A rapid protocol to distinguish between Citri Exocarpium Rubrum and Citri Reticulatae Pericarpium based on characteristic fingerprint and UHPLC-Q-TOF MS methods

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Table.S1 The content of hesperidin in 15 batches of CER and CRP.

Sample	Sample No.	Origins	hesperidin%
CER	J1	Jinhua,Zhejiang	3.76
CER	J2	Jinhua,Zhejiang	4.12
CER	J3	Jinhua,Zhejiang	4.85
CER	J4	Jinhua,Zhejiang	3.90
CER	J5	Jinhua,Zhejiang	4.41
CER	J6	Chengdu,Sichuan	3.44
CER	J7	Chengdu,Sichuan	3.06
CER	J8	Chengdu,Sichuan	3.78
CER	J9	Chengdu,Sichuan	3.85
CER	J10	Chengdu,Sichuan	3.38
CER	J11	Xinhui,Guangdong	3.34
CER	J12	Xinhui,Guangdong	3.97
CER	J13	Xinhui,Guangdong	4.14
CER	J14	Xinhui,Guangdong	4.88
CER	J15	Xinhui,Guangdong	4.07
CRP	C1	Linyi,Shandong	3.56
CRP	C2	Linyi,Shandong	4.18
CRP	C3	Linyi,Shandong	4.10
CRP	C4	Linyi,Shandong	3.62
CRP	C5	Linyi,Shandong	3.73

CRP	C6	Xinhui,Guangdong	4.08
CRP	C7	Xinhui,Guangdong	3.78
CRP	C8	Xinhui,Guangdong	4.46
CRP	C9	Xinhui,Guangdong	4.86
CRP	C10	Xinhui,Guangdong	4.65
CRP	C11	Suizhou,Hubei	3.14
CRP	C12	Suizhou,Hubei	3.52
CRP	C13	Suizhou,Hubei	4.79
CRP	C14	Suizhou,Hubei	4.31
CRP	C15	Suizhou,Hubei	4.04

Table.S2 The origins and batches of CER and CRP.

Sample No.	Origins	Samples
J1	Jinhua,Zhejiang	Citri Exocarpium Rubrum
J2	Jinhua,Zhejiang	Citri Exocarpium Rubrum
J3	Jinhua,Zhejiang	Citri Exocarpium Rubrum
J4	Jinhua,Zhejiang	Citri Exocarpium Rubrum
J5	Jinhua,Zhejiang	Citri Exocarpium Rubrum
J6	Chengdu,Sichuan	Citri Exocarpium Rubrum
J7	Chengdu,Sichuan	Citri Exocarpium Rubrum
J8	Chengdu,Sichuan	Citri Exocarpium Rubrum
J9	Chengdu,Sichuan	Citri Exocarpium Rubrum
J10	Chengdu,Sichuan	Citri Exocarpium Rubrum
J11	Xinhui,Guangdong	Citri Exocarpium Rubrum
J12	Xinhui,Guangdong	Citri Exocarpium Rubrum
J13	Xinhui,Guangdong	Citri Exocarpium Rubrum
J14	Xinhui,Guangdong	Citri Exocarpium Rubrum
J15	Xinhui,Guangdong	Citri Exocarpium Rubrum
C1	Linyi,Shandong	Citri Reticulatae Pericarpium
C2	Linyi,Shandong	Citri Reticulatae Pericarpium
C3	Linyi,Shandong	Citri Reticulatae Pericarpium

C4	Linyi,Shandong	Citri Reticulatae Pericarpium
C5	Linyi,Shandong	Citri Reticulatae Pericarpium
C6	Xinhui,Guangdong	Citri Reticulatae Pericarpium
C7	Xinhui,Guangdong	Citri Reticulatae Pericarpium
C8	Xinhui,Guangdong	Citri Reticulatae Pericarpium
C9	Xinhui,Guangdong	Citri Reticulatae Pericarpium
C10	Xinhui,Guangdong	Citri Reticulatae Pericarpium
C11	Suizhou,Hubei	Citri Reticulatae Pericarpium
C12	Suizhou,Hubei	Citri Reticulatae Pericarpium
C13	Suiz hou,Hubei	Citri Reticulatae Pericarpium
C14	Suizhou,Hubei	Citri Reticulatae Pericarpium
C15	Suizhou,Hubei	Citri Reticulatae Pericarpium

Table.S3 The content of 12 chemical markers in 6 unknown samples.

(mg/g)

Name	Unknown1	Unknown2	Unknown3	Unknown4	Unknown5	Unknown6
Caffeoylquinic acid A	0.24	0.66	0.31	0.64	0.68	0.29
Caffeoylquinic acid B	0.58	0.92	0.44	0.72	0.95	0.36
Caffeoylquinic acid C	1.15	1.20	0.57	0.81	1.35	0.79
Caffeoylquinic acid D	1.28	0.66	1.25	1.23	1.29	1.21
Vicenin-2	0.46	0.84	0.51	0.52	0.65	0.49
Melitidin	0.11	0.25	0.09	0.12	0.23	0.11
Nobiletin	0.21	0.30	0.20	0.18	0.29	0.19
3,5,6,7,8,3’,4’-heptemethoxyflavone	0.24	0.37	0.23	0.24	0.39	0.23
Natsudaidain	0.04	0.1	0.06	0.05	0.07	0.05
Narirutin 4’-glucoside	1.94	0.86	1.95	1.92	0.77	2.17
Naringin	8.53	2.18	8.10	8.80	2.23	8.92
Hesperidin	6.58	3.94	6.35	6.72	5.23	6.73

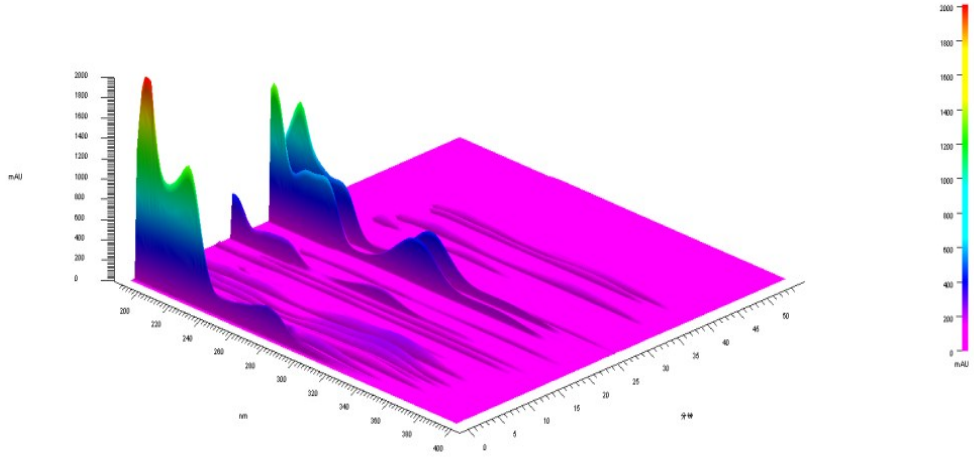

Fig.S1 The UV full-wavelength scanning of CER sample.

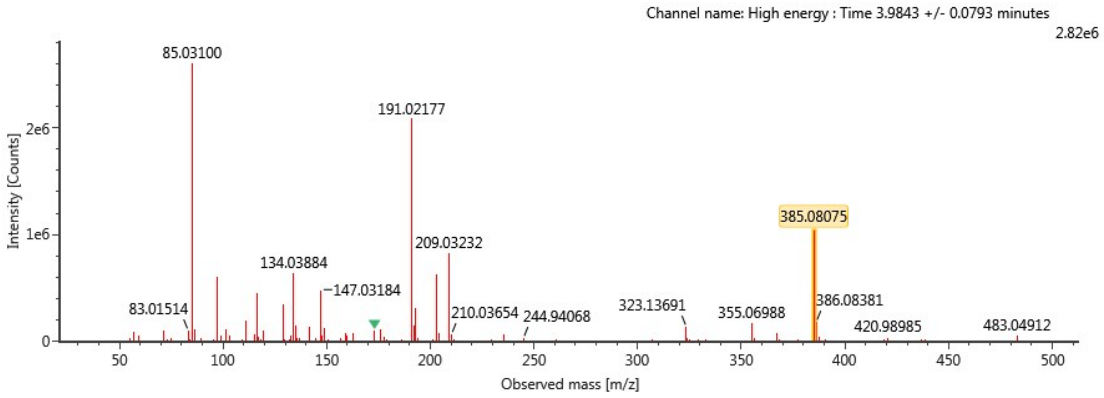

Fig. S2 The fragments of caffeoylquinic acid A in negative ion mode.

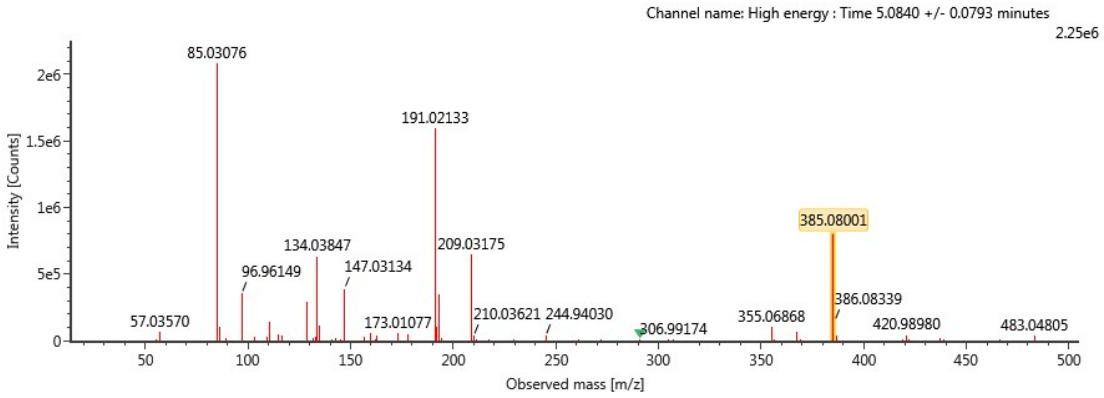

Fig. S3 The fragments of caffeoylquinic acid B in negative ion mode.

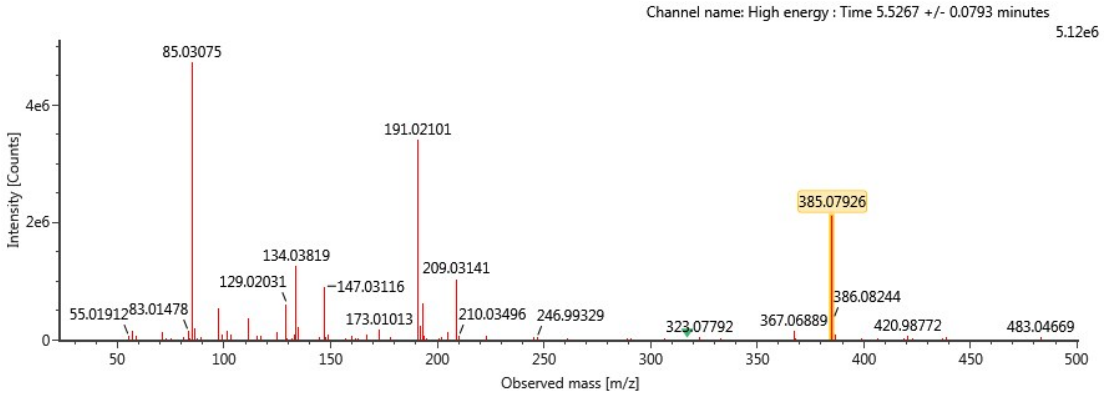

Fig. S4 The fragments of caffeoylquinic acid C in negative ion mode.

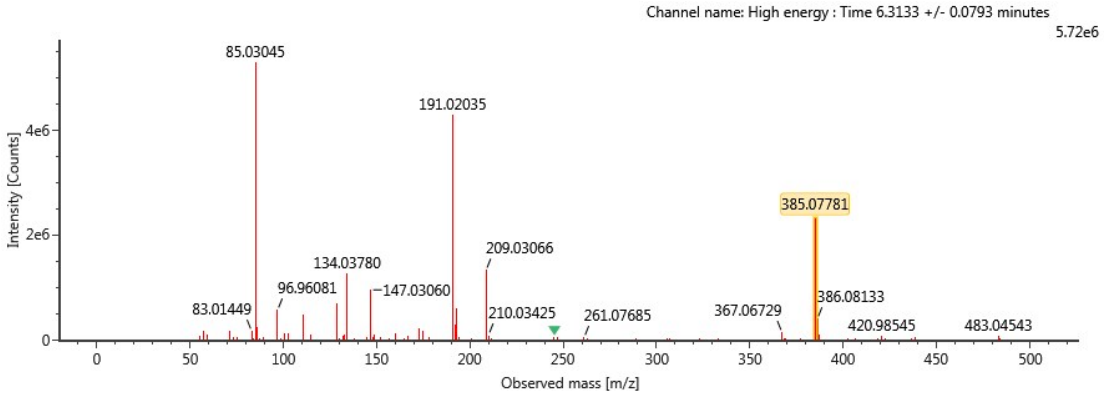

Fig. S5 The fragments of caffeoylquinic acid D in negative ion mode.

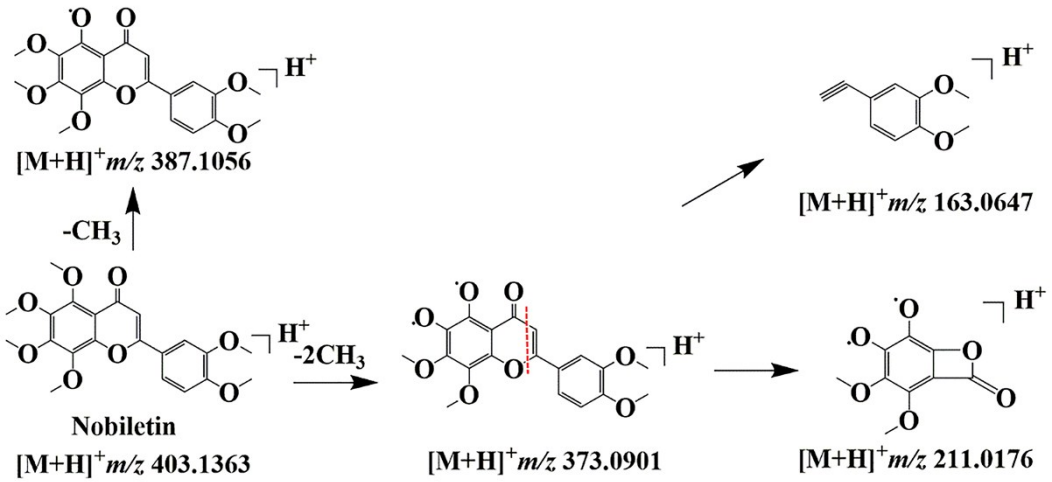

Fig. S6 The possible fragmentation pattern of nobiletin.

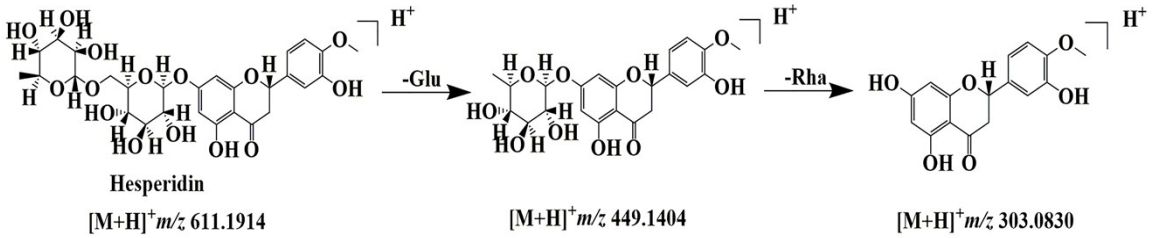

Fig. S7 The possible fragmentation pattern of hesperidin.

