

## ELECTRONIC SUPPLEMENTARY INFORMATION

**Structural, optical and photoconductivity characteristics of pristine FeO.Fe<sub>2</sub>O<sub>3</sub> and NTPI- FeO.Fe<sub>2</sub>O<sub>3</sub> nanocomposite : Aggregation induced emission enhancement of fluorescent organic nanoprobe of thiophene appended phenanthrimidazole derivative**

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**Table S1.** Mulliken atomic charges of imidazole and NTPI–FeO clusters

S. No.	NTPI		NTPI – Fe <sub>3</sub> O		NTPI - Fe <sub>3</sub> O <sub>2</sub>		Fe <sub>3</sub> O		Fe <sub>3</sub> O <sub>2</sub>	
	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges
1	C	-0.165846	C	-0.356634	C	-0.358075	Fe	0.201842	Fe	0.295833
2	C	-0.020017	C	-0.190746	C	-0.192971	Fe	0.201842	Fe	0.35550
3	C	0.091927	C	0.290008	C	0.293930	Fe	0.133372	Fe	0.295264
4	C	0.054434	C	0.230049	C	0.229985	O	-0.537056	O	-0.473185
5	C	-0.164052	C	-0.392355	C	-0.393260	-	-	O	-0.473462
6	C	-0.123220	C	-0.273607	C	-0.275235	-	-	-	-
7	C	0.076139	C	-0.168760	C	-0.171854	-	-	-	-
8	C	0.056737	C	0.239887	C	0.242327	-	-	-	-
9	C	0.054156	C	0.375230	C	0.346743	-	-	-	-
10	C	0.043543	C	0.185252	C	-0.173750	-	-	-	-
11	C	-0.118636	C	-0.379689	C	-0.334825	-	-	-	-
12	C	-0.136509	C	-0.248757	C	-0.257757	-	-	-	-
13	C	-0.122520	C	-0.275214	C	-0.277936	-	-	-	-
14	C	-0.167788	C	-0.378910	C	-0.382422	-	-	-	-
15	N	-0.458478	N	-0.243153	N	-0.245643	-	-	-	-
16	H	0.160180	C	0.211610	C	0.2032292	-	-	-	-
17	H	0.118590	N	-0.188467	N	-0.142357	-	-	-	-
18	H	0.085122	H	0.269848	H	0.282498	-	-	-	-
19	H	0.134020	H	0.237376	H	0.236218	-	-	-	-
20	H	0.116408	H	0.183247	H	0.183053	-	-	-	-
21	H	0.119096	H	0.245027	H	0.244682	-	-	-	-

22	H	0.117207	H	0.235671	H	0.234246	-	-	-	-
23	H	0.133285	H	0.239881	H	0.229799	-	-	-	-
24	C	0.123205	H	0.237846	H	0.234774	-	-	-	-
25	C	-0.042711	H	0.243137	H	0.241249	-	-	-	-
26	C	-0.093889	C	0.214015	C	0.212934	-	-	-	-
27	C	-0.192817	C	0.090784	C	0.089290	-	-	-	-
28	C	0.100219	C	-0.276006	C	-0.275773	-	-	-	-
29	C	-0.141056	C	-0.375372	C	-0.376900	-	-	-	-
30	H	0.158321	C	0.482809	C	-0.483317	-	-	-	-
31	C	-0.097245	C	-0.260571	C	-0.260593	-	-	-	-
32	H	0.175541	H	0.263846	H	0.268883	-	-	-	-
33	C	-0.157033	C	-0.240854	C	-0.241581	-	-	-	-
34	C	-0.138355	H	0.313446	H	0.313469	-	-	-	-
35	H	0.133856	C	-0.465817	C	-0.466382	-	-	-	-
36	C	-0.127776	C	-0.469669	C	-0.470986	-	-	-	-
37	H	0.131874	H	0.238577	H	0.238545	-	-	-	-
38	H	0.132801	C	-0.237363	C	-0.238545	-	-	-	-
39	H	0.132802	H	0.240892	H	-0.239661	-	-	-	-
40	H	0.127472	H	0.245202	H	0.244413	-	-	-	-
41	C	-0.56855	H	0.247783	H	0.246819	-	-	-	-
42	C	0.045418	H	0.236084	H	0.234969	-	-	-	-
43	C	-0.159111	C	-0.179484	C	-0.205901	-	-	-	-
44	H	0.1525570	C	-0.322126	C	-0.328059	-	-	-	-
45	C	-0.450263	C	-0.224671	C	-0.229920	-	-	-	-
46	H	0.135959	H	0.275906	H	0.275068	-	-	-	-
47	H	0.211524	C	-0.534165	C	-0.548426	-	-	-	-
48	S	0.531206	H	0.255784	H	0.253765	-	-	-	-

