Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Tuning of energy levels, transport properties and device performance of naphthalenediimide derivatives by introduction of Michael addition reaction

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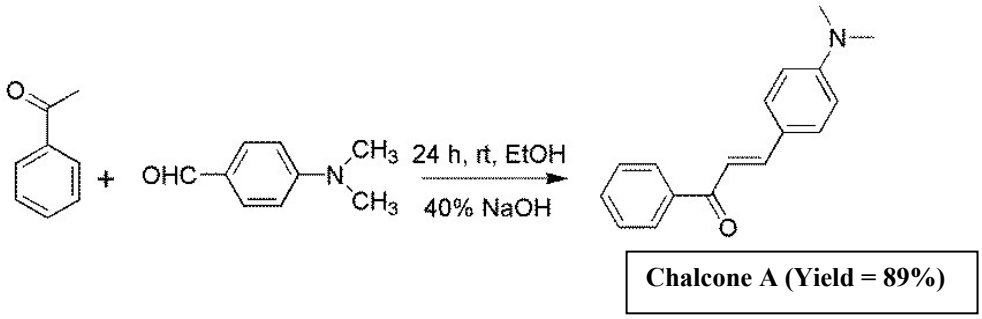

Figure S1(a). General synthesis scheme of chalcone A.

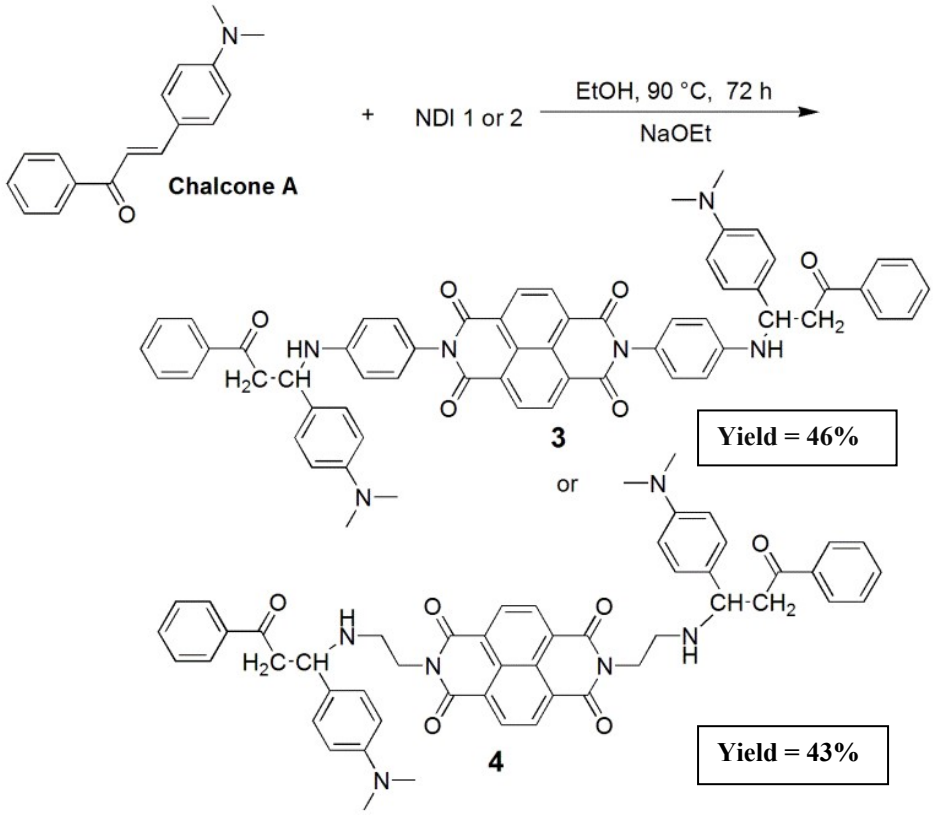

Figure S1(b). Synthesis scheme of Michael addition products **3** and **4** from 0.022 mM chalcone A and 0.022mM NDI in the presence of EtOH with NaOEt as catalyst.

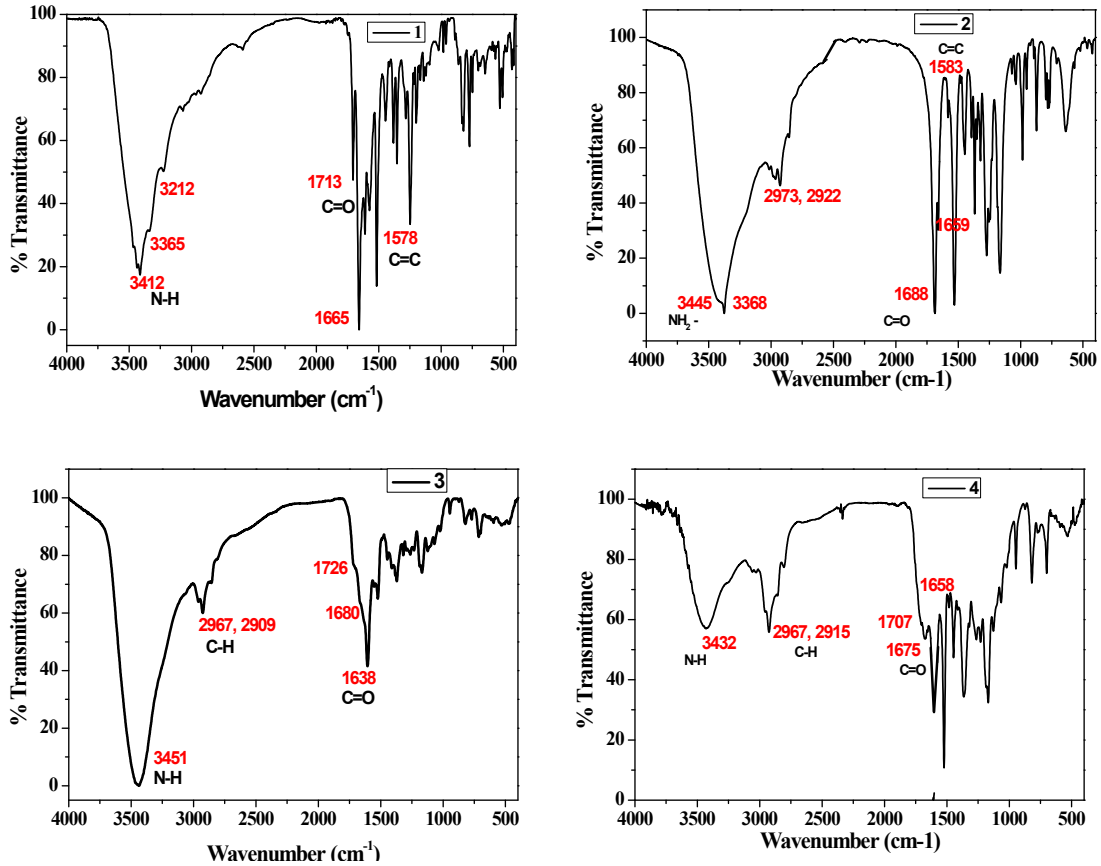

Figure S2(a). FTIR spectra of products **1**, **2**, **3** and **4**.

