

**Quantitative and Qualitative analysis of Ochratoxin-A using Fluorescent  
CQDs @ DNA-based Nanoarchitecture Assembly to Monitor the Food Safety  
and Quality**

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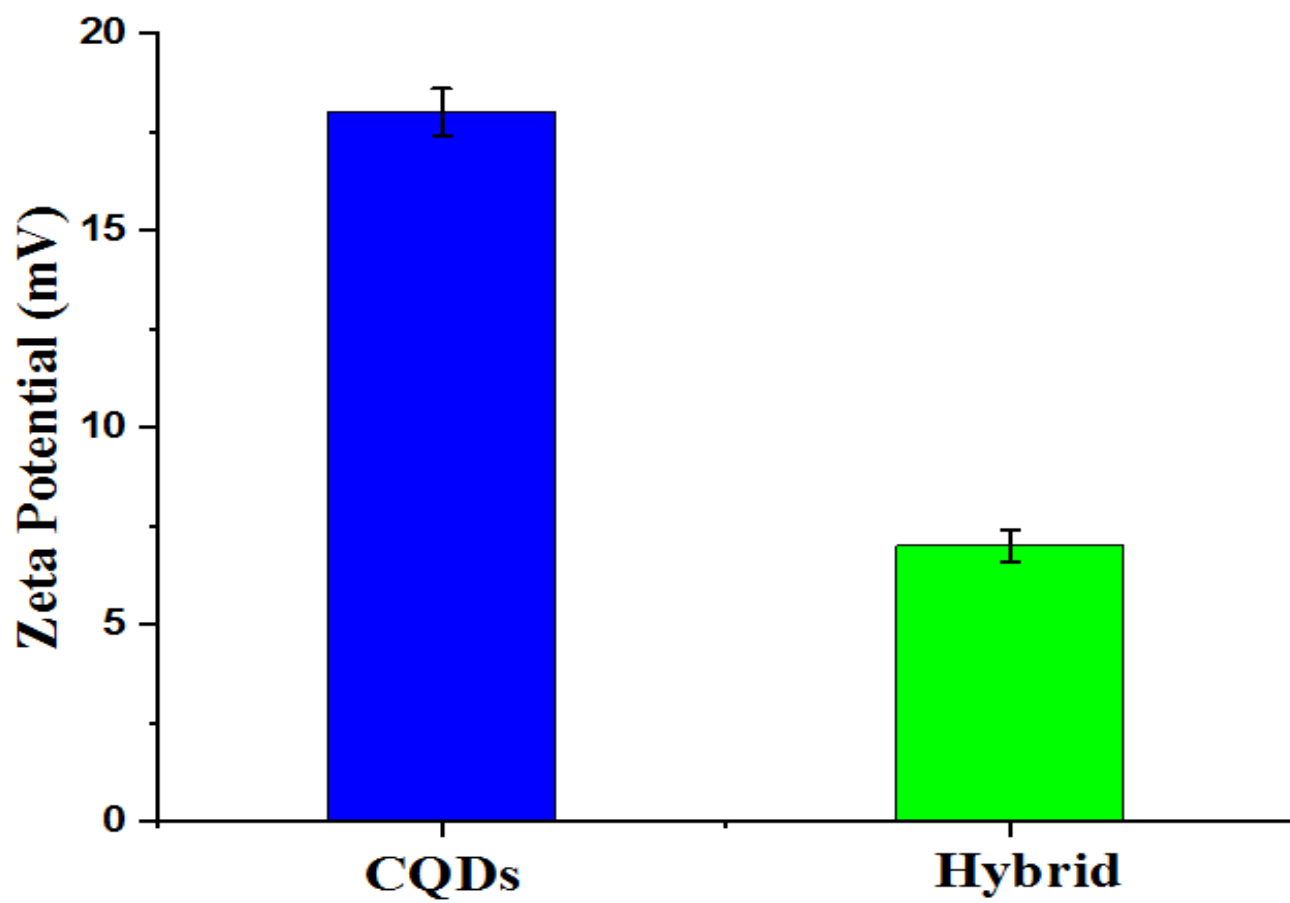
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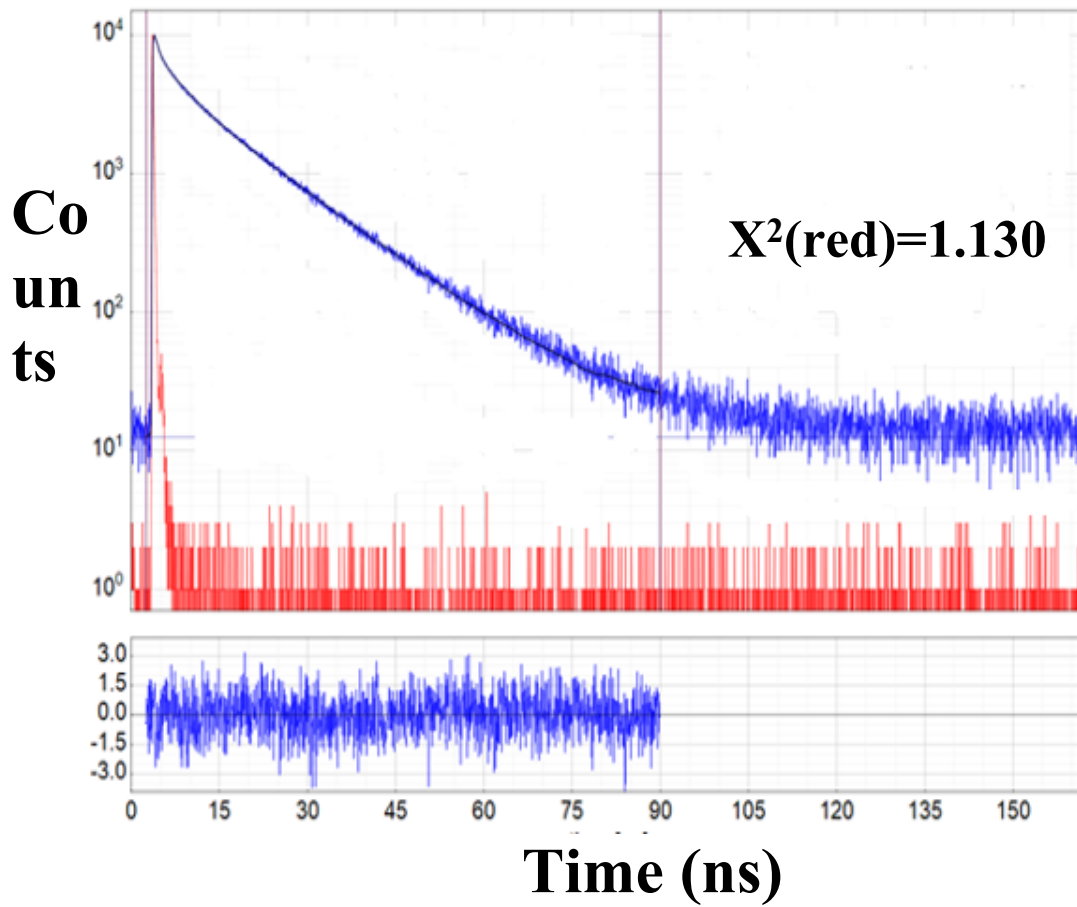
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# Supporting Information

<b>Figure No.</b>	<b>Description</b>
<b>S1</b>	Zeta potential of synthesized CQDs and Hybrid assembly.
<b>S2</b>	Time resolved fluorescence spectrum of CQDs.
<b>S3</b>	Linear regression analysis for interaction of CQDs with DNA.
<b>S4</b>	BH plot for CQD-DNA interaction (Fluorescence).
<b>S5</b>	UV-Visible absorption spectrum of CQDs on addition of DNA (0-10 $\mu$ M).
<b>S6</b>	UV-Visible absorption spectrum of CQDs alone and in the presence of OTA.
<b>S7</b>	UV-Visible absorption spectrum of DNA alone and in the presence of OTA.
<b>S8</b>	Interaction of OTA with CQDs alone.
<b>S9</b>	Competitive binding studies of CQDs@DNA-based nanoarchitecture assembly containing OTA over other selected Toxins and pesticides.
<b>S10</b>	Time dependent recognition studies of OTA with different concentrations
<b>S11</b>	BH plot for Hybrid-OTA interaction (Fluorescence)
<b>S12</b>	FT-IR data of Hybrid assembly.
<b>S13</b>	FT-IR data of Hybrid-OTA
<b>S14</b>	Effect of pH on CQDs@DNA-based nanoarchitecture assembly (hybrid; 1 $\mu$ M) alone and in the presence of OTA in an aqueous system
<b>S15</b>	Stability Studies of hybrid assembly kept at -20 °C w.r.t time.
<b>S16</b>	Stability Studies of hybrid assembly kept at 15 °C w.r.t time.
<b>S17</b>	Stability Studies of hybrid assembly kept at 30-33 °C w.r.t time.
<b>S18</b>	FT-IR data of DNA.
<b>S19</b>	A) HRTEM images of CQDs-DNA hybrid; B) HRTEM image of CQDs-DNA hybrid after addition of OTA.
<b>S20</b>	Fluorescence intensity change of CQDs on addition of DNA; Fluorescence intensity change of hybrid on addition of OTA (under UV light 255 nm).
<b>S21</b>	Fluorescence spectrum of OTA (10 $\mu$ M solution).



