Supplementary Materials

11-Keto-α-boswellic Acid, a Novel Triterpenoid from *Boswellia* spp. with Chemotaxonomic Potential and Antitumor Activity against Triple-Negative Breast Cancer Cells

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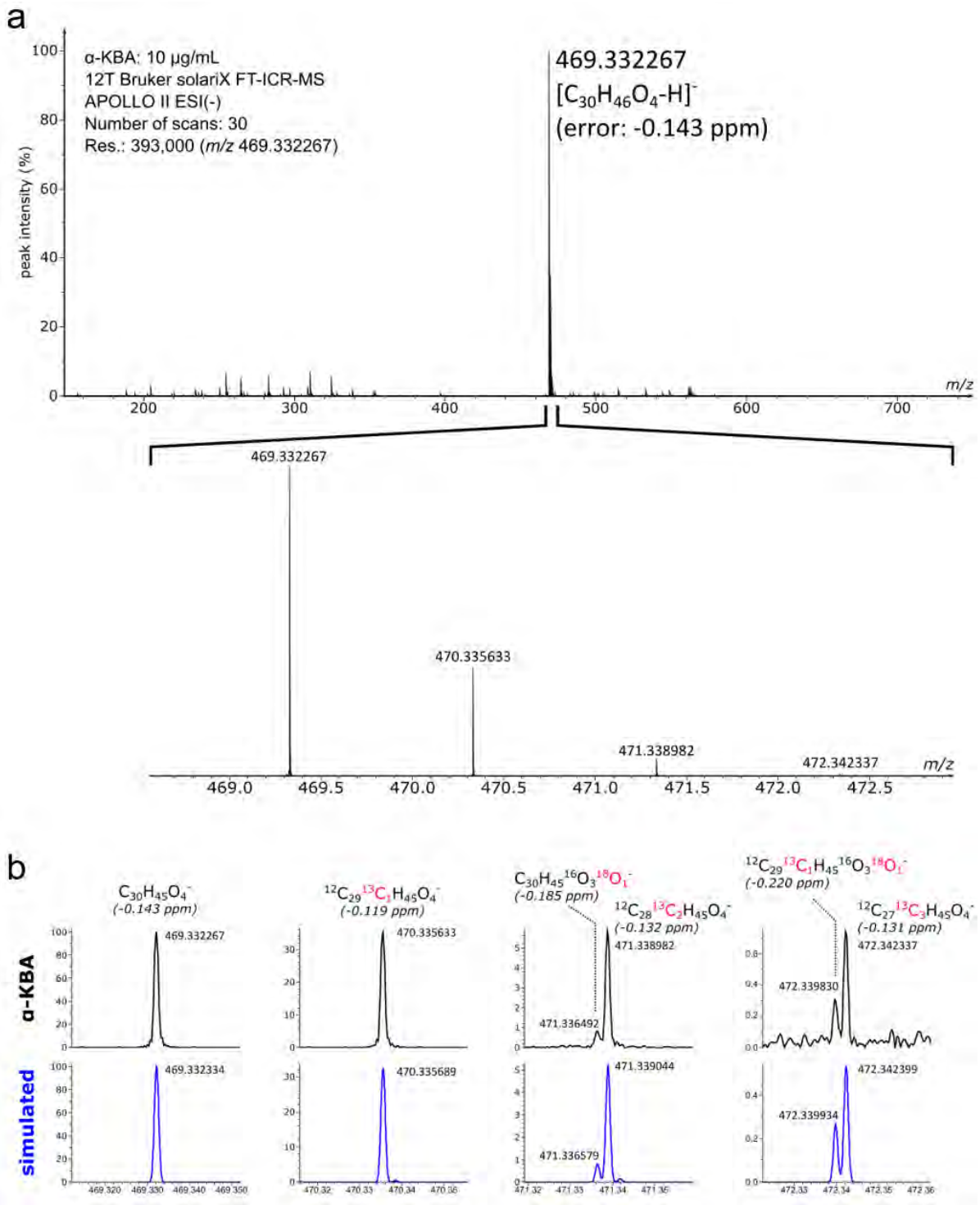

Figure S1. High-resolution mass spectrometry (HR-MS) of α-KBA. (**a**) HR mass spectrum with an exact mass at *m/z* 469.332267 for $[M\text{-}H]^-$ (calcd.: 469.332333, error: -0.143 ppm). (**b**) The isotope pattern and the individual exact masses corresponded to predicted data.

