

Supplementary materials

Development and Validation of a Novel LC-MS/MS Method for the Simultaneous Determination of Abemaciclib, Palbociclib, Ribociclib, Anastrozole, Letrozole, and Fulvestrant in Plasma Samples: A Prerequisite for Personalized Breast Cancer Treatment

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Section 1. Chromatograms and MS/MS spectra of the analyzed single-point patient samples:

Patient 1 (ABE + LET)

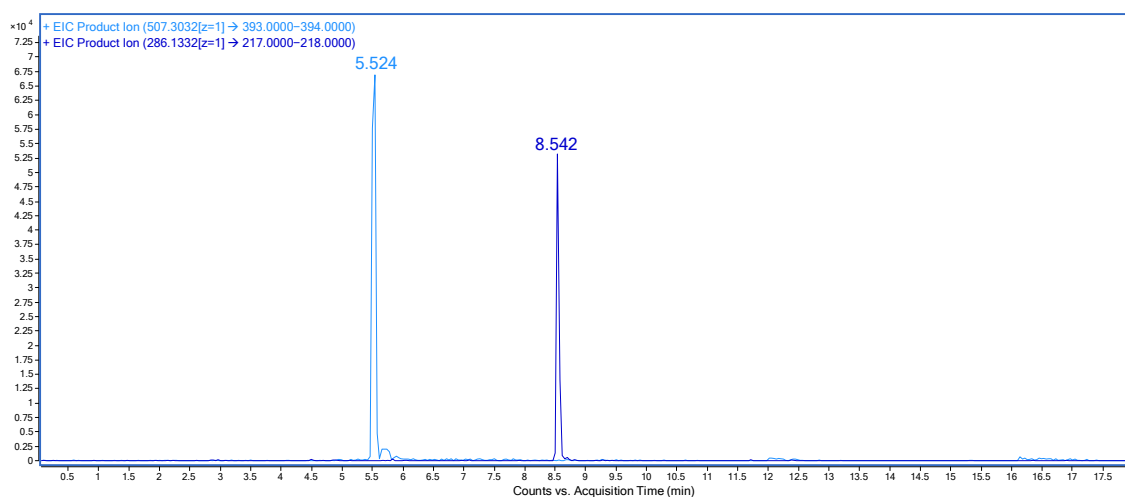


Figure S1. EIC of ABE (transition m/z 507.3→393.2) and LET (transition m/z 286.1→217.1).

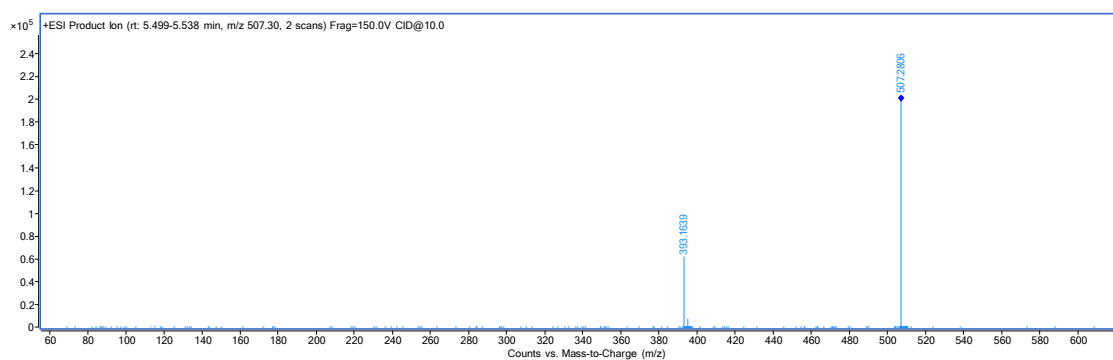


Figure S2. Mass spectrum of peak 1 (ABE, tr 5.524 min).

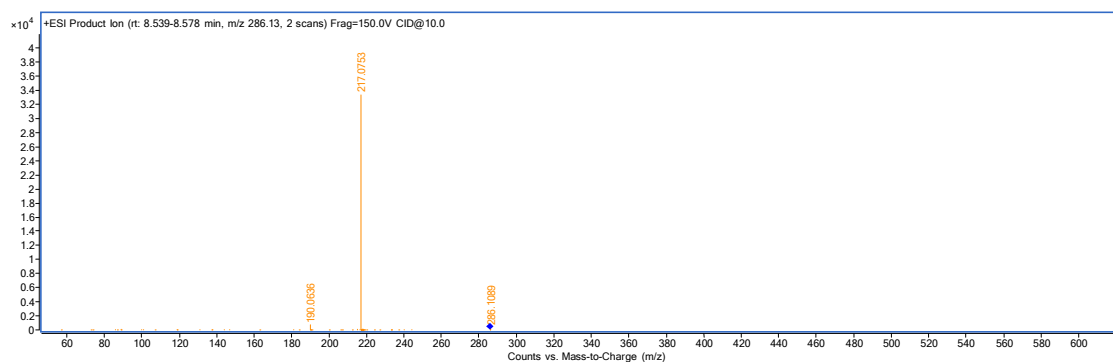


Figure S3. Mass spectrum of peak 2 (LET, tr 8.542 min).

Patient 2 (RIB + LET)

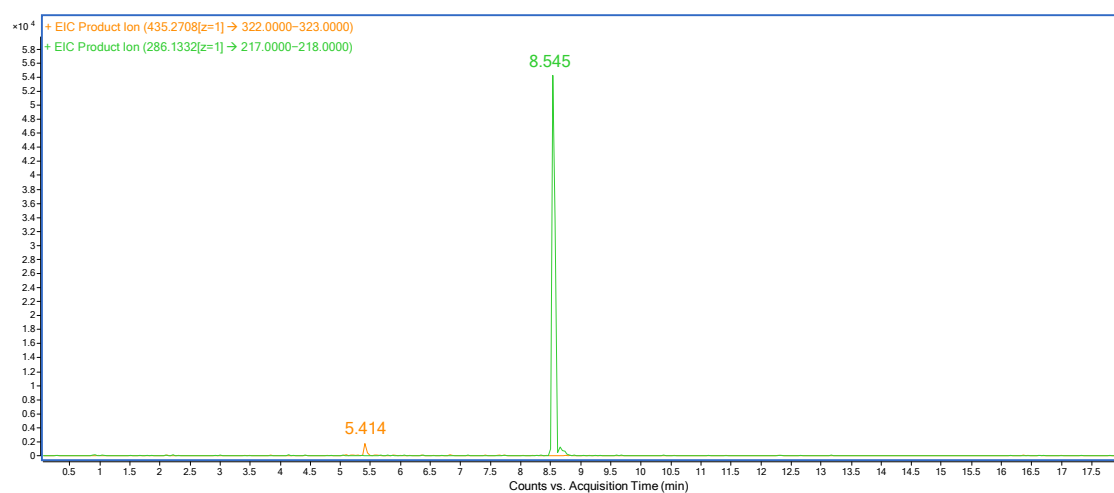


Figure S4. EIC of RIB (transition m/z 435.3→322.1) and LET (transition m/z 286.1→217.1).

