

Supplementary materials

Metabolites of Medicarpin and Their Distributions in Rats

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1. The EICs of 165 metabolites in rats (Figure S1–S44)

(1) metabolites (M1–M3) having the skeleton of medicarpin

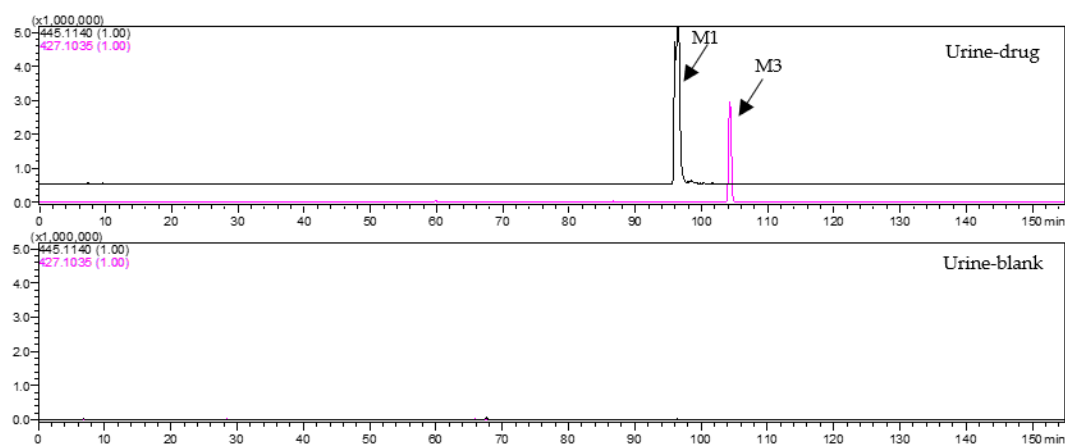


Figure S1. EICs of m/z 445.1140 and m/z 427.1035 in drug urine and blank urine in ESI- mode.

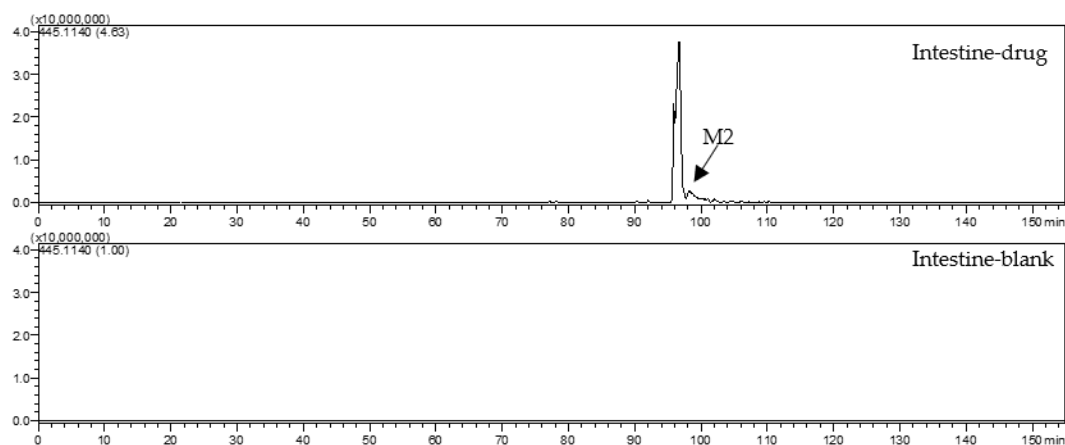


Figure S2. EICs of m/z 445.1140 in drug intestine and blank intestine in ESI- mode.

(2) metabolites (M4-M10) having the skeleton of hydrogenated medicarpin

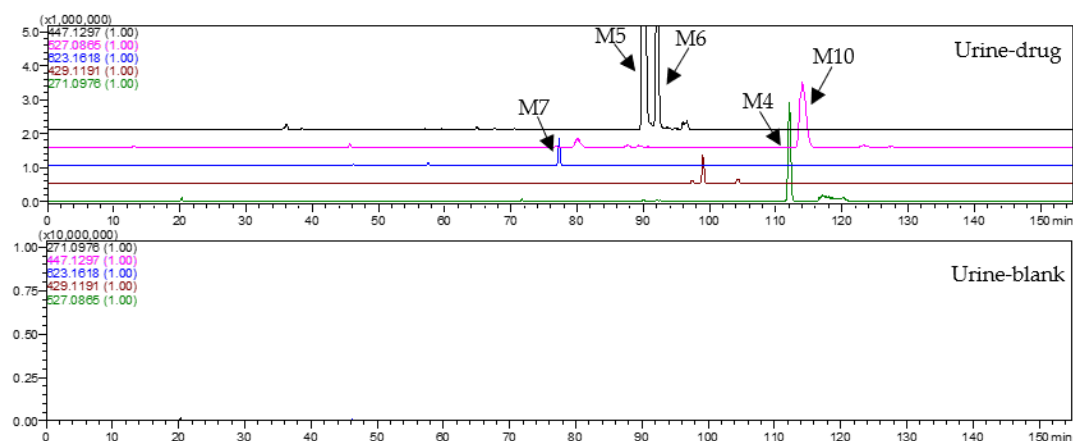


Figure S3. EICs of m/z 447.1297, m/z 527.0865, m/z 623.1618, m/z 429.1191 and m/z 271.0976 in drug urine and blank urine in ESI- mode.

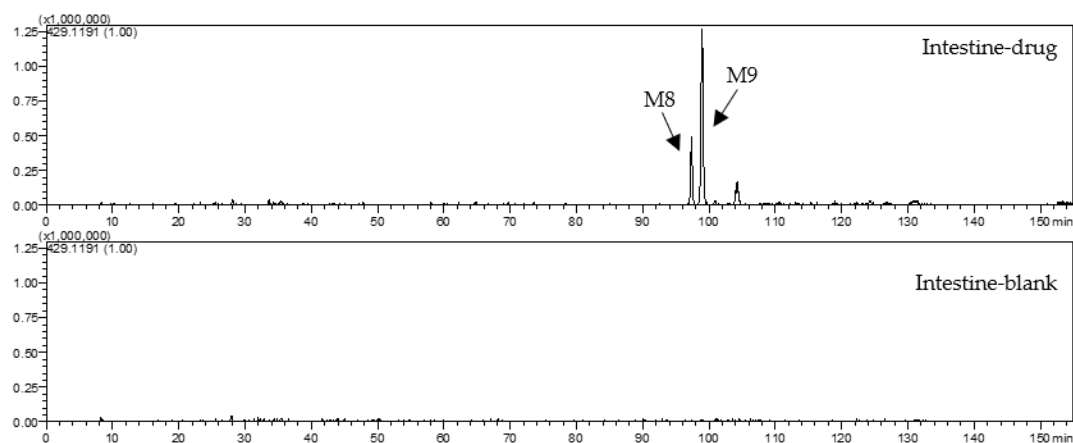


Figure S4. EICs of m/z 429.1191 in drug intestine and blank intestine in ESI- mode.

(3) metabolites (M11-M26) having the skeleton of demethylated medicarpin

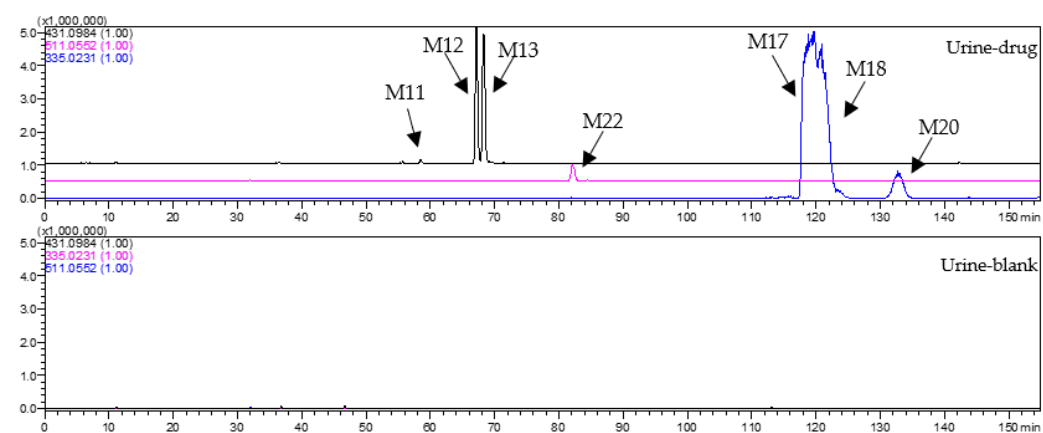


Figure S5. EICs of m/z 431.0984, m/z 511.0552 and m/z 335.0231 in drug urine and blank urine in ESI- mode.

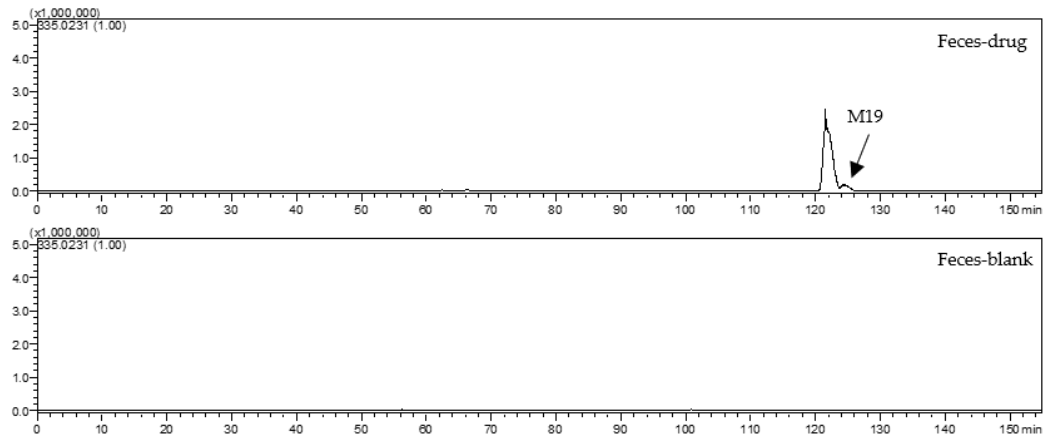


Figure S6. EICs of m/z 335.0231 in drug feces and blank feces in ESI- mode.

