

Supporting Information for

A Smartphone-Based VOC Sensor Using Colorimetric Polydiacetylenes

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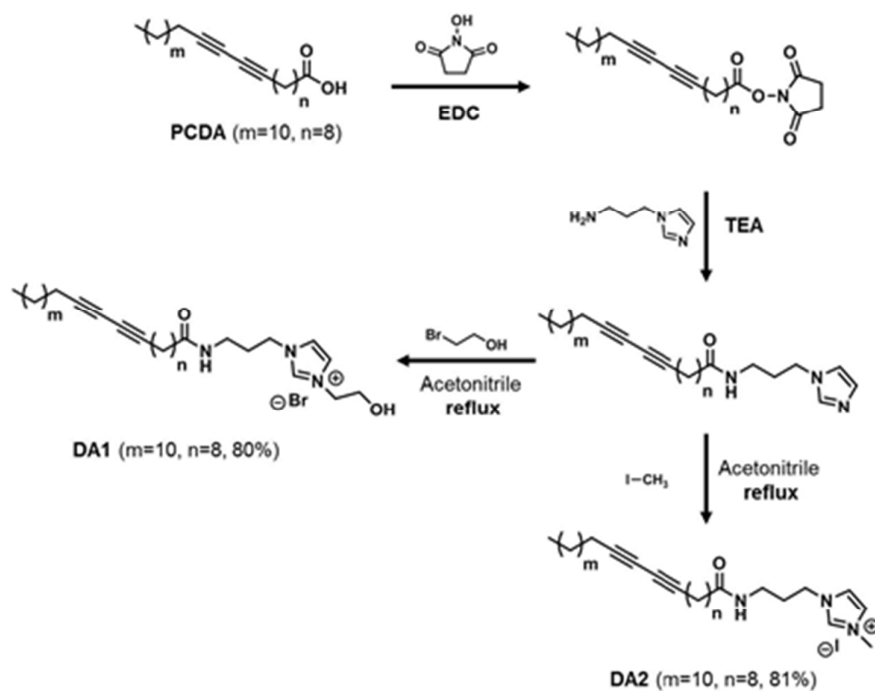
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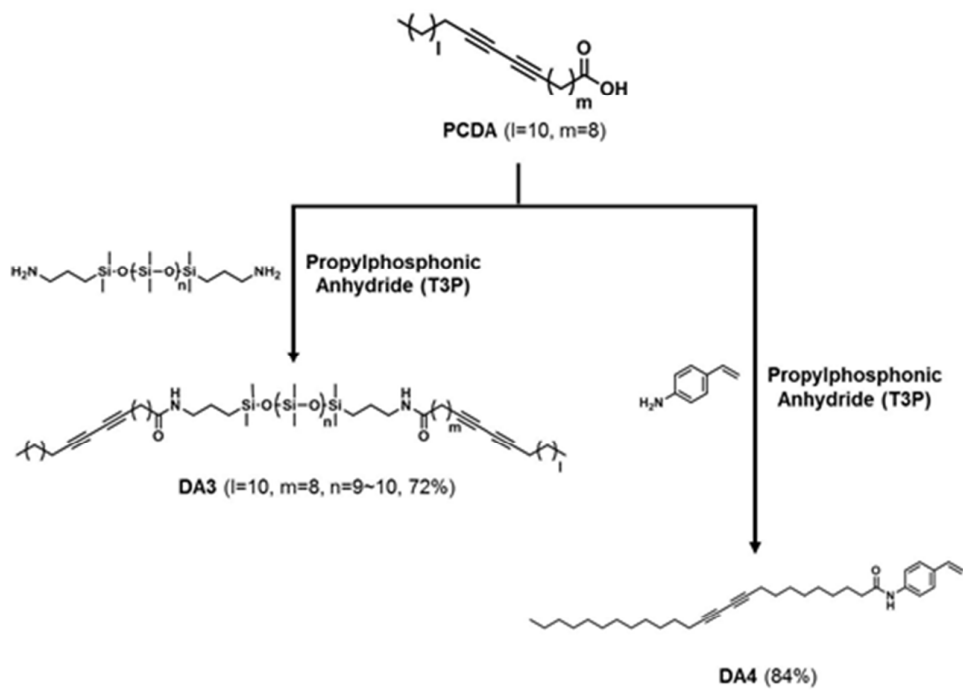
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Scheme S1. Synthesis of DA1 and DA2.