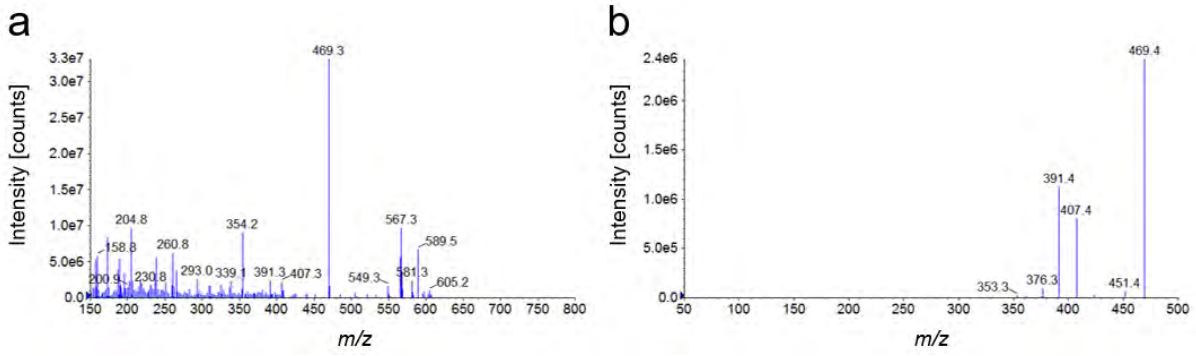

Figure S2. Tandem mass spectrometry (MS/MS) of α-KBA. (**a**) Mass spectrum with *m*/*z* 469.3 ([M-H]$^-$) as precursor ion. (**b**) Product ion mass spectrum with characteristic fragments at *m*/*z* 353.3, 376.3, 391.4, 407.4, and 451.4.