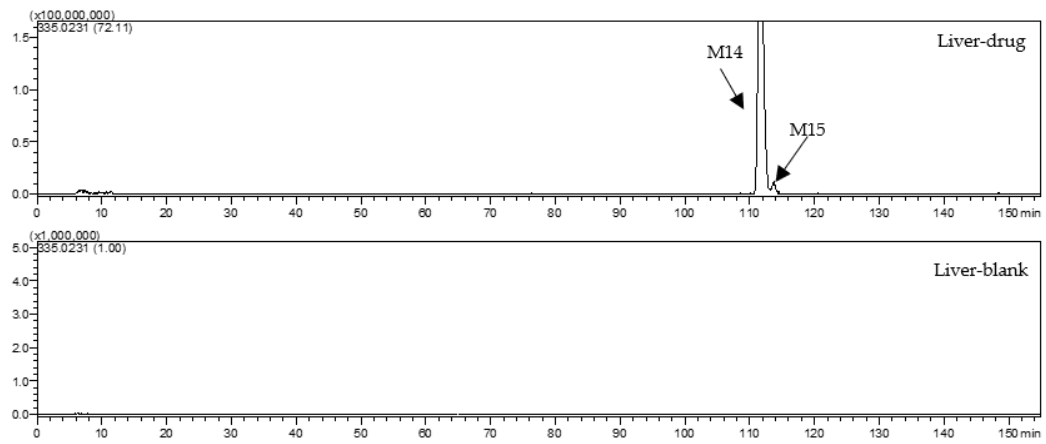


Figure S7. EICs of m/z 335.0231 in drug liver and blank liver in ESI- mode.

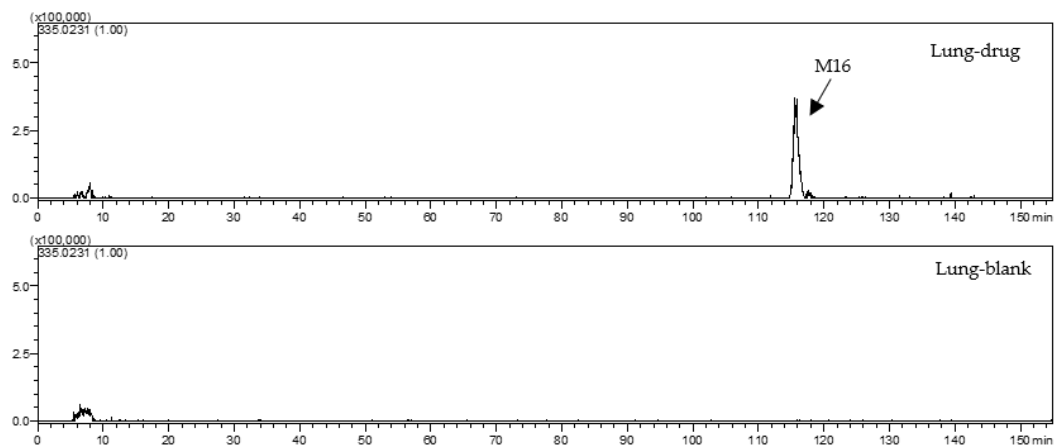


Figure S8. EICs of m/z 335.0231 in drug lung and blank lung in ESI- mode.

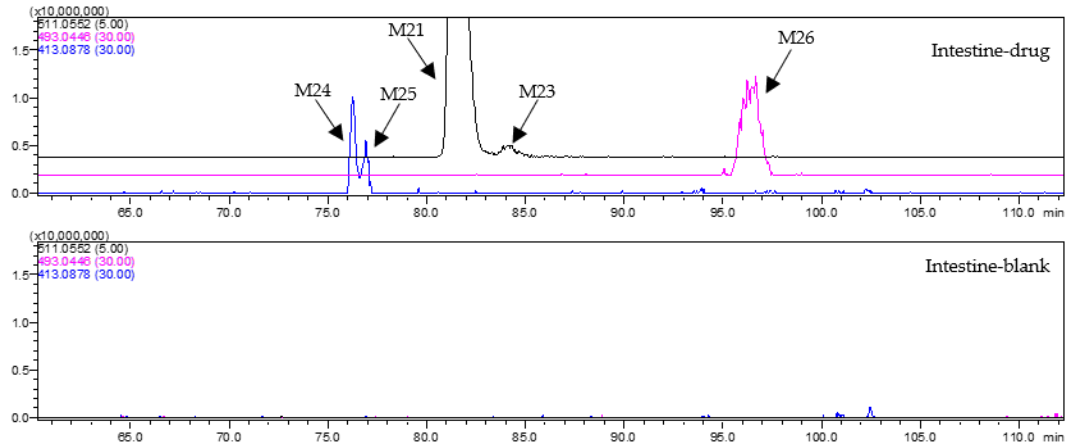


Figure S9. EICs of m/z 511.0552, m/z 493.0446 and m/z 413.0873 in drug intestine and blank intestine in ESI- mode.

(4) metabolites (M27–M52) having the skeleton of demethylated and hydrogenated medicarpin

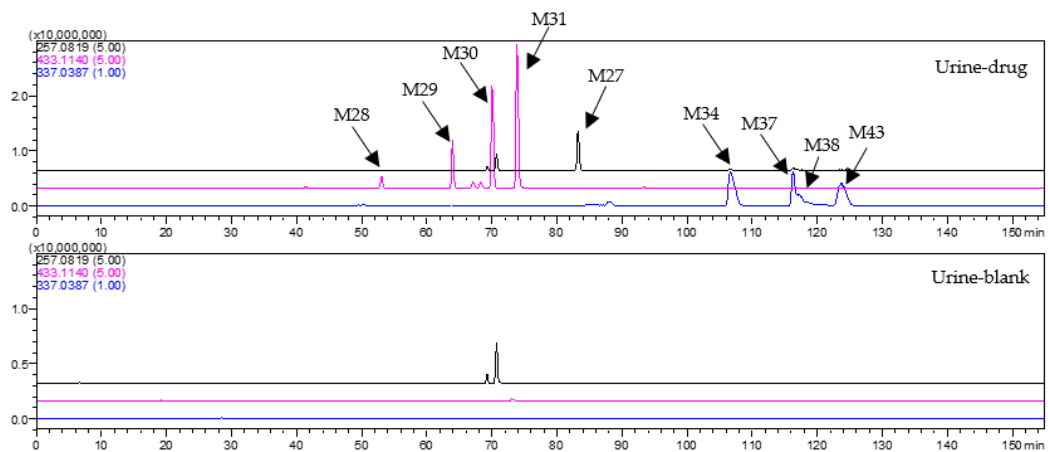


Figure S10. EICs of m/z 257.0819, m/z 433.1140 and m/z 337.0387 in drug urine and blank urine in ESI- mode.

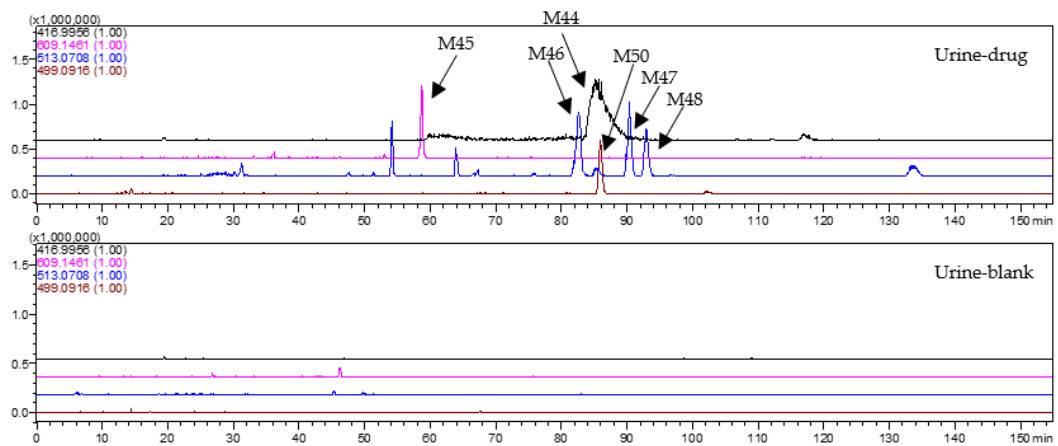


Figure S11. EICs of m/z 416.9956, m/z 609.1461, m/z 513.0708 and m/z 499.0916 in drug urine and blank urine in ESI- mode.

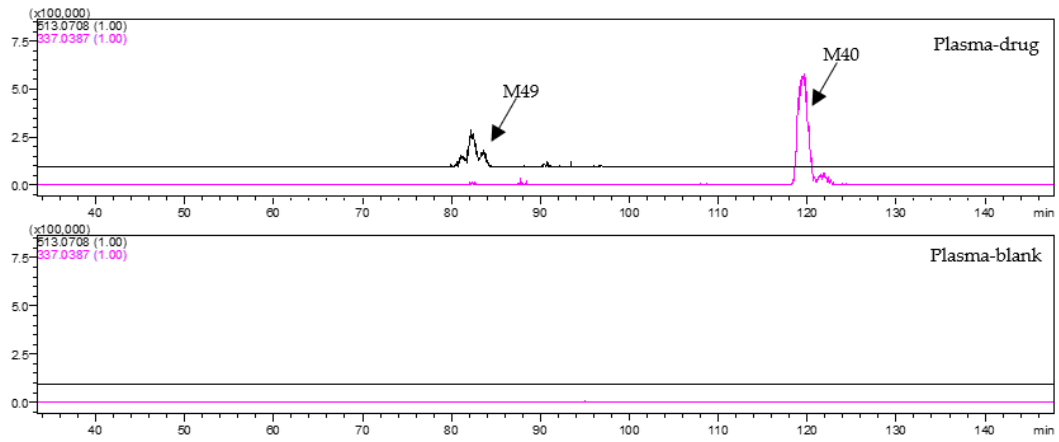


Figure S12. EICs of m/z 513.0708 and m/z 337.0387 in drug plasma and blank plasma in ESI- mode.

