Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPLEMENTARY MATERIAL

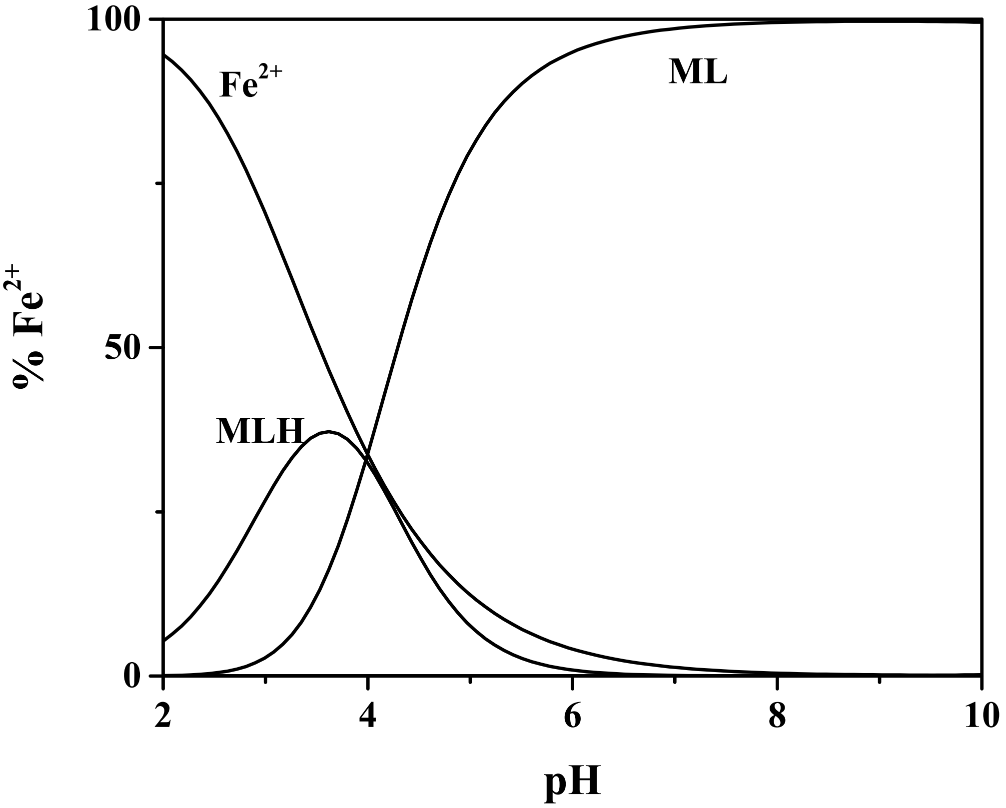

Figure S1. Distribution diagram of $M_pL_qH_r$ species as a function of pH in the Fe^{2+}/*8-HQA* system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. $c_{8\text{-}HQA}$ = 0.5 mmol dm^{-3}, $c_{Fe^{2+}}$ = 0.5 mmol dm^{-3}.

