Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Data

A novel carbon quantum dots for fluorescent detection of phenol and insight into the mechanism

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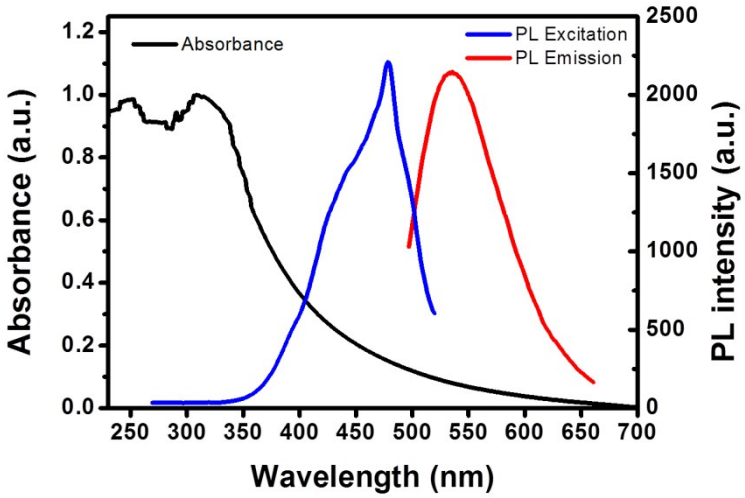

Fig. S1 UV-Vis absorption (Abs), PL excitation (Ex, λ_{em}=530 nm) and PL emission (Em, λ_{ex}=470 nm) of the CQDs (in water, pH = 7).

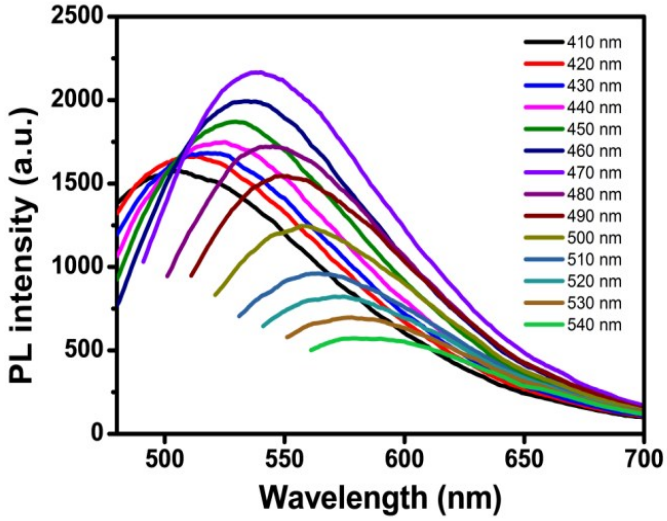

Fig. S2 The emission curves of CQDs with the different excitation wavelength from 410 nm to 540 nm (in water, pH = 7)