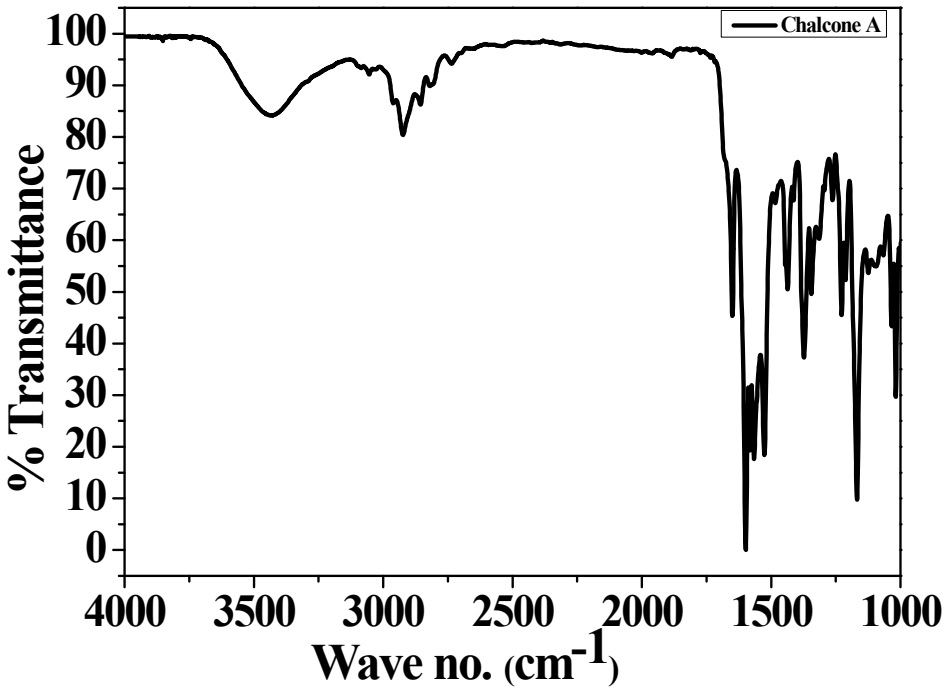

Figure S**2 (b)**. FTIR spectrum of chalcone A

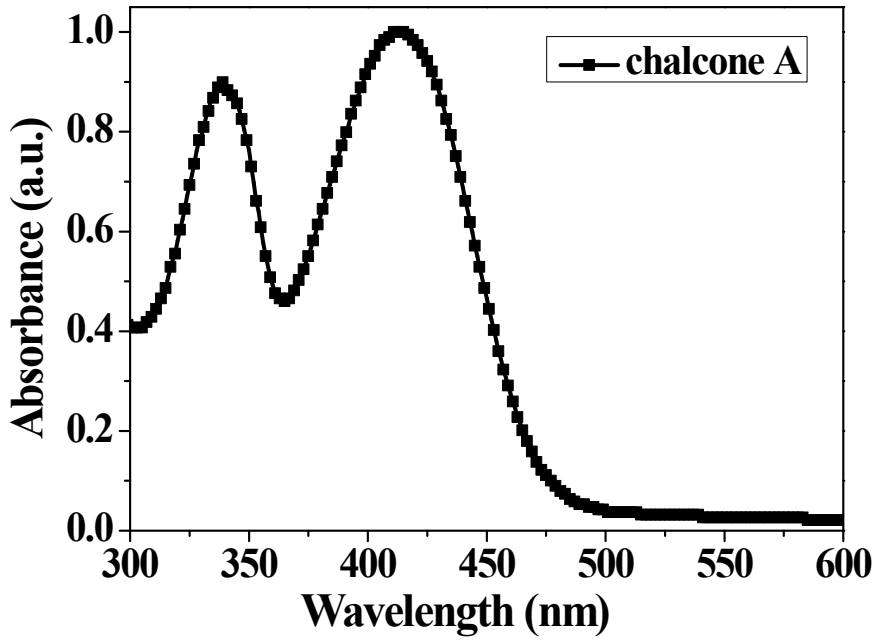

Figure S3. UV-Visible absorption spectrum of chalcone **A**

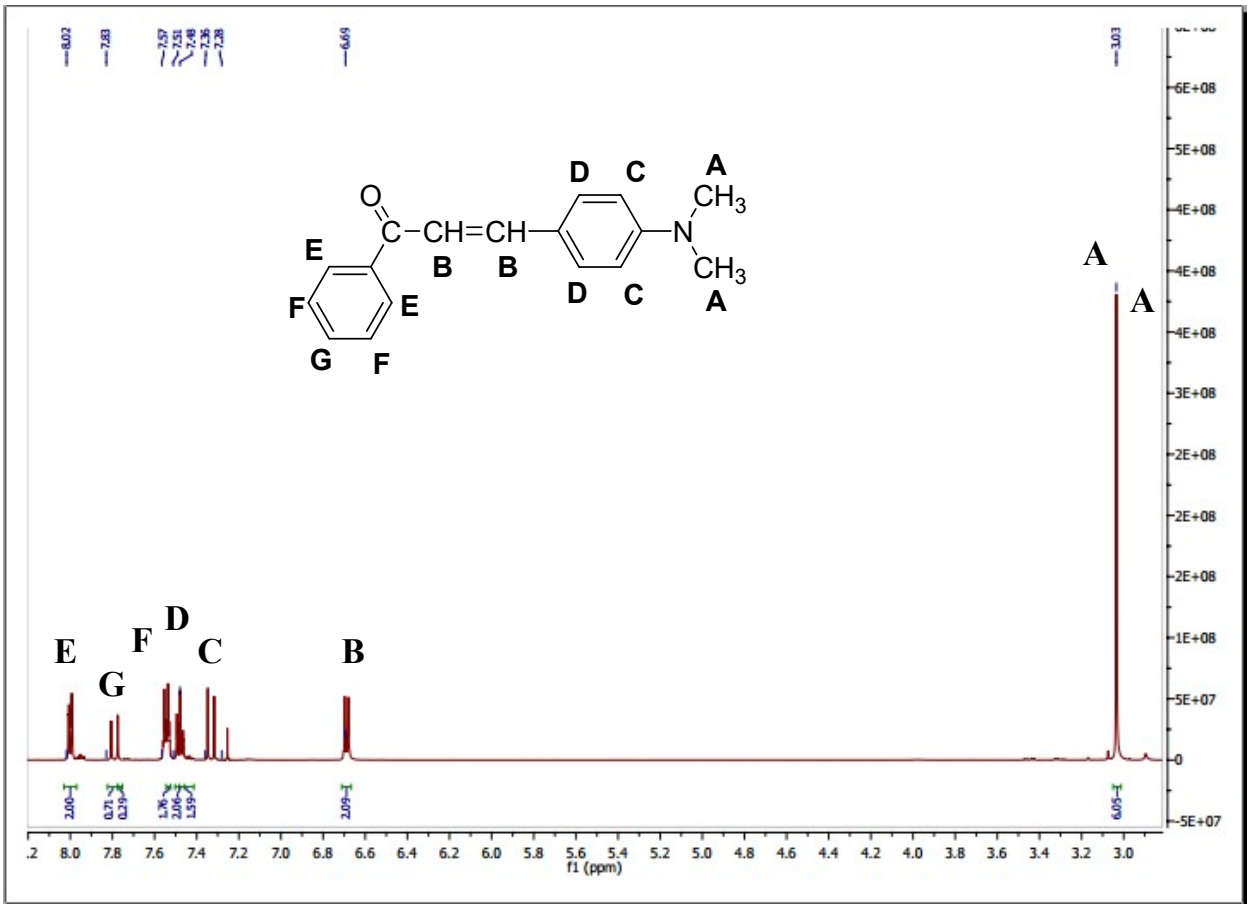

Figure S4. ^{1}H NMR spectrum of chalcone **A**

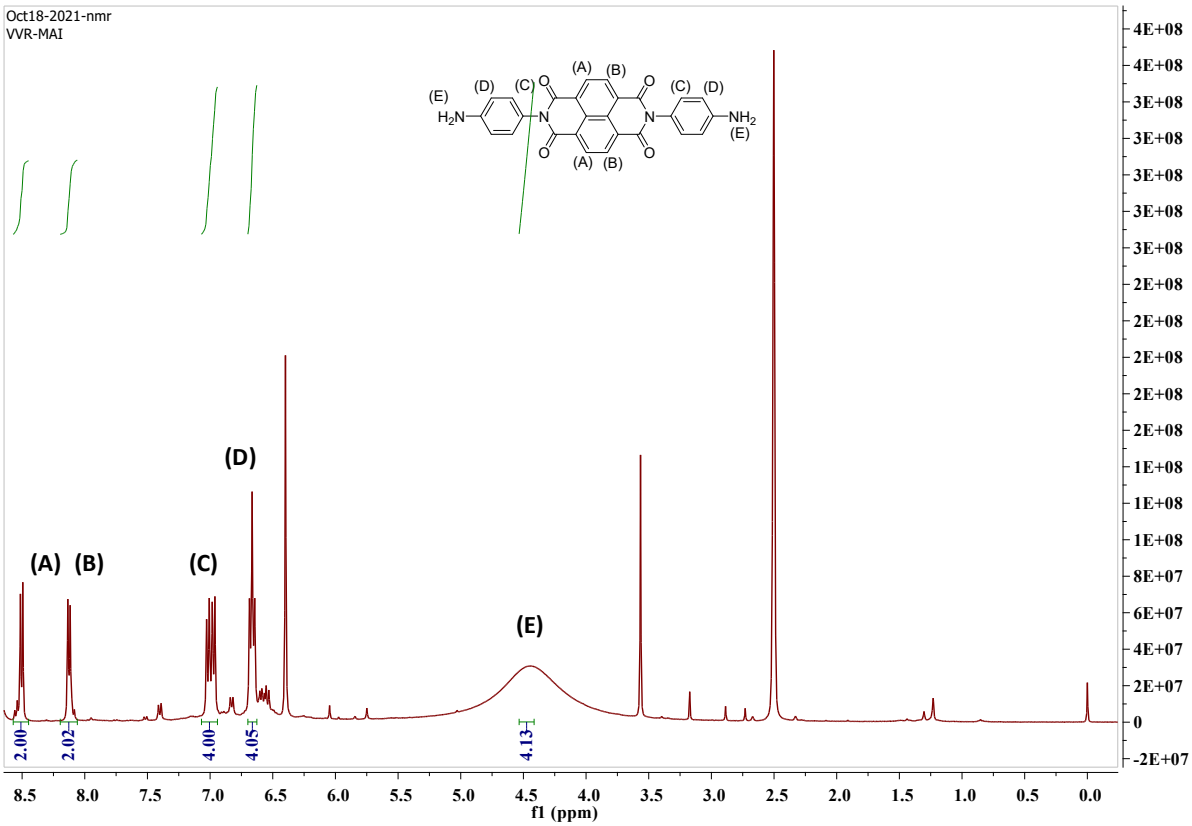

