

## Supplementary Information

### Preferential targeting cancer-related i-motif DNAs by the plant flavonol fisetin for theranostics applications

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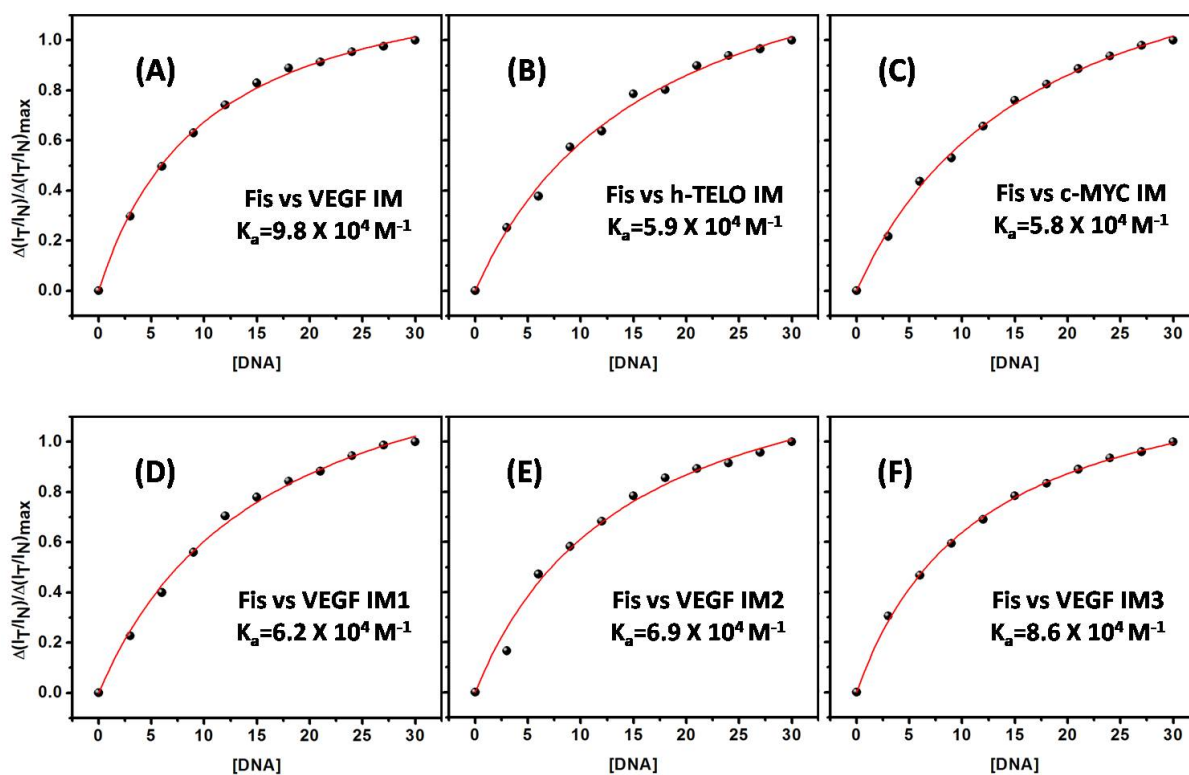
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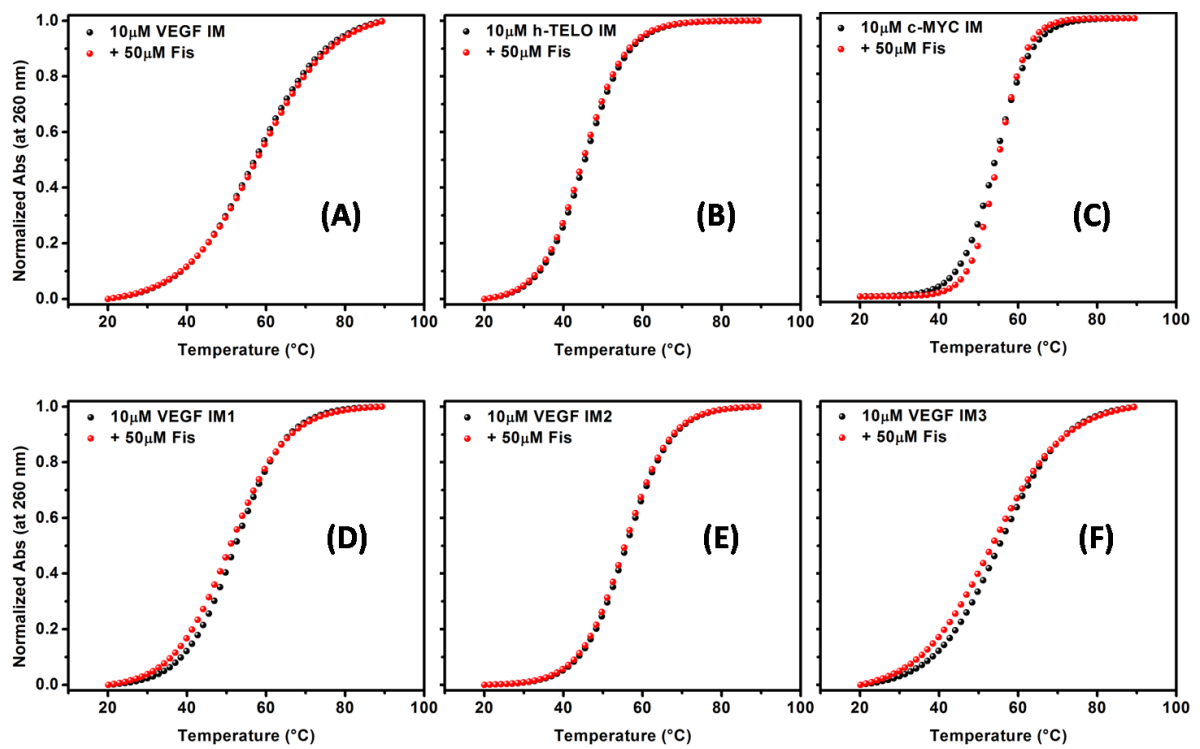
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**Figure S1:**



