

Electronic Supplementary Information

Efficient acceptorless dehydrogenation of hydrogen-rich *N*-heterocycles photocatalyzed by Ni(OH)₂@CdSe/CdS quantum dots

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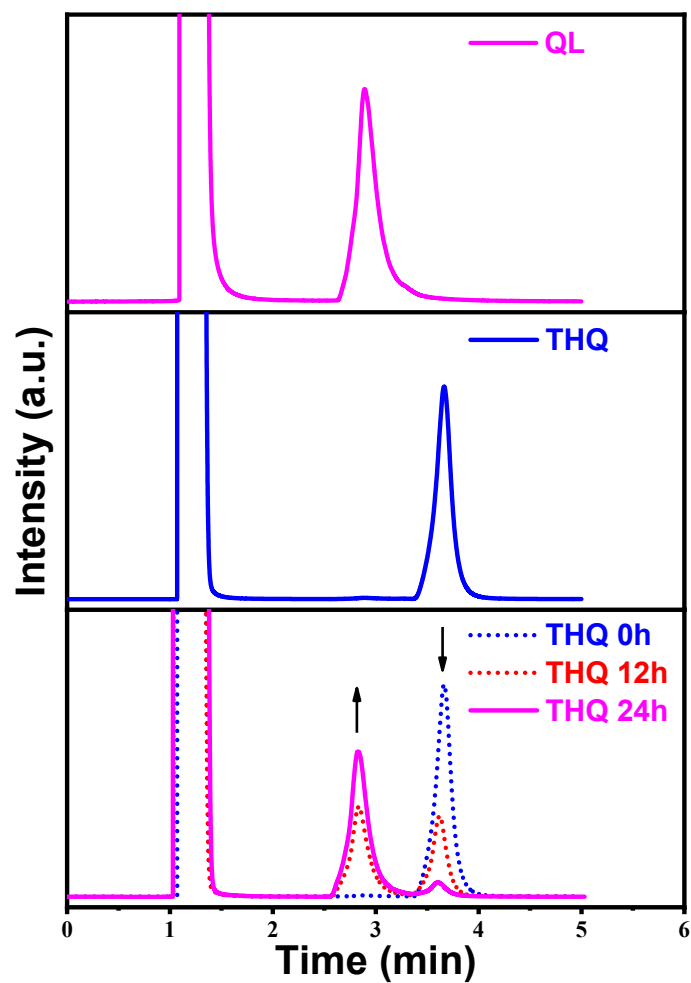


Figure S1. GC-FID analyses for THQ and QL. Experimental conditions were as follows: [CdSe/CdS QDs] = 2.8 mg/mL; [NiCl₂] = 1.6 mM; [THQ] = 20 mM; H₂O/CH₃CN (v/v = 2/3, 5 mL); the photocatalytic reactions were performed under blue LED irradiation ($\lambda = 420$ nm, I = 50 mW/cm²).

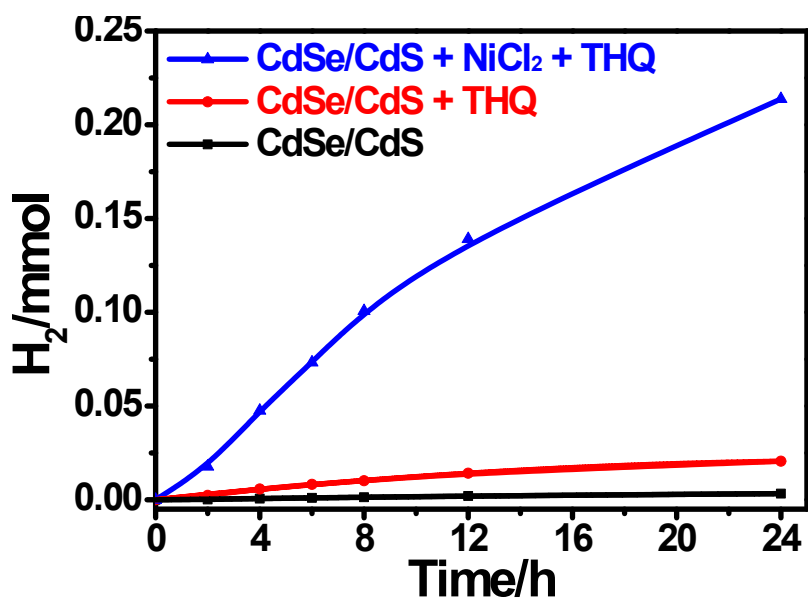


Figure S2. Time dependent photocatalytic hydrogen release over Ni(OH)₂@CdSe/CdS QDs. Experimental conditions were as follows: [CdSe/CdS] = 2.8 mg/mL, [NiCl₂] = 1.6 mM, [THQ] = 20 mM, H₂O/CH₃CN (v/v) = 2/3, the photocatalytic reactions were performed under blue LED irradiation ($\lambda = 420$ nm, I = 50 mW/cm²).

