Conserved binding of GCAC motifs by MEC-8, couch potato and the RBPMS protein family

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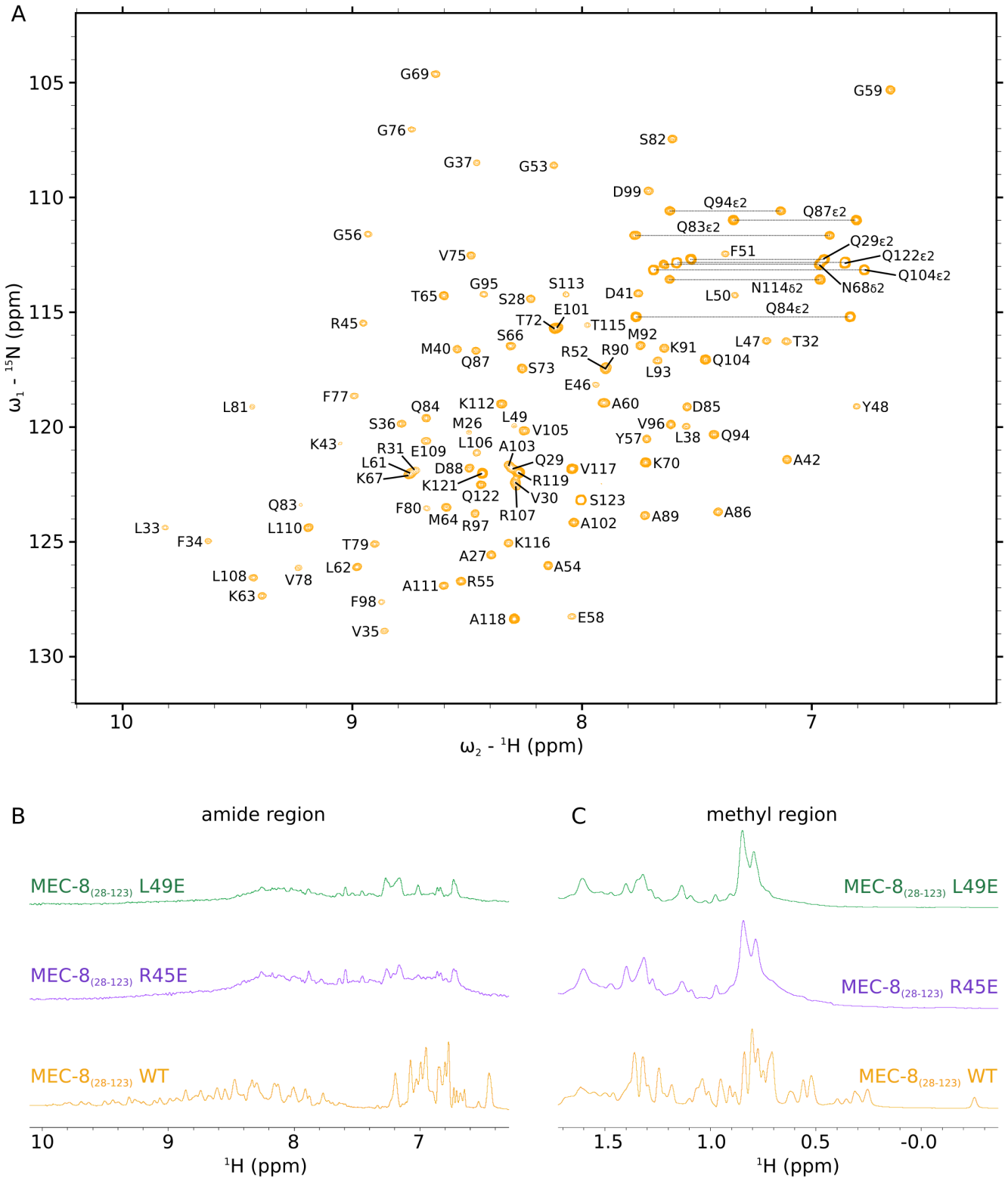
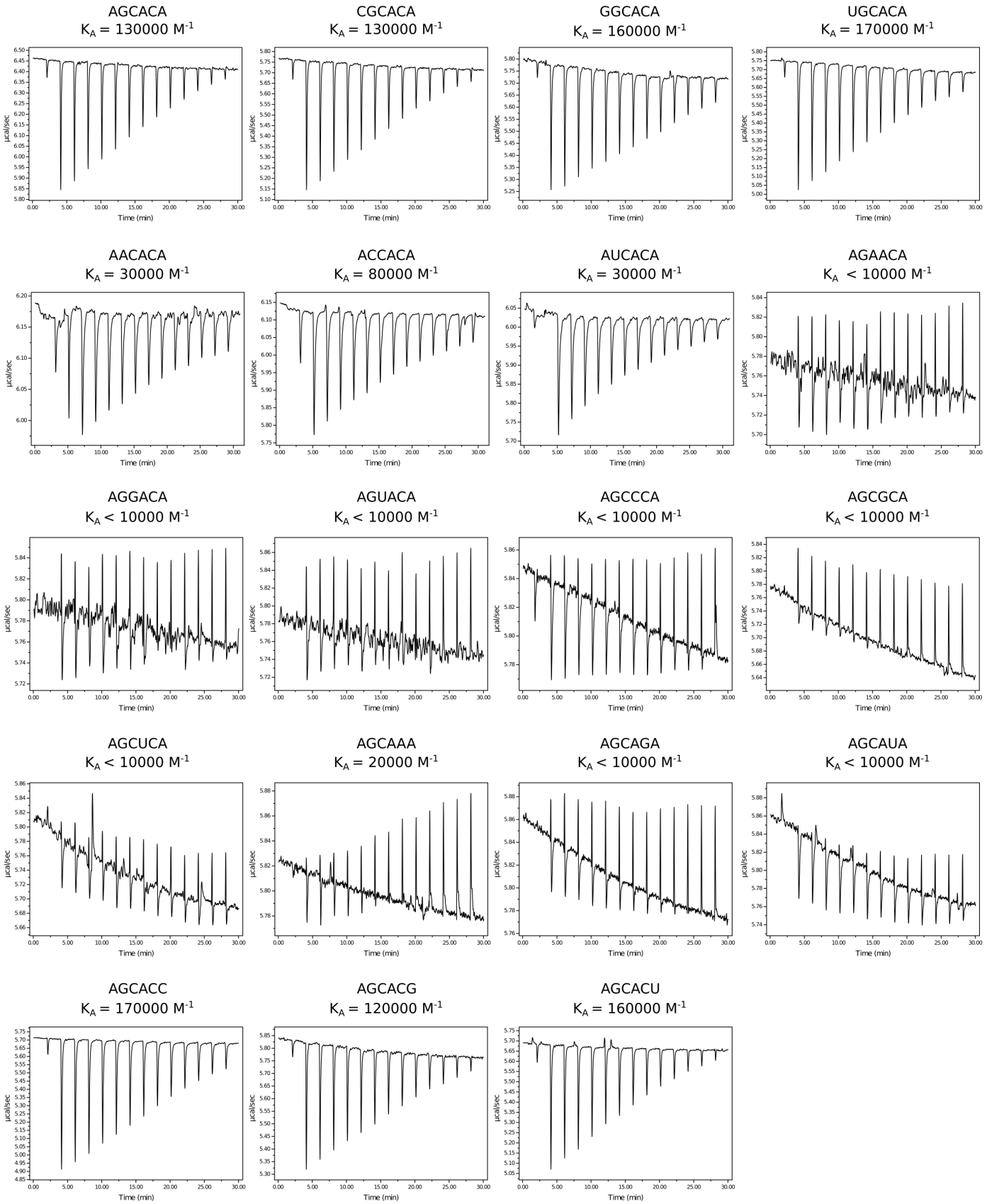
SUPPLEMENTARY TABLE S1. Data collection and refinement statistics.