Scheme S2. Synthesis of DA3 and DA4.

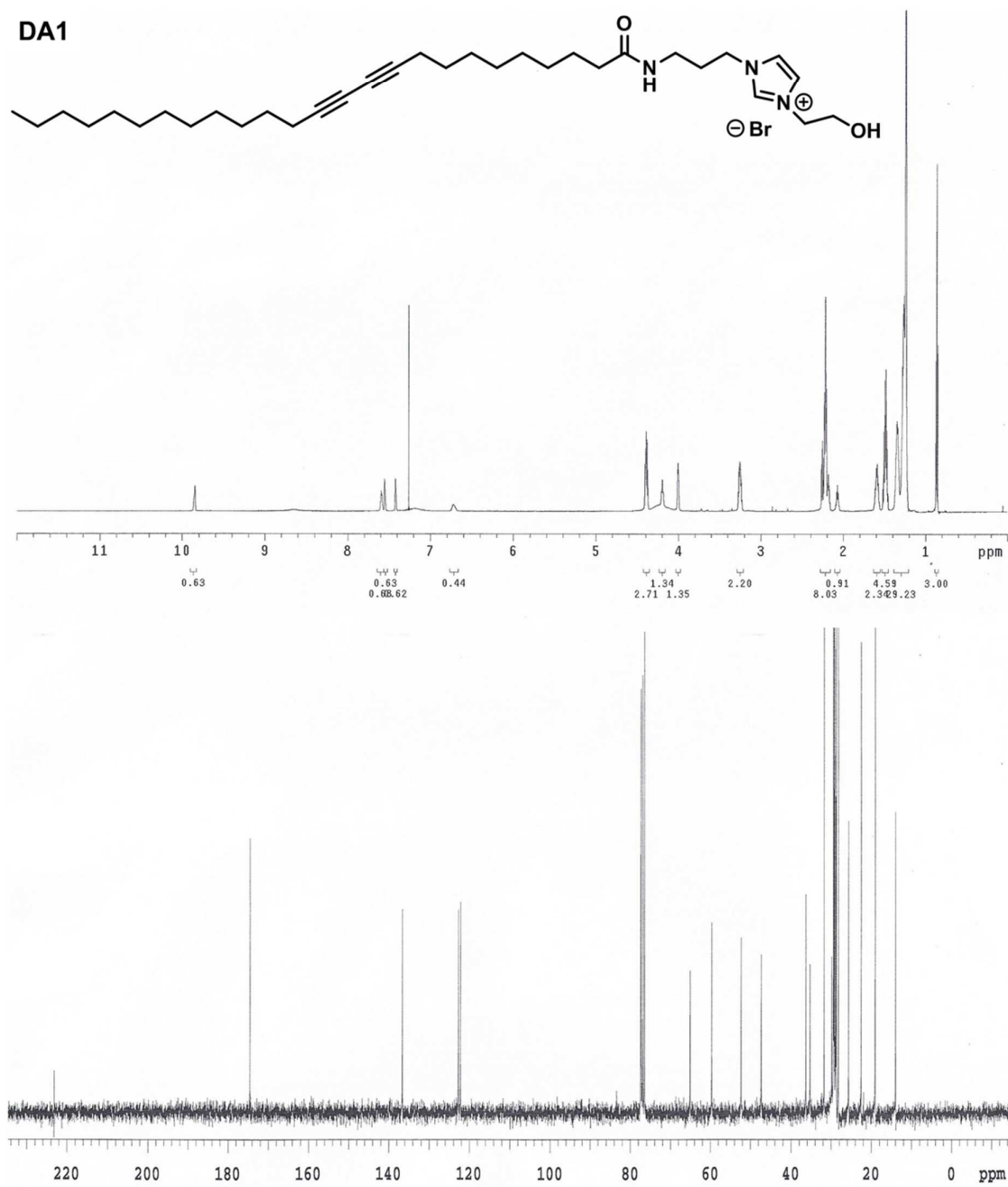


Figure S1. ¹H (top, 300 MHz) and ¹³C (bottom, 75 MHz) NMR spectra of DA1 in CDCl₃.