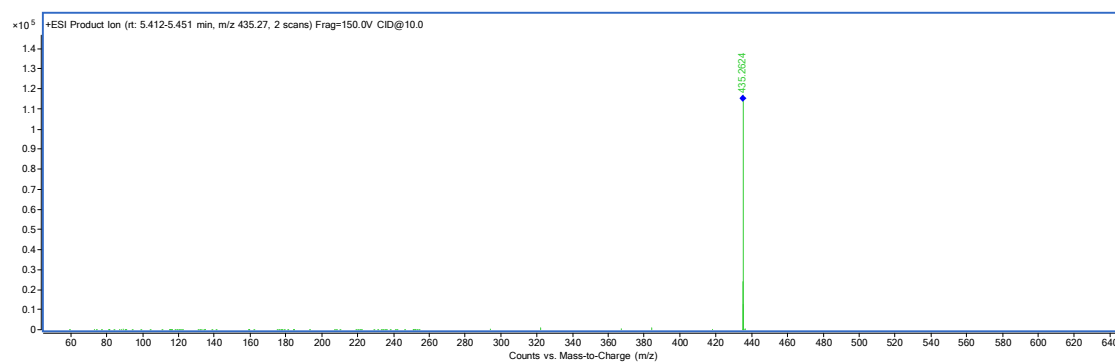


Figure S5. Mass spectrum of peak 1 (RIB, tr 5.414 min).

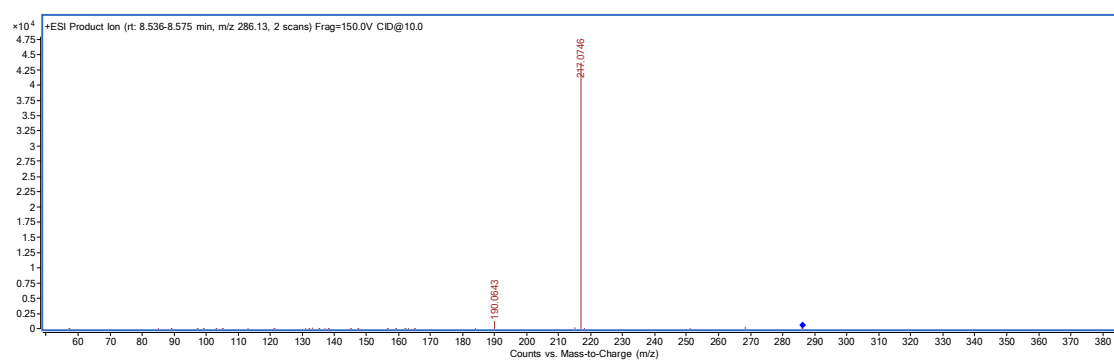


Figure S6. Mass spectrum of peak 2 (LET, tr 8.545 min).

Patient 3 (RIB + LET)

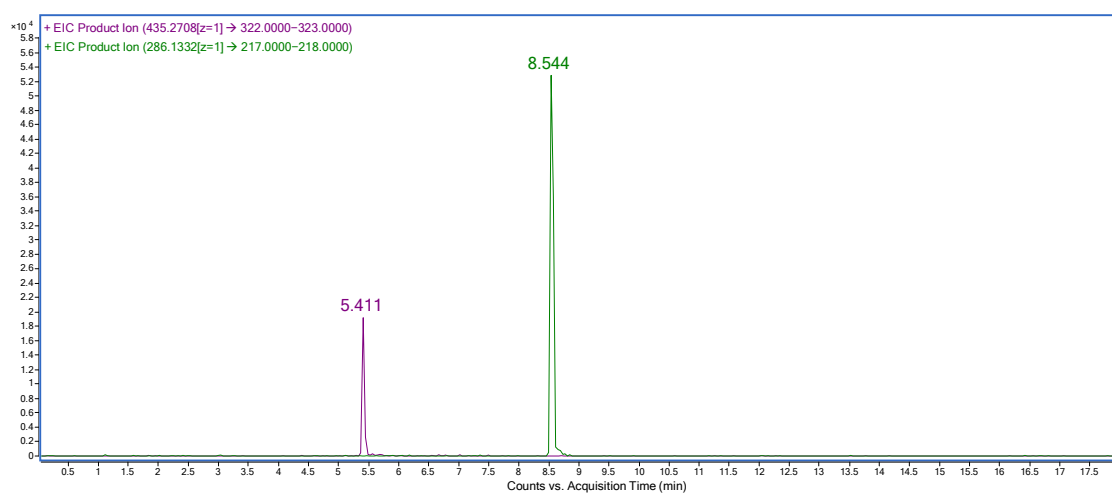


Figure S7. EIC of RIB (transition m/z 435.3→322.1) and LET (transition m/z 286.1→217.1).