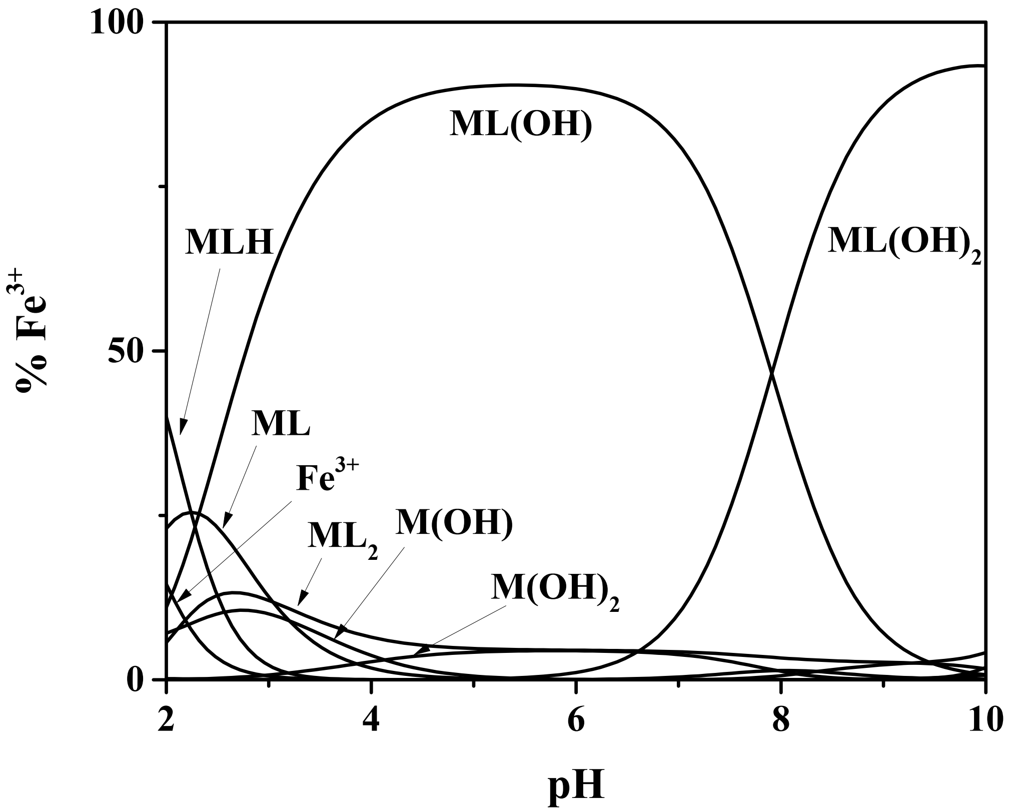

Figure S2. Distribution diagram of $M_pL_qH_r$ species as a function of pH in the Fe^{3+}/*8-HQA* system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. $c_{8\text{-}HQA}$ = 0.5 mmol dm^{-3}, $c_{Fe^{3+}}$ = 0.5 mmol dm^{-3}.

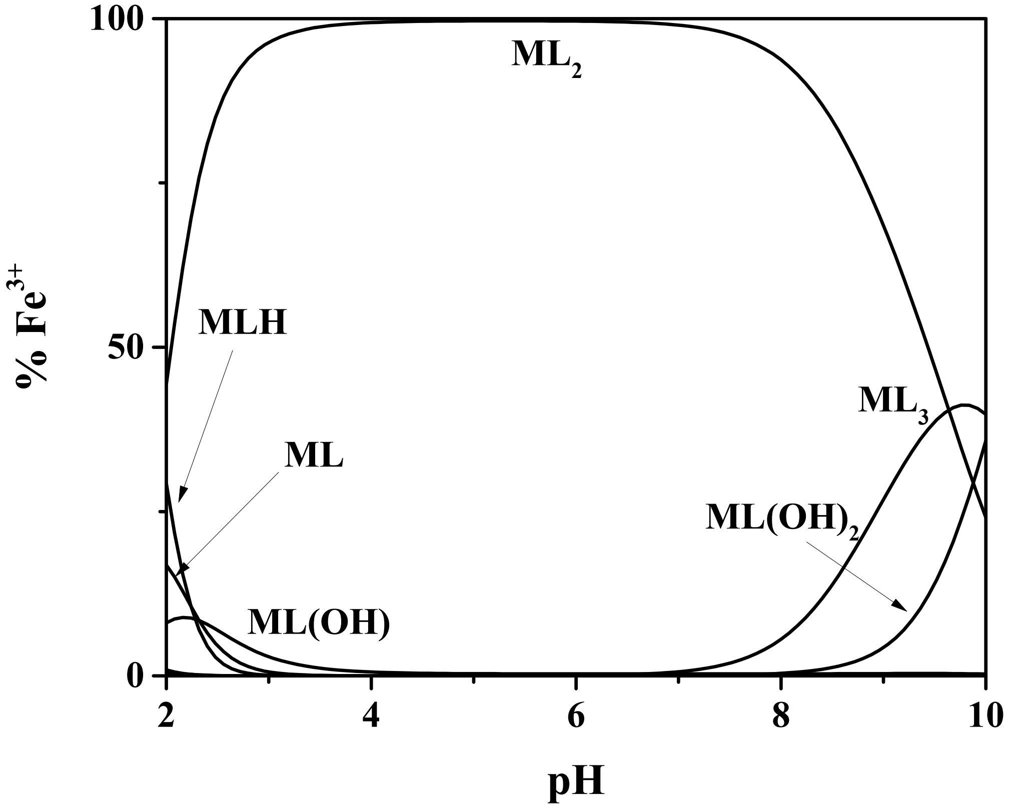

Figure S3. Distribution diagram of $M_pL_qH_r$ species as a function of pH in the Fe^{3+}/*8-HQA* system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. $c_{8\text{-}HQA}$ = 1.5 mmol dm^{-3}, $c_{Fe^{3+}}$ = 0.5 mmol dm^{-3}, considering the ML_3 species in the model.

