Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary information

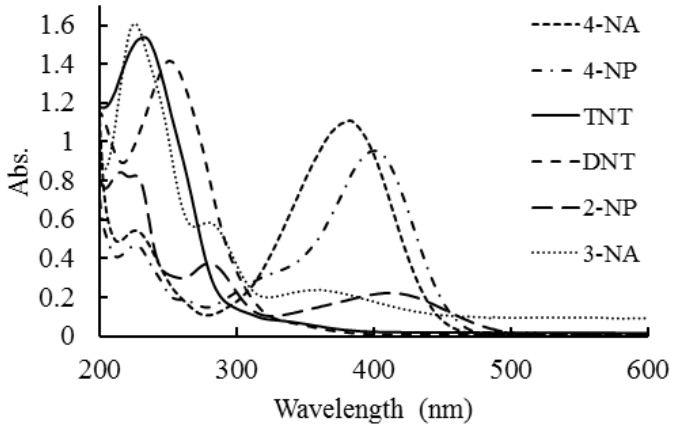

Fig. S1. Absorption Spectra of different nitro-compound at the same concentration (pH=7.4).

Table S1. The Stern-Volmer constants and R-square values for CQDs and CdTe QDs in the presence of nitro-compounds.

	CQD		CdTe	
	K_{SV}	R^2	K_{SV}	R^2
2-NP	0.0037	0.9969	0.0093	0.9673
3-NA	0.0038	0.9910	0.0098	0.9808
4-NA	0.0262	0.9910	0.0401	0.9823
4-NP	0.0171	0.9961	0.0255	0.9862
DNT	0.0011	0.9734	0.0260	0.9890
TNT	0.0013	0.9927	0.0523	0.9409

M-file

All calculations were performed in MATLAB 7.5.0. As an example, the program codes (M-file) used to simulate the fluorescence quenching data sets for *case II* in the Table 1 and with the spectral overlapping in the emission spectra is presented in the following M-file. This M-file simulate the fluorescence quenching of *F1*, *F2* and hybrid of *F1-F2* in the presence of *Q1* (using eq. (2)) and in the presence of both *Q1* and *Q2* (using eq. (3)).

```
clear
clc
x=400:700;                          % wavelength (nm)
I0(1,:)=gaussmf(x,[40 510]);        % emission spectra of F1
I0(2,:)=gaussmf(x,[40 590]);        % emission spectra of F2
Ksv11=2;                            % Stern-Volmer constant for complex formation of F1 with Q1
Ksv12=0.5;                          % Stern-Volmer constant for complex formation of F1 with Q2
Ksv21=0.5;                          % Stern-Volmer constant for complex formation of F2 with Q1
Ksv22=2;                            % Stern-Volmer constant for  complex formation of F2 with Q2

%%%% fluorescence quenching of F1, F2 and hybrid of F1-F2 in the presence of Q1
Q1=[0:0.1:1]';                      % concentration of Q1

for i=1:length(Q1)
    I_F1(i,:)=I0(1,:)./(1+Ksv11*Q1(i));
    I_F2(i,:)=I0(2,:)./(1+Ksv21*Q1(i));
    I_hybride(i,:)= I_F1(i,:)+I_F2(i,:);
end

figure(1),plot(x, I_F1,'b'), title('fluorescence quenching of F1 in the presence of Q1')
figure(2),plot(x, I_F2,'b'), title('fluorescence quenching of F2 in the presence of Q1')
figure(3),plot(x, I_hybride,'b'), title('fluorescence quenching of F1-F2 hybrid in the presence of Q1')

%%%% fluorescence quenching of hybrid of F1-F2 in the presence of Q1 and Q2
%%%% 36 spectrum according to a full factorial design for six concentration levels of Q1 and Q2
Q1=[0:0.2:1]';                      % concentration of Q1
Q2=[0:0.2:1]';                      % concentration of Q2
[C1,C2]=meshgrid(Q1,Q2);

for i=1:length(C1(:))
    I_F1(i,:)=I0(1,:)./(1+Ksv11*C1(i)+ Ksv12*C2(i));
    I_F2(i,:)=I0(2,:)./( 1+Ksv21*C1(i)+ Ksv22*C2(i));
    I_hybride(i,:)= I_F1(i,:)+I_F2(i,:);
end

figure(4),plot(x, I_F1,'b'), title('fluorescence quenching of F1 in the presence of Q1 and Q2')
figure(5),plot(x, I_F2,'b'), title('fluorescence quenching of F2 in the presence of Q1 and Q2')
figure(6),plot(x, I_hybride,'b'), title('fluorescence quenching of F1-F2 hybrid in the presence of Q1 and
Q2')
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For simulating the data with different selectivity and spectral overlapping cases, the values of *Ksv* and peak maxima of the spectra were changed according to the Table 1 and Fig. 1, respectively. For simulating of validation set the concentration of Q1 and Q2 were changed to [0.1; 0.3; 0.5]. White noise with a standard deviation of 0.1% of the maximum values of data was added to all simulated data sets. (**I=I+(0.001*max(max(I))*randn(size(I)))**