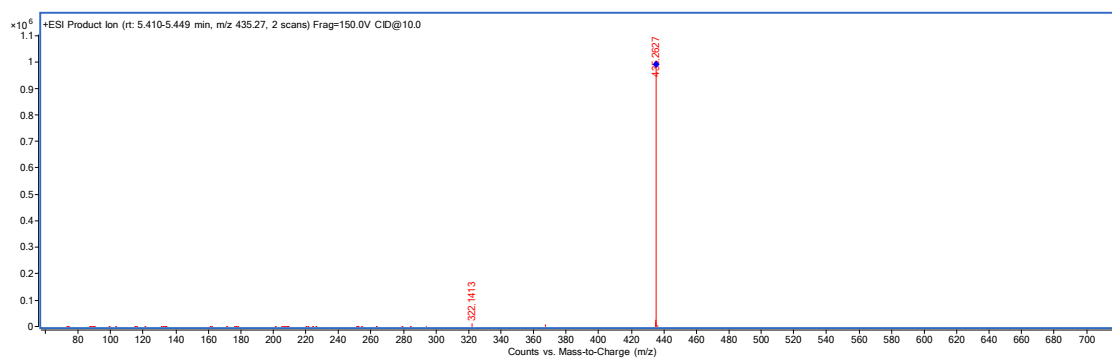


Figure S8. Mass spectrum of peak 1 (RIB, tr 5.411 min).

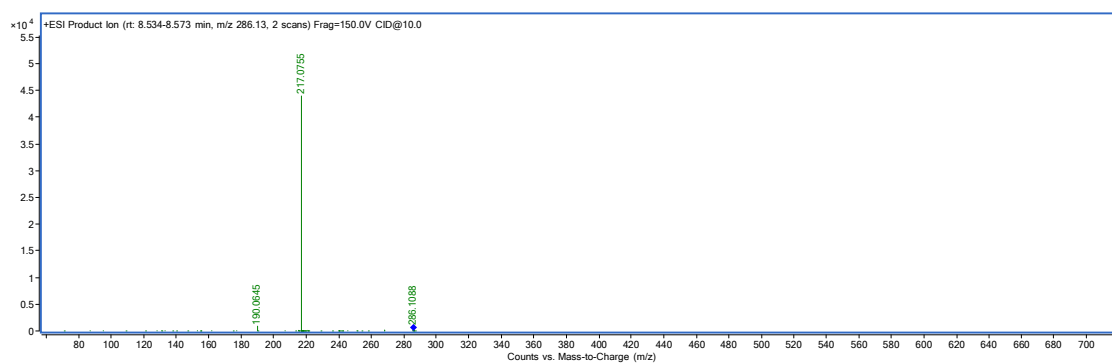


Figure S9. Mass spectrum of peak 2 (LET, tr 8.544 min).

Patient 4 (RIB + LET)

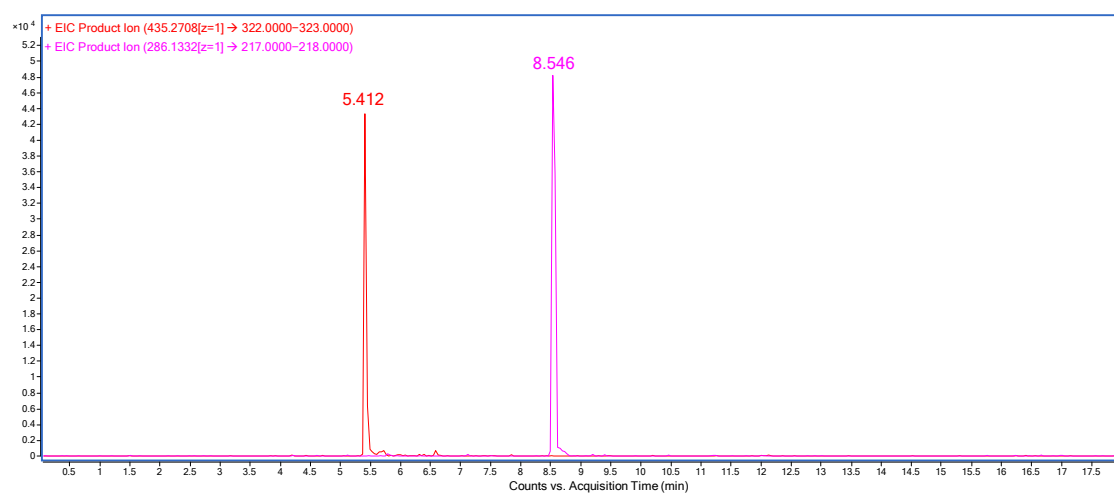


Figure S10. EIC of RIB (transition m/z 435.3 \rightarrow 322.1) and LET (transition m/z 286.1 \rightarrow 217.1).

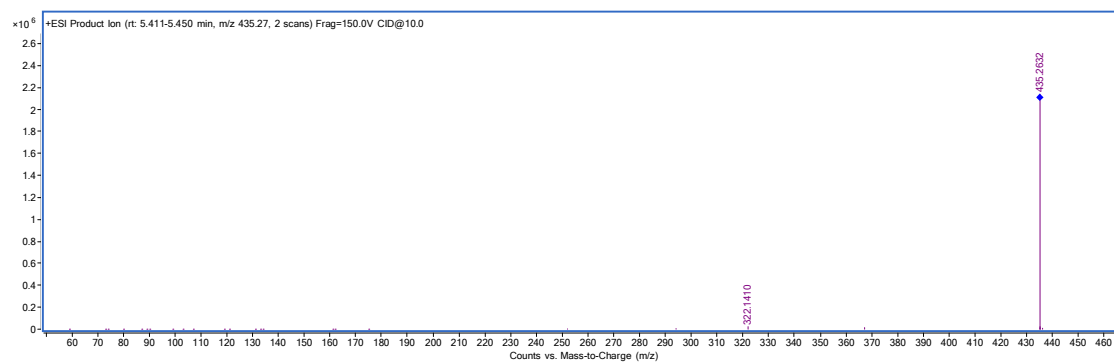


Figure S11. Mass spectrum of peak 1 (RIB, tr 5.412 min).

