Supporting Information

Three-Dimensional Zeolitic Imidazolate Framework-8 as Sorbent Integrated with Active Capillary Plasma Mass Spectrometry for Rapid Assessment of Low-Level Wine and Grape Quality-Related Volatiles

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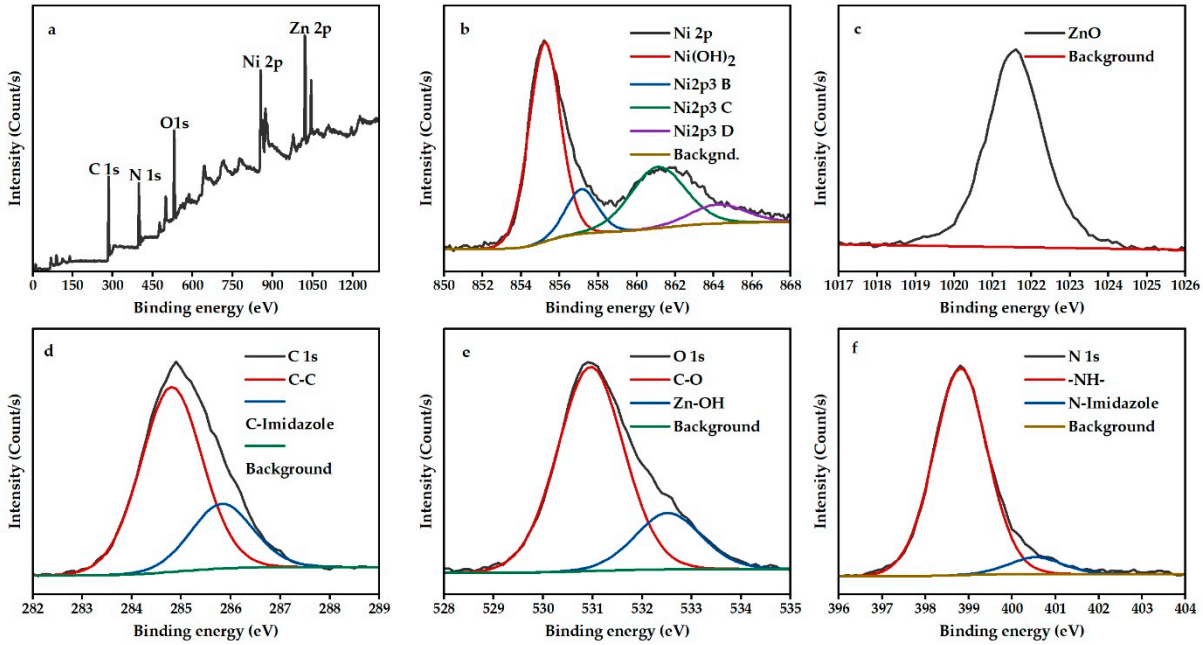


Figure S1. Surface elemental binding energies & distributions: (a) XPS survey spectrum of ZIF-8/NF, high-resolution and energy spectra of ZIF-8/NF (b) Ni 2p, (c) Zn 2p, (d) C 1s, (e) O 1s and (f) N 1s regions.