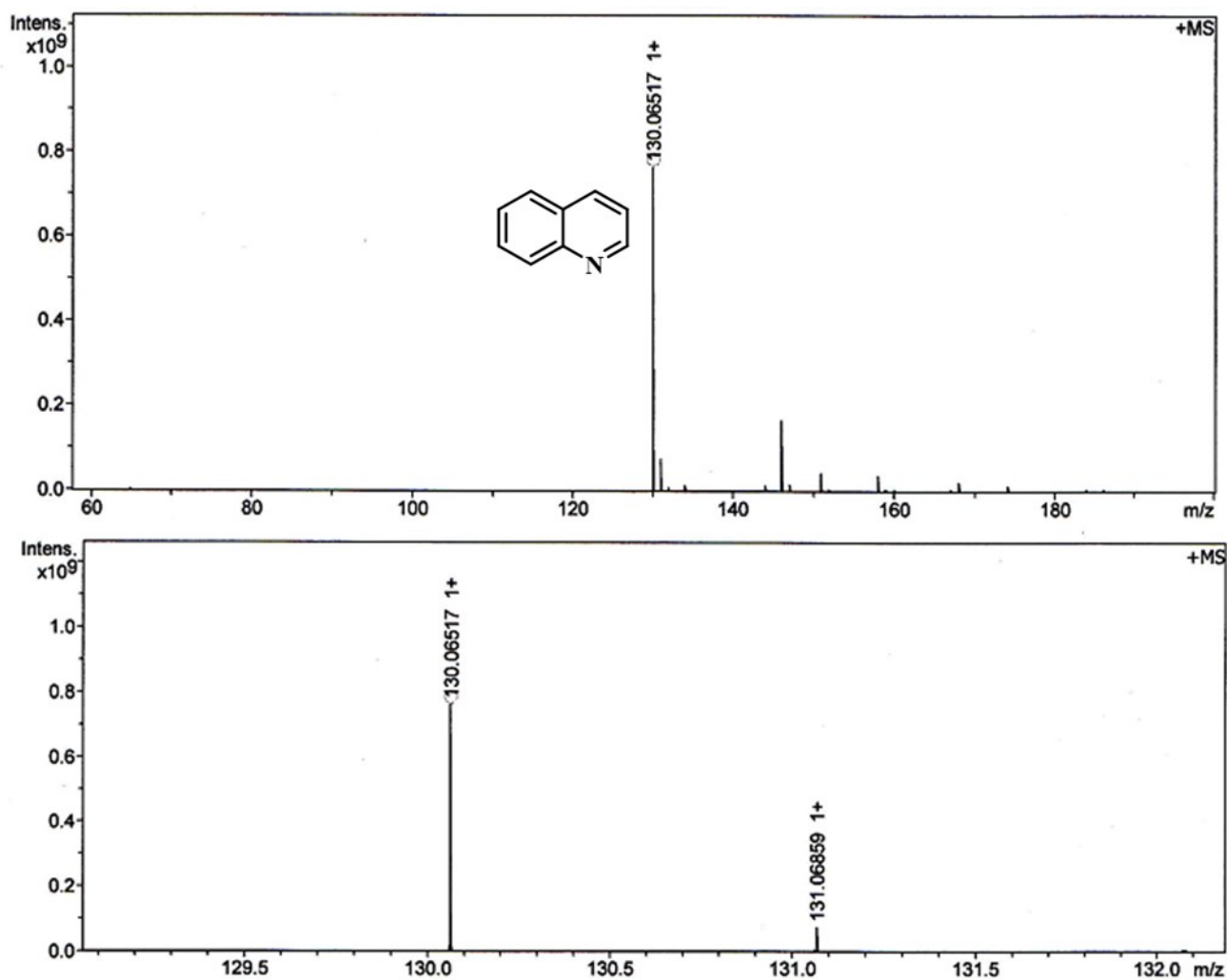


Figure S3. ESI-MS of the reaction solution (Table 1 entry 1).

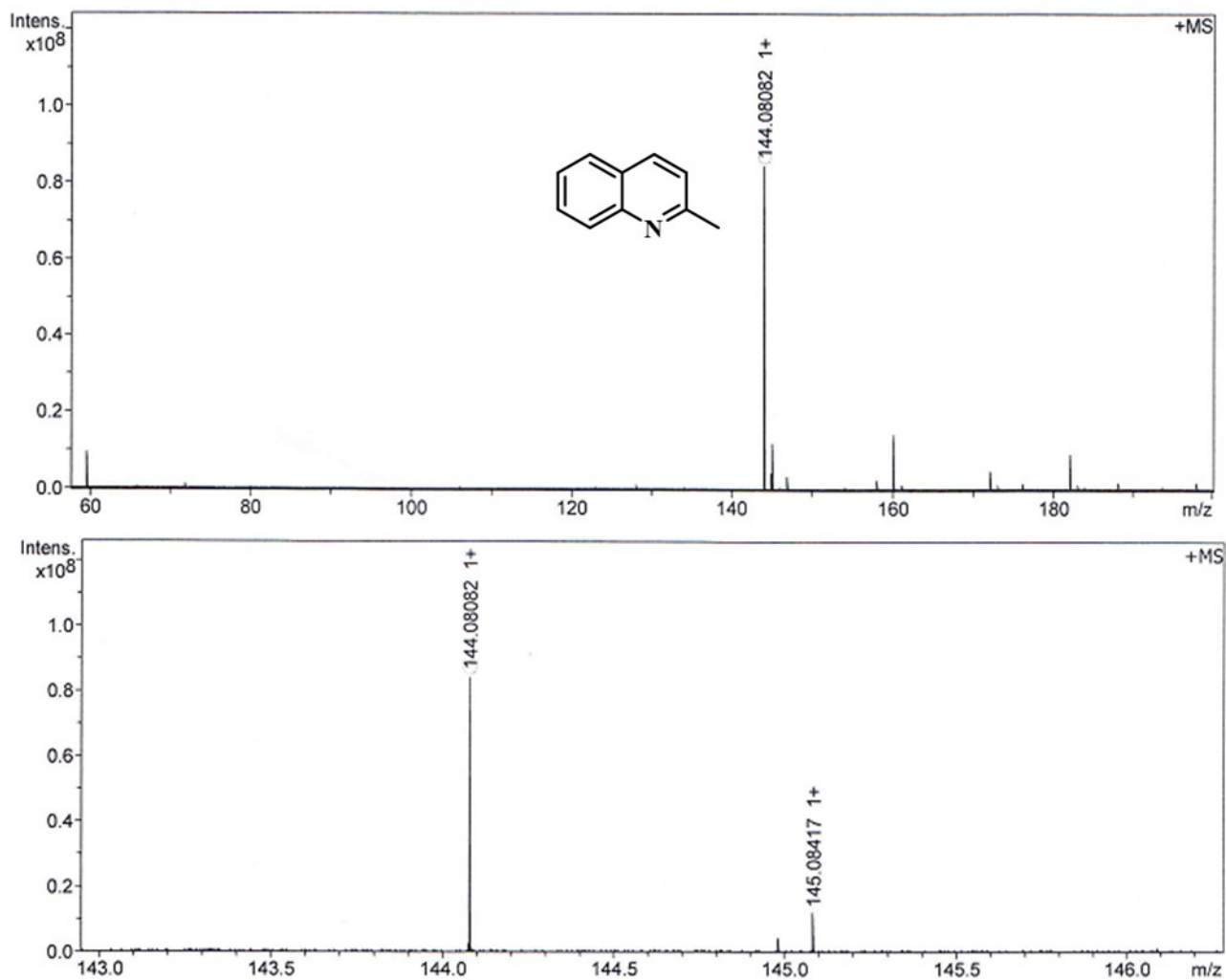


Figure S4. ESI-MS of the reaction solution (Table 1 entry 2).

