

Electronic Supplementary Information (ESI)

Selective 1D TOCSY NMR method for the determination of glutathione in white wine[§]

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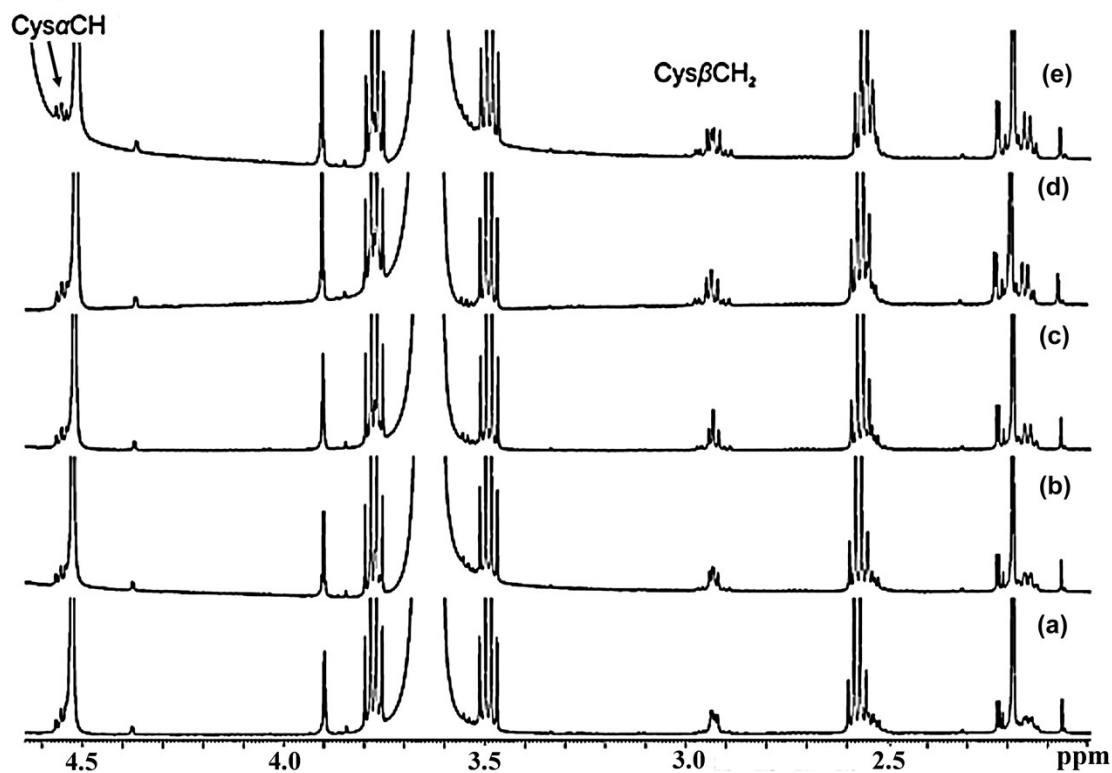


Fig. S1 Selected region of 500 MHz ¹H NMR spectra of model wine (pD = 3.5) with 2 mM of glutathione at various temperatures: 288 K (a), 293 K (b), 298 K (c), 303 K (d) and 308 K (e) (acquisition time = 2.74 s, relaxation delay = 5 s, numbers of scans = 64, experimental time ≈ 8.3 min).

