

Supporting Information

Preparation of Imidazole-Modified Paper Membrane for Selective Extraction of Gallic Acid and its Structural and Functional Analogues from *Pomegranate Peel*

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Table S1 Method comparison for analysis of gallic acid (GA) or other phenolic acids

Literature	Adsorption Method	Adsorbent materials	Sample	Method parameters or others
<i>Food Anal. Meth.</i> 2020 , 13 (1), 155-165,	d-SPE (dispersive solid-phase extraction)	Mixture of diatomaceous earth (DE) and graphitized carbon black (GCB)	<i>Myrciaria cauliflora</i> peel	Linear range: 0.1–137 µg/kg by UHPLC-MS/MS
<i>J. Chromatogr. A</i> 2014 , 1342, 44-53,	d-SPE	C-18 (50 mg)	wine	Linear range:0.1-50 µg/mL by LC-MWD (-multi-wavelength detection)
<i>J. Chromatogr. A</i> 2016 , 1453, 1-9,	In-syringe extraction	Ni-Co layered double hydroxides (LDH)	fruit juice	Linear range: 1-500 µg/L by LC-UV
<i>J. Chromatogr. B</i> 2017 , 1041, 98-103,	SPE (solid-phase extraction)	MIP (molecularly imprinting polymer)	phyllanthus urinaria L.	Purification
<i>Anal. Bioanal. Chem.</i> 2015 , 407 (25), 7681-7690,	SPE	MIP	pomegranate rind	Linear range: 0.005–1.0 µg/mL and 5.0–1000µg/mL by LC-UV
<i>J. Sep. Sci.</i> 2011 , 34 (19), 2602-2610,	SPE	MIP (200 mg)	<i>Rhizoma homalomenae</i>	Recovery 40% for GA by LC-DAD
<i>Food Chem.</i> 2017 , 226, 23-31	SPE	Sephadex LH-20 (820 mg)	wine	Recovery 44%-99% by LC-MS/MS
<i>J. Pharm. Biomed. Anal.</i> 2017 , 135, 87-96,	µ-SPE (micro SPE)	Ika Ultra-Turrax® Tube Drive	sea algae	Linear range: 0.2-5 ng/mL by LC-MS/MS
This work	MSPE (membrane SPE)	Imidazole-Modified Paper Membrane	<i>Pomegranate Peel</i>	Linear range (separated): 0.5-5 ng/mL, 5-100 ng/mL, 100-500 ng/mL by LC-UV

Table.S2 CFD simulation parameters

Item	Detailed settings
Geometry (membrane zone)	Cylinder: radius:12.5 mm, height:2 mm upper surface-inlet, lower surface-outlet built in 2D axial symmetry model
Boundary conditions	Inlet: velocity inlet Outlet: pressure outlet
Initial conditions	Concentration = 0 (in all zone at time = 0)
Compounds information	Molecular weight: 170.12 g/mol Diffusion coefficient: 10^{-8} m ² /s
Sample description	Concentration: 20 µg/mL Solvent: water (density: 1000.0 kg/m ³) Volume: 5 mL Flow time: 300 second Injection: Concentration × Rectangular wave
Porous medium (all zone)	Fluid: Velocity: 0.0034 cm/s (calculated by volume, flow time and geometry size) Diffusion: by solvent, others-default Porous zone: Porosity:0.6 (estimated) Adsorption: (temperature impact was not considered) Base density: 1200 kg/m ³ (estimated) Langmuir model: $C_{p,i} = \frac{K_i \times C_{max,i} \times C_i}{1 + K_L \times C_i}$ where $C_{p,i}$ – absorbed concentration on filter (mol/kg) C_i – concentration left in free solution (mol/kg) K_i – Langmuir constant for compound i(m ³ /mol) $C_{max,i}$ – the maximum absorbed amount for compound i(mol/kg), $i = 1-8$ $C_{max,i} = N_i \times S / M_i$, where N_i – monolayer capacity for compound i (g/m ²) S – BET specific surface area (m ² /g), in this work, the value 10 m ² /g was used.
Meshing	Extremely fine, controlled by physical field
Solution	Transient, time step:1s within 0-300s
Convergence	Yes
Others	1. For calculating the recovery, the field probe was used for later integral calculus. 2. For obtaining the breakthrough curve, point diagram of concentration vesus time at the center of the outlet was obtained in the postprocessing.

