Supplementary files for Inhibitory effects of selected dietary flavonoids on the formation of total heterocyclic amines and 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) in roast beef patties and in chemical models

Qin Zhu,[a] Shuang Zhang,[b] Mingfu Wang,[c] Jie Chen[b,d,*], and Zong-Ping Zheng[b,*]

[a]College of Life and Environmental Sciences, Hangzhou Normal University, Hangzhou, Zhejiang, 310036, People's Republic of China

[b]State Key Laboratory of Food Science and Technology, Jiangnan University, Wuxi, Jiangsu 214122, People's Republic of China

[c]School of Biological Sciences, The University of Hong Kong, Hong Kong, People's Republic of China

[d]Synergetic Innovation Center of Food Safety and Nutrition, Jiangnan University, Wuxi, Jiangsu, 214122, People's Republic of China

Validation of the method

Validation of the method

Linear regression was performed using the concentrations and peak area ratios of the standards and IS. The linear ranges were determined according to the regression correlation coefficient for each concentration range. The limit of detection (LODs) and limit of quantification (LOQs) were determined by diluting the standard solutions or the blank sample spiked with the HAs standards at concentration levels similar to a specified signal to noise (S/N) ratio (3 and 10 for the LODs and LOQs, respectively).

Table S1. Regression equation, linear ranges, correlative coefficient, limit of detection, limits of quantitation of seven HAs

HAAs	Regression line	Linear ranges (ng/mL)	Correlation coefficient (R^2)	Limits of detection (ng/g)	Limits of quantitation (ng/mL)
Norharman	y = 11.103x + 22.375	0.49~249.50	0.9915	0.056	1.09
1,5,6-TMIP	y = 10.168x + 53.458	0.99~508.00	0.9986	0.052	0.70
Harman	y = 31.679x + 34.792	0.36~183.75	0.9967	0.038	2.32
PhIP	y = 4.3468x + 148.46	0.86~442.50	0.9836	0.162	0.57
MeIQx	y = 32.913x + 17.958	1.01~517.00	0.9997	0.221	0.68
DMIP	y = 9.9411x - 0.0417	0.83~424.50	0.9975	0.065	0.48
4,8-DiMeIQx	y = 21.909x + 292.83	0.51~131.50	0.9889	0.029	0.29

Table S2. Recovery and RSD of seven HAs

HAs	Spiked level					
	1 ng/g		2 ng/g		4 ng/g	
	recovery（%）	RSD（%）	recovery（%）	RSD（%）	recovery（%）	RSD（%）
Norharman	67.7	3.3	85.5	3.3	90.0	8.2
1,5,6-TMIP	70.5	6.7	62.3	8.2	65.5	5.5
Harman	80.5	12.6	66.7	5.4	82.2	5.2
PhIP	67.2	3.6	59.9	5.8	54.8	7.2
MeIQx	83.1	3.5	70.7	6.0	80.9	20.2
DMIP	35.2	3.2	25.4	6.9	18.2	5.8
4,8-DiMeIQx	74.3	4.8	60.2	5.2	53.5	6.5

