Supplemental Information

Surface engineering of zinc phthalocyanine organic thin-film transistors results in part-per-billion sensitivity towards cannabinoid vapor

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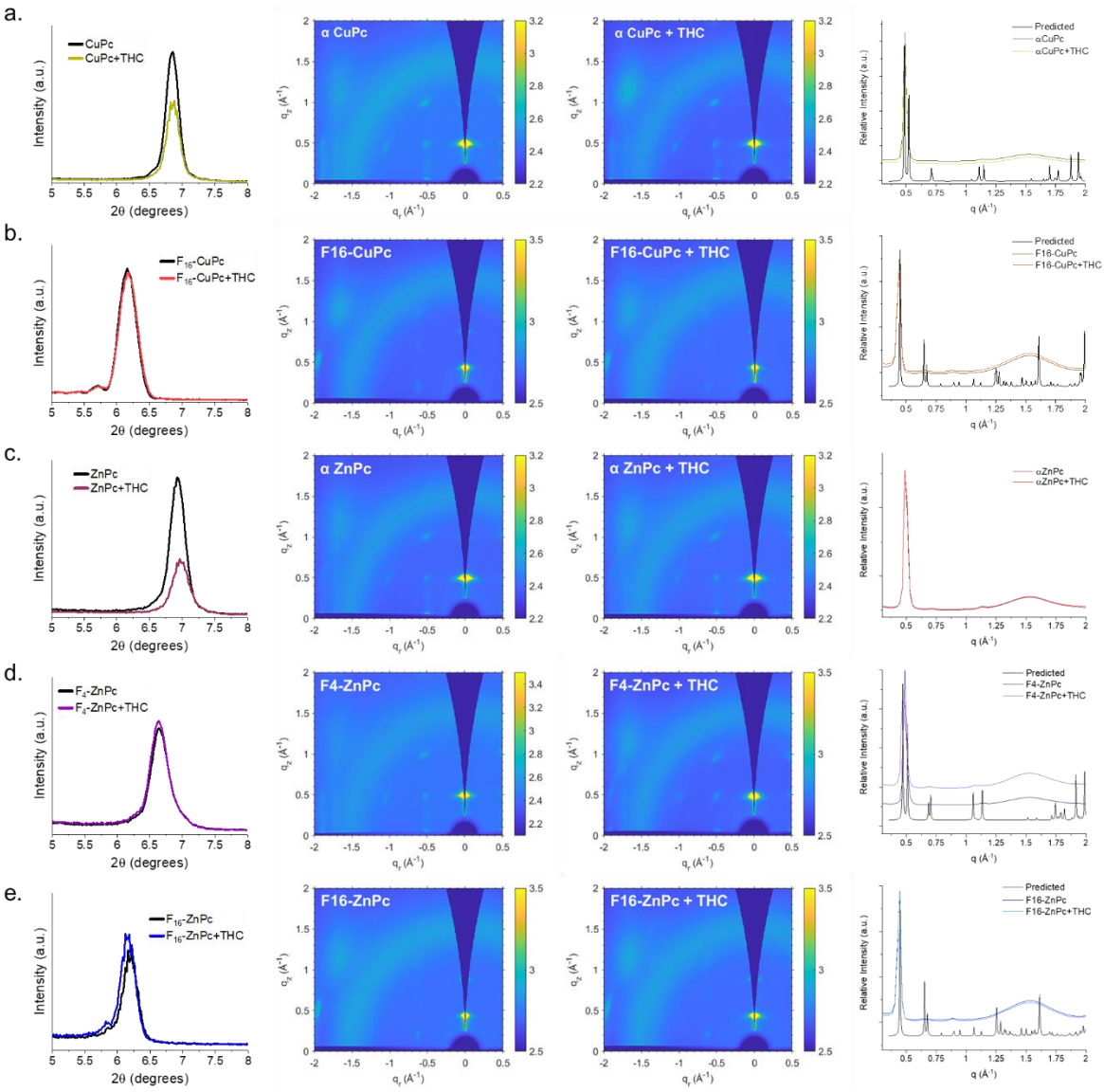

Figure S1. XRD, 2D scattering patterns (θ = 0.3°), and diffraction patterns predicted from single crystal and determined by GIWAXS of pre- and post- exposure films to THC vapor (a) α-CuPc (CCDC #219250) [1], (b) F_{16}-CuPc (CCDC #698474) [2], (c) α-ZnPc, (d) F_4-ZnPc (CCDC #1818040)[3], and (e) F_{16}-ZnPc (CCDC #1013162)[4].

