	125.805	C(24)-N(29)	1.408
	C(8)-C(7)-N(29)-C(20)	123.957	C(7)-N(29)	1.470
	C(18)-N(36)-C(35)	119.188	C(35)-N(36)	1.428
	C(18)-N(36)-C(37)	119.870	N(36)-C(37)	1.426
	C(19)-C(18)-N(36)-C(37)	129.783	C(18)-N(36)	1.433

Q205



Q197



Q198

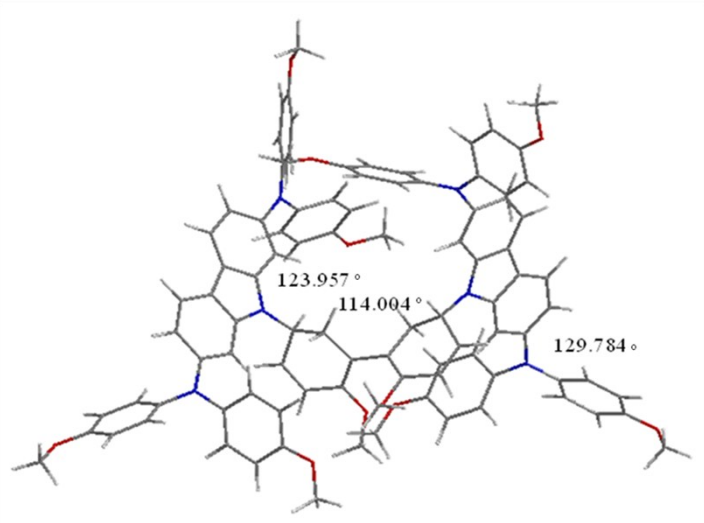
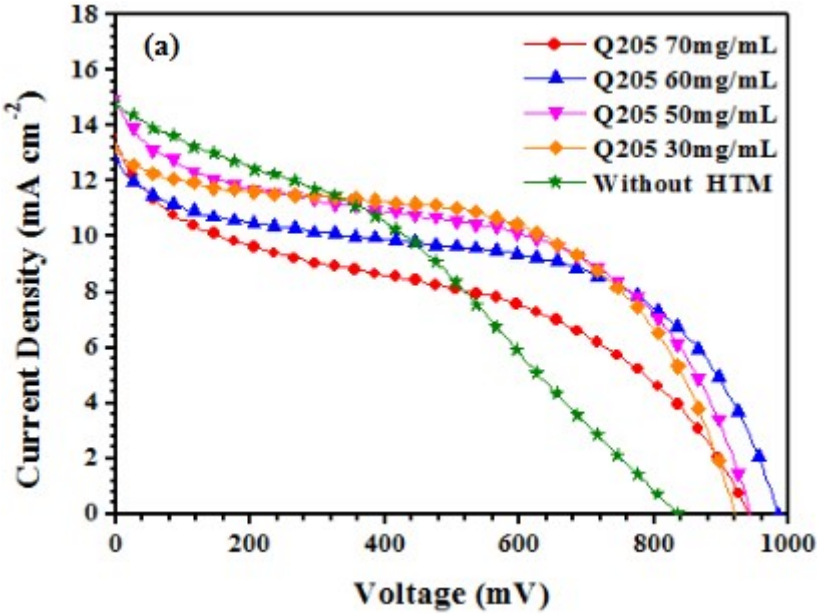
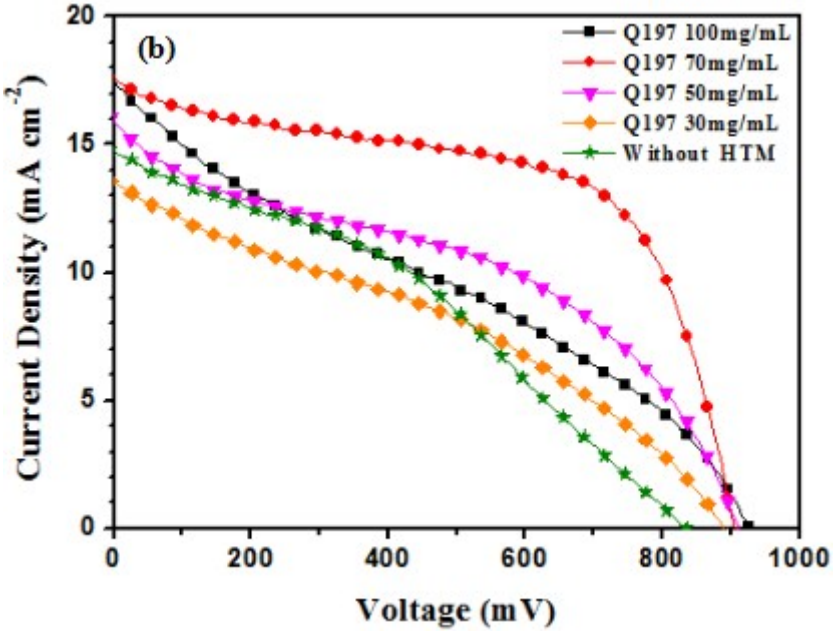


