

**Table S1**

Composition of SJIT.

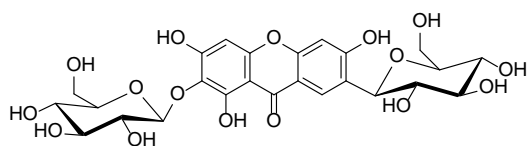
| Herbal medicine               | English name        | Scientific name                        | Family       | Using part       | Origin           | Amount (g) |
|-------------------------------|---------------------|--|--------------|------------------|------------------|------------|
| Ziziphi Semen                 | Ziziphus Seed       | <i>Ziziphus jujuba</i> Mill.           | Rhamnaceae   | Seed             | China            | 2666.67    |
| Cnidii Rhizoma                | Cnidium Rhizome     | <i>Cnidium officinale</i> Mak.         | Umbelliferae | Rhizome          | Yeongyang, Korea | 666.67     |
| Anemarrhenae Rhizoma          | Anemarrhena Rhizome | <i>Anemarrhena asphodeloides</i> Bunge | Asparagaceae | Rhizome          | Uiryeong, Korea  | 666.67     |
| Poria Sclerotium              | Poria               | <i>Poria cocos</i> Wolf                | Polyporaceae | Sclerotium       | Bonghwa, Korea   | 666.67     |
| Glycyrrhizae Radix et Rhizoma | Licorice            | <i>Glycyrrhiza uralensis</i> Fisch.    | Leguminosae  | Root and rhizome | China            | 333.32     |
|                               |                     |  |              | Total            |                  | 5000.00    |

**Table S2**

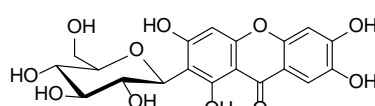
LC-MS/MS MRM analysis conditions for quantification of markers in SJIT.

| UPLC conditions  |   | MS conditions        |                                      |
|------------------|---|----------------------|--------------------------------------|
| UPLC system      | Acquity UPLC I-Class  | MS system            | Xevo TQ-XS                           |
| Column           | Acquity UPLC BEH C <sub>18</sub> column (2.1 mm × 100 mm, 1.7 μm) | MS software          | MassLynx v4.2                        |
| Column temp.     | 45 °C   | Ion source           | ESI <sup>+</sup> or ESI <sup>-</sup> |
| Sample temp.     | 5 °C  | Acquisition mode     | MRM                                  |
| Injection volume | 2.0 μL  | Capillary voltage    | 3.0 kV                               |
| Flow rate        | 0.3 mL/min  | Cone gas flow        | 50 L/h                               |
| Mobile phase A   | 0.1% (v/v) aqueous formic acid                                    | Desolvation gas flow | 700 L/h                              |
| Mobile phase B   | Acetonitrile  | Desolvation temp.    | 500 °C                               |
|                  | Time (min)  | A (%)                | B (%)                                |
|                  | Initial   | 80                   | 20                                   |
|                  | 14.0  | 5                    | 95                                   |
| Gradient         | 15.0  | 0                    | 100                                  |
|                  | 15.1  | 80                   | 20                                   |
|                  | 18.0  | 80                   | 20                                   |

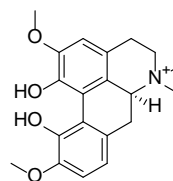
ESI; electrospray ionization, MRM; multiple reaction monitoring



