

Profiling and Preparation of Metabolites from Pyragrel in Human Urine by Online Solid-Phase Extraction Coupled with High Performance Liquid Chromatography Tandem Mass Spectrometry Followed by a Macroporous Resin-Based Purification Approach

Xin Zhao ^{1,†}, Jingjing Jiang ^{2,†}, Guang Yang ², Jie Huang ³, Guoping Yang ³, Guangwei He ⁴, Zhaoxing Chu ⁴, Taijun Hang ^{1,*} and Guorong Fan ^{2,5,6,*}

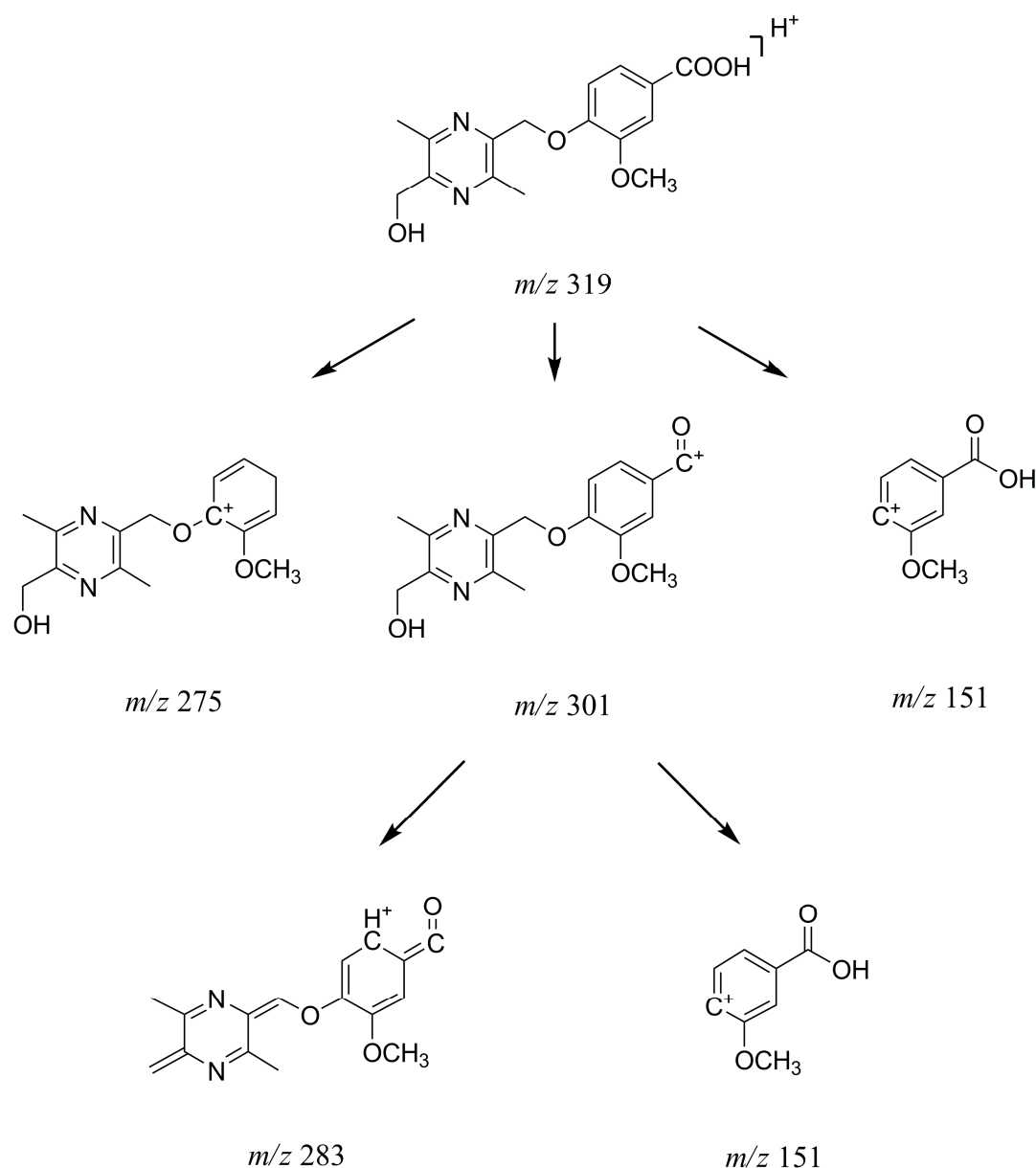


Fig. S1 Inferred fragmentation patterns of metabolite M2.

