pharmaceutics

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Supplementary Materials: Multifaced Role of Dual Herbal Principles Loaded-Lipid Nanocarriers in Providing High Therapeutic Efficacity

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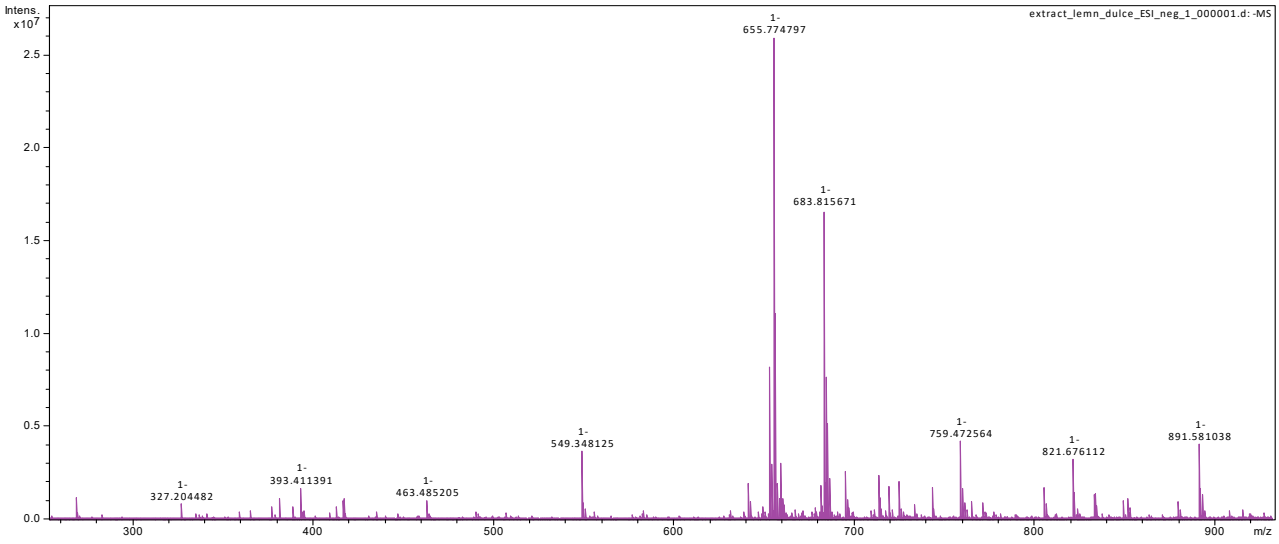
Experimental method. High Resolution Mass Spectrometer with 15T superconducting magnet (solariX-XR, QqqFT-ICR HR, Bruker Daltonics) of Fourier-Transform-Ion-Cyclotron-Resonance (FT-ICR) type was used. The herbal extract was introduced by direct infusion, negative ESI ionization, with a sample flow rate of 120 μL/h, with a spray gas pressure (N_2) of 2.5 bar at 200 °C and a flow rate of 7 L/min. The spectra were recorded over a mass range between 122 and 1000 uam at a source voltage of 5500 V.

By ESI-HR-MS analysis of *Glycyrrhiza glabra* extract, the ion corresponding to *glycyrrhizic acid* in negative ionization was obtained at [M-1] 821.67, *m/z* (Figure S1). The parent ion of Glycyrrhizic Acid (protonated precursor ions $[M–H]^-$ from *m/z* 821.67 was also reported in several literature references [1,2].

A fragmentation of the precursor ion was also made, the fragmentation spectrum is shown in Figure S2.

The MS/MS spectrum was recorded using the fragmentation technique (FSCID source) with a 30 V collision energy using the precursor ion *m/z* = 821.68 and a narrow isolation window of 0.03 *m/z*; the RF collision amplitude of 1700 Vpp and the RF frequency was 1.4 MHz.



