

# Supplementary Materials: *Marrubium vulgare* L. Leave Extract: Phytochemical Composition, Antioxidant and Wound Healing Properties

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## Table of Contents

1. NMR analysis.....	S2
2. MS experiments.....	S4

# 1. NMR analysis

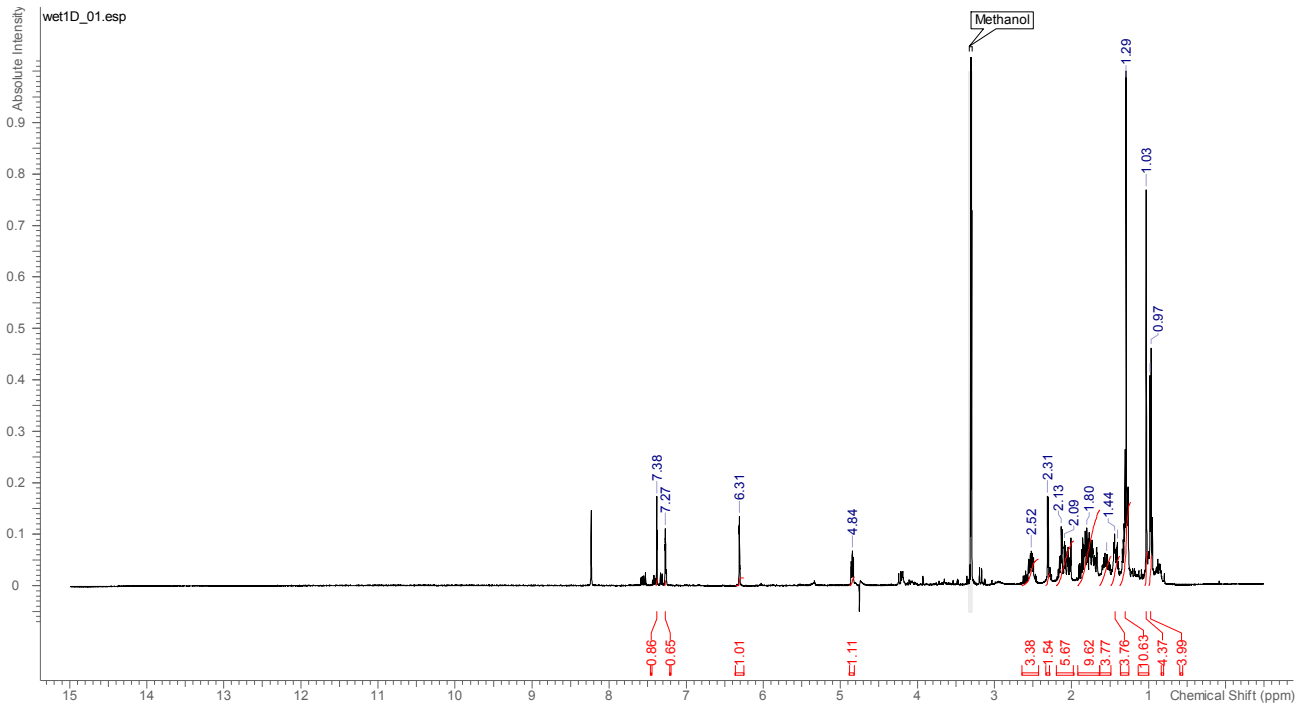


Figure S1.  $^1\text{H}$  spectrum of marrubiin.