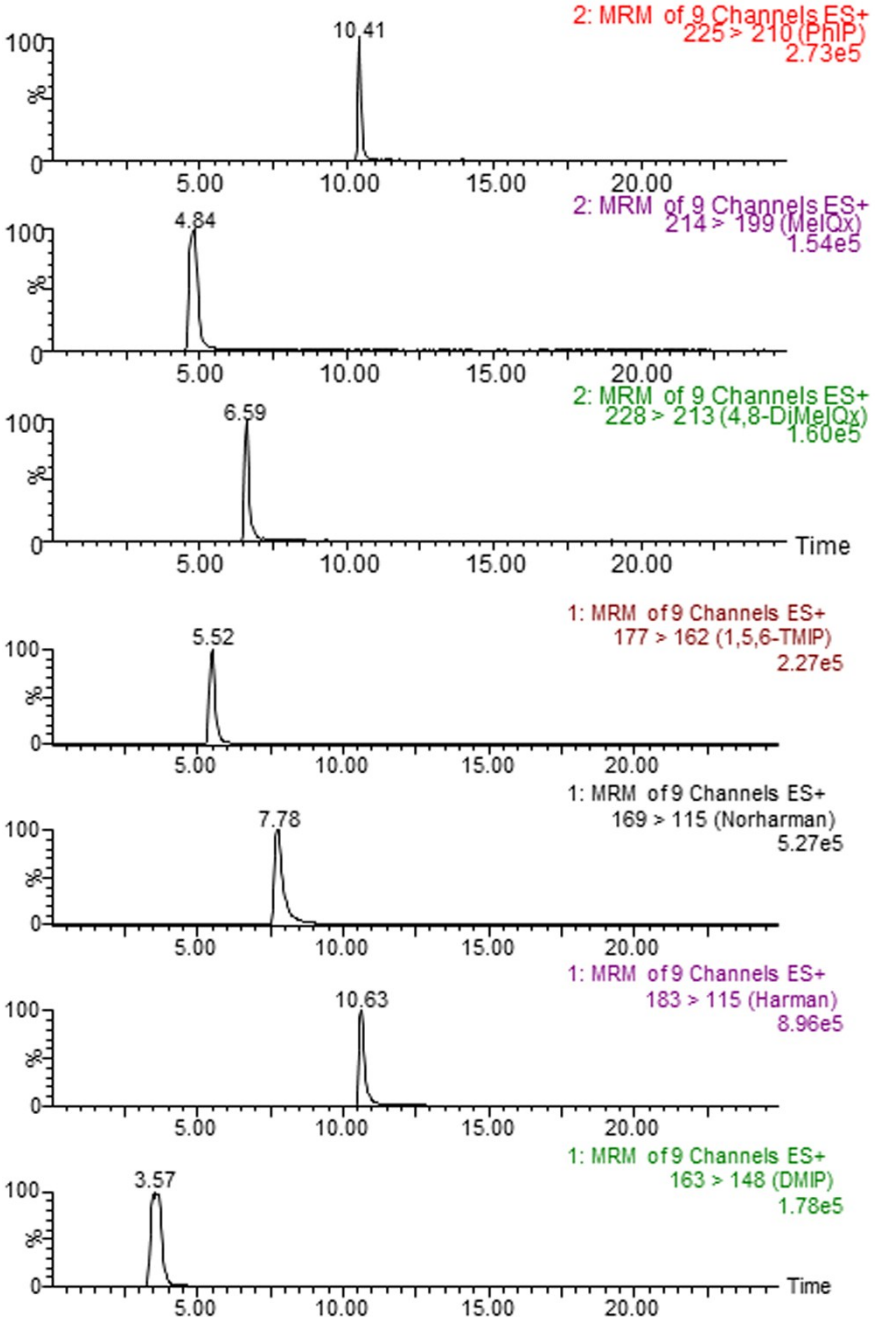

Figure S1. MRM chromatogram of seven heterocyclic amines standards

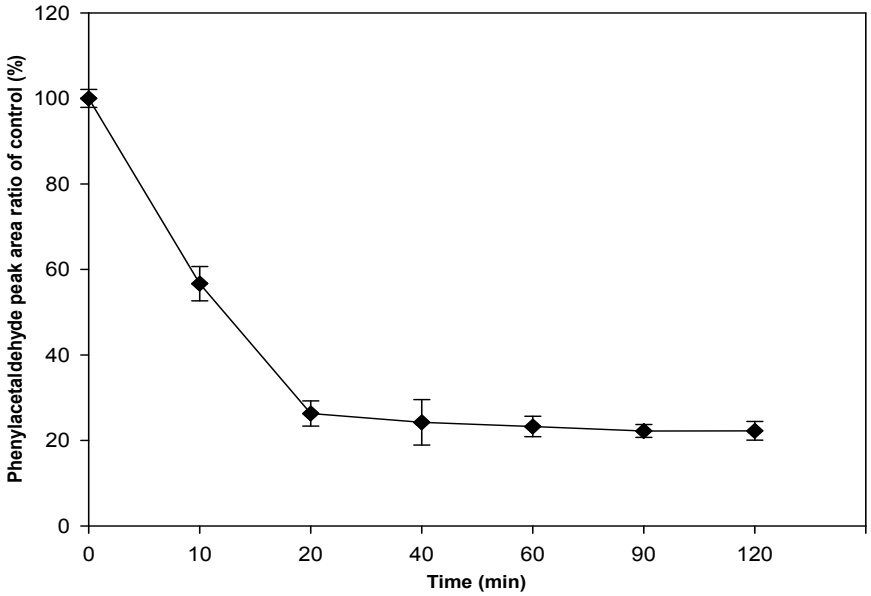

Figure S2. Changes in the relative content of phenylacetaldehyde with time in model system

