Supporting Information

CATECHIN DEGRADATION WITH CONCURRENT FORMATION OF HOMO- AND HETERO- CATECHIN DIMERS DURING *IN VITRO* DIGESTION.

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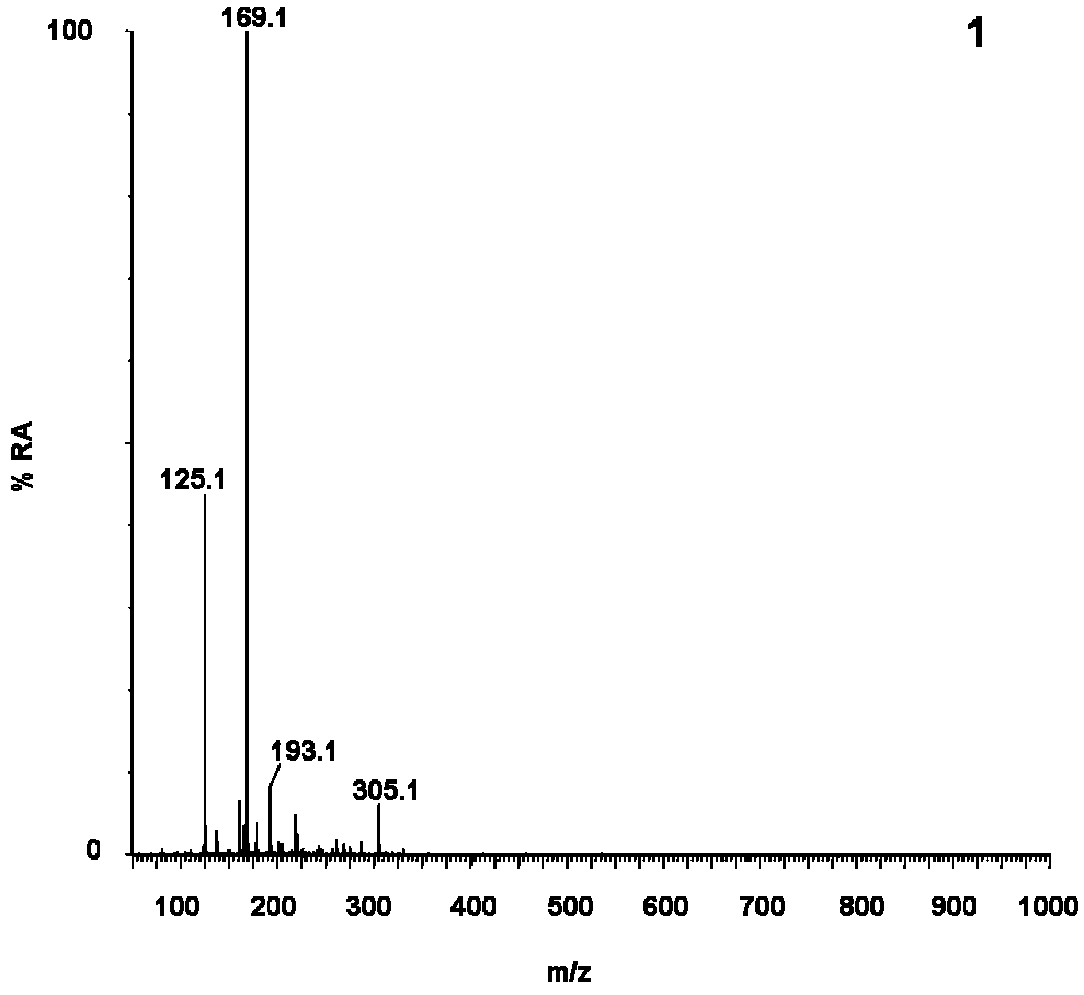
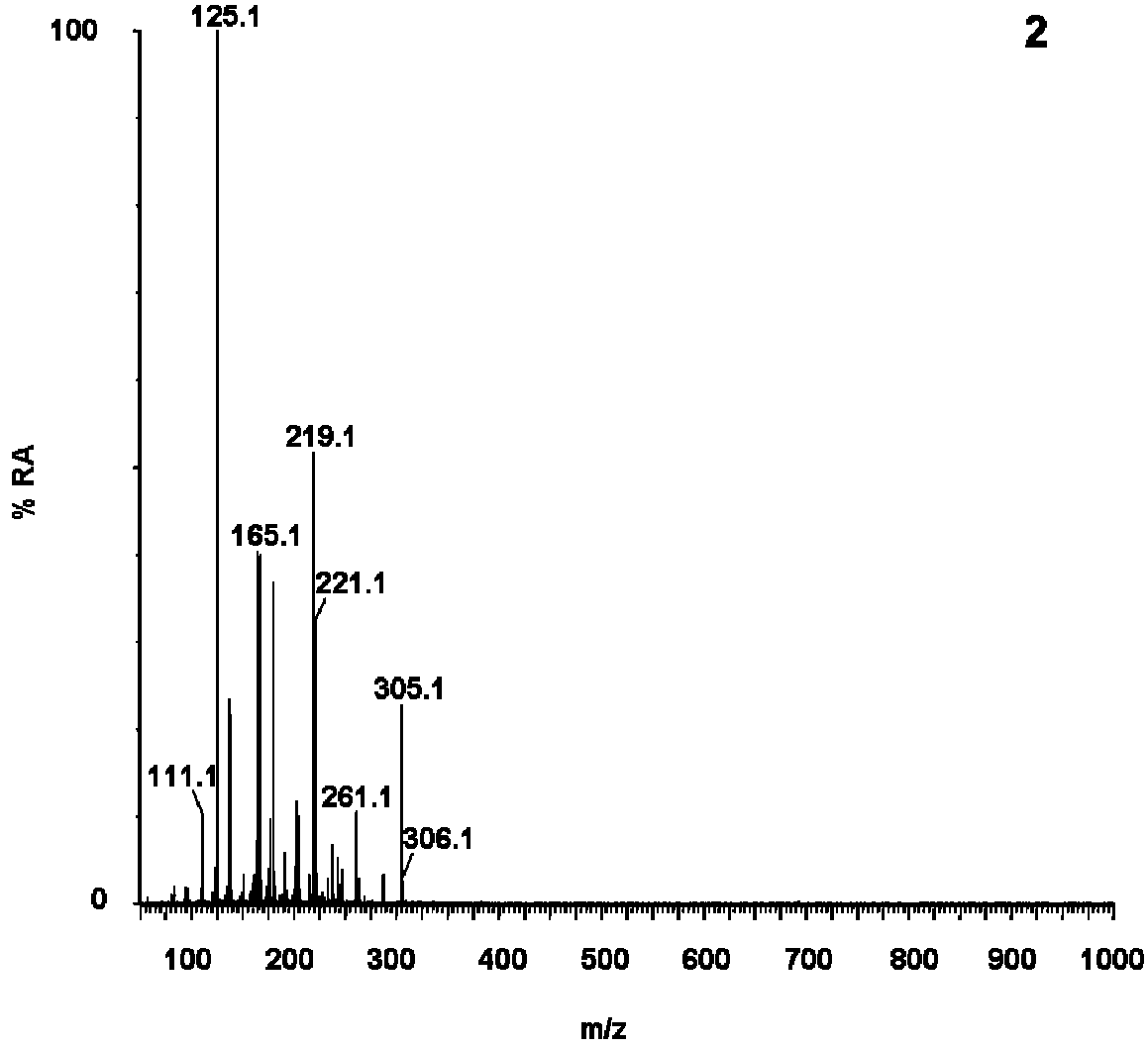
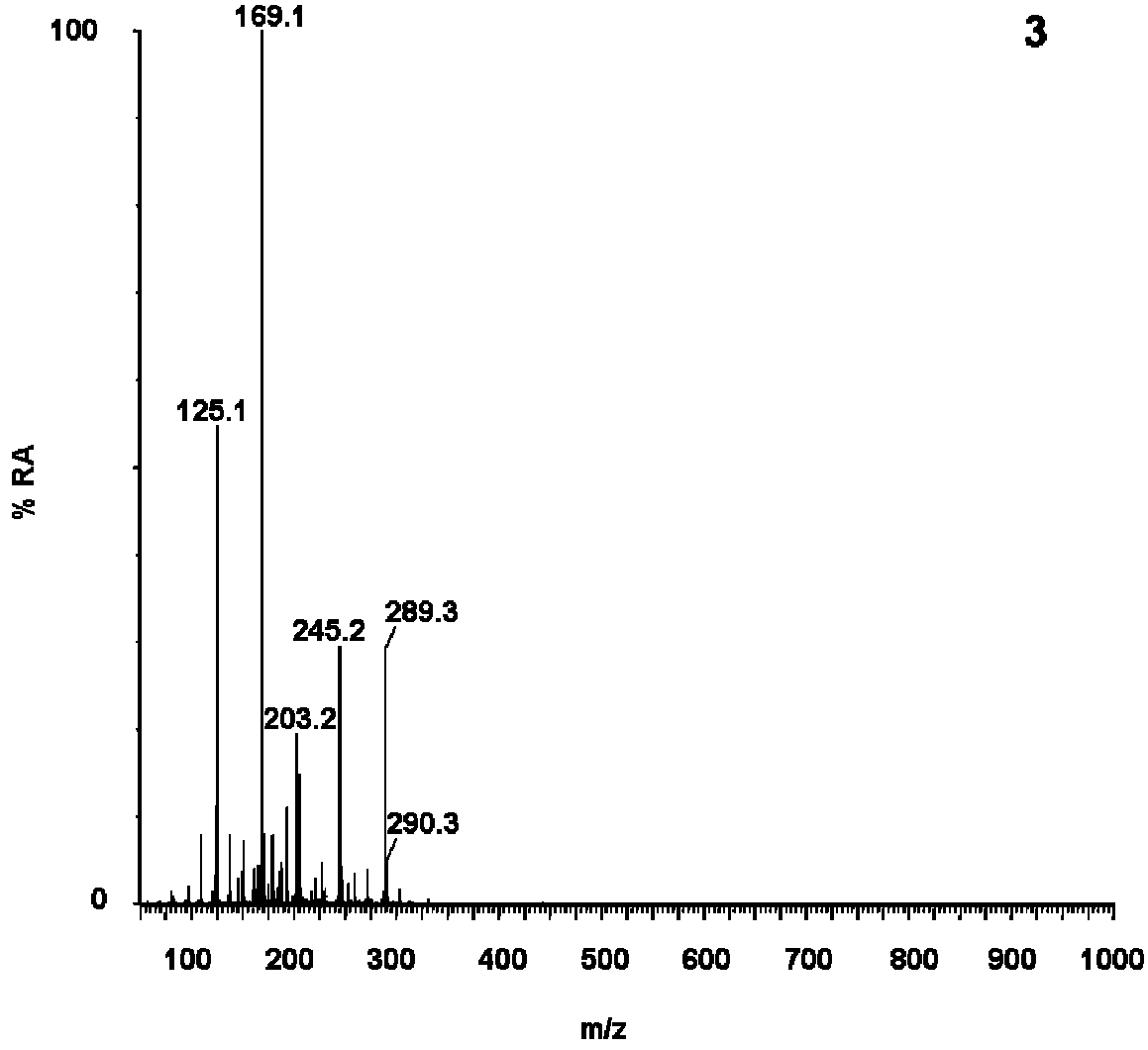
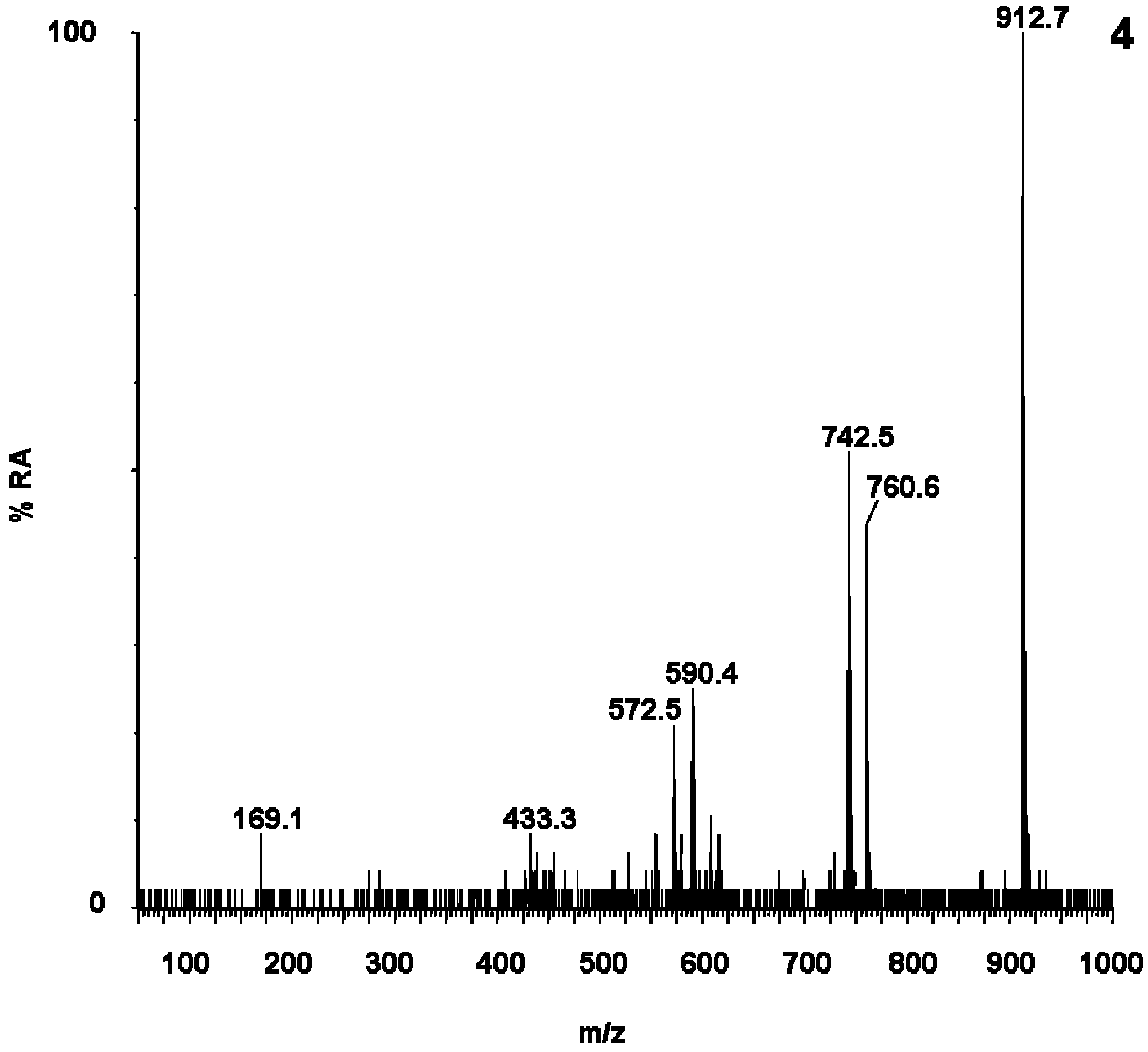
Figures S1-S19. CAD-MS/MS spectra (fragment ion relative abundance, % RA, versus mass-to-charge ratio, m/z) obtained for all species detected following simulated digestion of catechins individually and/or in combination: native catechins (EGCG, **1**; ECG, **2**; EGC, **3**), catechin epimers (GC, **7**; CG, **13**), and homo- and hetero-catechin dimers (m/z 913, **4** and **5**; m/z 883, **6**; m/z 609, **8** and **9**; m/z 579, **10**-**12**; m/z 761, **14** and **15**; m/z 731, **16** and **17**; m/z 897, **18** and **19**). Figure numbers refer to the corresponding compound numbers. Refer to Table 2 for compound identities and CAD parent ion collision energies. Note that the parent ion is not always observed in CAD-MS/MS spectra.

