Supplemental information

Unraveling the binding mode of a methamphetamine aptamer: A spectroscopic and calorimetric study

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Supporting Information

Unravelling the binding mode of a methamphetamine aptamer: a spectroscopic and calorimetric investigation

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Binding constant equation related to the "**Lock and Key**" equilibrium is the following: $K_D{}^{obs} = \frac{k_{off}}{k_{on}}$.

Binding constant equations related to the "**Conformational Selection**" equilibrium are the following: $K_D{}^{obs} = K_{disso}\,(1 + K_{iso})$ where $K_{disso} = \frac{k'_{off}}{k'_{on}}$ and $K_{iso} = \frac{k'_{rev}}{k'_{for}}$. Binding constant equations related to the "**Induced Fit**" equilibrium are the following: $K_D{}^{obs} = K_{disso}\,\frac{K_{iso}}{(1+K_{iso})}$ where $K_{disso} = \frac{k''_{off}}{k''_{on}}$ and $K_{iso} = \frac{k''_{rev}}{k''_{for}}$.

Equation S1. Binding constant equations related to the Lock-and-Key, Conformational Selection, and Induced Fit binding models.

Aptamer identification	Sequence 5'-3'
Aptamer-1	ATACGAGCTTGTTCAATAGCGTTTAGGCGTTCATTCATCCCGCTATCTGGCTGTATCGTGATAGTAAGAGCAATC
Aptamer-2	ATACGAGCTTGTTCAATAGCGTTTCTATCTGGCTGTATCGTGATAGTAAGAGCACTAATGATAGTAAGAGCAATC
Aptamer-3	ATACGAGCTTGTTCAATAGCGTTTAGCGTTCAATTCATCCCGCTATCCTGGCTGTATCGTGATAGTAGAACAATC
Aptamer-4	ATACGAGCTTGTTCAATAGCGTTTTACGTTCAATTCATCCCGCTATCTGGCTGTATCGTGATAGTAAGAGCAATC
Aptamer-2-40mer	GCGTTTCTATCTGGCTGTATCGTGATAGTAAGAGCACTAA
Mutated-Aptamer-2-40mer	GCGTTTCGTCCTGGCTGTATCGTGATAGTAAGAGCACTAA