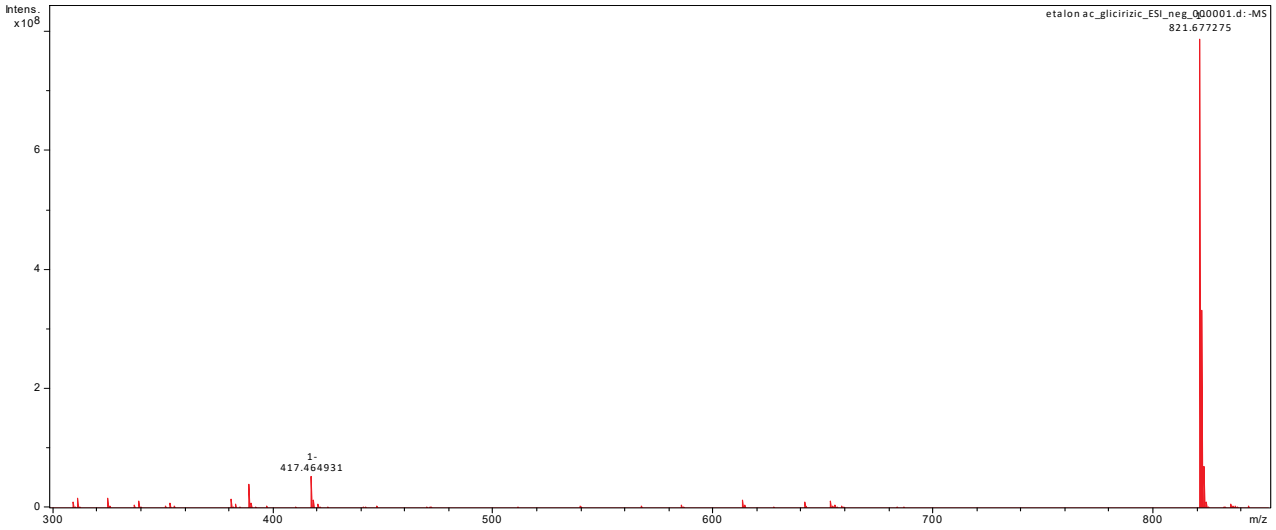


Figure S1. ESI-HR-Mass Spectrum of: (**a**). *Glycyrrhiza glabra extract* (GlyG) with Glycyrrhizic Acid parent ion (protonated precursor ions $[M–H]^-$ at m/z 821.67; (**b**). Glycyrrhizic Acid (standard), with protonated precursor ions $[M–H]^-$ at *m/z* 821.67.

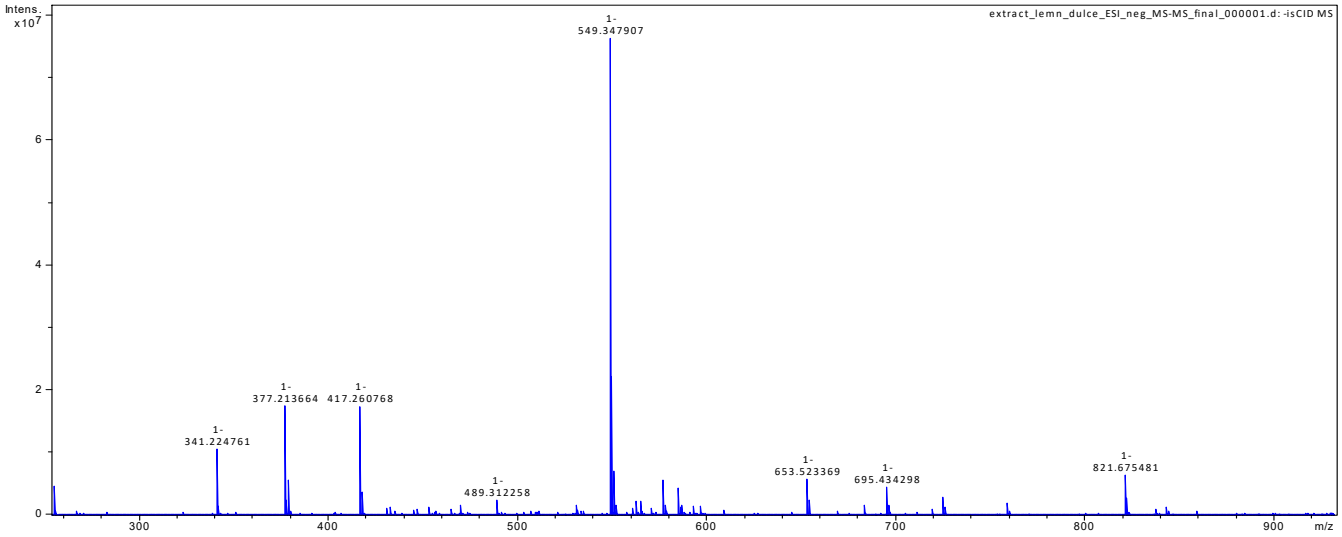


Figure S2. MS/MS Spectrum of *Glycyrrhiza glabra extract* obtained by fragmentation technique, using the precursor ion *m/z* = 821.68.

References

1. Ahmad, N.; Al-Subaiec, A.M.; Ahmad, R.; Sharma, S.; Alam, M.A.; Ashafaq, M; Rub, R.A.; Ahmad, F.J. Brain-targeted glycyrrhizic-acid-loaded surface decorated nanoparticles for treatment of cerebral ischaemia and its toxicity assessment. *Nanomed. Biotechnol*. **2019**, *47*, 475–490. doi: 10.1080/21691401.2018.1561458.
2. Qiao, X.; Song, W.; Ji S., Wang; Q., Guo, D.; Ye, M. Separation and characterization of phenolic compounds andtriterpenoid saponins in licorice (Glycyrrhiza uralensis) using mobilephase-dependent reversed-phase reversed-phase comprehensivetwo-dimensional liquid chromatography coupled with massspectrometry. *J. Chromatogr. A*. **2015**, *1402*, 36–45.