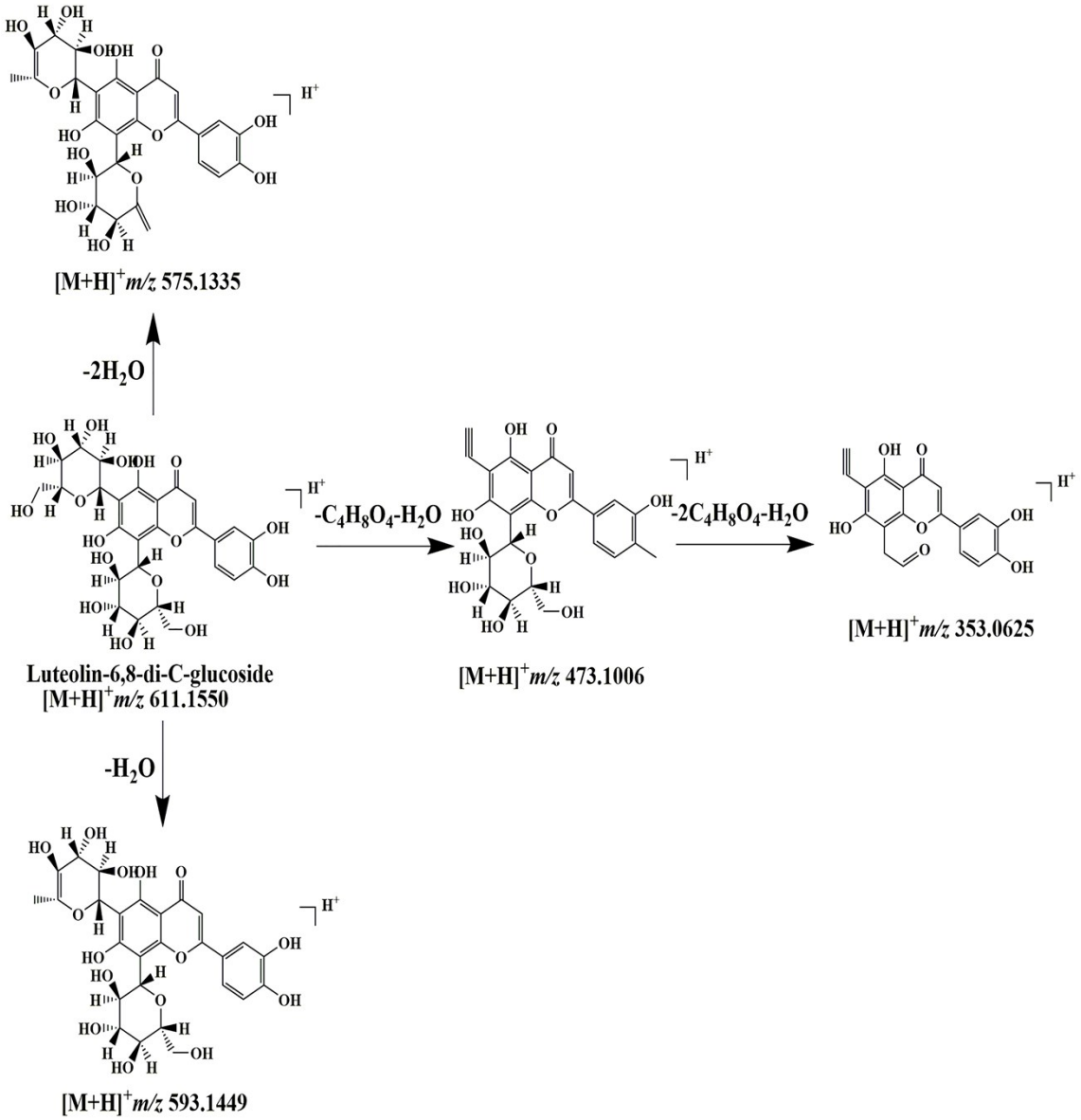

Fig. S8 The possible fragmentation pattern of luteolin-6, 8-di-C-glucoside.

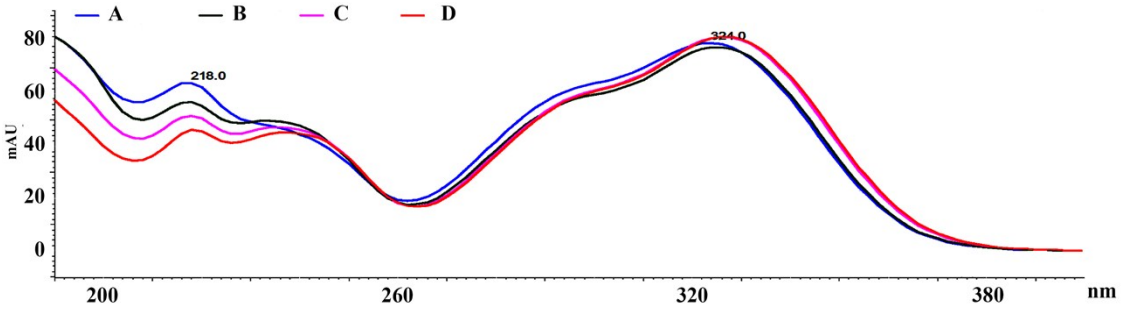

Fig.S9 The UV full-wavelength scanning of caffeoylquinic acid (A, B, C and D).

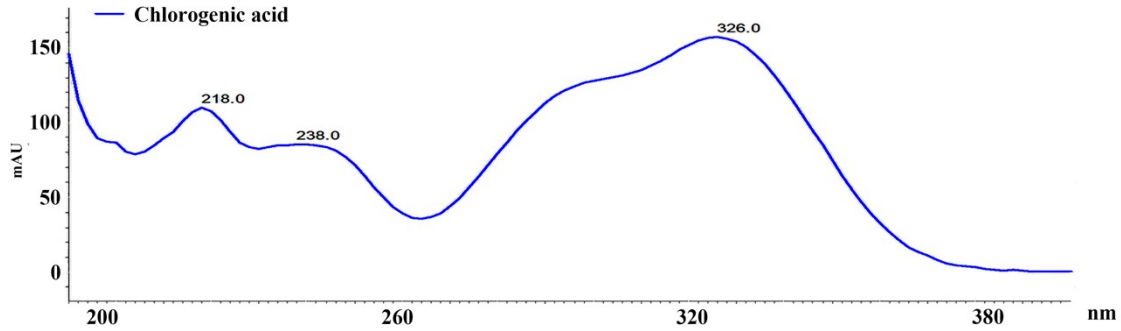

Fig.S10 The UV full-wavelength scanning of chlorogenic acid.

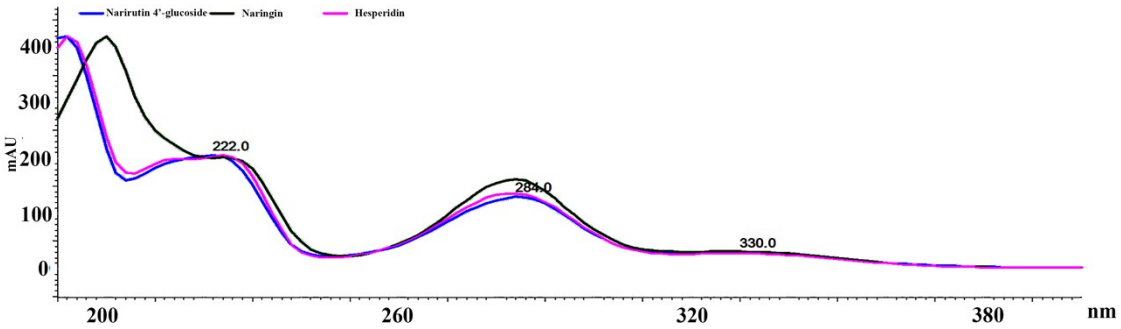

Fig. S11 The UV full-wavelength scanning of narirutin 4'-glucoside, naringin and hesperidin.

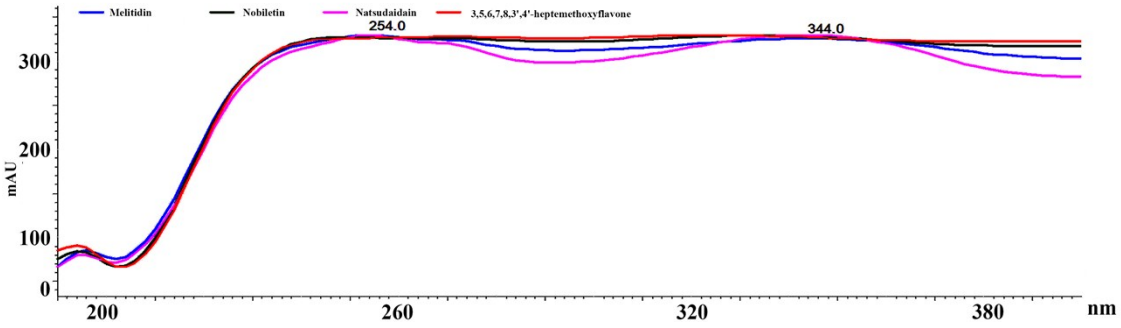

Fig. S12 The UV full-wavelength scanning of melitidin, nobiletin, natsudaidain and

3, 5, 6, 7, 8, 3’, 4’-heptemethoxyflavone.

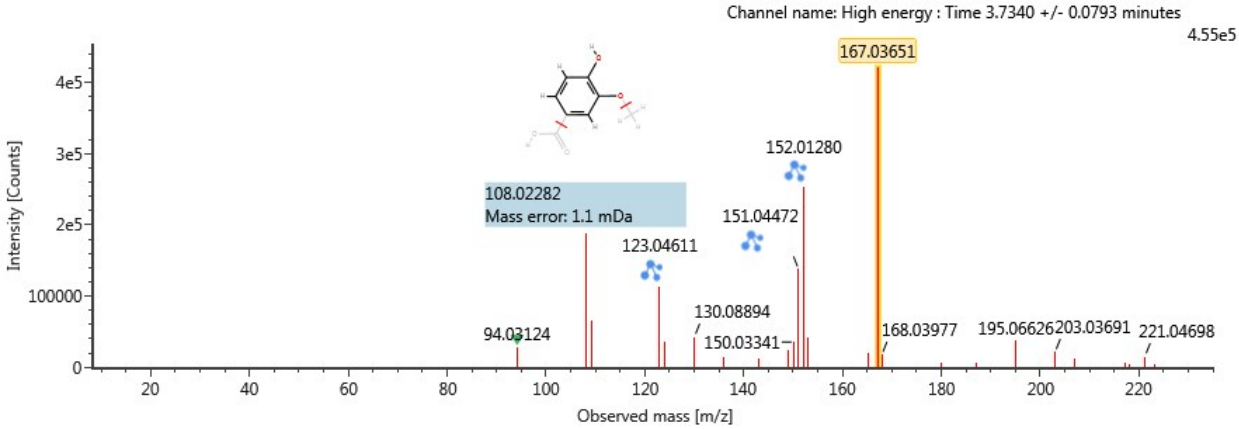

Fig. S13 The fragments of vanillic acid in negative ion mode.

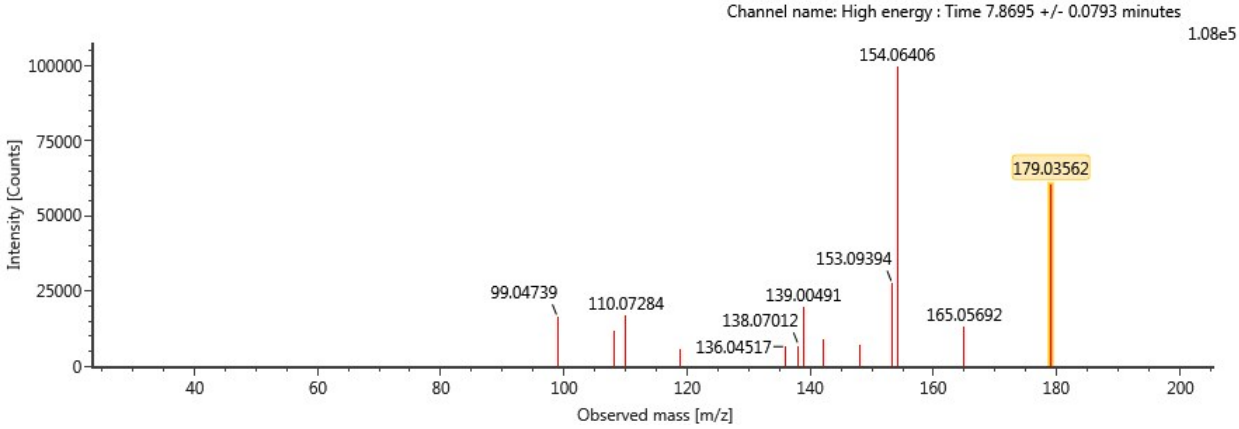

Fig. S14 The fragments of caffeic acid in negative ion mode.

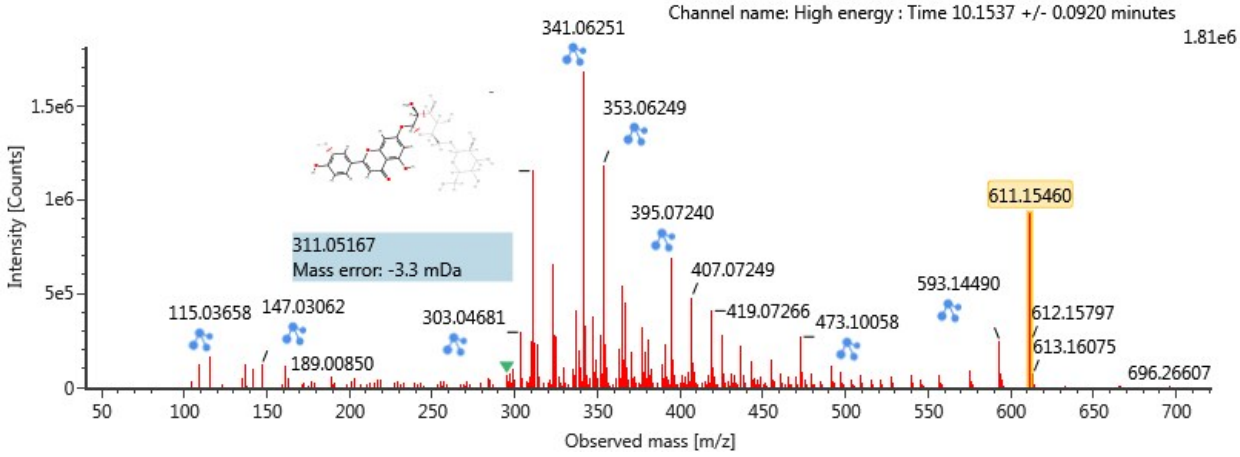

Fig. S15 The fragments of luteolin-6, 8-di-C-glucoside in positive ion mode.

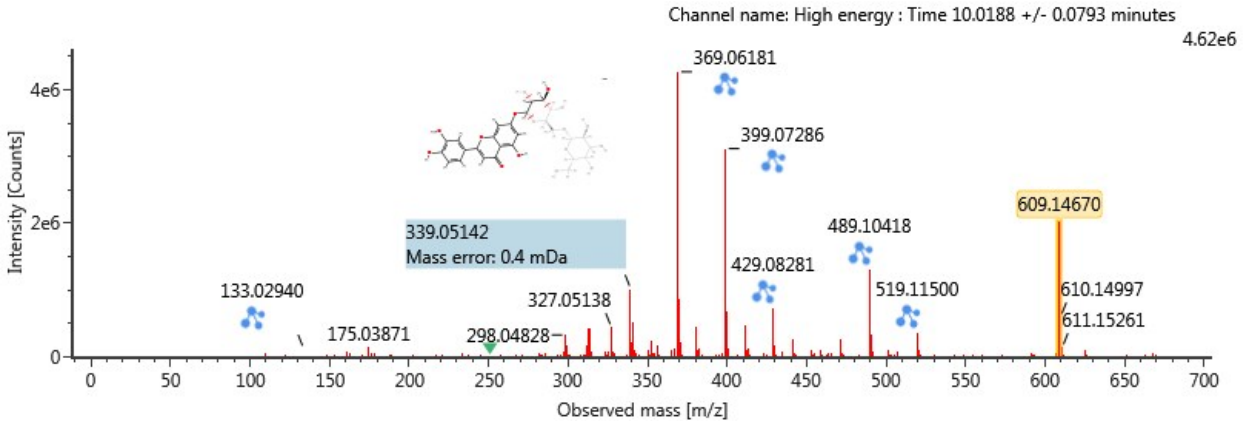

Fig. S16 The fragments of luteolin-6, 8-di-C-glucoside in negative ion mode.

