

Supplemental Material

Title: Metabolic profiling of nuciferine *in vivo* and *in vitro*

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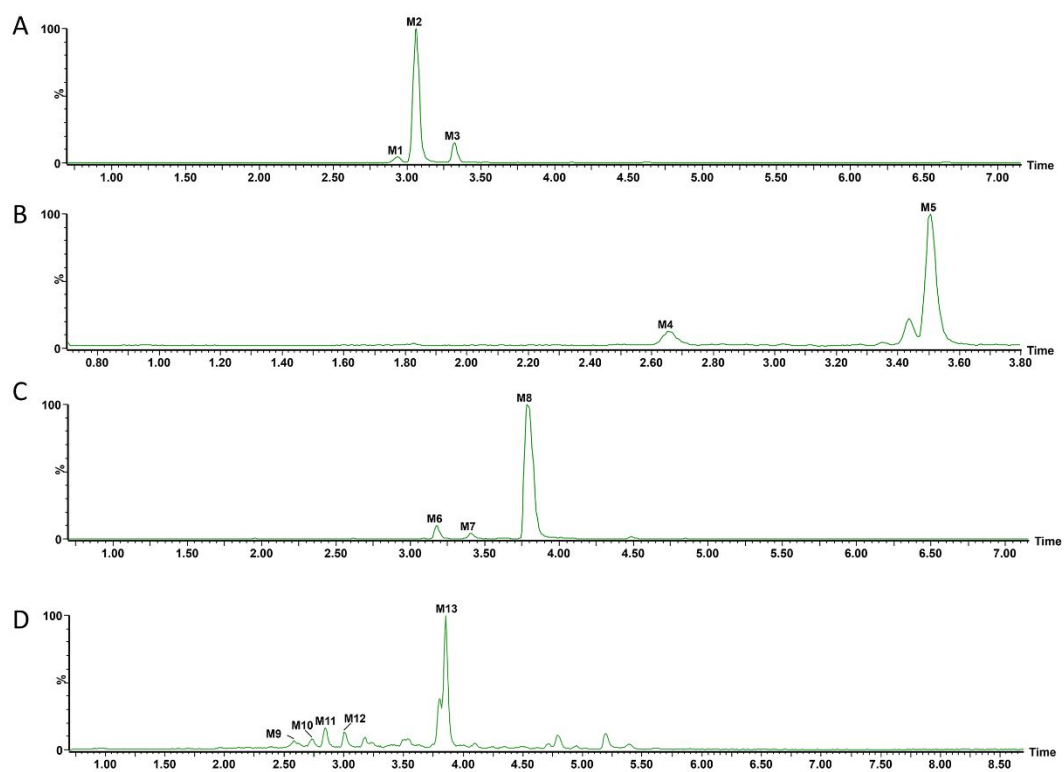
Xiuwei Yang, Yingtao Zhang, Youbo Zhang

Supplemental Table 1. ADMET Properties of CYPs

Enzyme	Substr	Sites
CYP1A2	Yes (88%)	C17, C15, N
CYP2A6	Yes (69%)	C17, C8
CYP2B6	Yes (79%)	C17, C8, C15, C10, C19
CYP2C8	Yes (77%)	C17, C19, C8, C18
CYP2C9	Yes (61%)	C17, C19, C8, C18
CYP2C19	Yes (71%)	C17, C19
CYP2D6	Yes (82%)	C19, C17, C18, C15
CYP2E1	Yes (90%)	C17, C19, C18
CYP3A4	Yes (98%)	C17, C19, C8, C18, N, C7

