Supporting Information

Chemical Emissions from Organic Light-Emitting Diode Screens during Use and Thermal Treatment

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MATERIALS AND METHODS

Section S1. Screen Samples

The OLED screens had an active display area of 259.0 × 175.0 mm (measured), a typical brightness of 400 cd m^{-2}, and a resolution of 1920 (RGB) × 1080 pixels. The screen weight is 67.28 g, with a density of 1484.44 g/m^2. The power supply unit delivered 66 W (11 V, 6 A) via a USB interface. The five screens were all sourced from the same manufacturer, brand, and batch. This study employed only one commercially available OLED screen type, which may limit sample representativeness. The screen structure and major component/materials categories included substrate (glass or polymer[1]), electrode layer (indium tin oxide[2]), functional layers, encapsulation layer (epoxy resin or UV adhesive)[3, 4], polarizer (PVA/TAC) or optical film, protective film (PET, PC), flexible printed circuits (FPCs) (PI, PET), and connectors (PVC). Accordingly, the present analysis should be regarded as an initial characterization based on one commercially available OLED screen sample, rather than as broadly representative of all OLED screens.

Section S2. Instrumental Analysis

The instrumental conditions for gas chromatography–high-resolution mass spectrometry (GC–HRMS) followed a previously established method.[1] Briefly, analyses were performed using a Q–Exactive mass spectrometer coupled to a Trace 1310 gas chromatograph and a TriPlus RSH autosampler (all from Thermo Fisher Scientific, Waltham, MA, USA). Separation was achieved using a TraceGOLD TG-5SiLMS semi-polar column (30 m × 0.25 mm i.d., 0.25 µm film thickness; Thermo Fisher Scientific). The GC oven temperature program was: 70 °C (0.5 min), ramp to 80 °C at 10 °C min^{-1}, ramp to 310 °C at 6 °C min^{-1}, and hold at 310 °C for 10.2 min. The mass spectrometer was operated in electron ionization (EI) mode. Data were acquired in full-scan mode over a mass range of m/z 50–500 at a resolving power of 60,000 (at m/z 200).

Section S3. Data Processing

In this study, suspect screening was conducted for compound identification using Compound Discoverer (v3.3; Thermo Fisher Scientific) against the NIST and Wiley mass spectral libraries. Preliminary candidate compounds were first screened using library match criteria of Score ≥ 90 and SI ≥ 750. To further support assignment, a C8–C40 n-alkane standard mixture (1 ppm) was analyzed alongside the sample batches, and experimentally measured retention indices (RIs) were calculated in the software. For candidate compounds with reference RI values available in the libraries, RI agreement was evaluated using the relative RI deviation, defined as $|RI_{measured} - RI_{reference}| / RI_{reference} \times 100\%$. For candidate compounds lacking experimental RI values in the libraries, RI values were additionally predicted using the Multimodal Machine Learning model developed by Matyushin et al,[5] and the predicted RI values were compared with the experimentally measured RI values as an auxiliary criterion for assignment. A relative RI deviation threshold of 10% was used as an upper screening criterion for RI-assisted candidate filtering. Candidate compounds supported by both library matching and RI agreement, but lacking confirmation by authentic standards, were assigned CL2, whereas compounds meeting the library match criteria but lacking usable RI information for RI-based filtering were assigned CL3. Selected candidates were further confirmed using authentic standards. Compounds that met the mass spectral and RI criteria and matched the retention time/RI of the authentic standard were assigned CL1.

