Submission for *Chemical Research in Toxicology*

A Novel Endogenous Cyclic Glutathione Adduct Formed During Oxidative Stress: Supplementary Data

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Running title: A Novel Endogenous Glutathione-adduct

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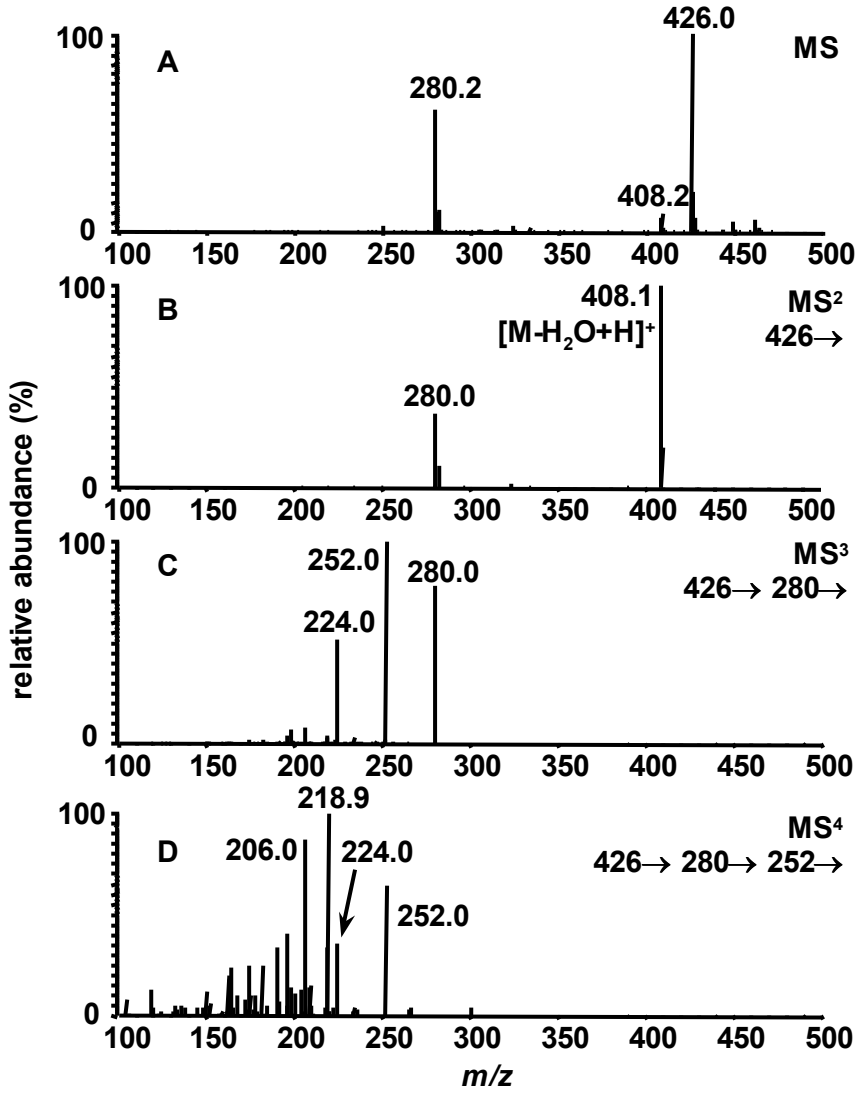

Figure S1: MS^n analyses of adduct IIa from the equine liver GST-mediated reaction between GSH and ONE. (A) MS^1, (B) MS^2, (C) MS^3, (D) MS^4.