Table S1. Full Meth-aptamer sequences used in the study. Buffer conditions are 2 mM Tris-HCl pH 7.5, 10 mM NaCl, 0.5 mM KCl, 0.2 mM MgCl$_2$ and 0.1 mM CaCl$_2$.
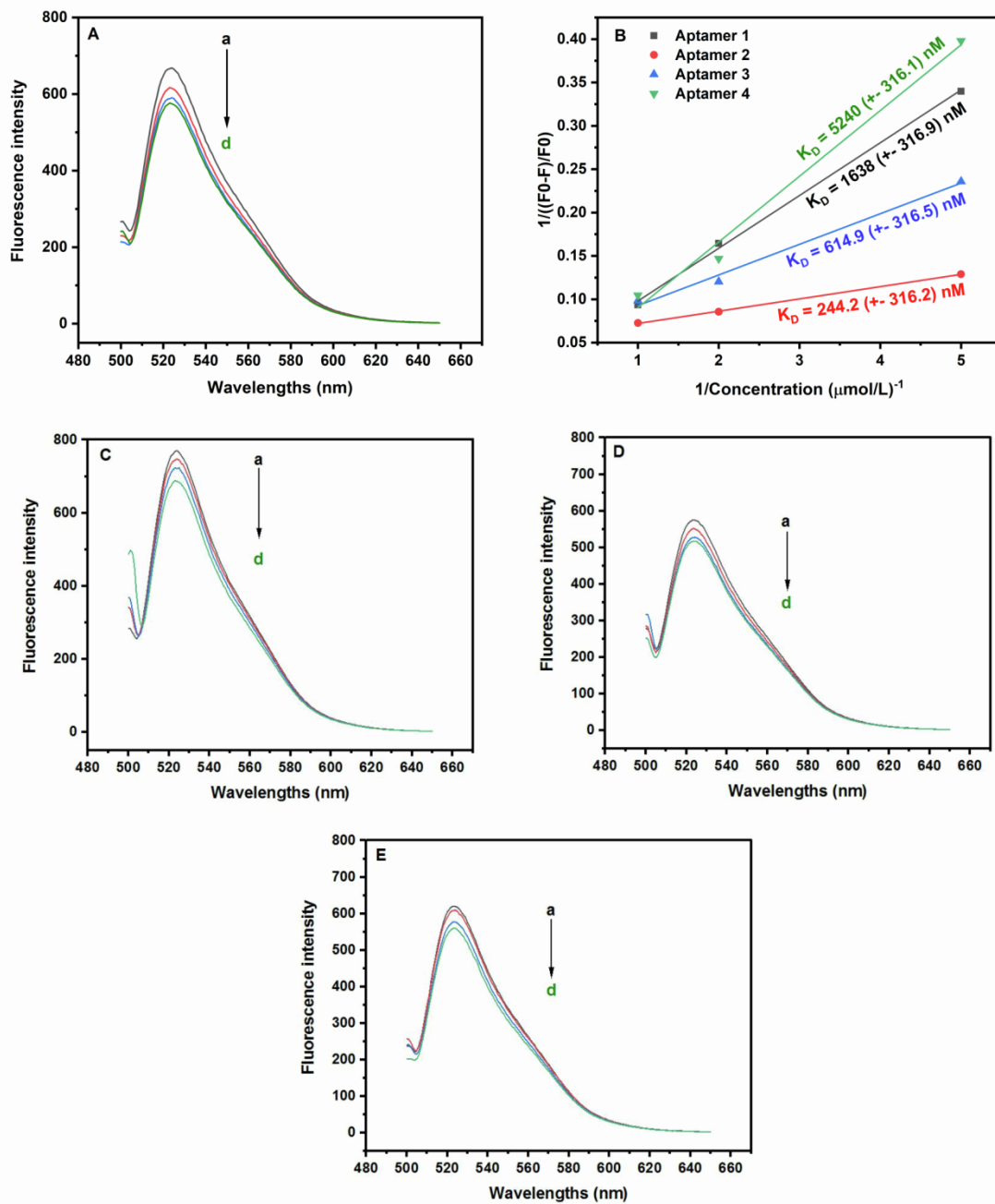
Figure S1. Meth titration (0 µM (a), 0.2 µM (b), 0.5 µM (c) and 1 µM (d)) for the Meth aptamers family. A