**Figure S1:** Zeta potential of synthesized CQDs and Hybrid assembly.



**Figure S2:** Time resolved fluorescence spectrum of CQDs.

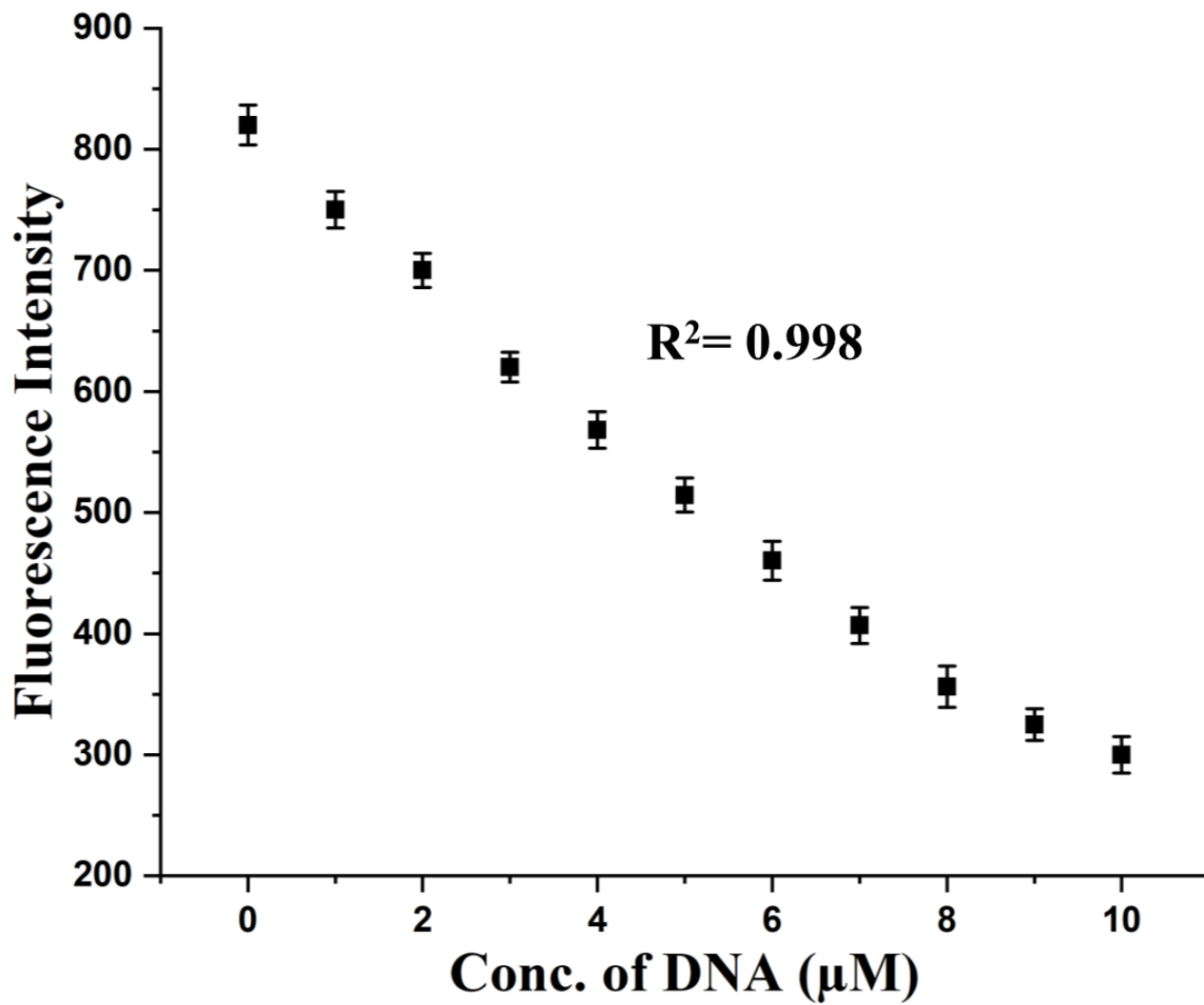
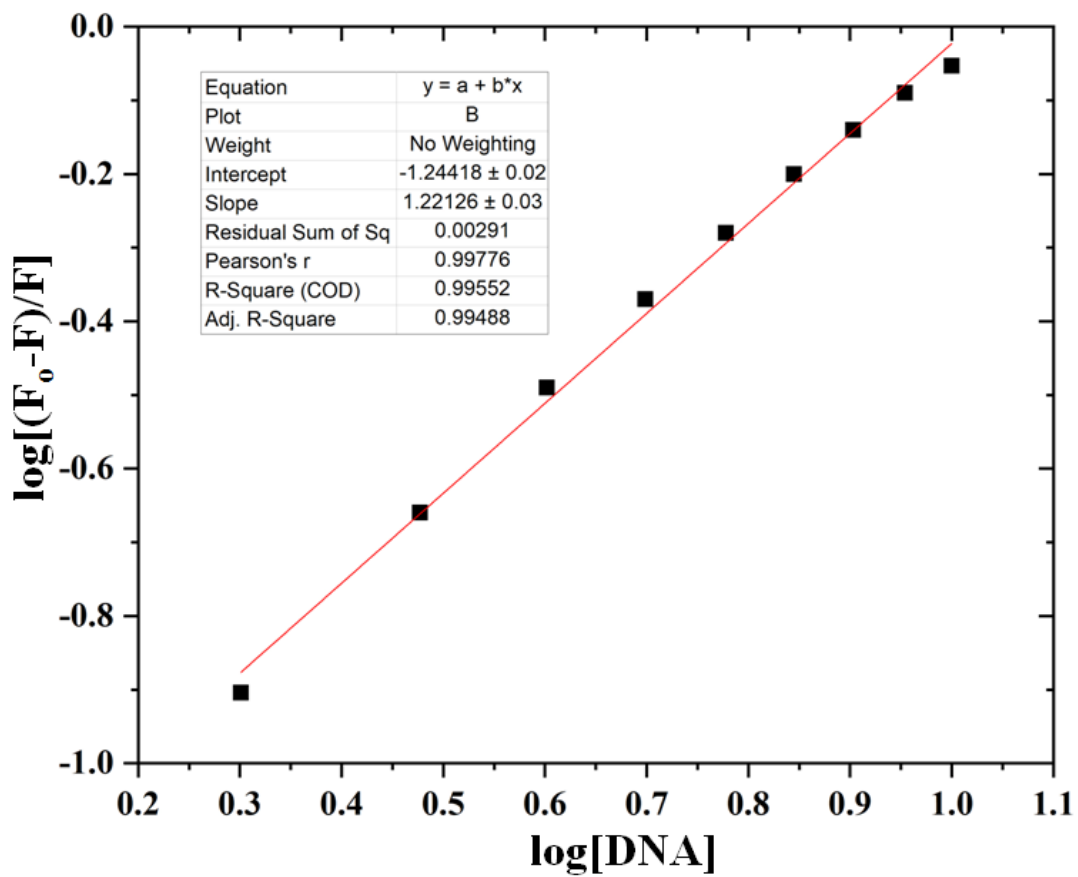
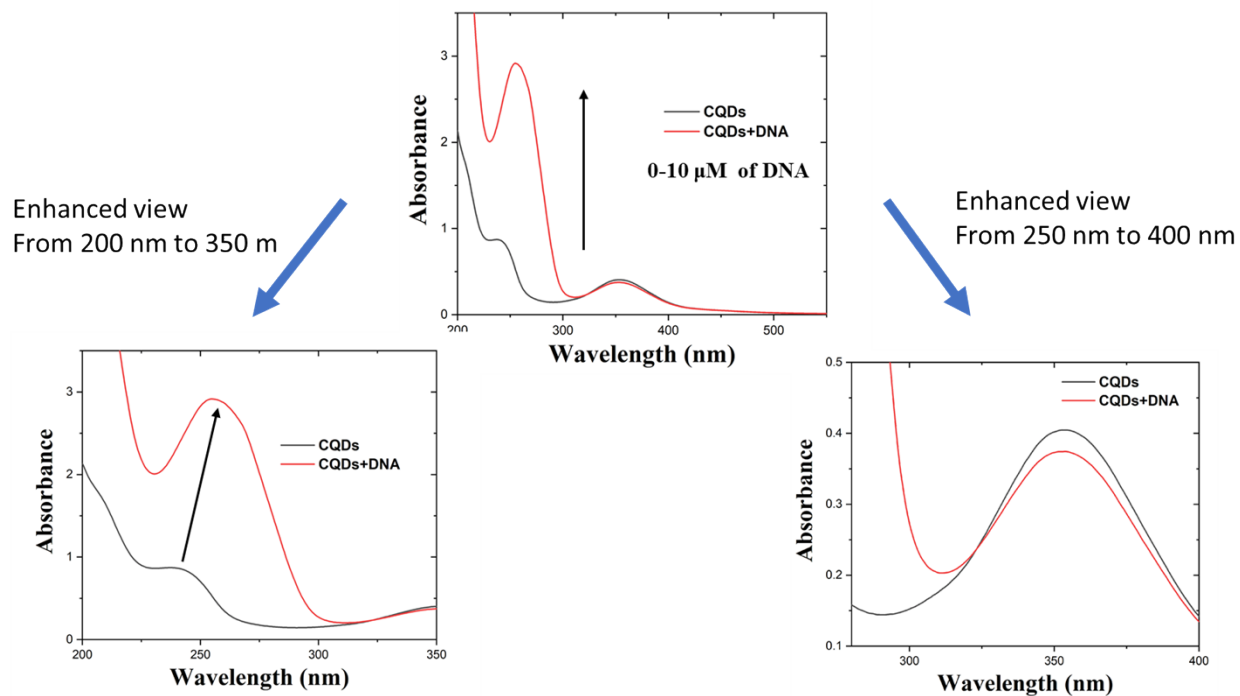