Figure S5. ^{1}H NMR spectrum of **1**

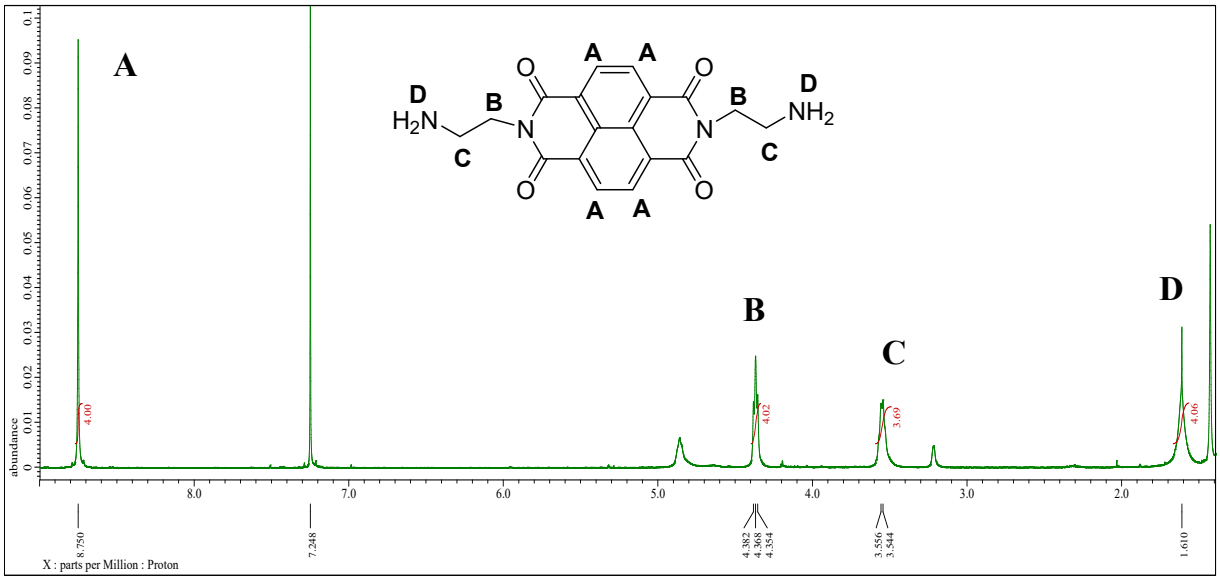

Figure S6. ^{1}H NMR spectrum of **2**

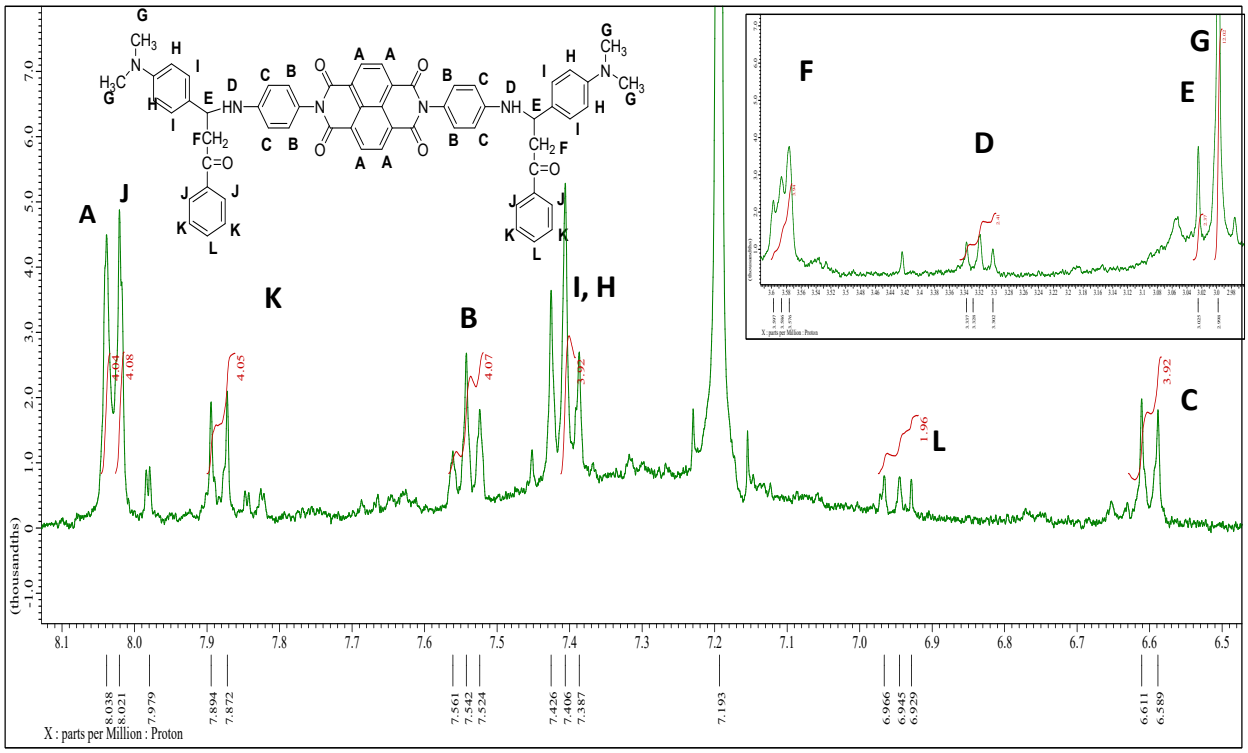

Figure S7. [1]H NMR spectrum of product **3**

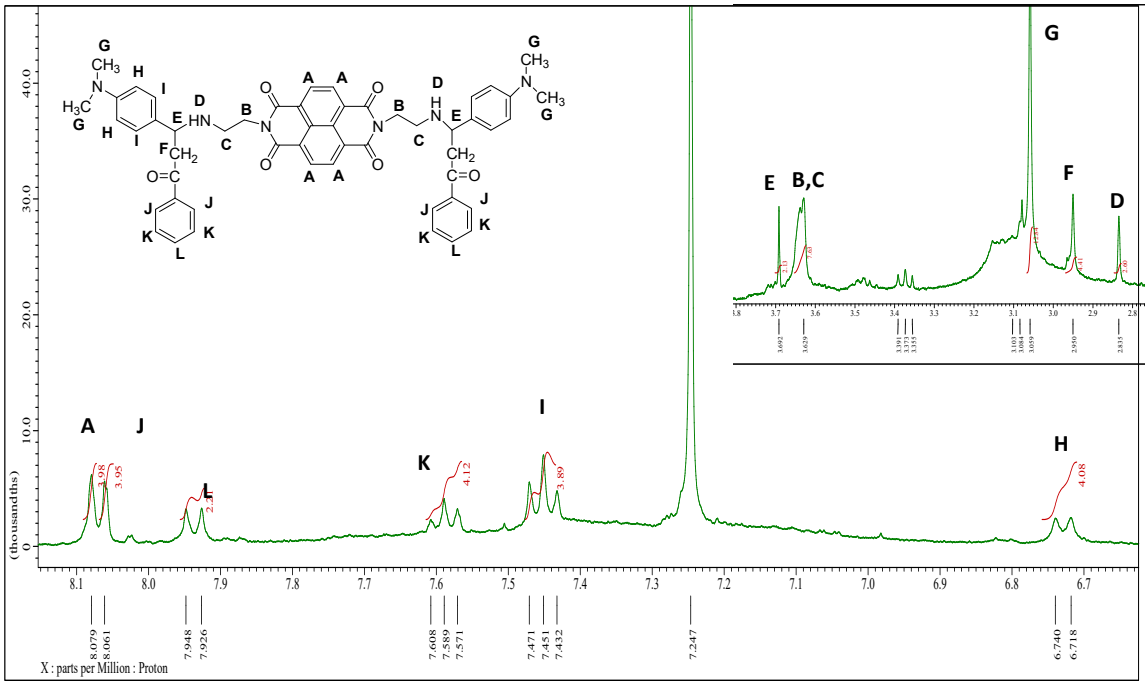

Figure S8. 1 H NMR spectrum of product 4

