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

A New Tripodal-3-Hydroxy-4-Pyridinone for Iron and Aluminium Sequestration. Synthesis, Complexation and *in Vivo* Studies

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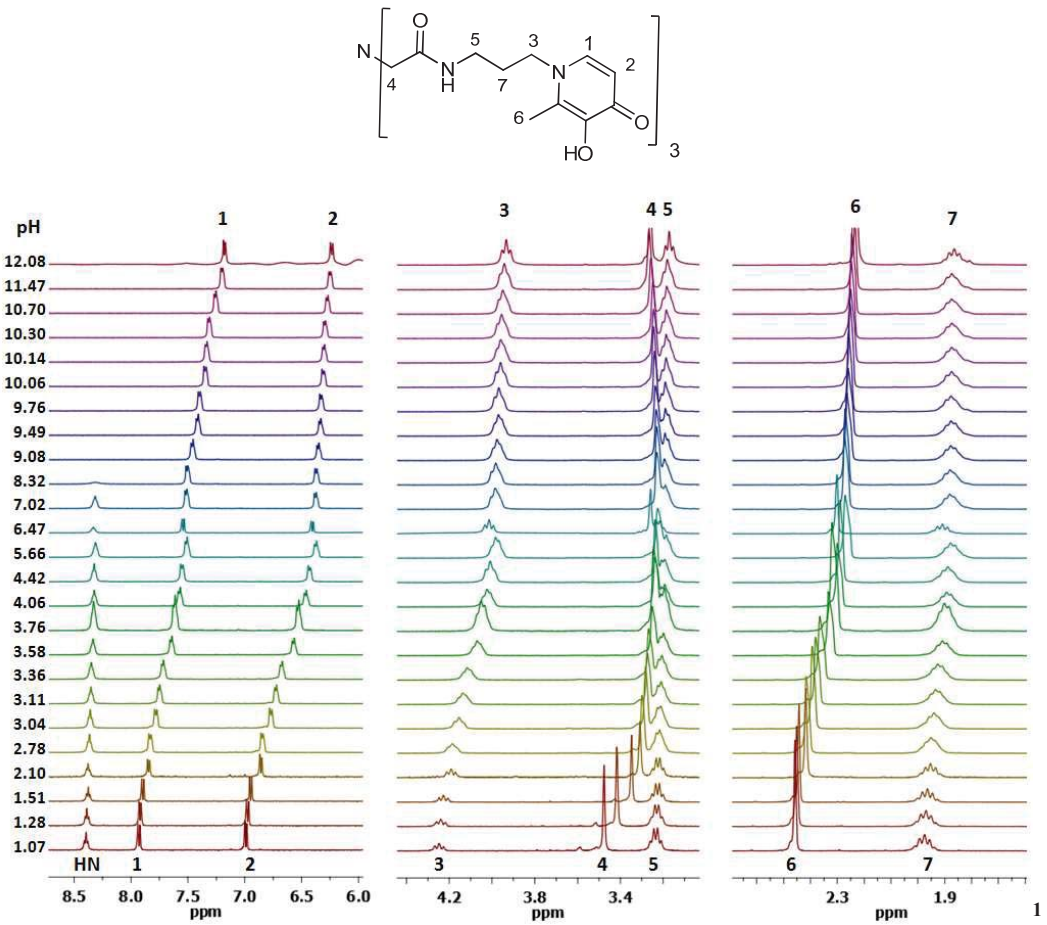

Figure S1. ^{1}H NMR spectra of NTA(PrHP)$_3$ 0.002 M collected at increasing pH values.

[1]