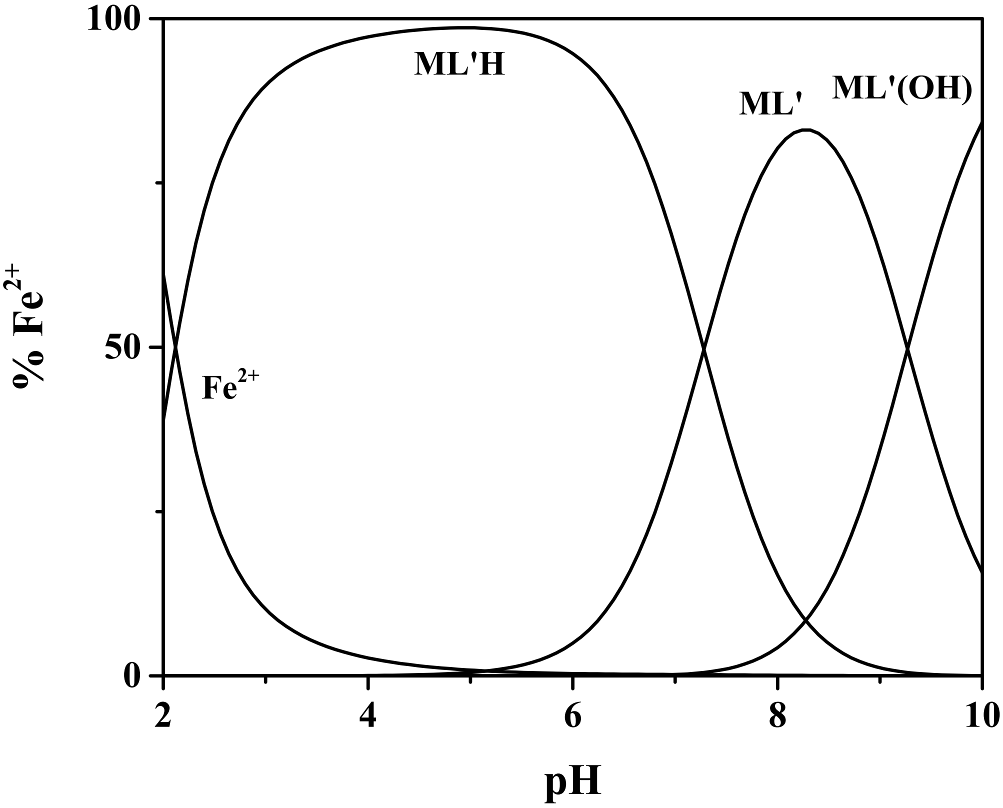

Figure S4. Distribution diagram of $M_pL'_qH_r$ species as a function of pH in the Fe^{2+}/EDTA system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. c_{EDTA} = 0.5 mmol dm^{-3}, $c_{Fe^{2+}}$ = 0.5 mmol dm^{-3}.