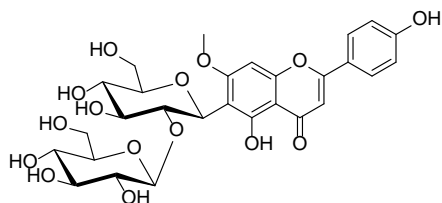
Neomangiferin



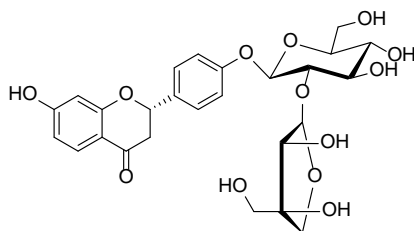
Mangiferin



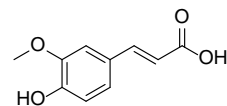
Magnoflorine



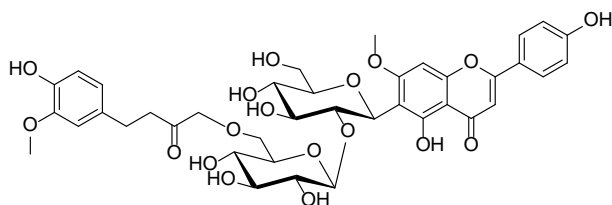
Spinosin



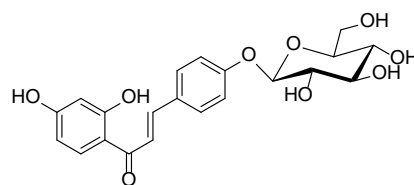
Liquiritin apioside



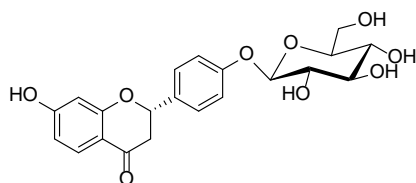
Ferulic acid



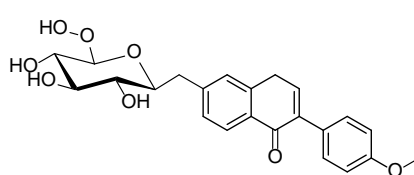
6'''-Ferylloyl spinosin



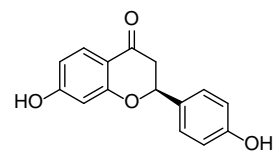
Isoliquiritin



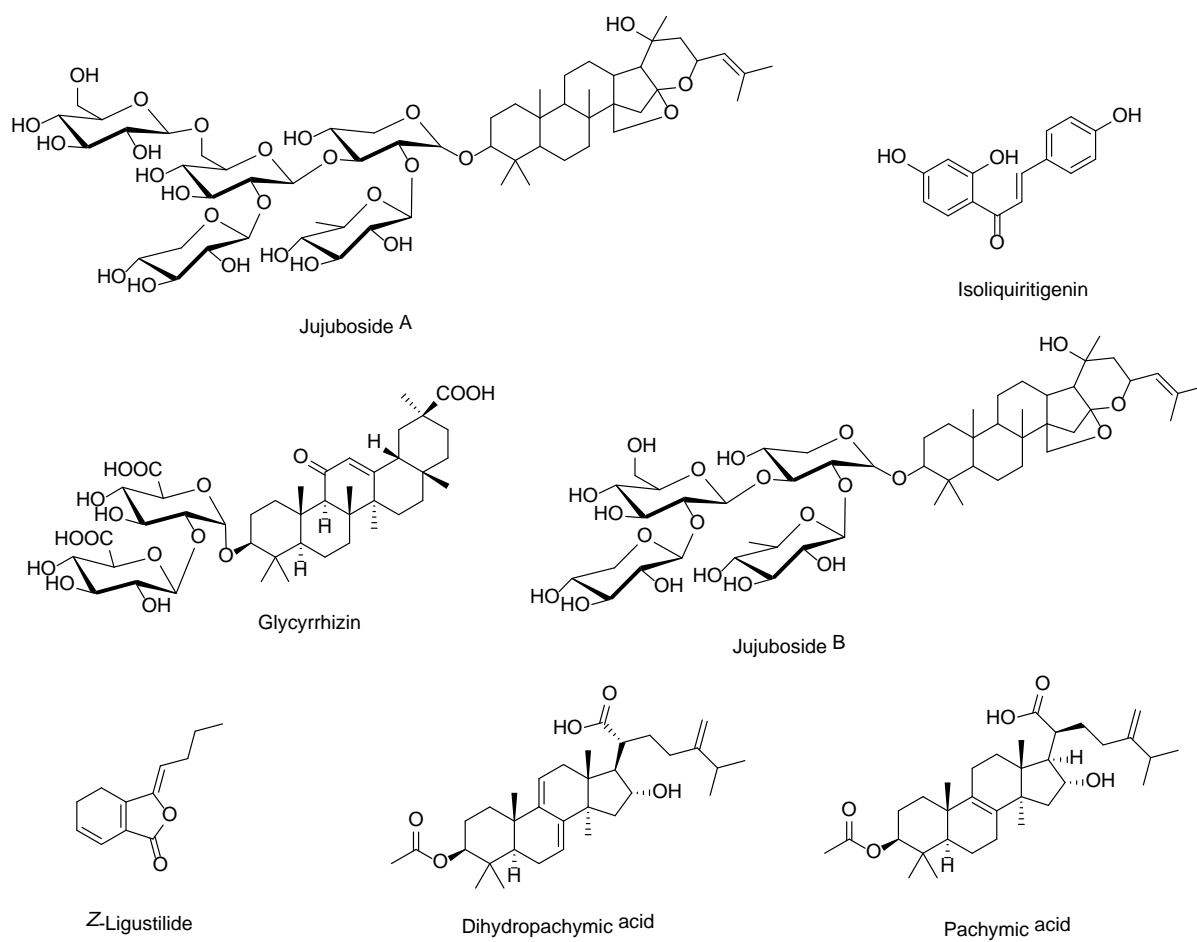
Liquiritin



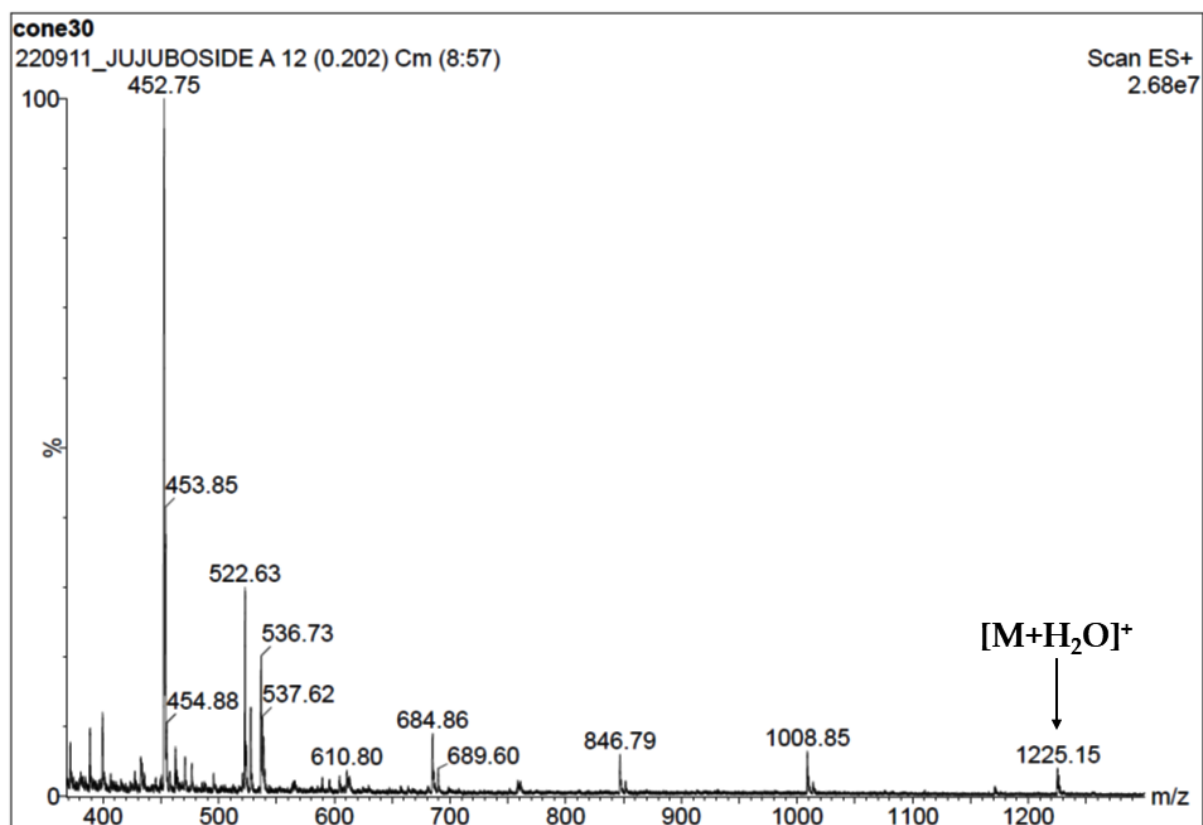
Ononin



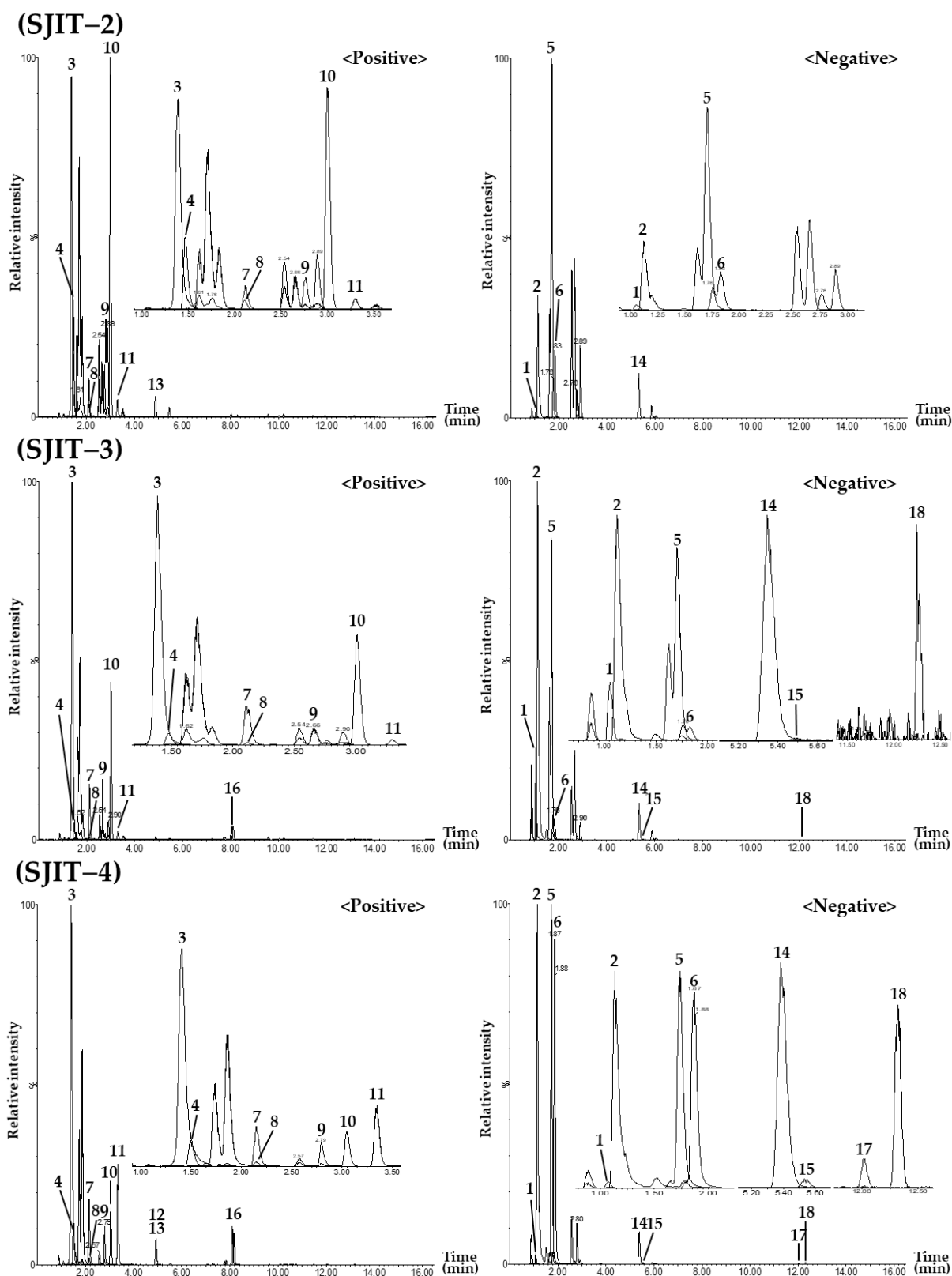
Liquiritigenin



**Figure S1.** Chemical structures of the eighteen target components in SJIT.



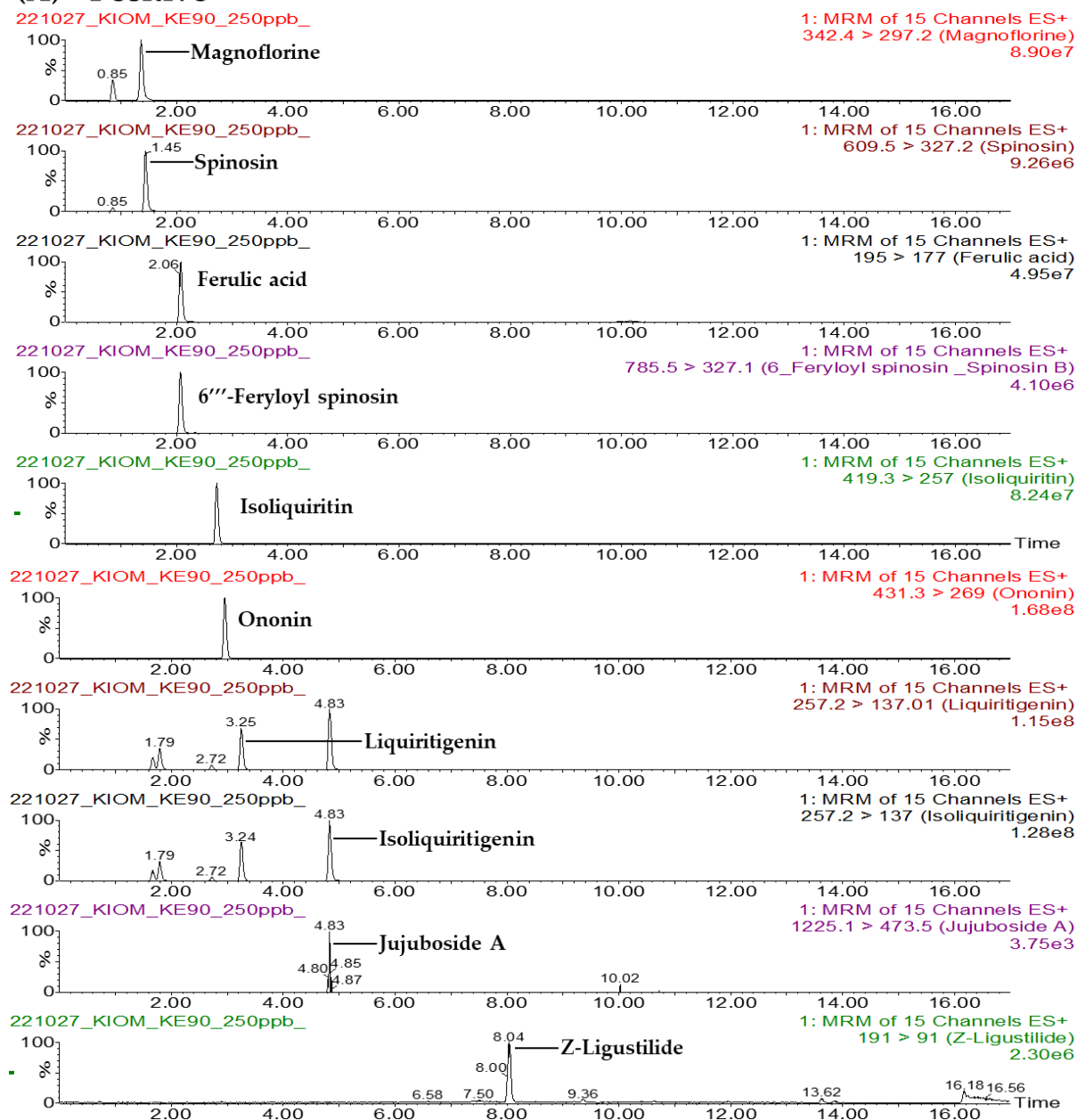
**Figure S2.** Precursor ion spectrum of jujuboside A.



**Figure S3.** Total ion chromatograms of SJIT-2 to SJIT-4 samples by the UPLC-MS/MS MRM method. Neomangiferin (1), mangiferin (2), magnoflorine (3), spinosin (4), liquiritin apioside (5), liquiritin (6), ferulic acid (7), 6'''-feruloyl spinosin (8), isoliquiritin (9), ononin (10), liquiritigenin (11), jujuboside A

(12), isoliquiritigenin (13), glycyrrhizin (14), jujuboside B (15), *Z*-ligustilide (16), dehydropachymic acid (17), and pachymic acid (18).