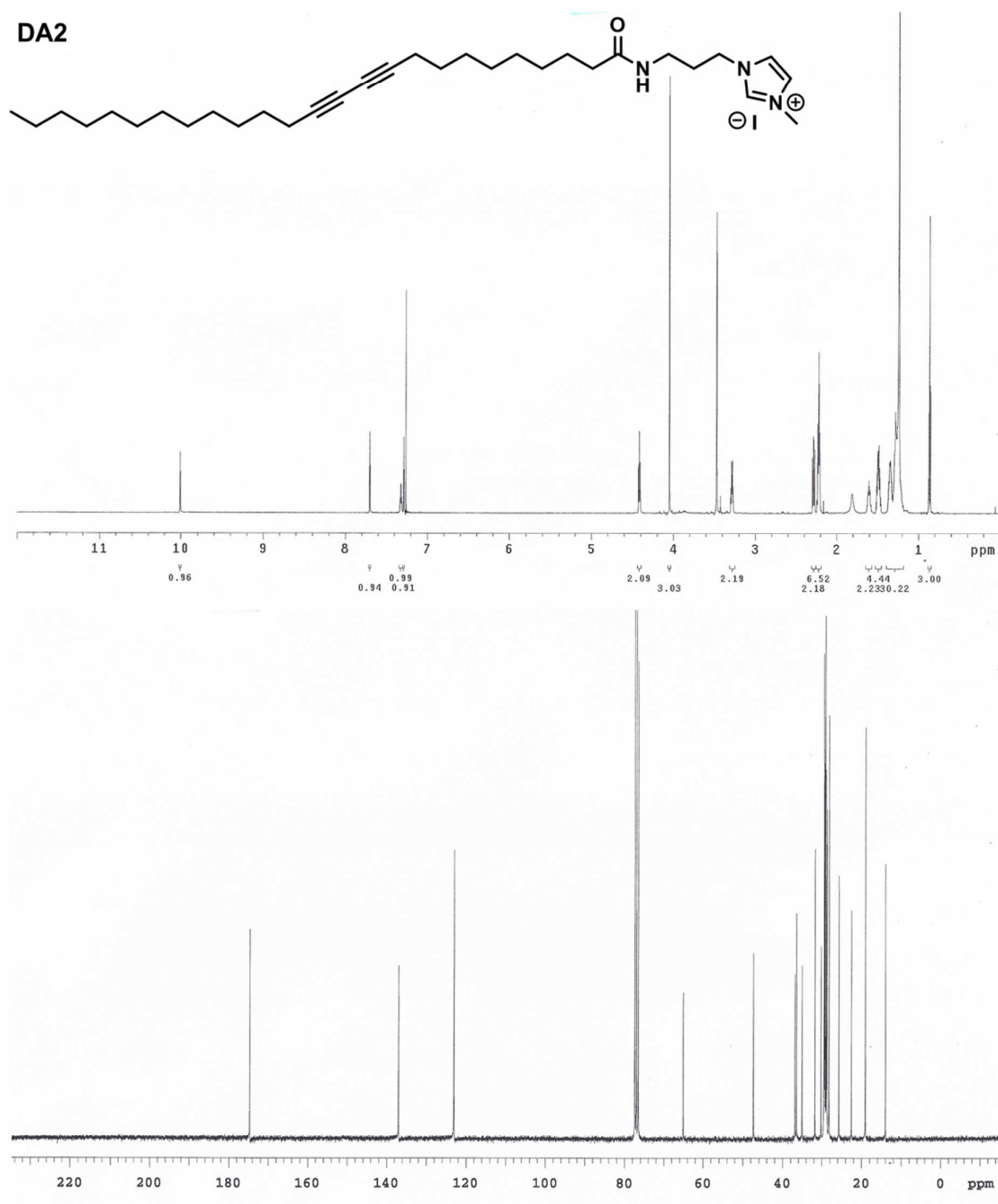


Figure S2. ^1H (top, 300 MHz) and ^{13}C (bottom, 75 MHz) NMR spectra of DA2 in CDCl_3 .