Fig. S2. Representative dihedral angles of **Q205**, **Q197** and **Q196**.


(a)
Q205 70mg/mL
Q205 60mg/mL
Q205 50mg/mL
Q205 30mg/mL
Without HTM
Current Density (mA cm-2)
Voltage (mV)
0
2
4
6
8
10
12
14
16
18
0
200
400
600
800
1000


(b)
Q197 100mg/mL
Q197 70mg/mL
Q197 50mg/mL
Q197 30mg/mL
Without HTM
Current Density (mA cm-2)
Voltage (mV)
0
5
10
15
20
0
200
400
600
800
1000

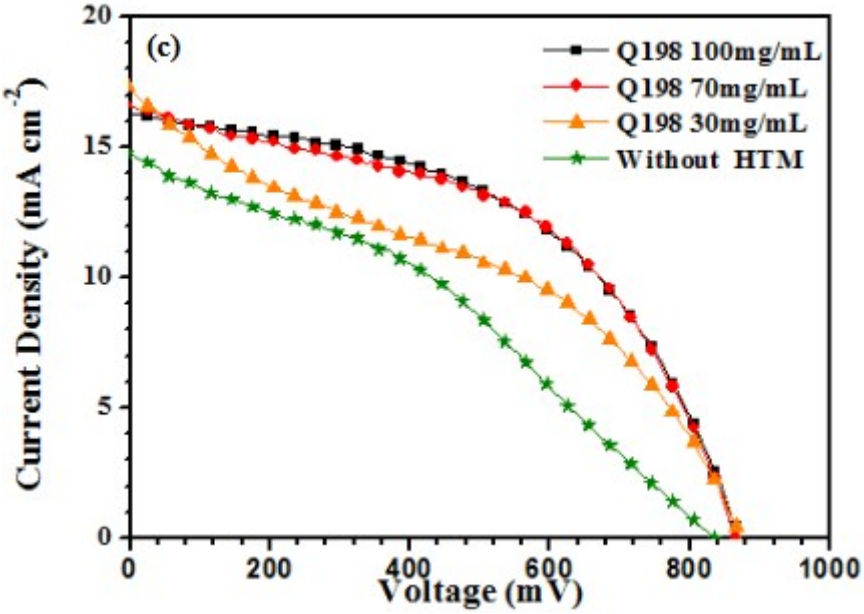
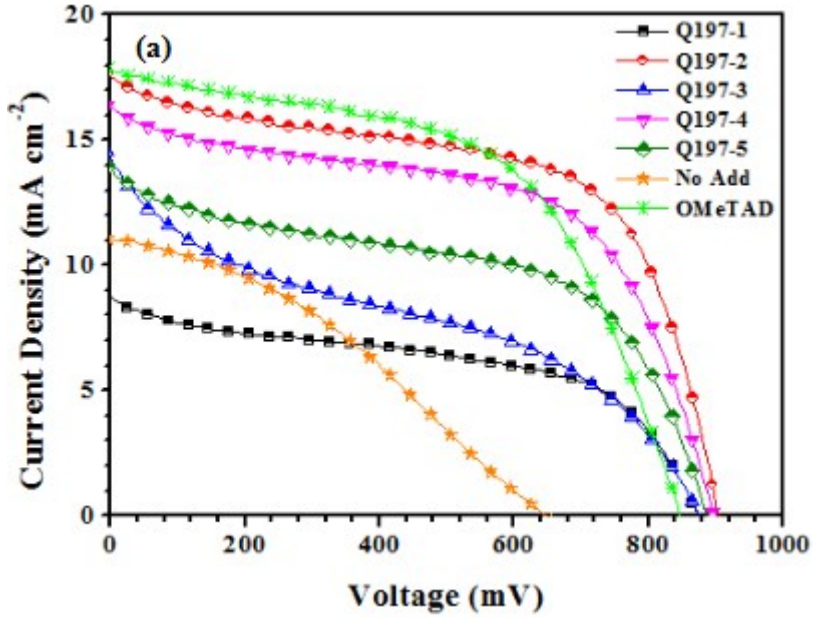
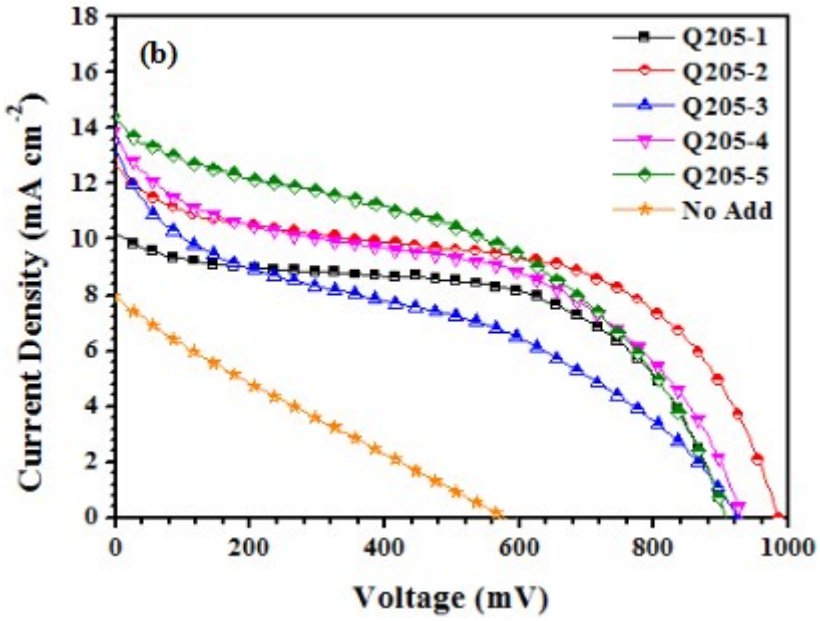


Fig. S3. *J–V* characteristics of PSCs based on different concentrations of (a) **Q205,** (b) **Q197** and (c) **Q198** doping with proportion of 30 mM Li-TFSi and 200 mM TBP.





