Table S3

The possible metabolic pathways of three different types of compounds.

No.	Metabolic pathway	Formula change	Δm(Da)	A	P	T
1	Deglucosidation	$-C_6H_{10}O_5$	-162.0528	√		
2	Derhamnosation	$-C_6H_{10}O_4$	-146.0579	√		
3	Dexylosation/arabinosation	$-C_5H_8O_4$	-132.0423	√		
4	Tri-deoxidation	− 3O	-47.9847		√	
5	Decarboxylation	–CO2	-43.9898	√	√	√
6	Di-deoxidation	− 2O	-31.9898	√	√	
7	Dehydration	$-H_2O$	-18.0105	√		
8	Deoxidation	− O	-15.9949	√	√	
9	Deoxidation + Hydrogenation	$-O + H_2$	-13.9793	√	√	
10	Di-desaturation	$-H_4$	-4.0312	√		
11	Methylation + Dehydration	$+ CH_2- H_2O$	-3.9949	√		
12	Desaturation	$-H_2$	-2.0156	√		
13	Methylation + Deoxidation	$+ CH_2 - O$	-1.9793	√		
14	Hydrogenation	$+ H_2$	+2.0156	√	√	√
15	Di-hydrogenation	$+ H_4$	+4.0312			√
16	Methylation	$+ CH_2$	+14.0156	√	√	
17	Hydroxylation	+ O	+15.9949			√
18	Methylation + Hydrogenation	$+CH_2 + H_2$	+16.0312	√	√	
19	Internal Hydrolysis	$+ H_2O$	+18.0105			√
20	Di-methylation	$+C_2H_4$	+28.0312	√	√	
21	Demethylation to Carboxylic Acid	$- H_2 + O_2$	+29.9742	√		
22	Methylation + Deoxidation	$+ CH_2 + O$	+30.0100	√		
23	Di-hydroxylation	+ 2O	+31.9898			√
24	Hydroxylation + Internal Hydrolysis	$+ O + H_2O$	+34.0054			√
25	Acetylation	$+ C_2H_2O$	+42.0105	√	√	
26	Tri-methylation	$+C_3H_6$	+42.0468	√	√	
27	Methylation + Acetylation	$+ CH_2 + C_2H_2O$	+56.0261	√		
28	Acetylation + Deoxidation	$+ C_2H_2O + O$	+58.0049	√		
29	Deoxidation + Sulfate Conjugation	$+ SO_3 - O$	+63.9619	√		
30	Di-methylation + Acetylation	$+ C_2H_4 + C_2H_2O$	+70.0417	√		
31	Sulfate Conjugation	$+ SO_3$	+79.9568	√	√	√
32	Hydrogenation + Sulfate Conjugation	$+ SO_3 +H_2$	+81.9724	√	√	√
33	Methylation + Sulfate Conjugation	$+ CH_2 + SO_3$	+93.9724	√	√	
34	Deoxidation + Glucuronidation	$+ C_6H_8O_6 - O$	+160.0369	√		
35	Glucosidation	$+ C_6H_{10}O_5$	+162.0528	√	√	√
36	Glucuronidation	$+ C_6H_8O_6$	+176.0318	√	√	√
37	Hydrogenation + Glucuronidation	$+ C_6H_8O_6 + H_2$	+178.0474	√	√	√
38	Hydroxylation + Dehydrogenation + Glucuronidation	$+ C_6H_6O_6 + O$	+190.0111			√
39	Methylation + Glucuronidation	$+ C_6H_8O_6 + CH_2$	+190.0474	√	√	
40	Hydroxylation + Glucuronidation	$+ C_6H_8O_6 + O$	+192.0267			√
41	Di-methylation + Glucuronidation	$+ C_8H_{12}O_6$	+204.063	√		
42	Dihydroxylation + dehydrogenation + Glucuronidation	$+ C_6H_6O_8$	+206.0060			√
43	Dihydroxylation + Glucuronidation	$+ C_6H_8O_8$	+208.0216			√

Note: A: Phenolic acids; P: Phthalides; T: Tanshinones