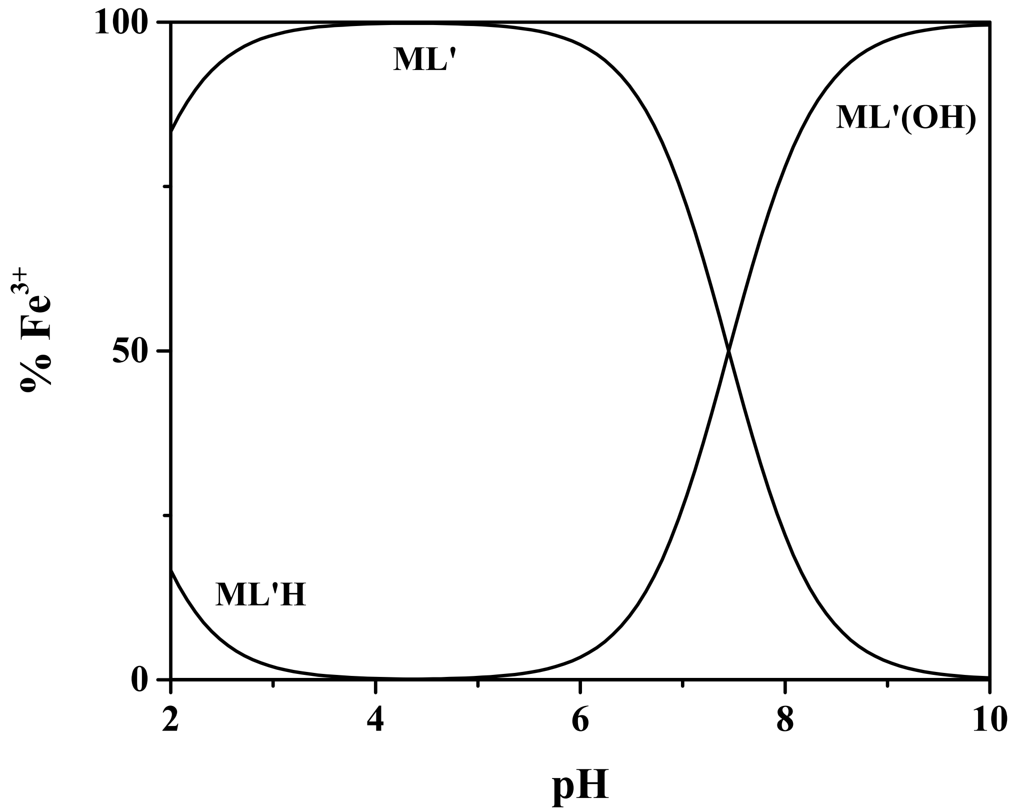

Figure S5. Distribution diagram of $M_pL'_qH_r$ species as a function of pH in the Fe^{3+}/EDTA system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. c_{EDTA} = 0.5 mmol dm^{-3}, $c_{Fe^{3+}}$ = 0.5 mmol dm^{-3}.