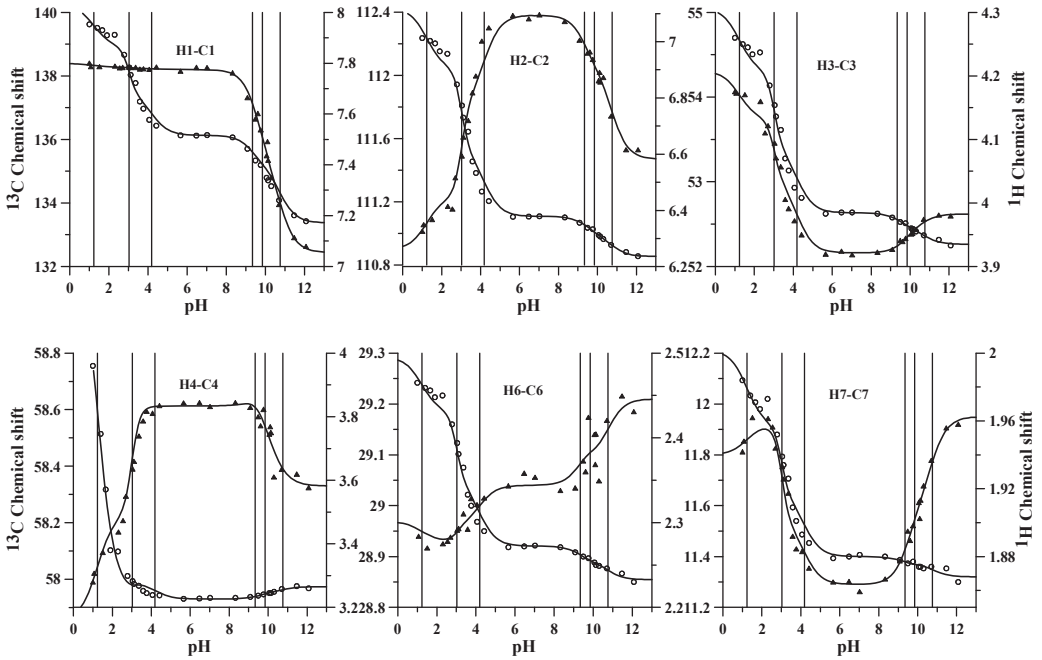

Figure S2. ^{13}C (▲) and ^{1}H (○)experimental chemical shifts of the various carbon atoms and protons in $NTA(PrHP)_3$, and the simulated trends as continuous lines, calculated using the protonation constants in Table 1

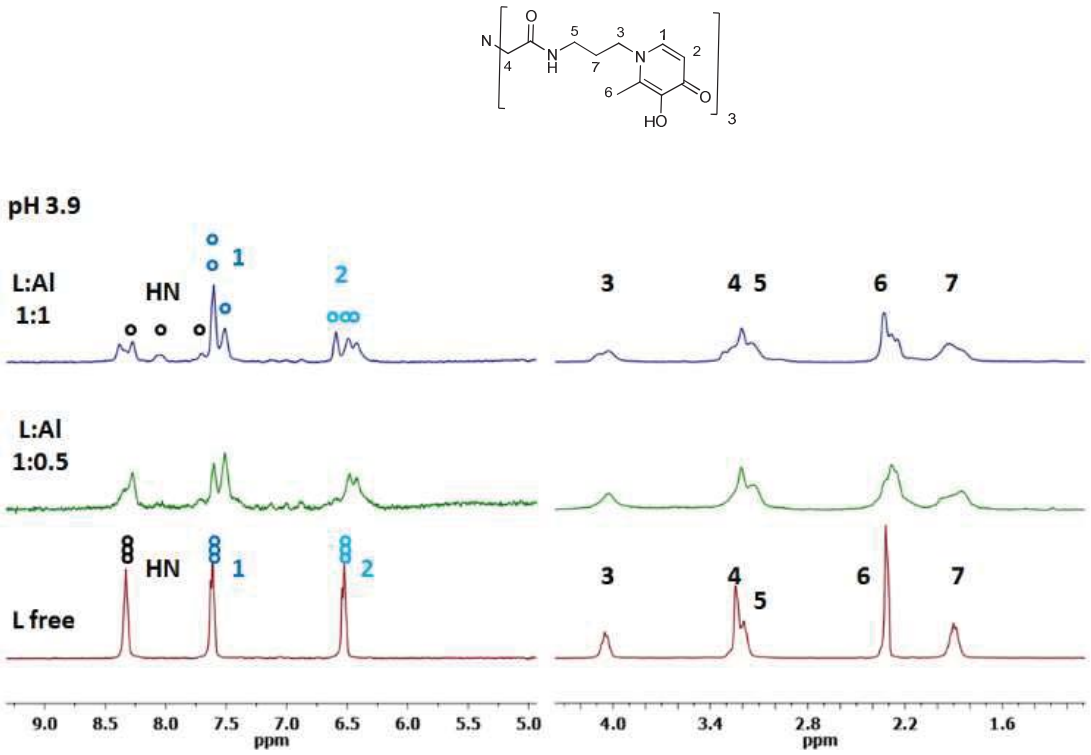

Figure S3. 1D ^{1}H NMR of NTA(PrHP)$_3$:Al(III) system at different metal to ligand (L) molar ratios at pH 3.9.