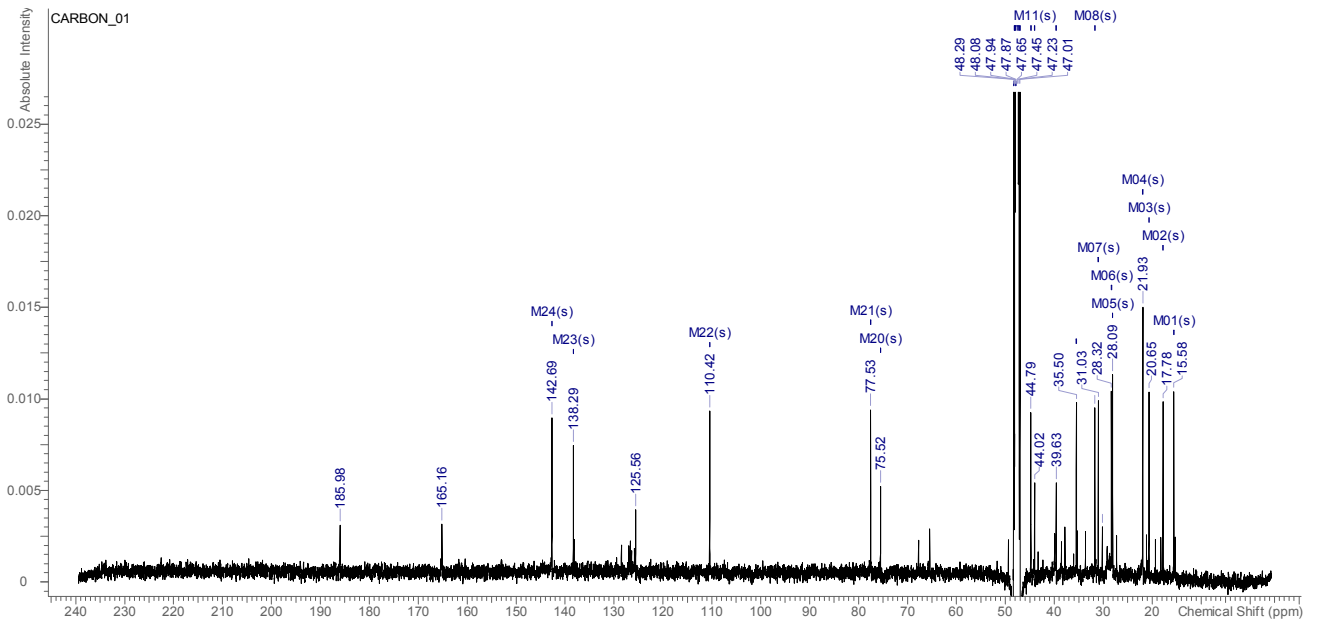
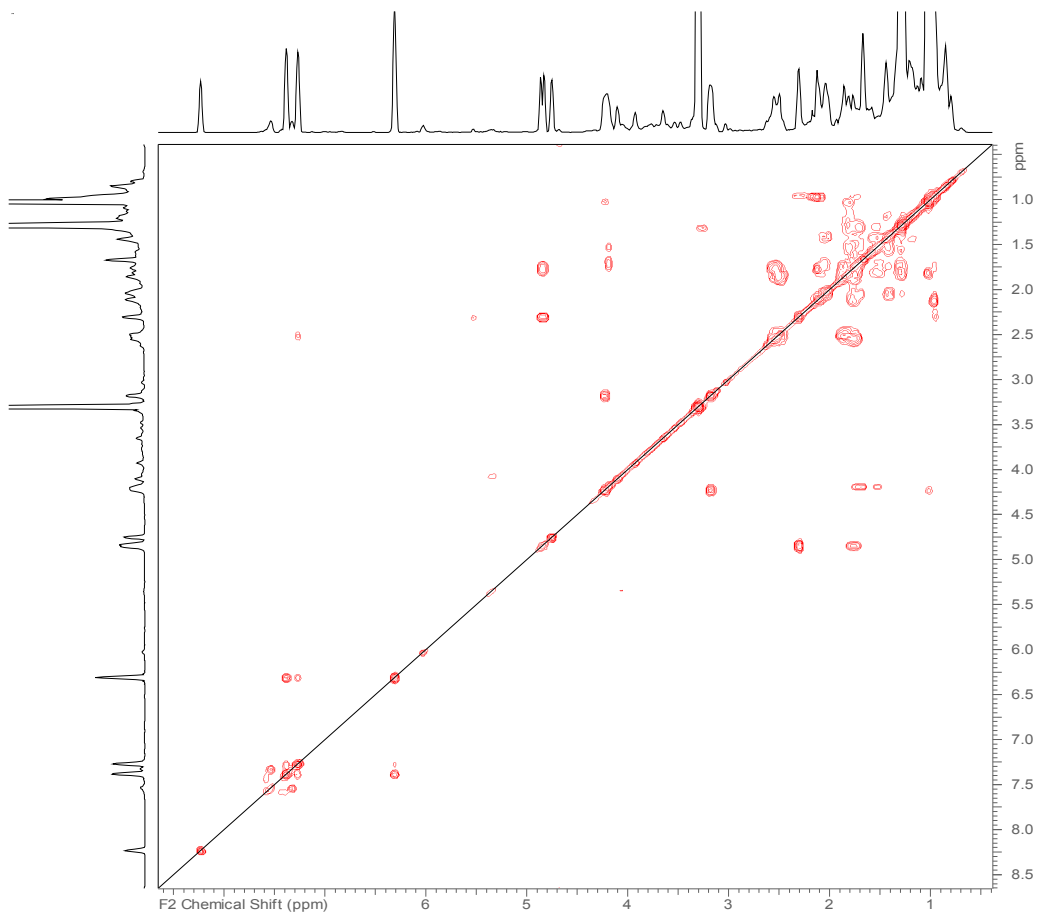
