Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary information

Design and Synthesis of Multifaceted Rhodanine Linked Thiophene as SnO_x–Perovskite Dual Interface Modifier Facilitating Enhanced Device Performance Through Improved Fermi Level Alignment, Defect Passivation and Reduced Energy Loss

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Supplementary Figures

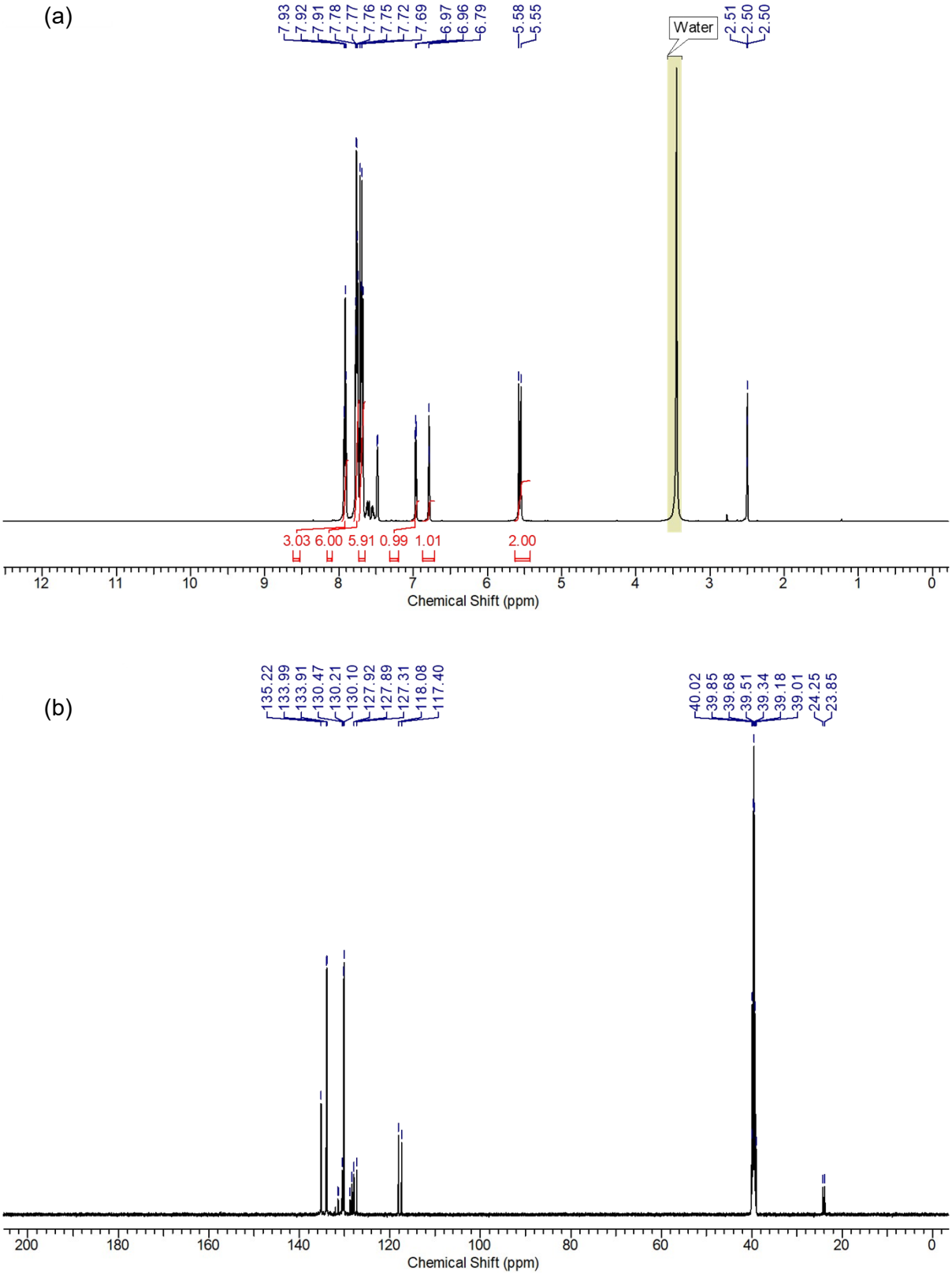


Fig. S1 (a) ^{1}H-NMR data of the compound **2** and (b) ^{13}C-NMR data of the compound **2.**