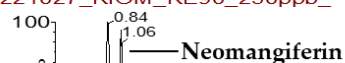
## (A) - Positive





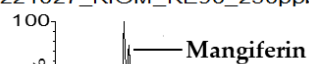
## (A) - Negative

221027\_KIOM\_KE90\_250ppb\_



2: MRM of 13 Channels ES-  
583.3 > 331 (Neomangiferin)  
1.70e6

221027\_KIOM\_KE90\_250ppb\_



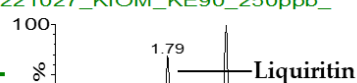
2: MRM of 13 Channels ES-  
421.1 > 301 (Mangiferin)  
8.38e6

221027\_KIOM\_KE90\_250ppb\_



2: MRM of 13 Channels ES-  
549.3 > 255 (Liquiritin apioside)  
8.94e6

221027\_KIOM\_KE90\_250ppb\_



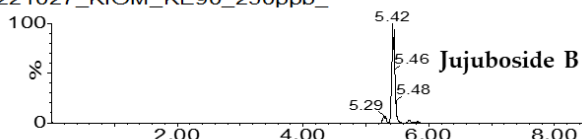
2: MRM of 13 Channels ES-  
417.4 > 255.2 (Liquiritin)  
1.40e7

221027\_KIOM\_KE90\_250ppb\_



2: MRM of 13 Channels ES-  
821.9 > 351.2 (Glycyrrhizin)  
2.64e5

221027\_KIOM\_KE90\_250ppb\_



2: MRM of 13 Channels ES-  
1043.8 > 911.5 (Jujuboside\_B)  
3.84e5

221027\_KIOM\_KE90\_250ppb\_



2: MRM of 13 Channels ES-  
525.7 > 59 (Dehydropachymic acid)  
1.99e5

221027\_KIOM\_KE90\_250ppb\_

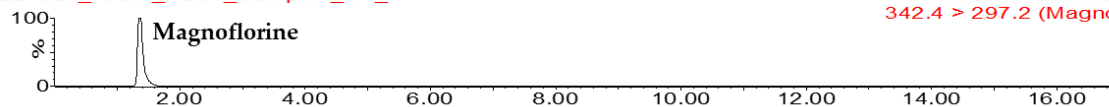


2: MRM of 13 Channels ES-  
527.6 > 465.4 (Pachymic acid)  
4.56e5

## (B) - Positive

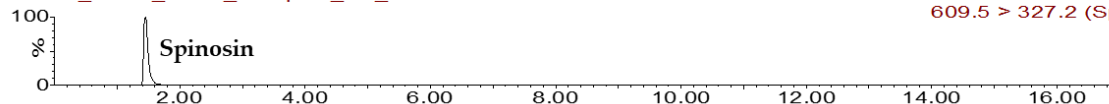
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
342.4 > 297.2 (Magnoflorine)  
1.27e9