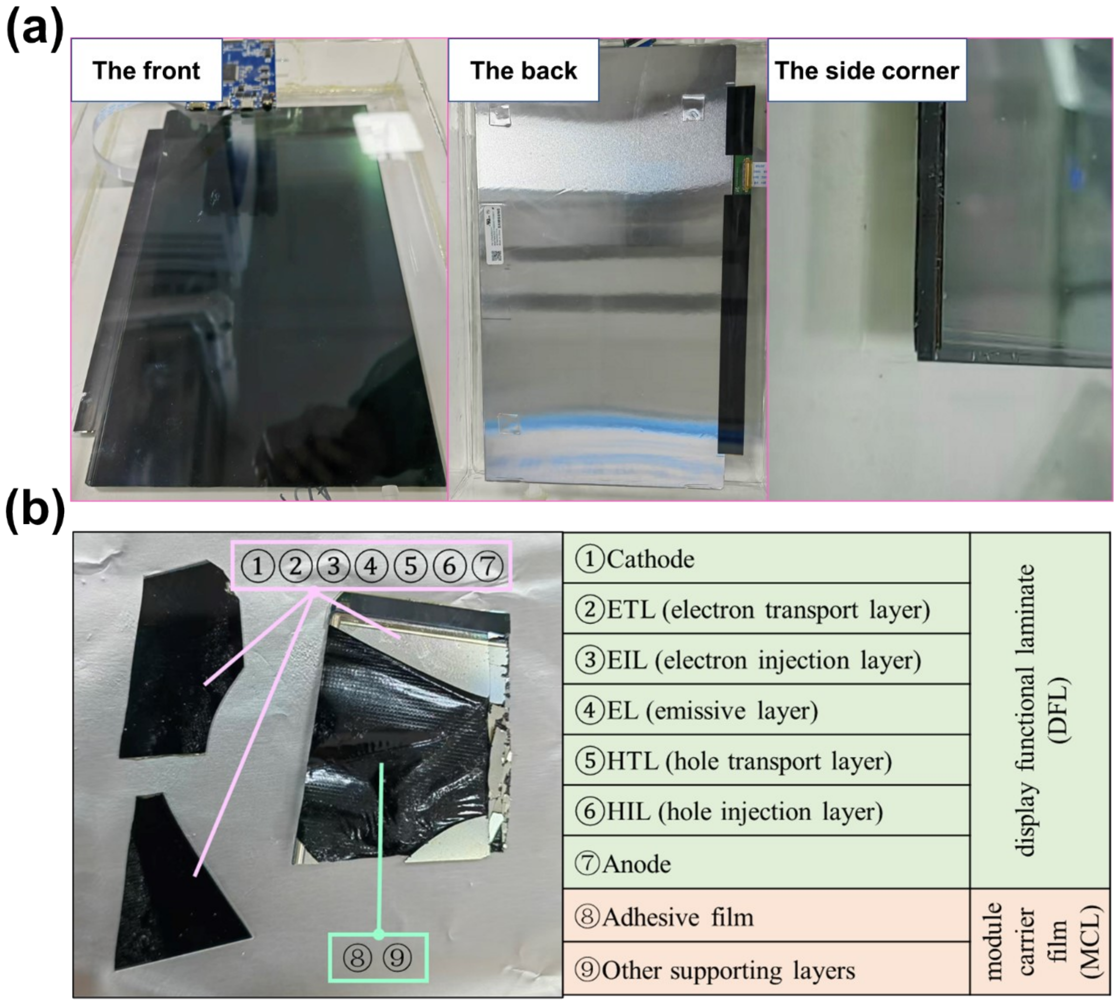

Figure S1. Physical appearance and structure of the OLED screen. (a) Front view, back view, and side corners of the screen and (b) Illustration of the manual separation of the module carrier film (MCL) and display functional laminate (DFL).