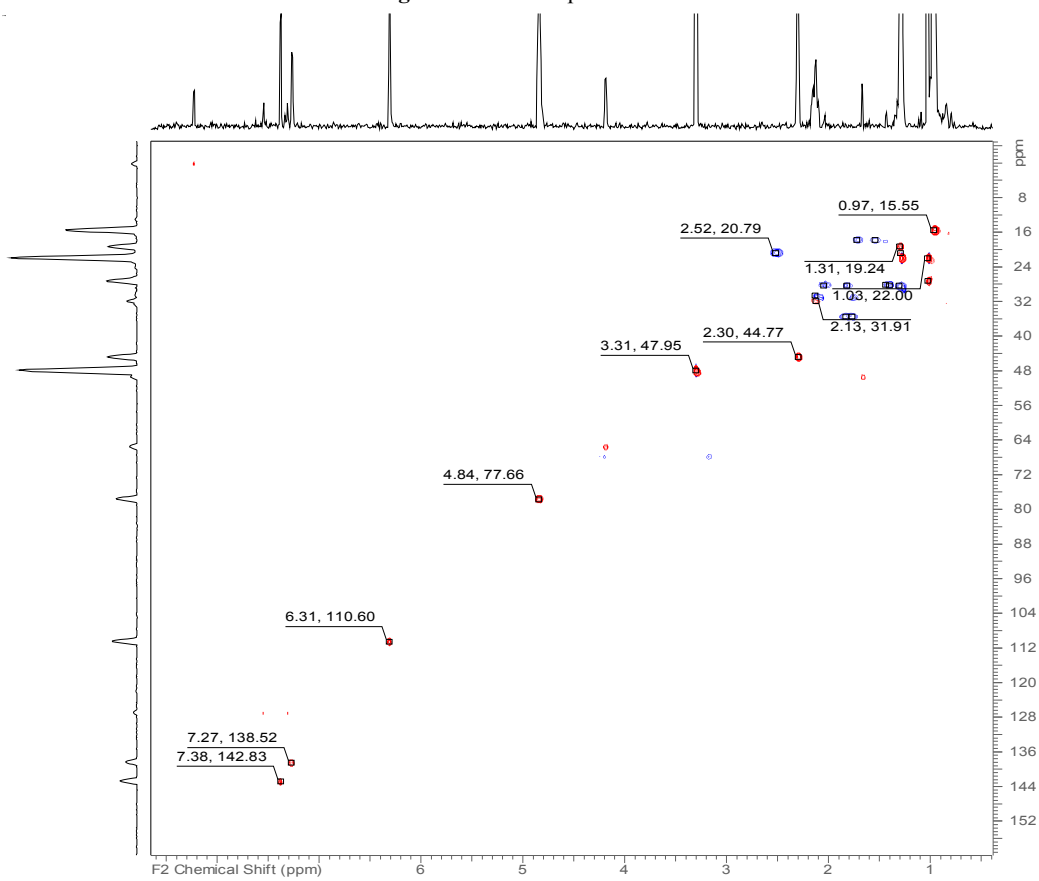


