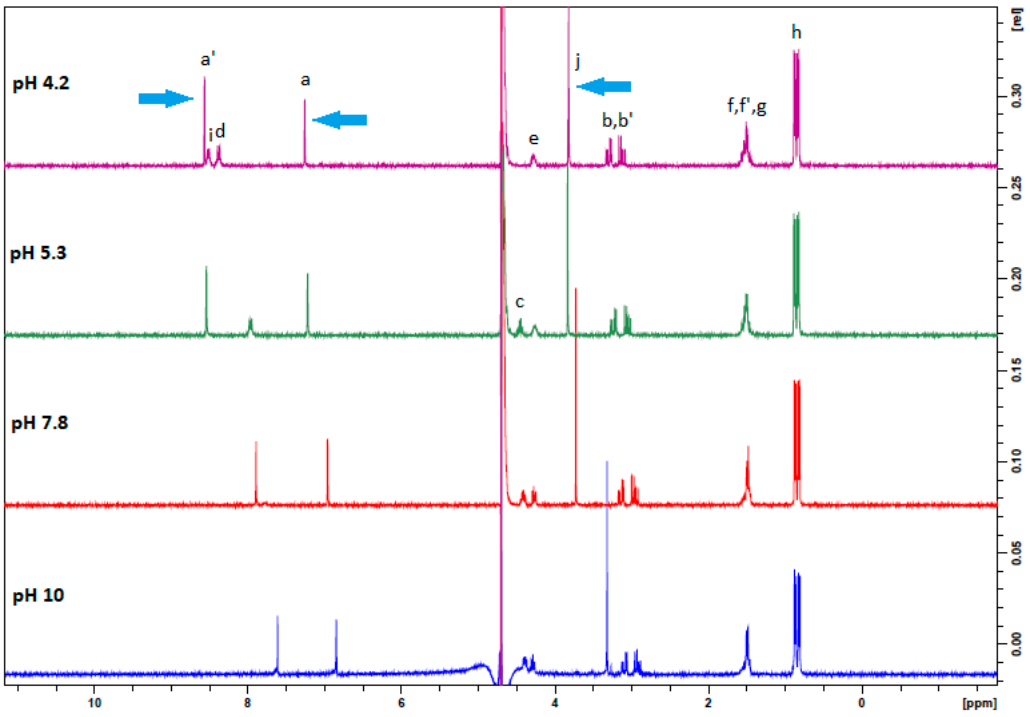
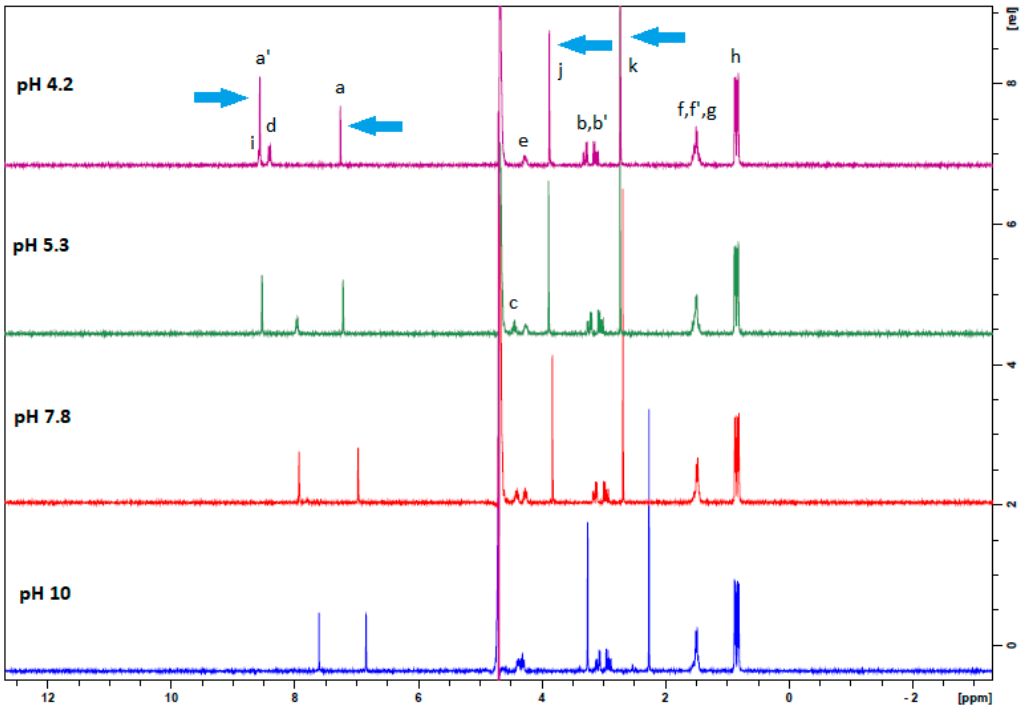
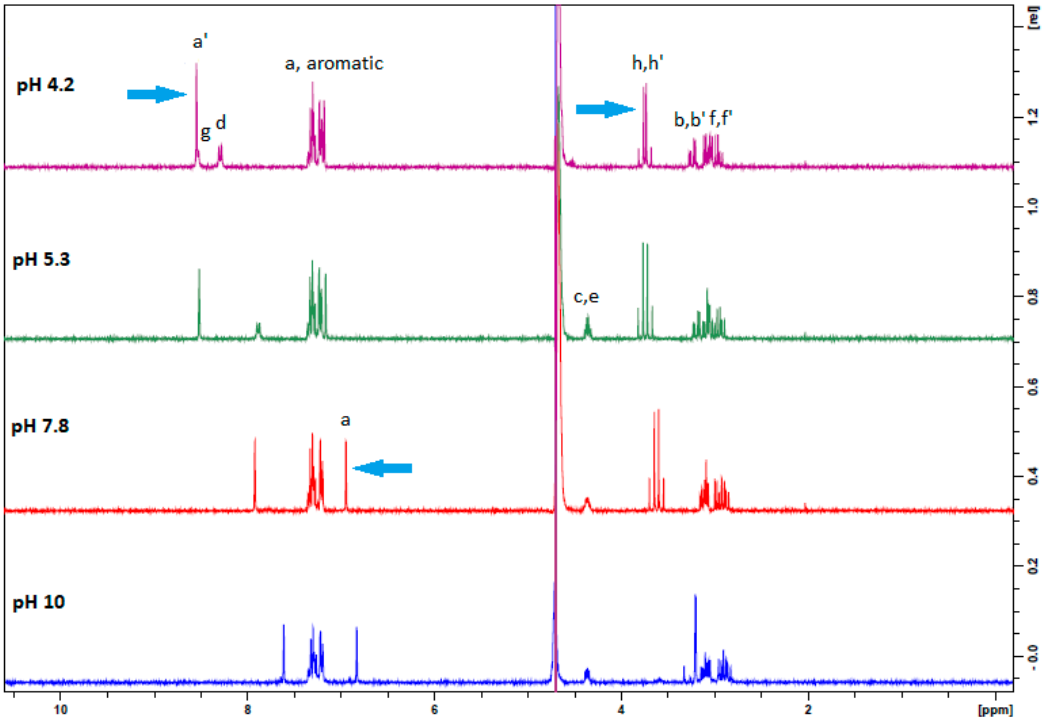
Supplementary Information