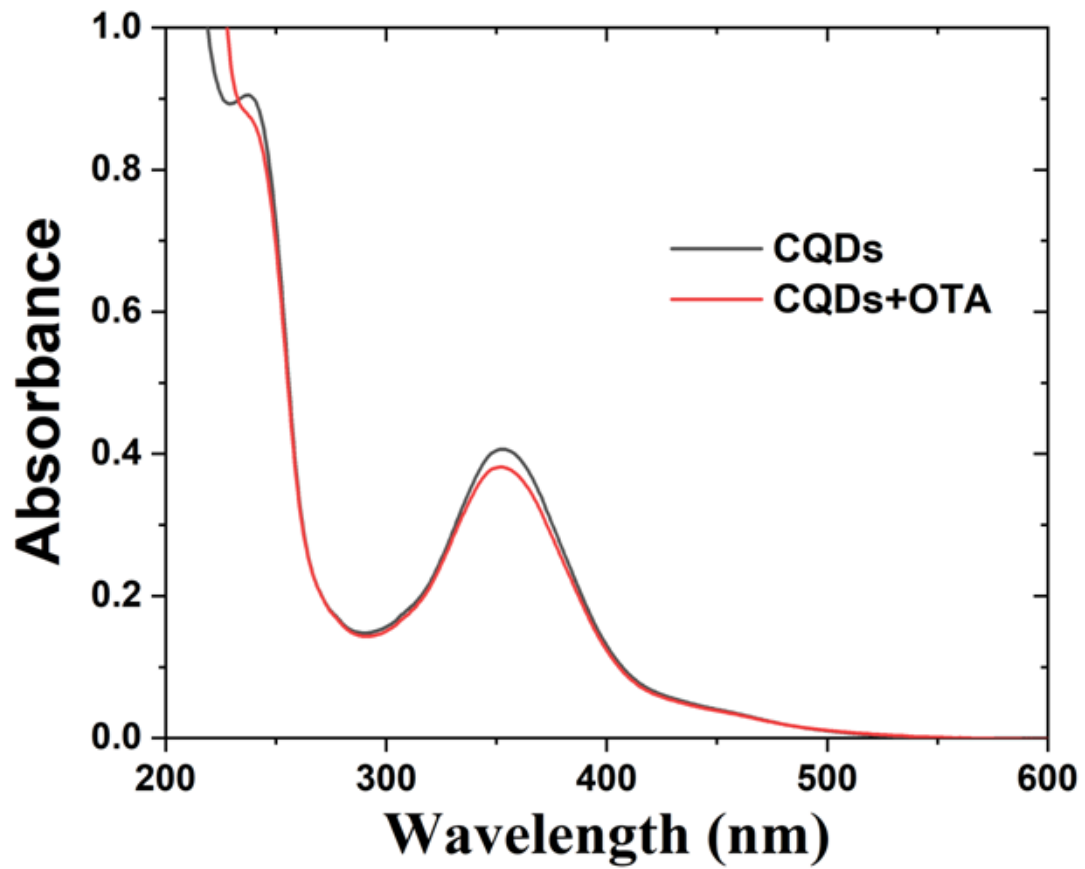
Figure S3: Linear regression analysis for interaction of CQDs with (0-10 µM) solution DNA.