Figure S2.  $^{13}\text{C}$  spectrum of Marrubiin.



**Figure S3.** COSY spectrum of marrubiin.



**Figure S4.** HSQC spectrum of marrubiin.

## 2. MS experiments

F: ITMS - c ESI Full ms2 887.17@cid35.00 [240.00-900.00]

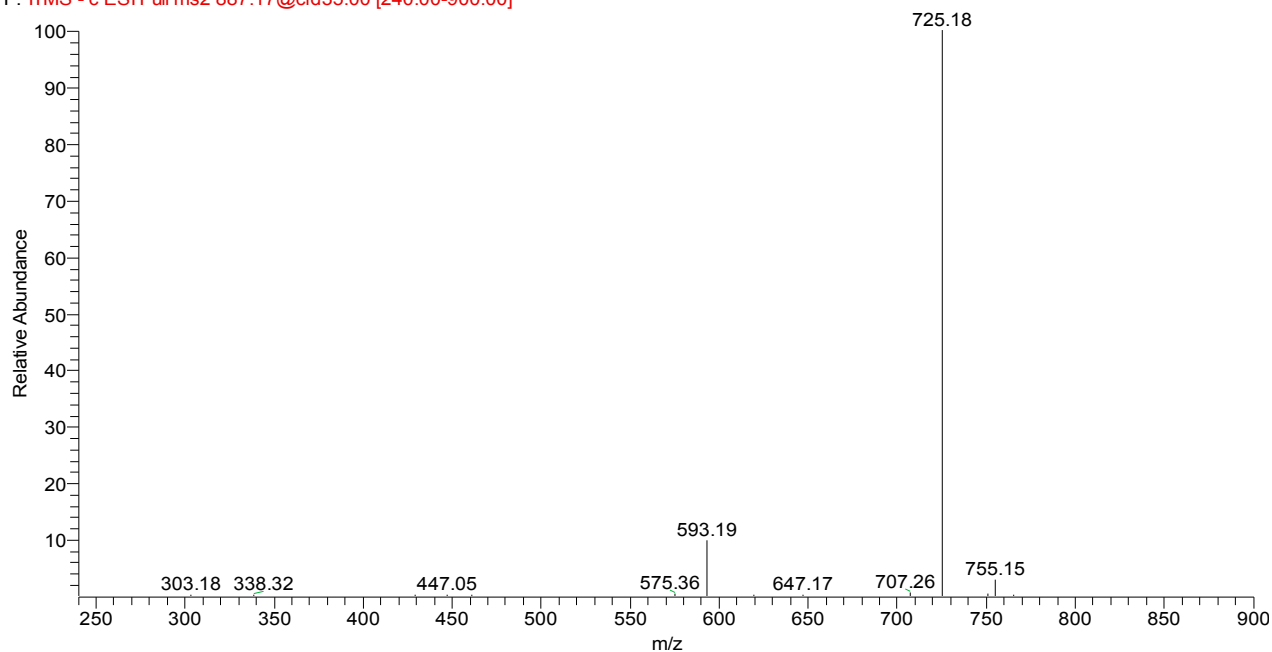


Figure S5. MS/MS spectrum negative ions of compound with retention time ( $t_R$ ) of 5.58 min, parent ion m/z 887.17.

F: ITMS + c ESI d Full ms2 906.00@cid35.00 [235.00-920.00]

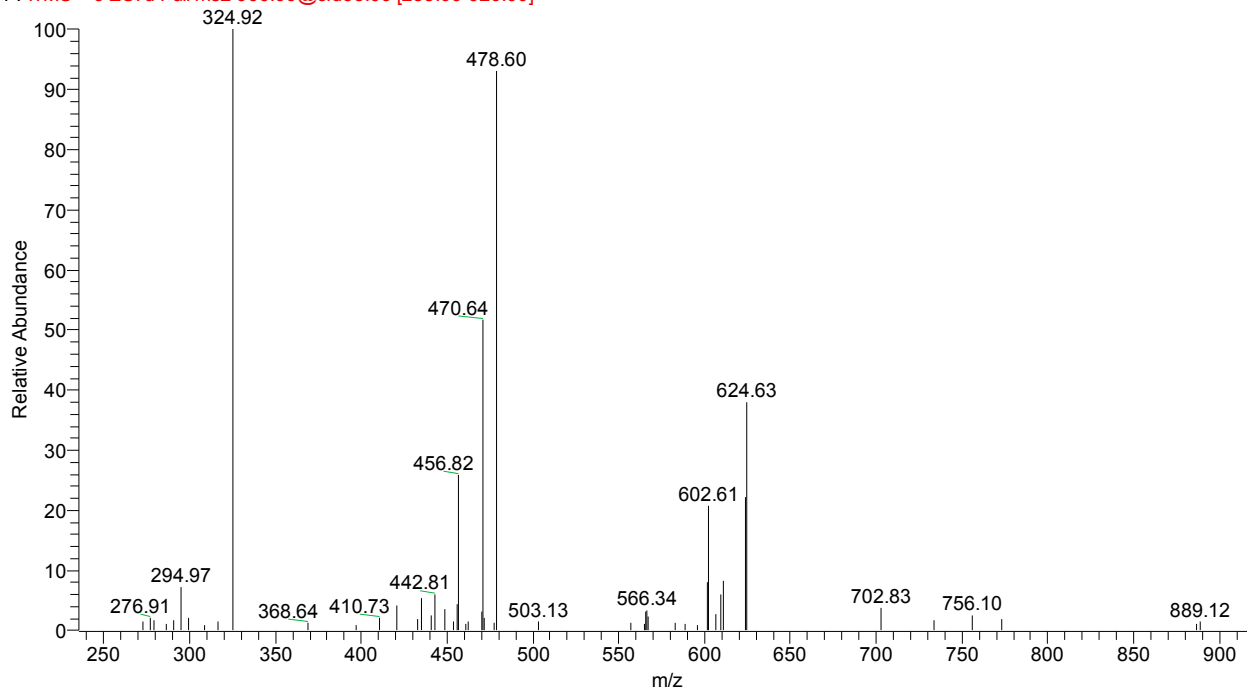


Figure S6. MS/MS spectrum positive ions of compound with retention time ( $t_R$ ) of 5.58, parent ion m/z 906.00.

