Electronic Supplementary Information

Optimal molecule-matching co-sensitization system for the improvement of photovoltaic performances of DSSCs

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1. Molecular structure confirmation

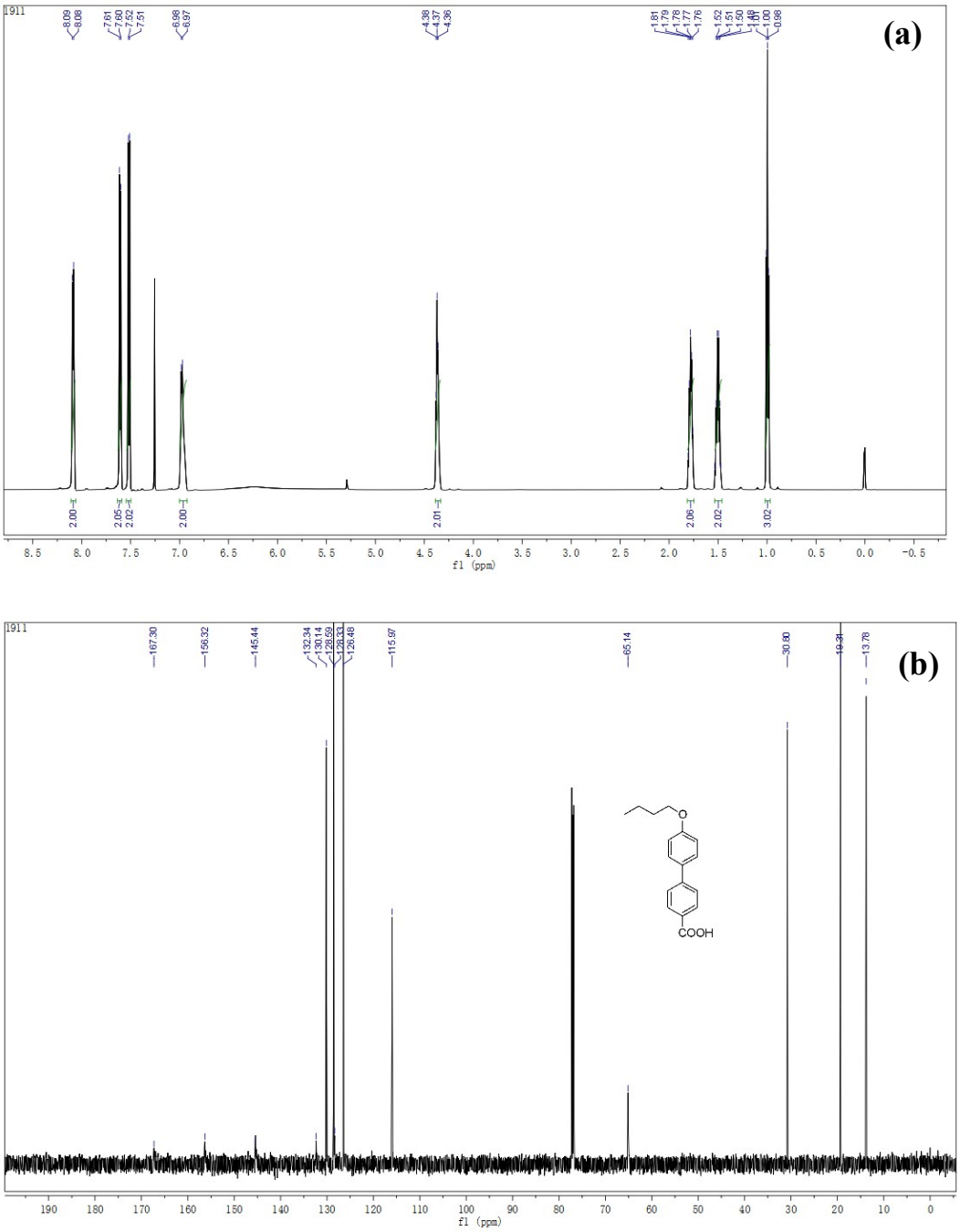

Fig. S1. (a) ^{1}H NMR and (b) ^{13}C NMR of compound **4OBA**.

