## Bifunctional <sup>64</sup>Cu-labelled macrobicyclic cage amine isothiocyanates for immuno-positron emission tomography

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Figure S2: <sup>1</sup>H NMR spectrum of [Mg(CH<sub>3</sub>)(NCS-OEG)sar](CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>



Figure S3: Structure of the water soluble bis(thiosemicarbazone) Na[H<sub>2</sub>L]



**Figure S4:** Section of interest of an absorbance spectrum (around 280 nm) of a solution containing Trastuzumab (25  $\mu$ L) in 50 mM MOPS buffer (3000  $\mu$ L, pH 7.1).



**Figure S5:** Section of interest of overlayed absorbance spectra (around 280 nm) of solutions formed as a result of titration of  $(CH_3)(p-NCS-Ph)$ sar-trastuzumab (4 µL each aliquot) into 50 mM MOPS buffer (918 µL).



**Figure S6:** Section of interest of overlayed absorbance spectra (around 460 nm) of the solutions used in determination of ligand to antibody ratio.