

Supplementary Information

A Systematic Strategy for the Metabolites of Amentoflavone *in Vivo* and *in Vitro* Based on UHPLC-Q-TOF-MS/MS Analysis

Baolin Wang^{a,b}, Yimeng Lu^a, Xiaolong Hu^a, Jiahao Feng^a, Wei Shen^a, Rong Wang^a,
Hao Wang^{a,□}

^a State Key Laboratory of Natural Medicines, Department of TCM Pharmaceuticals,
School of Traditional Chinese Pharmacy, China Pharmaceutical University, Nanjing
210009, People's Republic of China

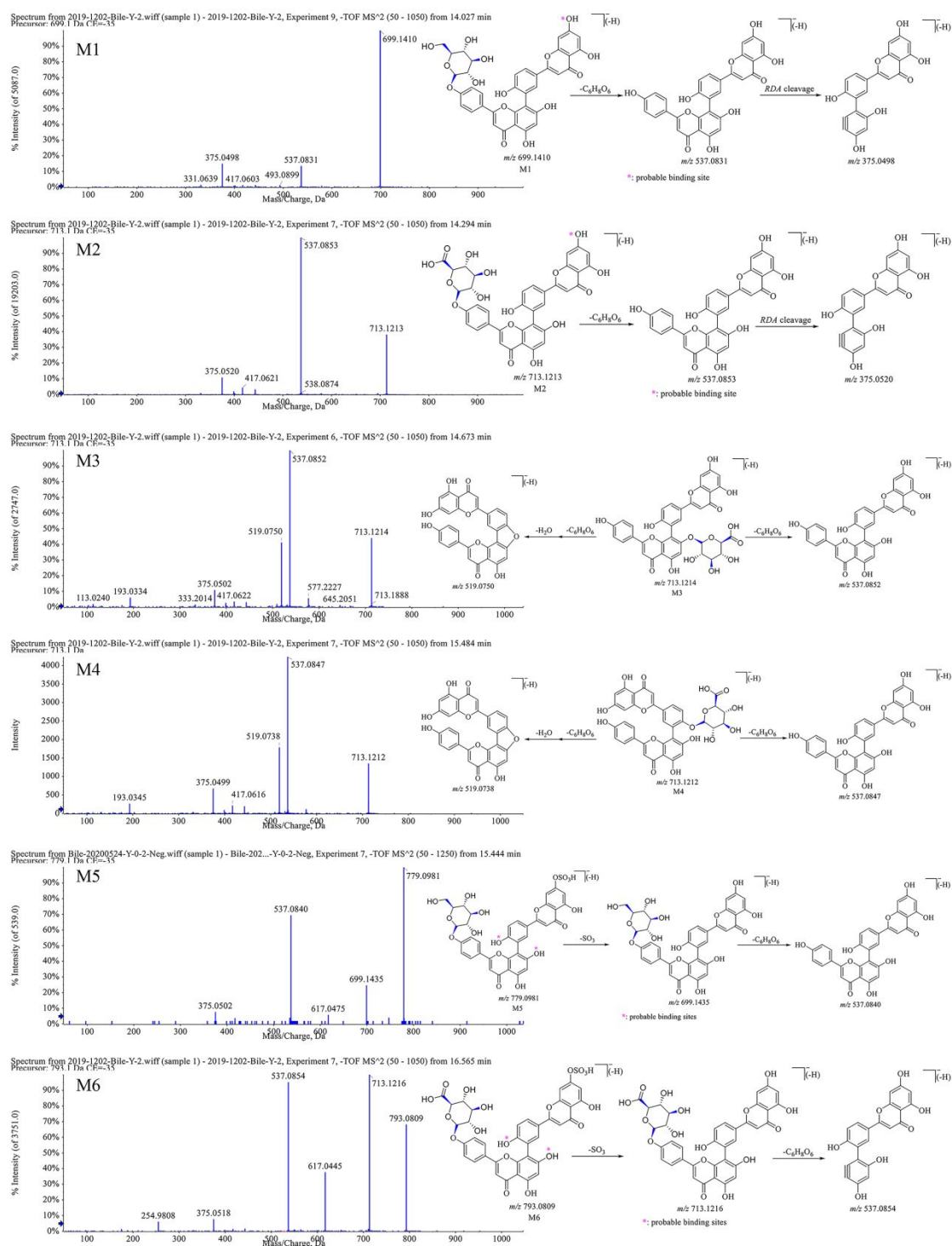
^b Nanchang Key Laboratory of Quality Control and Safety Evaluation of TCM,
Nanchang Institute for Food and Drug Control, Nanchang 330012, People's Republic
of China

