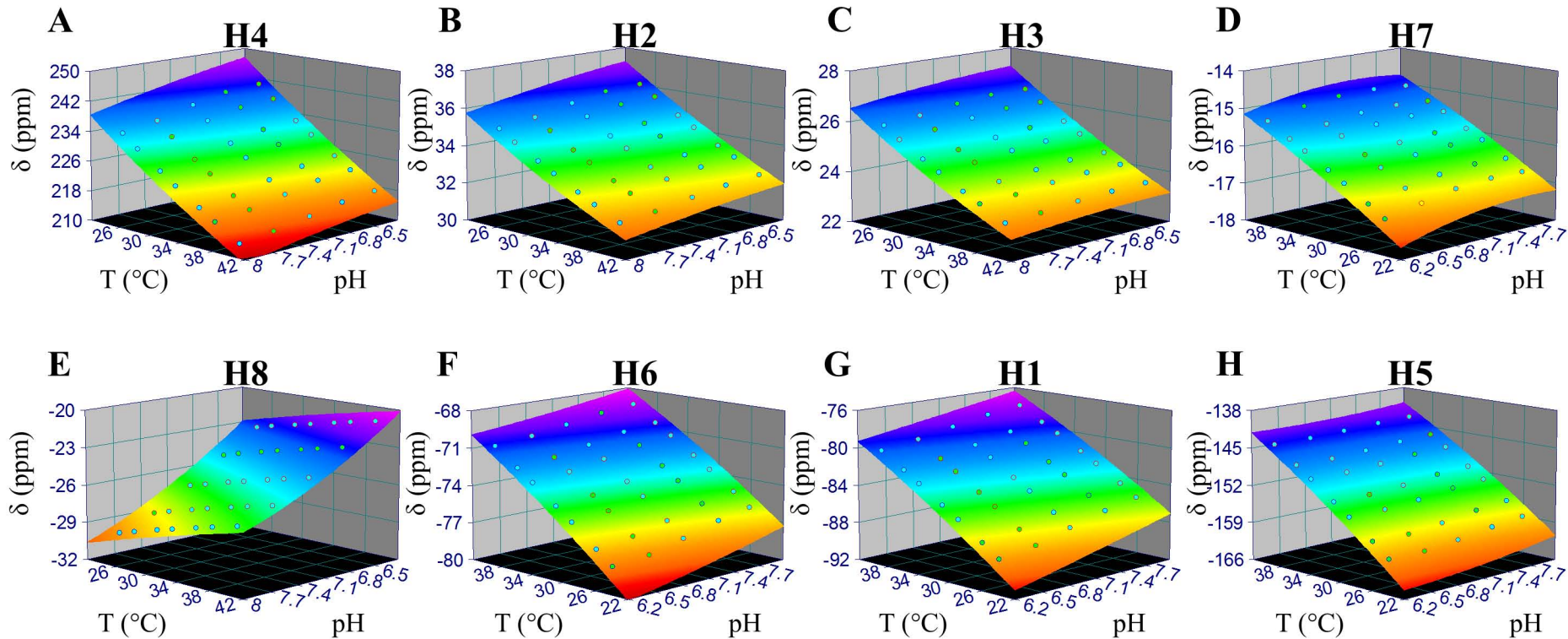
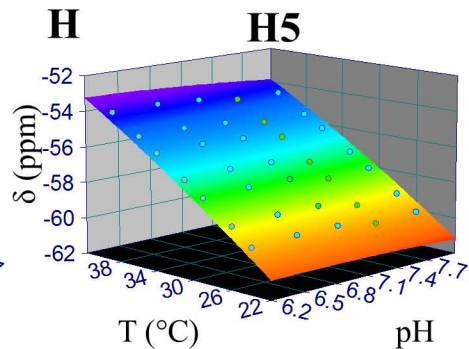
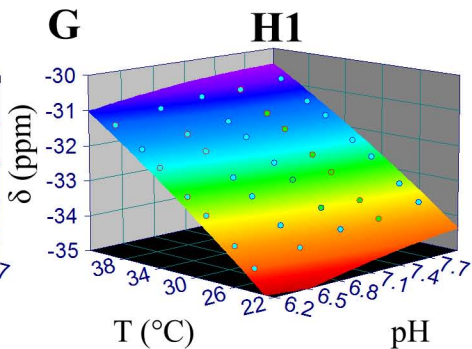
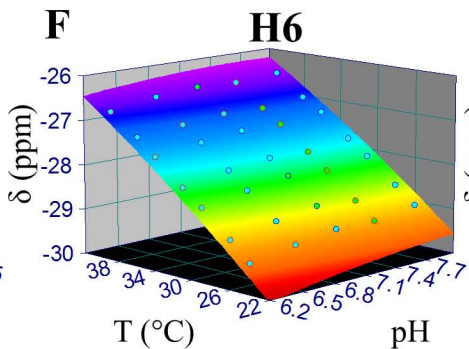
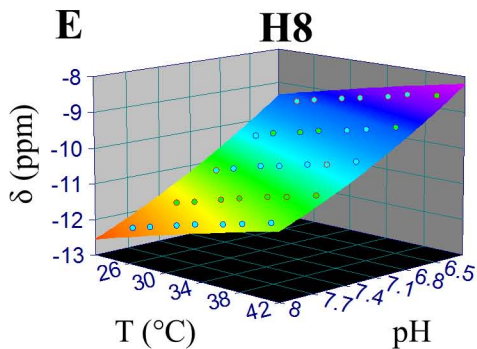
