Supporting Information

Rapid covalent ligation of fluorescent peptides to water solubilized quantum dots.

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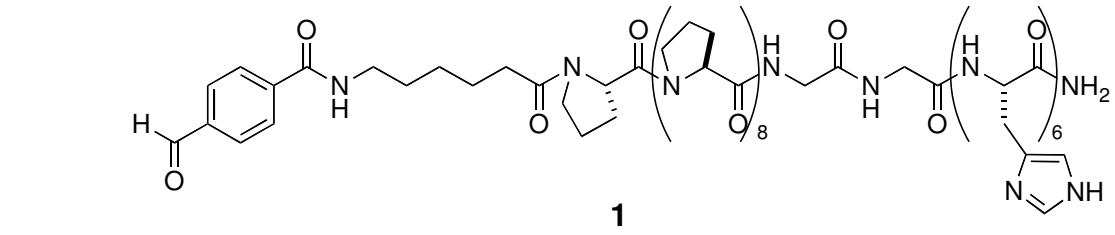

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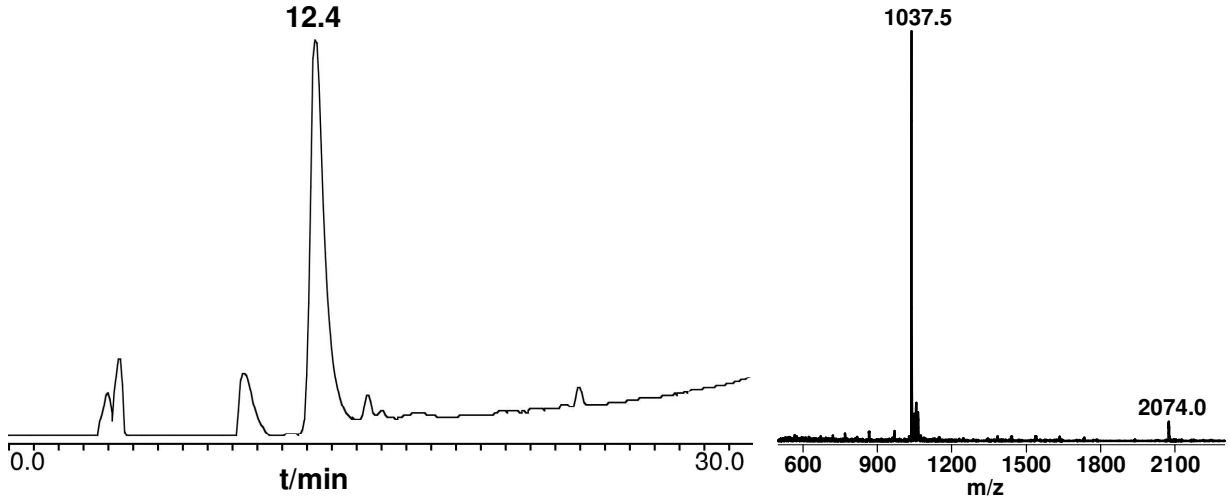

Figure S1. HPLC trace of the coupling reaction between Ahx-$Pro_9Gly_2His_6$ and succinimidyl 4-formylbenzoate (left). Mass of the compound at 12.4 min (right) matches the expected product **1**. Mass calcd. for $C_{99}H_{130}N_{31}O_{20}$ $[M+H]^+$ *m/z*=2074.0, found: 2074.0