**Figure S1:** Binding isotherm plots to determine the affinity binding constant ( $K_a$ ) from fluorescence titration experiment.

**Figure S2:**



**Figure S2:** UV melting curves of different i-motif DNA (10 μM) structures in the absence and presence (50 μM) of Fis.

Figure S3:

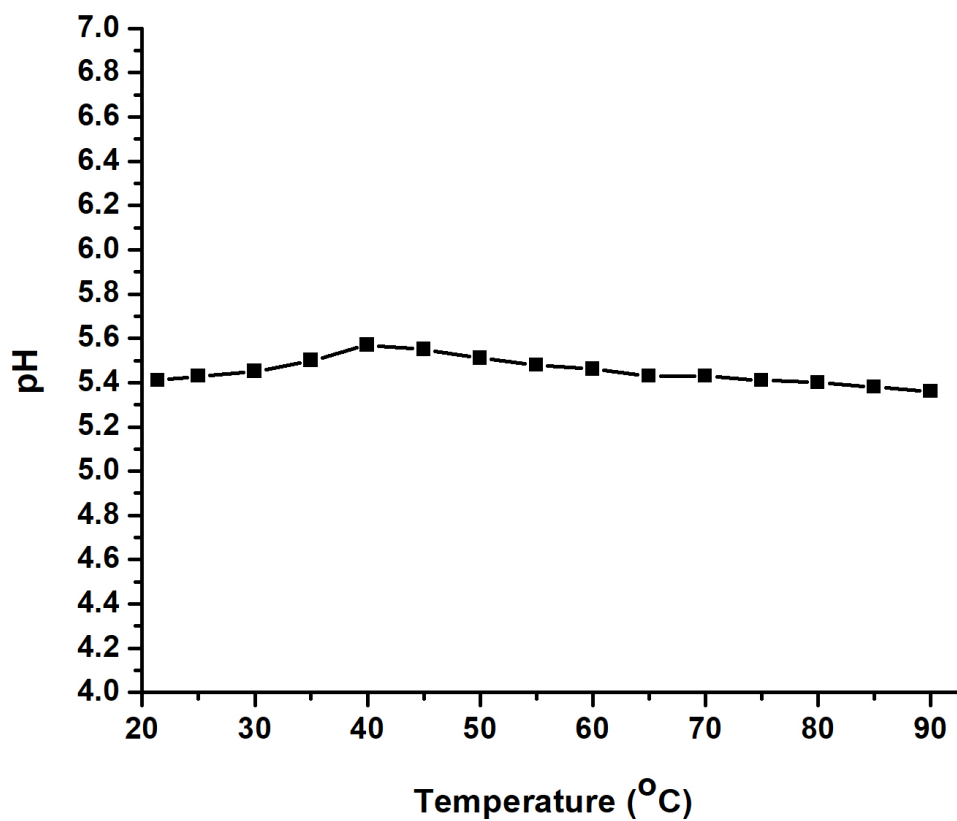
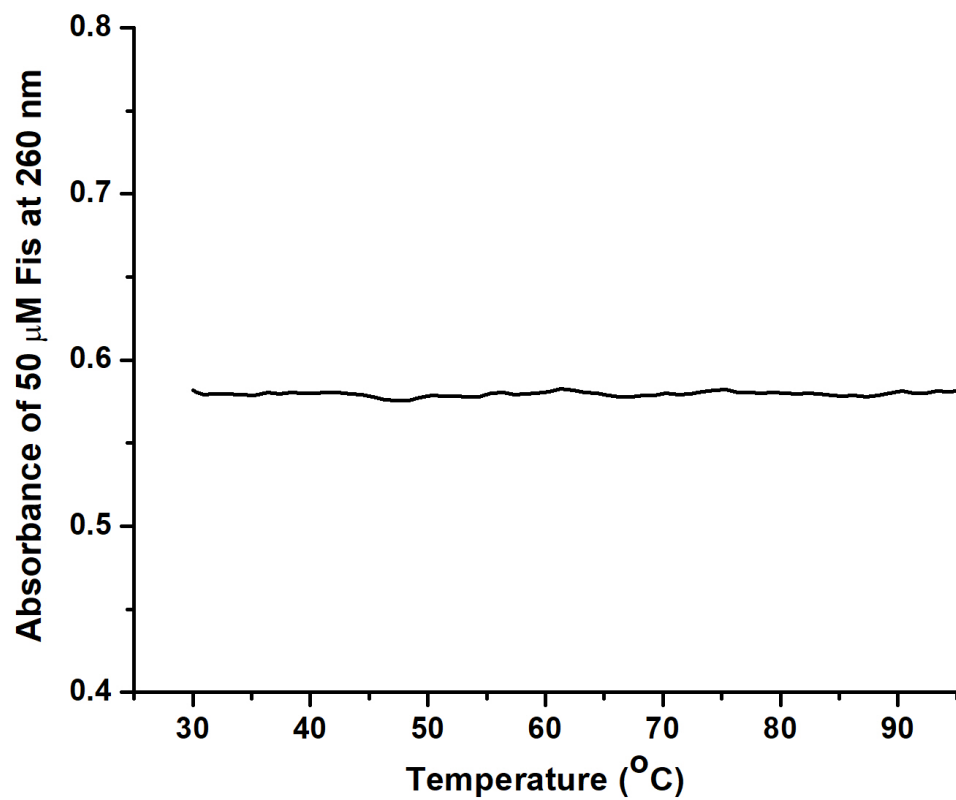


Figure S3: Monitoring the pH change of phosphate buffer (50 mM KCl, 10 mM  $\text{KH}_2\text{PO}_4$ , and 1 mM  $\text{K}_2\text{EDTA}$ ; pH 5.4) over the temperature range 20 to 90°C.

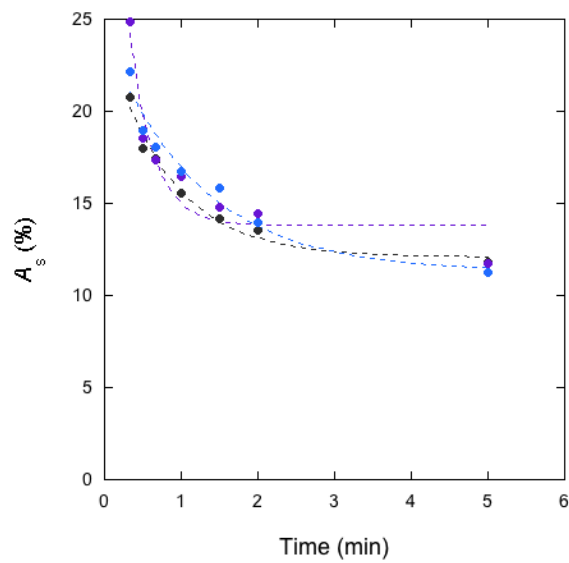
Figure S4:



