

# MoS<sub>2</sub> Quantum-dots as Label-free Fluorescent Nanoprobe for Highly Selective Detection of Methyl Parathion Pesticide

*Nafiseh Fahimi-Kashani<sup>†</sup>, Ali Rashti<sup>†</sup>, M. Reza Hormozi-Nezhad<sup>\*,†,‡</sup> and VahidehMahdavi<sup>‡†</sup>*

*<sup>†</sup>Department of Chemistry, Sharif University of Technology, Tehran 11155-9516, Iran*

*<sup>‡</sup>Institute of Nanoscience and Nanotechnology, Sharif University of Technology, Tehran, Iran*

*<sup>‡†</sup>Pesticide Research Department, Research Institute of Plant Protection, Tehran 147574-4741, Iran*

The quantum yield(QY) of MoS<sub>2</sub> QDs is determined relative to reference quinine sulfate of known QY (0.546). The QY for the MoS<sub>2</sub> QDs sample can be calculated as<sup>1</sup>

$$QY = QY_{ref} \frac{\eta^2 I A_{ref}}{\eta_{ref}^2 I_{ref} A}$$

where QY<sub>ref</sub> is the quantum yield of the reference compound, η and η<sub>ref</sub> are the refractive index of the sample and reference solution, I and I<sub>ref</sub> are the integrated intensities (areas) of sample and standard spectra, and A and A<sub>ref</sub> represent the absorbance of sample and standard.

**Table S1. Quantum yield of MoS<sub>2</sub> QDs**

sample	Integrated Emission Intensity	Absorbance at 324 nm	Refractive Index of Solvent (η)	Quantum Yield
Quinine sulfate	29180.25	0.01412	1.33	0.546 <sup>2</sup>
MoS <sub>2</sub> QDs	1385.1	0.01437	1.33	0.025

