Fig. S1 The separation effect of compounds 10 ~ 30.

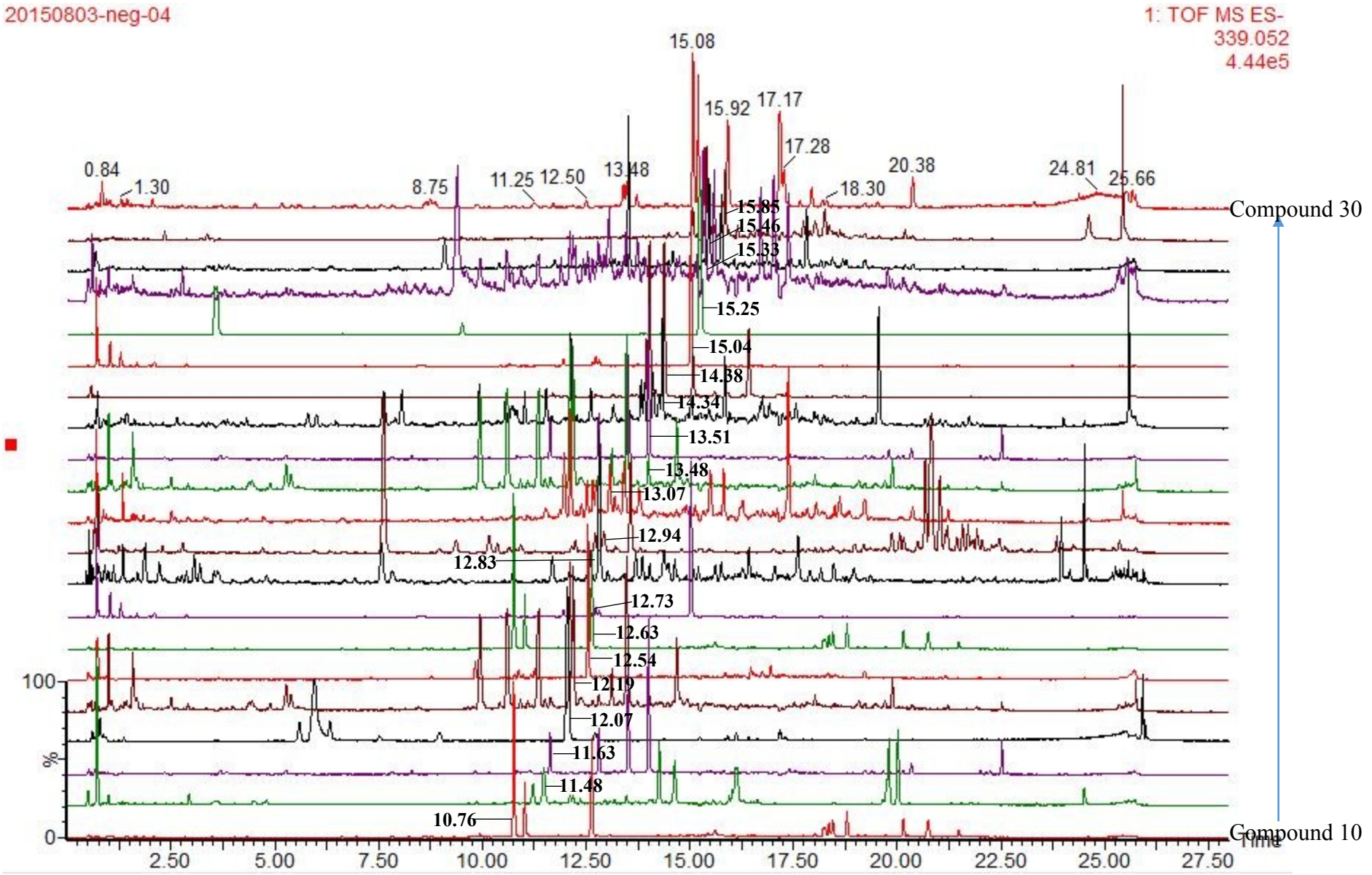
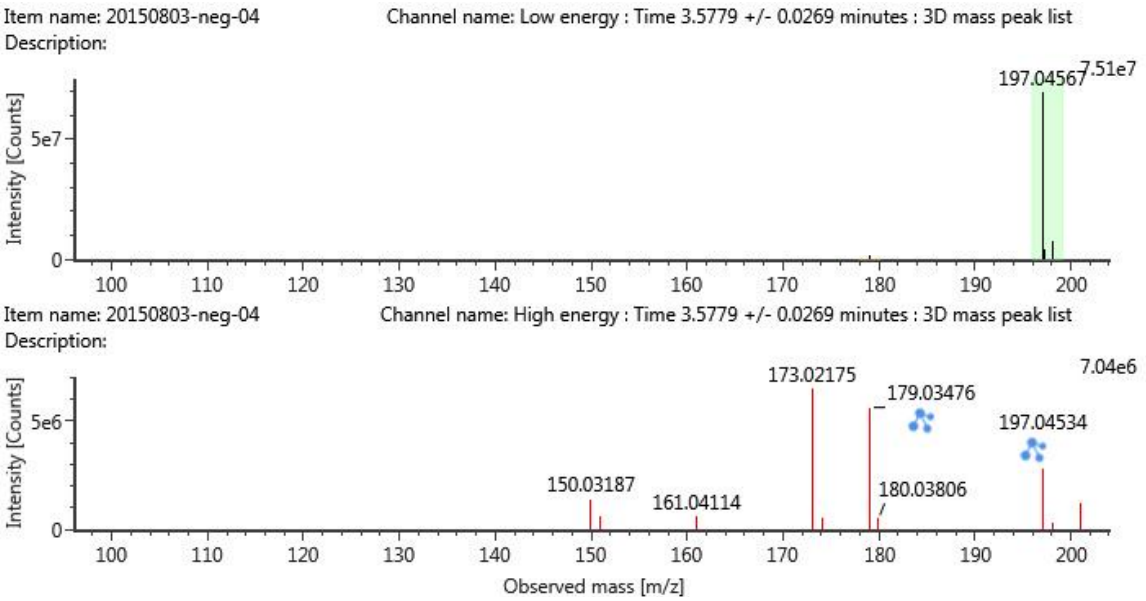
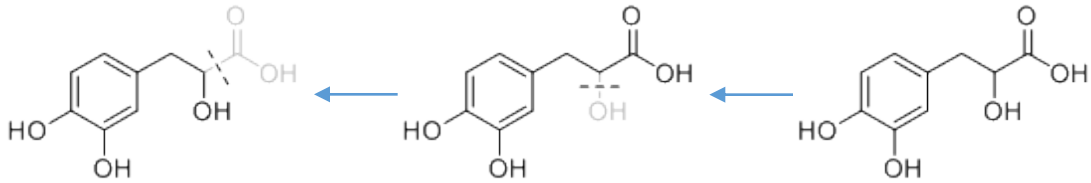


Fig. S2 The mass spectra and proposed fragmentation pathway of other compounds in DHI.

(4) Danshensu





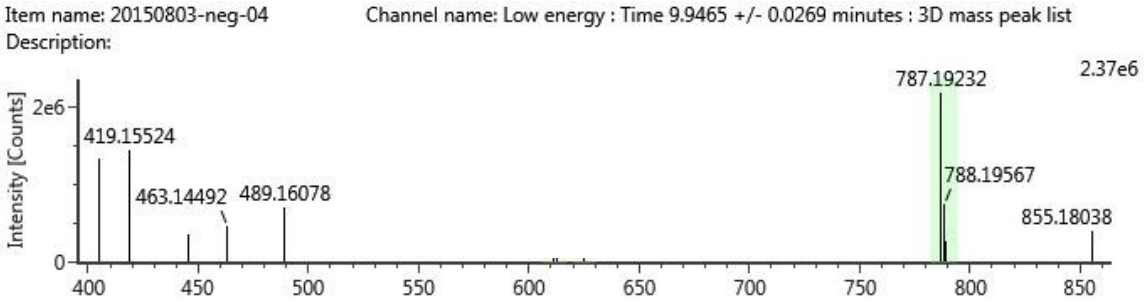
$[M–H–COOH]^-$
151.03857
Mass error: -1.5 mDa

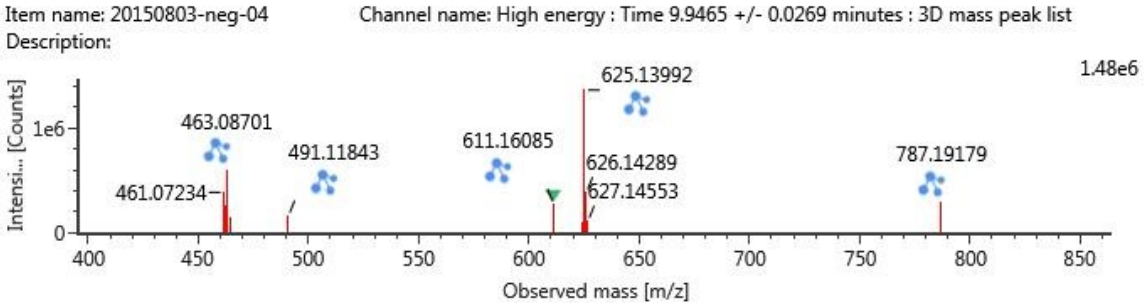
$[M–H–H_2O]^-$
179.03476
Mass error: -0.2 mDa

$[M–H]^-$
197.04534
Mass error: -0.2 mDa

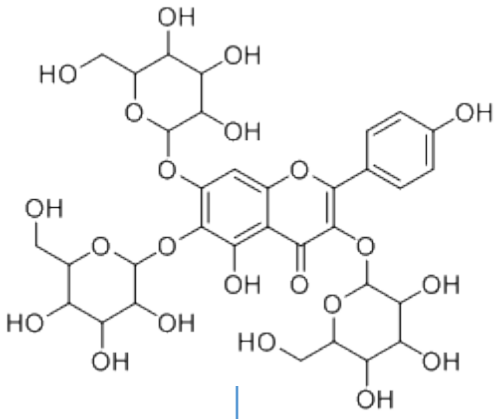
Fig. S2 (continued)

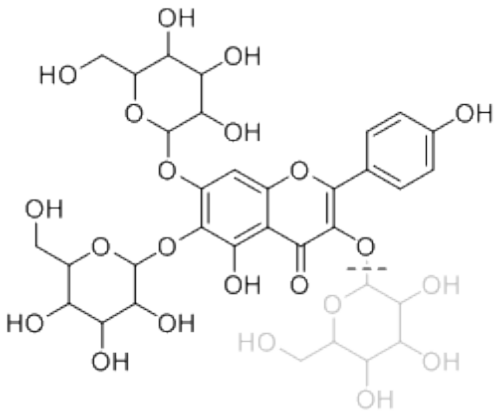
(9) 6-hydroxykaempferol-3,6,7-tri-O-glucoside



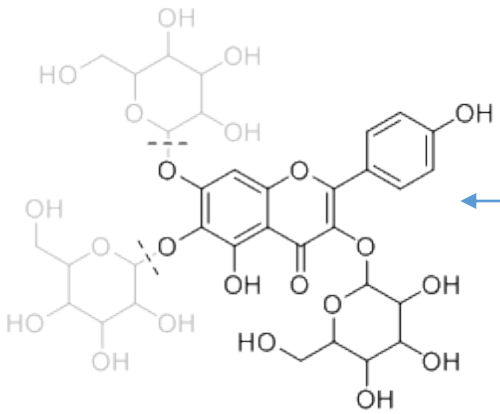


$[M–H]^-$
787.19179
Mass error: -2.1 mDa

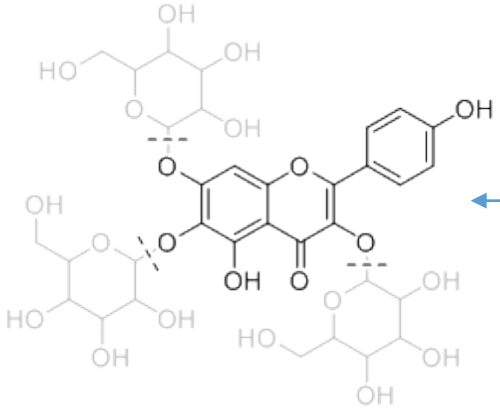




$[M–H–glu]^-$
625.13992
Mass error: -1.1 mDa



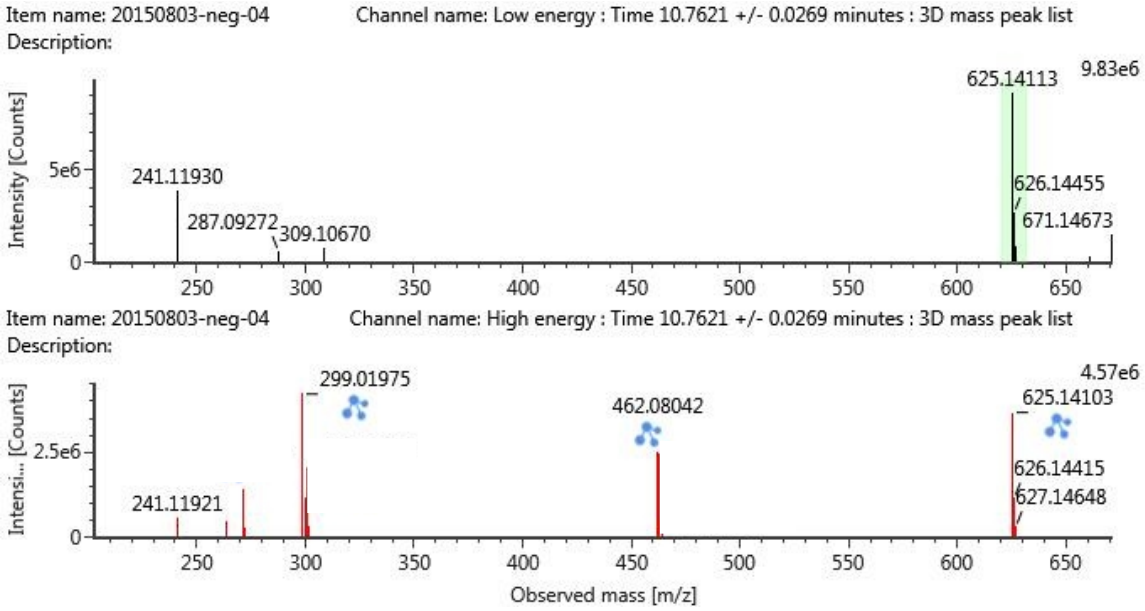
$[M–H–2glu]^-$
463.08701
Mass error: -1.2 mDa

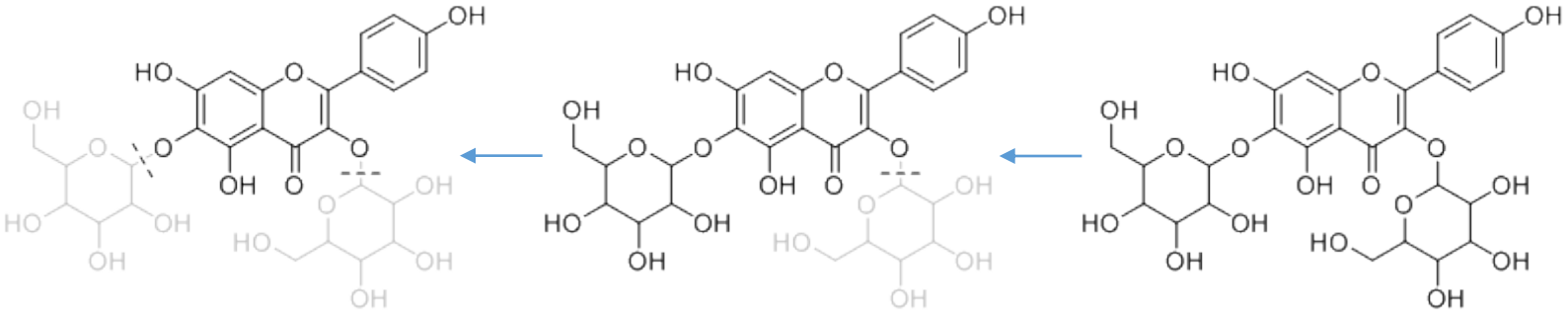


$[M–H–3glu]^-$
301.03426
Mass error: -1.1 mDa

Fig. S2 (continued)

