Supplementary material

Green electrochemical nanosensor platform design for mexiletine detection based on *Citrus reticulata* peels mediated iron nanoparticles and quantum dots and investigation of adsorption mechanism by DFT-D3 method

Ipek Kucuk[1,2], Cigdem Kanbes-Dindar[1], Didem Nur Unal[1,2], Burcin Bozal-Palabiyik[1], Arzu Karayel[3]*, Bengi Uslu[1]*

[1]Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06560, Ankara, Türkiye
[2]Ankara University, The Graduate School of Health Sciences, 06110, Ankara, Türkiye
[3] Hitit University, Faculty of Arts and Sciences, Department of Physics, Çorum, Türkiye

*Corresponding author email: buslu@pharmacy.ankara.edu.tr, karayelarzu@gmail.com

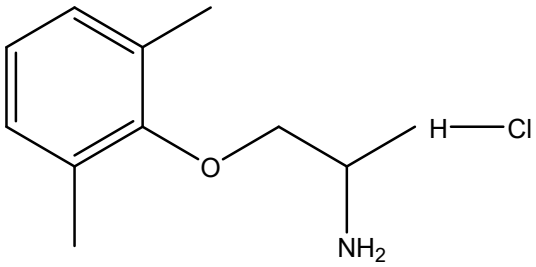

Figure. S1. Chemical structure of MXL.

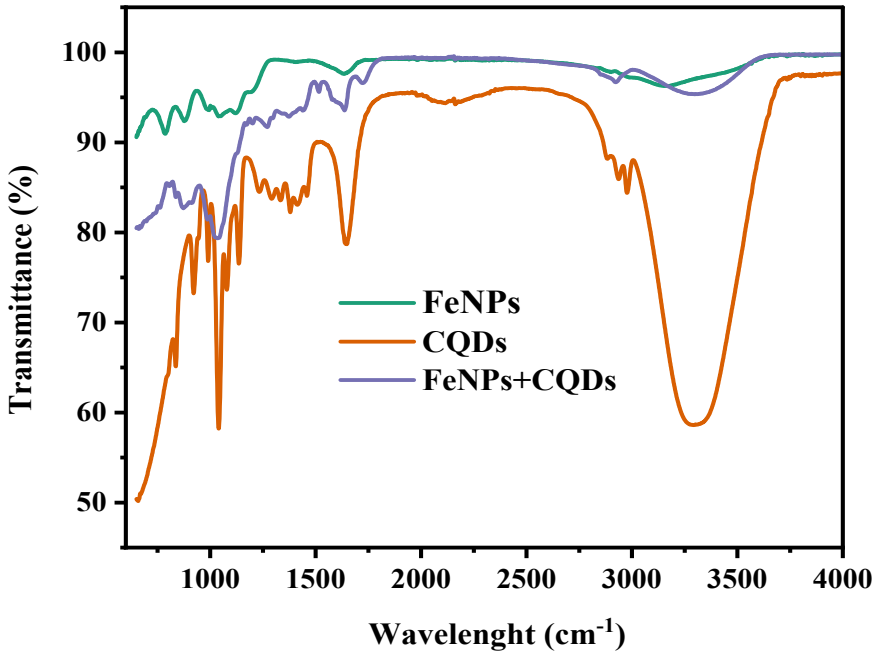

Figure. S2. FTIR spectrum of green FeNPs, CQDs and FeNPs-CQDs composite.