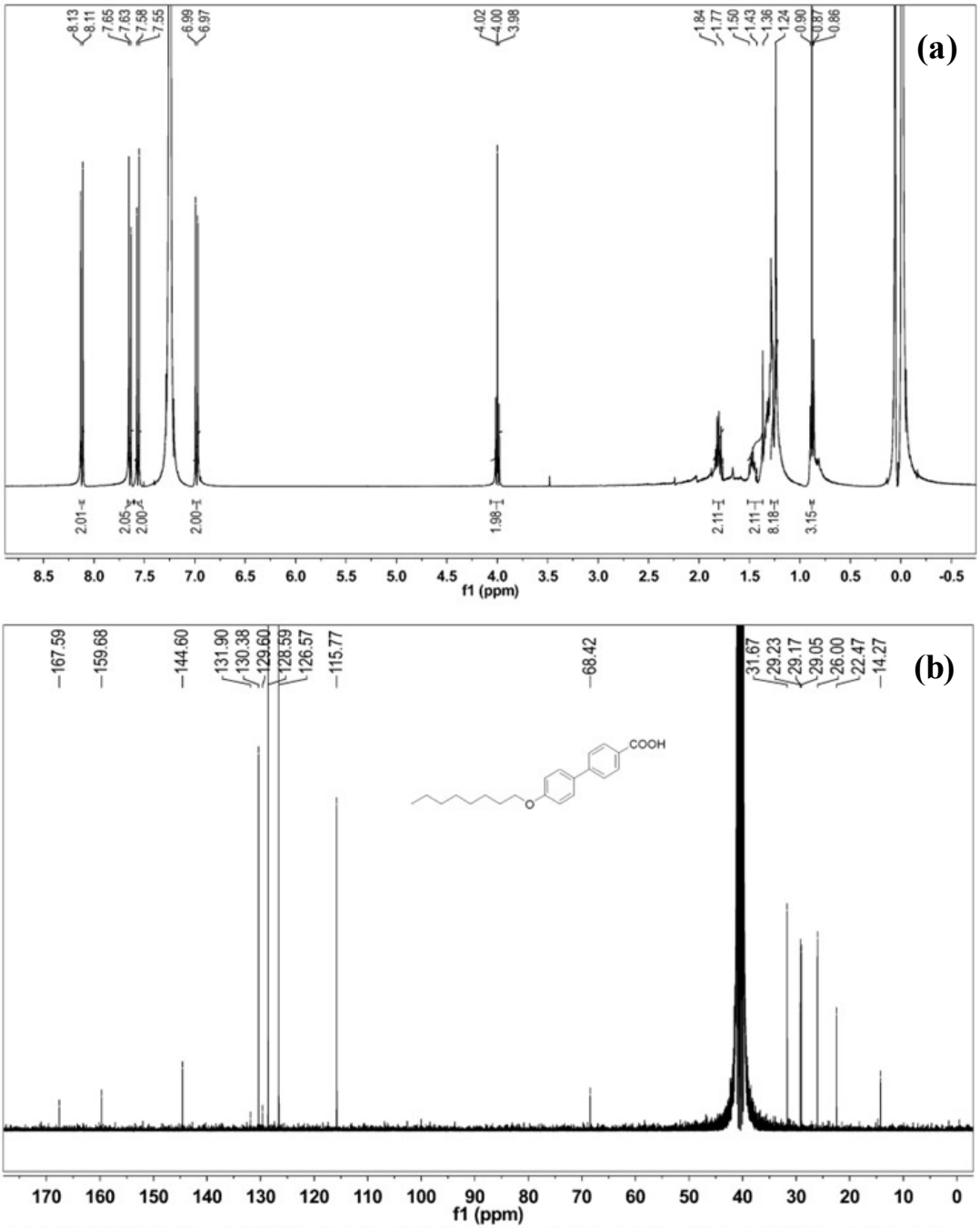

Fig. S2. (a) ^{1}H NMR and (b) ^{13}C NMR of compound **8OBA**.

