
**LC-MS/MS BASED DEREPLICATION OF ISOQUINOLINE-DERIVED
ALKALOIDS FROM THE TRUNK BARK OF *Unonopsis rufescens* (Baill.) R.E.Fr.
(Annonaceae)**

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Received: 02/02/2025; accepted: 05/15/2025; published online: 06/17/2025

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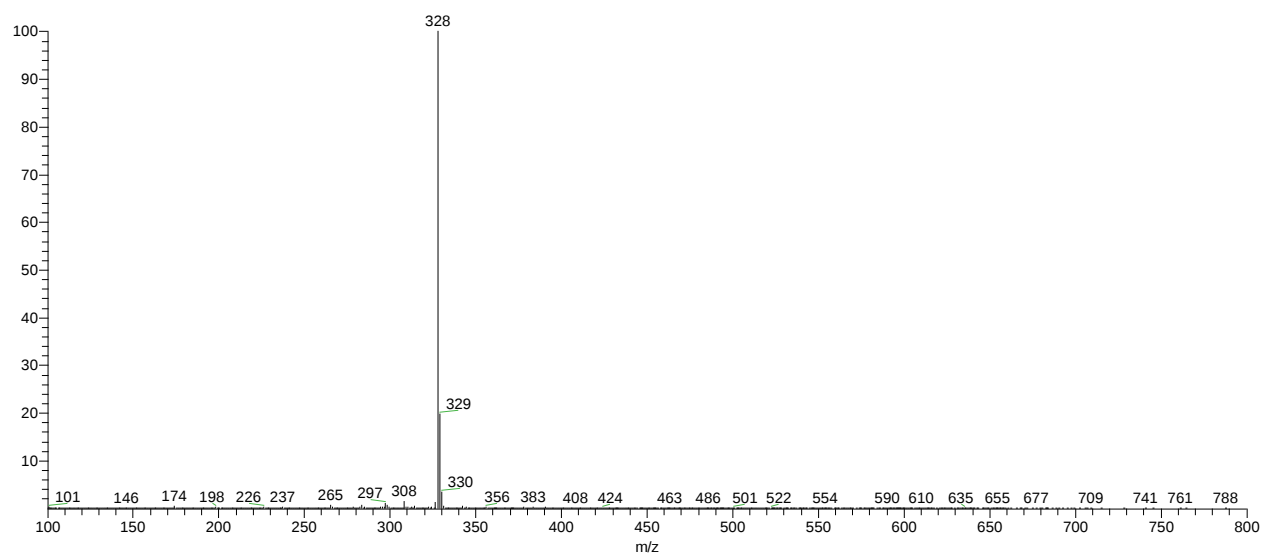


Figure 1S. Mass spectrum of the compound **1** ($t_R = 4.23$ min)

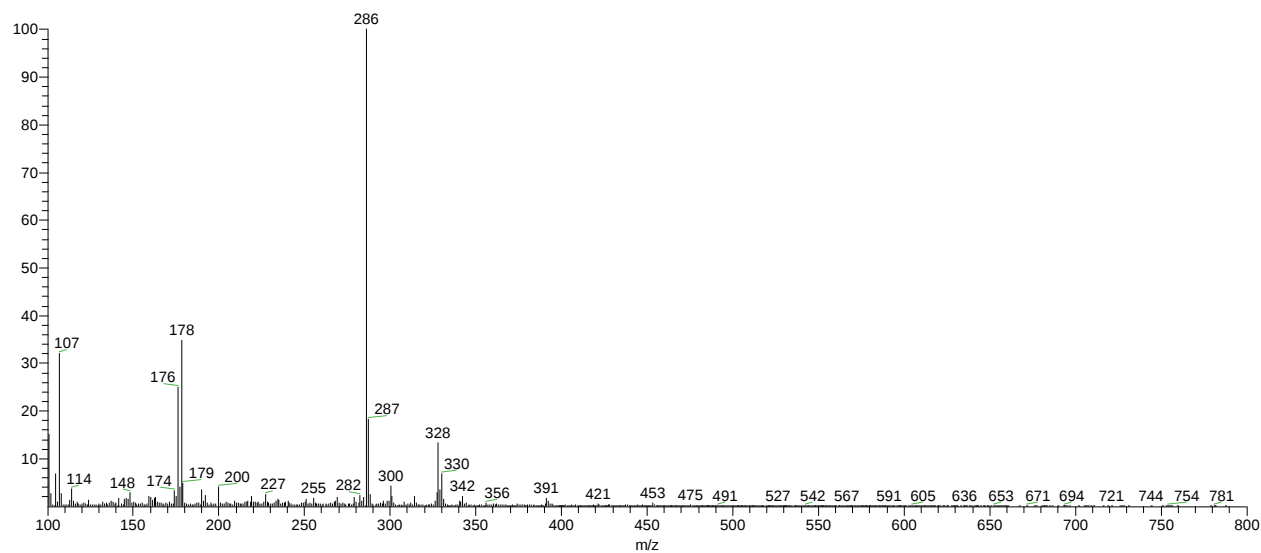


Figure 2S. Mass spectrum of the compound **2** ($t_R = 5.49$ min)

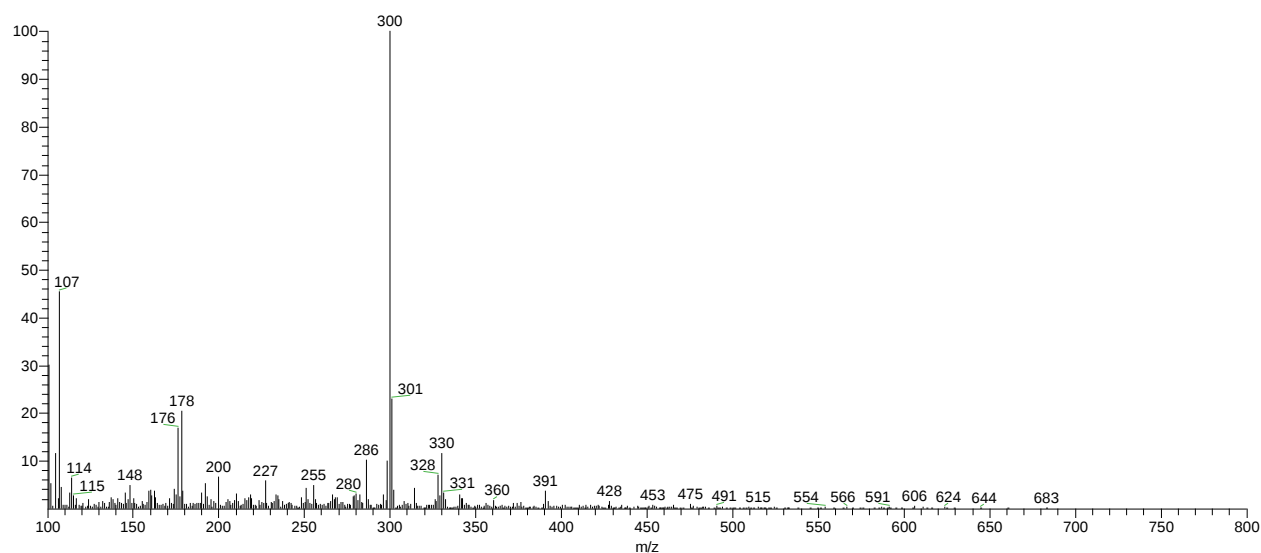


Figure 3S. Mass spectrum of the compound **3** ($t_R = 5.68$ min)

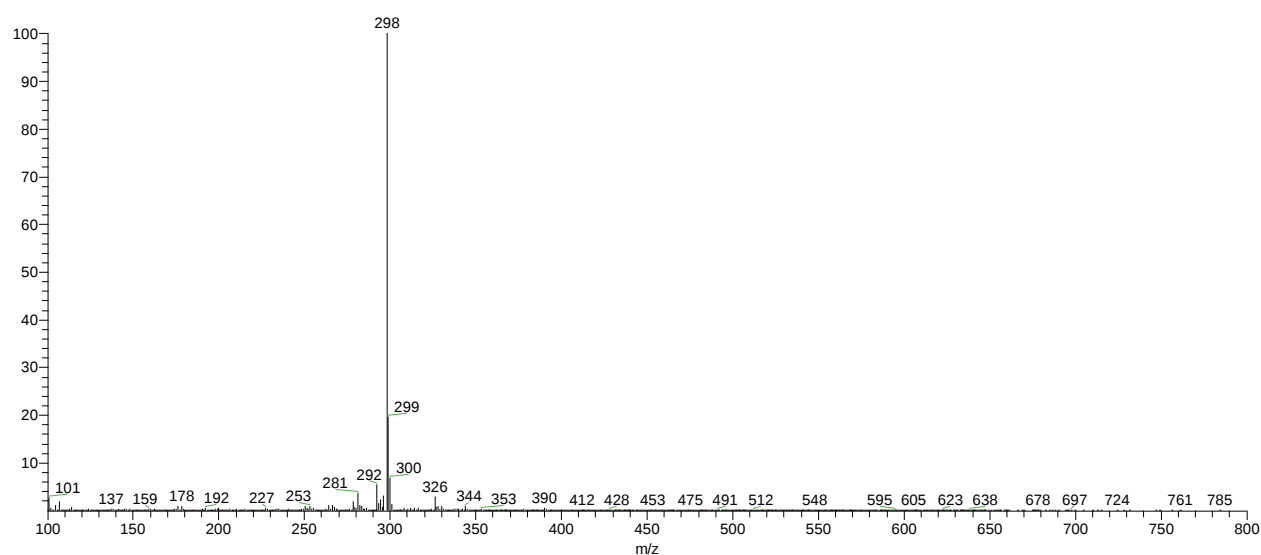


Figure 4S. Mass spectrum of the compound **4** ($t_R = 5.78$ min)

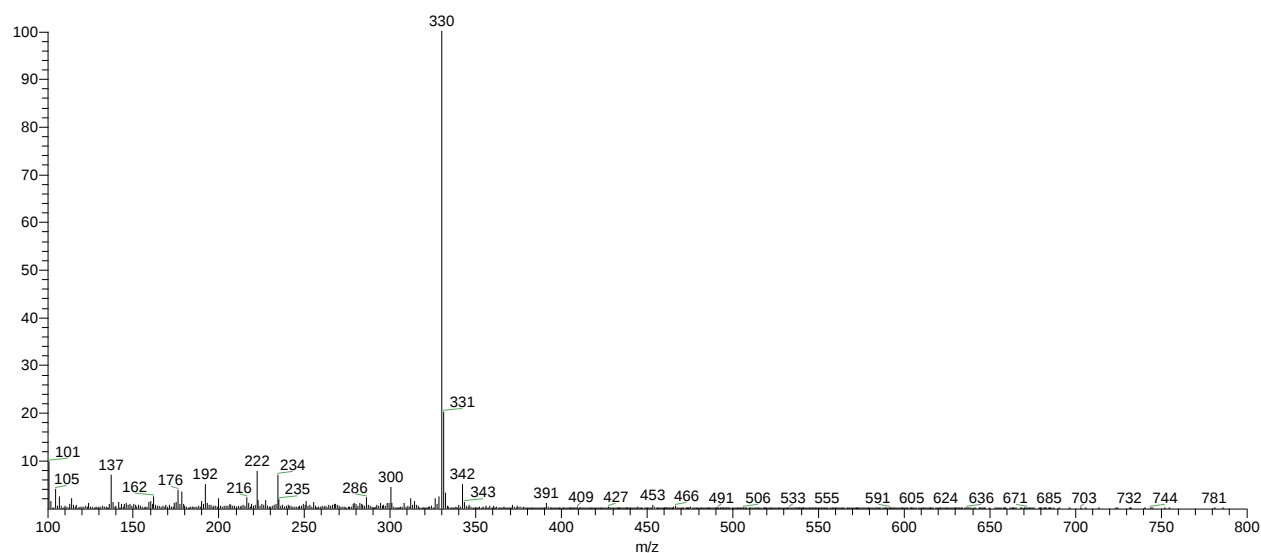


Figure 5S. Mass spectrum of the compound **5** ($t_R = 6.35$ min)

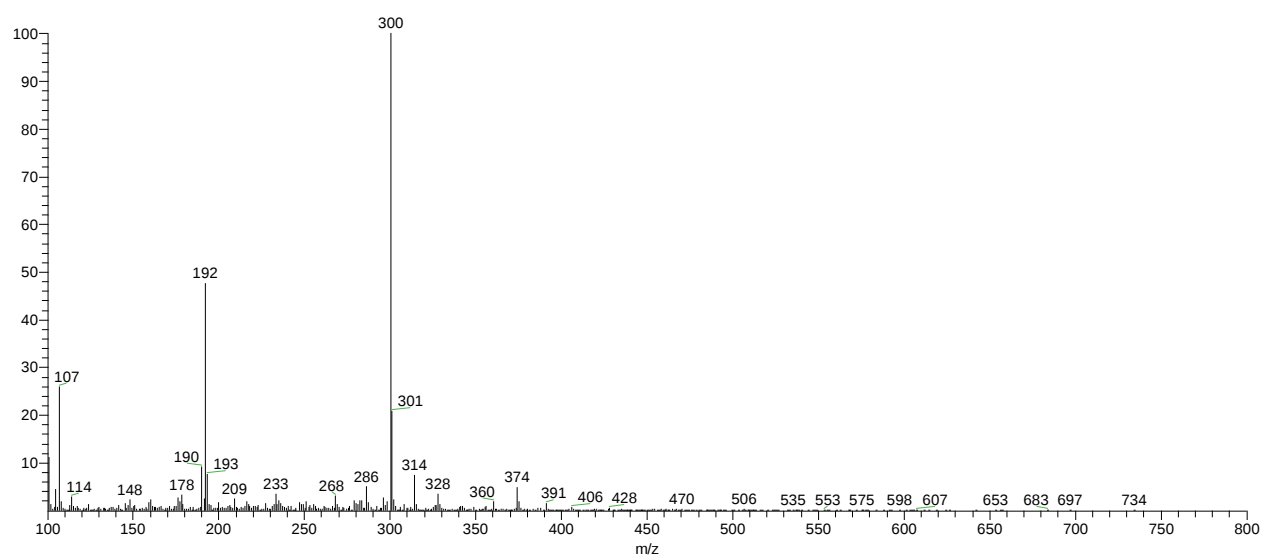


Figure 6S. Mass spectrum of the compound **6** ($t_R = 7.09$ min)

