

New Journal of Chemistry

Electronic Supplementary Information

Chemical Transformation of Ginsenoside Re by a Heteropoly Acid Investigated Using HPLC-MSⁿ/HRMS

Yang Xiu,^a Huan-Xi Zhao,^a Yue Gao,^a Wen-Long Liu^a and Shu-Ying Liu^{*a,b}

Jilin Ginseng Academy, Changchun University of Chinese Medicine, Changchun 130117, P. R. China, and Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022, P. R. China..

* Corresponding author. E-mail: syliu@ciac.ac.cn.

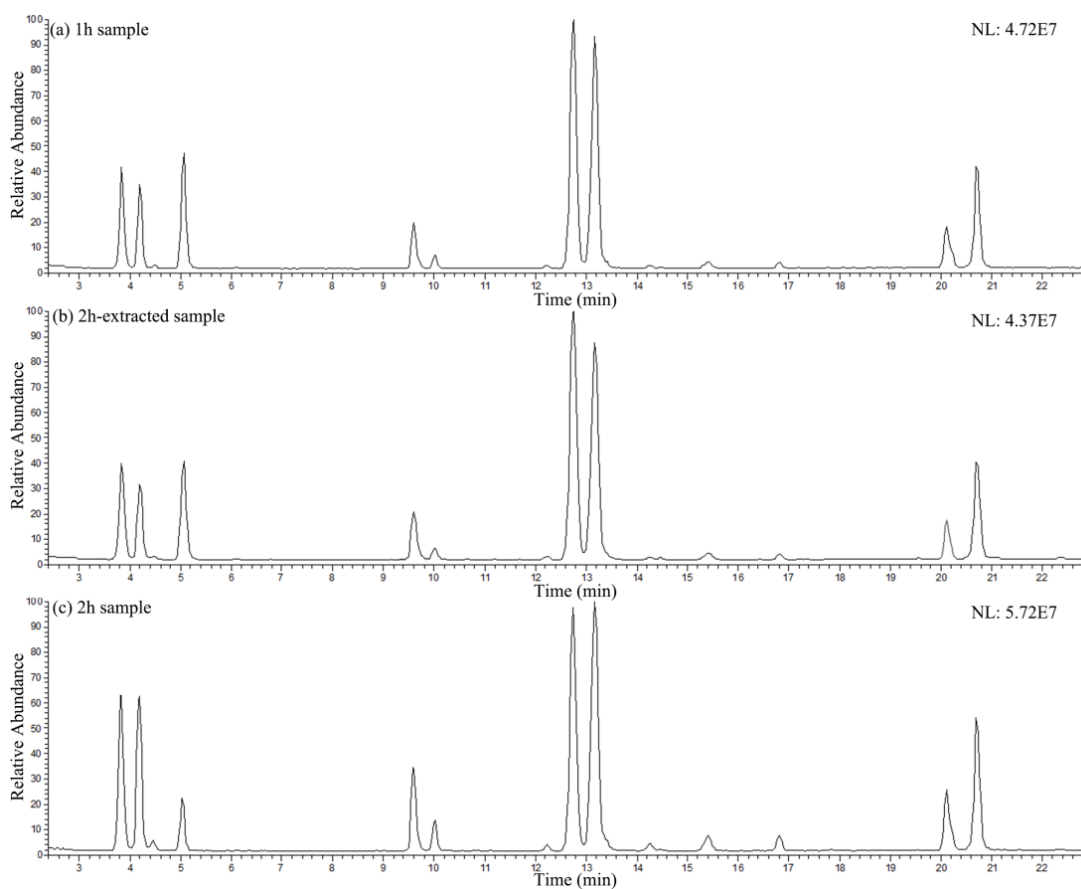


Fig. S1 TIC of the products of ginsenoside Re chemical transformation by H₃PW₁₂O₄₀ for (a) 1h, (b) 2h with extraction of catalyst at 1h and (c) 2h.