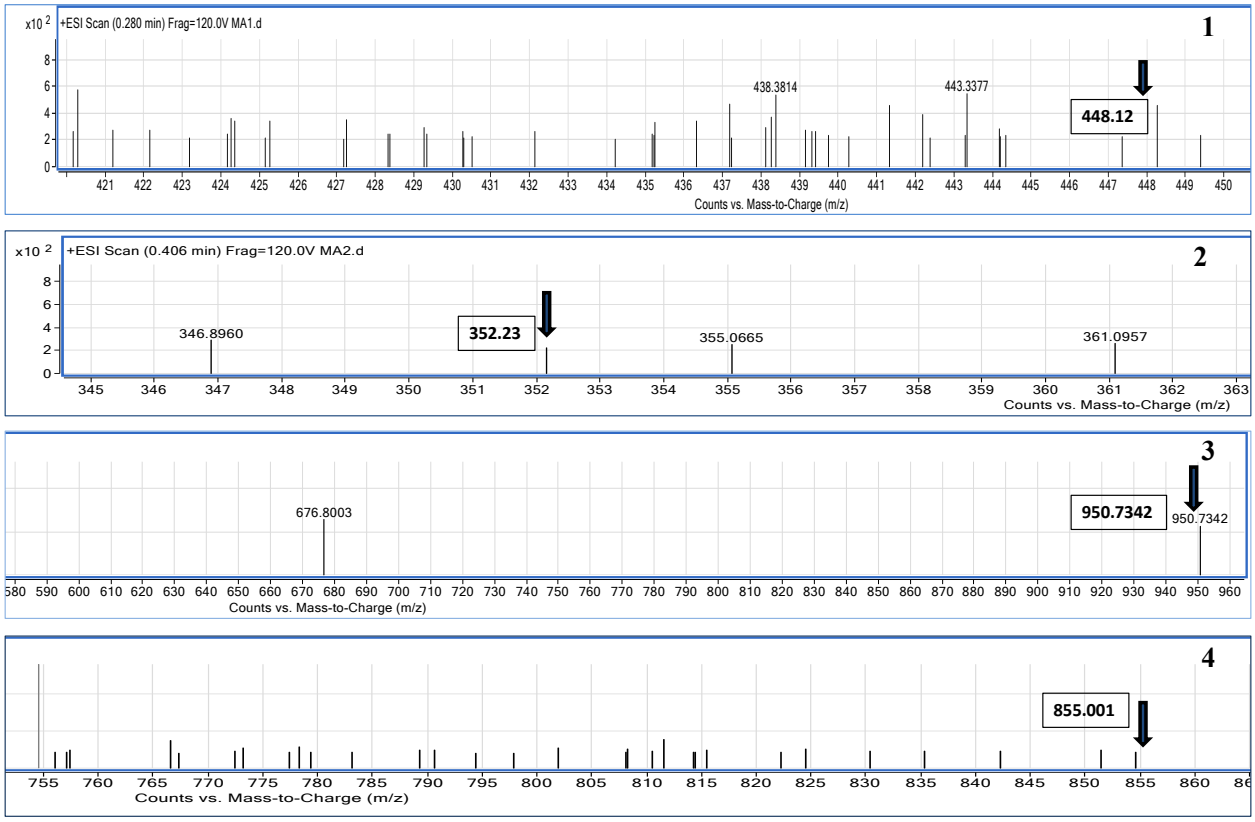

Figure S9. Mass spectrum analysis of products **1, 2, 3** and **4**.

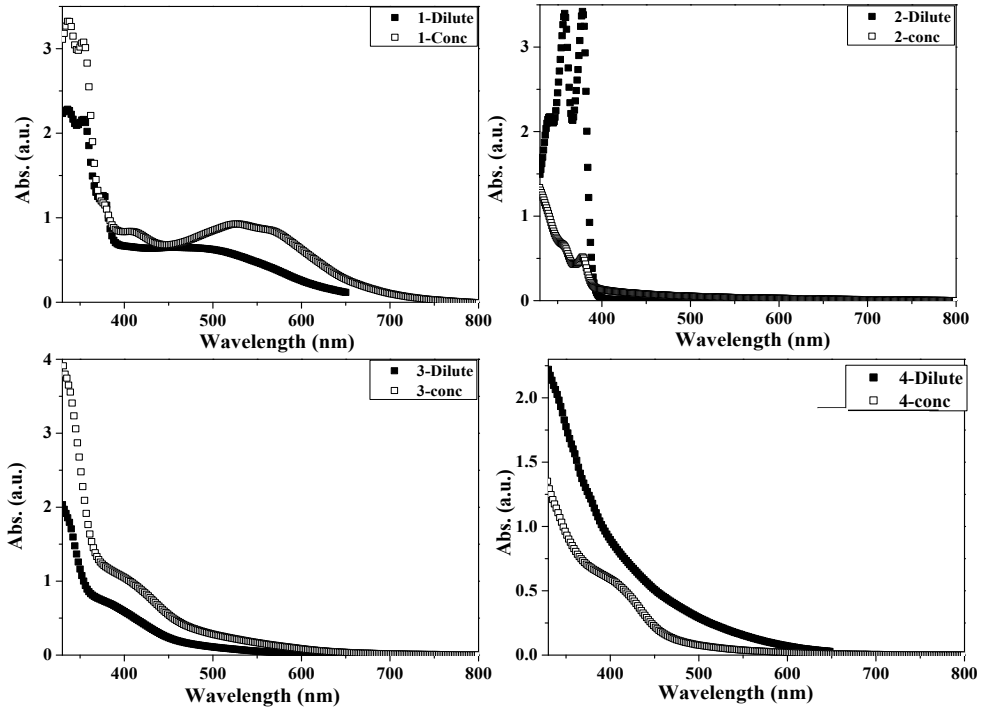

Figure S10. Comparative absorption spectra of the products **1, 2, 3** and **4** in THF for dilute (1 µM) and concentrated (1mM) solutions.