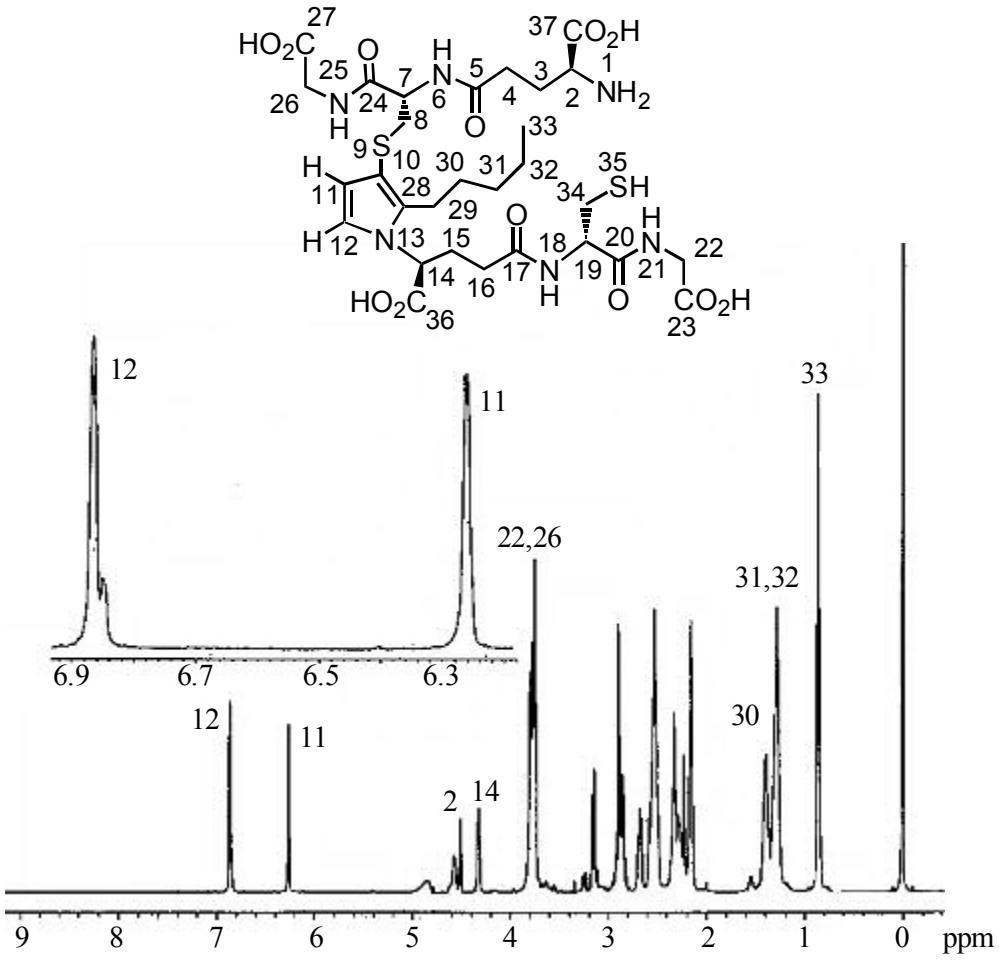

Figure S2: The ^{1}H NMR spectrum of adduct Ia.