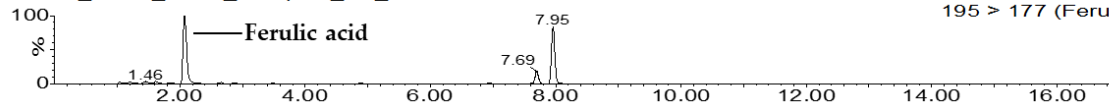
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
609.5 > 327.2 (Spinosin)  
2.89e8



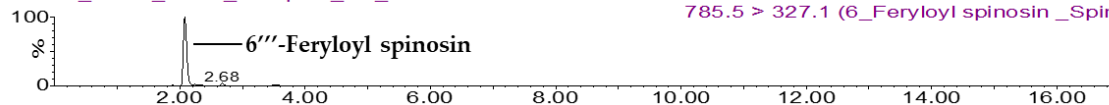
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
195 > 177 (Ferulic acid)  
2.40e8



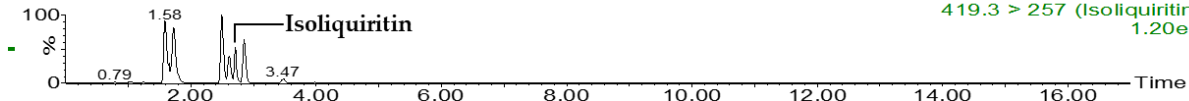
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
785.5 > 327.1 (6-Feryloyl spinosin \_Spinosin B)  
3.56e7



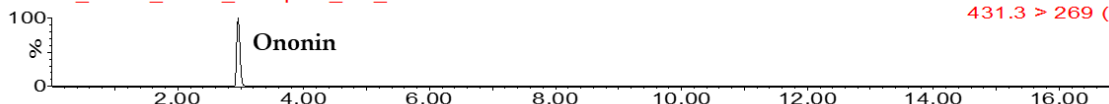
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
419.3 > 257 (Isoliquiritin)  
1.20e8



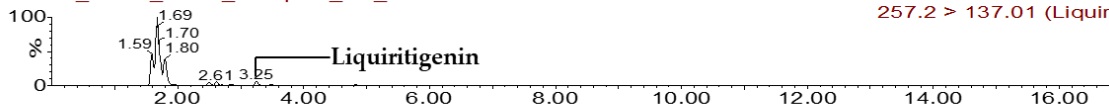
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
431.3 > 269 (Ononin)  
7.72e8



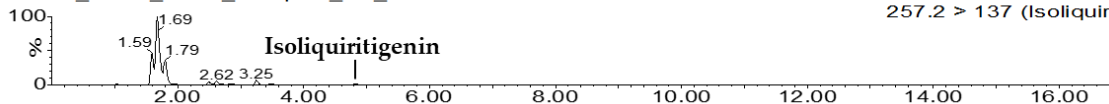
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
257.2 > 137.01 (Liquiritigenin)  
9.77e8



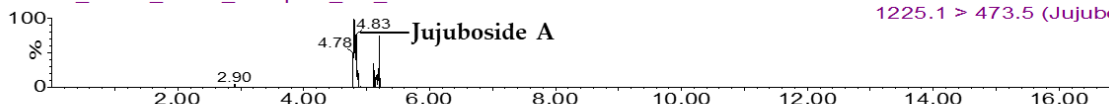
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
257.2 > 137 (Isoliquiritigenin)  
1.01e9



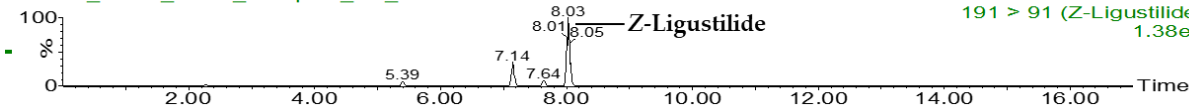
221027\_KIOM\_KE90\_Sample1\_D1\_1

1: MRM of 15 Channels ES+  
1225.1 > 473.5 (Jujuboside A)  
4.54e3



221027\_KIOM\_KE90\_Sample1\_D1\_1

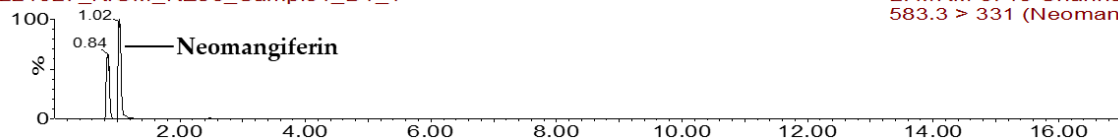
1: MRM of 15 Channels ES+  
191 > 91 (Z-Ligustilide)  
1.38e8



## (B) - Negative

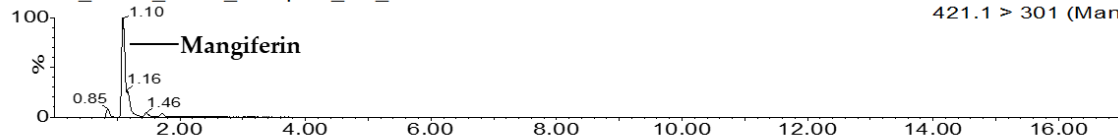
221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
583.3 > 331 (Neomangiferin)  
1.33e7



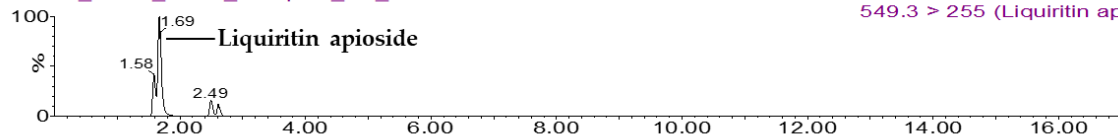
221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
421.1 > 301 (Mangiferin)  
1.74e8



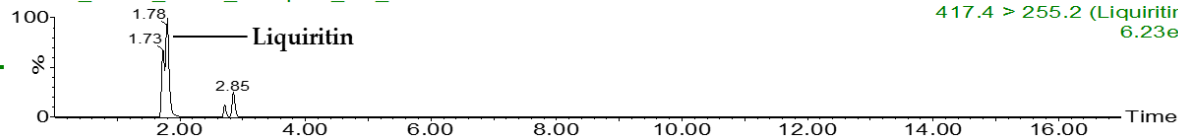
221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
549.3 > 255 (Liquiritin apioside)  
3.14e8



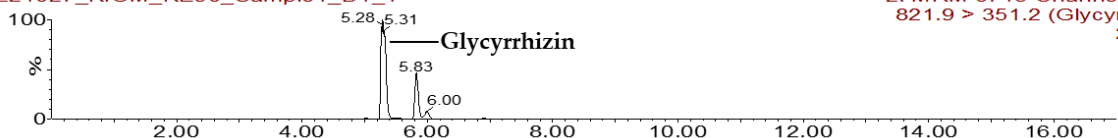
221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
417.4 > 255.2 (Liquiritin)  
6.23e7



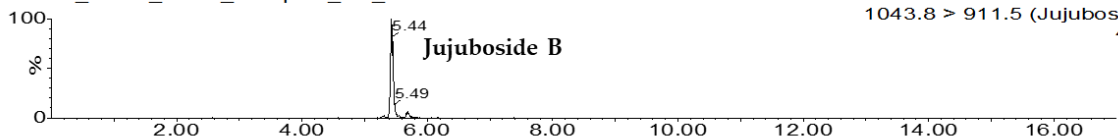
221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
821.9 > 351.2 (Glycyrrhizin)  
2.48e7