*Corresponding author

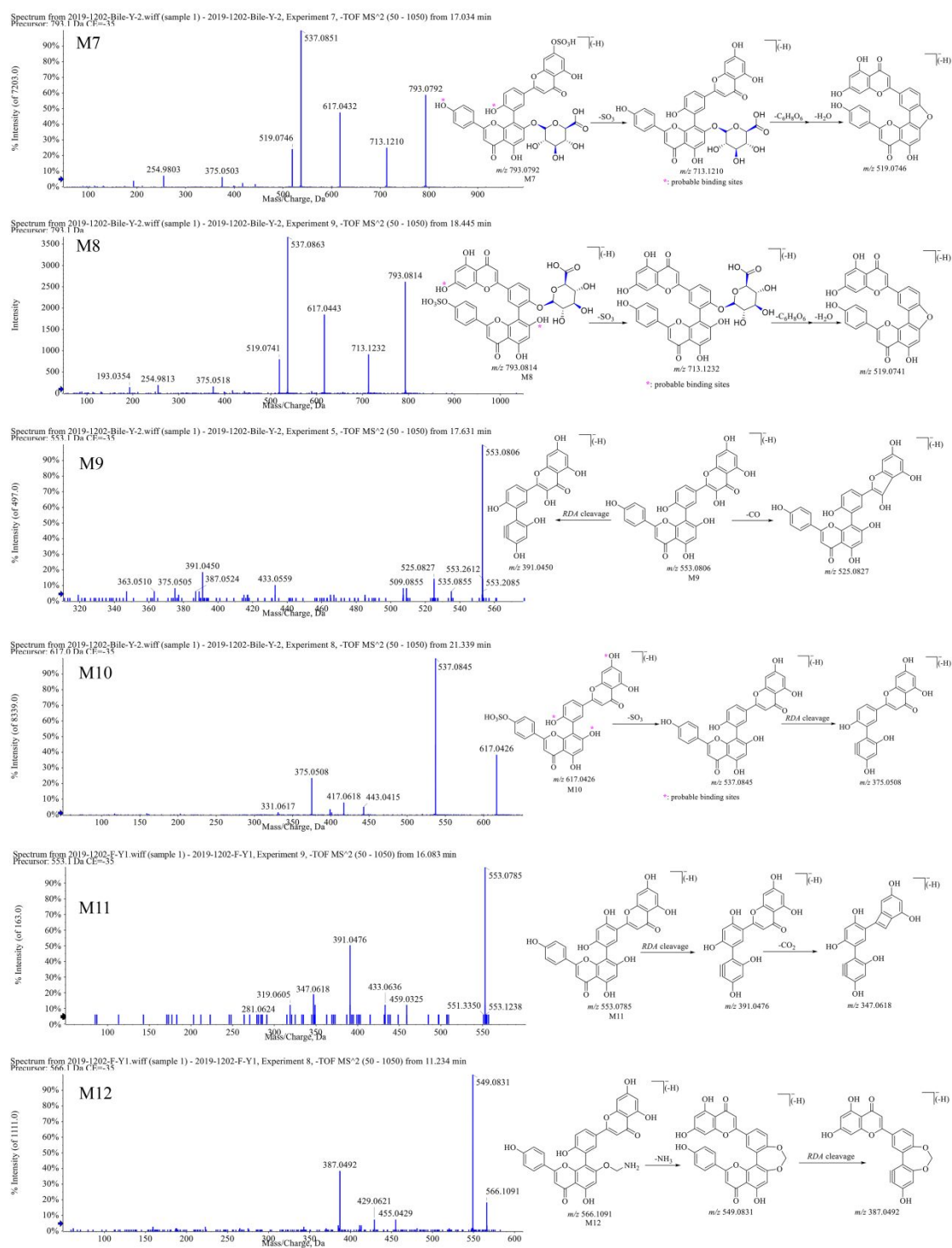
Tel: +86-025-83271328; Fax: +86-025-83271328; Email: wanghao@cpu.edu.cn (H.
Wang).