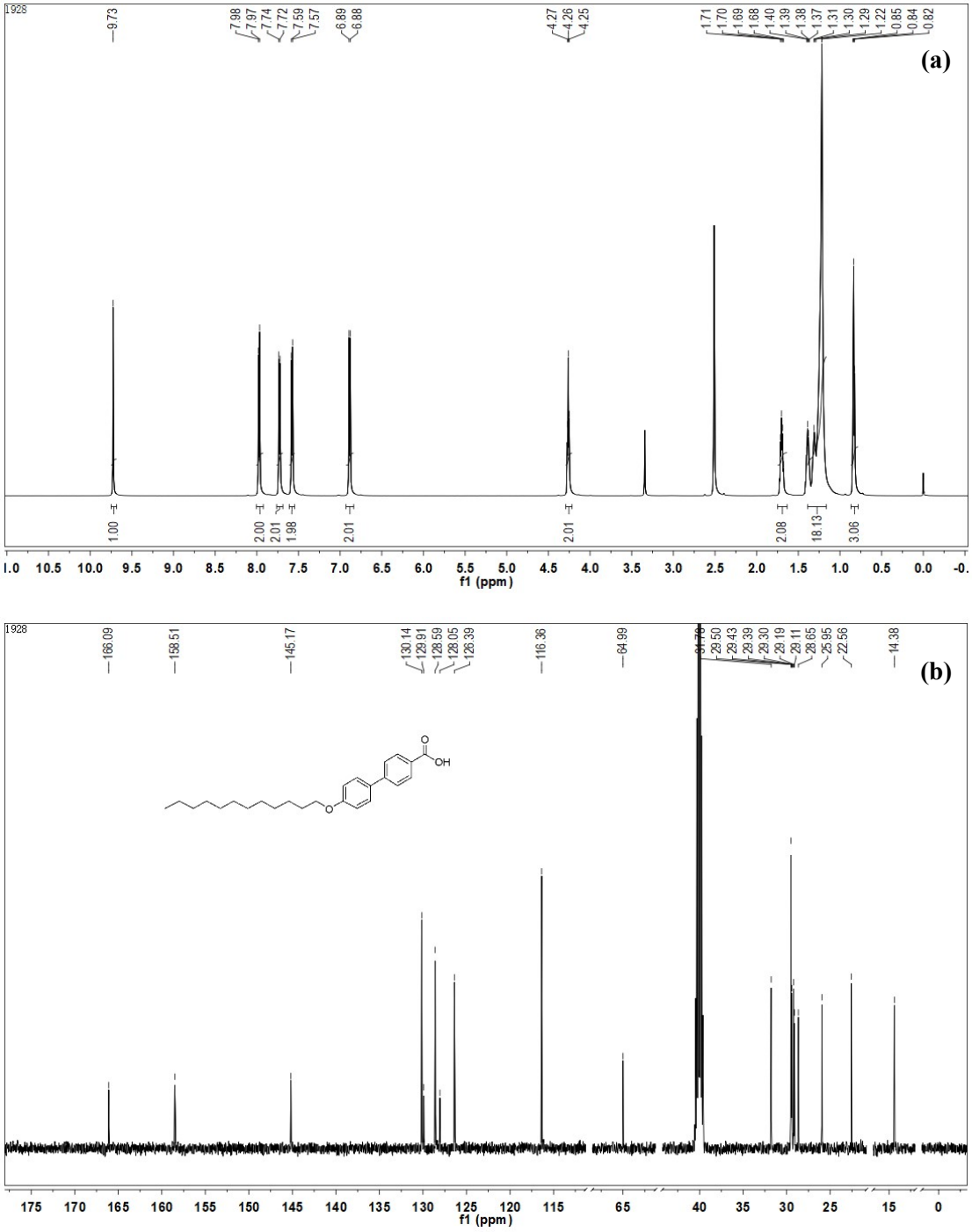

Fig. S3. (a) ^{1}H NMR and (b) ^{13}C NMR of compound **12OBA**.

