Development of a QuEChERS-Based Method for the Determination of Carcinogenic 2-Nitrofluorene and 1-Nitropyrene in Rice Grains and Vegetables: A Comparative Study with Benzo[*a*]pyrene

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Table S1. Linear Regression Parameters of the Calibration Curves and Limit of Quantitation (LOQ) of the Developed HPLC-FLD Method.

NPAHs/PAHs	Log K_{ow}[a]	TEF[b]	Linear range (mg/L)	R^2	LOQ (μg/L)	LOQ_m[c] (μg/kg)	LOD_m (μg/kg)
2-Nitrofluorene	3.37	0.01	0.005–1.01	0.9995	4.3	0.43	0.12
1-Nitropyrene	4.69	0.1	0.005-1.00	0.9994	2.5	0.25	0.08
Benzo[*a*]pyrene	6.30	1	0.005-1.02	0.9996	1.6	0.16	0.05

[a] Log K_{ow} is the octanol-water partition coefficient. [b]TEF is the toxicity equivalency factors. [c] The LOQ_m is the sample extract based on 10 g of sample.

Table S2. Comparison of d-SPE-Based QuEChERS Extraction Method with SPE Method for Rice and Vegetable Analysis.

	QuEChERs method			SPE method		
	Rice	Celery	Cabbage	Rice	Celery	Cabbage
2-Nitrofluorene	0.69±0.03	<LOQ	ND	0.78±0.04	ND	ND
1-Nitropyrene	<LOQ	25.27±2.37	0.51±0.07	<LOQ	25.42±2.32	0.45±0.02
Benzo[*a*]pyrene	0.22±0.01	0.34±0.12	<LOQ	0.21±0.00	0.49±0.08	ND

The data represent mean ± SD for three independent determinations.

Table S3. Mean LB and UB Concentrations for 2-Nitrofluorene, 1-Nitropyrene, and Benzo[*a*]pyrene in each Food Categories (μg/kg).

	2-Nitrofluorene		**1-Nitropyrene**		**Benzo[*a*]pyrene**	
	LB	UB	LB	UB	LB	UB
Rice	0.82	0.88	0.49	0.53	0.39	0.43
Vegetable	0.38	0.51	0.46	0.49	0.33	0.36
root and tuberous	0.60	0.63	0.78	0.78	0.48	0.48
fruit	0.86	0.94	0.48	0.50	0.36	0.41
bulb and stem	0.02	0.22	0.24	0.34	0.44	0.44
leafy	0.02	0.22	0.31	0.35	0.15	0.19

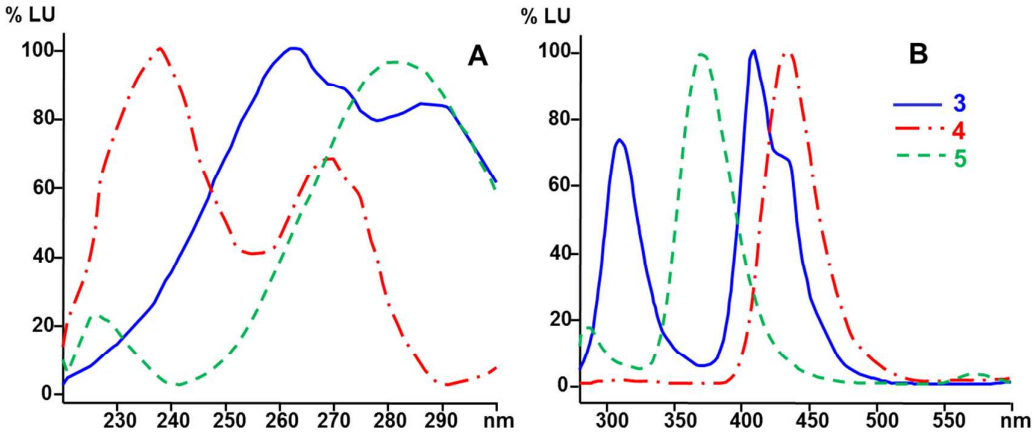

Figure S1. Fluorescence excitation (A) and emission (B) spectra of PAHs and the amino-PAHs formed by Fe/H^+-induced nitro-reduction of nitro-PAHs.

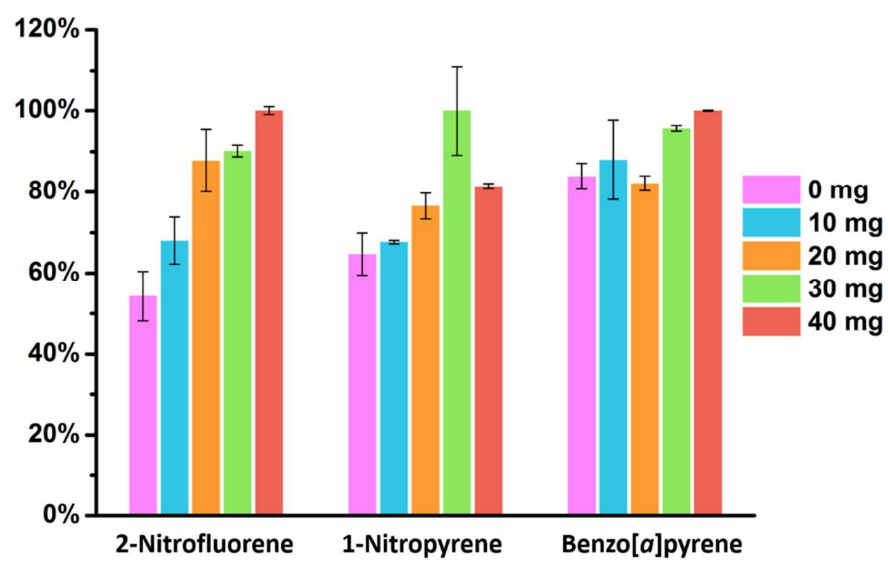

Figure S2. Effect of different amount of PSA on the recoveries of 2-nitrofluorene, 1-nitropyrene, and benzo[*a*]pyrene from sample extracts.