Supplementary Figure Captions

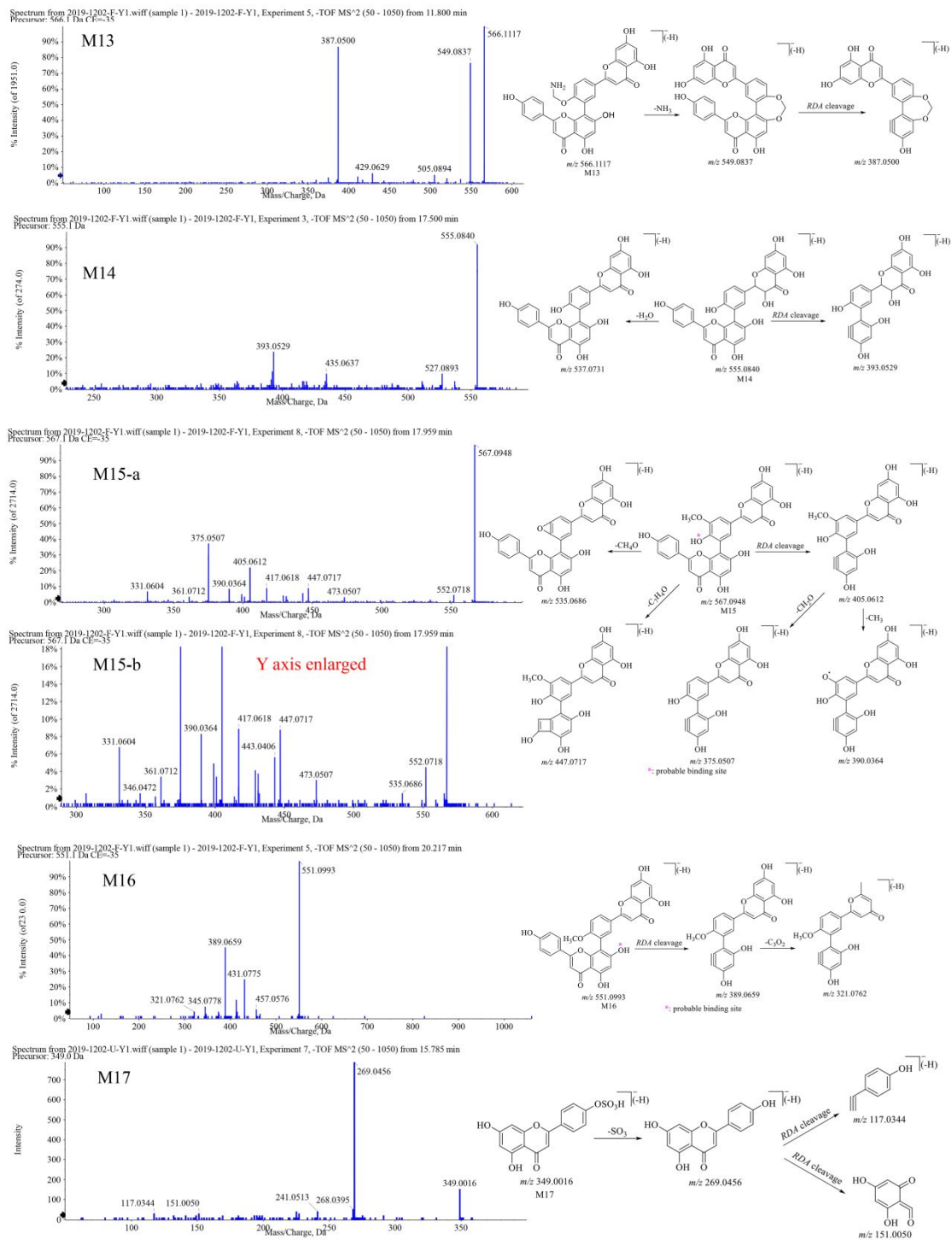
Supplementary Figure 1-1: The MS/MS spectra of M1-6 -----	3
Supplementary Figure 1-2: The MS/MS spectra of M7-12 -----	4
Supplementary Figure 1-3: The MS/MS spectra of M13-17 -----	5
Supplementary Figure 1-4: The MS/MS spectra of M18-22 -----	6
Supplementary Figure 1-5: The MS/MS spectra of M23-28 -----	7
Supplementary Figure 1-6: The MS/MS spectra of M29-34 -----	8
Supplementary Figure 1-7: The MS/MS spectra of M35-40 -----	9
Supplementary Figure 1-8: The MS/MS spectra of M41-43 -----	10