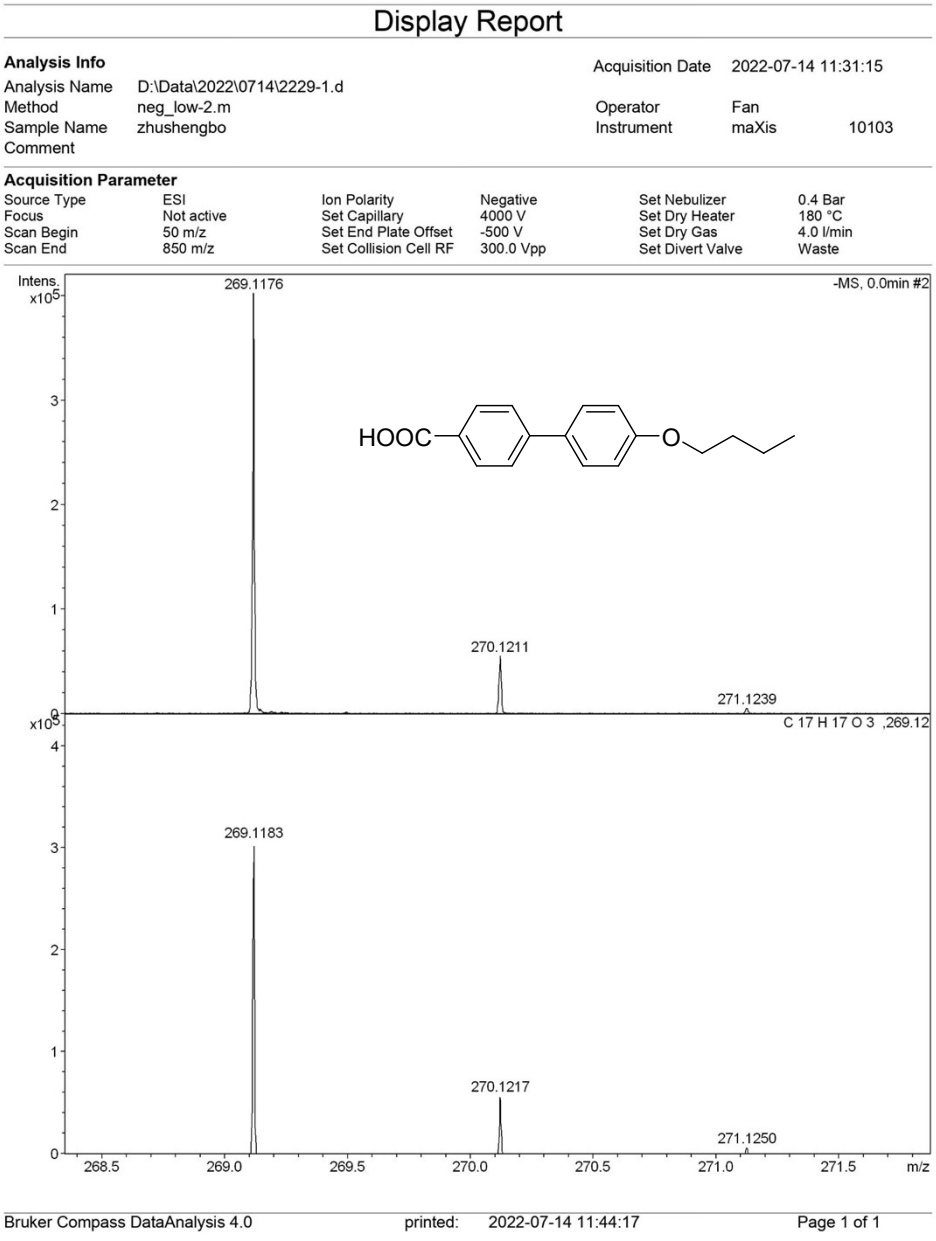

Fig. S4. HRMS of **4OBA**.