Table S3 Searching results in MS library

Number	Name	CAS	ESI mode*	RT/min	Mw	m/z	m/z range (EIC)	Peak area
1	Catechin	7295-85-4	+	2.49	290.0790	291.0860	291.0802-291.0981	126252741
2	Ellagic acid	476-66-4	+	7.09	302.0063	303.0149	303.0088-303.0210	131585576
3	Quercetin 3-O- galactoside	482-36-0	+	7.71	464.0955	465.1030	465.0937-465.1123	117938614
4	Corilagin	23094-69-1	-	3.9	634.0860	633.0743	633.0616-633.08706	456040405
5	Gallic acid	149-91-7	-	1.26	170.0251	169.0145	169.0111-169.0179	602067382
6	beta-Glucogallin	13405-60-2	-	1.15	332.0743	331.069	331.0624-331.0756	142691542

*ESI mode: “+” meant positive, “-” meant negative.

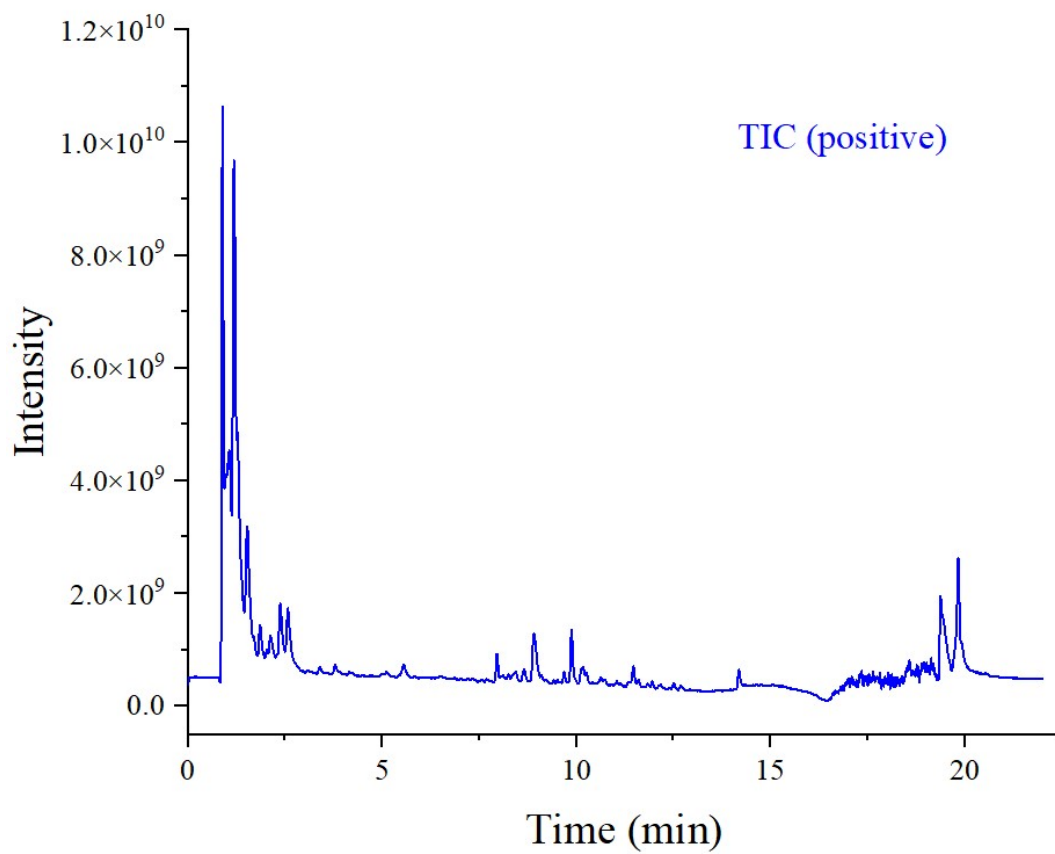


Fig.S1 TIC (positive mode) of LC-TOF/MS for the MSPE-proposed *Pomegranate Peel* extract