**Figure S4:** Benesi–Hildebrand plot for CQD-DNA interaction (Fluorescence).

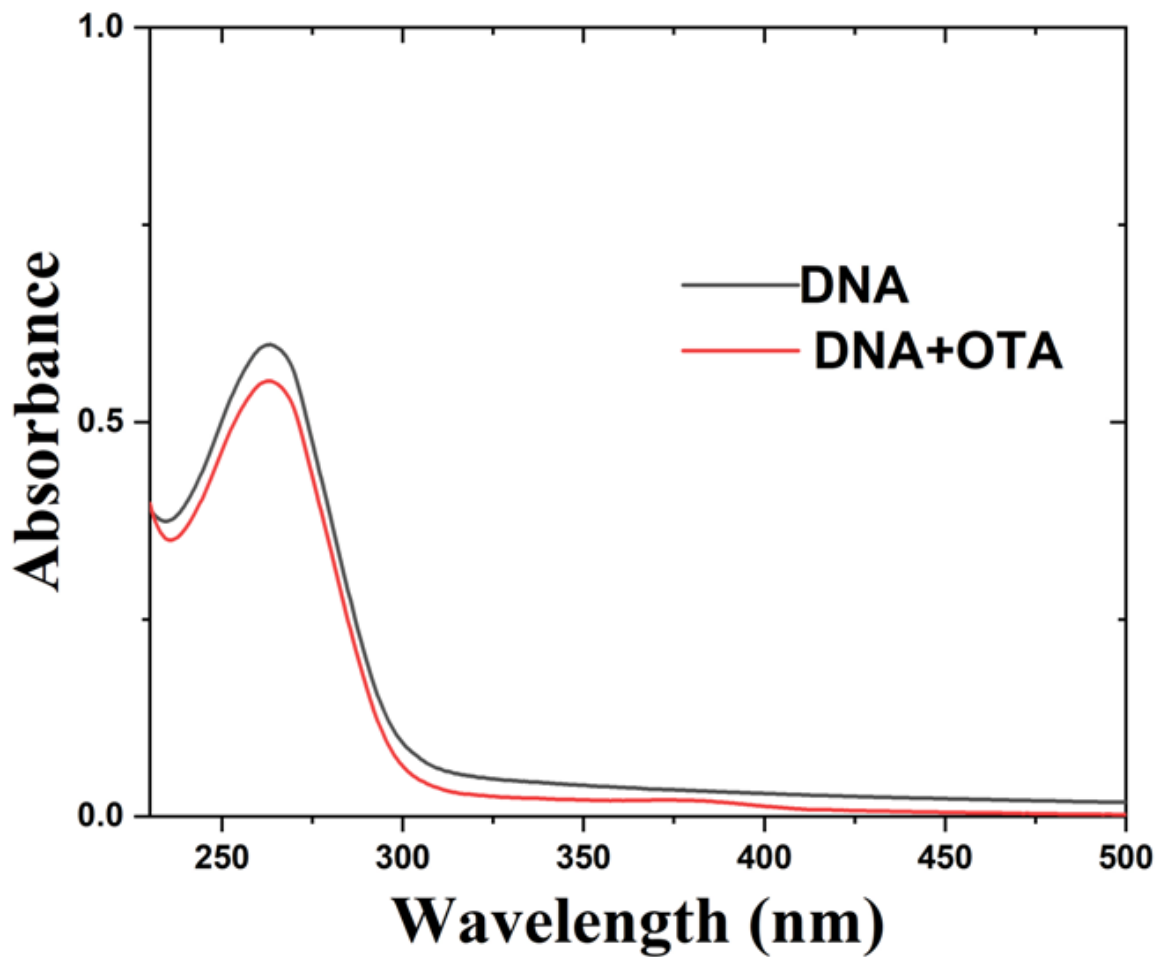


**Figure S5:** UV-Visible absorption spectrum of CQDs on addition of DNA (0-10  $\mu$ M).

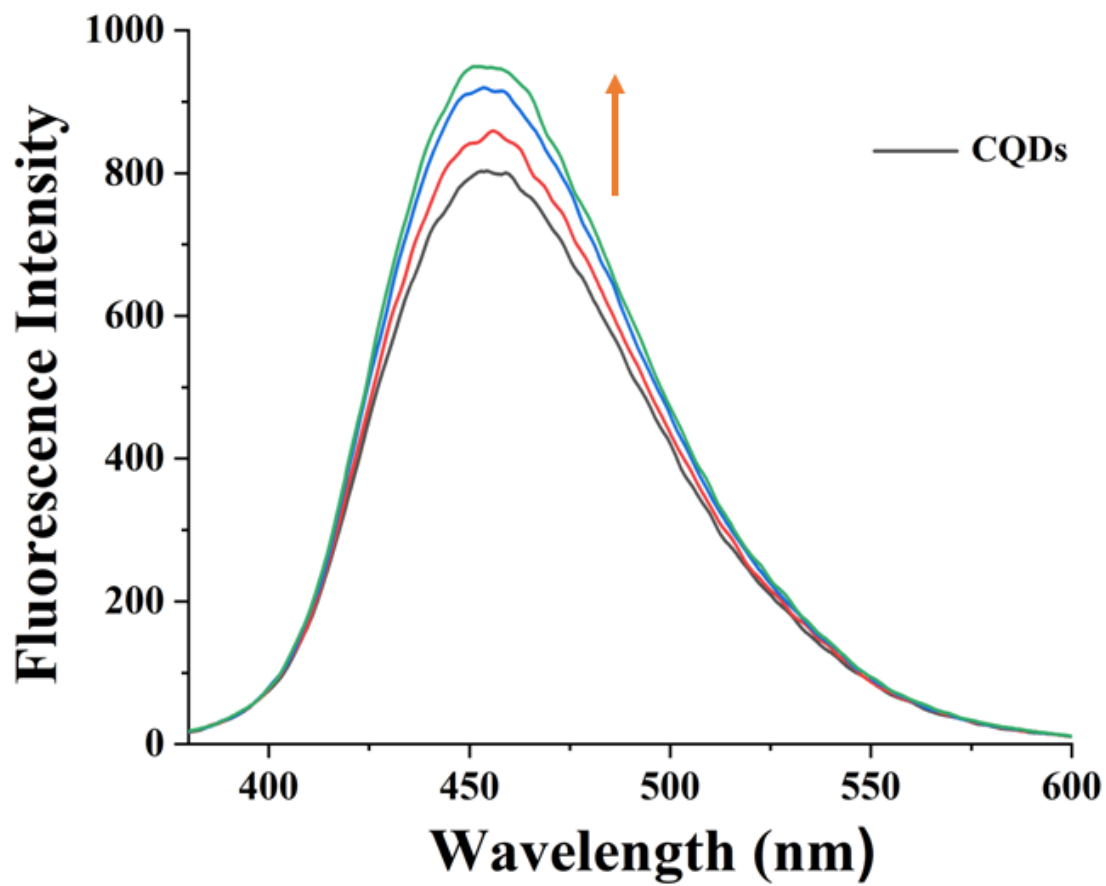


**Figure S6:** UV-Visible absorption spectrum of CQDs alone and in the presence of 10  $\mu\text{M}$  solution of OTA





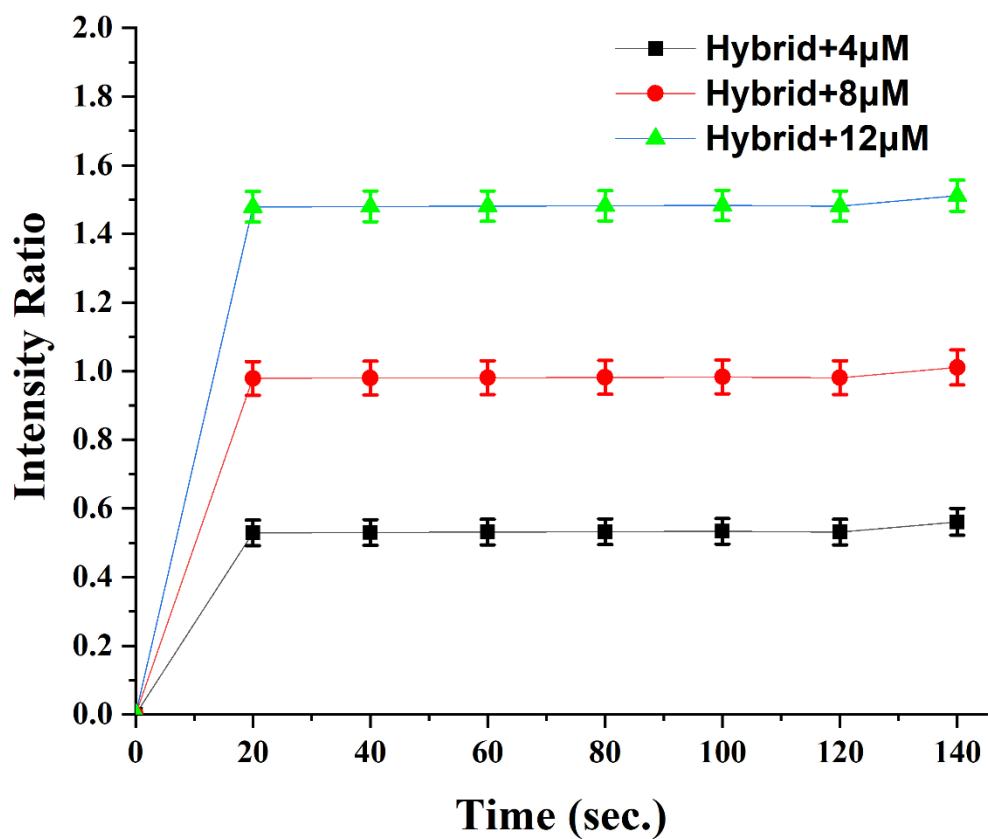
**Figure S7:** UV-Visible absorption spectrum of DNA alone and in the presence of OTA (50  $\mu$ L of 1mM solution)