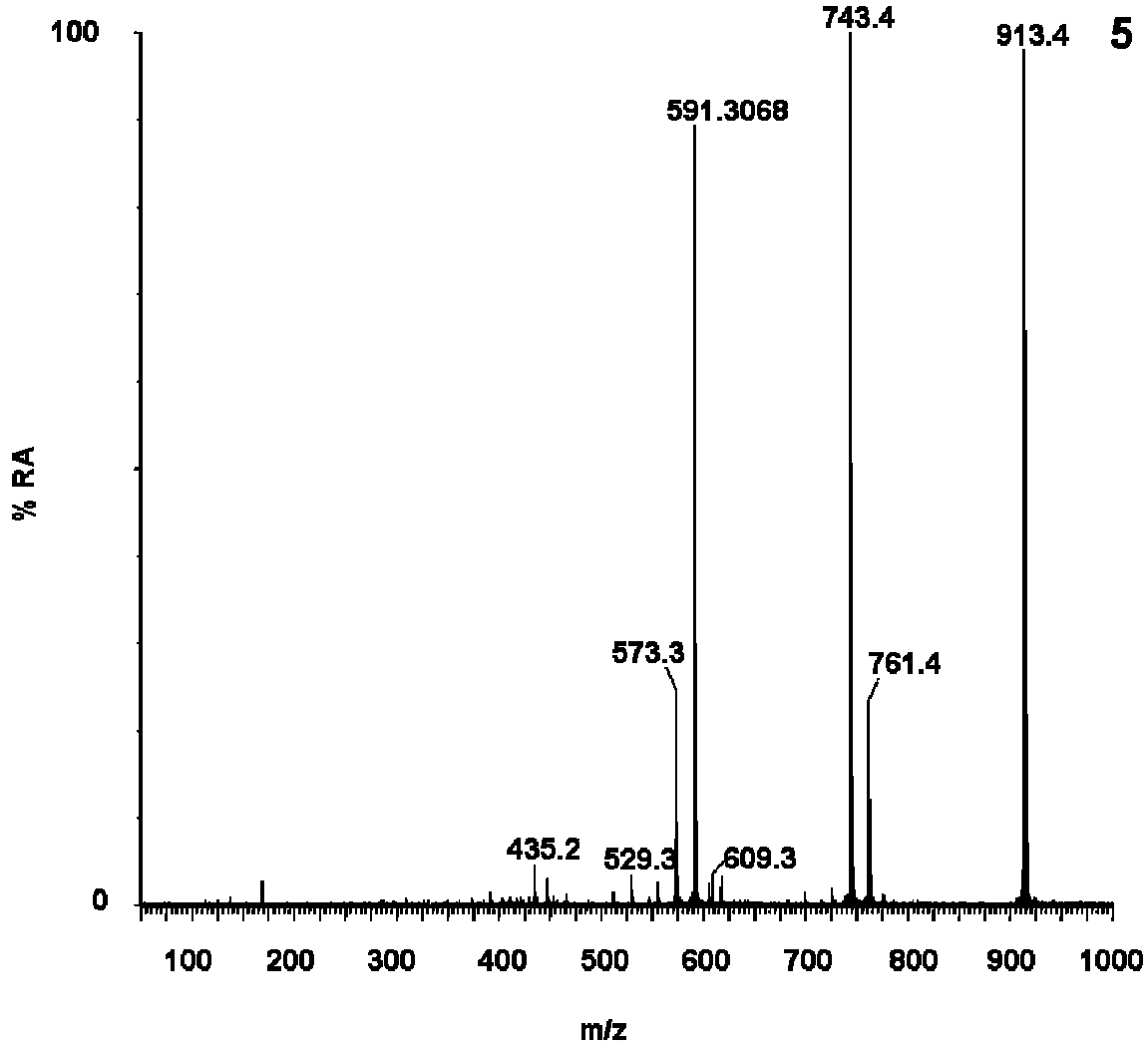
Figures S20-S25. HPLC-ECD elution profiles (response at 200 mV) of undigested catechin raw material (— — —), the subsequent digesta extract (———), and a digestive blank extract (no RM added) (— – – —) from EGCG (S20), EGC (S21), ECG (S22), combined EGCG-EGC (S23), combined EGCG-ECG (S24), and combined EGC-ECG (S25) raw material formulations. Peak scale is −0.1-1.0 μA. Refer to Table 2 for identities of numbered peaks.

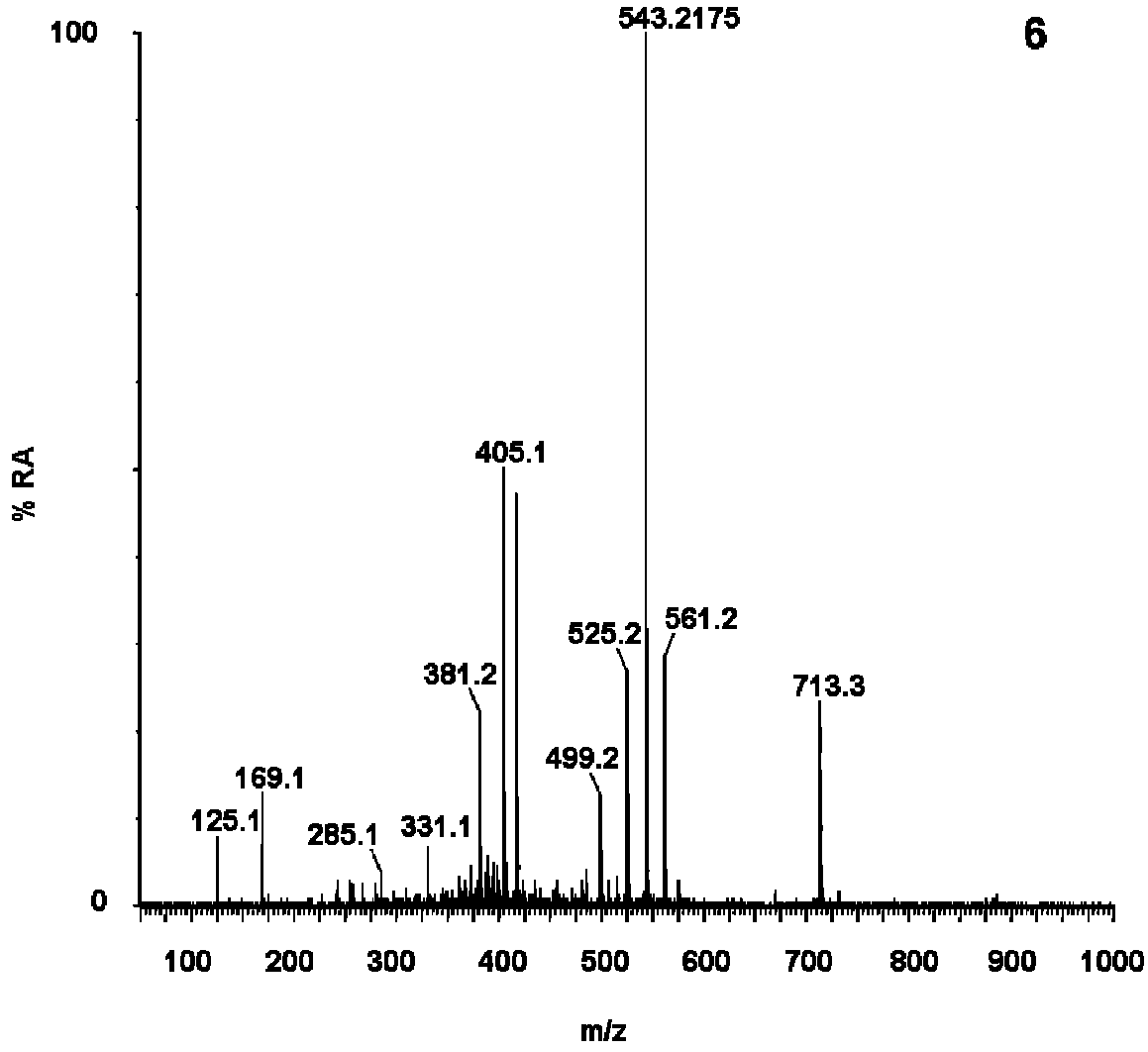

100
169.1
1
% RA
125.1
193.1
305.1
0
100
200
300
400
500
600
700
800
900
1000
m/z