**Figure S1**

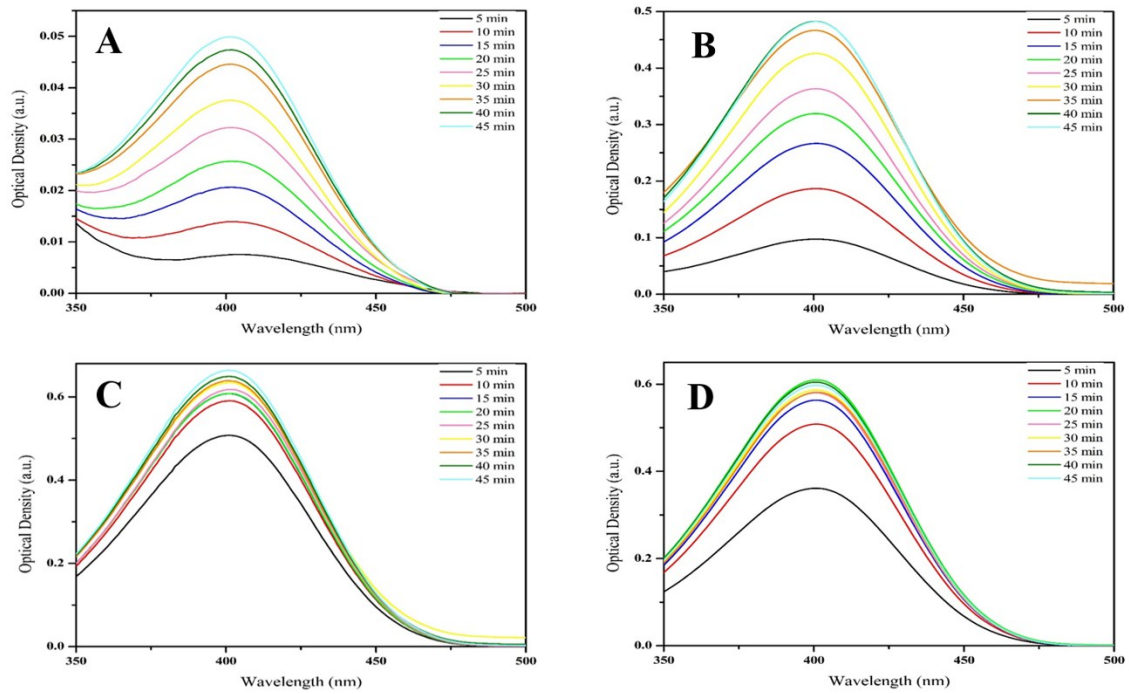


Figure S1 UV-Vis spectra of hydrolyzed MP ( $5 \mu\text{g}\cdot\text{mL}^{-1}$ ) at time intervals of 5 min at A) 25°C B) 50°C C) 75°C D) 95°C.

**Figure S2**

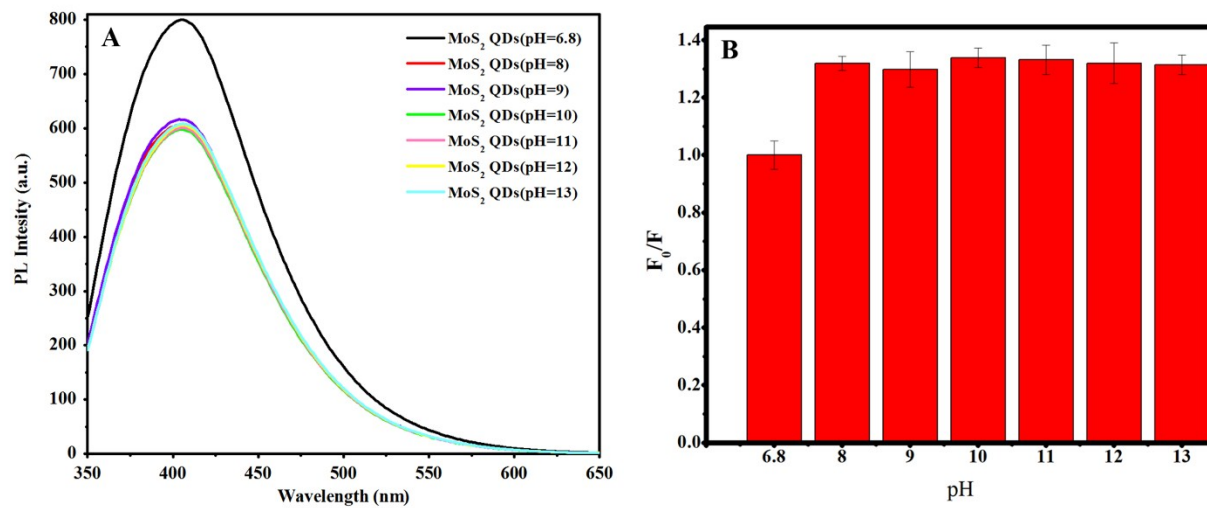


Figure S2 A) PL spectra of MoS<sub>2</sub> QDs in different pH and B) corresponding ratio of Original MoS<sub>2</sub> QDs PL intensity to MoS<sub>2</sub> QDs PL intensities at different pHs (415 nm). A decrease in PL intensities of MoS<sub>2</sub> QDs is observed with an increase pH. However, MoS<sub>2</sub> QDs are stable with Variation of pH in the range of 8 to 13.