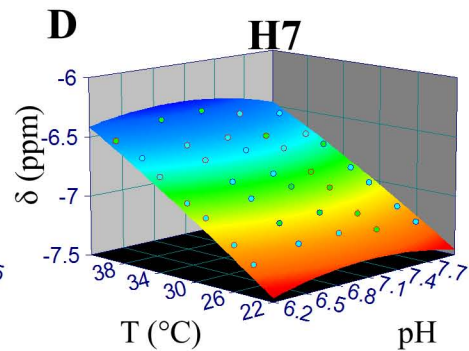
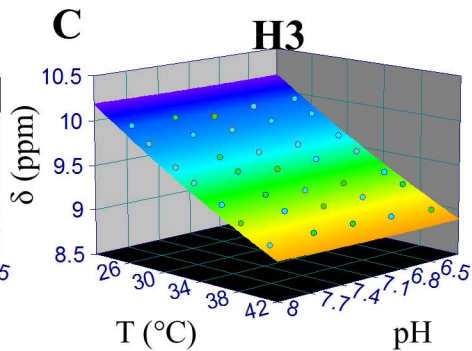
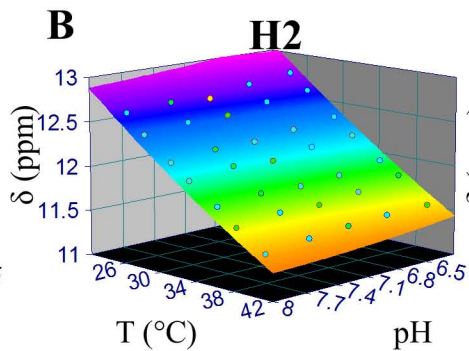
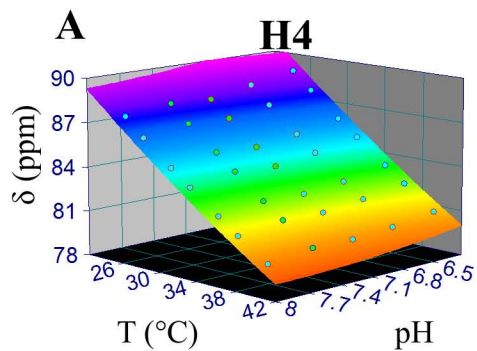