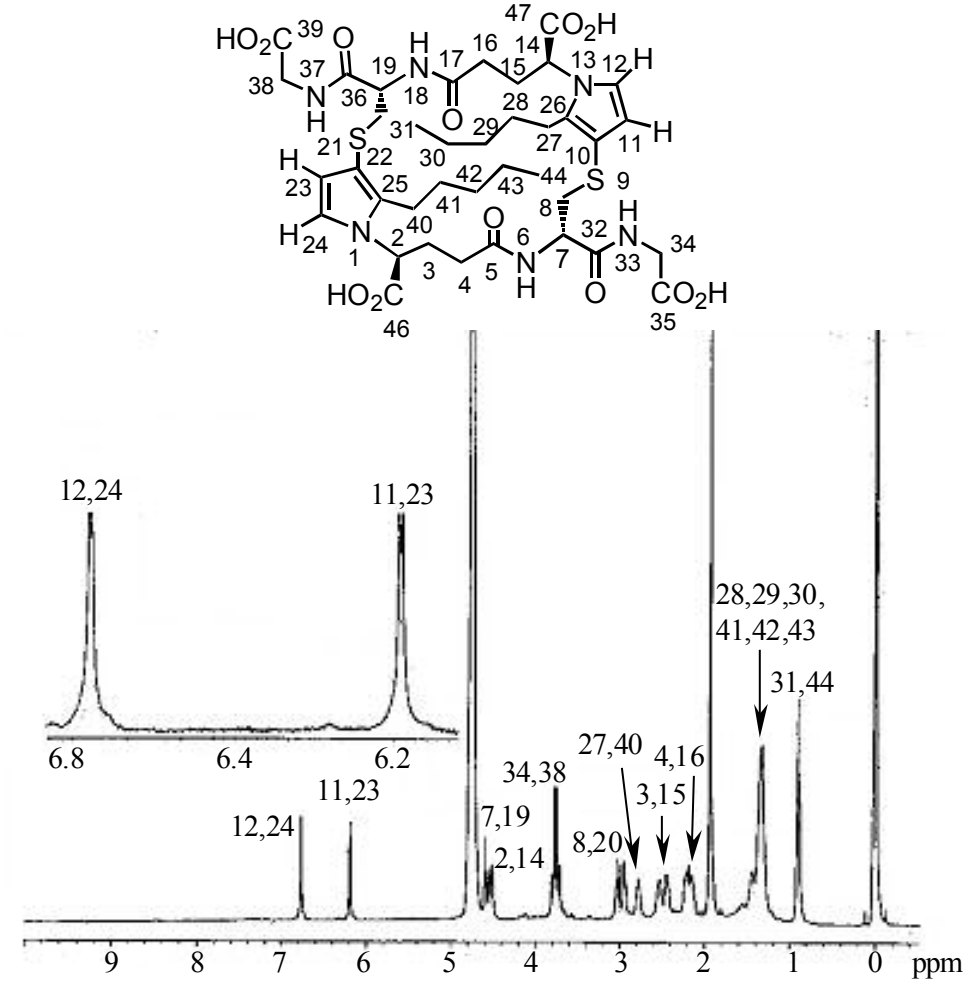

Figure S3 ^{1}H NMR spectrum of adduct III.

