Supporting Information

for

Glyco-*β*-Cyclodextrin Capped Quantum Dots: Synthesis, Cytotoxicity and Optical Detection of Carbohydrate-Protein Interactions

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1. UV-visible and fluorescence spectra.

Absorbance measurements of QD solutions were performed by a Thermo scientific UV-visible scan spectrophotometer. Fluorescence emission spectra were recorded on a Fluoromax-4 spectrofluorometer. Uv-visible spectra of both modified and QD-TOPO showed a broad absorption band. Upon excitation at the 400 nm, a maximum emission at 640 nm was observed (Fig S1). Quantum yields have been calculated using the equation.

$$\Phi_{comp}/\Phi_{ref} = A_{comp} \text{ X } [C]_{ref} / A_{ref} \text{ X } [C]_{comp}$$

where [C] refers to the concentration of the samples and A to the area of the emission spectra. Quantum yield was determined relative to that of fluorescein at 470 nm (0.093) (Table S1). [1]

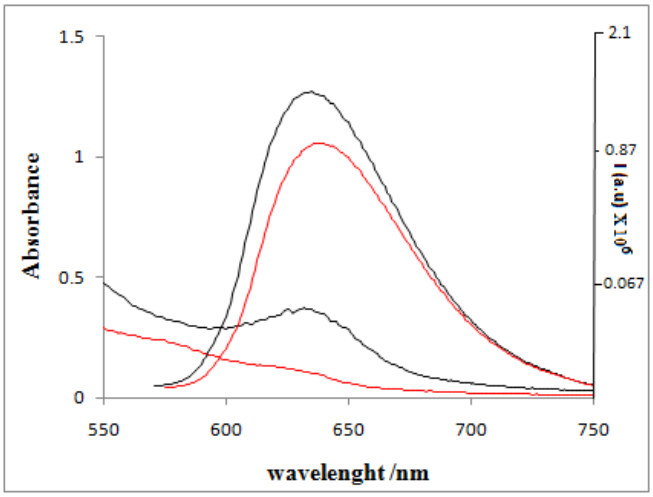


Figure S1. Normalized UV-visible and fluorescence spectra of QD-TOPO (black line) and QD-1 (black line) of the compound.

Compound	λ_{max}	QY (Φ)
1	641	0.42
2	641	0.38
3	643	0.39
QD-TOPO	643	0.29

Table S1. Photophysical properties of comp **1-3** and QD-TOPO. The quantum yields (QYs) of glycol-QDs in water were measured relative to the value of fluorescein.

2. FT-IR spectroscopic studies.

In Figure S2, IR spectrum of free QD_{640}-TOPO shows a peak corresponding to CH_2 stretching mode for TOPO at 2925 cm^{-1}. Whereas, *β*- CD-modified QDs (**QD-1**; Figure S2b) spectrum strongly resembles that of free *β*-CDs with the broad band at ~3300 $cm^{-1}$from the O-H vibration and an intense stretching vibration band at 1086 and 1044cm^{-1} that corresponds to glycosidic

bond, and slightly shifted CH_2 stretching mode at 2974 cm^{-1} from TOPO inclusion confirming that the surface of QDs has been modified by *β*–CDs (Table S2).