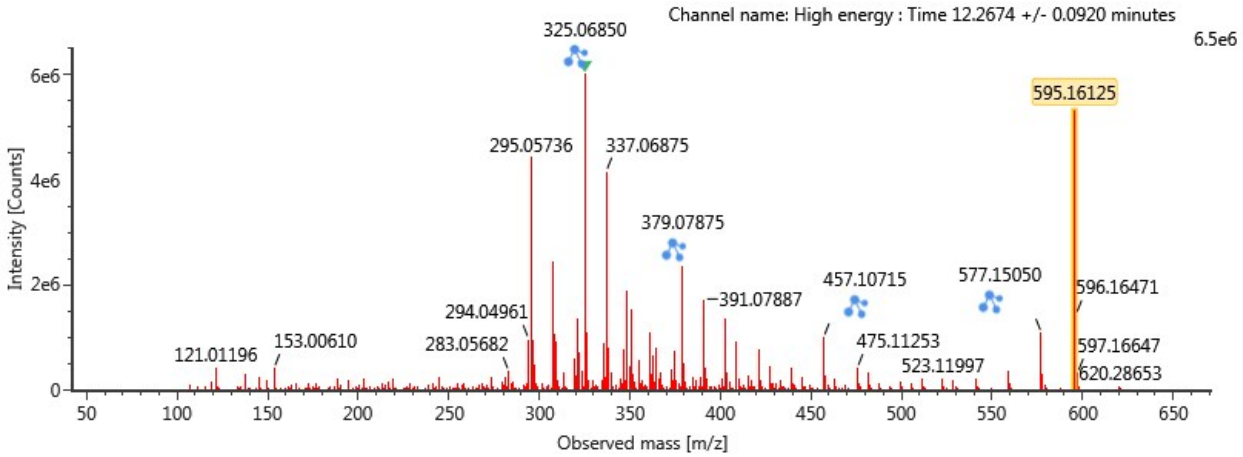

Fig. S17 The fragments of vicenin-2 in positive ion mode.

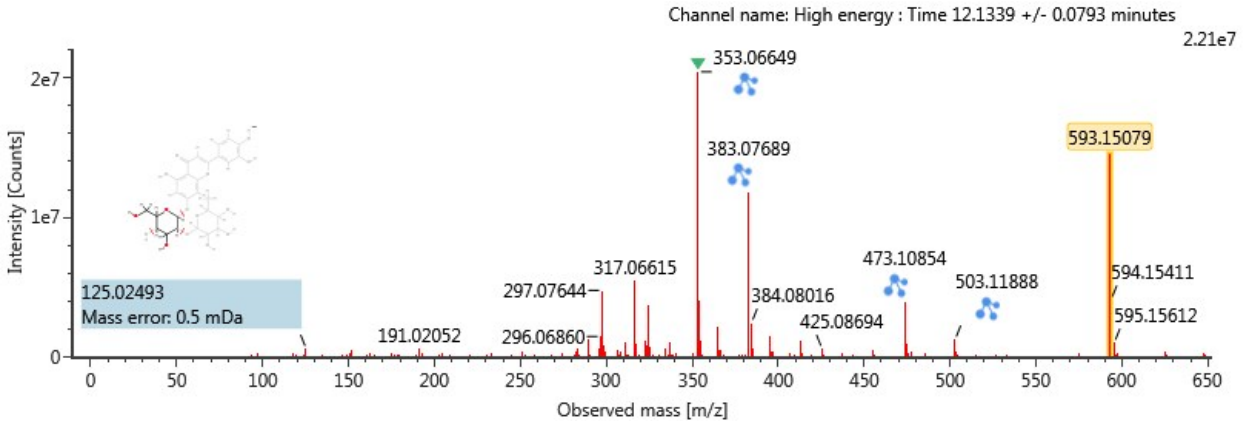

Fig. S18 The fragments of vicenin-2 in negative ion mode.

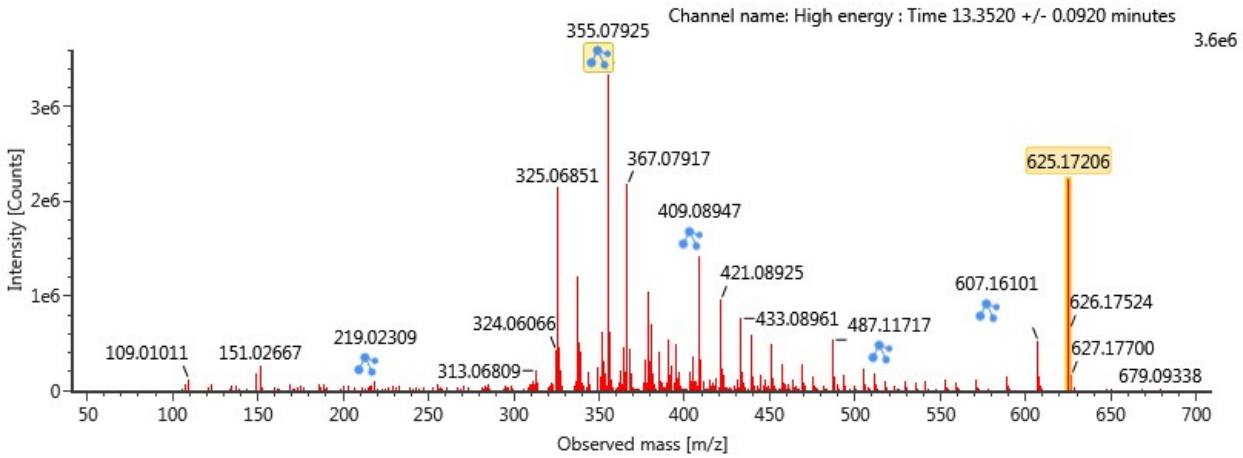

Fig. S19 The fragments of chrysoeriol-6, 8-di-C-glucoside in positive ion mode.

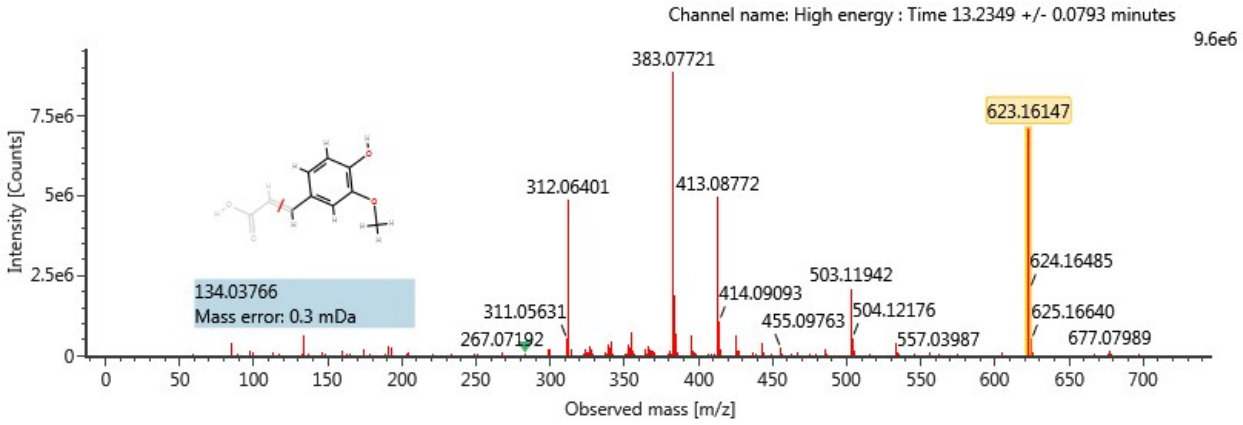

Fig. S20 The fragments of chrysoeriol-6, 8-di-C-glucoside in negative ion mode.

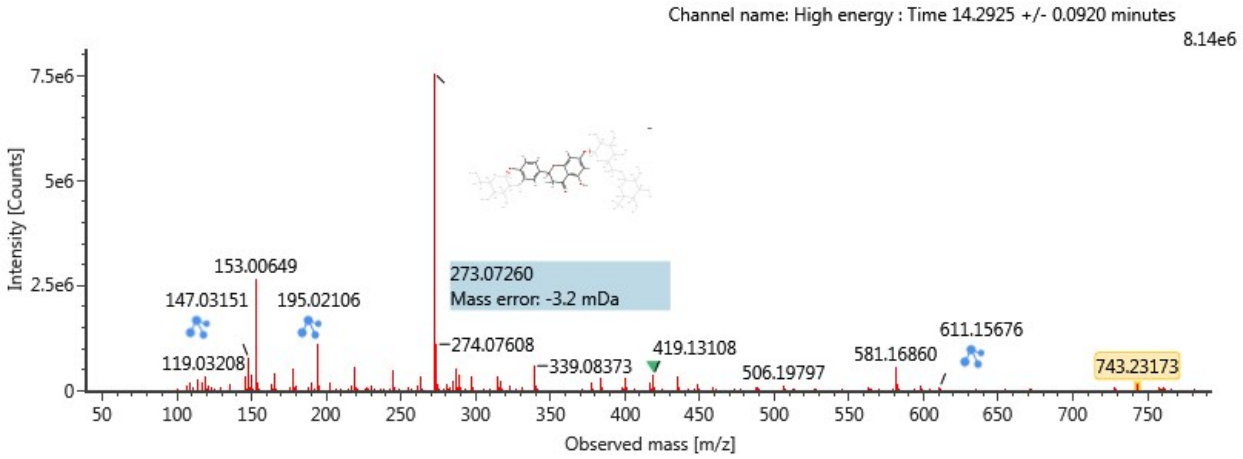

Fig. S21 The fragments of narirutin 4'-glucoside in positive ion mode.

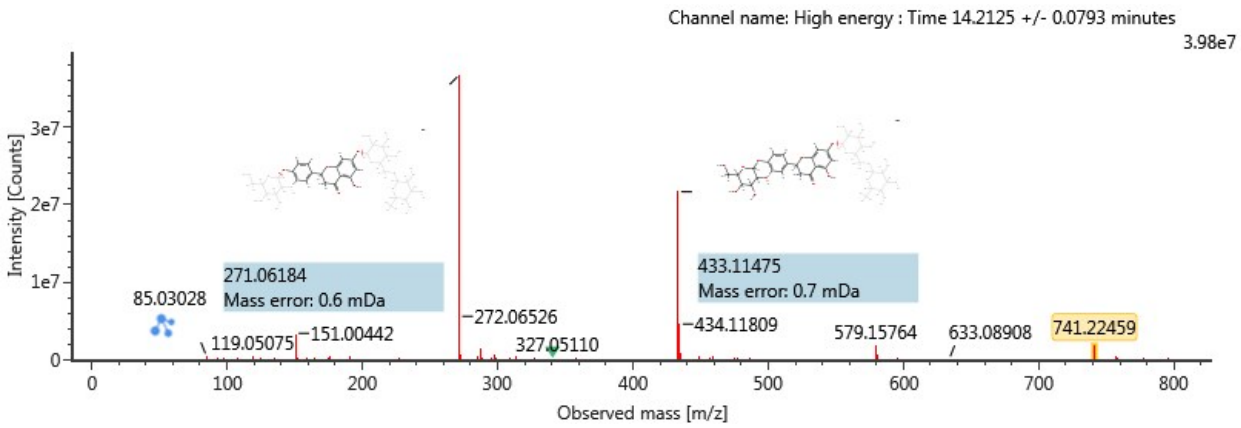

Fig. S22 The fragments of narirutin 4'-glucoside in negative ion mode.

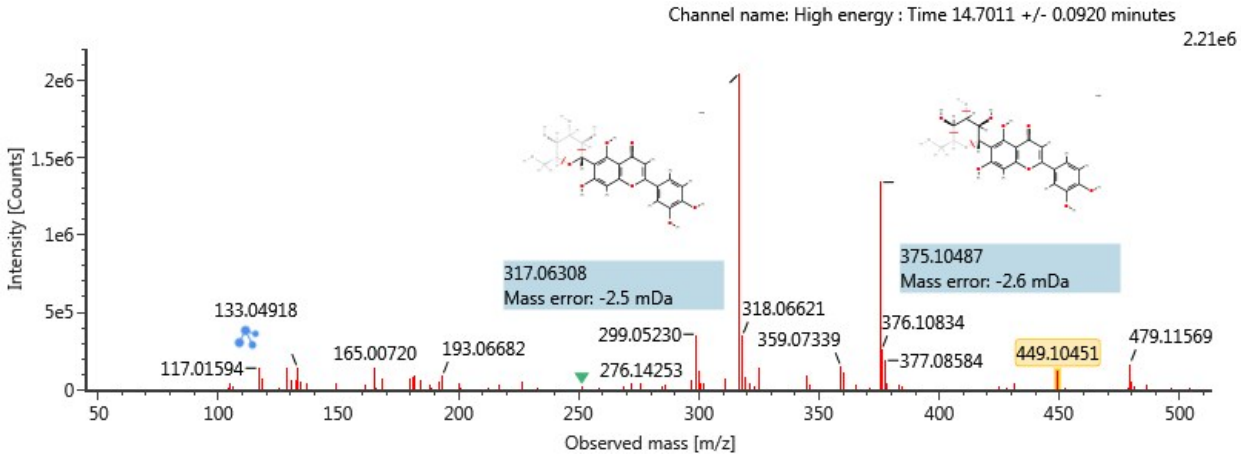

Fig. S23 The fragments of isoorientin in positive ion mode.

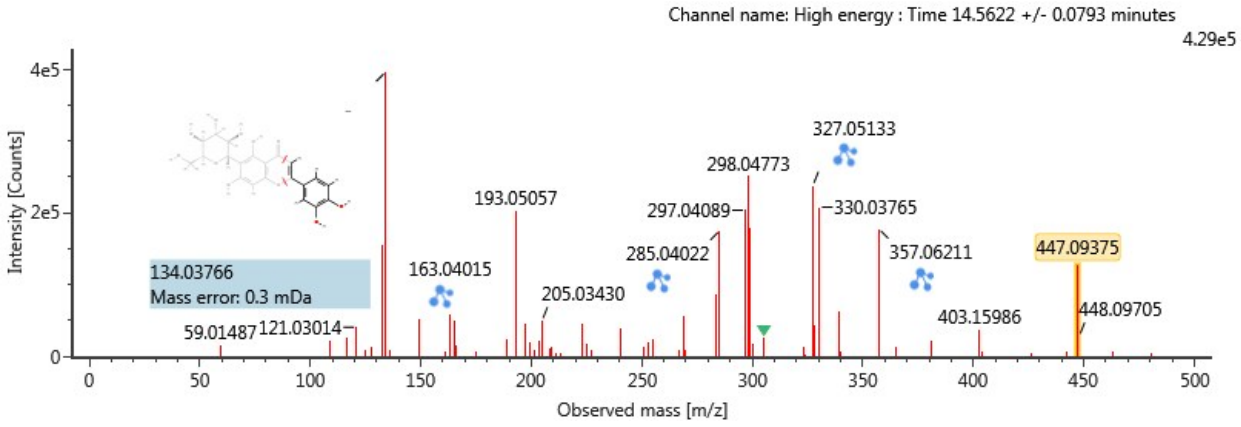

Fig. S24 The fragments of isoorientin in negative ion mode.

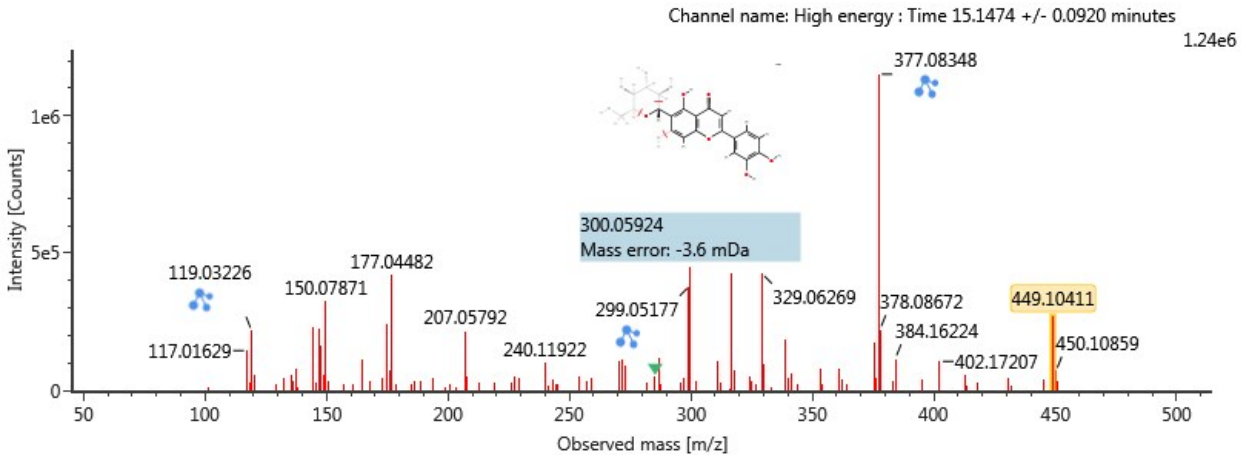

Fig. S25 The fragments of orientin in positive ion mode.