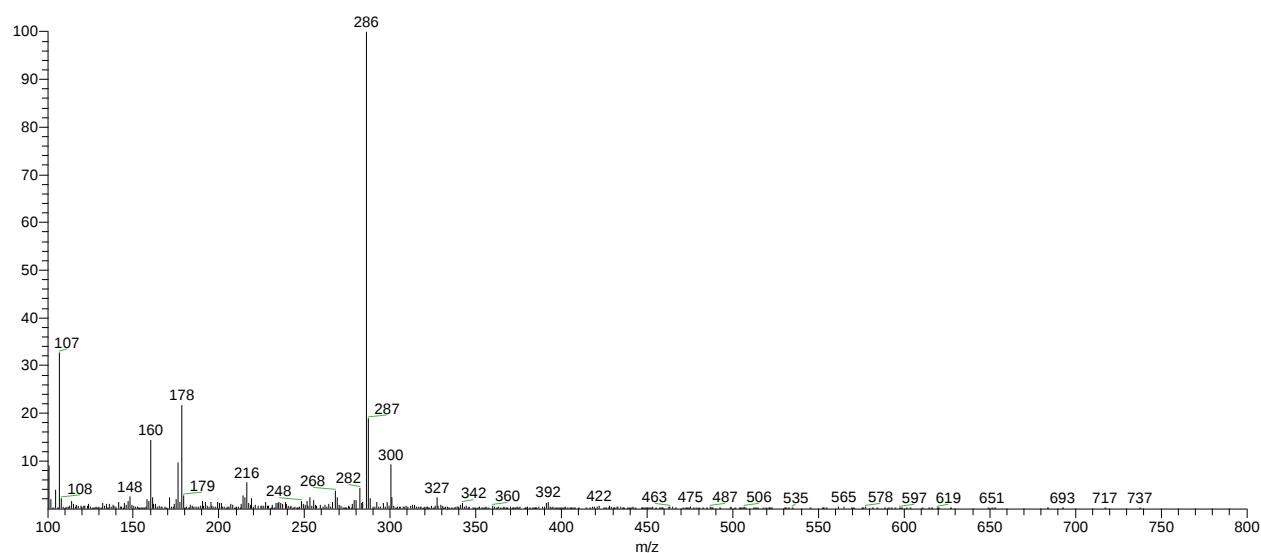


Figure 7S. Mass spectrum of the compound **7** ($t_R = 7.69$ min)

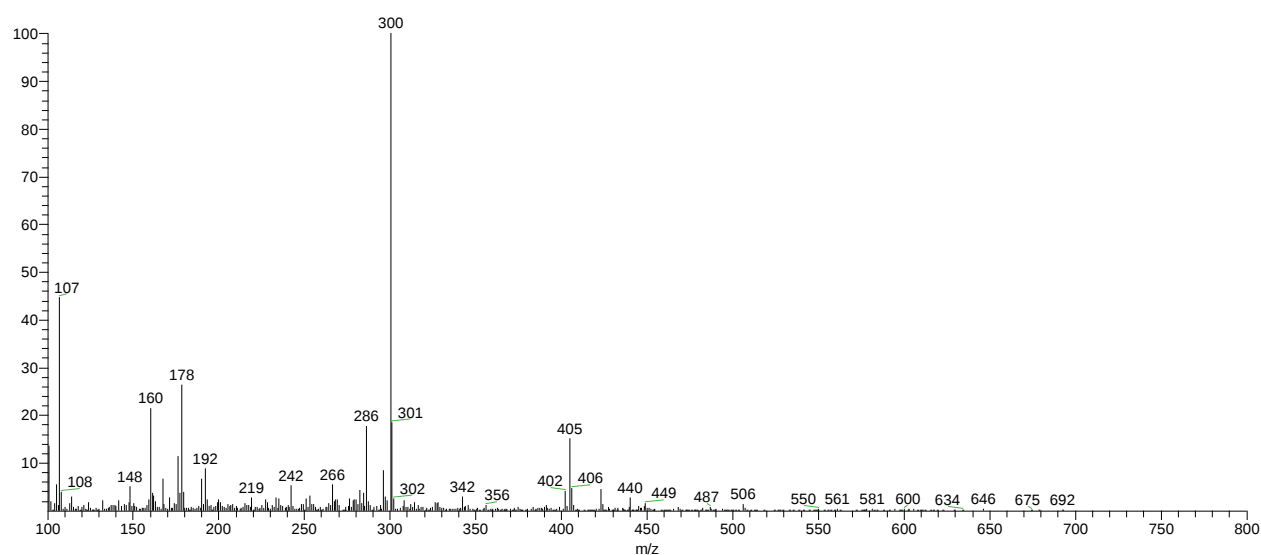


Figure 8S. Mass spectrum of the compound **8** ($t_R = 7.74$ min)

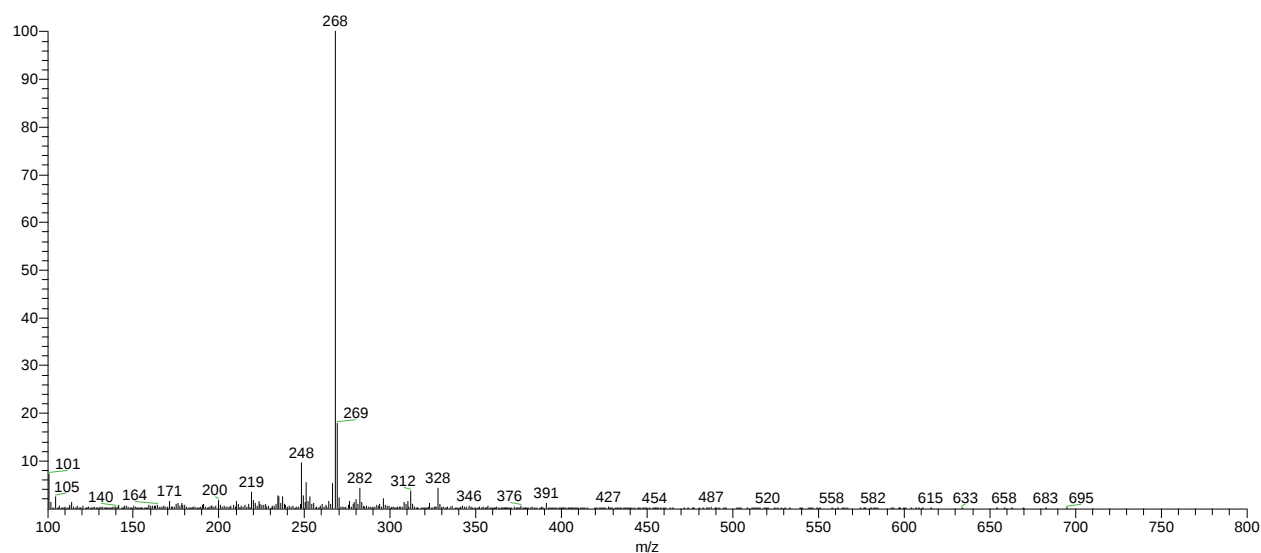


Figure 9S. Mass spectrum of the compound **9** ($t_R = 8.19$ min)

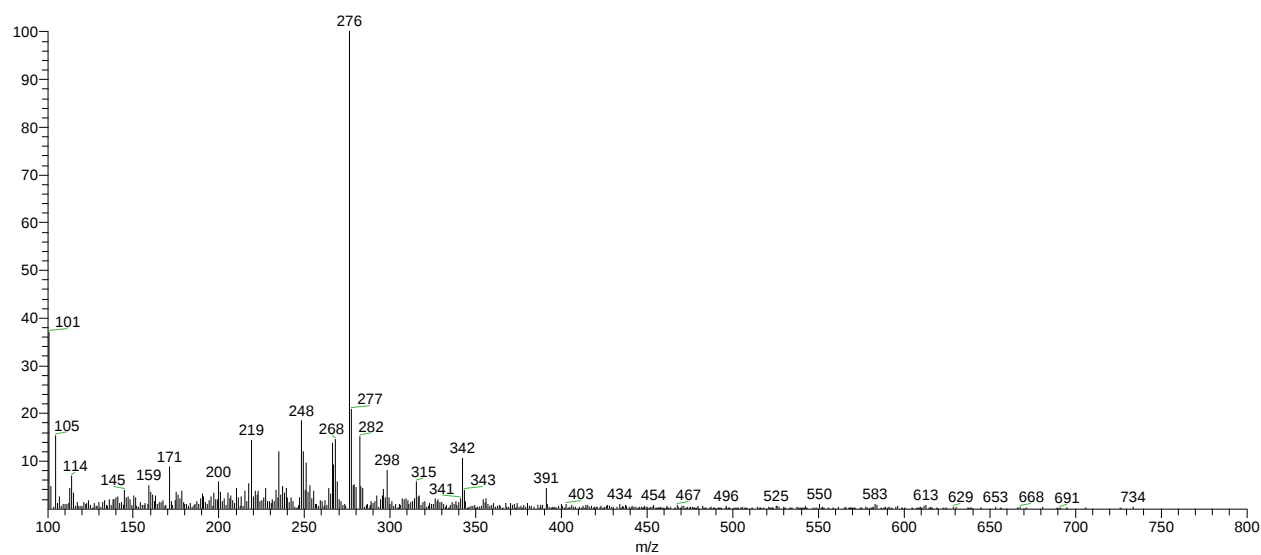


Figure 10S. Mass spectrum of the compound **10** ($t_R = 8.32$ min)

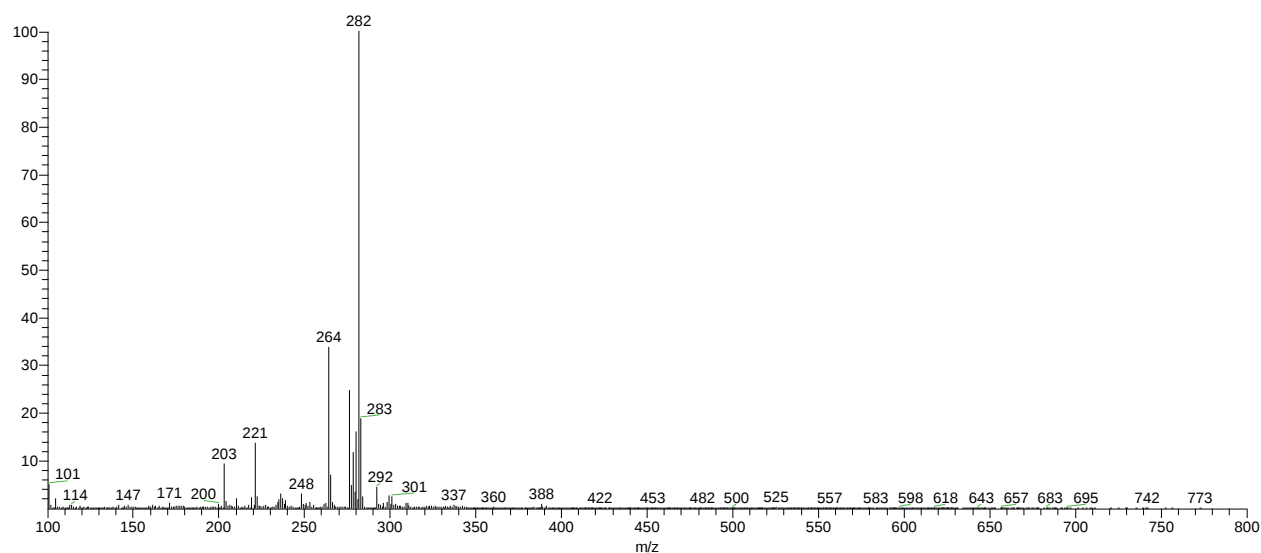


Figure 11S. Mass spectrum of the compound **11** ($t_R = 8.75$ min)

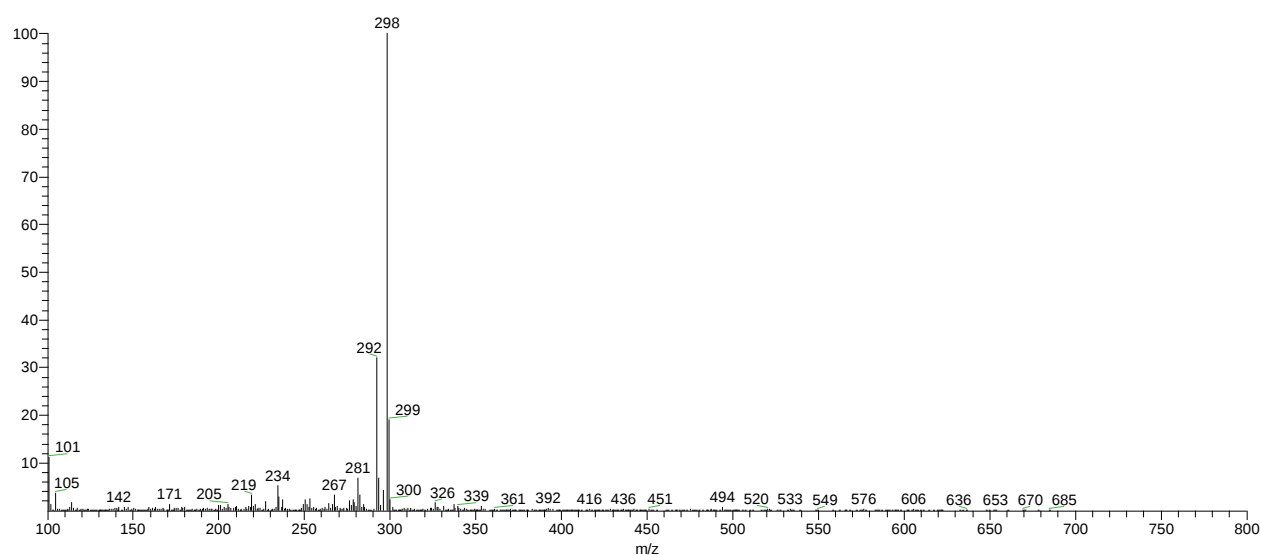


Figure 12S. Mass spectrum of the compounds **12** and **13** ($t_R = 10.25$ min)

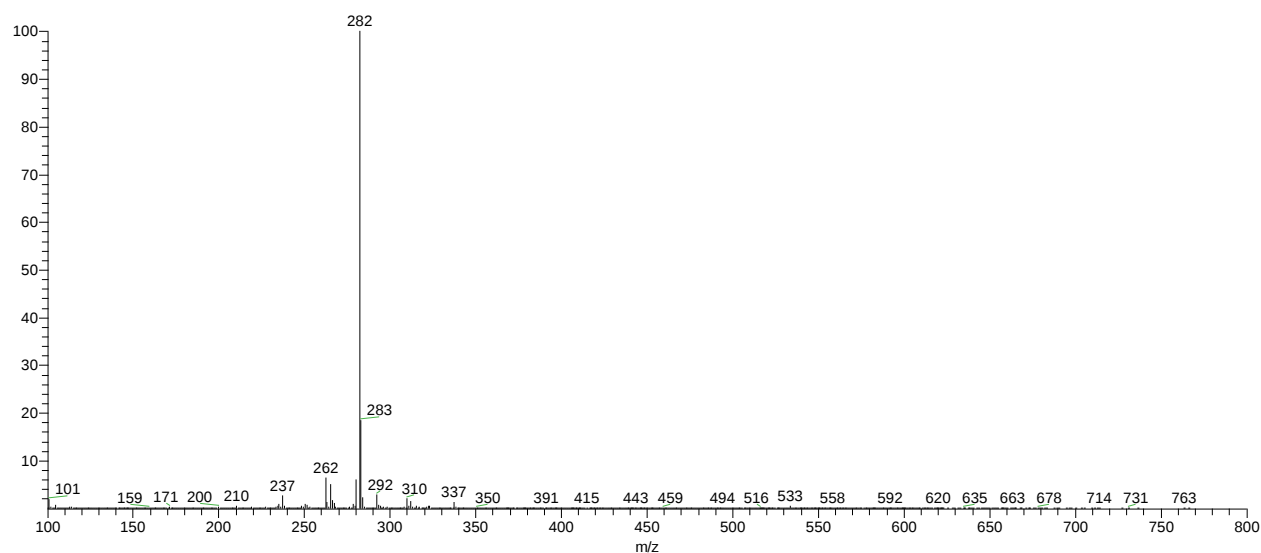


Figure 13S. Mass spectrum of the compound **14** ($t_R = 10.56$ min)