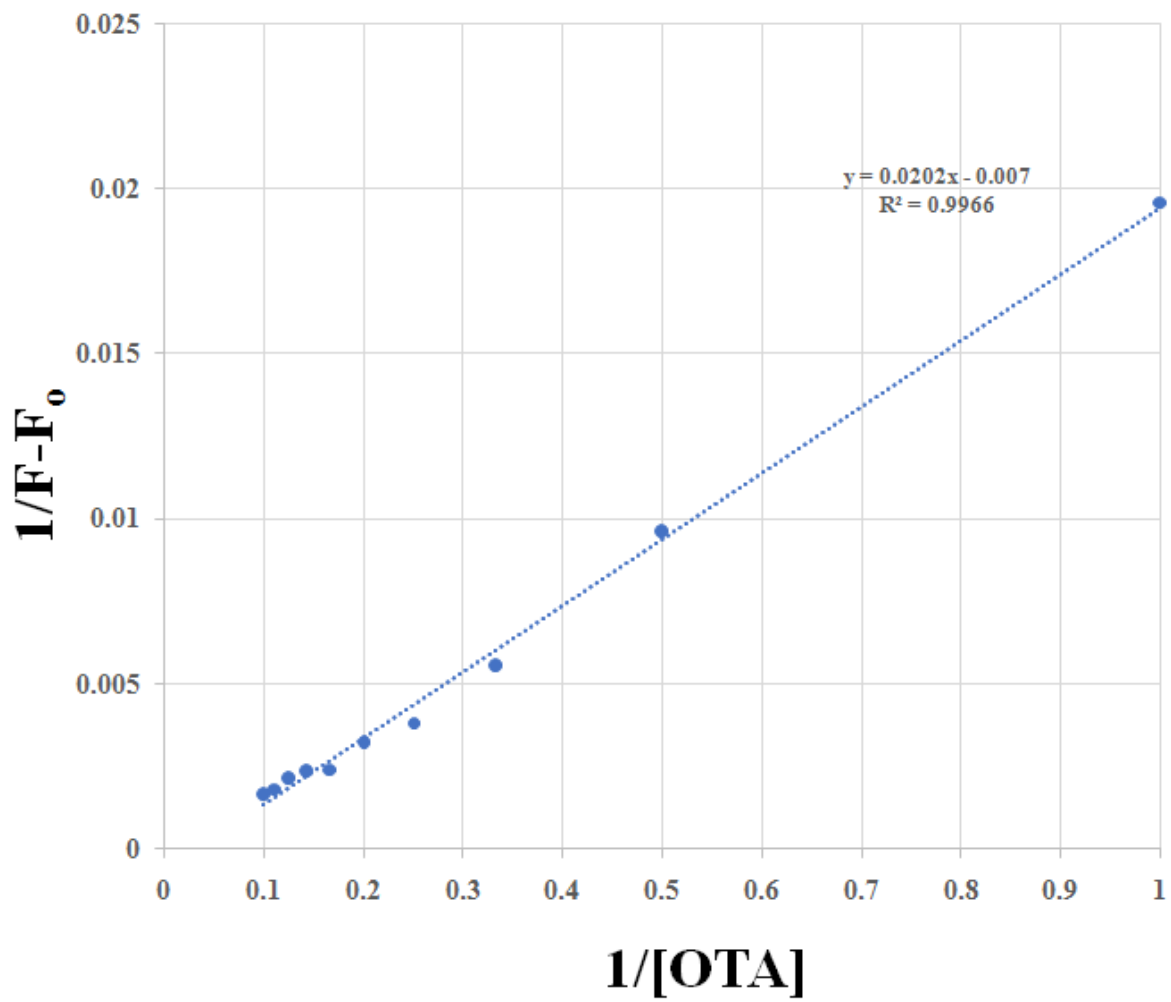
**Figure S8:** Interaction of OTA (0-50  $\mu\text{L}$  of 1mM solution) with CQDs alone.



**Figure S9:** Competitive binding studies of CQDs@DNA-based nanoarchitecture assembly containing OTA over other selected Toxins and pesticides (1mM) (in triplicate).



**Figure S10:** Time dependent recognition studies of OTA with different concentrations (4 μM, 8 μM, 12 μM) (in triplicate).



**Figure S11:** BH plot for Hybrid-OTA interaction (Fluorescence).

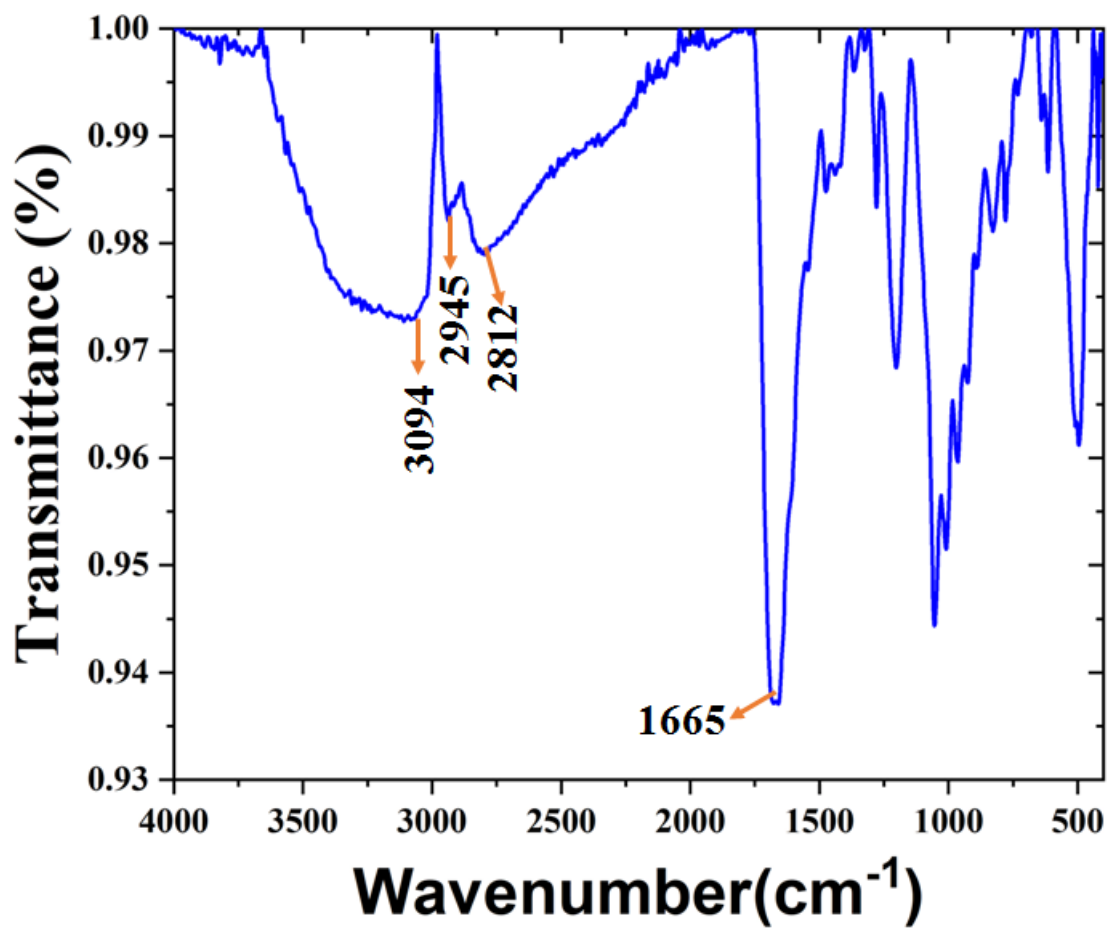


Figure S12: FT-IR data of Hybrid assembly.