F: ITMS - c ESI Full ms2 755.22@cid35.00 [205.00-900.00]

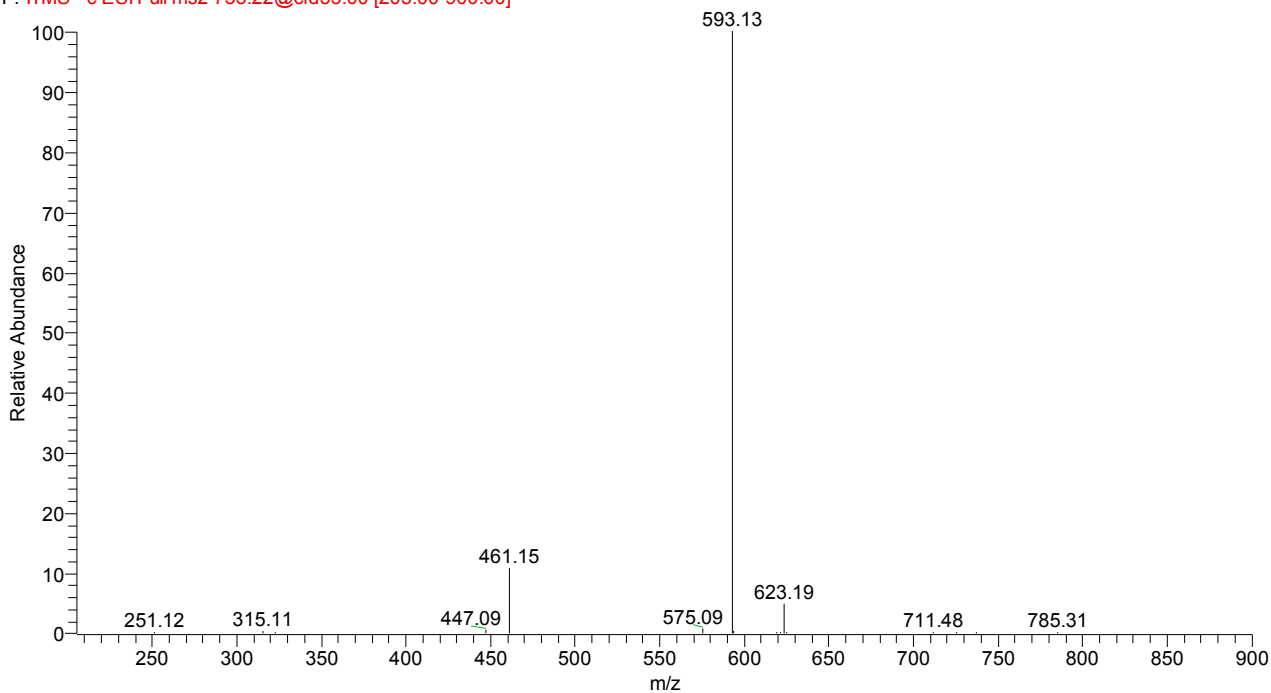


Figure S7. MS/MS spectrum negative ions of compound with retention time ( $t_R$ ) of 5.79, parent ion m/z 755.22.

F: ITMS + c ESI d Full ms2 773.92@cid35.00 [200.00-785.00]

