

## Supporting information

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

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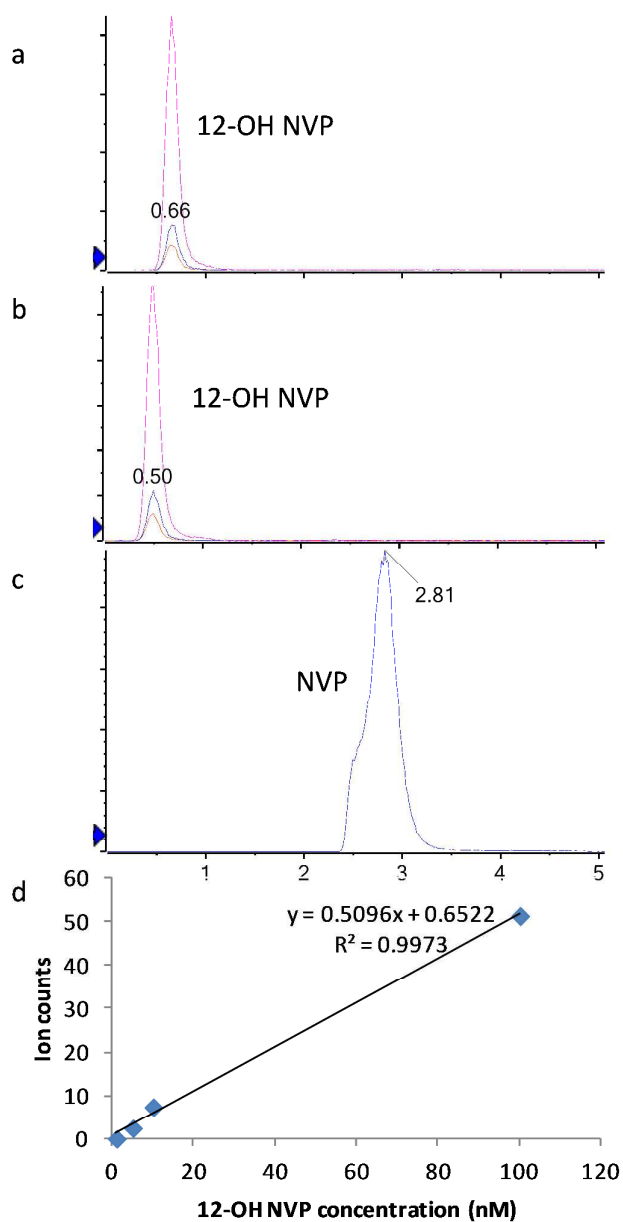
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**Figure S1.** Quantitative analysis of NVP and 12-OH-NVP metabolite in plasma from HIV patients receiving NVP. 12-OH-NVP standard (a), 12-OH-NVP (b) and NVP (c) detected in patient plasma, standard curve was constructed with synthetic 12-OH-NVP ranging from 1 nM to 1  $\mu$ 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).

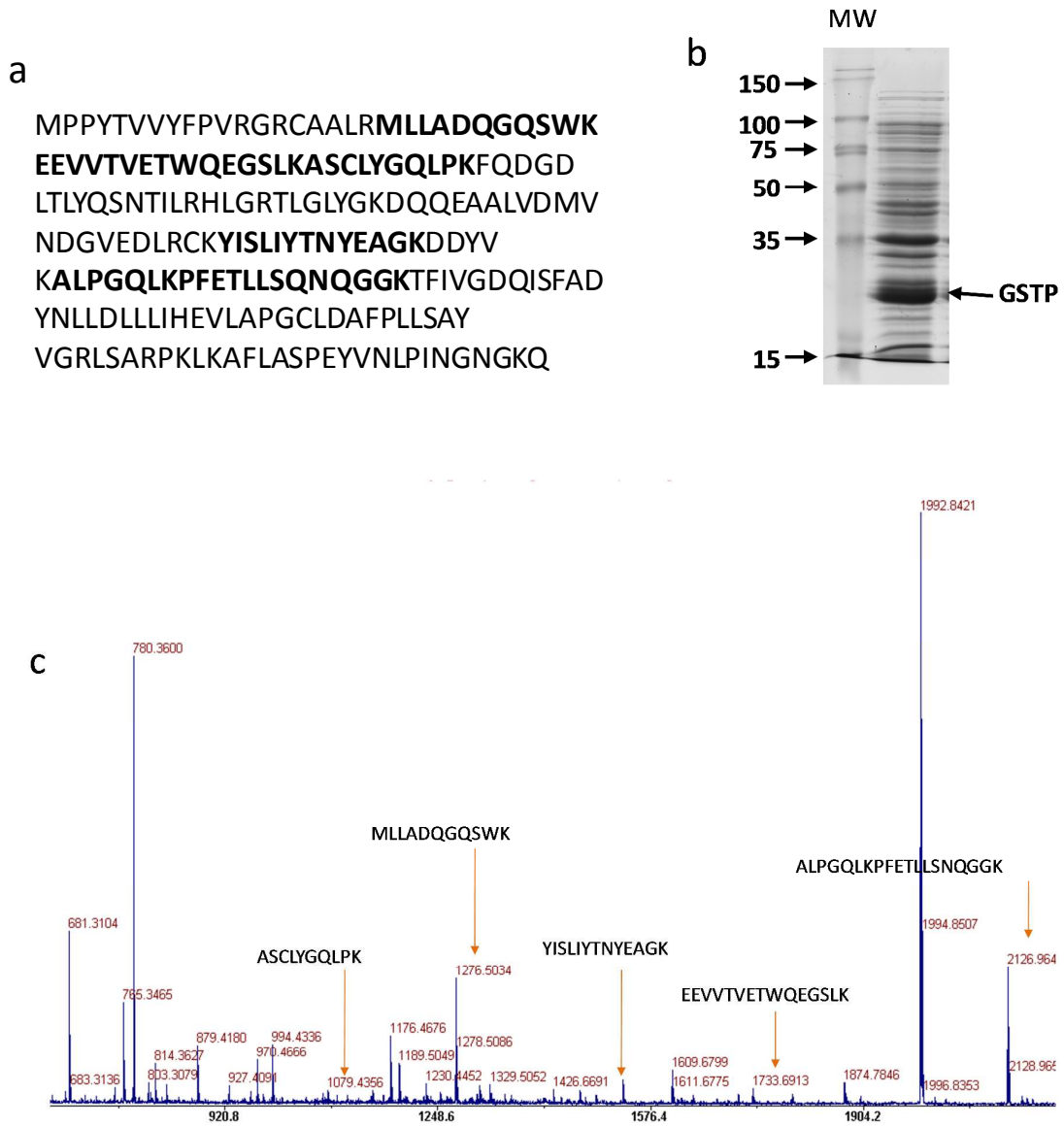
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**Figure S1**