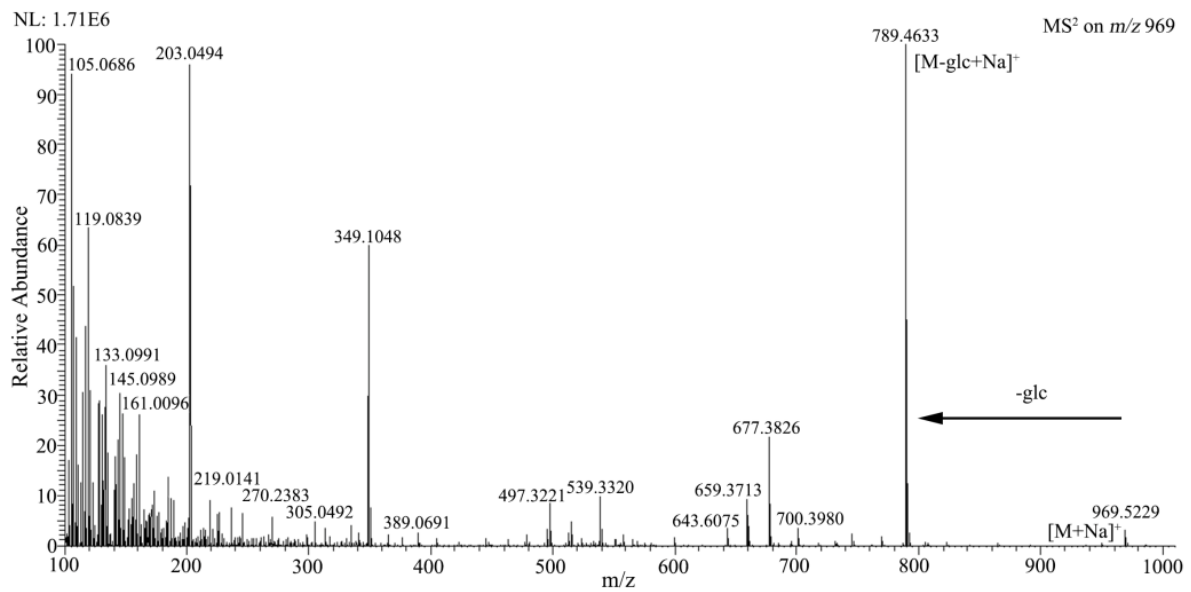


Fig. S2 High-resolution MS² spectrum from the [M+Na]⁺ ion at *m/z* 969 of ginsenoside Re.