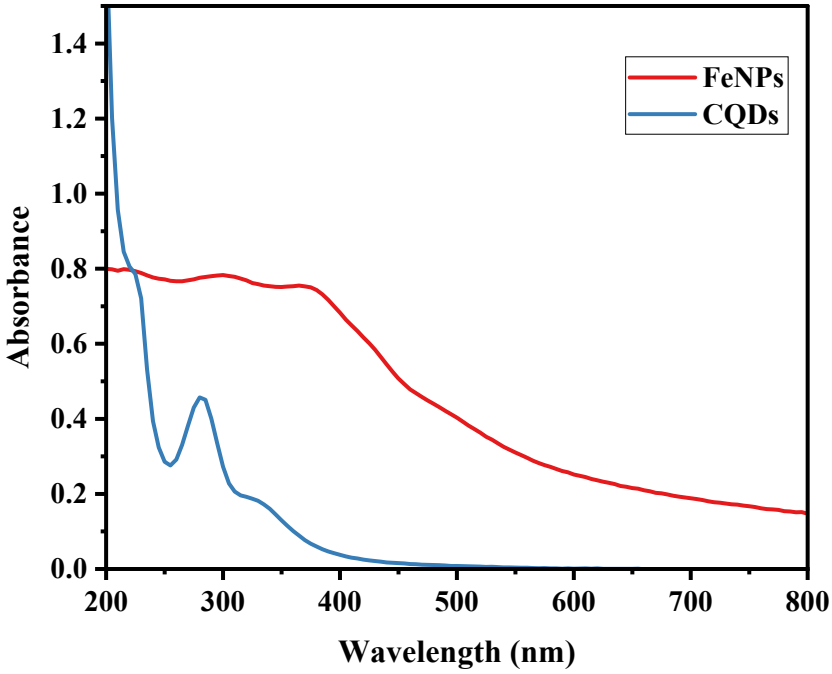

Figure. S3. UV-vis spectrum of green FeNPs and CQDs.

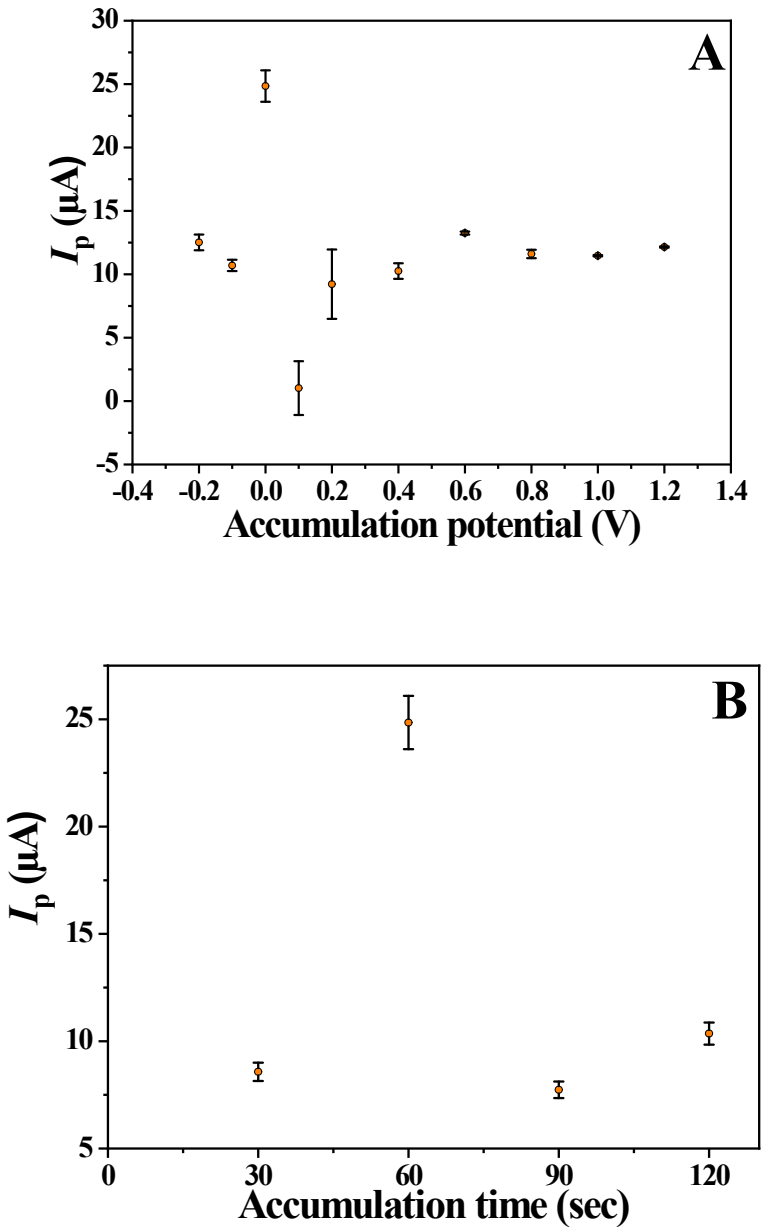

Figure. S4. Effect of accumulation potential (accumulation time: 60 s) (A) and time (accumulation potential: 0 V) (B) on MXL signal at CQDs/FeNPs/GCE.