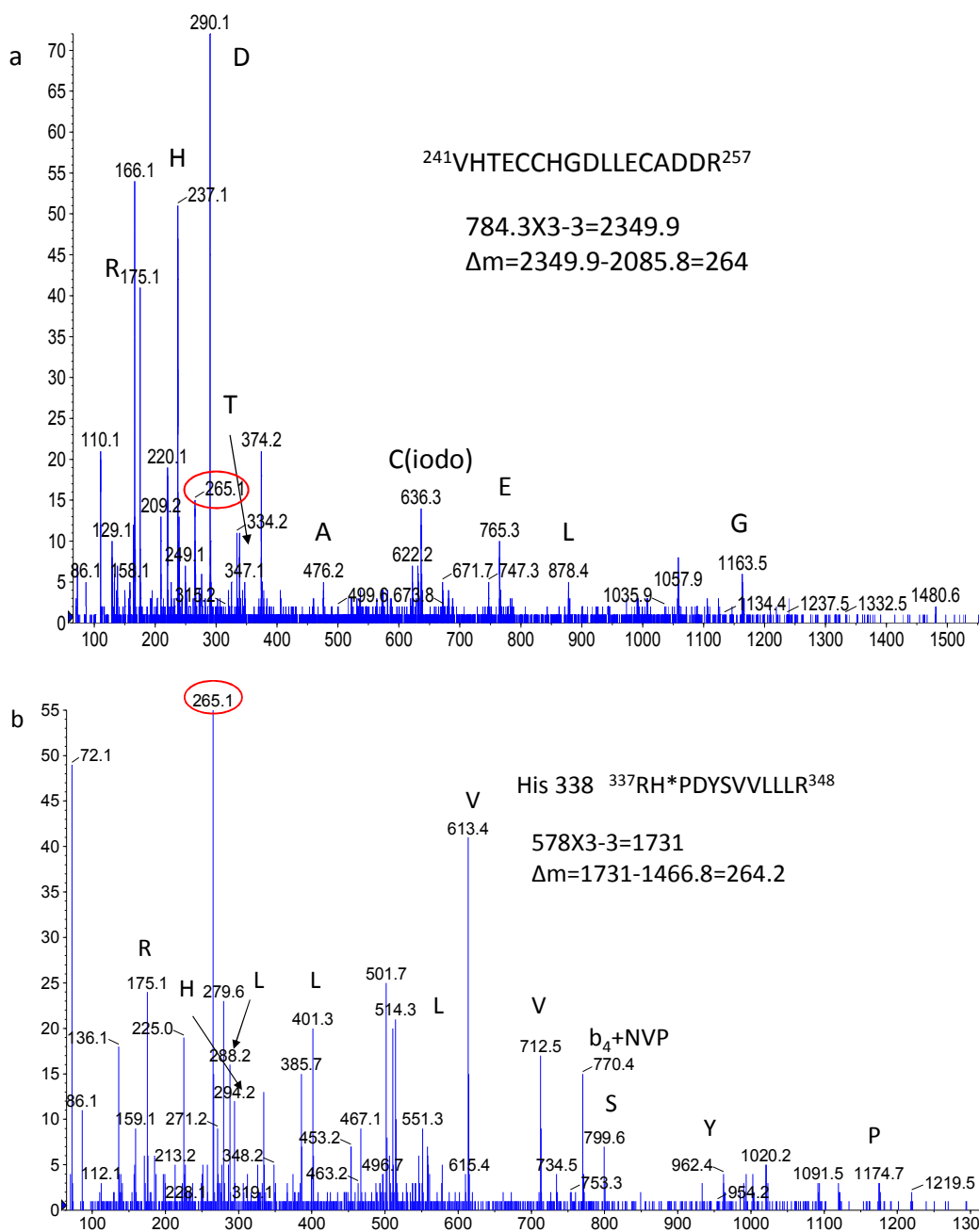
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Figure S2



**Figure S2. Characterization 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



**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);