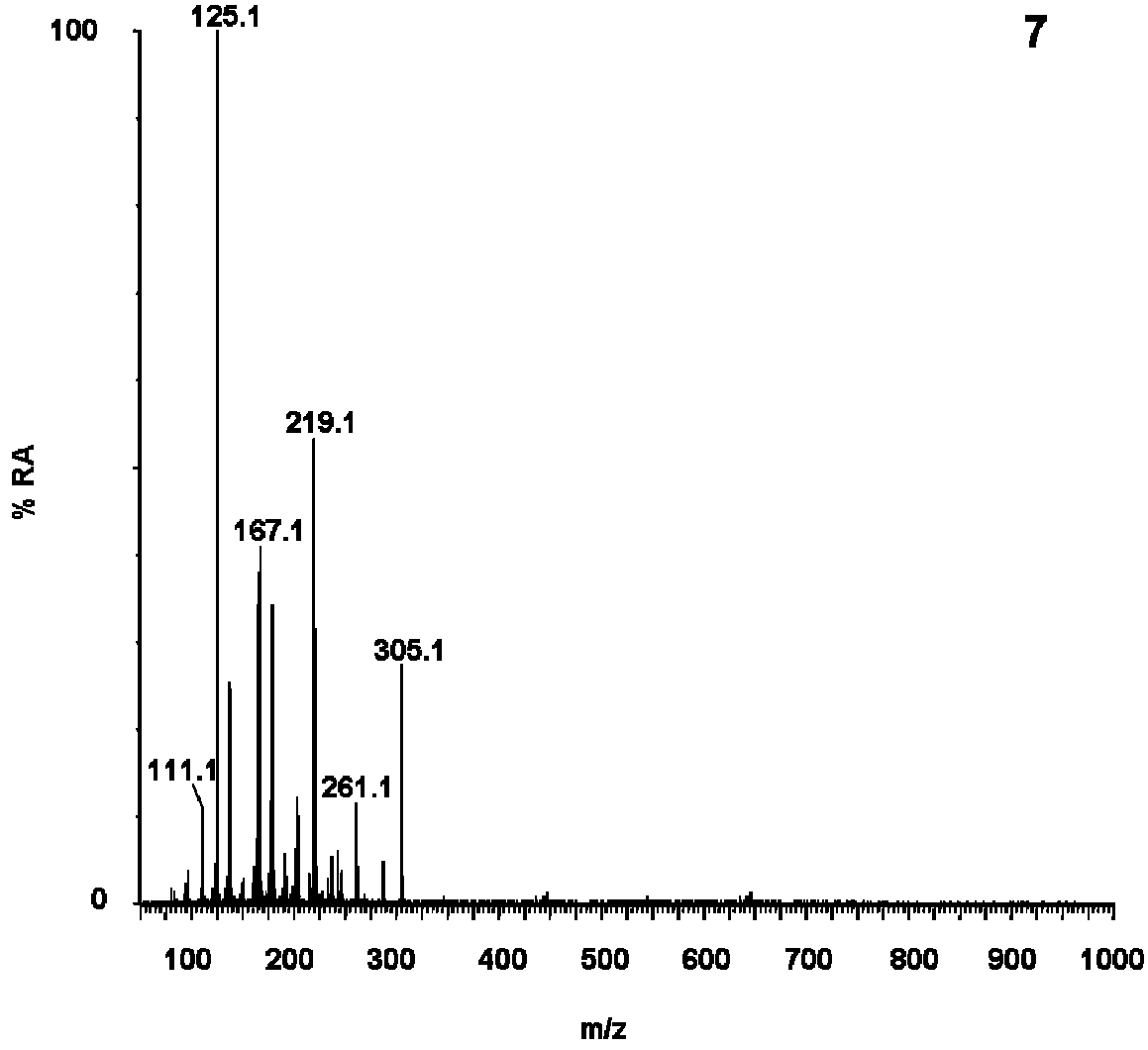

2
100
0
% RA
125.1
219.1
165.1
221.1
305.1
111.1
261.1
306.1
100
200
300
400
500
600
700
800
900
1000
m/z

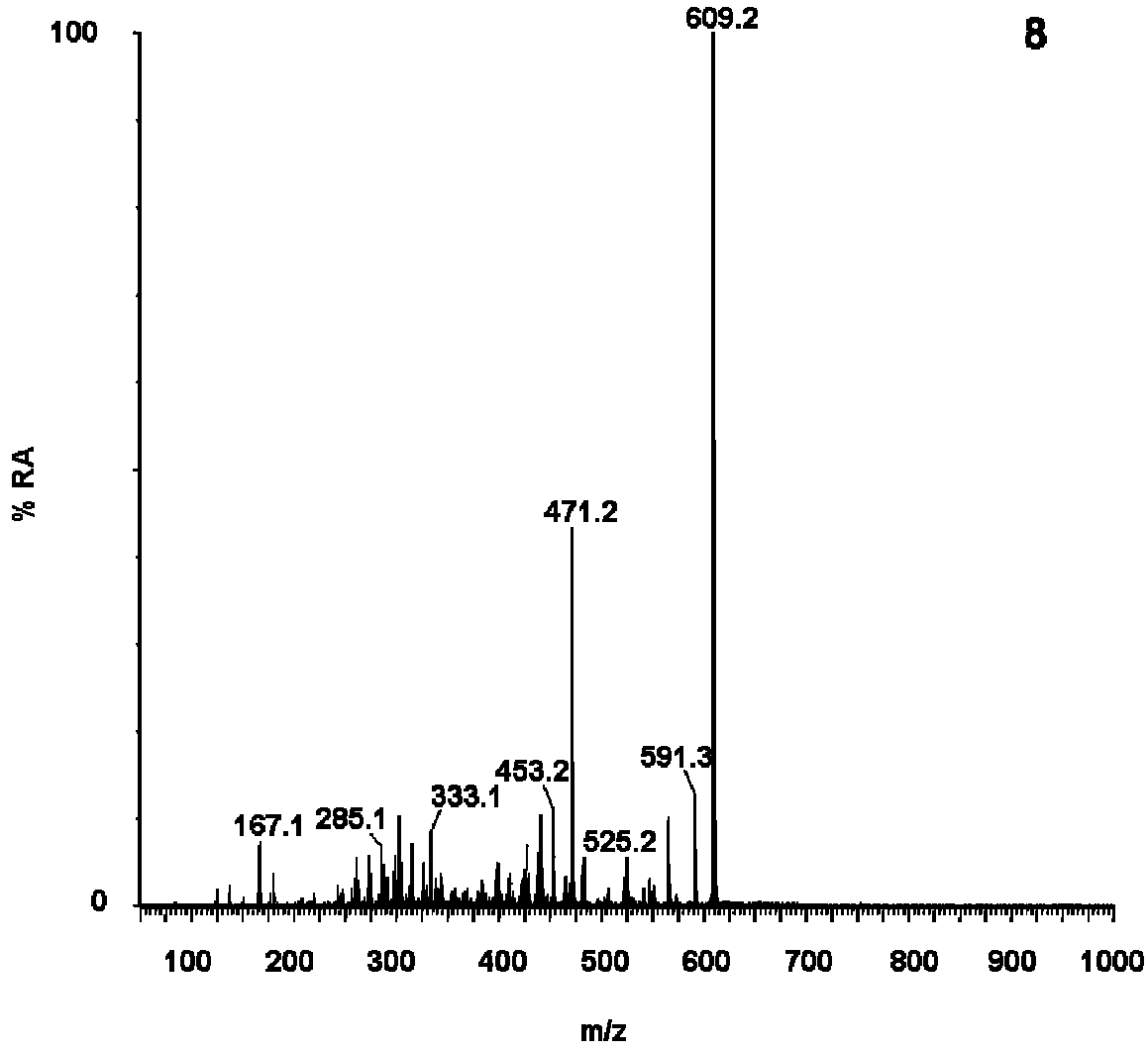

3
100
0
% RA
169.1
125.1
245.2
289.3
203.2
290.3
100
200
300
400
500
600
700
800
900
1000
m/z


4
912.7
100
742.5
760.6
% RA
590.4
572.5
169.1
433.3
0
100
200
300
400
500
600
700
800
900
1000
m/z


100
0
% RA
743.4
913.4
5
591.3068
573.3
761.4
435.2
529.3
609.3
100
200
300
400
500
600
700
800
900
1000
m/z


6
543.2175
100
% RA
405.1
525.2
561.2
381.2
713.3
499.2
169.1
125.1
285.1
331.1
0
100
200
300
400
500
600
700
800
900
1000
m/z


7
100
125.1
219.1
167.1
305.1
111.1
261.1
0
% RA
100
200
300
400
500
600
700
800
900
1000
m/z