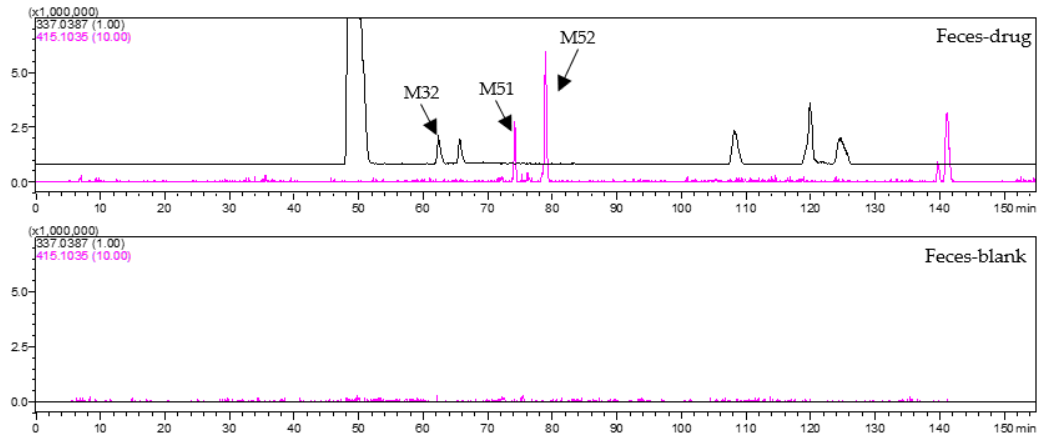


Figure S13. EICs of m/z 337.0387 and m/z 415.1035 in drug feces and blank feces in ESI- mode.

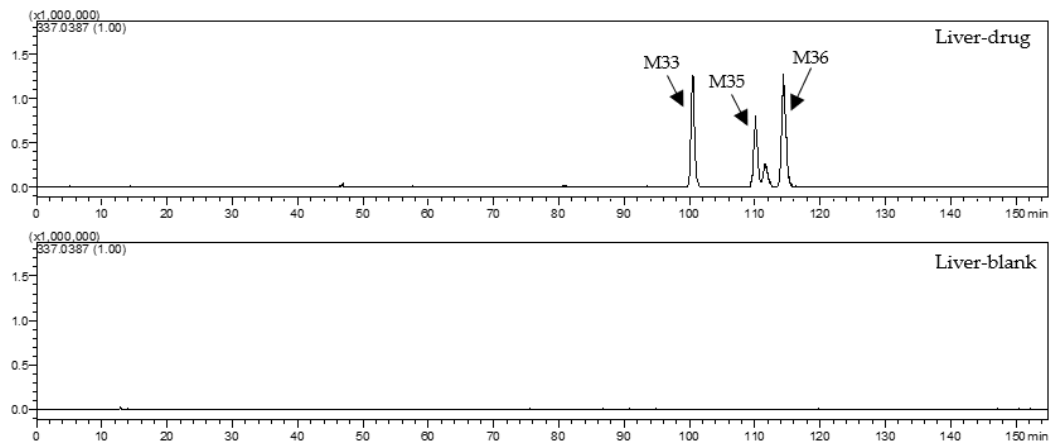


Figure S14. EICs of m/z 337.0387 in drug liver and blank liver in ESI- mode.

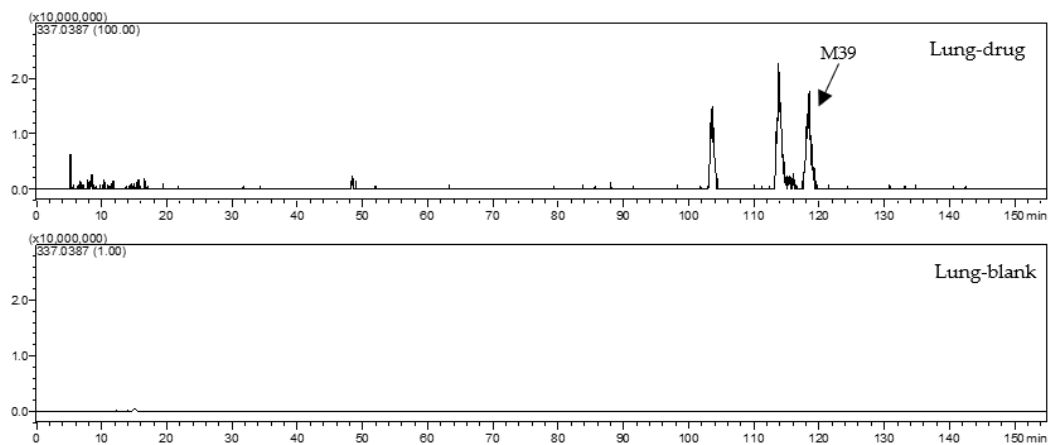


Figure S15. EICs of m/z 337.0387 in drug lung and blank lung in ESI- mode.

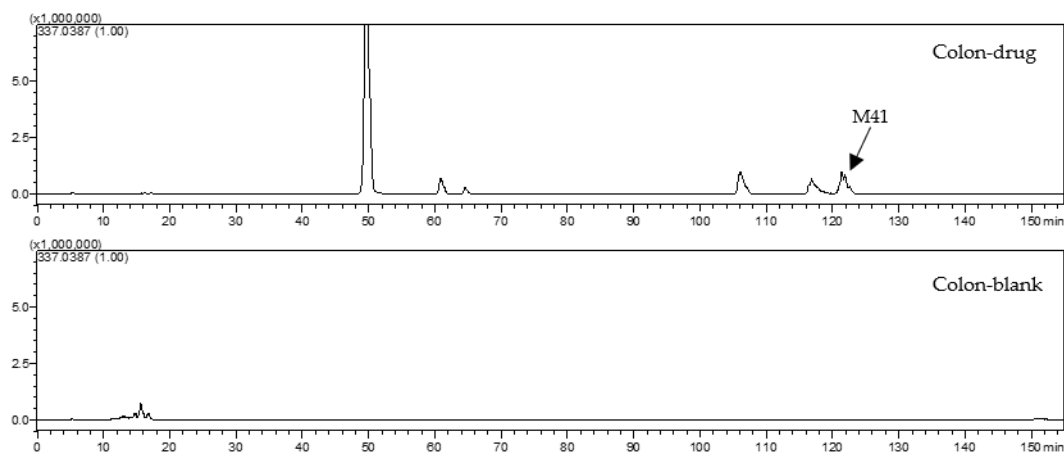


Figure S16. EICs of m/z 337.0387 in drug colon and blank colon in ESI- mode.

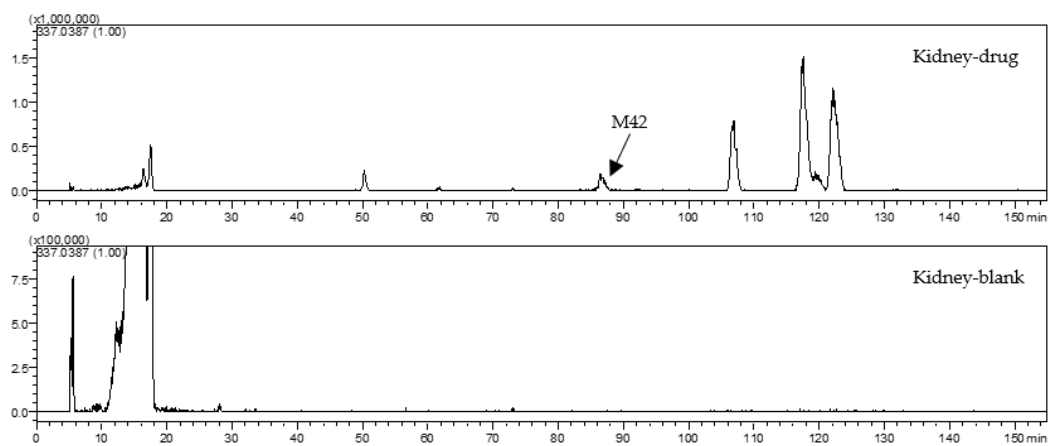


Figure S17. EICs of m/z 337.0387 in drug kidney and blank kidney in ESI- mode.

(5) metabolites (M53–M75) having the skeleton of demethylated and hydroxylated medicarpin

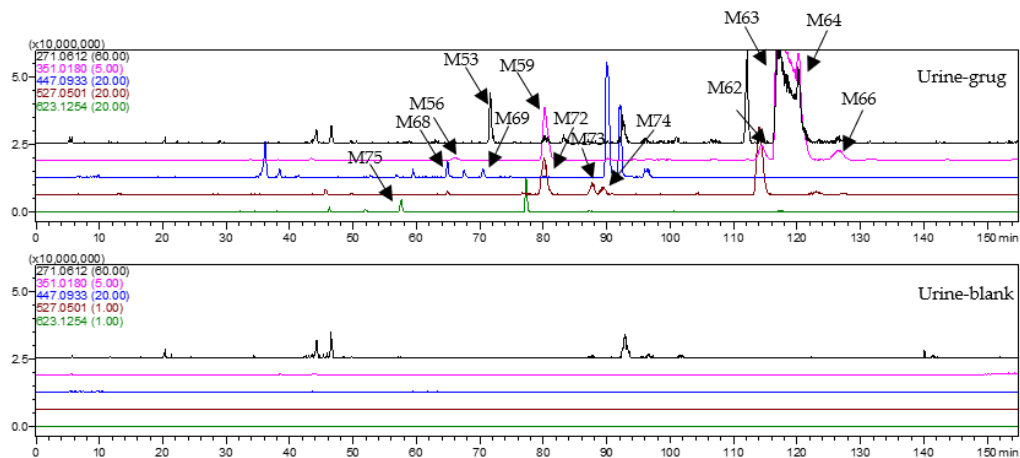


Figure S18. EICs of m/z 271.0612, m/z 351.0180, m/z 447.0933, m/z 527.0501 and m/z 623.1254 in drug urine and blank urine in ESI- mode.

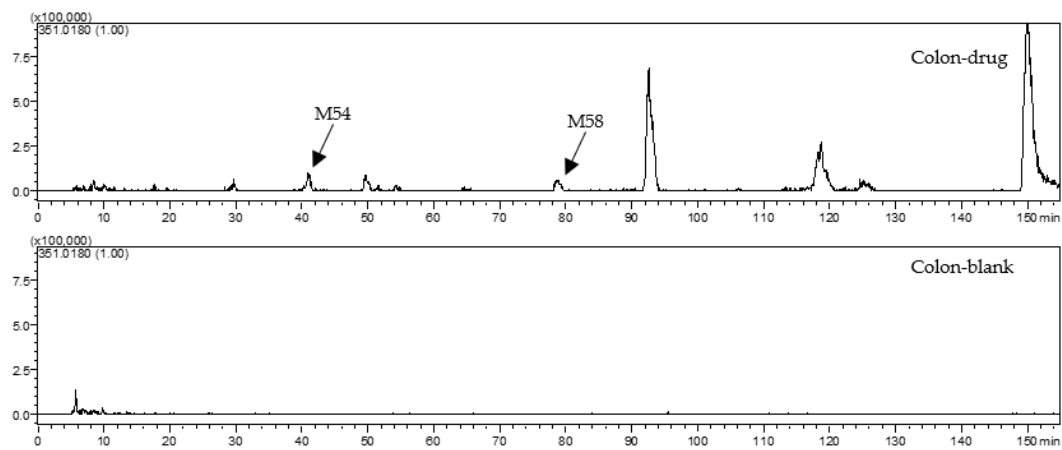


Figure S19. EICs of m/z 351.0180 in drug colon and blank colon in ESI- mode.