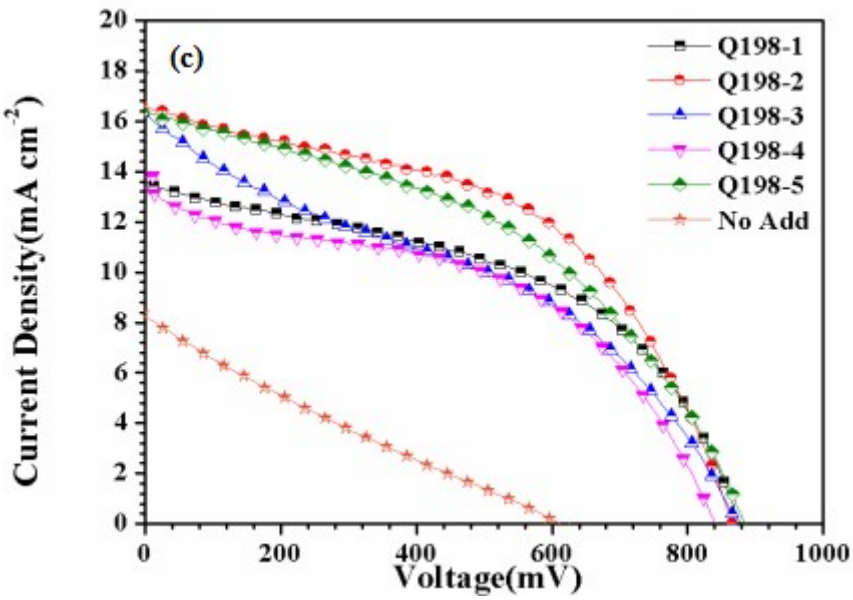


Fig. S4. *J–V* characteristics of PSCs based on (a) **Q197** (70mg/mL), (b) **Q205** (60mg/mL) and (c) **Q198** (70mg/mL) doping with different proportions of Li-TFSi/TBP. 1: 60 mM/200 mM; 2: 30 mM/200 mM; 3: 15 mM/200 mM; 4: 30 mM/120 mM; 5: 30 mM/60 mM.

Table S2. *J-V* characteristics of photovoltaic measurements of **Q197**.

Condition	Li-TFSI/mM	TBP/mM	*J*sc/mA·cm^{-2}	*V*oc/V	*FF*	η %
100mg/mL	30	200	17.14	933	0.35	5.59
70mg/mL	30	200	15.31	903	0.58	8.08
50mg/mL	30	200	14.30	909	0.41	5.29
30mg/mL	30	200	13.63	884	0.34	4.09
Pure $MAPbI_3$	Without HTM		14.92	832	0.34	4.27
1	60	200	9.072	872	0.49	3.91
2	30	200	15.31	903	0.58	8.08
3	15	200	14.36	872	0.33	4.18
4	30	120	16.53	897	0.56	8.38
5	30	60	13.98	886	0.51	6.37
Without doping	---	---	11.14	645	0.34	2.45
Spiro-OMeTAD	30	120	17.53	850	0.55	8.13

Table. S3. *J-V* characteristics of photovoltaic measurements of **Q205**.