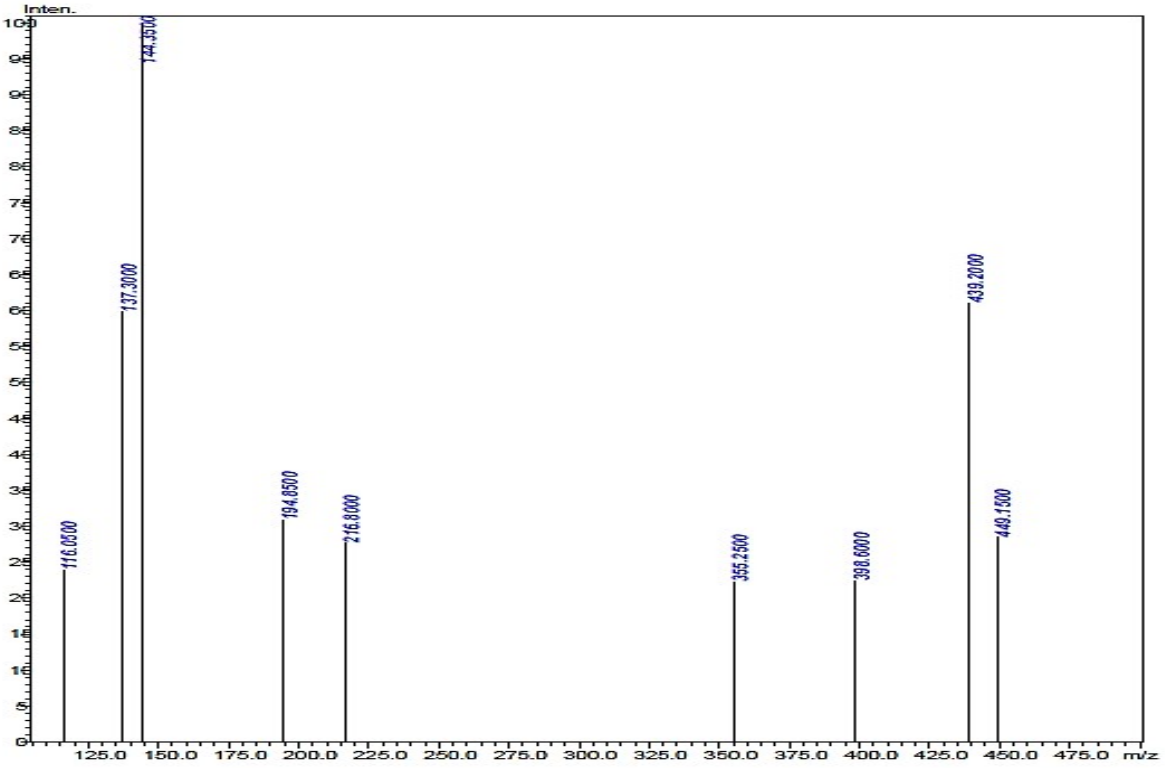


Fig. S2 HPLC-MS data of the compound **2.**

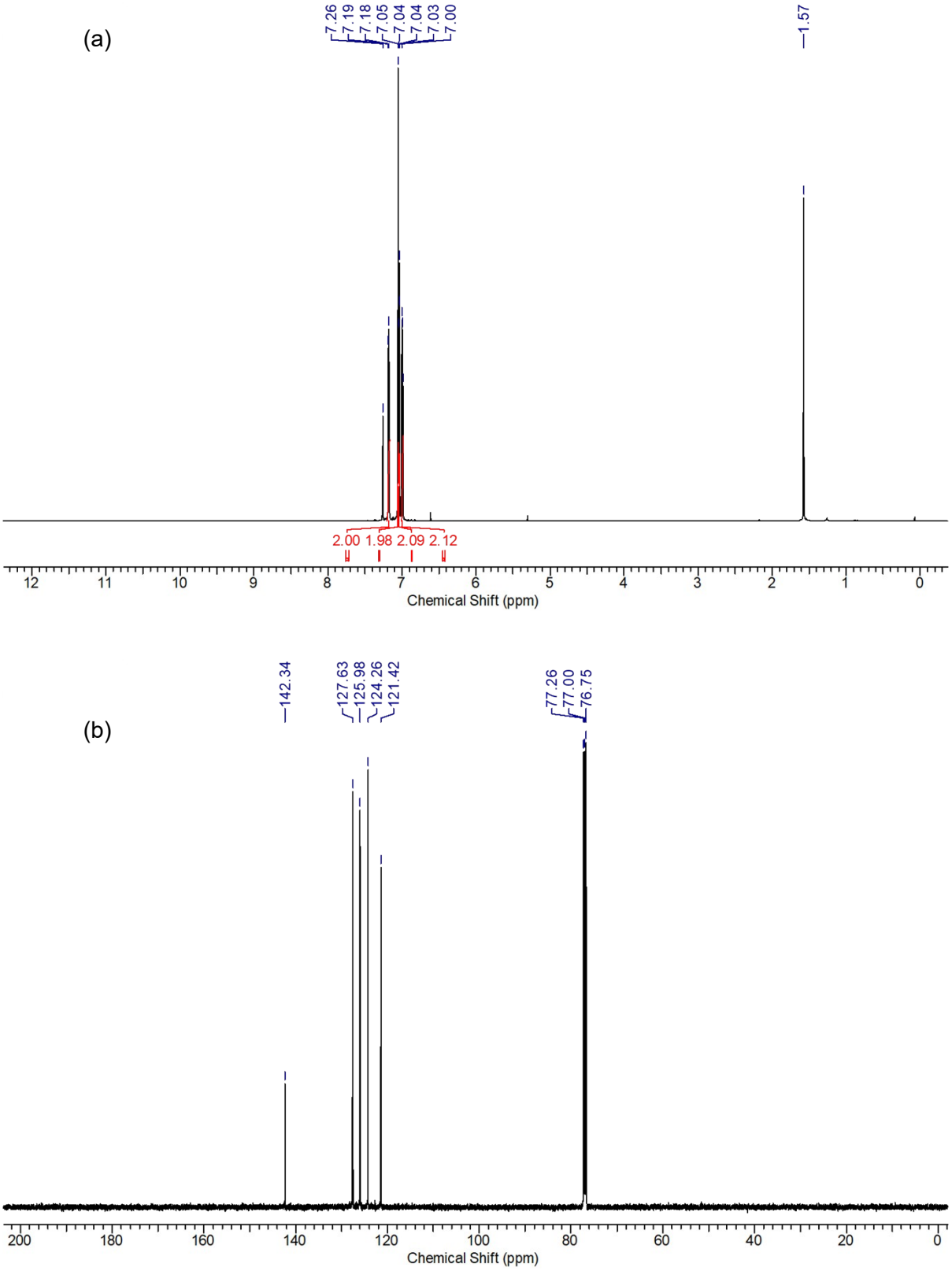


Fig. S3 (a) ^{1}H-NMR data of the compound **3** and (b) ^{13}C-NMR data of the compound **3**.

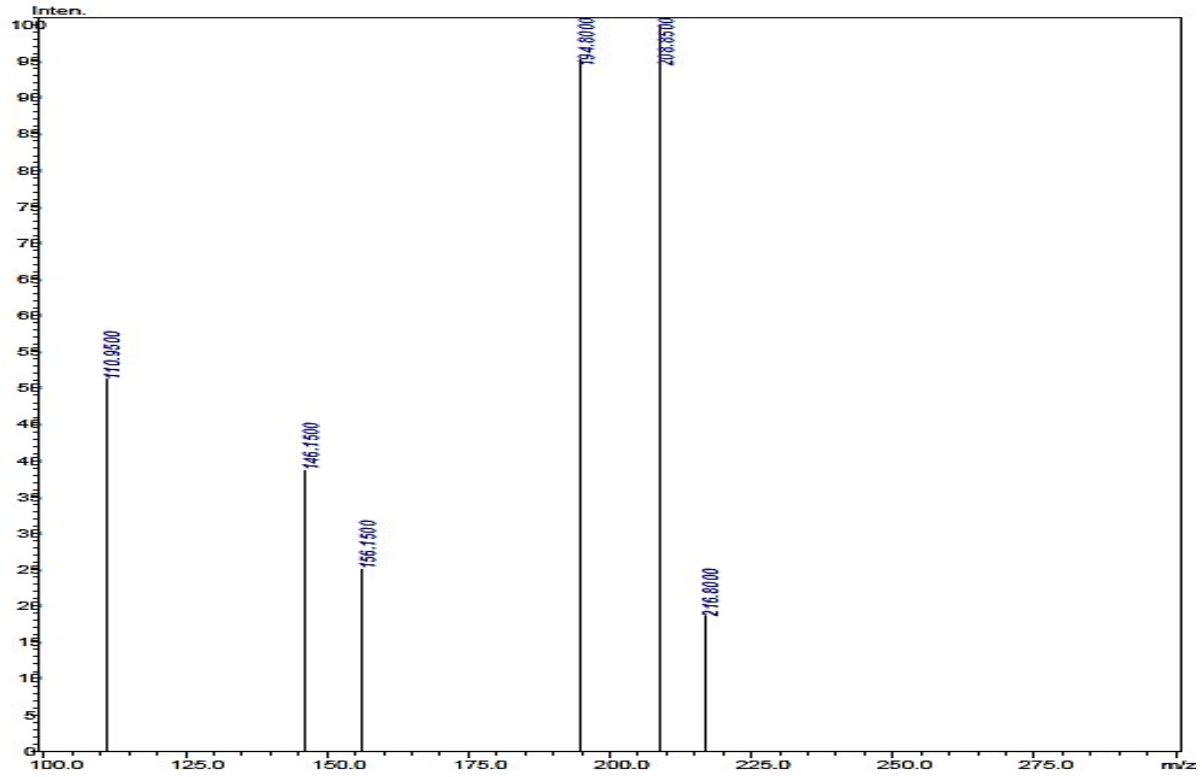


Fig. S4 HPLC-MS data of the compound **3**.