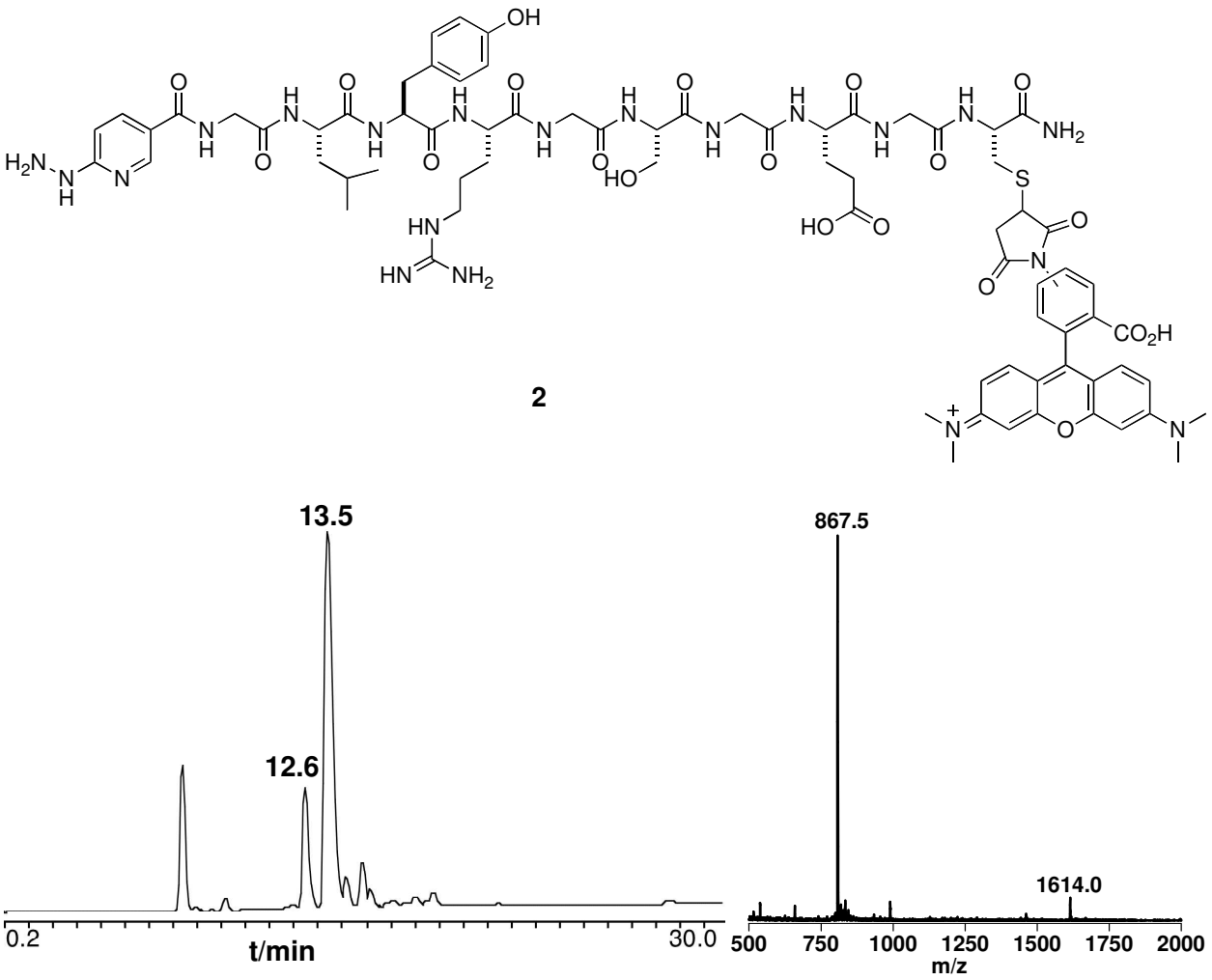

Figure S2. HPLC trace of the labeling reaction between *HYNIC*-GLYRGSGEGC and (5,6)-Maleimide TAMRA (left). Mass of the isomer 5,6-compounds at 12.6 and 13.5 min (right) match the expected product **2**. Mass calcd for $C_{74}H_{94}N_{20}O_{20}S$ $[M+H]^+$ *m/z*=1614.7, found: 1614.0

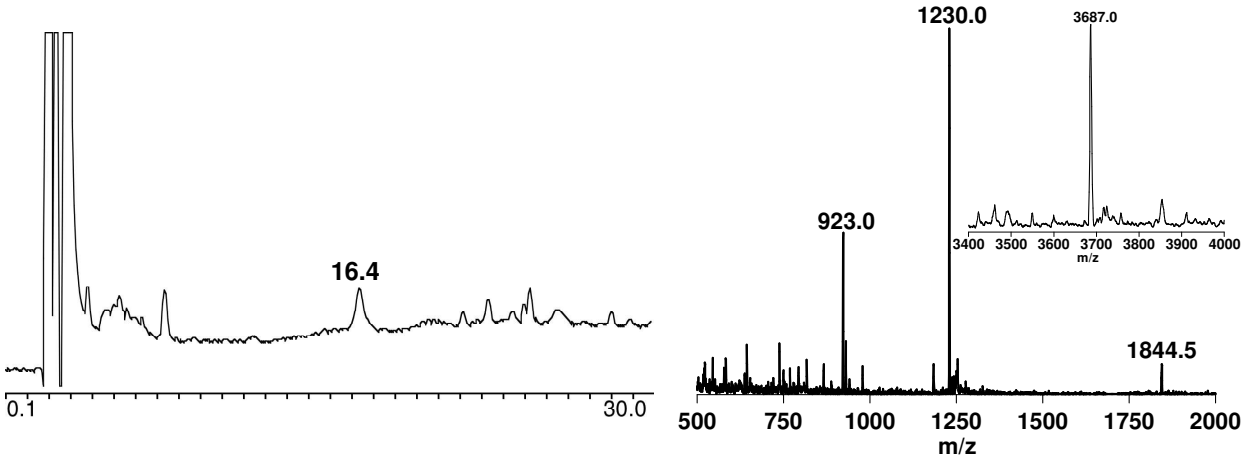

Figure S3. Crude HPLC and Ms spectrum of the compound at 16.4 min peak. The compound corresponds to the hydrolyzed maleimide form of the product. Mass calcd for $C_{173}H_{223}N_{51}O_{40}S$ $[M+H]^+$ *m/z*=3687.7, found: 3687.0

QDs (1 μM final concentration) were incubated in 50-100 mM HEPES buffer pH 7.0 with peptide **1** (30 μM) for 30 min. Following the self-assembling, aniline (~100 mM) and peptide **2** (30 μM) were added and the reaction was gently shaken overnight. Then, it was filtered through PD-10 column and the conjugate peptide **3**:QD collected. Next, imidazole (0.5 M final concentration) was added to the solution and stirred for another 5 h more. Following, the solution was spun out in a Microcon Ultracel filter (Millipore, cut off 10000) and the filtered injected in HPLC.