Supplementary Fig.1

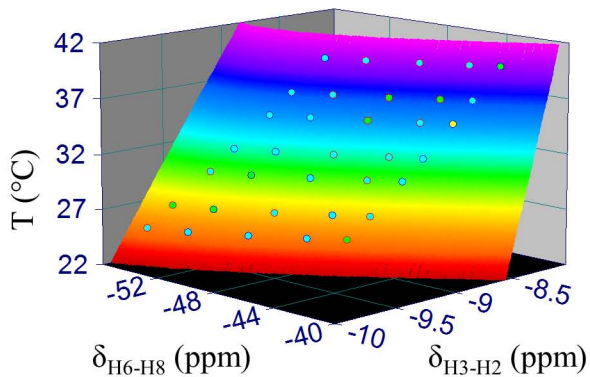
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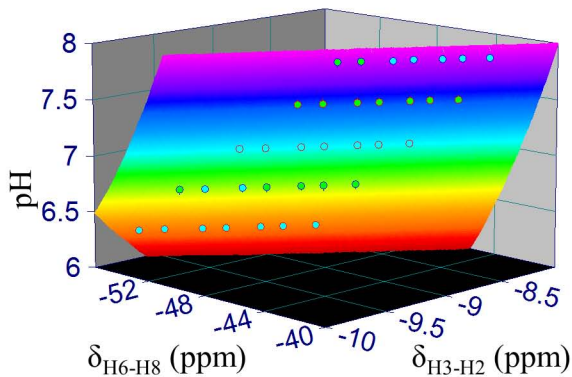
Supplementary Fig.2**Top**