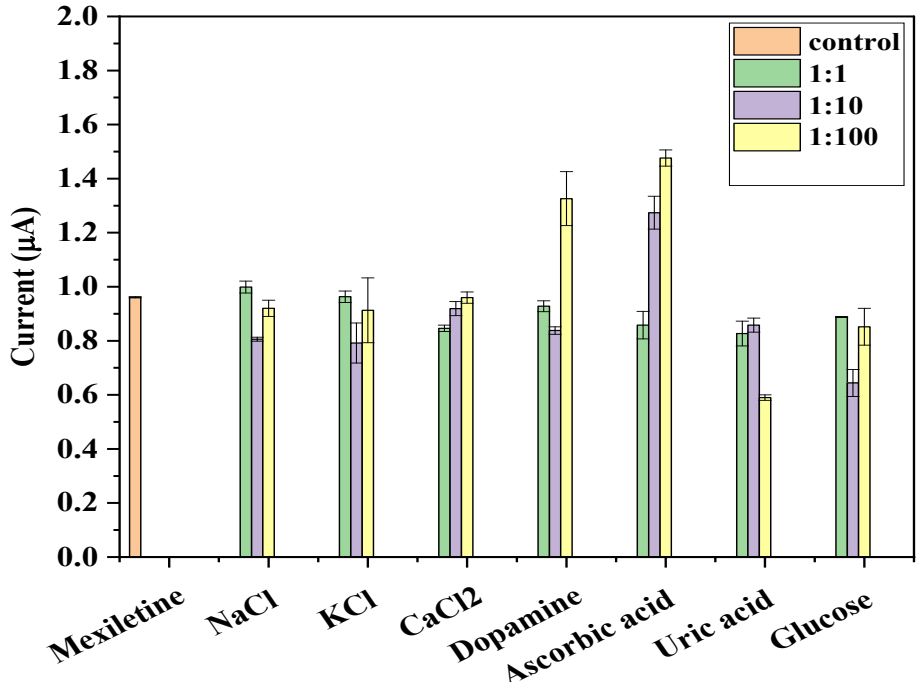

Figure. S5. Interference effect of different compounds onto the MXL signal in the molar ratio of 1:1, 1:10 and 1:100.

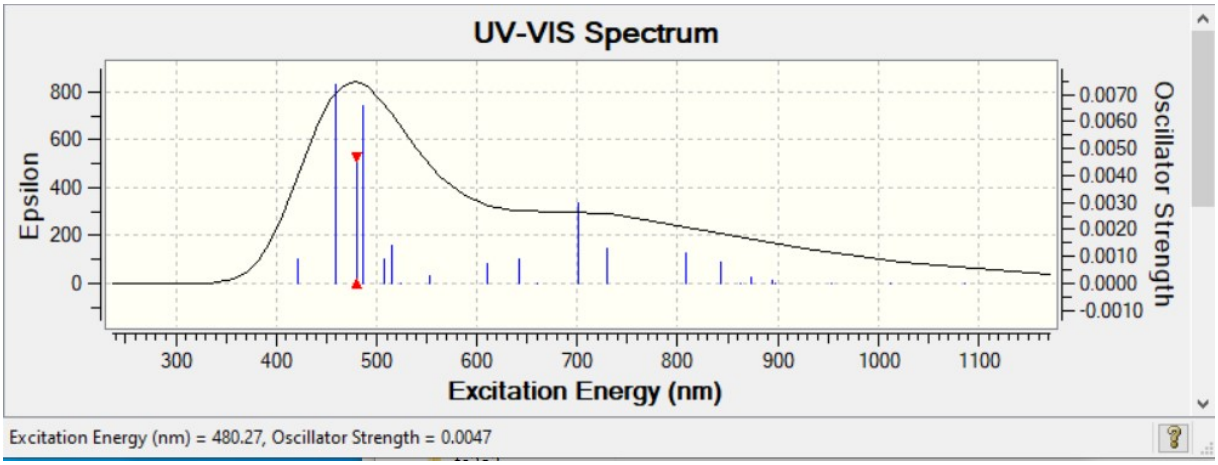

Figure. S6. Calculated UV-vis spectrum of $Fe_2O_3{-}(OH)_4$ at B3LYP-D3/LanL2DZ level.