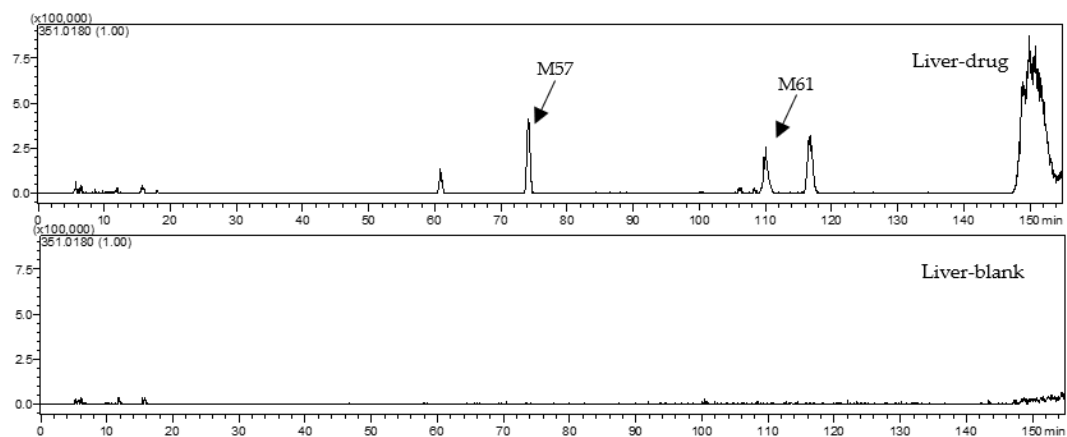


Figure S20. EICs of m/z 351.0180 in drug liver and blank liver in ESI- mode.

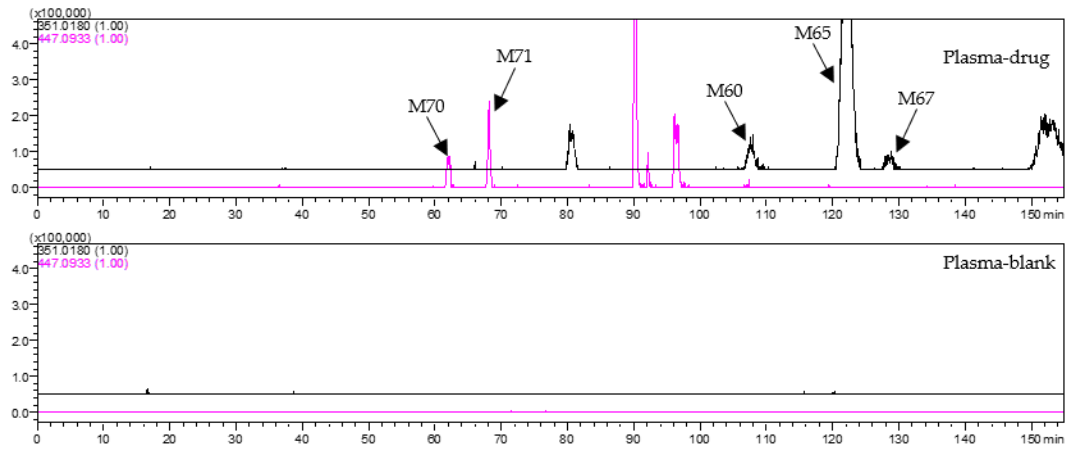


Figure S21. EICs of m/z 351.0180 and 447.0933 in drug plasma and blank plasma in ESI- mode.

(6) metabolites (M76–M107) having the skeleton of hydroxylated medicarpin

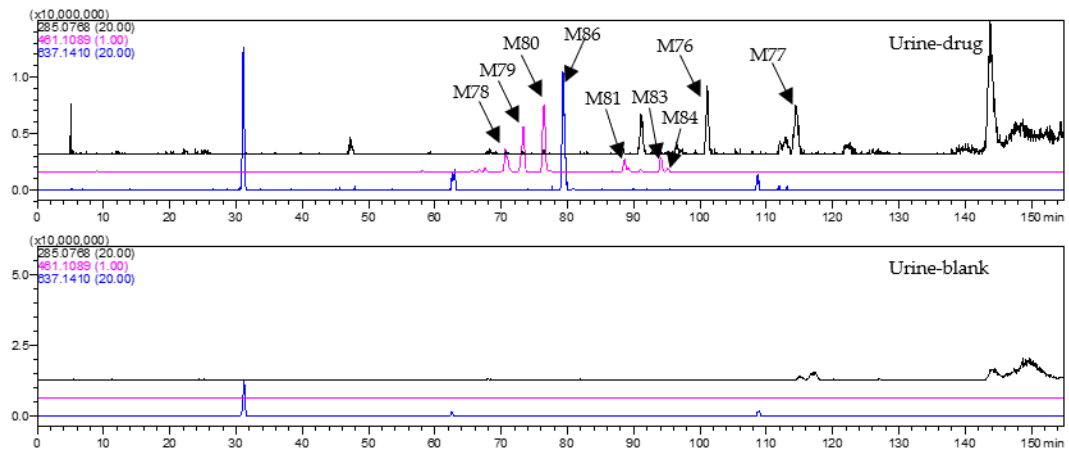


Figure S22. EICs of m/z 285.0768, m/z 461.1089 and m/z 637.1410 in drug urine and blank urine in ESI- mode.

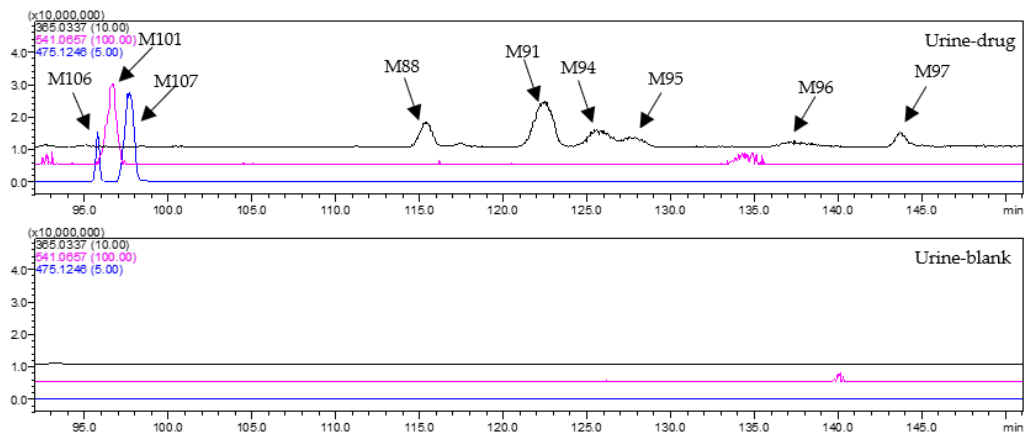


Figure S23. EICs of m/z 365.0337, m/z 541.0657 and m/z 475.1246 in drug urine and blank urine in ESI- mode.

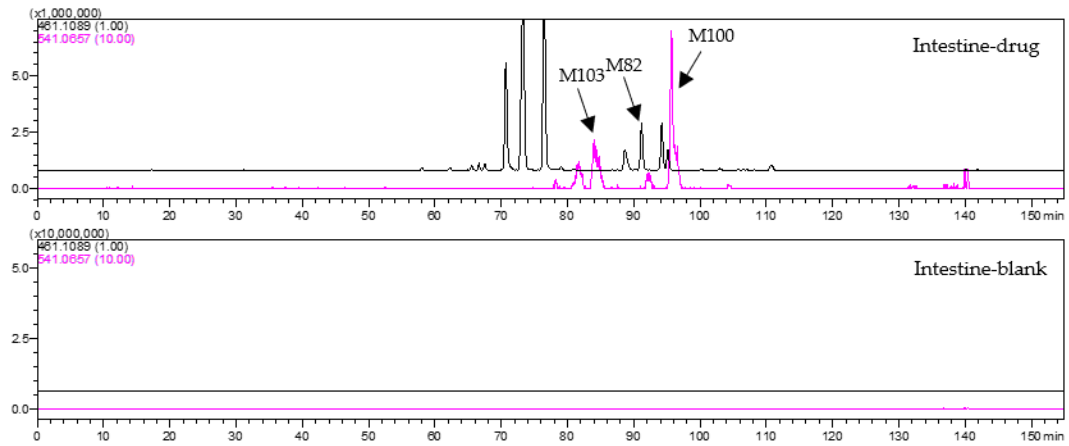


Figure S24. EICs of m/z 461.1089 and 541.0657 in drug intestine and blank intestine in ESI- mode.

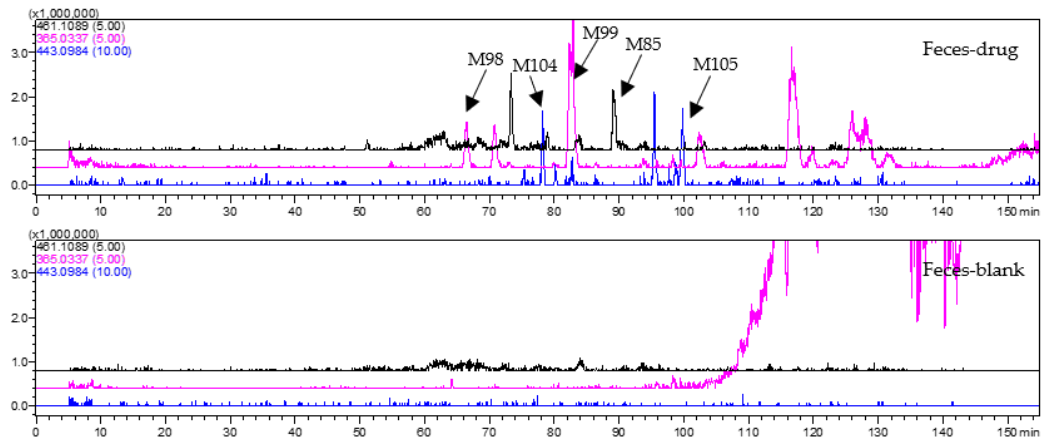


Figure S25. EICs of m/z 461.1089, m/z 365.0337 and m/z 443.0984 in drug feces and blank feces in ESI- mode.