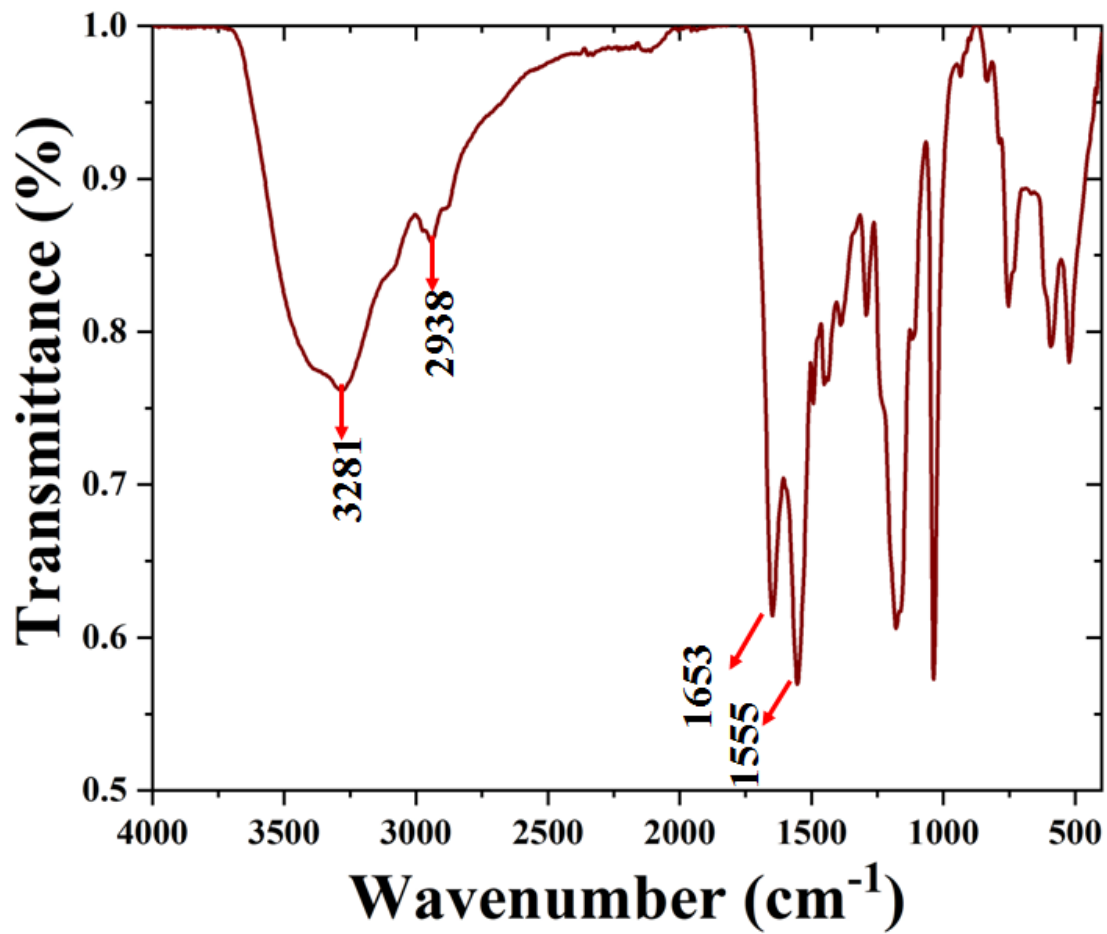
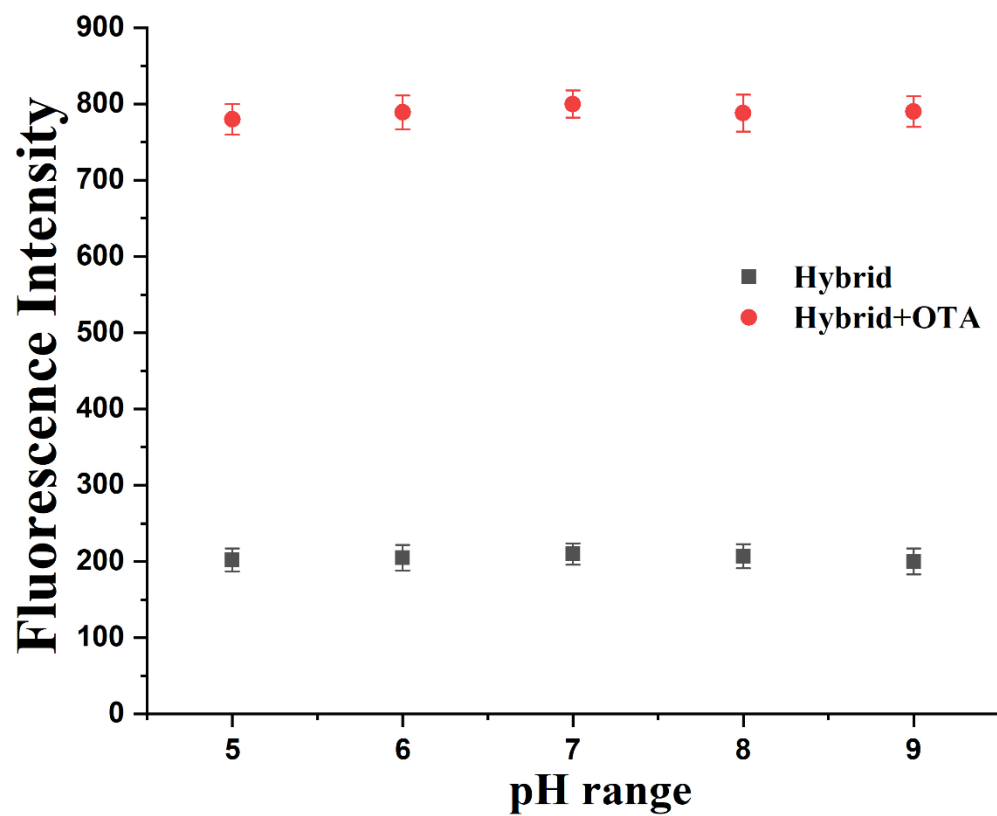
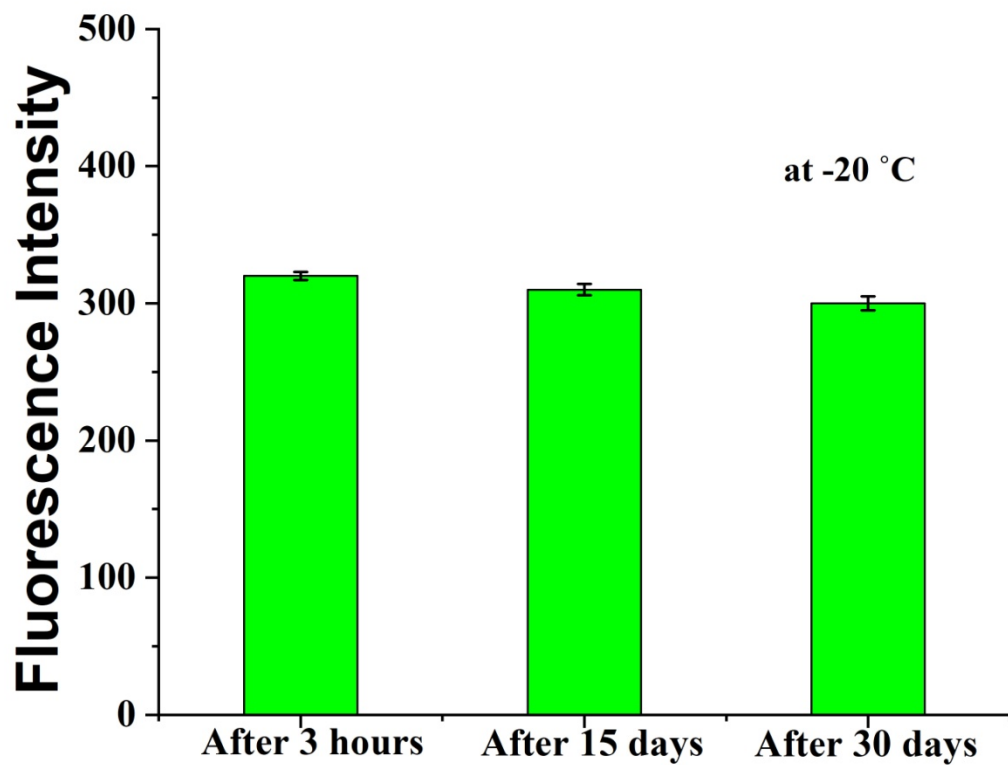


