

Supporting information

Detection of drug bioactivation *in vivo*: Mechanism of nevirapine-albumin conjugate formation in patients

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Figure S1. Quantitative analysis of NVP and 12-OH-NVP metabolite in plasma from HIV patients receiving NVP. 12-OH-NVP standard (a), 12-OH-NVP (b) and NVP (c) detected in patient plasma, standard curve was constructed with synthetic 12-OH-NVP ranging from 1 nM to 1 μ M (in 50% methanol/0.1% TFA) (d).

Figure S2. Characterisation of human GSTP expressed in *E.coli*. Amino acid sequence of human GSTP is listed (a); Crude GSTP was resolved by SDS-PAGE using 10% gel (b); peptide mass fingerprinting by MALDI-MS to characterize GSTP (c).

Figure S3. MS/MS analysis of NVP-modified HSA peptides identified *in vitro*. MS/MS spectra of tryptic peptide ²⁴¹VHTECCHGDLLECADDR²⁵⁷ modified by NVP at either His242 or His247. Characteristic fragment ions from NVP group are circled (a); MS/MS spectra of tryptic peptide ³³⁷RH*PDYSVLLLR³⁴⁸ modified by NVP at His338 marked with an * (b);

Figure S1

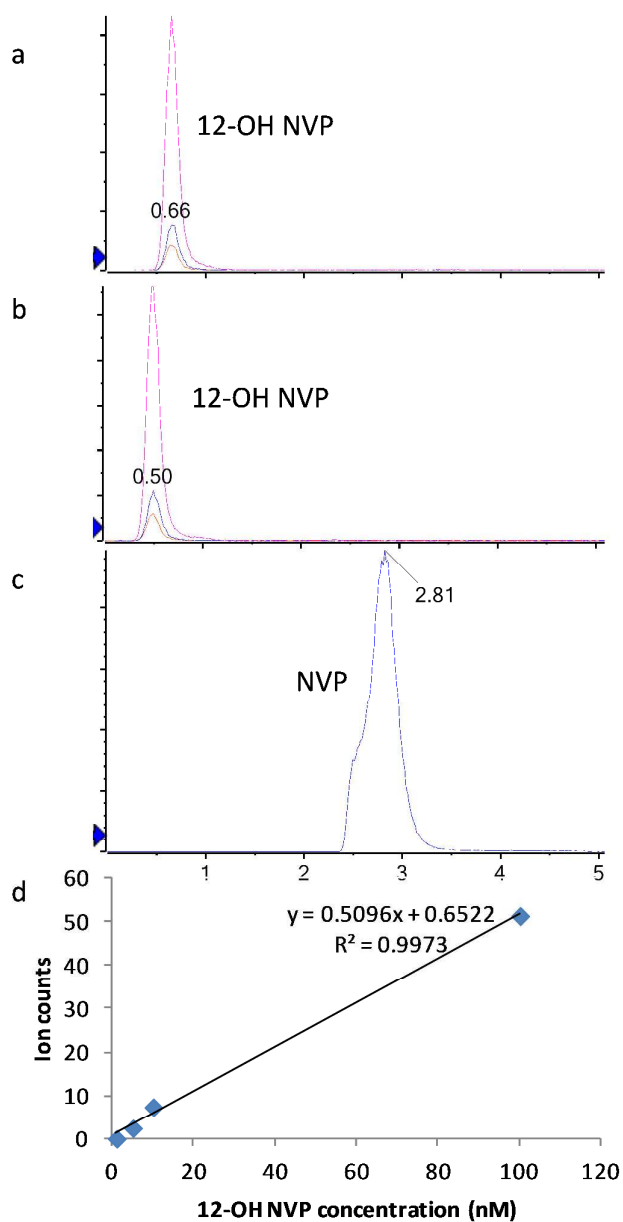