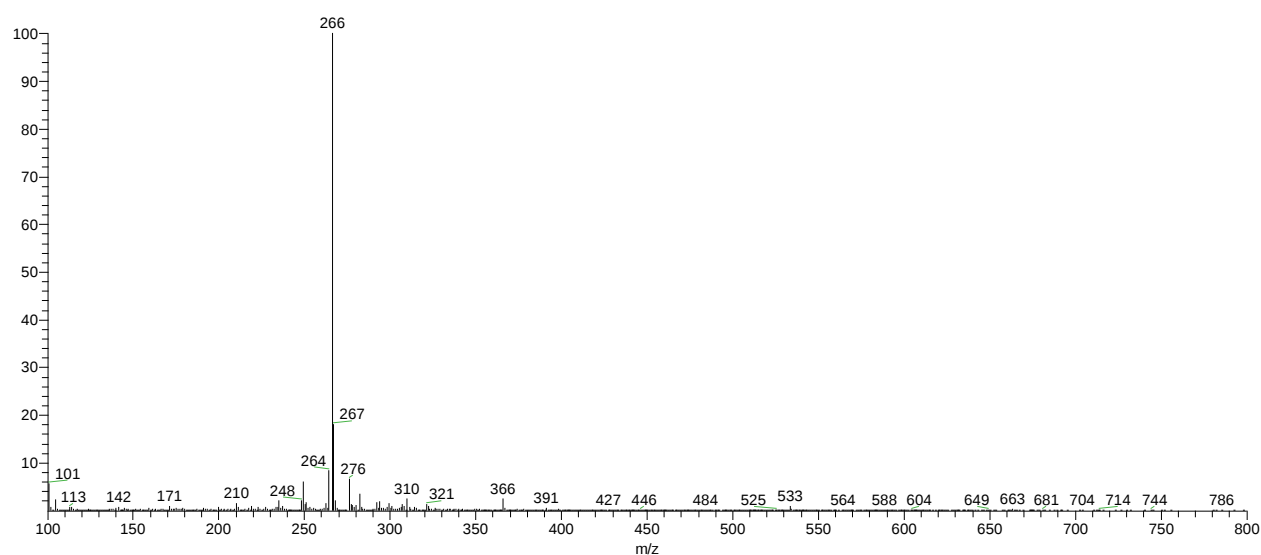


Figure 14S. Mass spectrum of the compound **15** ($t_R = 10.72$ min)

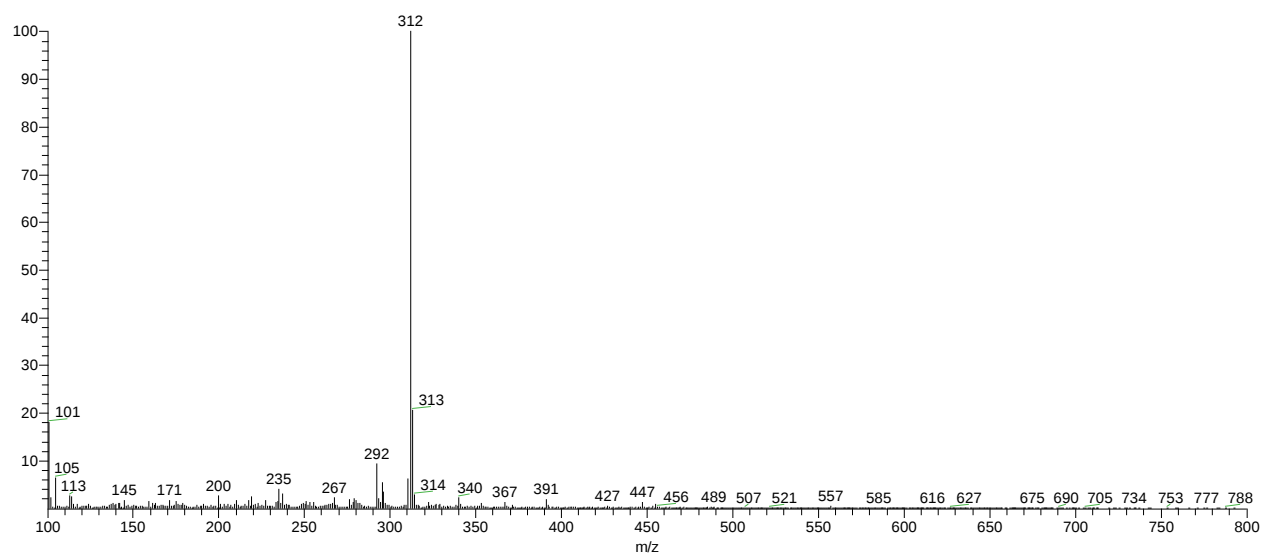


Figure 15S. Mass spectrum of the compound **16** ($t_R = 11.90$ min)

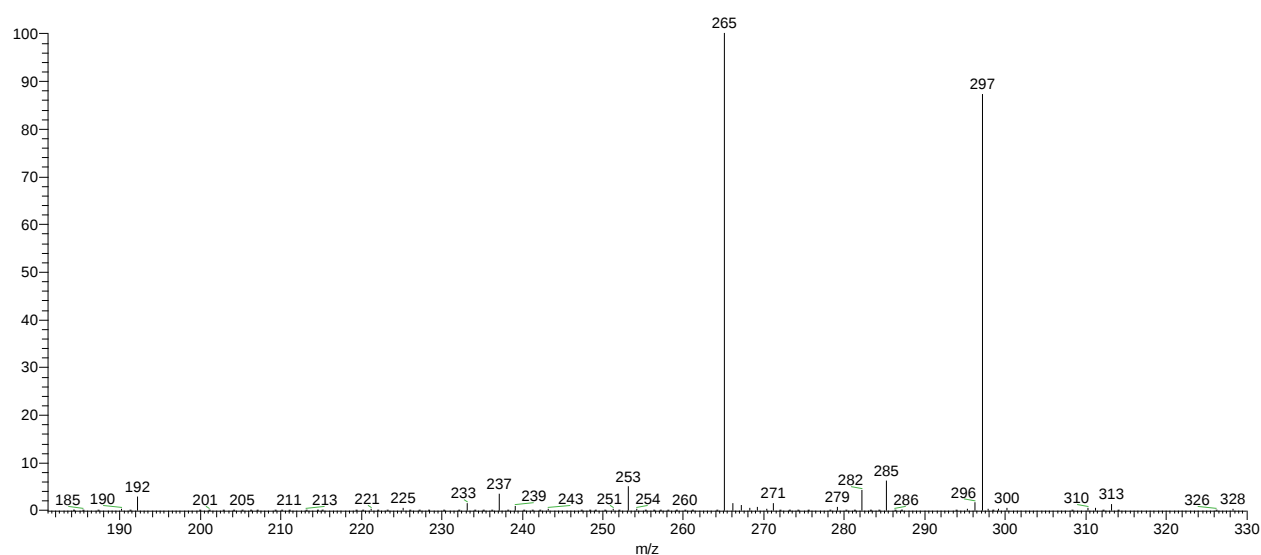


Figure 16S. MS^2 spectrum of the ion at m/z 328 (compound **1**)

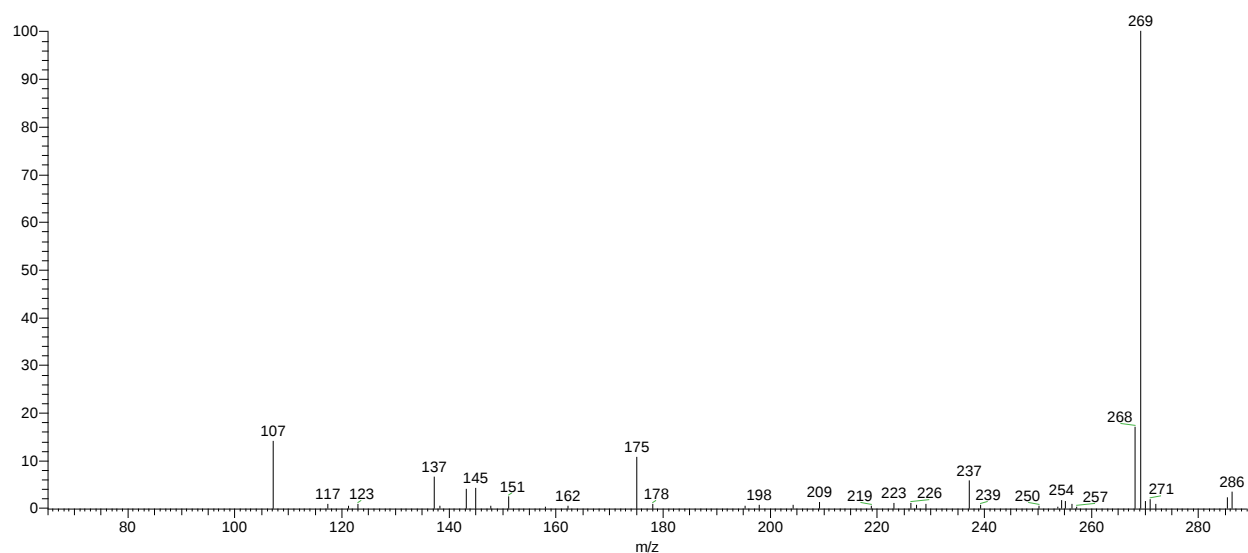


Figure 17S. MS² spectrum of the ion at m/z 286 (compound 2)

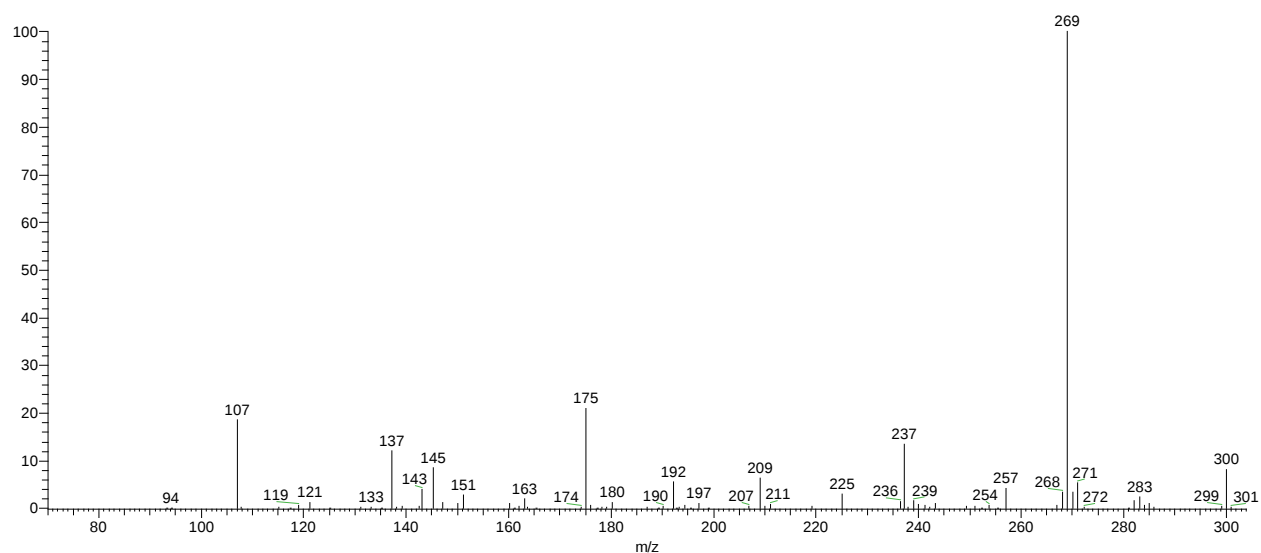


Figure 18S. MS² spectrum of the ion at m/z 300 (compound 3)

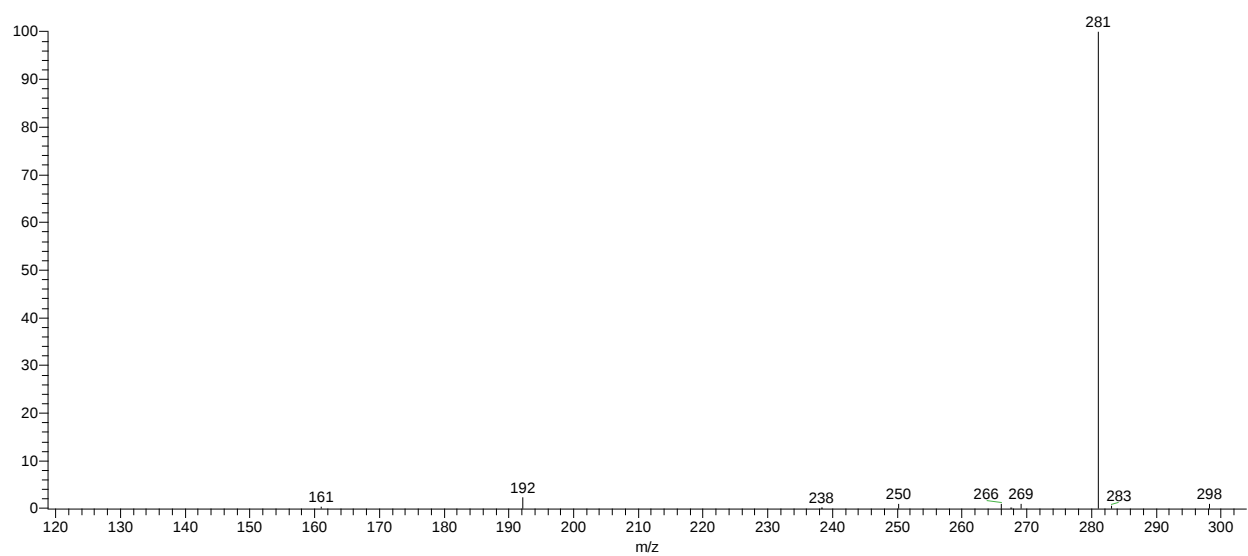


Figure 19S. MS² spectrum of the ion at m/z 298 (compound 4)