8
100
0
% RA
609.2
471.2
591.3
453.2
333.1
285.1
167.1
525.2
100
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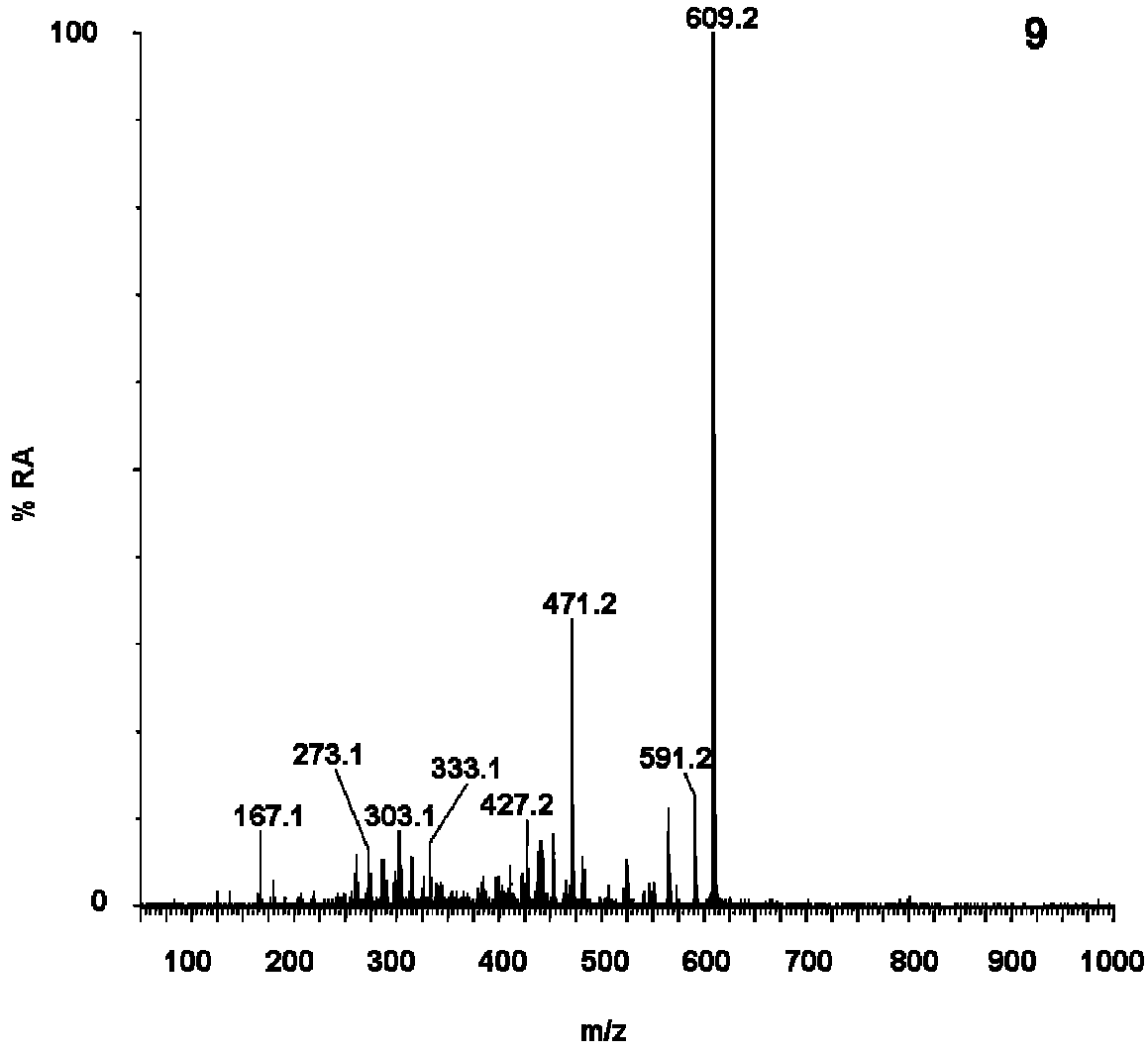
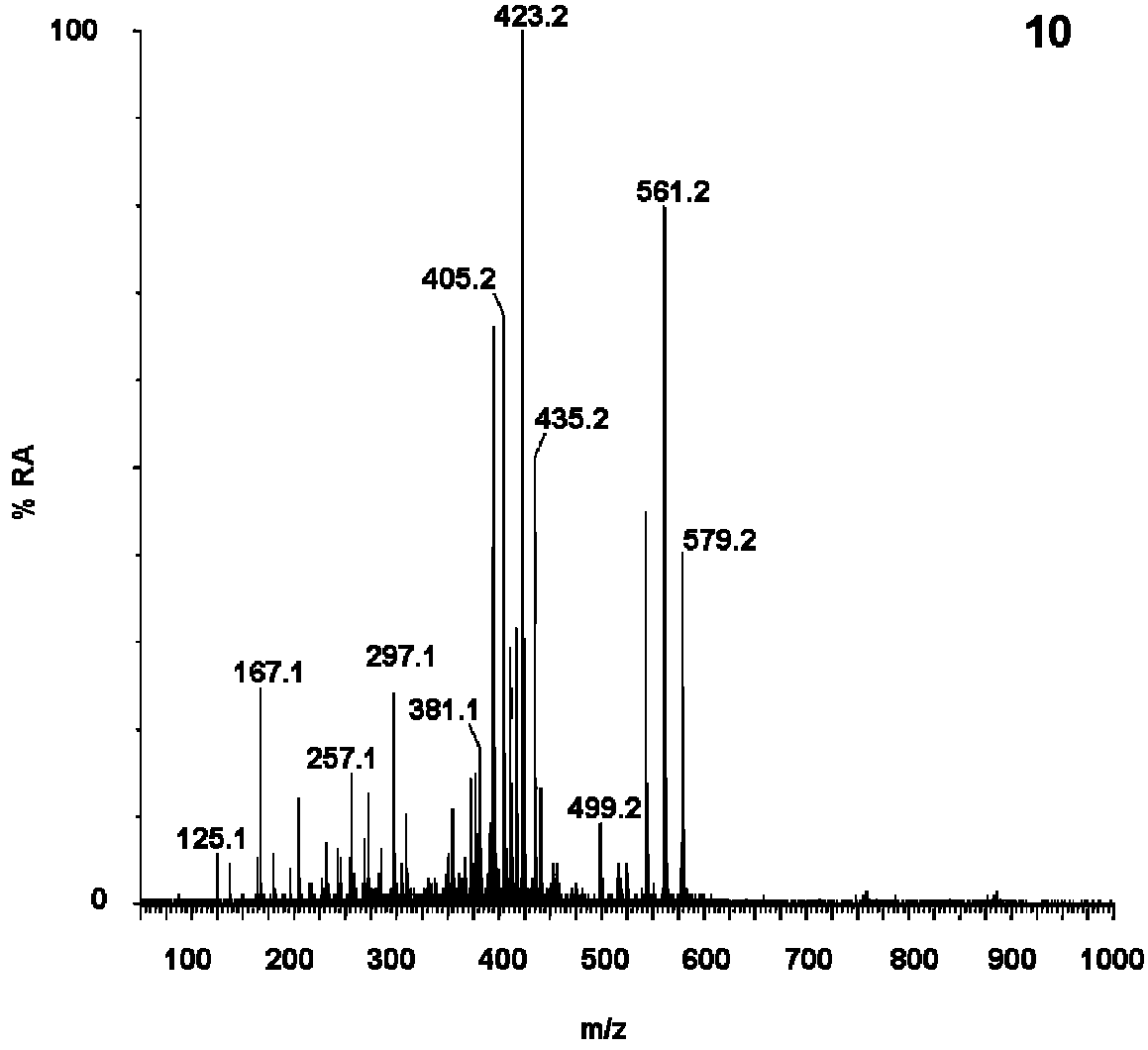
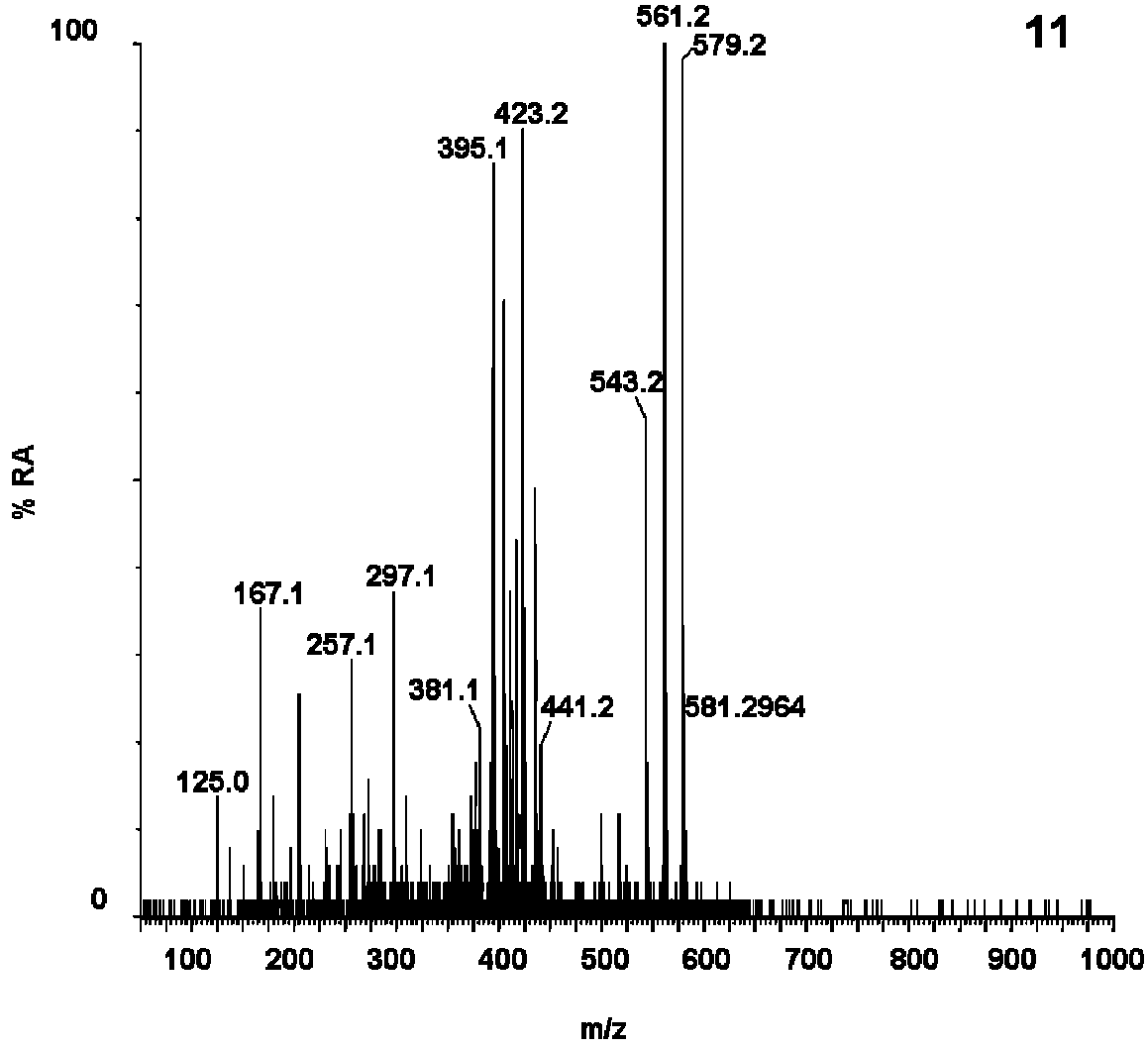
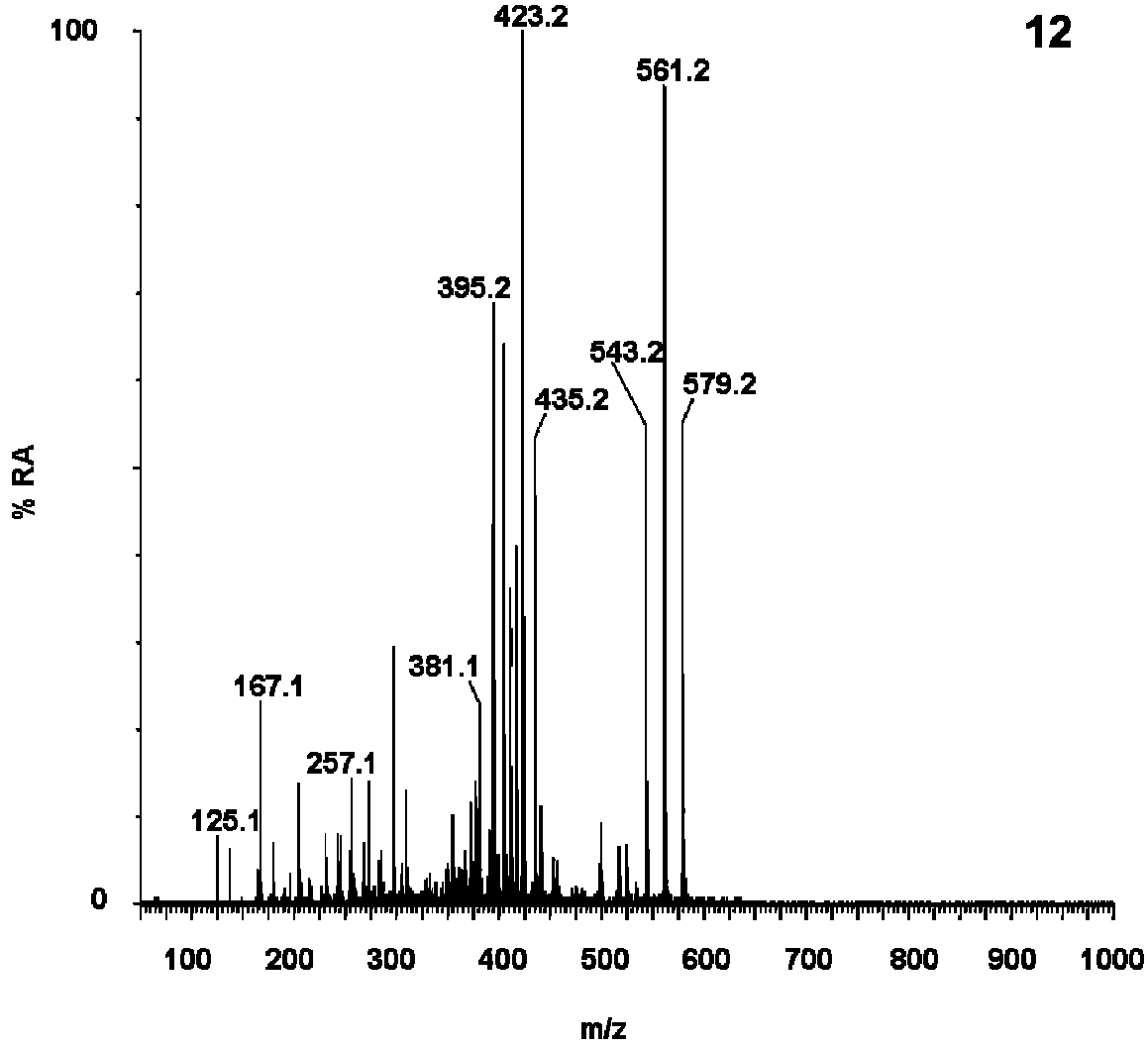
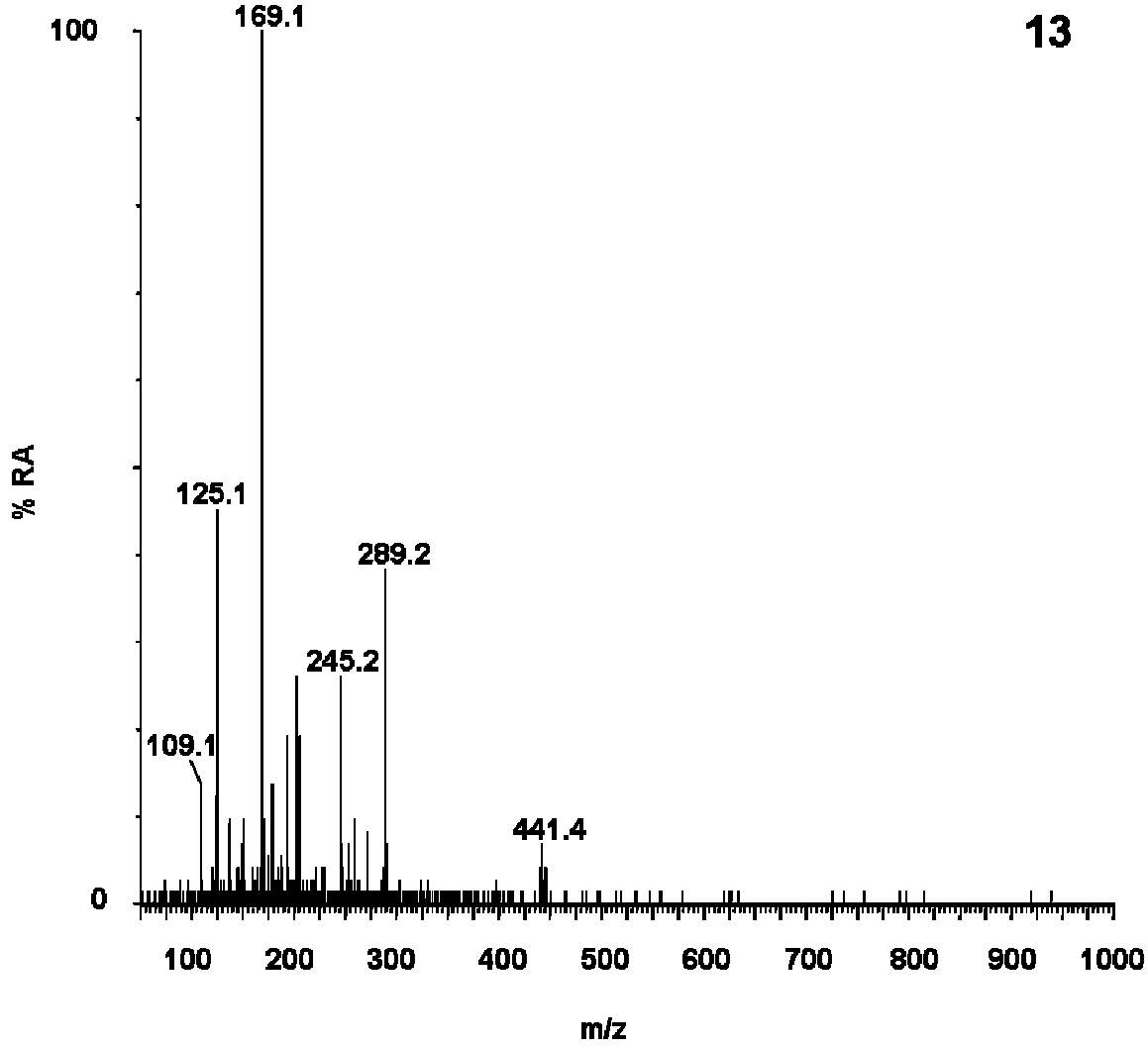
300
400
500
600
700
800
900
1000
m/z