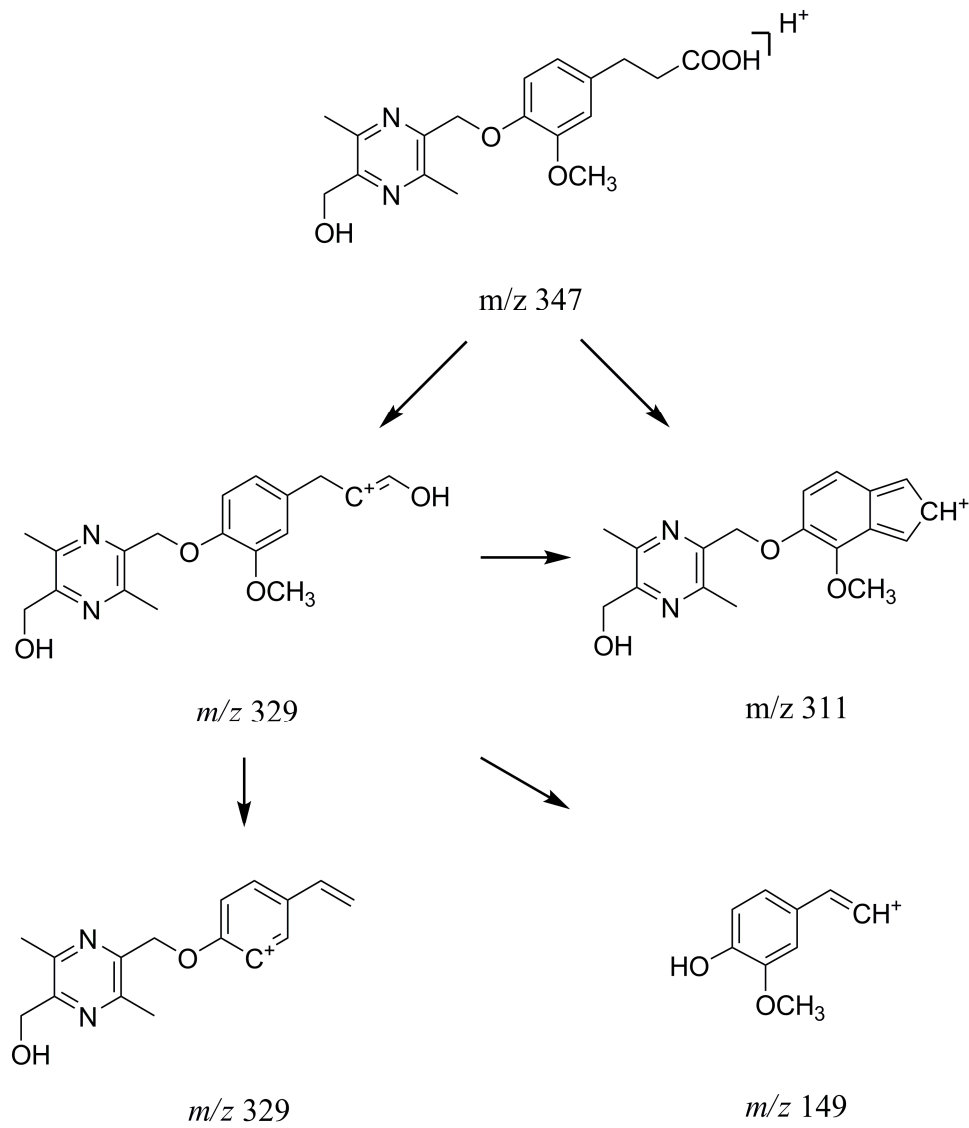


Fig. S2 Inferred fragmentation patterns of metabolite M3.