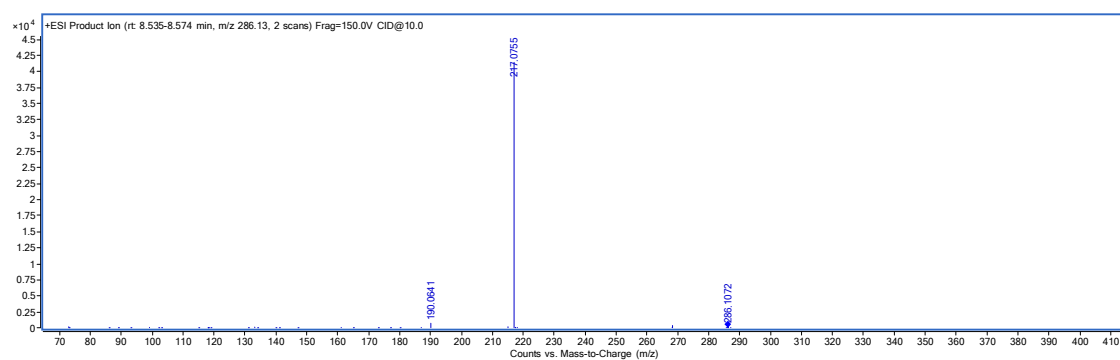


Figure S12. Mass spectrum of peak 2 (LET, tr 8.546 min).

Patient 5 (RIB + ANA)

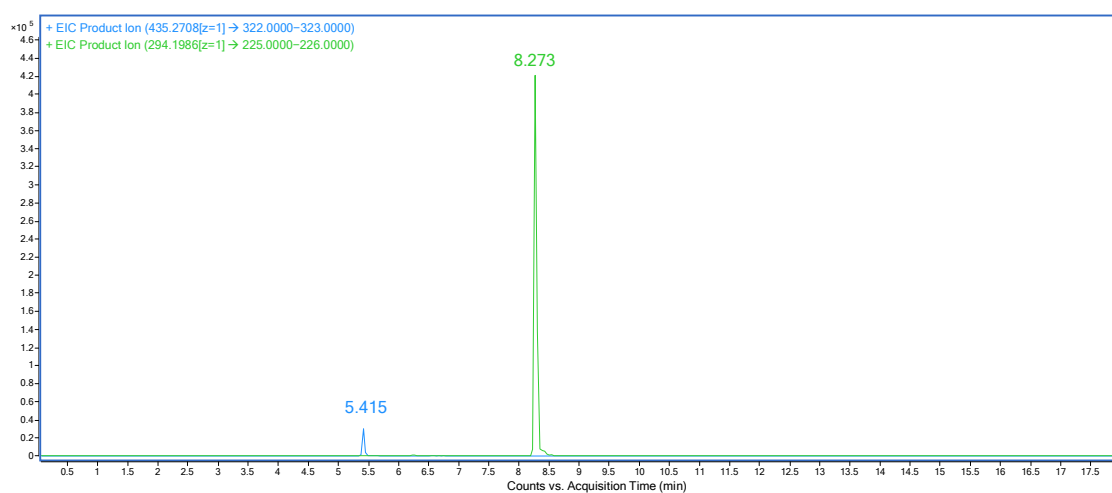


Figure S13. EIC of RIB (transition m/z 435.3→322.1) and ANA (transition m/z 294.2→225.1).

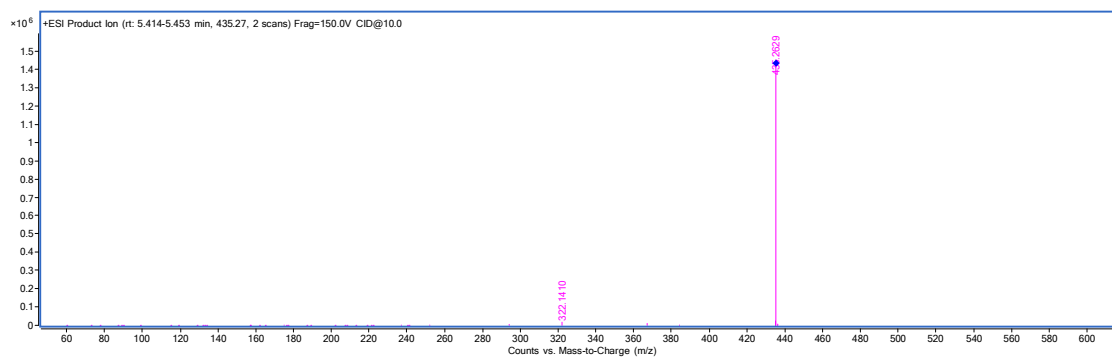


Figure S14. Mass spectrum of peak 1 (RIB, tr 5.415 min).

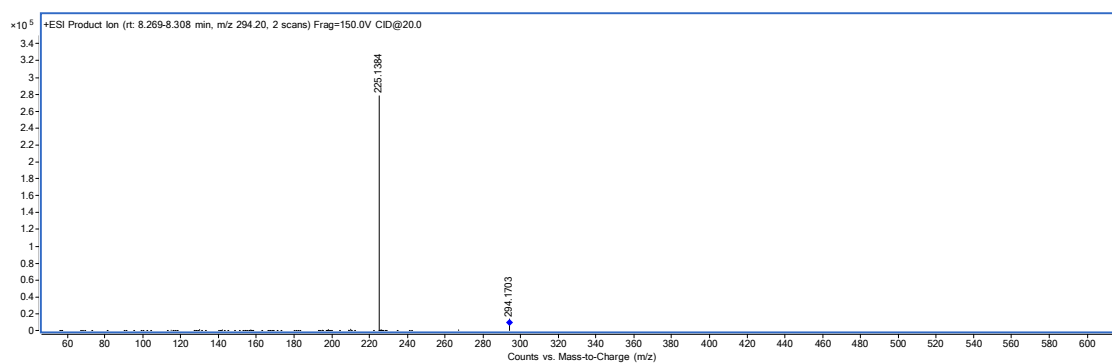


Figure S15. Mass spectrum of peak 2 (ANA, tr 8.273 min).

