

Supporting information

# A Novel Ferrocene-linked Thionine as a Dual Redox Mediator for the Electrochemical Detection of Dopamine and Hydrogen Peroxide

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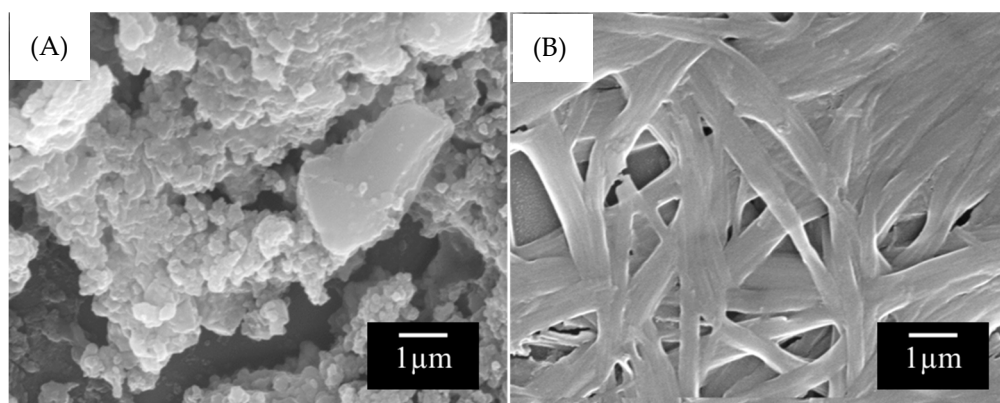
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**Figure S1.** SEM images of (A) FcDA, and (B) TH.