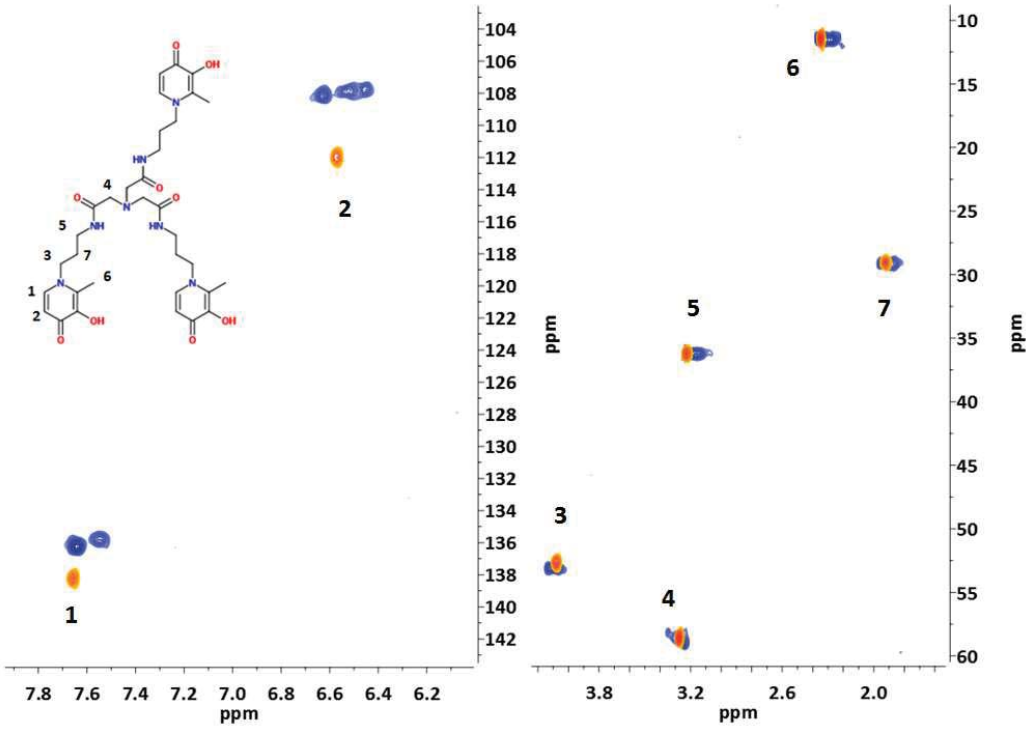

Figure S4. 2D HSQC ^{1}H NMR of the NTA(PrHP)$_3$:Al(III) system at pH 3.9.

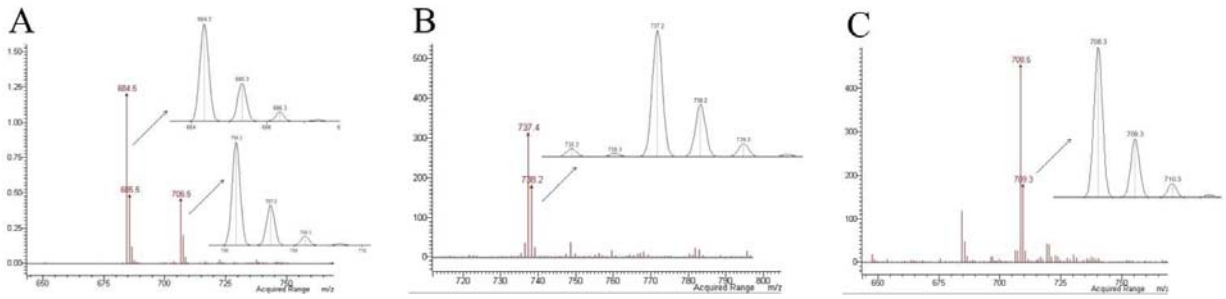

Figure S5. Expanded range of ESI-MS experimental and simulated (up) spectrum of A) ligand $[LH_4]^+$; B) $[FeLH]^+$ complex and C) $[AlLH]^+$ complex.