	MEC-8 RRM1	**MEC-8 RRM1 + AGCACATTTTTTTTAGCACA**
PDB ID	5BJR	5TKZ
Data collection		
Beamline	ESRF ID23-2	ESRF ID23-2
Space group	*I* 2 2 2	*P* 32 2 1
Cell dimensions		
a, b, c (Å)	52.59, 96.42, 109.99	52.19, 52.19, 156.53
α, β, γ (°)	90, 90, 90	90, 90, 120
Wavelength (Å)	0.873	0.873
Resolution (Å) [a]	35.36–2.60 (2.69–2.60)	25.74–1.53 (1.58–1.53)
R_{merge} (%) [a]	8.5 (34.4)	3.4 (35.9)
$I/\sigma I$ [a]	6.00 (2.68)	8.03 (2.26)
Observations [a]	17121 (1703)	76451 (7524)
Unique reflections [a]	8854 (872)	38386 (3768)
Completeness (%) [a]	99.06 (99.54)	99.99 (100.00)
Multiplicity [a]	1.9 (2.0)	2.0 (2.0)
Refinement		
Resolution (Å) [a]	35.36–2.60 (2.76–2.60)	25.74–1.53 (1.58–1.53)
Number of reflections	8842	38385
R_{work}/R_{free} (%)	23.7/28.5	23.3/27.1
Unit cell content / No. atoms		
Protein/nucleic acid	1328	1606
Solvent	37	134
Ions (NH_4)	15	
Average B, all atoms ($Å^2$)	48.5	38.4