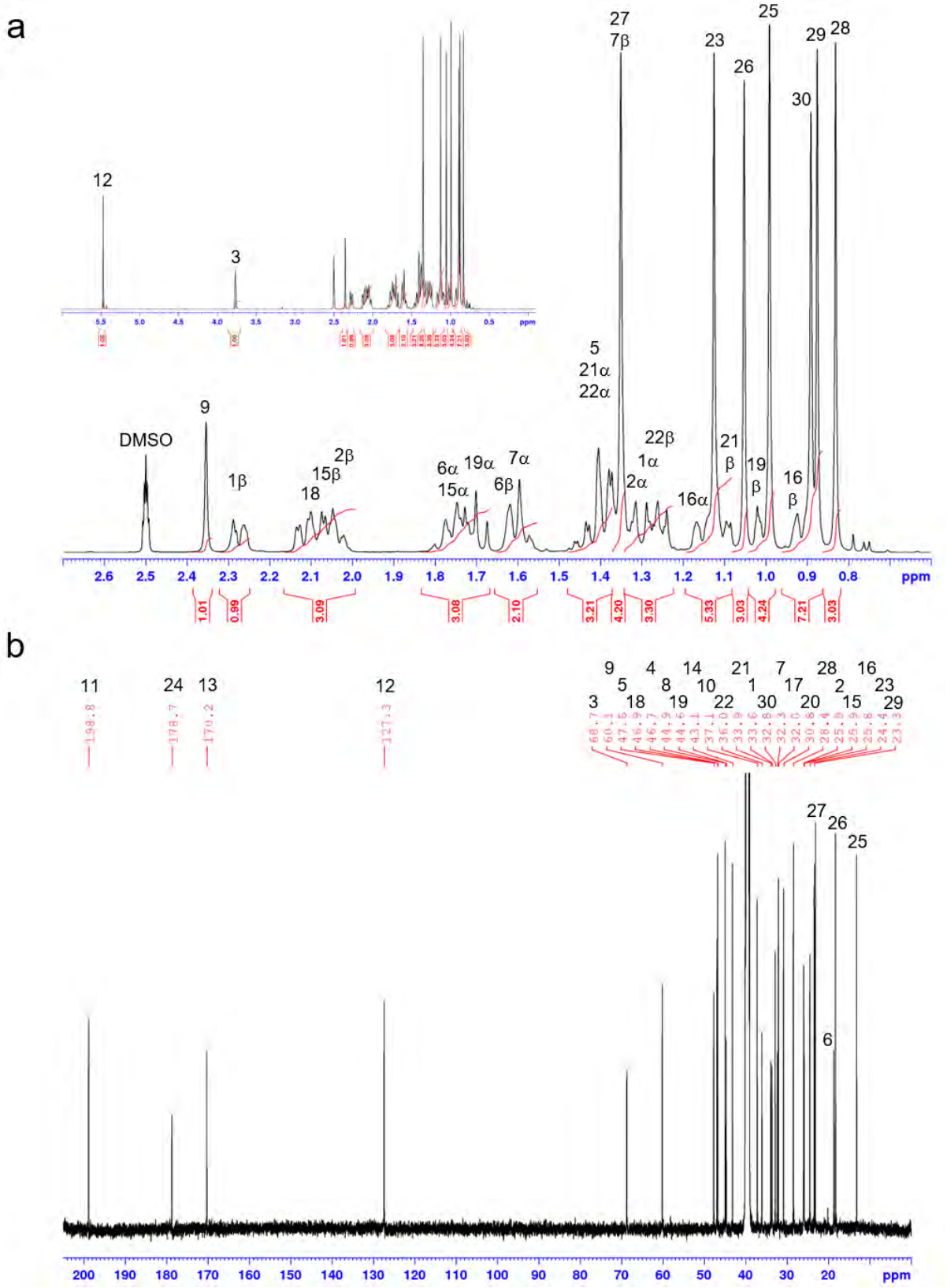

Figure S3. ^{1}H and ^{13}C NMR spectra of α-KBA (in DMSO-d_6). (**a**) ^{1}H NMR spectrum. (**b**) ^{13}C NMR spectrum. Assigment of signals according to Figure 3a and Table 1 of the main text.