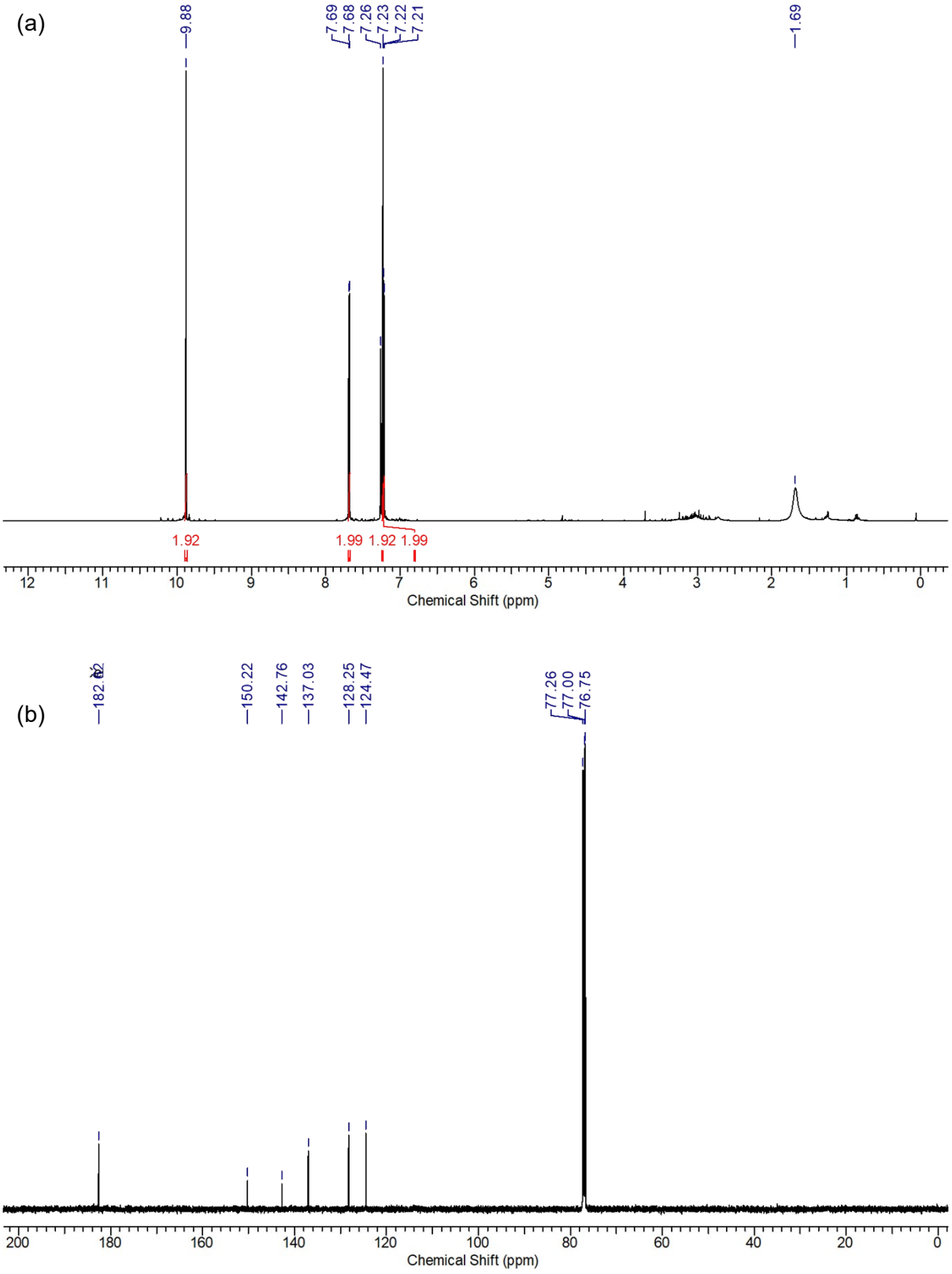


Fig. S5 (a) ^{1}H-NMR data of the compound **4** and (b) ^{13}C-NMR data of the compound **4**.

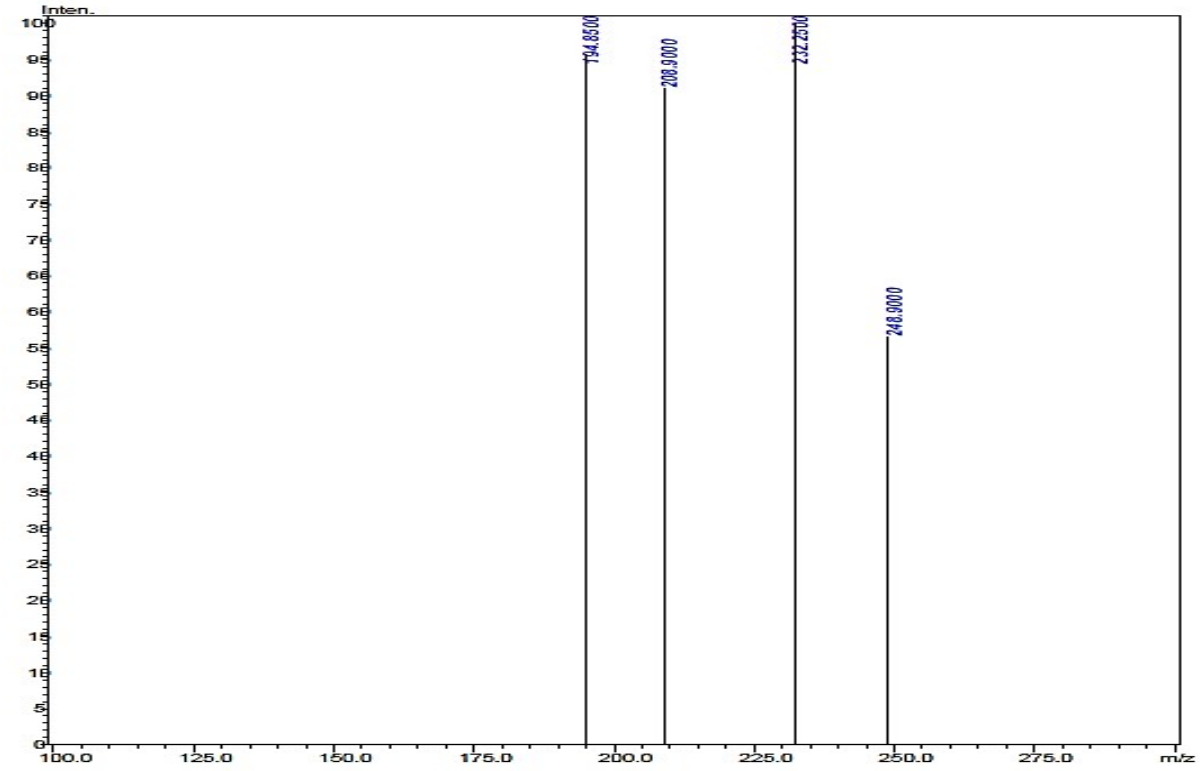


Fig. S6 HPLC-MS data of the compound **4**.

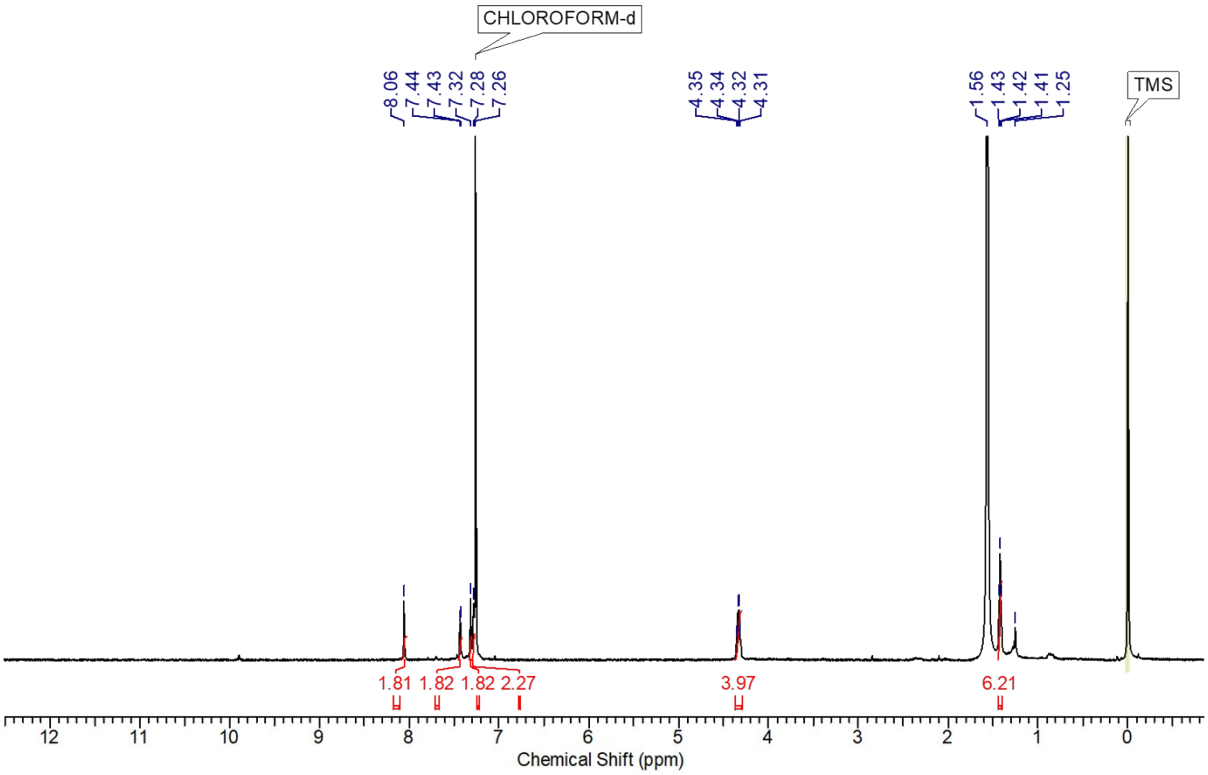


Fig. S7 ^{1}H-NMR data of the compound **AA6**.