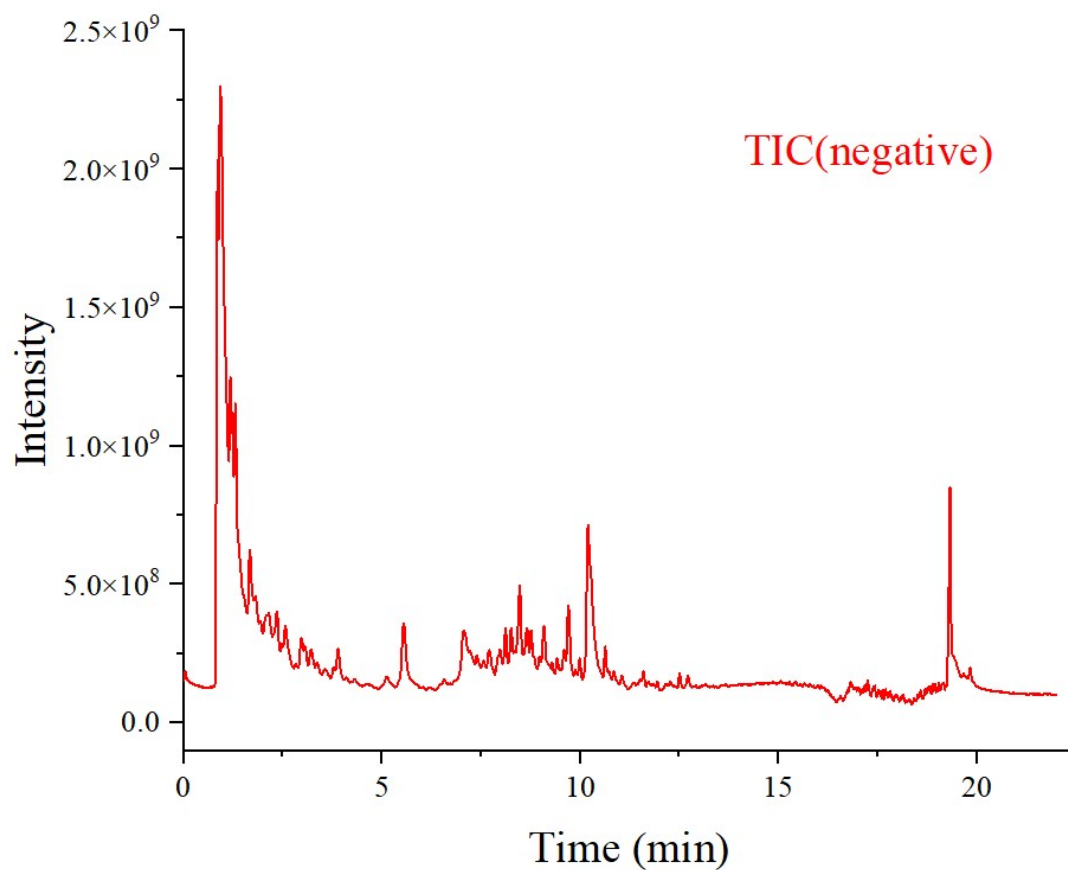


Fig.S2 TIC (negative mode) of LC-TOF/MS for the MSPE-proposed *Pomegranate Peel* extract