49			H	0.301850	H	0.298433	-	-	-	-
50	-	-	S	0.438568	S	0.488043	-	-	-	-
51	-	-	Fe	0.0151939	Fe	0.238848	-	-	-	-
52	-	-	Fe	0.052177	Fe	0.030576	-	-	-	-
53	-	-	Fe	0.107875	Fe	0.409408	-	-	-	-
54	-	-	O	-0.528712	O	-0.509375	-	-	-	-
55	-	-	-	-	O	-0.410890	-	-	-	-

S. No.	Fe <sub>3</sub> O <sub>3</sub>		Fe <sub>4</sub> O		Fe <sub>4</sub> O <sub>2</sub>		Fe <sub>4</sub> O <sub>3</sub>		Fe <sub>4</sub> O <sub>4</sub>	
	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges
1	Fe	0.440286	Fe	0.144470	Fe	0.373271	Fe	0.339690	Fe	0.290203
2	Fe	0.435227	Fe	0.187534	Fe	0.193631	Fe	0.335945	Fe	0.398816
3	Fe	0.43980	Fe	-0.506458	O	-0.480634	O	-0.466934	O	-0.423475
4	O	-0.437237	Fe	0.096910	Fe	0.195597	Fe	0.251163	Fe	0.464195
5	O	-0.437889	O	0.077544	Fe	0.122972	Fe	0.294147	Fe	0.451254
6	O	-0.440206		-	O	-0.404842	O	-0.396407	O	-0.369995
7	-	-	-	-	-	-	O	-0.357603	O	-0.366521
8	-	-	-	-	-	-	-	-	O	-0.444478

**Figure S1.** LC- Mass spectrum of NTPI –FeO.Fe<sub>2</sub>O<sub>3</sub> composite

**Figure S2.** Photographs of enhancement of nanoaggregates of NTPI with Fe<sup>3+</sup> ion (a) Test strip ; (b) 10<sup>-3</sup> M Fe<sup>3+</sup> ; (c) 10<sup>-5</sup> M Fe<sup>3+</sup> ; (d) 10<sup>-7</sup> M Fe<sup>3+</sup> ; e) 10<sup>-8</sup> M Fe<sup>3+</sup>