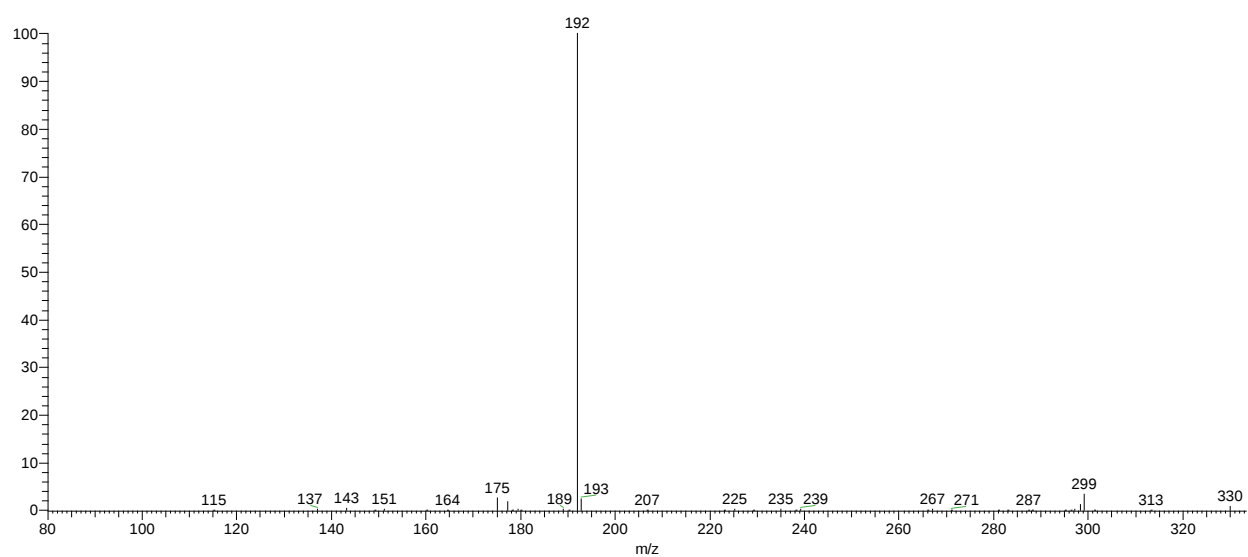


Figure 20S. MS² spectrum of the ion at m/z 330 (compound 5)

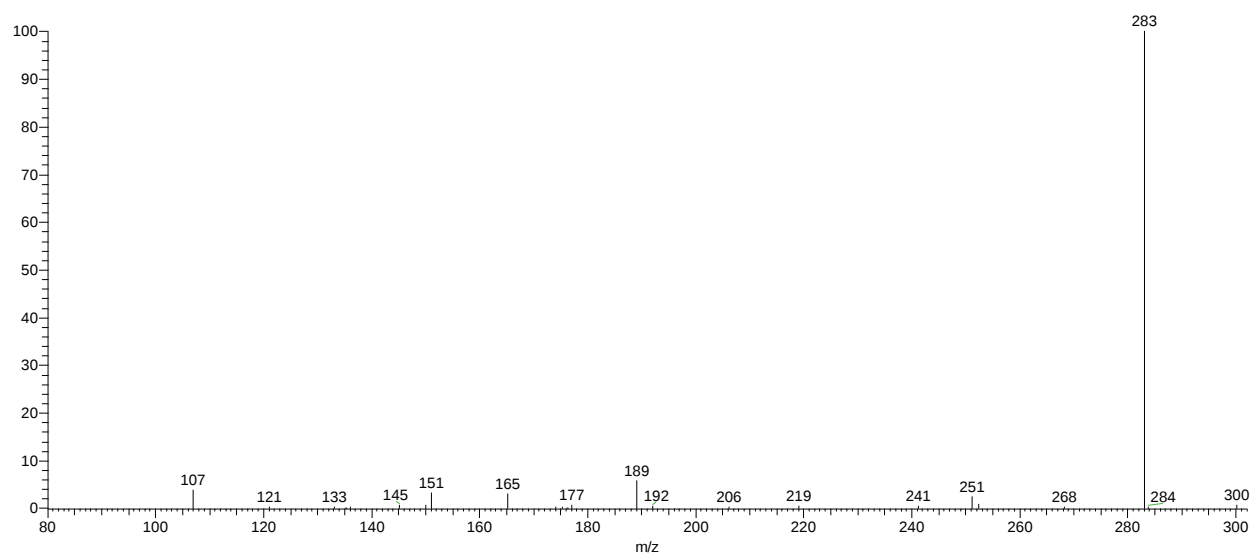


Figure 21S. MS² spectrum of the ion at m/z 300 (compound 6)

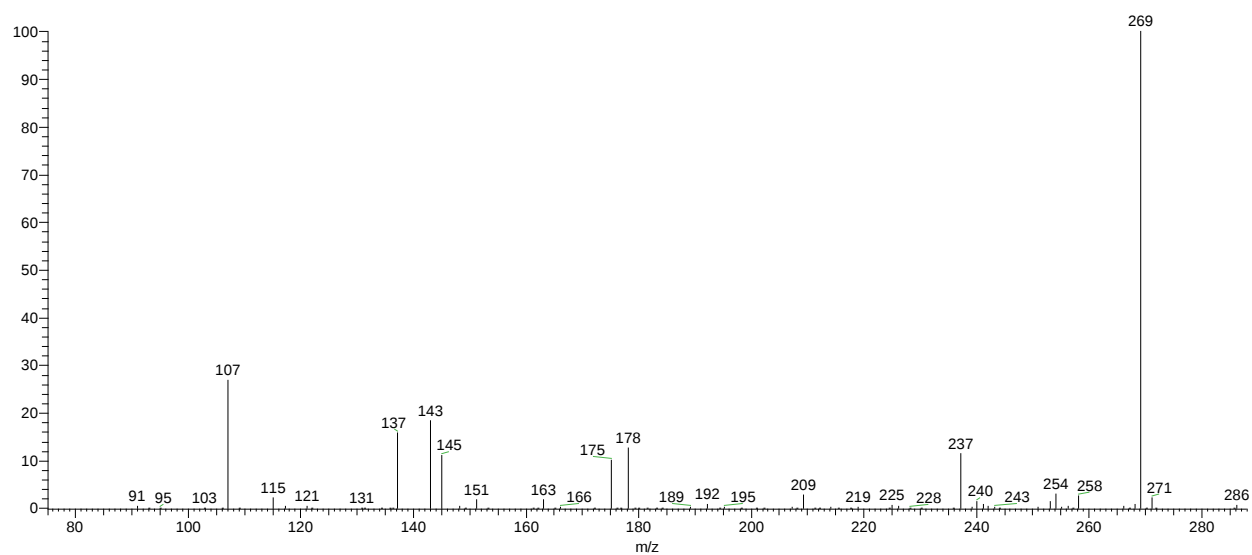


Figure 22S. MS² spectrum of the ion at m/z 286 (compound 7)

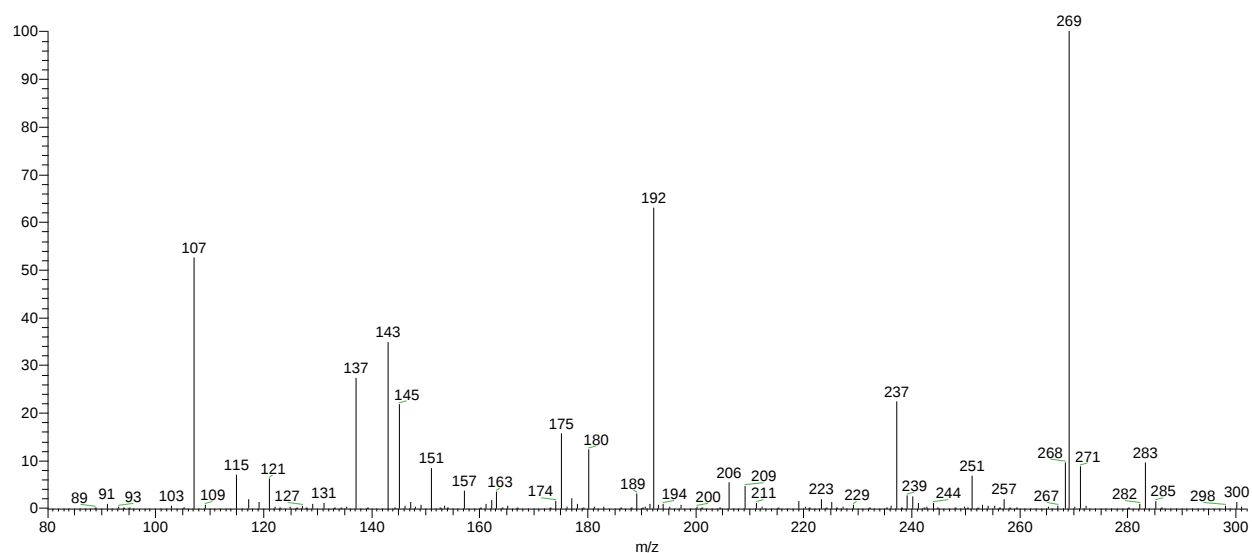


Figure 23S. MS² spectrum of the ion at m/z 300 (compound 8)

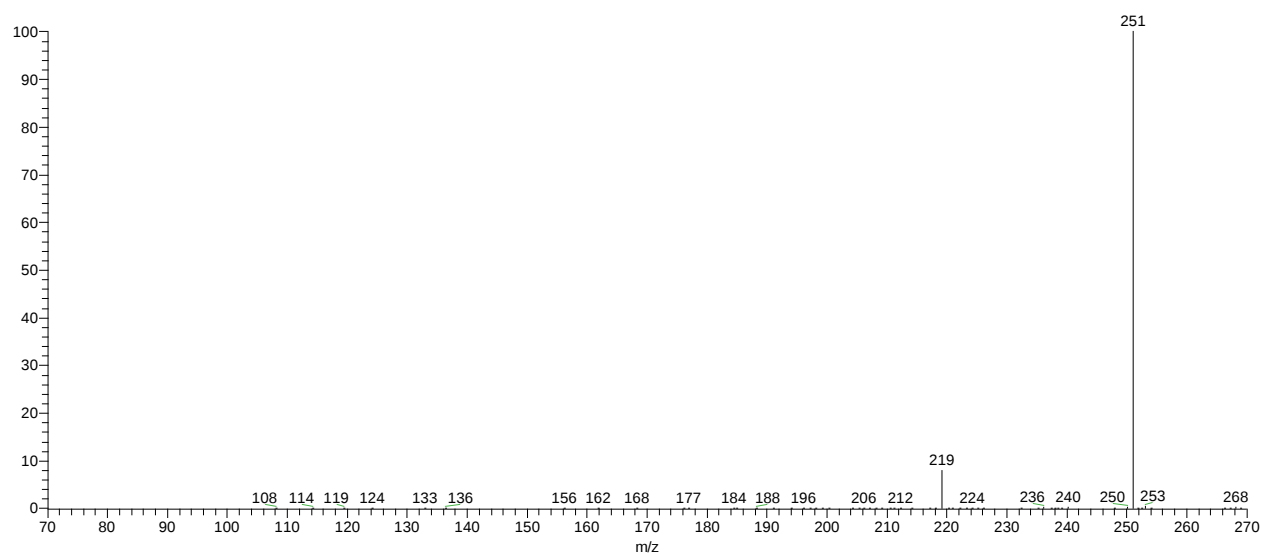


Figure 24S. MS² spectrum of the ion at m/z 268 (compound 9)

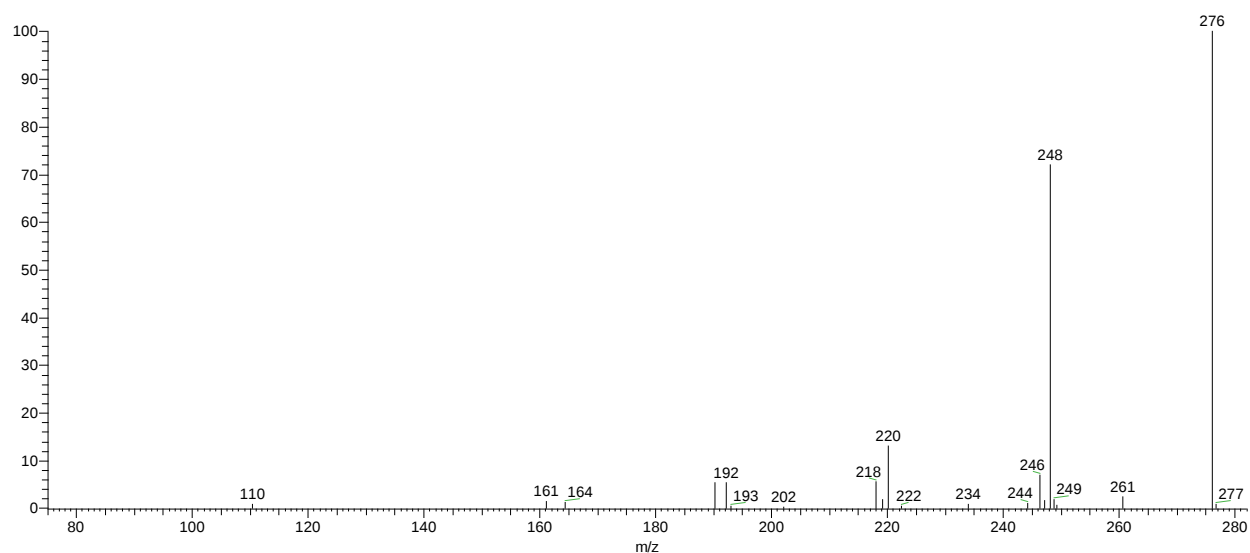


Figure 25S. MS² spectrum of the ion at m/z 276 (compound 10)

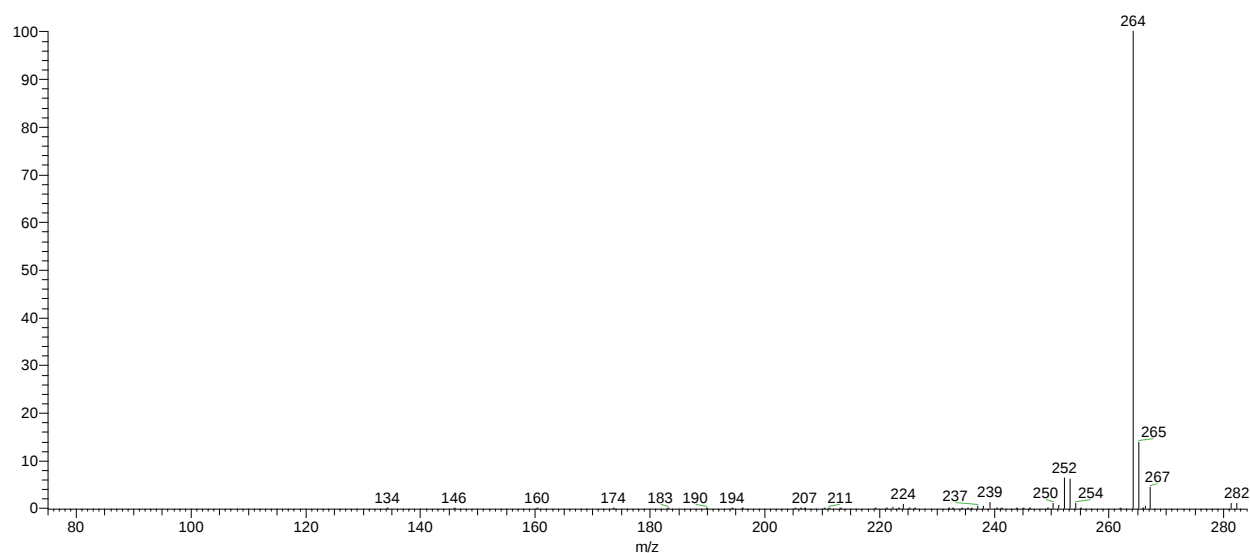


Figure 26S. MS² spectrum of the ion at m/z 282 (compound 11)