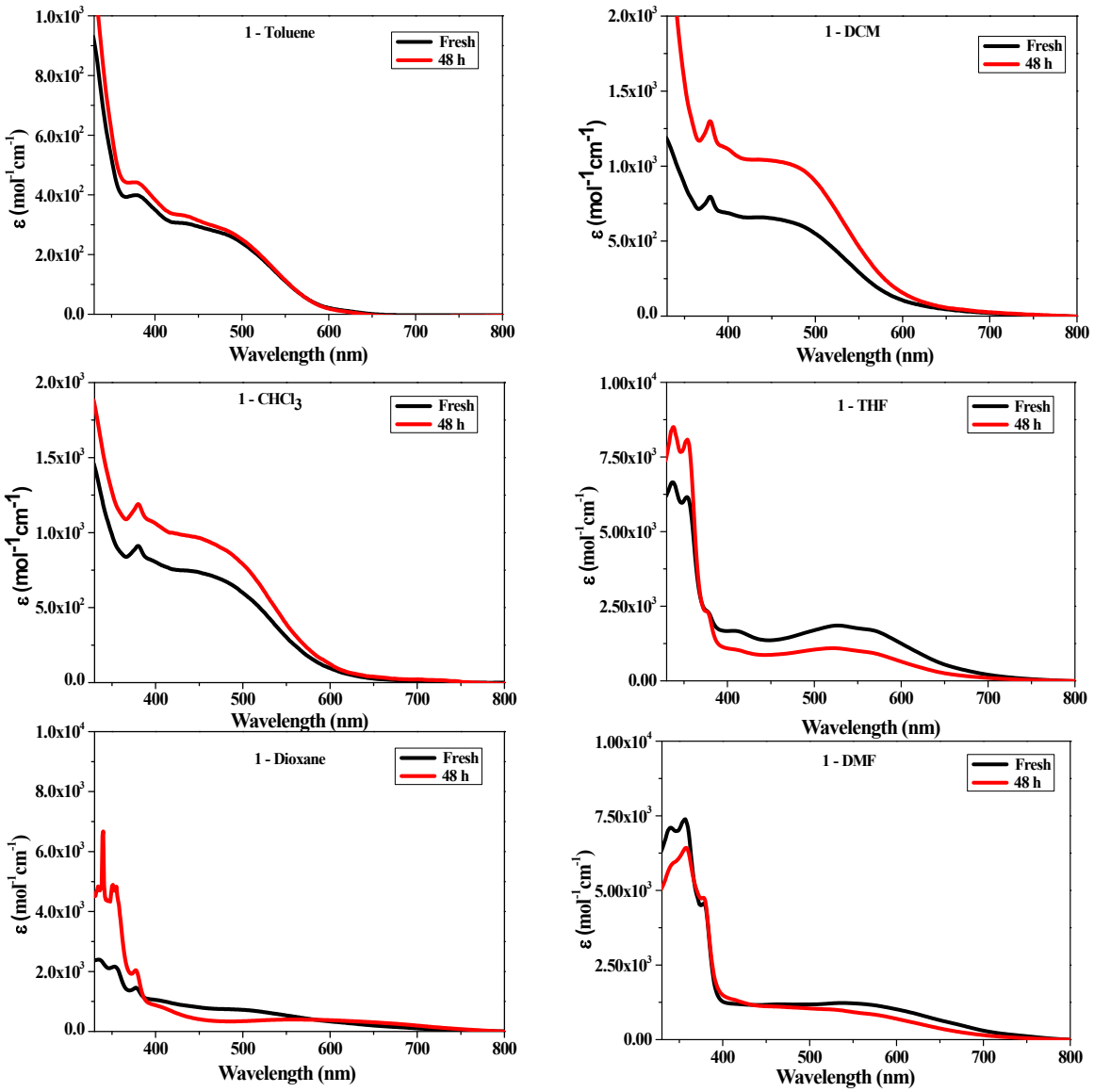

Figure S11. UV-Vis absorption of **1** (fresh and 48 h aged) in different solvents

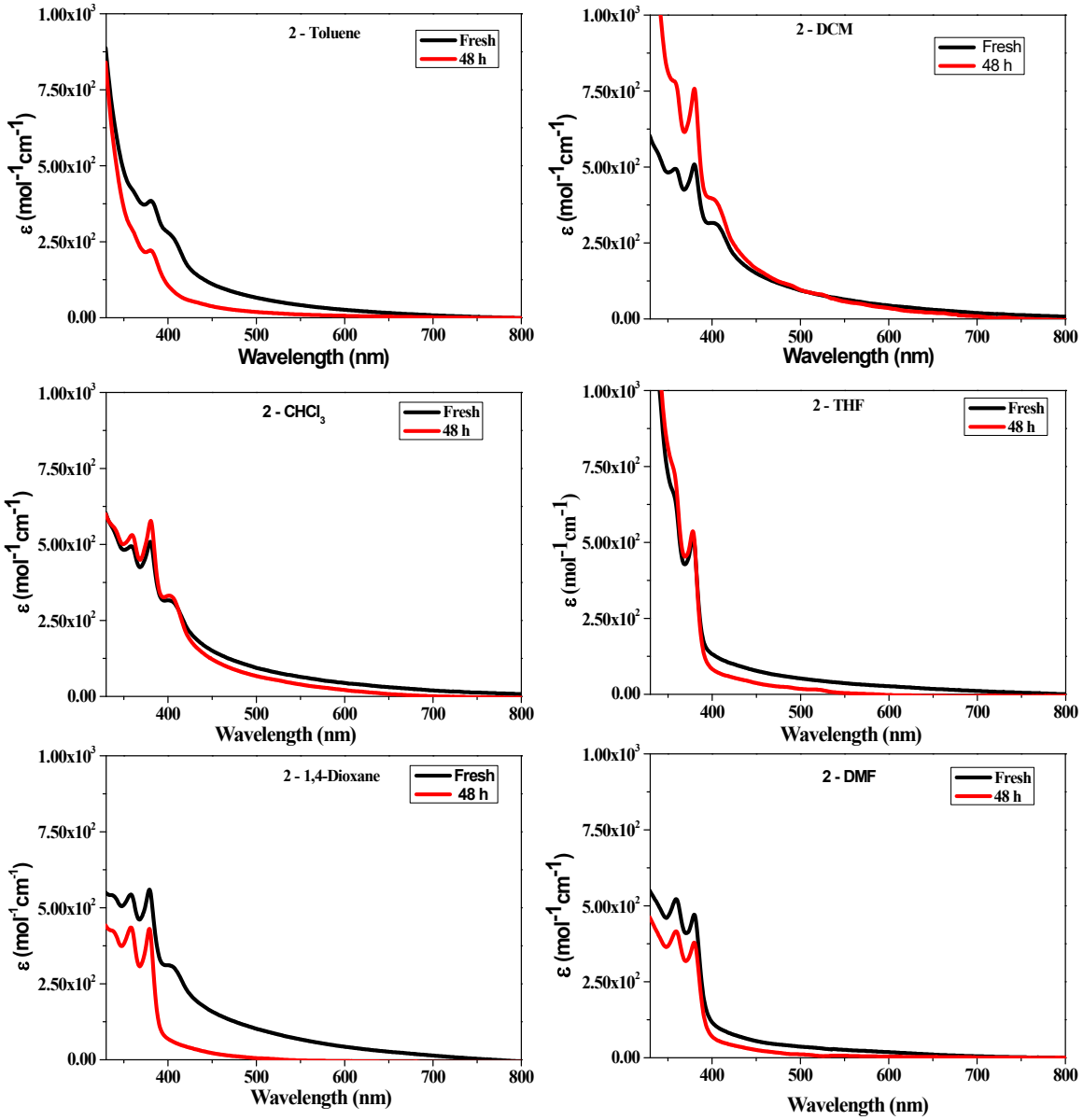

Figure S12. UV-Vis absorption of 2 (fresh and 48 h aged) in different solvents.