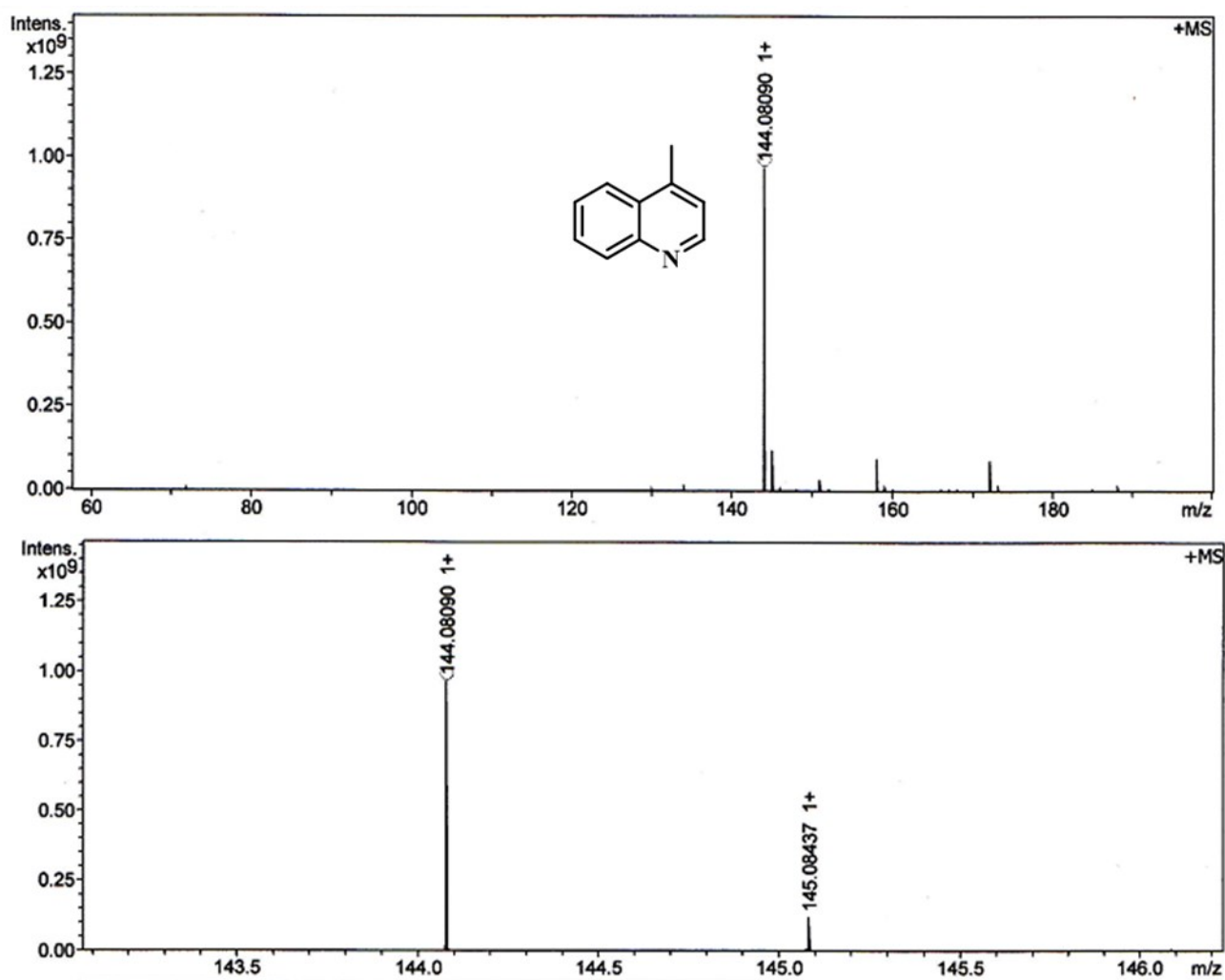


Figure S5. ESI-MS of the reaction solution (Table 1 entry 3).

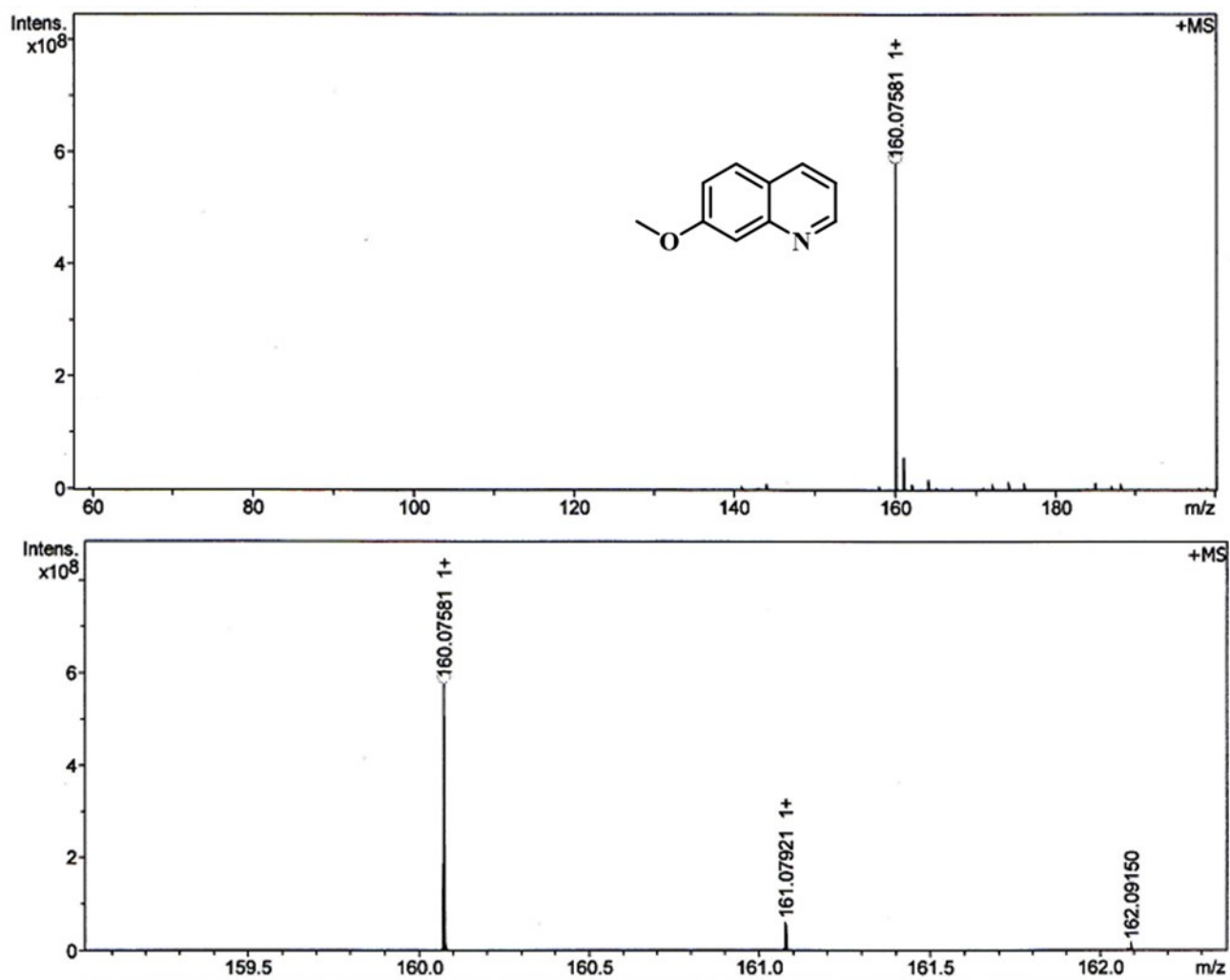


Figure S6. ESI-MS of the reaction solution (Table 1 entry 4).