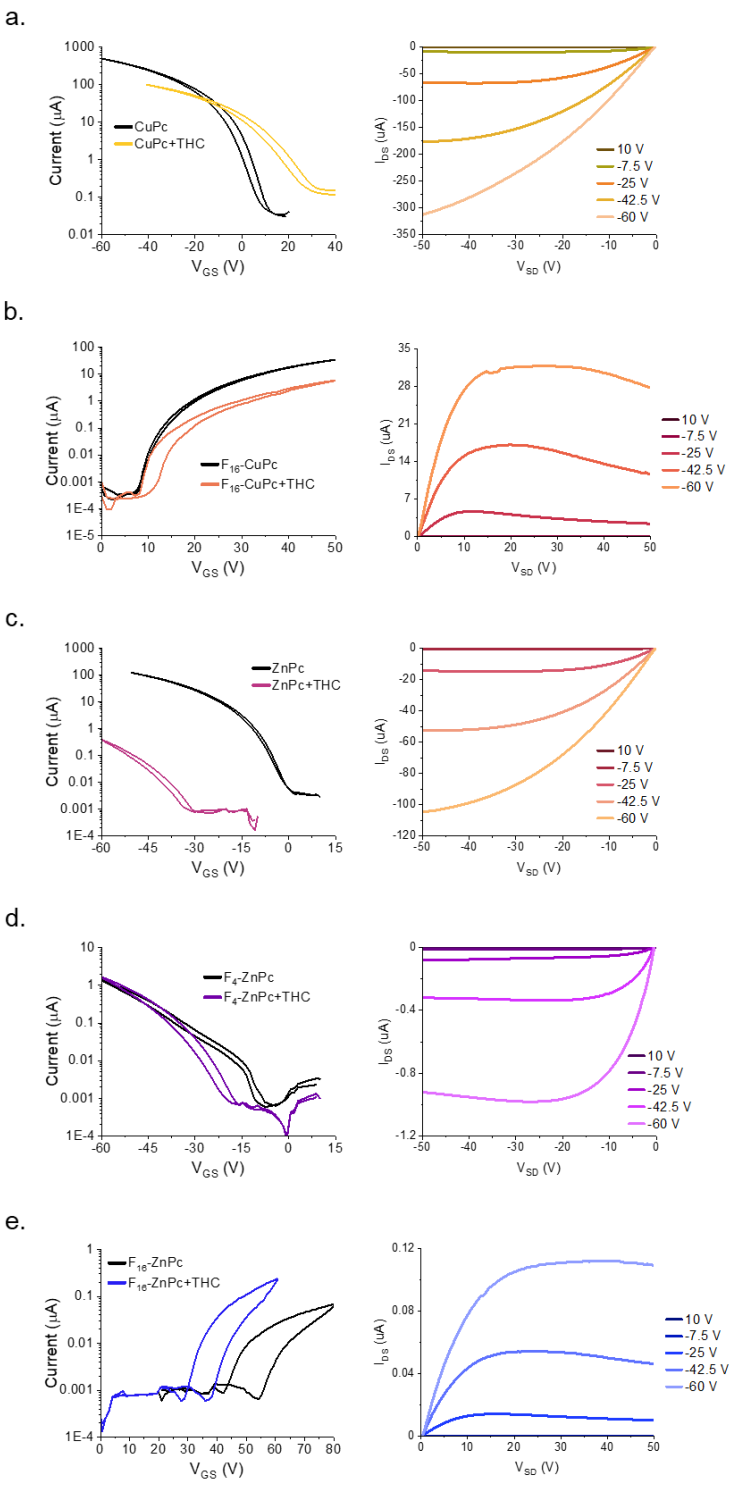

Figure S2. Characteristic transfer and output curves of Pc thin-films pre- and post- exposure to THC vapor. Twenty (a) CuPc, (b) F_{16}-CuPc, (c) ZnPc, (d) F_4-ZnPc, and (e) F_{16}-ZnPc OTFTs were characterized and then exposed to 4 ppm THC vapor over a period of 90 seconds.