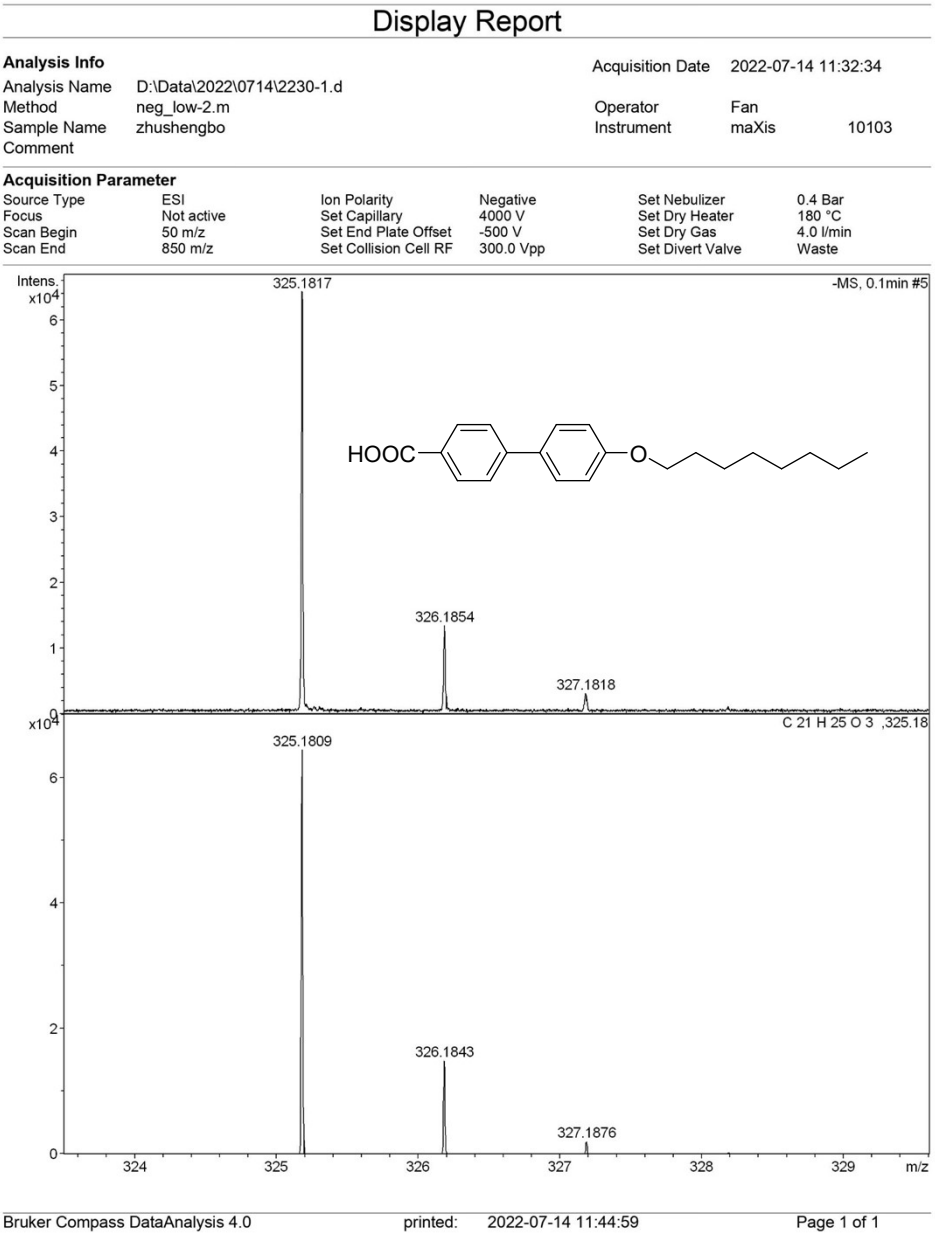

Fig. S5. HRMS of **8OBA**.