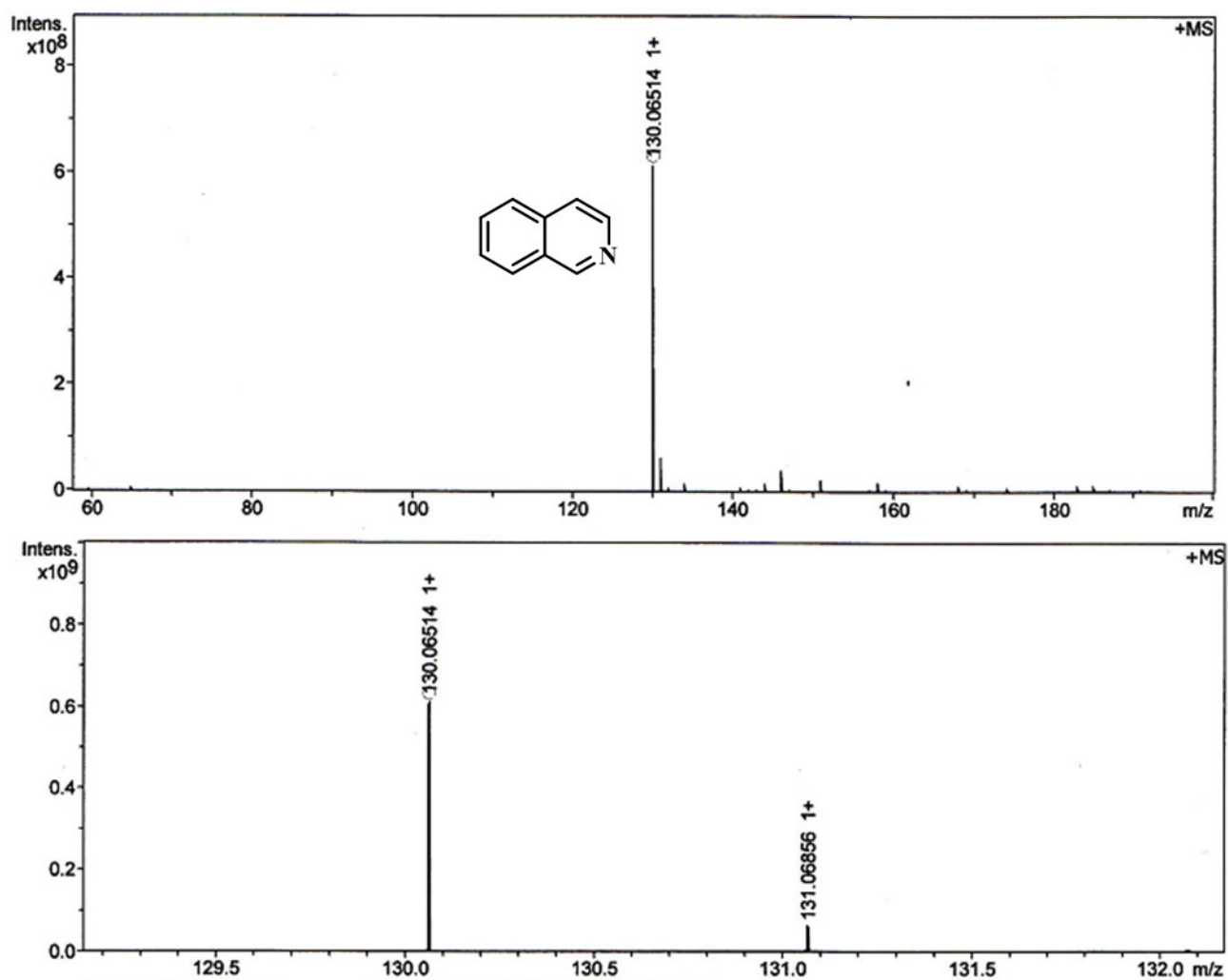


Figure S7. ESI-MS of the reaction solution (Table 1 entry 5).