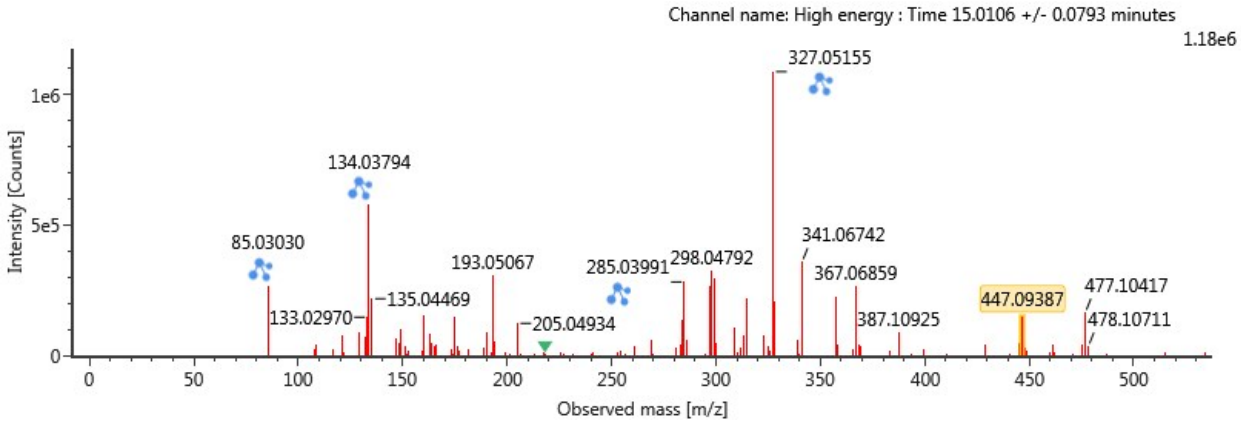

Fig. S26 The fragments of orientin in negative ion mode.

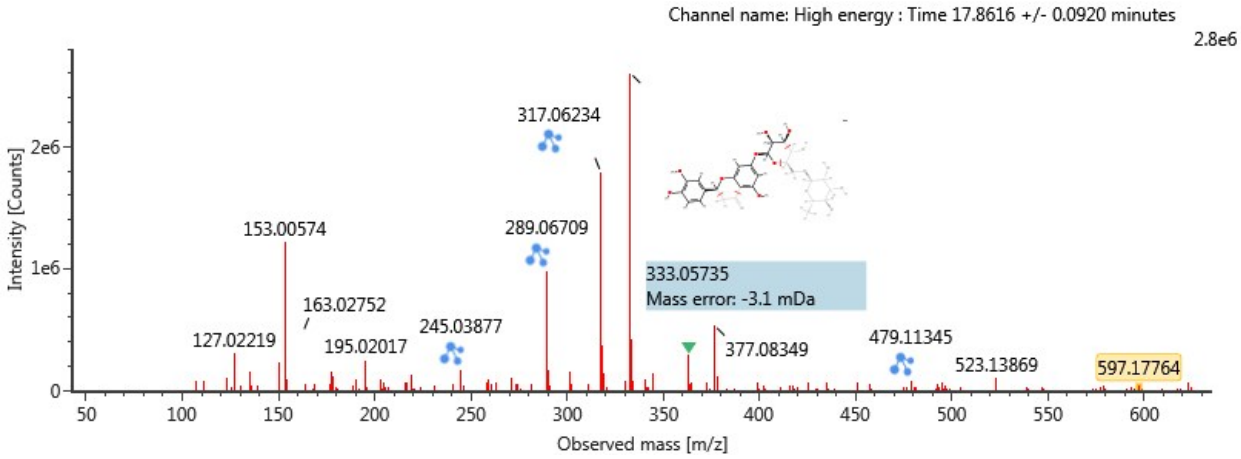

Fig. S27 The fragments of eriocitrin in positive ion mode.

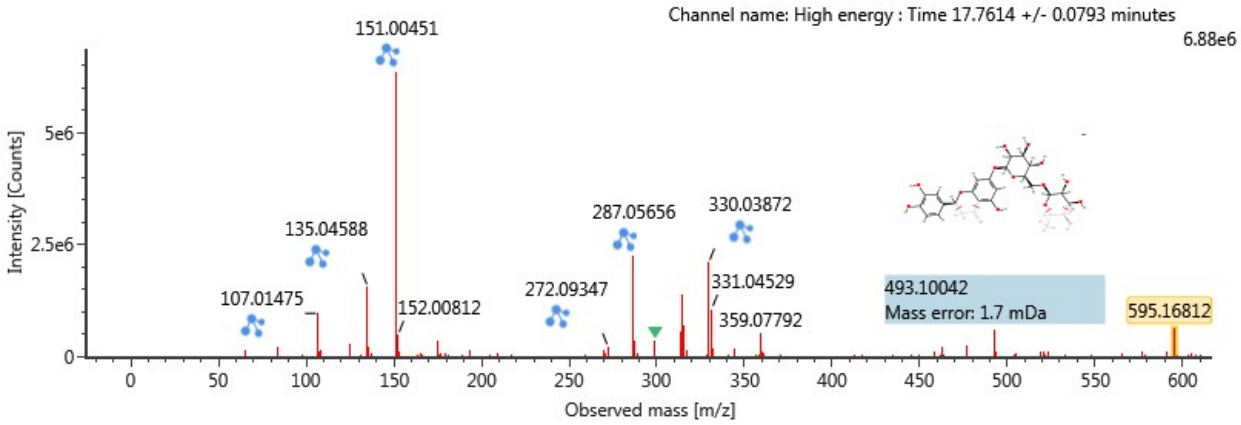

Fig. S28 The fragments of eriocitrin in negative ion mode.

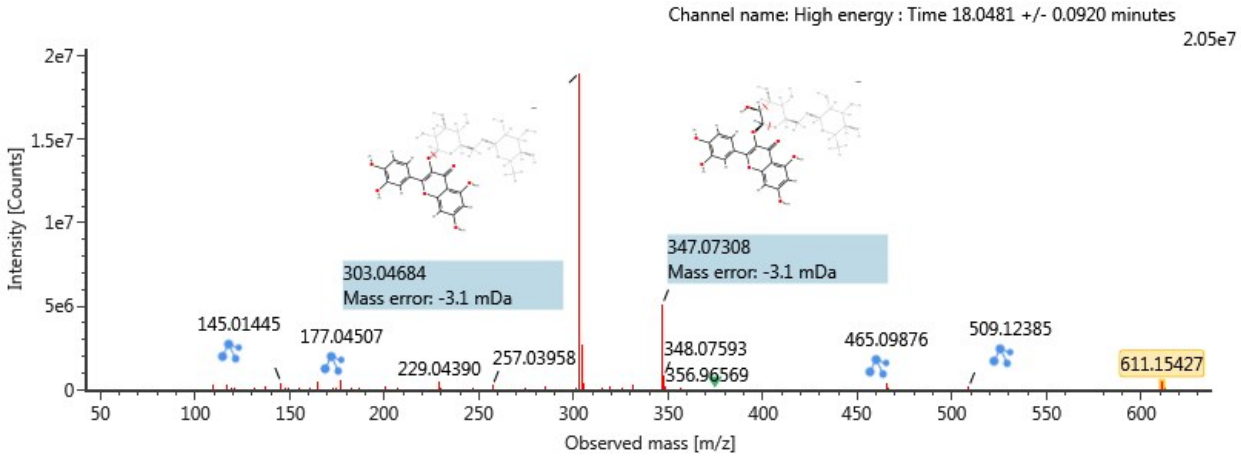

Fig. S29 The fragments of rutin in positive ion mode.

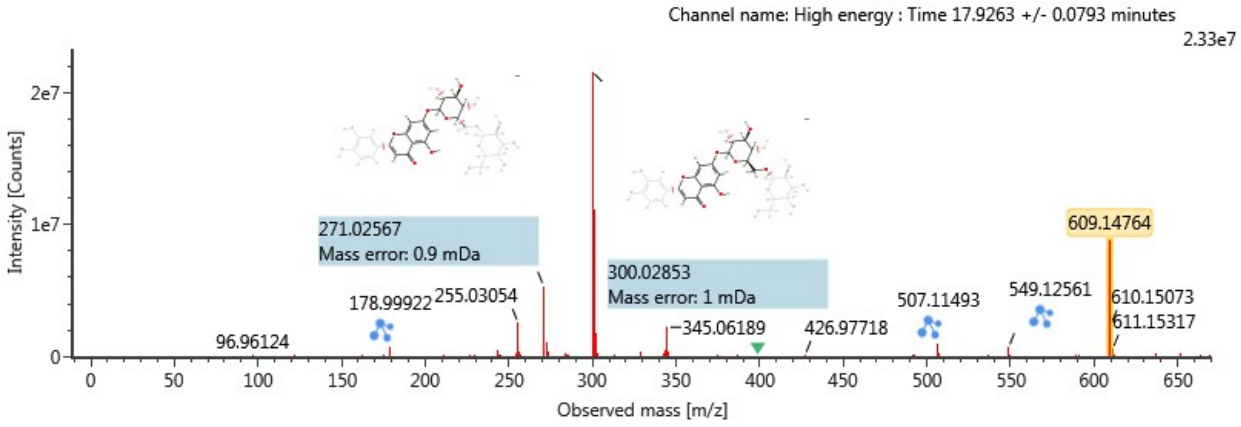

Fig. S30 The fragments of rutin in negative ion mode.

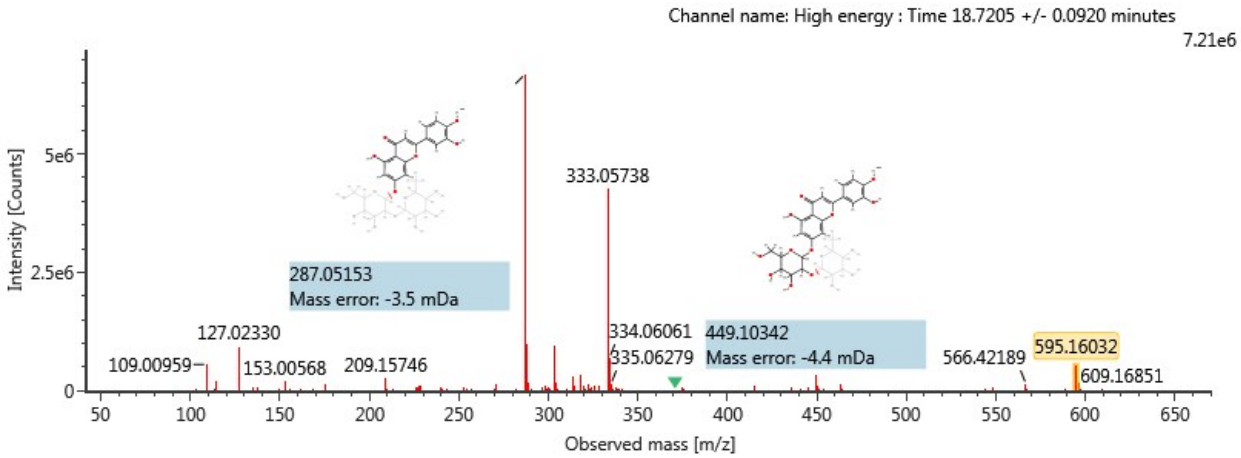

Fig. S31 The fragments of lonicerin in positive ion mode.

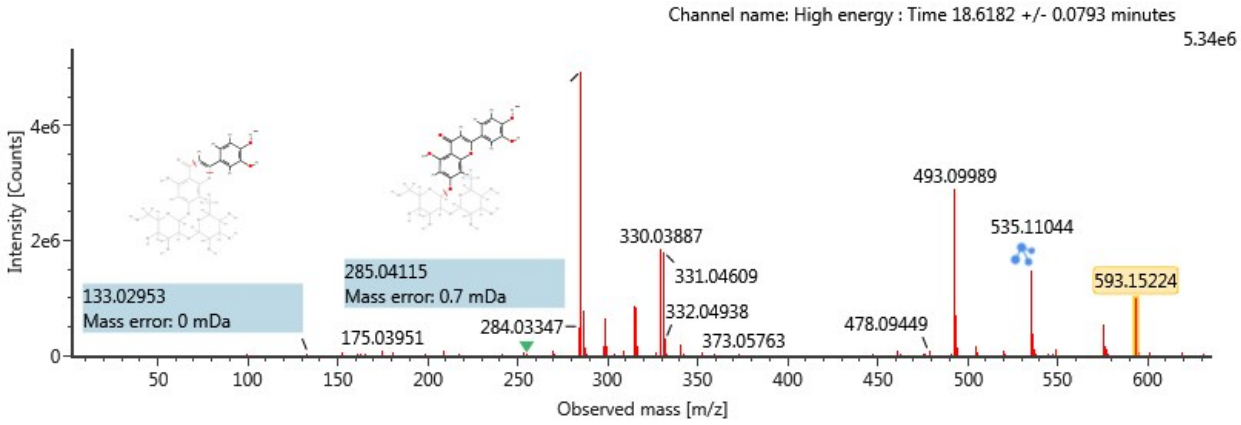

Fig. S32 The fragments of lonicerin in negative ion mode.

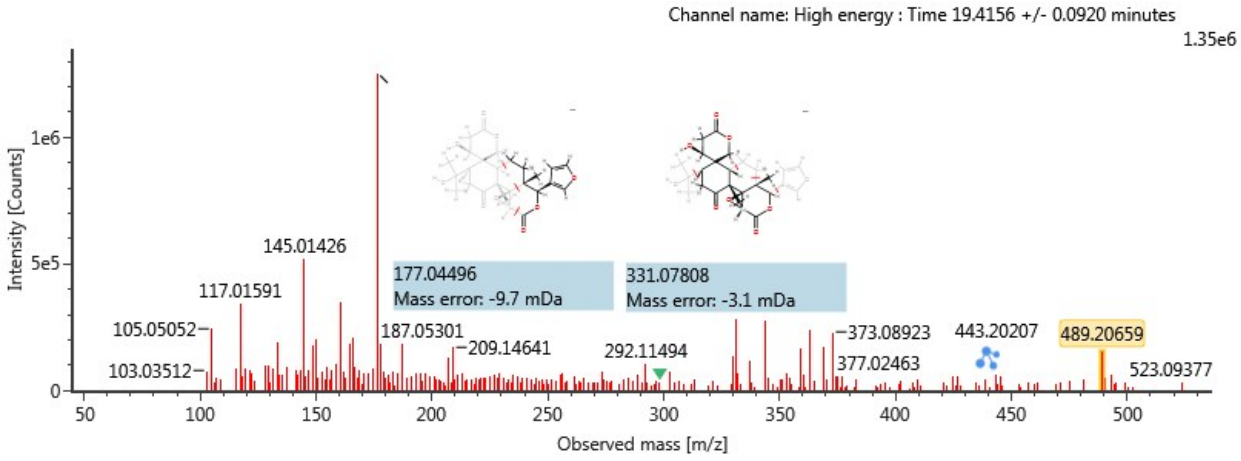

Fig. S33 The fragments of isolimonic acid in positive ion mode.

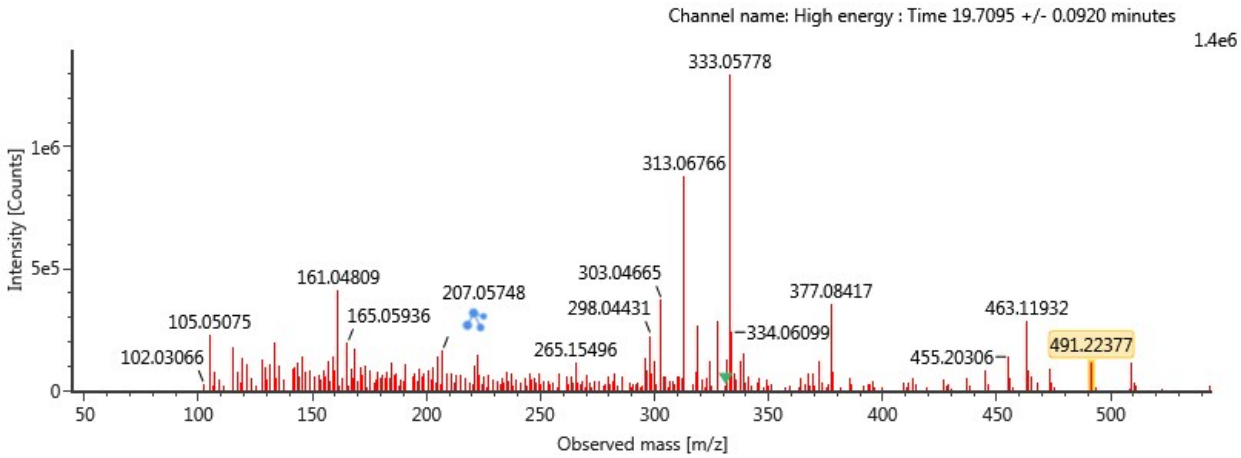

Fig. S34 The fragments of deacetylnomilinic acid in positive ion mode.