**Figure S3**

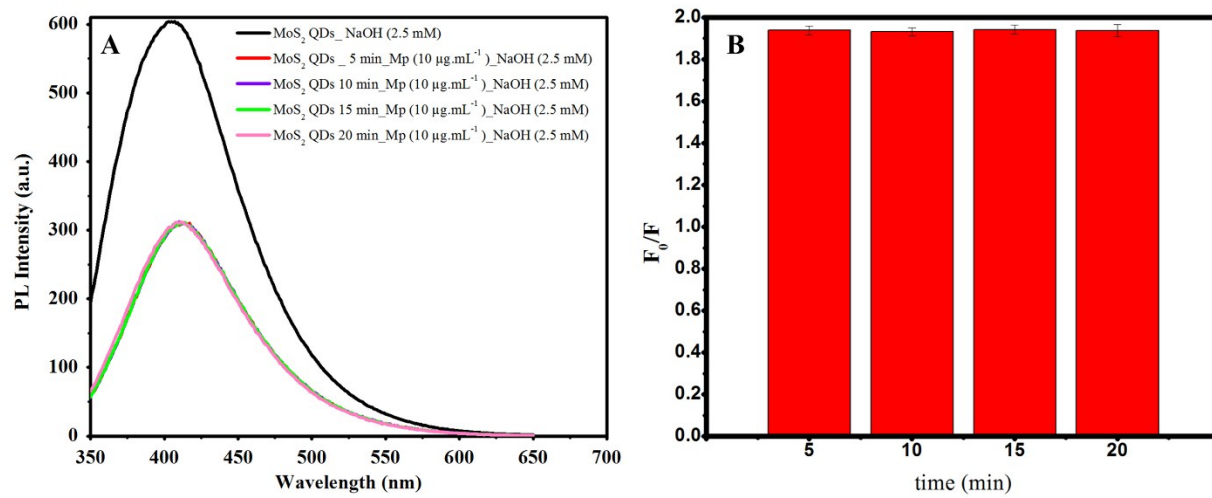


Figure S3 Effect of time on sensor PL response in presence of 10 µg.mL<sup>-1</sup> MP and 2.5 mM hydroxide ions.

Figure S4

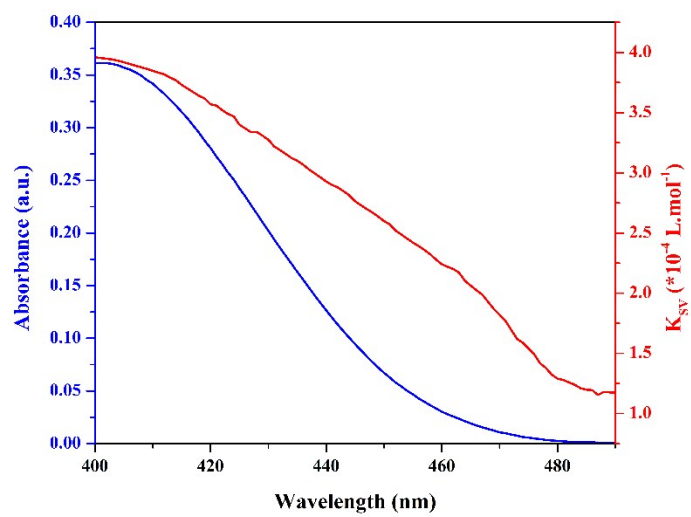


Figure S4 Plot of Stern–Volmer constants for p-NP quenching of MoS<sub>2</sub> QDs against emission wavelengths, and UV–vis spectra of p-NP in the 400–500 nm wavelength region.

**Figure S5**

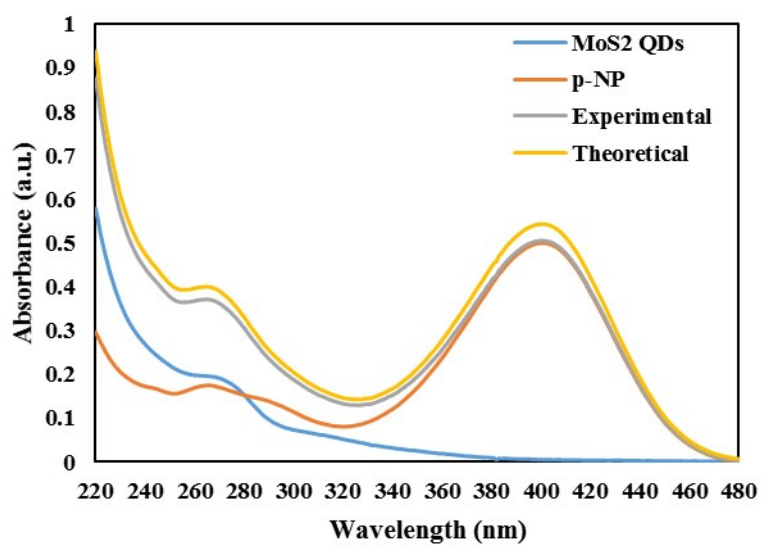


Figure S5 UV-vis spectra of MoS<sub>2</sub> QDs and p-NP, as well as the theoretical and experimental profiles based on the sum of the MoS<sub>2</sub> QDs and p-NP spectra.