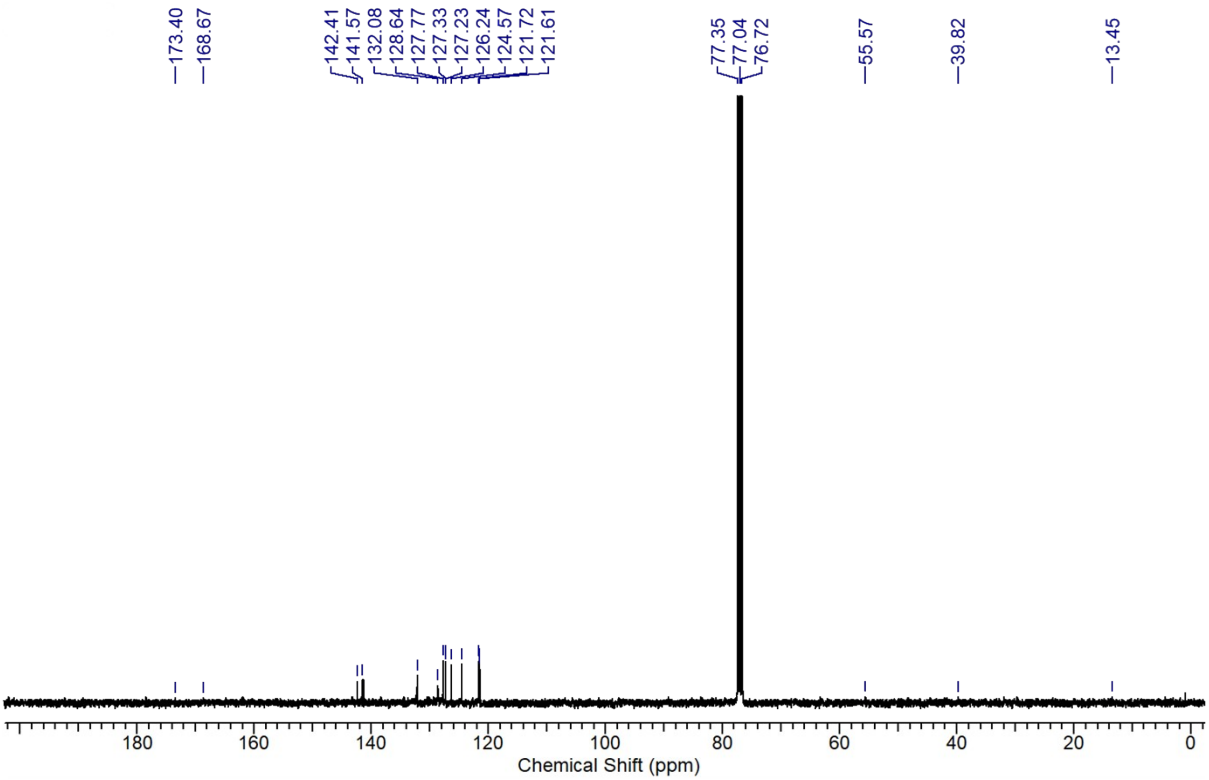


Fig. S8 ^{13}C-NMR data of the compound **AA6.**

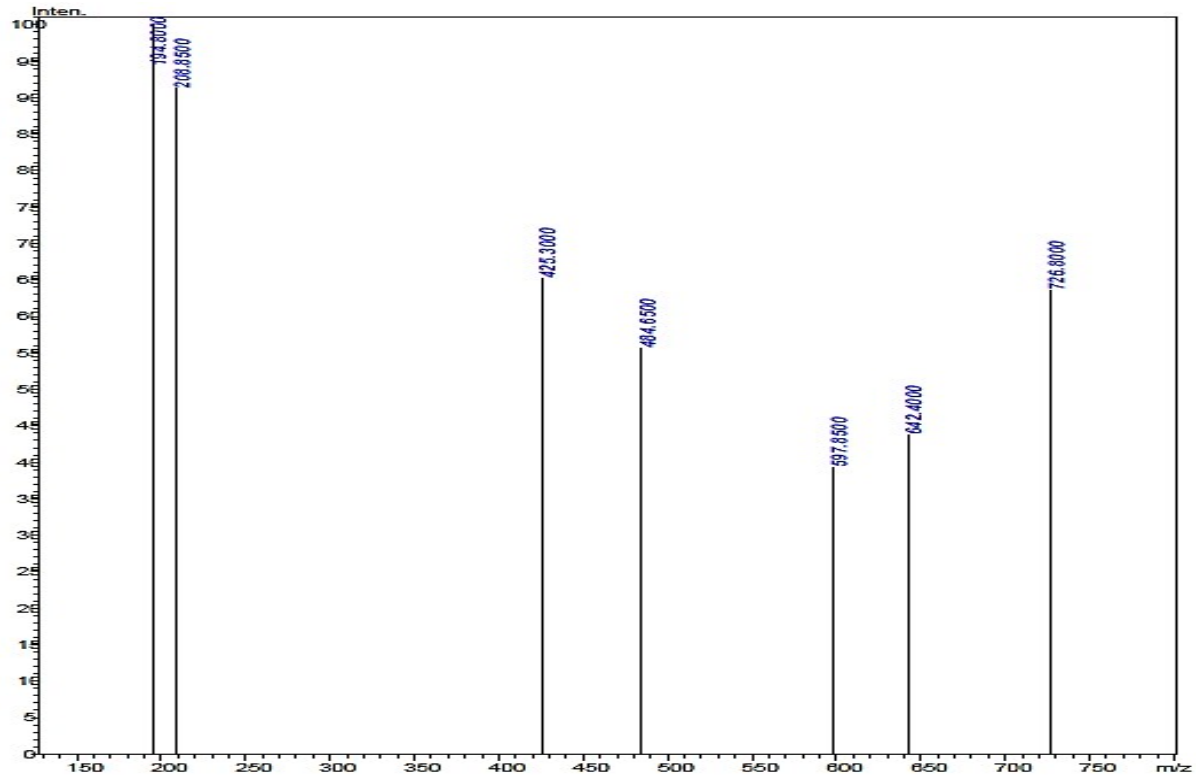


Fig. S9 HPLC-MS data of the compound **AA6.**

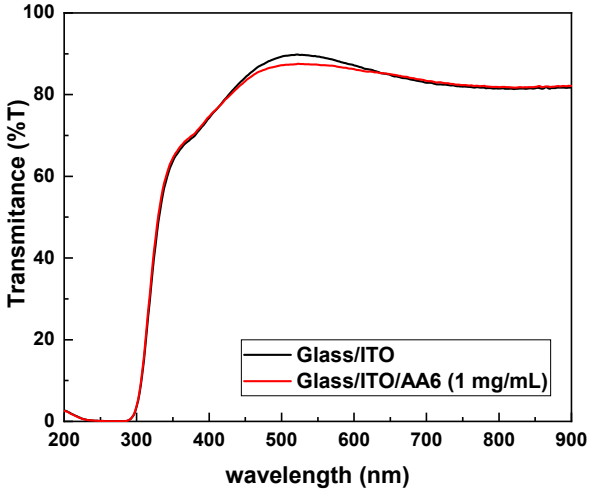


Fig. S10 UV-Vis. %T spectra of AA6 coated on ITO/Glass substrate.

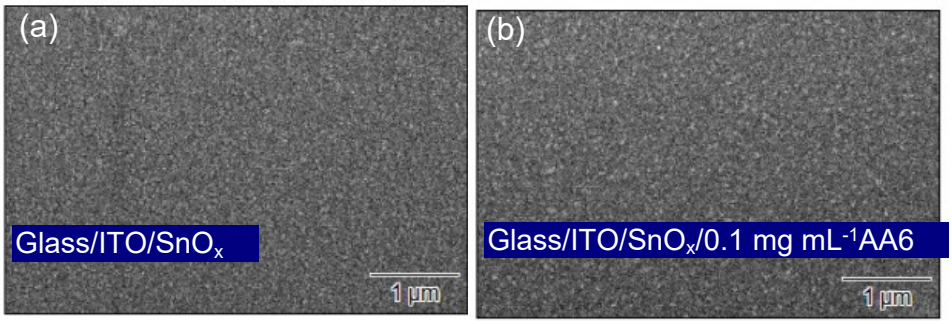


Fig. S11 (a) SEM analysis of SnO_x. (b)AA6 passivated SnO_x thin films.

