Determination of Particle Size Distribution of Water-Soluble CdTe Quantum Dots by Optical Spectroscopy

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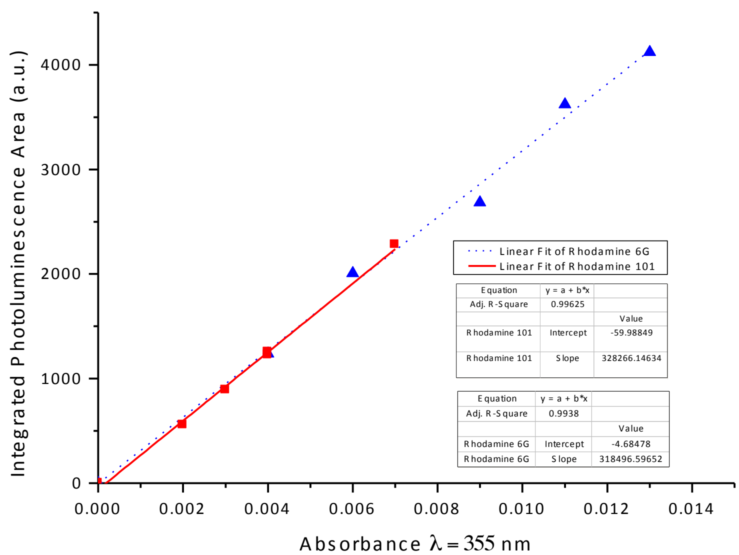

Figure S1. Calibration curves for the fluorescence quantum yield of rhodamine 6G (97%) in aqueous media by using rhodamine 101(100%) as reference.

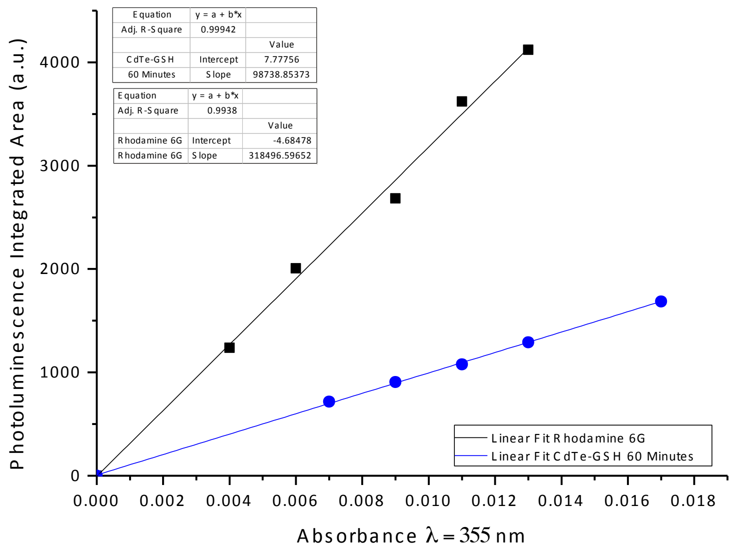

Figure S2. Calibration curves for the fluorescence quantum yield of rhodamine 6G (97%) and CdTe-GSH (60 minutes of synthesis) in aqueous media.