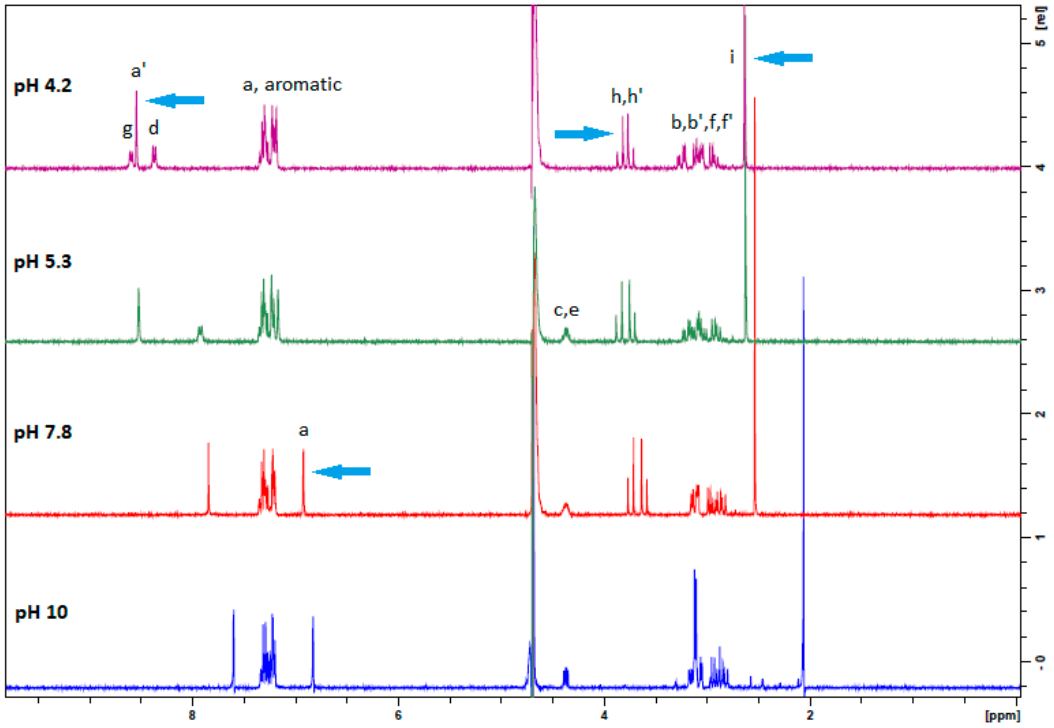
(a)