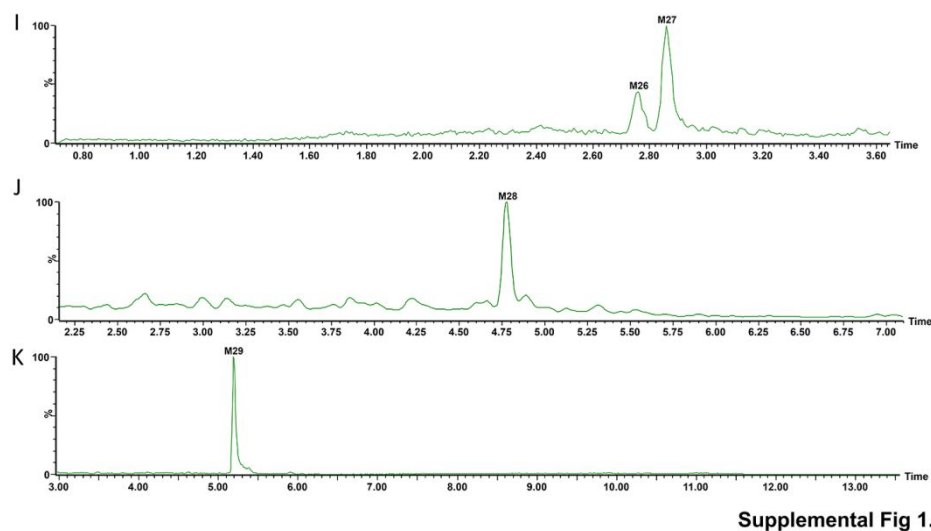
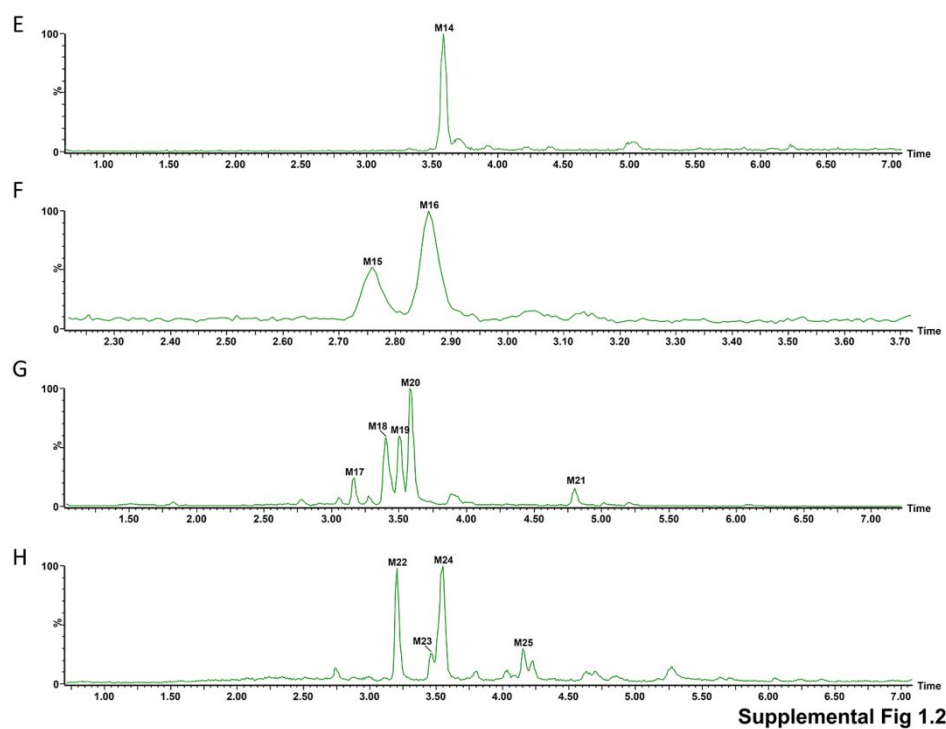
Supplemental Table 2. ADMET Properties of UGTs

Enzyme	UGT1A1	UGT1A3	UGT1A4	UGT1A6	UGT1A8	UGT1A9	UGT1A10	UGT2B7	UGT2B15
Substr	No (98%)	No (98%)	Yes (98%)	No (97%)	No (98%)	No (96%)	No (97%)	No (96%)	No (98%)