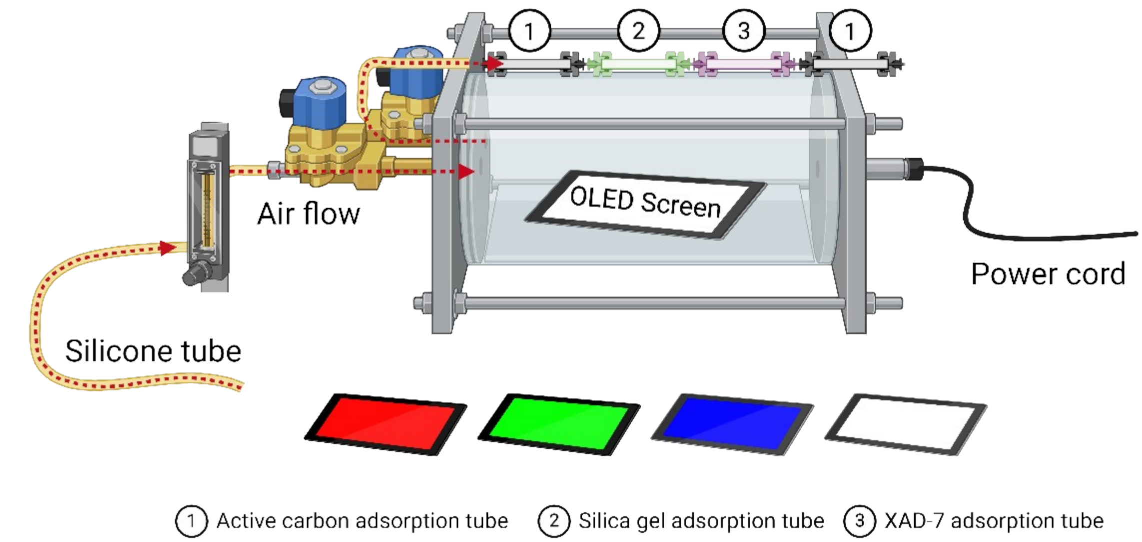

Figure S2. Schematic of the custom-built compound-collection device used to capture emissions from OLED screens during normal operation.