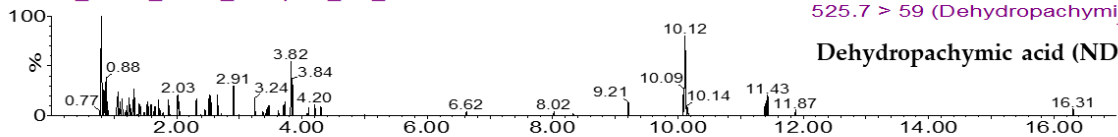
221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
1043.8 > 911.5 (Jujuboside B)  
4.38e5



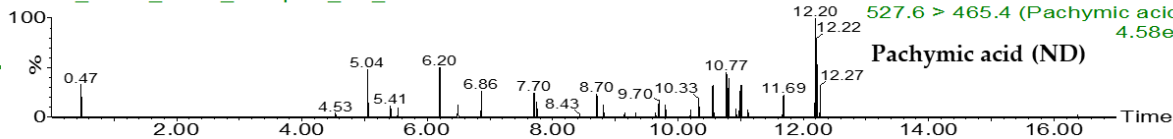
221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
525.7 > 59 (Dehydropachymic acid)  
7.22e3

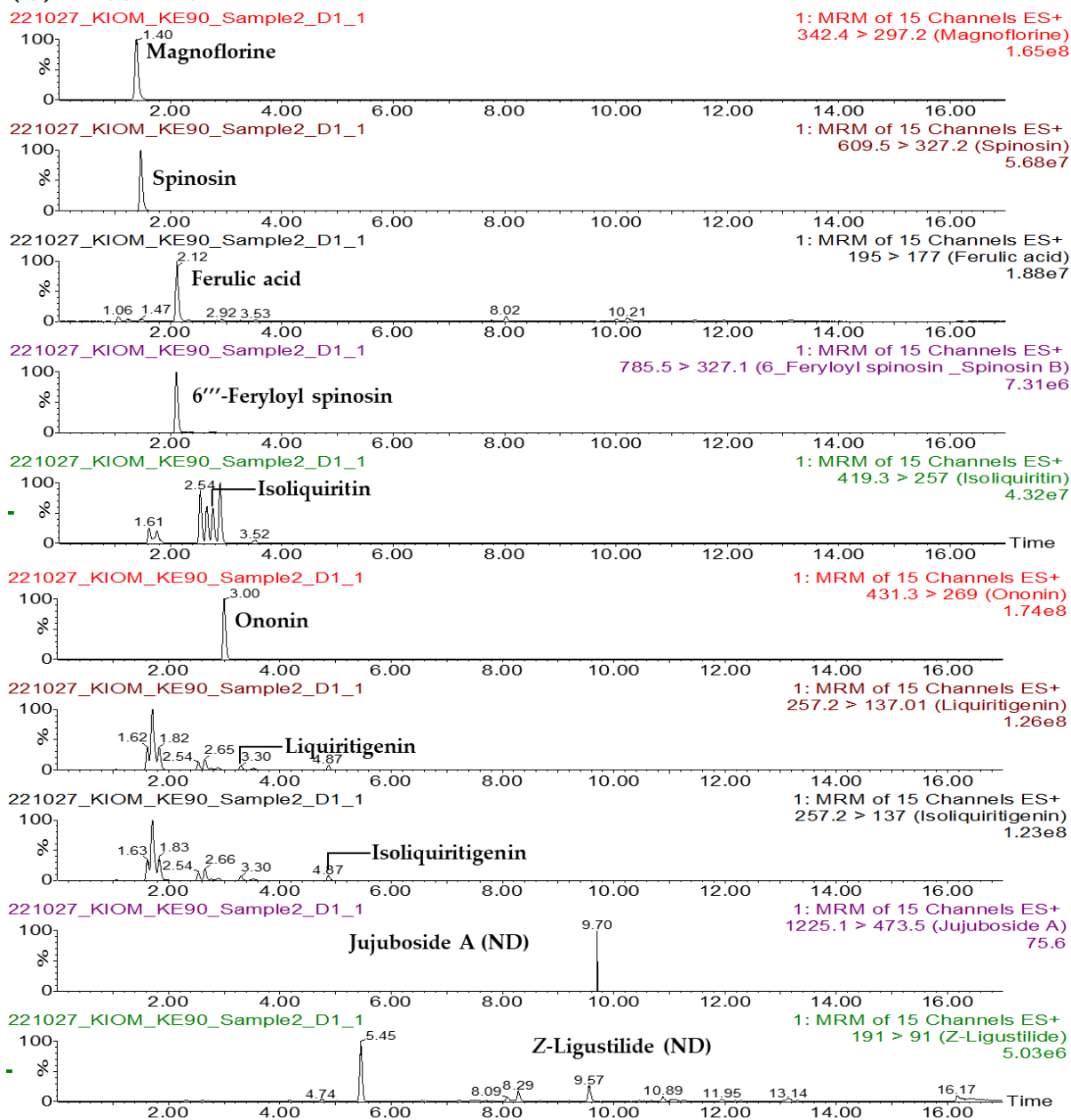


221027\_KIOM\_KE90\_Sample1\_D1\_1

2: MRM of 13 Channels ES-  
527.6 > 465.4 (Pachymic acid)  
4.58e3

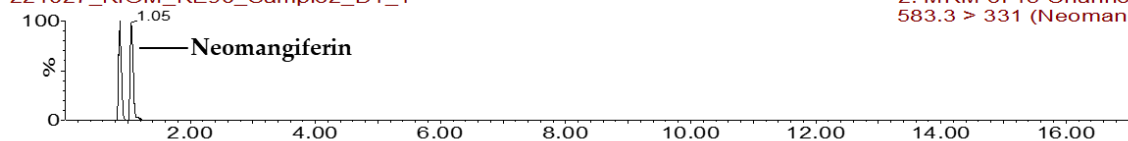


## (C) - Positive



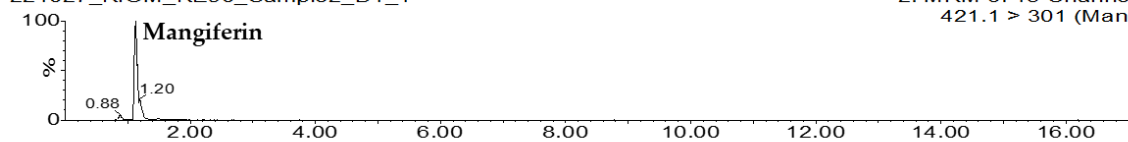
# (C) - Negative

221027\_KIOM\_KE90\_Sample2\_D1\_1



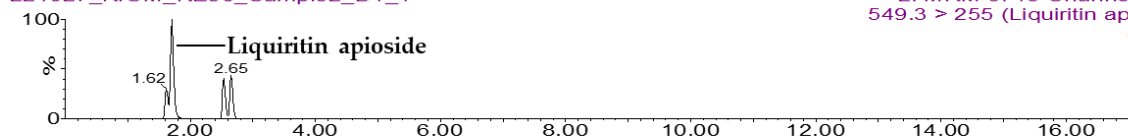
2: MRM of 13 Channels ES-  
583.3 > 331 (Neomangiferin)  
1.20e6