Table S1 EDX percentage of all possible elements in SnO_x and AA6 passivated SnO_x thin films.

Element	SnO_x	SnO_x/0.05 mg mL^{-1} AA6	SnO_x/ 0.1 mg mL^{-1} AA6	SnO_x/0.2 mg mL^{-1} AA6
	wt. %	wt. %	wt. %	wt. %
C	6.89	6.47	6.94	6.15
N	3.29	2.54	0.61	2.14
O	50.24	49.47	51.69	51.65
S	**0.02**	**0.09**	**0.3**	**0.41**
Sn	39.56	41.45	40.45	39.65
Total	100.00	100.00	100.00	100.00

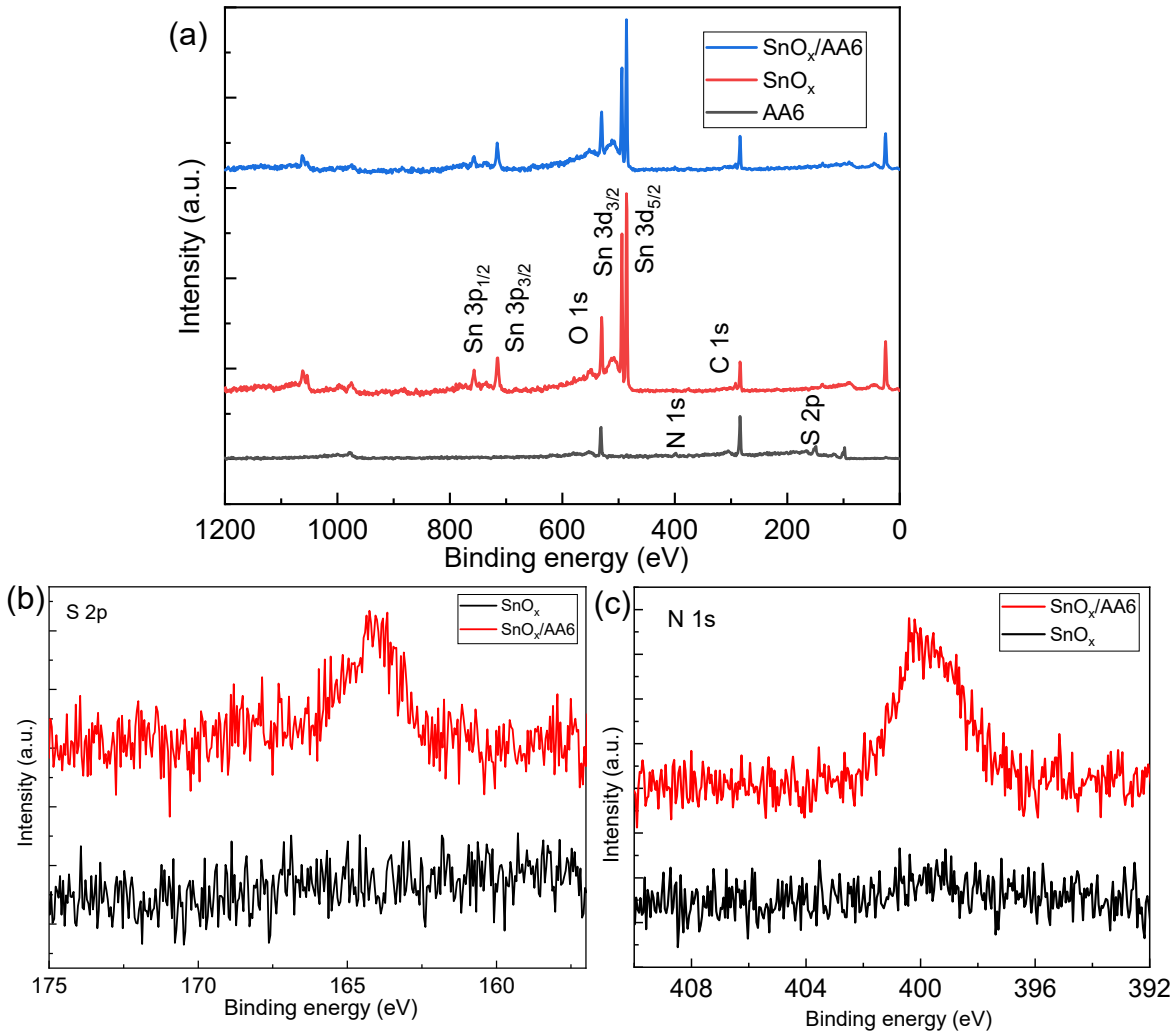


Fig. S12 (a) XPS survey scan of AA6, SnO_x & SnO_x/AA6 thin films. (b) S 2p plots for SnO_x and AA6 passivated SnO_x films. (c) corresponding N1s plot.

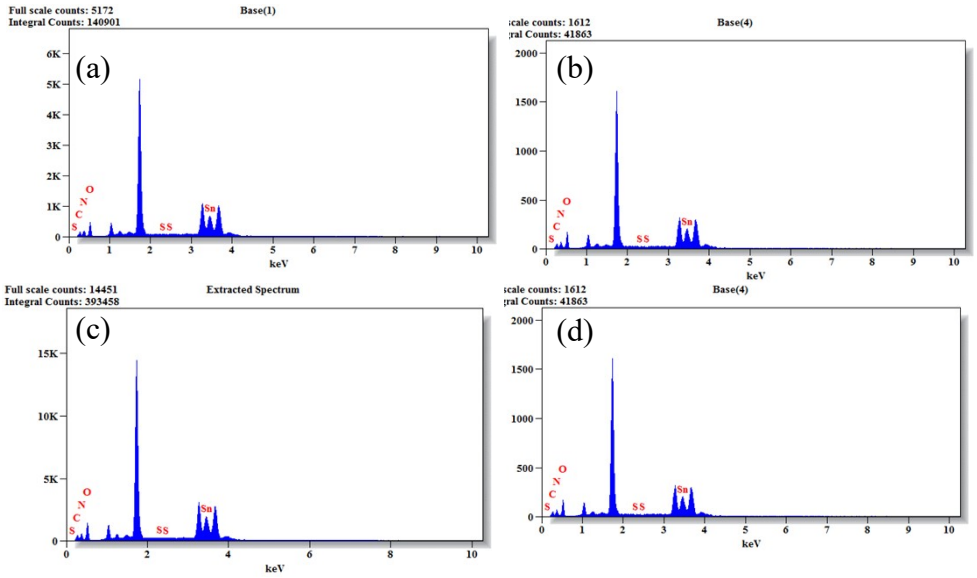


Fig. S13 EDX plot for SnO_x and AA6 passivated SnO_x films as follows. (a) SnO_x. (b) SnO_x/0.05 mg mL^{-1} AA6. (c) SnO_x/0.1 mg mL^{-1} AA6. (d) SnO_x/0.2 mg mL^{-1} AA6.