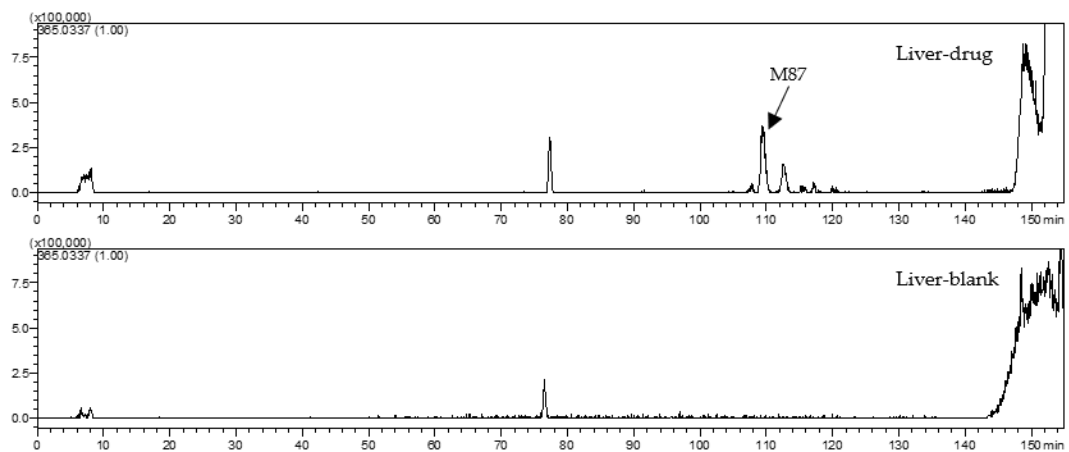


Figure S26. EICs of m/z 365.0337 in drug liver and blank liver in ESI- mode.

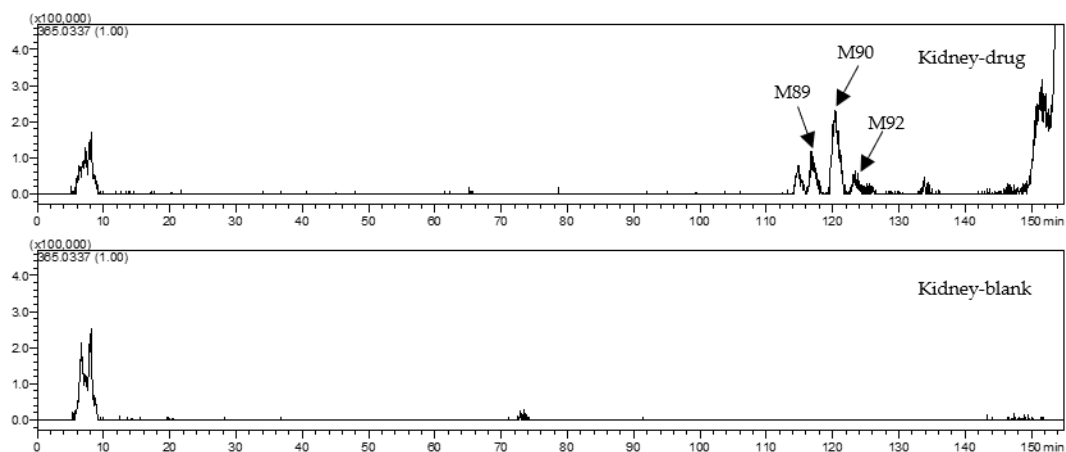


Figure S27. EICs of m/z 365.0337 in drug kidney and blank kidney in ESI- mode.

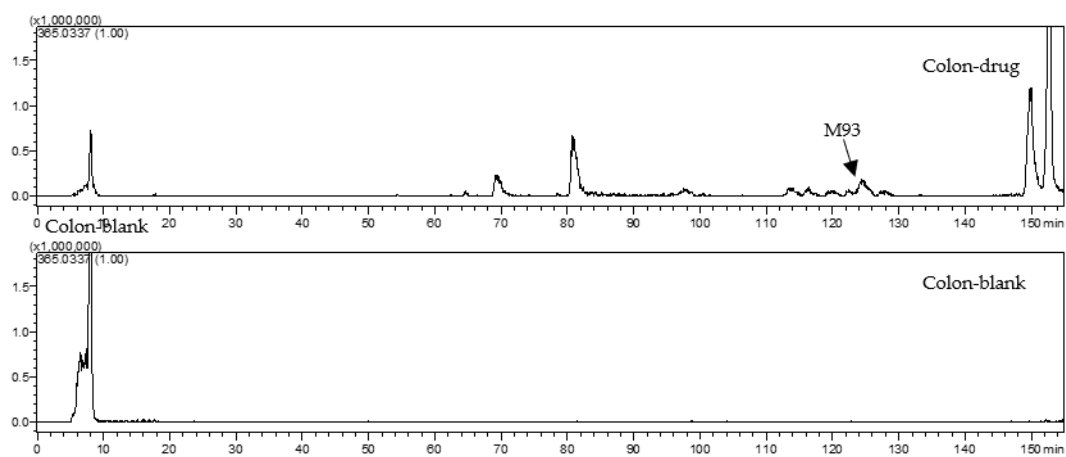


Figure S28. EICs of m/z 365.0337 in drug colon and blank colon in ESI- mode.

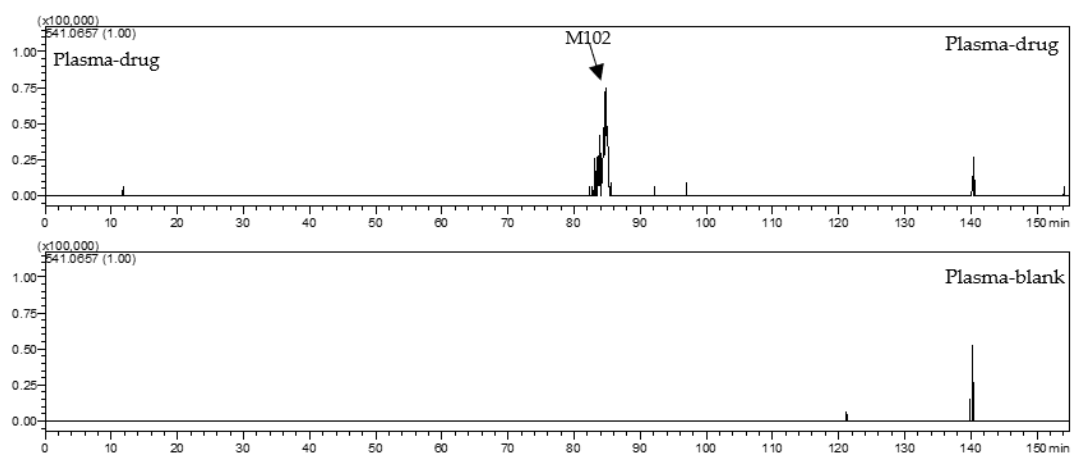


Figure S29. EICs of m/z 541.0657 in drug plasma and blank plasma in ESI- mode.

(7) metabolites (M108–M138) having the skeleton of hydrogenated and hydroxylated medicarpin

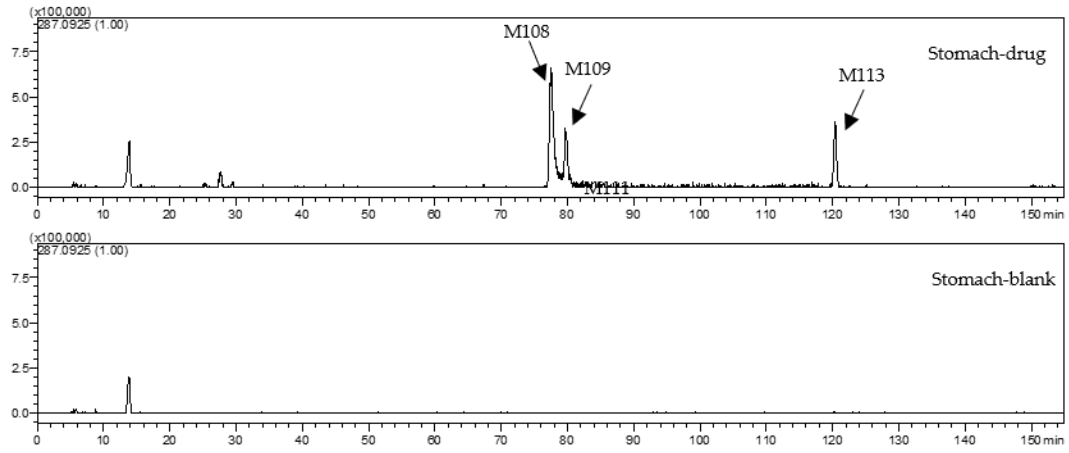


Figure S30. EICs of m/z 287.0925 in drug stomach and blank stomach in ESI- mode.

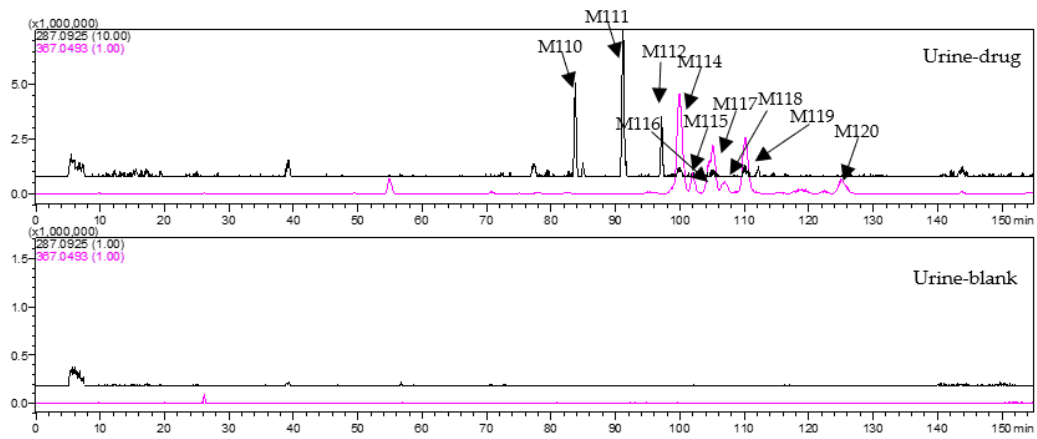


Figure S31. EICs of m/z 287.0925 and 367.0493 in drug urine and blank urine in ESI- mode.