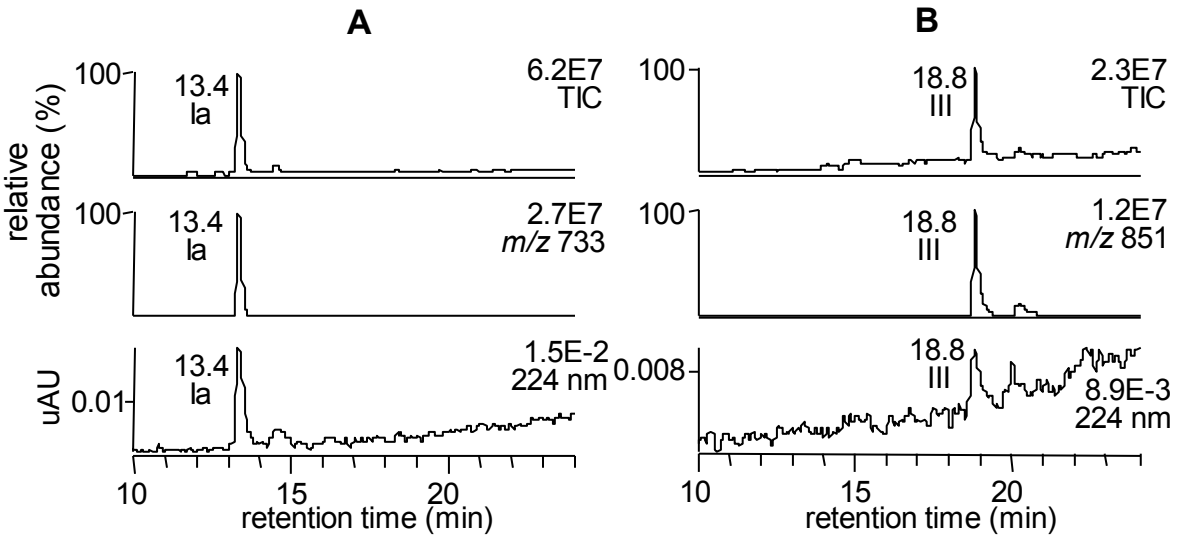

Figure S4 LC-MS Analysis of (system 1) of the reaction between adduct Ia and 3-[$^2H_1$]-ONE. (A) Adduct Ia purified from the reaction between GSH and 3-[$^2H_1$]-ONE (B). LC-MS analysis of the reaction between adduct Ia and 3-[$^2H_1$]-ONE at 37 ^oC overnight showing the exclusive formation of adduct III.

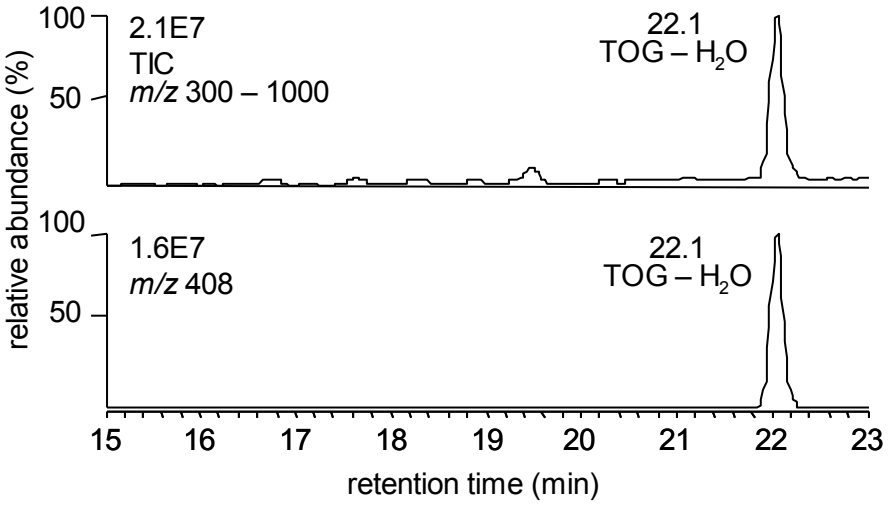

Figure S5: LC-MS analysis (system 1) of dehydrated adduct IIb from the reaction of TOG with 1 % TFA.