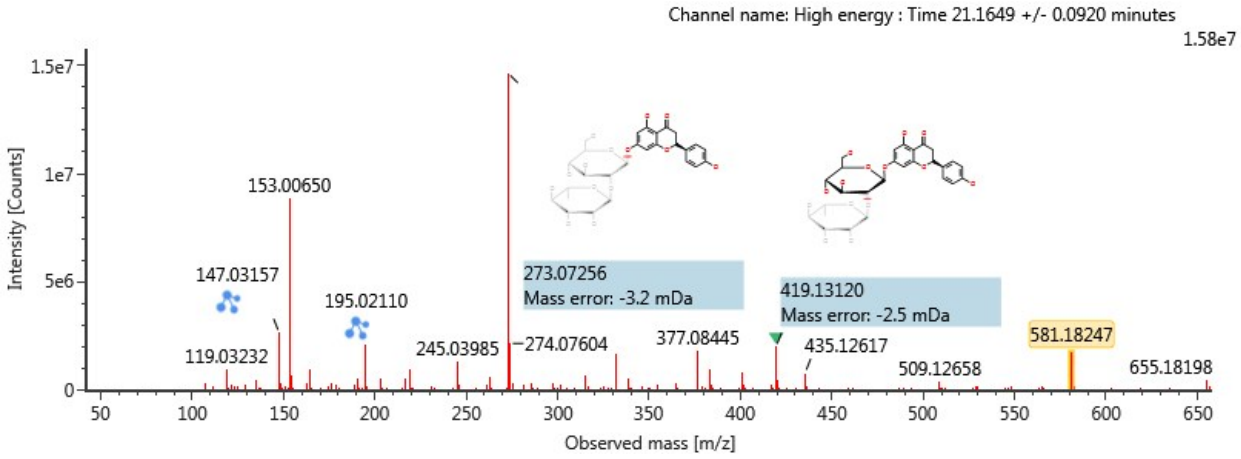

Fig. S35 The fragments of naringin in positive ion mode.

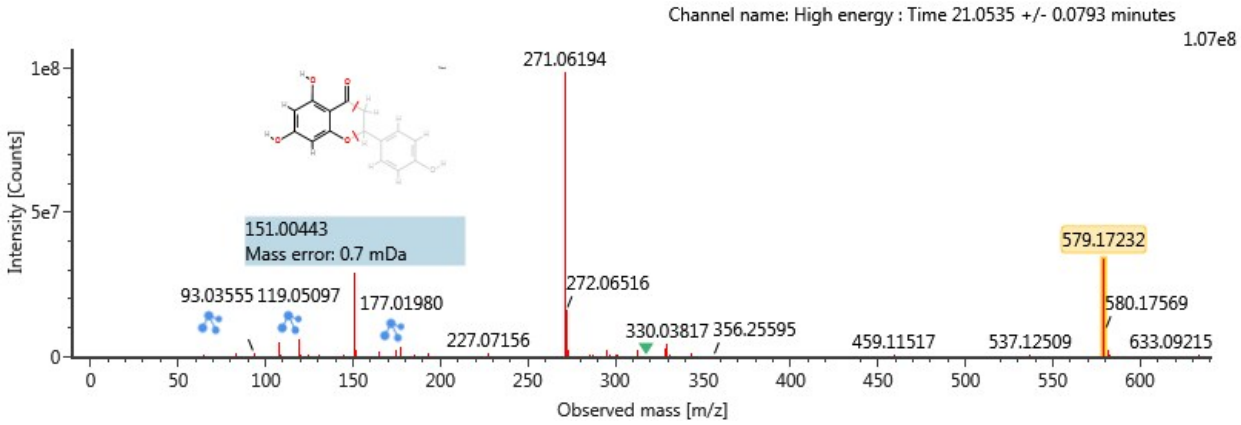

Fig. S36 The fragments of naringin in negative ion mode.

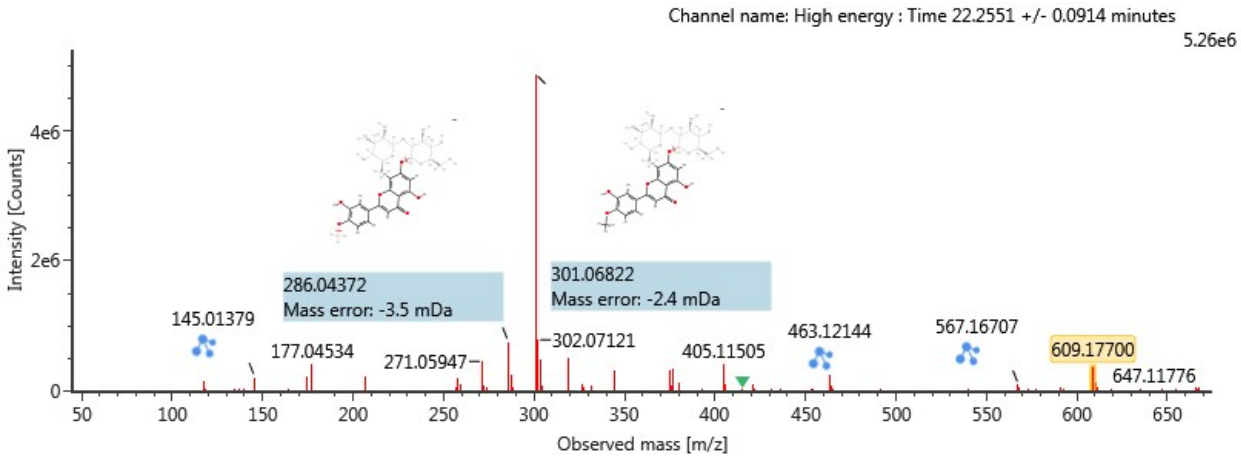

Fig. S37 The fragments of diosmin in positive ion mode.

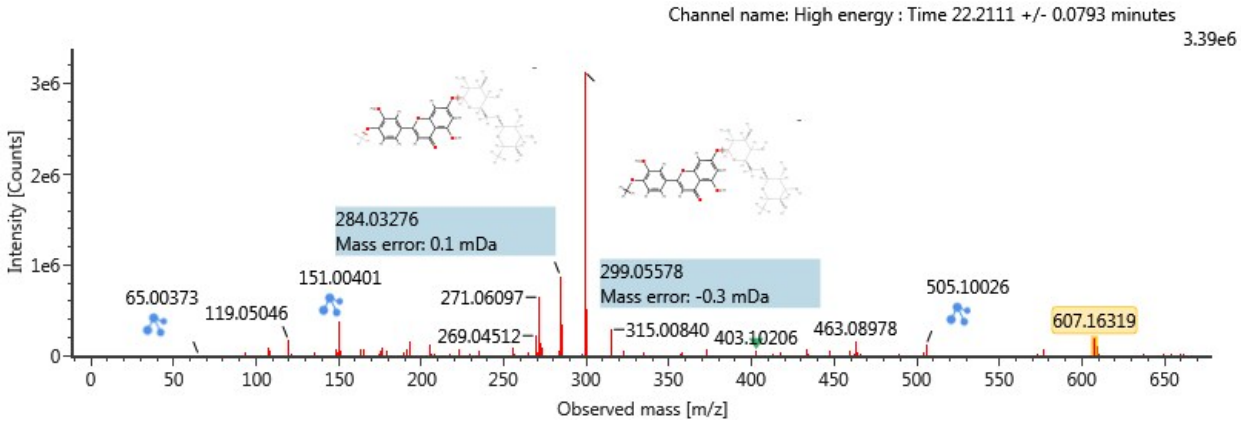

Fig. S38 The fragments of diosmin in negative ion mode.

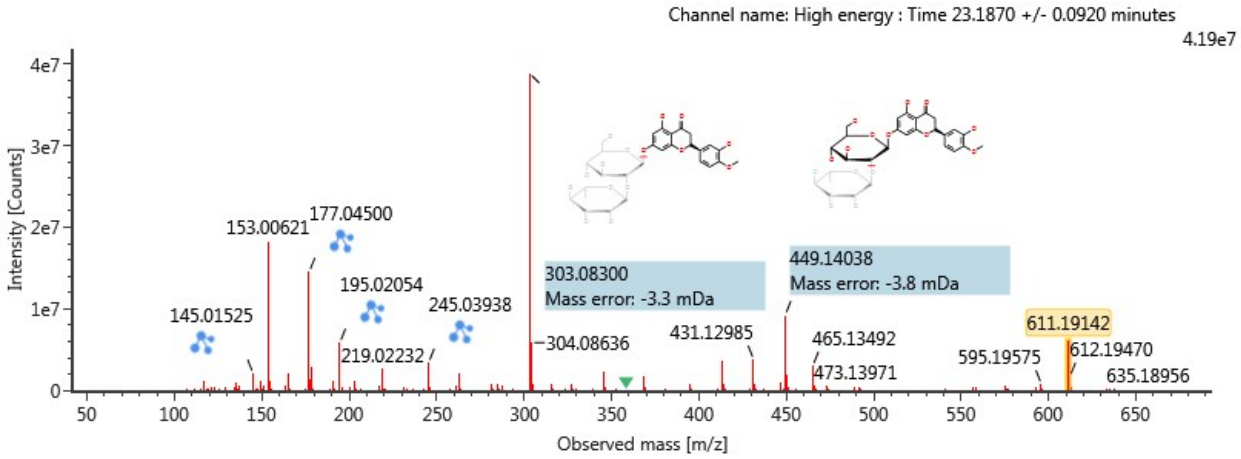

Fig. S39 The fragments of hesperidin in positive ion mode.

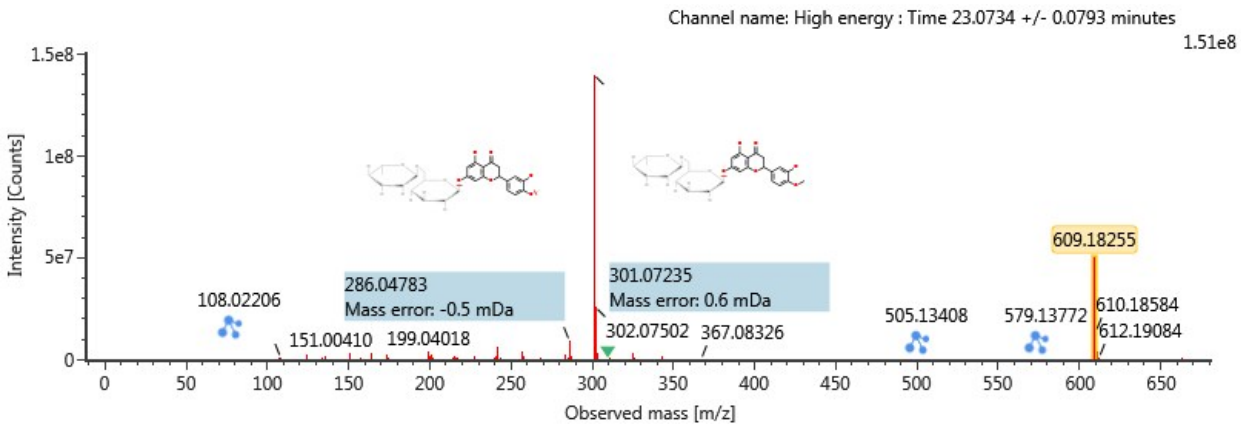

Fig. S40 The fragments of hesperidin in negative ion mode.

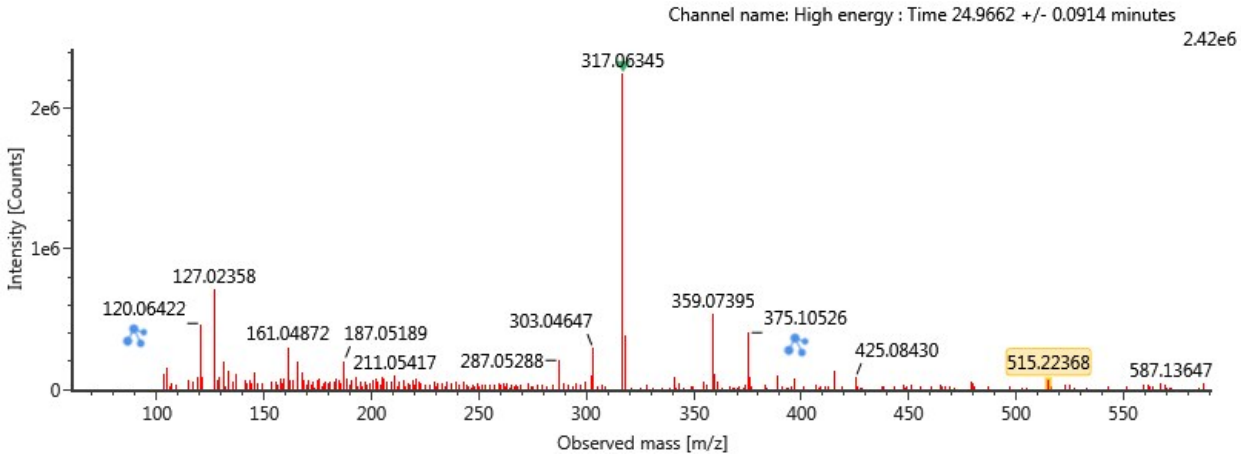

Fig. S41 The fragments of nomilin in positive ion mode.

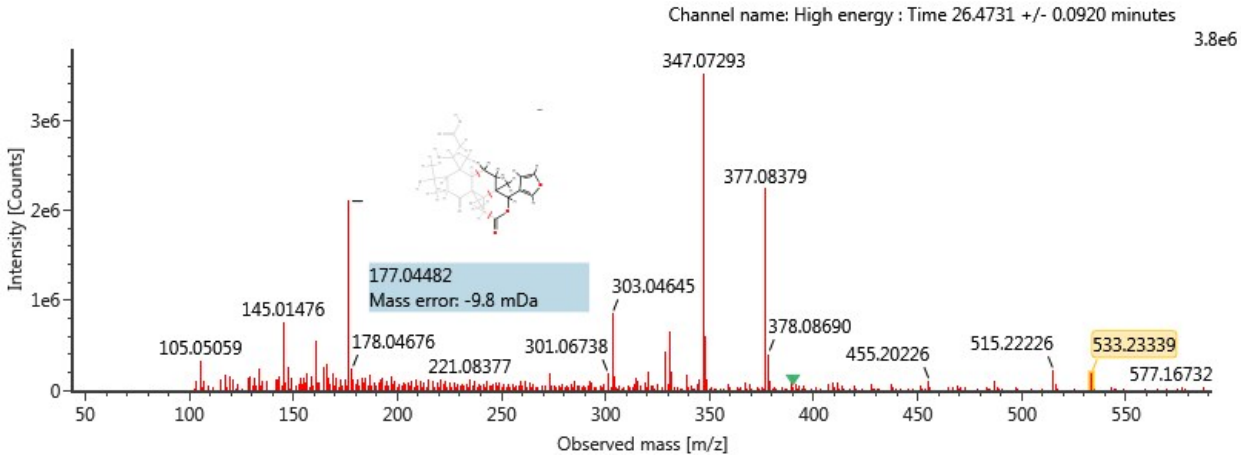

Fig. S42 The fragments of nomilinic acid in positive ion mode.

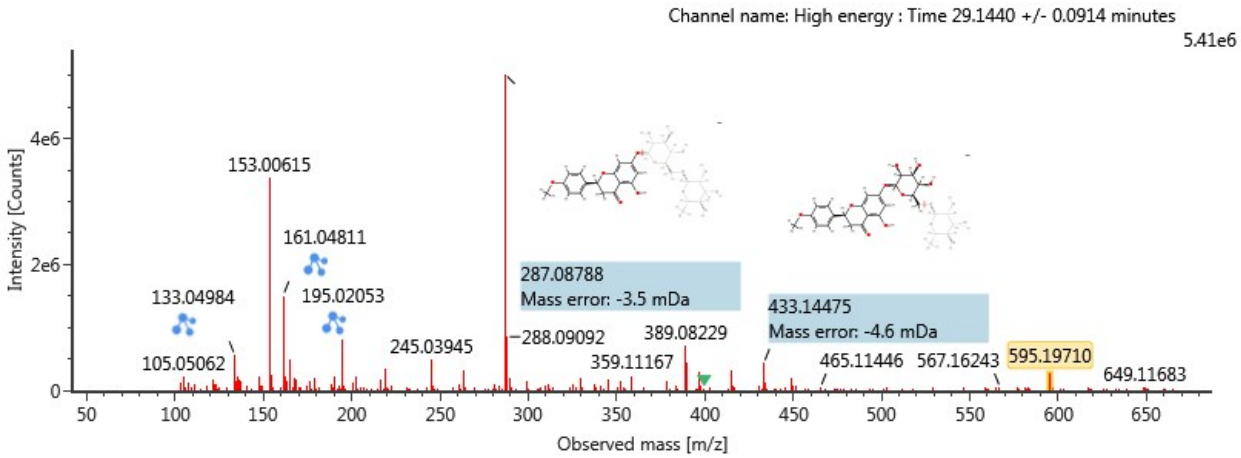

Fig. S43 The fragments of poncirin in positive ion mode.