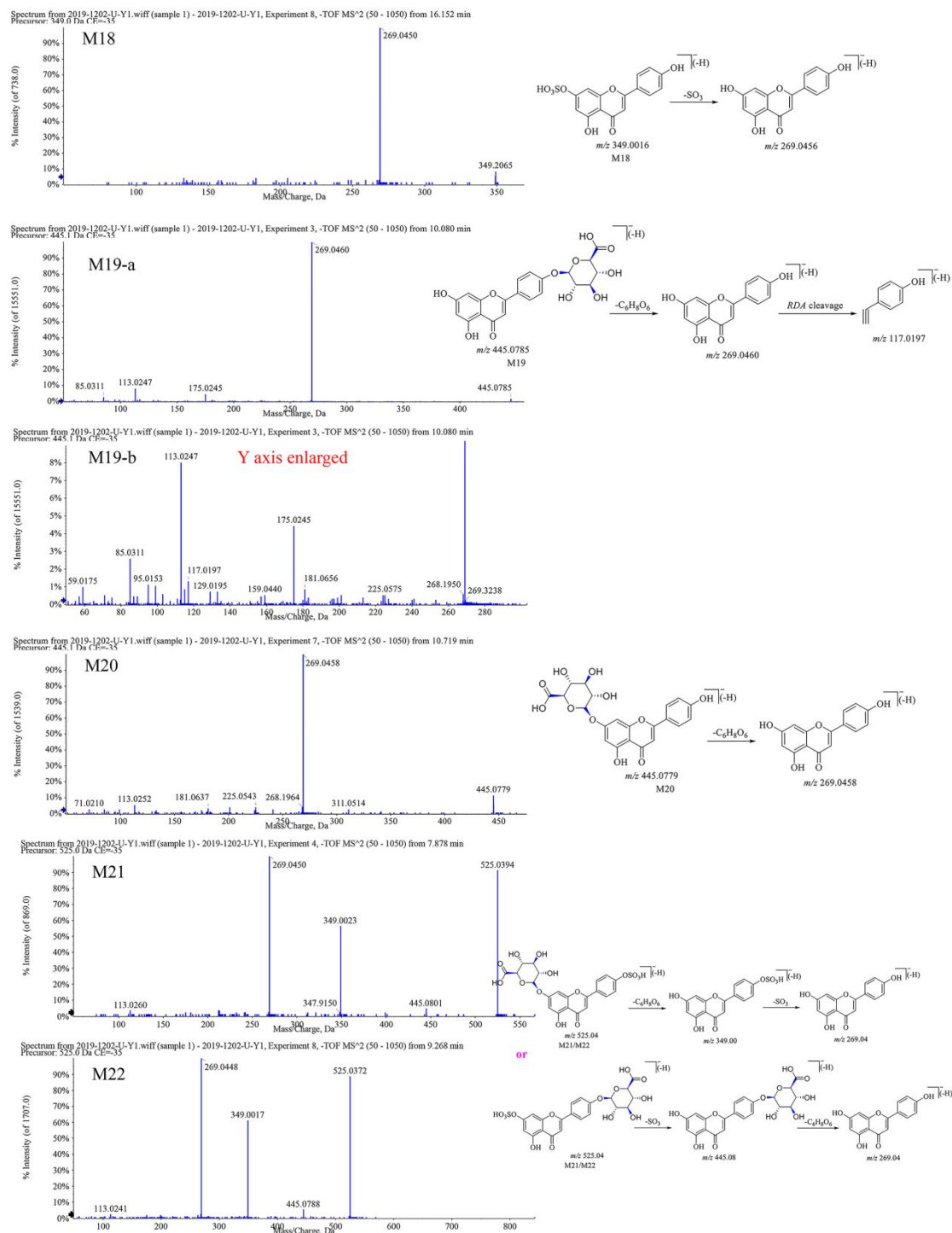
Supplementary Figure 1-1



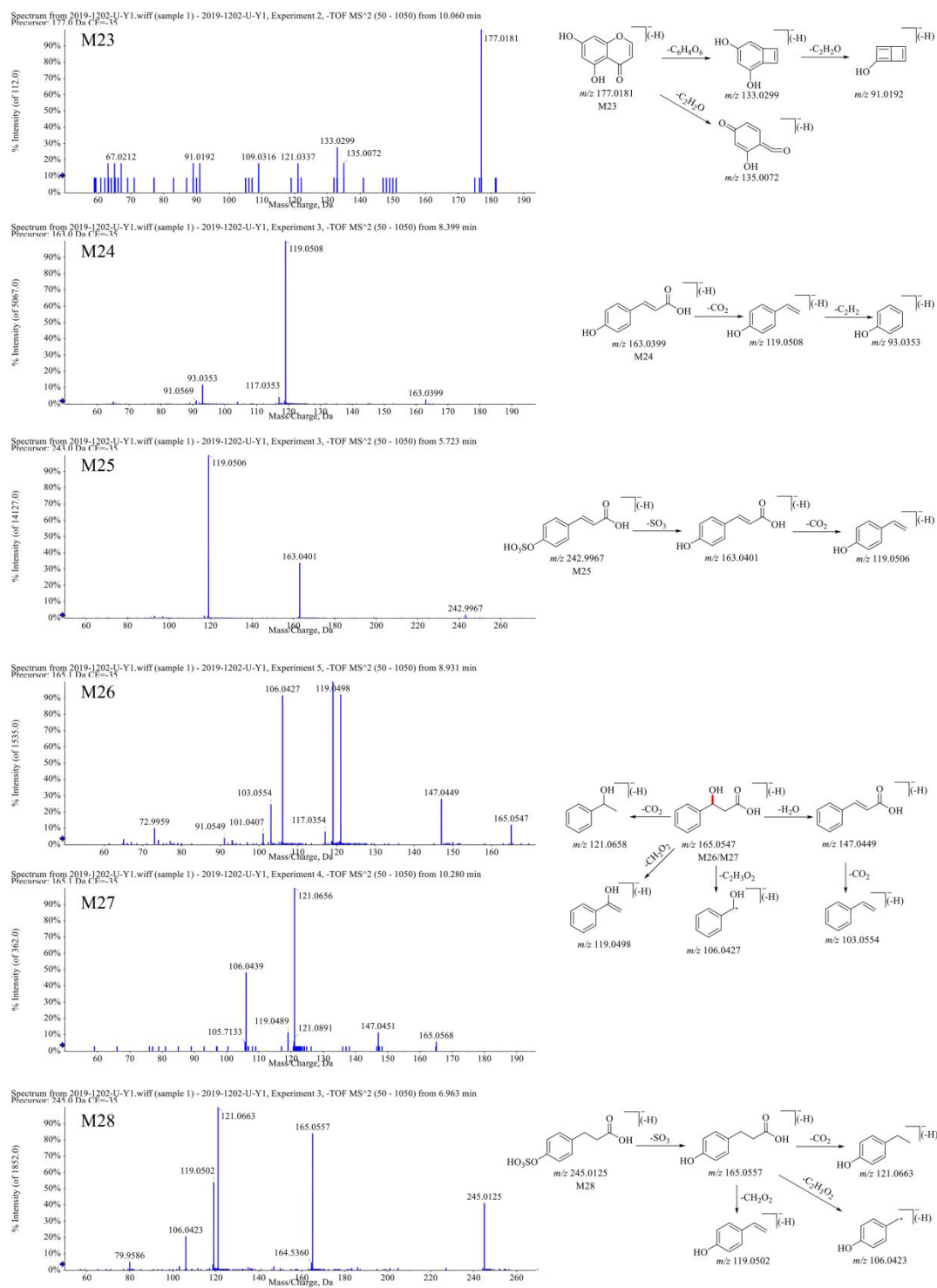
Supplementary Figure 1-2