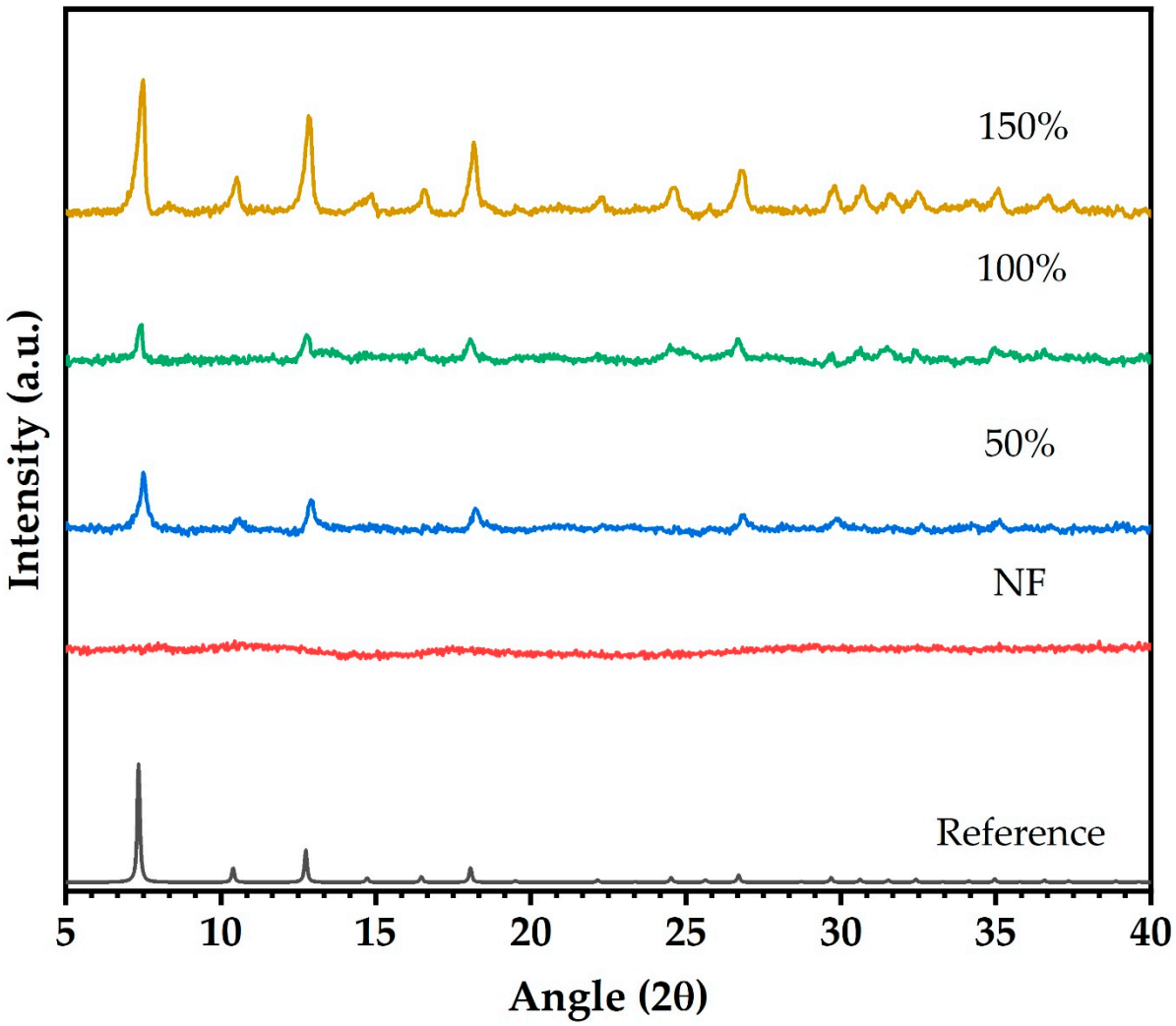


Figure S2. XRD patterns of ZIF-8/NF using different weight percent with identical mole ratio.