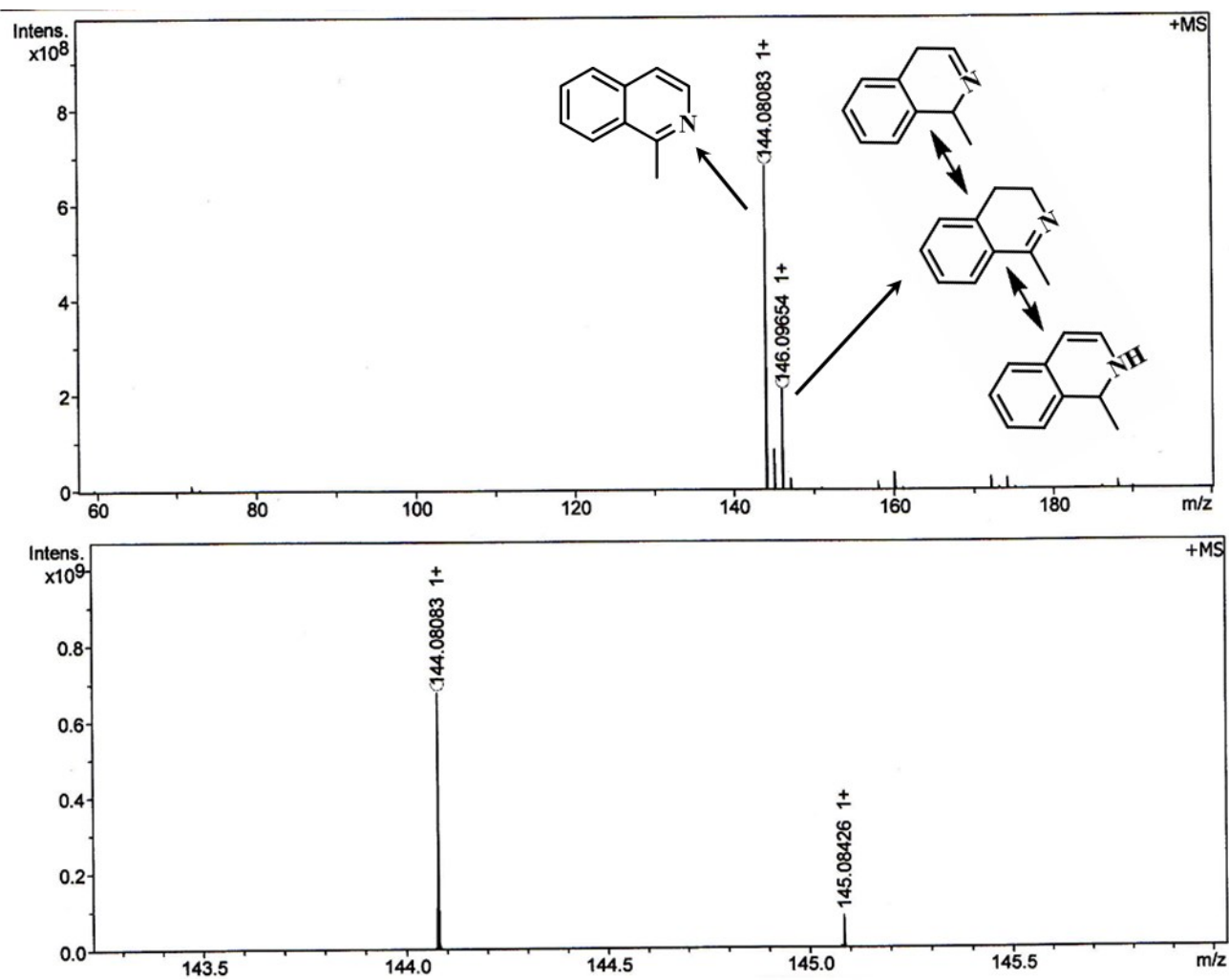


Figure S8. ESI-MS of the reaction solution (Table 1 entry 6).

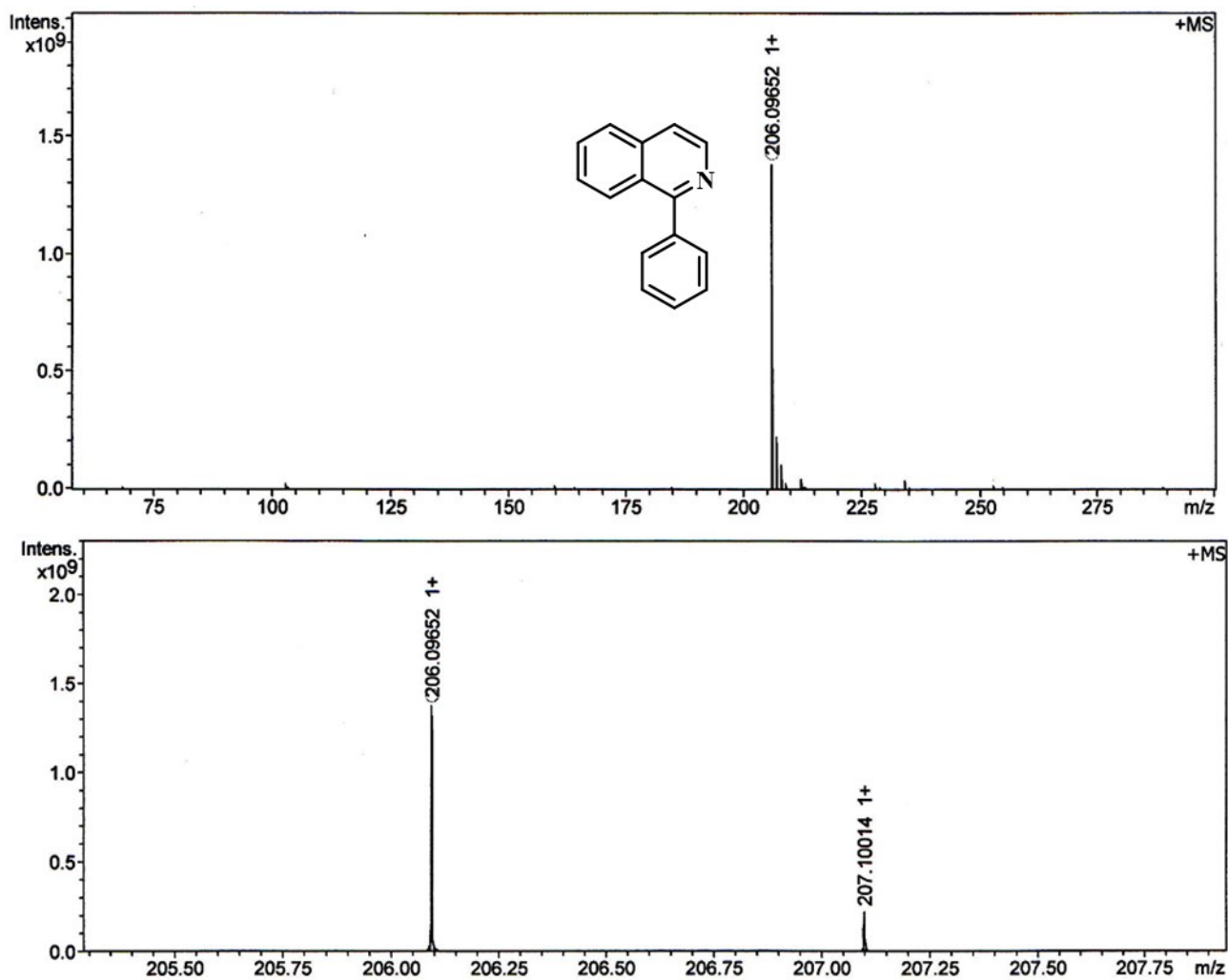


Figure S9. ESI-MS of the reaction solution (Table 1 entry 7).

