Electronic Supplementary Information

Detection of Sulfur Mustard Simulant by Trisaryl Phosphoric Triamide-Based Resin Using Quartz Crystal Microbalance Sensor

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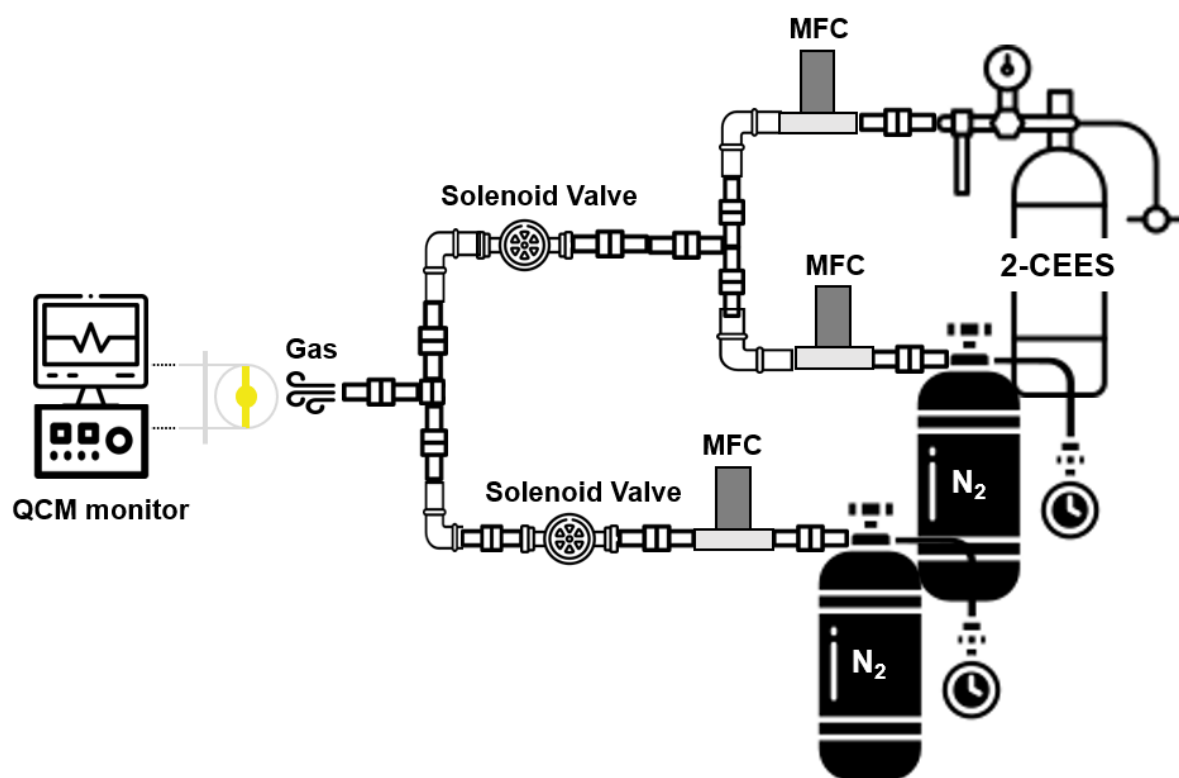*E-mail : songcs@skku.edu