(10) 6-hydroxykaempferol-3,6-di-O-glucoside





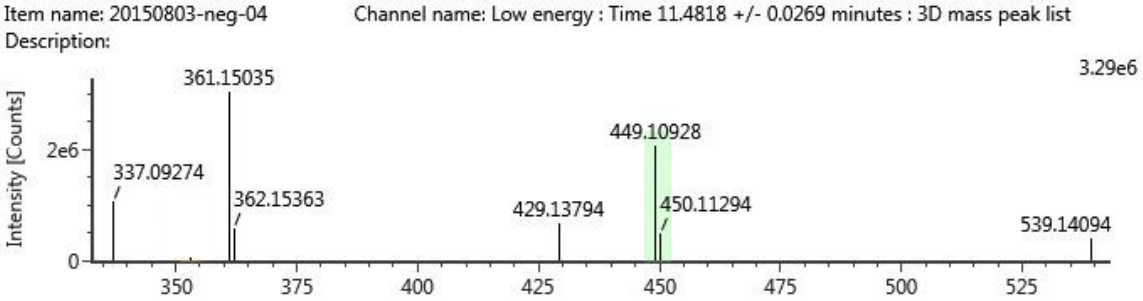
[M–H–2glu]⁻
299.01975
Mass error: 0 mDa

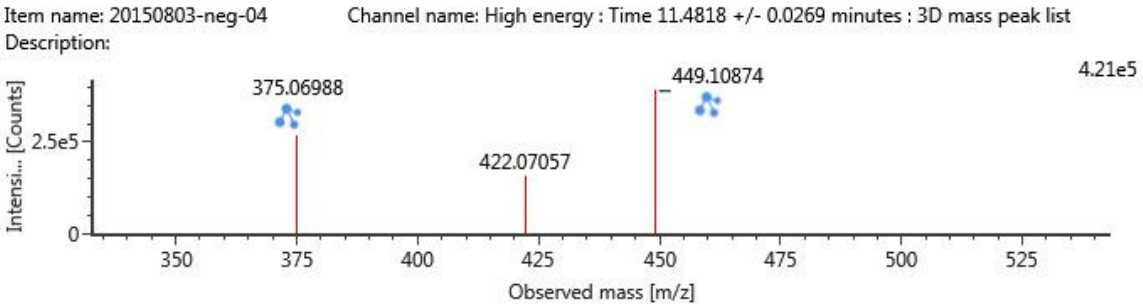
[M–H–glu]⁻
462.08042
Mass error: 0 mDa

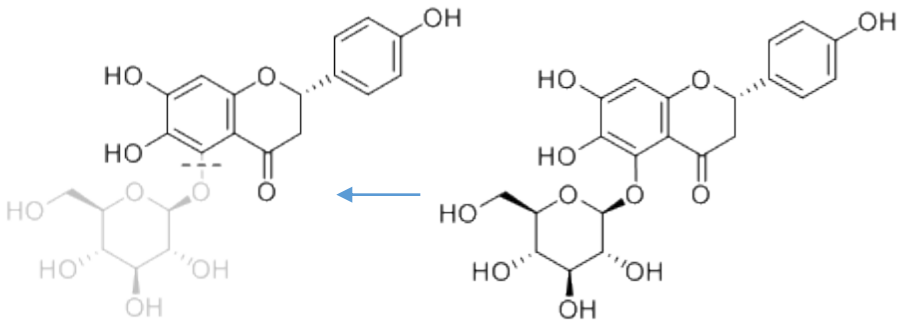
[M–H]⁻
625.14103
Mass error: 0 mDa

Fig. S2 (continued)

(11) neocarthamin





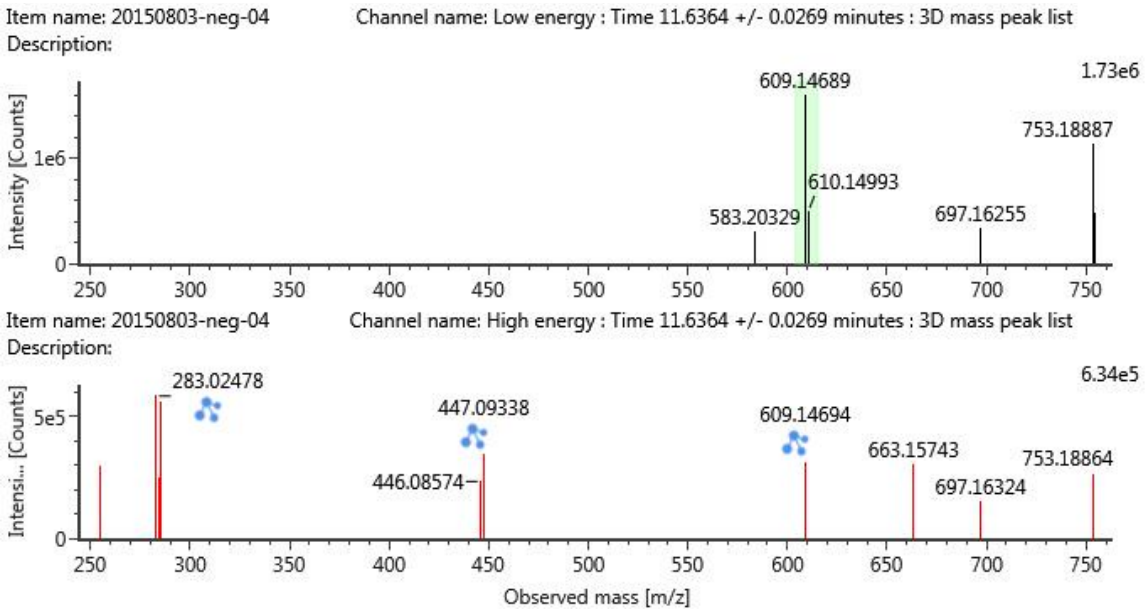


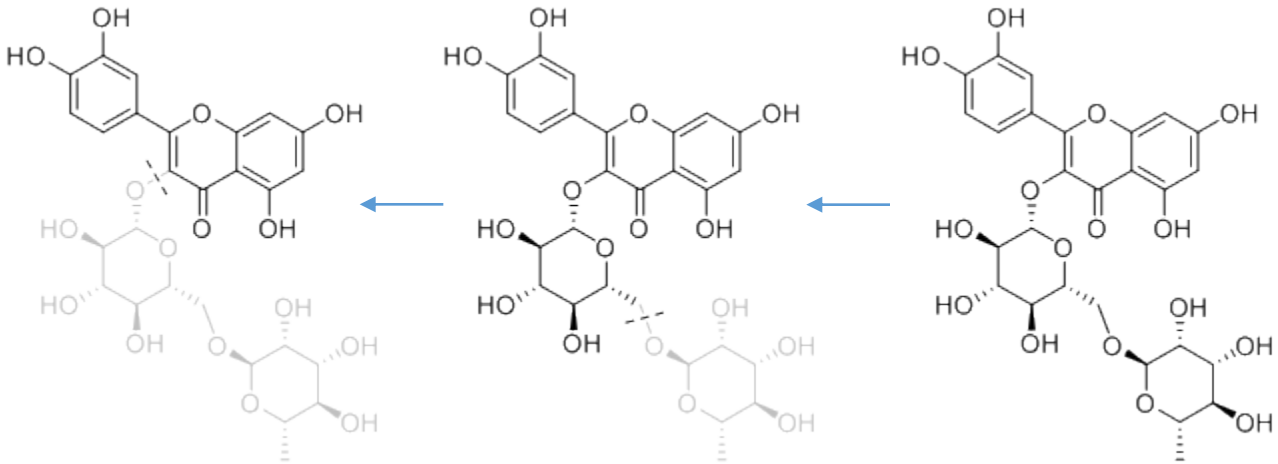
$[M–H–glu–H_2O]^-$
269.04535
Mass error: -0.2 mDa

$[M–H]^-$
449.10874
Mass error: -0.2 mDa

Fig. S2 (continued)

(12) rutin





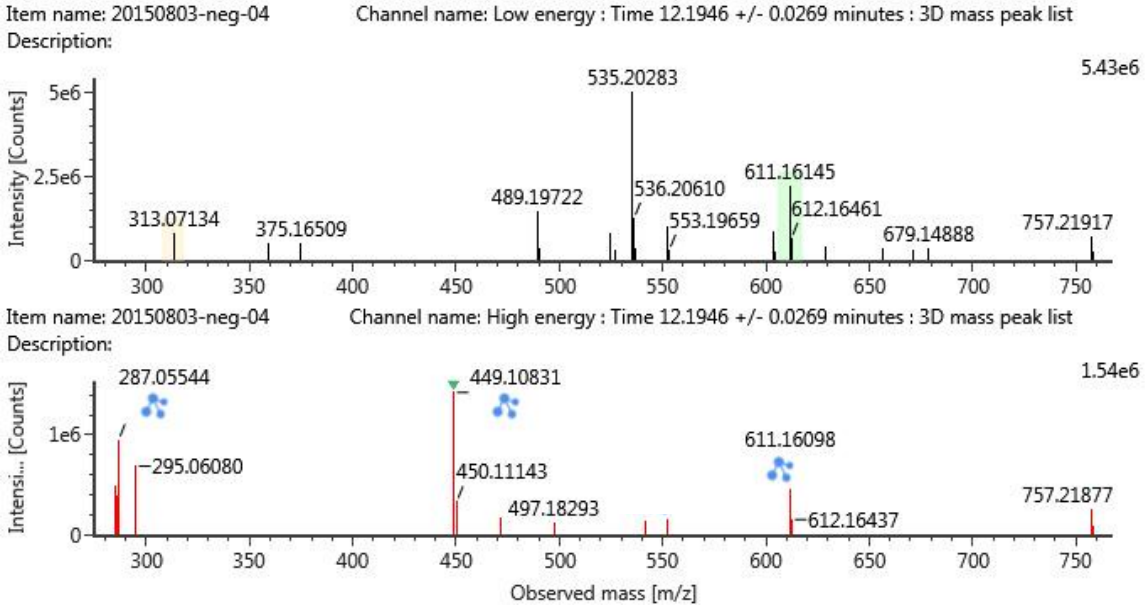
[M–H–2glu]$^-$
283.02478
Mass error: 0 mDa

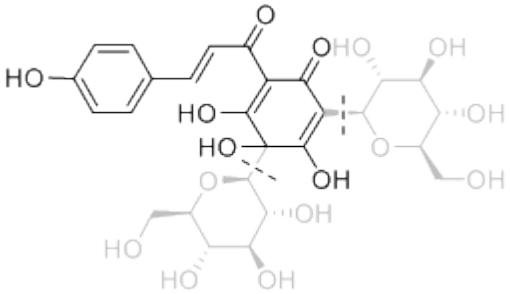
[M–H–glu]$^-$
447.09338
Mass error: 0.1 mDa

[M–H]$^-$
609.14694
Mass error: 0.8 mDa

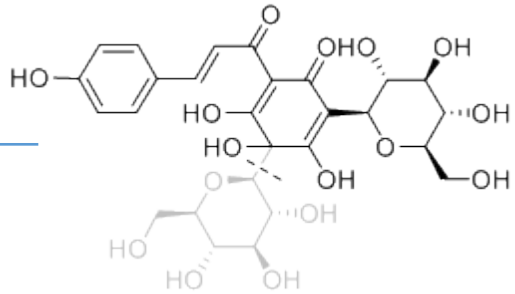
Fig. S2 (continued)

(14) hydroxysafflor yellow A

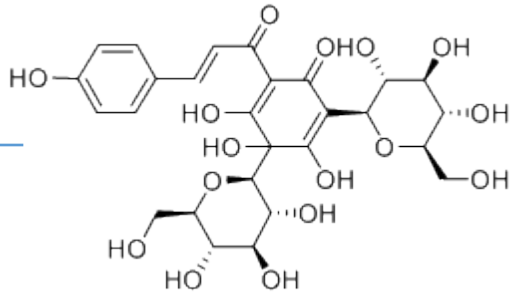




$[M–H–2glu]^-$
287.05544
Mass error: -0.7 mDa



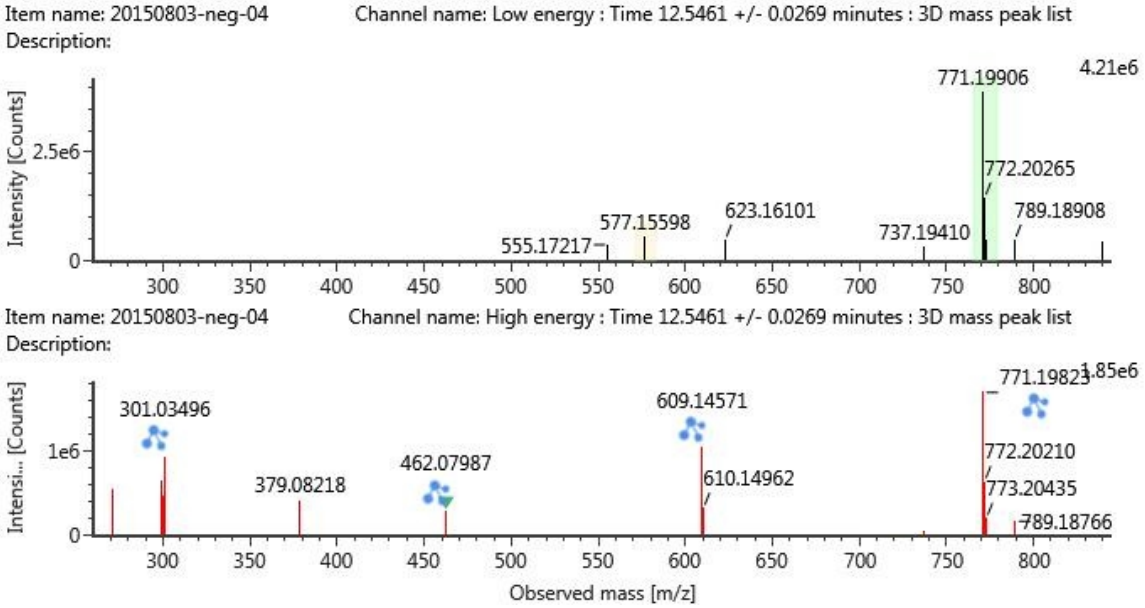
$[M–H–glu]^-$
449.10831
Mass error: -0.6 mDa

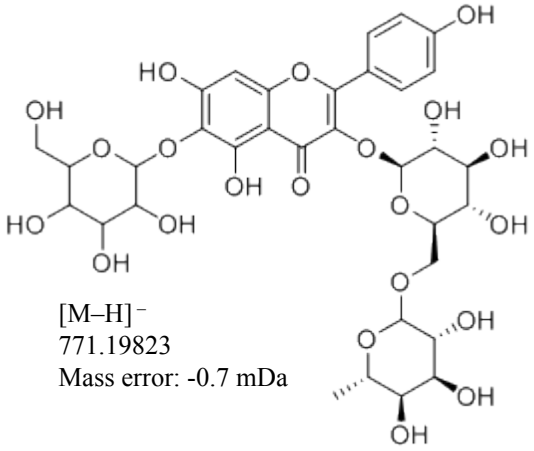


$[M–H]^-$
611.16098
Mass error: -0.8 mDa

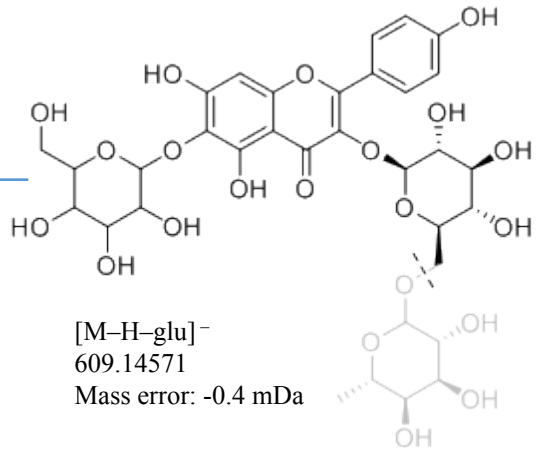
Fig. S2 (continued)