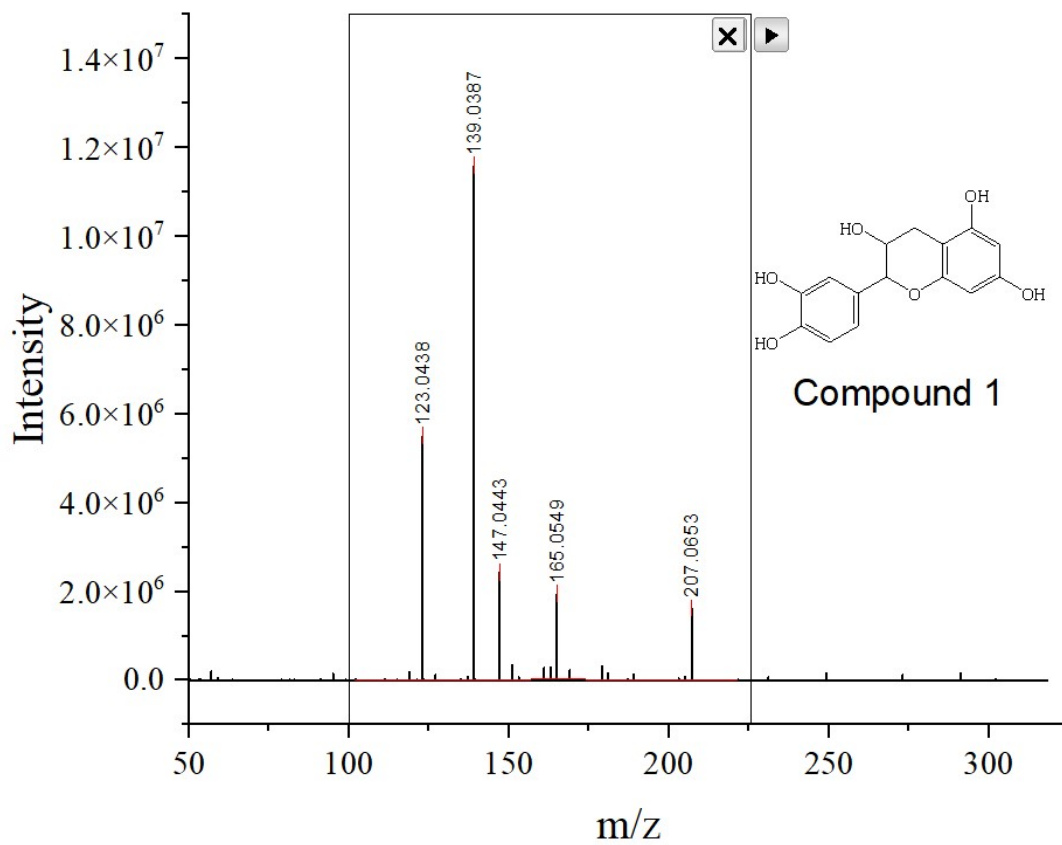


Fig.S3 Secondary MS result for compound 1 (Catechin)

The rectangle in the figure (Fig.S3-S8) was added by origin software to marking peaks automatically