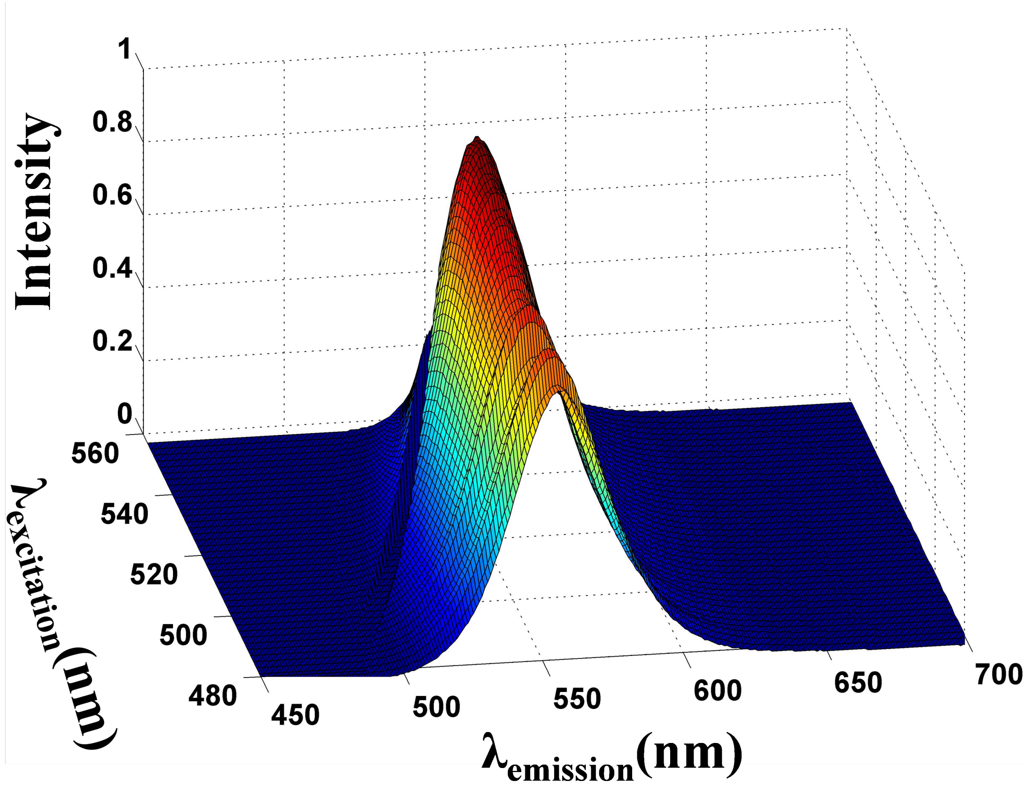

Figure S3. Fluorescence spectra of CdTe QDs (30 minutes of synthesis) obtained after excitation at different wavelengths.