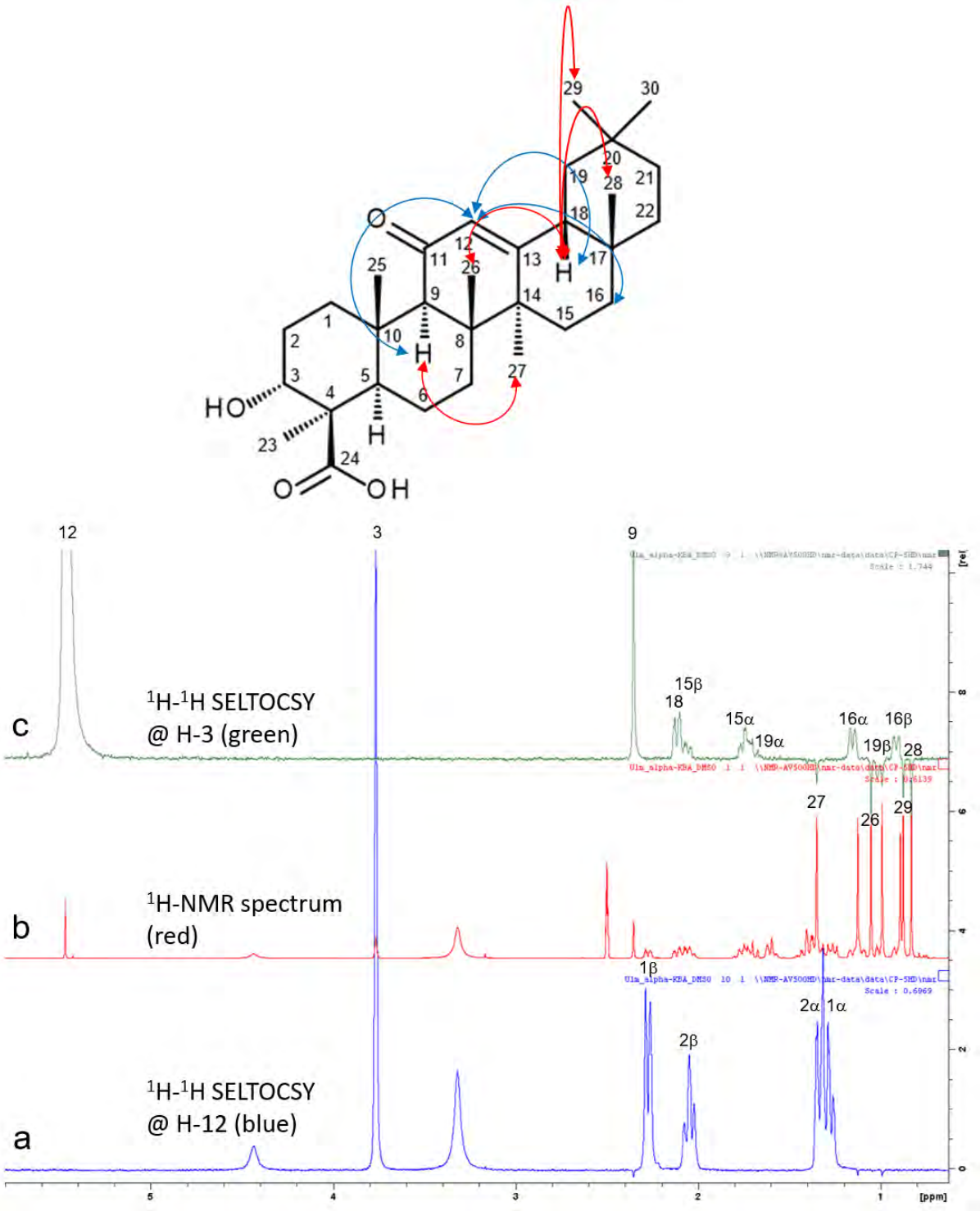

Figure S4. ^{1}H, ^{1}H SELTOCSY (selective total correlation spectroscopy) spectra of α-KBA (in DMSO-d_6). Comparison of the ^{1}H NMR spectrum (**b**) with ^{1}H, ^{1}H SELTOCSY spectra. (**a**) Transmitter frequency at δ_H 3.77 (H-3). (**c**) Transmitter frequency at δ_H 5.47 (H-12).