(b)

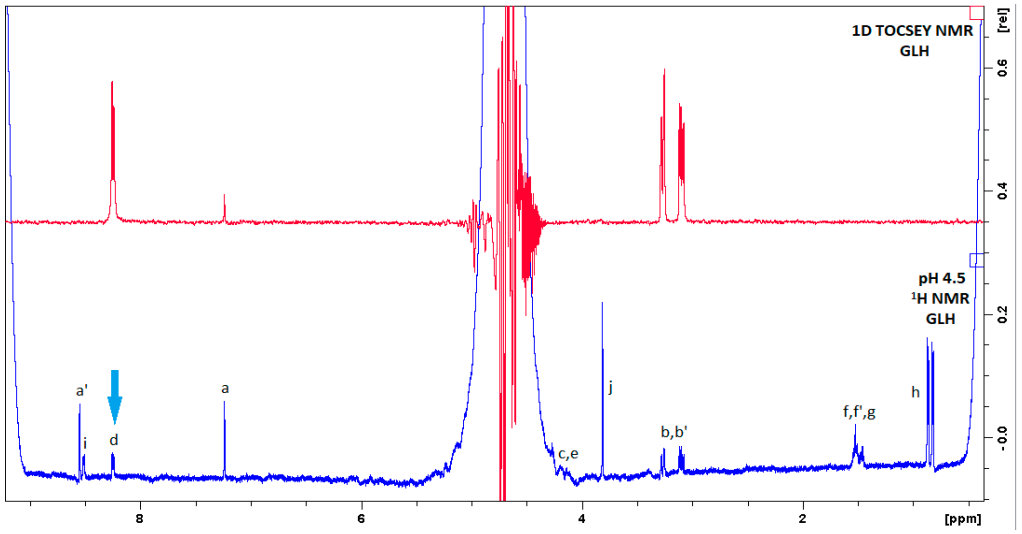


(c)