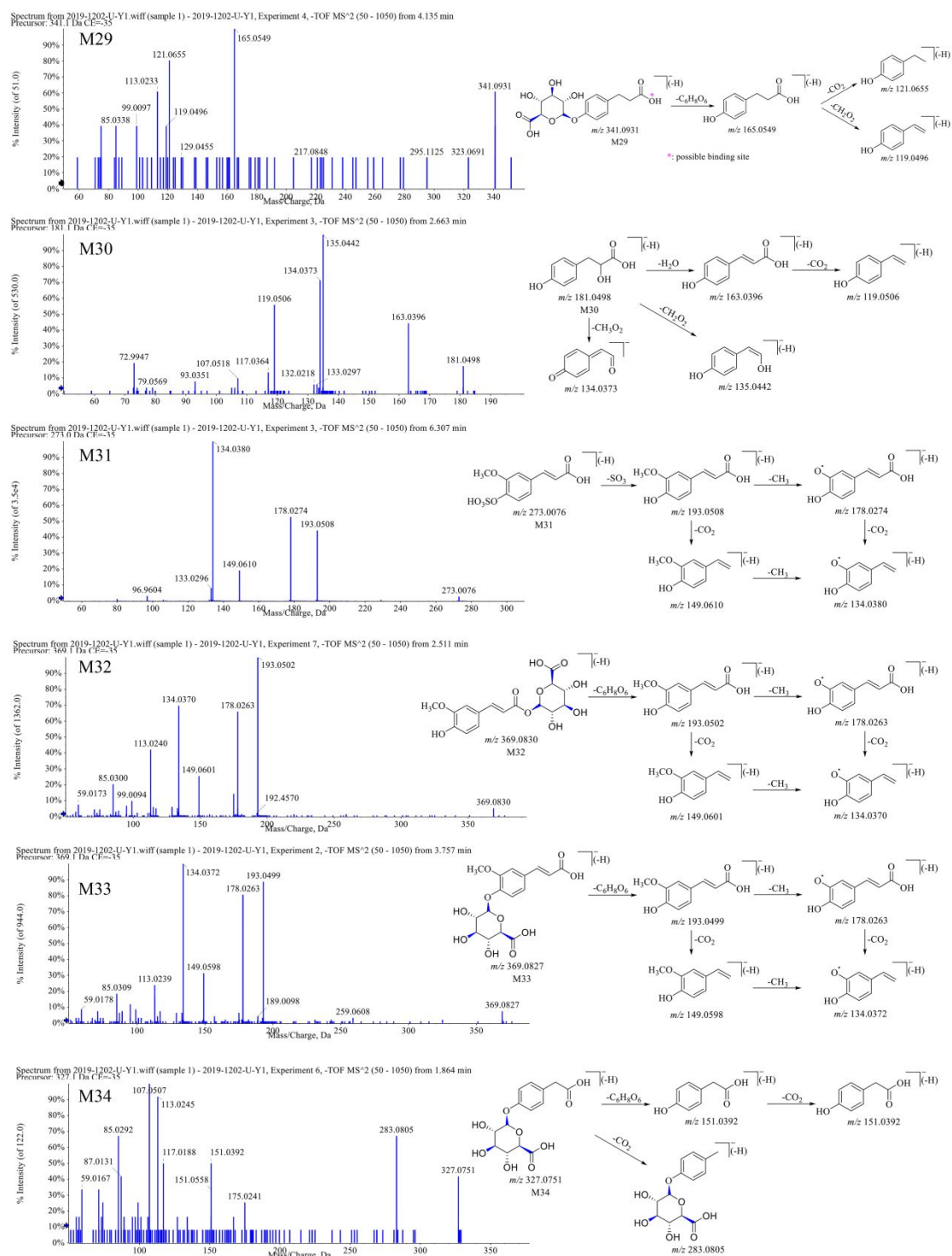
Supplementary Figure 1-3



Supplementary Figure 1-4

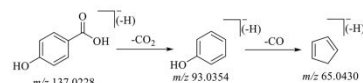
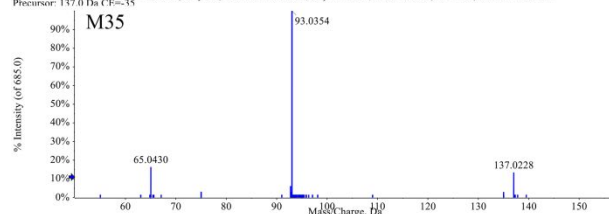


Supplementary Figure 1-5

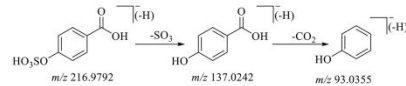
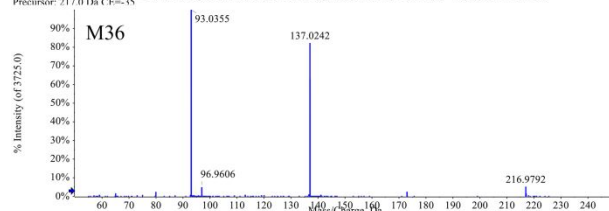


