

Supporting Information

Inhibitory effects of iron-based carbonaceous nanocomposites on mushroom tyrosinase activity: molecular aspects and mechanistic insights.

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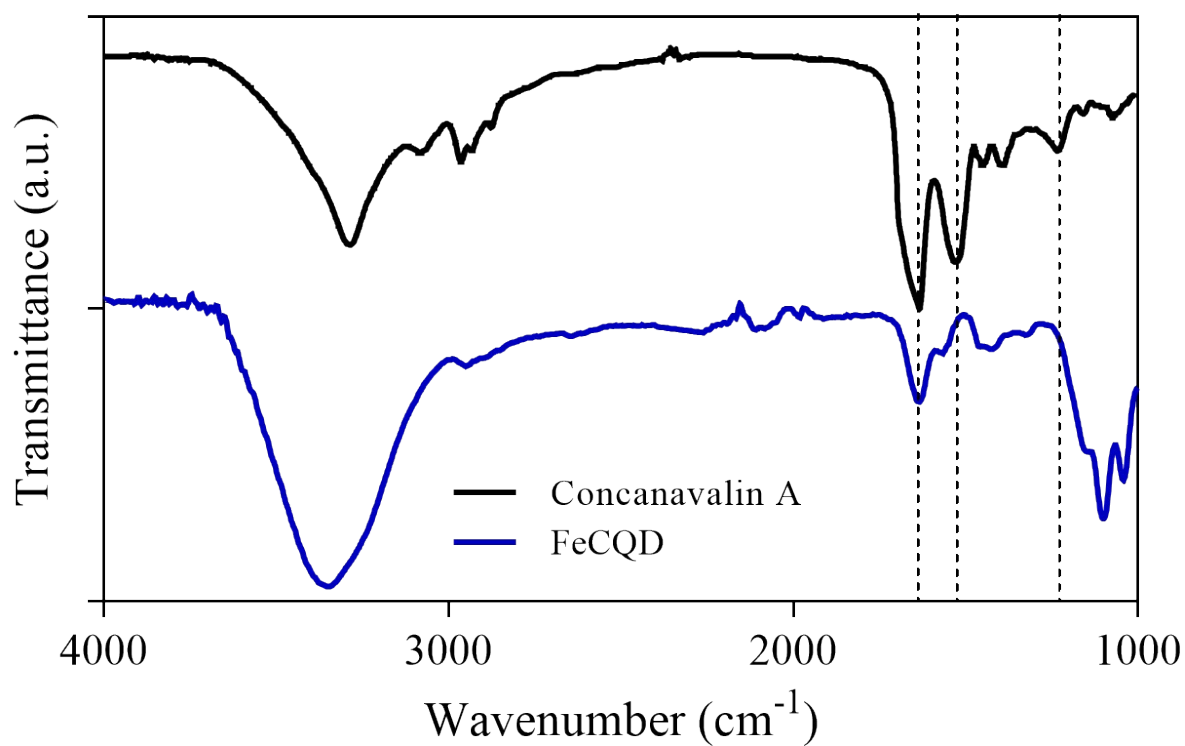


Figure S1. FTIR spectra of the protein Concanavalin A (red) and the synthesized CDs (blue), showing similarities and differences between the spectra.

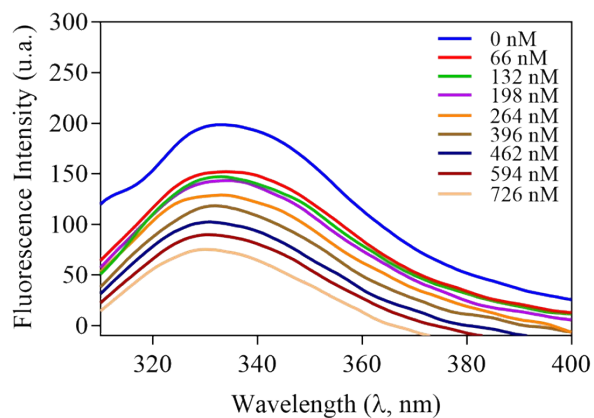
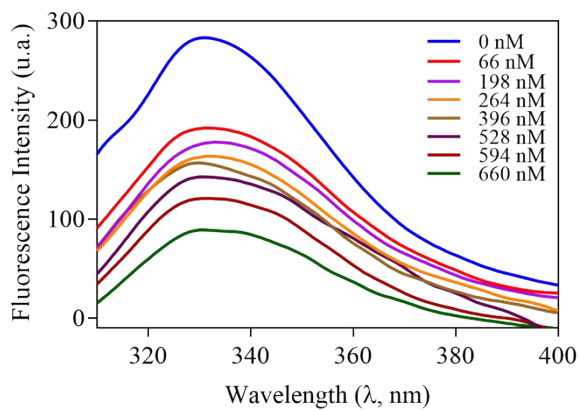


Figure S2. Fluorescence quenching of Tyrosinase by CDs in two temperatures: 303K(a), and 313K(b); showing the fluorescence intensity decrease due to the CDs titration.