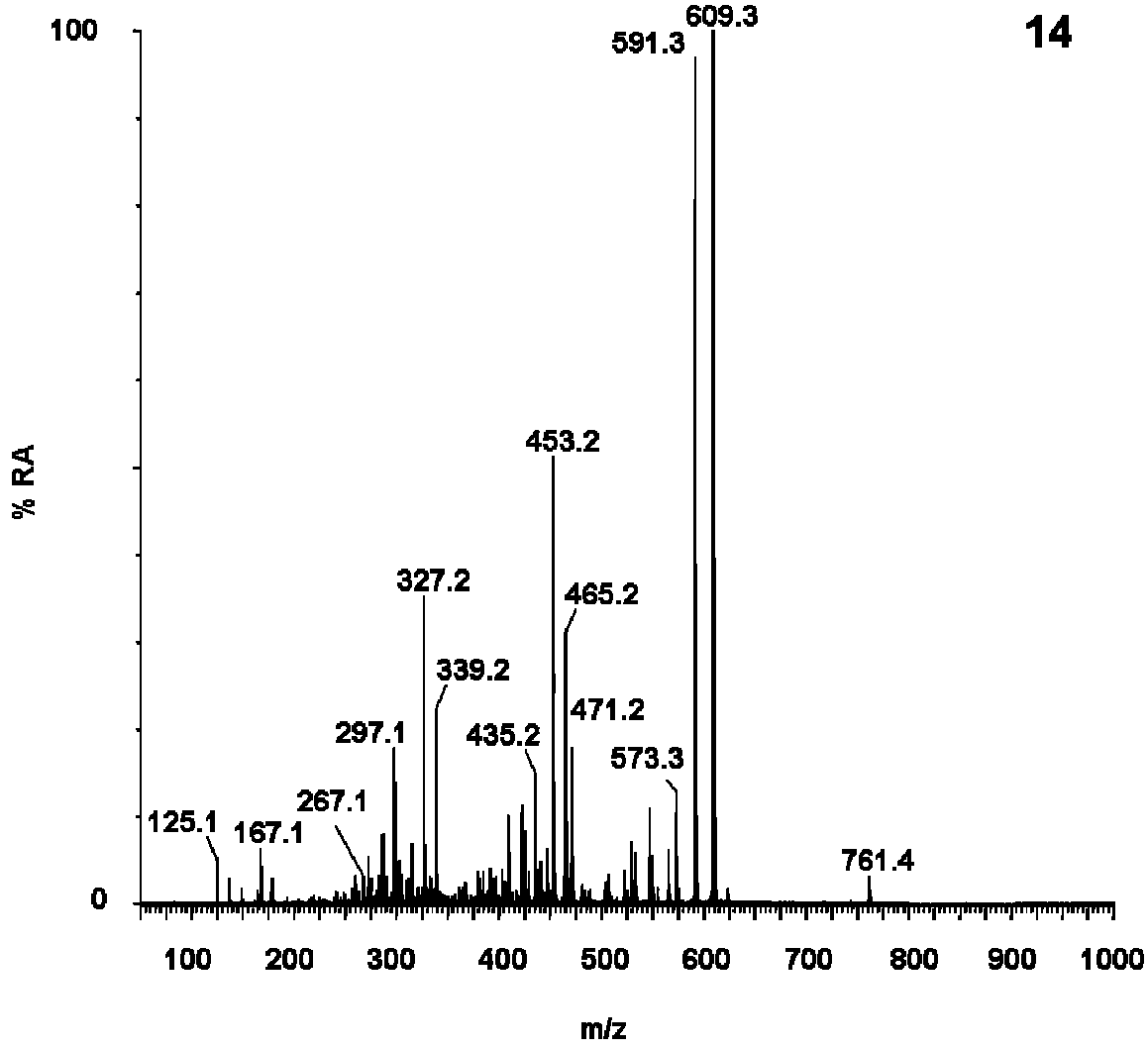

9
609.2
100
% RA
471.2
273.1
333.1
591.2
167.1
303.1
427.2
0
100
200
300
400
500
600
700
800
900
1000
m/z


10
100
0
% RA
423.2
561.2
405.2
435.2
579.2
297.1
167.1
381.1
257.1
499.2
125.1
100
200
300
400
500
600
700
800
900
1000
m/z


11
100
0
% RA
561.2
579.2
423.2
395.1
543.2
297.1
167.1
257.1
381.1
441.2
581.2964
125.0
100
200
300
400
500
600
700
800
900
1000
m/z


12
100
0
% RA
423.2
561.2
395.2
543.2
579.2
435.2
381.1
167.1
257.1
125.1
100
200
300
400
500
600
700
800
900
1000
m/z


13
100
169.1
125.1
289.2
245.2
109.1
441.4
0
% RA
100
200
300
400
500
600
700
800
900
1000
m/z