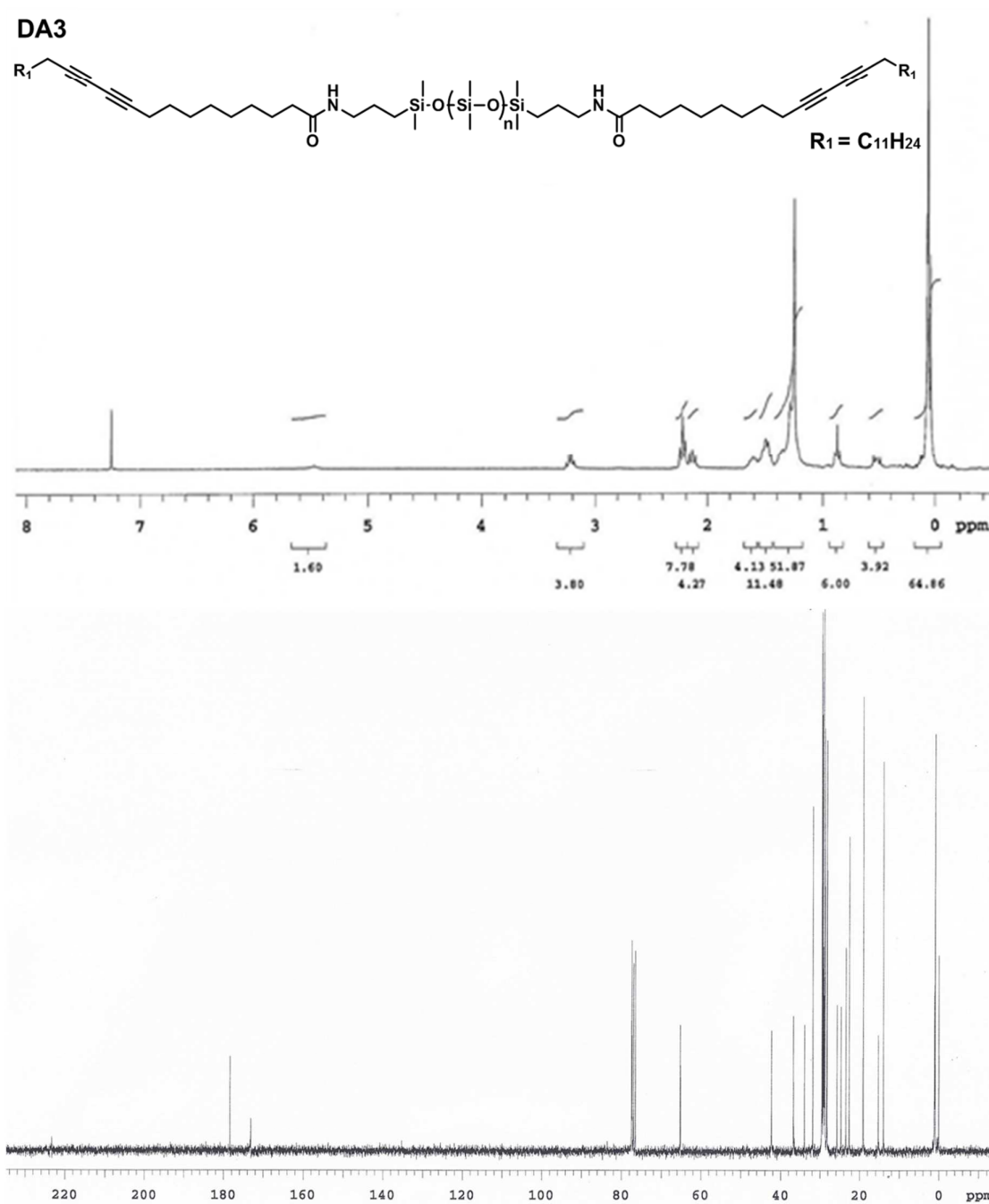


Figure S3. 1H (top, 300 MHz) and ^{13}C (bottom, 75 MHz) NMR spectra of DA3 in $CDCl_3$.