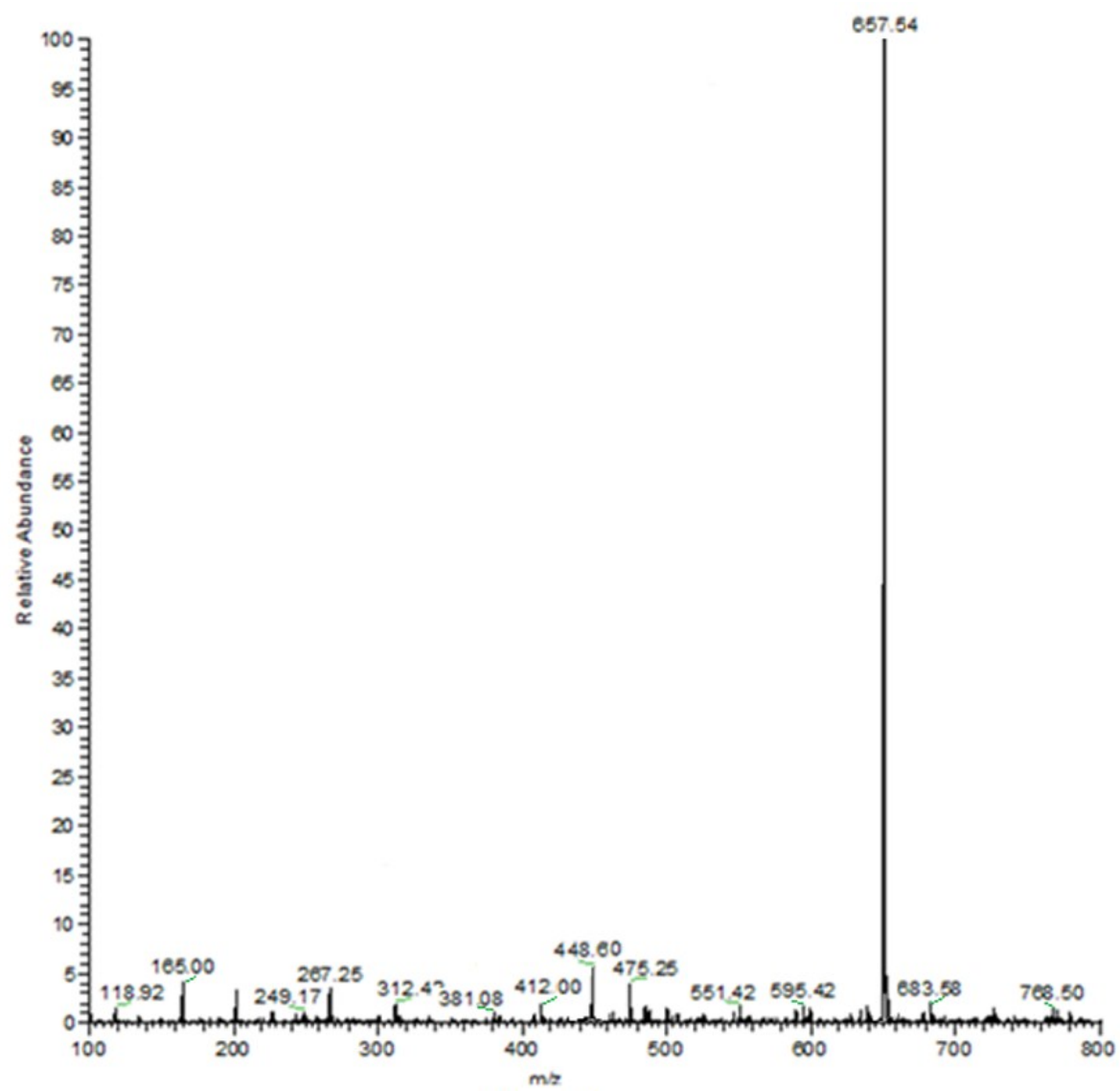
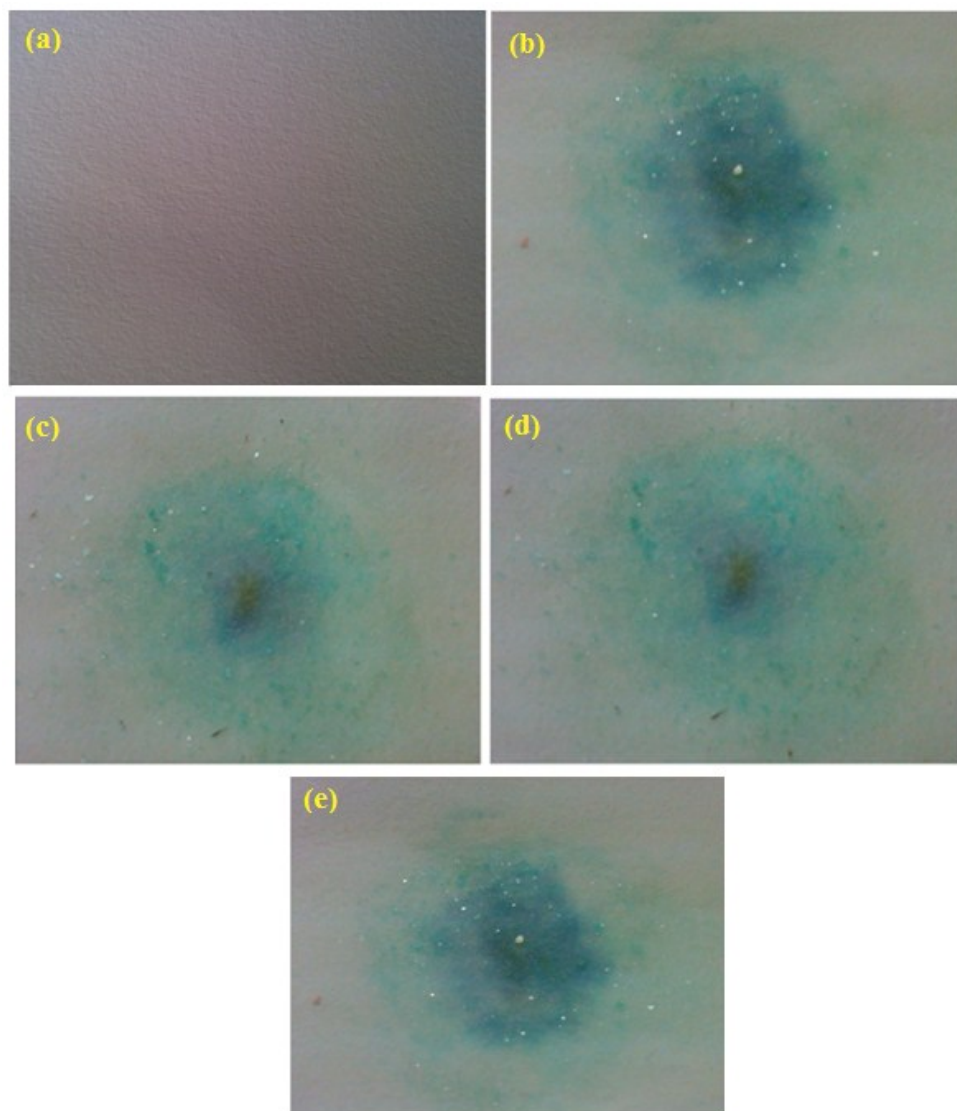


Figure S1



**Figure S2**