fluorescence decrease at 520 nm is monitored for (A) Aptamer-2, (C) Aptamer-1, (D) Aptamer-3 and (E) Aptamer-4. (B) Linearization of the Langmuir isotherm for each aptamer.
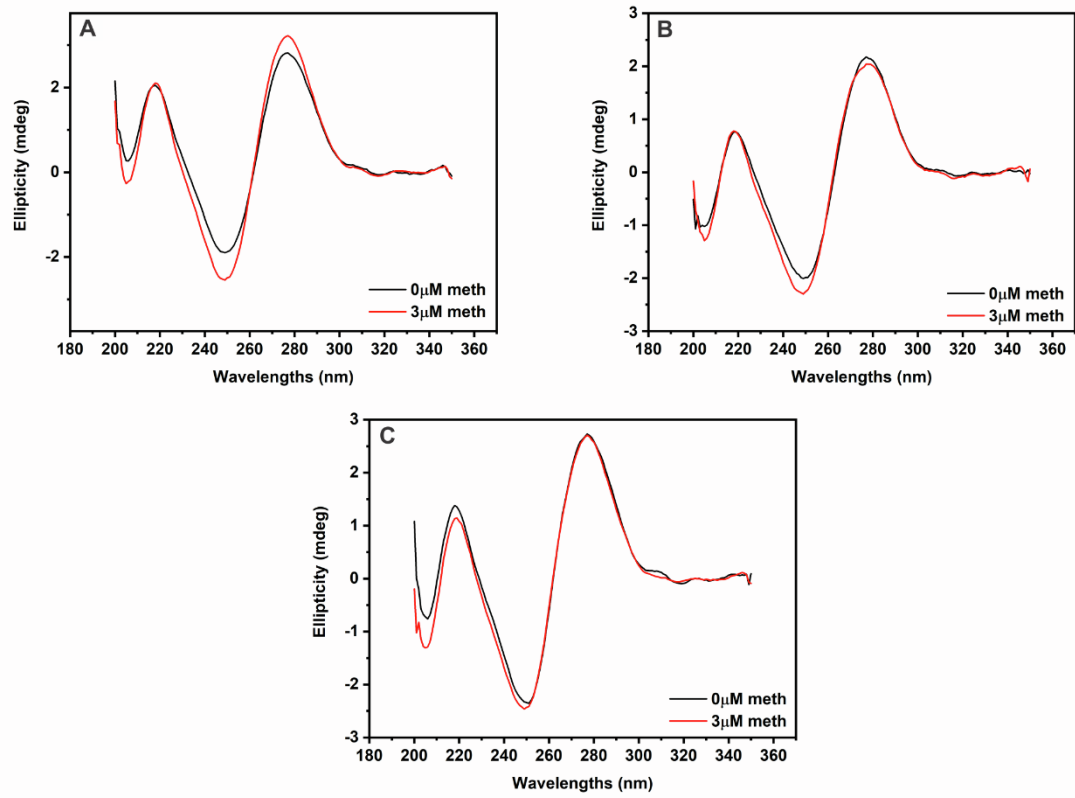
Figure S2. CD experiments for the three other Meth aptamers (A) Aptamer-1, (B) Aptamer-3 and (C) Aptamer-4.