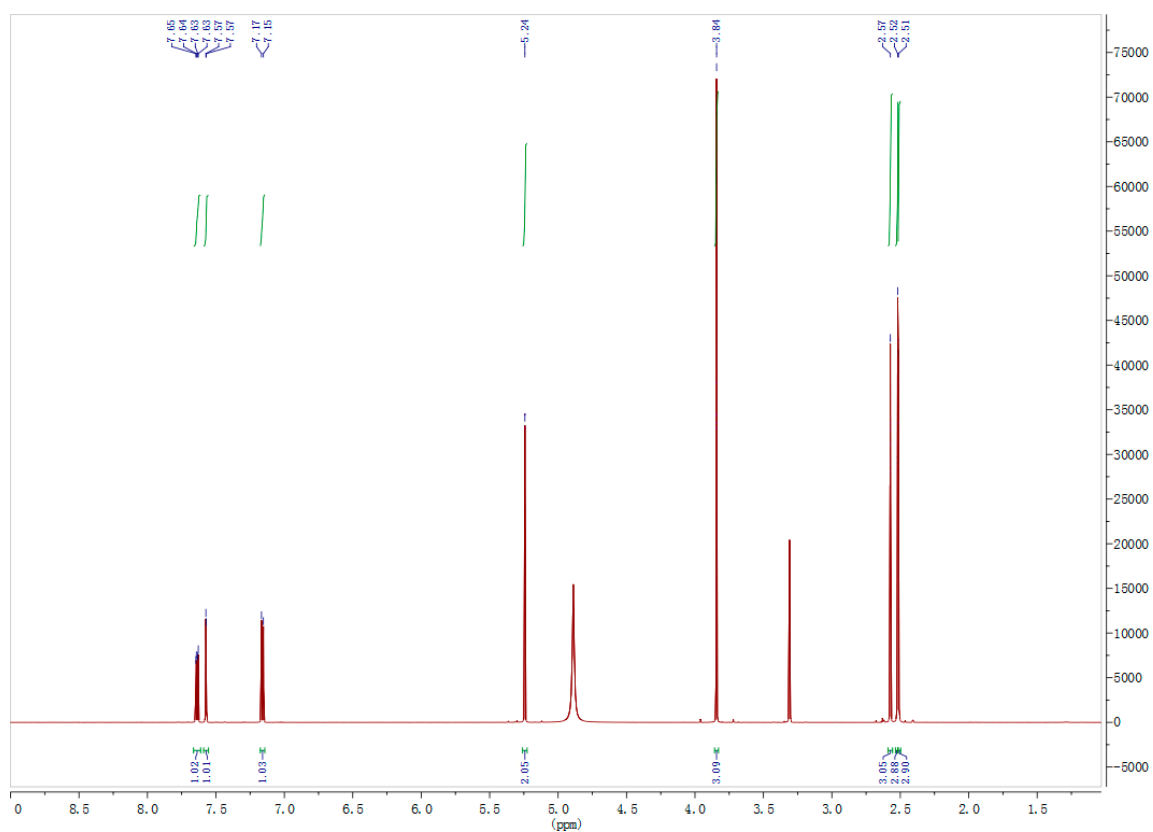


Fig. S3 ^1H NMR spectrum of metabolite M4.