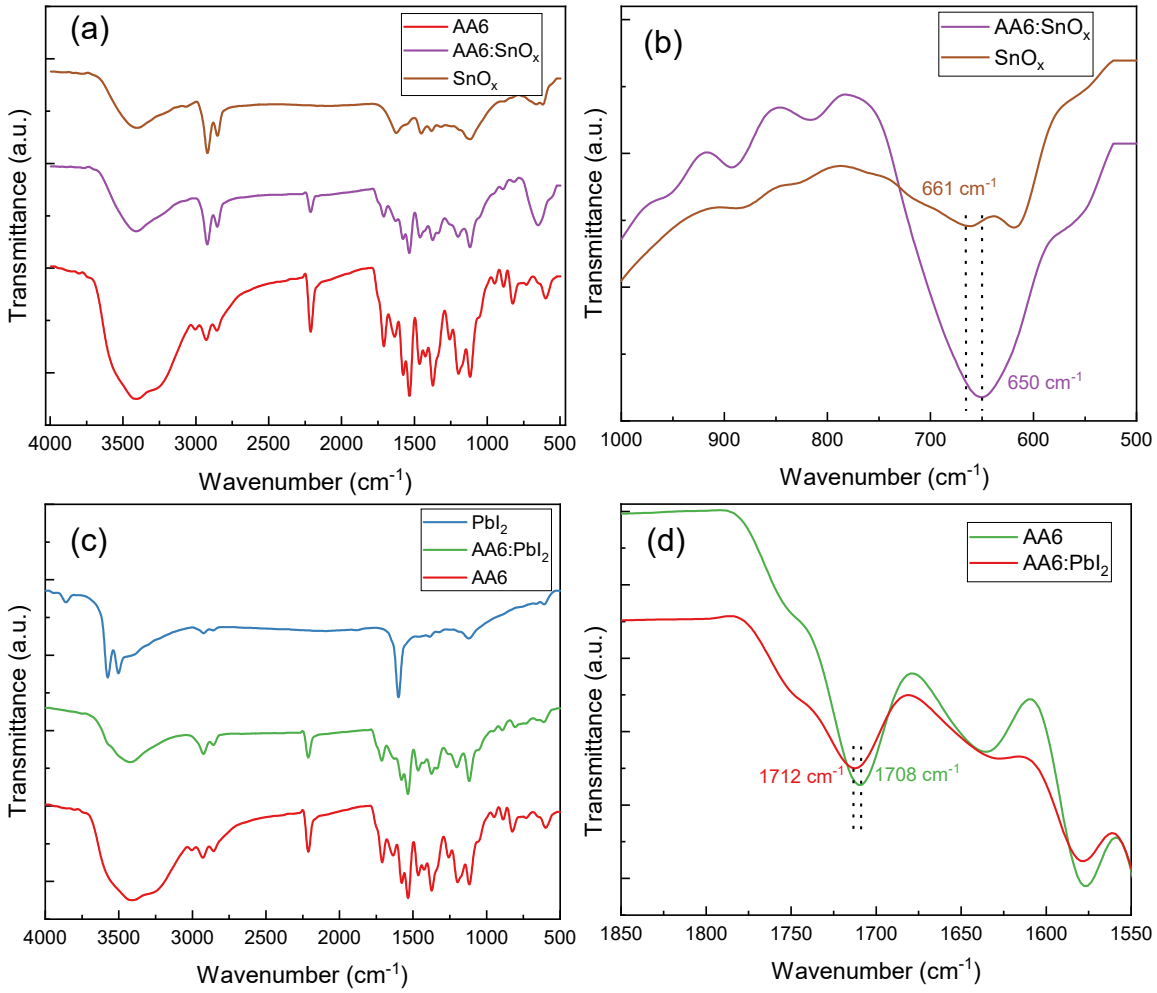


Fig. S14 FTIR spectra of (a) SnO_x, AA6 and SnO_x:AA6 mixed samples. (b) Zoomed view of Sn–O vibration peak. (c) FTIR spectra of PbI_2, AA6 and AA6:PbI_2 mixed samples. (d) Zoomed view of -C=O stretching vibration peak.

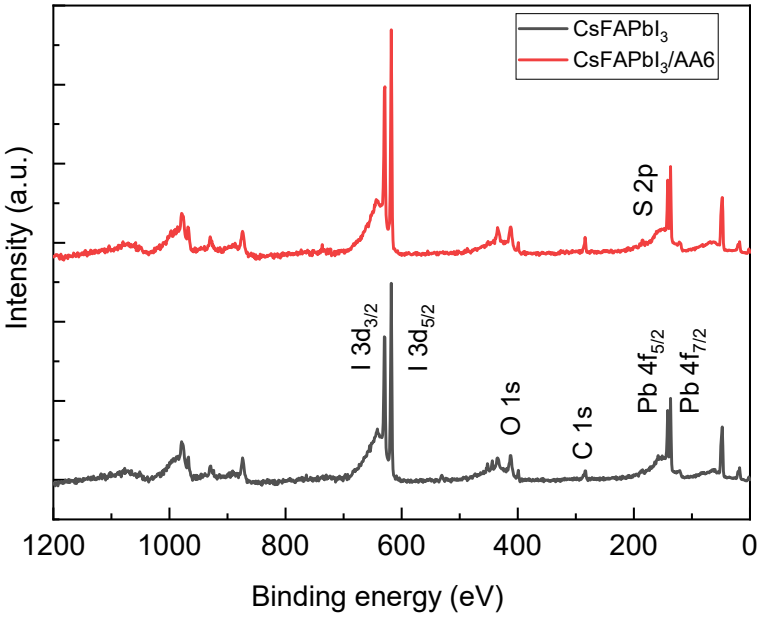


Fig. S15 XPS survey scan of $CsFAPbI_3$ and $CsFAPbI_3$/AA6 thin films.

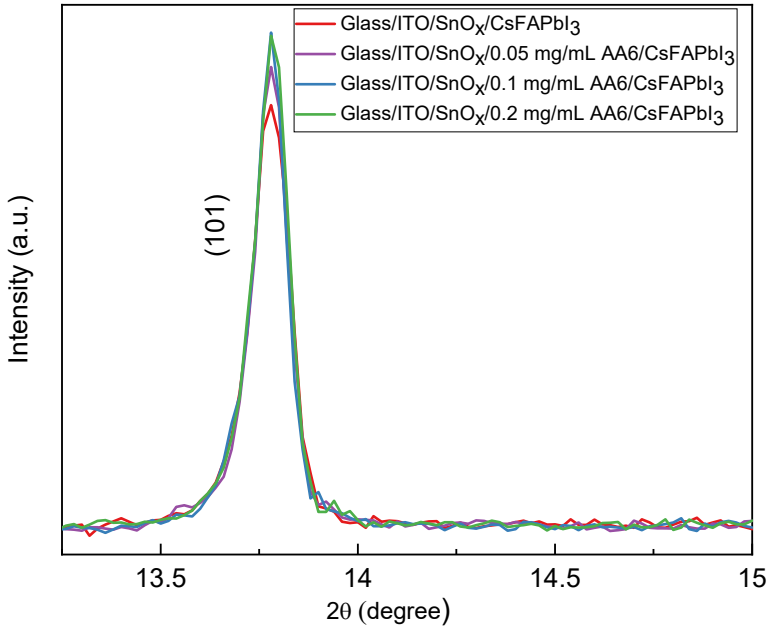


Fig. S16 XRD spectra of $CsFAPbI_3$ (101) plane intensity comparison.

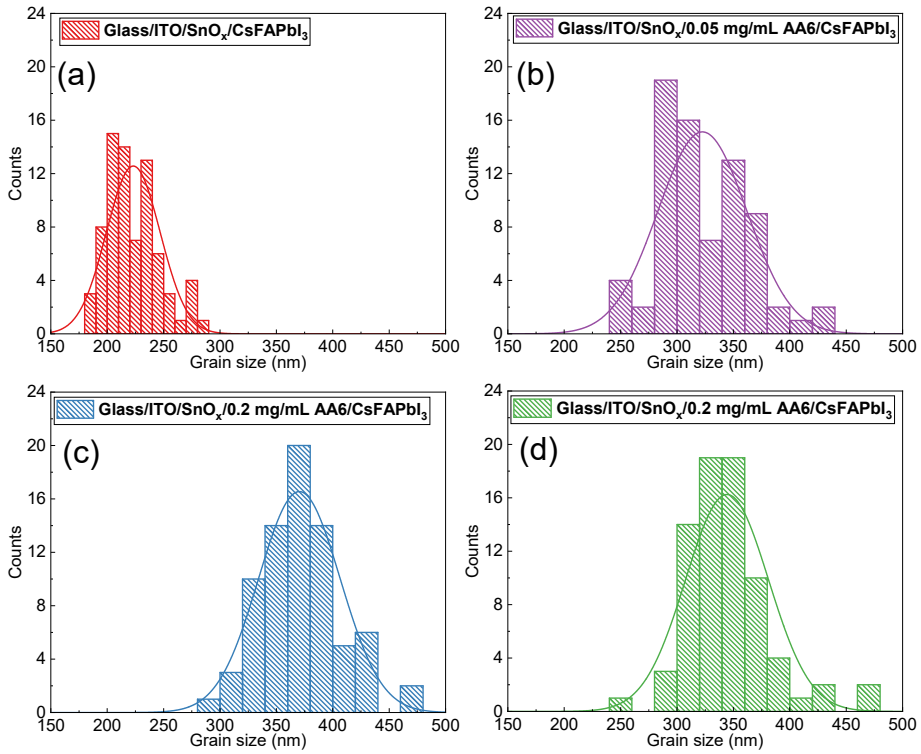


Fig. S17 (a) SEM grain size histogram plots of $CsFAPbI_3$ and (b–d) AA6 passivated $CsFAPbI_3$ films, grain size was calculated from ImageJ software with an average of randomly measured 75 grains.