R.m.s. deviations		
Bond lengths (A)	0.002	0.009
Bond angles (°)	0.571	1.177
Ramachandran plot		
Favored (%)	100	99.43
Allowed (%)	0	0.57
Outliers (%)	0	0

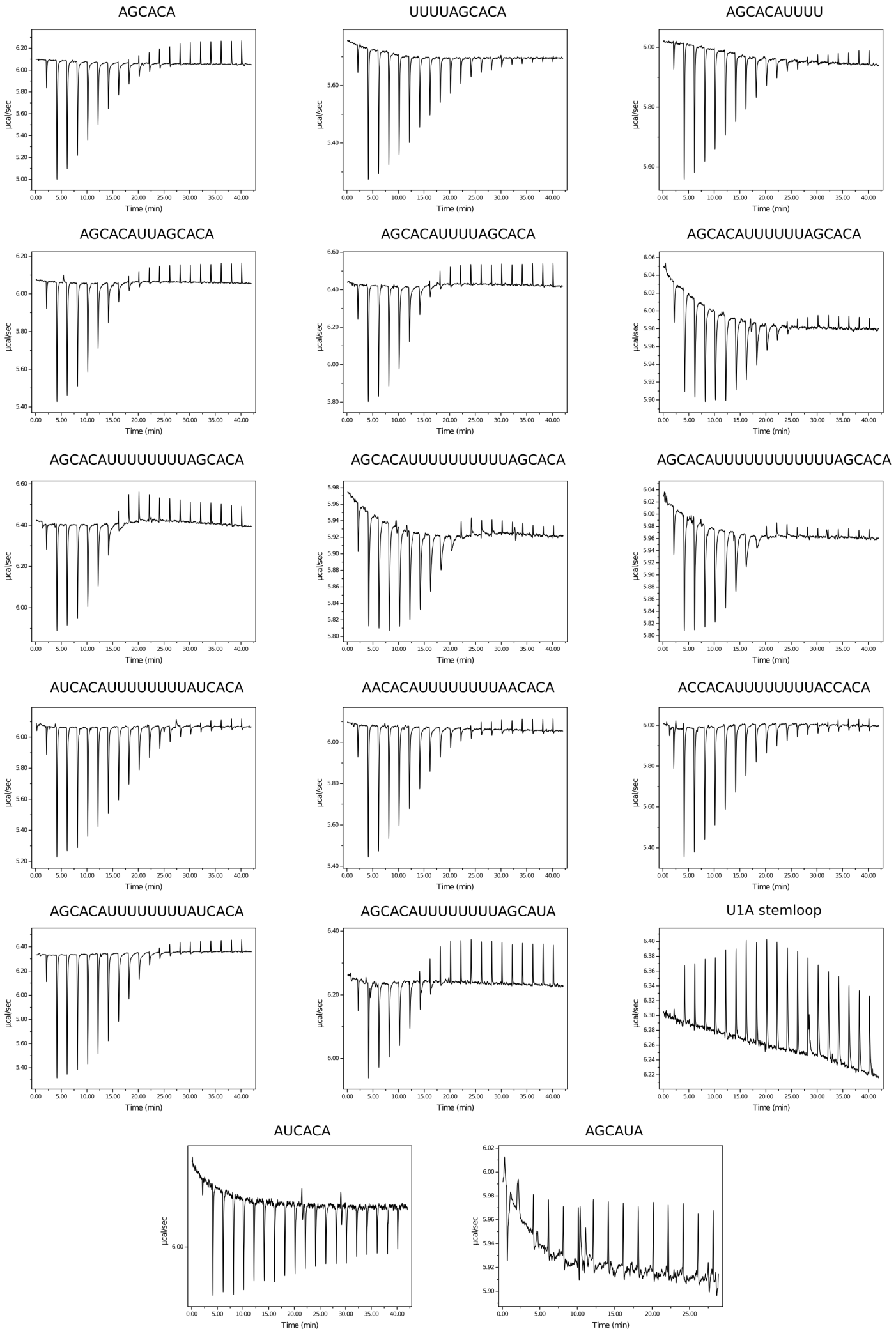
[a] Data in parentheses refer to the highest resolution shell



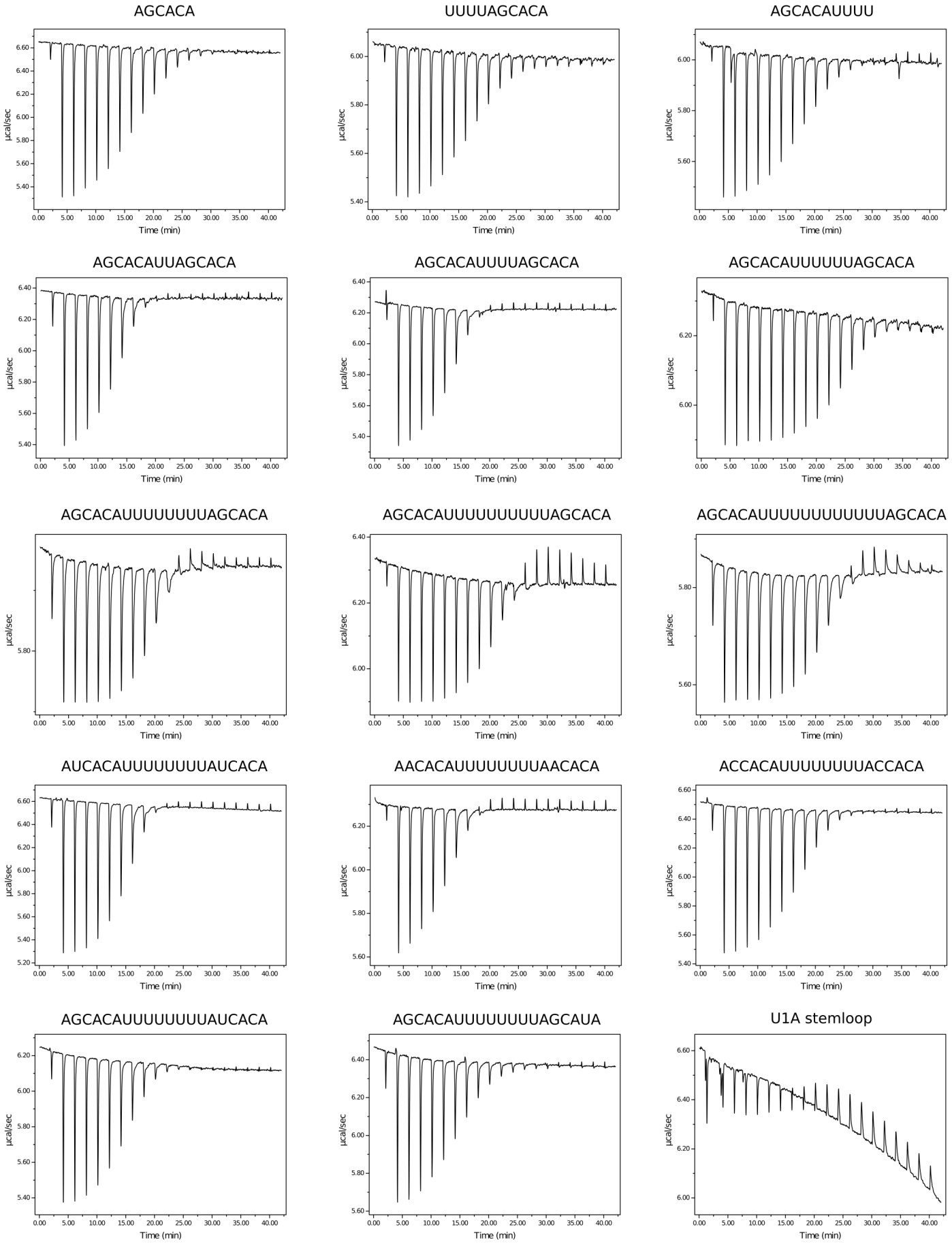
SUPPLEMENTARY FIGURE S1. NMR spectroscopy data for MEC-8 RRM1. (*A*) ^{1}H,^{15}N-HSQC spectrum at 298 K for 500 μM ^{15}N MEC-8$_{(28\text{-}123)}$ in 50 mM TRIS (pH 7.5) and 150 mM NaCl, with 10% D_2O (v/v). Crosspeaks for backbone amides, as well as sidechain asparagine and glutamine amides, have been annotated with residue type and number. (*B*,*C*) Selected regions of 1D ^{1}H spectra for wildtype MEC-8$_{(28\text{-}123)}$, as well as mutants Arg45Glu and Leu49Glu. Both dimerization surface mutants result in destabilization of the protein fold.