Supplementary Fig.3 Top

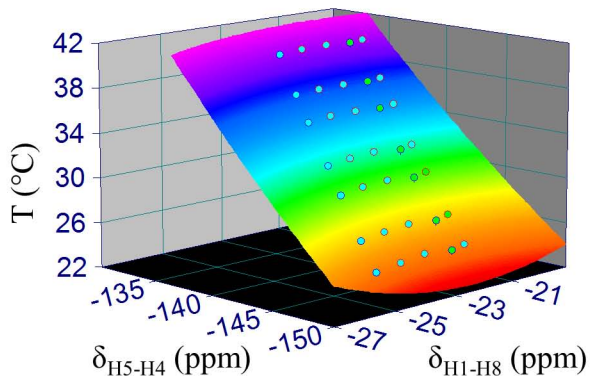
A Tm-DOTA-4AmP⁵⁻



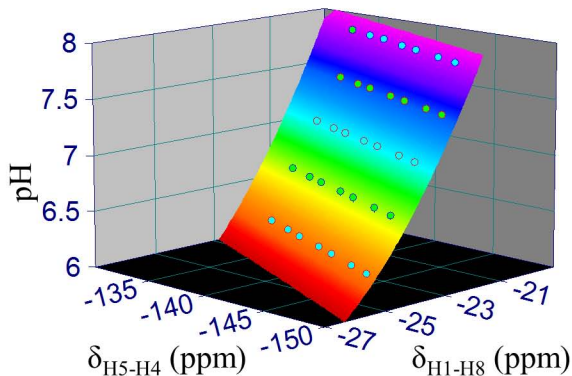
B Tm-DOTA-4AmP⁵⁻