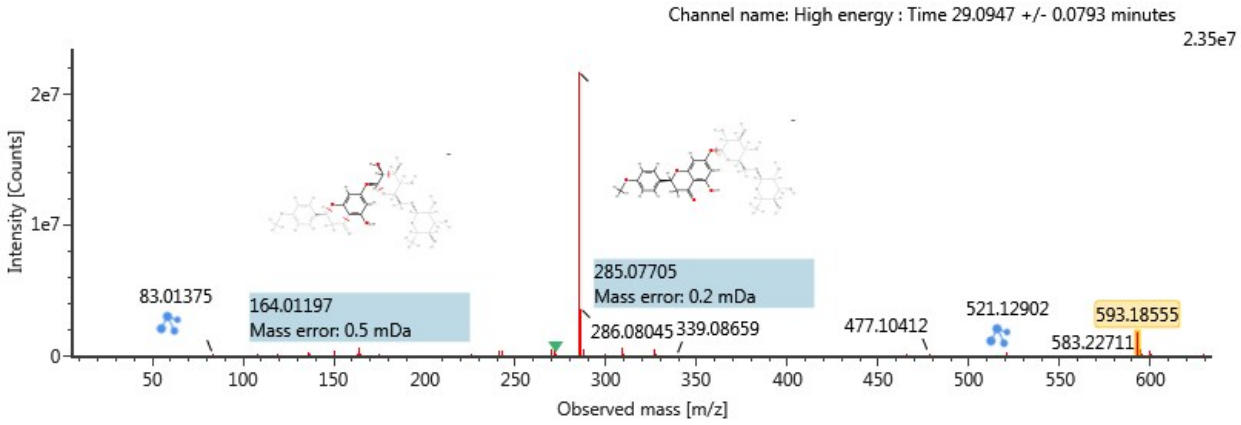

Fig. S44 The fragments of poncirin in negative ion mode.

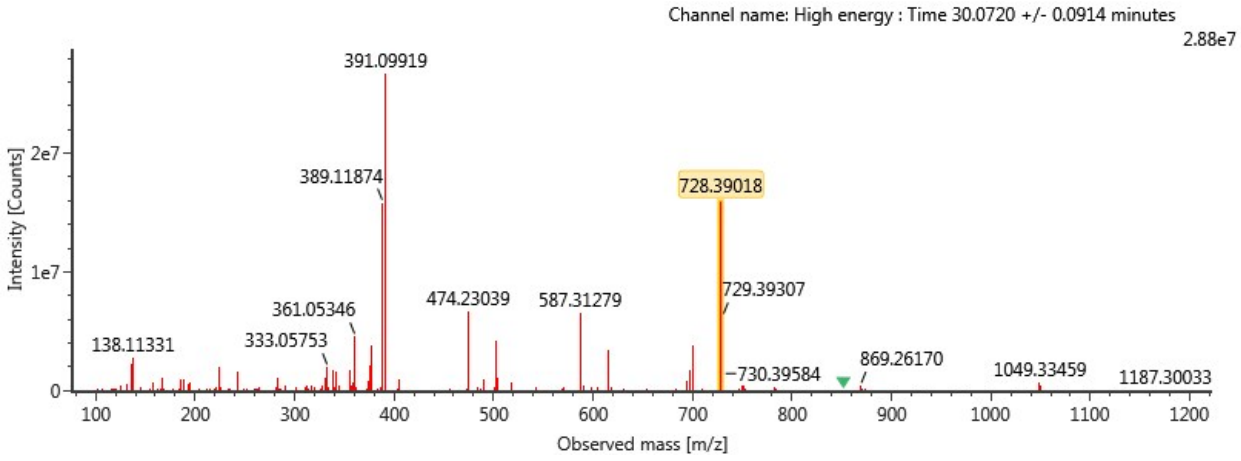

Fig. S45 The fragments of citrusin Ⅲ in positive ion mode.

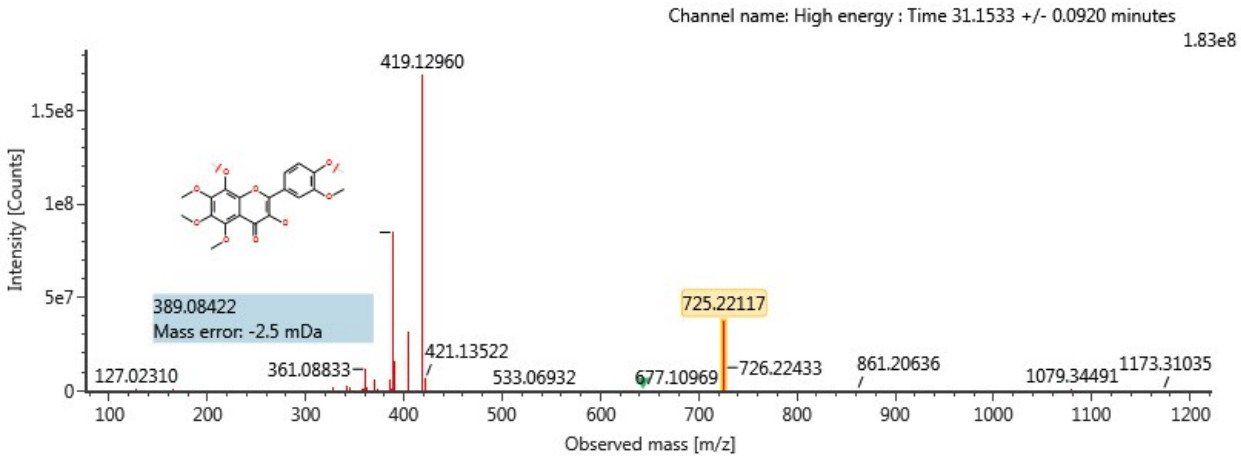

Fig. S46 The fragments of melitidin in positive ion mode.

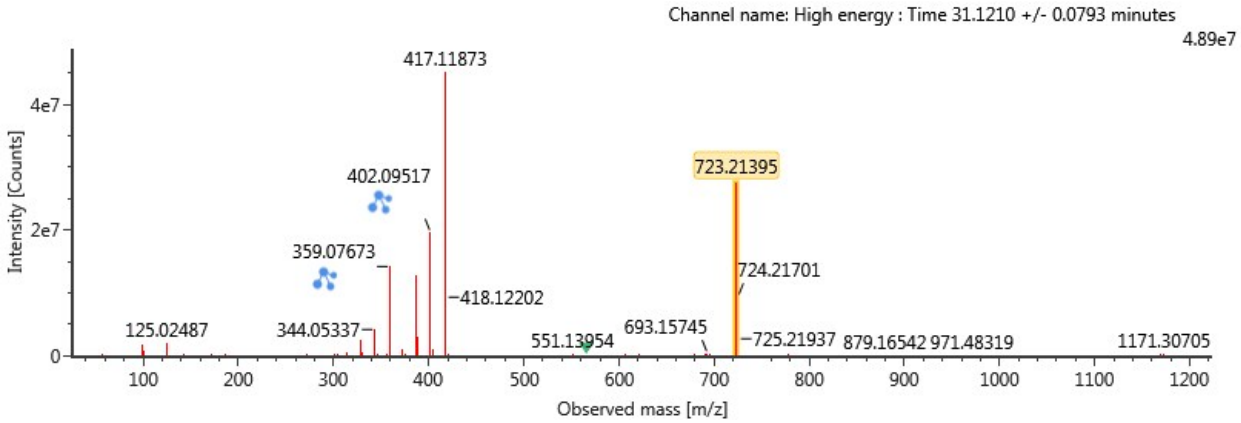

Fig. S47 The fragments of melitidin in negative ion mode.

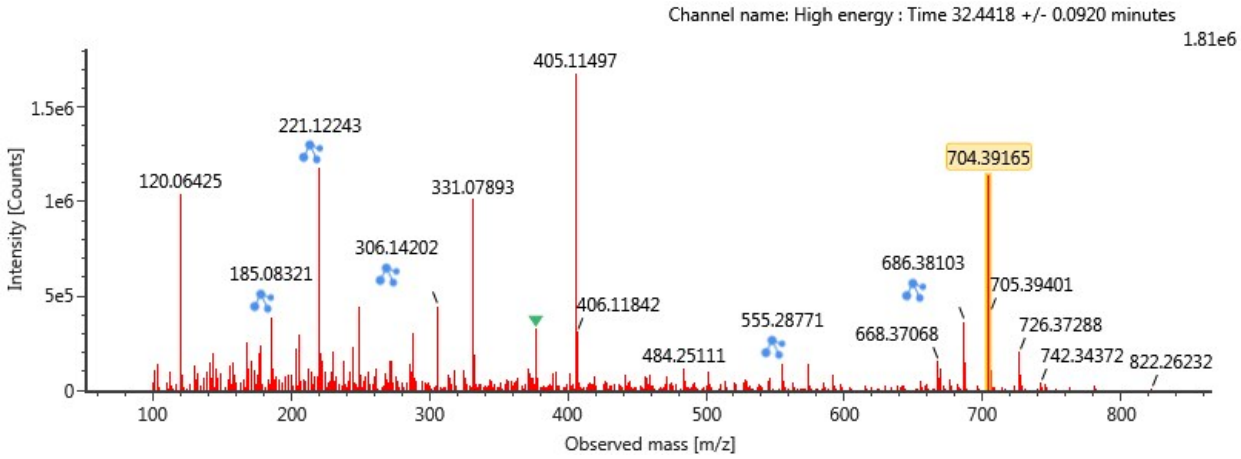

Fig. S48 The fragments of citrusin I in positive ion mode.

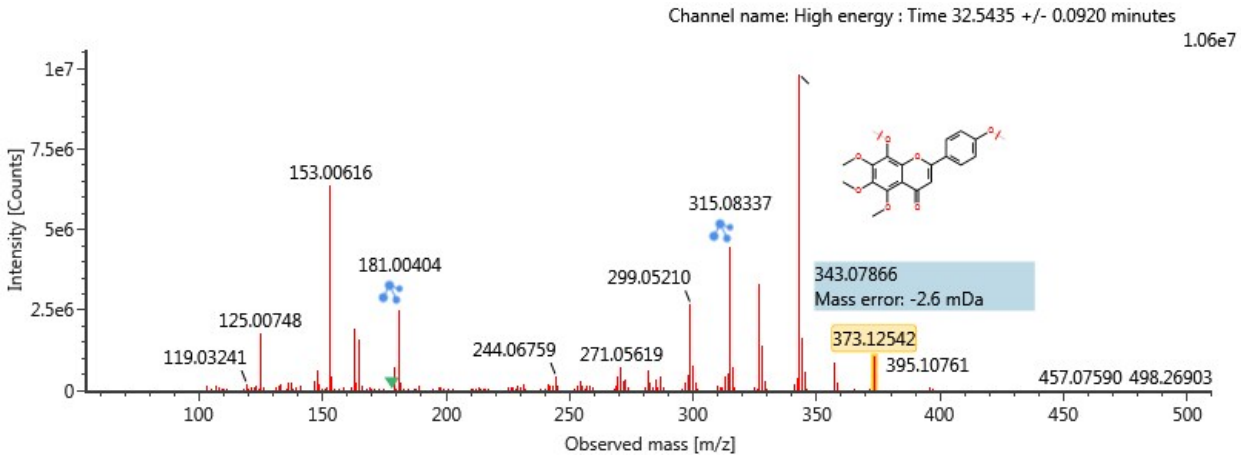

Fig. S49 The fragments of isosinensetin in positive ion mode.

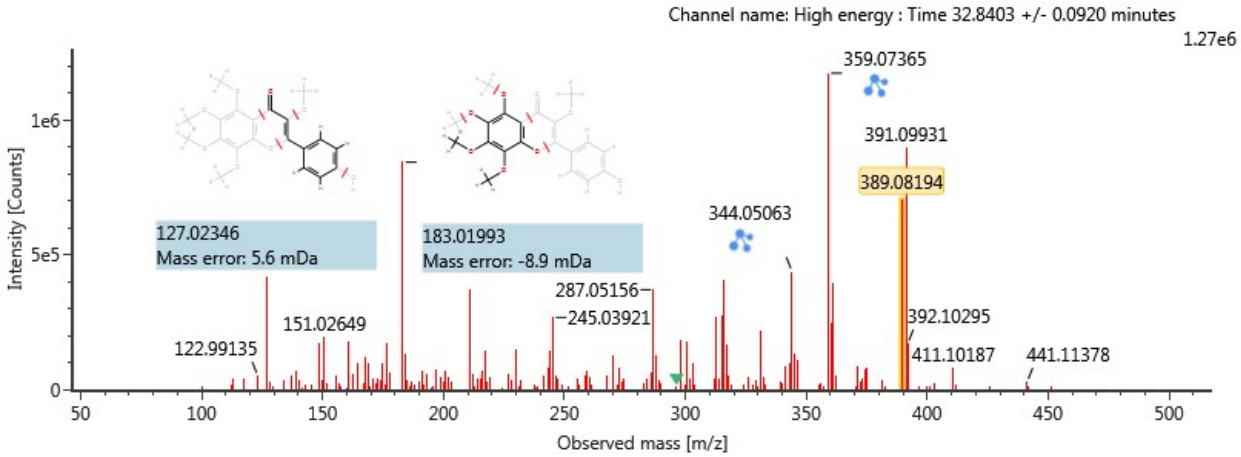

Fig. S50 The fragments of 3'-hydroxy- 5,6,7,8,4'- pentamethoxyflavanone in positive ion mode.

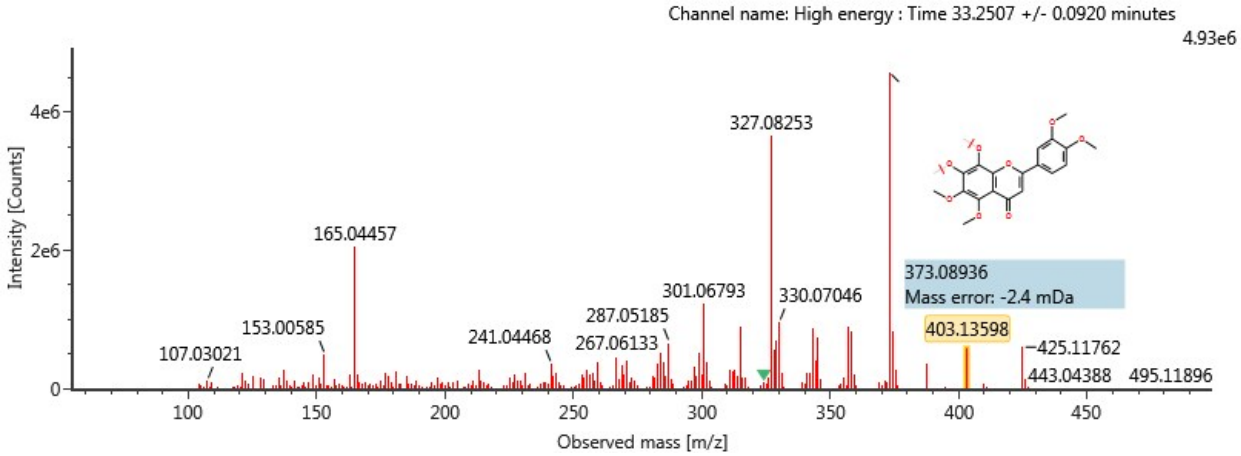

Fig. S51 The fragments of 5, 7, 8, 3', 4', 5'-hexamethoxyflavone in positive ion mode.