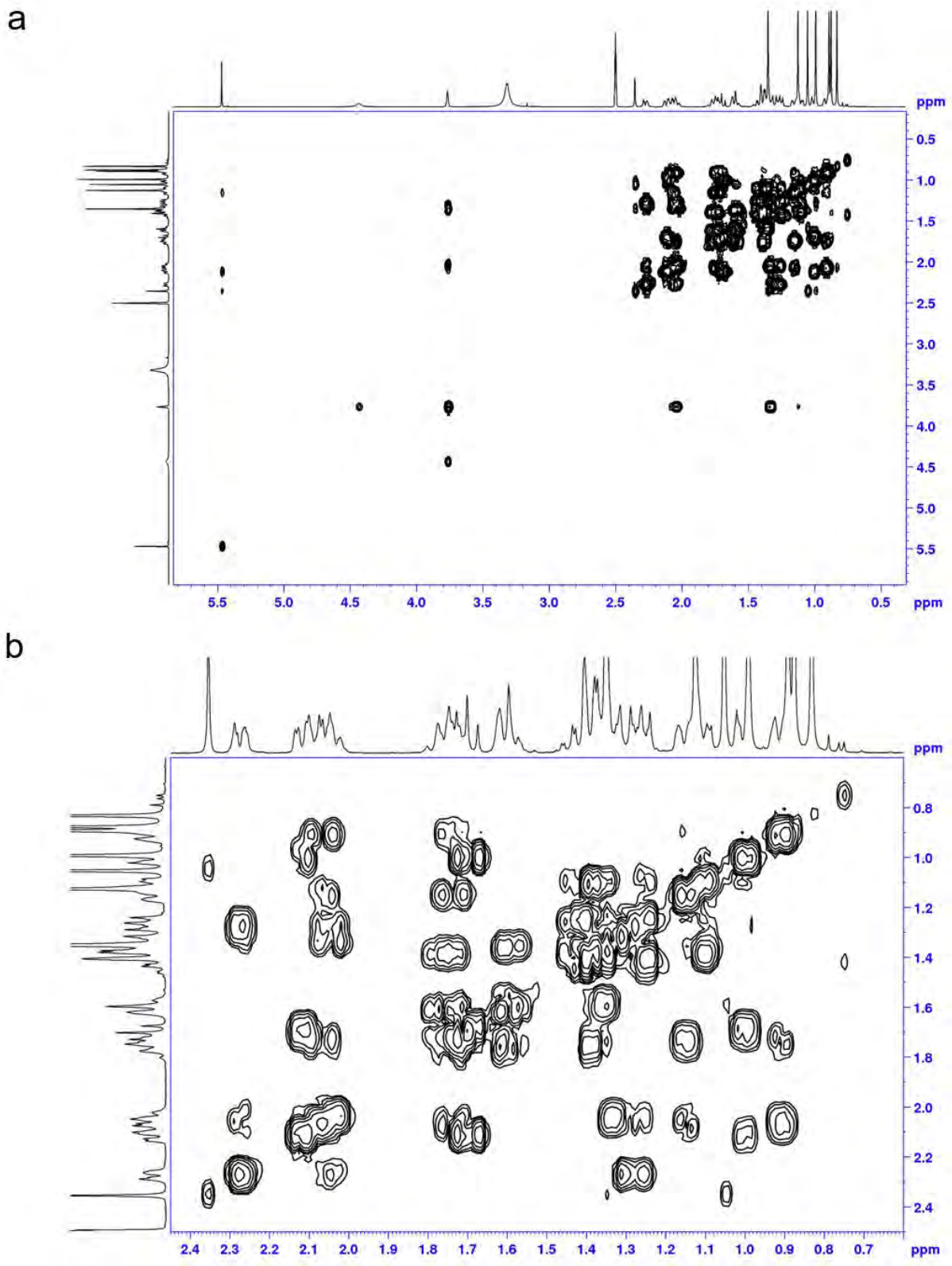

Figure S5. ^{1}H, ^{1}H COSY (correlation spectroscopy) spectrum of α-KBA (in DMSO-d_6). (**a**) Full spectrum. (**b**) Enlarged section.