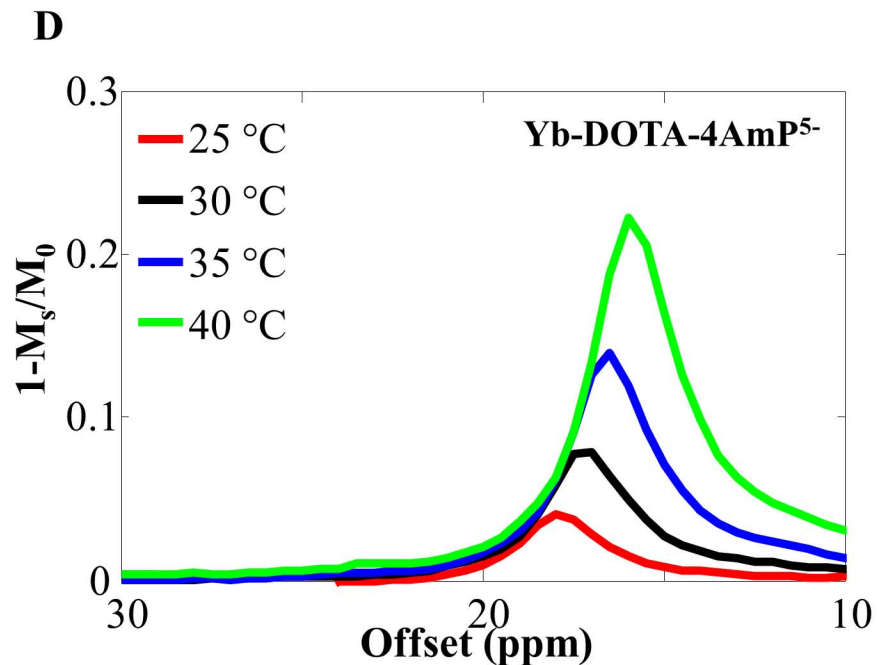
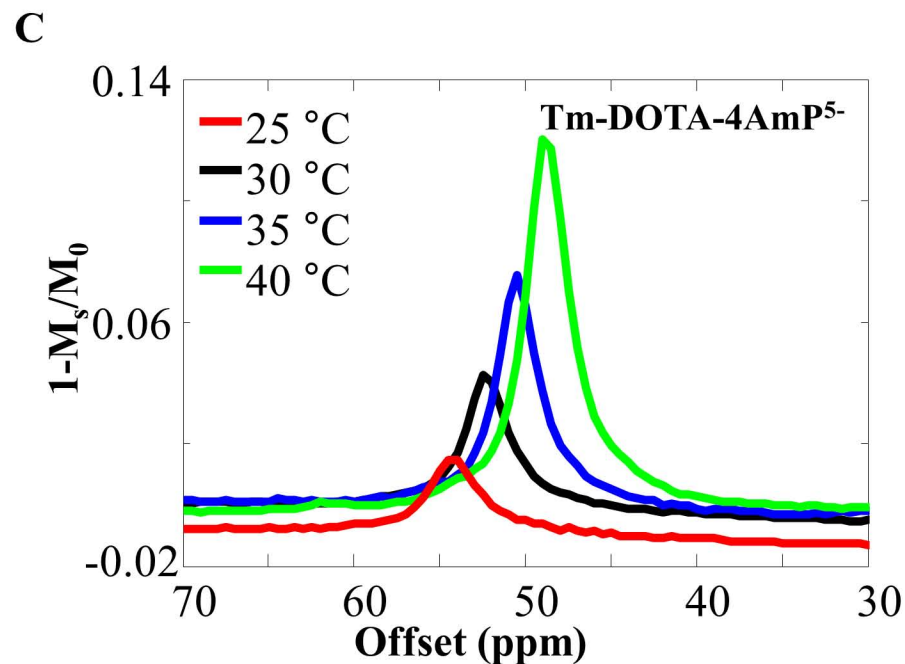
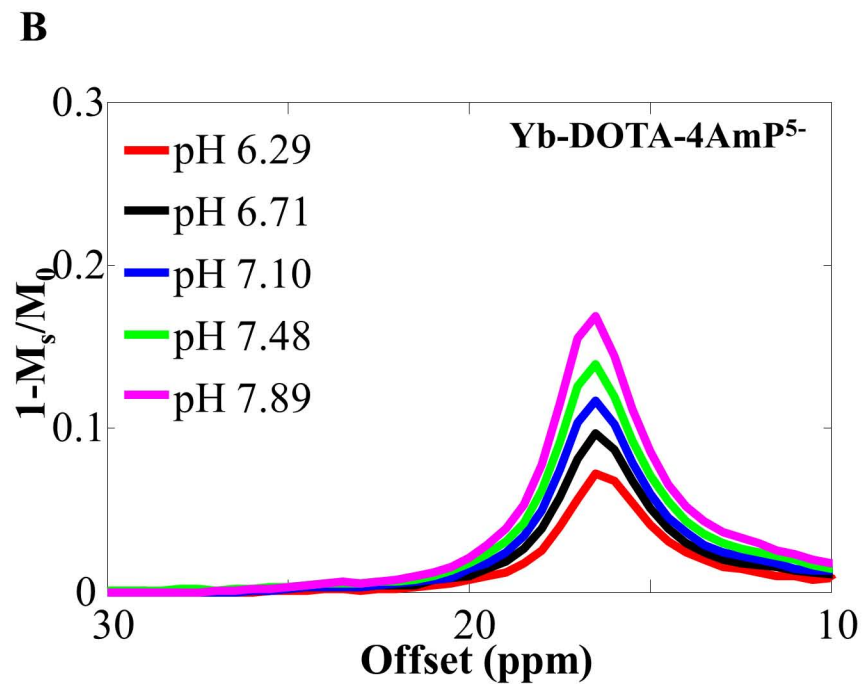
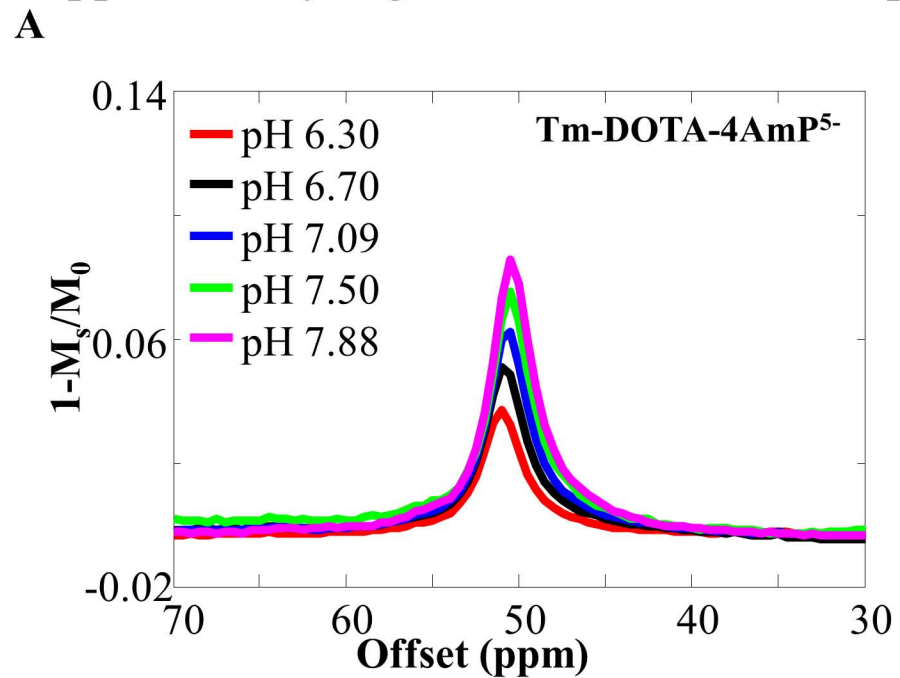