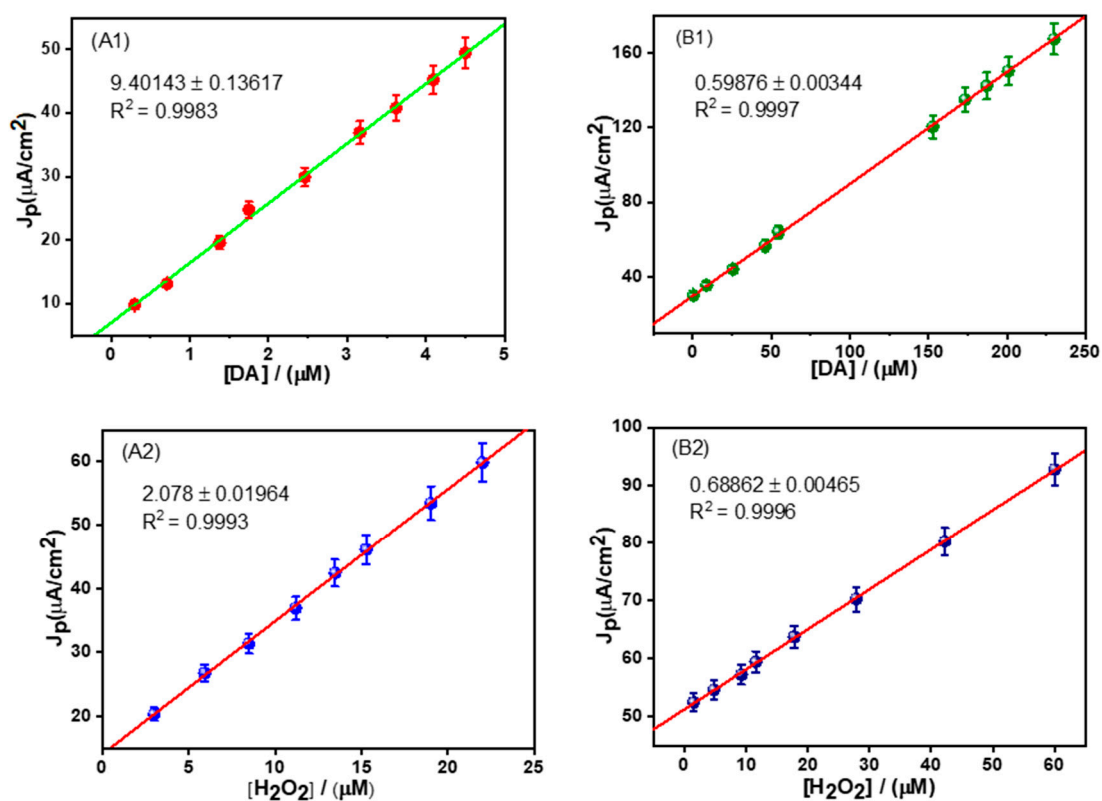
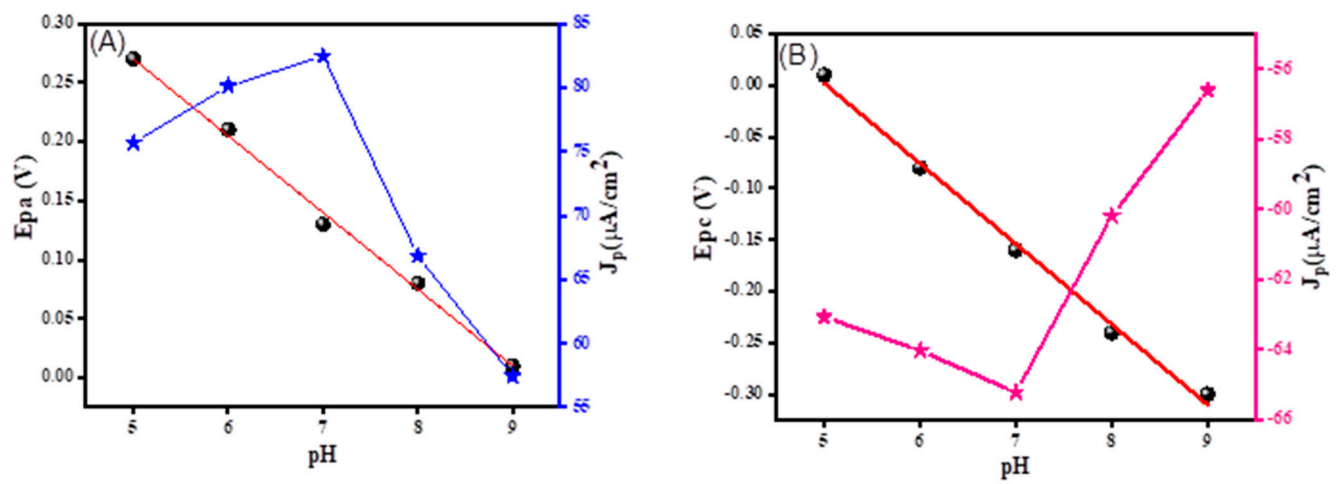
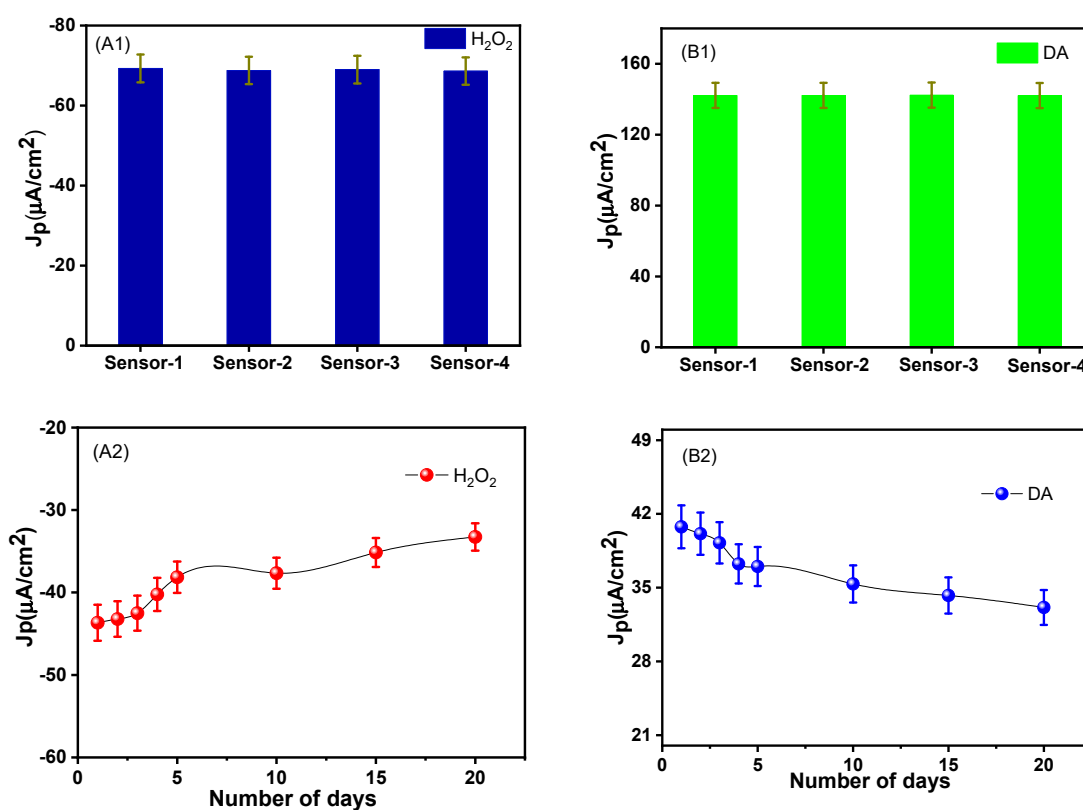