221027\_KIOM\_KE90\_Sample2\_D1\_1



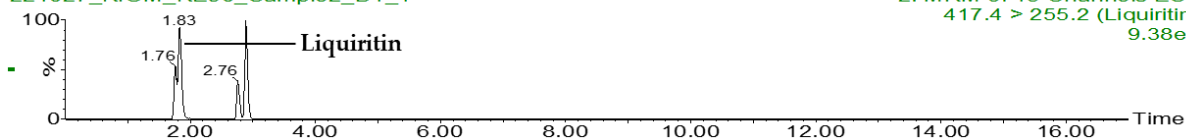
2: MRM of 13 Channels ES-  
421.1 > 301 (Mangiferin)  
1.58e7

221027\_KIOM\_KE90\_Sample2\_D1\_1



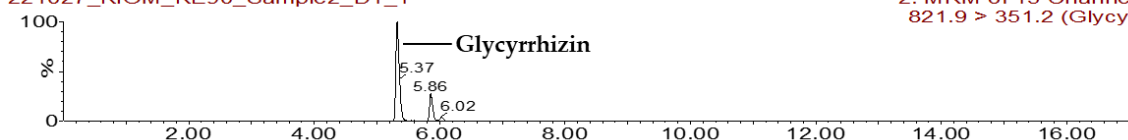
2: MRM of 13 Channels ES-  
549.3 > 255 (Liquiritin apioside)  
4.66e7

221027\_KIOM\_KE90\_Sample2\_D1\_1



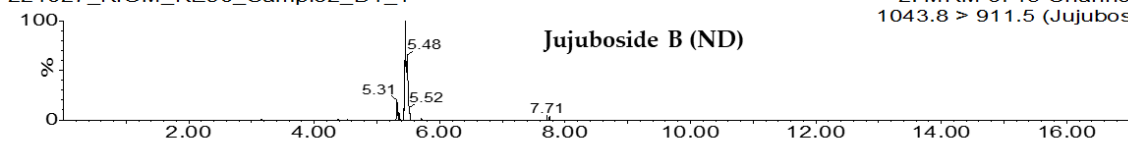
2: MRM of 13 Channels ES-  
417.4 > 255.2 (Liquiritin)  
9.38e6

221027\_KIOM\_KE90\_Sample2\_D1\_1



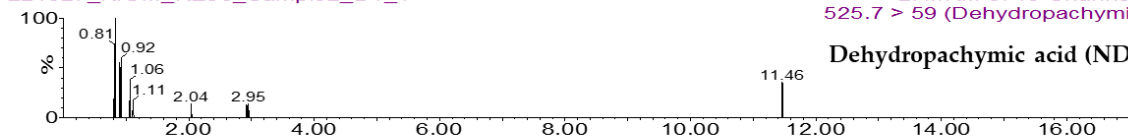
2: MRM of 13 Channels ES-  
821.9 > 351.2 (Glycyrrhizin)  
5.74e6

221027\_KIOM\_KE90\_Sample2\_D1\_1



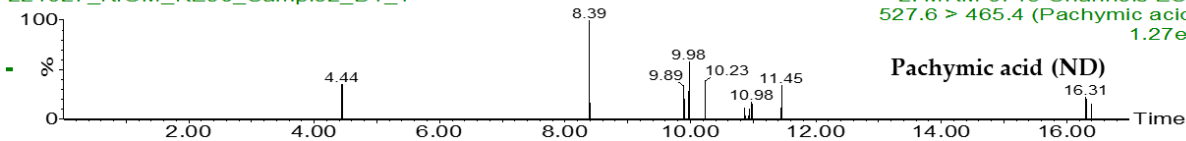
2: MRM of 13 Channels ES-  
1043.8 > 911.5 (Jujuboside\_B)  
2.20e4

221027\_KIOM\_KE90\_Sample2\_D1\_1



2: MRM of 13 Channels ES-  
525.7 > 59 (Dehydropachymic acid)  
1.23e3

221027\_KIOM\_KE90\_Sample2\_D1\_1

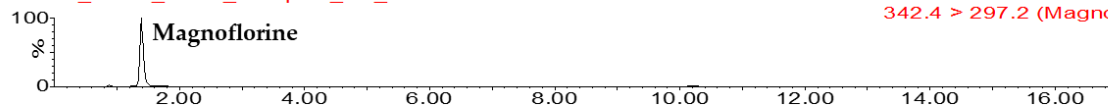


2: MRM of 13 Channels ES-  
527.6 > 465.4 (Pachymic acid)  
1.27e3

## (D) - Positive

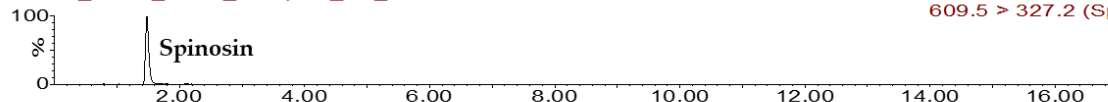
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
342.4 > 297.2 (Magnoflorine)  
2.38e8



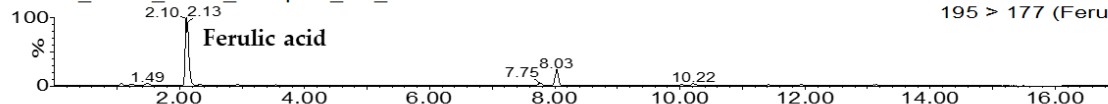
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
609.5 > 327.2 (Spinosin)  
1.13e7



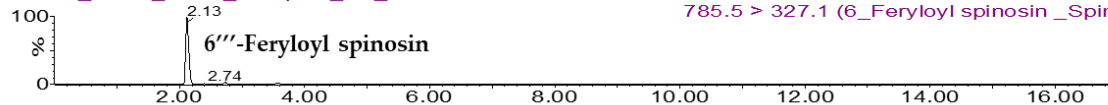
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
195 > 177 (Ferulic acid)  
3.71e7



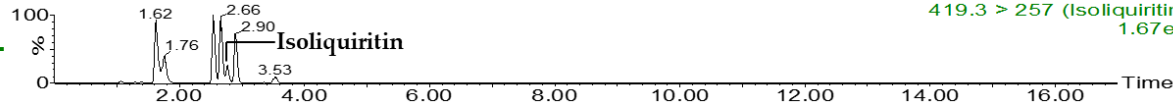
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
785.5 > 327.1 (6-Feryloyl spinosin \_Spinosin B)  
2.31e6



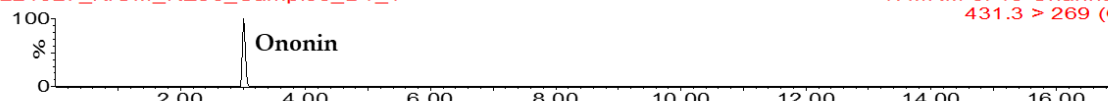
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
419.3 > 257 (Isoliquiritin)  
1.67e7



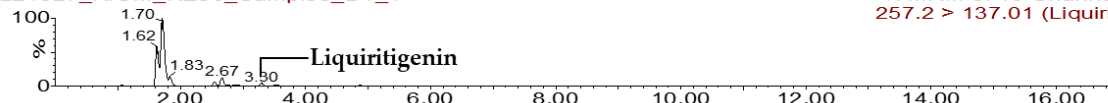
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
431.3 > 269 (Ononin)  
1.05e8



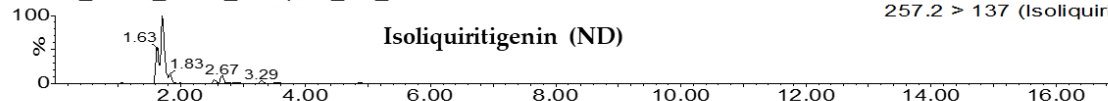
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
257.2 > 137.01 (Liquiritigenin)  
1.18e8



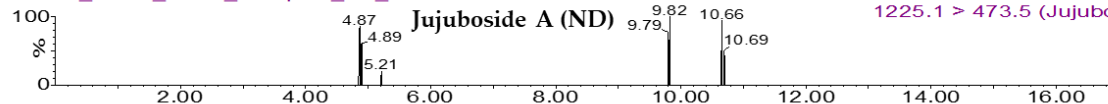
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
257.2 > 137 (Isoliquiritigenin)  
1.22e8