Supplementary Figure 1-6

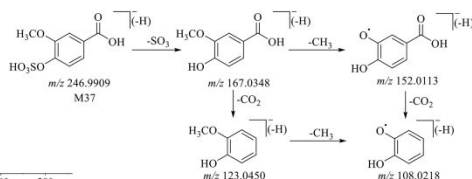
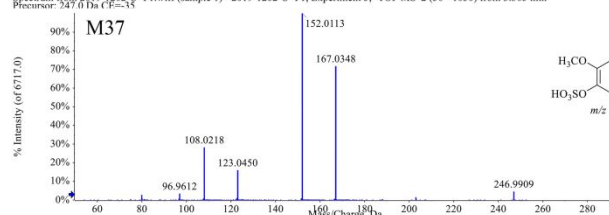
Spectrum from 2019-1202-U-Y1.wiff (sample 1) - 2019-1202-U-Y1, Experiment 3, -TOF MS² (50 - 1050) from 11.613 min
Precursor: 137.0 Da C₇H₅O₃



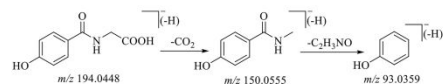
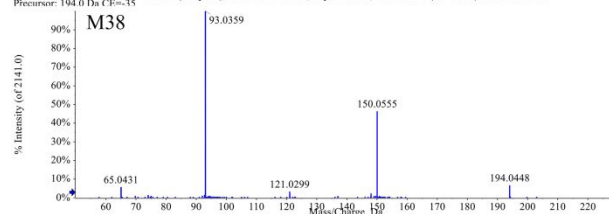
Spectrum from 2019-1202-U-Y1.wiff (sample 1) - 2019-1202-U-Y1, Experiment 4, -TOF MS² (50 - 1050) from 2.933 min
Precursor: 216.9 Da C₇H₅O₄S



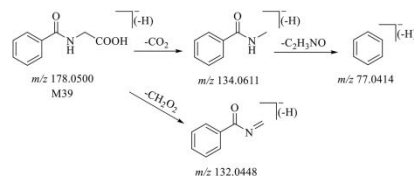
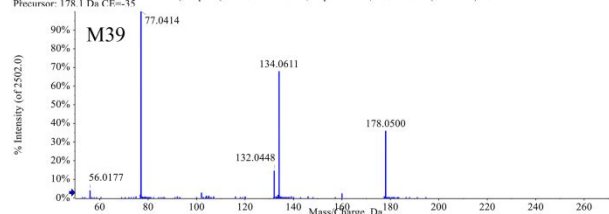
Spectrum from 2019-1202-U-Y1.wiff (sample 1) - 2019-1202-U-Y1, Experiment 5, -TOF MS² (50 - 1050) from 3.305 min
Precursor: 246.9 Da C₉H₇O₅S



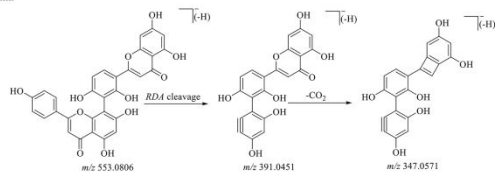
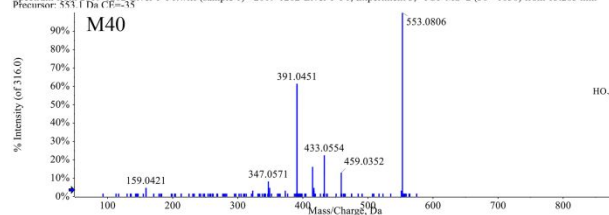
Spectrum from 2019-1202-U-Y1.wiff (sample 1) - 2019-1202-U-Y1, Experiment 3, -TOF MS² (50 - 1050) from 8.622 min
Precursor: 194.0 Da C₈H₇O₃N



