Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information for

Influence of pH and Mg(II) on the catalytic core domain 5 of a bacterial group II intron

M. Pechlaner, A. Dominguez-Martin and R.K.O. Sigel

Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland.

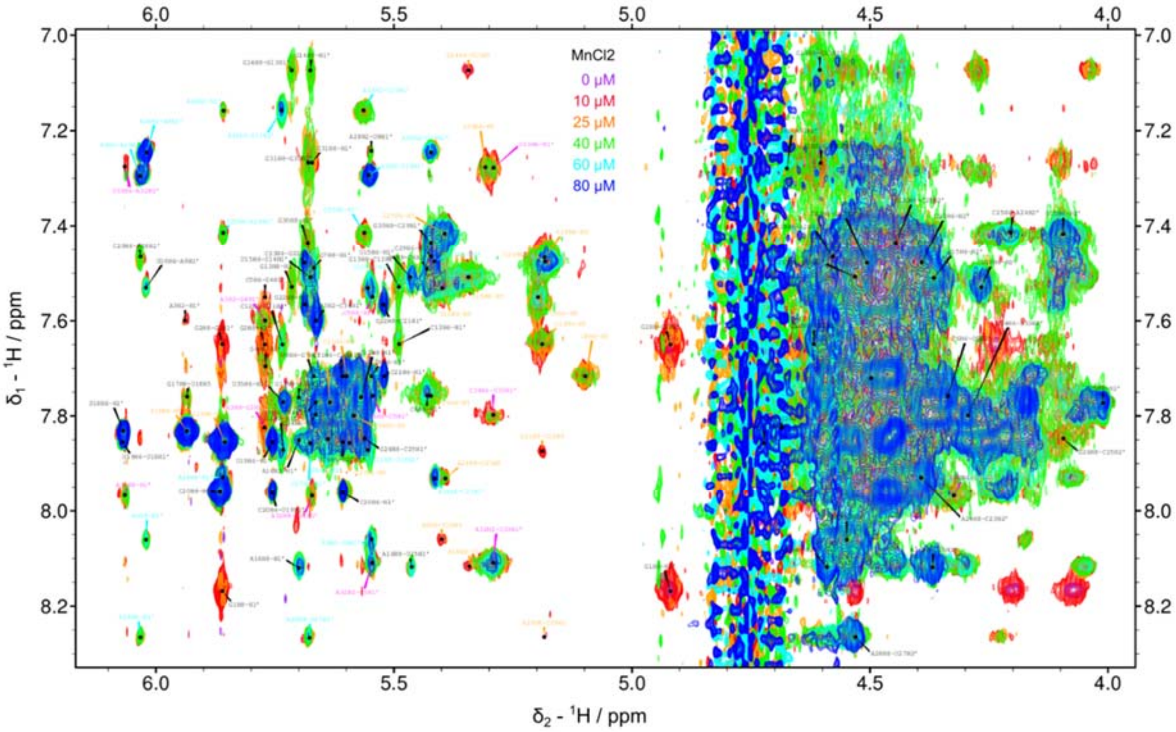

Figure S1. Overlay of ^{1}H,^{1}H-NOESY spectra of *Av*D5 in the presence of increasing amounts of $MnCl_2$. The regions connecting base to sugar protons are shown.

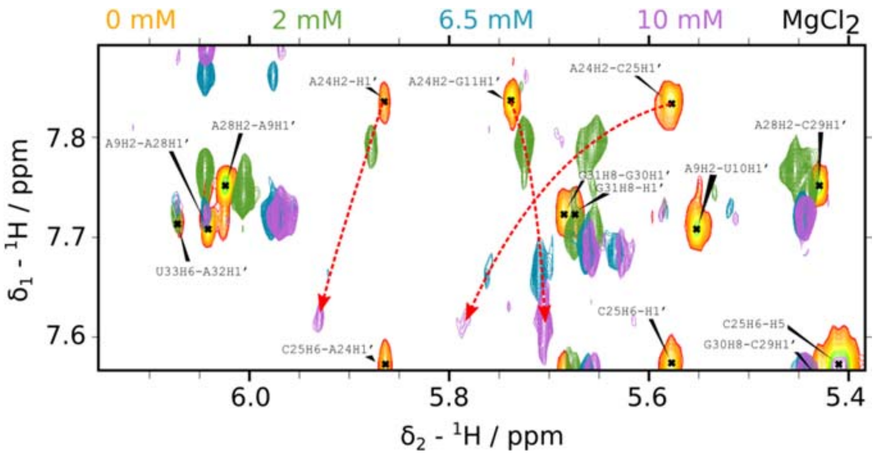

Figure S2. Small section of an overlay of ^{1}H,^{1}H-NOESY spectra in the presence of increasing amounts of $MgCl_2$. Red arrows mark the movement of three A24H2 cross-peaks. Only A24H2-C25H1' is significantly decreased at high $MgCl_2$ concentration.