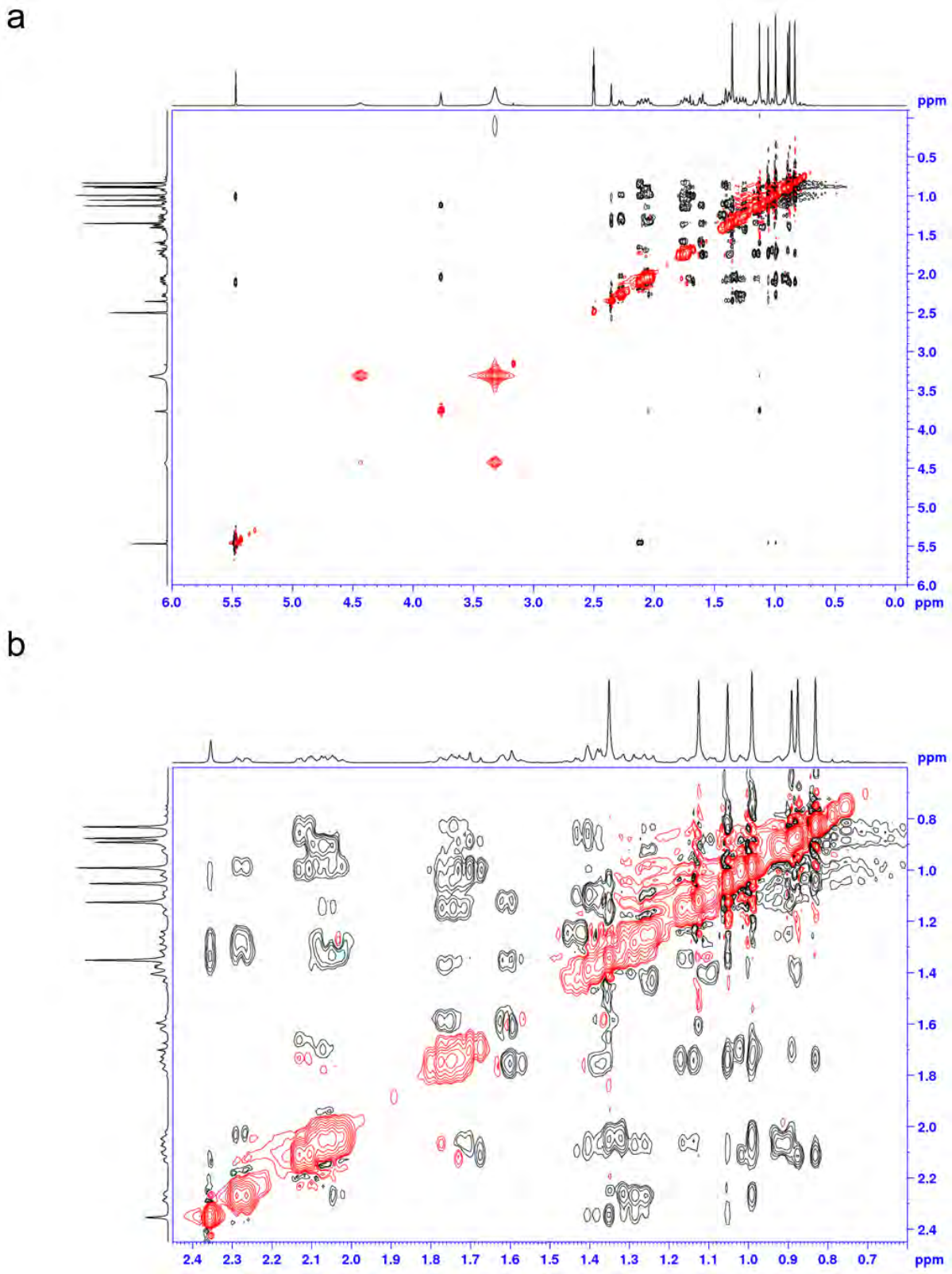

Figure S6. ^{1}H, ^{1}H ROESY (rotating frame Overhauser enhancement spectroscopy) spectrum of α-KBA (in DMSO-d_6). (**a**) Full spectrum. (**b**) Enlarged section.