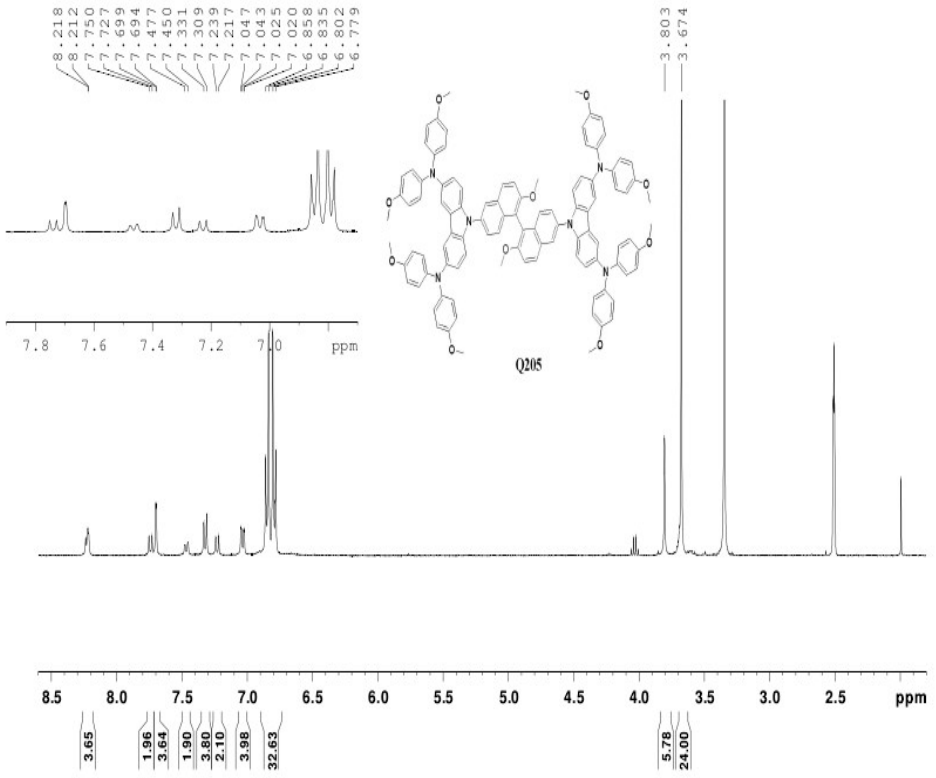
Condition	Li-TFSI/mM	TBP/mM	*J*sc/mA·cm^{-2}	*V*oc/V	*FF*	η %
70mg/mL	30	200	13.17	939	0.37	4.55
60mg/mL	30	200	13.23	984	0.50	6.51
50mg/mL	30	200	13.87	943	0.46	6.08
30mg/mL	30	200	12.33	907	0.44	4.92
Pure $MAPbI_3$	Without HTM		14.92	832	0.34	4.27
1	60	200	11.79	903	0.55	5.83
2	30	200	13.23	984	0.50	6.51
3	15	120	12.42	931	0.39	4.54
4	30	120	13.56	929	0.43	5.36
5	30	300	14.29	906	0.44	5.66
Without doping	---	---	7.86	580	0.23	1.04