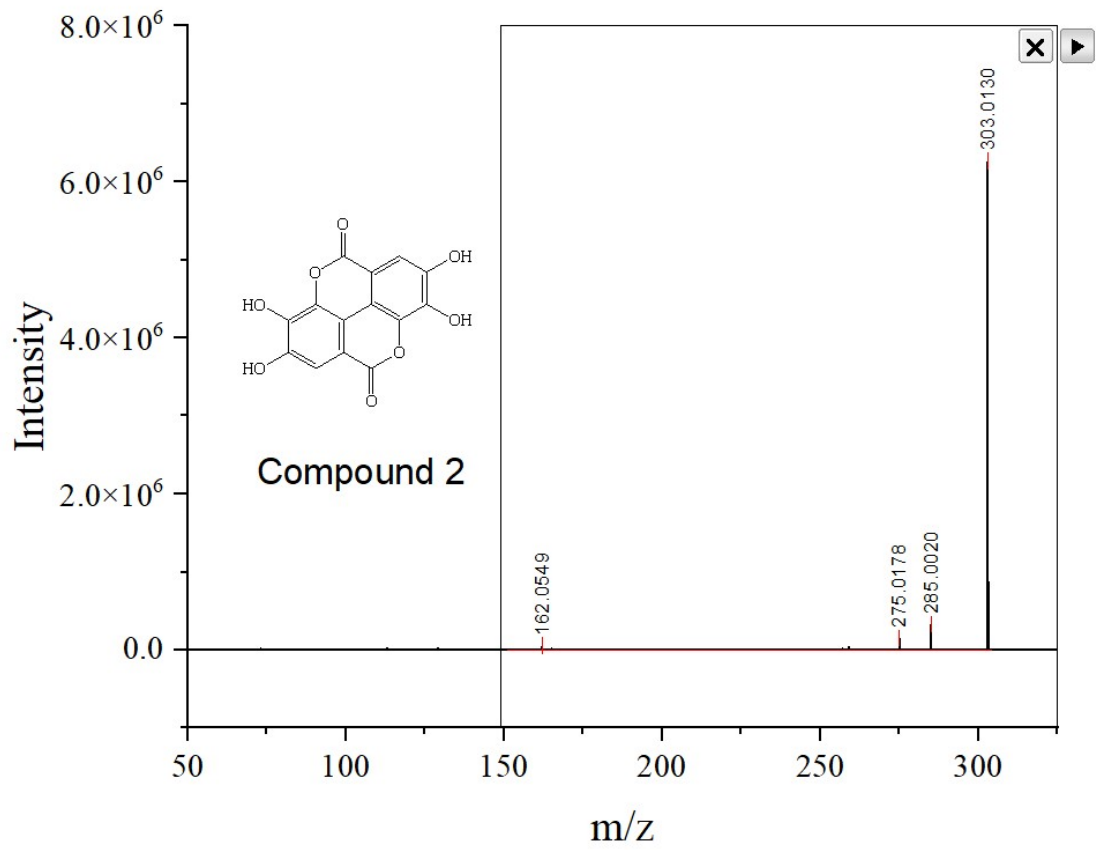


Fig.S4 Secondary MS result for compound 2 (Ellagic acid)

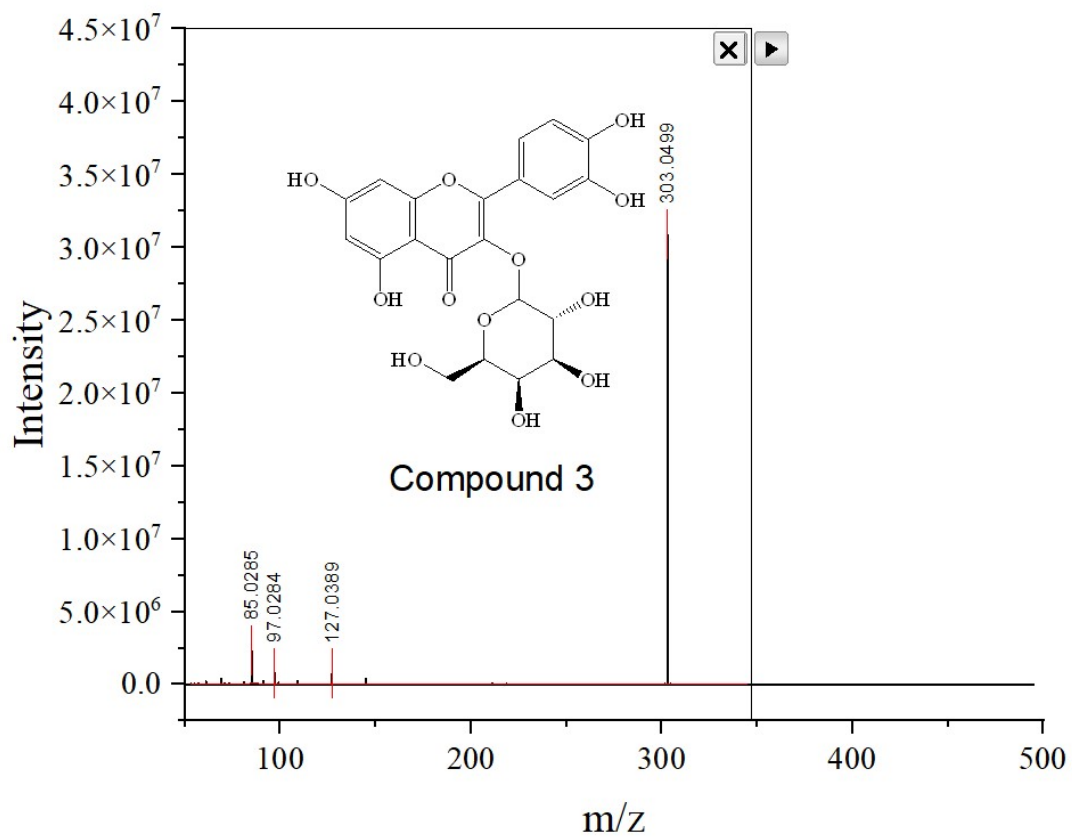


Fig.S5 Secondary MS result for compound 3 (Quercetin 3-O-galactoside)