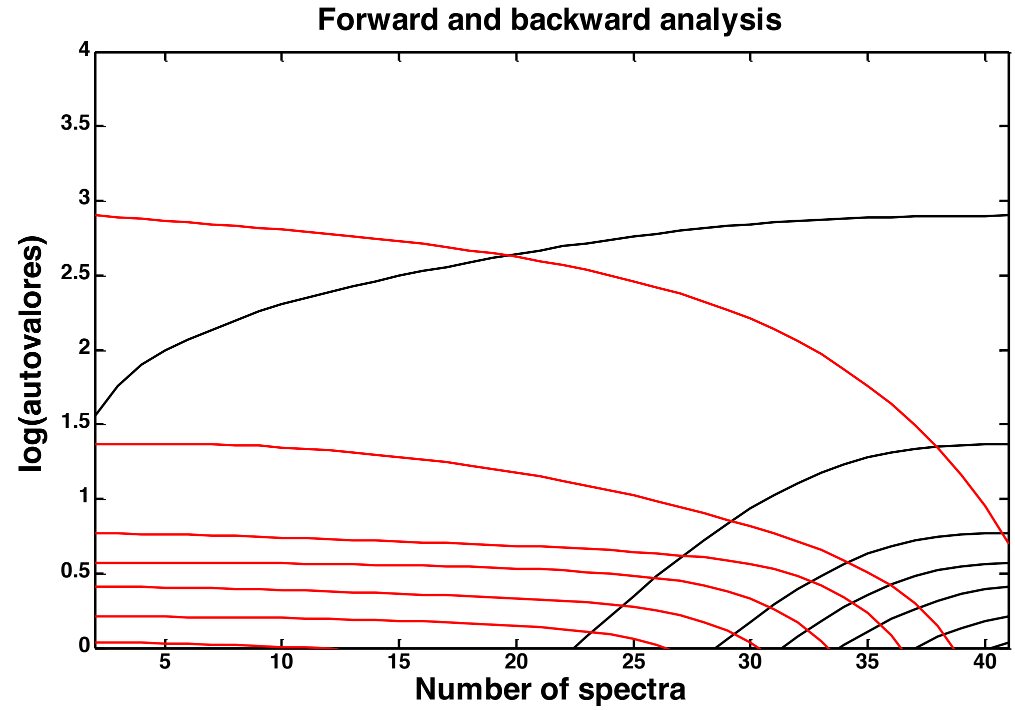

Figure S4. Forward and backward analysis for the CdTe QDs (30 minutes of synthesis).

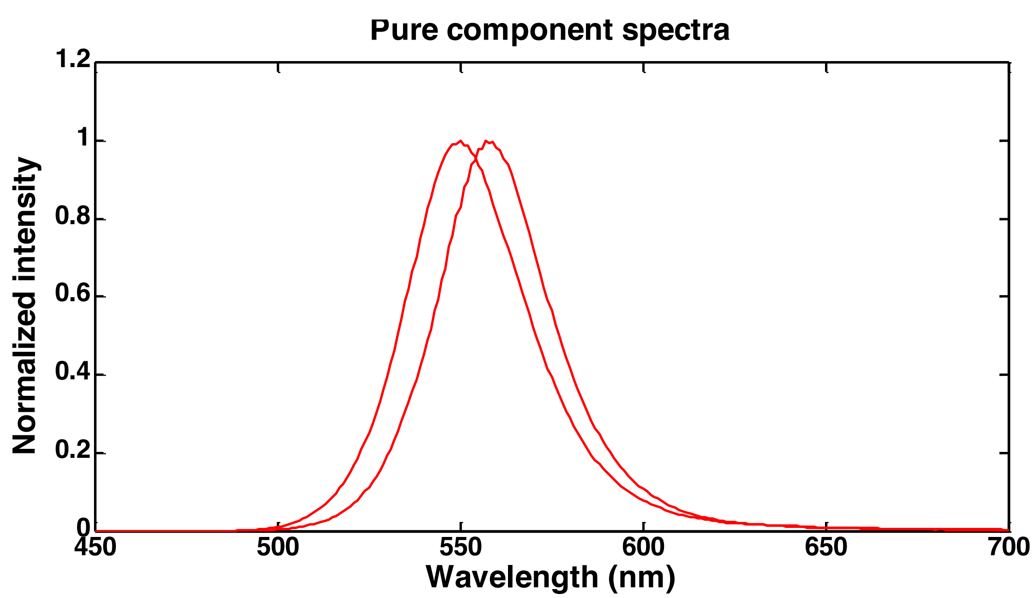

Figure S5. Pure component spectra obtained from the EFA-MCR method for the CdTe QDs (30 minutes of synthesis).