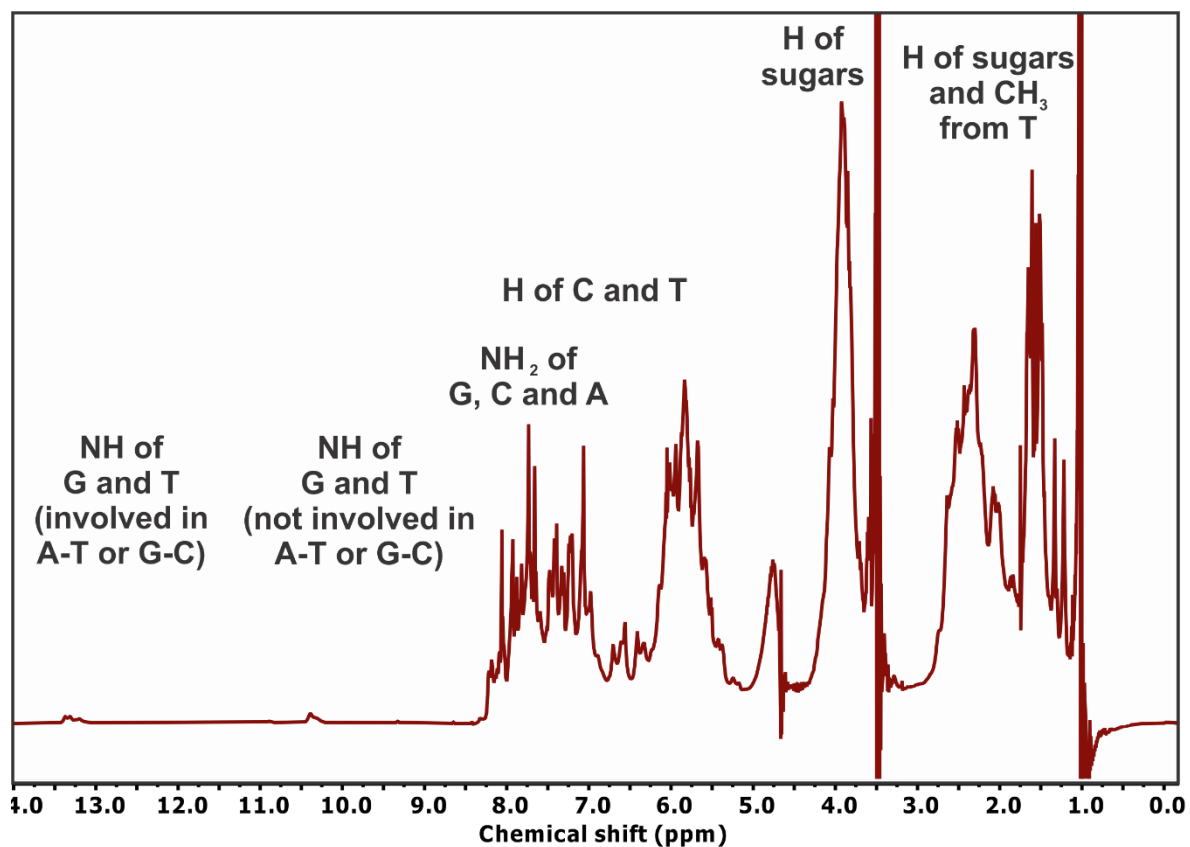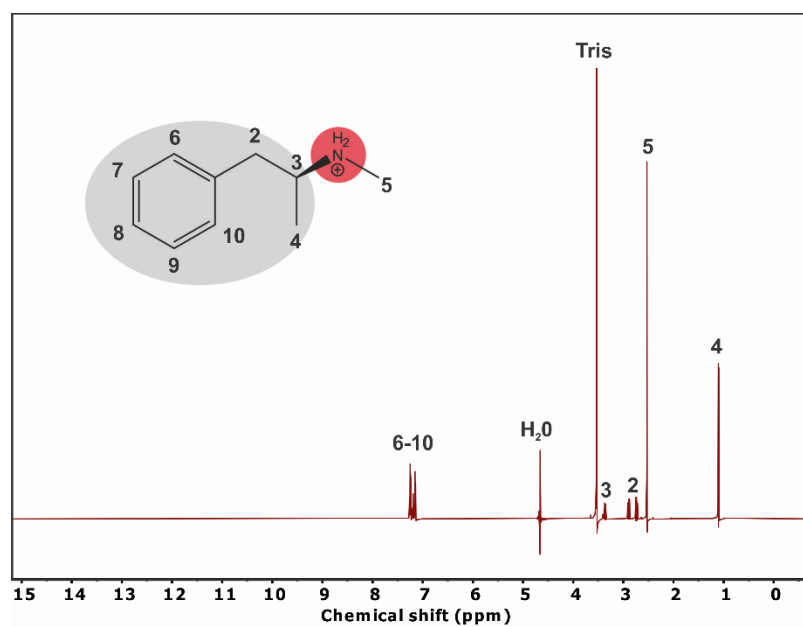
Figure S3. Aptamer-2-40mer ^{1}H-NMR spectrum.
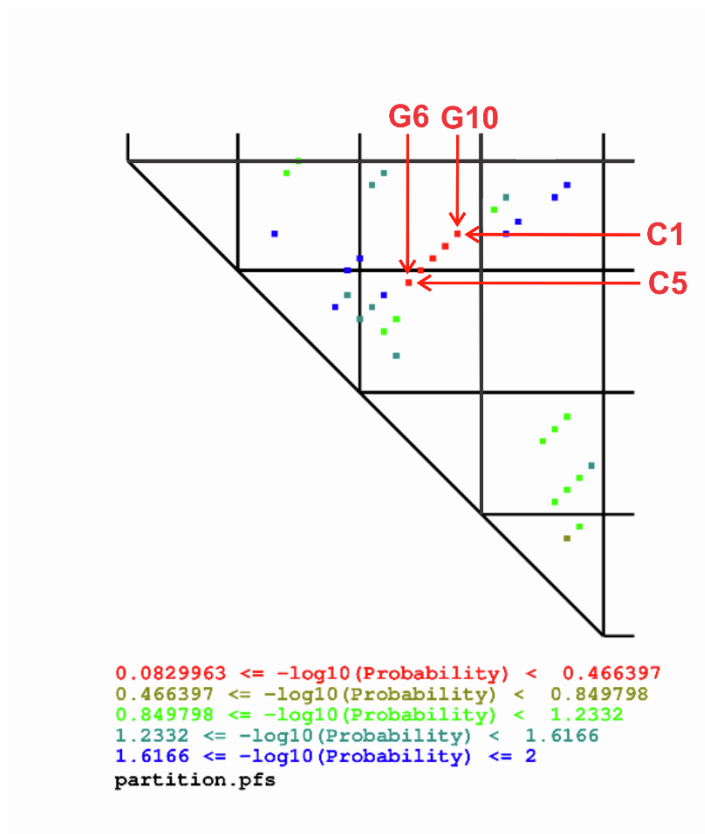

Figure S4. Meth ^{1}H-NMR spectrum.

Figure S5. Partition results for Aptamer-2-40mer obtained from *RNAstructure*.