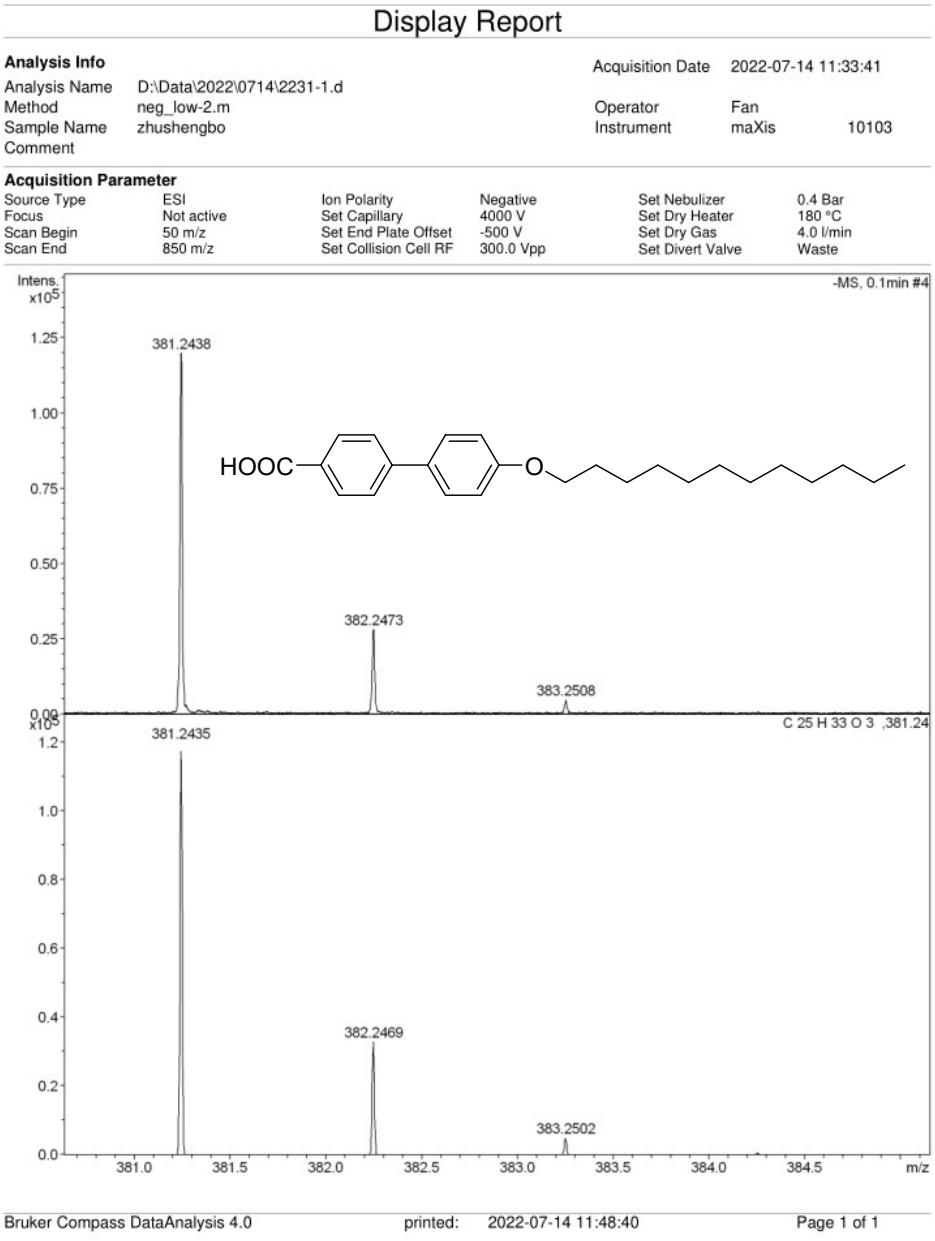

Fig. S6. HRMS of **12OBA**.

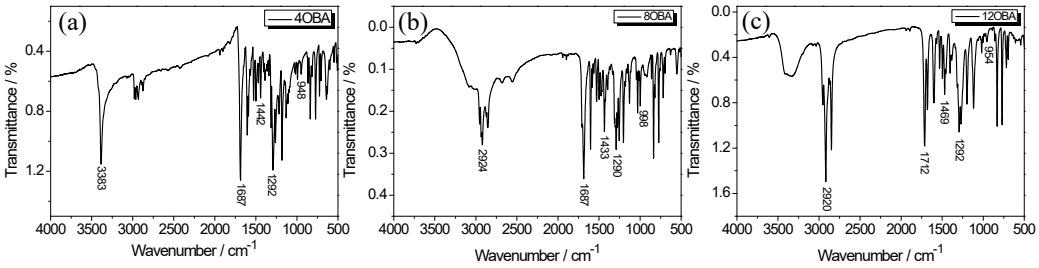

Fig. S7. FT-IR spectra of (a) **4OBA**, (b) **8OBA** and (c) **12OBA**.

2. Thermal stability

It is crucial to study the thermal behavior of sensitizers, and good thermal behavior is a prerequisite for organic materials used in photovoltaic applications. The thermal properties of the co-sensitizers **nOBA** (n=4, 8 and 12) are studied by differential scanning calorimetry (DSC) and thermogravimetric analyses (TGA) at the heating rate of 10 °C min^{-1} under an argon atmosphere. The DSC and TGA curves of **nOBA** (n=4, 8 and 12) are shown in Fig. S8 and S9, respectively. All the co-sensitizers **nOBA** (n=4, 8 and 12) exhibit satisfactory thermal stability with high thermal decomposition (T_d) temperatures at 255 °C (**4OBA**), 280 °C (**8OBA**) and 310° C (**12OBA**) (*Mater. Chem. Front.*, 2022, **6**, 580-592; *Phys. Chem. Chem. Phys.*, 2020, **22**, 23169-23184; *Thermochim. Acta*, 2006, **440**, 181-187). The test results are as follows:

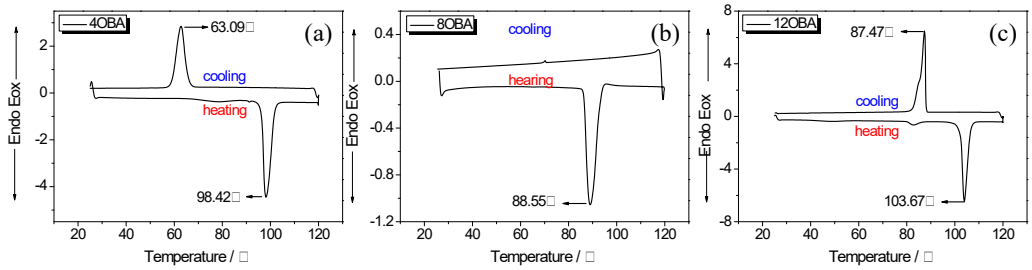

Fig. S8. DSC curves of (a) **4OBA**, (b) **8OBA** and (c) **12OBA**.