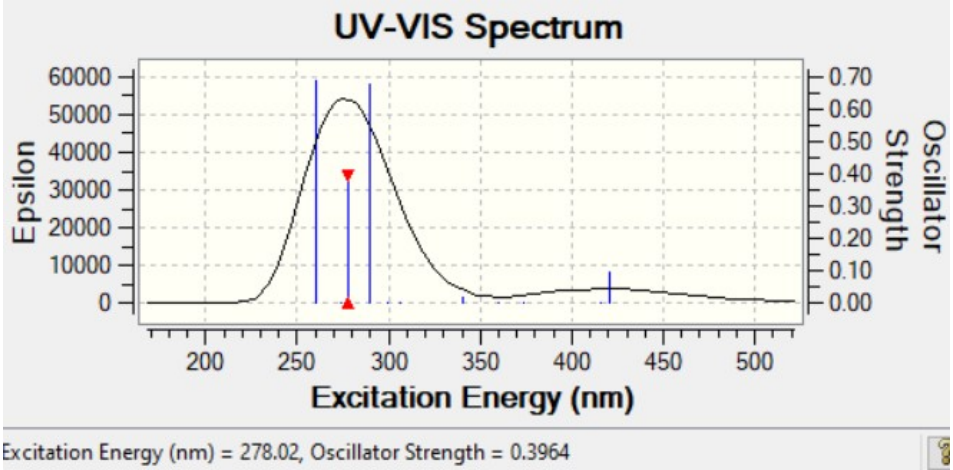

Figure. S7. Calculated UV-vis spectrum of CQDs at B3LYP-D3/LanL2DZ level.

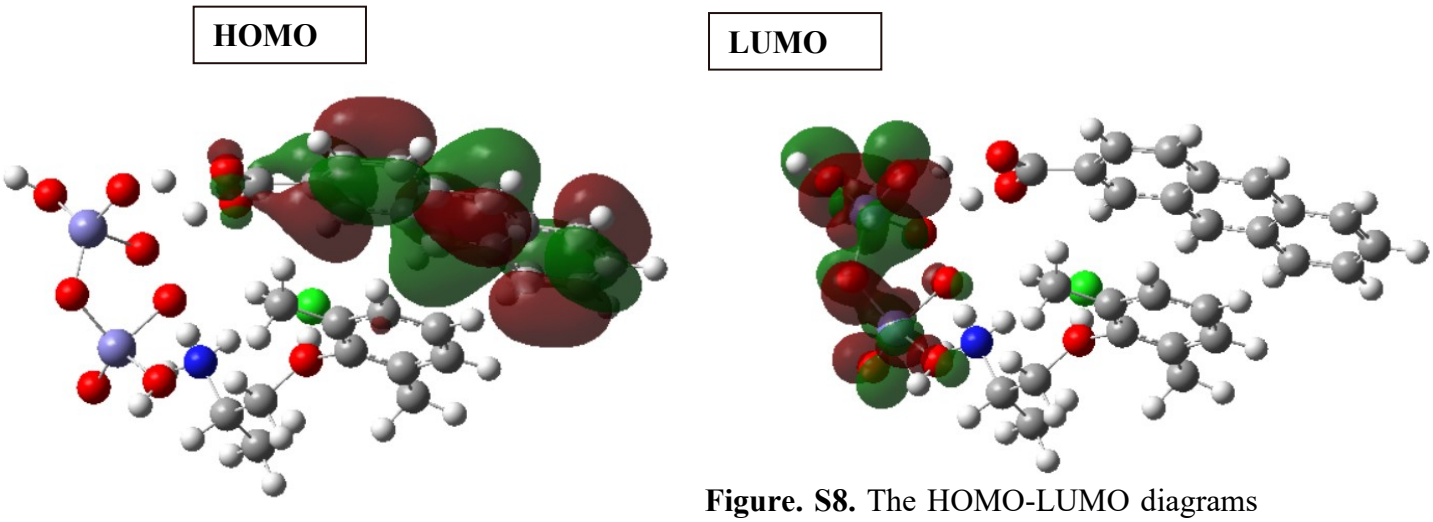

Figure. S8. The HOMO-LUMO diagrams of the complex at B3LYP-D3/LanL2DZ level in solvent phase. Atom colors: carbon in gray, nitrogen in dark-blue, oxygen in red, chlorine in green, iron in purple and hydrogen in white.