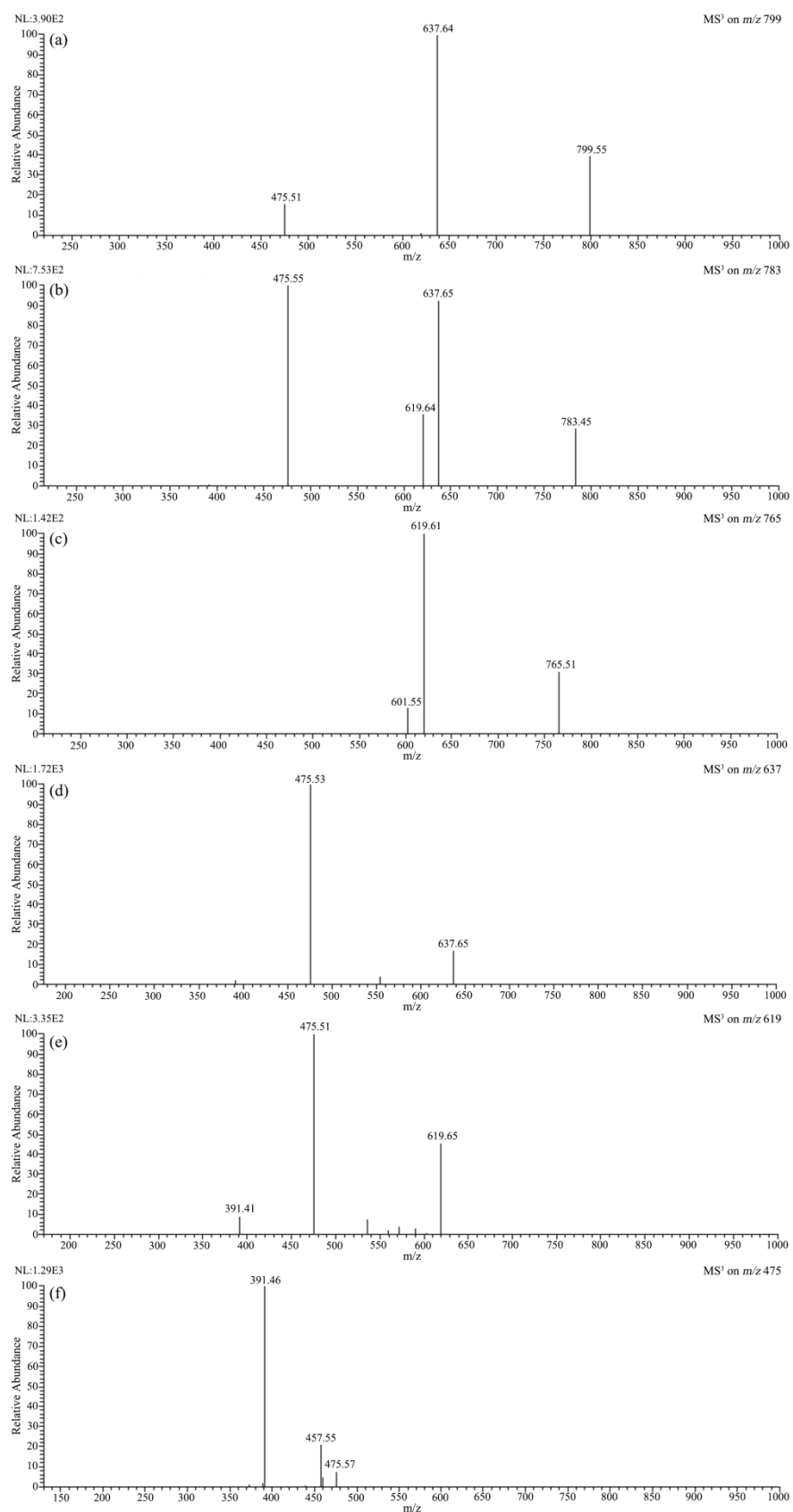


Fig. S3 MS³ spectra on the ions at m/z (a) 799, (b) 783, (c) 765, (d) 637, (e) 619 and (f) 475 from the [M+HCOO]⁻ ion of ginsenoside Re.