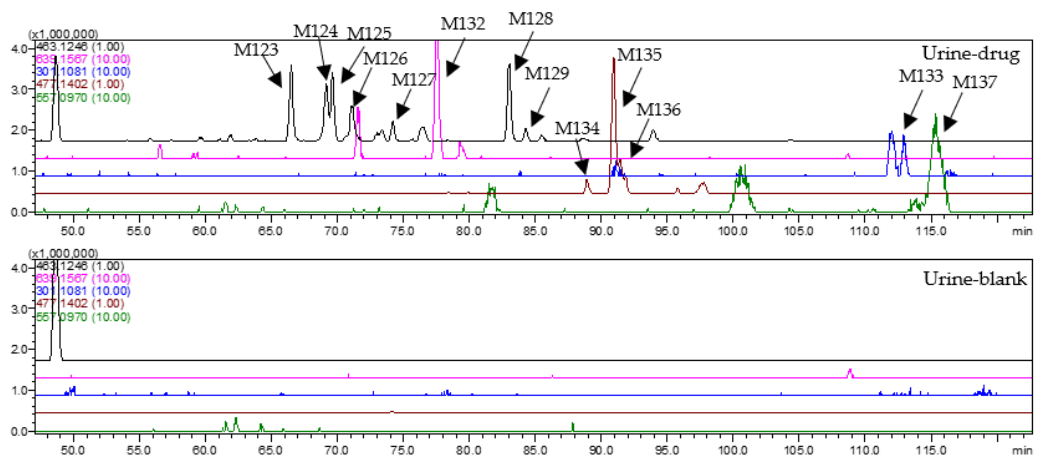


Figure S32. EICs of m/z 463.1246, m/z 639.1567, m/z 301.1081, m/z 477.1402 and m/z 557.0970 in drug urine and blank urine in ESI- mode.

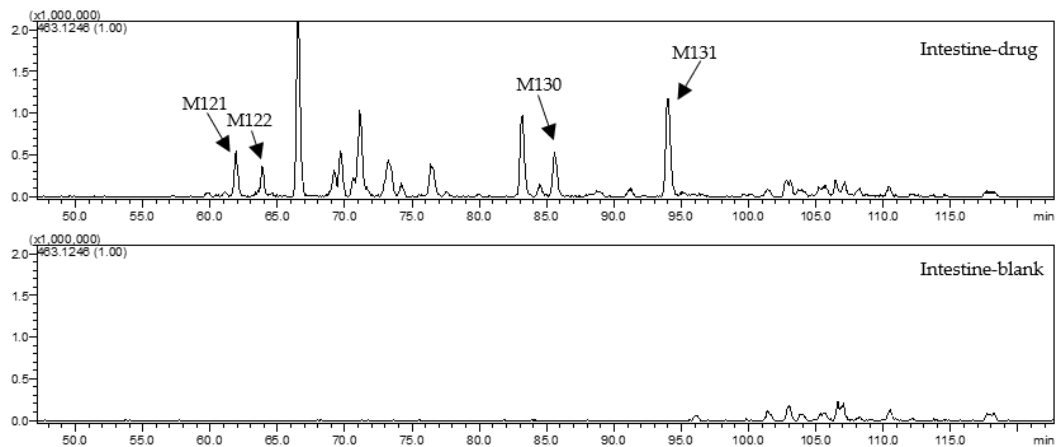


Figure S33. EICs of m/z 463.1246 in drug intestine and blank intestine in ESI- mode.

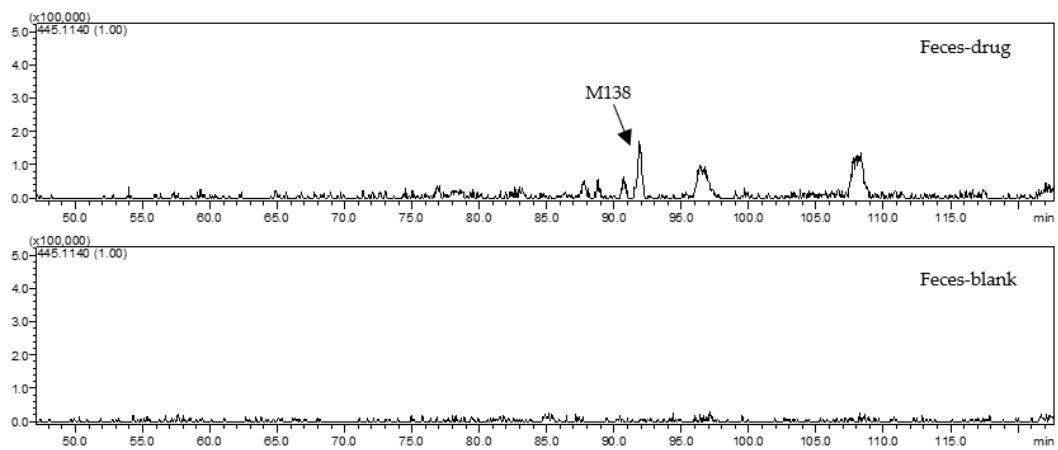


Figure S34. EICs of m/z 445.1140 in drug feces and blank feces in ESI- mode.

(8) metabolites (M139–M149) having the skeleton of demethylated, hydrogenated and hydroxylated medicarpin

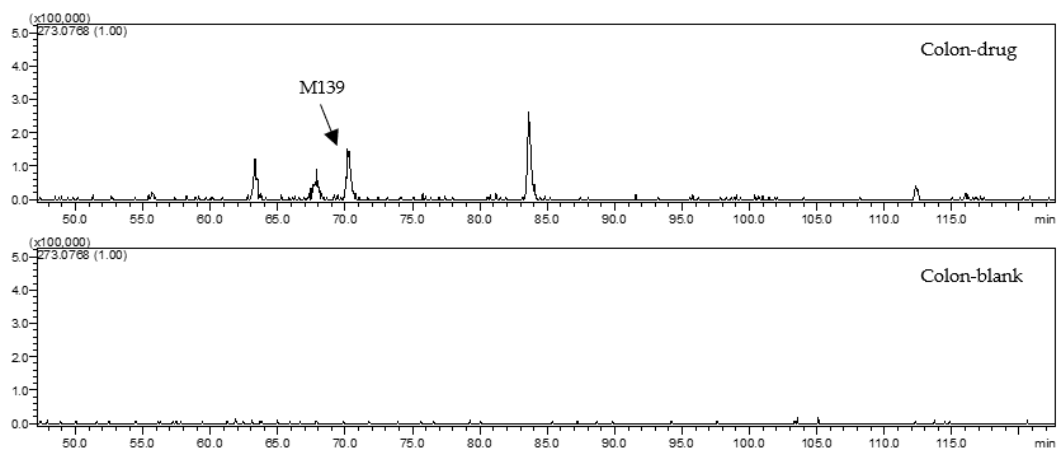


Figure S35. EICs of m/z 273.0768 in drug colon and blank colon in ESI- mode.

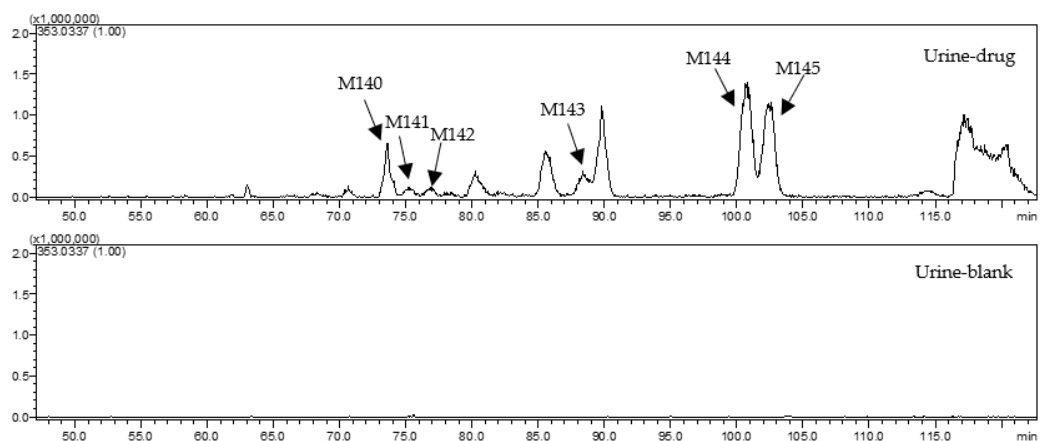


Figure S36. EICs of m/z 353.0337 in drug urine and blank urine in ESI- mode.

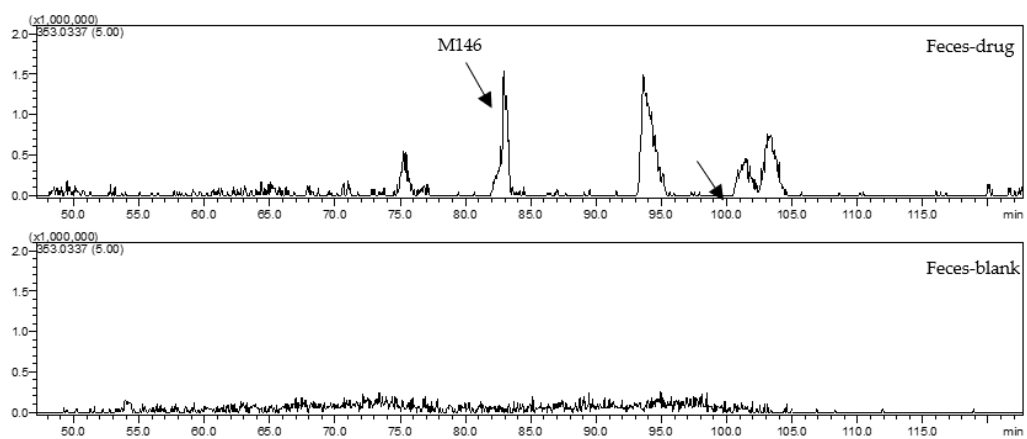


Figure S37. EICs of m/z 353.0337 in drug feces and blank feces in ESI- mode.