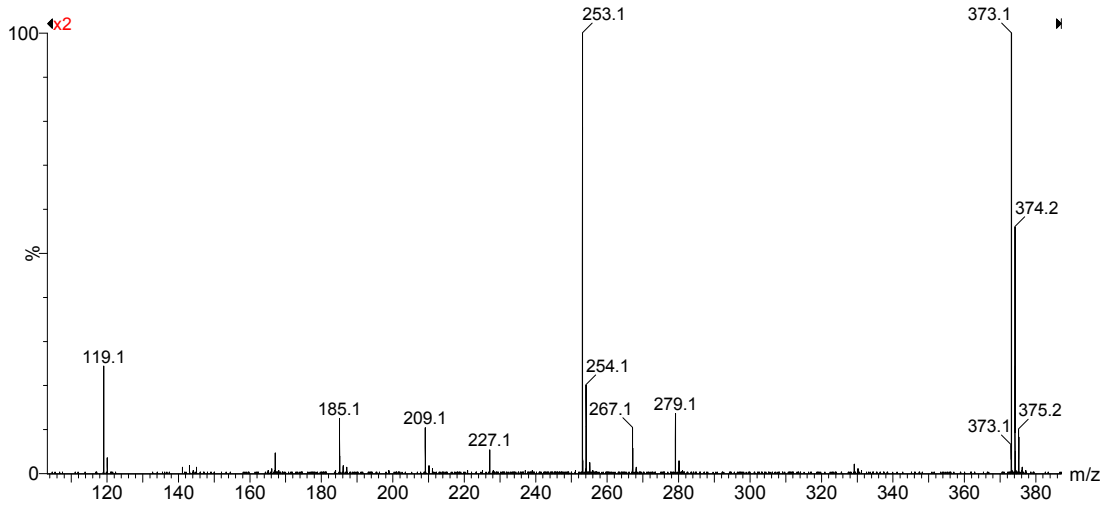

Figure S3. LC-MS/MS^2 spectrum of naringenin-phenylacetaldehyde adduct

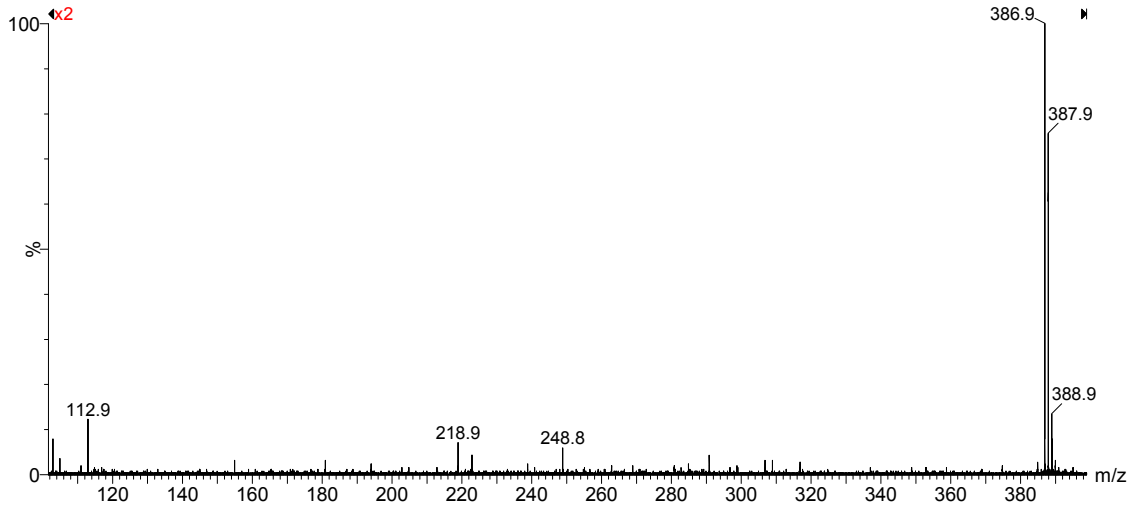

Figure S4. LC-MS/MS^2 spectrum