Patient 6 (RIB + EXE)

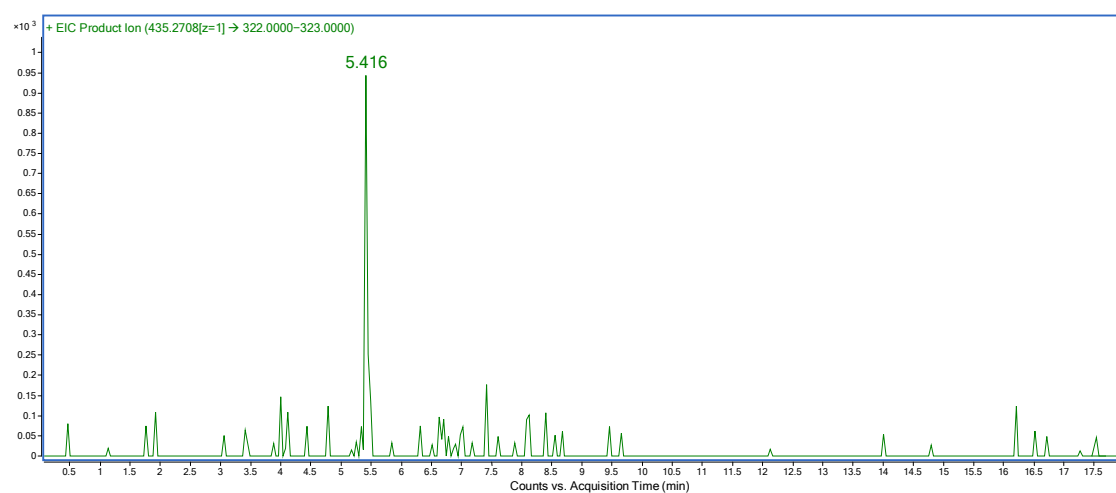


Figure S16. EIC of RIB (transition m/z 435.3 \rightarrow 322.1).

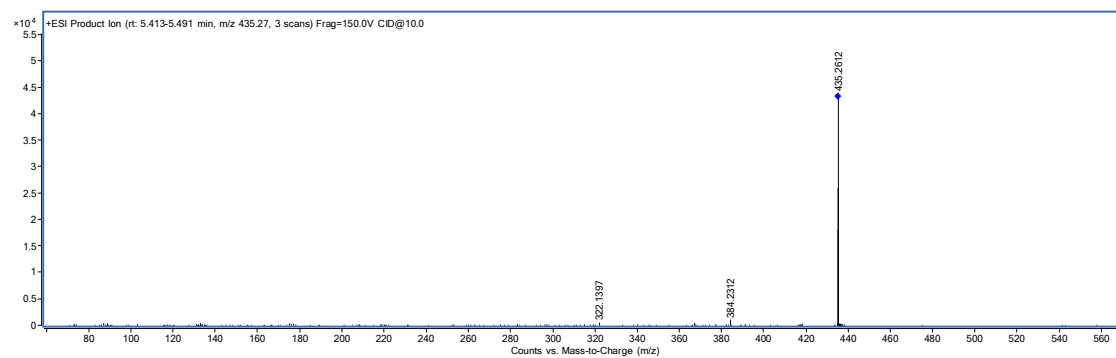


Figure S17. Mass spectrum of the peak (RIB, tr 5.416 min).

Patient 7 (RIB + FUL)

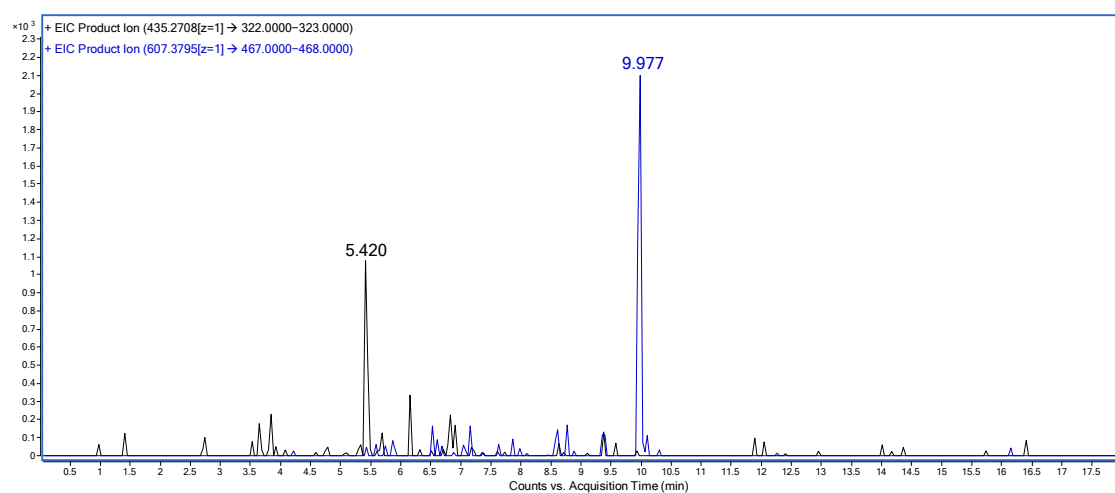


Figure S18. EIC of RIB (transition m/z 435.3 \rightarrow 322.1) and FUL (transition m/z 607.4 \rightarrow 467.2).

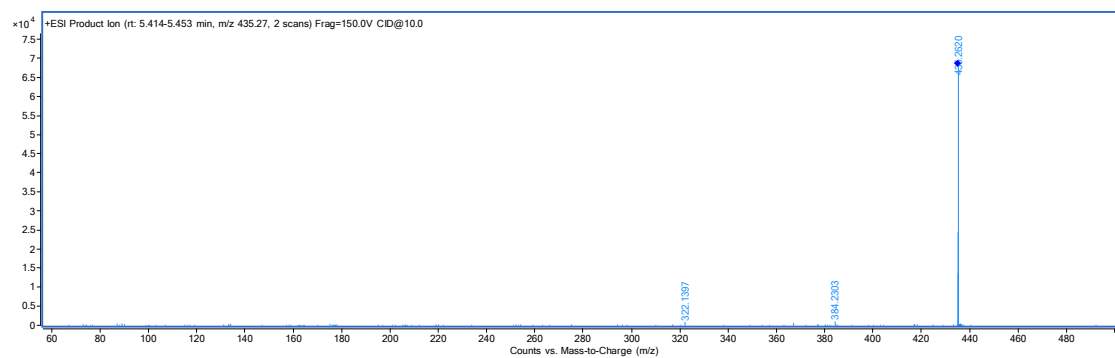


Figure S19. Mass spectrum of peak 1 (RIB, tr 5.420 min).

