Supplementary Materials

Sniff Species: SURMOF-Based Sensor Array Discriminates Aromatic Plants Beyond the Genus Level

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1. X-Ray Diffractograms

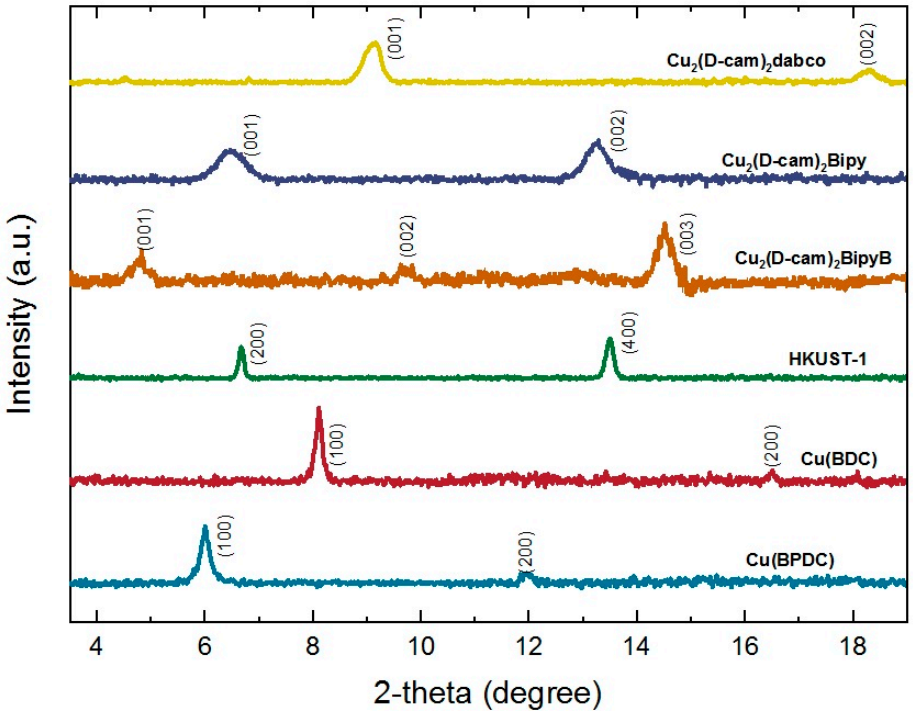

Figure S1. The X-ray diffractograms of the SURMOFs thin films of the sensor array used in the e-Nose system. e.g. $Cu_2(DCam)_2(dabco)$, $Cu_2(DCam)_2$ (BiPy), $Cu_2(DCam)_2$ (BiPyB), HKUST-1, Cu(BDC), Cu(BPDC). The data indicates crystalline. oriented growth of the MOF films with the targeted structure.