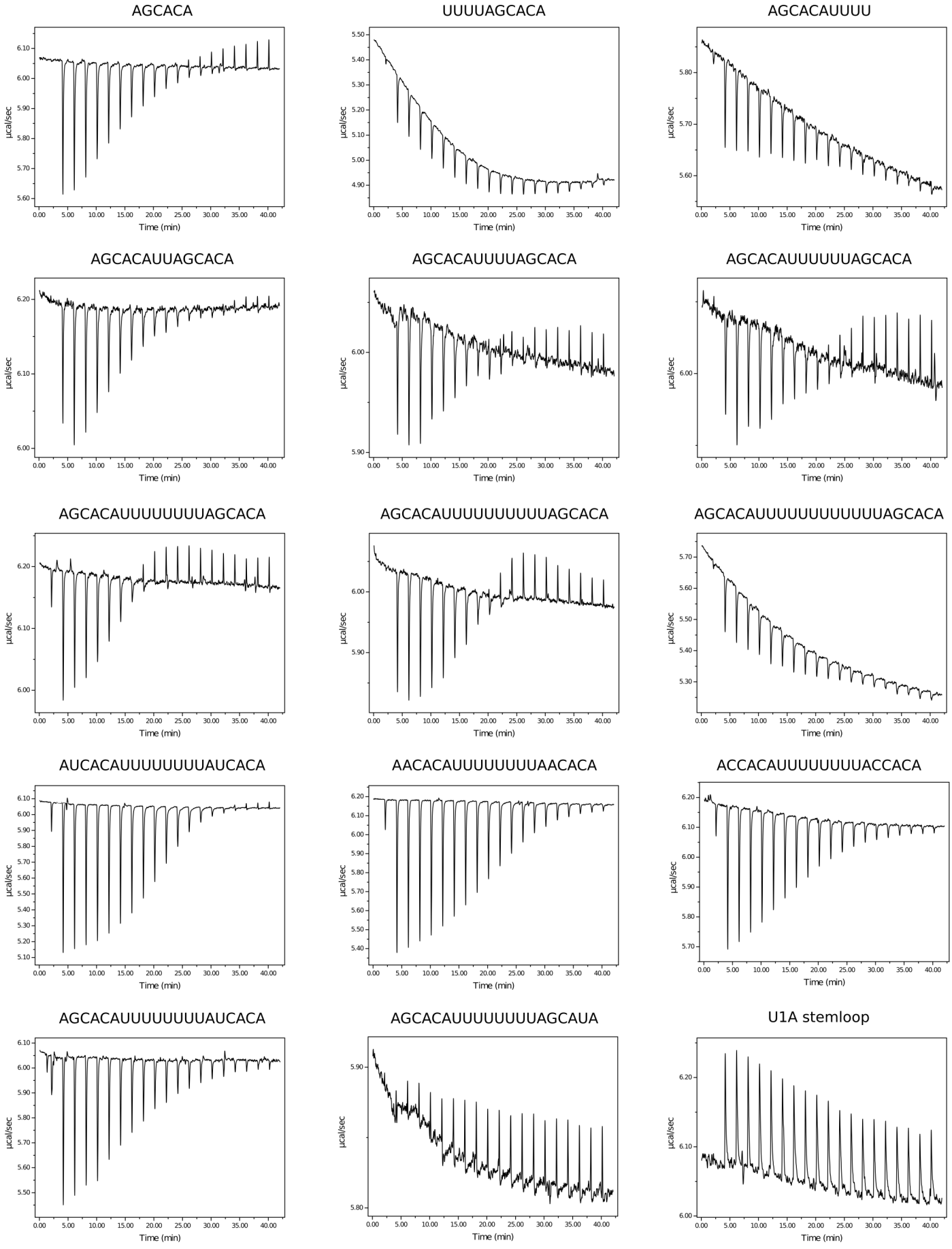
SUPPLEMENTARY FIGURE S2. Representative raw ITC data and derived K_A values used to define the initial affinity-weighted sequence motif of MEC-8 RRM1 as shown in Fig. 1F.



SUPPLEMENTARY FIGURE S3. Representative raw ITC data for RNA ligand binding by MEC-8 RRM1 from Table 1.



SUPPLEMENTARY FIGURE S4. Representative raw ITC data for RNA ligand binding by couch potato RRM from Table 2.



SUPPLEMENTARY FIGURE S5. Representative raw ITC data for RNA ligand binding by RBPMS RRM from Table 2.