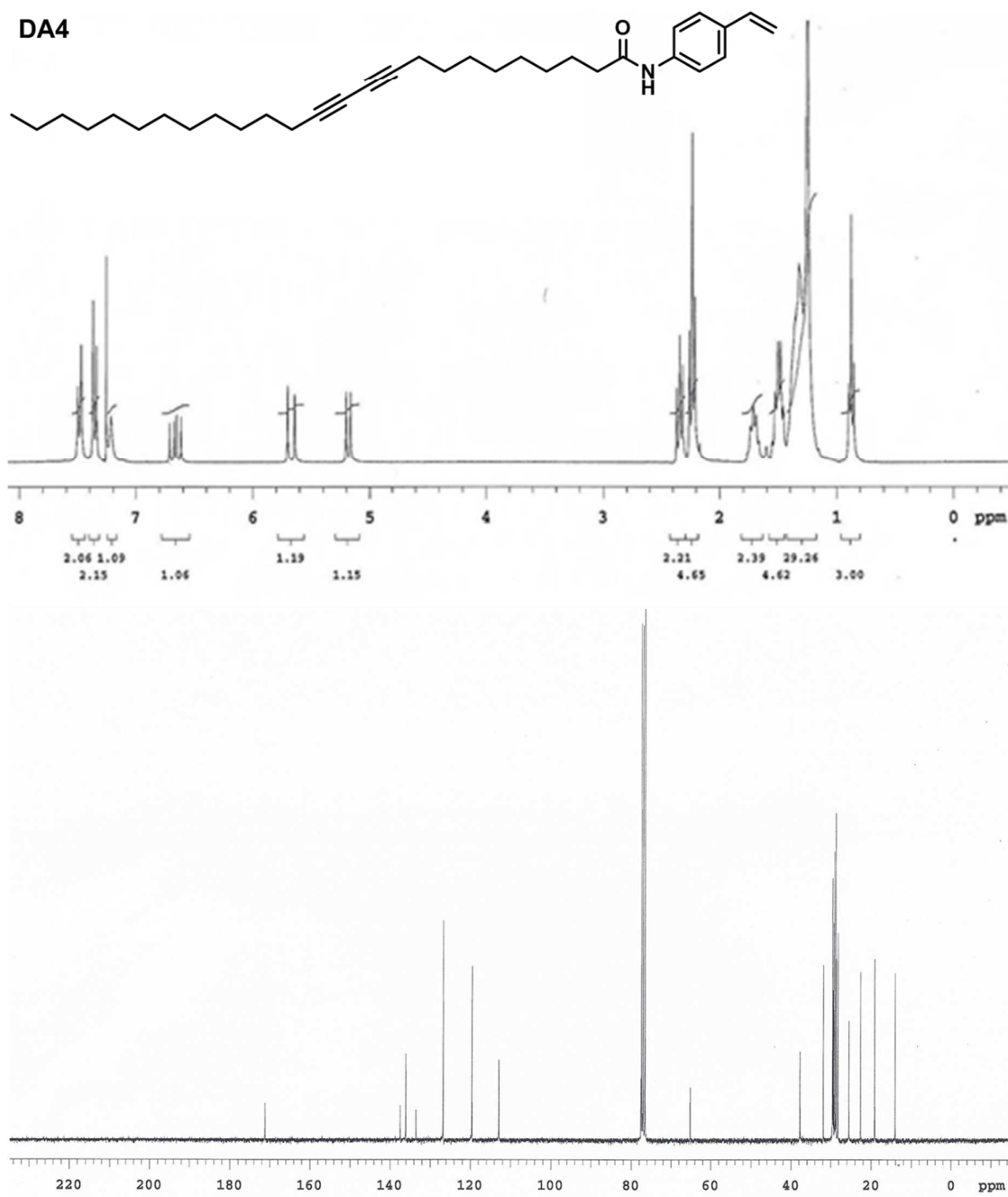


Figure S4. ^1H (top, 300 MHz) and ^{13}C (bottom, 75 MHz) NMR spectra of DA4 in CDCl_3 .