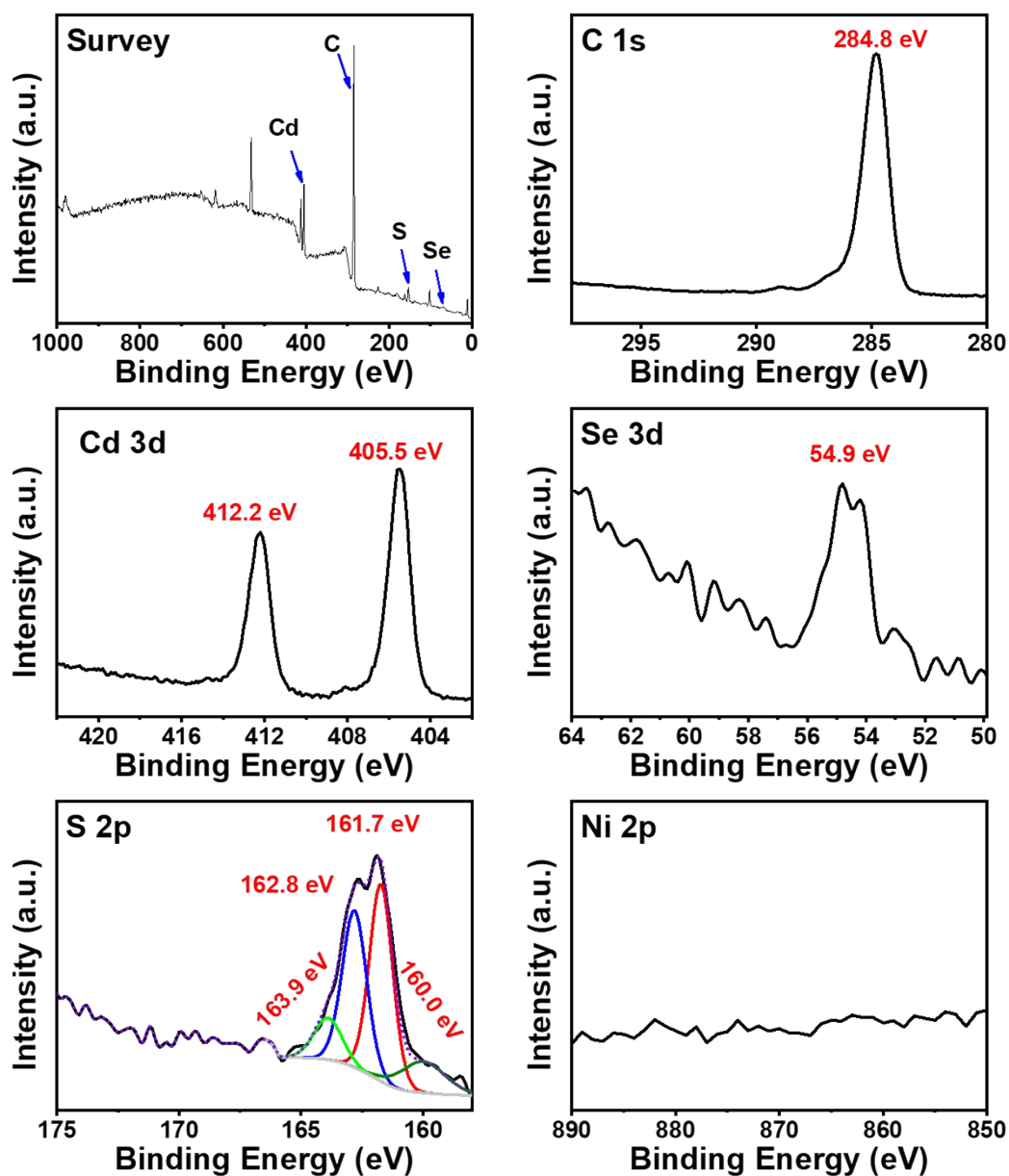


Figure S10. XPS spectrum of CdSe/CdS QDs; high-resolution XPS spectra of C 1s, Cd 3d, Se 3d, S 2p, Ni 2p.