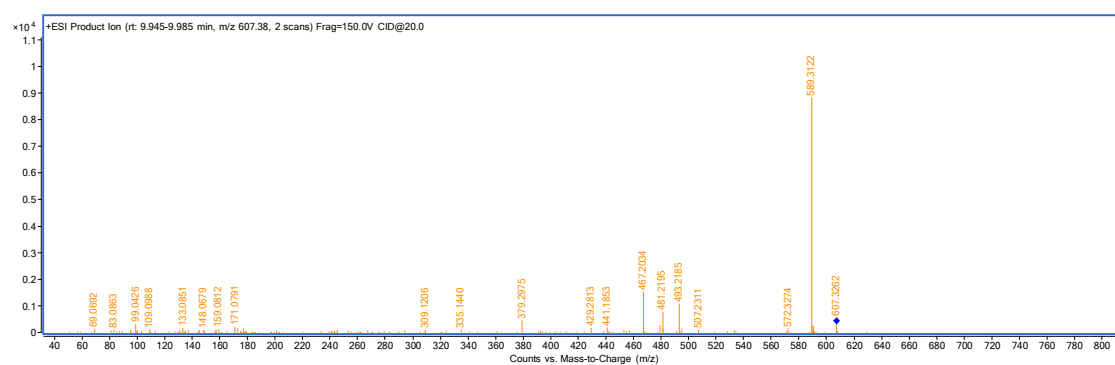


Figure S20. Mass spectrum of peak 2 (FUL, tr 9.977 min).

Patient 8 (PAL + FUL)

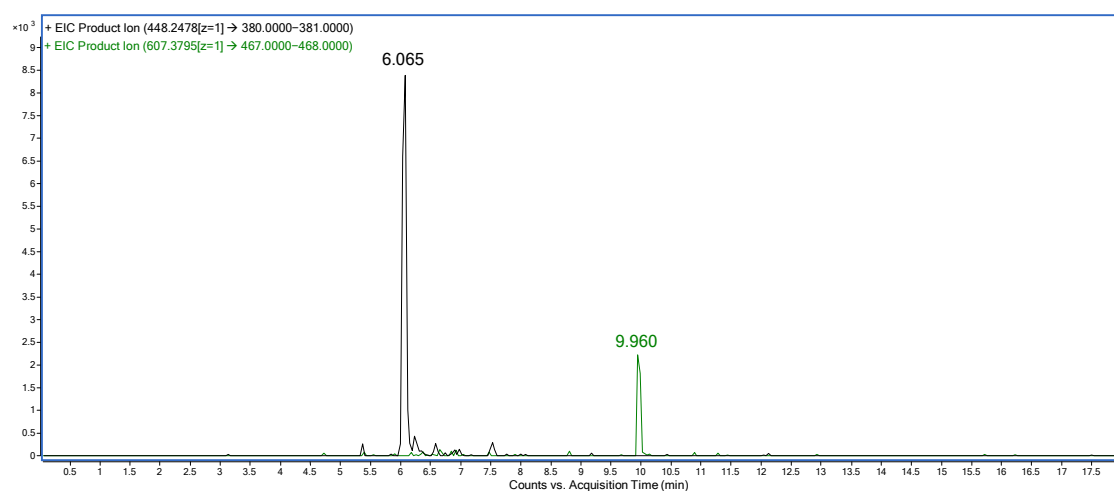


Figure S21. EIC of PAL (transition m/z 448.3→380.2) and FUL (transition m/z 607.4→467.2).

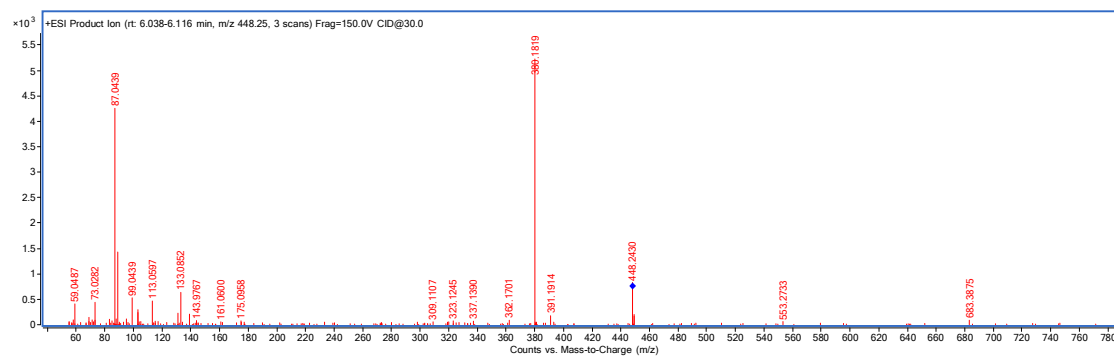


Figure S22. Mass spectrum of peak 1 (PAL, tr 6.065 min).

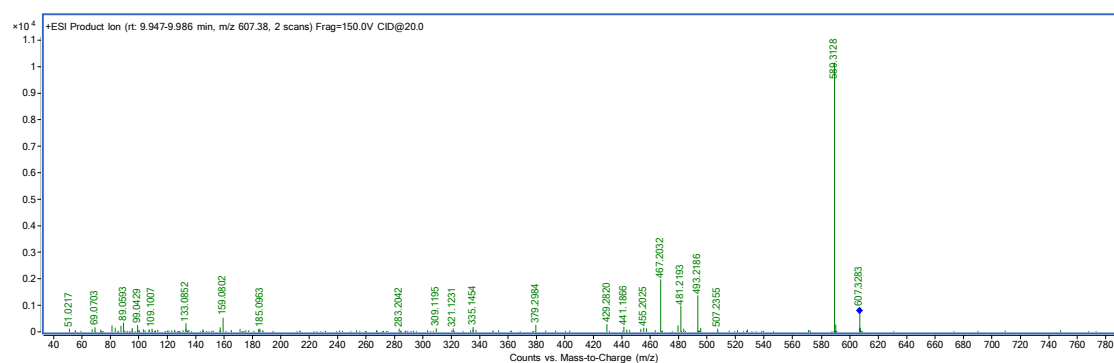


Figure S23. Mass spectrum of peak 2 (FUL, tr 9.960 min).