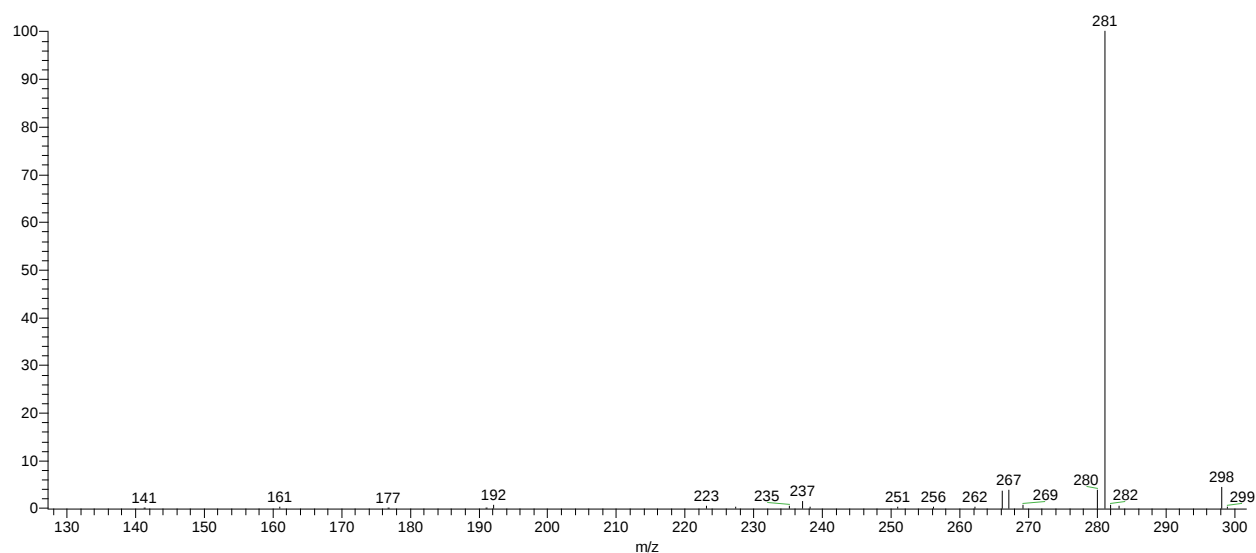


Figure 27S. MS² spectrum of the ion at m/z 298 (compound 12)

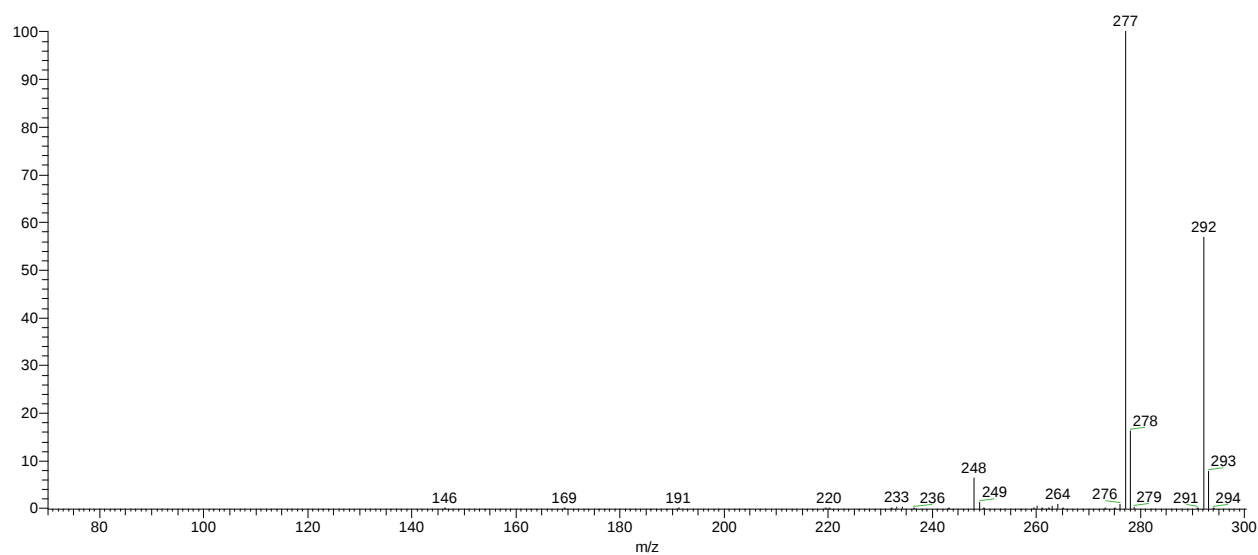


Figure 28S. MS² spectrum of the ion at m/z 292 (compound 13)

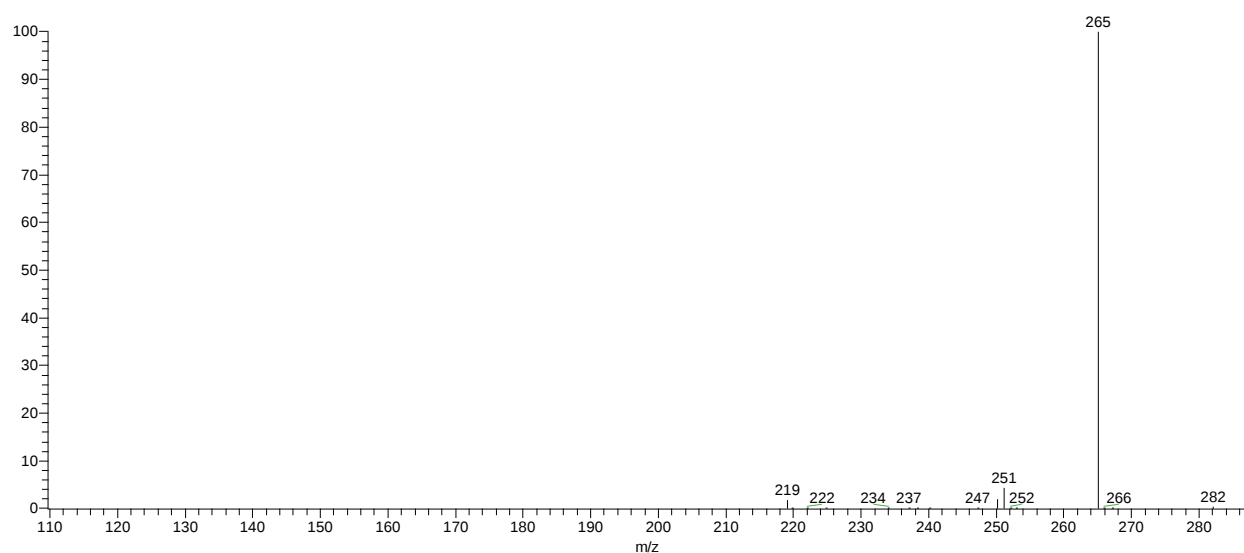


Figure 29S. MS² spectrum of the ion at m/z 282 (compound 14)

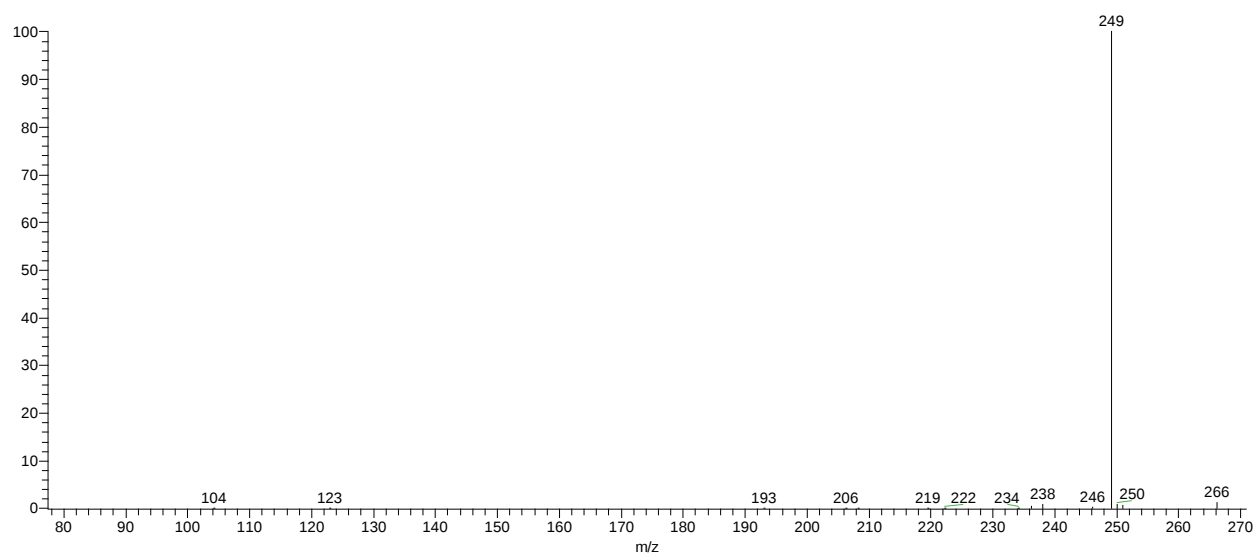


Figure 30S. MS² spectrum of the ion at m/z 266 (compound 15)

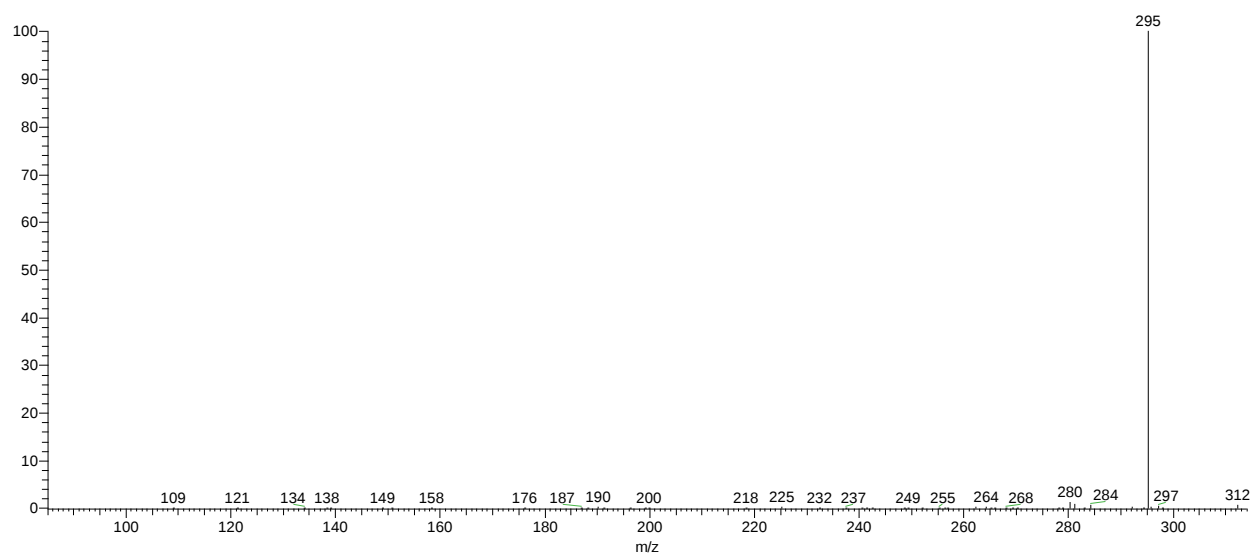


Figure 31S. MS² spectrum of the ion at m/z 312 (compound 16)

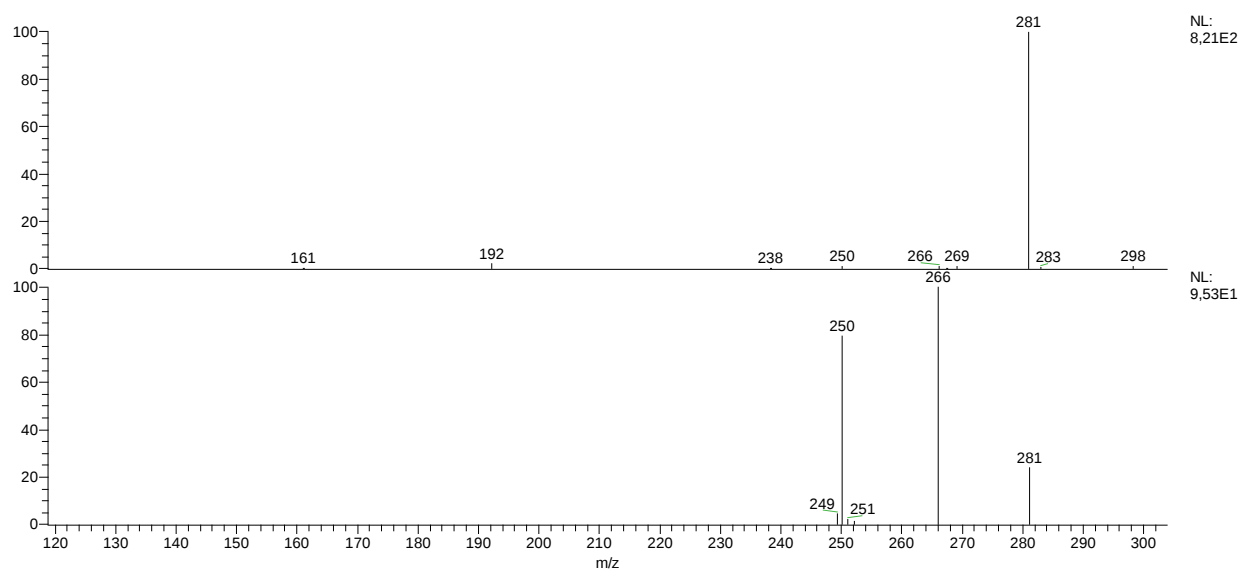


Figure 32S. MS² and MS³ spectra of the ion at m/z 298 (compound 4)