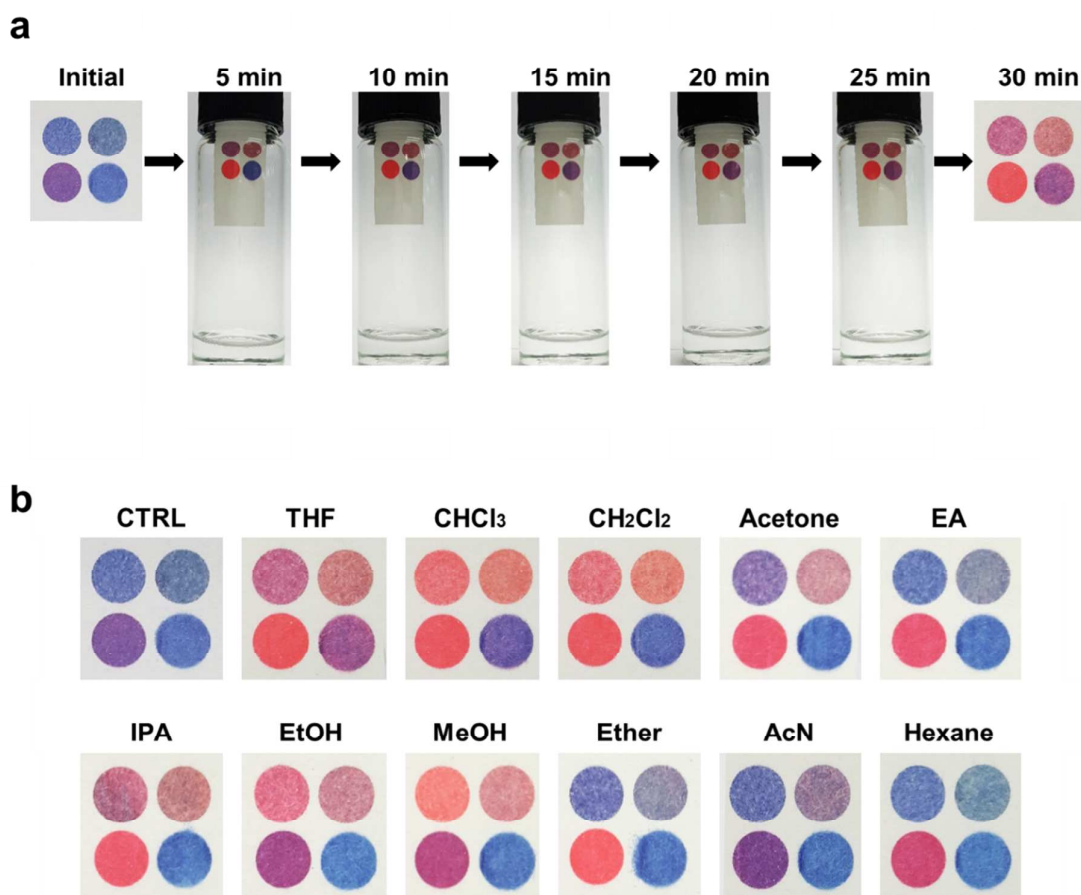


Figure S5. Vapochromic responses of the PDA array sensor. (a) Photographs showing the color change of the PDA sensor upon exposure to the THF vapor at ambient conditions. (b) Different color patterns when the PDA sensors were exposed to the eleven VOC gases.