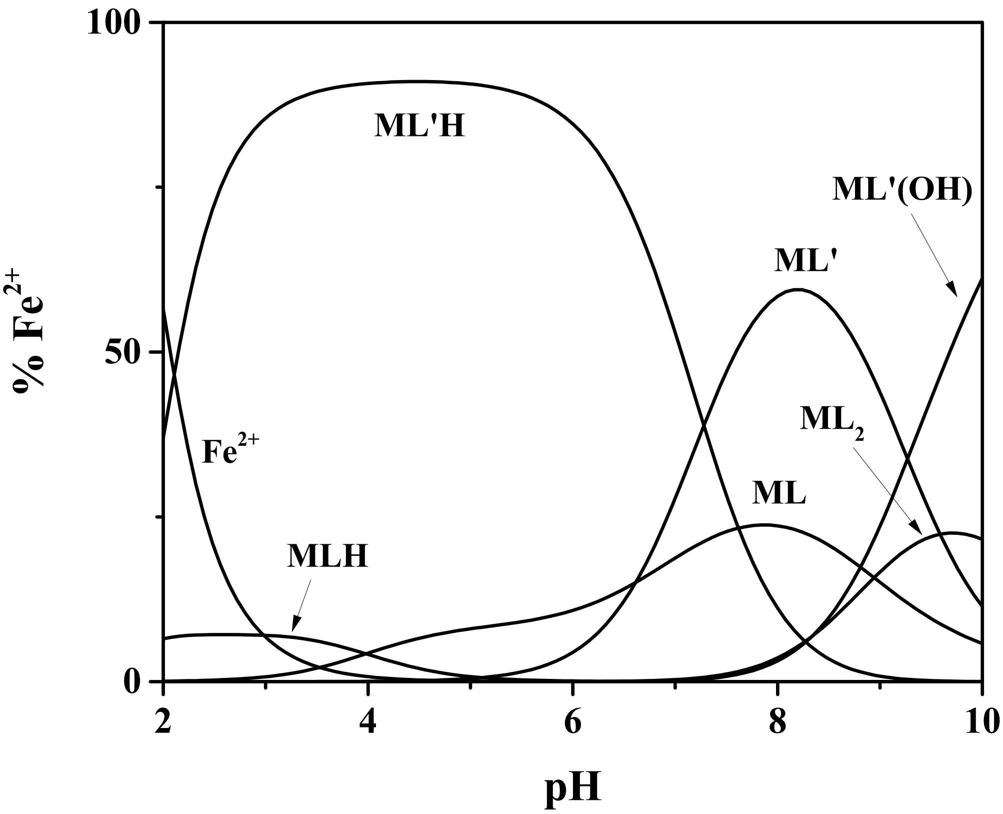

Figure S6. Distribution diagram of $M_pL_qL'_{q'}H_r$ species as a function of pH in the Fe^{2+}/*8-HQA*/EDTA system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. $c_{8\text{-}HQA}$ = 0.5 mmol dm^{-3} , c_{EDTA} = 0.5 mmol dm^{-3}, $c_{Fe^{2+}}$ = 0.5 mmol dm^{-3}. L ≡ *8-HQA*, L' ≡ EDTA.

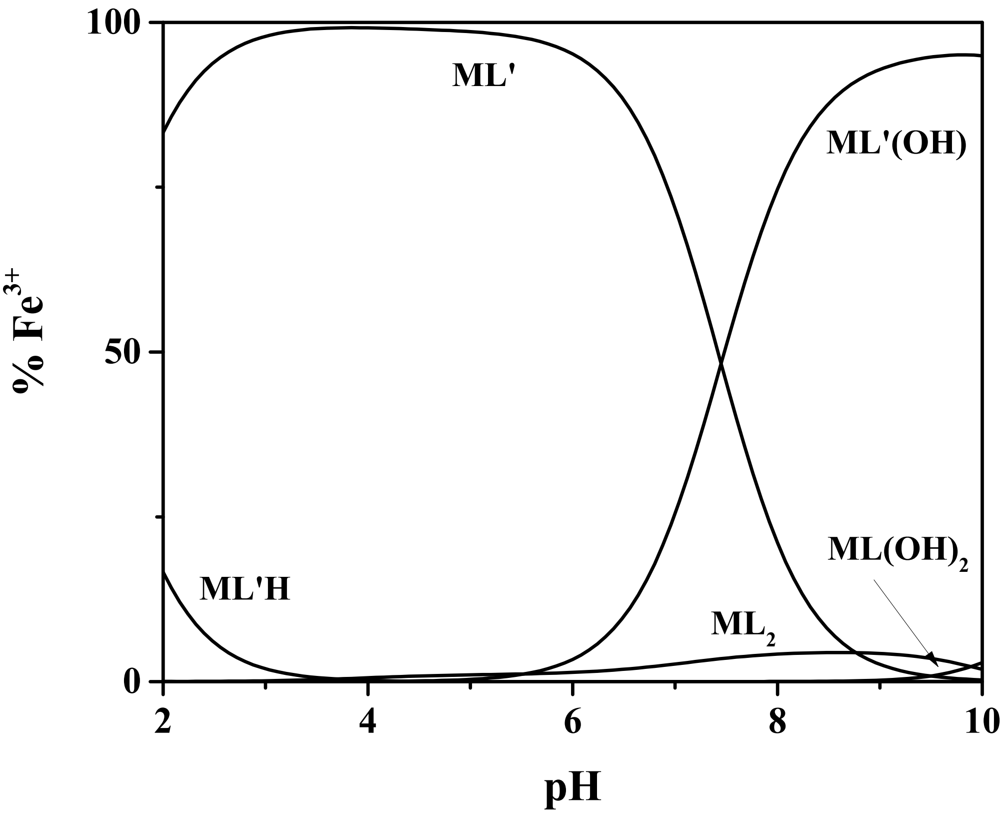

Figure S7. Distribution diagram of $M_pL_qL'_{q'}H_r$ species as a function of pH in the Fe^{3+}/*8-HQA*/EDTA system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. $c_{8\text{-}HQA}$ = 0.5 mmol dm^{-3} , c_{EDTA} = 0.5 mmol dm^{-3}, $c_{Fe^{3+}}$ = 0.5 mmol dm^{-3}. L ≡ *8-HQA*, L' ≡ EDTA.