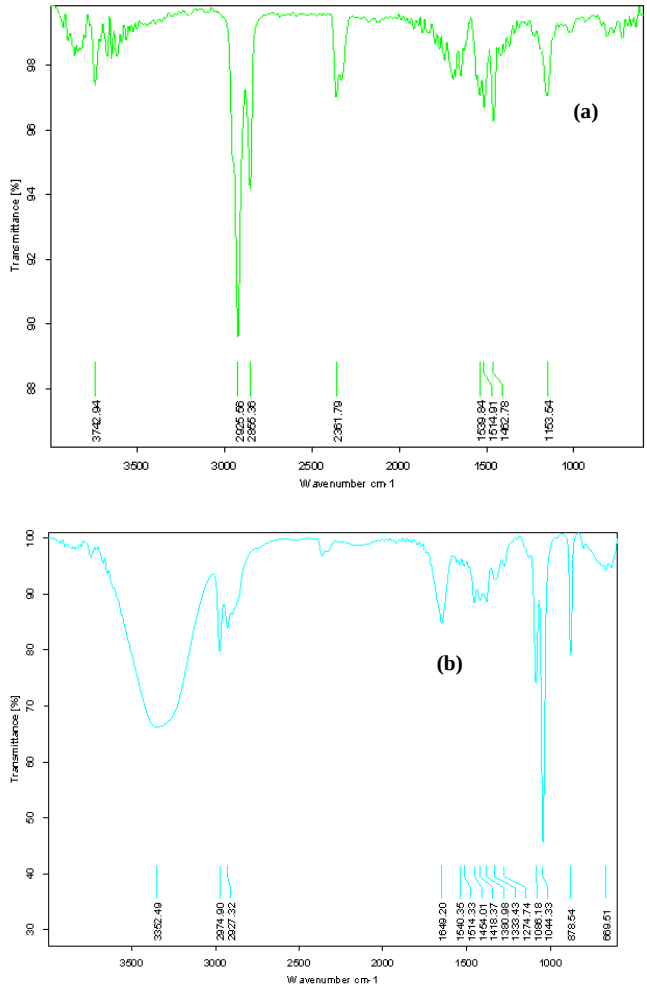


Figure S2. FTIR spectra of (a) QD_{640}-TOPO (green color) and (b) **1 (**bright turquoise color)

Compound	**FT-IR frequency (cm^{-1})**
QD_{640}-TOPO	2925, 2855 (CH-stretch),
β- CDs	3284 (OH- br stretch), 1031 (C-O-C stretch)
1	3352 (OH-br stretch), 2974, 2927 (CH-stretch), 1086, 1044 (C-O-C stretch)

Table S2. Characteristic IR frequencies of glyco-QDs

3. ^{1}H-NOESY spectra

The formation of host-guest complexes was further characterized by ^{1}H-NOESY NMR spectroscopy. ^{1}H NMR of the complex showed a slightly different chemical shift compared to the native compound due to strong host-guest interactions. The 2D NOESY spectra (Fig S4-S6**)** prove intermolecular correlations between the TOPO and *β*-CD groups in D_2O. Figure S3 displayed the H-proton of the *β*-CD and TOPO and the cross peaks in 2D NOESY indicate strong nuclear overhauser effect (NOE) correction between the inner core proton **H3** and **H5** of *β*-CD with aliphatic chain of TOPO moiety at 1.22 and 0.87 ppm respectively. However, it was difficult to identify **H3** and **H5** of *β*CDman and *β*CDgal. Instead, our attention was drawn on to the protons of TOPO as we observed a strong NOE interaction with protons from the *β*CDman and *β*CDgal region. It was observed that proton **1, 2, 3** of TOPO showed a strong overhauser effect with *β*-CD protons and a weak or no interaction with proton **4-8**, indicating the *β*-CD inner core is in close proximity to aliphatic part. of TOPO moieties (Fig **S4**). Finally, above results correlates to Dan Grustein et al work.[2]

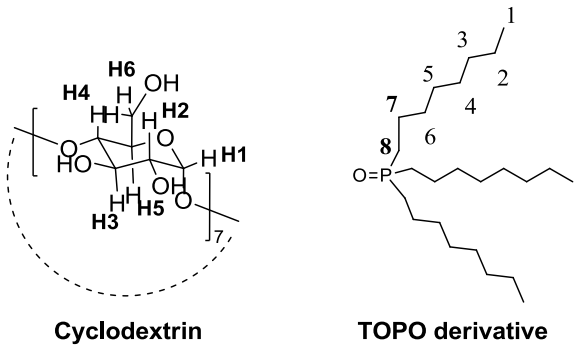


Figure S3. Proton designation of the relevant molecule moiety involved in host-guest complex.