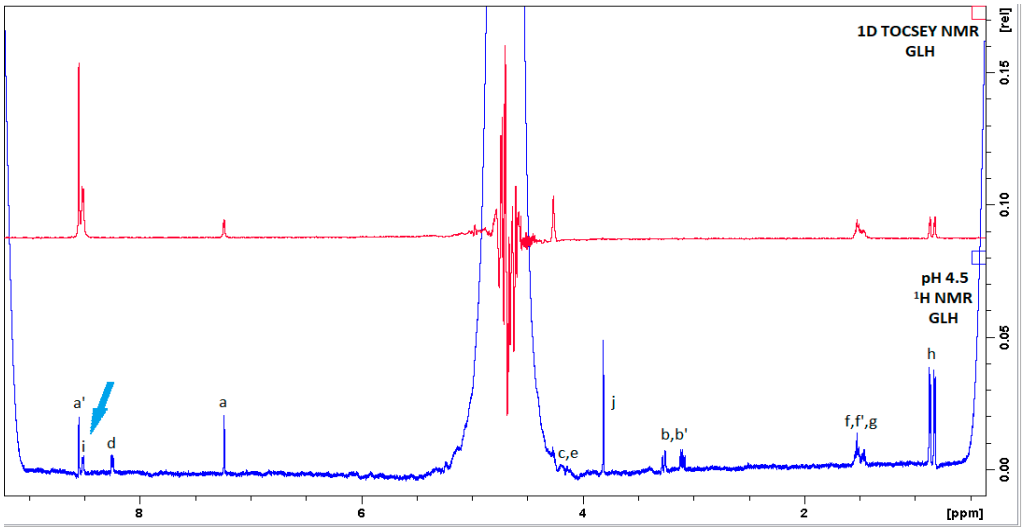


(d)

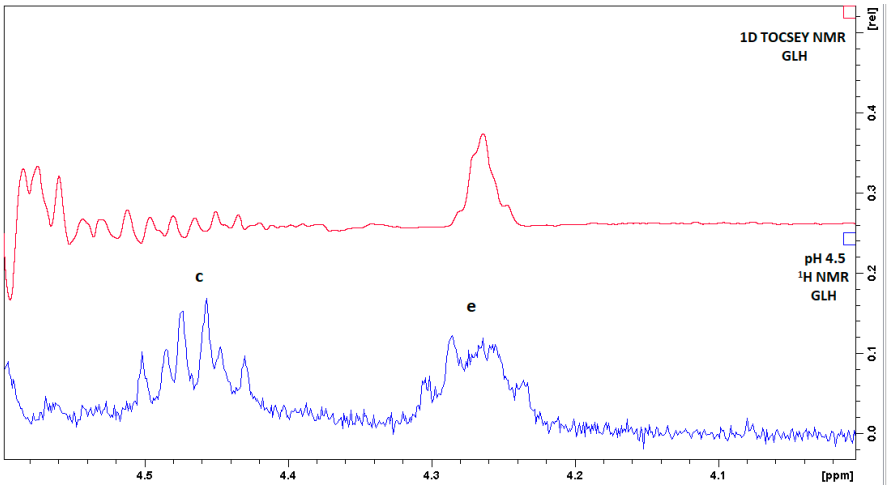
Figure S1: ^{1}H NMR spectra of (a) GLH, (b) Sar-LH, (c) GFH and (d) Sar-FH at increasing pH values from 2-11. An arrow has been added to indicate the shifting of peaks over increasing pH values.



(a)



(b)



(c)

Figure S2. 1D selective gradient TOCSY NMR spectra (red) and ^{1}H NMR spectra (blue) of GLH at pH 4.5. (a) full spectrum of the irradiated amide-NH peak **d** at 8.246 ppm, (b) full spectrum of the

irradiated amide-NH peak **i** at 8.511 ppm and (c) section of the spectrum of the irradiated amide-NH peak **i** at 8.511 ppm. An arrow has been added to indicate the irradiated amide-N.