Table S4. J-V characteristics of photovoltaic measurements of **Q198**.

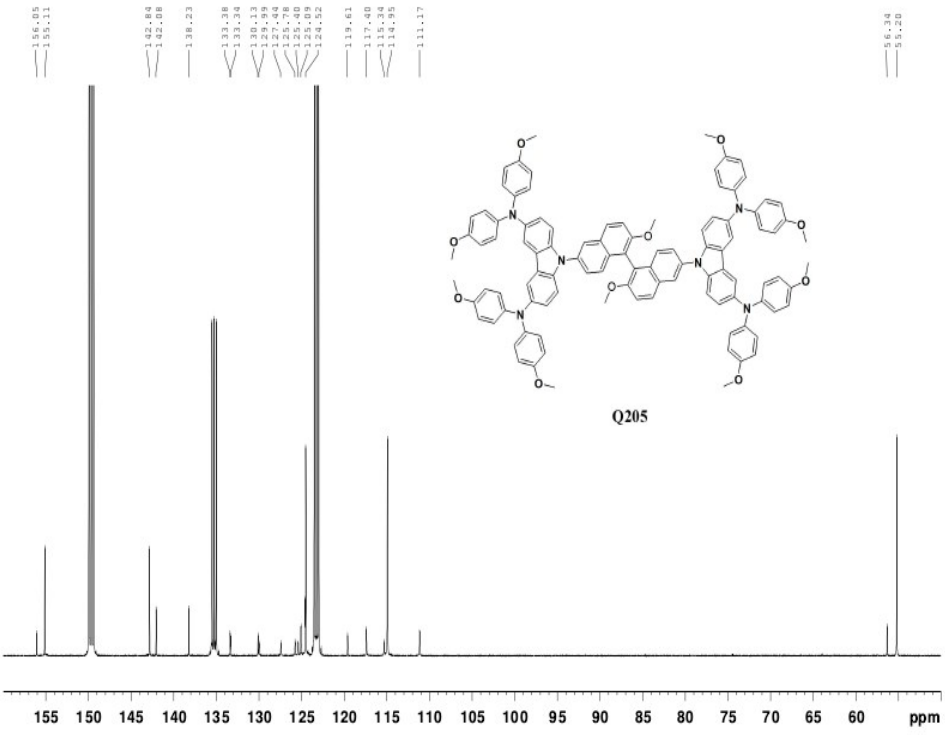
Condition	Li-TFSI/mM	TBP/mM	*J*sc/mA·cm^{-2}	*V*oc/V	*FF*	η %
100mg/mL	30	200	14.60	869	0.37	4.74
70mg/mL	30	200	16.69	863	0.49	7.08
30mg/mL	30	200	16.44	869	0.49	7.04
Pure $MAPbI_3$	Without HTM		14.92	832	0.34	4.27
1	60	200	14.67	876	0.45	5.73
2	30	200	16.69	863	0.49	7.08
3	15	120	16.33	870	0.37	5.23
4	30	120	13.56	840	0.46	5.19
5	30	300	16.33	881	0.44	6.30
Without doping	---	---	8.22	609	0.22	1.12