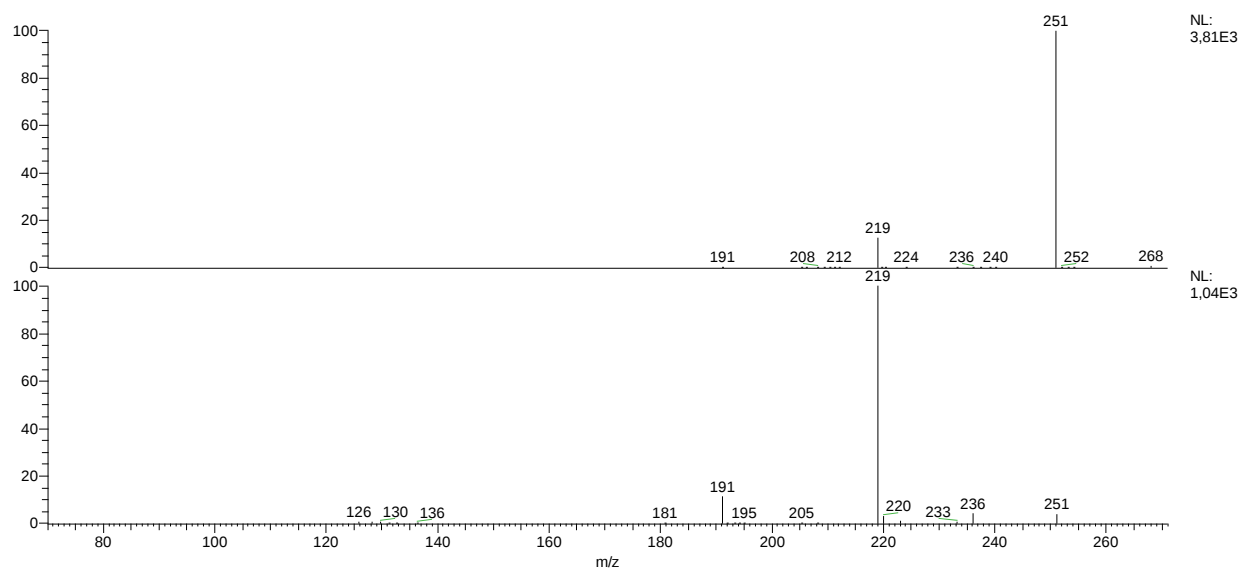


Figure 33S. MS² and MS³ spectra of the ion at m/z 268 (compound 9)

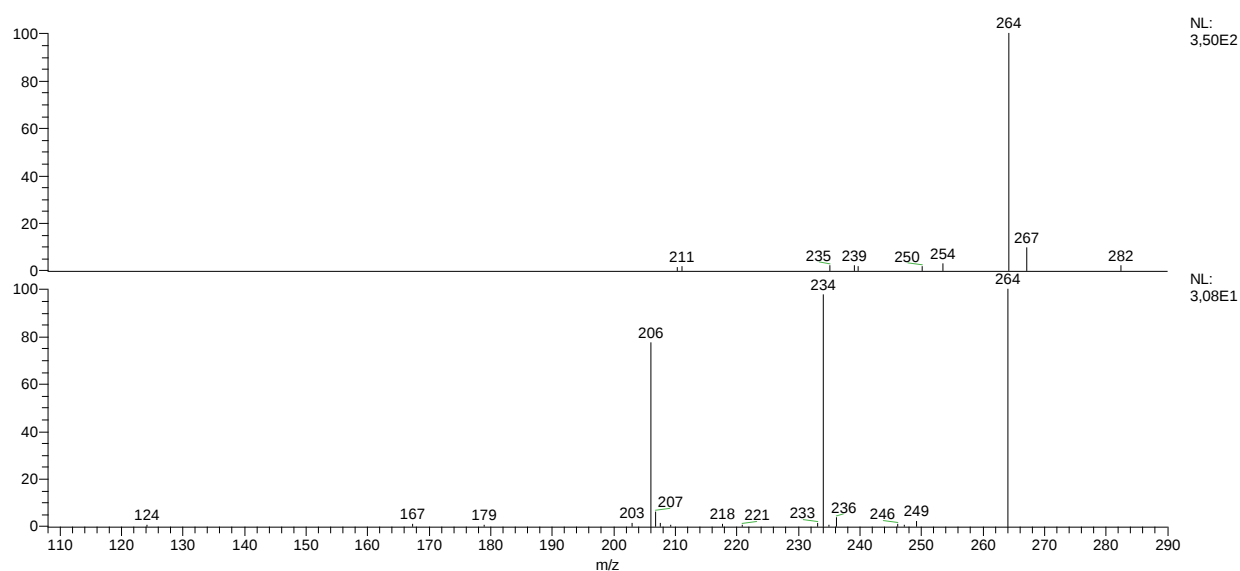


Figure 34S. MS² and MS³ spectra of the ion at m/z 282 (compound 11)

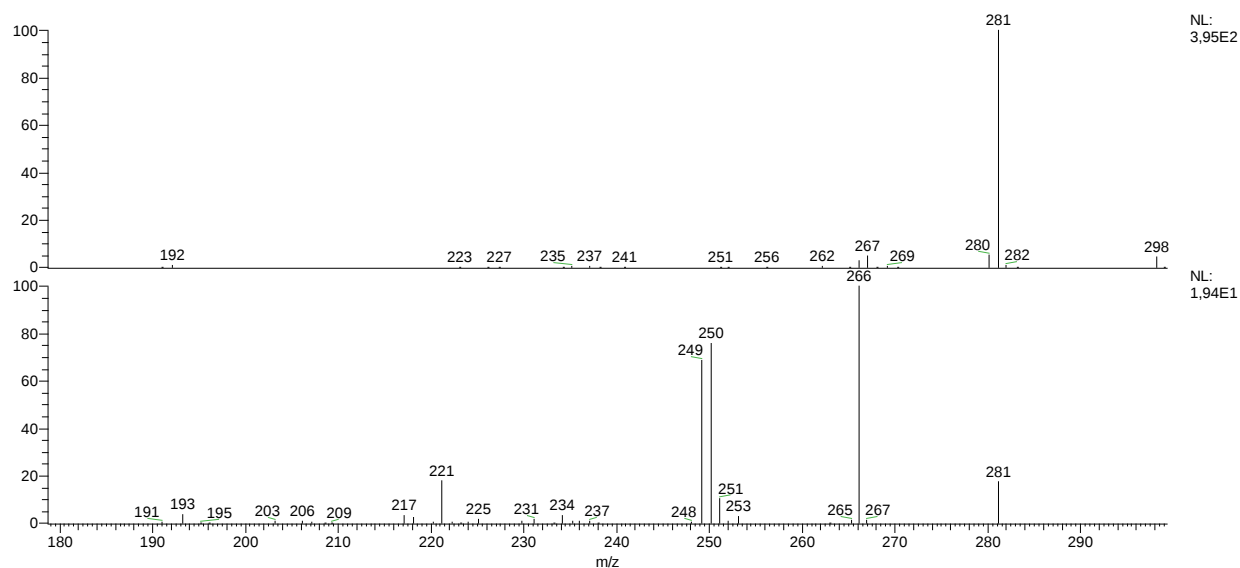


Figure 35S. MS² and MS³ spectra of the ion at m/z 298 (compound 12)

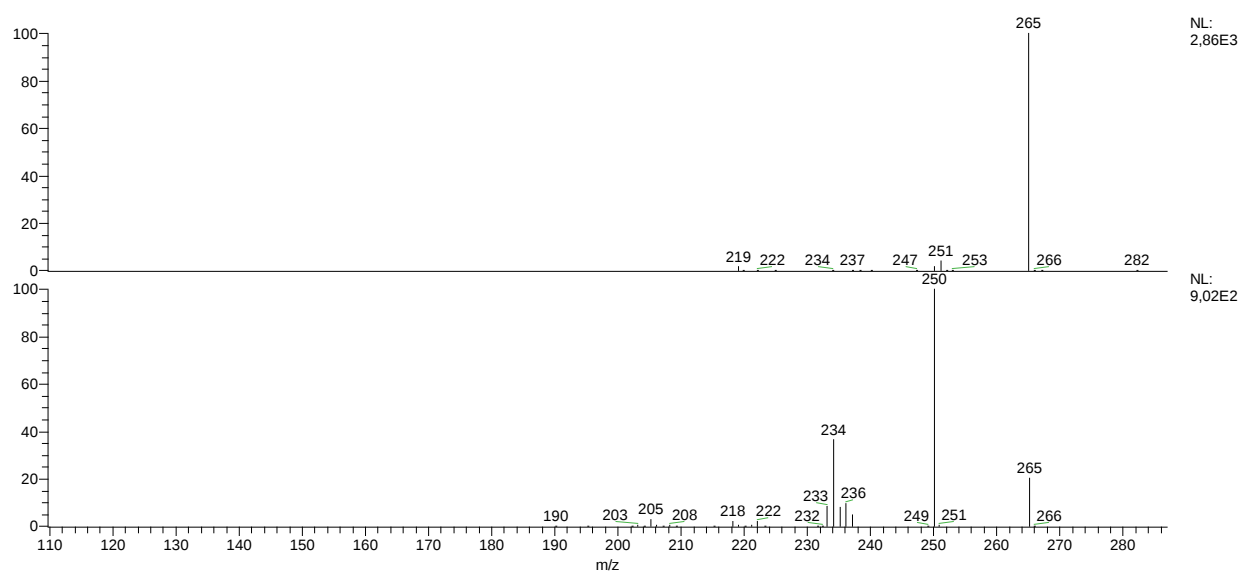


Figure 36S. MS² and MS³ spectra of the ion at m/z 282 (compound 14)

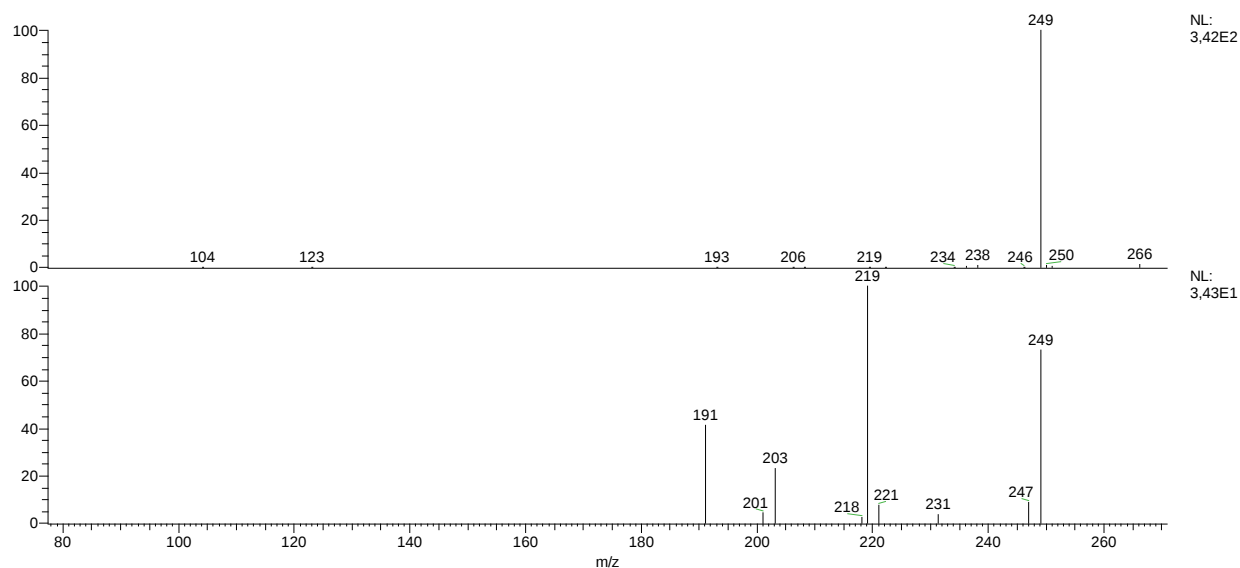


Figure 37S. MS² and MS³ spectra of the ion at m/z 266 (compound 15)

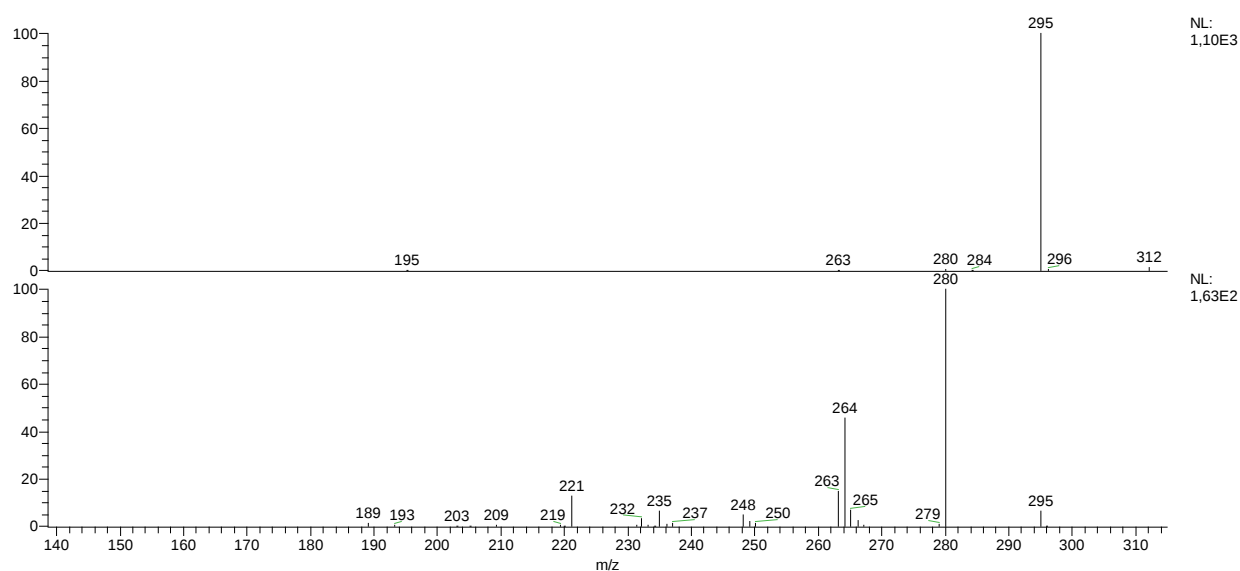


Figure 38S. MS² and MS³ spectra of the ion at m/z 312 (compound 16)

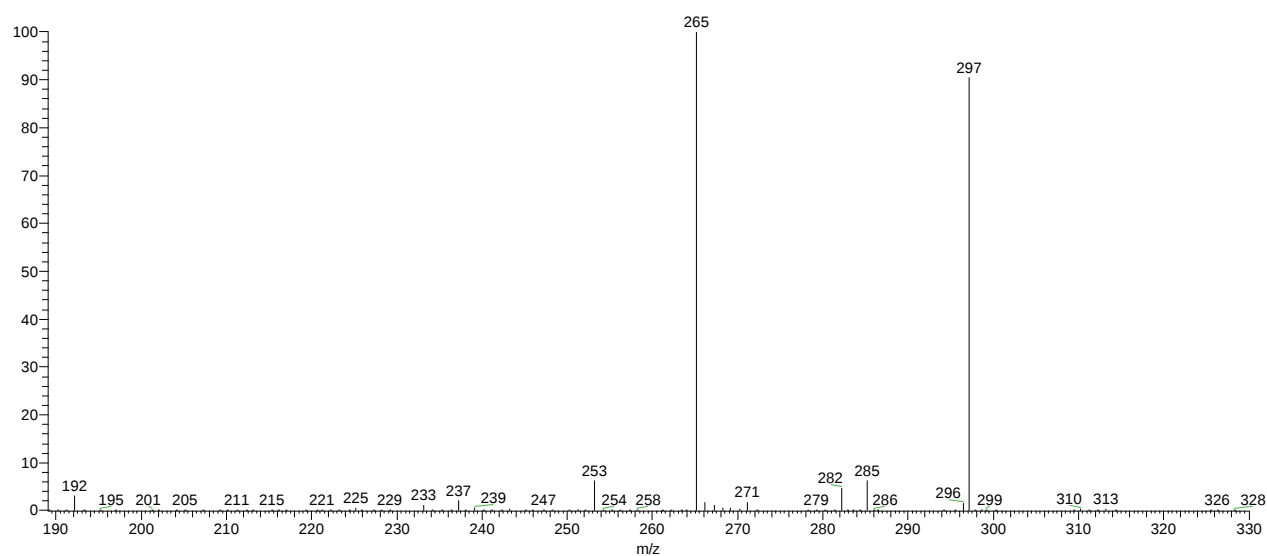


Figure 39S. MS² spectrum of the pallidine standard (m/z 328)