Patient 9 (PAL + FUL)

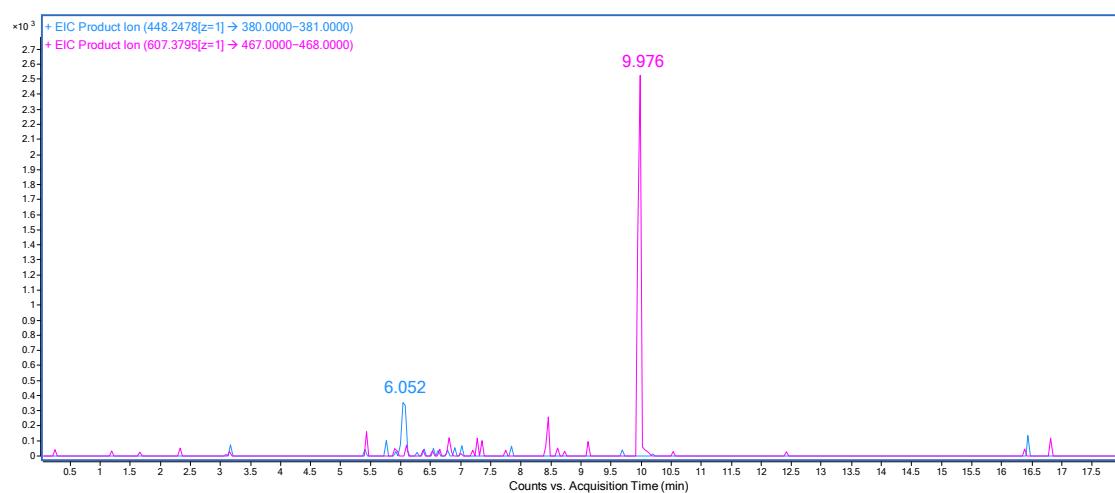


Figure S24. EIC of PAL (transition m/z 448.3 \rightarrow 380.2) and FUL (transition m/z 607.4 \rightarrow 467.2).

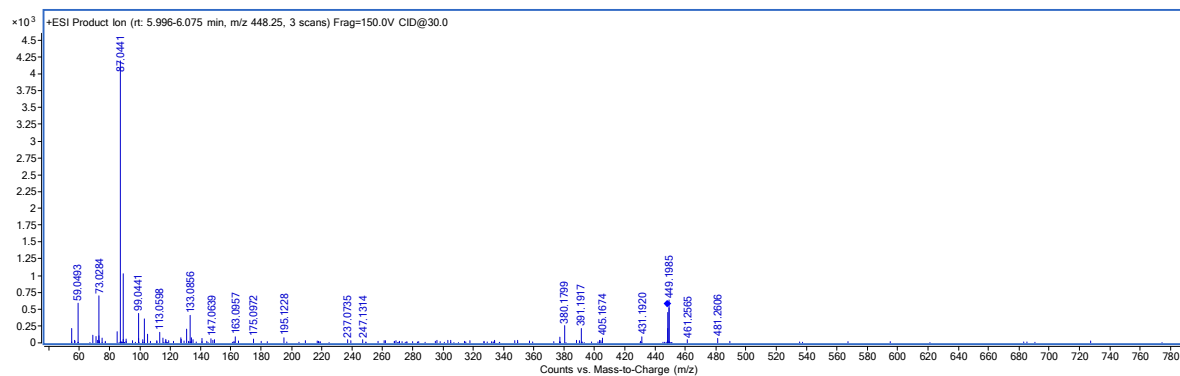


Figure S25. Mass spectrum of peak 1 (PAL, tr 6.052 min).

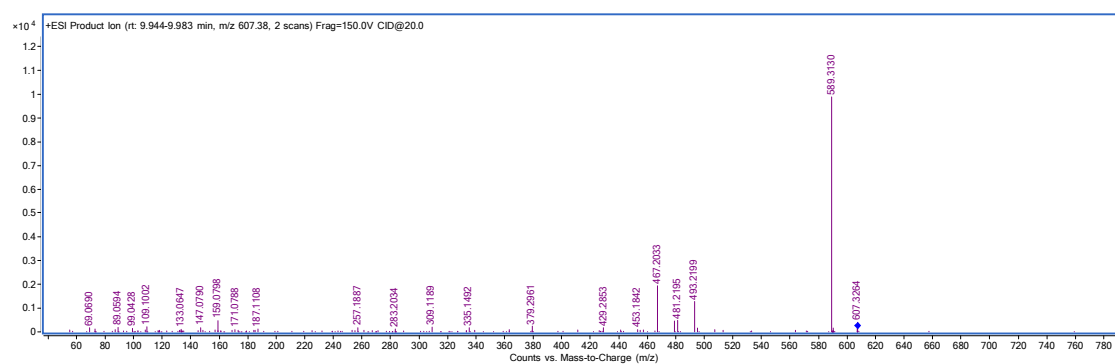


Figure S26. Mass spectrum of peak 2 (FUL, tr 9.976 min).

Patient 10 (PAL + FUL)

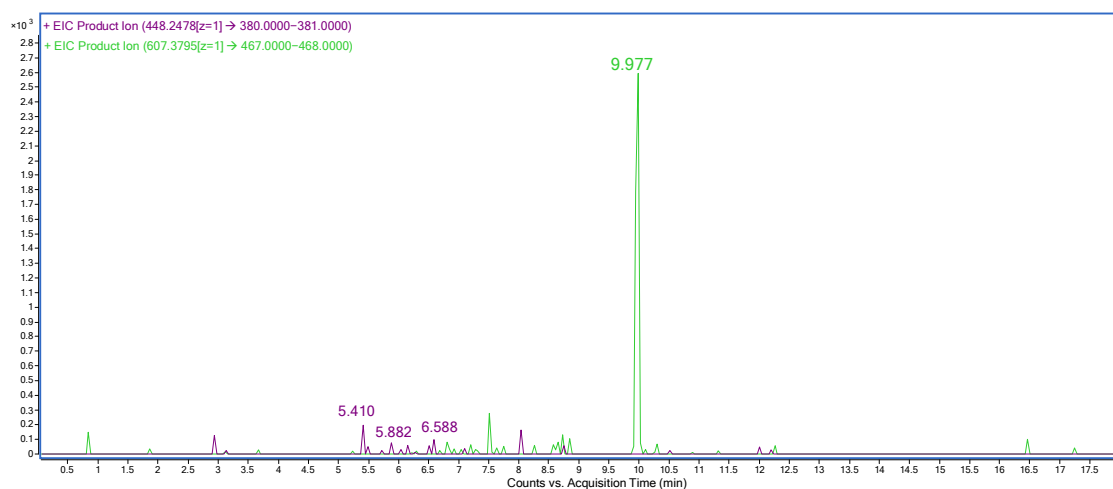


Figure S27. EIC of PAL (transition m/z 448.3→380.2) and FUL (transition m/z 607.4→467.2).