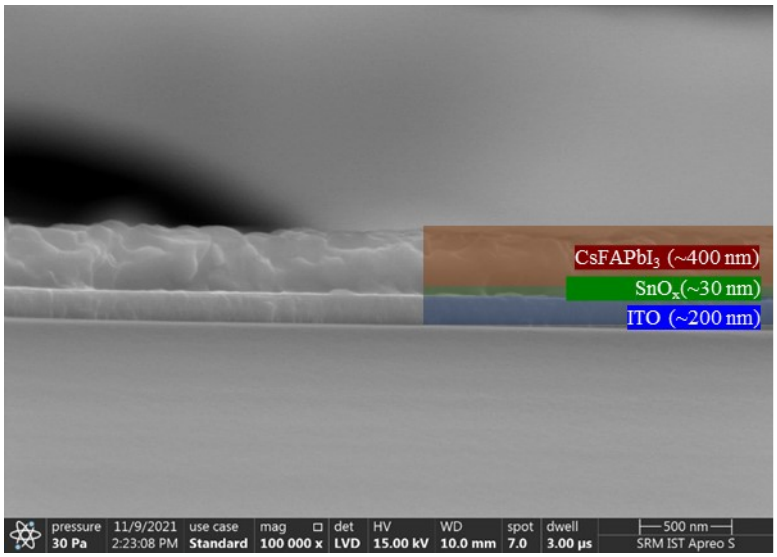


Fig. S18 Cros-section SEM of Glass/ITO/SnO_x/$CsFAPbI_3$.

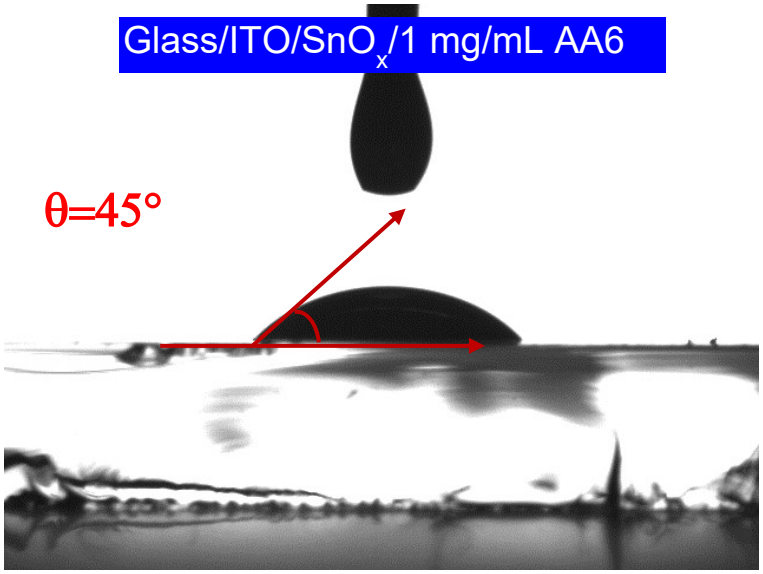


Fig. S19 Perovskite ink-based contact angle measurements for glass/ITO/SnO_x/1 mg mL^{-1} AA6.

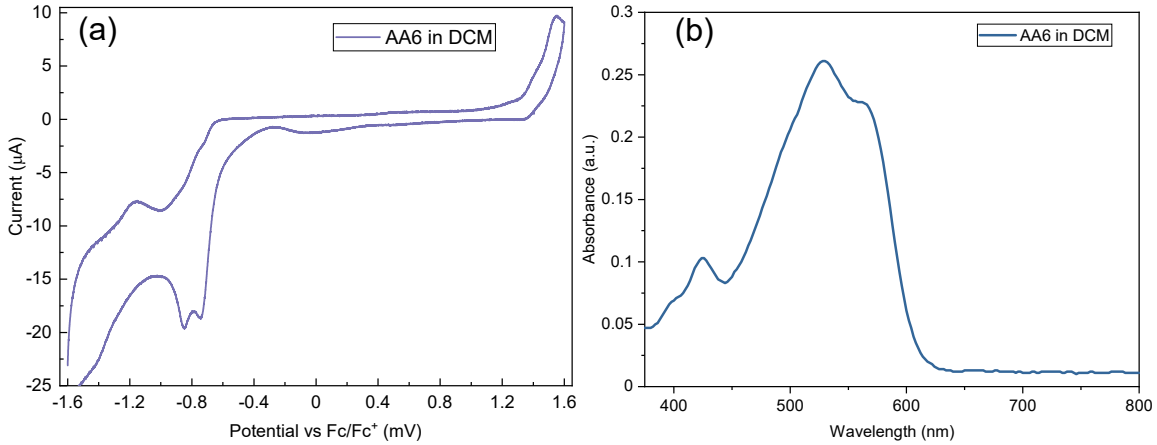


Fig. S20 (a) CV analysis of AA6 molecule (in DCM). (b) UV-Vis. spectra of AA6 molecule (in DCM).

