In *vitro* selection and characterization of a single-stranded DNA aptamer against the herbicide atrazine

Supporting Information

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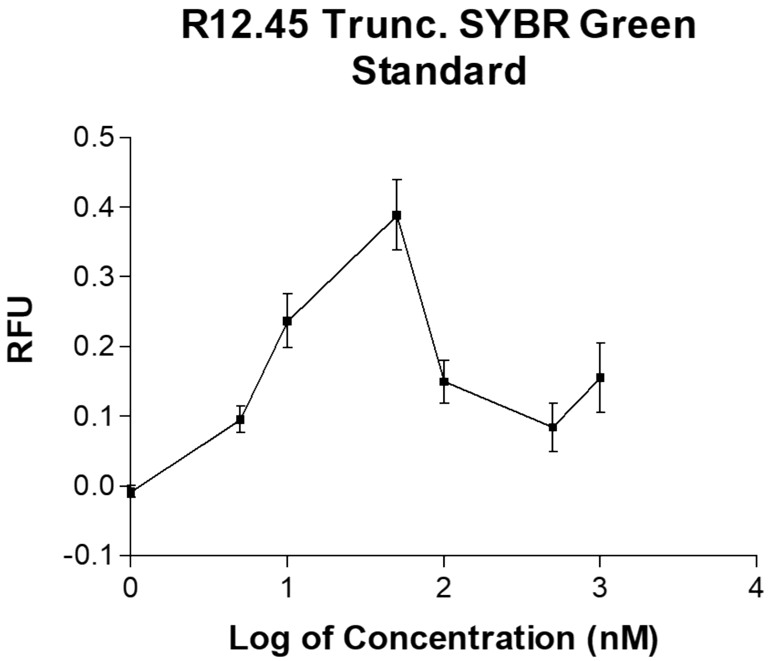
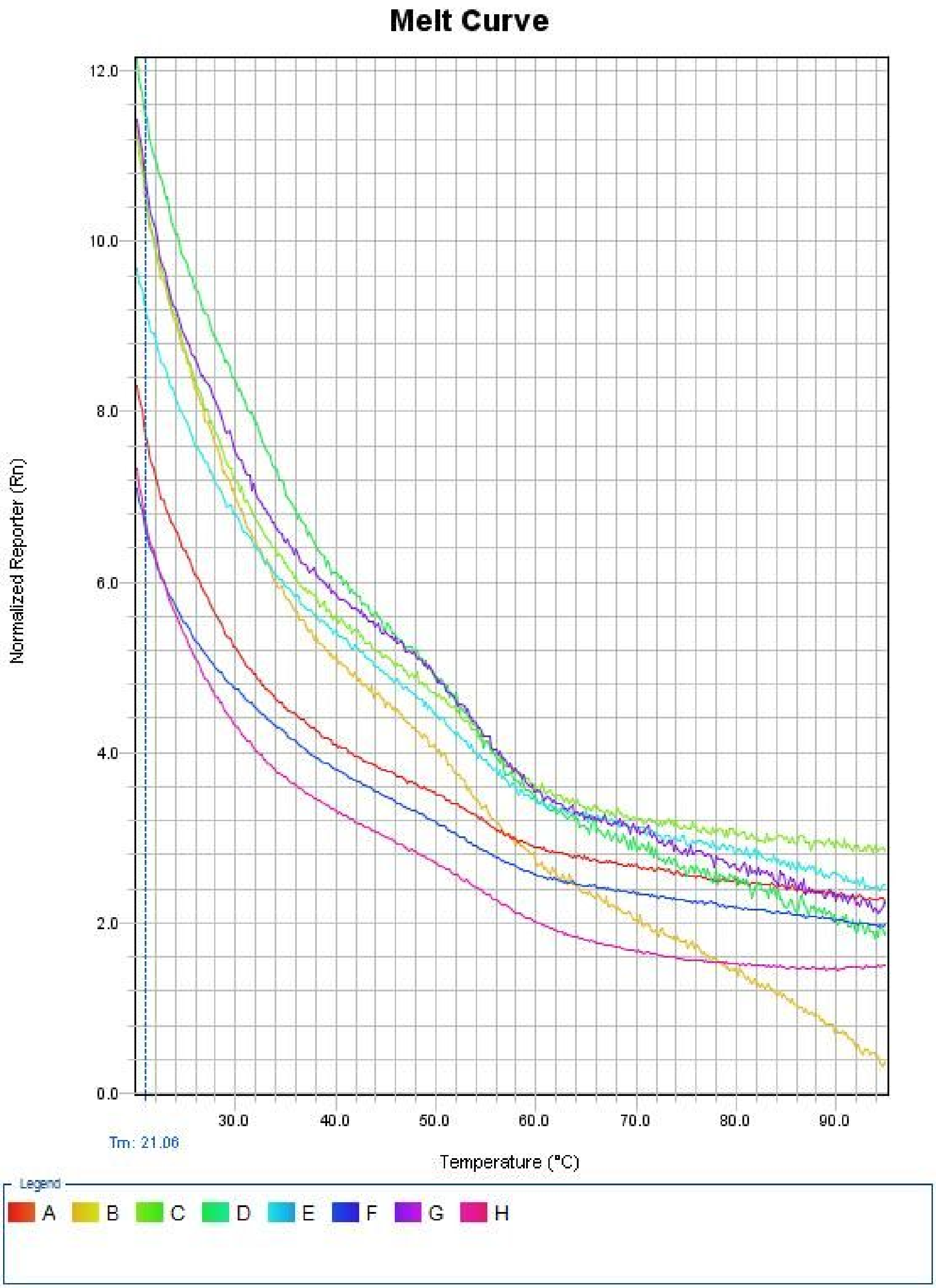
Supporting Table 1. Binding thermodynamic values of ITC experiments