Table S1. K_D [mM] of different residues in *Av*D5 as determined by ISTAR.[a]

	G1	G2	A3	G4	C5	C6	G7	U8	A9
H1'	n.a.	n.a.	**5.17 +/- 1.17**	n.a.	**3.48 +/- 0.37**	2.23 +/- 0.35	n.a.	**2.32 +/- 0.31**	**4.70 +/- 0.62**
H2'	n.a.	**5.24 +/- 0.43**	-	-	**3.88 +/- 0.25**	**5.13 +/- 0.32**	5.49 +/- 0.27	**2.61 +/- 0.53**	n.a.
H2/H5	-	-	**2.01 +/- 0.26**	-	n.a.	2.53 +/- 0.70	-	n.a.	**5.22 +/- 0.52**
H6/H8	1.42 +/- 0.25	n.a.	n.a.	n.a.	2.06 +/- 0.90	n.a.	n.a.	5.31 +/- 0.85	**5.74 +/- 0.65**

	U35	C34	U33	A32	G31	G30	C29	A28	U27
H1'	n.a.	n.a.	1.42 +/- 0.11	n.a.	**3.86 +/- 0.18**	4.01 +/- 0.30	n.a.	n.a.	**8.13 +/- 0.52**
H2'	n.a.	n.a.	**5.73 +/- 1.06**	**16.00 +/- 4.46**	1.37 +/- 0.28	**4.66 +/- 0.27**	5.49 +/- 0.39	**4.63 +/- 0.82**	**5.39 +/- 0.41**
H2/H5	39.14 +/- 17.06	n.a.	n.a.	n.a.	-	-	n.a.	**3.50 +/- 0.81**	**5.77 +/- 0.71**
H6/H8	9.49 +/- 1.44	1.87 +/- 0.31	1.31 +/- 0.40	n.a.	**1.80 +/- 0.20**	n.a.	1.04 +/- 0.07	n.a.	n.a.

	U10	G11	C12	G13	G14	U15	A16	G17
H1'	**4.93 +/- 0.62**	**4.22 +/- 0.23**	1.88 +/- 0.42	n.a.	n.a.	**9.77 +/- 1.12**	n.a.	**17.79 +/- 4.10**
H2'	n.a.	**4.89 +/- 0.49**	1.46 +/- 0.37	**5.48 +/- 0.53**	**10.10 +/- 1.14**	n.a.	n.a.	**20.75 +/- 8.06**
H2/H5	n.a.	-	n.a.	-	-	**16.97 +/- 2.78**	9.11 +/- 2.26	-
H6/H8	n.a.	**5.37 +/- 0.67**	2.41 +/- 0.24	n.a.	**6.25 +/- 0.53**	n.a.	n.a.	n.a.

	G26	C25	A24	C23	G22	C21	C20	U19	U18
H1'	**2.02 +/- 0.39**	**3.51 +/- 0.41**	**10.20 +/- 2.25**	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
H2'	n.a.	**5.42 +/- 0.53**	**20.56 +/- 8.49**	**4.76 +/- 0.38**	4.57 +/- 0.58	**16.37 +/- 4.81**	n.a.	n.a.	n.a.
H2/H5	-	**5.96 +/- 0.63**	**13.38 +/- 2.80**	n.a.	-	n.a.	**22.13 +/- 6.36**	30.13 +/- 13.33	n.a.
H6/H8	n.a.	**5.57 +/- 0.67**	**10.59 +/- 1.68**	**15.48 +/- 6.59**	n.a.	**11.31 +/- 1.24**	**13.44 +/- 2.35**	3.47 +/- 0.51	n.a.

[a] M. I. C. Erat, J. Coles, C. Finazzo, B. Knobloch and R. K. O. Sigel, *Coord. Chem. Rev.*, **2012**, *256*, 279-288.

n.a. … K_D not used in analysis because either curves cannot be fitted or there is too little change in chemical shift to fit data reliably.

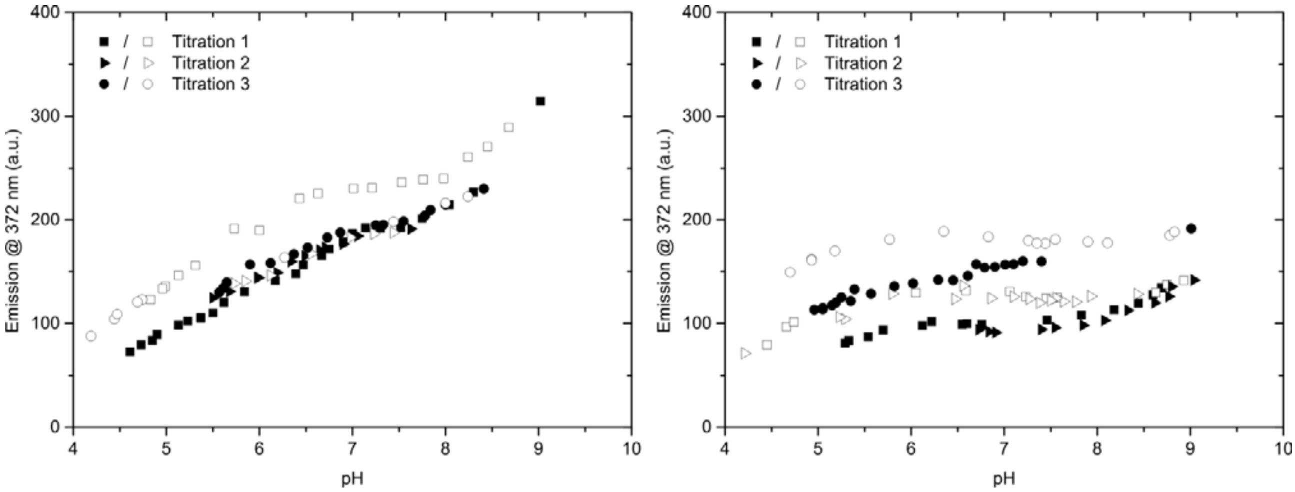

Figure S3. Fluorescence emission of *Av*D5-AP3 at 372 nm in dependence of pH in the absence (left) or in the presence (right) of 6 mM Mg(II). Solid and open data points represent measurements in opposite pH directions, i.e. increasing and decreasing, respectively.