2. Frequency Shifts

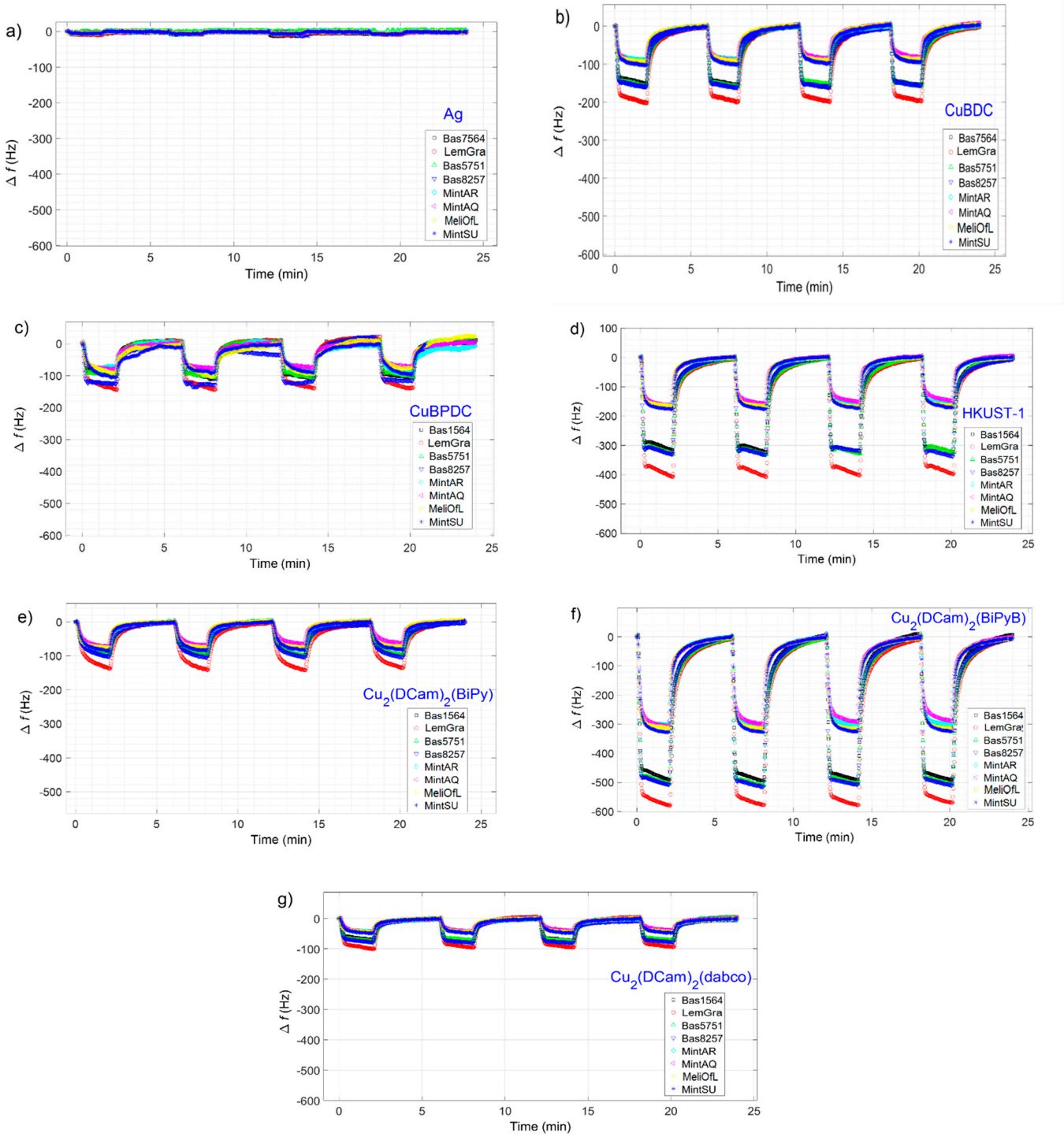

Figure S2. Resonance frequency shifts of the sensor array with 7 different sensing materials (see Table 1 for abbreviations) during 4 cycles of exposure to the individual Basel/Mint/Lemon Grass/Melissa O.L. leaves.