(15) 6-hydroxykaempferol-3-O-rutinoside-6-O-glucoside

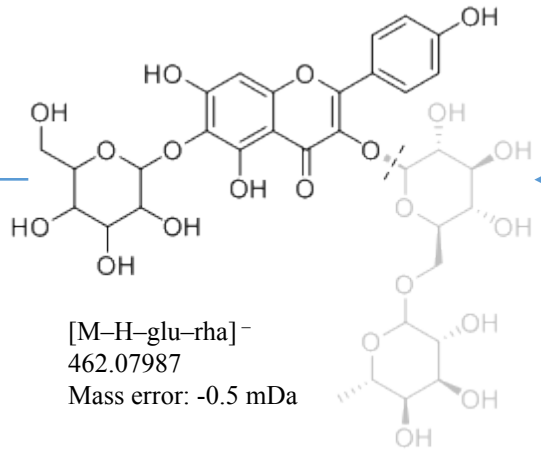




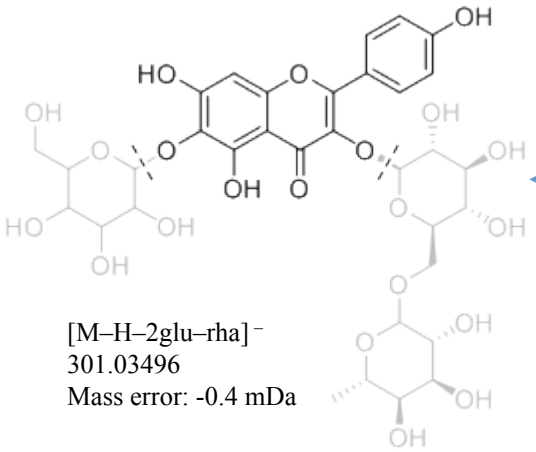
$[M–H]^-$
771.19823
Mass error: -0.7 mDa



$[M–H–glu]^-$
609.14571
Mass error: -0.4 mDa



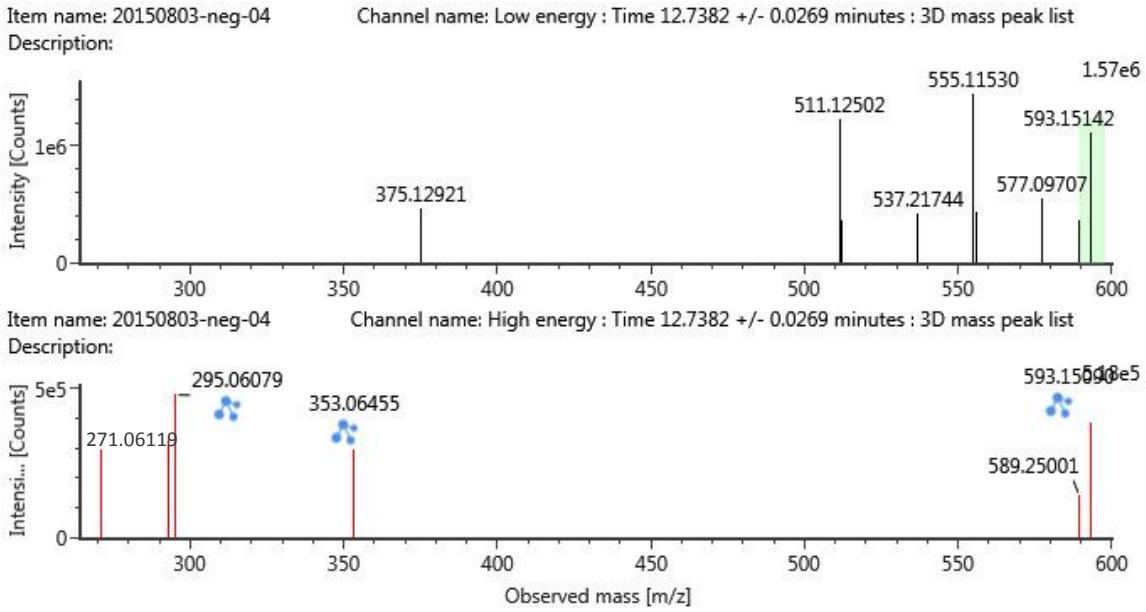
$[M–H–glu–rha]^-$
462.07987
Mass error: -0.5 mDa

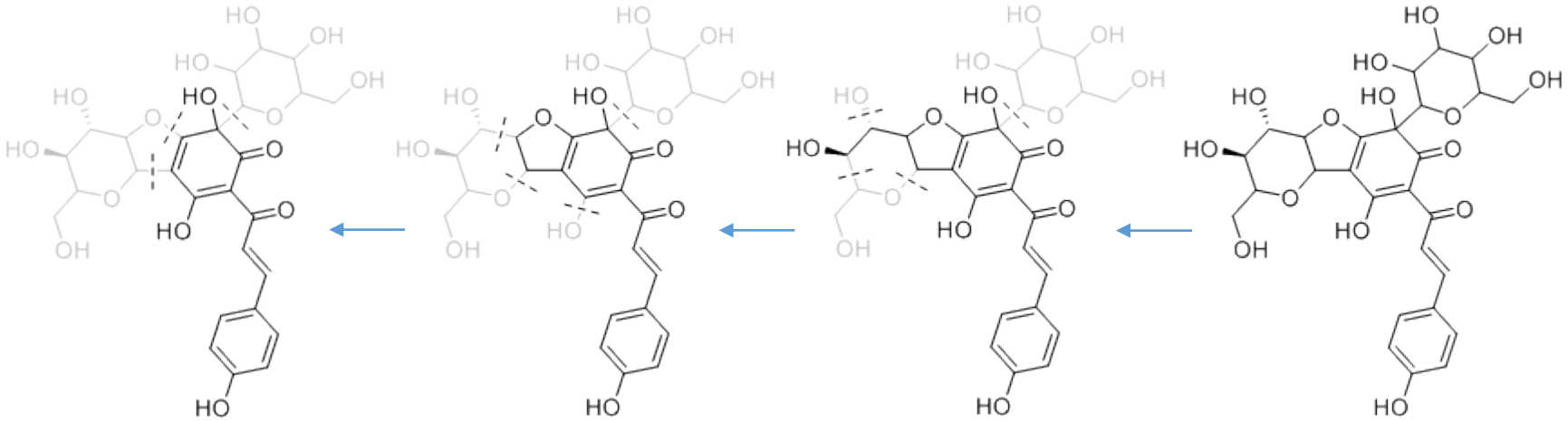


$[M–H–2glu–rha]^-$
301.03496
Mass error: -0.4 mDa

Fig. S2 (continued)

(17) safflor yellow A





$[M–H–glu–C_6H_8O_5]^-$
271.06119
Mass error: 0 mDa

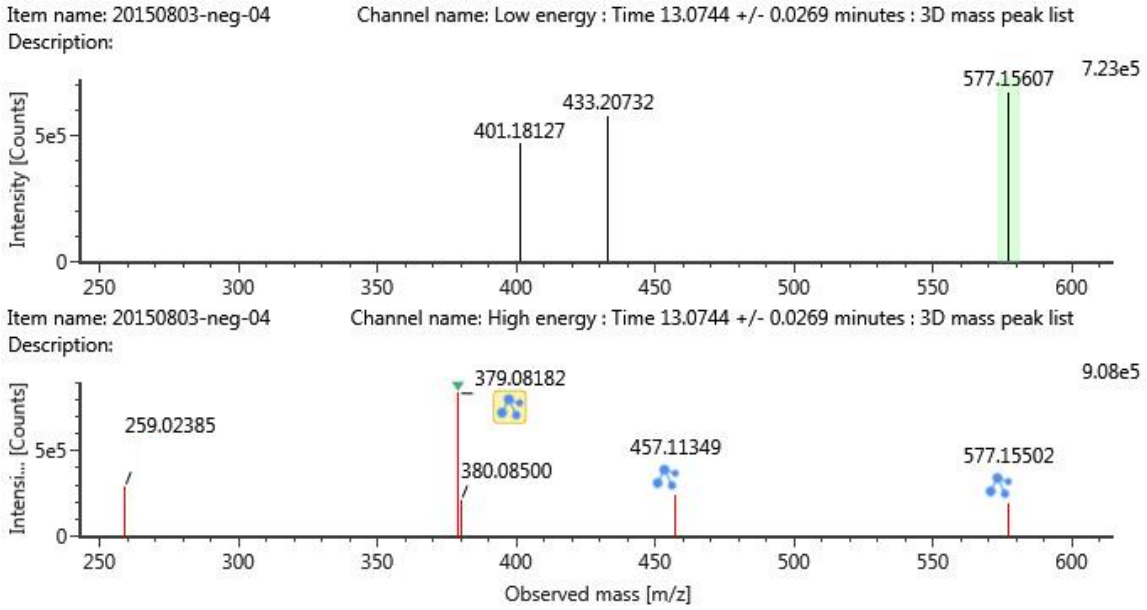
$[M–H–glu–H_2O–C_4H_7O_4]^-$
295.06079
Mass error: -0.4 mDa

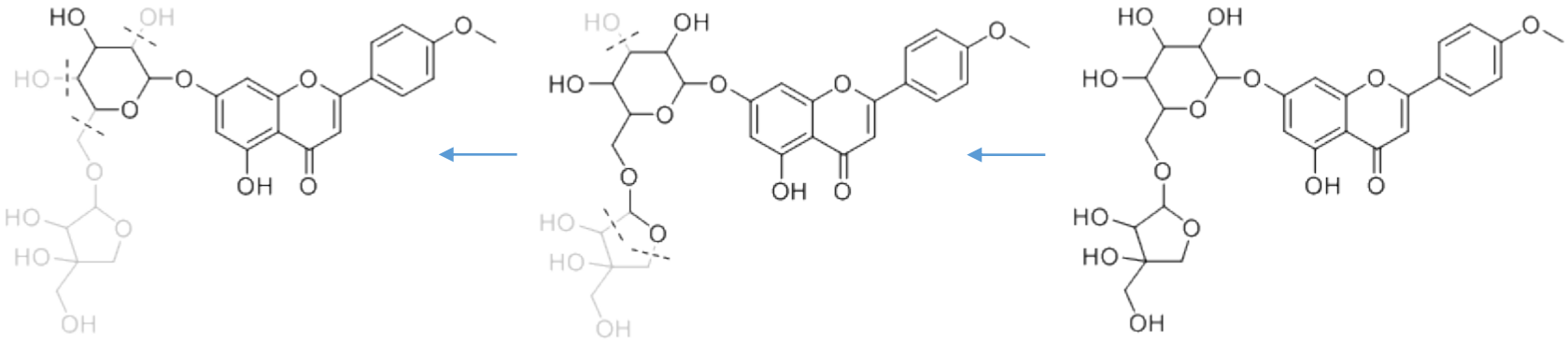
$[M–H–glu–H_2O–C_2H_4O_2]^-$
353.06455
Mass error: -2.1 mDa

$[M–H]^-$
593.15090
Mass error: -0.3 mDa

Fig. S2 (continued)

(20) 5,7-dihydroxy-4′-methoxyflavone-7-O-β-D-apiofuranosyl-(1-6)-O-β-D-glucoside





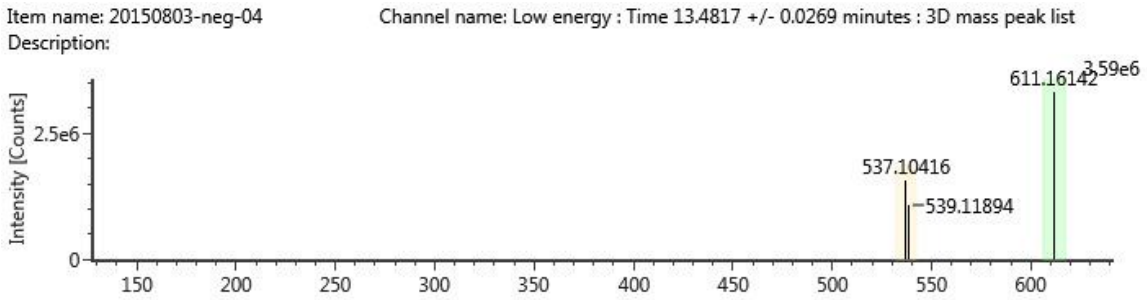
$[M–H–C_6H_{11}O_5–2H_2O]^-$
379.08182
Mass error: -0.5 mDa

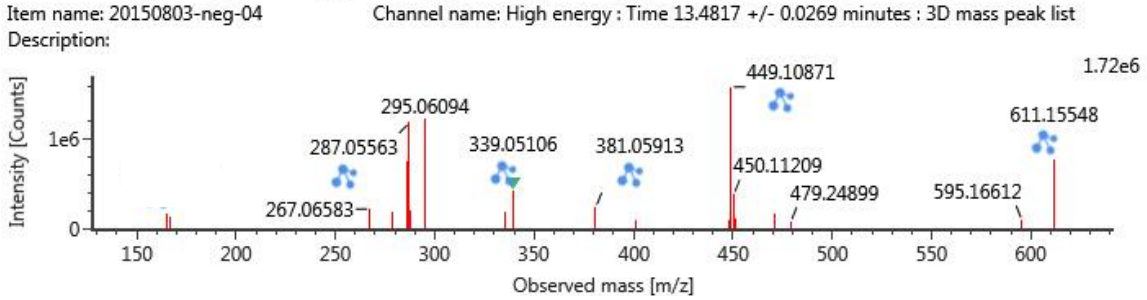
$[M–H–C_4H_8O_4]^-$
457.11349
Mass error: -0.5 mDa

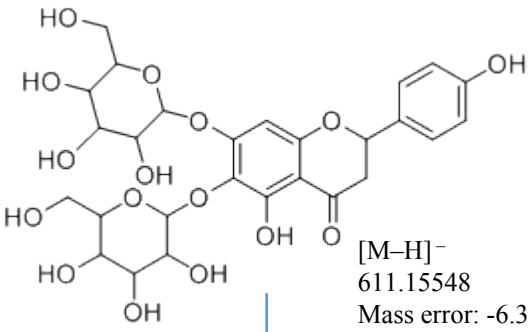
$[M–H]^-$
577.15502
Mass error: -1.3 mDa

Fig. S2 (continued)

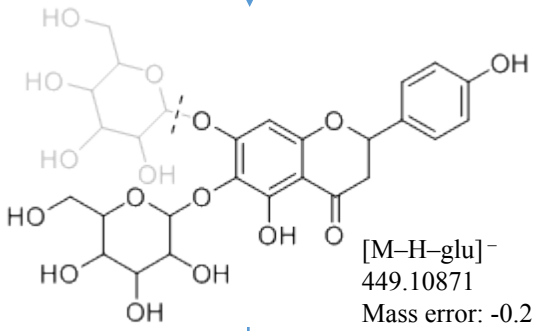
(21) 5,6,7,4′-tetrahydroxyflavanone 6,7-di-O-β-D-glucoside



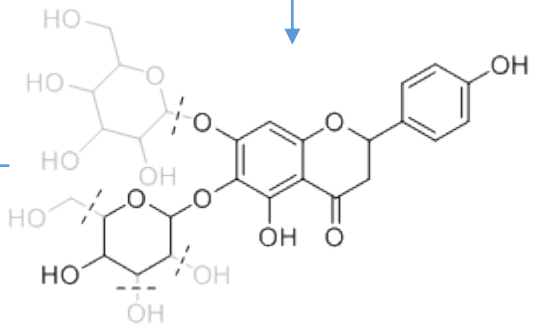




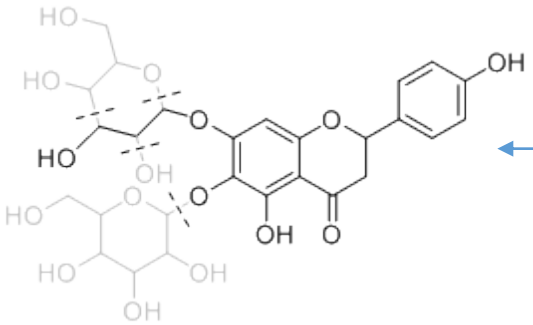
$[M–H]^-$
611.15548
Mass error: -6.3 mDa



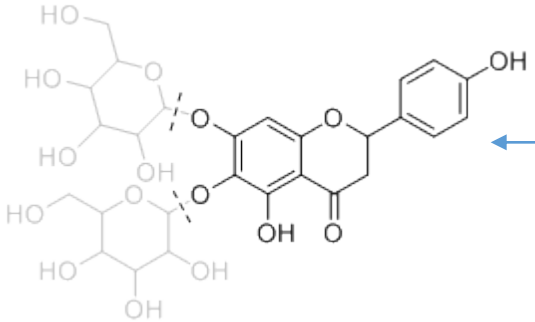
$[M–H–glu]^-$
449.10871
Mass error: -0.2 mDa