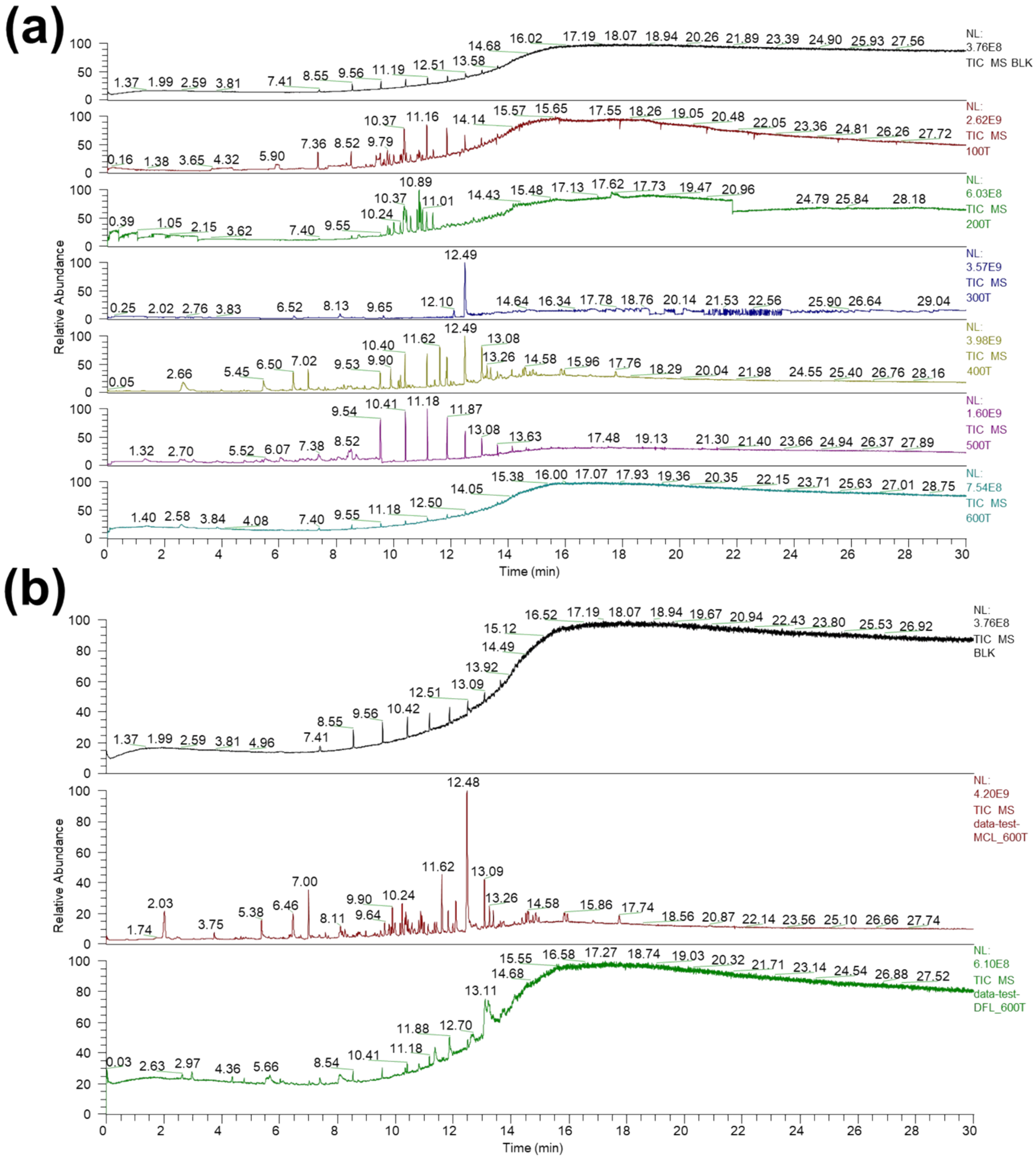

Figure S3. Chromatograms of samples under different pyrolysis conditions: (a) temperature-programmed pyrolysis and (b) high-temperature pyrolysis.