Table S1. XYZ coordinates of CQDs (X, Y, and Z in Å).

C	-2.68093400	0.07769900	0.00000600
C	-1.61922000	-0.81497400	0.00001600
C	-0.26602900	-0.34220200	0.00001100

C	-0.02119900	1.09122300	-0.00000600
C	-1.15187300	1.98426700	-0.00001600
C	-2.44120200	1.49918200	-0.00001300
C	0.82932400	-1.23138800	0.00002000
C	1.30654600	1.55972000	-0.00001200
C	2.40353200	0.67133300	-0.00000500
C	2.15853200	-0.76185500	0.00001200
C	3.28454100	-1.65788900	0.00001800
H	3.09912200	-2.73004300	0.00003200
C	4.57807100	-1.17016500	0.00000800
C	4.82031100	0.24675200	-0.00000900
C	3.76377000	1.13898300	-0.00001400
H	0.64296900	-2.30407700	0.00003700
H	-1.81477300	-1.88311200	0.00003500
H	-0.96924000	3.05649500	-0.00002700
H	-3.30045700	2.16283200	-0.00003100
H	1.49183600	2.63251800	-0.00001900
H	5.42285400	-1.85431000	0.00001000
H	5.84479900	0.61062700	-0.00001500
H	3.94759700	2.21137100	-0.00002500
C	-4.08804000	-0.38282100	0.00000600
O	-5.09160100	0.35520700	0.00008400
O	-4.21535800	-1.77101800	-0.00009000
H	-5.16582000	-2.02301000	-0.00007600

Table S2. XYZ coordinates of Fe_2O_3 NPs (X, Y, and Z in Å).

Fe	1.42973900	-0.02819300	-0.24667400
O	0.80335500	0.27148700	1.46820800
O	-0.63194900	0.21844100	1.52654700

O	-0.07043100	0.09305100	-1.02030700
Fe	-1.52958000	0.01110300	0.07543400
O	2.10949800	-1.60304800	-0.02211500
H	2.46277600	-2.05656300	-0.82585000
O	2.48346200	1.34041700	-0.33705900
H	2.54794500	1.90572900	0.46778500
O	-2.37622200	1.38243800	-0.53935700
H	-2.02219800	1.81520100	-1.35054200
O	-2.02047300	-1.60619700	-0.32897700
H	-2.77055700	-1.99274200	0.18533800

Table S3. XYZ coordinates of MXL (X, Y, and Z in Å).

C	1.85257060	1.20094442	0.30121568
C	1.02356684	0.12952308	-0.08130651
C	1.50015133	-1.12971188	-0.49938918

C	2.90041763	-1.29651141	-0.54896037
C	3.76501436	-0.24802885	-0.18404696
C	3.24583057	0.98792805	0.24304666
H	3.30822785	-2.25346927	-0.86590737
H	4.84132454	-0.39702318	-0.22353804
H	3.91871765	1.78959402	0.53871543
C	1.26689979	2.52279490	0.75680766
H	1.03937021	3.17322652	-0.10028915
H	0.33504001	2.37103266	1.31168497
H	1.97270681	3.06092831	1.39868786
C	0.54685653	-2.26049525	-0.83130680
H	-0.32692722	-1.91785547	-1.39765108
H	1.05620642	-3.04170651	-1.40579576
H	0.15759579	-2.70967653	0.09184650
O	-0.39587670	0.31610096	-0.01162579
C	-1.03646012	0.88728751	-1.23180879
C	-2.55799263	0.71177522	-1.15890179
N	-2.89569126	-0.72478187	-1.20460566
H	-3.81700705	-0.91959787	-1.58729117
H	-2.74077708	-1.21436442	-0.32357427
C	-3.17959217	1.48983500	0.03020271
H	-4.27345832	1.41847019	-0.00981392
H	-2.90329834	2.55321595	-0.00089363
H	-2.85003578	1.07188240	0.98728750
H	-0.75374540	1.94612050	-1.27473111
H	-0.63547700	0.34671242	-2.09546108
H	-2.92857565	1.15874565	-2.09438320
Cl	-1.58396219	-1.26103110	1.99161807
H	-0.99925425	-0.42608593	0.94553249