Figure S2. Linear plot for different concentrations of DA (A1, B1) and  $H_2O_2$  (A2, B2) measured from Figure 4.



**Figure S3.** Linear plot for different pH in the detection of DA (A) and H<sub>2</sub>O<sub>2</sub> (B) measured from Figure 5(B1,B2).



**Figure S4.** Reproducibility and Stability of GC/TH-FcDA electrode in the presence of  $H_2O_2$  (A1,A2) and DA

(B1,B2)

**Table S1.** A. Comparison of analytical parameters for DA detection at GC/TH-FcDA. B. Comparison of analytical parameters for  $H_2O_2$  detection at GC/TH-FcDA.

A						
Modified electrode Material	Technique	Linear range (μM)	LOD (μM)	Sensitivity (μM/μA/cm²)	Electrolyte	Ref
Fe <sub>3</sub> O <sub>4</sub> @APTES/SPCE	DPV	1-200	0.034	-	pH 6.5	12
L <sub>j</sub> -LaMnO <sub>3</sub> /GCE	CA	1-600	0.032	1	0.1 M KOH	13
Cu/Cu <sub>x</sub> O NPs/PGE	DPV	0.3-53	1.07	0.51	pH 5.8	14
GO/WO <sub>3</sub> /GCE	CA	0.3 -1245	0.306	0.392	pH 7	15
Graphene-GQDs/GCE	DPV	0.1-100	0.03	14.25	pH 6	16

La-doped MTO/GCE	CA	5 - 50	1.32	-	pH 7	17
MoS <sub>2</sub> /CC	CV	250 – 4000	0.3	0.77	pH 7.4	18
GCE/Poly(Co-TABAPc)	CV	0.1–4	30	0.016	pH 7	20
	AMP	0.1–1	20	0.024		
GCE/TH/Fc	CA	0.569 - 515	0.19	0.142	pH 7	19
<b>GC/TH-FcDA</b>	DPV	0.3 - 230	0.07	0.59	pH 7	This work
<b>B</b>						
Modified electrode Material	Technique	Linear range (μM)	LOD (μM)	Sensitivity (μM/μA/cm <sup>2</sup> )	Electrolyte	Ref
γ-Fe <sub>2</sub> O <sub>3</sub> /Fe <sub>3</sub> O <sub>4</sub> /GC E	CA	0.2 – 8000	0.05	-	pH 7.3	12
NiCo-DH/AuPt@CC	CA	10 – 670	0.145	-	pH 7.4	21
CuO/g-C <sub>3</sub> N <sub>4</sub> /GCE	DPV	0.5 - 50	0.31	3.327	pH 7	22
Bi <sub>2</sub> Te <sub>3</sub> /GCE	CA	-	0.016	4900	0.1 M K <sub>2</sub> SO <sub>4</sub>	23
AuNPs-PB-GO/GCE	CA	3.8-5400	1.3	87.6	0.5 M KCl	24
Cu-TCPP MOF/Cu <sub>5</sub> .4O/GCE	SWV	0.1 – 590	0.13	-	pH 7.4	25
AuNPs-Psi/GCE	LSV	2000 – 13810	14.84	10.65	pH 7	26
	SWV	500 - 6910	15.16	10.41		
GCE/TH/Fc	CA	0.569 - 785	0.19	0.128	pH 7	19
<b>GC/TH-FcDA</b>	DPV	1.5 - 60	0.49	0.68	pH 7	This-work