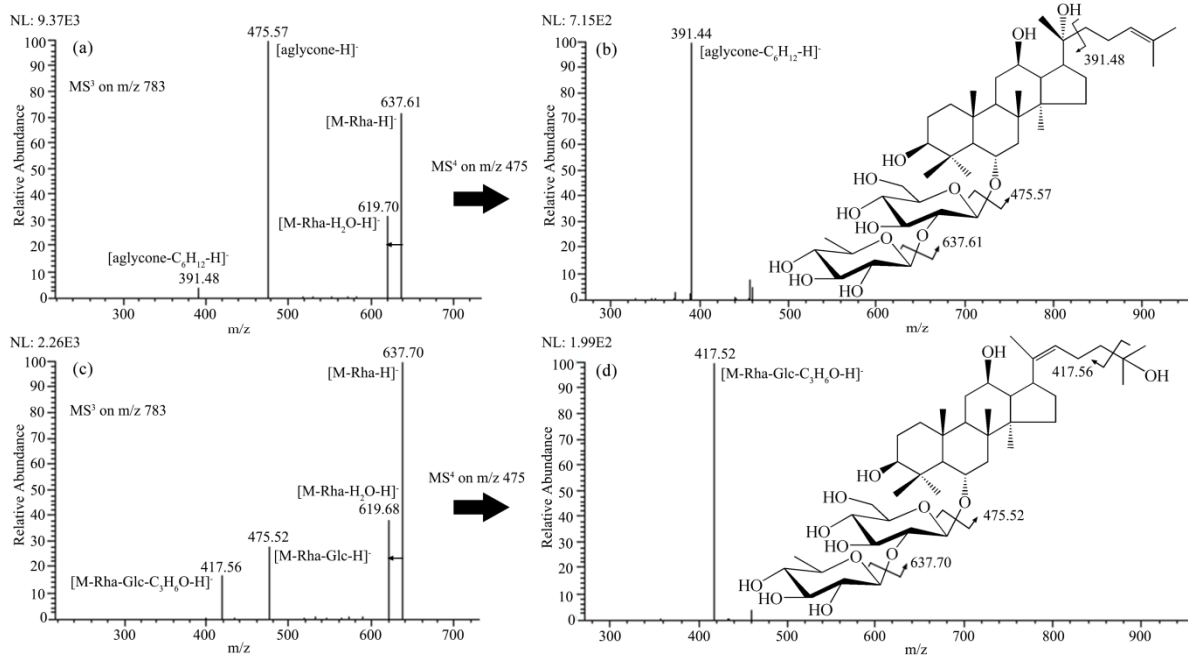


Fig. S4 MS³ spectra on the ions at m/z 783 from the [M+HCOO]⁻ ion of (a) ginsenoside 20(R)-Rg₂ and (c) 25-OH-F₄. Fragmentation pathways and MS⁴ spectra on the ions at m/z 475 from the [M+HCOO]⁻ ion of (b) ginsenoside 20(R)-Rg₂ and (d) 25-OH-F₄.