Table S5. Photovoltaic parameters from eight cells with **Q197**.

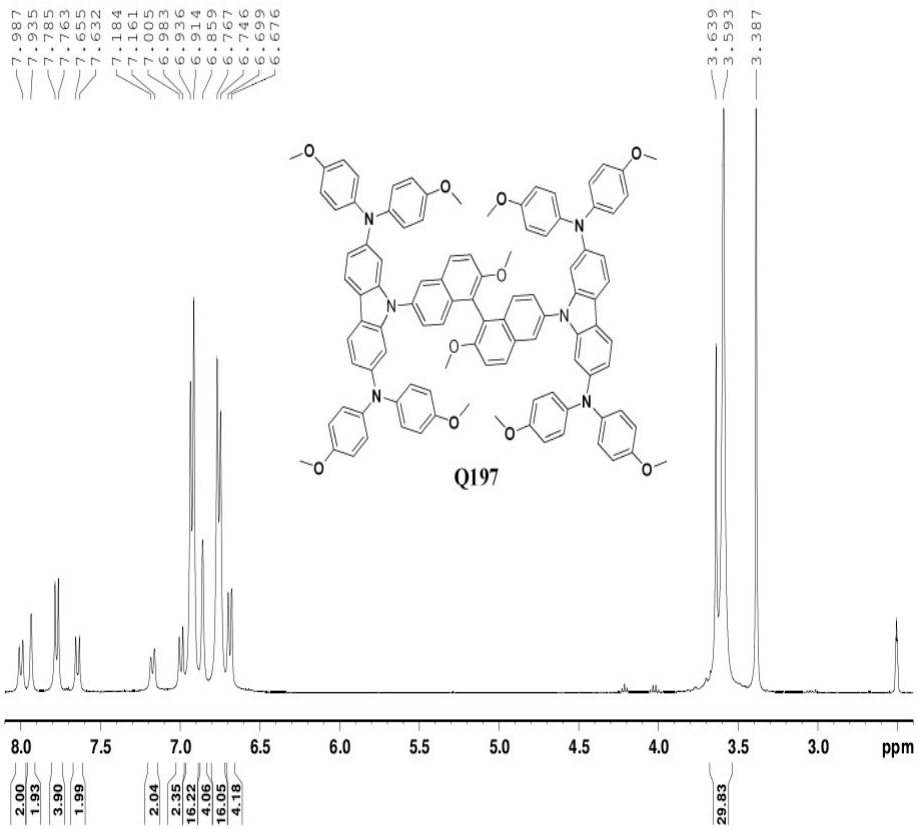
Condition	*J*sc/mA·cm^{-2}	*V*oc/V	*FF*	η %
1	17.12	934	0.49	7.85
2	16.76	890	0.47	7.00
3	15.82	913	0.52	7.48
4	16.53	897	0.56	8.38
5	15.21	897	0.60	8.13
6	15.46	890	0.56	7.72
7	15.97	886	0.48	6.80
8	16.89	913	0.48	7.33
average	16.22	903	0.52	7.59