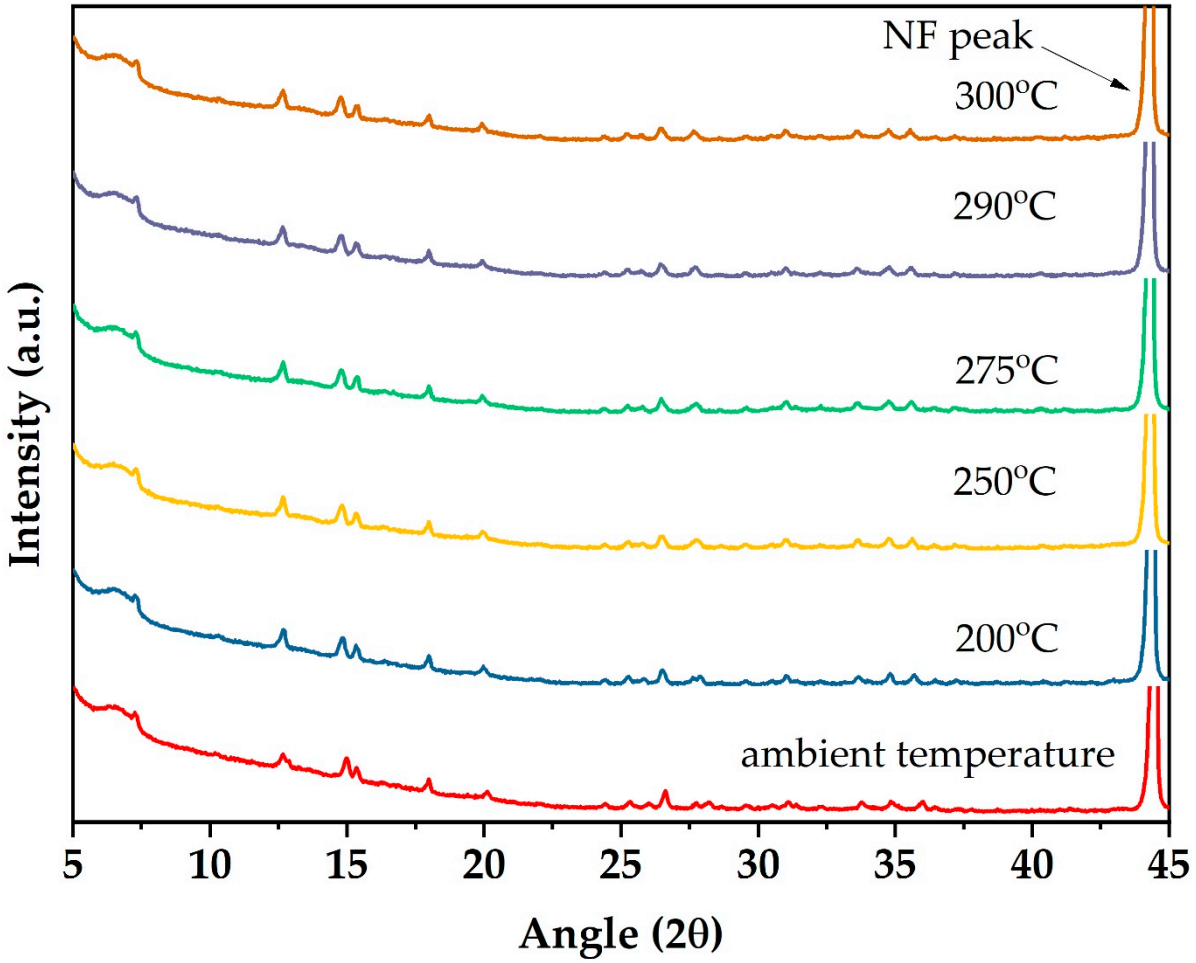


Figure S3. Temperature dependent study of ZIF-8/NF using non-ambient XRD technique.