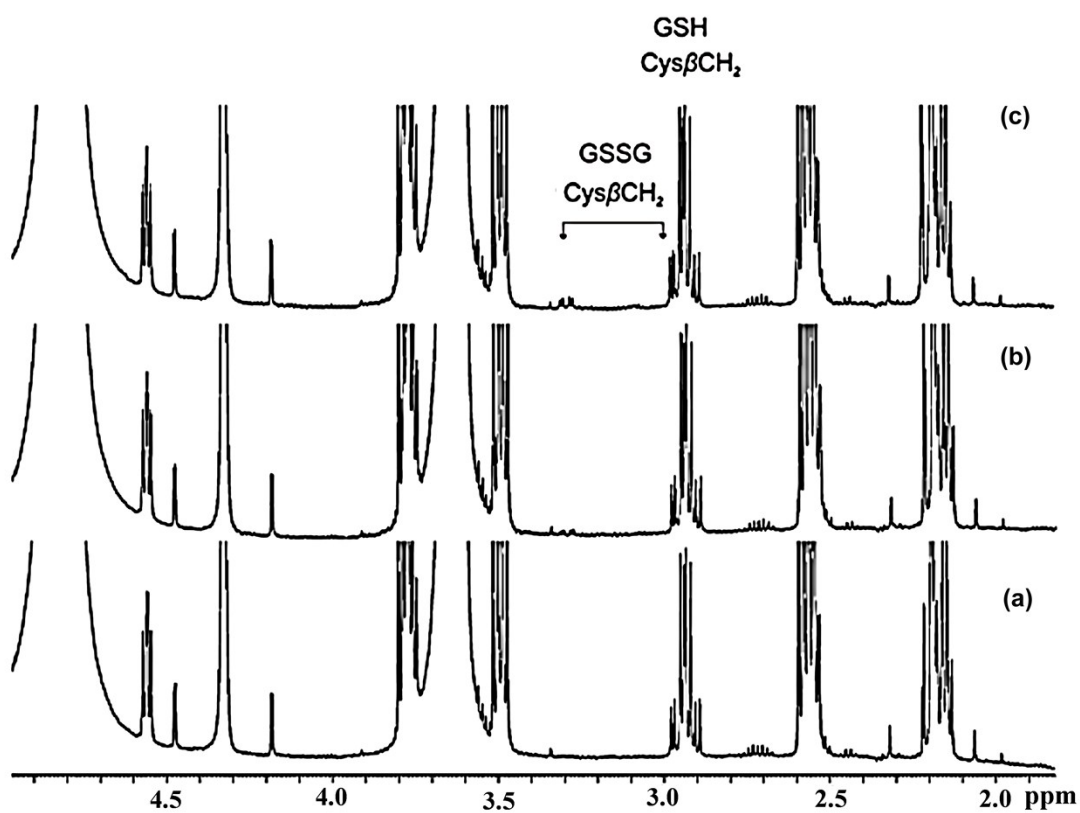


Fig S2 Selected region of 500 MHz ¹H NMR spectra of model wine with 2.1 mM of GSH at pD=5.0, recorded at different time intervals: (a) immediately after preparation of the solution, (b) and (c) after 14 h and 34 h, respectively (T = 298 K, acquisition time = 2.74 s, relaxation delay = 5 s, number of scans = 64, experimental time ≈ 8.3 min).