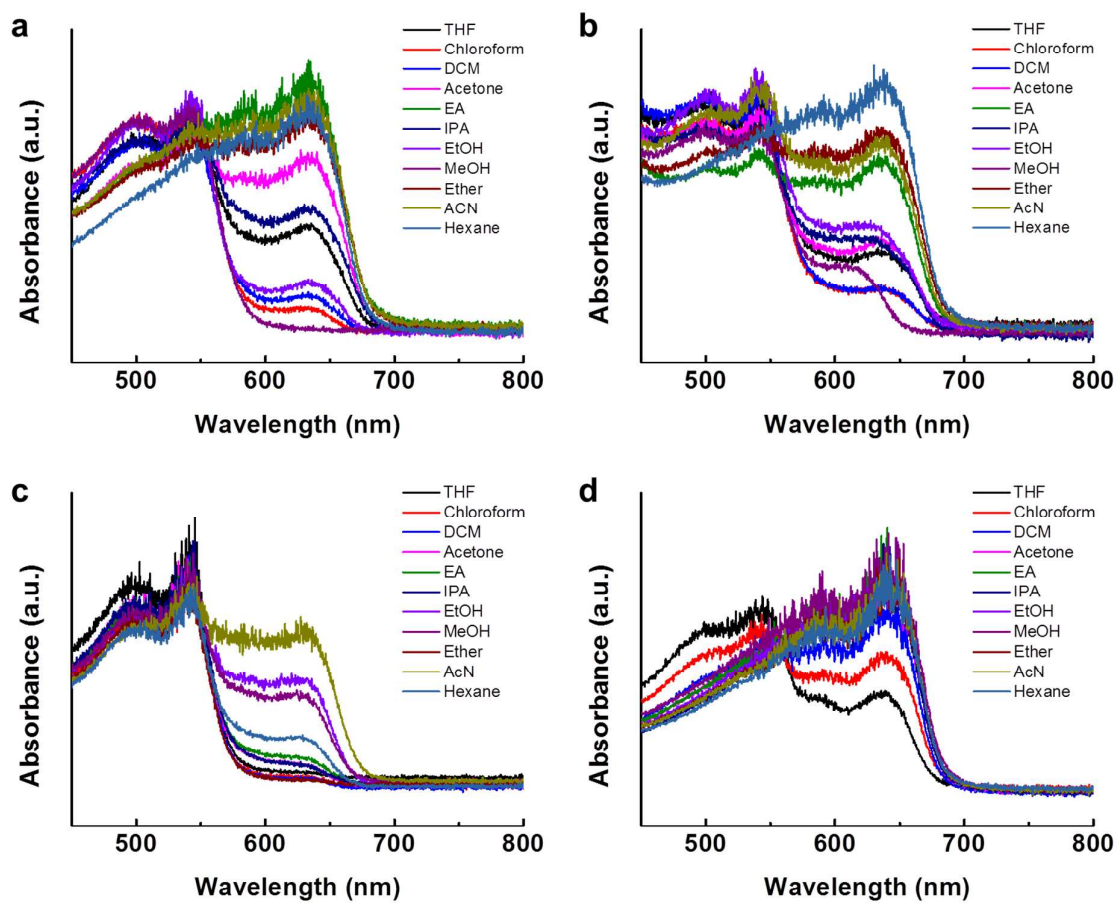


Figure S6. UV-vis absorbance spectra for vapochromic responses of (a) PDA1, (b) PDA2, (c) PDA3 and (d) PDA4 upon exposure to VOC gases.

a

R value	THF	CHCl ₃	CH ₂ Cl ₂	Acetone	EA	IPA	EtOH	MeOH	Ether	AcN	Hexane
PDA1	145-165	180-200	178-195	108-128	85-105	123-158	160-185	185-205	80-108	80-105	82-105
PDA2	150-170	170-190	175-195	151-171	105-125	130-155	130-155	145-170	95-120	100-120	88-112
PDA3	170-200	185-205	188-208	175-195	170-190	140-192	105-128	115-135	183-203	82-105	142-161
PDA4	107-127	85-110	77-97	70-95	70-95	65-90	65-90	65-90	65-85	65-85	67-87

b

H value	THF	CHCl ₃	CH ₂ Cl ₂	Acetone	EA	IPA	EtOH	MeOH	Ether	AcN	Hexane
PDA1	322-338	345-355	340-360	250-260	221-231	320-340	335-350	345-360	225-245	225-240	210-235
PDA2	340-360	350-360	350-360	340-350	225-240	335-350	345-355	345-360	230-250	270-285	202-220
PDA3	340-360	345-360	345-355	240-350	338-353	340-350	300-315	315-330	340-360	260-280	330-345
PDA4	290-310	235-255	220-235	215-230	217-227	215-230	215-225	215-230	215-235	215-230	210-230

Table S1. Database of the normalized R (a) and H (b) values for vapochromic responses of PDAs.