Table S1. Calculated transfer data pre- and post- THC vapor exposure for morphologically different films[a]

	Low		Med		High		Very High	
	Baseline	+THC	Baseline	+THC	Baseline	+THC	Baseline	+THC
Peak Mobility [10^{-2} cm^2/Vs]	2.5±0.2	1.8±0.3	2.4±0.1	2.0±0.2	2.9±0.2	2.6±0.2	2.7±0.1	2.7±0.1
Voltage Threshold [V]	-2.8±0.4	-19.3±2.1	-8.2±0.7	-12.6±0.8	-6.8±1.0	-8.9±0.8	-11.4±1.1	-8.2±1.2
Defect Density [$10^{12}/cm^2V$]	12.3±1.3	21.4±2.3	13.7±0.8	15.4±1.0	7.51±0.5	12.5±0.8	4.23±0.4	9.9±0.7
Maximum Hysteresis [V]	1.6	6.1	1.3	2.5	1.1	3.2	0	2.1
On/Off Ratio	$4•10^3$	$2•10^3$	$4•10^3$	$4•10^3$	$1•10^4$	$7•10^3$	$7•10^4$	$2•10^4$

a. Mobility, voltage threshold, and defect density was calculated from the transfer data of 18 OTFTs for each condition and averaged.

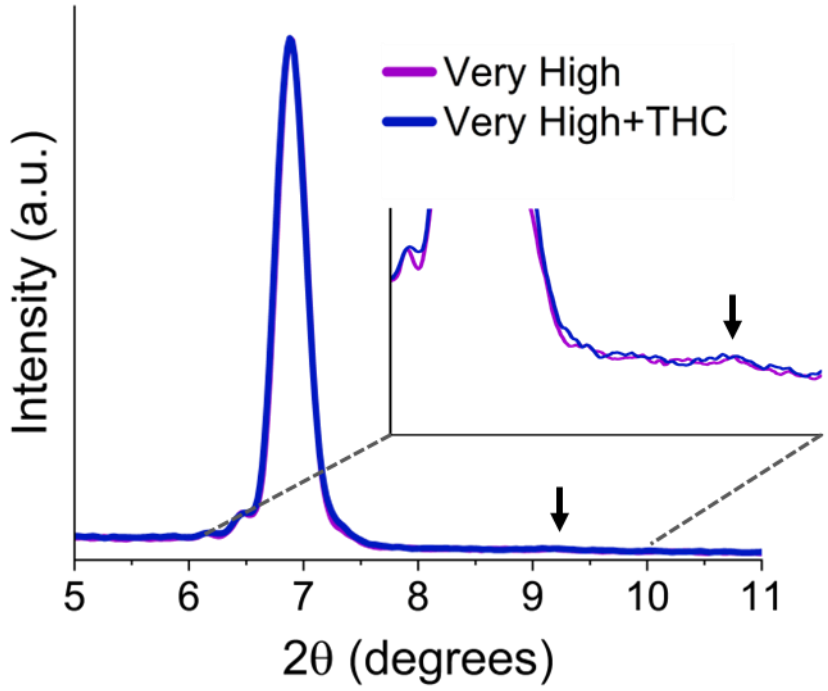

Figure S3. XRD spectra of very high crystallinity ZnPc thin-films pre- and post-THC vapor exposure, with inset showing spectra between 6 and 10 degrees 2θ. ZnPc thin-films were deposited at a rate of 0.2 Å/s and 180°C with a pre-deposited monolayer of p-sexiphenyl (p-6P) before being exposed to 400 ppb THC vapor over 90 seconds.