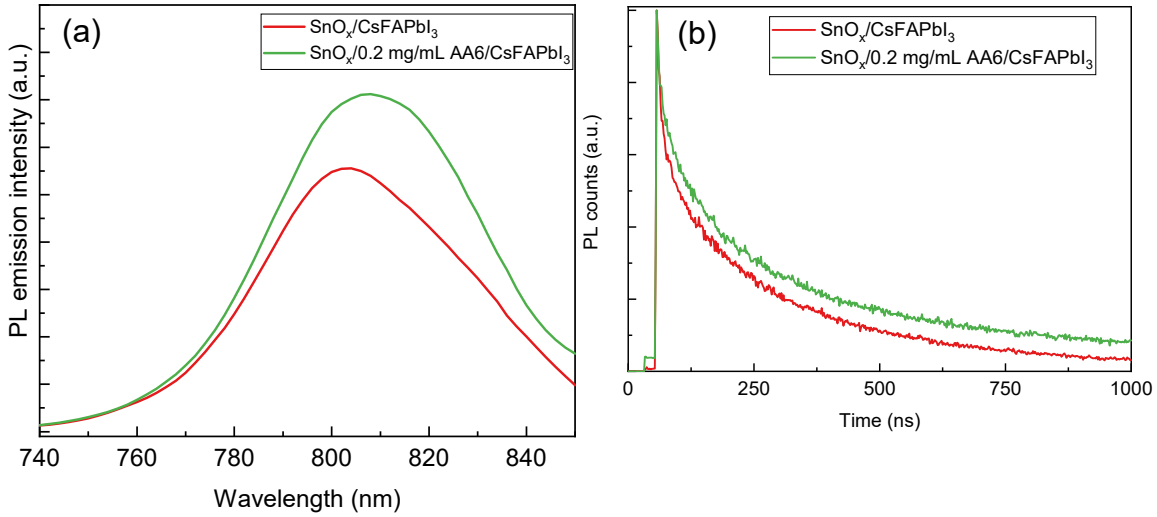
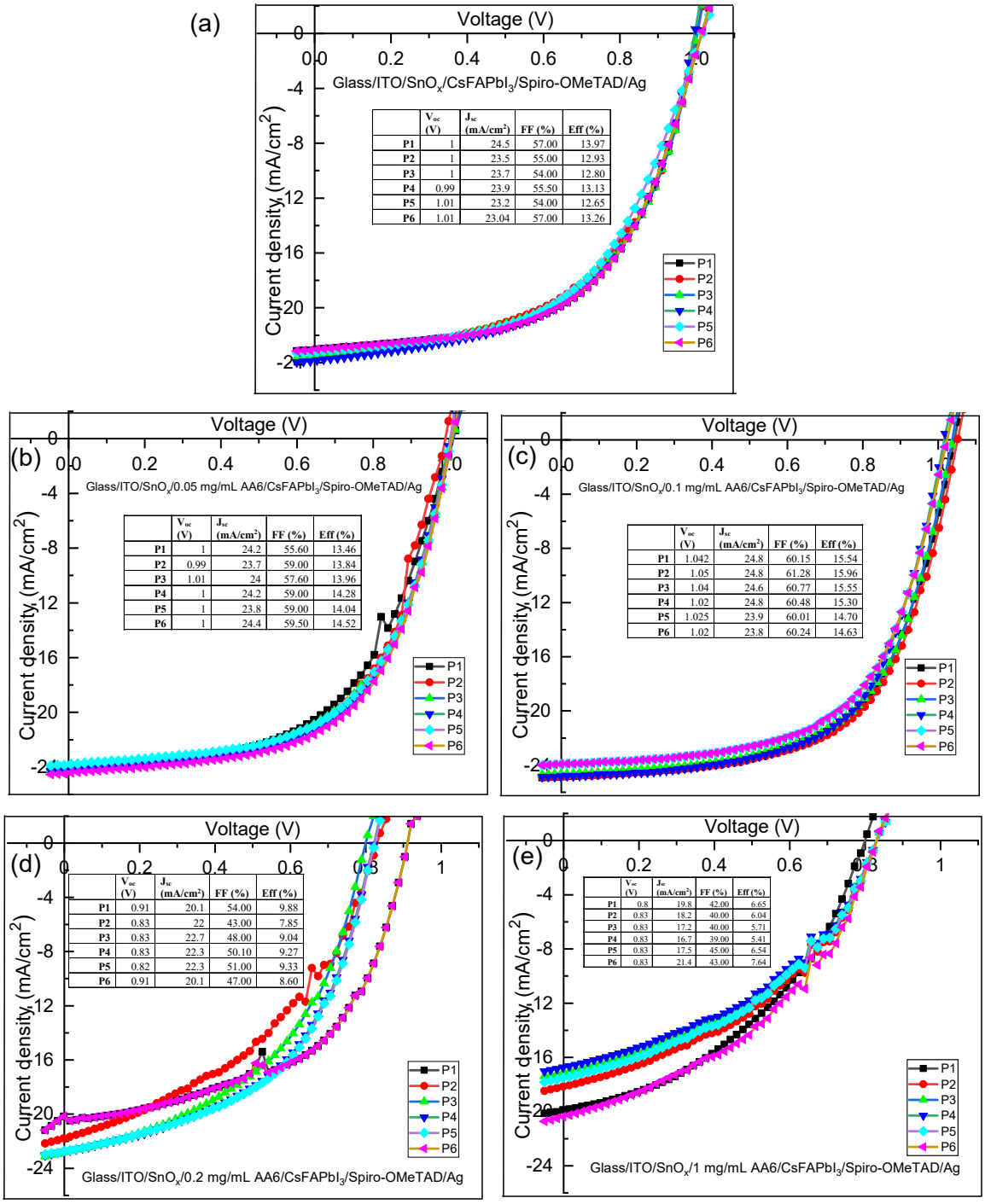


Fig. S21 (a) Steady state PL analysis of $CsFAPbI_3$ coated on SnO_x and 0.2 mg mL^{-1} AA6 passivated SnO_x films. (b) corresponding lifetime analysis.



	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Eff (%)
P1	1	24.5	57.00	13.97
P2	1	23.5	55.00	12.93
P3	1	23.7	54.00	12.80
P4	0.99	23.9	55.50	13.13
P5	1.01	23.2	54.00	12.65
P6	1.01	23.04	57.00	13.26

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Eff (%)
P1	1	24.2	55.60	13.46
P2	0.99	23.7	59.00	13.84
P3	1.01	24	57.60	13.96
P4	1	24.2	59.00	14.28
P5	1	23.8	59.00	14.04
P6	1	24.4	59.50	14.52

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Eff (%)
P1	1.042	24.8	60.15	15.54
P2	1.05	24.8	61.28	15.96
P3	1.04	24.6	60.77	15.55
P4	1.02	24.8	60.48	15.30
P5	1.025	23.9	60.01	14.70
P6	1.02	23.8	60.24	14.63

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Eff (%)
P1	0.91	20.1	54.00	9.88
P2	0.83	22	43.00	7.85
P3	0.83	22.7	48.00	9.04
P4	0.83	22.3	50.10	9.27
P5	0.82	22.3	51.00	9.33
P6	0.91	20.1	47.00	8.60

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Eff (%)
P1	0.8	19.8	42.00	6.65
P2	0.83	18.2	40.00	6.04
P3	0.83	17.2	40.00	5.71
P4	0.83	16.7	39.00	5.41
P5	0.83	17.5	45.00	6.54
P6	0.83	21.4	43.00	7.64

Fig. S22 Representative J-V plots of AA6 passivated PSC. (a) bare SnO_x. (b) SnO_x/0.05 mg mL^{-1} AA6. (c) SnO_x/0.1 mg mL^{-1} AA6. (d) SnO_x/0.2 mg mL^{-1} AA6 and (e) SnO_x/1 mg mL^{-1} AA6.

Table S2 Sn $3d_{5/2}$ peak fitting parameters of SnO_x & SnO_x/AA6.

	SnO_x	SnO_x/AA6
Sn^{4+} peak [eV]	486.6	486.5
Sn^{2+} peak [eV]	487.1	487
Sn^{0} peak [eV]	485.8	485.4
Sn^{4+} peak area	49819	36077
Sn^{2+} peak area	13706	7256
Sn^{0} peak area	5333	1899
Sn^{4+} FWHM	1.18	1.22
Sn^{2+} FWHM	1.74	1.81
Sn^{0} FWHM	2	1.56
Sn^{4+} percentage	72	80
Sn^{2+} percentage	20	16
Sn^{0} percentage	8	4

Table S3 O 1s peak fitting parameters of SnO_x & SnO_x/AA6.

	SnO_x	SnO_x/AA6
Lattice oxygen peak [eV]	530.7	530.7
Amorphous oxygen peak [eV]	532.1	532.1
Sn-O-S or Sn-O-N peak [eV]	-	532
Lattice oxygen peak area	13153	9202
Amorphous oxygen peak area	6735	3639
Sn-O-S or Sn-O-N peak area	-	913
Lattice oxygen FWHM	1.45	1.44
Amorphous oxygen FWHM	1.54	1.9
Sn-O-S or Sn-O-N FWHM	-	0.98
Lattice oxygen percentage	66	67
Amorphous oxygen percentage	33	26
Sn-O-S or Sn-O-N percentage	-	7

Table S4 TRPL lifetime parameters of $CsFAPbI_3$ on SnO_x and AA6 passivated SnO_x.

Samples	τ_1 (ns)	I1 (%)	τ_2 (ns)	I2 (%)	τ_{avg} (ns)
Glass/ITO/SnO_x/$CsFAPbI_3$	65	8	305	92	301
Glass/ITO/SnO_x/0.05 mg mL^{-1} AA6/$CsFAPbI_3$	60	9	260	91	256
Glass/ITO/SnO_x/0.1 mg mL^{-1} AA6/$CsFAPbI_3$	25	6	180	94	179
Glass/ITO/SnO_x/0.2 mg mL^{-1} AA6/$CsFAPbI_3$	56	6	310	94	304

* Where τ_1 and τ_2 indicate fast decay and slow decay lifetime component of perovskite absorber, I_1 and I_2 refer to corresponding amplitude and τ_{avg} represents average PL lifetime.