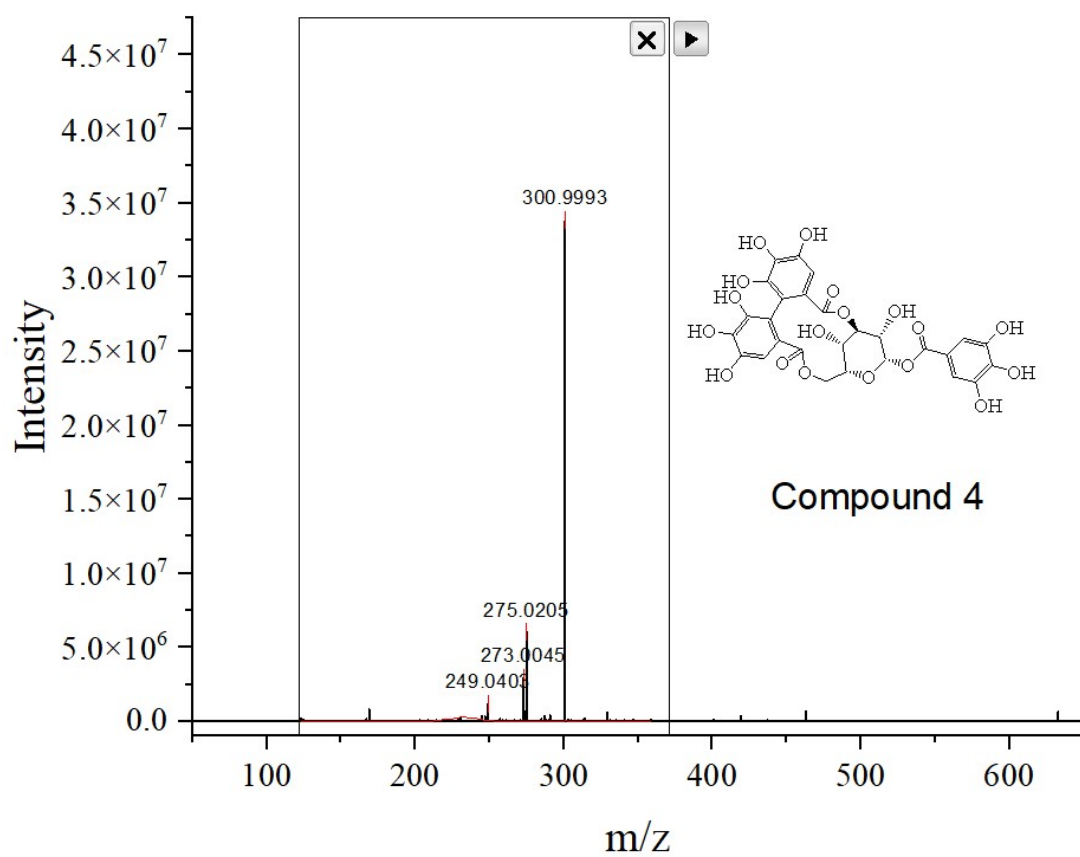


Fig.S6 Secondary MS result for compound 4 (Corilagin)