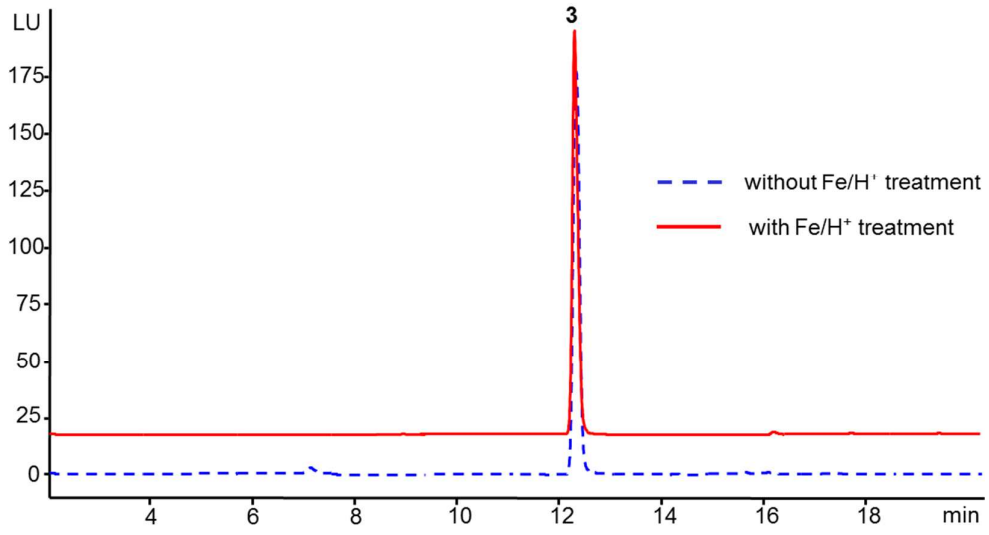

Figure S3. Effect of the Fe/H^+-treatment on benzo[*a*]pyrene concentration. The analysis showed benzo[*a*]pyrene was unaffected as the nitro-PAHs are being reduced to fluorescing amino-PAHs by the Fe/H^+-induced nitro-reduction.

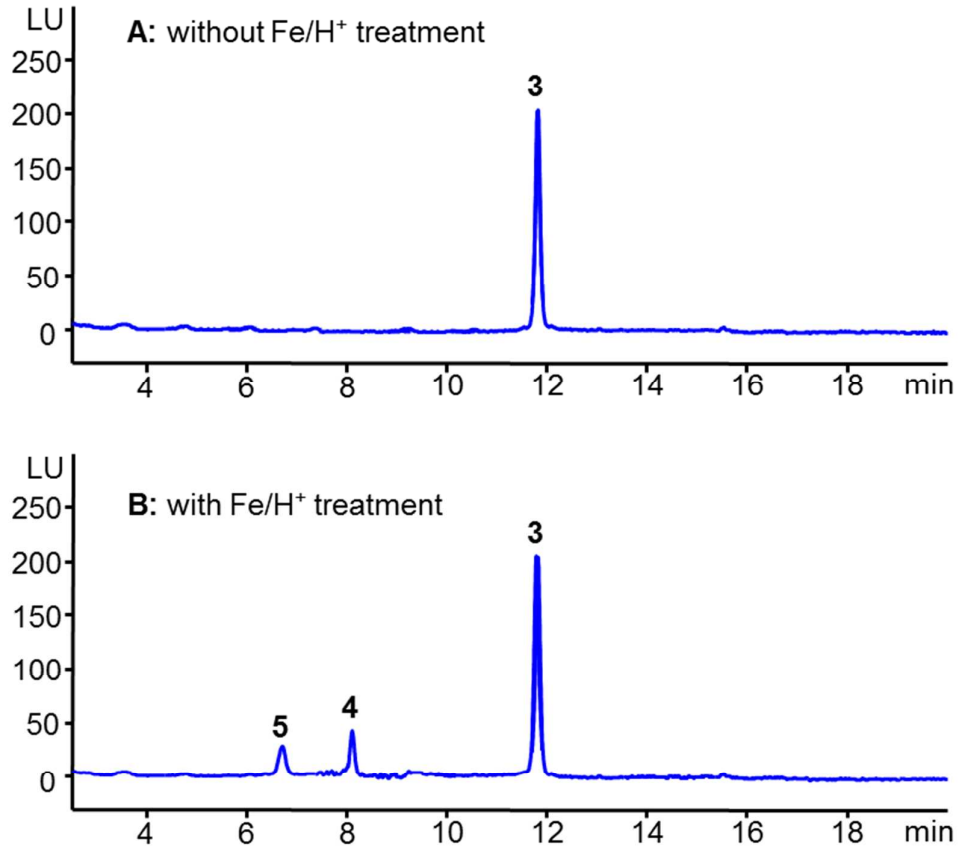

Figure S4. Chromatograms from HPLC-FLD analysis of vegetable sample with and without Fe/H^+ treatment.