Supplementary Material (ESI) for Molecular BioSystems

Human serum albumin modifications associated with reductive radical stress

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SUPPORTING INFORMATION

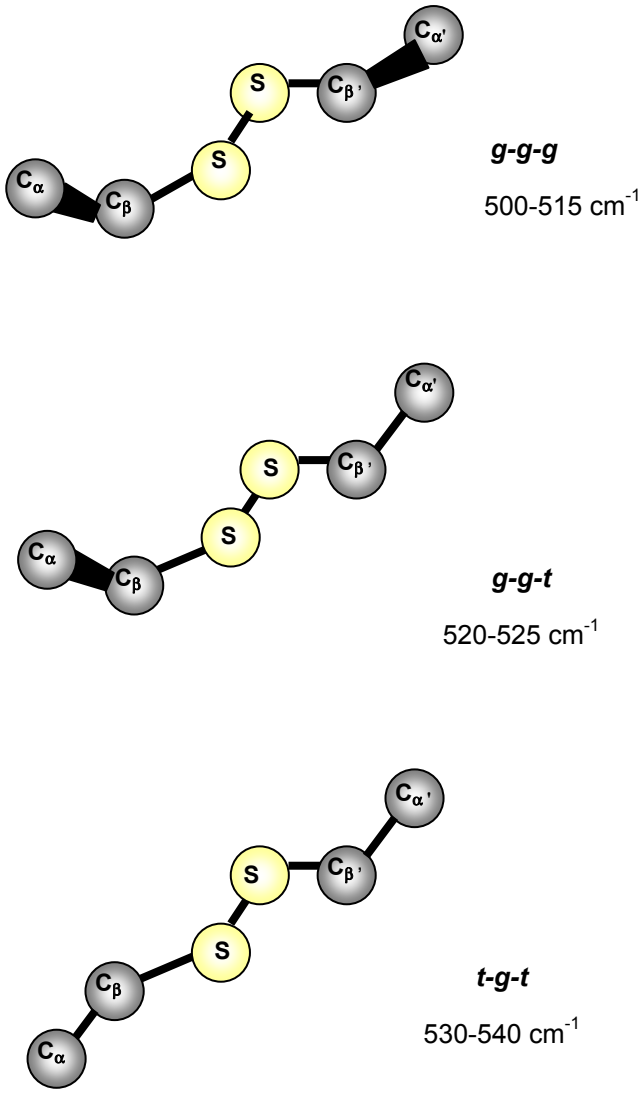

Figure S1. Conformations of the C_α-C_β-S-S-$C_{\beta'}$-$C_{\alpha'}$ moiety. *Gauche-gauche gauche*, *ggg*; *gauche-gauche-trans*, *ggt*; *trans-gauche-trans*, *tgt.* The Raman wavenumber of the corresponding S-S stretching vibration, which changes as a function of the internal rotation about C-S and C-C bonds of the C_α-C_β-S-S-$C_{\beta'}$-$C_{\alpha'}$ moiety, is also indicated.

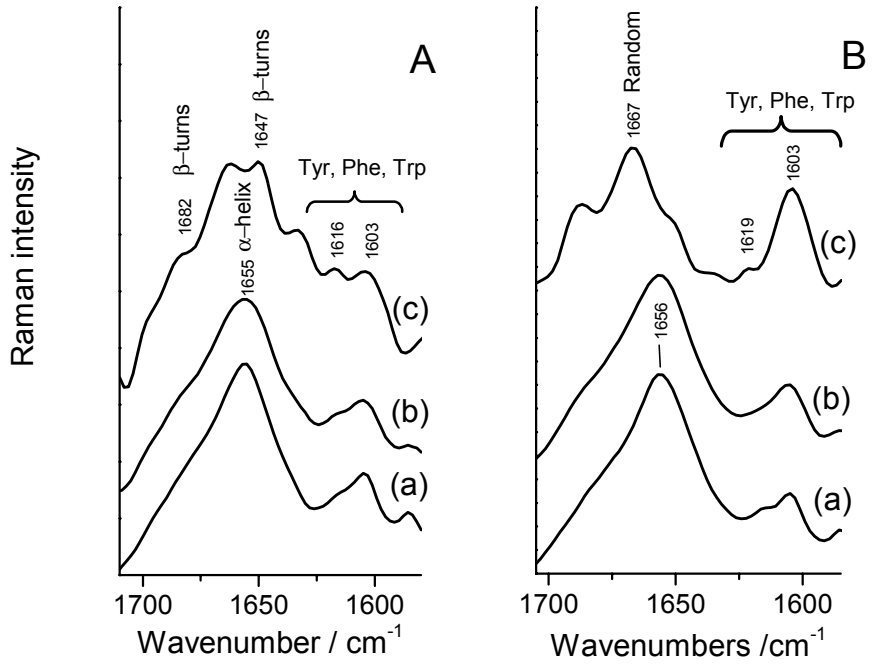

Figure S2. The Raman spectra of HSA samples in the 1550-1700 cm^{-1} region for (A) Ar-flushed aqueous solutions containing 0.2 M *t*-BuOH and (B) Ar-flushed aqueous solutions following different irradiation doses, (a) 0, (b) 50 and (c) 300 Gy.