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Figure S1. The custom-designed gas line and QCM setup employed for measuring 2-CEES gas in our experiments.
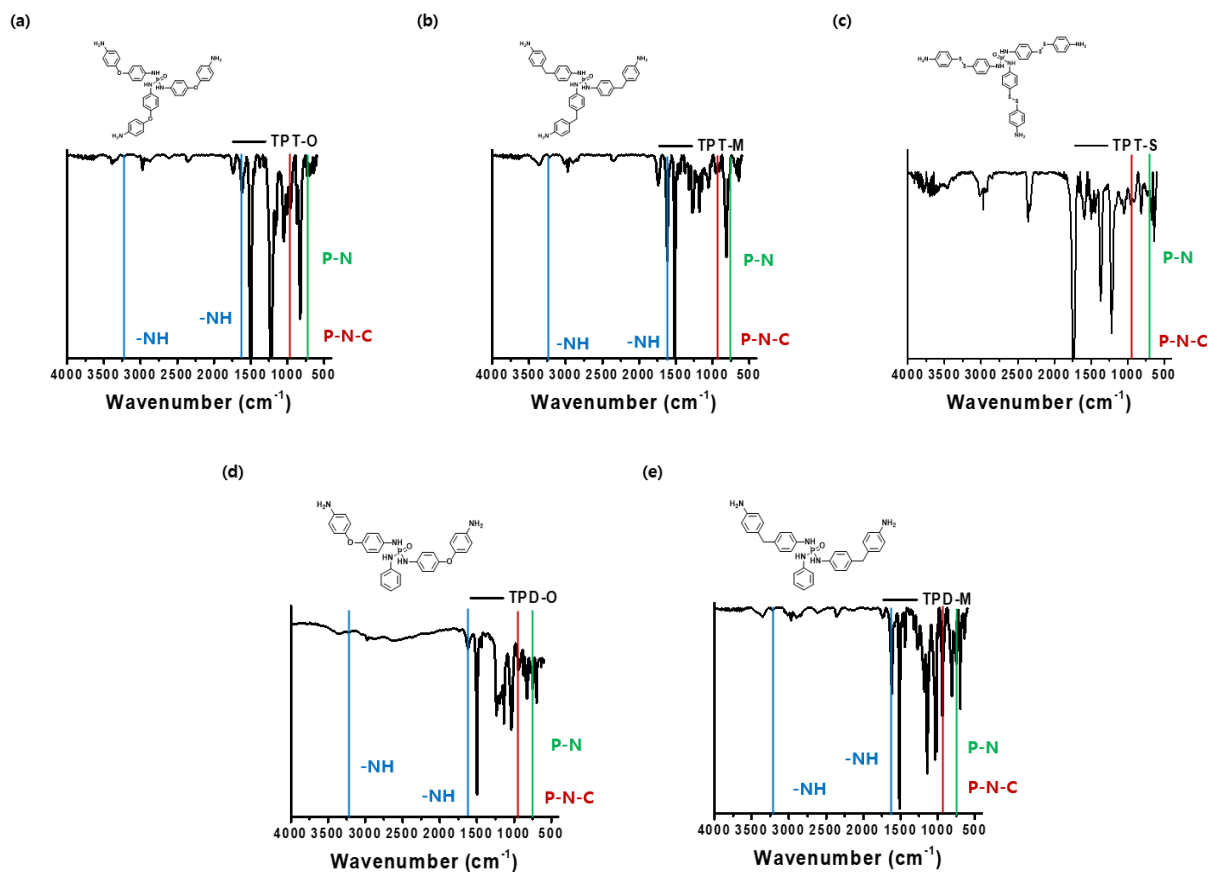
Figure S2. FT-IR spectra after the first synthetic process: (a) TPT-O, (b) TPT-M, (c) TPT-S, (d) TPD-O, and (e) TPD-M.. The absorption peaks were noted at 954 cm^{-1}, 760 cm^{-1}, 1623^{-1} and 3215cm^{-1} which were assigned for the bending vibration peaks of P-N-C, P-N, -NH, and the stretching vibration absorption of -NH, respectively.