Figure S13: FT-IR data of Hybrid-OTA

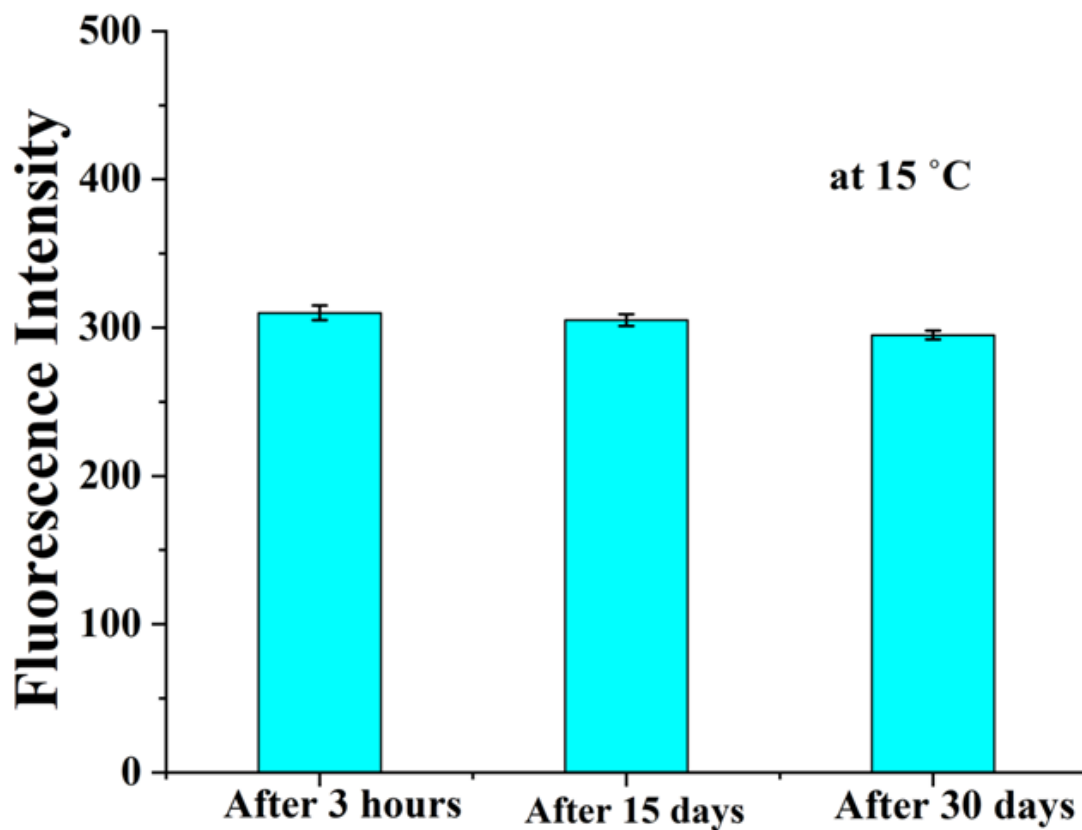


**Figure S14:** Effect of pH on CQDs@DNA-based nanoarchitecture assembly (hybrid) alone and in the presence of 10  $\mu\text{M}$  OTA in an aqueous system (in triplicate).

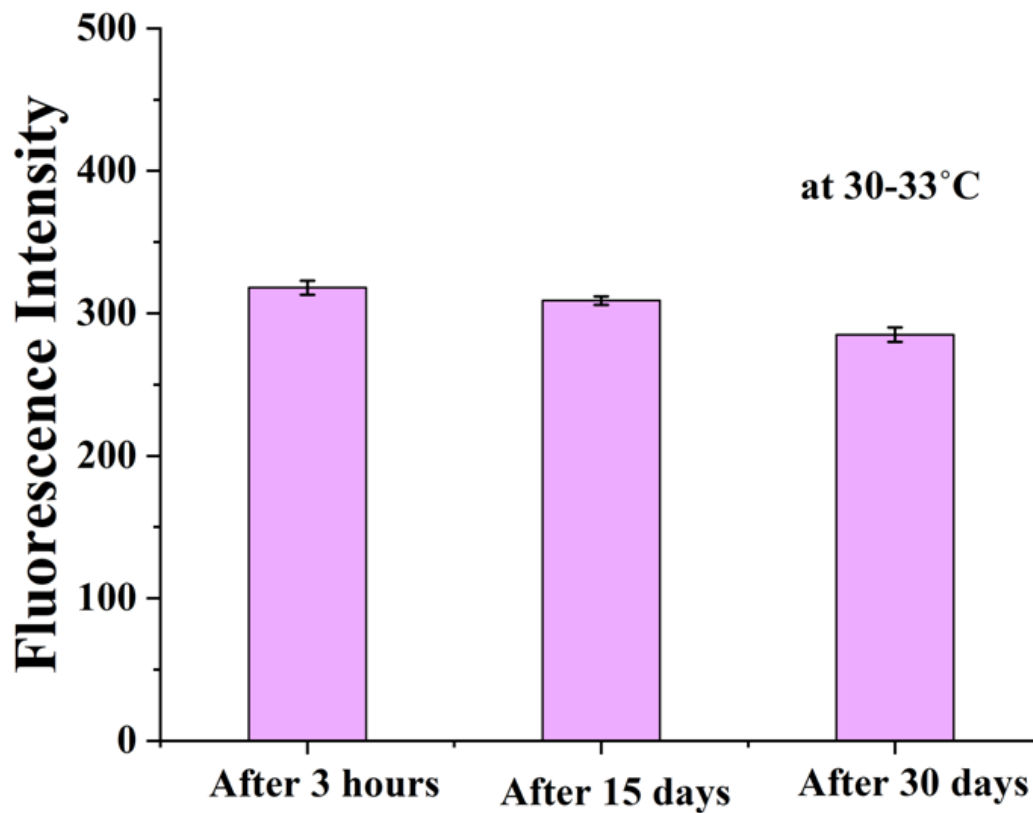




**Figure S15:** Stability Studies of hybrid assembly kept at -20 °C w.r.t time (in triplicate).



**Figure S16:** Stability Studies of hybrid assembly kept at 15 °C w.r.t time (in triplicate).



**Figure S17:** Stability Studies of hybrid assembly kept at 30-33 °C w.r.t time (in triplicate).

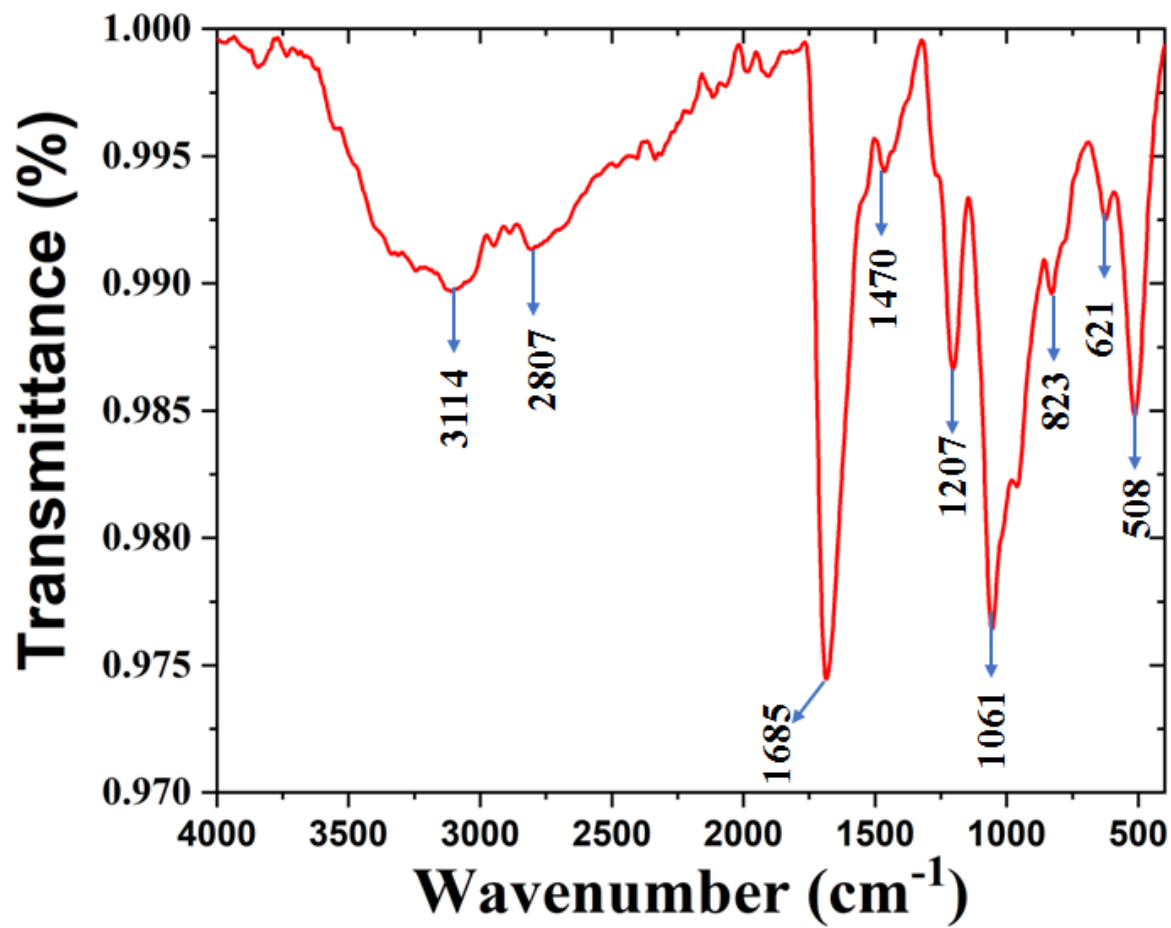


Figure S18: FT-IR data of DNA.