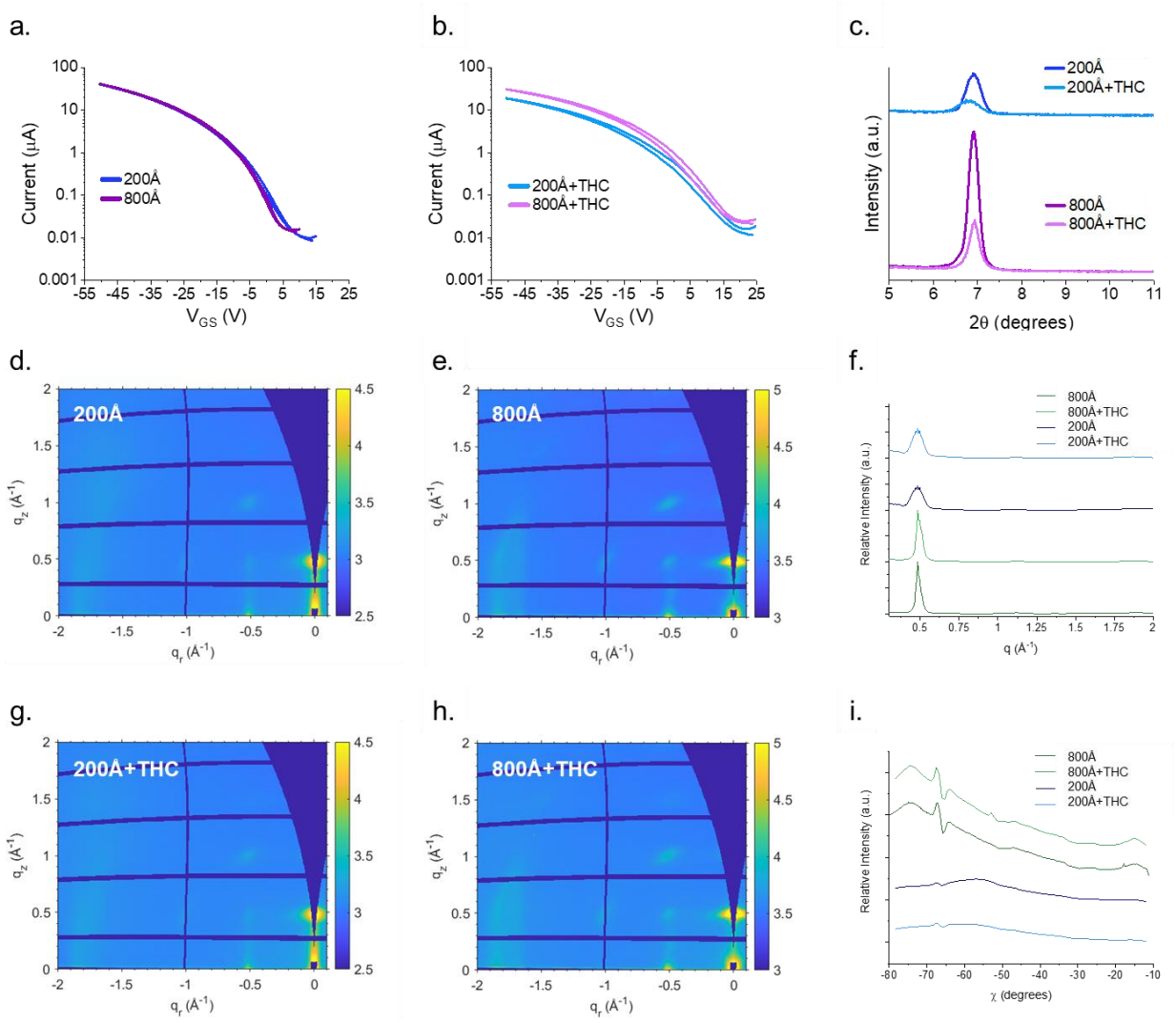

Figure S4. Effects of thickness on THC vapor sensitivity of ZnPc thin films. Transfer curves of 200 and 800 Å ZnPc OTFTs (a) pre- and (b) post- THC vapor exposure. (c) XRD spectra of thin-films pre- and post-exposure.2D scattering patterns (θ = 0.1°) of (d, g) 200 and (e, h) 800 Å α-ZnPc pre- and post- exposure to THC vapor. (f) Diffraction patterns determined by GIWAXS and (i) linecut profiles with respect to χ using a *q* range between 1.9-2.1 Å^{-1}.