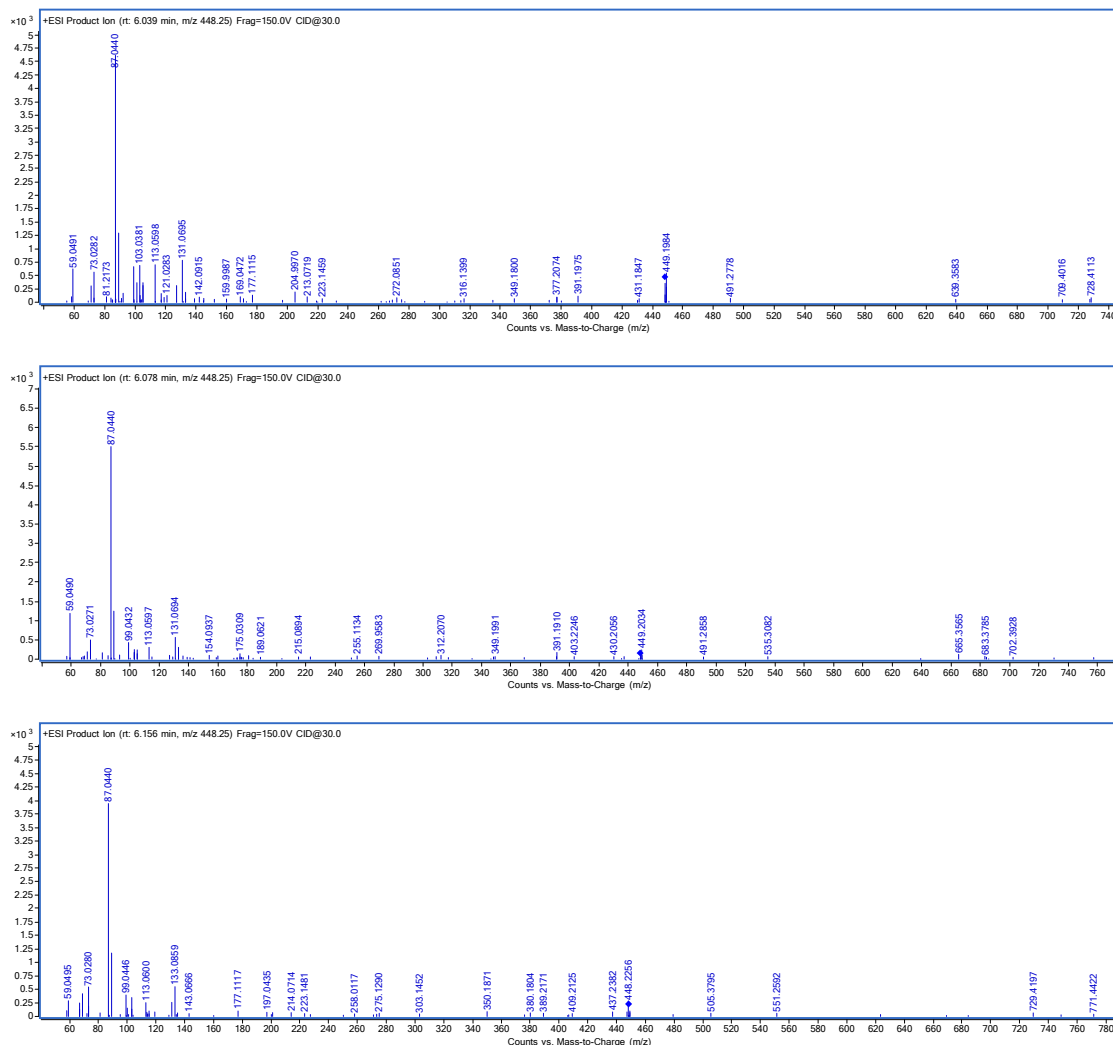


Figure S28. Mass spectra around the retention time of PAL, 6.0 min.

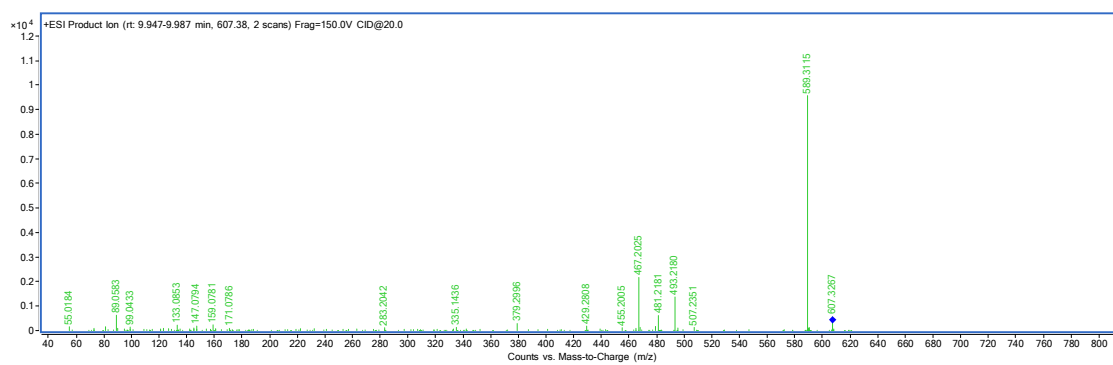


Figure S29. Mass spectrum of the peak (FUL, tr 9.977 min).

Section 2. Results of the pharmacokinetic study:

Table S1. Exact RIB plasma concentrations measured at each timepoint.

t (h)	C_{RIB} (ng/mL)
0.00	944.84
0.25	1051.75
0.50	1235.13
1.00	1519.81
3.00	1830.10
6.00	1713.58
12.00	1501.88