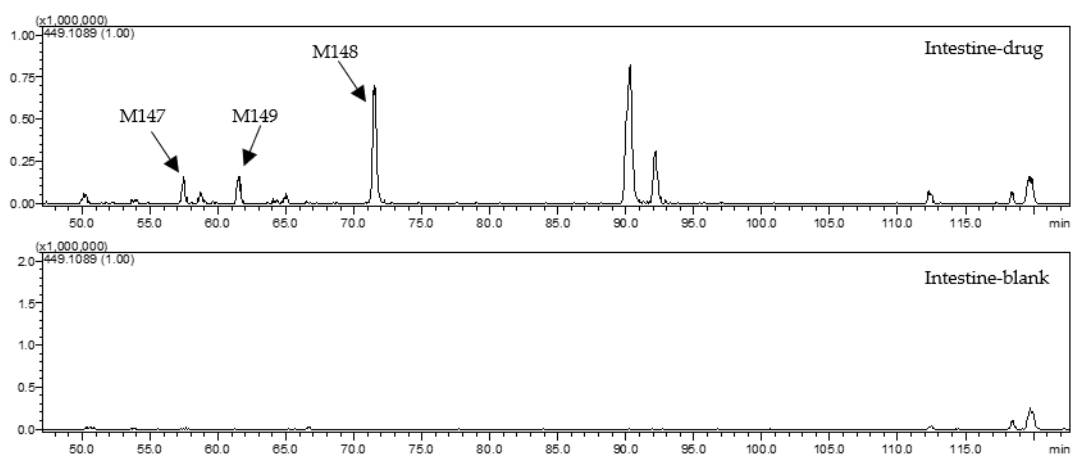


Figure S38. EICs of m/z 449.1089 in drug intestine and blank intestine in ESI- mode.

(9) metabolites (M150–M156) having the skeleton of demethylated and dihydroxylated medicarpin

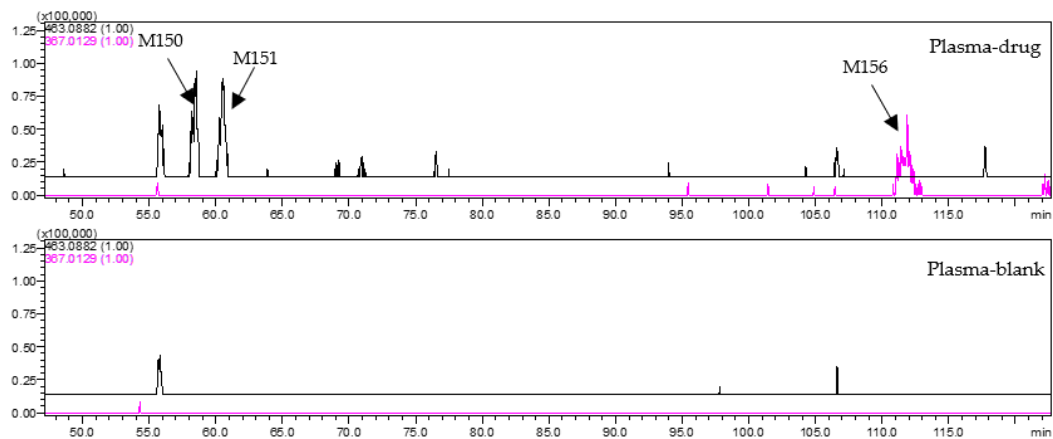


Figure S39. EICs of m/z 463.0882 and 367.0129 in drug plasma and blank plasma in ESI- mode.

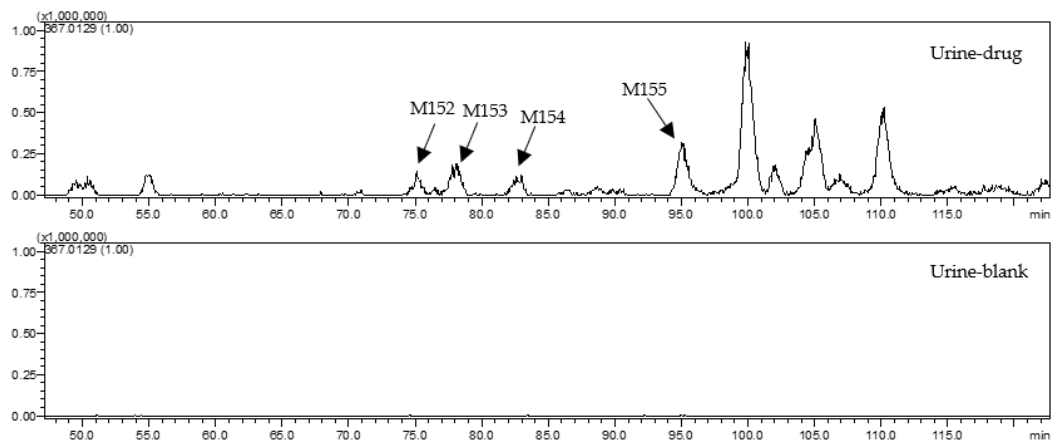


Figure S40. EICs of m/z 367.0129 in drug urine and blank urine in ESI- mode.

(10) metabolites (M157–M161) having the skeleton of dihydroxylated medicarpin

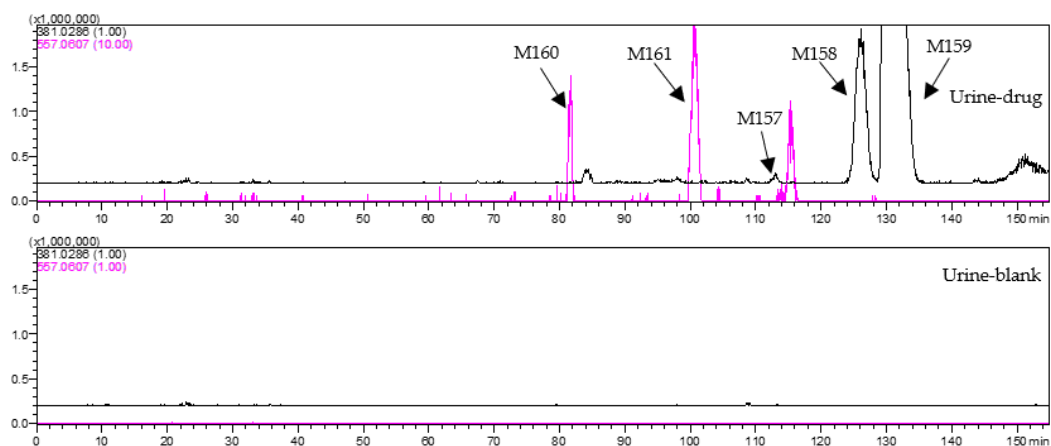


Figure S41. EICs of m/z 381.0286 and 557.0607 in drug urine and blank urine in ESI- mode.

(11) metabolite (M162) having the skeleton of hydrogenated and dihydroxylated medicarpin

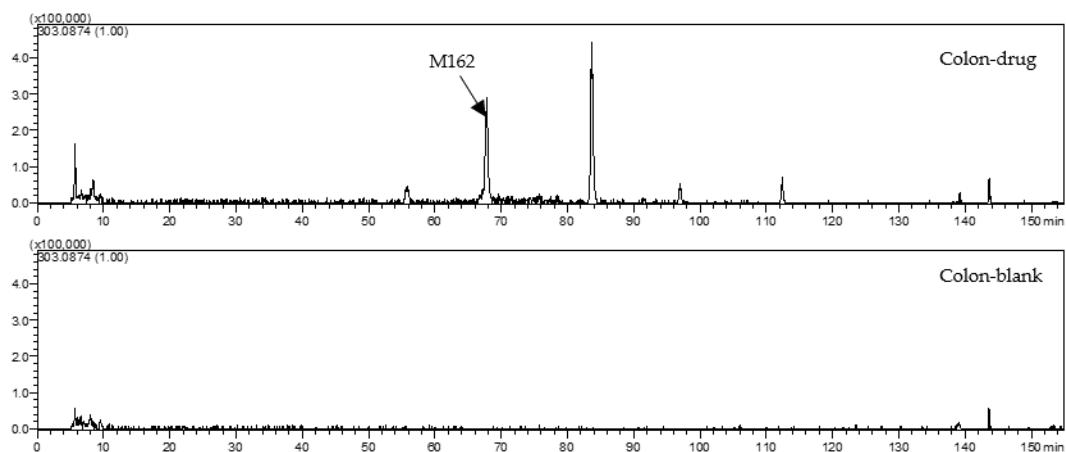


Figure S42. EICs of m/z 303.0874 in drug colon and blank colon in ESI- mode.

(12) metabolites (M163–M164) having the skeleton of hydrogenated and trihydroxylated medicarpin

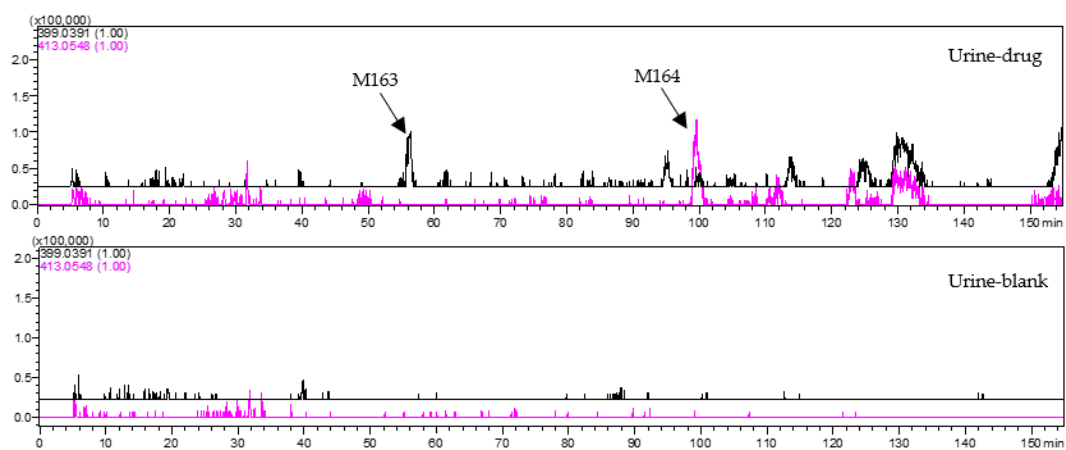


Figure S43. EICs of m/z 399.0391 and 557.0607 in drug urine and blank urine in ESI- mode.