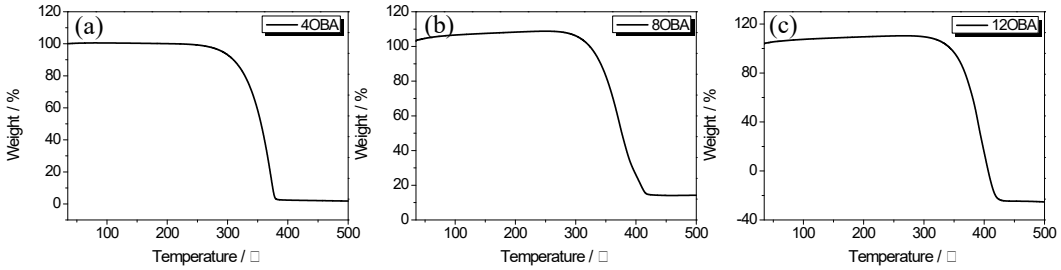

Fig. S9. TGA curves of (a) **4OBA**, (b) **8OBA** and (c) **12OBA**.

3. Application evaluation

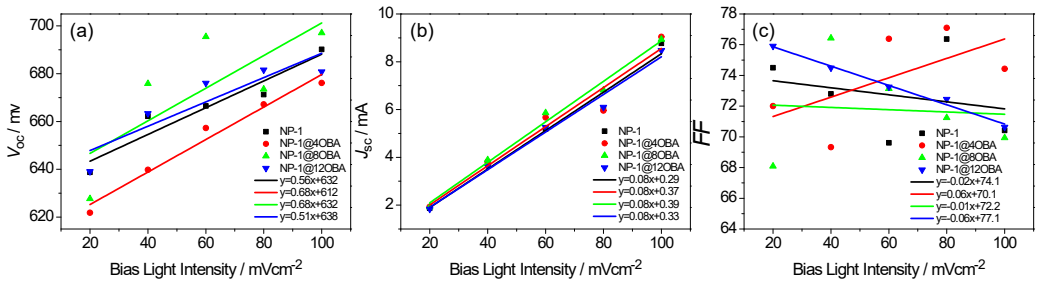

Fig. S10. (a) V_{oc}, (b) J_{sc} and (c) *FF* of DSSCs under different irradiations.

In addition to testing the photovoltaic parameters under different irradiation conditions, their durability was also tested. The following figure shows the 1000 h durability of the DSSC devices. The results are shown in Fig. S11 and Table S3.