**Table S2.** Cartesian coordinates of the molecules.

<u>Dopamine (E= -517.05647668 Hartrees)</u>
N,0,0.9413134941,2.3284959067,-0.8435697701
C,0,-0.0547587588,1.2525397238,-0.861837543
C,0,-1.1294896503,1.4998214291,0.2098012972
C,0,-2.1574467495,0.3917579538,0.2790414341
C,0,-1.8836330921,-0.780616316,1.0002802441

C,0,-2.799453457,-1.8265127495,1.0436734207
O,0,-2.5158297444,-2.9558063795,1.7538616575
C,0,-4.0190146371,-1.7089483704,0.3546625517
O,0,-4.857674478,-2.7983777721,0.463600185
C,0,-4.3050257643,-0.554112137,-0.3620500044
C,0,-3.3761913022,0.4911429425,-0.3989805841
H,0,1.6826268995,2.1244293094,-1.5096709094
H,0,0.5123621164,3.1964035364,-1.1594837038
H,0,0.460055632,0.3112253244,-0.6361312962
H,0,-0.5536254952,1.1084420062,-1.8367272536
H,0,-1.6307240444,2.4529381815,-0.0043531492
H,0,-0.6241094287,1.6209450904,1.1741664928
H,0,-0.9515382522,-0.8935364848,1.5462221704
H,0,-3.2736863322,-3.5528603927,1.6629041614
H,0,-5.6719212262,-2.6324565619,-0.0269766611
H,0,-5.2530363282,-0.4664419647,-0.888943536
H,0,-3.6110994011,1.3916277244,-0.9592892042
<u>Hydrogen peroxide (E= -151.54319300 Hartrees)</u>
O,0,-0.718451786,-0.1175410519,-0.0544959339
O,0,0.7182804842,0.1175465486,-0.0542849118
H,0,-1.0140016216,0.6668525257,0.4349664917
H,0,1.0137211477,-0.6670772701,0.4348764909
<u>Thionine (E= -1025.56236704 Hartrees)</u>
C,0,0.0381078325,0.344566668,-1.3633644918
C,0,-0.1545770431,-1.0569996177,-1.0835247307
S,0,-0.2231588336,-1.6353411898,0.5645104461
C,0,-0.0143285269,-0.1806195548,1.5107541846
C,0,0.1586096915,1.0975334767,0.8655851986
N,0,0.178586126,1.3090649538,-0.4518656246
C,0,0.0831676176,0.7396547649,-2.7400225561
C,0,-0.0496629514,-0.1646928556,-3.751231818
C,0,-0.2404597273,-1.5534767734,-3.4559520313
C,0,-0.2896835614,-1.9770456946,-2.1086910094
C,0,-0.0194031986,-0.288208217,2.8906467054
C,0,0.1461305884,0.8620765303,3.6946302061
C,0,0.3190994831,2.1394597805,3.06957974
C,0,0.3237800947,2.2430728279,1.7104347248
N,0,0.1429533859,0.7700568602,5.0384267194
N,0,-0.3706867822,-2.4393658184,-4.4621867459
H,0,0.2284051355,1.7955092074,-2.9396659459
H,0,-0.0125816195,0.1555062848,-4.7876784186
H,0,-0.4344022385,-3.0303325805,-1.8867620159
H,0,-0.1504039524,-1.2557852176,3.3662965666
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H,0,0.453062594,3.1991957775,1.2155660926
H,0,0.0234076206,-0.1146531029,5.5072417693
H,0,0.2606024526,1.5871461158,5.6174267188
H,0,-0.5060708684,-3.4229560468,-4.2860847973
H,0,-0.3364396704,-2.1432678924,-5.4254469856
<u>Ferrocenedicarboxylic acid (E= -2027.87503716 Hartrees)</u>
C,0,-0.757555,0.630403,1.497326
C,0,-0.033773,-0.459607,2.057883