$[M–H–glu–2H_2O–CH_2OH]^-$
381.05913
Mass error: -2.5 mDa



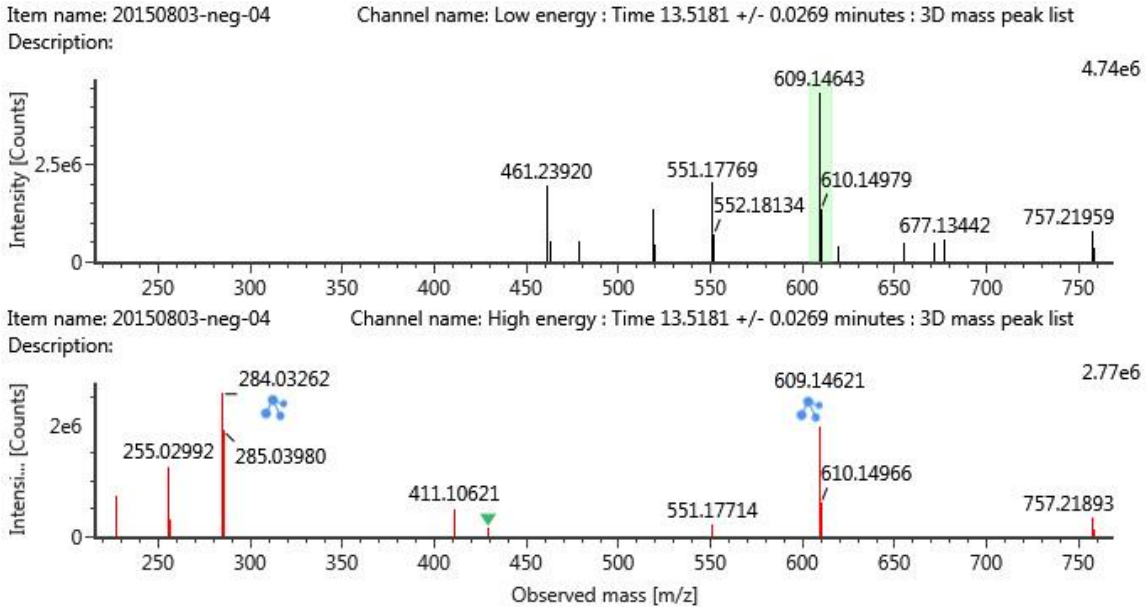
$[M–H–glu–H_2O–C_3H_6O_3]^-$
339.05106
Mass error: 0 mDa

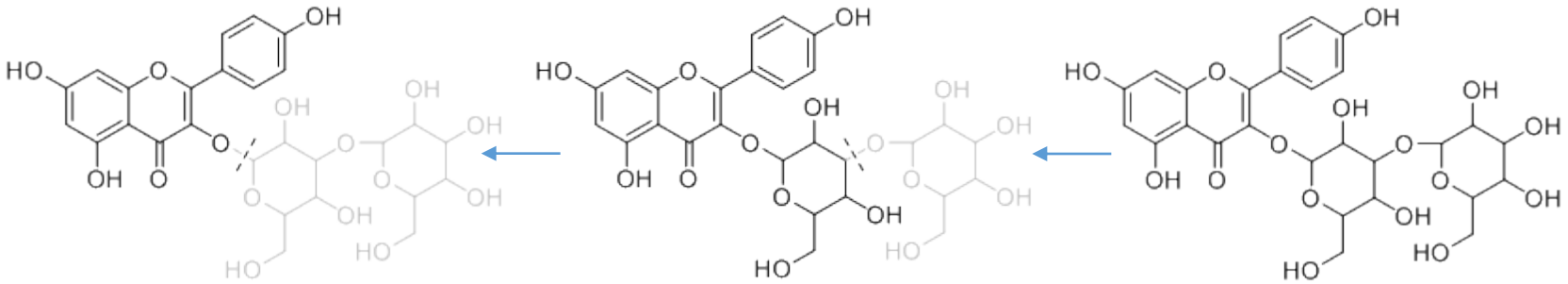


$[M–H–2glu]^-$
287.05563
Mass error: -0.5 mDa

Fig. S2 (continued)

(22) kaempferol-3-O-sophorose





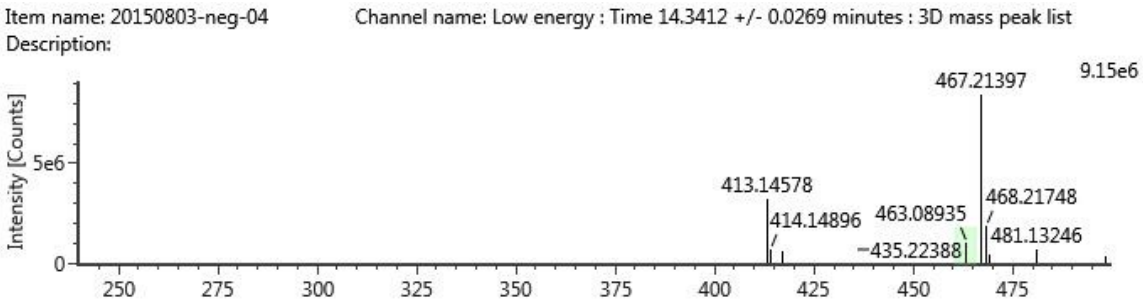
$[M–H–soph]^-$
284.03262
Mass error: 0 mDa

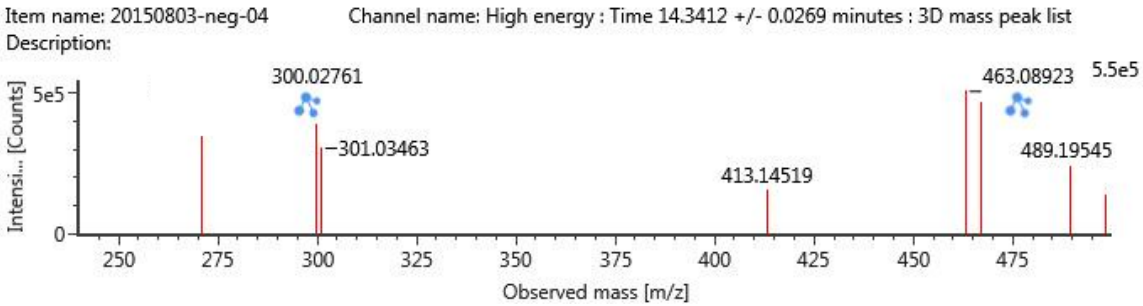
$[M–H–glu–H_2O]^-$
429.08340
Mass error: 0.7 mDa

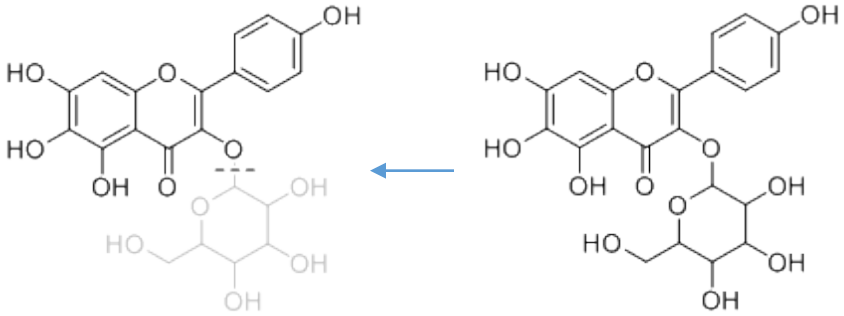
$[M–H]^-$
609.14621
Mass error: 0.1 mDa

Fig. S2 (continued)

(23) 6-hydroxykaempferol-3-O-glucoside





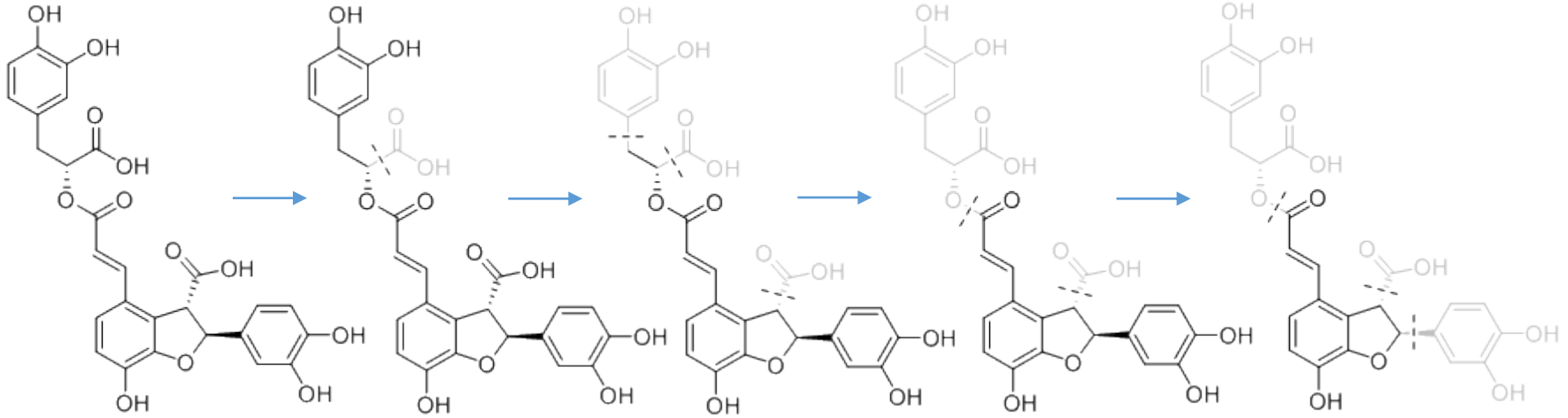


[M–H–glu]$^-$
300.02761
Mass error: 0.1 mDa

[M–H]$^-$
463.08923
Mass error: 1 mDa

Fig. S2 (continued)

(24) lithospermic acid



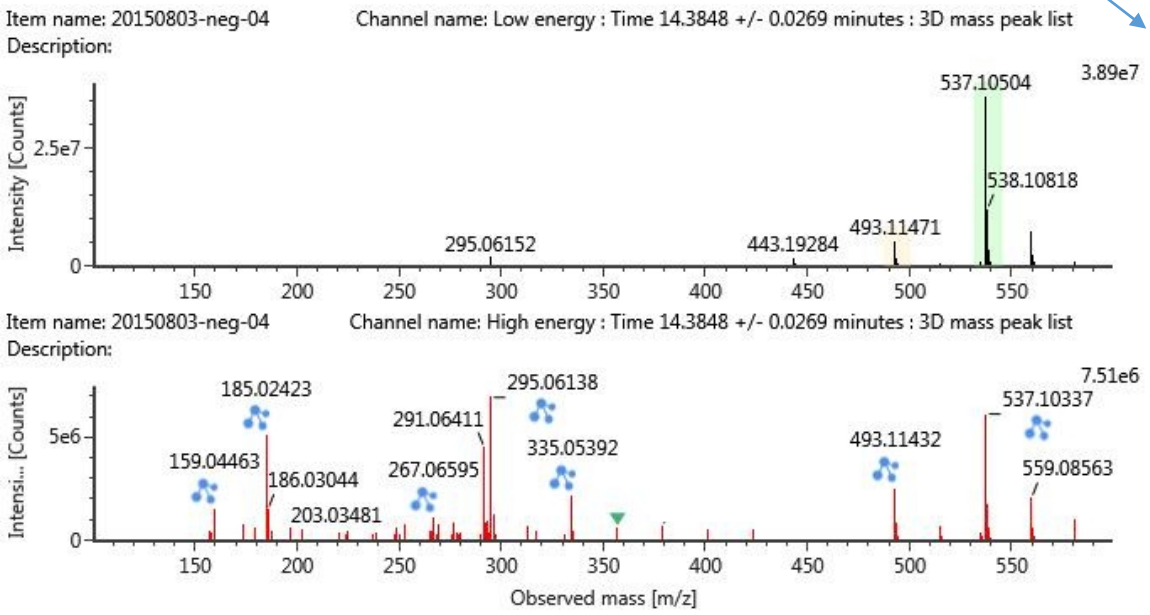
[M–H]$^-$
537.10337
Mass error: -0.5 mDa

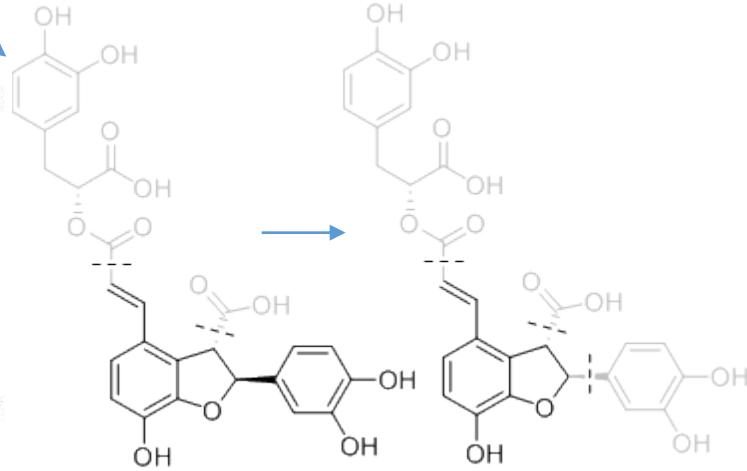
[M–H–CO–H$_2$O]$^-$
493.11432
Mass error: 0.3 mDa

[M–H–2CO–2H$_2$O–C$_6$H$_5$O$_2$]$^-$
335.05392
Mass error: -2.2 mDa

[M–H–CO–H$_2$O–C$_9$H$_9$O$_5$]$^-$
295.06138
Mass error: -0.2 mDa

[M–H–CO–H$_2$O–C$_9$H$_9$O$_6$–C$_6$H$_5$O$_2$]$^-$
185.02423
Mass error: -0.2 mDa



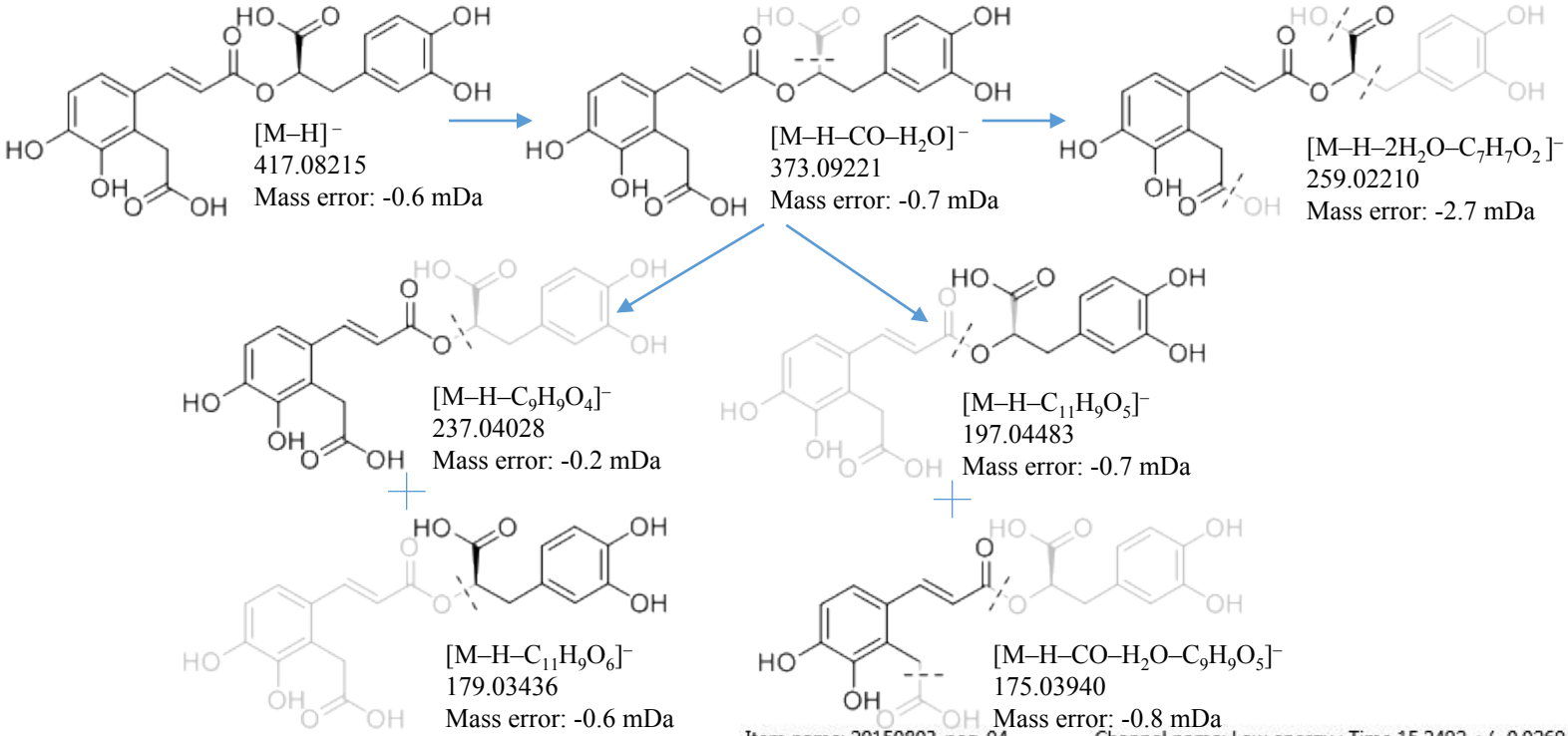


[M–H–CO–H$_2$O–C$_{10}$H$_9$O$_6$]$^-$
267.06595
Mass error: -0.3 mDa

[M–H–CO–H$_2$O–C$_{10}$H$_9$O$_6$–C$_6$H$_5$O$_2$]$^-$
159.04463
Mass error: -0.3 mDa