Supplemental Fig 1.1

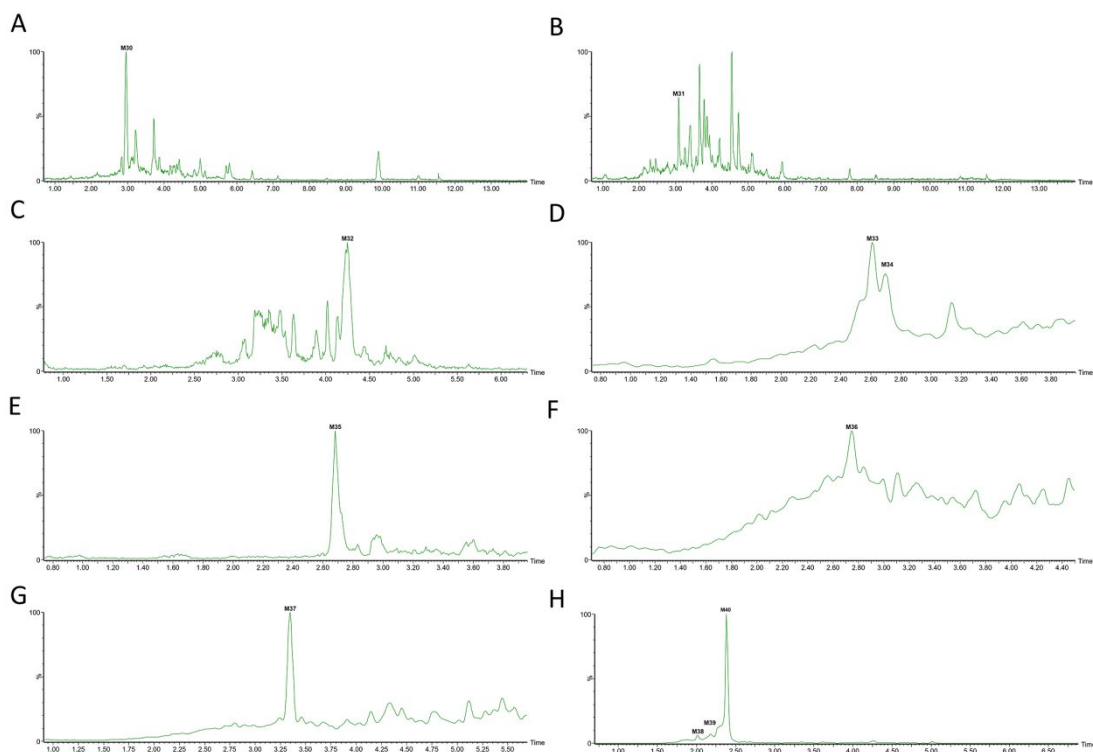
Supplemental Fig 1.1 Chromatograms of Phase I metabolites of NF: (A) M1, M2, M3; (B) M4, M5; (C) M6, M7, M8; (D) M9, M10, M11, M12, M13



Supplemental Fig 1.2
Chromatograms of

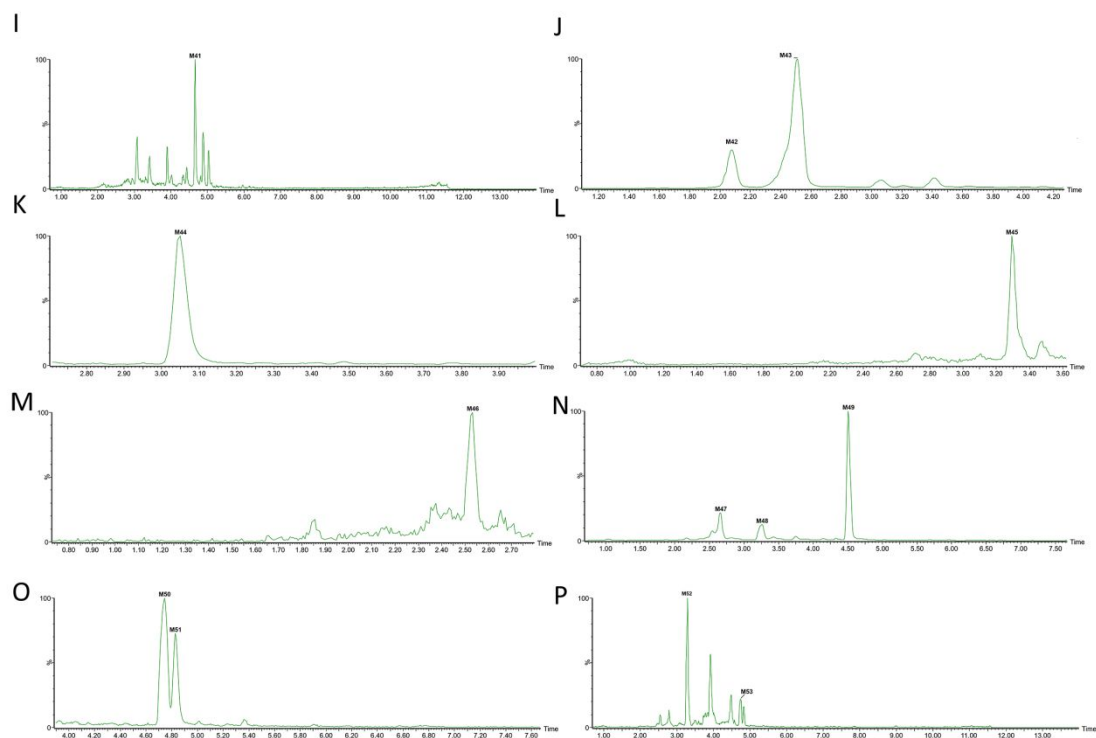
Phase I metabolites of NF: (E) M14; (F) M15, M16; (G) M17, M18, M19, M20, M21; (H) M22, M23, M24, M25