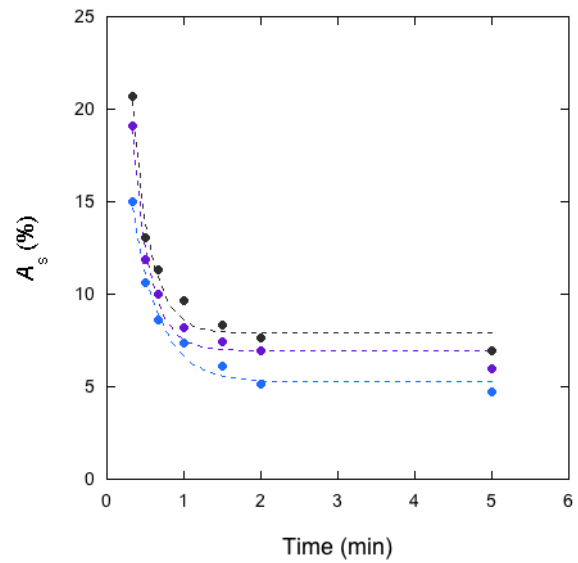
**Figure S4:** Monitoring the absorbance of Fis (50 μM) at 260 nm in phosphate buffer (50 mM KCl, 10 mM KH<sub>2</sub>PO<sub>4</sub>, and 1 mM K<sub>2</sub>EDTA; pH 5.4) over the temperature range.

Figure S5:

(A)

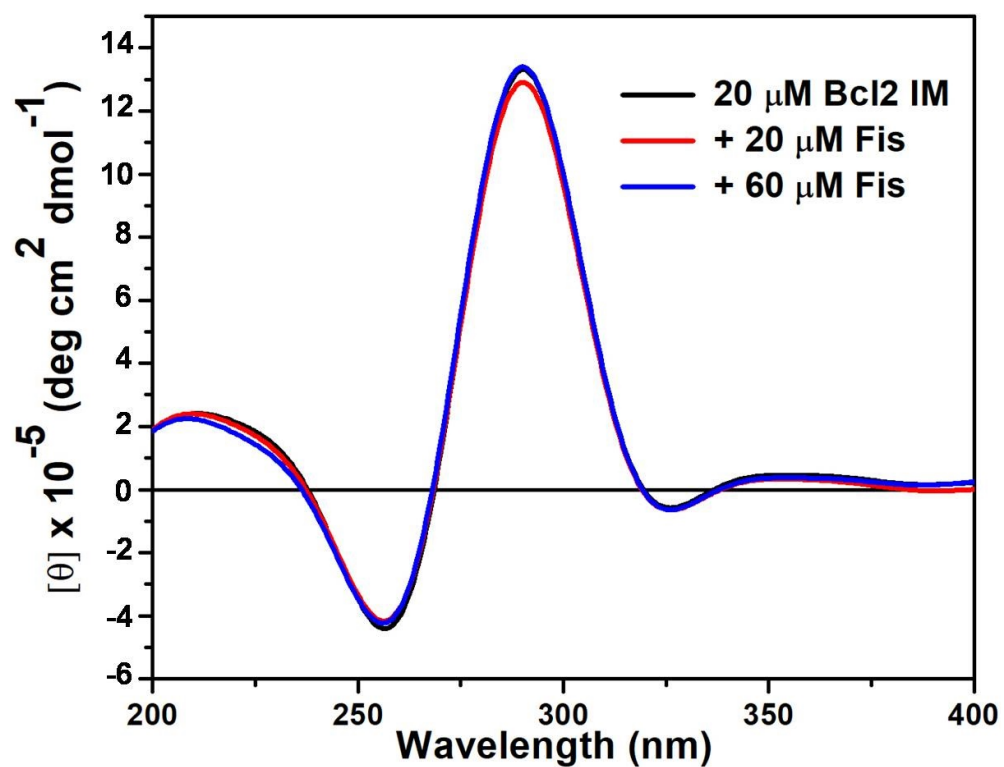


(B)



**Figure S5:** Analyses of resolving of stalled product in reactions of VEGF IM (A) in the absence of Fis and (B) presence of 100  $\mu\text{M}$  Fis. All the plots were from three independent assays. The dotted lines indicate each fitting curve. All the replication assays were carried in 40 mM MES (pH 6.0), 50 mM KCl, 8 mM  $\text{MgCl}_2$ , 1  $\mu\text{M}$  KF exo-, 1  $\mu\text{M}$  DNAs, and 250  $\mu\text{M}$  dNTPs at 37°C.

Figure S6:



**Figure S6:** CD spectra of Bcl2 IM DNA in the absence (black spectrum) and presence of different concentrations of Fis. All the experiments were performed in a buffer consisting of 50 mM KCl, 10 mM  $\text{KH}_2\text{PO}_4$ , and 1 mM  $\text{K}_2\text{EDTA}$  (pH 5.4) at 25°C.