I. The experiment

The interaction of Cu with thiols was studied by adding aliquots of a Cu(II) stock solution to a solution containing thiol (L-cysteine, glutathione, 3-mercaptopropionic acid, or thioacetic acid) buffered to pH = 8.4 with 0.1 M borate buffer. The Cu concentration of 100 µM was the same in all experiments, while the thiol concentrations ranged from 100 to 1000 µM. The kinetics of the reduction of Cu(II) and the oxidation of Cu(I) were studied by adding aliquots of the Cu–thiol solution to the mixture of BCS and EDTA (BCS assay). The BCS effectively binds Cu(I) in an orange complex with an absorption maximum (A_{max}) of 484 nm, while a masking ligand is necessary to avoid Cu(II) interference. The EDTA was used as the masking ligand for Cu(II) with a fivefold excess of EDTA over BCS, which has been found to be optimal for ensuring Cu(II) complexation while avoiding Cu(I) oxidation. A volume of 1 mL of the Cu–thiol model solution was added to the mixture containing 3 mL of BCS (1000 µM) and 0.15 mL of EDTA (0.1 M), resulting in a dilution factor (DF) of 4.15 in the Cu–thiol model solution and final concentrations of 723 µM BCS and 0.00361 M EDTA. The addition of the Cu–thiol solution to the mixture of BCS and EDTA resulted in the formation of an orange-colored solution with an absorption maximum (A_{max}) of 484 nm, indicating the presence of Cu(I) in the solution. Cu(I) concentrations were determined by measuring the A_{484} solution, calculating the Cu(I) concentration from the Cu(I)–BCS calibration curve, and correcting the Cu(I) concentration by a dilution factor of 4.15. For the Cu(I)–BCS calibration curve, one blank and five standard additions of Cu(I) were prepared. The blank solution contained 3 mL of 1000 µM BCS, 0.15 mL of 0.1 M EDTA, 0.1 mL of 1 M borate buffer, and MQ water with a final volume of 4.15 mL. The final concentrations of 723 µM BCS and 0.00361 M EDTA were the same as those used to measure the absorbance of Cu–thiol solutions. The Cu(I) standard solutions were prepared in the same way as the blank solution, adding five different Cu(I) aliquots that resulted in a linear absorbance over the concentration range studied, from 1.1 to 35.2 µM. The Cu(I) standard solution was freshly prepared before the experiment. In short the Cu(I) standard solution used for the calibration curve of the Cu(I)–bathocuproine complex was prepared by dissolving copper(I) chloride (CuCl; Thermo Fisher Scientific, Waltham, MA, USA) in a solution containing 1 M sodium chloride (NaCl; Grammol, North Salt Lake, UT, USA) and 0.1 M hydrochloric acid (HCl; Roth, Newport Beach, CA, USA), which was previously purged with high purity nitrogen to remove oxygen To better understand the reaction mechanism, in addition to monitoring the Cu(I) concentration, UV–Vis spectra of solutions containing Cu and L-cys were recorded at the same reaction time as was the Cu(I) determination. Copper reduction by individual thiol species was investigated by measuring the Cu(I) concentration with a UV–Vis spectrophotometer (Analytik Jena, Jena, Germany) in a 1 cm quartz cuvette.

II. The data

Interaction between Cu(II) and gluthathione (GSH)

The interaction between Cu(II) and gluthatione was investigated over time at Cu:GSH ratios of 1:1 and 1:10.

The raw spectrophotometry data are under the file: Cu(II) and gluthathione.zip

Under Cu and gluthathione.zip are 2 folders with the stoichiometry indicated as follows:

Cu GHS 1 to 1

Cu GHS1 to 10.

Under each folder the raw data are presented (spectrophotometric measurements with the .dat file extension). The file name consist of ligand name and the time frame when subsamples are taken. Also the raw spectrophotometric data for construction of Figure 2 are given (folder name: Figure 2).

Interaction between Cu(II) and L-Cysteine

The interaction between Cu(II) and L-Cysteine was investigated over time at Cu:L-Cys ratios of 1:1, 1:2.5, 1:5, and 1:10.

The raw spectrophotometry data are under the zip file: Cu (II) and L-Cysteine.zip.

Under Cu and L-Cysteine.zip are 4 folders with the Cu:L-Cys stoichiometry indicated as follows:

Cu Cys 1 to 1

Cu Cys 1 to 2.5
Cu Cys 1 to 5
Cu Cys 1 to 10.
Under each folder the raw data are accessible (spectrophotometric measurements with the .dat file extension). The file name consist of ligand name and the time frame when subsamples are taken. In the Cu Cys 1 to 1 and Cu Cys 1 to 10 folder the raw data for construction of the Figure 4 are given (folder name: Figure 4).

Interaction between Cu(II) and 3-mercaptopropionic acid (MPA)

The interaction between Cu(II) and 3-mercaptopropionic acid was investigated over time at Cu:MPA ratios of 1:1, 1:2.5, 1:5, and 1:10.
The raw spectrophotometry data are under the zip file: Cu(II) and 3-mercaptopropionic acid.zip.
Under Cu and 3-mercaptopropionic acid.zip are 4 folders with the Cu:MPA stoichiometry indicated as follows:
Cu MPA 1 to 1
Cu MPA 1 to 2.5
Cu MPA 1 to 5
Cu MPA 1 to 10.
Under each folder the raw data are accessible (spectrophotometric measurements with the .dat file extension). The file name consist of ligand name and the time frame when subsamples are taken. In the Cu MPA 1 to 1 and Cu MPA 1 to 10 folder the raw data for construction of the Figure 6 are given (folder name: Figure 6).

Interaction between Cu(II) and thioacetic acid (TAA)

The interaction between Cu(II) and thioacetic acid was investigated over time at Cu:TAA ratios of 1:1, 1:2.5, 1:5, and 1:10.
The raw spectrophotometry data are under the zip file: Cu(II) and thioacetic acid.zip.
Under Cu and thioacetic acid.zip are 4 folders with the Cu:TAA stoichiometry indicated as follows:
Cu TAA 1 to 1
Cu TAA 1 to 2.5
Cu TAA 1 to 5
Cu TAA 1 to 10.
Under each folder the raw data are accessible (spectrophotometric measurements with the .dat file extension). The file name consist of ligand name and the time frame when subsamples are taken. In the Cu TAA 1 to 5 the raw data for construction of the Figure 7 are given (folder name: Figure 7).