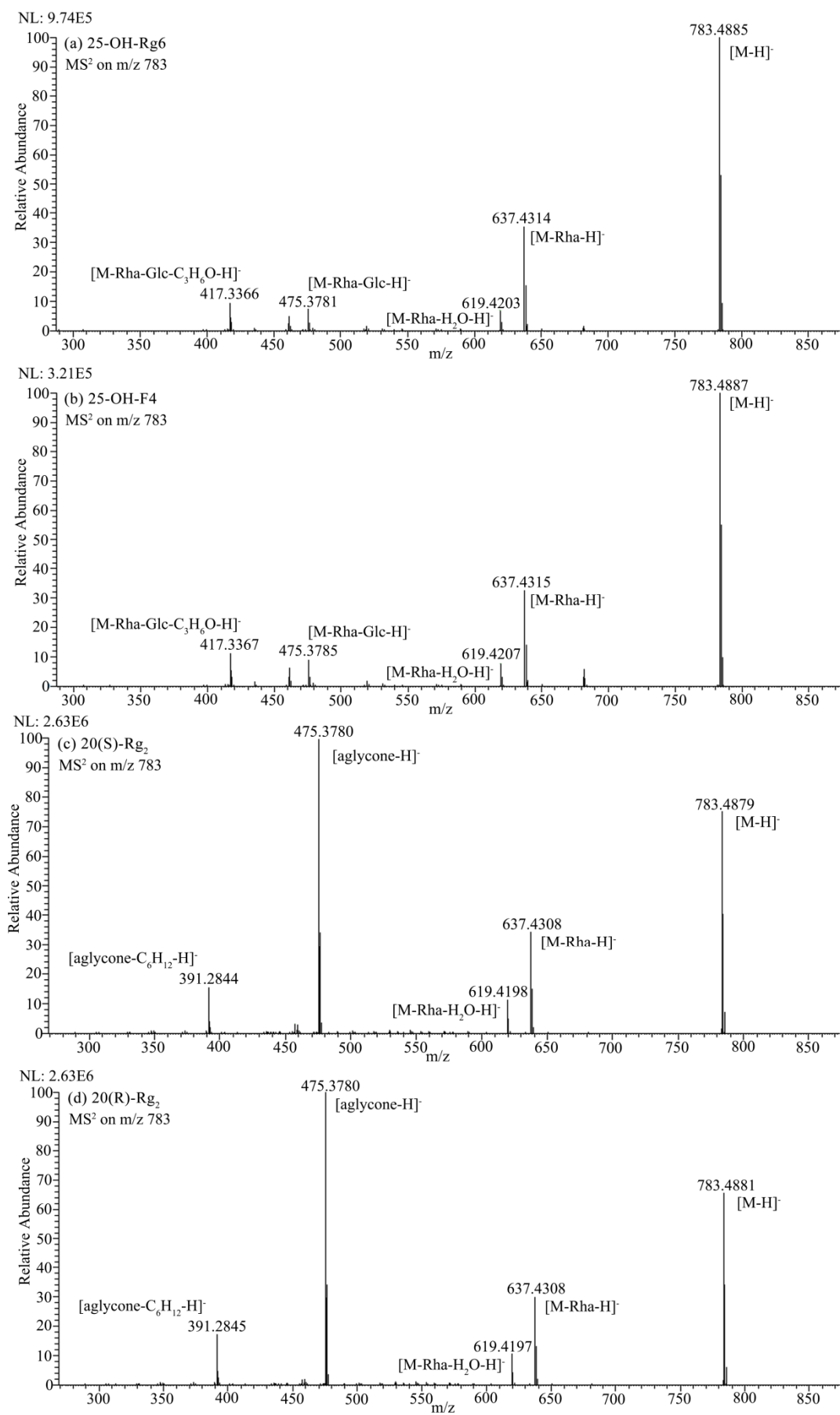


Fig. S5 High-resolution MS² spectra from the [M-H]⁻ ion of ginsenoside (a) 25-OH-F₄, (b) 25-OH-Rg₆, (c) 20(S)-Rg₂ and (d) 20(R)-Rg₂.

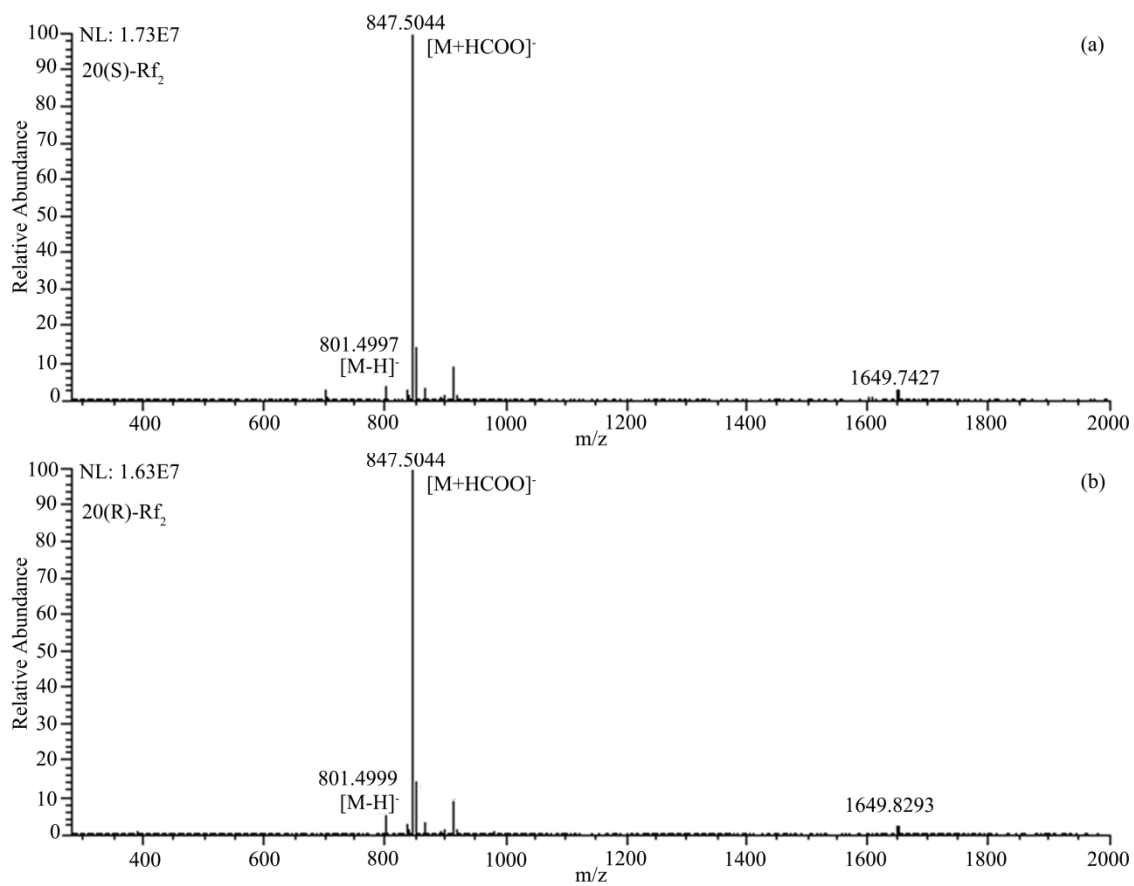


Fig. S6 High-resolution MS spectra of ginsenoside (a) 20(S)-Rf₂ and (b) 20(R)-Rf₂.

