

### Optimization of MS parameters

Flow injection analysis (FIA) of 10 µg/mL from each compound was conducted for source optimization. The parameters for EMS and IDA experiments are mentioned above.

**Table S1.** Parameters of EMS and IDA experiments.

Parameters	EMS	IDA-EPI
Mass range (m/z)	100-700	50-700
Scan period (s)	0.1513	
Number of scans	3	1
Scan rate (amu/s)	4000	1000
Curtain gas	30	30
CAD gas	Medium	High
Temperature (°C)	550	550
Gas 1	45	45
Gas 2	45	45
Ion spray	-4500	-4500
Declustering potential	-30	-30
Entrance potential	-7.5	-7.5
Collision energy	-10	-30
C2B	-300	-450
IPA threshold for EPI experiments		10000 counts
Peak selected for the EPI scan		Two most intense peaks
Q1 resolution		Low
Collision energy spray		10

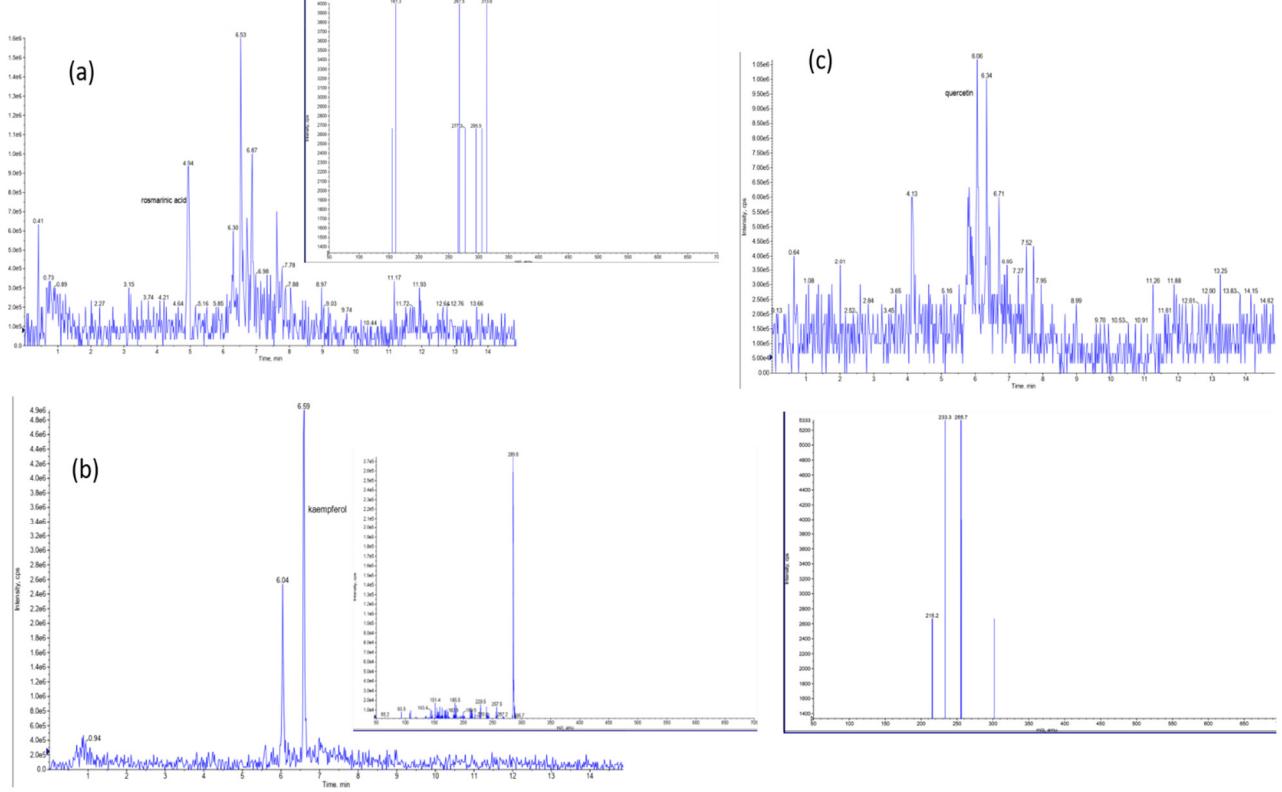
**Table S2.** Molecular target prediction probability values of examined phenolic compounds, derived from the application of open web-based tools Random Forest QSAR (<http://rfqsar.kaist.ac.kr/home.php>) (accessed on 1 December 2022) and Swiss Target Prediction (<http://www.swisstargetprediction.ch/>) (accessed on 1 December 2022).

Compounds	Probability Value		Probability Value	
	Random Forest QSAR	hCA-II	Swiss Target Prediction	hCA-XII
Apigenin		0.74	0.56	0.56
Caffeic acid		0.80	0.74	0.74
Chlorogenic acid		0.05	-	0.10
Kaempferol		0.83	1.00	1.00
Naringenin		-	0.10	0.91
Quercetin		0.83	1.00	1.00
Rosmarinic acid		0.65	0.17	0.12
Syringic acid		0.80	1.00	1.00

**Table S3.** Results of total phenolic content (TPC), antiradical (ABTS) and antioxidant activity (FRAP) of banana flesh samples during storage at  $18.0 \pm 0.5$  °C.

Days	Total Phenolic Content (TPC) (mg GAE / g of banana flesh)	Antiradical activity (ABTS) (mg TE / g of banana flesh)	Antioxidant activity (FRAP) (mg Fe(II) / g of banana flesh)
2	0.309±0.063a	0.971±0.080a	2.846±0.275a
4	0.157±0.053bc	0.405±0.070b	1.507±0.273be
7	0.118±0.020b	0.385±0.036b	1.195±0.105c
9	0.122±0.027bc	0.407±0.036b	1.324±0.121cb
11	0.152±0.020bc	0.408±0.047b	1.416±0.147cbd
14	0.180±0.026c	0.444±0.024bc	1.620±0.127de
17	0.384±0.037d	0.500±0.041c	1.649±0.166de
21	0.467±0.043e	0.578±0.061d	1.762±0.196e

a-e: Different letters in the results of each analysis indicate that the values of the samples differ significantly.



**Figure S1.** Representative chromatographs and EMS mass spectra of indicative elucidated compounds.  
 (a) rosmarinic acid; (b) kaempferol; (c) quercetin.