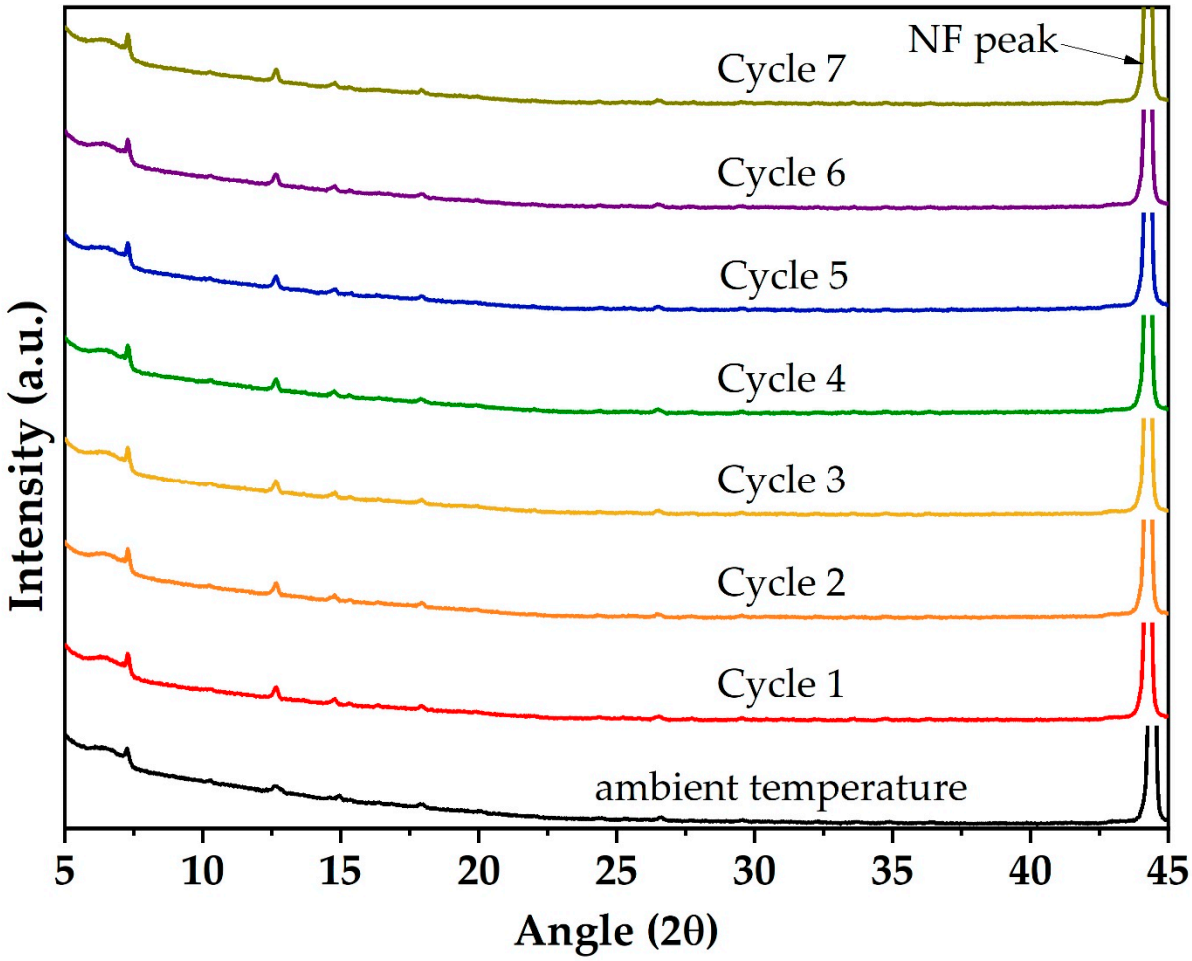
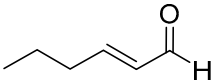
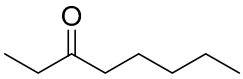
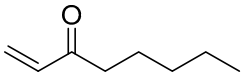
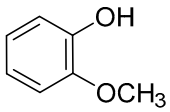
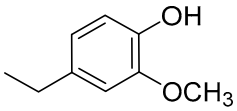


Figure S4. Non-ambient XRD patterns of ZIF-8/NF at 280°C for 7 repeated cycles.

Table S1. The calibration using TD-GC/MS.

Compound	Tenax-TA				ZIF-8/NF			
	Calibration range (ng/L)	Calibration equation	R^2	LOD (ng/L)	Calibration range (ng/L)	Calibration equation	R^2	LOD (ng/L)
1-octen-3-ol	0.89 – 8.05	$y = 5197x - 4161$	0.977	2.7	0.89 – 8.05	y = 1955x – 713	0.980	4.5
1-octen-3-one	0.85 – 7.66	$y = 5042x - 3642$	0.992	2.6	0.85 – 7.66	y = 1636x – 733	0.992	2.6
3-octanone	0.87 – 7.84	$y = 4256x - 1906$	0.990	2.6	0.87 – 6.10	y = 4788x – 1410	0.994	2.6

Table S2. List of common phytosanitary volatiles in grapes and wines.

Analytes	Chemical Structure	Vapor pressure (mmHg) at 25°C
(E)-2-Hexenal		4.60E+00
3-Octanone		2.00E+00
1-Octen-3-one		1.10E+00
Guaiacol		7.60E-02
4-Ethylguaiacol		1.70E-02