Fig. S2 (continued)

(26) salvianolic acid D



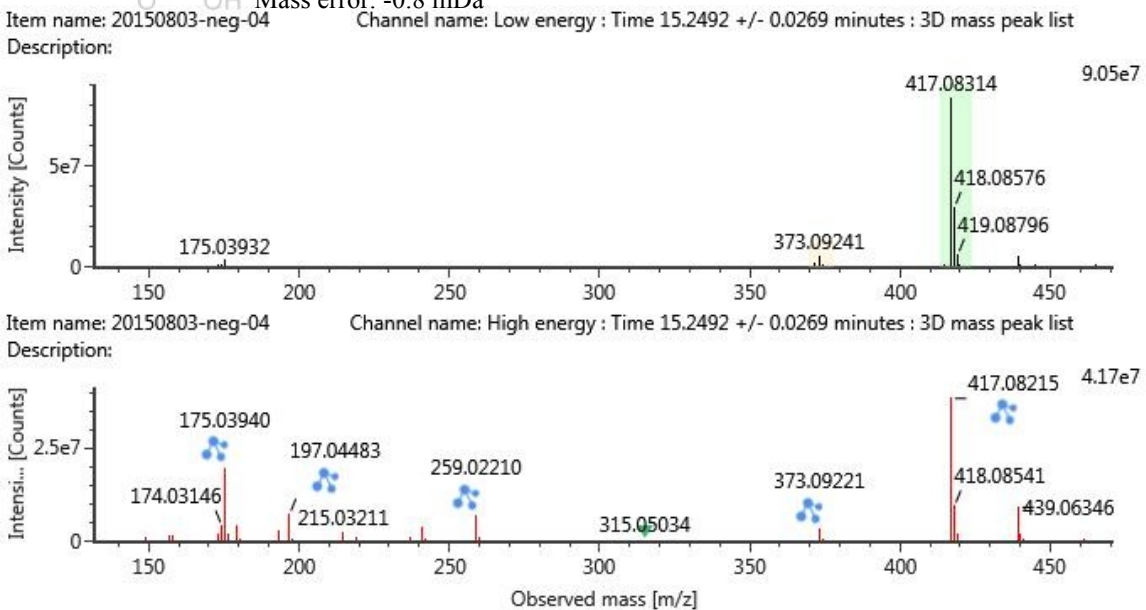
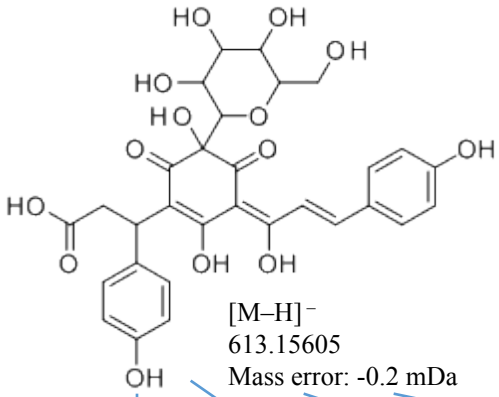
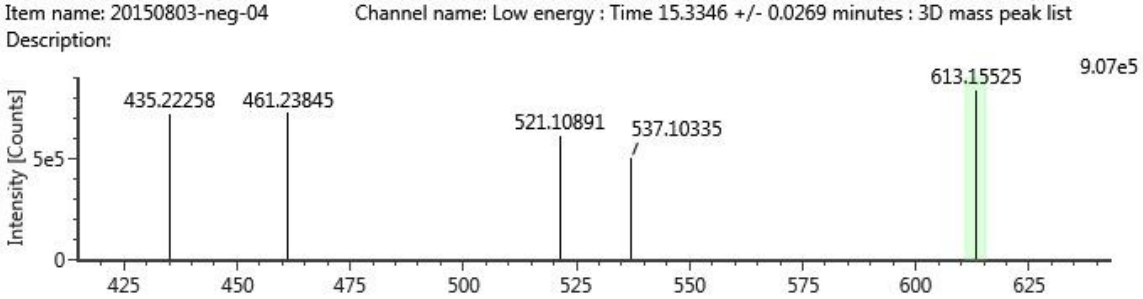


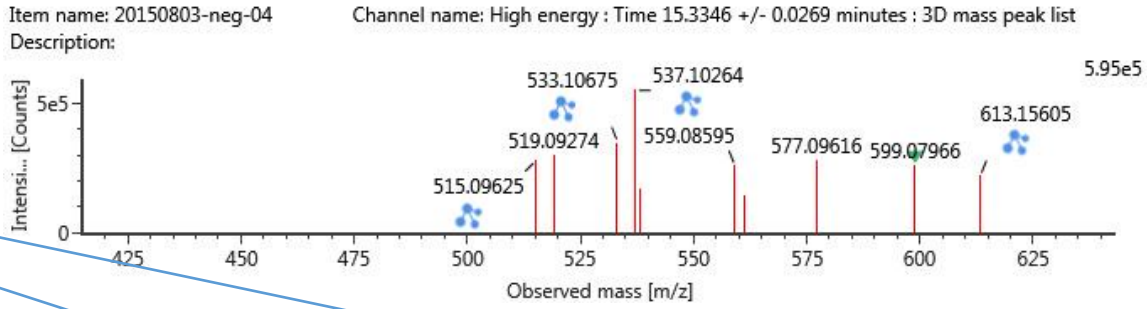
Fig. S2 (continued)

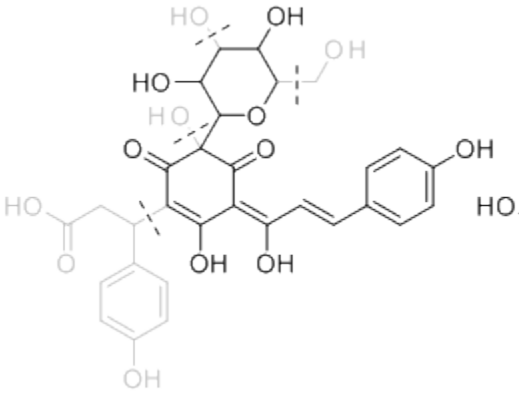
(27) safflomin C



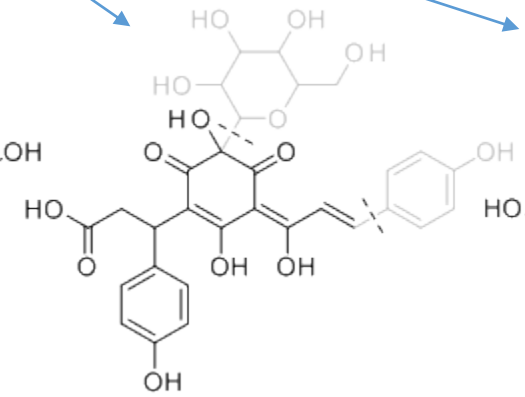
$[M–H]^-$
613.15605
Mass error: -0.2 mda



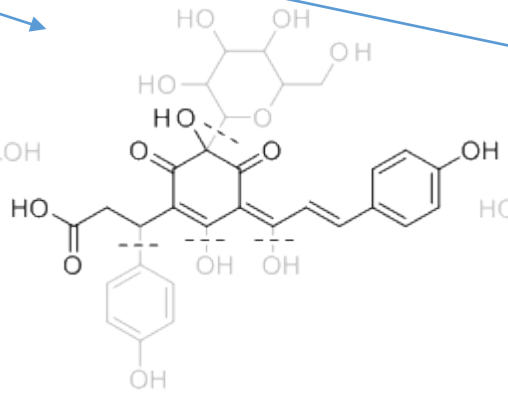




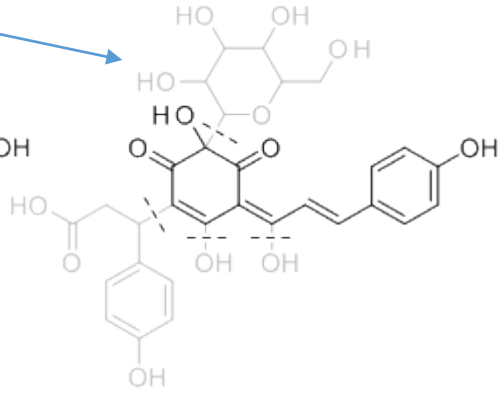
$[M–H–2H_2O–CH_2OH–C_9H_9O_3]^-$
379.04315
Mass error: -2.8 mda



$[M–H–C_6H_{11}O_5–C_6H_5O]^-$
357.06106
Mass error: -0.5 mda



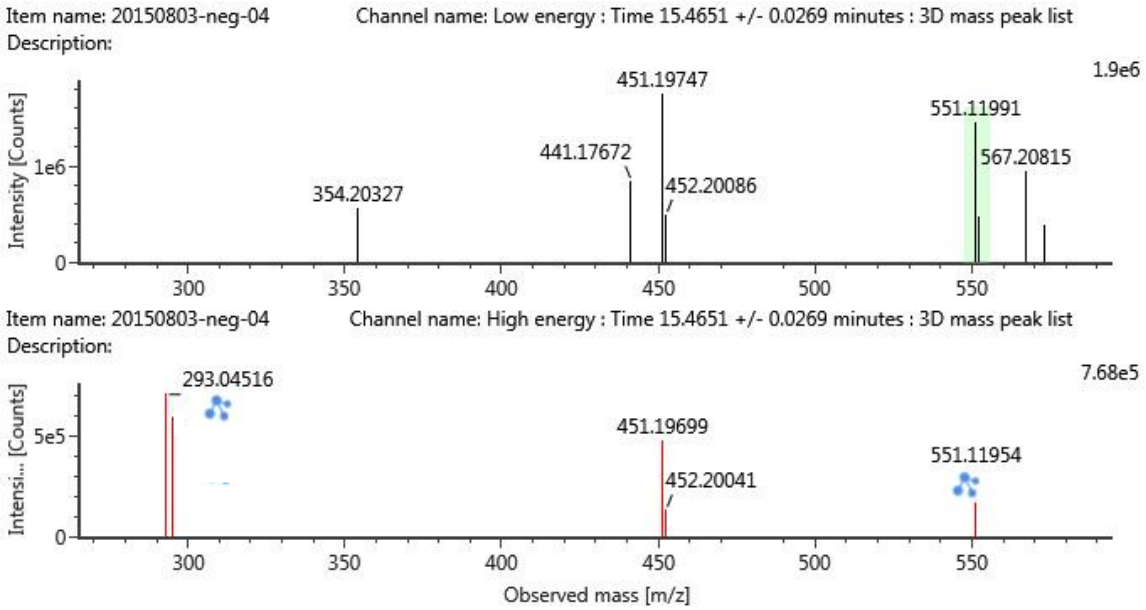
$[M–H–C_6H_{11}O_5–C_6H_5O–2H_2O]^-$
321.03995
Mass error: -0.5 mda

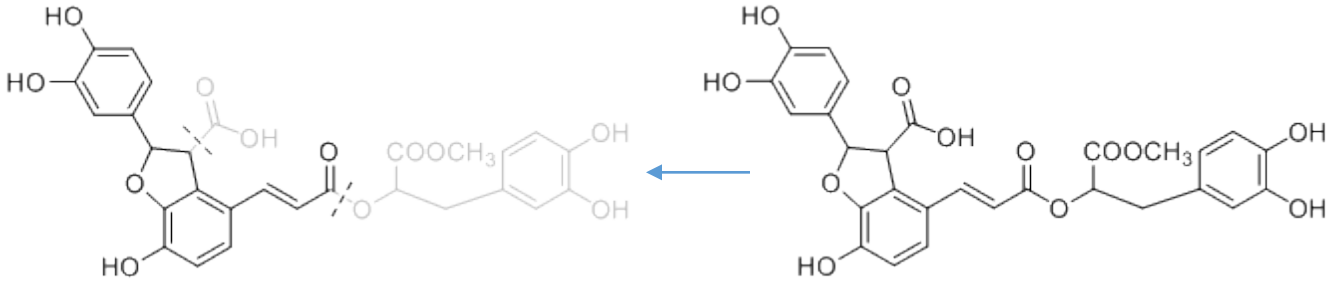


$[M–H–C_6H_{11}O_5–C_9H_9O_3–2H_2O]^-$
253.04970
Mass error: -0.9 mda

Fig. S2 (continued)

(28) litherospermic acid monomethyl ester



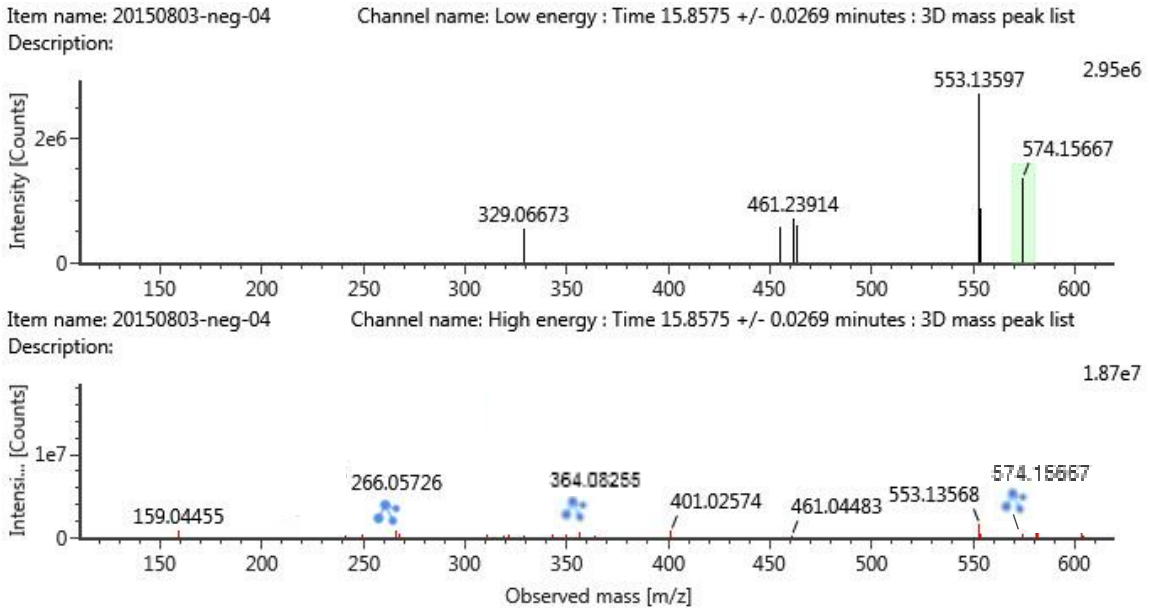


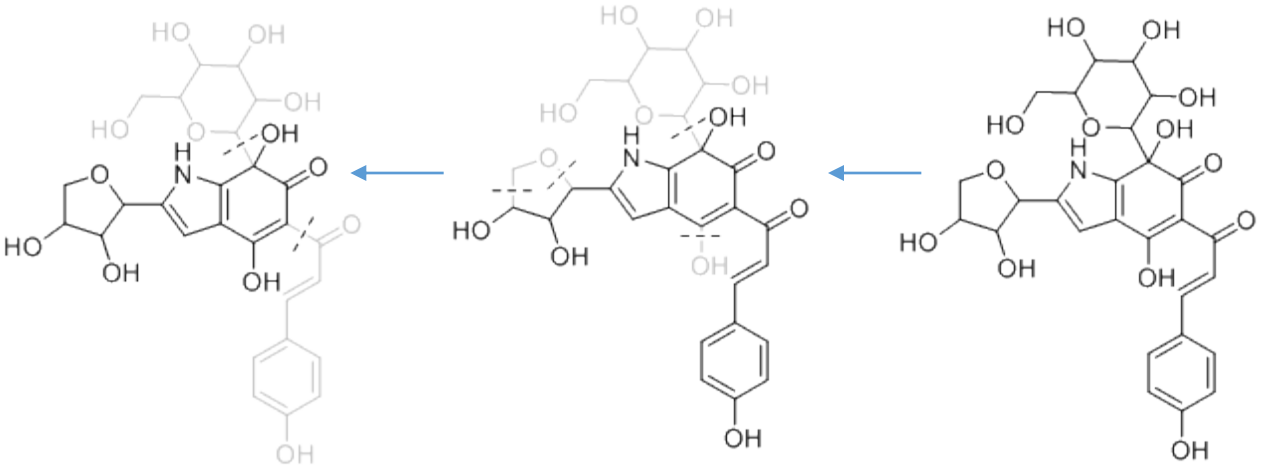
$[M–H–CO–H_2O–C_{10}H_{11}O_5]^-$
293.04516
Mass error: -0.4 mDa