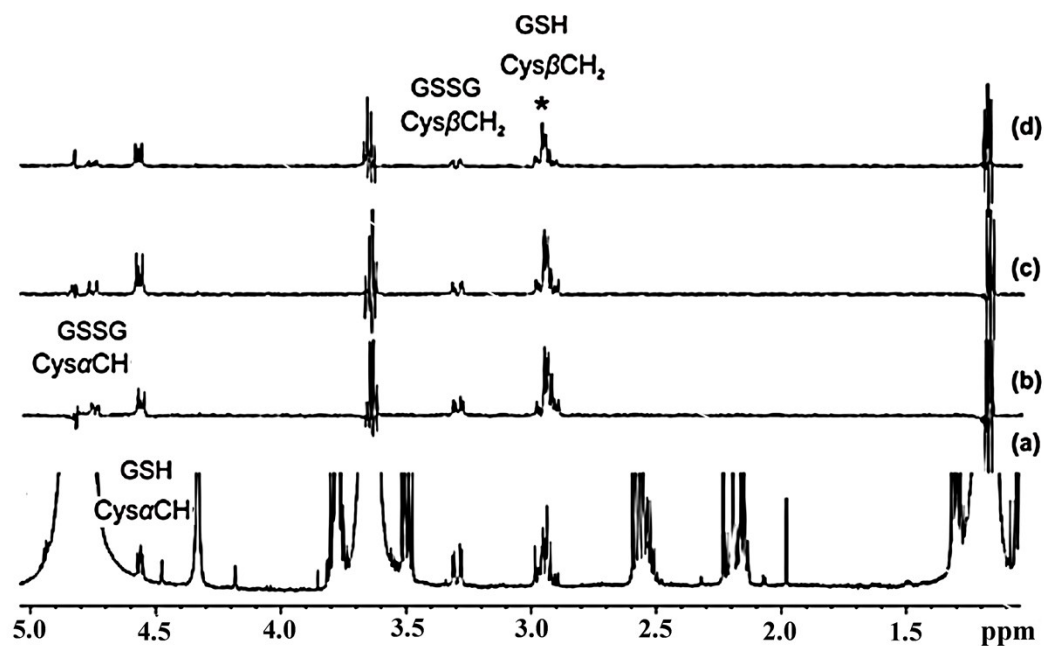


Fig S3 (a) Selective region of 500 MHz ^1H NMR spectrum of model wine with a mixture of reduced (1.4 mM) and oxidized (2 mM) glutathione, at pD = 5.0 ($T = 298\text{ K}$, acquisition time = 2.74 s, relaxation delay = 5 s, numbers of scans = 64, experimental time $\sim 8\text{ min}$). (b) - (d). A series of selective 1D TOCSY spectra of the solution (a) with mixing times $\tau_m = 38\text{ ms}$ (b), 50 ms (c), and 150 ms (d), with the selective pulse at 2.95 ppm (denoted with an asterisk) ($T = 298\text{ K}$, acquisition time = 2.74 s, relaxation delay = 15 s, number of scans = 16, experimental time $\approx 4.7\text{ min}$).

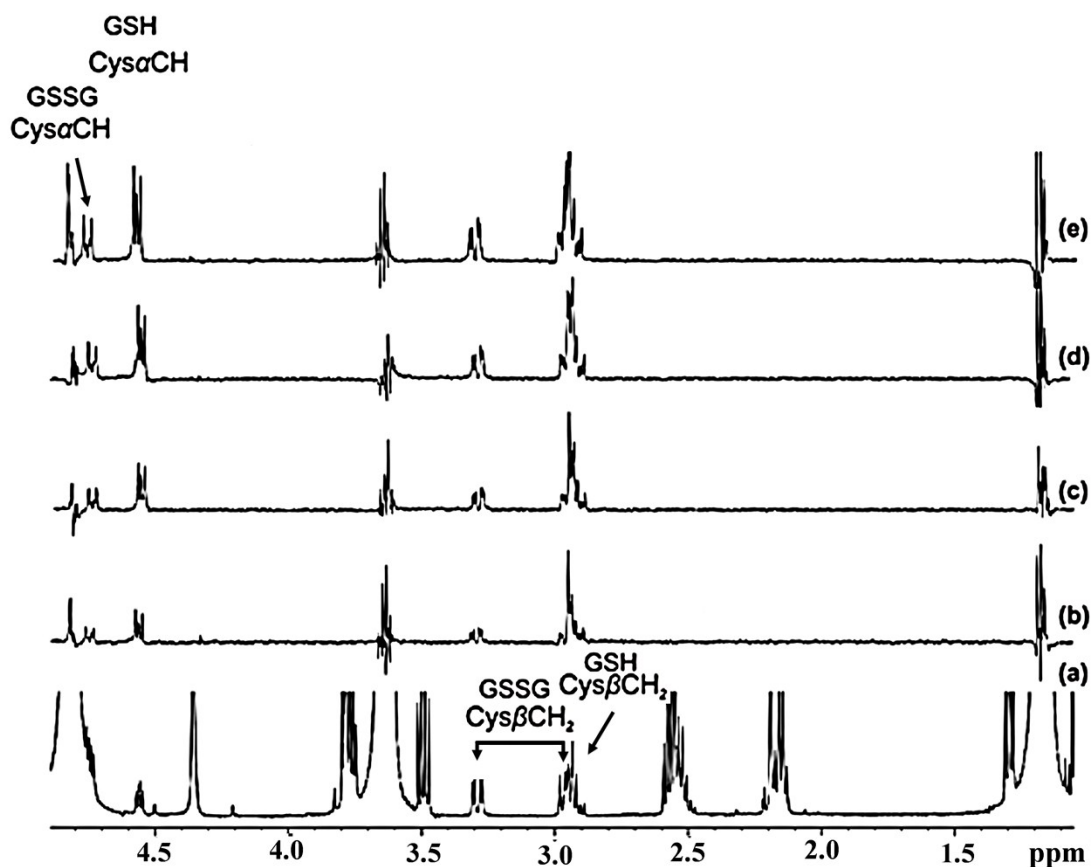


Fig. S4 (a) Selective region of 500 MHz ^1H NMR spectrum of model wine with a mixture of reduced (0.68 mM) and oxidized (0.68 mM) glutathione, at pD = 5.0 (T= 298 K, acquisition time = 2.74. s, relaxation delay = 5 s, number of scans= 8, experimental time = 1 min). (b) – (e) A series of selective 1D TOCSY spectra of the solution (a) used for the calibration curve: 0.68 (b), 1.29 (c), 1.85 (d) and 2.67 (e) mM for GSH and 0.68 (b), 1.30 (c), 1.86 (d) and 2.69 (e) mM for GSSG) (T= 298 K, acquisition time= 2.74 s, relaxation delay= 15 s, number of scans= 16, mixing time τ_m = 50 ms, experimental time \approx 6 min).