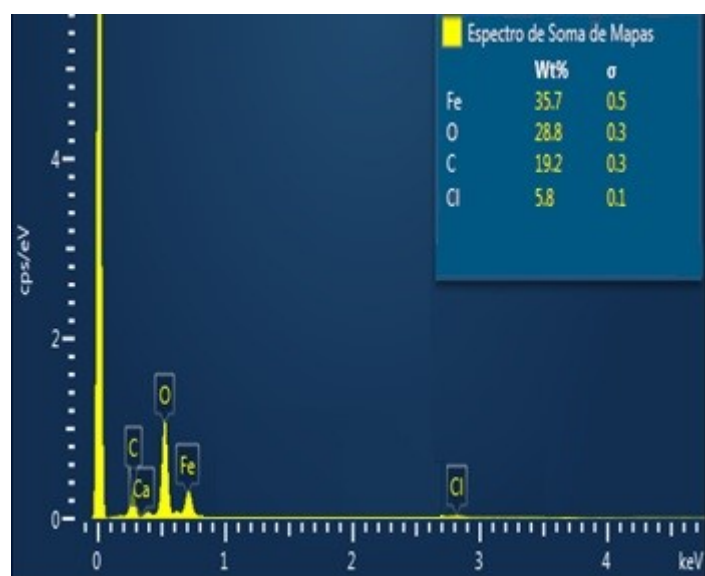


Figure S3: EDS spectrum of FeCQD.

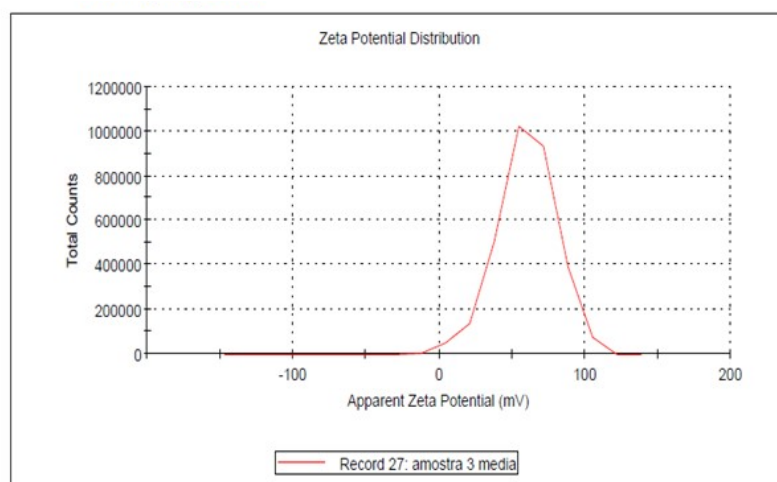


Figure S4: Zeta potential of FeCQD in PBS.

Supplementary Script: *Color_h*.