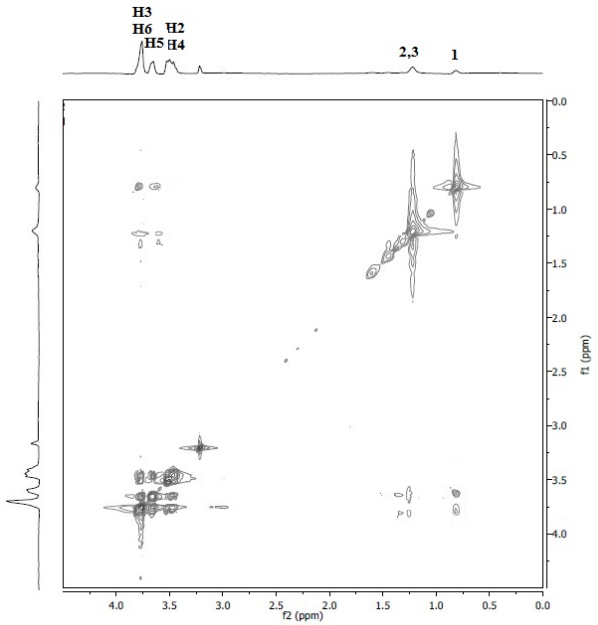


Figure S4. ^{1}H-NOESY spectra of **QD-1**

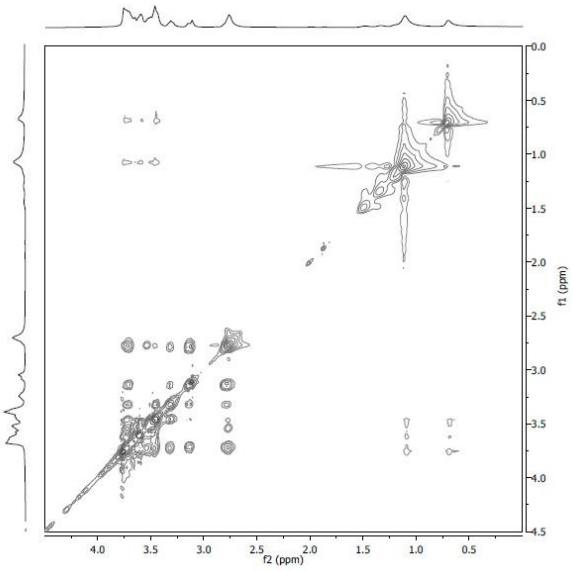


Figure S5. ^{1}H-NOESY spectra of **QD-2**

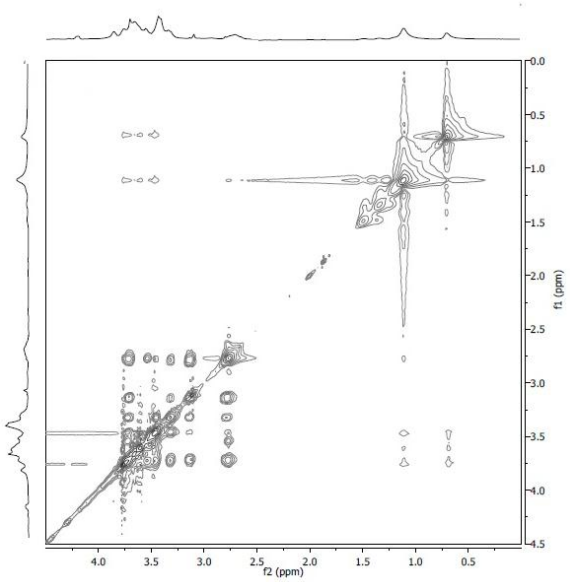


Figure S6. ^{1}H-NOESY spectra of **QD-3**

4. EDX analysis.

The EDX mappings nanoparticles was performed with Ametec/EDAX Analytical System Genesis Version 5 apparatus. The voltage was 10 kV in high-current mode. Nanoparticles were positioned at 65° to the detector. Figure S7 clearly showed peaks of functionalization of QD increases the peak intensity of oxygen and carbon indicating the presence of CD moiety on top of QDs.

