Electronic Supporting Information

Magnetic $BiFeO_3$ nanoparticles (BFO MNPs): a sustainable and efficient catalyst for green synthesis of highly substituted imidazole derivatives

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Fig. **S1**. Synthesis of diverse imidazole derivatives using bismuth ferrite nanoparticles in solvent-free systems.

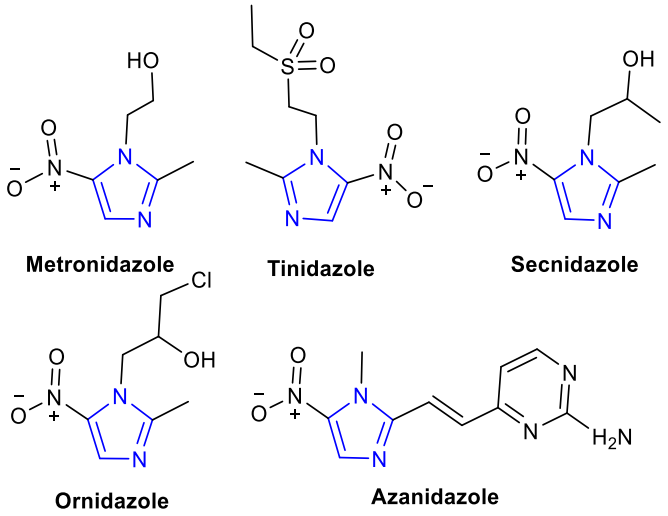


Fig. S2. Exemplary of biologically Active imidazole derivatives.

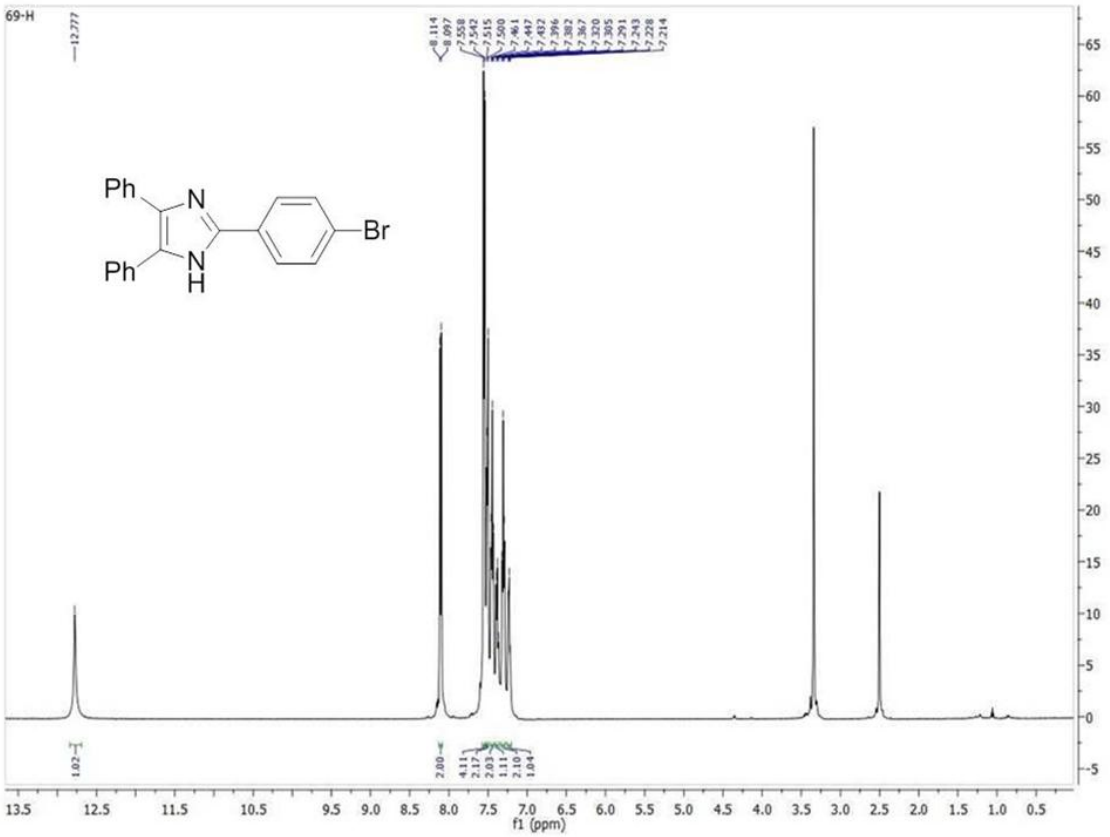


Fig. S3: ^{1}H NMR of 2-(4-bromophenyl)-4,5-diphenyl-1*H*-imidazole (**4c**).