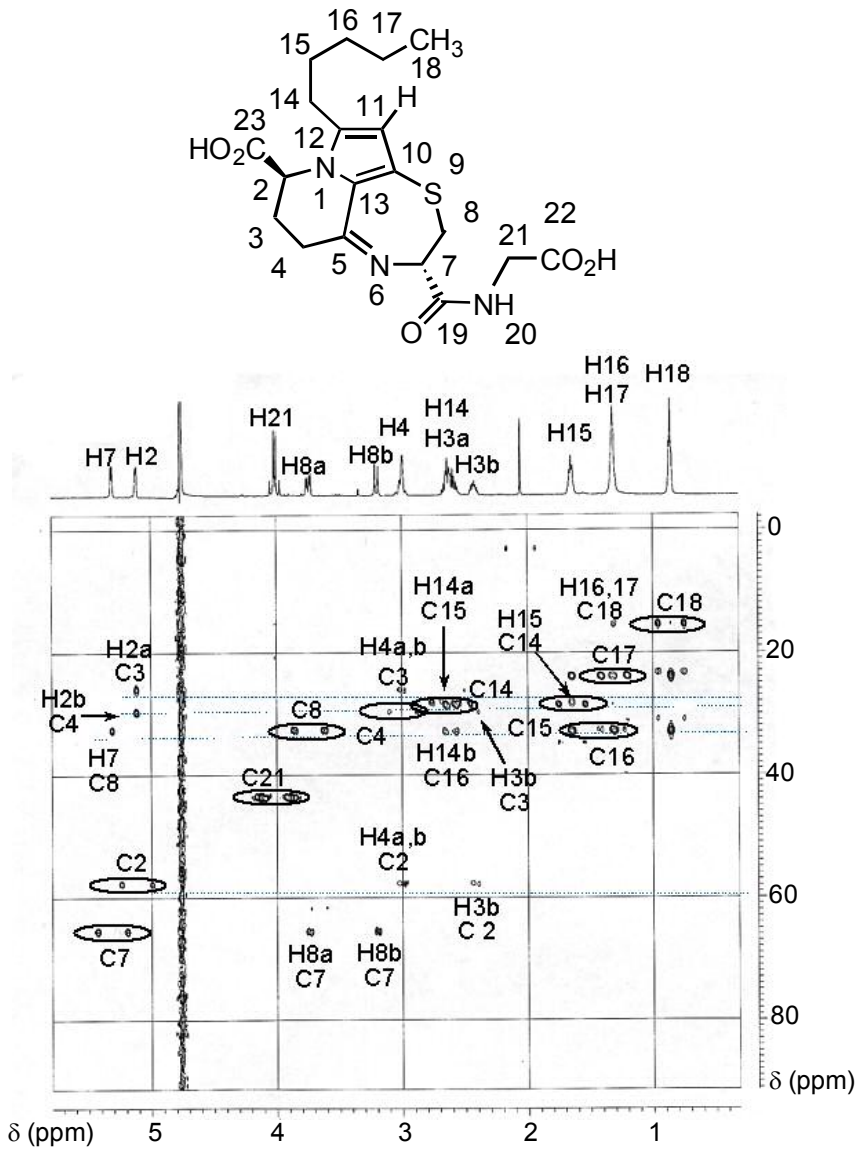

Figure S6: HMQC spectrum of dehydrated Adduct IIb.

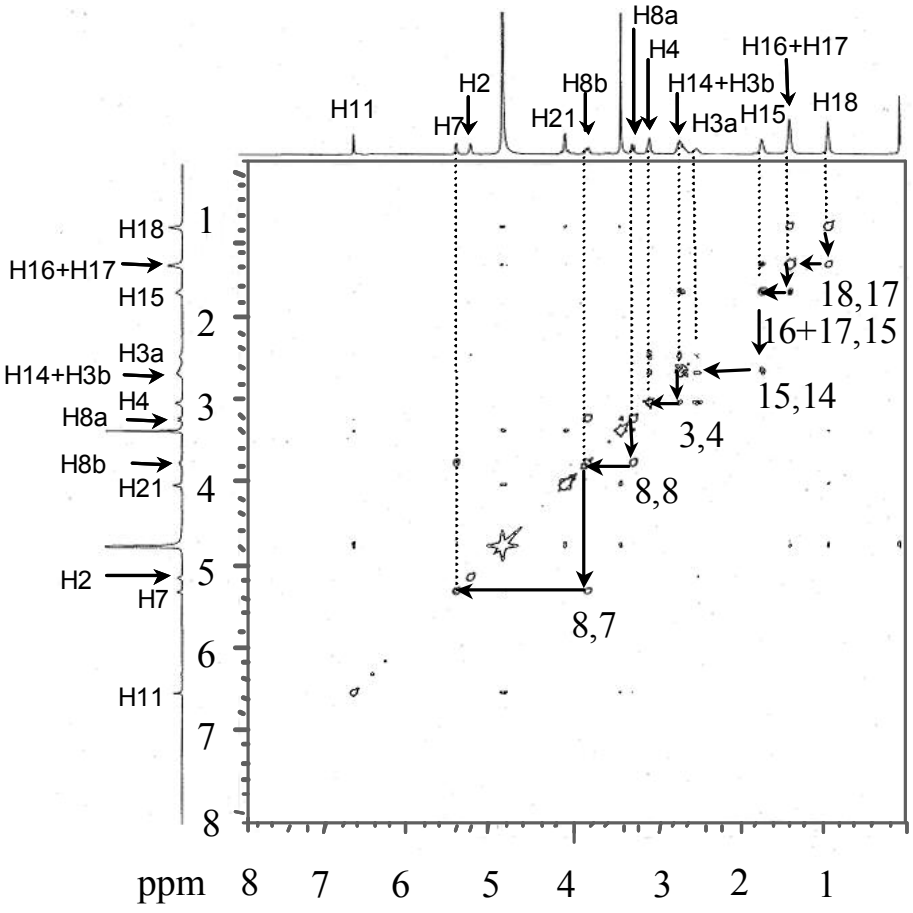

Figure S7: 2D COSY spectrum of dehydrated Adduct IIb.