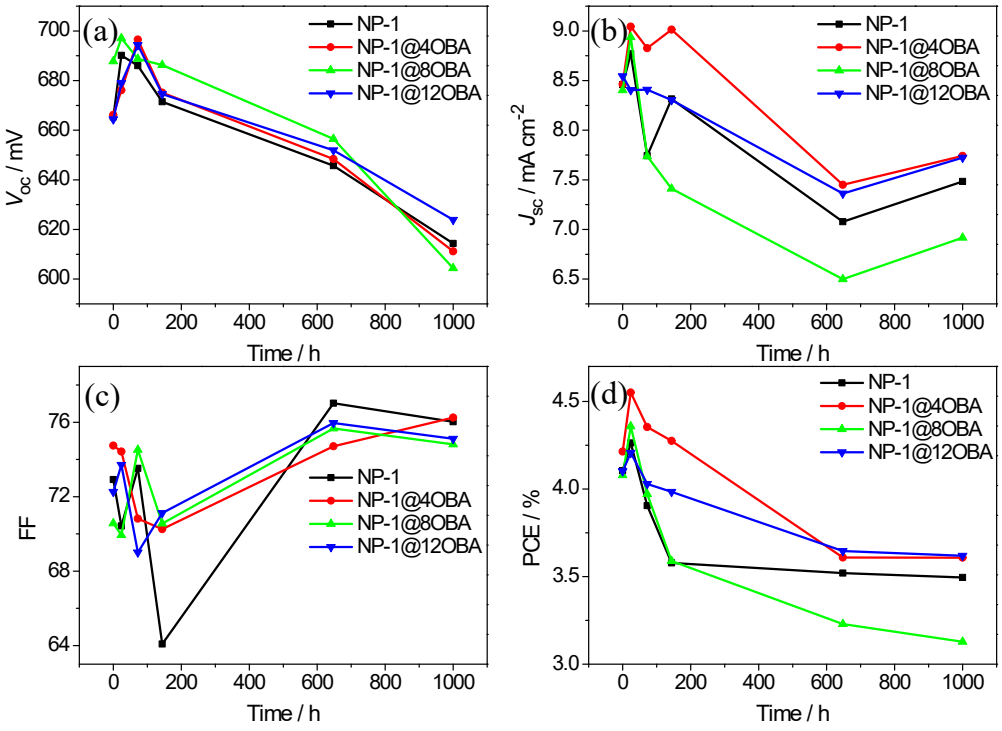

Fig. S11. Durability of (a) V_{oc}, (b) J_{sc}, (c) *FF* and (d) PCE of DSSCs based on **NP-1**, **NP-1@4OBA**, **NP-1@8OBA**, **NP-1@12OBA** for 1000 h.

Table S1 The length (*L*), height (*H*) and width (*W*) of the three-dimensional structures, and the ratio of *H* and *W*.

Dye	*L*(Å)	*H*(Å)	*W*(Å)	*H/W*
NP-1	21.67	10.07	4.64	2.17
4OBA	17.91	5.61	3.38	1.66
8OBA	22.93	6.05	3.42	1.77
12OBA	28.33	6.31	3.31	1.91

Table S2 Photovoltaic performances of DSSCs under different irradiation.

Devices	Bias Light Intensity / mW cm^{-2}	V_{oc} / mV	J_{sc} / mA cm^{-2}	*FF* / %	PCE / %
NP-1	20	638.72	1.87	74.50	0.89
	40	662.19	3.74	72.80	1.80
	60	666.49	5.18	69.61	2.40
	80	671.23	6.03	76.36	3.09
	100	690.18	8.77	70.42	4.26
NP-1@4OBA	20	621.80	1.93	72.00	0.86
	40	639.81	3.82	69.33	1.69
	60	657.26	5.67	76.38	2.84
	80	667.19	5.96	77.10	3.06
	100	676.13	9.04	74.43	4.55
NP-1@8OBA	20	627.67	1.92	68.09	0.82
	40	675.87	3.89	76.43	2.01
	60	695.48	5.86	73.14	2.98
	80	673.55	6.81	71.24	3.27
	100	697.11	8.94	69.94	4.36
NP-1@12OBA	20	639.06	1.83	75.91	0.89
	40	663.37	3.62	74.49	1.79
	60	676.09	5.26	73.25	2.60
	80	681.62	6.10	72.45	3.01
	100	680.84	8.47	70.64	4.07

Table S3 The length (L), Durability data of V_{oc}, J_{sc}, *FF*, PCE for DSSCs based on **NP-1**, **NP-1@4OBA**, **NP-1@8OBA**, **NP-1@12OBA** for 1000 h.

Devices	Time / h	V_{oc} / mV	J_{sc} / mA cm^{-2}	*FF* / %	PCE / %
NP-1	0	665.35	8.46	72.92	4.10
	24	690.18	8.77	70.42	4.26
	72	685.97	7.74	73.53	3.91
	144	671.44	8.31	64.09	3.58
	648	645.70	7.08	77.02	3.52
	1000	614.35	7.48	76.02	3.50
NP-1@4OBA	0	666.20	8.46	74.75	4.21
	24	676.13	9.04	74.43	4.55
	72	696.49	8.83	70.82	4.35
	144	675.16	9.01	70.25	4.28
	648	648.37	7.45	74.71	3.61
	1000	611.19	7.74	76.25	3.61
NP-1@8OBA	0	687.78	8.40	70.57	4.08
	24	697.11	8.94	69.94	4.36
	72	688.77	7.74	74.52	3.97
	144	686.27	7.41	70.56	3.59
	648	656.49	6.50	75.67	3.23
	1000	604.41	6.92	74.81	3.13
NP-1@12OBA	0	664.40	8.54	72.26	4.10
	24	679.01	8.41	73.71	4.21
	72	694.32	8.41	69.01	4.03
	144	674.58	8.30	71.12	3.98
	648	651.94	7.36	75.96	3.65
	1000	623.89	7.72	75.11	3.62