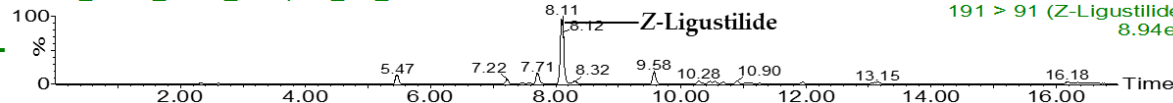
221027\_KIOM\_KE90\_Sample3\_D1\_1

1: MRM of 15 Channels ES+  
1225.1 > 473.5 (Jujuboside A)  
1.24e3



221027\_KIOM\_KE90\_Sample3\_D1\_1

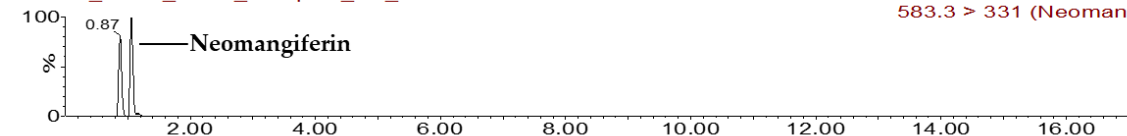
1: MRM of 15 Channels ES+  
191 > 91 (Z-Ligustilide)  
8.94e6



## (D) - Negative

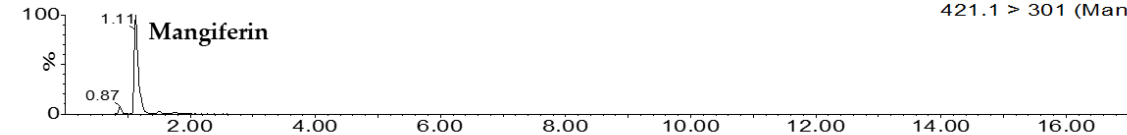
221027\_KIOM\_KE90\_Sample3\_D1\_1

2: MRM of 13 Channels ES-  
583.3 > 331 (Neomangiferin)  
1.39e7



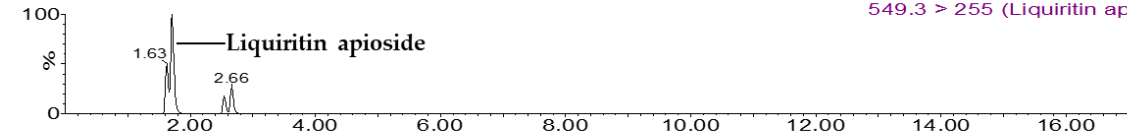
221027\_KIOM\_KE90\_Sample3\_D1\_1

2: MRM of 13 Channels ES-  
421.1 > 301 (Mangiferin)  
5.40e7



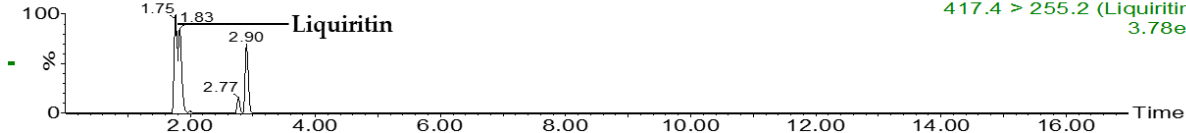
221027\_KIOM\_KE90\_Sample3\_D1\_1

2: MRM of 13 Channels ES-  
549.3 > 255 (Liquiritin apioside)  
4.55e7



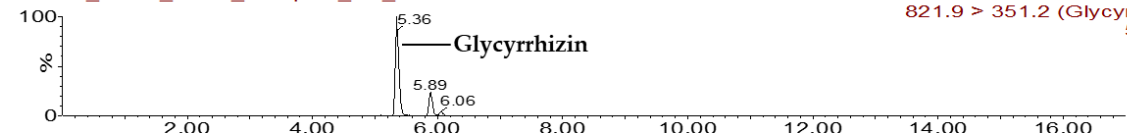
221027\_KIOM\_KE90\_Sample3\_D1\_1

2: MRM of 13 Channels ES-  
417.4 > 255.2 (Liquiritin)  
3.78e6



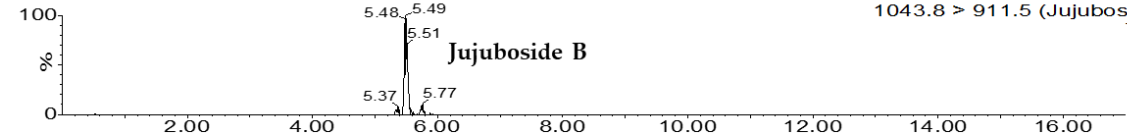
221027\_KIOM\_KE90\_Sample3\_D1\_1

2: MRM of 13 Channels ES-  
821.9 > 351.2 (Glycyrrhizin)  
5.57e6



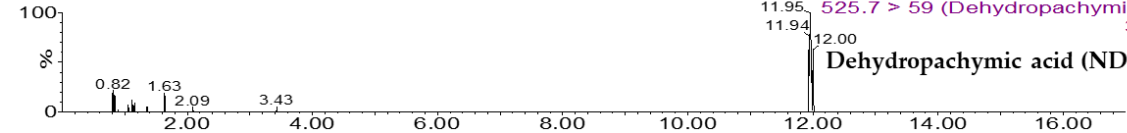
221027\_KIOM\_KE90\_Sample3\_D1\_1

2: MRM of 13 Channels ES-  
1043.8 > 911.5 (Jujuboside B)  
7.20e4



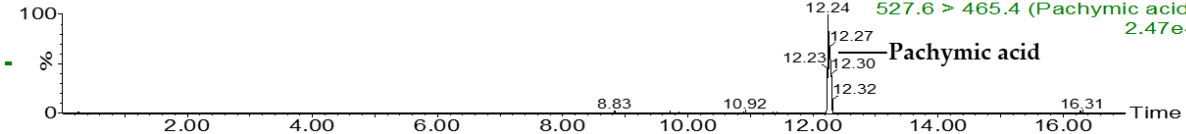
221027\_KIOM\_KE90\_Sample3\_D1\_1

2: MRM of 13 Channels ES-  
525.7 > 59 (Dehydropachymic acid)  
3.49e3



221027\_KIOM\_KE90\_Sample3\_D1\_1

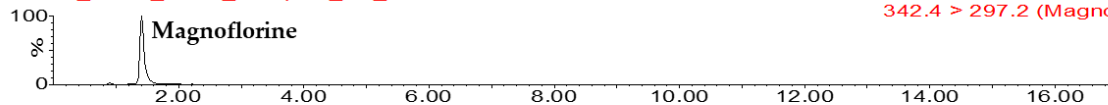
2: MRM of 13 Channels ES-  
527.6 > 465.4 (Pachymic acid)  
2.47e4



## (E) - Positive

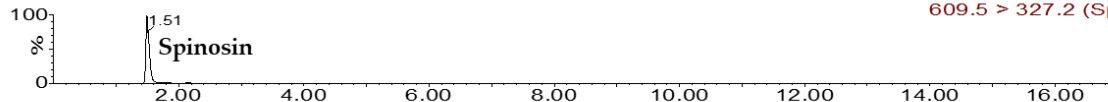
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
342.4 > 297.2 (Magnoflorine)  
1.11e9



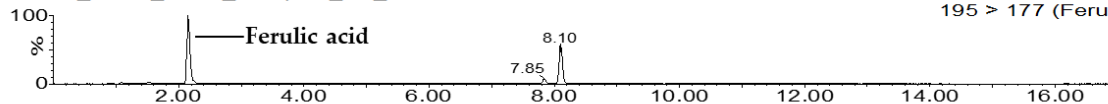
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
609.5 > 327.2 (Spinosin)  
1.33e8