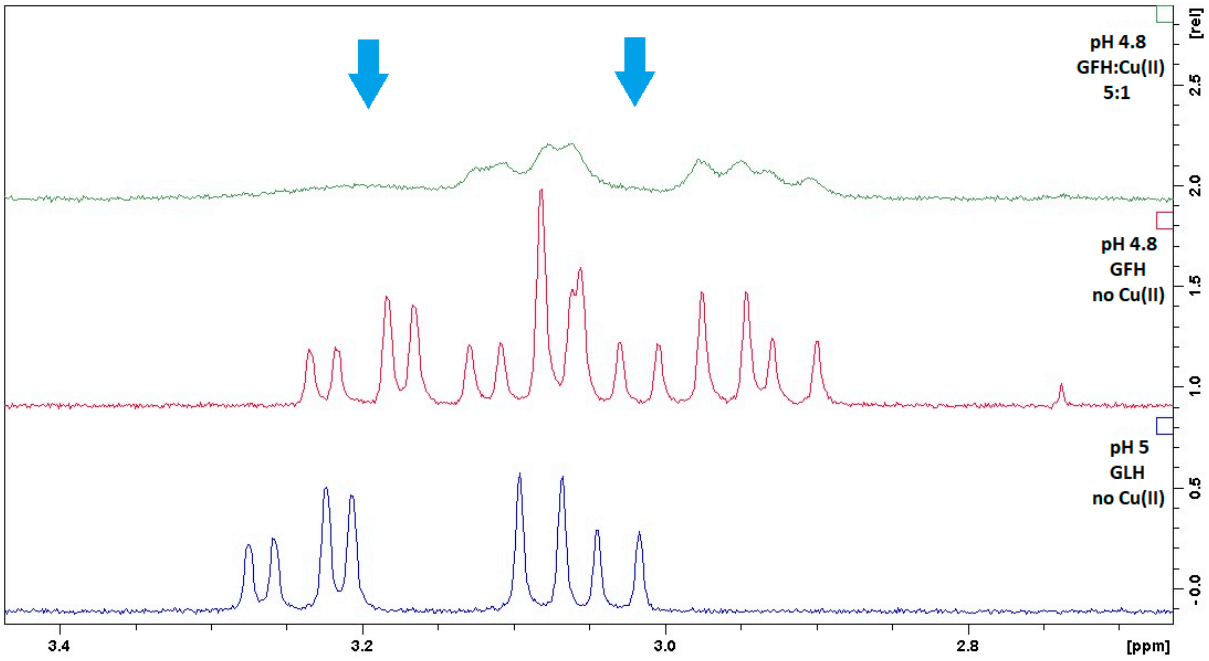


Figure S3. The ^{1}H NMR spectra (blue) of the ligand GFH and the ^{1}H NMR spectra (red) after GFH has been titrated with copper(II) to reach a 5:1 ligand copper(II) ratio at a pH of 4.8 in 90 % water and 10 % D_2O. ^{1}H NMR spectra (green) with arrows pointing to the significant broadening of peaks **b** and **b′**, after GFH has been titrated with copper(II).