**Figure S6**

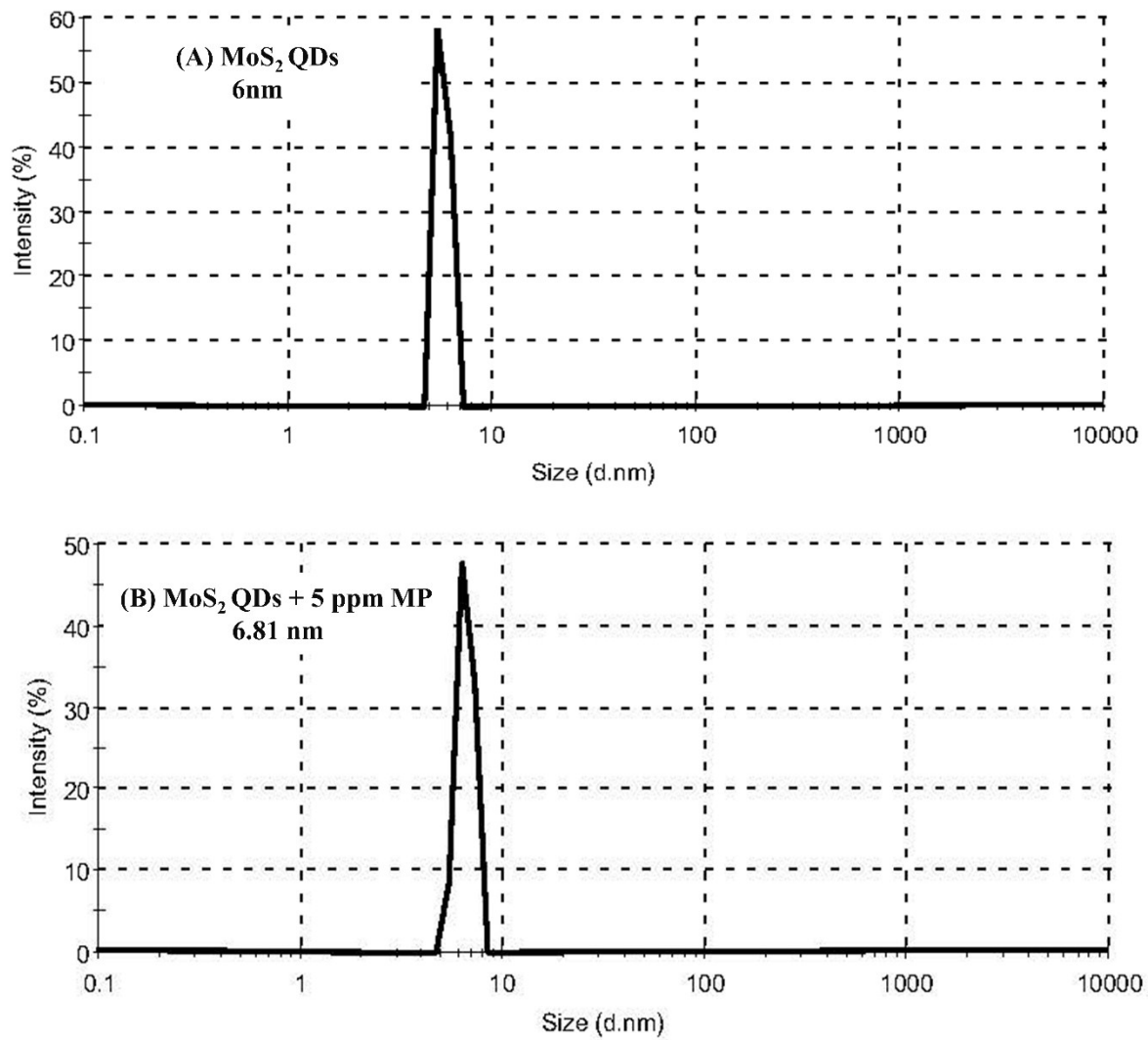


Figure S6 The hydrodynamic diameter of Synthesized MoS<sub>2</sub> QDs (A) and MoS<sub>2</sub> QDs in the presence of p-NP (B) measured by DLS method.



Figure S7

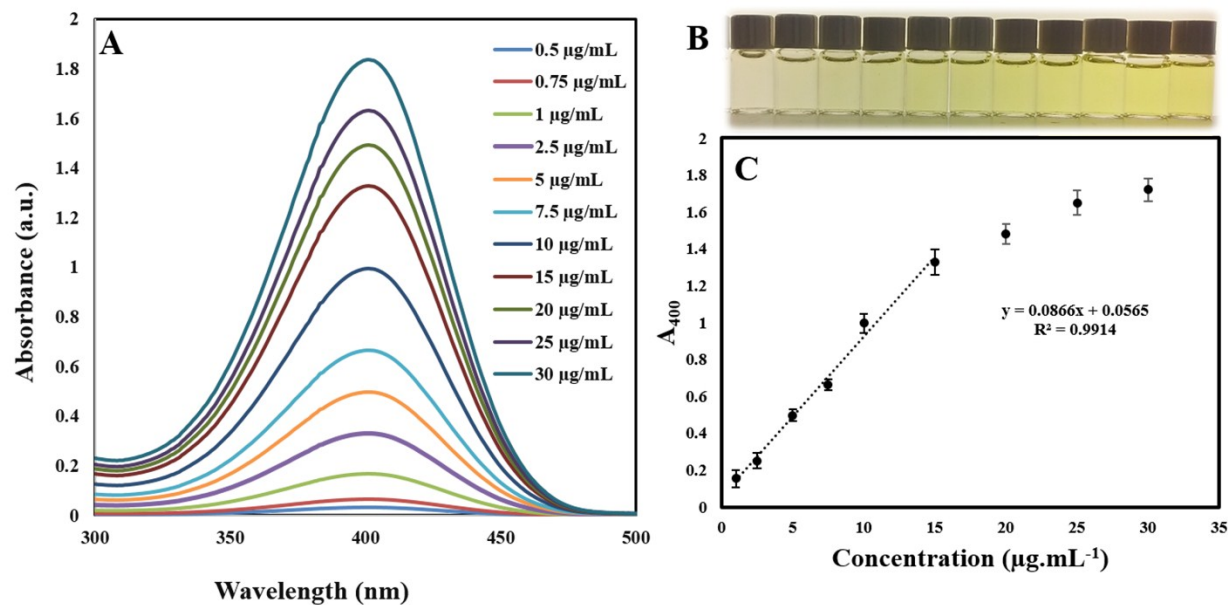


Figure S7 Colorimetric determination of MP. A) UV-Vis Spectra of p-NP formed through hydrolysis reaction of MPs at optimum condition by varying concentration of p-NP (hydrolyzed product of MP) B) Digital images of solutions at  $t = 30$  min according to increasing concentration of MPs. C) Calculated calibration curve for determination of MP showing a linear pattern at concentration ranges  $1 \mu\text{g}\cdot\text{mL}^{-1}$  to  $15 \mu\text{g}\cdot\text{mL}^{-1}$ .

## REFERENCES

- (1) Eaton, D. F. Pure Appl. Chem. 1988, 60, 1107–1114.
- (2) Brouwer, A. M. Pure Appl. Chem. 2011, 83, 2213–2228