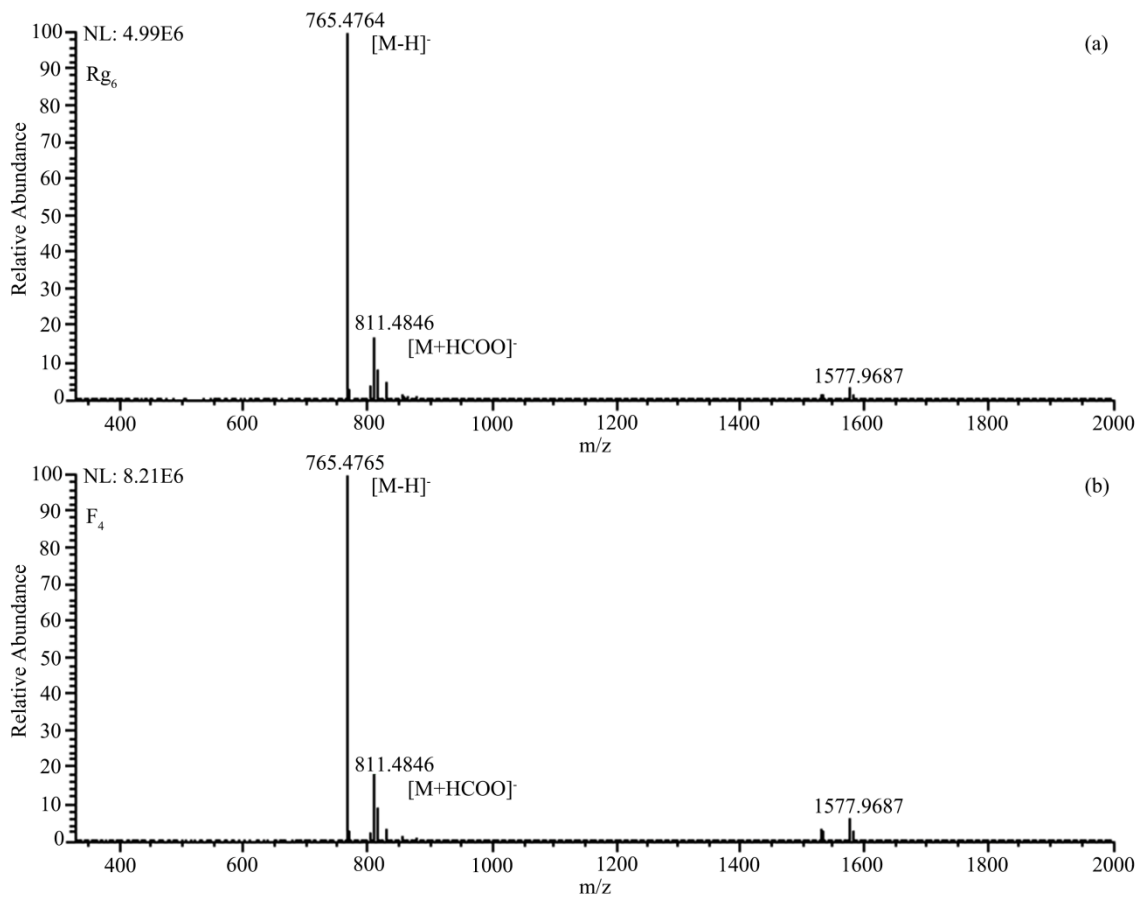


Fig. S7 High-resolution MS spectra of ginsenoside (a) Rg_6 and (b) F_4 .