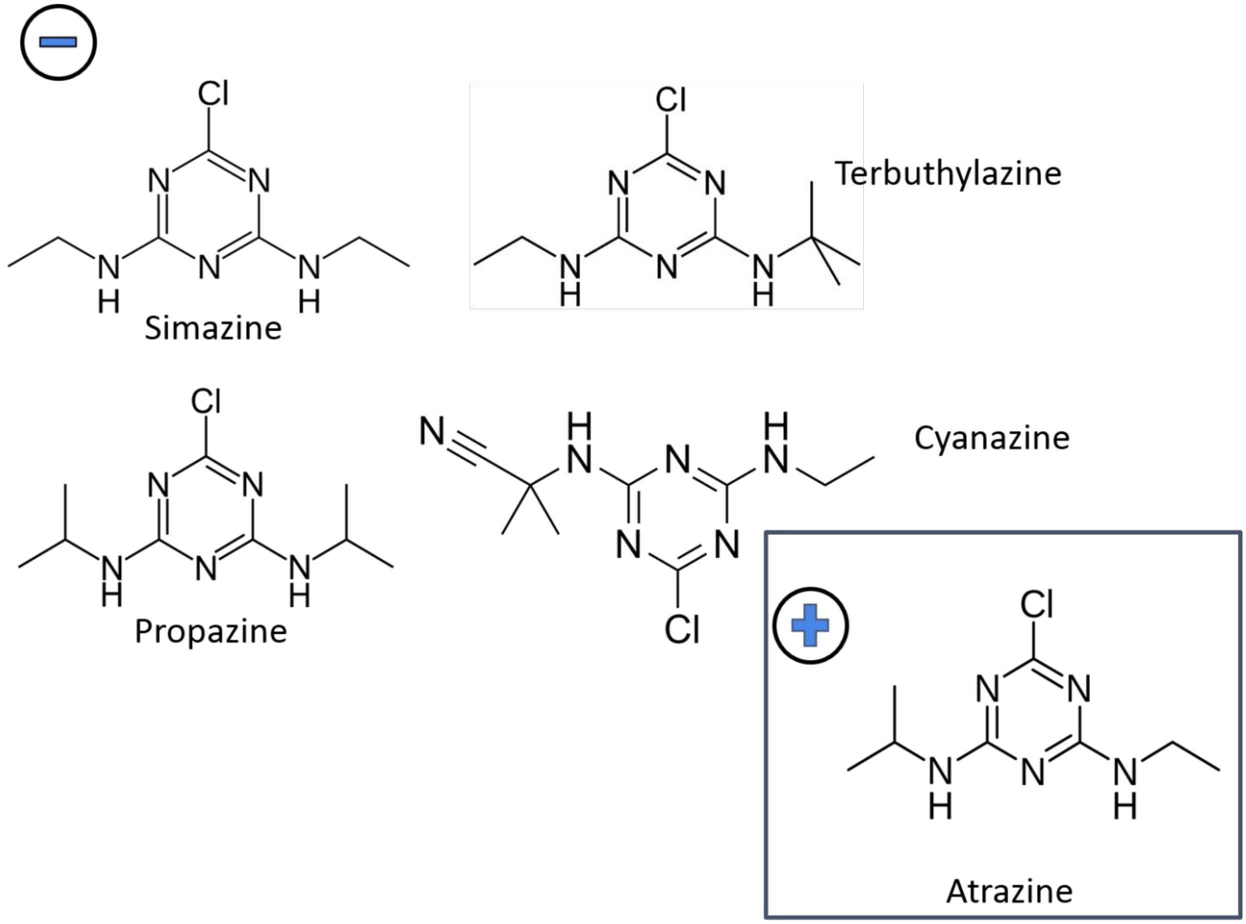
	Aptamer: atrazine molar Ratio = 1:5	Aptamer: atrazine molar Ratio = 1:10
n-value	$6.23 \times 10^{-2} \pm 1.7 \times 10^{-3}$	$3.00 \times 10^{-6} \pm 0.370$
K (M^{-1})	$2.70 \times 10^{8} \pm 0$	$2.60 \times 10^{6} \pm 8.20 \times 10^{6}$
K_d (nM)	3.70	384 ± 121
ΔH (kcal/ mol)	$-2.78 \pm 9.15 \times 10^{-2}$	$-2.69 \times 10^{3} \pm 3.32 \times 10^{9}$
ΔS (cal/ mol/ deg)	29.2	-9.01×10^{4}
c value	162	0.000039