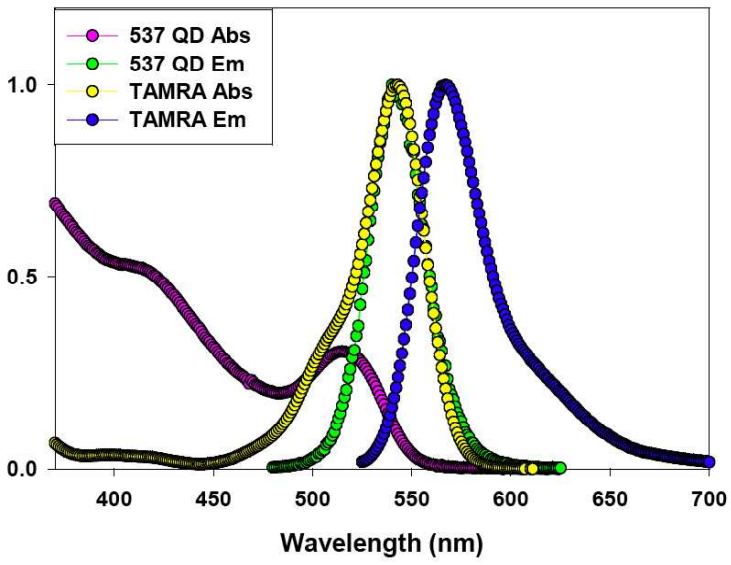

Figure S4. Spectral overlap of QDs and fluorophores used in this study. Normalized absorption and emission of 537 nm QDs and tetramethylrhodamine (TAMRA) are shown. 537 nm QDs has a quantum yield ~20%, QD ε_{350} = 520,000; TAMRA ε_{555} = 65,000. R_0 for the QD-dye pair is 5.0 nm.

Peptide:QD ligation.

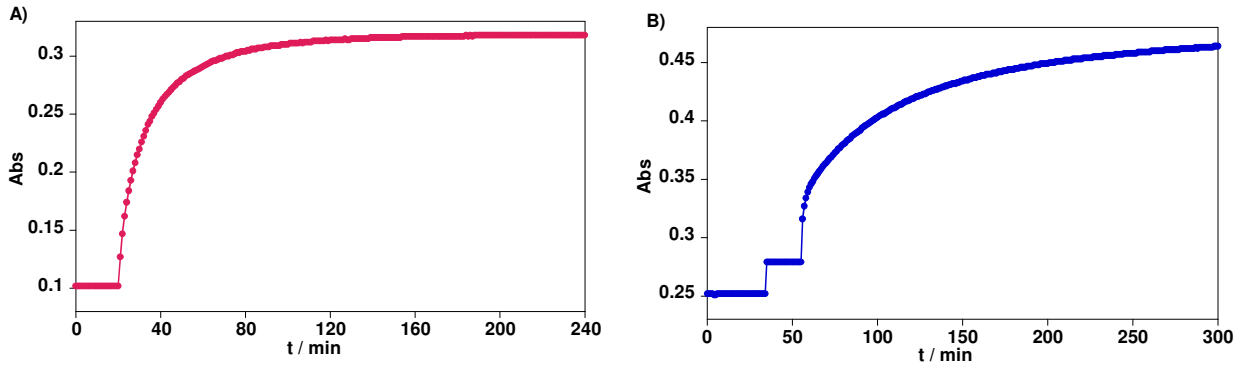

Figure S5. UV trace of the ligation reactions: A) between **1** (22 µM) and **2** (14.9 µM) in presence of 100 mM of aniline and absence of QDs. B) between **1** (21 µM) self-assembled to QDs (0.9 µM) and **2** (14 µM) in presence of ~100 mM of aniline: first 34 min complex peptide **1**:QDs, followed by the addition of peptide **2**. Aniline was added to reaction mixtures at 20 min after addition of peptide **2** .

Absorbance was normalized by subtracting the contribution of the QDs and TAMRA absorptions (aniline does not absorb at 354 nm), followed by dividing by the highest abs value (end time point) and multiplying the result by the conversion percentage at that end time point (1 for reaction in absence of QDs and 0.95 with QDs).