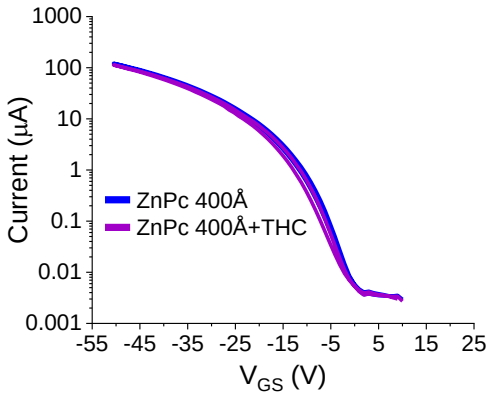

Figure S5: Initially screened ZnPc OTFT transfer curves pre- and post- exposure to 40 ppb THC vapor for 90 seconds. Films were deposited at a rate of 0.2 Å/s.

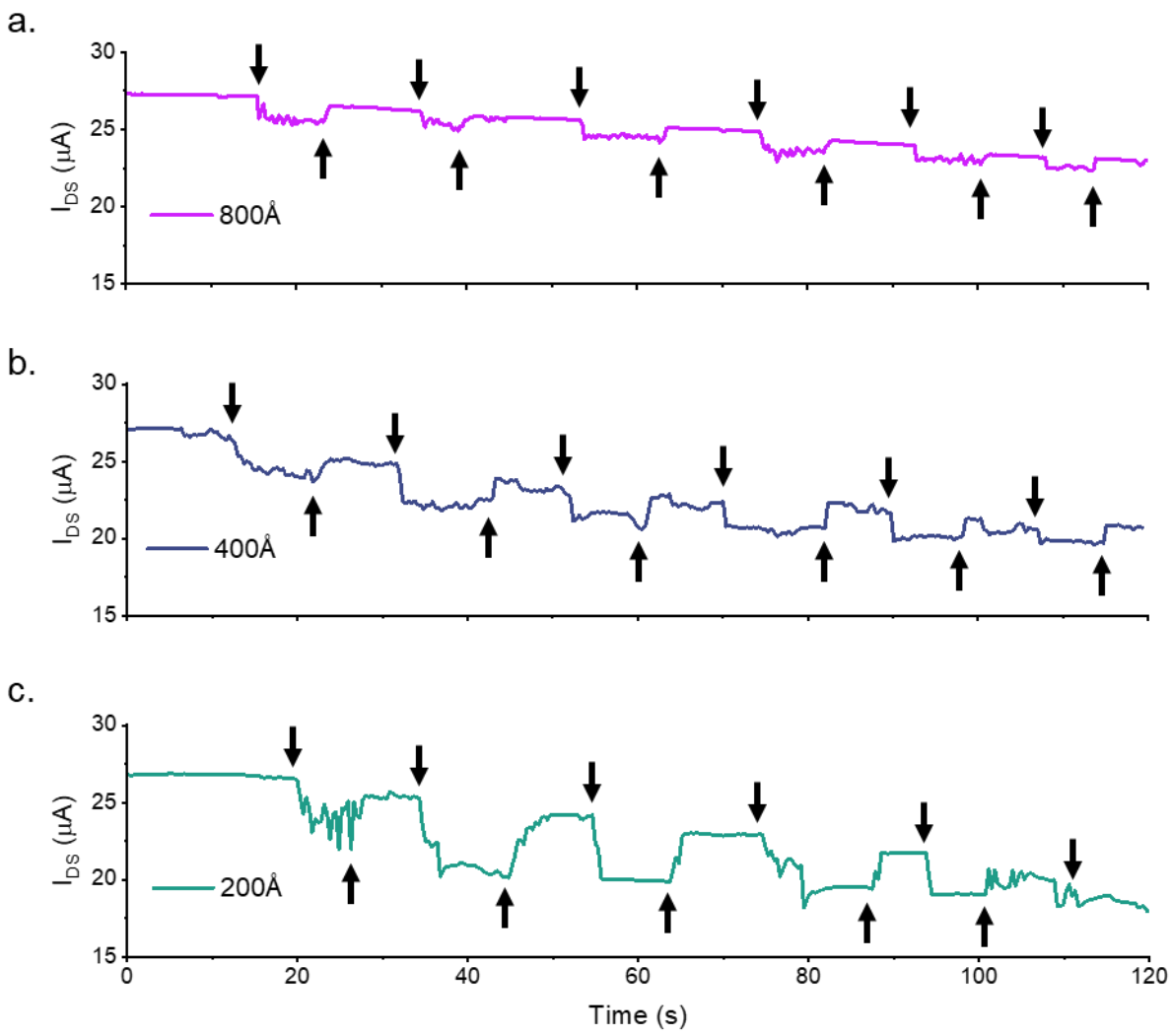

Figure S6. Periodic in-situ THC vapor exposure and detection. The effects of periodic THC exposure on (a) 800, (b) 400, and (c) 800 Å ZnPc OTFTs. A V_{SD} of -50 V was held and a V_{GS} of -40 V and was pulsed at