(13) metabolite (M165) has the skeleton of demethylated, hydrogenated and dihydroxylated medicarpin

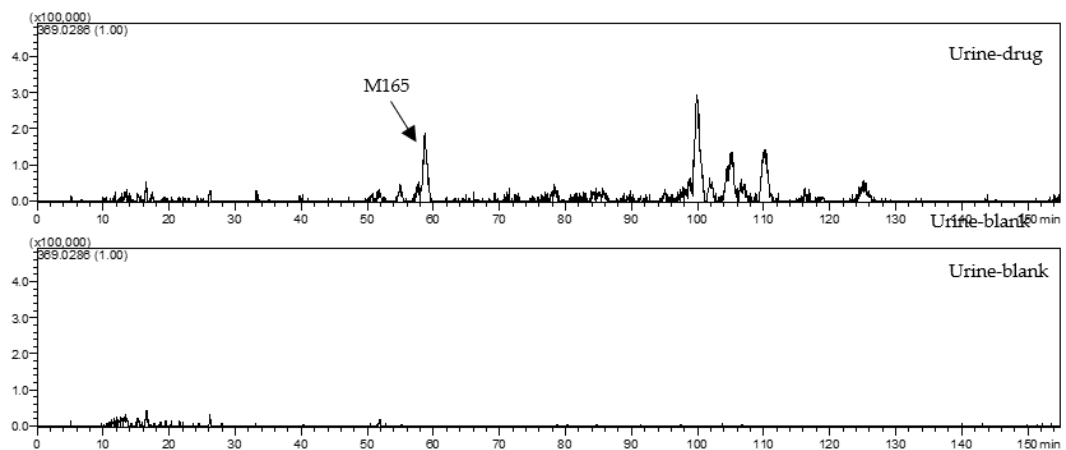


Figure S44. EICs of m/z 369.0286 in drug urine and blank urine in ESI- mod.

2. The MS spectra of M4, M10, M37, M112, M114, M115, M144 and M159 (Figure S45–S52)

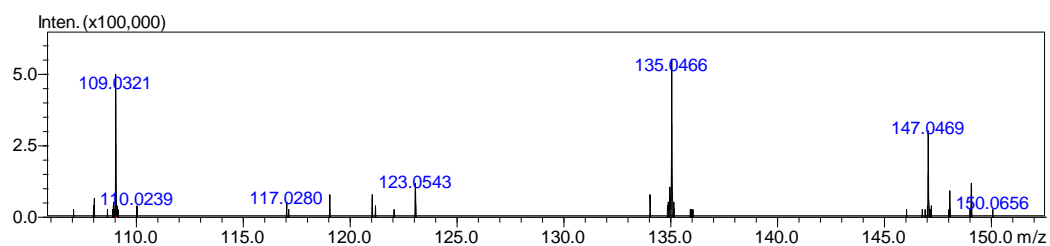


Figure S45. The MS² spectrum of M4.

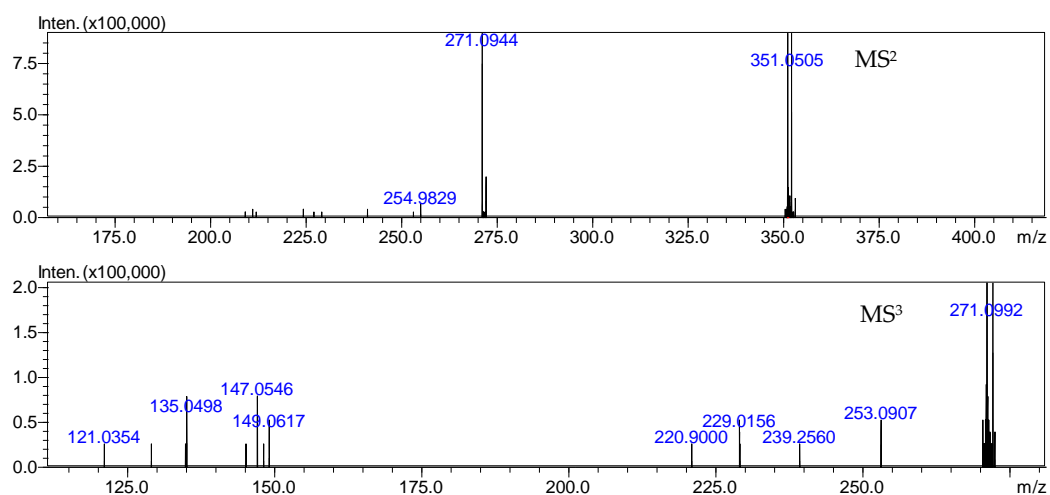


Figure S46. The MS² and MS³ spectra of M10.

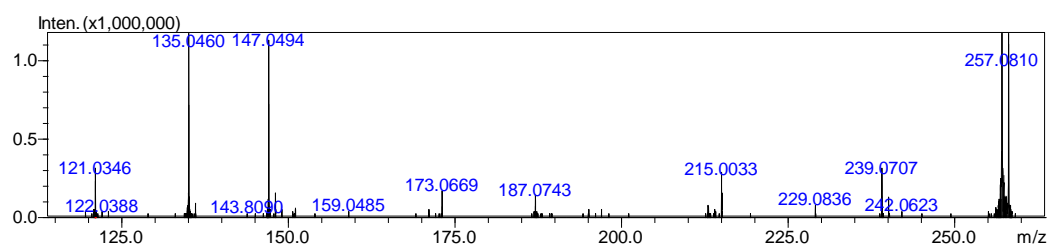


Figure S47. The MS² spectrum of M37.

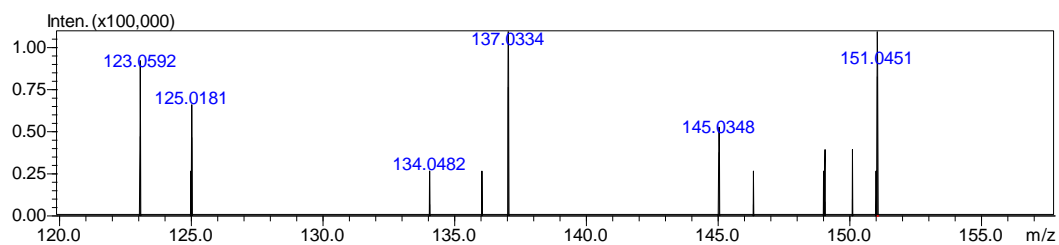


Figure S48. The MS² spectra of M112.

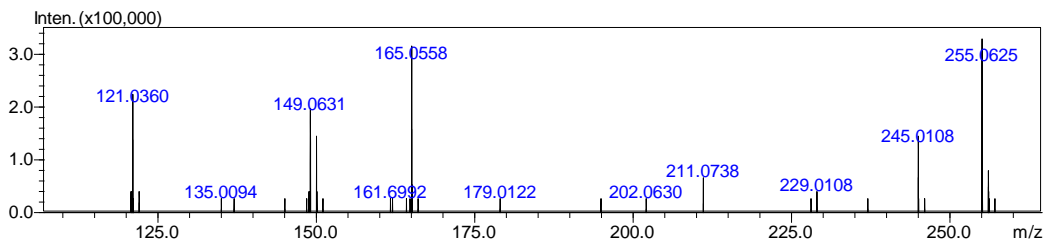


Figure S49. The MS² spectrum of **M114**.

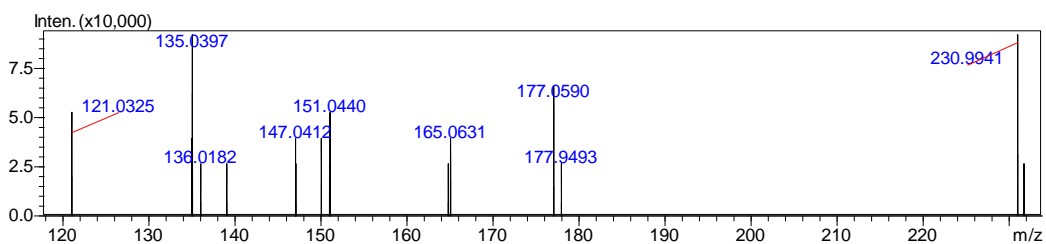


Figure S50. The MS² spectrum of **M115**.

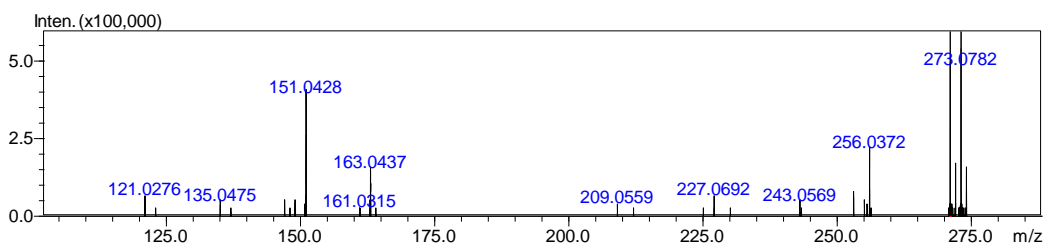


Figure S51. The MS² spectrum of **M144**.

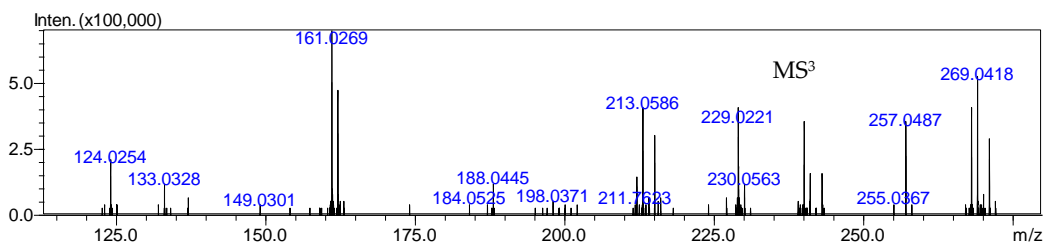
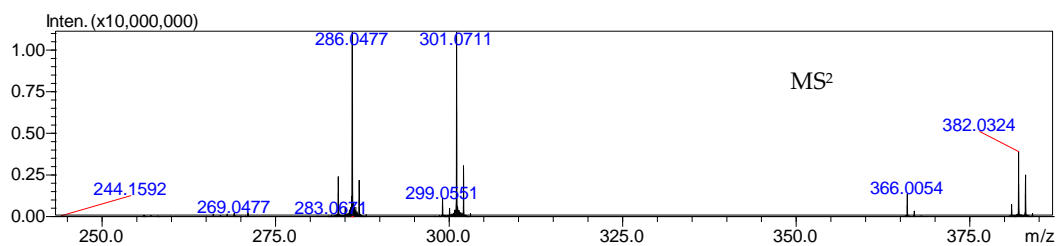


Figure S52. The MS² and MS³ spectra of **M159**.