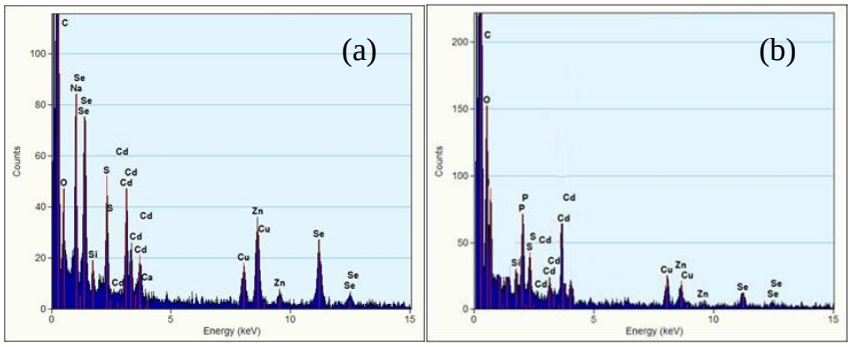
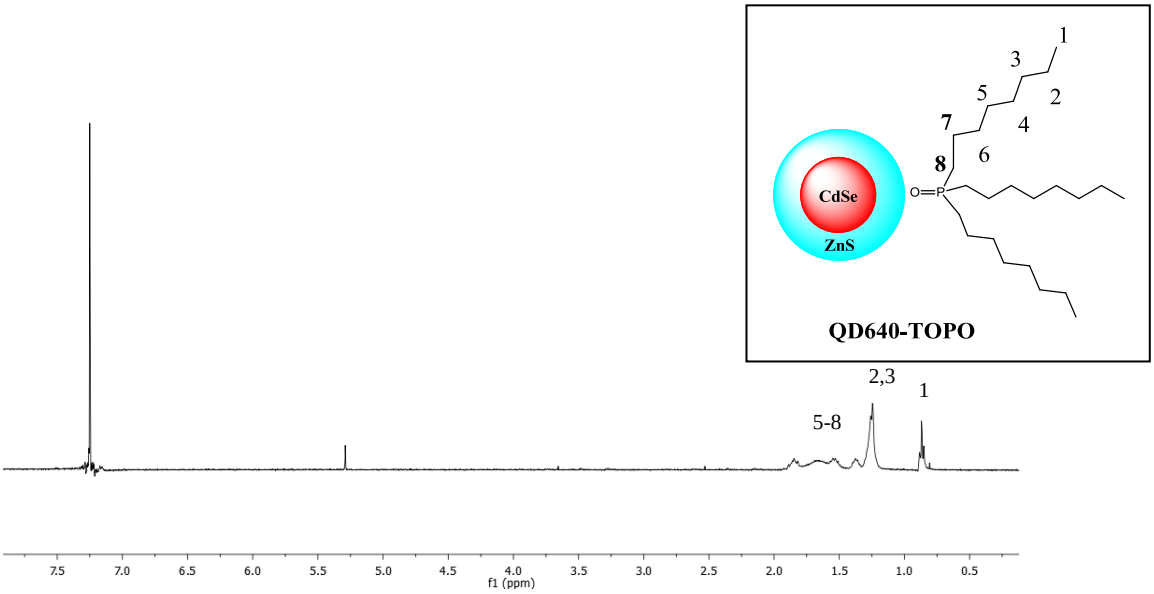
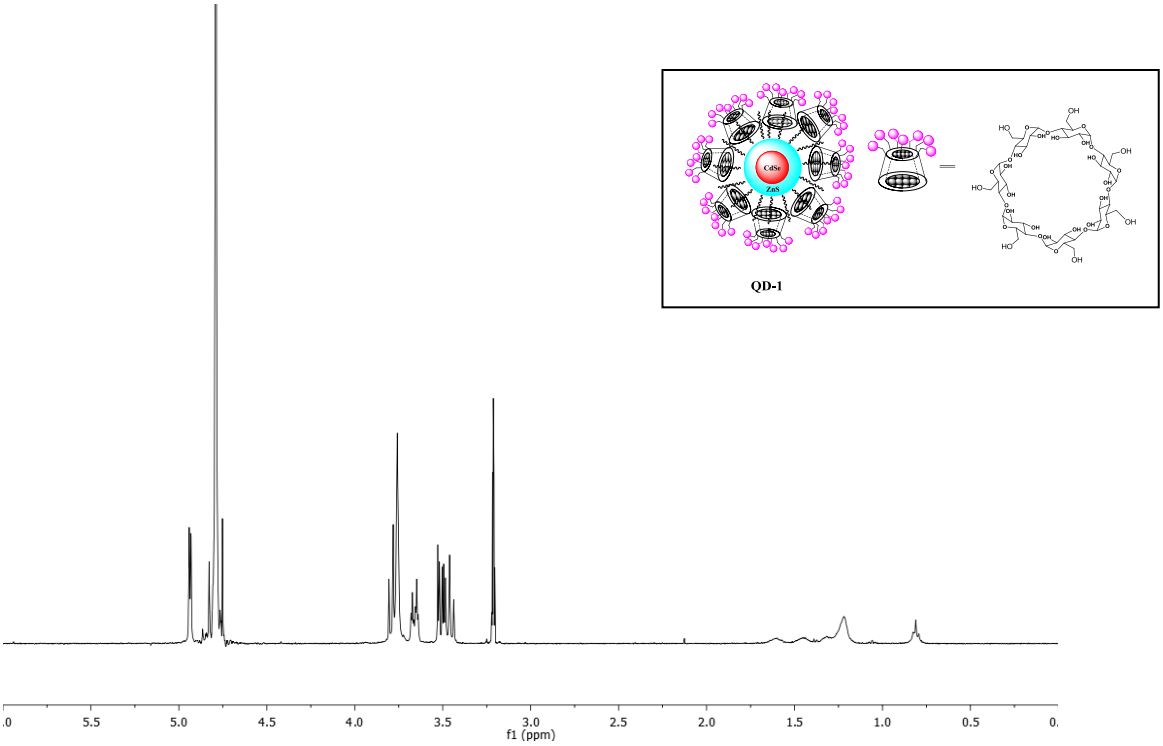