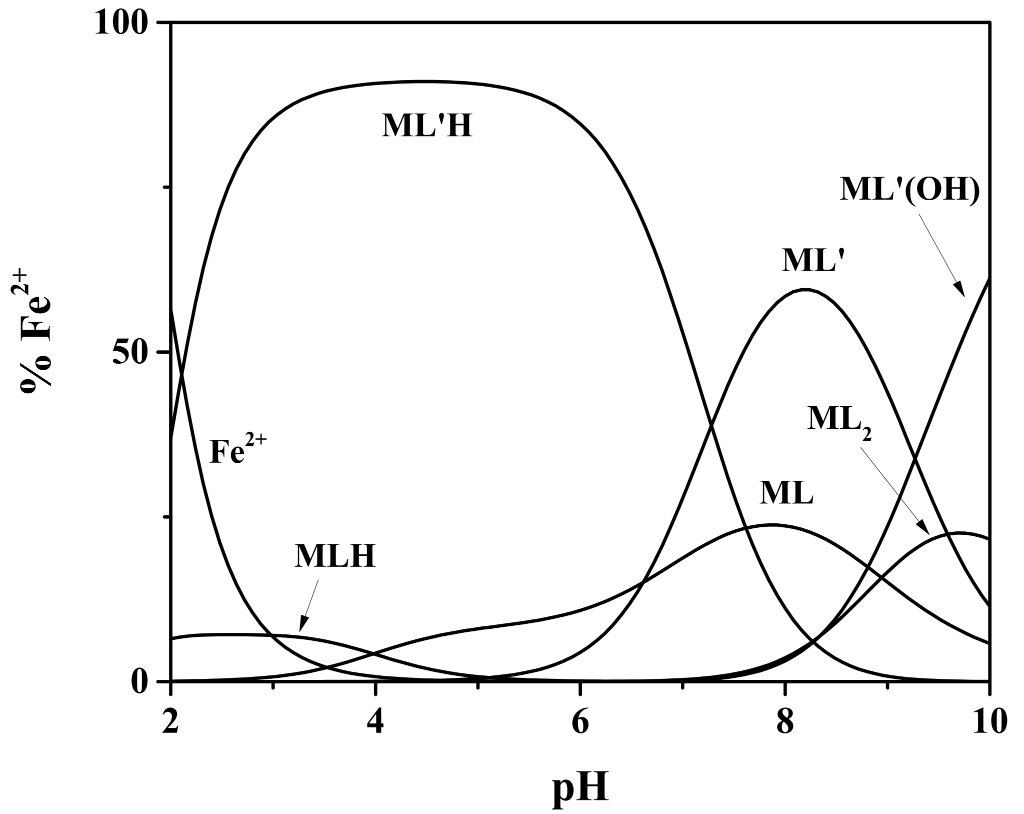

Figure S8. Distribution diagram of $M_pL_qL'_{q'}H_r$ species as a function of pH in the Fe^{2+}/*8-HQA*/EDTA system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. $c_{8\text{-}HQA}$ = 1.0 mmol dm^{-3} , c_{EDTA} = 0.5 mmol dm^{-3}, $c_{Fe^{2+}}$ = 0.5 mmol dm^{-3}. L ≡ *8-HQA*, L' ≡ EDTA.