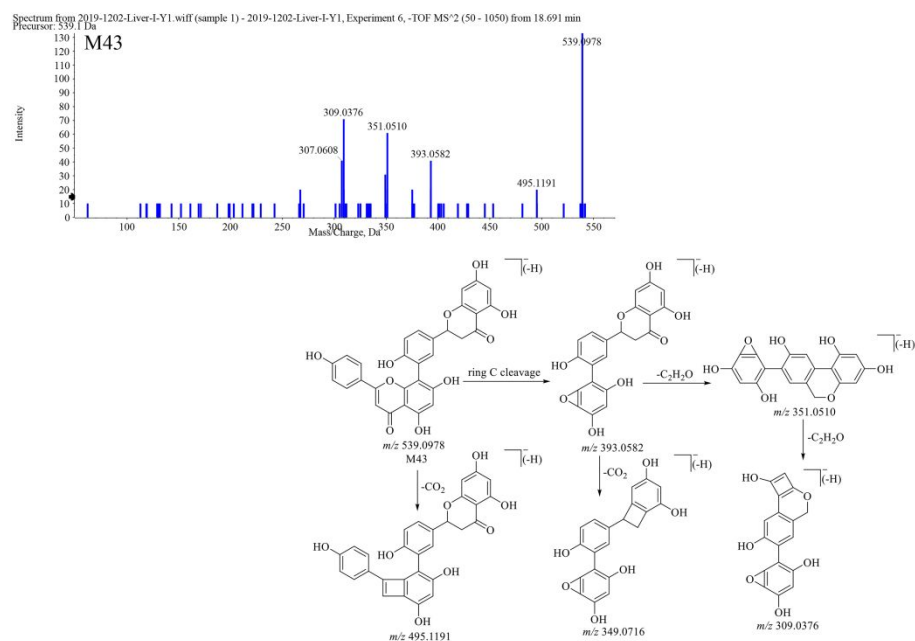
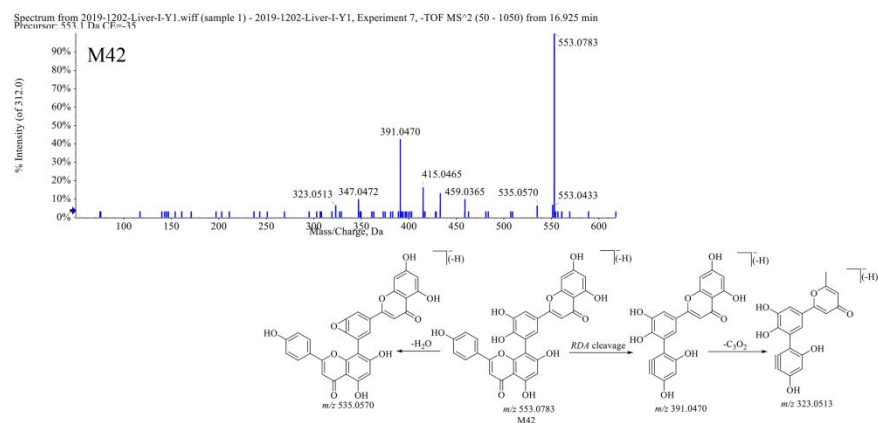
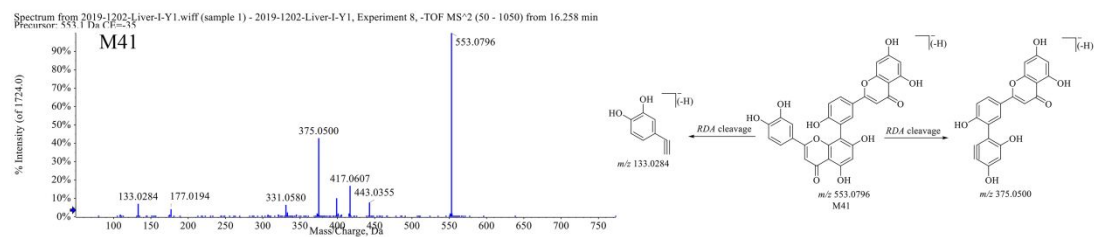
Spectrum from 2019-1202-U-Y1.wiff (sample 1) - 2019-1202-U-Y1, Experiment 4, -TOF MS² (50 - 1050) from 5.744 min
Precursor: 178.0 Da C₈H₇O₃N



Spectrum from 2019-1202-Liver-I-Y1.wiff (sample 1) - 2019-1202-Liver-I-Y1, Experiment 5, -TOF MS² (50 - 1050) from 15.285 min
Precursor: 553.0 Da C₂₁H₁₅O₁₀



Supplementary Figure 1-7



Supplementary Figure 1-8