$[M–H]^-$
551.11954
Mass error: 0 mDa

Fig. S2 (continued)

(29) cartormin





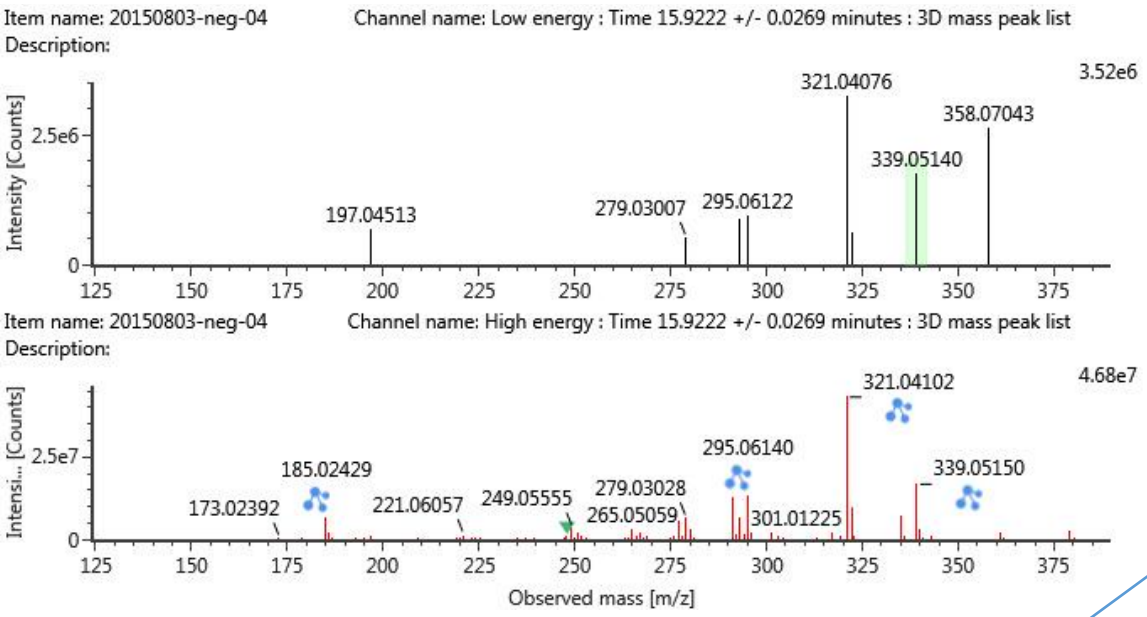
$[M–H–glu–C_9H_7O_2]^-$
266.05726
Mass error: -0.4 mDa

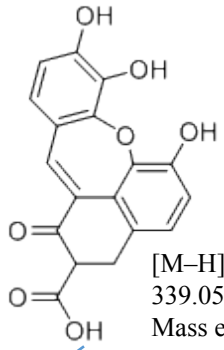
$[M–H–glu–H_2O–CH_2O]^-$
364.0825
Mass error: -0.1 mDa

$[M–H]^-$
574.15657
Mass error: 0 mDa

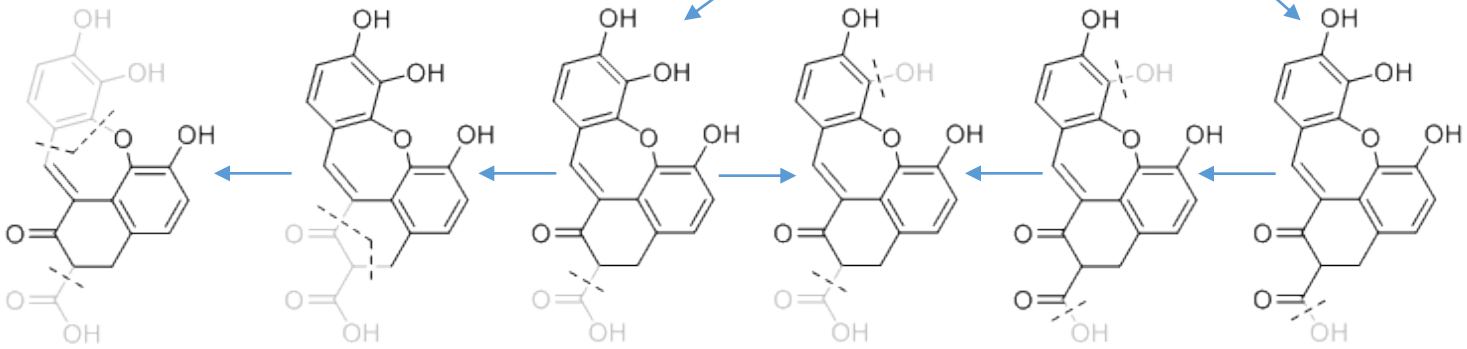
Fig. S2 (continued)

(30) salvianolic acid G





$[M–H]^-$
339.05150
Mass error: 0.5 mDa



$[M–H–CO–H_2O–C_6H_4O_2]^-$
185.02429
Mass error: -0.1 mDa

$[M–H–C_3H_2O_3]^-$
253.04957
Mass error: -1.1 mDa

$[M–H–CO–H_2O]^-$
295.06140
Mass error: 0.2 mDa

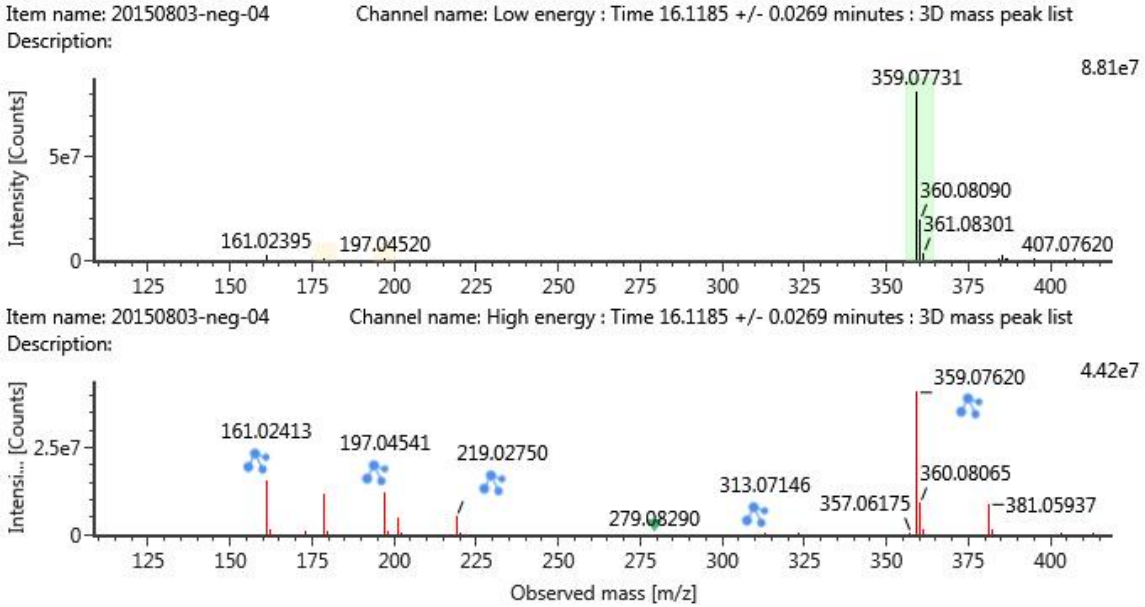
$[M–H–CO–2H_2O]^-$
277.05073
Mass error: 0.1 mDa

$[M–H–2H_2O]^-$
303.03006
Mass error: 0.2 mDa

$[M–H–H_2O]^-$
321.04102
Mass error: 0.6 mDa

Fig. S2 (continued)

(31) rosmarinic acid



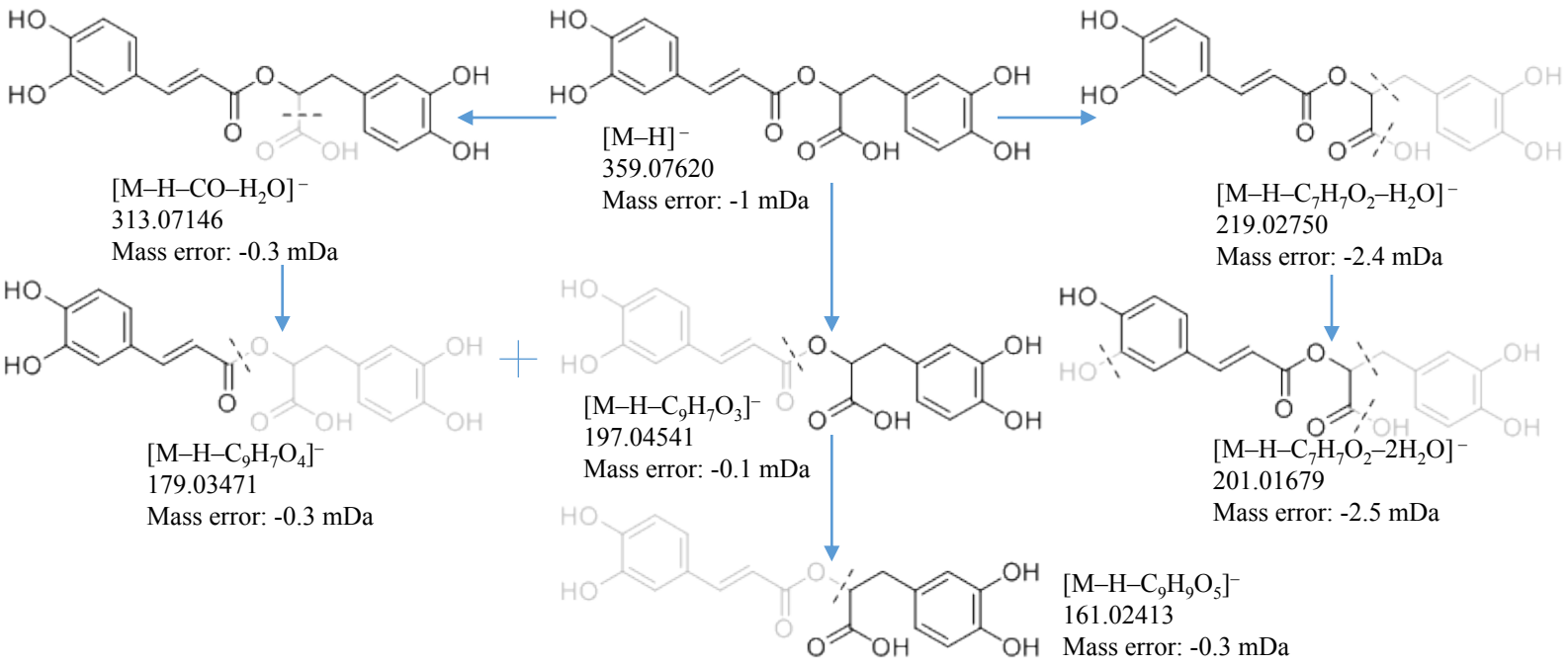
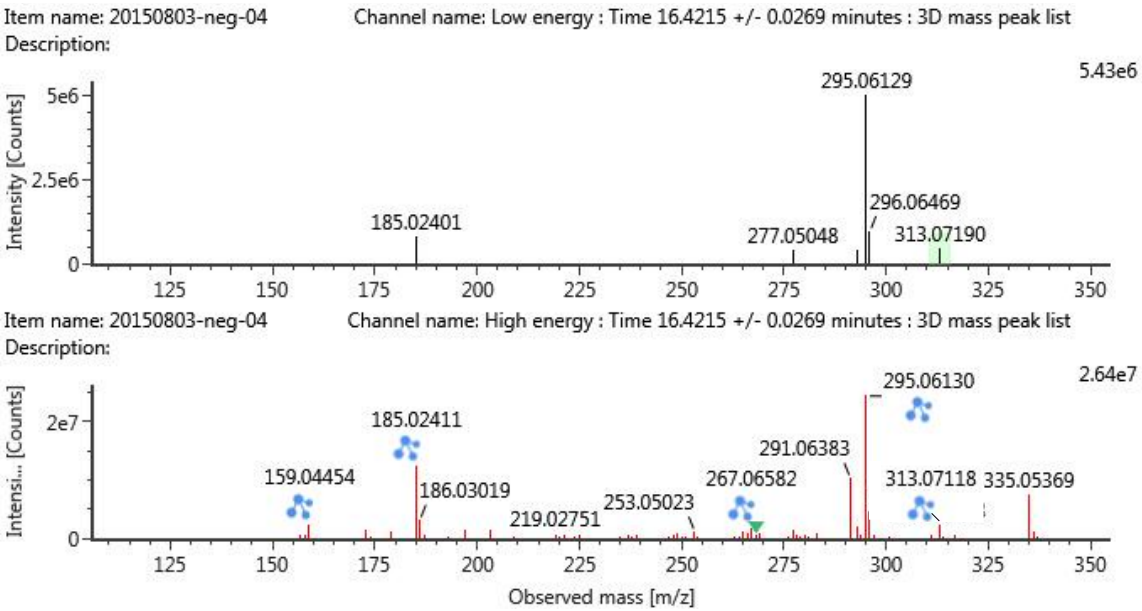
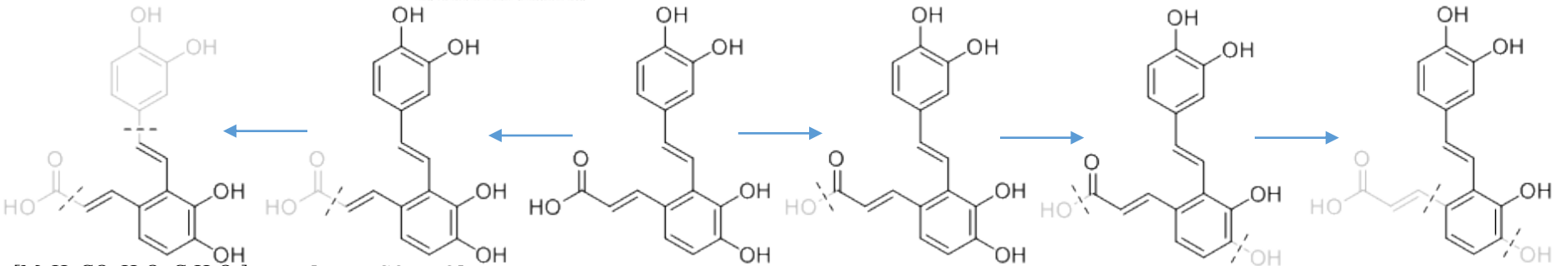


Fig. S2 (continued)

(32) salvianolic acid F





$[M–H–CO–H_2O–C_6H_5O_2]^-$
159.04454
Mass error: -0.6 mDa

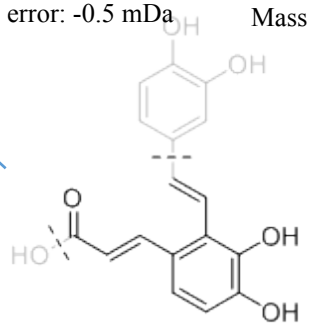
$[M–H–CO–H_2O]^-$
267.06582
Mass error: -0.5 mDa