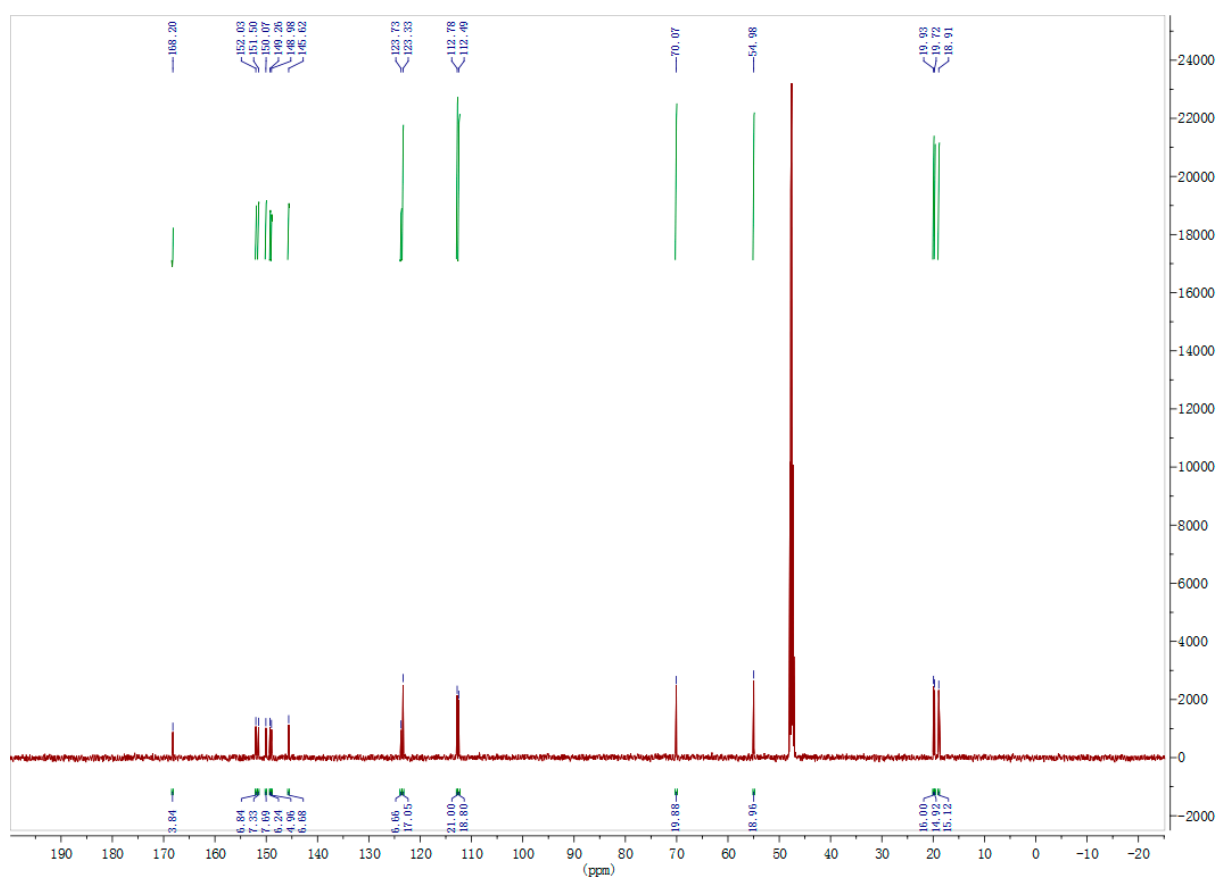


Fig. S4 ^{13}C NMR spectrum of metabolite M4.