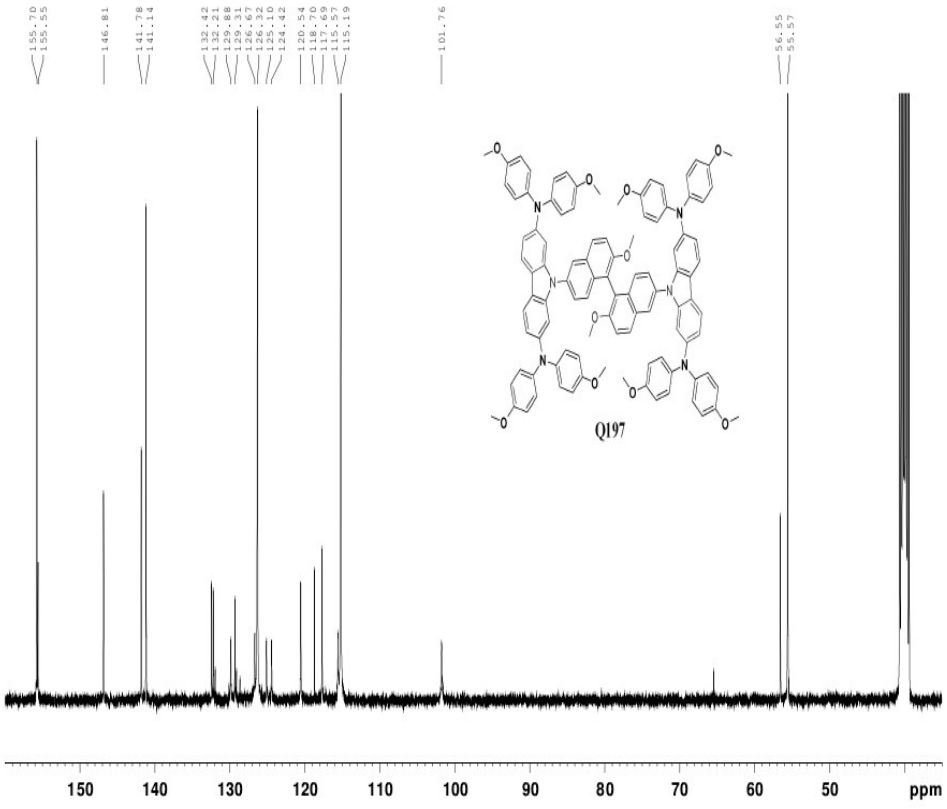
^{1}H NMR (DMSO-d_6) spectra of **Q205**



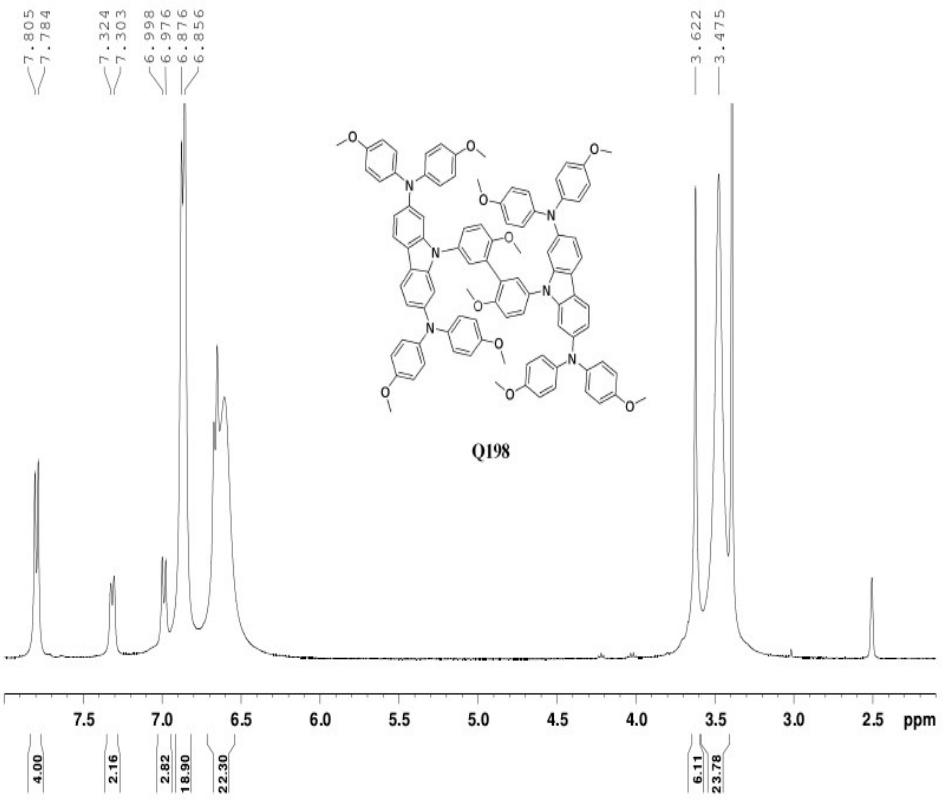
^{13}C NMR (Pyridine -d_6) spectra of **Q205**