$[M–H]^-$
313.07118
Mass error: -0.6 mDa

$[M–H–H_2O]^-$
295.06130
Mass error: 0.1 mDa

$[M–H–2H_2O]^-$
277.05024
Mass error: -0.4 mDa

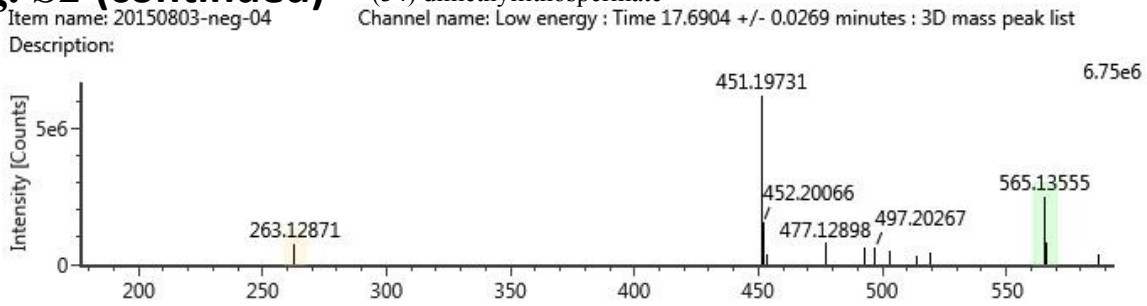
$[M–H–CO–2H_2O–C_2H_2]^-$
225.05474
Mass error: -1 mDa

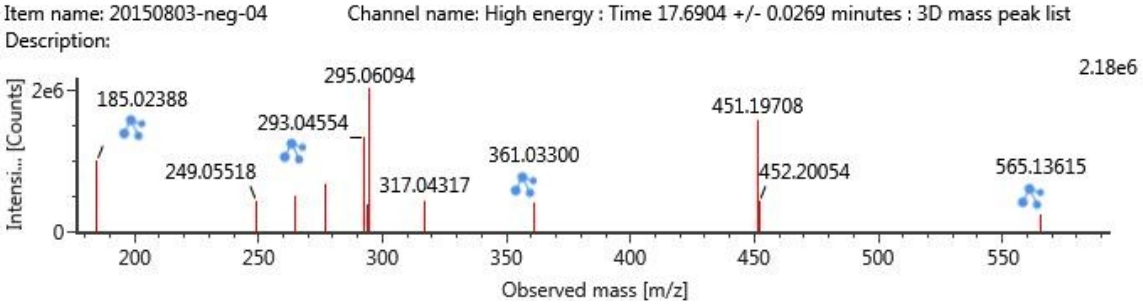


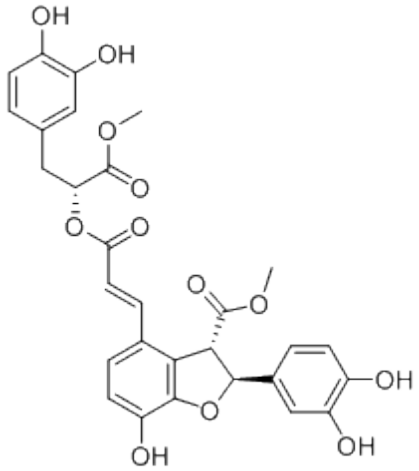
$[M–H–H_2O–C_6H_5O_2]^-$
185.02411
Mass error: -0.3 mDa

Fig. S2 (continued)

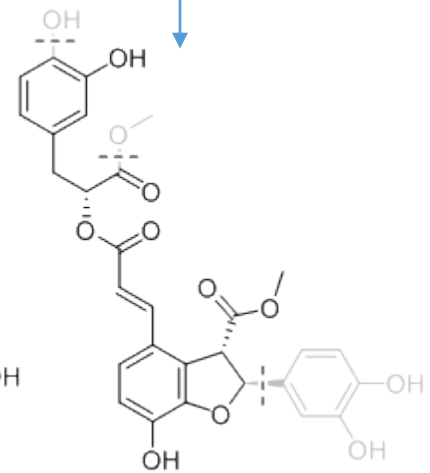
(34) dimethyllithospermate



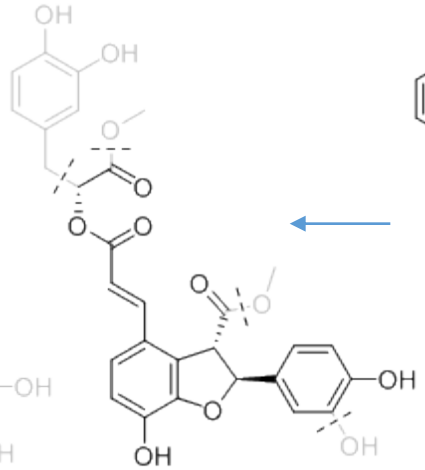




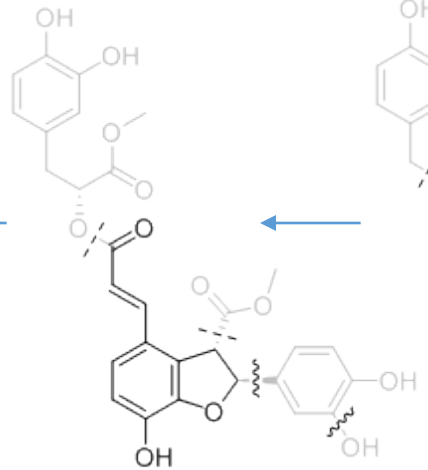
$[M–H]^-$
565.13615
Mass error: 1 mDa



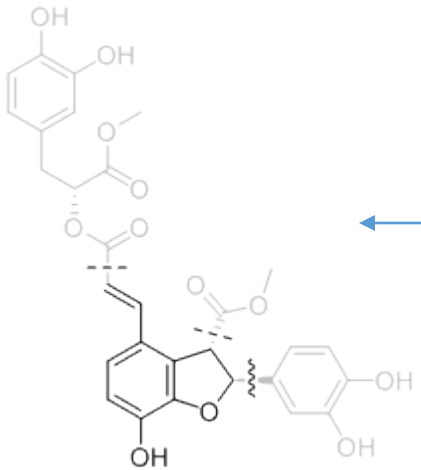
$[M–H–C_6H_5O_2–CH_3O–H_2O]^-$
407.07492
Mass error: -2.3 mDa



$[M–H–C_7H_7O_2–H_2O–2CH_3O]^-$
361.03300
Mass error: -2.4 mDa



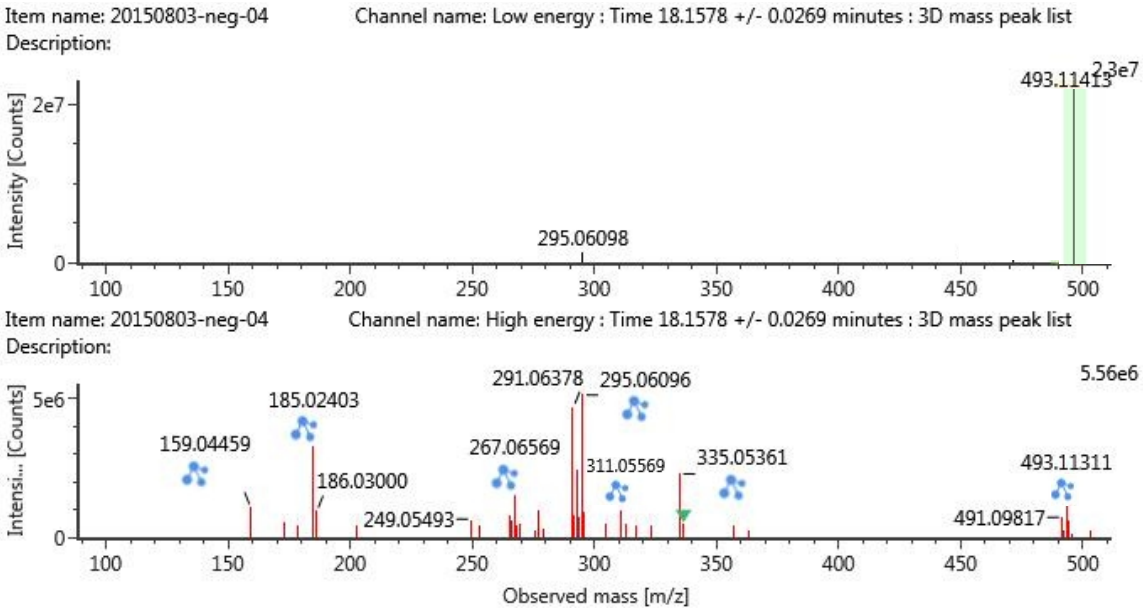
$[M–H–C_{10}H_{11}O_5–CO_2CH_3]^-$
293.04554
Mass error: 0 mDa
$[M–H–C_{10}H_{11}O_5–CO_2CH_3–C_6H_5O_2]^-$
185.02388
Mass error: -0.5 mDa
$[M–H–C_{10}H_{11}O_5–CO_2CH_3–H_2O]^-$
277.05024
Mass error: -0.4 mDa



$[M–H–C_{11}H_{11}O_6–CO_2CH_3]^-$
265.04994
Mass error: -0.7 mDa
$[M–H–C_{11}H_{11}O_6–CO_2CH_3–C_6H_5O_2]^-$
159.04435
Mass error: -0.8 mDa

Fig. S2 (continued)

(35) salvianolic acid A



$[M–H–C_9H_9O_5–C_6H_5O_2]^-$
185.02403, 173.02335
Mass error: -0.4 mDa

$[M–H–C_7H_7O_2–2H_2O]^-$
335.05361
Mass error: -2.5 mDa

$[M–H]^-$
493.11311
Mass error: -0.9 mDa

$[M–H–C_9H_9O_4–C_6H_5O_2]^-$
203.0342
Mass error: –0.7 mDa

$[M–H–C_9H_9O_4]^-$ + $[M–H–C_{17}H_{14}O_6]^-$
311.05569 + 179.03427
Mass error: -0.4 mDa, -0.7 mDa

$[M–H–C_9H_9O_5]^-$, $[M–H–C_9H_9O_5–H_2O]^-$
295.06096, 277.05009
Mass error: -0.2 mDa, -0.5 mDa

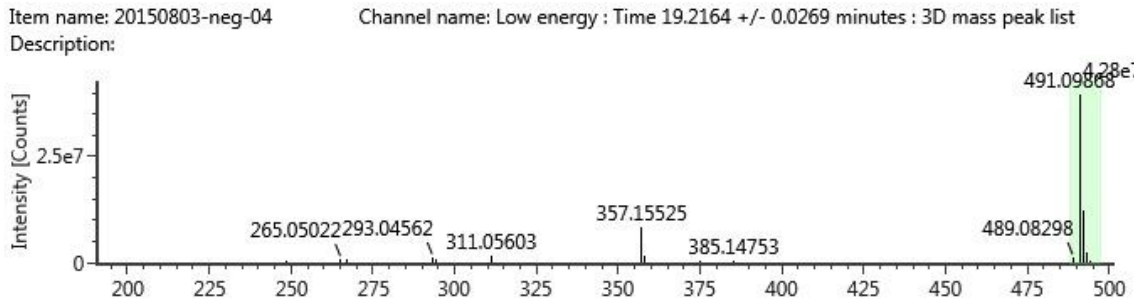
$[M–H–C_8H_7O_2–2H_2O]^-$
323.05493
Mass error: -1.2 mDa

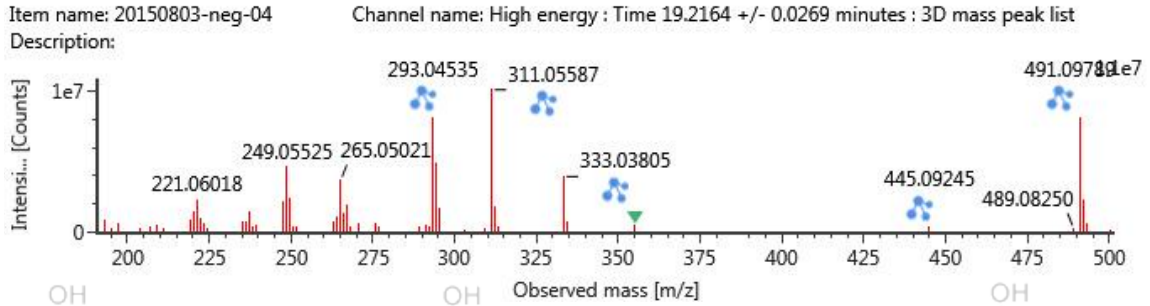
$[M–H–C_{10}H_9O_6–C_6H_5O_2]^-$
159.04459
Mass error: -0.6 mDa

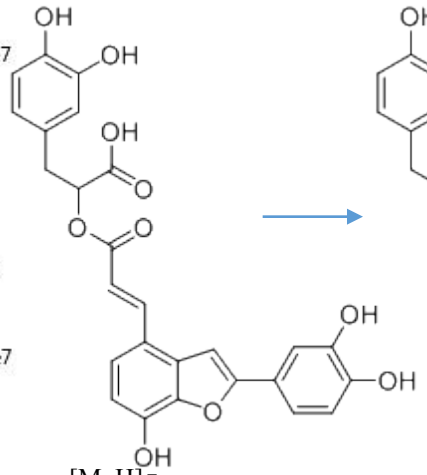
$[M–H–C_{10}H_9O_6]^-$
267.06569
Mass error: -0.6 mDa

Fig. S2 (continued)

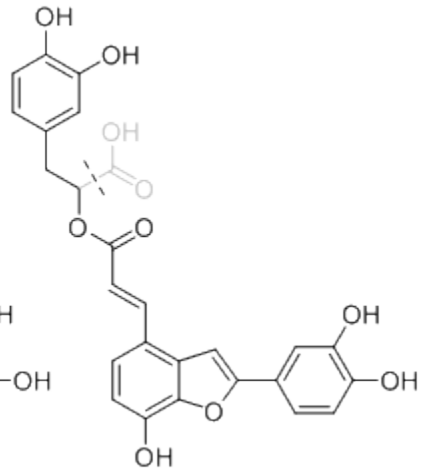
(36) salvianolic acid C



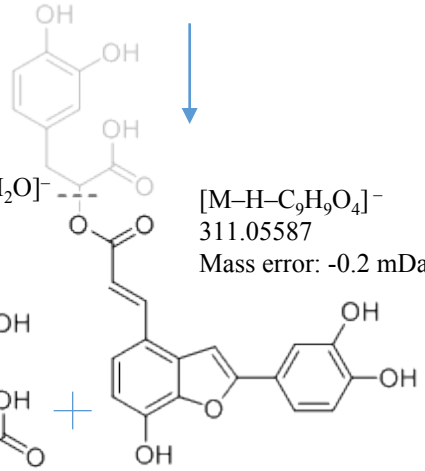




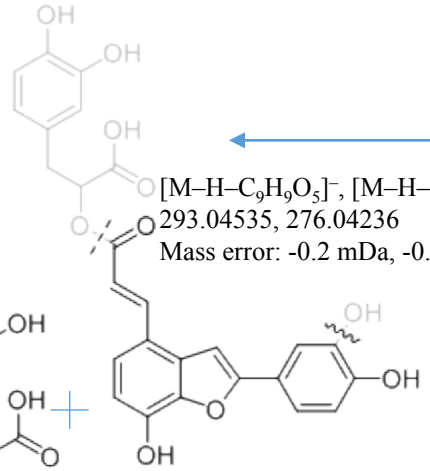
$[M–H]^-$
491.09789
Mass error: -0.5 mDa



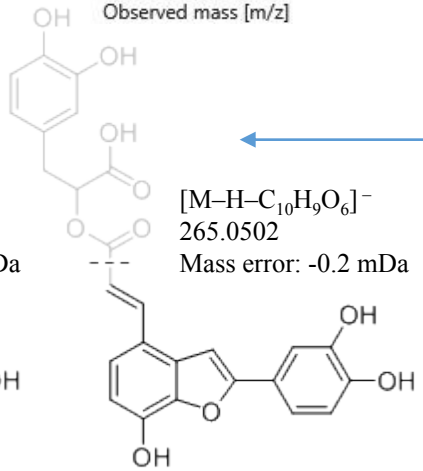
$[M–H–CO–H_2O]^-$
445.09245
Mass error: -0.4 mDa



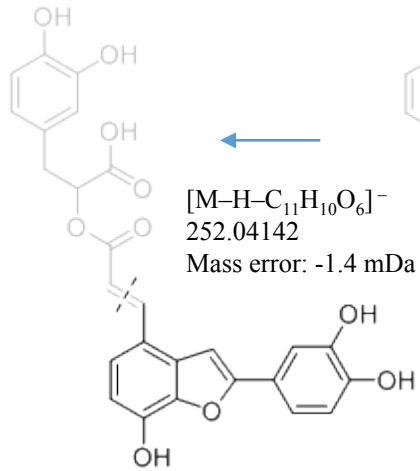
$[M–H–C_9H_9O_4]^-$
311.05587
Mass error: -0.2 mDa