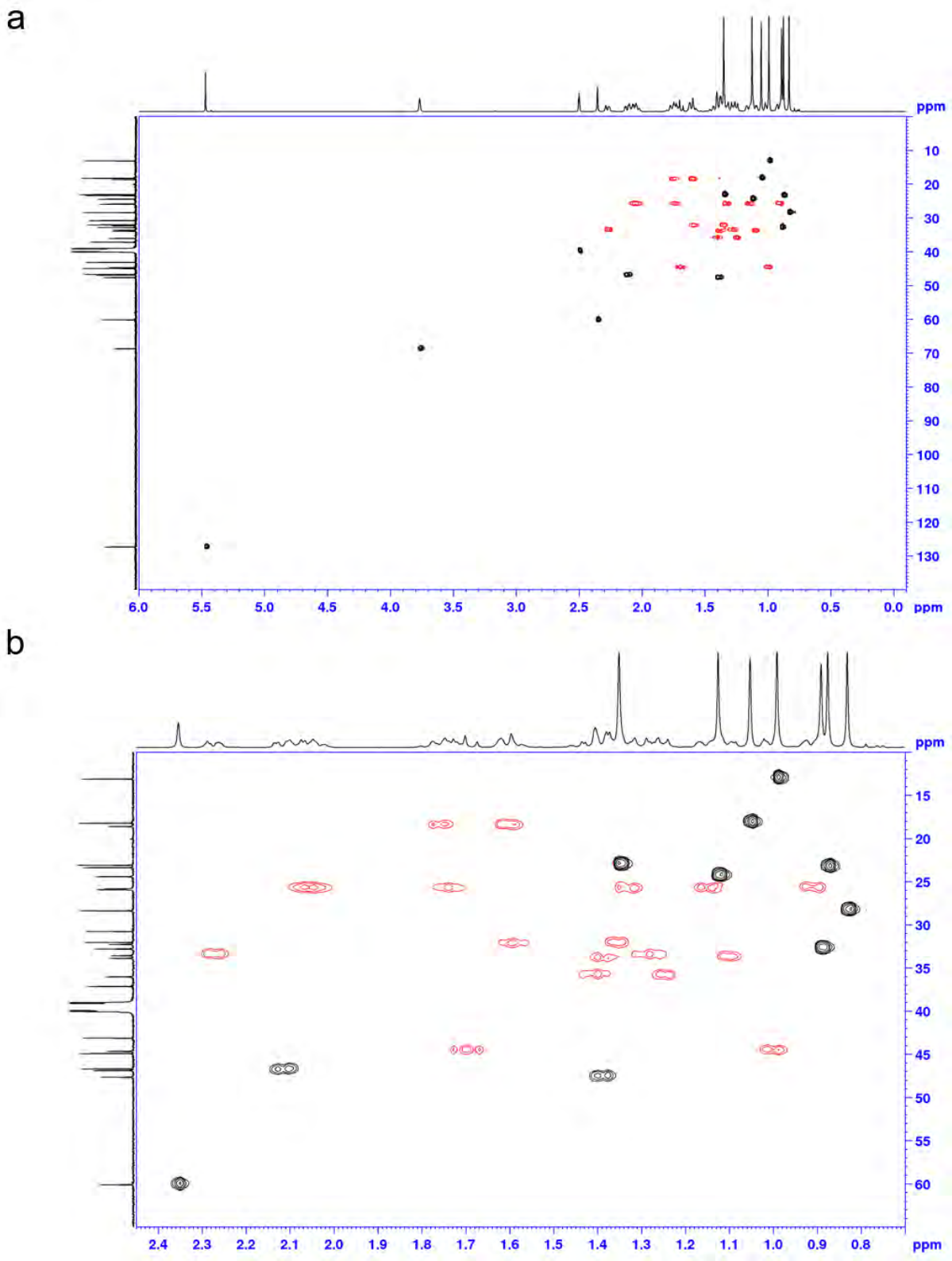

Figure S7. ^{1}H, ^{13}C HSQC (heteronuclear single quantum coherence spectroscopy) spectrum of α-KBA (in DMSO-d_6). (**a**) Full spectrum. (**b**) Enlarged section.