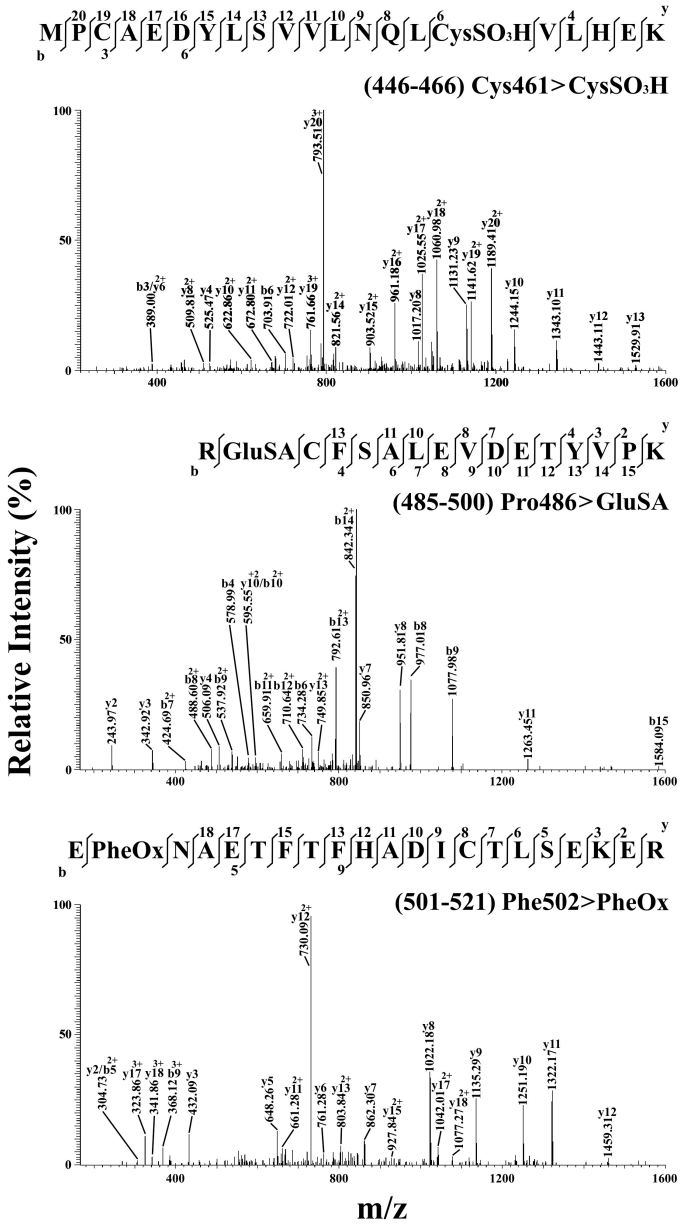

Figure S3. Tandem mass spectrometry analysis of some oxidized peptides present in the tryptic digest of irradiated HSA samples. Newly formed amino acids are shown with a three-letter abbreviation. The fragmentation mass spectrum of the triply charged ion at *m/z* 837.6 associated with the peptide (446-466)Cys461>$CysSO_3H$ is shown in panel A. The fragmentation mass spectrum of the triply charged ion at *m/z* 643.1 associated with the peptide (485-500)Pro486>GluSA is shown in panel B. The fragmentation mass spectrum of the triply charged ion at *m/z* 854.5 associated with the peptide (501-521)Phe502>PheOx, is shown in panel C.

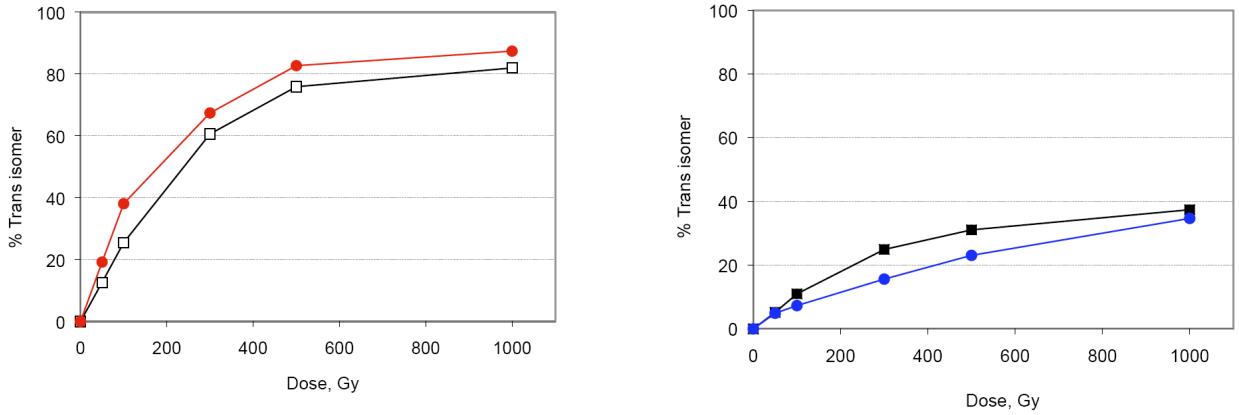

Figure S4. Dose dependence of the formation of elaidate (trans isomer) residues from γ-irradiation of POPC vesicles (2 mM) containing 0.6 mg/mL HSA (9.2 μM, ●) or BSA (9 μM, □) in the presence of 0.2 M *t*-BuOH as additive in aqueous Ar-flushed solutions or containing 0.6 mg/mL HSA (9.2 μM, ●) or BSA (9 μM, ■) in aqueous Ar-flushed solutions. Reported values represent the mean of three independent measurements ($p < 0.05$); errors are ± 2%.