Supplemental Fig 1.3 Chromatograms of Phase I metabolites of NF: (I) M26, M27; (J) M28; (K) M29



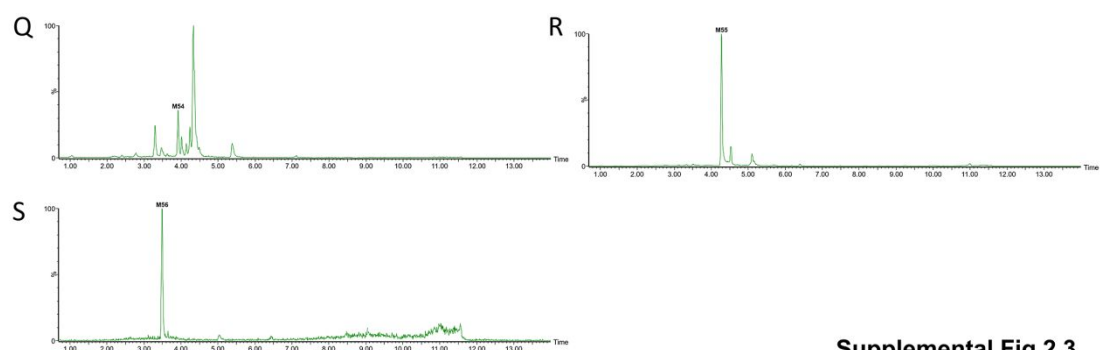
Supplemental Fig 2.1

Supplemental Fig 2.1 Chromatograms of Phase II metabolites of NF: (A) M30; (B) M31; (C) M32; (D) M33, M34; (E) M35; (F) M36; (G) M37; (H) M38, M39, M40



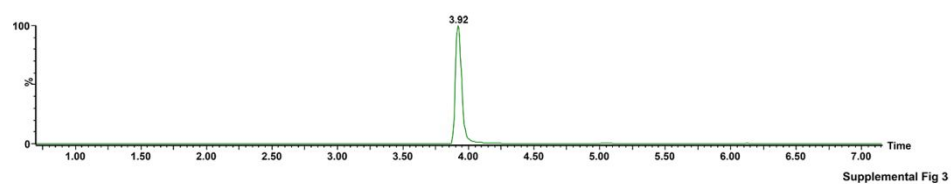
Supplemental Fig 2.2

Supplemental Fig 2.2 Chromatograms of Phase II metabolites of NF: (I) M41; (J) M42, M43; (K) M44; (L) M45; (M) M46; (N) M47, M48, M49; (O) M50, M51; (P) M52, M53



Supplemental Fig 2.3

Supplemental Fig 2.3 Chromatograms of Phase II metabolites of NF: (Q) M54; (R) M55; (S) M56



Supplemental Fig 3

Supplemental Fig 3 Chromatograms of NF