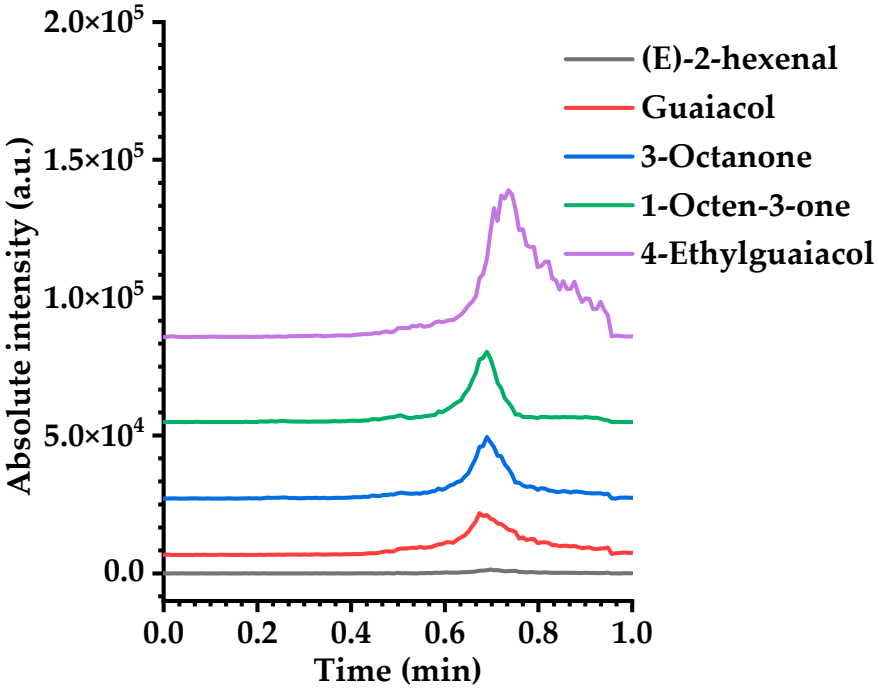


Figure S5. The extracted chromatogram at 280°C desorption temperature using ZIF-8/NF.

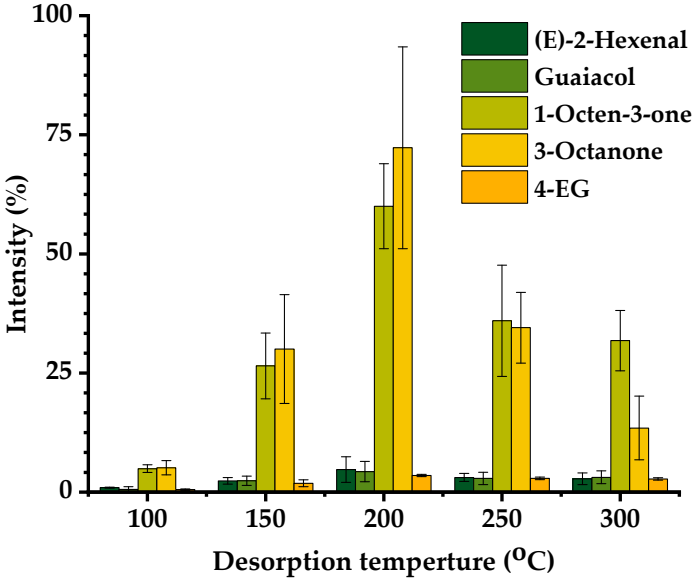


Figure S6. Desorption temperature dependent study of selected analytes using

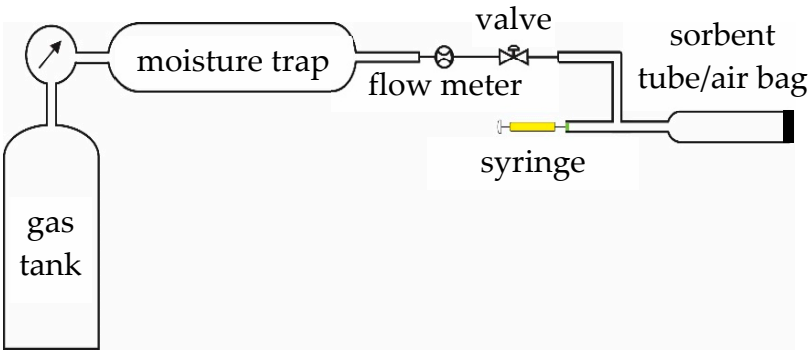


Figure S7. Schematic diagram for gas sampling.

The customized gas sample set up has thermal block with a digital temperature controller. The thermal block fits with Swagelok® Tube Fitting, union tee, ¼" tube OD. One end is capped with stainless steel plug for ¼" and 11-mm high temperature resistant GC inlet septa (Agilent, Australia). This part served as the sample injector/inlet. The second end is connected to a high purity nitrogen gas that passes through from moisture trap and digital airflow controller. The third end is the volatile outlet which can be connected to sample gas bag or thermal desorption tube.