**Supplementary Material**

**Supplementary Fig. 1.** Overview of various methods used for glutathione conformational studies: simulation, *in vitro* sample to *in vivo* conditions.

**Supplementary Fig. 2.** *In vitro* aqueous GSH sample study using NMR. A) 2D NMR showing J-coupled GSH Cysteine –Hα and –Hβ peaks in aqueous sample. B) 1D NMR spectra of GSH Cysteine –Hα and –Hβ peaks in the same aqueous sample. The chemical spectra is referenced with respect to acetone D6 (δ-2.04 ppm) as external reference [18] (copyright permission obtained from the publisher).

**Supplementary Fig. 1**



**Supplementary Fig. 2**