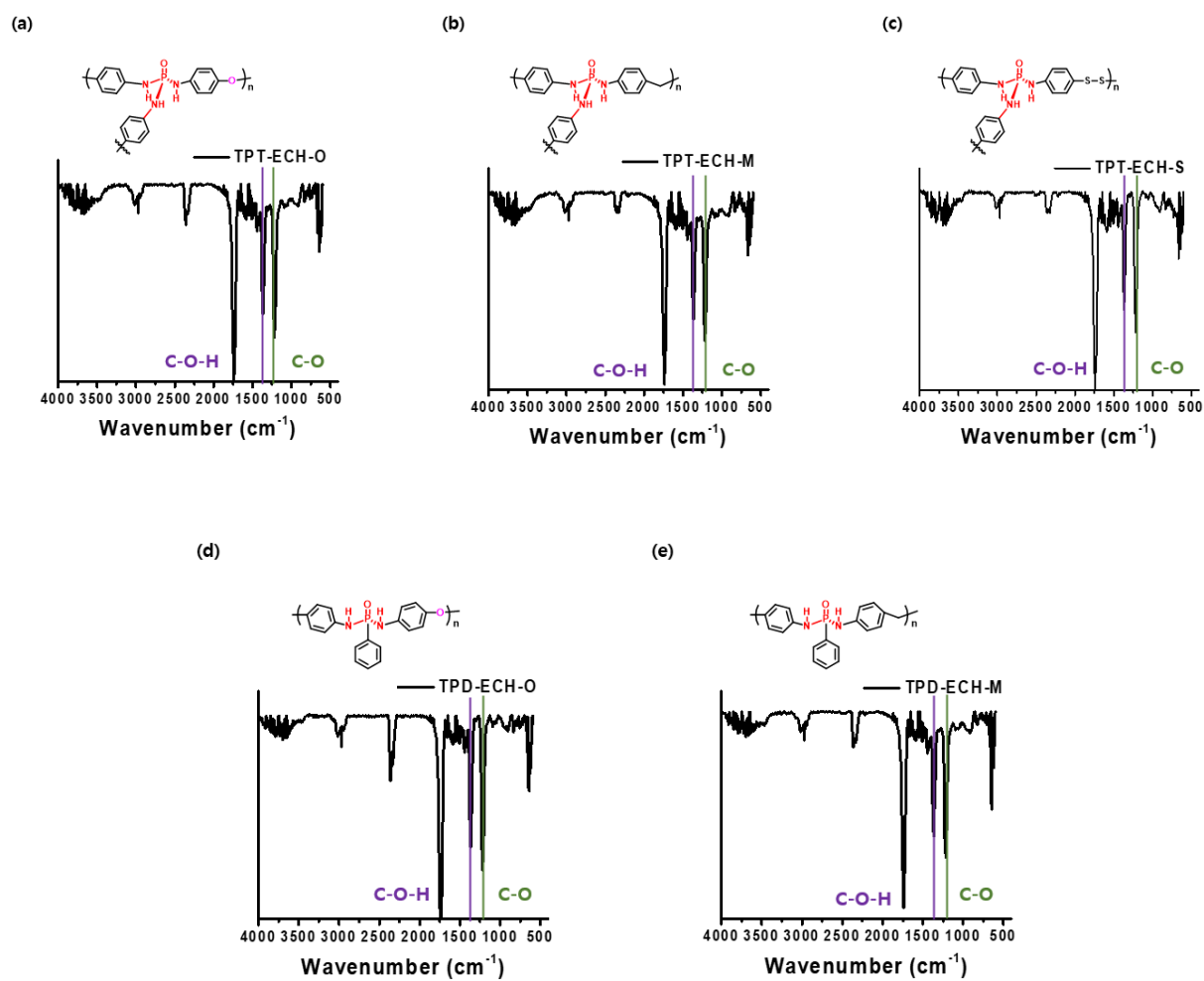
Figure S3. FT-IR spectra after the epoxy curing reaction: (a) TPT-ECH-O, (b) TPT-ECH-M, (c) TPT-ECH-S, (d) TPD-ECH-O, and (e) TPD-ECH-M. The absorption peaks were noted at 1365 cm^{-1} and 1221cm^{-1} which were assigned for the bending vibration peaks of C-O-H and C-O, respectively.
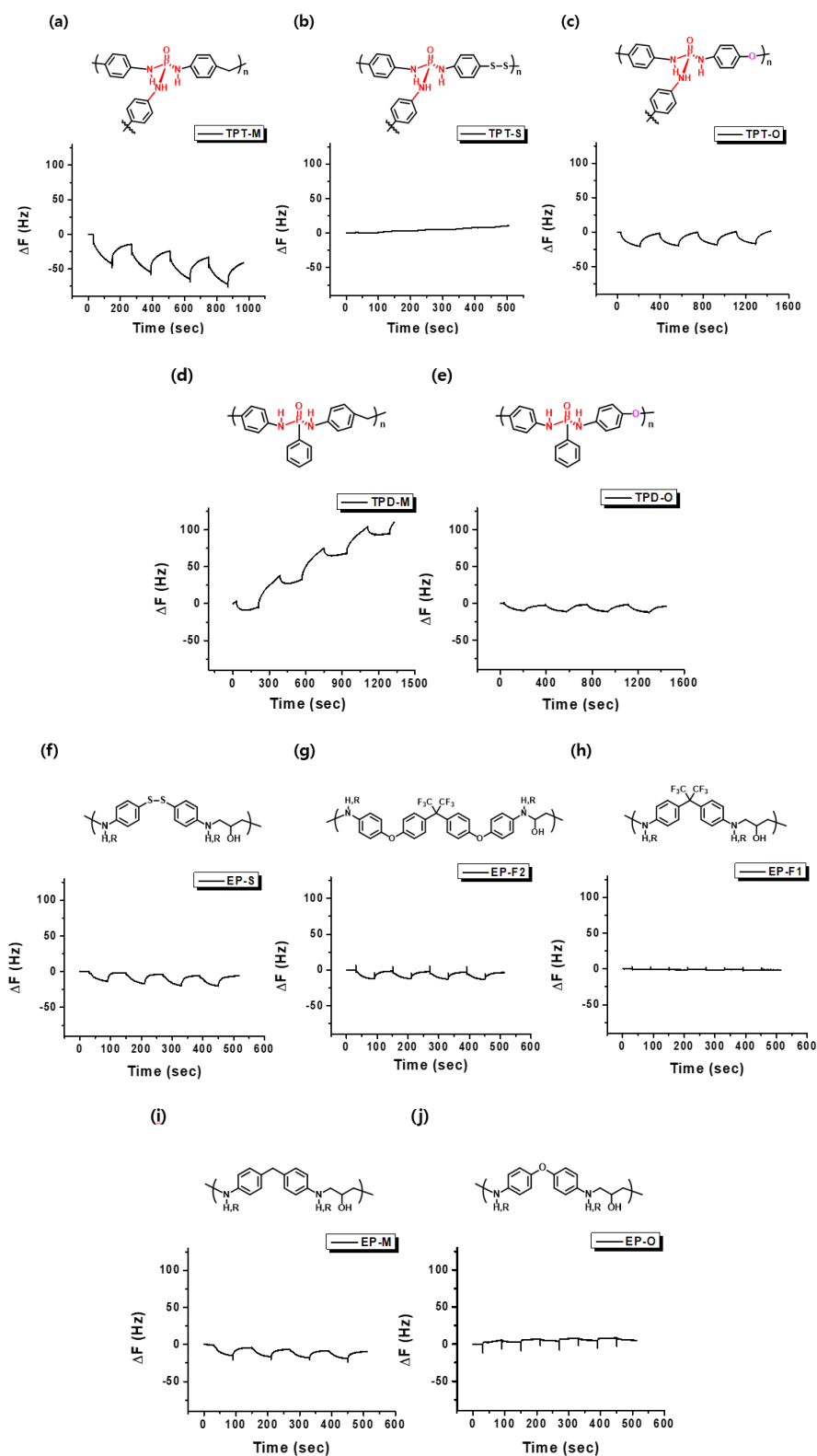
Figure S4. Comparison of QCM signals of TPT-M (a), TPT-S (b), TPT-O (c), TPD-M (d), TPD-O (e), EP-S (f), EP-F2 (g), EP-F1 (h), EP-M, and EP-O (j) for 10 ppm of 2-CEES gas.