3. Nonlinear Least Square Fit

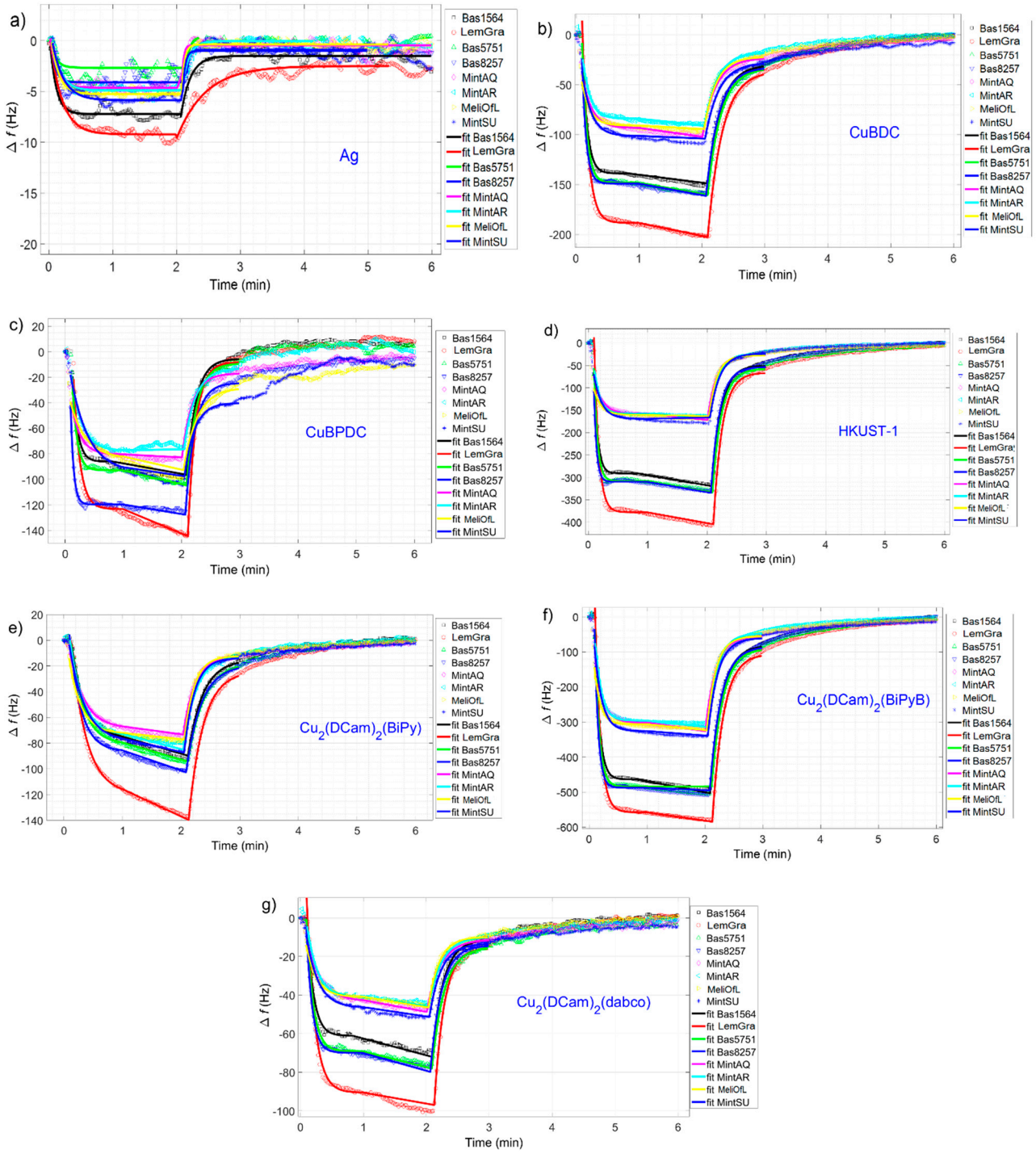

Figure S3. Nonlinear Least square fit to an exponential rise function describing (Adsorption process) and an exponential drop function as (desorption process) to find response time values of the sensor array.

Table S1. The response times calculated from Nonlinear Least square fit to an exponential rise function describing (Adsorption process) and an exponential drop function as (desorption process).

Sensor array	Bas1564 5τ(s)		LemGra 5τ (s)		Bas5751 5τ (s)		Bas8257 5τ (s)		MintAQ 5τ (s)		MintAR 5τ (s)		MeliOfL 5τ (s)		MintSU 5τ (s)	
	Ads.	Des.	Ads.	Des.	Ads.	Des.	Ads.	Des.	Ads.	Des.	Ads.	Des.	Ads.	Des.	Ads.	Des.
Ag	23.6	61.2	43.0	75.3	10.9	31.5	8.4	27.1	34.2	13.5	20.7	50.9	27.3	14.2	73.4	21.4
Cu(BDC)	23.1	61.9	28.2	58.4	22.4	62.2	19.4	59.3	45.4	62.3	35.8	62.9	39.1	58.8	44.1	62.1
Cu(BPDC)	26.4	47.1	32.9	39.8	24.0	48.3	15.5	46.4	47.3	53.6	55.5	59.2	78.8	77.3	91.2	51.5
HKUST-1	17.8	43.6	23.1	43.1	17.4	45.4	13.5	42.7	42.0	44.1	28.6	45.0	37.4	42.6	39.9	45.5
$Cu_2(Dcam)_2(BiPy)$	64.8	75.3	78.6	74.3	66.3	80.9	59.2	76.8	76.6	57.5	66.8	64.9	62.5	50.9	79.8	52.8
$Cu_2(Dcam)_2(BiPyB)$	23.3	56.3	27.8	57.5	22.2	58.3	18.6	57.9	40.2	50.7	32.2	53.2	30.5	45.8	38.5	51.3
$Cu_2(Dcam)_2(dabco)$	31.1	51.5	38.5	46.9	31.5	55.8	27.4	51.3	66.3	62.5	49.6	62.6	49.9	50.6	56.9	55.6

4. Change in the k-NN accuracies with increasing number of nearest neighbor

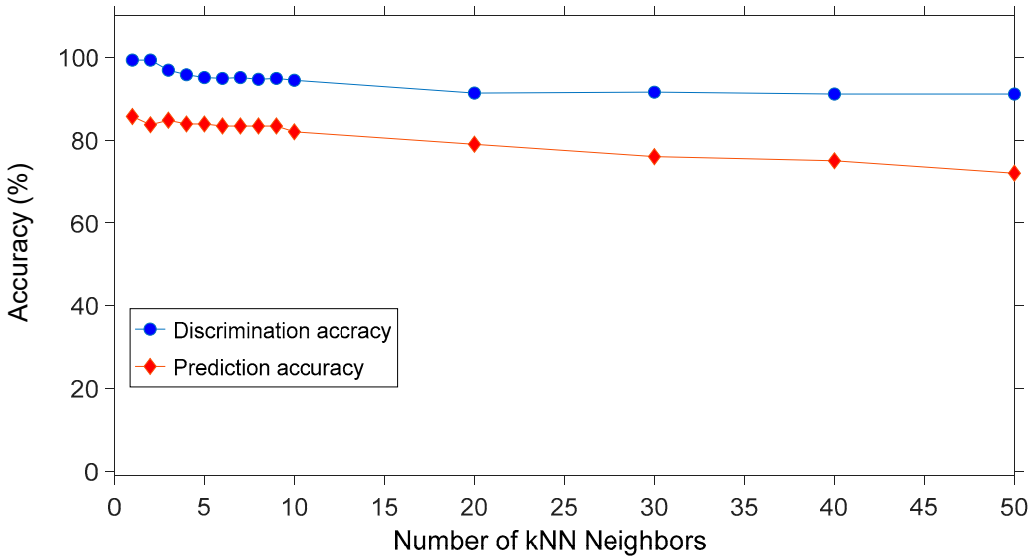

Figure S4. The change in the k-NN discrimination and prediction accuracies with increasing number of nearest neighbor between 2 and 50.