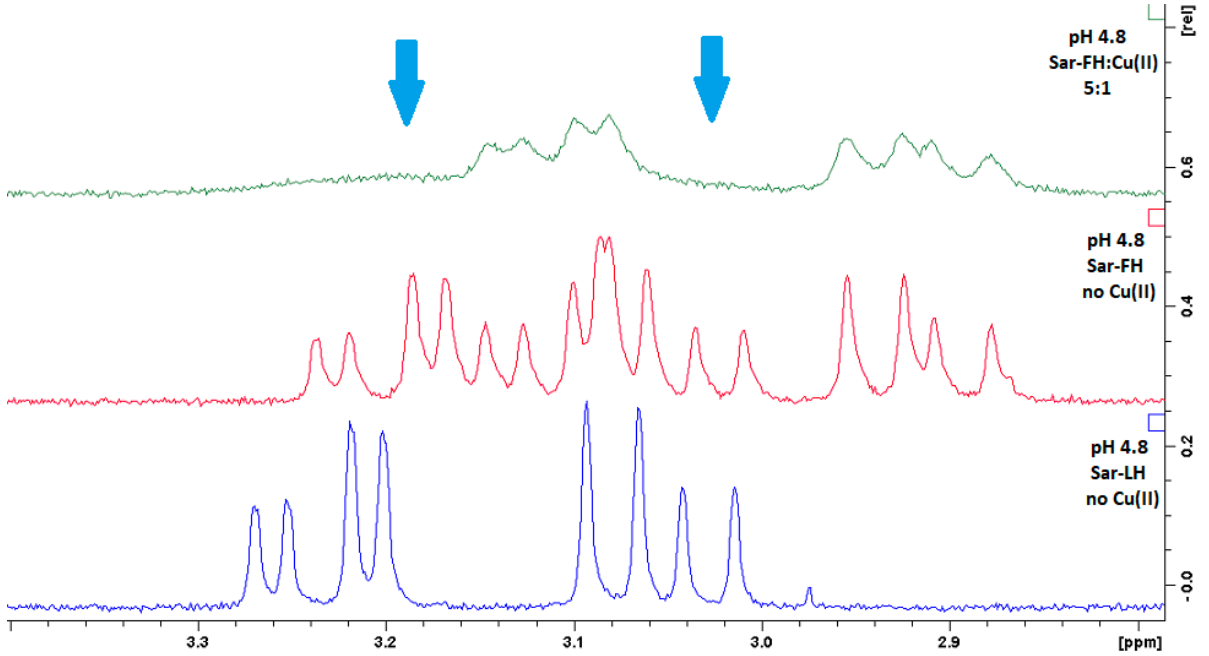


Figure S4. The ^{1}H NMR spectra (blue) of the ligand Sar-FH and the ^{1}H NMR spectra (red) after Sar-FH has been titrated with copper(II) to reach a 5:1 ligand copper(II) ratio at a pH of 4.8 in 90 % water

and 10 % D_2O. ^1H NMR spectra (green).with arrows pointing to the significant broadening of peaks **b** and **b′**, after Sar-FH has been titrated with copper(II)

Table S1. Structural assignments of m/z base peaks that were found in the ESI-MS spectrum for Cu-GLH, Cu-Sar-FH and Cu-GFH at pH 5 (positive mode) with a 1:1 ratio and concentration of 1 mM for GLH, Sar-FH and GFH, and 0.7 mM for copper(II) in aqueous solution

Complex	m/z	Assignment
Cu-GLH	326.24	$(LH+H)^{1+}$
	348.08	$(LH+Na)^{1+}$
	370.06	$(L+2Na)^{1+}$
	371.04	uncomplexed ligand
	387.07	$(MLH_{-2}+2H)^{1+}$
		$(MLH_{-1}+H)^{1+}$
	388.05	$(M^{I}LH_{-2}+3H)^{1+}$
		$(M^{I}LH_{-1}+2H)^{1+}$
Cu-Sar-FH	368.03	$(L+Na$-benzene ring decomposition$)^{1+}$
	374.12	$(LH+H)^{1+}$
	396.10	$(LH+Na)^{1+}$
	408.00	$(M^{I}LH_{-2}+2H$-benzene ring decomposition$)^{1+}$
	418.22	$(L+2Na)^{1+}$
	430.12	$(M^{I}LH_{-2}+H+Na$-benzene ring decomposition$)^{1+}$
	435.02	$(MLH_{-2}+2H)^{1+}$
	436.07	$(M^{I}LH_{-2}+3H)^{1+}$
Cu-GFH	354.94	$(MLH_{-2}+H$-imidazole$)^{1+}$
	360.19	$(LH+H)^{1+}$
	370.97	$(MLH_{-2}+H$-imidazole$+H_2O)^{1+}$
	382.10	$(LH+Na)^{1+}$
	404.15	$(L+2Na)^{1+}$
	421.02	$(MLH_{-2}+2H)^{1+}$
	422.07	$(M^{I}LH_{-2}+3H)^{1+}$