a rate of 20 milliseconds on 80 milliseconds off over a period of 120 seconds. 40 ppb THC vapor was introduced to a 50 mL chamber.

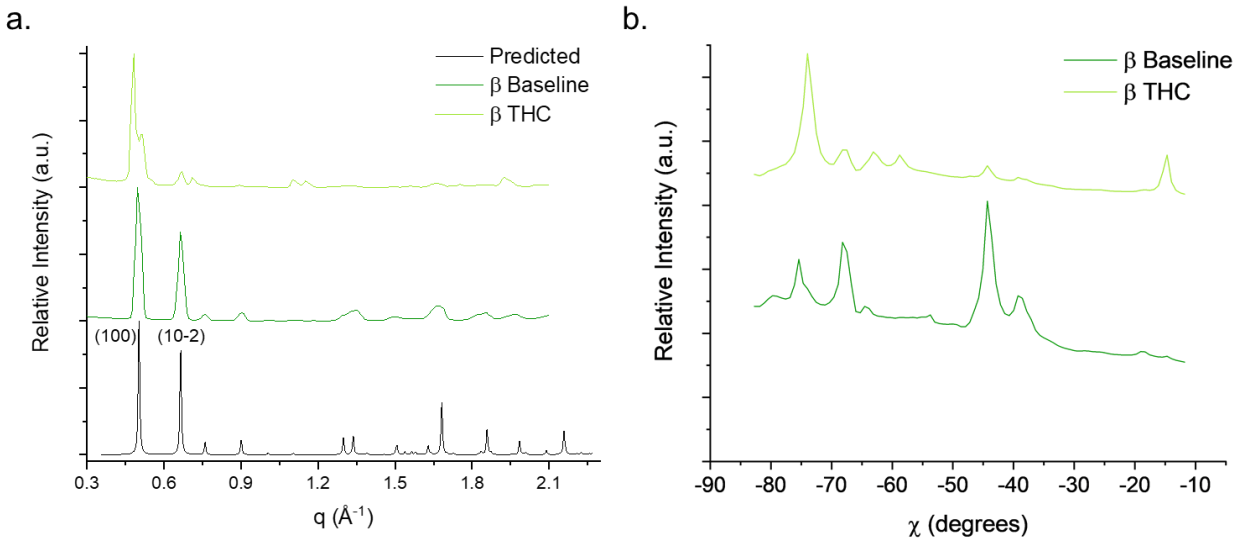

Figure S7. (a) Diffraction pattern of β-ZnPc predicted from single crystal (CCDC #2098417)[3] and β-ZnPc pre- and post- exposure to THC vapor determined by GIWAXS. (b) Linecut profiles of pre- and post- exposed β-ZnPc with respect to χ using a *q* range between 1.9-2.1 $Å^{-1}$.