of kaemferol-phenylacetaldehyde adduct

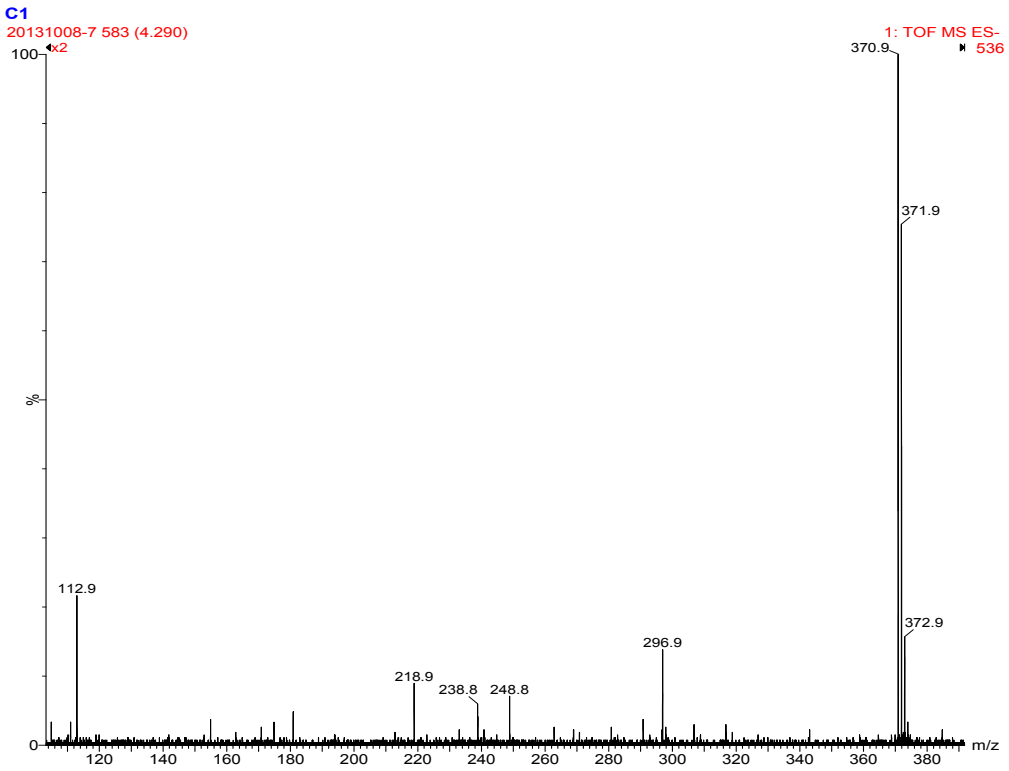

Figure S5. LC-MS/MS^2 spectrum of apigenin-phenylacetaldehyde adduct

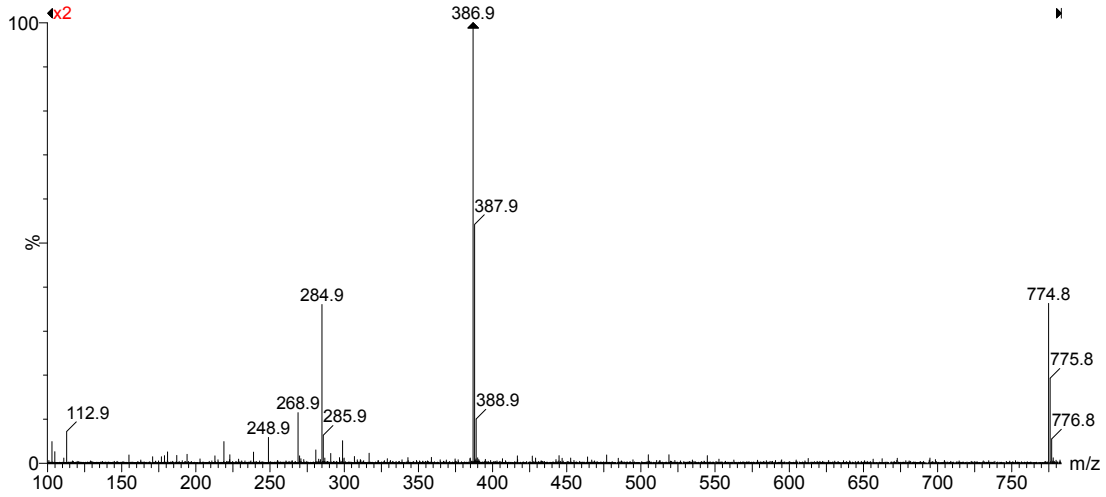