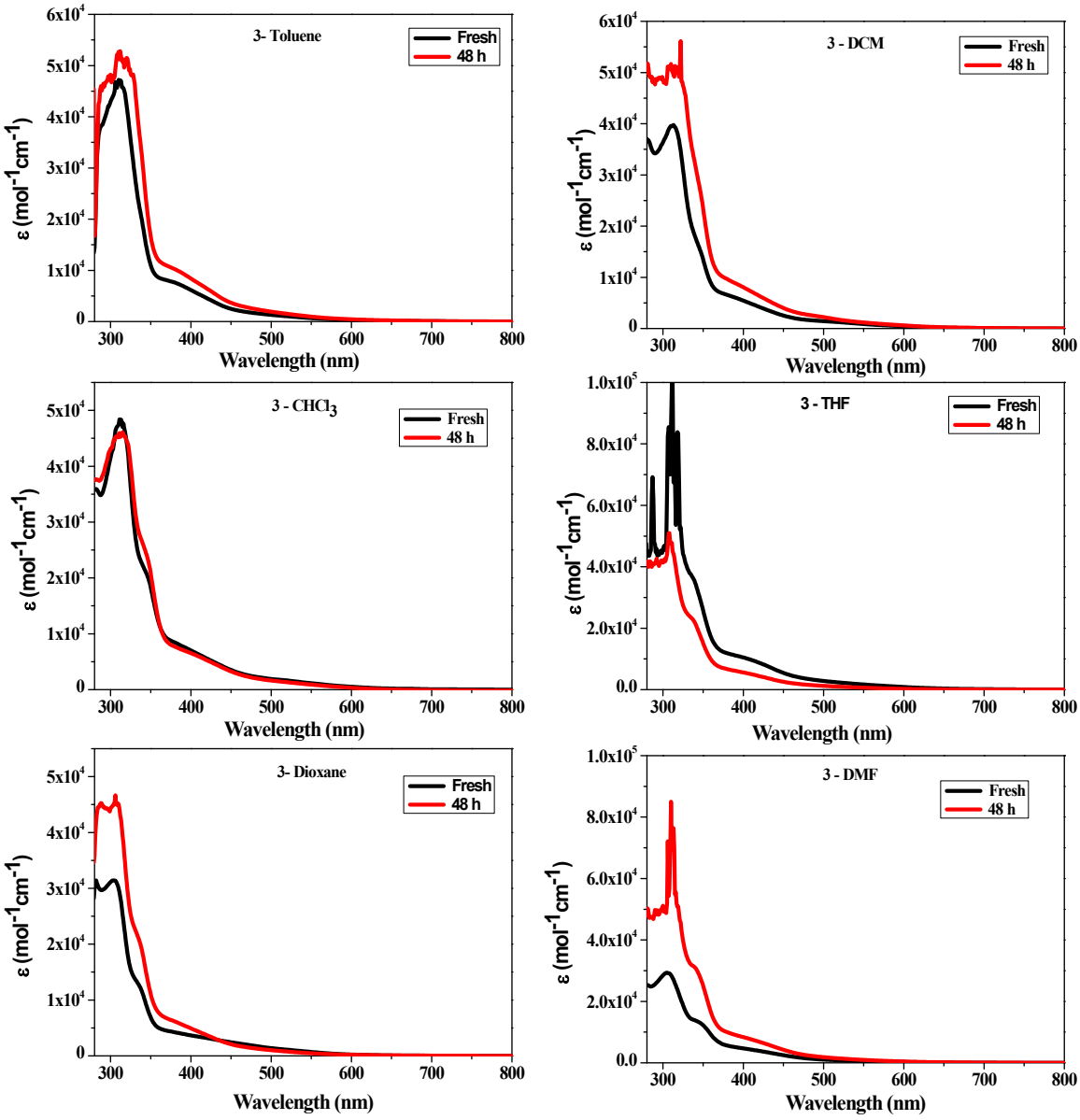

Figure S13. UV-Vis absorption of **3** (fresh and 48 h aged) in different solvents.

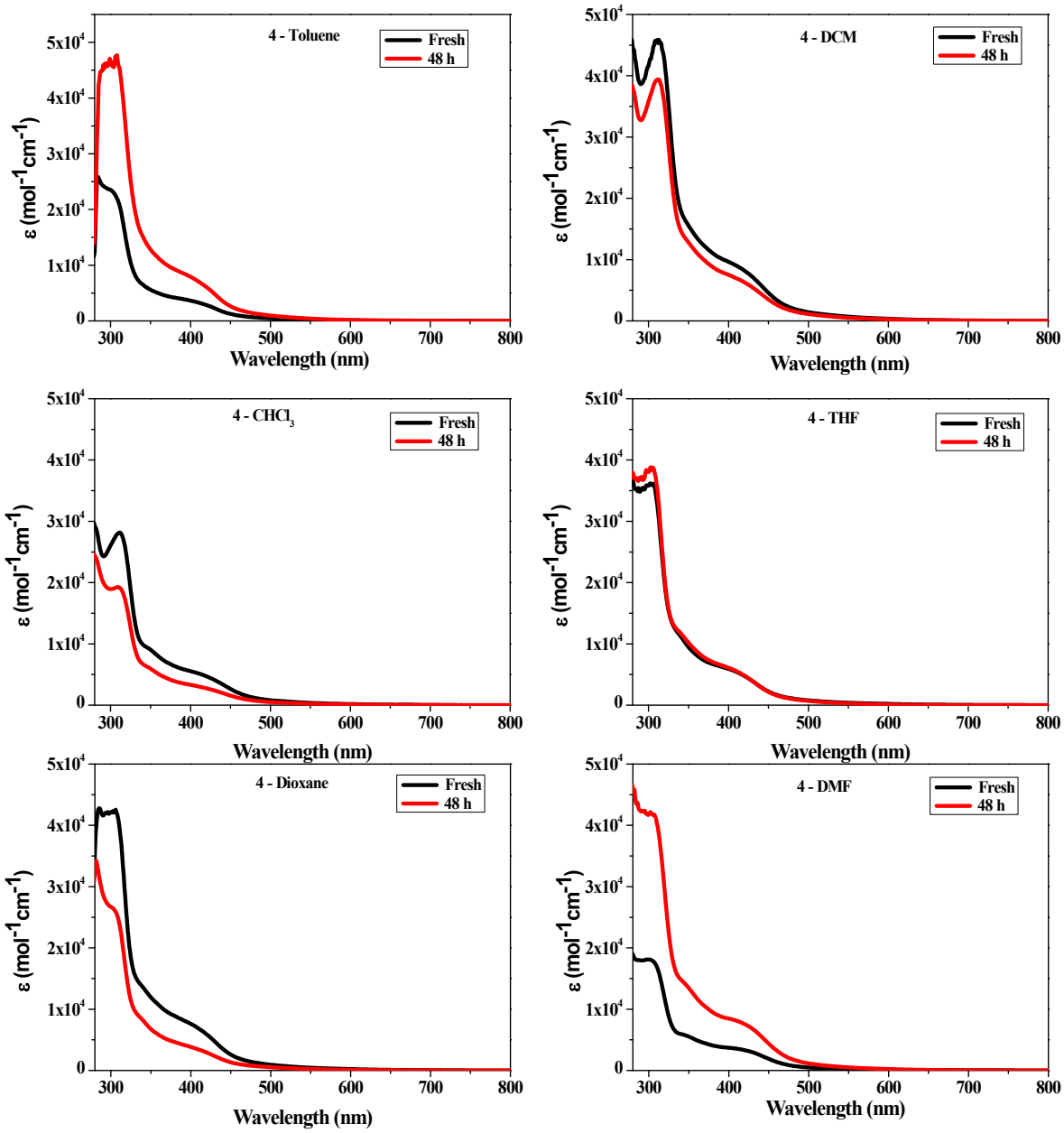

Figure S14. UV-Vis absorption of fresh and 48 h aged samples of **4** in different solvents

Table S1. Position of absorption maximum of 1, 2, 3 and 4 in different solvents in their fresh and 48 h aged samples

1	**toluene**	**DCM**	**$CHCl_3$**	**THF**	**Dioxane**	**DMF**
fresh	319,379	319,379, 467	319,379, 467	335,378, 412,526	335,377, 500	338,379, 549
48 h	319,382	316,379, 480	317,377, 480	337,377, 543	339,377, 589	339,357, 380,552
2	**toluene**	**DCM**	**$CHCl_3$**	**THF**	**Dioxane**	**DMF**
fresh	381	340,358, 378,401	336,357, 378	356, 378	336,358, 378	359, 379
48 h	379	359, 381, 406	337, 357, 380,403	357, 377	337,360, 379	359, 380
3	**toluene**	**DCM**	**$CHCl_3$**	**THF**	**Dioxane**	**DMF**
fresh	311,378	311,347, 439	310,348, 397	305,336, 392	302,335, 410	305,347, 410
48 h	321,388	309,320, 485	313,348, 397	312,341, 424	306,338, 397	315,342, 413
4	**toluene**	**DCM**	**$CHCl_3$**	**THF**	**Dioxane**	**DMF**
fresh	296,396	310,414	311,351, 418	304,341, 406	306,341, 402	302,343, 419
48 h	306,407	312,417	311,347, 422	306,341, 406	305,344, 408	306,343, 427