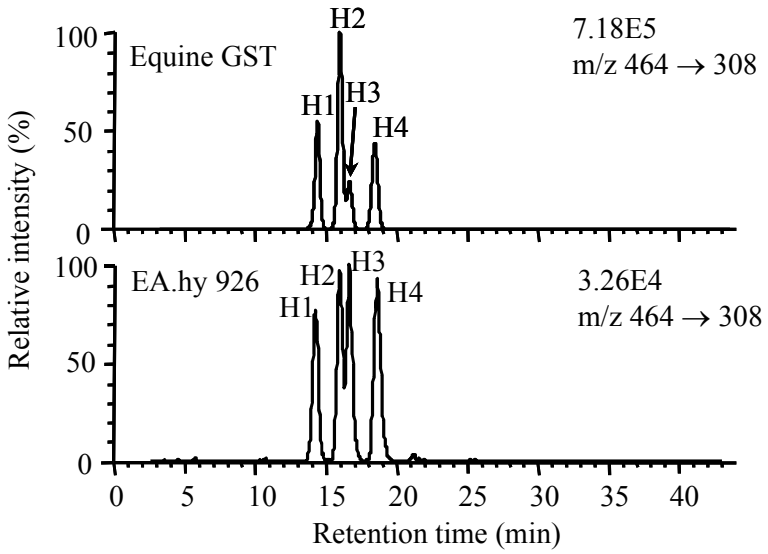

Figure S8: Separation (using LC system 6) of four (H1-H4) of the potential eight diastereomers formed in the incubation of HNE with GSH in the presence of equine GS (upper) (upper). Analysis of the HNE-GSH-adduct diastereomers formed when EA.hy 926 cells were treated with HNE (lower).

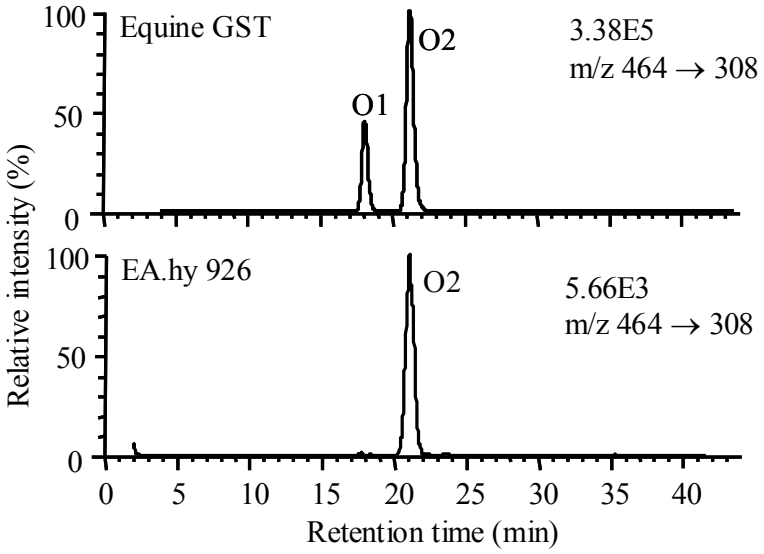

Figure S9: Separation (using LC system 6) of two (O11 and O2) of the potential four diastereomers formed in the incubation of ONO with GSH in the presence of equine GS (upper) (upper). Analysis of the ONO-GSH-adduct diastereomers formed when EA.hy 926 cells were treated with ONO (lower).