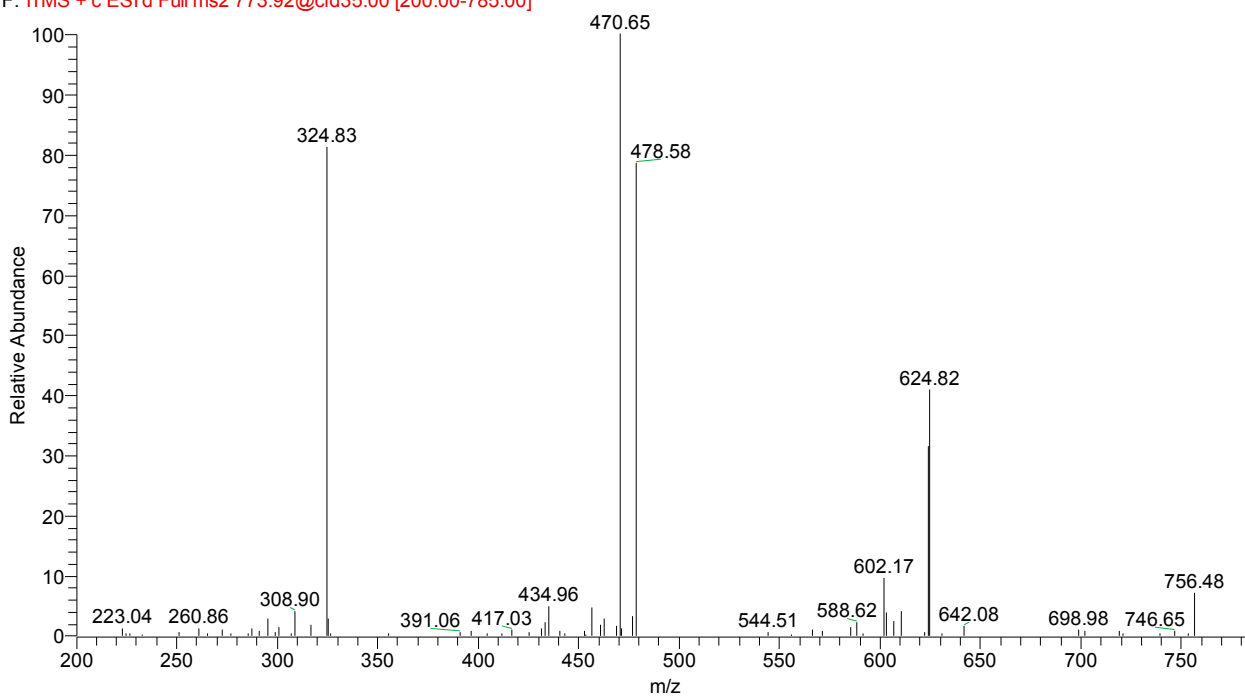


Figure S8. MS/MS spectrum positive ions of compound with retention time ( $t_R$ ) of 5.79, parent ion m/z 773.92.

Marrubium\_1613\_170928165552 #150-155 RT: 5.68-5.78 AV: 2 NL: 2.95E3  
F: ITMS - c ESI Full ms2 755.22@cid35.00 [205.00-900.00]

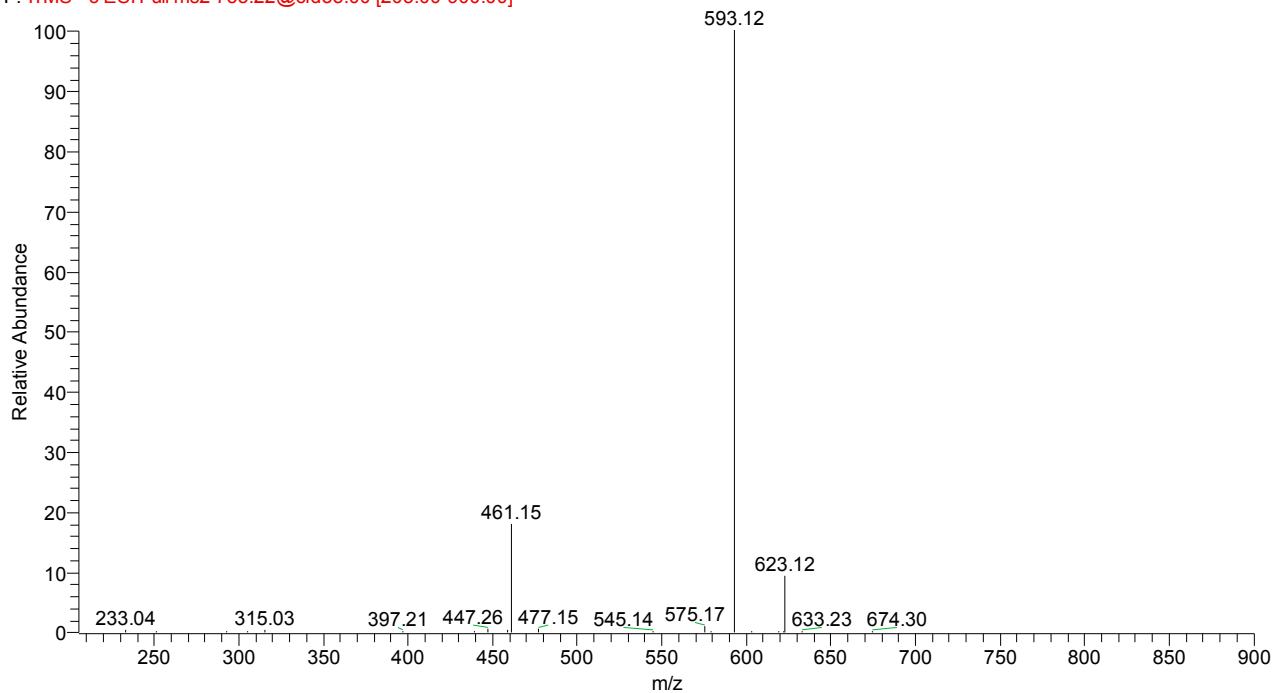


Figure S9. MS/MS spectrum negative ions of compound with retention time ( $t_R$ ) of 6.16 parent ion m/z 755.22.