### **Limit of detection (LOD)**

Limit of detection is calculated from fluorescence titration data. The fluorescence spectrum of hybrid was measured six times and standard deviation of blank measurement was calculated. In order to calculate slope, the fluorescence intensity data at 460 nm was plotted against concentration of OTA. Detection limit was calculated using the  $3\sigma$  method.

$$\text{LOD} = 3\sigma/m$$

Where  $\sigma$  = standard deviation

$m$  = slope of graph between fluorescence intensity vs concentration of OTA

$$\text{LOD} = 0.801/56.4 \times 10^{-6} \text{ M}$$

$$= 0.014 \times 10^{-6} \text{ M}$$

$$= \mathbf{14 \text{ nM}}$$

### **Limit of Quantification (LOQ)**

The limit of quantification was calculated using the  $10\sigma$  method.

$$\text{LOD} = 10\sigma/m$$

$$\text{LOQ} = 2.67/56.4 \times 10^{-6} \text{ M}$$

$$= 0.047 \times 10^{-6} \text{ M}$$

$$= \mathbf{47 \text{ nM}}$$

**Working range of sensor** from titration experiment is (1-10  $\mu\text{M}$ ) (**Figure S9**).

### Quantum yield of CQDs

The quantum yield (QY) of CQDs was calculated with the following equation, where 'cqds' and 'st' corresponds to the cqds sample and reference standard, QS (quinine sulphate), respectively. The QY ( $\Phi$ ) of QS in 0.1 M H<sub>2</sub>SO<sub>4</sub> is determined to be 54%.

$$\Phi_{\text{CQDs}} = \Phi_{\text{st}} \cdot \left( \frac{A_{\text{st}}}{A_{\text{cqds}}} \right) \cdot \left( \frac{F_{\text{cqds}}}{F_{\text{st}}} \right) \cdot \left( \frac{n_{\text{st}}^2}{n_{\text{cqds}}^2} \right)$$

Where:

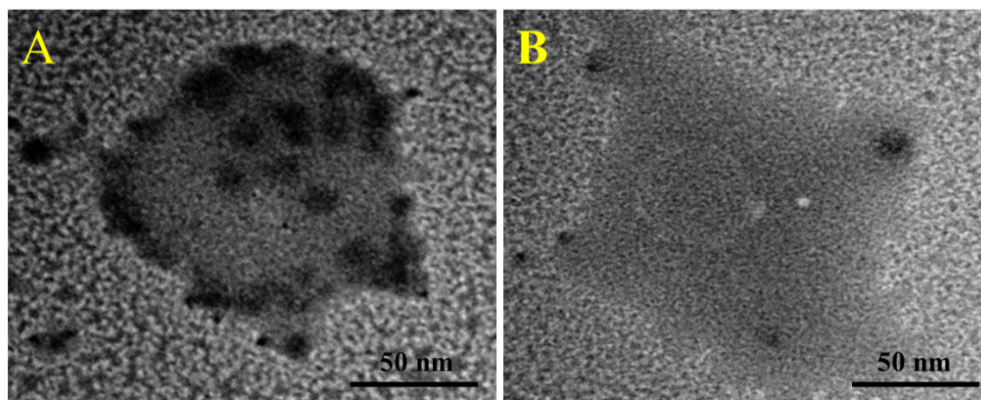
$\Phi_{\text{cqds}}$  = quantum yield of CQDs

$\Phi_{\text{st}}$  = quantum yield of standard

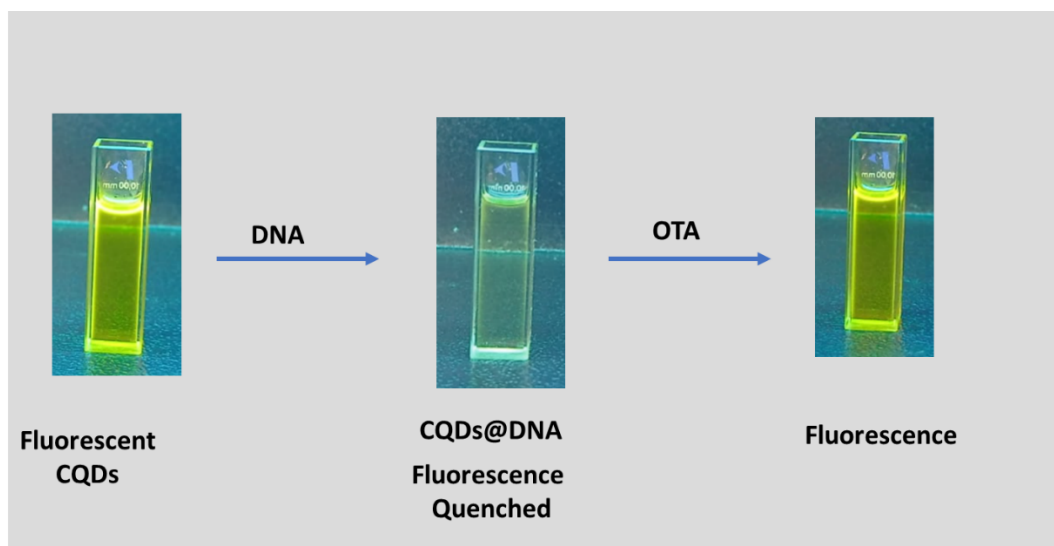
$F_{\text{cqds}}$  = Fluorescence intensity of CQDs

$F_{\text{st}}$  = Fluorescence intensity of standard

$n$  = refractive index

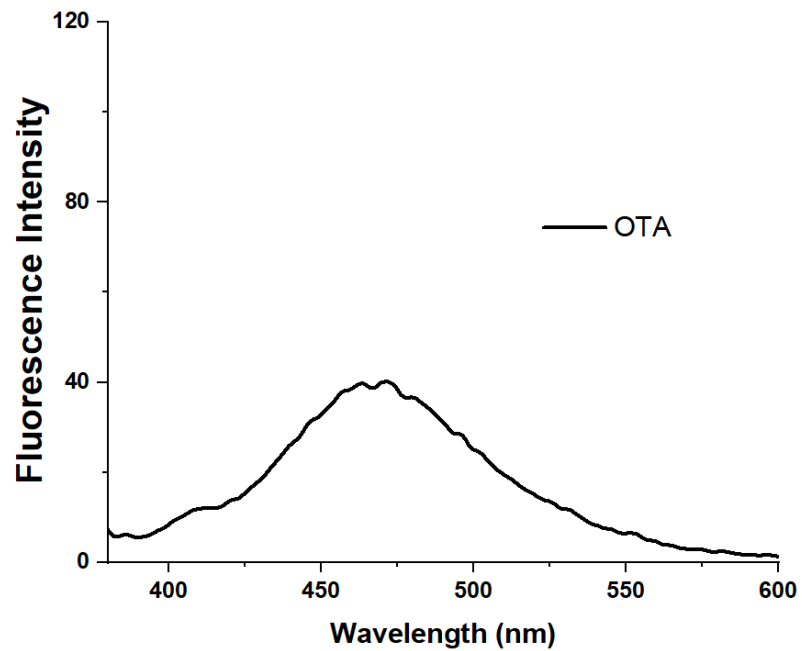


**Figure S19:** **A)** HRTEM images of CQDs-DNA hybrid; **B)** HRTEM image of CQDs-DNA hybrid after addition of OTA.



**Figure S20:** Fluorescence intensity change of CQDs on addition of DNA; Fluorescence intensity change of hybrid on addition of OTA (under UV light 255 nm).





**Figure S21:** Fluorescence spectrum of OTA (10 $\mu$ M solution).