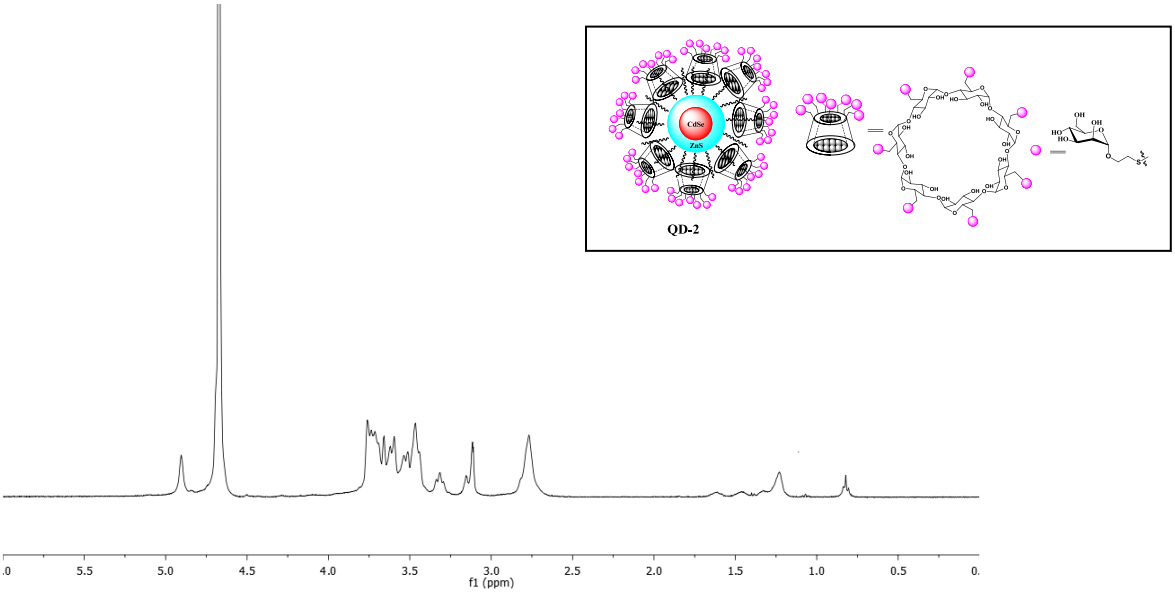
Figure S7. EDX spectra of Compound QD-TOPO (a) and **QD-1** (b).