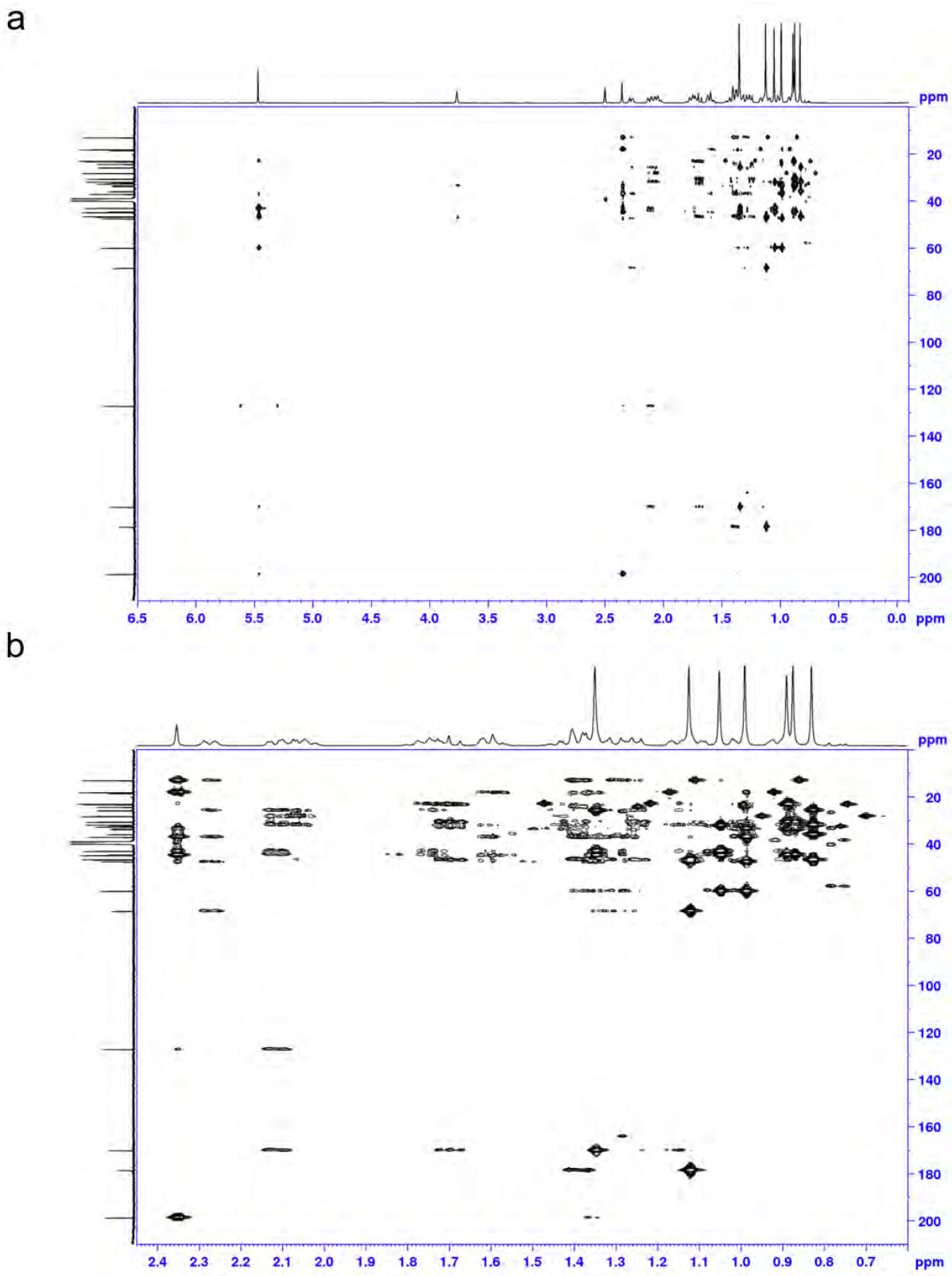

Figure S8. ^{1}H, ^{13}C HMBC (heteronuclear multiple bond correlation spectroscopy) spectrum of α-KBA (in DMSO-d_6). (**a**) Full spectrum. (**b**) Enlarged section.