Table S1. a) ^{13}C individual chemical shifts of the different carbon atoms of the $NTA(PrHP)_3$ ligand (see Scheme 1 for atom numbering) of the variously protonated species, calculated by HypNMR program;[22] b) variations of the individual chemical shifts connected to each deprotonation step.

a) Individual chemical shift (δ, ppm)

Species	C1	C2	C3	C4	C5	C6	C7
L^{3-}	132.440	111.467	58.332	52.622	36.384	29.211	11.950
LH^{2-}	135.213	112.029	58.419	52.479	36.372	29.095	11.628
LH_2^-	136.700	112.067	58.665	52.255	36.336	29.119	11.492
LH_3	138.207	112.379	58.613	52.162	36.333	29.039	11.295
LH_4^+	138.252	111.809	58.612	53.061	36.130	28.965	11.541
LH_6^{3+}	138.270	111.227	58.231	53.739	36.077	28.927	11.923
LH_7^{4+}	138.392	110.896	57.854	54.306	36.283	28.970	11.805

b) Variation of individual chemical shift (Δδ, ppm)

Protonation	C1	C2	C3	C4	C5	C6	C7
$L^3 \rightarrow LH^{2-}$	2.773	0.562	0.087	-0.146	-0.012	-0.116	-0.323
$LH^{2-} \rightarrow LH_2^-$	1.487	0.038	0.246	-0.221	-0.036	0.024	-0.136
$LH^{2-} \rightarrow LH_3$	1.507	0.311	-0.052	-0.093	-0.003	-0.080	-0.197
$LH_3 \rightarrow LH_4^+$	0.045	-0.570	-0.002	0.899	-0.204	-0.074	0.247
$LH_4^+ \rightarrow LH_6^{3+}$	0.018	-0.582	-0.380	0.679	-0.053	-0.039	0.382
$LH_6^{3+} \rightarrow LH_7^{4+}$	0.122	-0.331	-0.377	0.566	0.206	0.044	-0.118

Table S2. a) ^{1}H individual chemical shifts of the protons of the NTA(PrHP)$_3$ ligand (see Scheme 1 for atom numbering) of the variously protonated species, calculated with HypNMR; b) variations of the individual chemical shifts connected to each deprotonation step.

a) ^{1}H individual chemical shift (δ, ppm)

Species	**H1**	**H2**	**H3**	**H4**	**H5**	**H6**	**H7**
L^{3-}	7.171	6.236	3.935	3.265	3.175	2.233	1.868
LH^{2-}	7.330	6.308	3.959	3.249	3.186	2.254	1.876
LH_2^{-}	7.405	6.330	3.967	3.238	3,194	2.254	1.874
LH_3	7.516	6.379	3.985	3.226	3.189	2.272	1.880
LH_4^{+}	7.684	6.621	4.092	3.280	3.200	2.350	1.917
LH_6^{3+}	7.867	6.903	4.206	3.248	3.218	2.431	1.957
LH_7^{4+}	8.030	7.121	4.307	4.395	3.267	2,495	2,002

b) Variation of individual chemical shift (Δδ, ppm)

Protonation	**H1**	**H2**	**H3**	**H4**	**H5**	**H6**	**H7**
$L^{3} \rightarrow LH^{2-}$	0.158	0.072	0.024	-0.016	0.011	0.021	0.008
$LH^{2-} \rightarrow LH_2^{-}$	0.076	0.022	0.009	-0.011	0.008	0.001	-0.003
$LH^{2-} \rightarrow LH_3$	0.111	0.049	0.017	-0.012	-0.005	0.018	0.006
$LH_3 \rightarrow LH_4^{+}$	0.168	0.242	0.108	0.054	0.011	0.077	0.037
$LH_4^{+} \rightarrow LH_6^{3+}$	0.182	0.282	0.114	-0.032	0.018	0.081	0.040
$LH_6^{3+} \rightarrow LH_7^{4+}$	0.163	0.219	0.101	1.147	0.049	0.065	0.045