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Figure S2

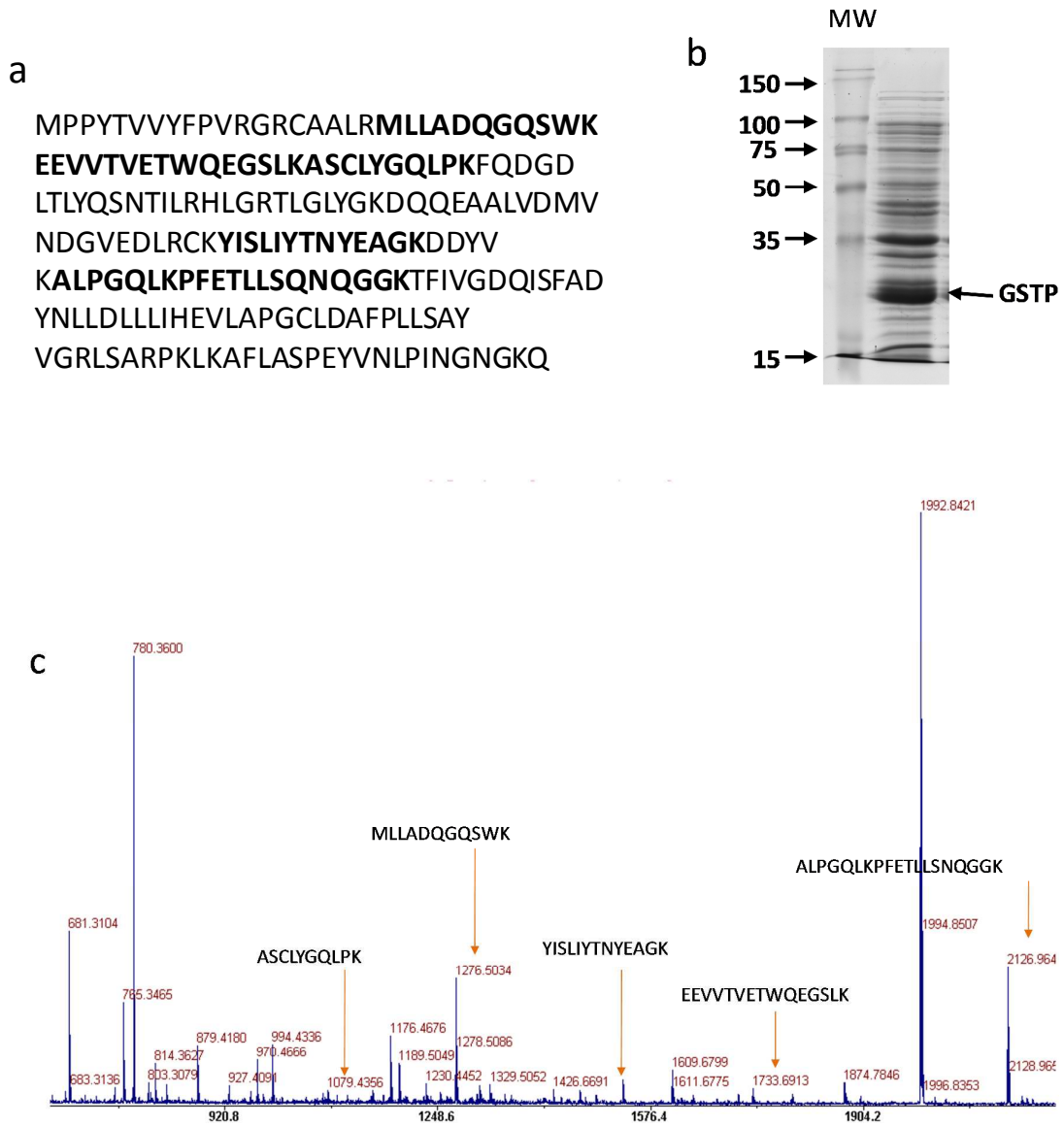


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Figure S3

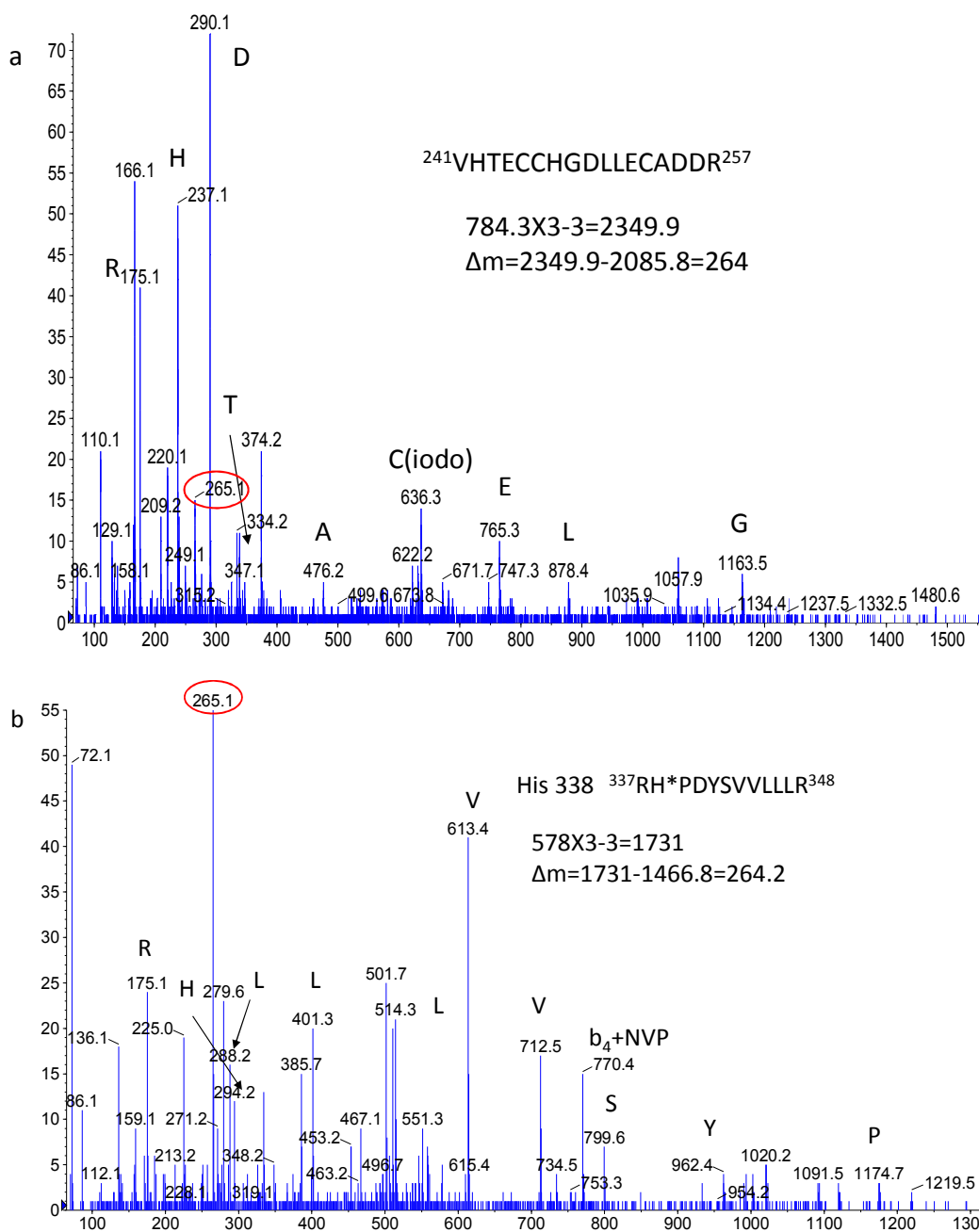


Figure S3. MS/MS analysis of NVP-modified HSA peptides identified *in vitro*. MS/MS spectra of tryptic peptide $^{241}\text{VHTECCHGDLLECADDR}^{257}$ modified by NVP at either His242 or His247. Characteristic fragment ions from NVP group are circled (a); MS/MS spectra of tryptic peptide $^{337}\text{RH}^*\text{PDYSVLLLLR}^{348}$ modified by NVP at His338 marked with an * (b);