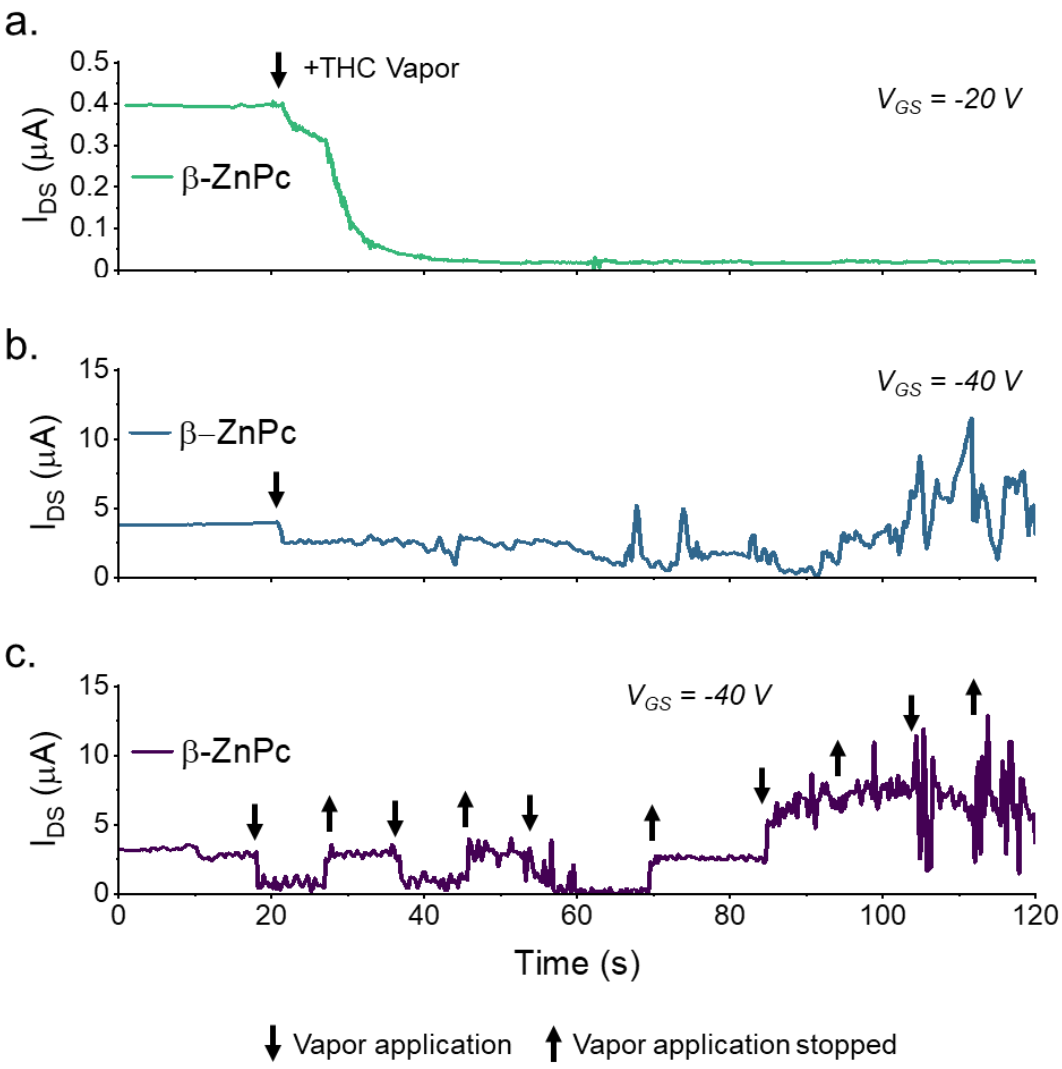

Figure S8. Continuous and periodic in-situ THC vapor exposure and detection. The effects of (a) continuous THC exposure when V_{GS} = -20V, (b) continuous THC exposure when V_{GS} = -40V, and (c) periodic THC exposure when V_{GS} = -20V on β-ZnPc OTFTs. A V_{SD} of -50 V was held and V_{GS} was pulsed at a rate of 20 ms on 80 ms off over a period of 120 seconds. 400 ppb THC vapor was introduced to a 50 mL chamber.

References

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