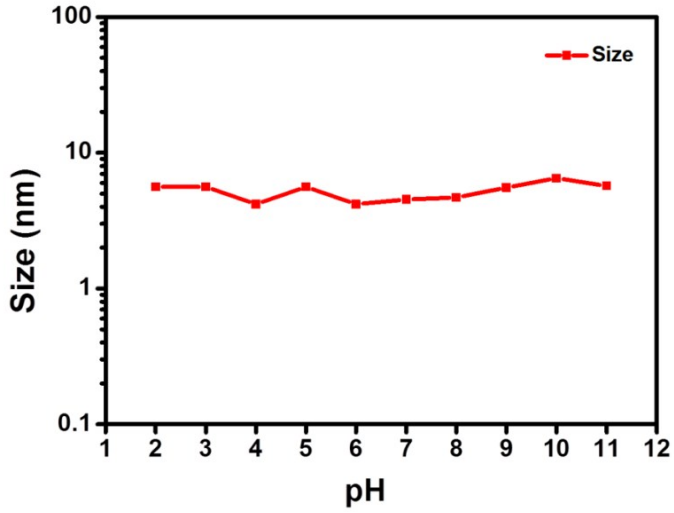

Fig. S3 The Size number of CQDs dispersed in different pH solutions

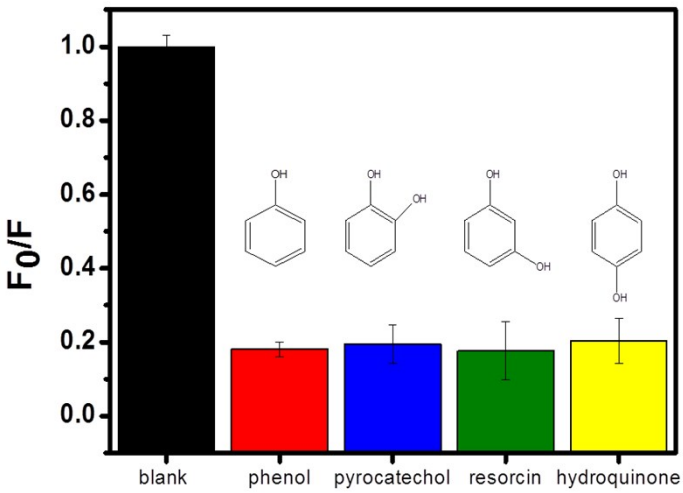

Fig. S4 fluorescence intensity ratios (F_0/F) of CQDs with phenol analogues

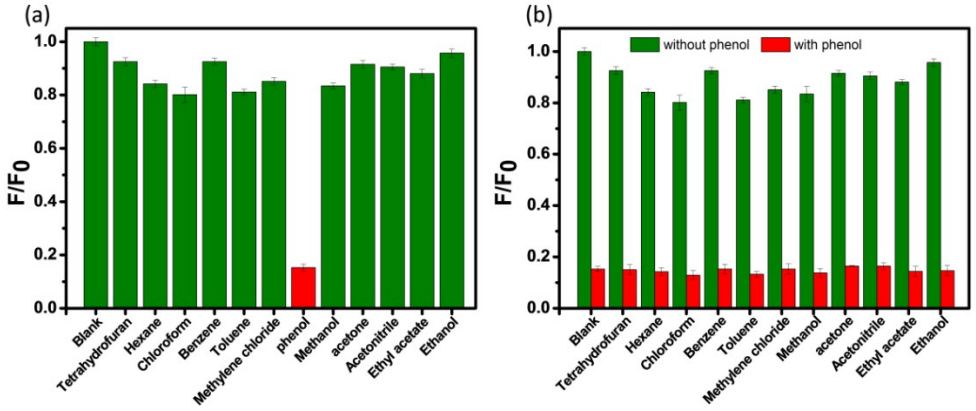

Fig. S5 (a)Fluorescence intensity ratios (F/F_0) of the CQDs in the presence and absence of different organic solvents; (b) Selectivity of CQDs toward phenol: Column diagrams of F/F_0 of CQDs-organic solvents at 530 nm. Green bars represent the addition of various organic solvents to the blank solution and red bars represent the subsequent addition of phenol to the solutions (CQDs-organic solvents- phenol) excitation wavelength at 470 nm.