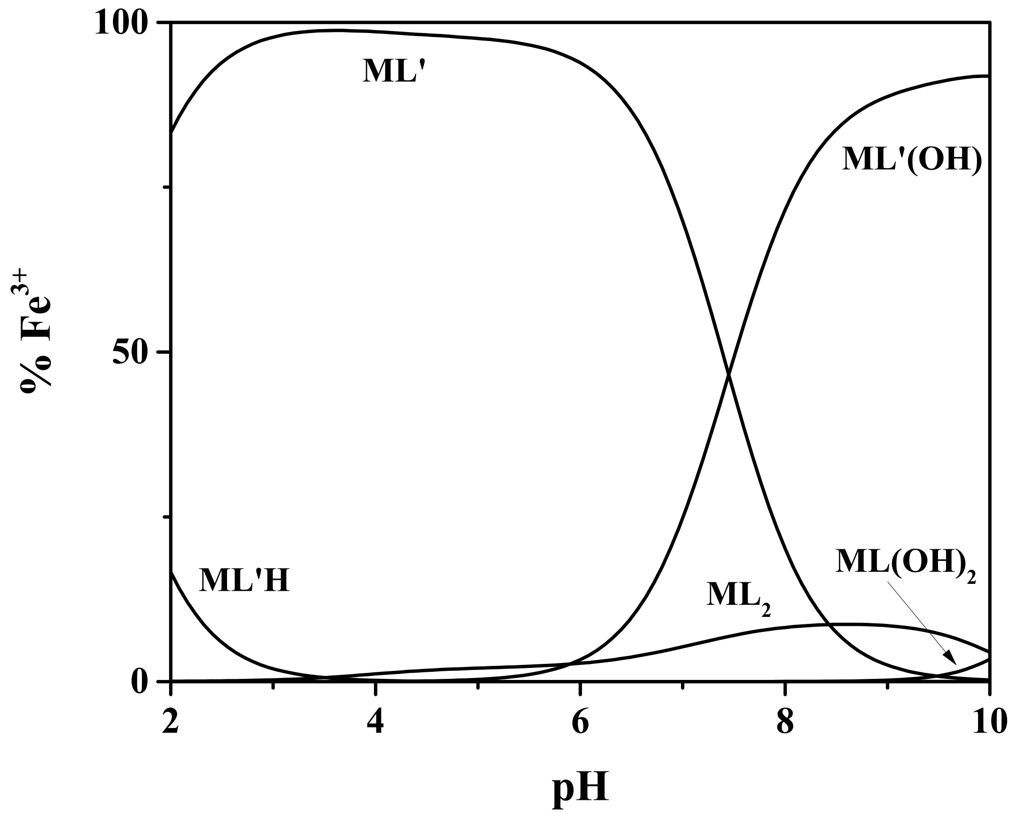

Figure S9. Distribution diagram of $M_pL_qL'_{q'}H_r$ species as a function of pH in the Fe^{3+}/*8-HQA*/EDTA system, in $KCl_{(aq)}$ at I = 0.2 mol dm^{-3} and at T = 298.15 K. $c_{8\text{-}HQA}$ = 1.0 mmol dm^{-3} , c_{EDTA} = 0.5 mmol dm^{-3}, $c_{Fe^{3+}}$ = 0.5 mmol dm^{-3}. L ≡ *8-HQA*, L' ≡ EDTA.