F: ITMS + c ESI d Full ms2 773.92@cid35.00 [200.00-785.00]

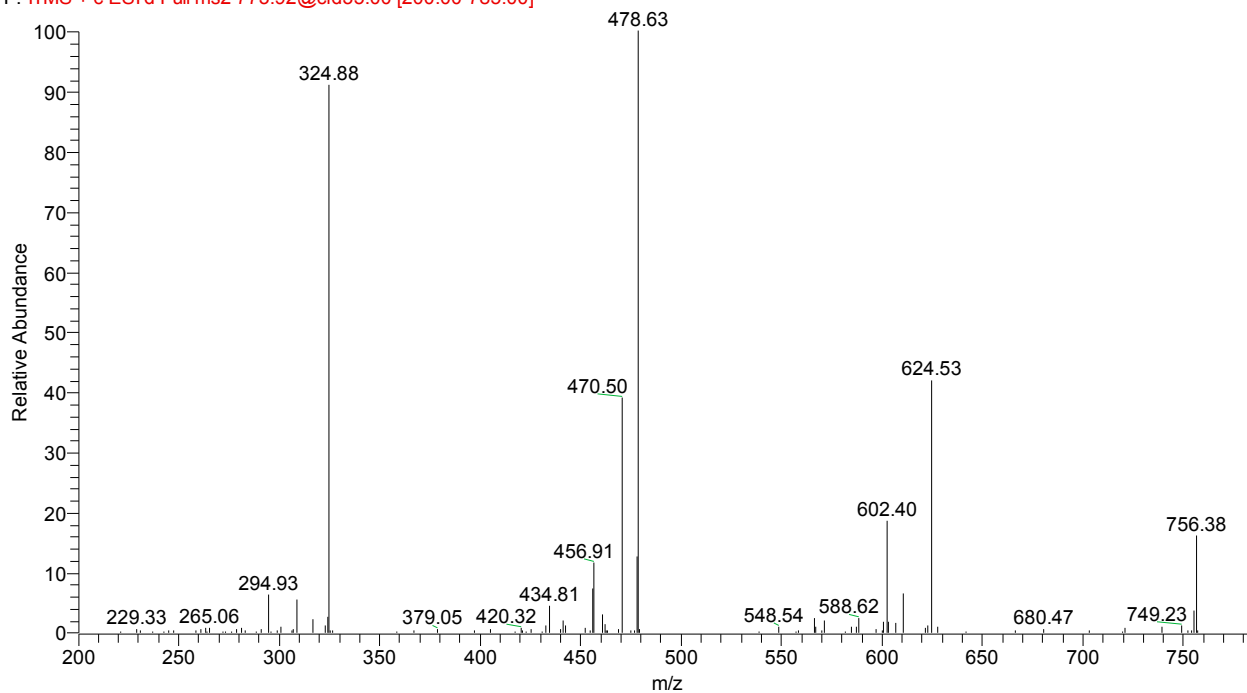


Figure 10. MS/MS spectrum positive ions of compound with retention time ( $t_R$ ) of 6.16 parent ion m/z 773.92.

F: ITMS - c ESI d Full ms2 623.16@cid35.00 [160.00-1260.00]