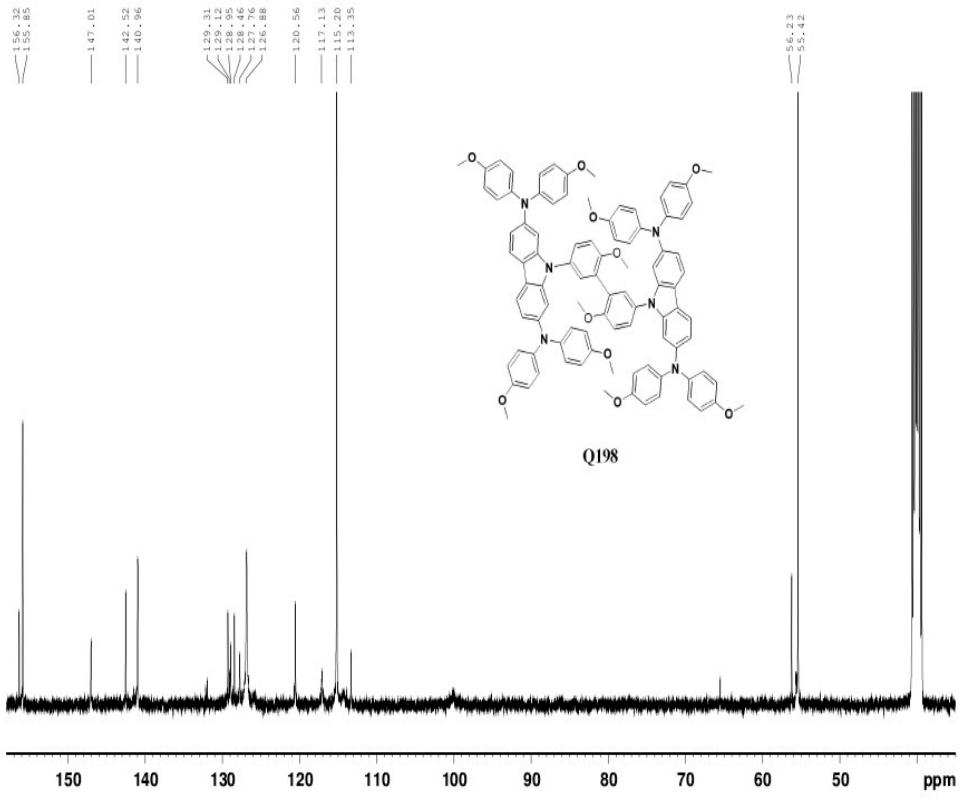
^{1}H NMR (DMSO-d_6) spectra of **Q197**



^{13}C NMR (DMSO-d_6) spectra of **Q197**



^{1}H NMR (DMSO-d_6) spectra of **Q198**



^{13}C NMR (DMSO-d_6) spectra of **Q198**