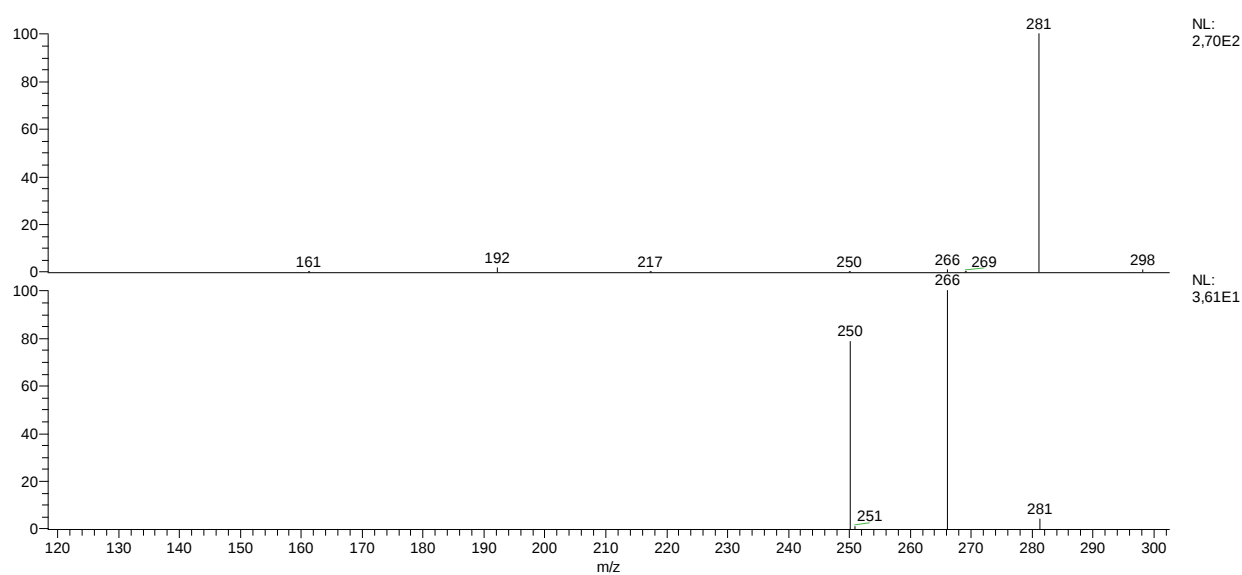


Figure 40S. MS² and MS³ spectra of the stepharine standard (m/z 298)

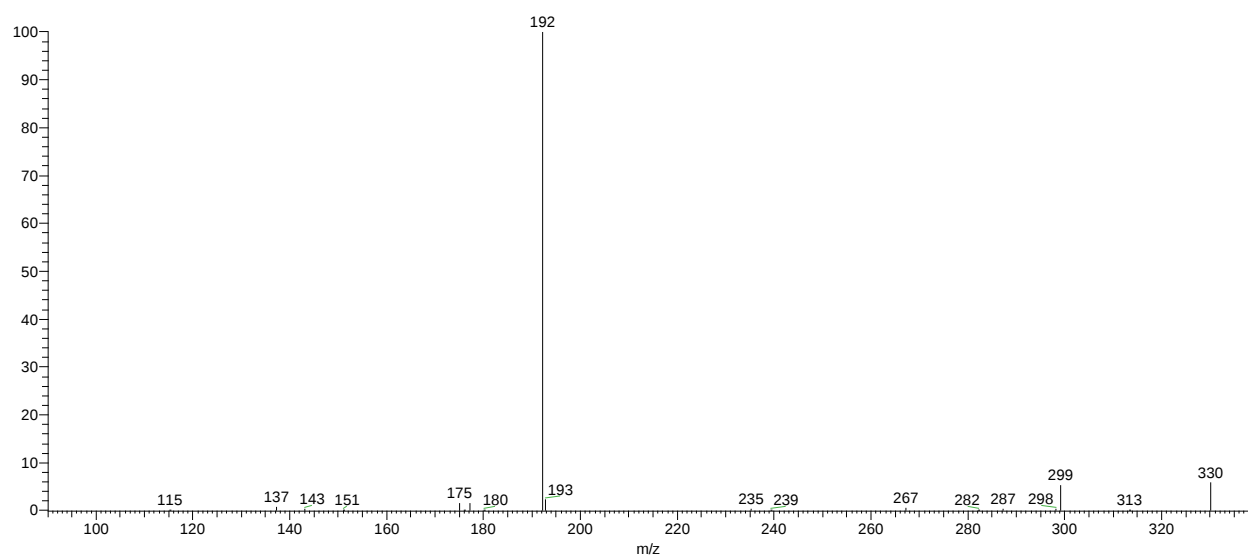


Figure 41S. MS² spectrum of the reticuline standard (m/z 330)

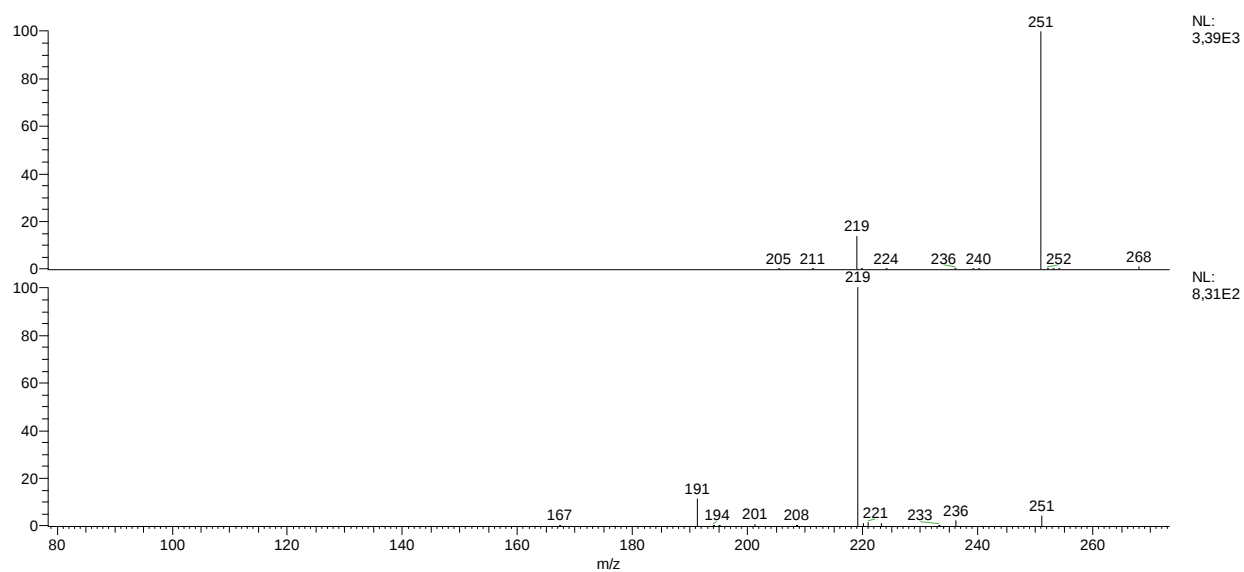


Figure 42S. MS² and MS³ spectra of the asimilobine standard (m/z 268)

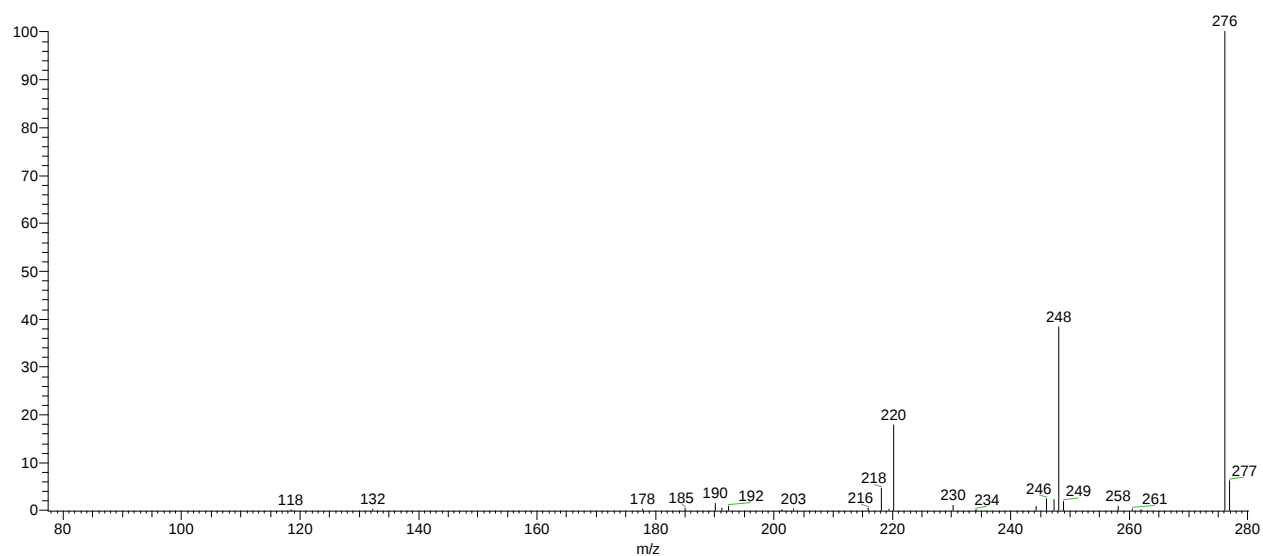


Figure 43S. MS² spectrum of the liriodenine standard (m/z 276)

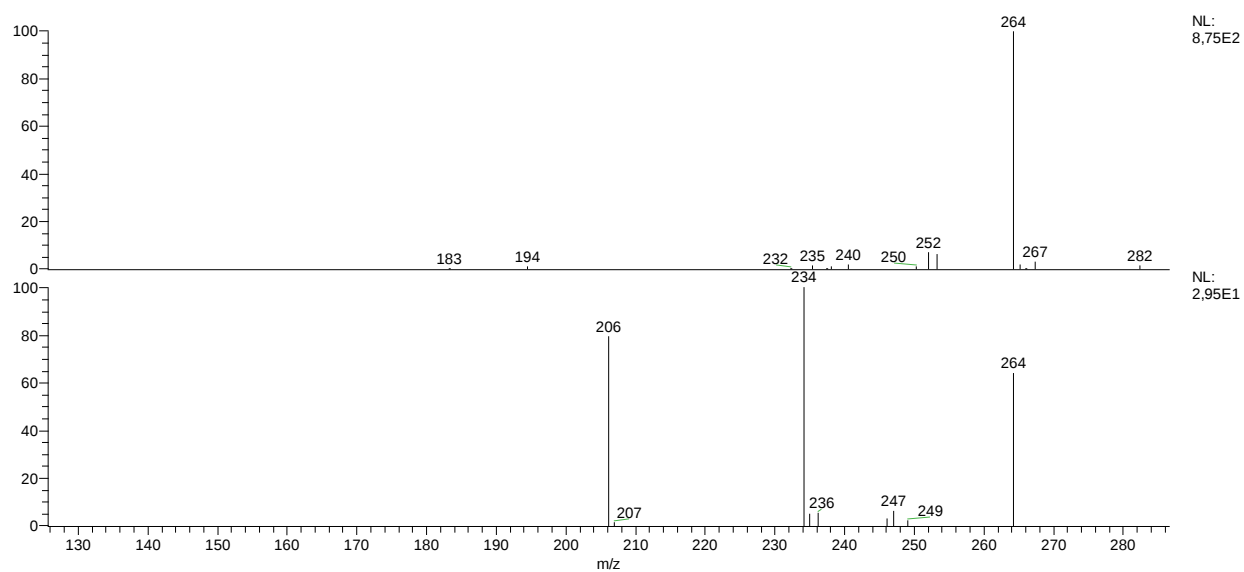


Figure 44S. MS² and MS³ spectra of the norushinsunine standard (m/z 282)

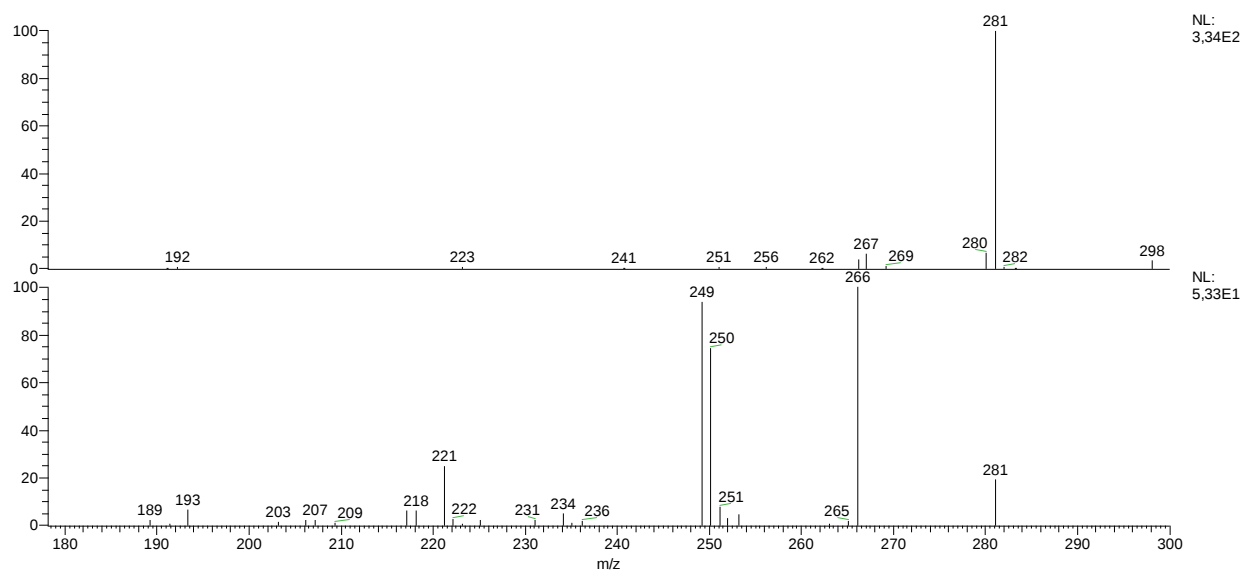


Figure 45S. MS² and MS³ spectra of the isopiline standard (m/z 298)

