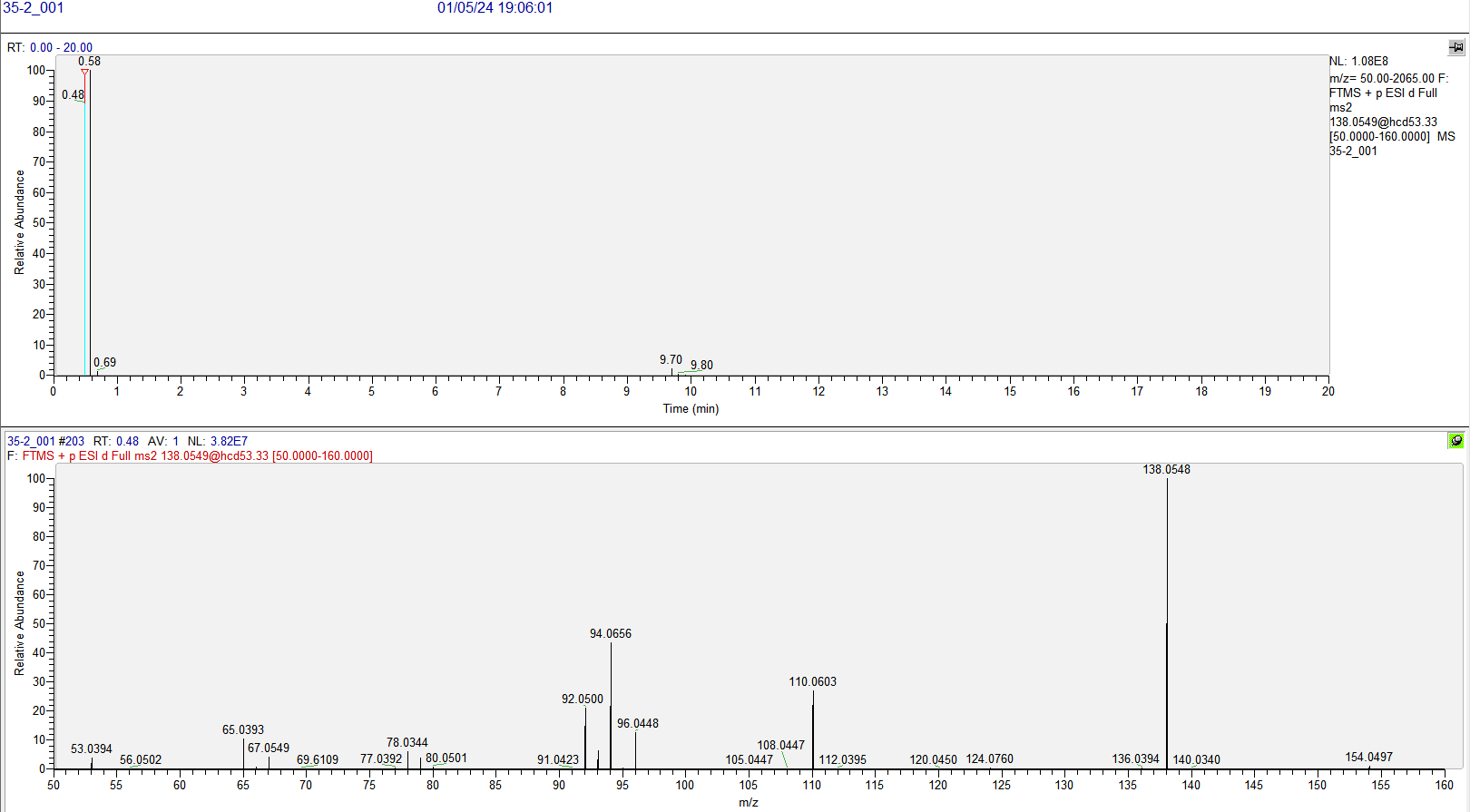
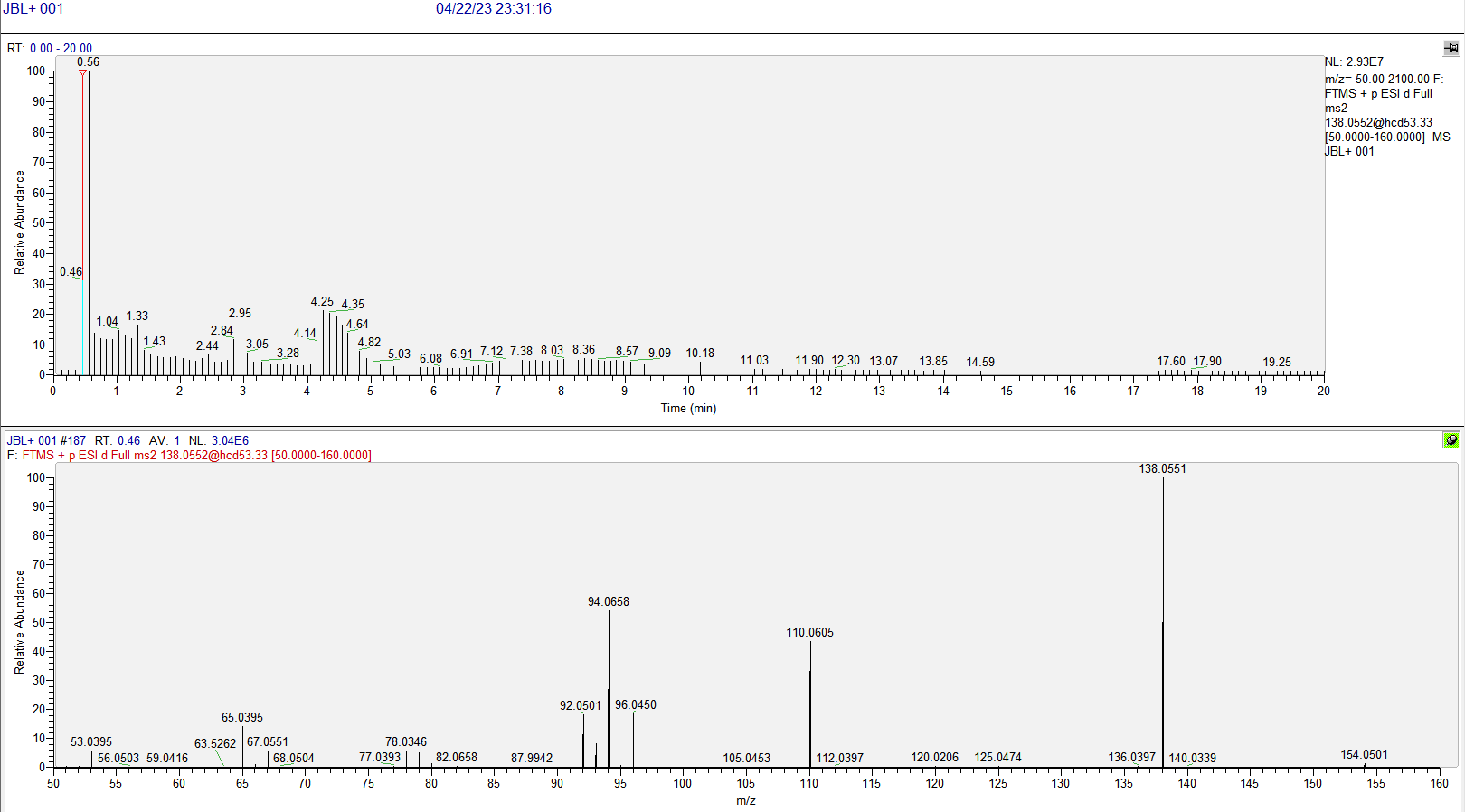
*Suppl. 2.1* Identification of trigonelline (CAS 535-83-1, C7H7NO2, M.W. 137.138).



**A**



**B**

**A**

**A**

**A**

Fig. S1.2.1 The main results of trigonelline (CAS 535-83-1, C7H7NO2) and its corresponding peak in the TIC diagram using UPLC-Q-Orbitrap-MS analysis. (**A**) The MS/MS fragments of standard trigonelline. (**B**) The MS/MS spectra from chromatographic peak in the JBL extract.

**Note**：The m/z values in purple are the calculated ones. The m/z calculation was based on the relative atomic masses of C (12.0000), H (1.007825), O (15.994915), and N (14.003074)[1]

**Identification**: As seen in Fig. S1.2.1, the extract ion peak, MS/MS spectra, and characteristic pears were highly similar. Thus, the chromatographic peaks in the JBL extracts were identified as trigonelline (CAS 535-83-1).

**References**:

[1] Jürgen H Gross, *Mass spectrometry*. 2013, Beijing: Science press.