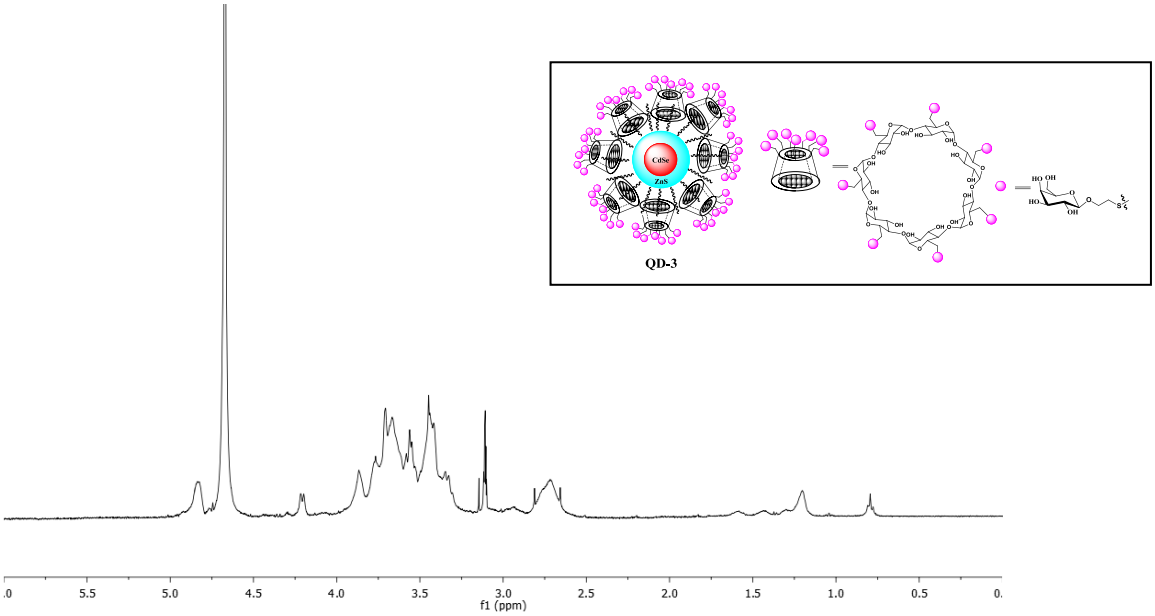
References.

1. M. M. Martin, *Chem. Phys. Lett*. **1975**. 35, 105-111
2. D. Grunstein, M. Maglinao, R. Kikkeri, M. Collot, K. Barylyuk, F. Kamena, B. Lepenies, R. Zenobi, P. H. Seeberger. *J. Am. Chem. Soc*, **2011**, 133(35):13957-66.






CdSe
ZnS
QD-2
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


CdSe
ZnS
QD-3
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)