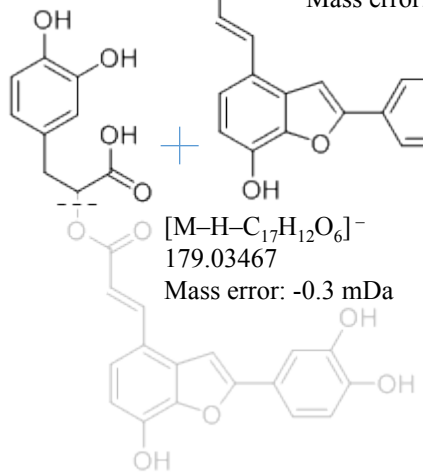
$[M–H–C_9H_9O_5]^-$, $[M–H–C_9H_9O_5–H_2O]^-$
293.04535, 276.04236
Mass error: -0.2 mDa, -0.5 mDa



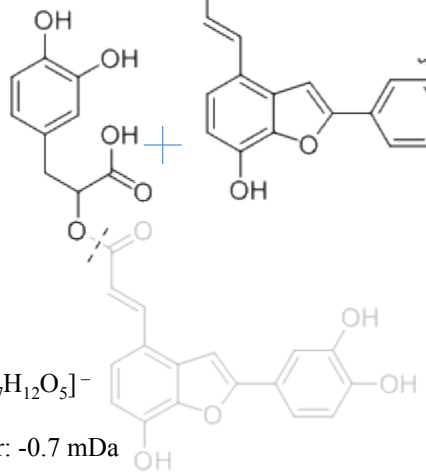
$[M–H–C_{10}H_9O_6]^-$
265.0502
Mass error: -0.2 mDa



$[M–H–C_{11}H_{10}O_6]^-$
252.04142
Mass error: -1.4 mDa



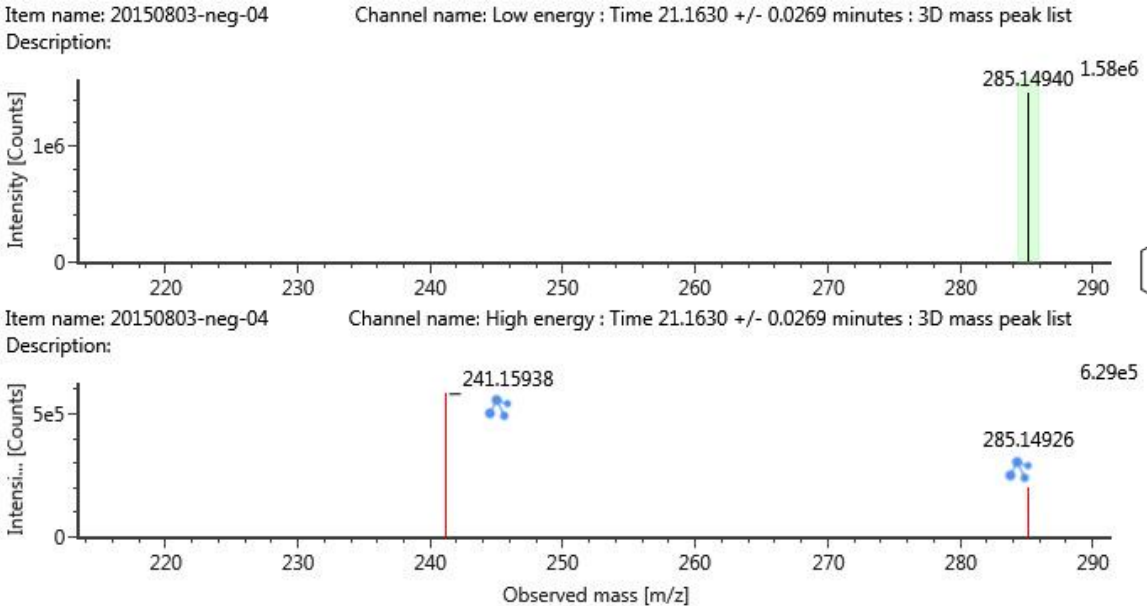
$[M–H–C_{17}H_{12}O_6]^-$
179.03467
Mass error: -0.3 mDa

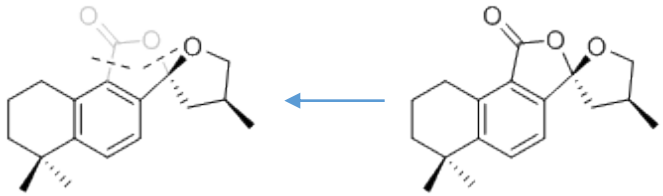


$[M–H–C_{17}H_{12}O_5]^-$
197.04481
Mass error: -0.7 mDa

Fig. S2 (continued)

(37) epicryptoacetalide

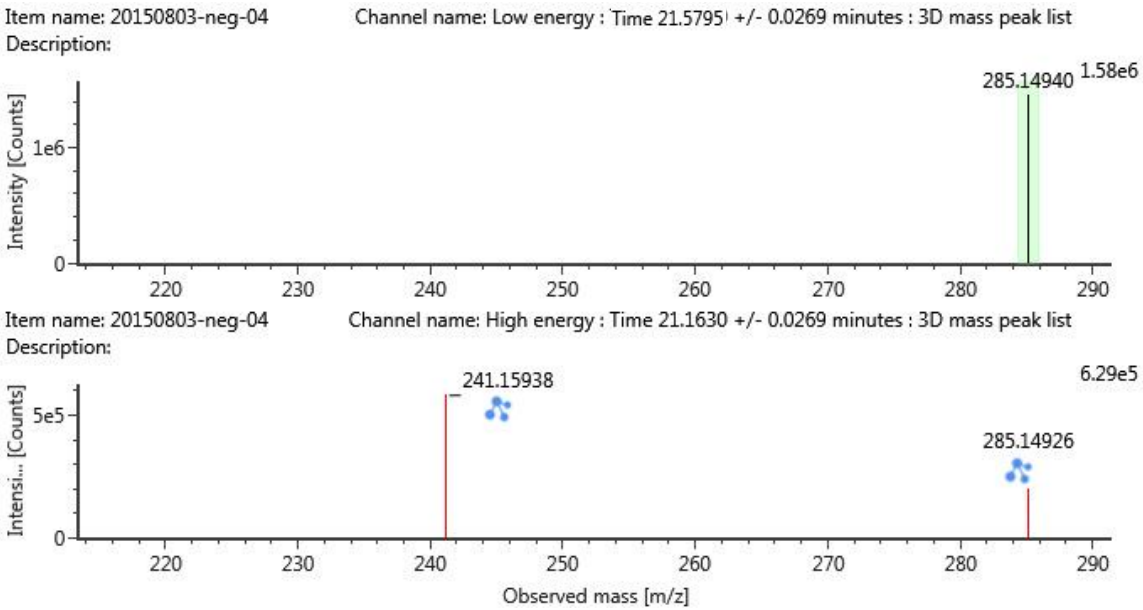


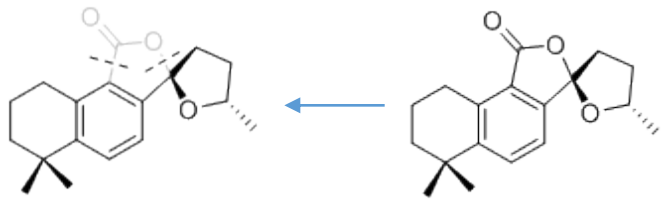


$[M–H–CO_2]^-$
241.15938
Mass error: -0.4 mDa

$[M–H]^-$
285.14926
Mass error: -0.4 mDa

(38) cryptoacetalide



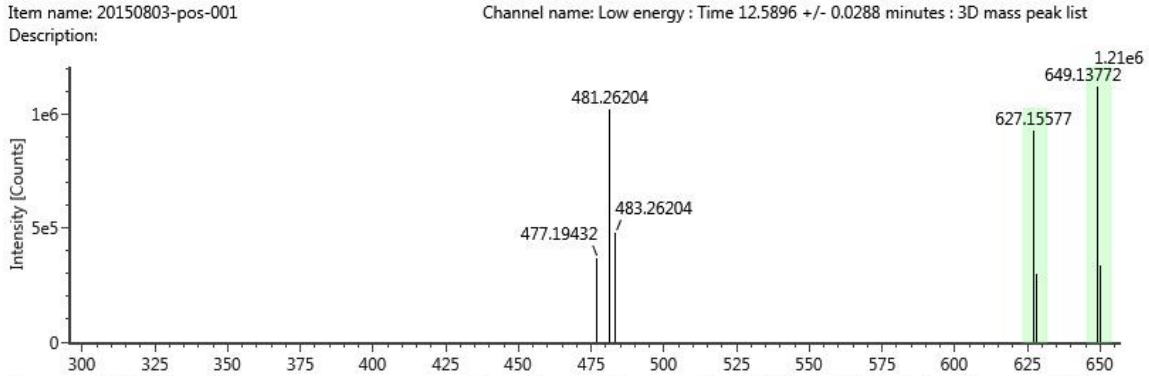


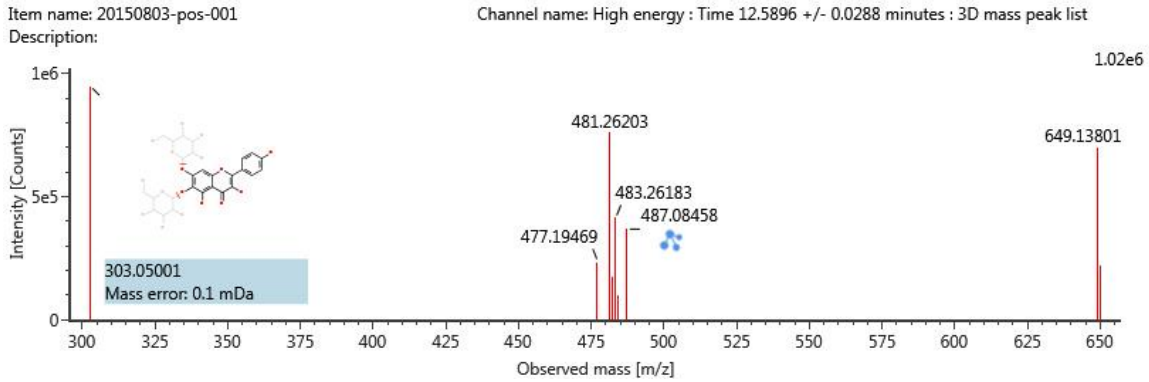
$[M–H–CO_2]^-$
241.15938
Mass error: -0.4 mDa

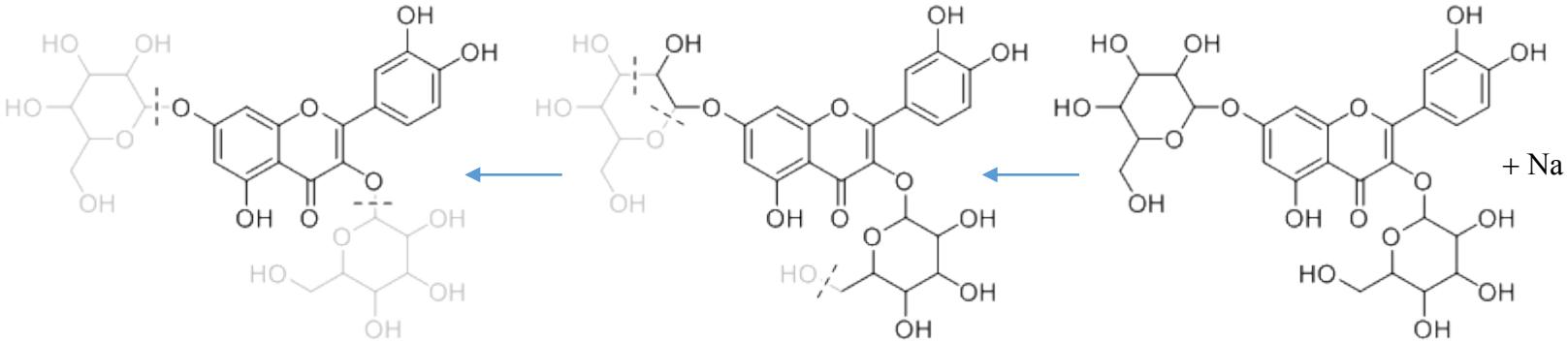
$[M–H]^-$
285.14926
Mass error: -0.4 mDa

Fig. S2 (continued)

(41) quercetin-3,7-di-O-glucoside







$[M+H-2glu]^+$
303.05001
Mass error: 0.1 mDa

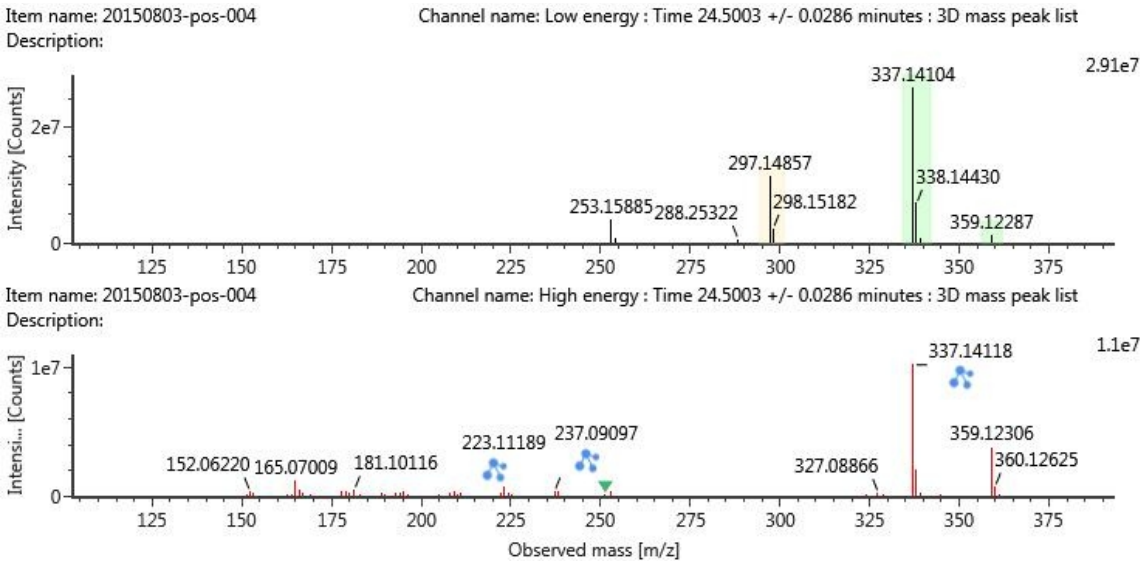
$[M+H-C_5H_8O_3-H_2O]^+$
487.08458
Mass error: -2.0 mDa

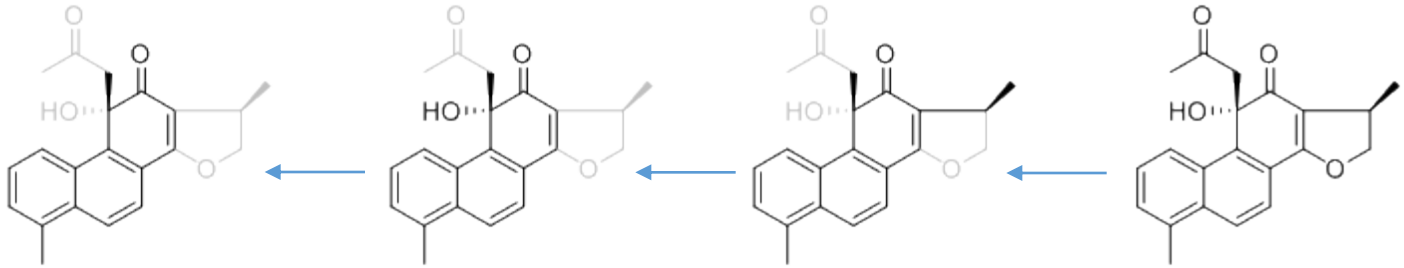
$[M+H]^+$
627.15632

$[M+Na]^+$
649.13801

Fig. S2 (continued)

(44) danshenol C





$[M+H–COCH_3–H_2O–C_3H_6O]^+$	$[M+H–COCH_3–C_3H_6O]^+$	$[M+H–COCH_3–H_2O–CH_2O]^+$	$[M+H]^+$	$[M+Na]^+$
223.11189	237.09097	251.14307	337.14118	359.12306
Mass error: 0.1 mDa	Mass error: 0 mDa	Mass error: 0 mDa	Mass error: -2.3 mDa	