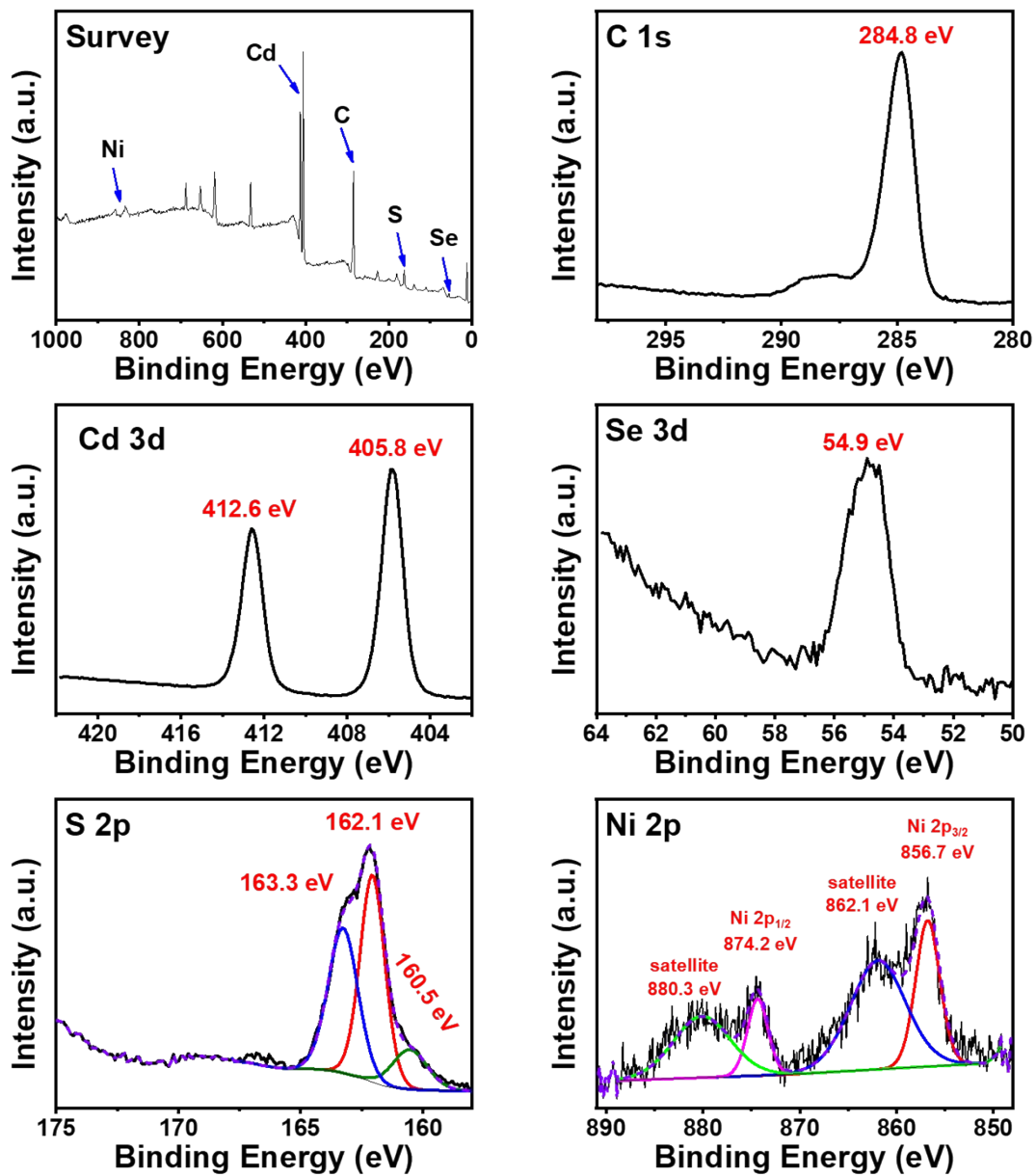


Figure S11. XPS spectra of Ni(OH)₂@CdSe/CdS QDs; high-resolution XPS spectra of C 1s, Cd 3d, Se 3d, S 2p, Ni 2p.

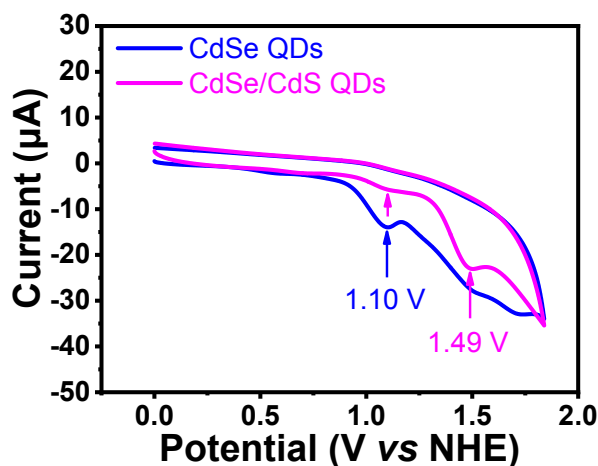


Figure S12. Cyclic voltammetry curve of CdSe (0.4 mg/mL, blue) and CdSe/CdS QDs (0.3 mg/mL, magenta) in degassed water without electrolyte, scan rate: 50 mV/s.

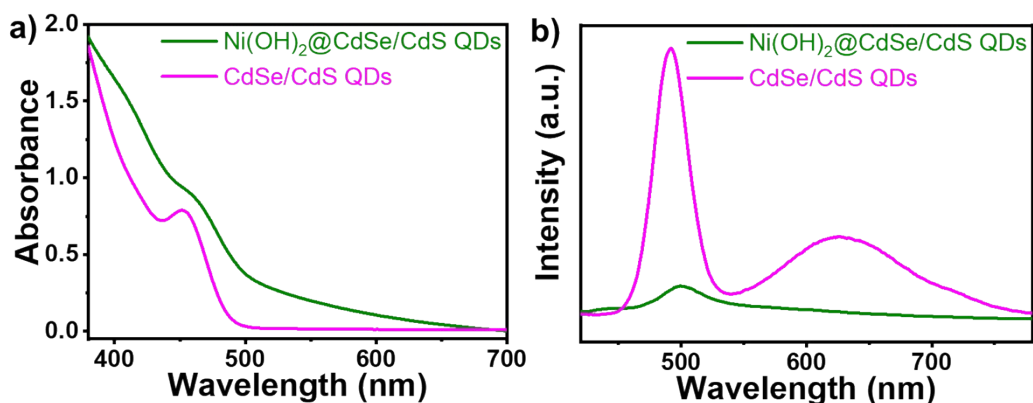


Figure S13. a) Absorption and b) normalized emission spectra of Ni(OH)₂@CdSe/CdS and CdSe/CdS QDs ($\lambda_{ex} = 400$ nm).

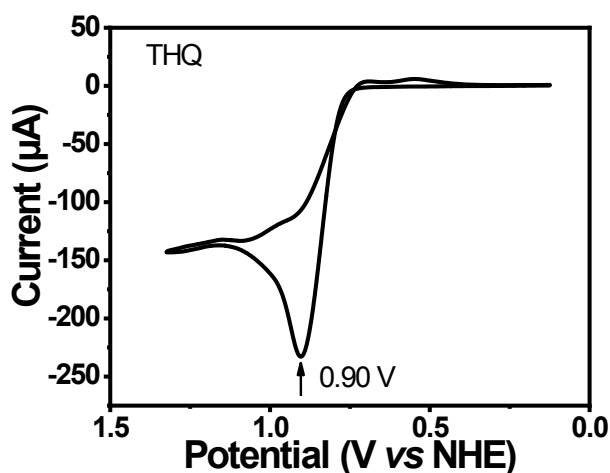


Figure S14. Cyclic voltammetry curve of THQ (1 mM) in degassed CH₃CN with 0.1 M NBu₄PF₆ as

electrolyte, scan rate: 50 mV/s.