H,0,0.843852,-0.381826,2.685448
C,0,-0.632822,-1.674342,1.605792
H,0,-0.292393,-2.673164,1.842158
C,0,-1.815144,0.084613,0.696085
C,0,-1.725743,-1.345073,0.758913
H,0,-2.383877,-2.029406,0.243623
C,0,0.757542,0.630635,-1.497172
C,0,0.033724,-0.459240,-2.057906
C,0,0.632747,-1.674058,-1.606061
H,0,0.292298,-2.672831,-1.842620
C,0,1.815127,0.084675,-0.696073
C,0,1.725692,-1.344980,-0.759141
H,0,2.383825,-2.029427,-0.243996
Fe,0,0.000026,-0.541283,-0.000001
H,0,-0.843876,-0.381290,-2.685487
H,0,-0.551919,1.682104,1.633452
C,0,2.797248,0.811388,0.124942
C,0,-2.797228,0.811438,-0.124873
O,0,-3.631750,0.292394,-0.839903
O,0,-2.679040,2.159417,-0.002786
O,0,3.631790,0.292262,0.839886
O,0,2.679066,2.159393,0.003055
H,0,3.362902,2.536942,0.580977
H,0,-3.362888,2.537056,-0.580630
H,0,0.551966,1.682360,-1.633192
<u>Ferrocenedicarboxylic acid linked with thionine (E= -3926.09245638 Hartrees)</u>
C,0,0.883195,0.091454,2.304717
C,0,-0.357083,0.784068,2.314382
H,0,-7.263936,2.875513,-0.790350
C,0,-0.276016,1.865274,1.385657
H,0,-1.075572,2.544881,1.124653
C,0,1.754102,0.758415,1.378408
C,0,1.020378,1.856500,0.803484
H,0,1.361715,2.537545,0.034587
C,0,-1.198322,-1.475832,0.009209
C,0,0.138723,-1.858979,-0.289110
C,0,0.650897,-0.955719,-1.268821
H,0,1.646139,-0.983488,-1.690557
C,0,-1.517240,-0.322014,-0.791080
C,0,-0.355425,-0.001302,-1.572893
H,0,-0.290239,0.819172,-2.272932
Fe,0,0.077375,0.074059,0.425605
H,0,0.682383,-2.673410,0.168821
H,0,-1.219631,0.525446,2.912902
C,0,-2.767802,0.467513,-0.854106
C,0,3.143042,0.314419,1.128268
O,0,3.534073,-0.822693,1.342512
O,0,-2.802876,1.645346,-1.170253
H,0,-1.836373,-1.949850,0.744105
C,0,-12.689465,-0.939641,0.120163
C,0,-11.439128,-1.601469,0.140147
C,0,-10.269645,-0.885426,-0.034739

C,0,-10.297936,0.549193,-0.241326
C,0,-11.586778,1.187334,-0.253262
C,0,-12.736668,0.482080,-0.080984
C,0,-7.973545,0.881500,-0.442309
C,0,-7.571693,-0.484106,-0.266646
C,0,-6.228070,-0.834876,-0.306560
H,0,-5.935774,-1.873273,-0.174561
C,0,-5.240432,0.143164,-0.525950
C,0,-5.620381,1.505977,-0.703125
C,0,-6.946993,1.846853,-0.658065
H,0,-11.409534,-2.676303,0.292853
H,0,-11.595790,2.260461,-0.408197
H,0,-13.700118,0.981782,-0.094302
H,0,-4.854535,2.245781,-0.881407
N,0,-9.241279,1.329224,-0.423499
S,0,-8.751993,-1.744492,-0.000707
N,0,-3.922751,-0.275892,-0.550831
N,0,-13.832435,-1.624060,0.286747
H,0,-13.836171,-2.623312,0.427963
H,0,-14.727843,-1.158774,0.271357
H,0,-3.772762,-1.268875,-0.428111
C,0,12.262593,-1.609212,-0.508802
C,0,10.933977,-1.931819,-0.148115
C,0,9.953158,-0.956696,-0.156104
C,0,10.264557,0.408536,-0.531964
C,0,11.625901,0.698893,-0.893566
C,0,12.588641,-0.261332,-0.885271
C,0,8.102665,1.303437,-0.259383
C,0,7.445822,0.098110,0.154136
C,0,6.087610,0.074479,0.461080
H,0,5.595886,-0.833646,0.782315
C,0,5.340873,1.260032,0.367311
C,0,5.976787,2.469085,-0.043954
H,0,10.693026,-2.952032,0.135752
H,0,11.846860,1.723111,-1.172529
H,0,13.611099,-0.022892,-1.160735
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H,0,7.810881,3.396047,-0.658161
N,0,9.405560,1.417845,-0.571481
S,0,8.329570,-1.401456,0.295263
N,0,3.990734,1.329557,0.658238
N,0,13.224413,-2.546487,-0.504483
H,0,13.032134,-3.501786,-0.242306
H,0,14.174756,-2.321868,-0.758844
H,0,3.580524,2.252801,0.610606
H,0,1.154836,-0.774187,2.891436
C,0,7.310250,2.486502,-0.345824