QDs size dispersion program

```
clear all;
format long;
%Graphic parameters
COR=['b' 'g' 'r' 'c' 'm' 'y' 'k'];k=7;
cor=COR(k);
ft=14;
aa=2.0;
axy=2.0;
ttitulo=11;
awords=1.5;
%**********************************************************************
%**********************************************************************
%Pathway
p=path;
path(p,'put the pathway');

arq_I=load('put the matrix M (n,m)');
arq_lamb=load('put the matrix W(m)');
arq_exc=load('put the excitation wavelength matrix');
arq_A=load('put the absorption spectrum data');
arq_lamp=load('put the lamp data intensity');

IF_exp= arq_I';
lamb_exp= arq_lamb';
lamb_exc=arq_exc(:)';
lamb_abs=arq_A(1,:)';
A_exp=arq_A(2,:) ';
I_lamp=arq_lamp(2,:)';
lamb_lamp=arq_lamp(1,:)';
%**********************************************************************
% Filter routine
N=length(A_exp);
N1=length(I_lamp);
[m,n]=size(IF_exp);
lamb_fluo_ini=lamb_exp(1);

for i=1:m
    for j=1:n
        if(lamb_exc(i)>lamb_fluo_ini)
            if((lamb_exc(i)>=((lamb_exp(j)+2)-7)) && lamb_exc(i) <=
((lamb_exp(j)+2)+0))
              M_aux(i,j)=IF_exp(i,j);
            else
                M_aux(i,j)=0.0;
            end
      end

    end
end
```

```
for i=1:m
   for j=1:n
     M_aux_2(i,j)=IF_exp(i,j)-M_aux(i,j);
    end
end

M_aux_2=IF_exp;

%****************************************************************
% Obtaining the absorbance value corresponding to the excitation wave-
length
for i=1:m
    for j=1:N
      if lamb_abs(j)==lamb_exc(i)
         A_exp_aux(i)=A_exp(j)+0.001;
      end
    end
end

%Storing the lamp data
lamb_lamp=round(lamb_lamp);
count=0.0;
AS=mean(I_lamp);
for i=1:m
   for j=1:N1
      if (lamb_lamp(j)==lamb_exc(i))
         I_lamp_aux(i)=I_lamp(j);
      end
   end
end

I_lamb_aux=I_lamp_aux/max(I_lamp_aux);

for i=1:m
          IF_exp_max(i)=max(IF_exp(i,:));

end

% Introducing the calibration curve (diameter versus fluorescence peak)
and finding the wavelength that corresponds to the fluorescence peak

aux_D=0.0;
for i=1:m
   for j=1:n
       if IF_exp(i,j)==IF_exp_max(i)
           lamb_exp_aux(i)=lamb_exp(j);
       end
   end
   D(i)= put the empirical equation (diameter versus fluorescence peak);
end

%*************************************************************************
```

```
% Introducing the calibration curve "fluorescence quantum yield versus
diameter"

aux_D=0.0;
for i=1:m
   for j=1:n
       if IF_exp(i,j)==IF_exp_max(i)
           lamb_exp_aux(i)=lamb_exp(j);
       end
   end
   QY_f(i)= put the empirical equation (QY versus diameter);;
end

QY=QY_f;

%**************************************************************************
% Obtaining the percentage of QDs present in solution

L=1; %comprimento da cubeta dado em cm
for i=1:m
          Epsilon(i)=10043*(D(i)^(2.12));
          C(i)=A_exp_aux(i)/(Epsilon(i)*L); %molar
    IF_int(i)=((IF_exp_max(i))/(I_lamp_aux(i)*QY(i)*Epsilon(i)*L*C(i)));
end

Q_QDs=((IF_int)/sum(IF_int))*100;

%**************************************************************************
%Finding QDs with the same diameter and adding them

j_aux=0.0;
count=0.0;
for i=1:m
    for j=1:m
       if(j~=i)
          if (j~=j_aux)
              if(D(j)==D(i))
               count=count+1.0;
               aux_D_s(count)=D(j);
               j_aux(count)=j;
               Q_QDs(i)=Q_QDs(i)+Q_QDs(j);
               Q_QDs(j)=0.0;
            end
          end
       end
    end
end



count=0.0;
for i=1:m
```

```
    if(Q_QDs(i)~=0.0)
        count=count+1.0;
        Q_QDs_aux(count)=Q_QDs(i);
        D_Q_QDs_aux(count)=D(i);
    end
end

%*************************************************************************
% Graphs
figure(1); bar(D_Q_QDs_aux,Q_QDs_aux,5,'r','linewidth',aa);hold on;
ylabel('P(%) ','fontsize',ft,'fontweight','bold');
set(h1,'linewidth',2,'fontsize',ft,'fontweight','bold');
```