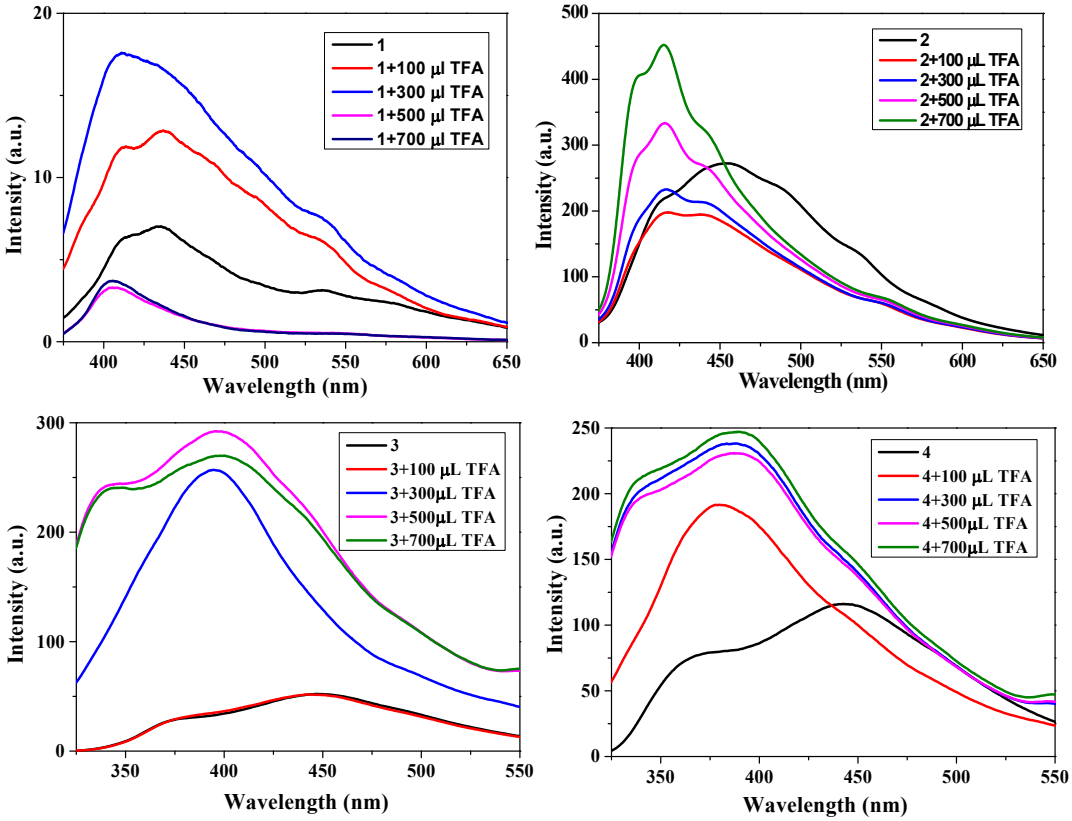

Figure S15. PL spectra of products in chloroform with addition of TFA.

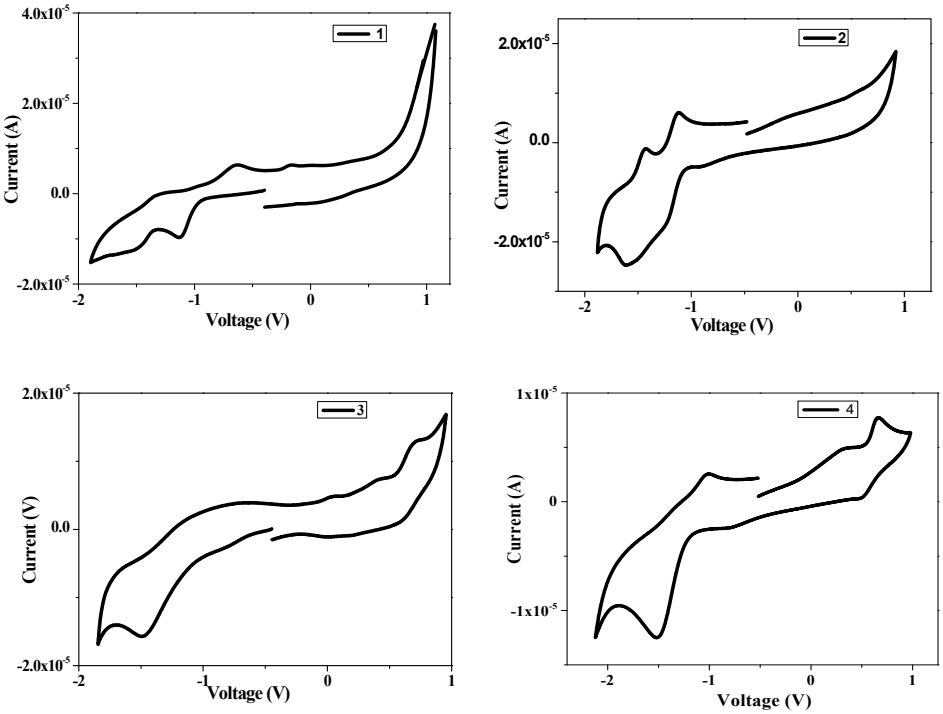

Figure S16. Cyclic voltammograms of 1, 2, 3 and 4 for the determination of HOMO-LUMO energy levels.

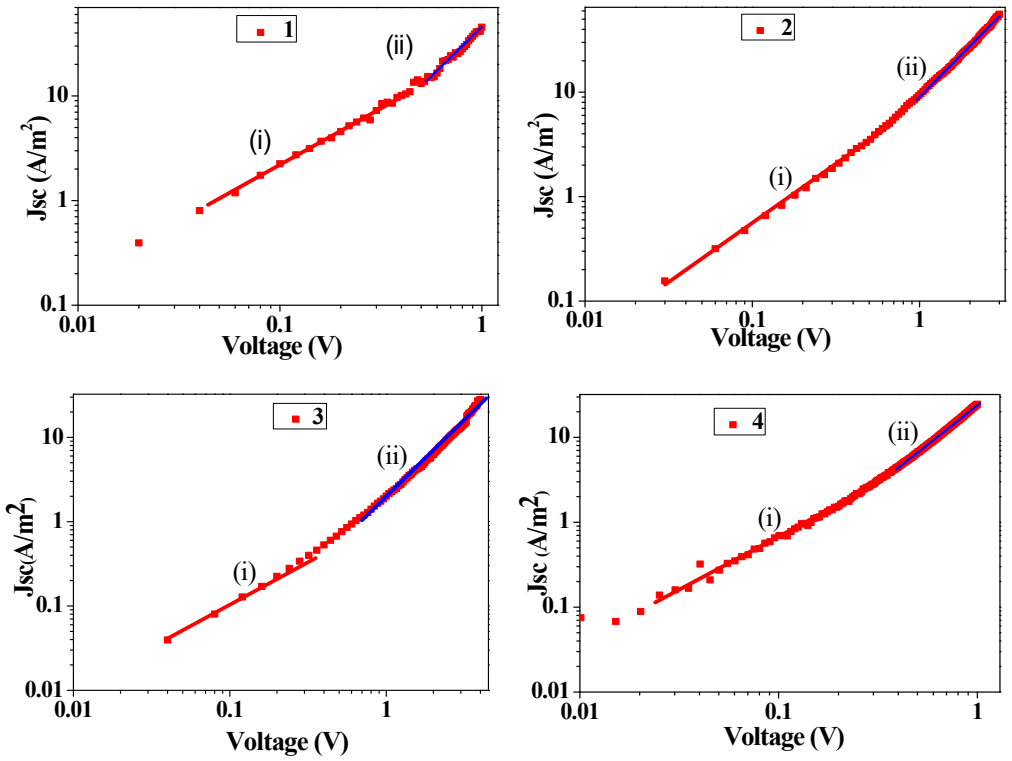

Figure S17. SCLC electron mobility measurement curves for **1**, **2**, **3** and **4.**