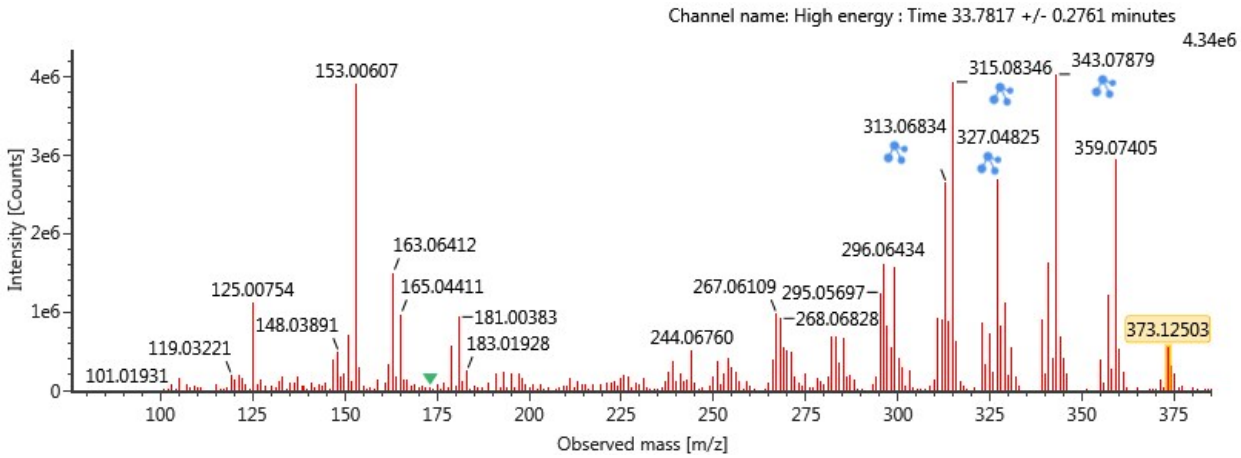

Fig. S52 The fragments of sinensetin in positive ion mode.

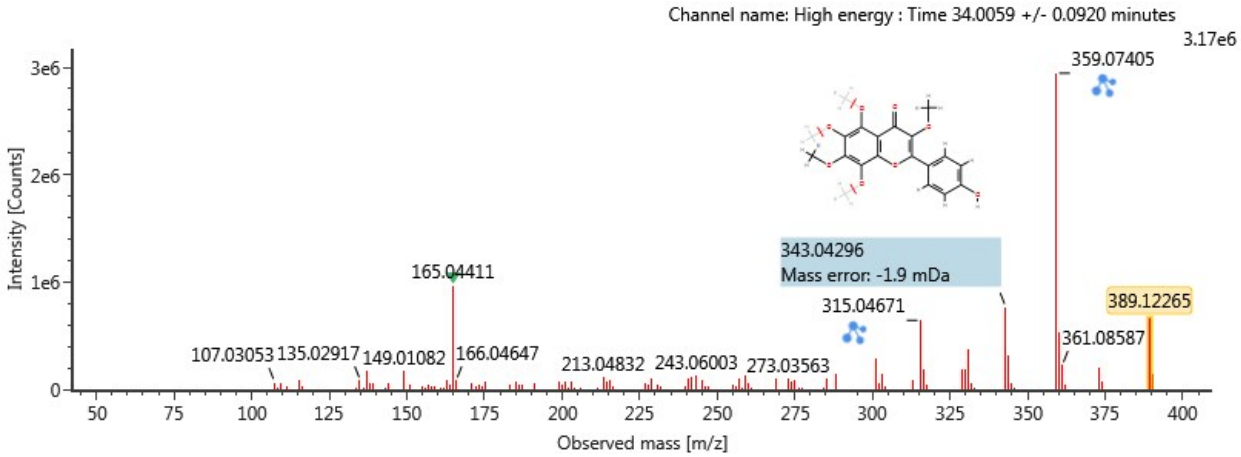

Fig. S53 The fragments of monohydroxy- pentamethoxyflavanone in positive ion mode.

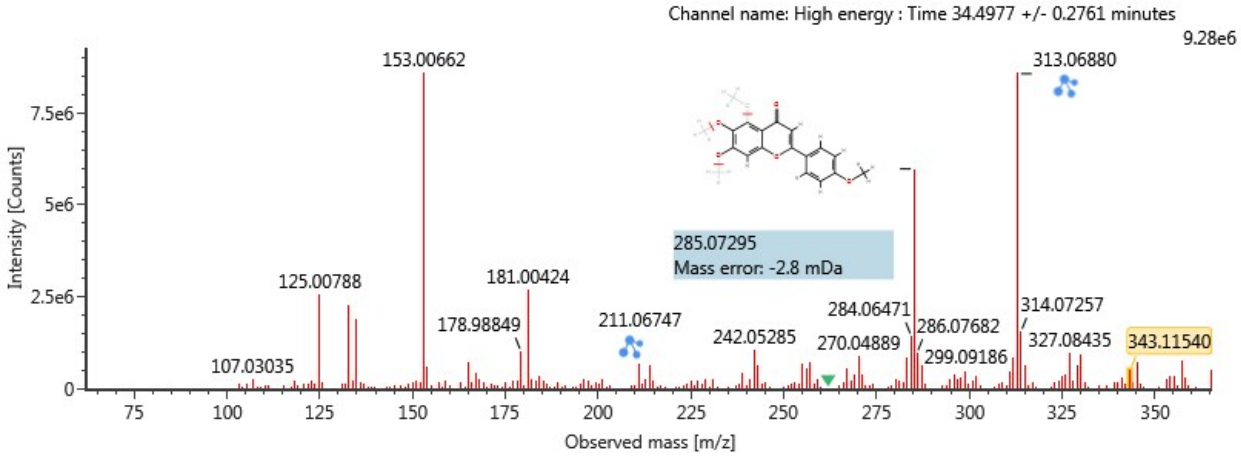

Fig. S54 The fragments of 5, 6, 7, 4'-tetramethoxyflavone in positive ion mode.

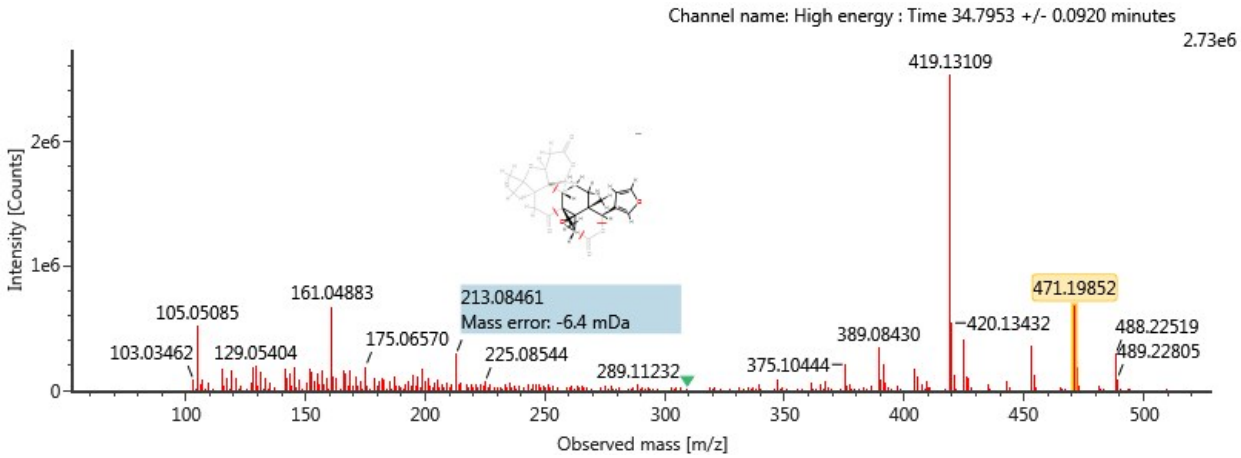

Fig. S55 The fragments of limonin in positive ion mode.

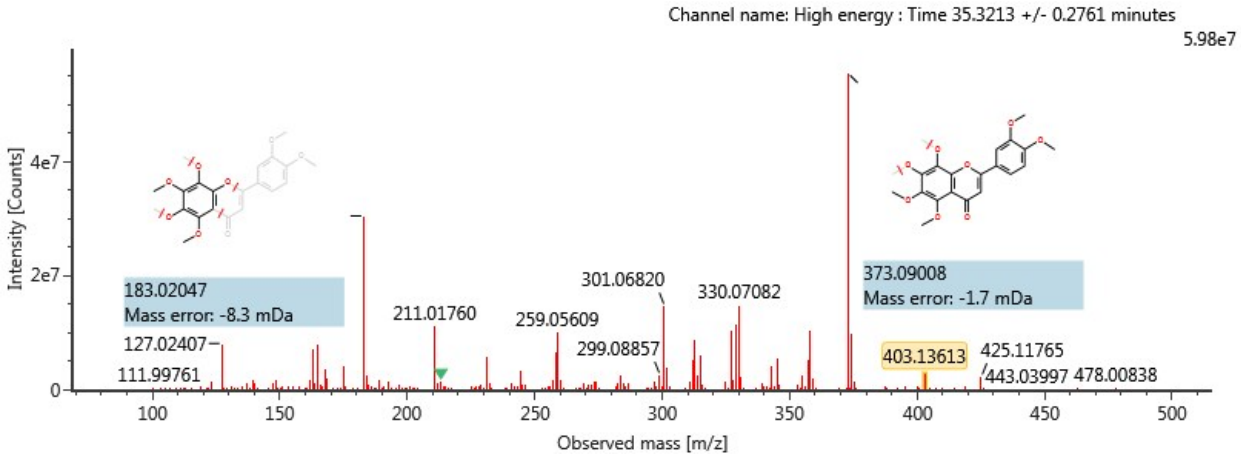

Fig. S56 The fragments of nobiletin in positive ion mode.

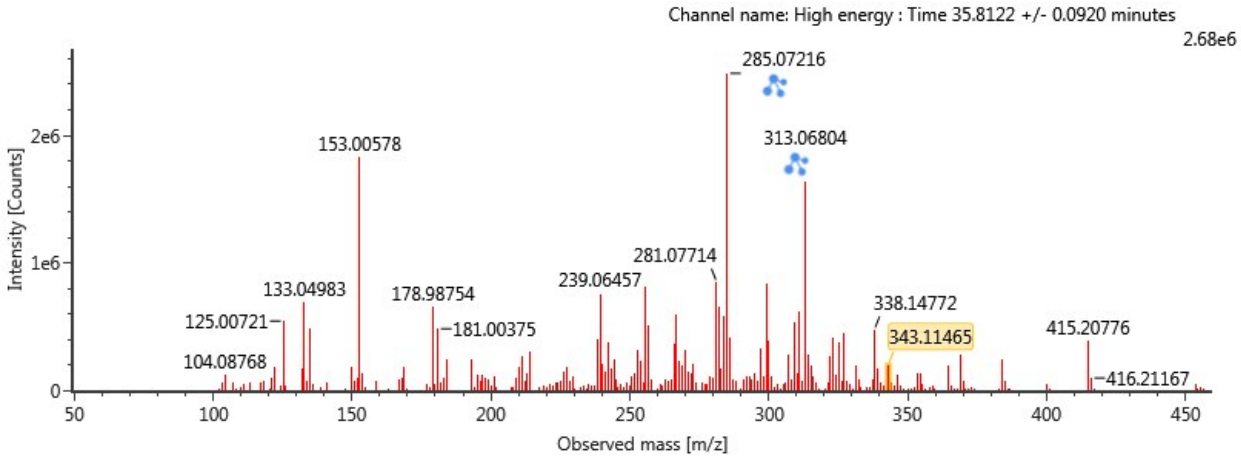

Fig. S57 The fragments of 5, 7, 8, 4'-tetramethoxyflavone in positive ion mode.

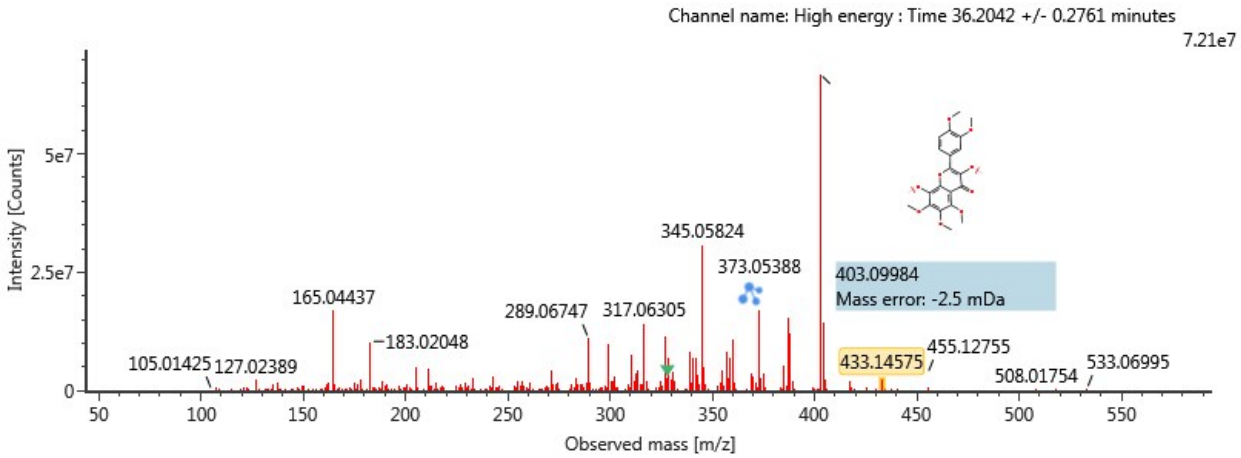

Fig. S58 The fragments of 3, 5, 6, 7, 8, 3', 4'-heptemethoxyflavone in positive ion mode.

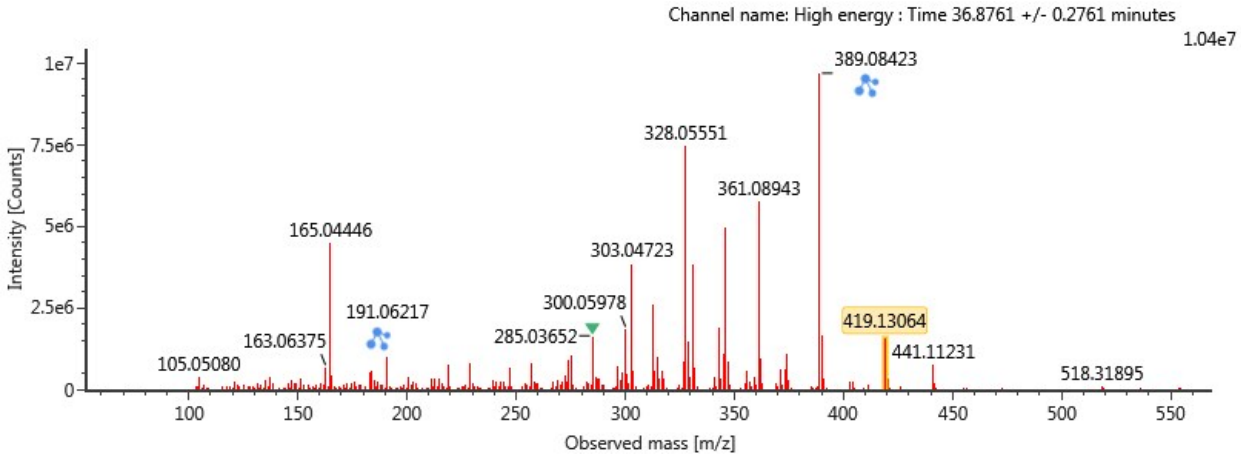

Fig. S59 The fragments of 5-hydroxy-3, 6, 7, 8, 3', 4'-pentamethoxyflavanone in positive ion mode.

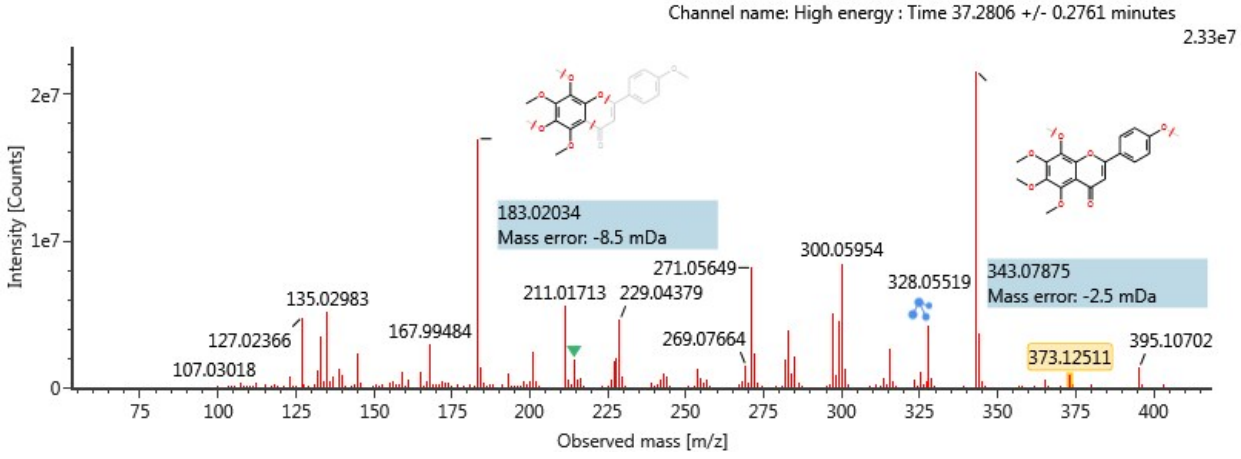

Fig. S60 The fragments of tangeritin in positive ion mode.