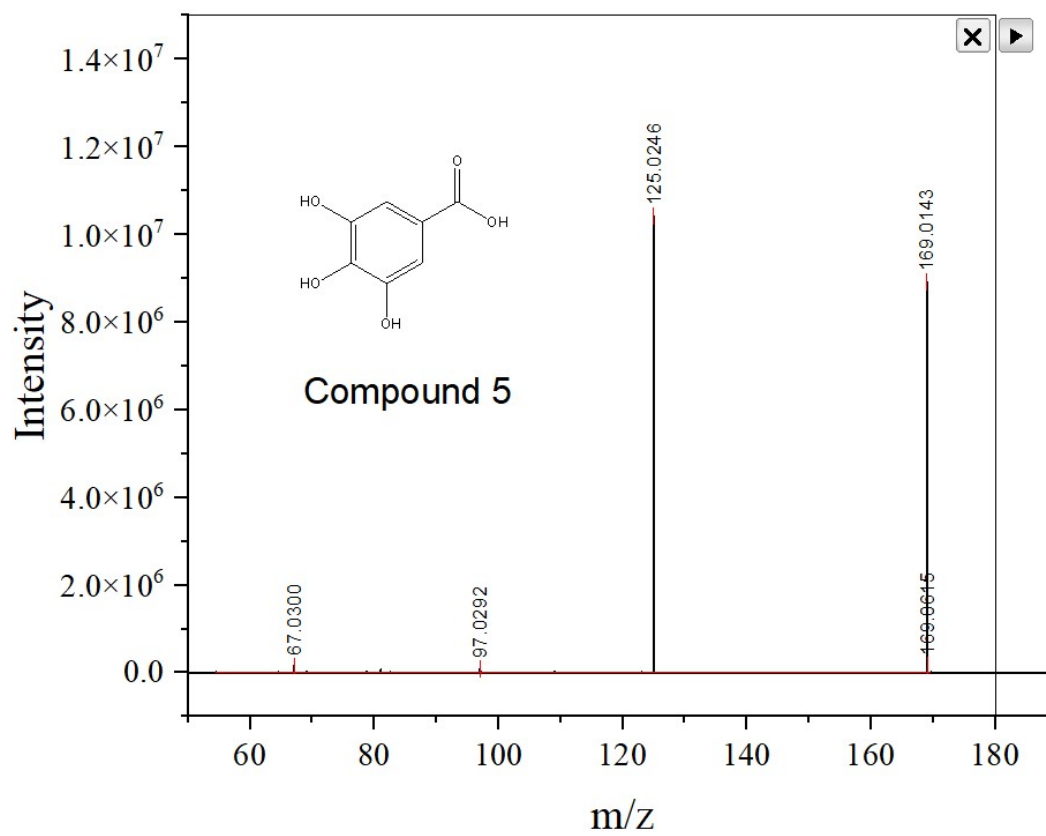


Fig.S7 Secondary MS result for compound 5 (Gallic acid)

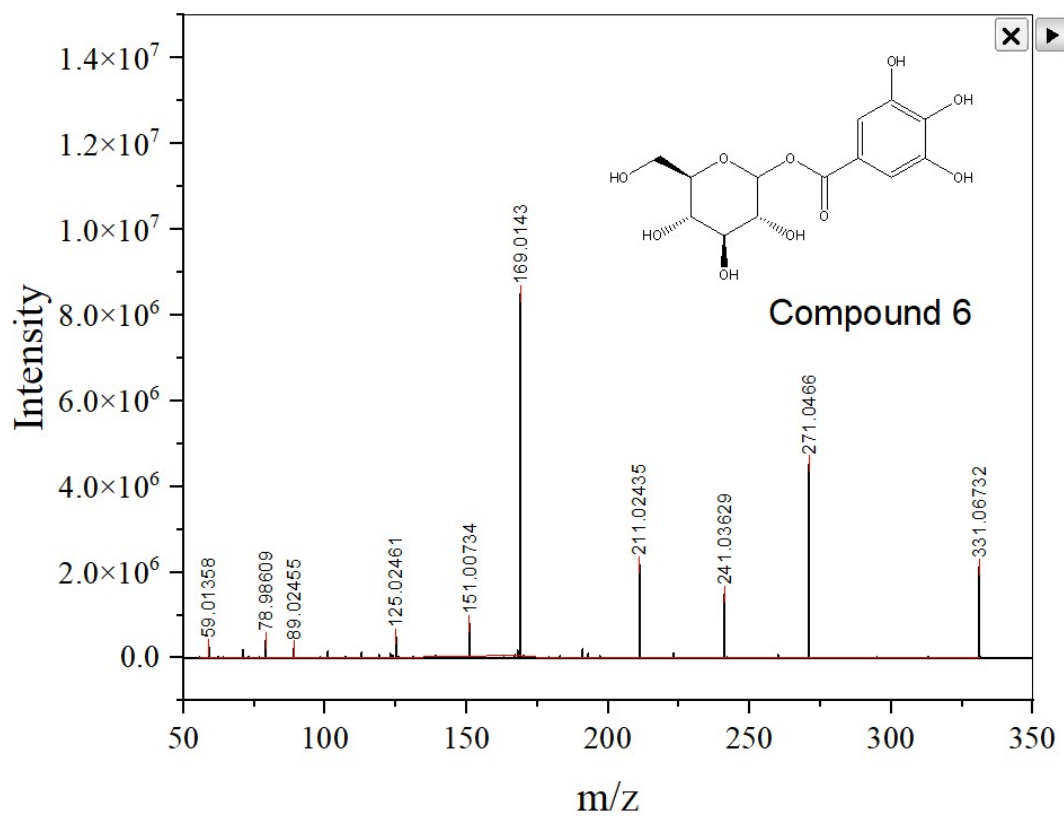


Fig.S8 Secondary MS result for compound 6 (beta-Glucogallin)