C Yb-DOTA-4AmP⁵⁻



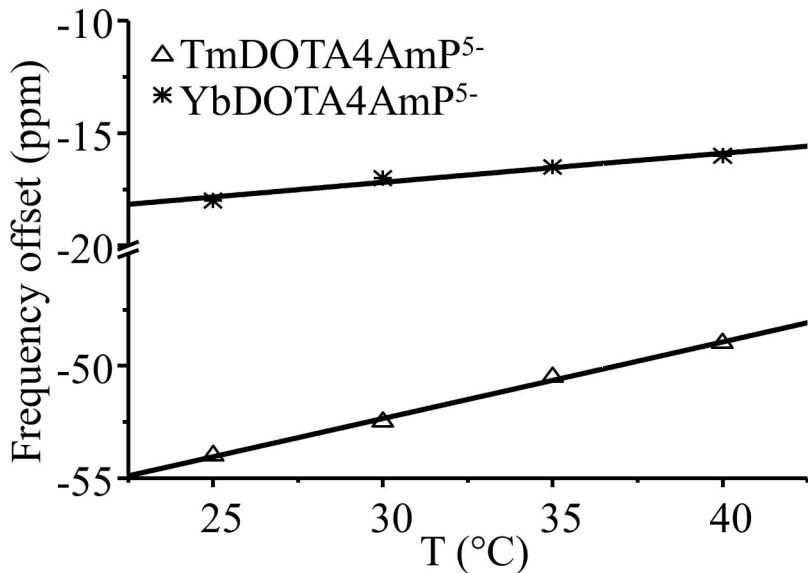
D Yb-DOTA-4AmP⁵⁻

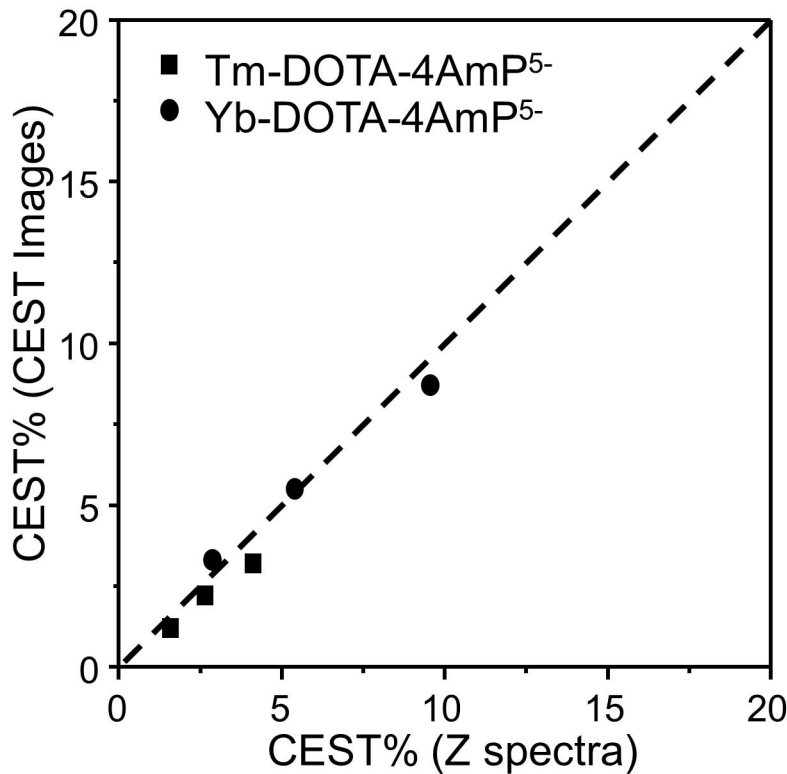


Supplementary Fig.4**Top**

Supplementary Fig.5

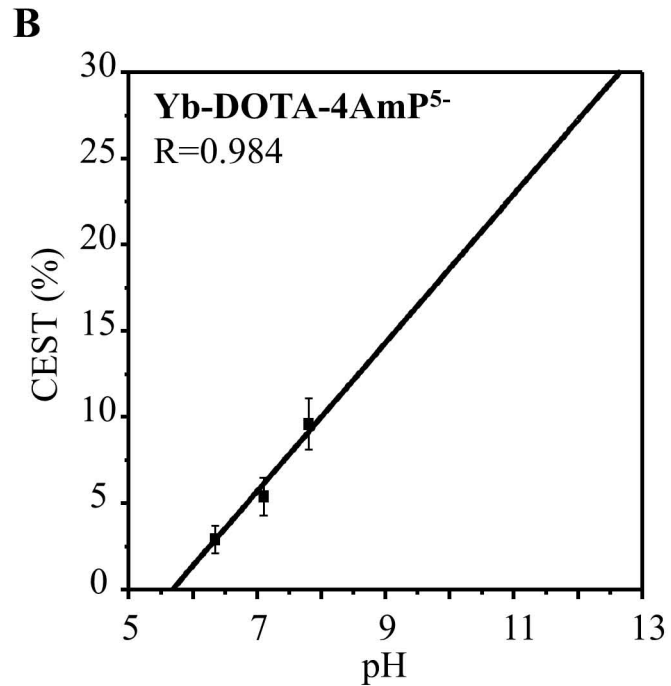
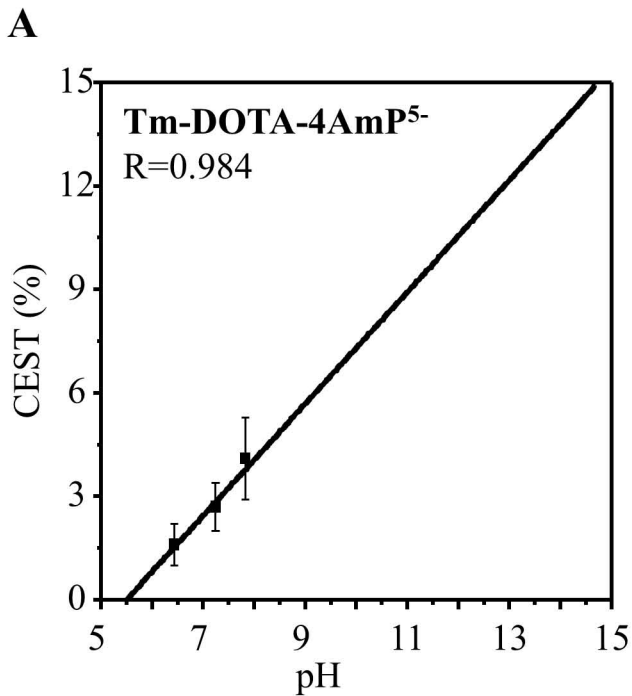
Top





Supplementary Fig.7

Top



Supplementary Table 1. Coefficients for T and pH dependence of chemical shift in ¹H resonances of Tm-DOTA-4AmP⁵⁻

Resonance	a	b	c	d	e	f	r²
H4	306.469	1.854	-2.930	-0.617	0.0123	0.0856	0.999
H2	46.149	0.583	-0.498	-0.121	0.00228	0.0144	0.999
H3	31.901	0.895	-0.383	-0.106	0.00185	0.0100	0.999
H7	-36.648	4.0964	0.210	-0.262	-0.000912	-0.00393	0.999
H8	40.928	-15.732	0.0702	0.769	-0.00115	0.023	0.998
-NH	-56.849	-3.398	0.690	0.312	-0.00294	-0.0192	0.999
H6	-100.557	0.0123	0.913	0.150	-0.00373	-0.0268	0.999
H1	-123.486	2.143	1.065	0.0585	-0.00425	-0.0330	0.999