14
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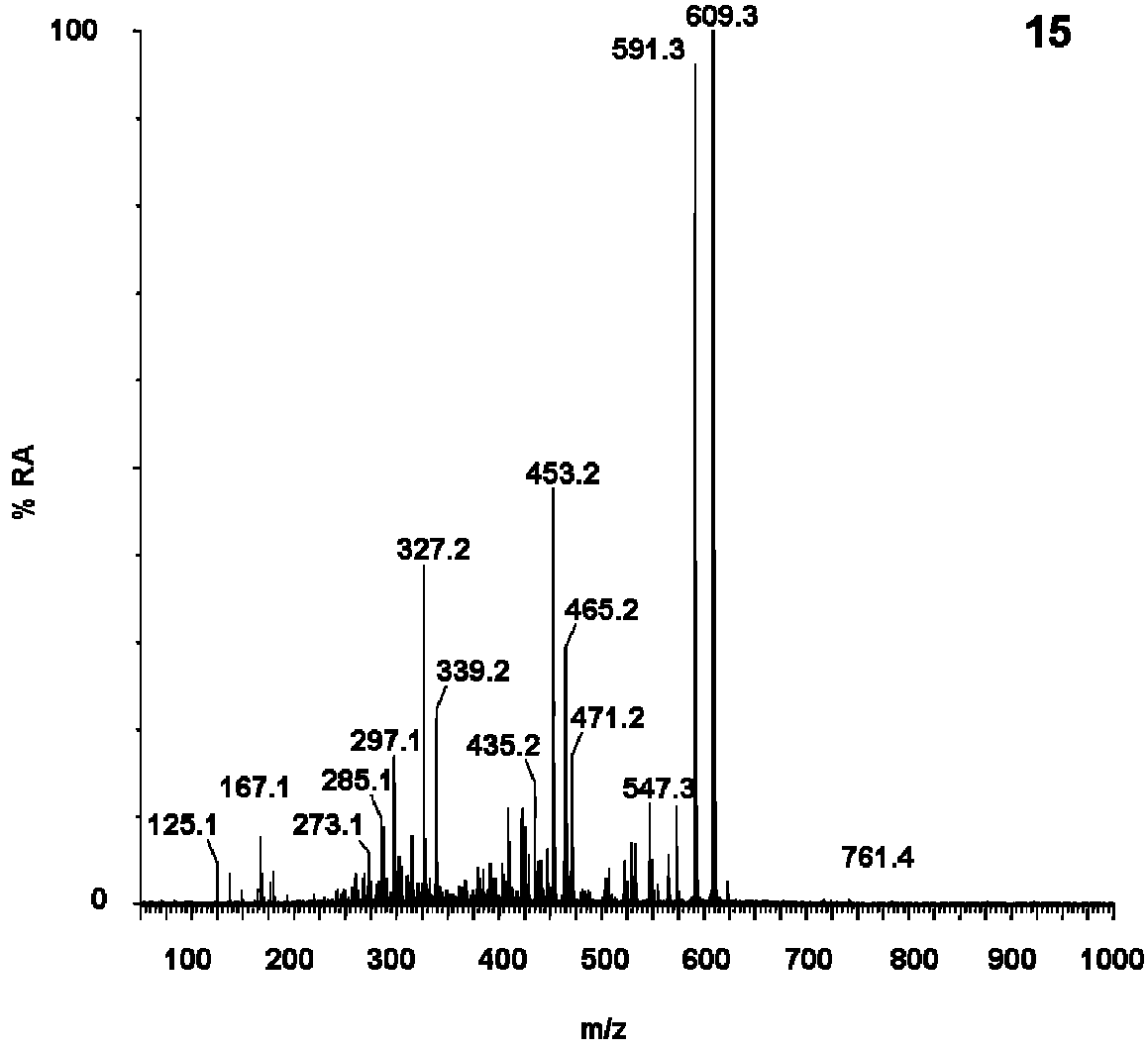
% RA
609.3
591.3
453.2
327.2
465.2
339.2
471.2
297.1
435.2
573.3
267.1
125.1
167.1
761.4
100
200
300
400
500
600
700
800
900
1000
m/z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100
0
% RA
609.3
591.3
453.2
327.2
465.2
339.2
471.2
297.1
435.2
285.1
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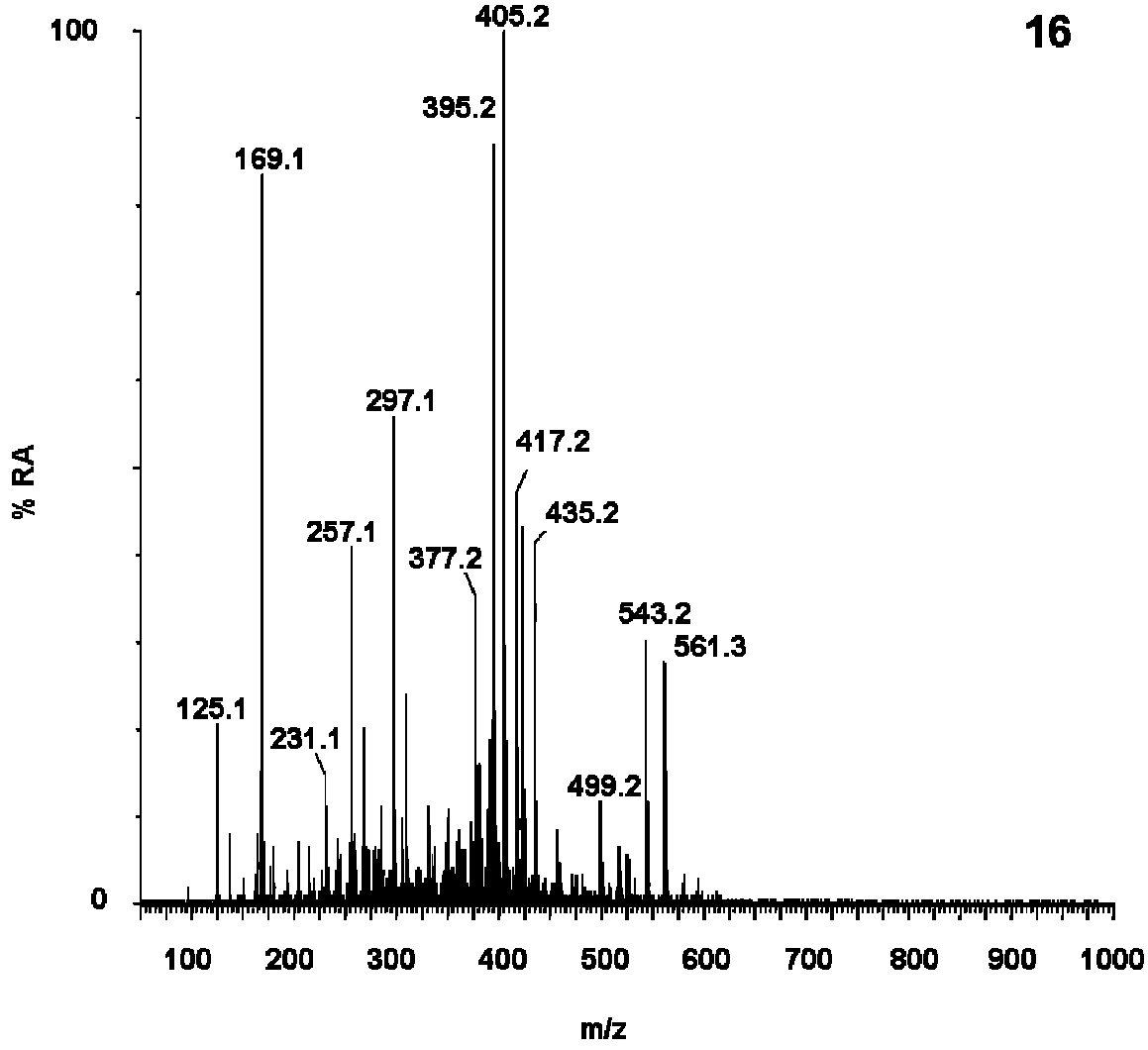
300
400
500
600
700
800
900
1000
m/z


16
100
0
% RA
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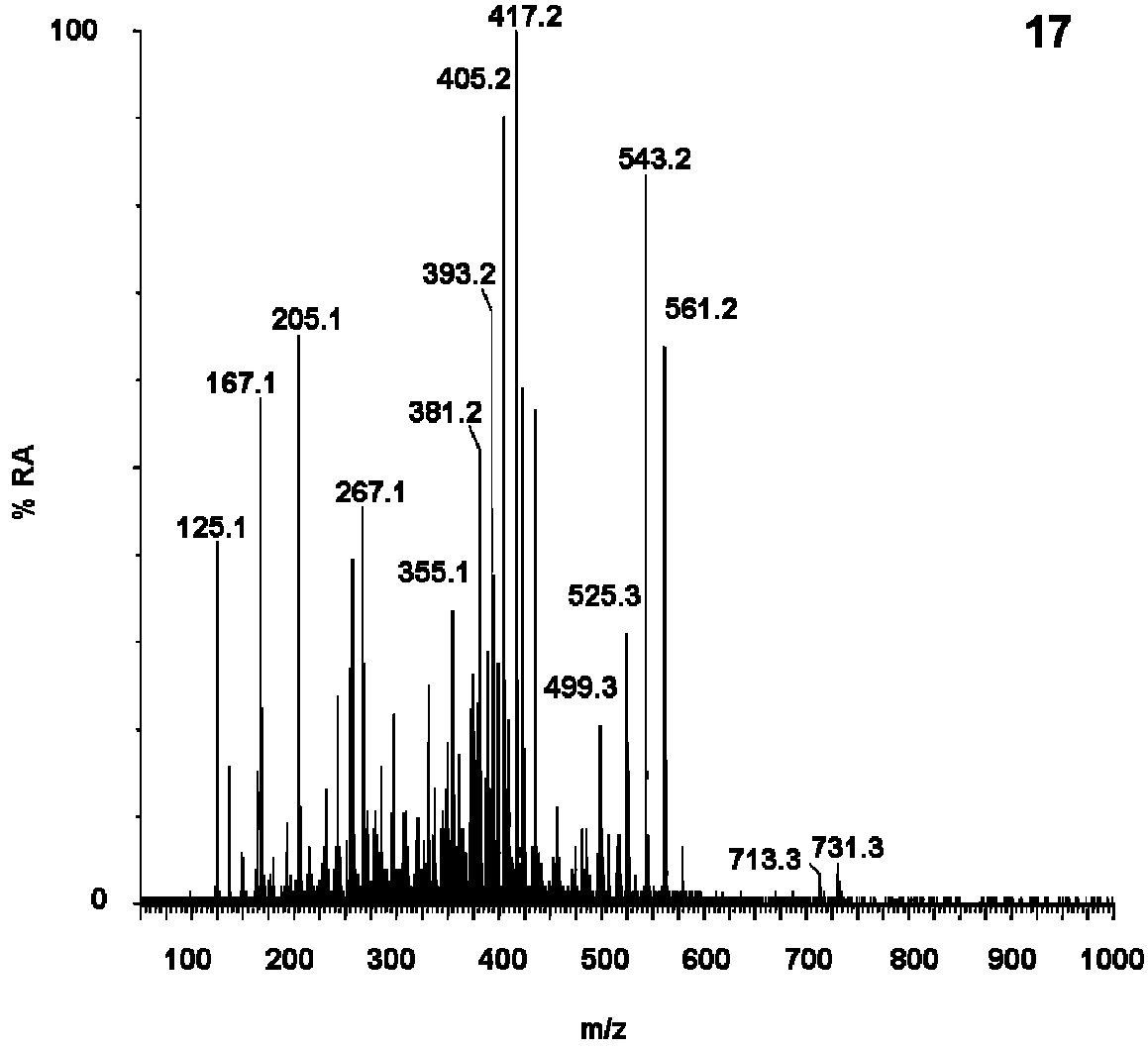
395.2
169.1
297.1
417.2
435.2
257.1
377.2
543.2
561.3
125.1
231.1
499.2
100
200
300
400
500
600
700
800
900
1000
m/z