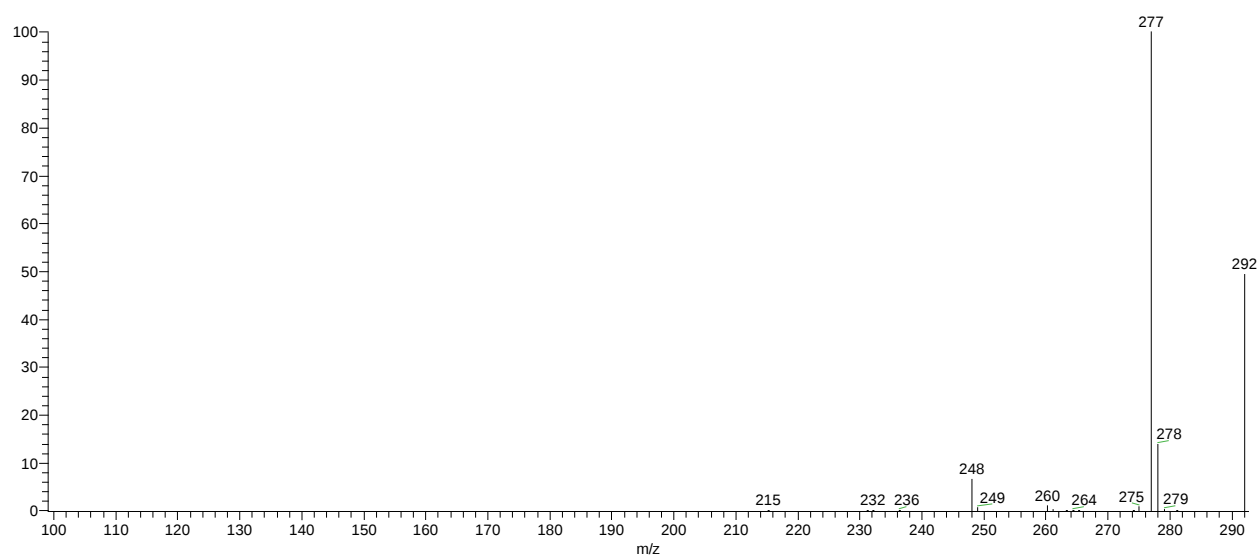


Figure 46S. MS² spectrum of the lysicamine standard (m/z 292)

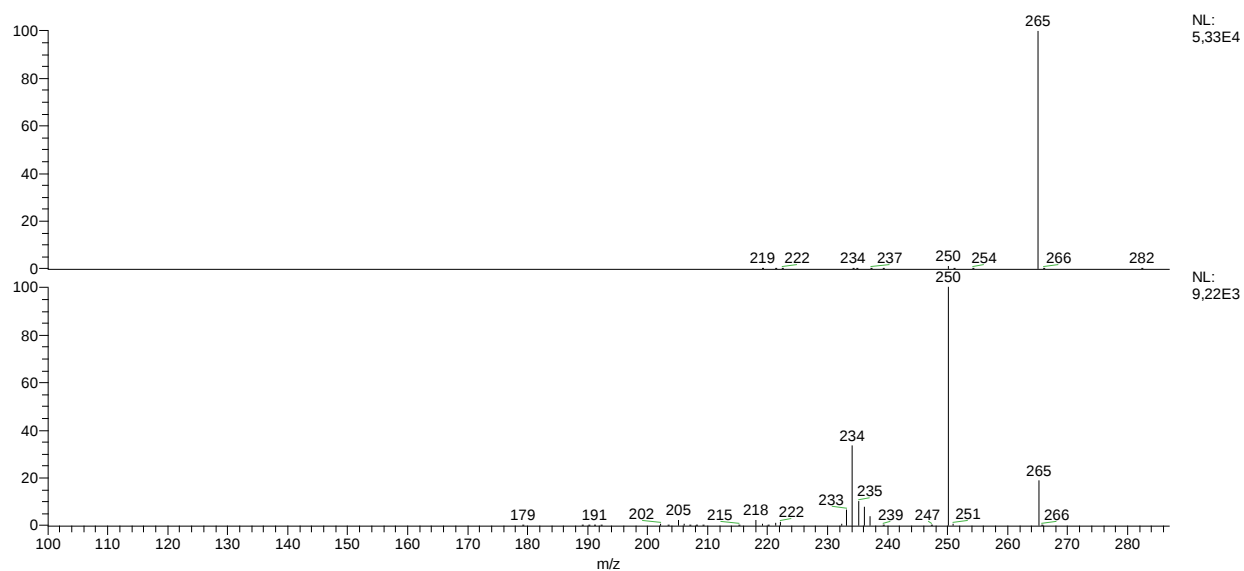


Figure 47S. MS² and MS³ spectra of the nornuciferine standard (m/z 282)

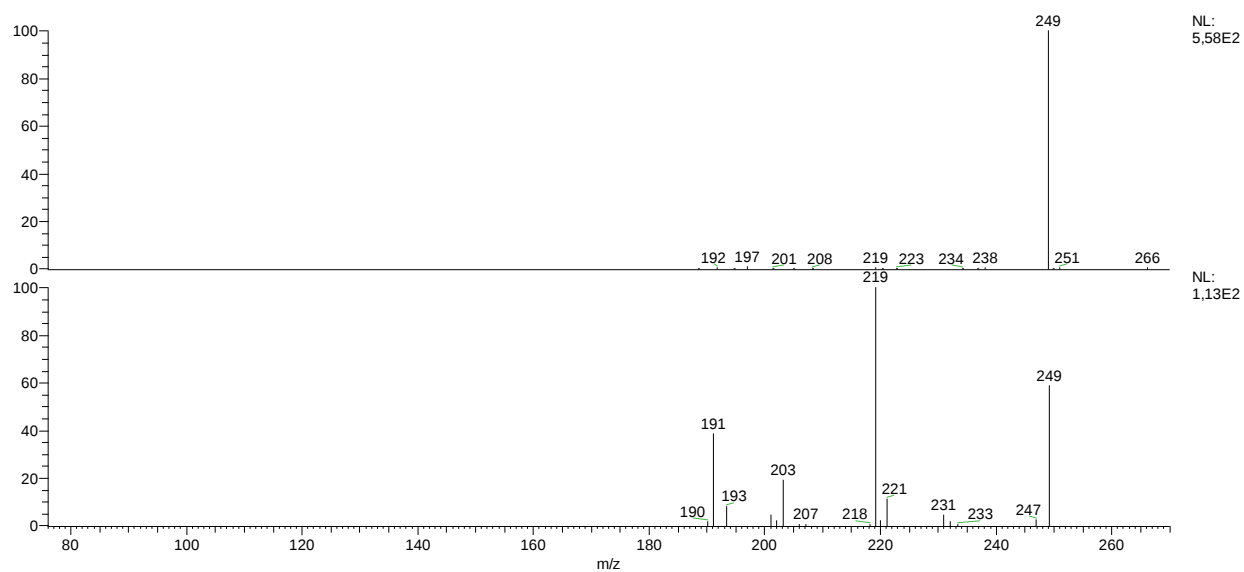


Figure 48S. MS² and MS³ spectra of the anonaine standard (m/z 266)

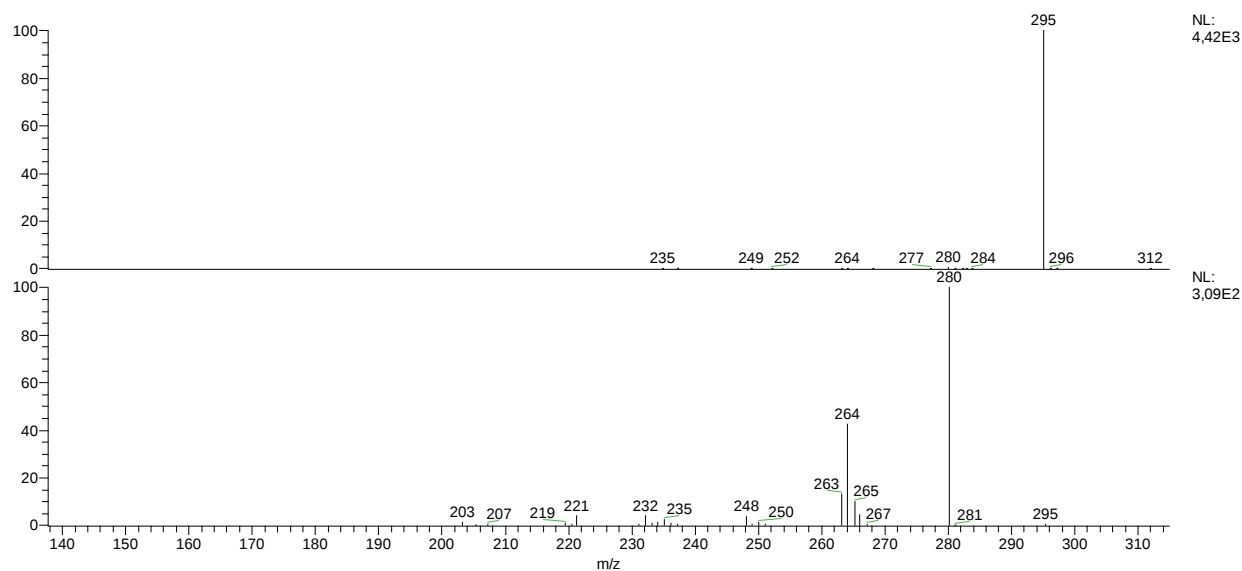


Figure 49S. MS² and MS³ spectra of the O-methylisopiline standard (m/z 312)

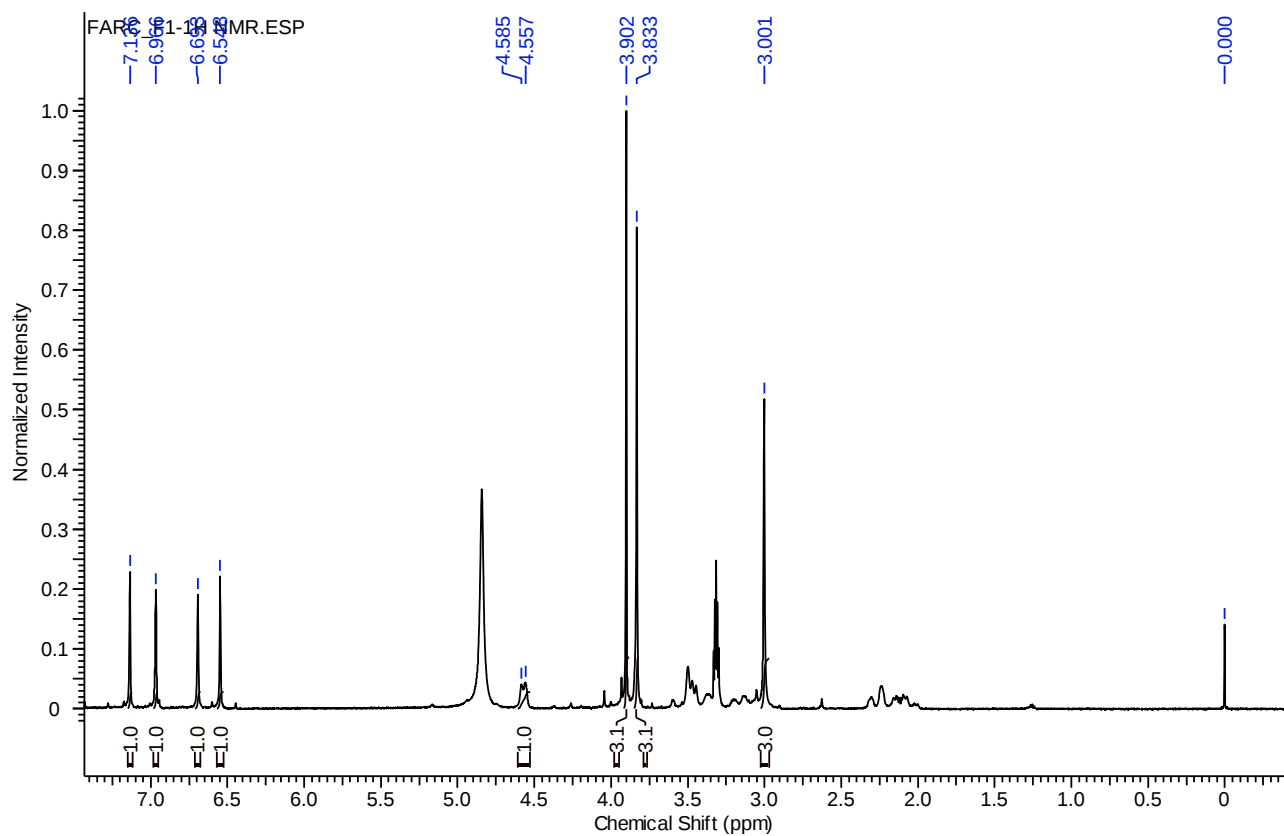
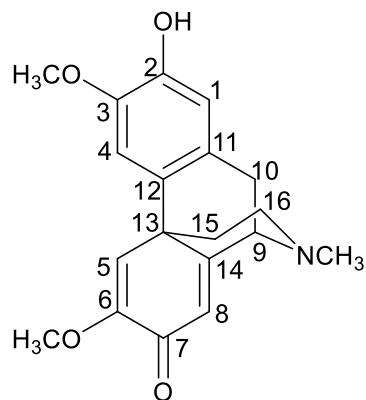


Figure 50S. ¹H NMR spectrum of compound **1** in CD₃OD at 600 MHz

Table 1S. ^1H NMR data (CD_3OD , 600 MHz) for compound **1**

Position	δ_{H} mult. (J in Hz) ^a	^1H δ (mult., J in Hz) ^b
1	6.69, s, 1H	6.72, s, 1H
2	—	—
3	—	—
4	7.14, s, 1H	7.29, s, 1H
5	6.97, s, 1H	6.95, s, 1H
6	—	—
7	—	—
8	6.55 s, 1H	6.51 s, 1H
9	4.57, d, 1H (5.6)	4.62, d, 1H (5.7)
10	—	—
11	—	—
12	—	—
13	—	—
14	—	—
15	—	—
16	—	—
3-OCH ₃	3.90, s, 3H	3.88, s, 3H
6-OCH ₃	3.83, s, 3H	3.78, s, 3H
N-CH ₃	3.00, s, 3H	3.01, s, 3H



^aExperiment performed at 600 MHz in CD_3OD ; ^bdata available in reference 1.

REFERENCE

1. da Silva, F. M. A.; da Silva Filho, F. A.; de Souza, C. A. S.; Maciel, J. B.; Costa, E. V.; Barison, A.; Koolen, H. H. F.; de Souza, A. D. L.; Pinheiro, M. L. B.; *Biochem. Syst. Ecol.* **2018**, *79*, 12. [[Crossref](#)]