H5	-186.904	-4.849	1.954	0.536	-0.00821	-0.0513	0.999
H3-H2	-14.249	0.312	0.115	0.015	-0.000429	-0.00441	0.997
H6-H8	-141.485	15.744	0.843	-0.619	-0.00258	-0.0498	0.997

Supplementary Table 2. Coefficients for T and pH dependence of chemical shift in ¹H resonances of Yb-DOTA-4AmP⁵⁻

Resonance	a	b	c	d	e	f	r²
H4	128.566	-5.396	-0.903	0.292	0.00391	0.0181	0.998
H2	17.793	-0.545	-0.135	0.0279	0.000657	0.00174	0.997
H3	12.754	-0.177	-0.103	0.0117	0.000550	0.000643	0.997
H7	-15.870	1.955	0.0843	-0.135	-0.000334	-0.00169	0.994
H8	13.972	-5.643	0.0352	0.261	-0.000382	0.00754	0.997
H6	-42.246	1.713	0.301	-0.0914	-0.00126	-0.00663	0.998
H1	-51.937	2.555	0.358	-0.132	-0.00145	-0.00890	0.998
H5	-78.871	1.887	0.631	-0.125	-0.00277	-0.0112	0.997
H1-H8	-65.909	8.198	0.323	-0.393	-0.00107	-0.0164	0.999
H5-H4	-207.442	7.282	1.535	-0.417	-0.00668	-0.0293	0.998