17
100
0
% RA
417.2
405.2
543.2
393.2
561.2
205.1
167.1
381.2
267.1
125.1
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500
600
700
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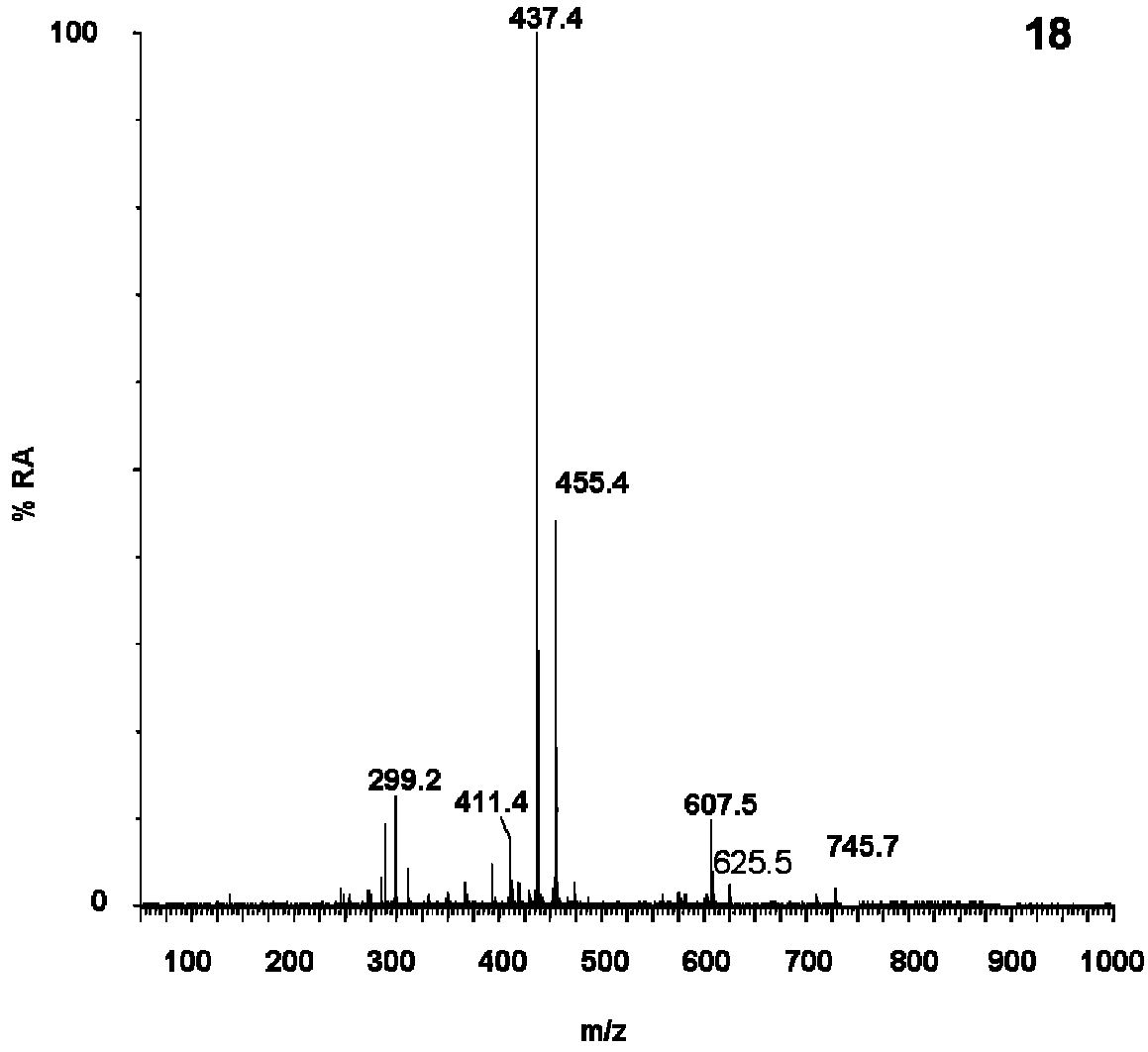
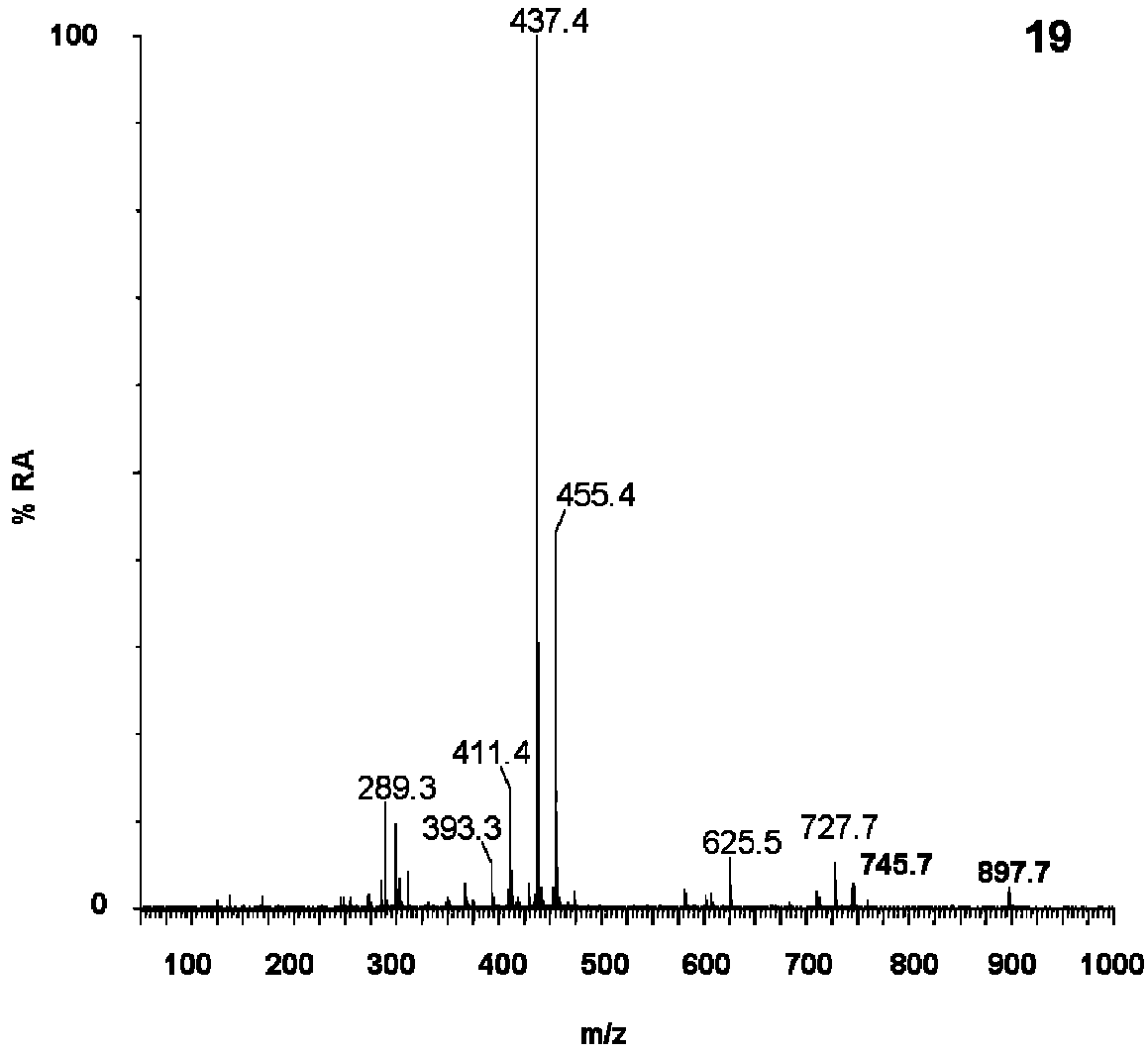
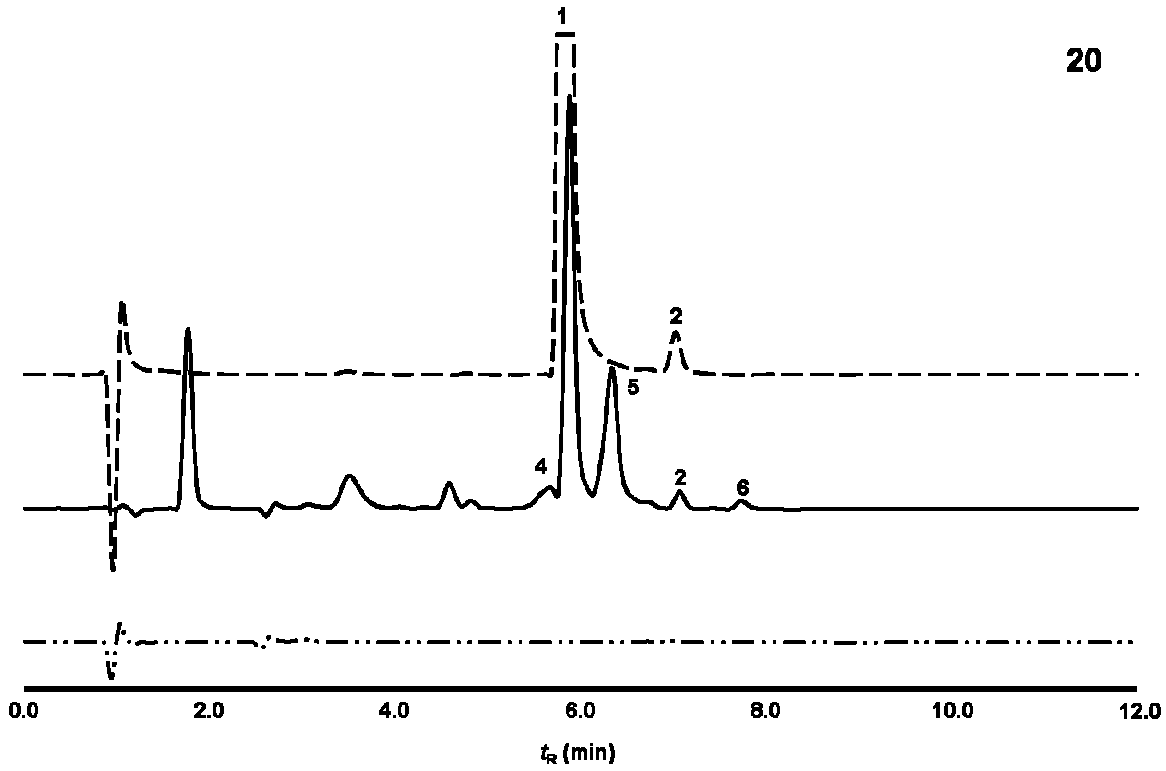
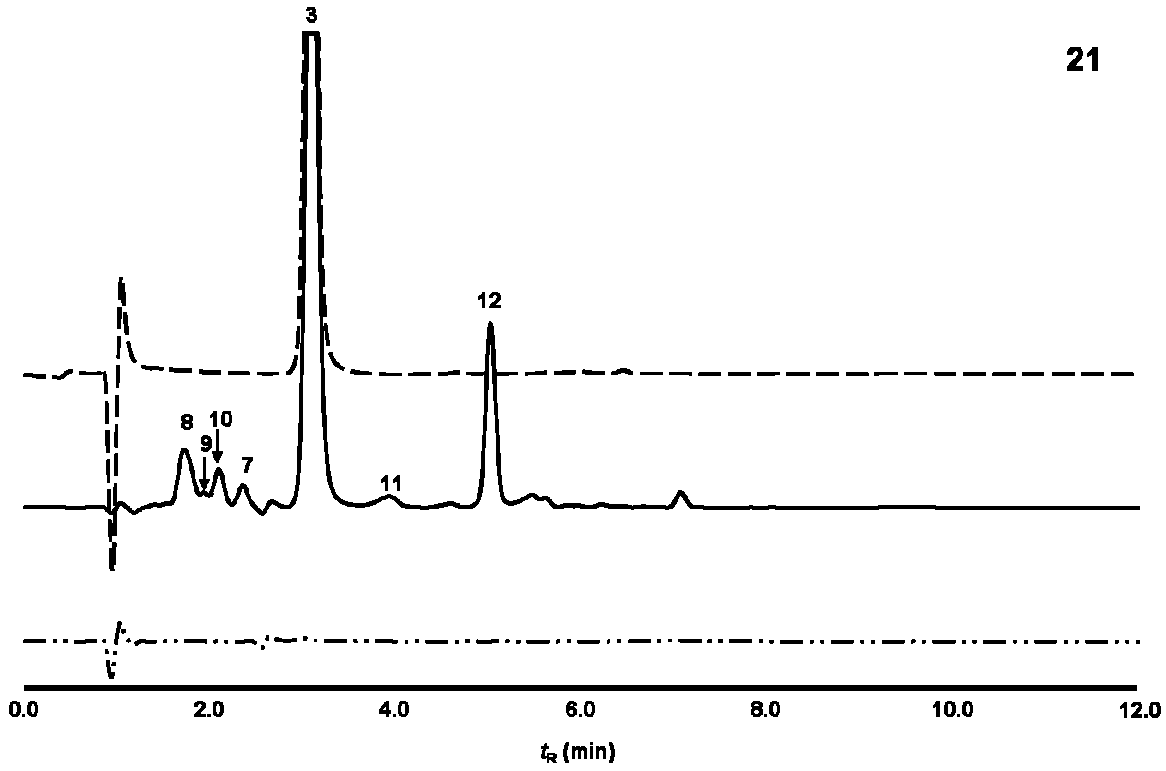
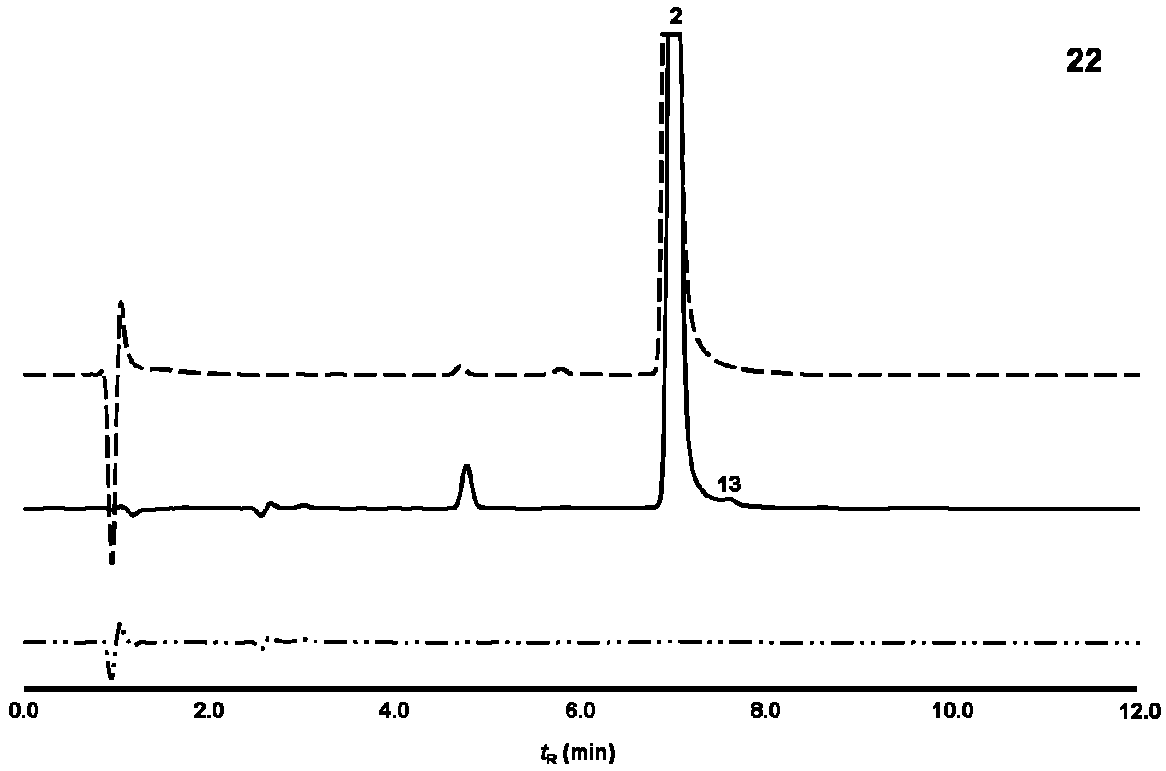
900
1000
m/z