Supporting Figure 1. Representative data from SG standard assay. Atrazine concentrations were: 1 nM, 5 nM, 10 nM, 50 nM, 100 nM, 500 nM, 1000 nM. RFU represents averaged normalized fluorescence responses with respect to plan binding buffer. All values were analyzed with one-way ANOVA: $F_{7, 8} = 14.84$, $p = 0.000529$. Similar upward trend at low concentrations, and downward trends were observed in three independent assays.



Supporting Figure 2. Data from SG standard melting experiment. A: buffer control (0 nM). Varying atrazine concentration were presented in B to H well. B: 1 nM, C: 5 nM, D: 10 nM, E: 50 nM, F: 100 nM, G: 500 nM, H: 1000 nM. Normalized fluorescence signals at low concentrations of atrazine were higher than signals of buffer control.



Supporting Figure 3. Chemical structures of all the herbicides used in the selection scheme. Negative sign denotes negative targets. Positive sign denotes the positive target.

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At-Apt-25    :                         CTACGCTAGCTTGTATGCCCATCTGACCTCTGTGCTGCTA
R12.23 Trunc.:                     TACTGTTTGCACTGGCGGATTTAGCCAGTCAGTG
R12.45 Trunc.: ACCGTCTGAGCGATTCGTACTTTATTCGGGAAGGGTATCAGCGGGG
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Supporting Figure 4. Sequence comparison of different atrazine binding aptamers. Only the variable region of At-Apt-25 was shown. A truncated R12.23 (34-mer) responsible for the primary stem-loop structure was shown. Highlighted regions represented sequence similarity between R12. 45 Trunc. and R12. 23 Trunc. Underlined regions represented sequence similarity between At-Apt-25, R12.23 Trunc. and R12.45 Trunc.