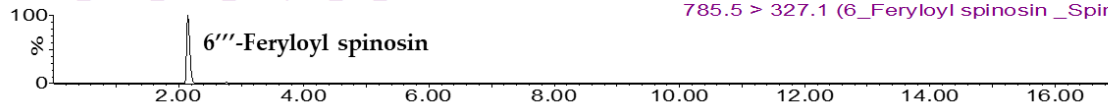
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
195 > 177 (Ferulic acid)  
2.02e8



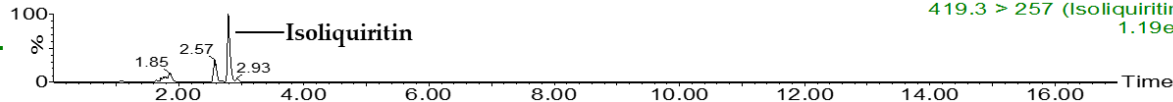
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
785.5 > 327.1 (6''-Feryloyl spinosin \_Spinosin B)  
2.22e7



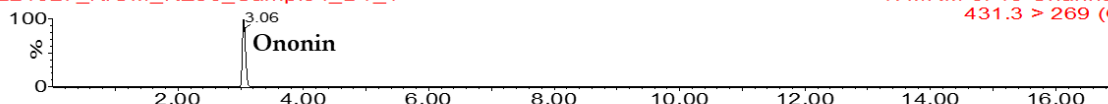
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
419.3 > 257 (Isoliquiritin)  
1.19e8



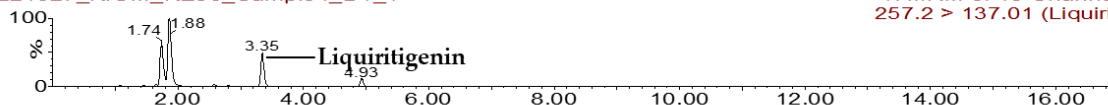
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
431.3 > 269 (Ononin)  
1.76e8



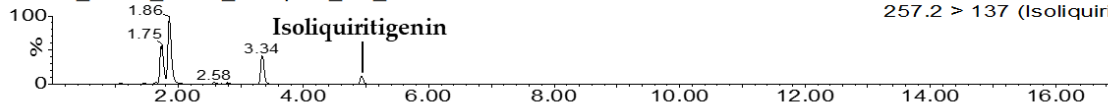
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
257.2 > 137.01 (Liquiritigenin)  
6.24e8



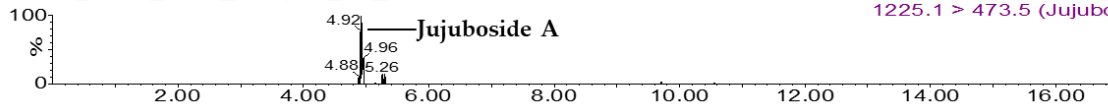
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
257.2 > 137 (Isoliquiritigenin)  
6.65e8



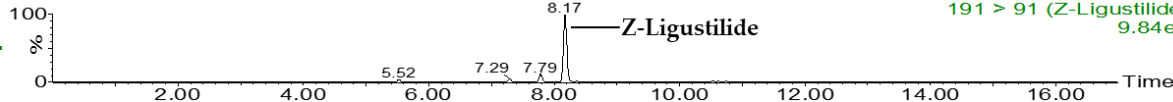
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
1225.1 > 473.5 (Jujuboside A)  
7.20e3



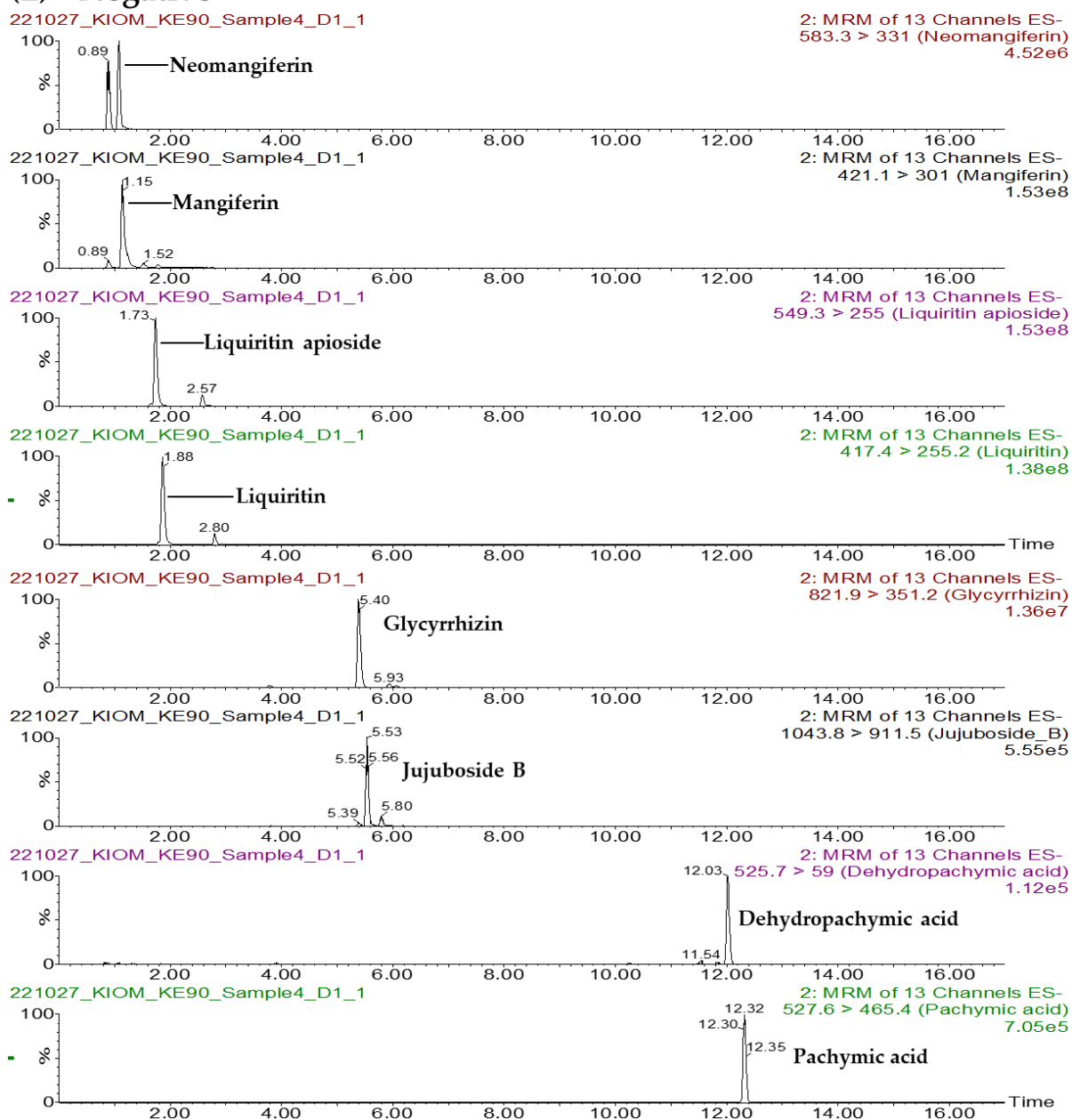
221027\_KIOM\_KE90\_Sample4\_D1\_1

1: MRM of 15 Channels ES+  
191 > 91 (Z-Ligustilide)  
9.84e7





## (E) - Negative



**Figure S4.** Extracted ion chromatograms of standard compounds (A) and SJIT-1 to SJIT-4 samples (B-E) by UPLC-MS/MS method. Compounds 1-18 as in Figure S2.