The Langmuir-isotherm analysis for the response of the receptors

The adsorption process of 2-CEES on each receptor can be described as follows, assuming non-dissociative adsorption of 2-CEES.

The equilibrium constant for 2-CEES adsorption (K) can be expressed in relation to the surface coverage (θ) and partial pressure of 2-CEES (P) as follows:

$$K = \theta \ (1-\theta)P$$

Rearrangement of this equation gives,

$$\theta = KP \ 1+KP$$

and taking the reciprocal of both side of equation gives,

$$1/\theta = (1 \ / \ K)(1/ \ P) +1$$

The surface coverage (θ) represents the ratio of adsorbed molecules on the surface to the number of molecules in a monolayer covering the surface sites, and it can be expressed in terms of ΔF as follows:

$$\theta = \Delta F \ / \ \Delta F_{Max}$$

When ΔF_{Max} represents the frequency change (ΔF) measured during QCM experiments when the receptor surface was fully covered with a monolayer of 2-CEES molecules, combining equations yields the linear relationship between ($1/\Delta F$) and ($1/P$) as follows:

$$1 \ / \ \Delta F = (1 \ / \ \Delta F_{Max} \times K \ )1 \ / \ P + 1 \ / \ \Delta F_{Max}$$

For each receptor case, the reciprocal of the 2-CEES concentration ($1/P$) was plotted against the inverse of ΔF ($1/\Delta F$) at each 2-CEES concentration, and each dataset was fitted using the linear least squares regression method. From the slope ($1/(\Delta F_{Max} \times K)$) and Y-axis intercept ($1/\Delta F_{Max}$) of the line fitted to each dataset, the equilibrium constant (K) of 2-CEES adsorption and ΔF_{Max} values were derived.