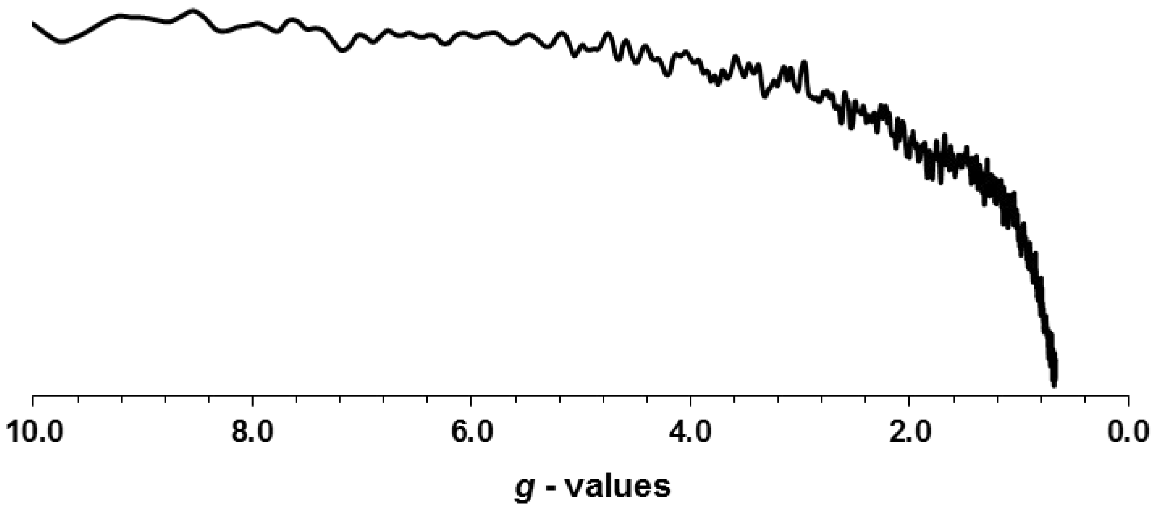

Figure S10. ESR spectra of Fe^{2+}/*8-HQA* system 1:1 c_L:c_M ratios. Experimental conditions: T = 100 K; pH = 7.0, c_L = c_M = 1.0 mmol dm^{-3}.

Table S1. Experimental details on the concentrations (in mmol dm^{-3}) of potentiometric titrations on the Fe/*8-HQA*/EDTA systems

Fe (M)	*8-HQA* (L)	EDTA (L’)	Ratio (M:L:L’)	Fe (M)	*8-HQA* (L)	EDTA (L’)	Ratio (M:L:L’)
1.5	1.5	--	1:1:0	1.5	0.8	0.8	2:1:1
1.2	1.2	--	1:1:0	1.2	0.6	0.6	2:1:1
1.0	1.0	--	1:1:0	1.0	0.5	0.5	2:1:1
1.0	1.5	--	1:1.5:0	1.5	1.5	0.8	2:2:1
0.8	1.2	--	1:1.5:0	1.2	1.2	0.6	2:2:1
0.6	1.0	--	1:1.5:0	1.0	1.0	0.5	2:2:1
0.8	1.5	--	1:2:0	1.5	0.8	1.5	2:1:2
0.6	1.2	--	1:2:0	1.2	0.6	1.2	2:1:2
0.5	1.0	--	1:2:0	1.0	0.5	1.0	2:1:2
0.5	1.5	--	1:3:0	0.8	1.5	1.5	1:2:2
0.4	1.2	--	1:3:0	0.6	1.2	1.2	1:2:2
1.5	1.5	1.5	1:1:1	0.5	1.0	1.0	1:2:2
1.2	1.2	1.2	1:1:1	0.5	1.5	0.5	1:3:1
1.0	1.0	1.0	1:1:1	0.4	1.2	0.4	1:3:1
1.0	1.5	1.0	1:1.5:1	0.5	0.5	1.5	1:1:3
0.8	1.2	0.8	1:1.5:1	0.4	0.4	1.2	1:1:3
0.6	1.0	0.6	1:1.5:1	1.5	0.5	0.5	3:1:1
1.0	1.0	1.5	1:1:1.5	1.2	0.4	0.4	3:1:1
0.8	0.8	1.2	1:1:1.5	0.5	1.5	1.0	1:3:2
0.6	0.6	1.0	1:1:1.5	0.4	1.2	0.8	1:3:2
1.5	1.0	1.0	1.5:1:1	0.5	1.0	1.5	1:2:3
1.2	0.8	0.8	1.5:1:1	0.4	0.8	1.2	1:2:3
1.0	0.6	0.6	1.5:1:1	1.5	0.5	1.0	3:1:2
0.8	1.5	0.8	1:2:1	1.2	0.4	0.8	3:1:2
0.6	1.2	0.6	1:2:1	1.5	1.0	0.5	3:2:1
0.5	1.0	0.5	1:2:1	1.2	0.8	0.4	3:2:1

0.8	0.8	1.5	1:1:2	1.0	0.5	1.5	2:1:3
0.6	0.6	1.2	1:1:2	0.8	0.4	1.2	2:1:3
0.5	0.5	1.0	1:1:2	1.0	1.5	0.5	2:3:1
				0.8	1.2	0.4	2:3:1

Table S2. Experimental details of HESI-HRMS measurements.

Time (min)	Flow (mL min^{-1})	MS Acquisition	Valve
0	0.1		Waste
0.5	0.1	X	Waste → MS
0.6	0.02	X	MS
4	0.02	X	MS → Waste
4.1	1		Waste
5	1		Waste
5.1	0.2		Waste
5.5			Waste → MS
5.8			MS → Waste
6	0.2		Waste