Figure S6. LC-MS/MS^2 spectrum of luteolin-phenylacetaldehyde adduct

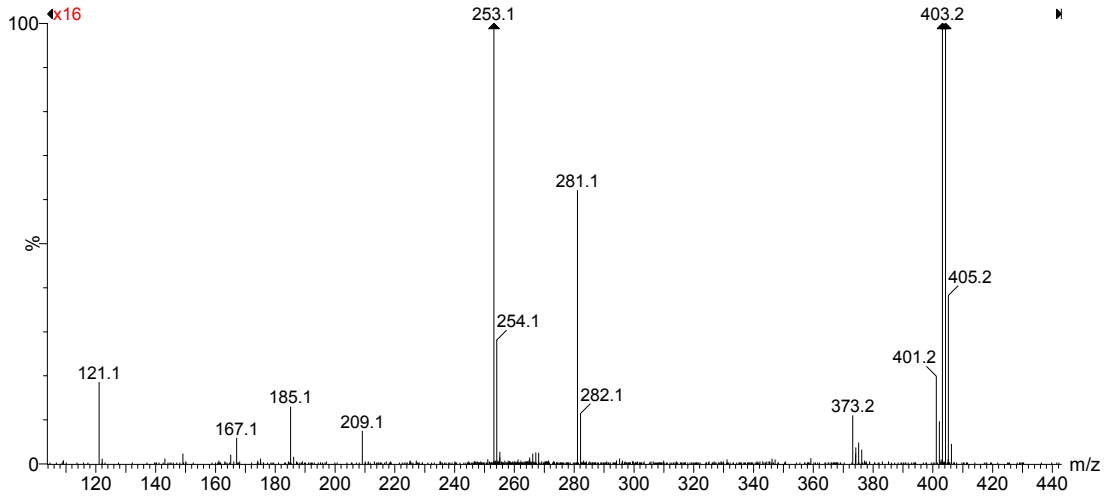

Figure S7. LC-MS/MS^2 spectrum of quercetin-phenylacetaldehyde adduct