This code can be found at https://pymolwiki.org/index.php/Color_h

```
# color_h
# -----

# PyMOL command to color protein molecules according to the Eisenberg
hydrophobicity scale

#

# Source: http://us.expasy.org/tools/pscale/Hphob.Eisenberg.html
# Amino acid scale: Normalized consensus hydrophobicity scale
# Author(s): Eisenberg D., Schwarz E., Komarony M., Wall R.
# Reference: J. Mol. Biol. 179:125-142 (1984)
#

# Amino acid scale values:
#

# Ala: 0.620
# Arg: -2.530
# Asn: -0.780
# Asp: -0.900
# Cys: 0.290
# Gln: -0.850
# Glu: -0.740
# Gly: 0.480
# His: -0.400
# Ile: 1.380
# Leu: 1.060
# Lys: -1.500
# Met: 0.640
# Phe: 1.190
```

```
# Pro: 0.120
# Ser: -0.180
# Thr: -0.050
# Trp: 0.810
# Tyr: 0.260
# Val: 1.080
#
# Usage:
# color_h (selection)
#
from pymol import cmd

def color_h(selection='all'):
    s = str(selection)
    print(s)
    cmd.set_color('color_ile', [0.996, 0.062, 0.062])
    cmd.set_color('color_phe', [0.996, 0.109, 0.109])
    cmd.set_color('color_val', [0.992, 0.156, 0.156])
    cmd.set_color('color_leu', [0.992, 0.207, 0.207])
    cmd.set_color('color_trp', [0.992, 0.254, 0.254])
    cmd.set_color('color_met', [0.988, 0.301, 0.301])
    cmd.set_color('color_ala', [0.988, 0.348, 0.348])
    cmd.set_color('color_gly', [0.984, 0.394, 0.394])
    cmd.set_color('color_cys', [0.984, 0.445, 0.445])
    cmd.set_color('color_tyr', [0.984, 0.492, 0.492])
    cmd.set_color('color_pro', [0.980, 0.539, 0.539])
    cmd.set_color('color_thr', [0.980, 0.586, 0.586])
    cmd.set_color('color_ser', [0.980, 0.637, 0.637])
```

```
cmd.set_color('color_his', [0.977, 0.684, 0.684])
cmd.set_color('color_glu', [0.977, 0.730, 0.730])
cmd.set_color('color_asn', [0.973, 0.777, 0.777])
cmd.set_color('color_gln', [0.973, 0.824, 0.824])
cmd.set_color('color_asp', [0.973, 0.875, 0.875])
cmd.set_color('color_lys', [0.899, 0.922, 0.922])
cmd.set_color('color_arg', [0.899, 0.969, 0.969])
cmd.color("color_ile", ("s" and resn ile))
cmd.color("color_phe", ("s" and resn phe))
cmd.color("color_val", ("s" and resn val))
cmd.color("color_leu", ("s" and resn leu))
cmd.color("color_trp", ("s" and resn trp))
cmd.color("color_met", ("s" and resn met))
cmd.color("color_ala", ("s" and resn ala))
cmd.color("color_gly", ("s" and resn gly))
cmd.color("color_cys", ("s" and resn cys))
cmd.color("color_tyr", ("s" and resn tyr))
cmd.color("color_pro", ("s" and resn pro))
cmd.color("color_thr", ("s" and resn thr))
cmd.color("color_ser", ("s" and resn ser))
cmd.color("color_his", ("s" and resn his))
cmd.color("color_glu", ("s" and resn glu))
cmd.color("color_asn", ("s" and resn asn))
cmd.color("color_gln", ("s" and resn gln))
cmd.color("color_asp", ("s" and resn asp))
cmd.color("color_lys", ("s" and resn lys))
cmd.color("color_arg", ("s" and resn arg))

cmd.extend('color_h', color_h)
```



```
def color_h2(selection='all'):  
    s = str(selection)  
    print(s)  
    cmd.set_color("color_ile2", [0.938, 1, 0.938])  
    cmd.set_color("color_phe2", [0.891, 1, 0.891])  
    cmd.set_color("color_val2", [0.844, 1, 0.844])  
    cmd.set_color("color_leu2", [0.793, 1, 0.793])  
    cmd.set_color("color_trp2", [0.746, 1, 0.746])  
    cmd.set_color("color_met2", [0.699, 1, 0.699])  
    cmd.set_color("color_ala2", [0.652, 1, 0.652])  
    cmd.set_color("color_gly2", [0.606, 1, 0.606])  
    cmd.set_color("color_cys2", [0.555, 1, 0.555])  
    cmd.set_color("color_tyr2", [0.508, 1, 0.508])  
    cmd.set_color("color_pro2", [0.461, 1, 0.461])  
    cmd.set_color("color_thr2", [0.414, 1, 0.414])  
    cmd.set_color("color_ser2", [0.363, 1, 0.363])  
    cmd.set_color("color_his2", [0.316, 1, 0.316])  
    cmd.set_color("color_glu2", [0.27, 1, 0.27])  
    cmd.set_color("color_asn2", [0.223, 1, 0.223])  
    cmd.set_color("color_gln2", [0.176, 1, 0.176])  
    cmd.set_color("color_asp2", [0.125, 1, 0.125])  
    cmd.set_color("color_lys2", [0.078, 1, 0.078])  
    cmd.set_color("color_arg2", [0.031, 1, 0.031])  
    cmd.color("color_ile2", "("+s+" and resn ile)")  
    cmd.color("color_phe2", "("+s+" and resn phe)")  
    cmd.color("color_val2", "("+s+" and resn val)")  
    cmd.color("color_leu2", "("+s+" and resn leu)")
```

```
cmd.color("color_trp2", "("+s+" and resn trp)")
cmd.color("color_met2", "("+s+" and resn met)")
cmd.color("color_ala2", "("+s+" and resn ala)")
cmd.color("color_gly2", "("+s+" and resn gly)")
cmd.color("color_cys2", "("+s+" and resn cys)")
cmd.color("color_tyr2", "("+s+" and resn tyr)")
cmd.color("color_pro2", "("+s+" and resn pro)")
cmd.color("color_thr2", "("+s+" and resn thr)")
cmd.color("color_ser2", "("+s+" and resn ser)")
cmd.color("color_his2", "("+s+" and resn his)")
cmd.color("color_glu2", "("+s+" and resn glu)")
cmd.color("color_asn2", "("+s+" and resn asn)")
cmd.color("color_gln2", "("+s+" and resn gln)")
cmd.color("color_asp2", "("+s+" and resn asp)")
cmd.color("color_lys2", "("+s+" and resn lys)")
cmd.color("color_arg2", "("+s+" and resn arg)")

cmd.extend('color_h2',color_h2)
```