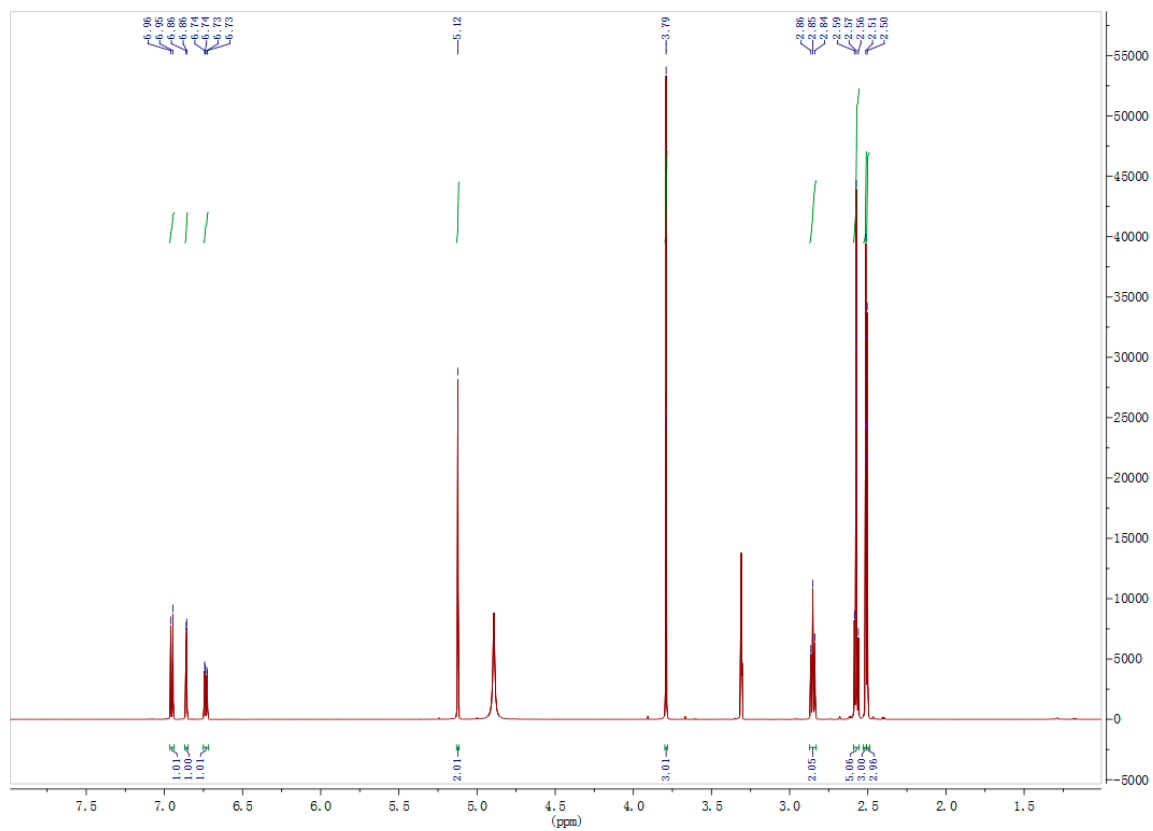


Fig. S5 ^1H NMR spectrum of metabolite M5.

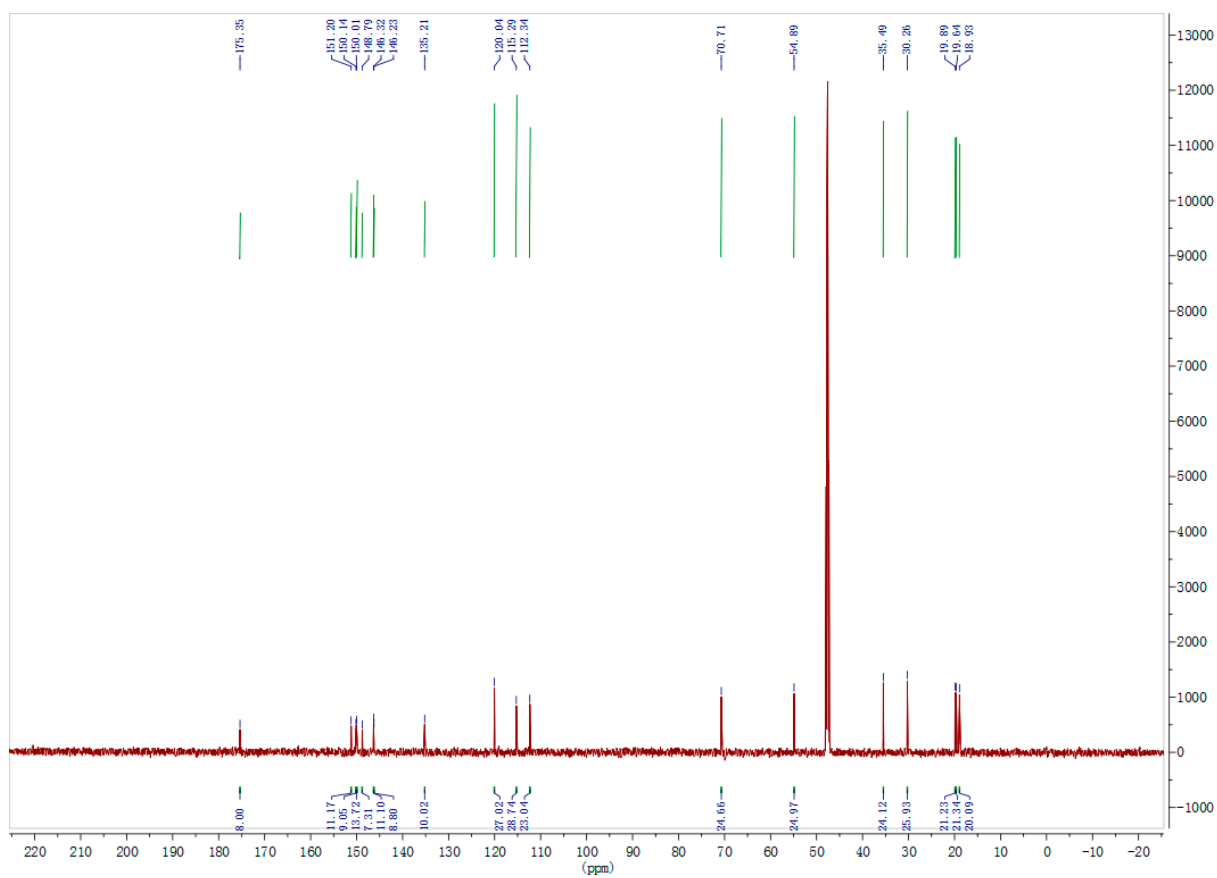


Fig. S6 ^{13}C NMR spectrum of metabolite M5.