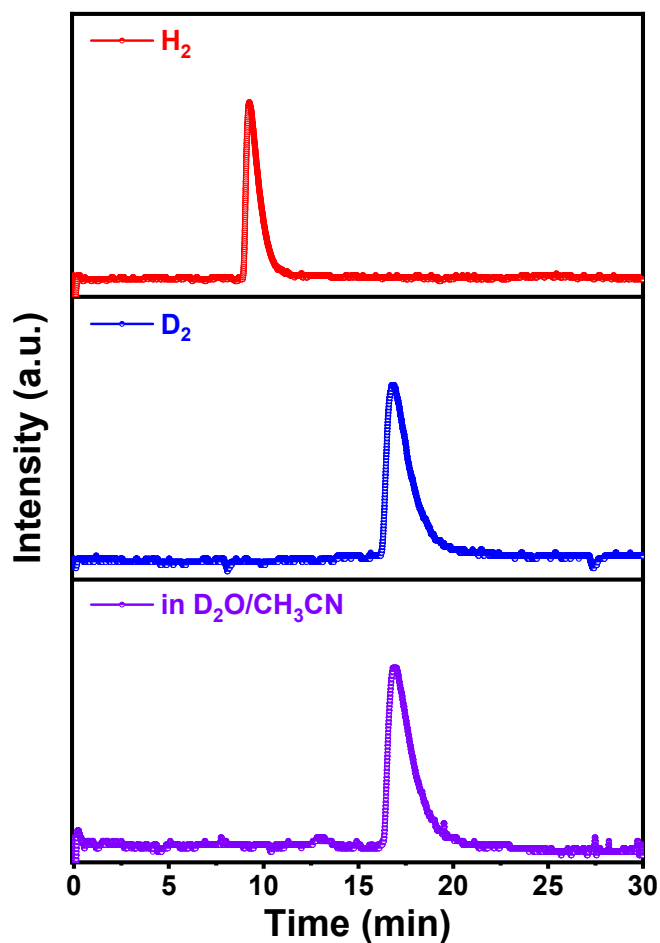


Figure S15. GC-TCD analyses using 15 % $\text{MnCl}_2@ \gamma\text{-Al}_2\text{O}_3$ as column packing for high purity H_2 (top), high purity D_2 (middle) and the gas phase of photocatalytic dehydrogenation of THQ in $\text{D}_2\text{O}/\text{CH}_3\text{CN}$ (bottom). Experimental conditions were as follows: $[\text{CdSe}/\text{CdS QDs}] = 2.8 \text{ mg/mL}$; $[\text{NiCl}_2] = 1.6 \text{ mM}$; $[\text{THQ}] = 20 \text{ mM}$; $\text{H}_2\text{O}/\text{CH}_3\text{CN}$ (v/v = 2/3, 5 mL); the photocatalytic reactions were performed under blue LED irradiation ($\lambda = 420 \text{ nm}$, $I = 50 \text{ mW/cm}^2$).

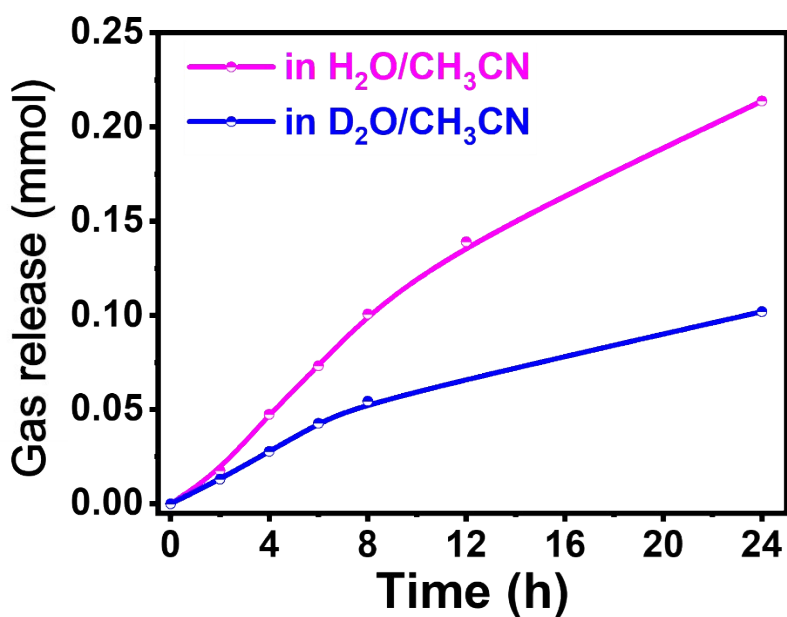


Figure S16. Time dependent photocatalytic H₂ or D₂ release over Ni(OH)₂@CdSe/CdS QDs. Experimental conditions were as follows: [CdSe/CdS] = 2.8 mg/mL, [NiCl₂] = 1.6 mM, [THQ] = 20 mM, H₂O or D₂O/CH₃CN (v/v) = 2/3, the photocatalytic reactions were performed under blue LED irradiation ($\lambda = 420$ nm, $I = 50$ mW/cm²).

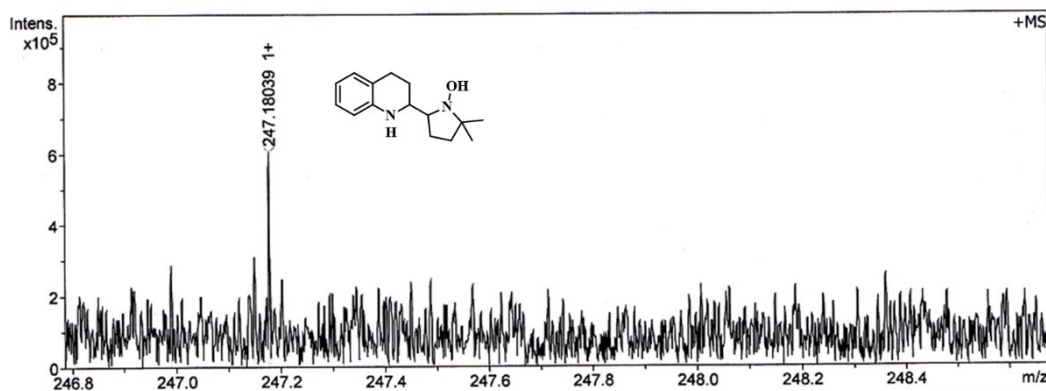


Figure S17. ESI-MS spectrum of adduct between the radical intermedia of THQ and DMPO.

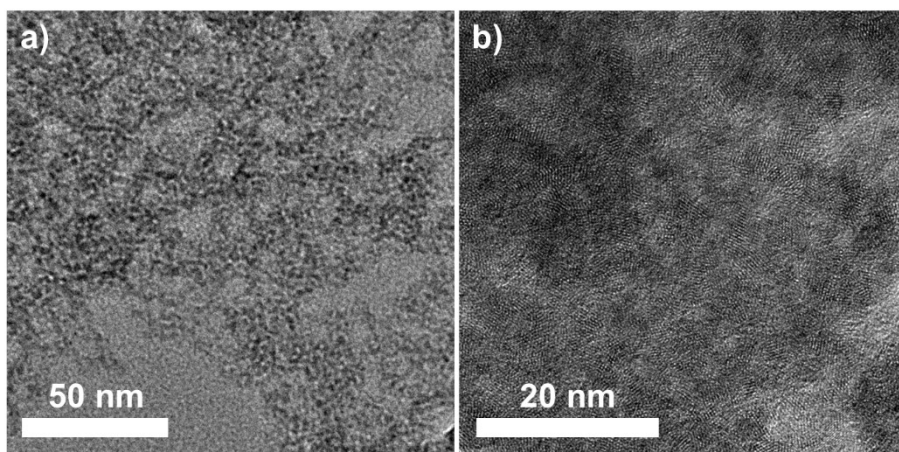


Figure S18. TEM images of a) CdSe and b) CdSe/CdS QDs.