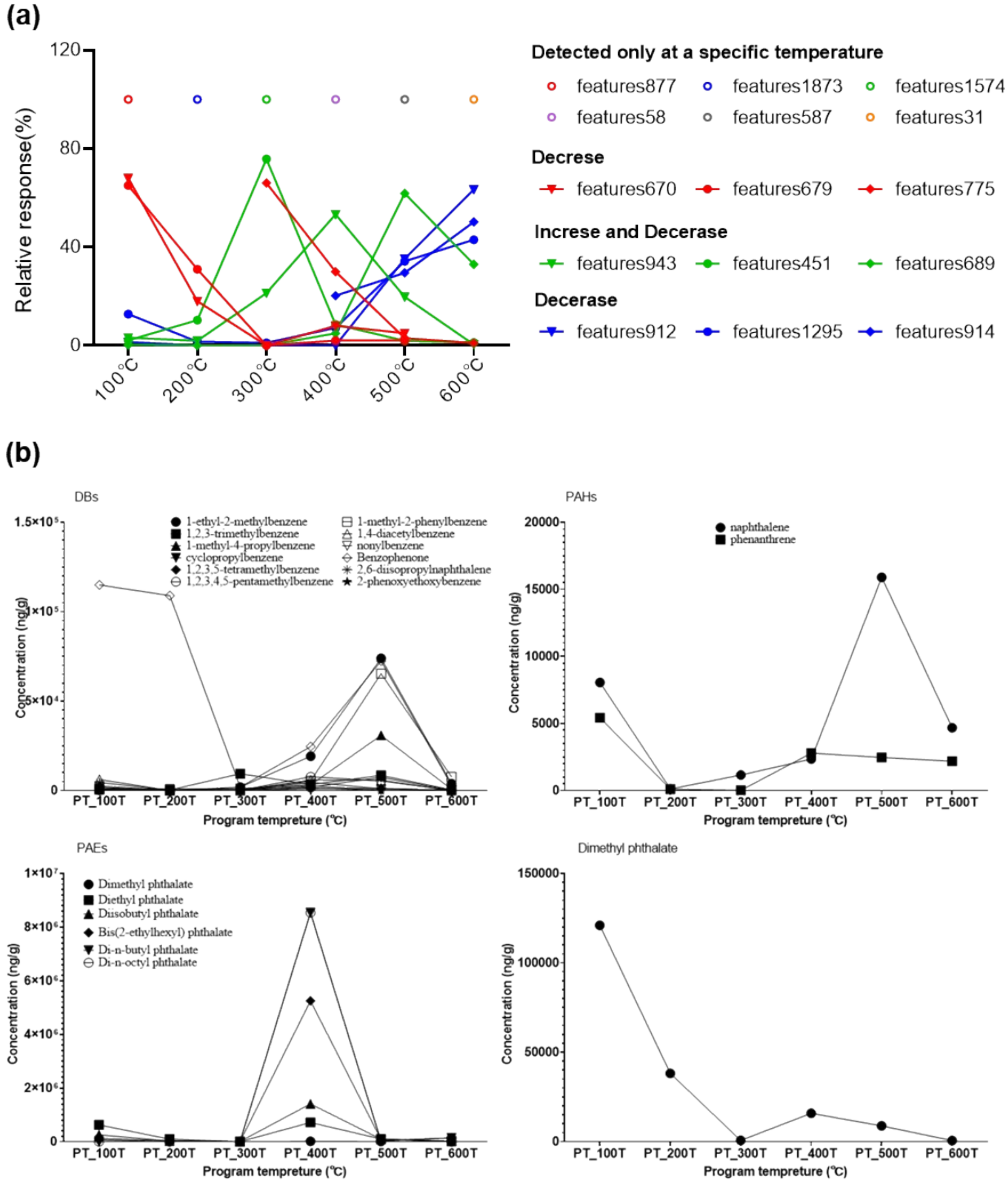

Figure S4. (a) Representative features illustrating distinct emission patterns across the TP-py process and (b) release trends of CL1 compounds across the TP-py process.

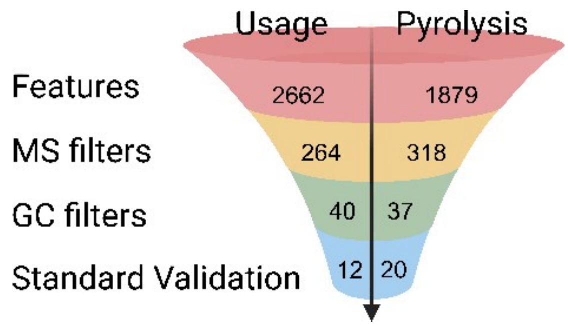

Figure S5. Stepwise data-processing workflow for suspect screening, showing the number of detected features, retained candidates, and compounds confirmed by authentic standards at each step.

Name	MS match score					RI		
	Total Score	HRF Score	RHRF Score	SI	RSI	Calculated RI	Predicted RI	delta RI
Naphthalene, 1-(2-propenyl)-	91.3	81.8	85.4	839	855	1398	1452.11	3.7%

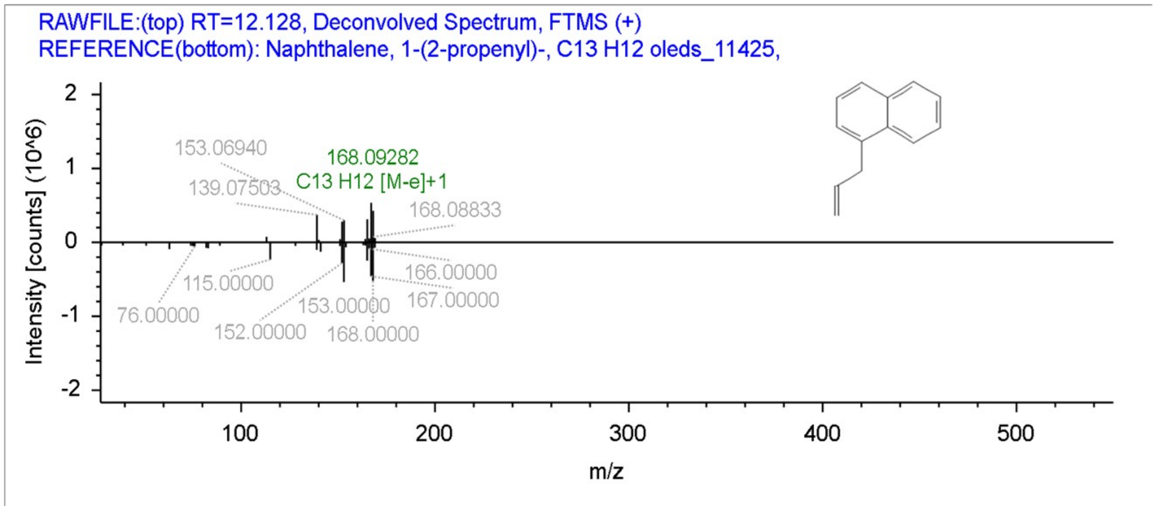

Figure S6. Tentative identification of an OLED-related chemical in pyrolysis treatment using an in-house established OLED-chemical spectral database.

REFERENCE

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