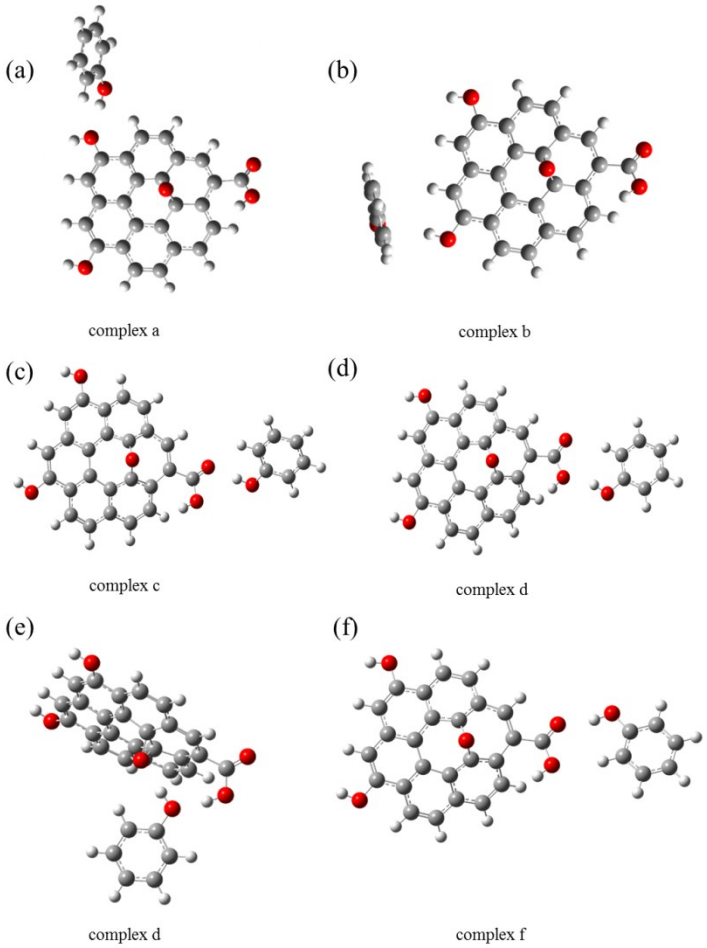

Fig. S6 Geometric optimization structure of different complexes (a-f) formed between CQDs and phenol

Table S1 The fluorescence quantum yield of CQDs

	I	*A*	η	*Φ* / %
Quinine sulfate	760863.603	0.0673	1.41	54.0
CQDs	175891.121	0.0598	1.33	12.5

Table S2 Comparison of different methods for phenol detection

Methods	Detection limit (μ M)	Ref
UV-vis	0.6	[1]
Electrochemistry	0.07	[2]
HPLC	0.03	[3]
CdTe QDs	0.5	[4]
Graphene quantum dots	1.27	[5]
Carbon quantum dots	0.076	This work

Table S3 The energies of six complexes and its relative values

	Energy (a.u.)	Relative values (a.u.)	Relative values (Kcal/mol)
complex a	-1643.49239	0.0001	0.1
complex b	-1643.48979	0.003	1.8
complex c	-1643.472988	0.019	12
complex d	-1643.48522	0.007	4.4
complex e	-1643.475889	0.016	10
complex f	-1643.49256	0	0

Table S4 the electronic excitation energies of CQDs and **complex**

Excited states	CQDs (eV)	**complex** (eV)
S_1	2.5184	2.4249
S_2	2.7745	2.9170
S_3	3.2667	2.9473
S_4	3.4593	3.2060
S_5	3.5969	3.3138
S_6	3.8016	3.4031
S_7	3.9017	3.4724
S_8	4.0014	3.5764
S_9	4.1175	3.7679
S_{10}	4.1940	3.9073

Table S5 The bond length and ^{1}H NMR chemical shifts for hydrogen bond in S_0 and S_1 state.

	S_0	S_1
Bond lengths/ Å		
C38=O41···H55-O54	1.89	1.57
^{1}H NMR/ ppm		
H55	23.14	17.87

References:

1. Y. Ni, Z. Xia and S. Kokot, A kinetic spectrophotometric method for simultaneous determination of phenol and its three derivatives with the aid of artificial neural network, *J Hazard Mater*, 2011, **192**, 722-729.
2. B. C. Janegitz, R. A. Medeiros, R. C. Rocha-Filho and O. Fatibello-Filho, Direct electrochemistry of tyrosinase and biosensing for phenol based on gold nanoparticles electrodeposited on a boron-doped diamond electrode, *Diam Relat Mater*, 2012, **25**, 128-133.
3. M. O. A. S. Ramiz S. J. Alkasir, Colorimetric paper bioassay for the detection of phenolic compounds, *Anal Chem*, 2012, **84**, 9729-9737.
4. J. Yuan, W. Guo and E. Wang, Utilizing a CdTe quantum dots−enzyme hybrid system for the determination of both phenolic compounds and hydrogen peroxide, *Anal Chem*, 2008, **80**, 1141-1145.

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