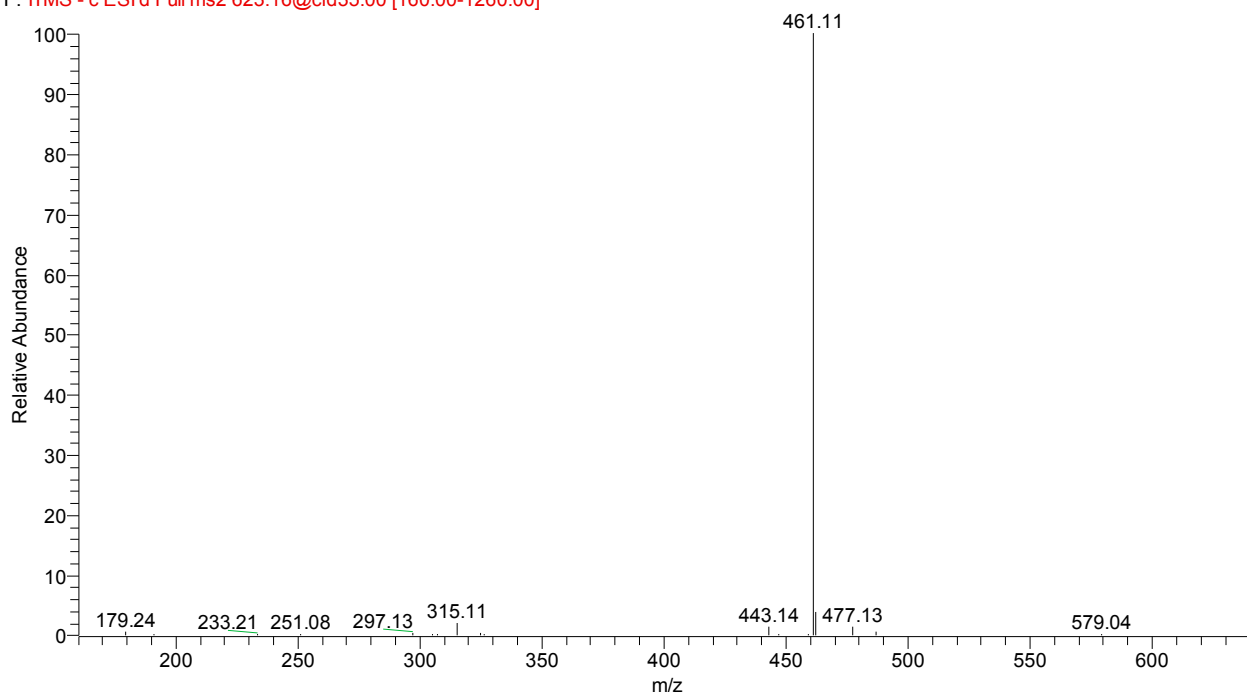


Figure S11. MS/MS spectrum negative ions of compound with retention time ( $t_R$ ) of 6.36, parent ion m/z 623.16.

F: ITMS + c ESI d Full ms2 641.89@cid35.00 [165.00-655.00]

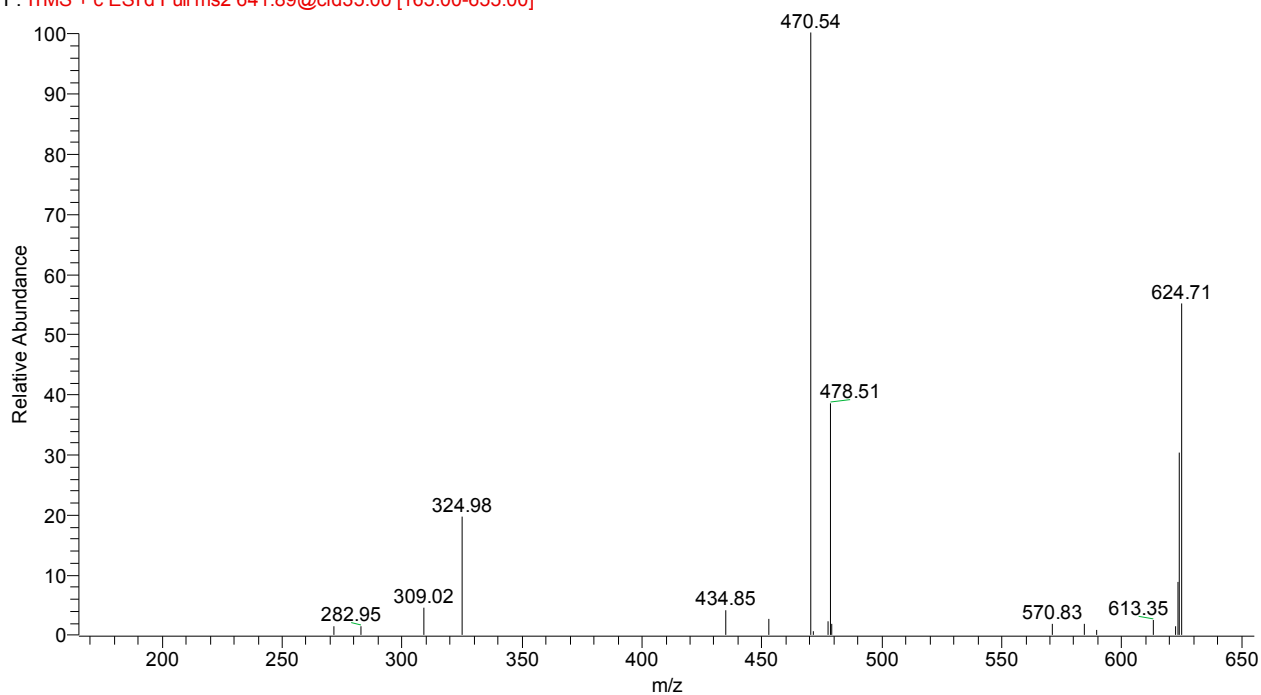


Figure S12. MS/MS spectrum positive ions of compound with retention time ( $t_R$ ) of 6.36, parent ion m/z 641.89.