Additionally, we computed the Gibbs free energy change (ΔG^o) of 2-CEES adsorption using the following equation:

$$\Delta G^o = -RT\ln K$$

Where R represents the gas constant (8.314 J/mol·K), T denotes the absolute temperature in Kelvins, and K is the adsorption constant.

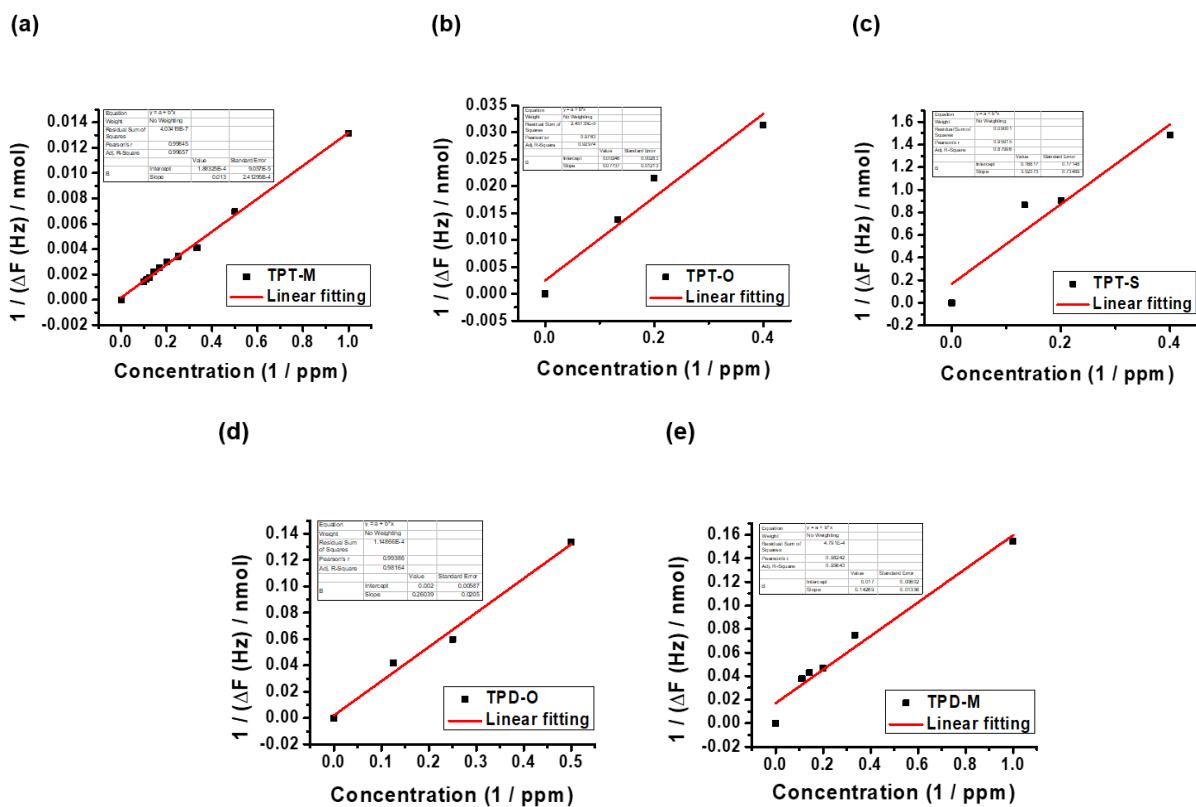**Figure S5.** Langmuir linear fitting data of receptors.

	$\triangle F_{max}$	K	$\triangle G°$	R^2
TPT-M	$5.31 * 10^3$	$1.42 * 10^{-2}$	$2.47 * 10^3$	0.998745
TPT-O	$4.03 * 10^2$	$3.23 * 10^{-3}$	$1.42 * 10^4$	0.92974
TPT-S	$5.95 * 10^0$	$4.71 * 10^{-2}$	$7.58 * 10^3$	0.87998
TPD-O	$5.00 * 10^2$	$7.70 * 10^{-3}$	$1.21 * 10^4$	0.98164
TPD-M	$5.88 * 10^1$	$1.19 * 10^{-1}$	$5.25 * 10^3$	0.95653
EP-S	N/A	N/A	N/A	N/A
EP-F2	N/A	N/A	N/A	N/A
EP-F1	N/A	N/A	N/A	N/A
EP-M	N/A	N/A	N/A	N/A
EP-O	N/A	N/A	N/A	N/A

Table S1. Langmuir isotherm fitting data of TPT-M receptor.