18
100
0
% RA
437.4
455.4
299.2
411.4
607.5
625.5
745.7
100
200
300
400
500
600
700
800
900
1000
m/z


19
100
0
% RA
437.4
455.4
411.4
289.3
393.3
625.5
727.7
745.7
897.7
100
200
300
400
500
600
700
800
900
1000
m/z


20
1
2
5
4
2
6
0.0
2.0
4.0
6.0
8.0
10.0
12.0
t_R (min)


21
3
12
8
9
10
7
11
0.0
2.0
4.0
6.0
8.0
10.0
12.0
t_R (min)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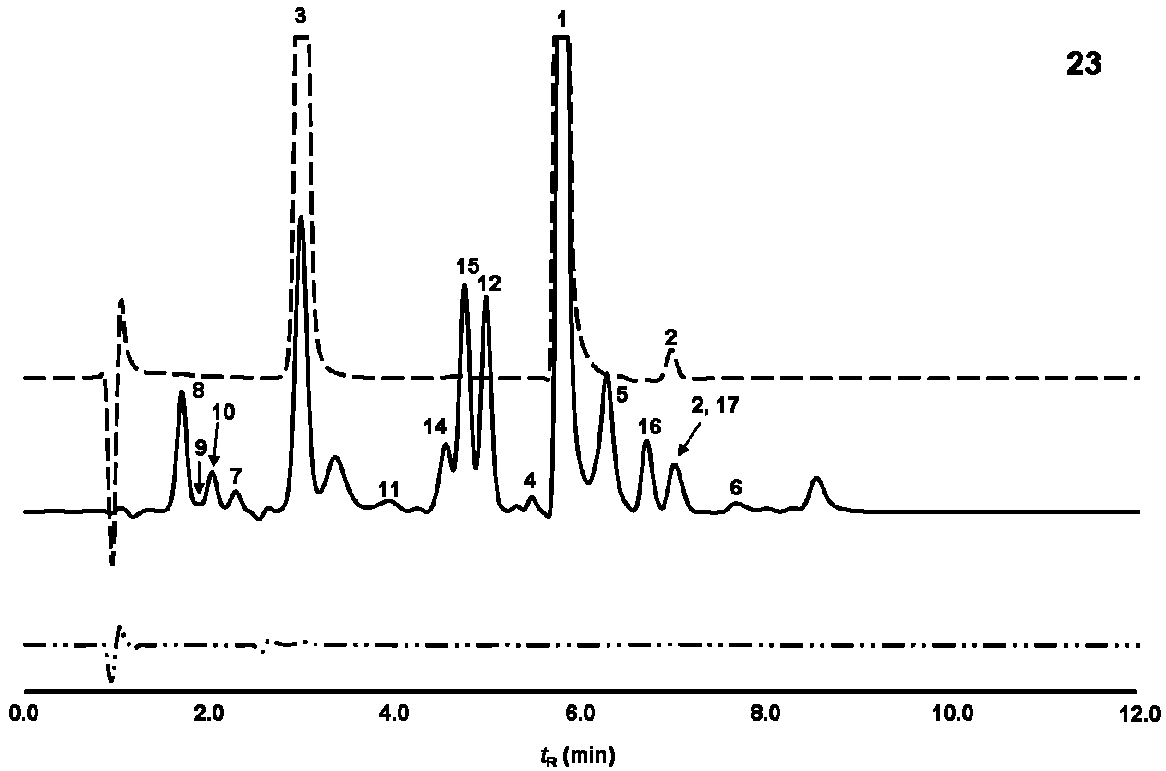
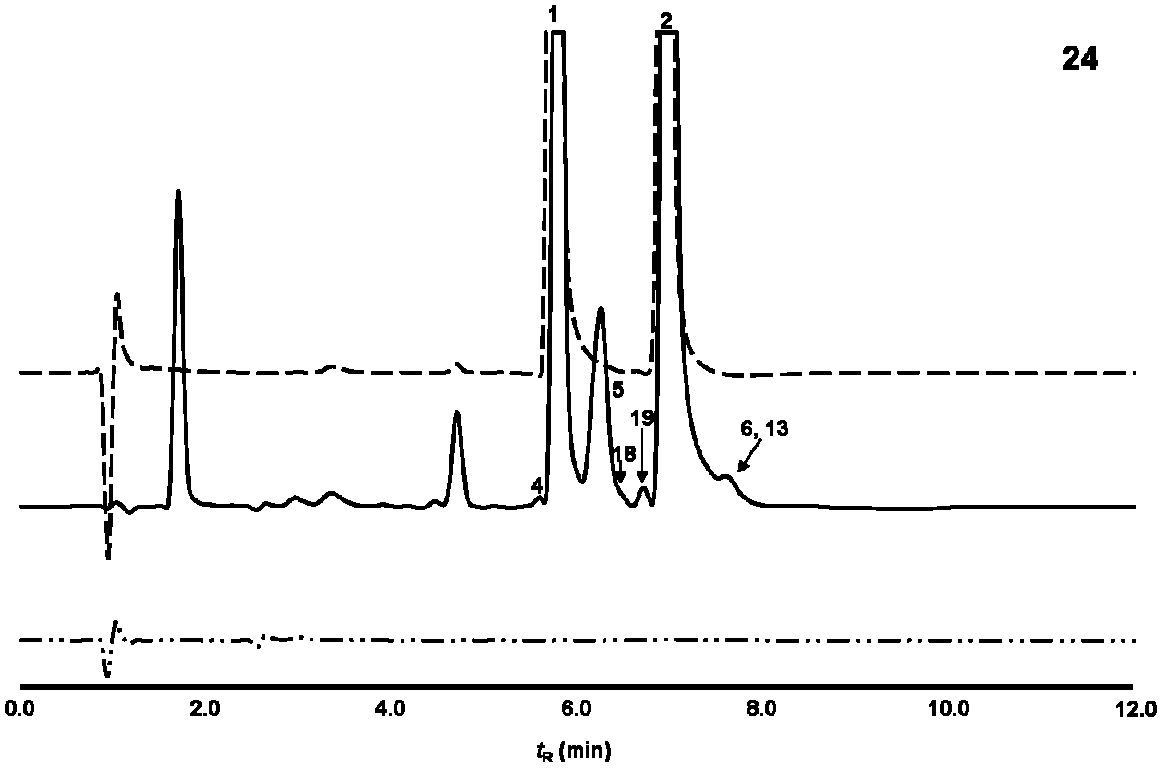
2
13
0.0
2.0
4.0
6.0
8.0
10.0
12.0
t_R (min)


23
3
1
15
12
2
8
10
9
7
14
11
4
5
16
2, 17
6
0.0
2.0
4.0
6.0
8.0
10.0
12.0
t_R (min)


24
1
2
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19
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6, 13
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8.0
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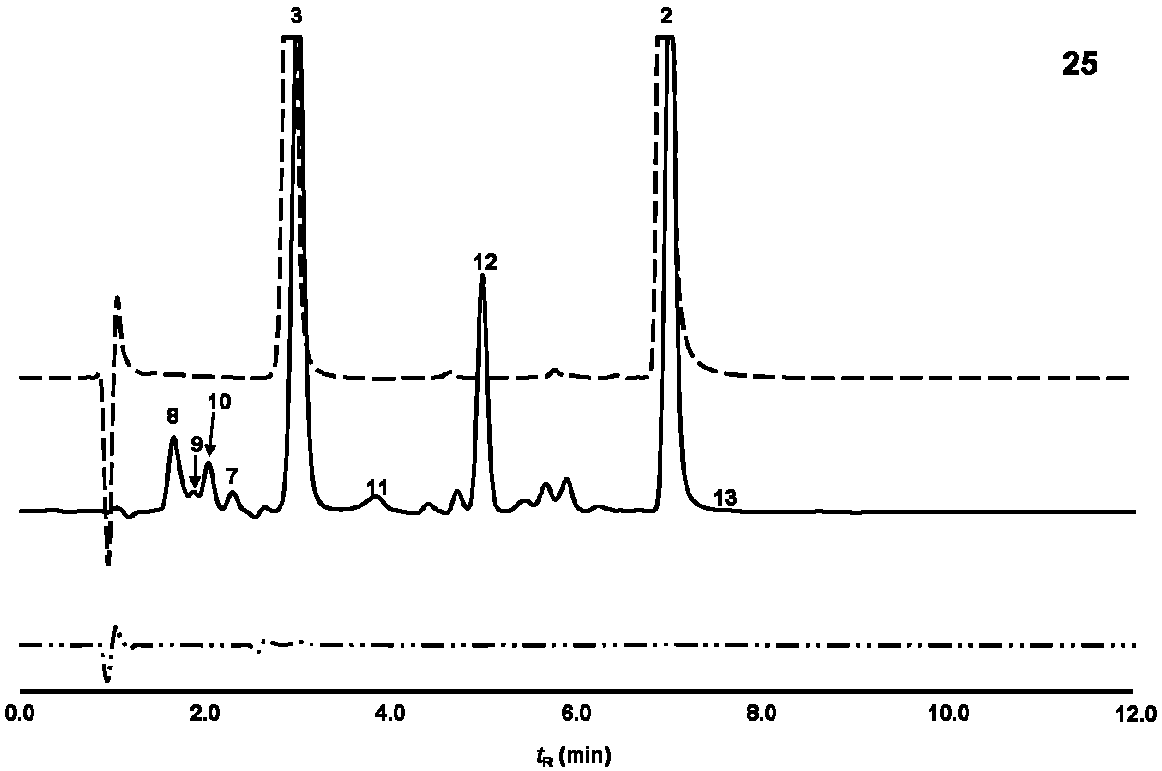
12.0
t_R (min)


25
3
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7
11
13
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2.0
4.0
6.0
8.0
10.0
12.0
t_R (min)