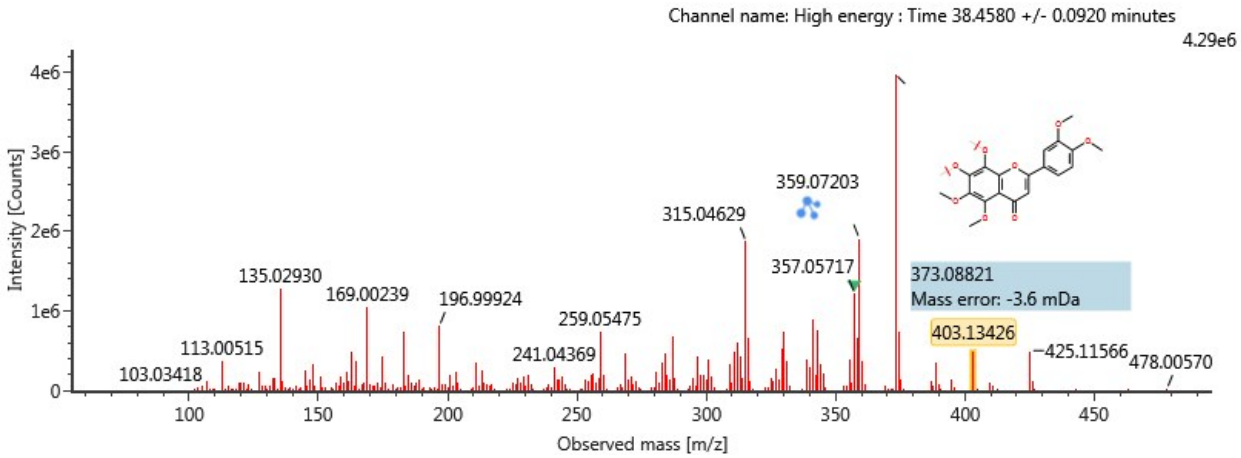

Fig. S61 The fragments of hexamethoxyflavone in positive ion mode.

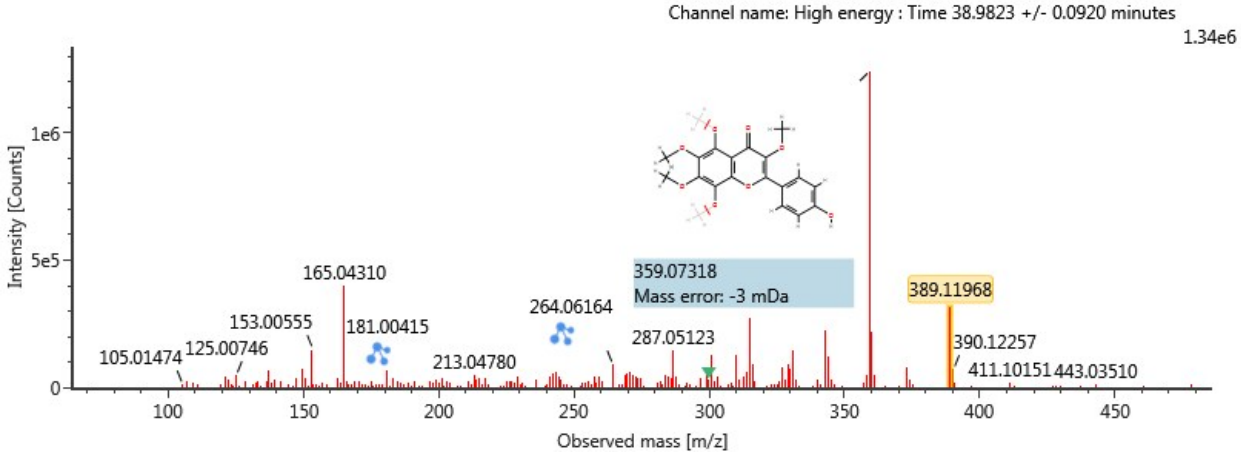

Fig. S62 The fragments of 5-hydroxy- 6, 7, 8, 3', 4'- pentamethoxyflavanone in positive ion mode.

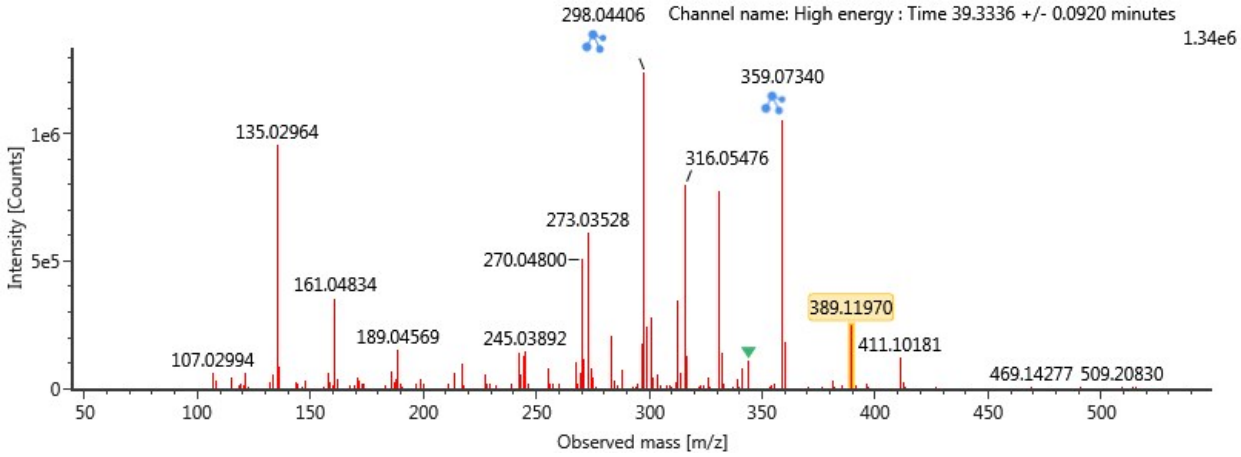

Fig. S63 The fragments of monohydroxy- pentamethoxyflavanone in positive ion mode.

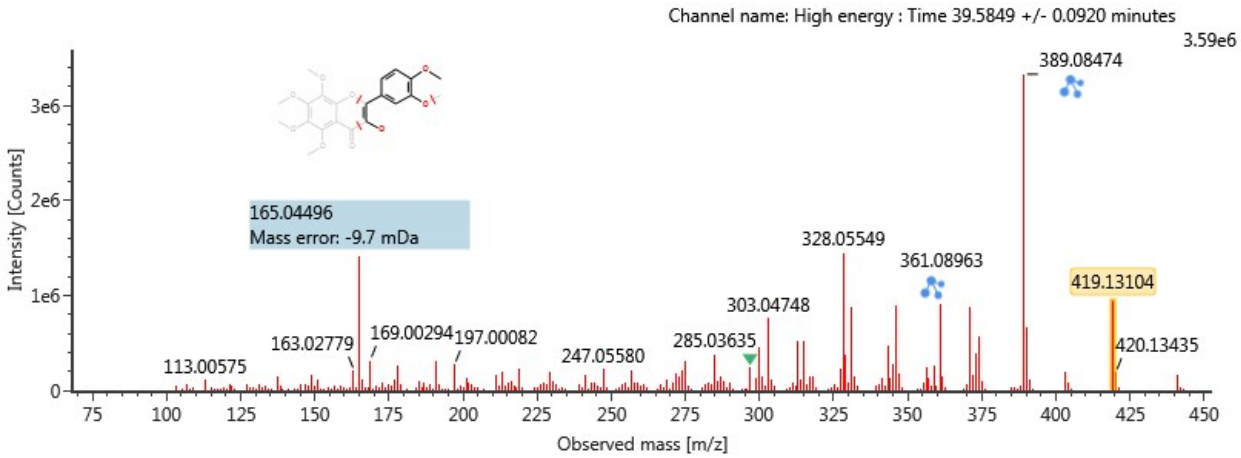

Fig. S64 The fragments of natsudaidain in positive ion mode.

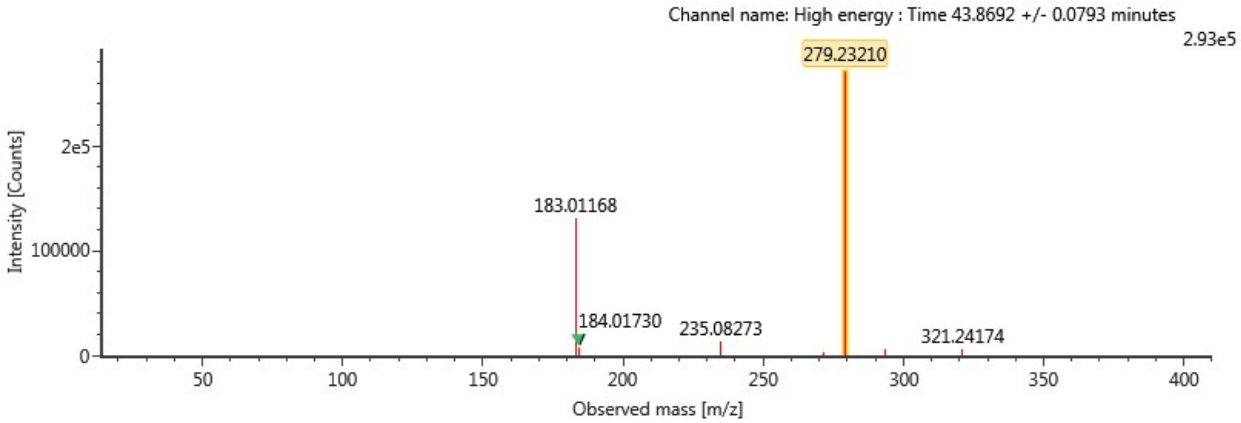

Fig. S65 The fragments of linolic acid in negative ion mode.

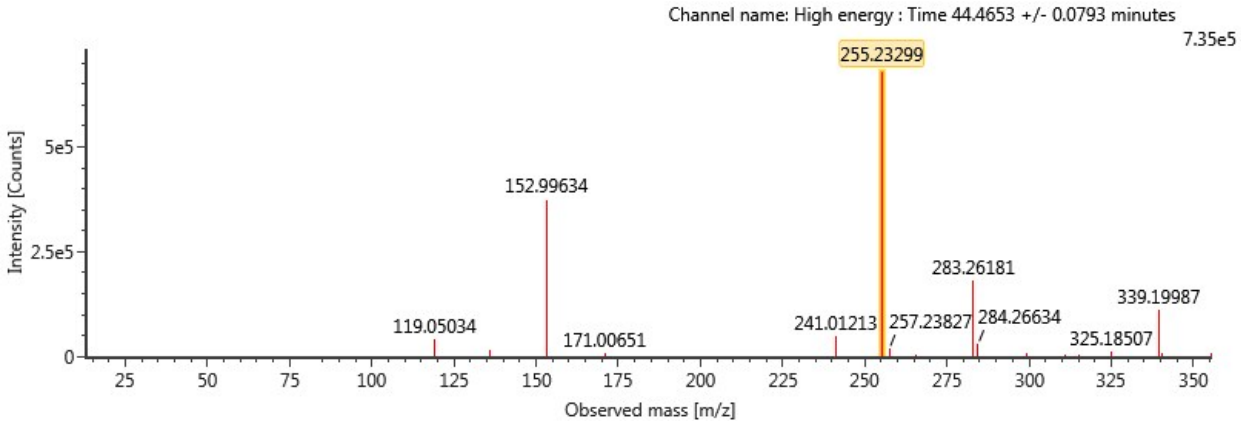

Fig. S66 The fragments of palmitic acid in negative ion mode.

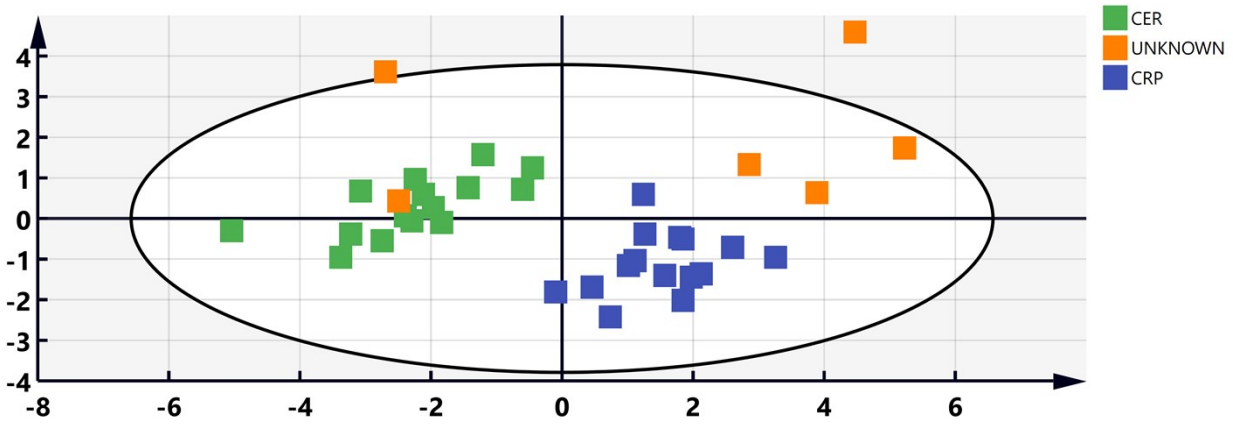

Fig. S67 The PCA score plot of 12 chemical markers in CER , CRP and unknown samples.

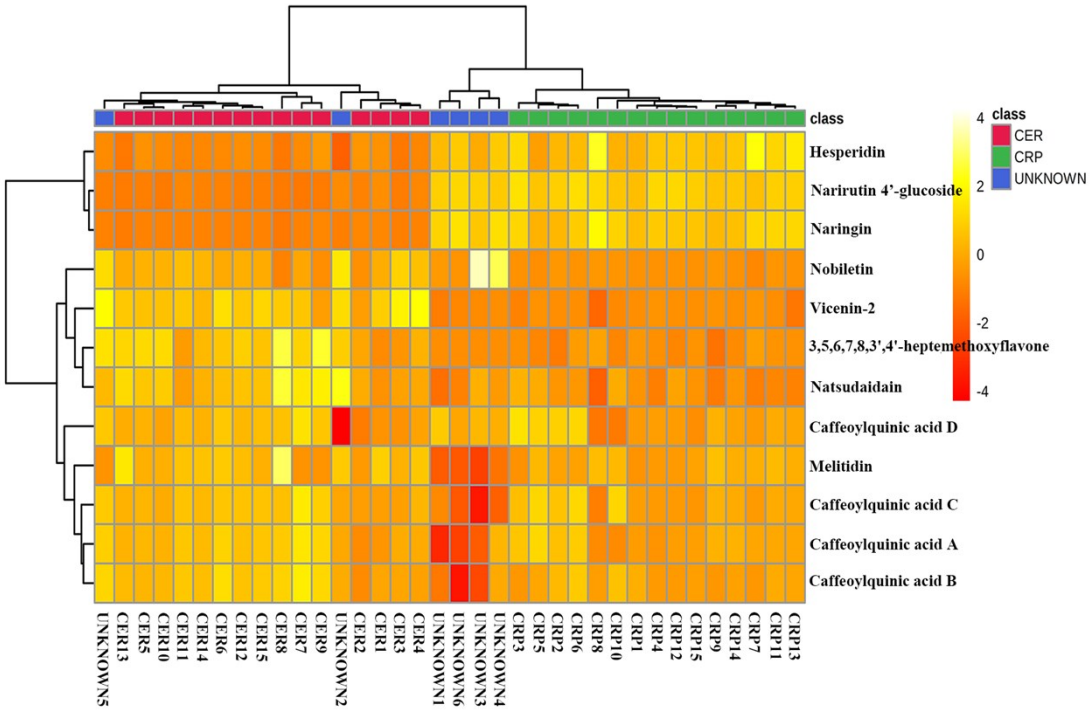

Fig. S68 Heat map of 12 chemical markers in CER , CRP and unknown samples.