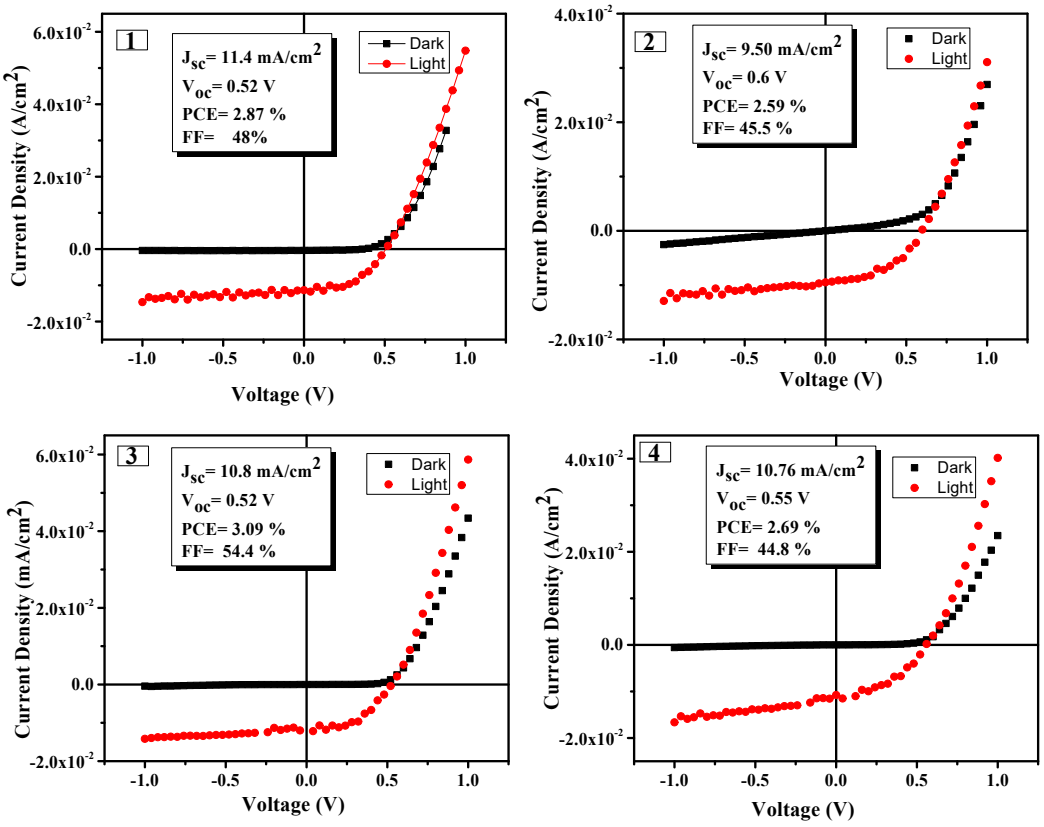

Figure S18. J-V characteristics of the Champion cell for products **1**, **2**, **3** and **4** with their Photovoltaic parameters J_{SC} (short-circuit current density), V_{oc}(open-circuit voltage), FF(fill factor), and PCE(power conversion efficiency) in the inset.

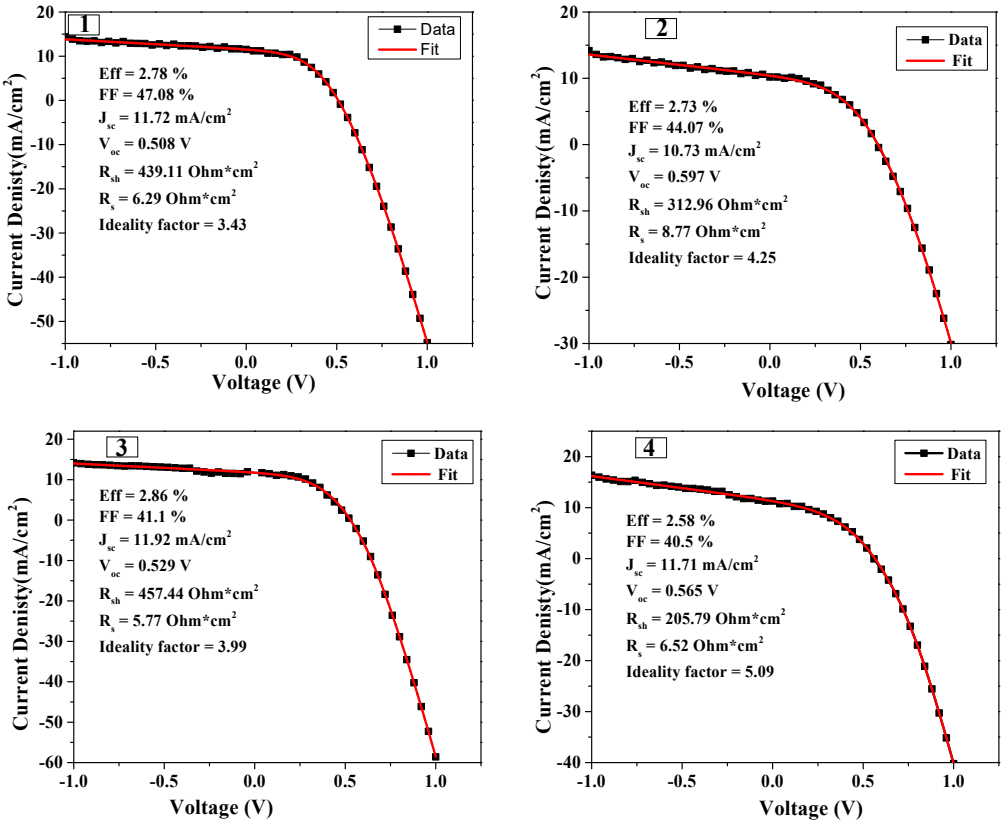

Figure S19. J-V characteristics of **1**, **2**, **3** and **4** devices with theoretical fitting showing Jsc, Voc, FF, PCE, ideality factor, shunt and series resistance.

Table S2. Photovoltaic parameters for **1**

Conc.	**Spin coating(rpm)**	**J_{sc} (mA/cm^2)**	**V_{oc} (mV)**	**FF**	**PCE (%)**
3 mg/mL	1000	11.4	0.52	0.48	2.87
		10.8	0.52	0.45	2.54
		10.4	0.52	0.48	2.61
5 mg/mL	1000	8.80	0.51	0.33	1.52
		8.68	0.52	0.37	1.49
		6.92	0.52	0.38	1.39
7 mg/ mL	1000	6.01	0.51	0.40	1.27
		7.06	0.49	0.33	1.19
		7.58	0.50	0.29	1.15

Table S3. Photovoltaic parameters for **2**

Conc.	Spin coating(rpm)	J_{sc} (mA/cm^2)	V_{oc} (mV)	FF	PCE (%)
3 mg/mL	1000	10.5	0.6	0.42	2.71
		9.38	0.6	0.42	2.38
		9.5	0.6	0.45	2.59
5 mg/mL	1000	7.41	0.51	0.35	1.33
		6.93	0.50	0.34	1.20
		7.85	0.49	0.30	1.19
7 mg/ mL	1000	5.78	0.51	0.30	0.89
		5.45	0.47	0.31	0.85
		4.77	0.42	0.33	0.68

Table S4. Photovoltaic parameters for **3**

Conc.	Spin coating(rpm)	J_{sc} (mA/cm^2)	V_{oc} (mV)	FF	PCE (%)
3 mg/mL	1000	10.7	0.54	51.2	3.00
		10.8	0.52	54.4	3.09
		9.35	0.54	54.4	2.73
5 mg/mL	1000	8.61	0.49	31.8	1.37
		7.47	0.50	36.4	1.36
		8.57	0.48	28.9	1.20
7 mg/ mL	1000	6.73	0.43	30.4	0.88
		6.28	0.42	27.3	0.72
		5.72	0.43	34.0	0.84

Table S5. Photovoltaic parameters for **4**

Conc.	Spin coating(rpm)	J_{sc} (mA/cm^2)	V_{oc} (mV)	FF	PCE (%)
3 mg/mL	1000	10.76	0.55	44.8	2.69
		10.14	0.51	46.0	2.39
		10.86	0.51	51.1	2.55
5 mg/mL	1000	8.69	0.52	35.8	1.63
		8.04	0.52	38.1	1.62
		8.67	0.51	35.4	1.58
7 mg/ mL	1000	7.88	0.52	33.6	1.38
		8.08	0.52	34.1	1.44
		6.96	0.52	37.2	1.35

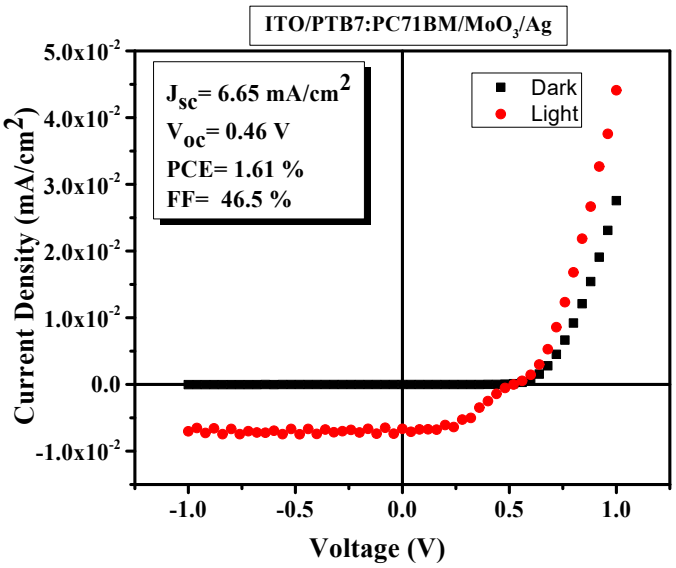

Figure S20. J-V characteristic for inverted organic solar cell device fabricated without ETL.