2-(4-Bromophenyl)-4,5-diphenyl-1*H*-imidazole (4c): White solid, M.P: 250-252 ^{o}C, ^{1}H NMR (500 MHz, DMSO-d_6, δ = ppm) δ: 7.22 (t, *J* = 7.5 Hz, 1H, ArH), 7.30 (t, *J* = 7.0 Hz, 2H, ArH), 7.38 (d, *J* = 7.0 Hz, 1H, Ar-H), 7.44 (t, *J* = 7.0 Hz, 2H, Ar-H), 7.50 (d, *J* = 7.5 Hz, 2H, Ar-H), 7.55 (m, 4H, Ar-H), 8.10 (d, *J* = 7.5 Hz, 2H, Ar-H), 12.77 (s, 1H, NH).

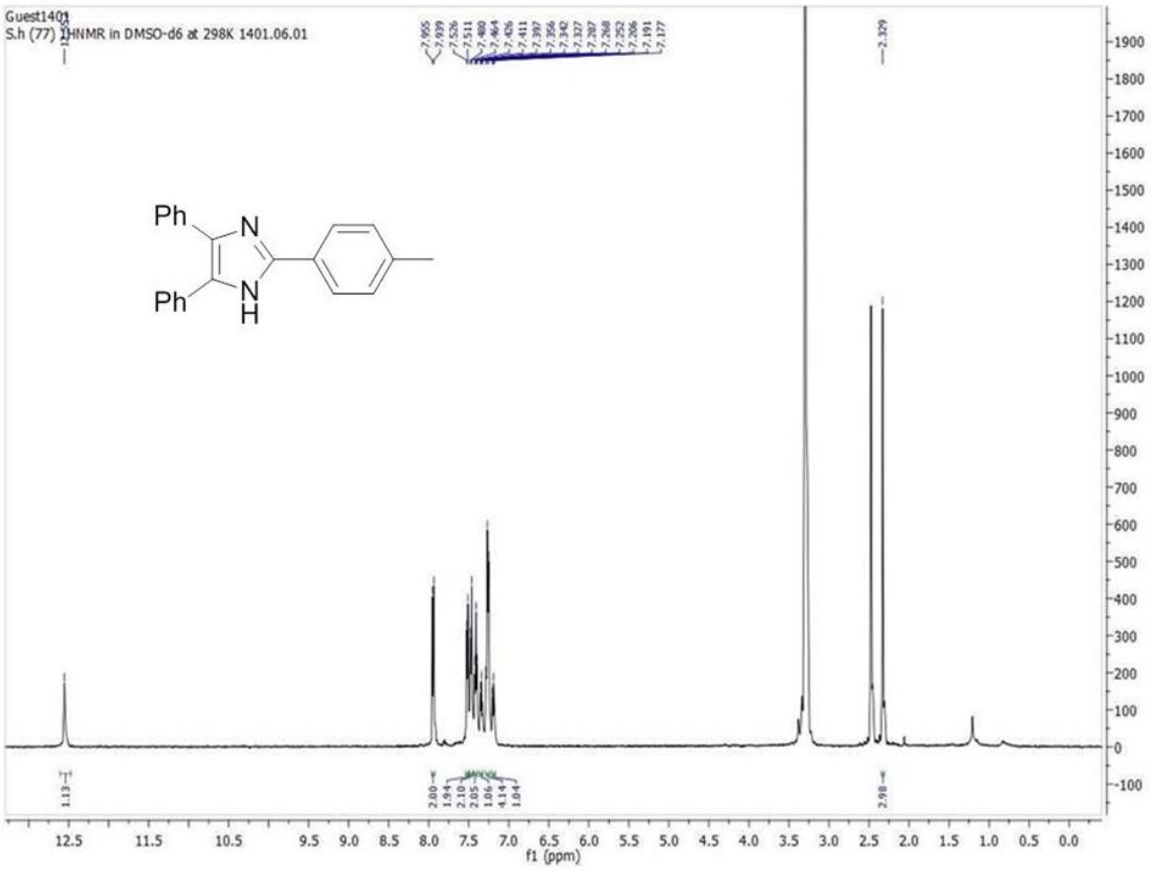


Fig. S4. ^{1}H NMR of 2-(4-methylphenyl)-4,5-diphenyl-1*H*-imidazole (**4i**).

2-(4-Methylphenyl)-4,5-diphenyl-1*H*-imidazole (4i): White solid, M.P: 232-230 ^{o}C, ^{1}H NMR (500 MHz, DMSO-d_6, δ = ppm) δ: 2.32 (s, 3H, CH_3), 7.19 (t, *J* = 7.5 Hz, 1H, ArH), 7.26 (m, 4H, ArH), 7.34 (d, *J* = 7.0 Hz, 1H, Ar-H), 7.41 (t, *J* = 7.5 Hz, 2H, Ar-H), 7.47 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.51 (d, *J* = 7.5 Hz, 2H, Ar-H), 7.94 (d, *J* = 8.0 Hz, 2H, Ar-H), 12.55 (s, 1H, NH).

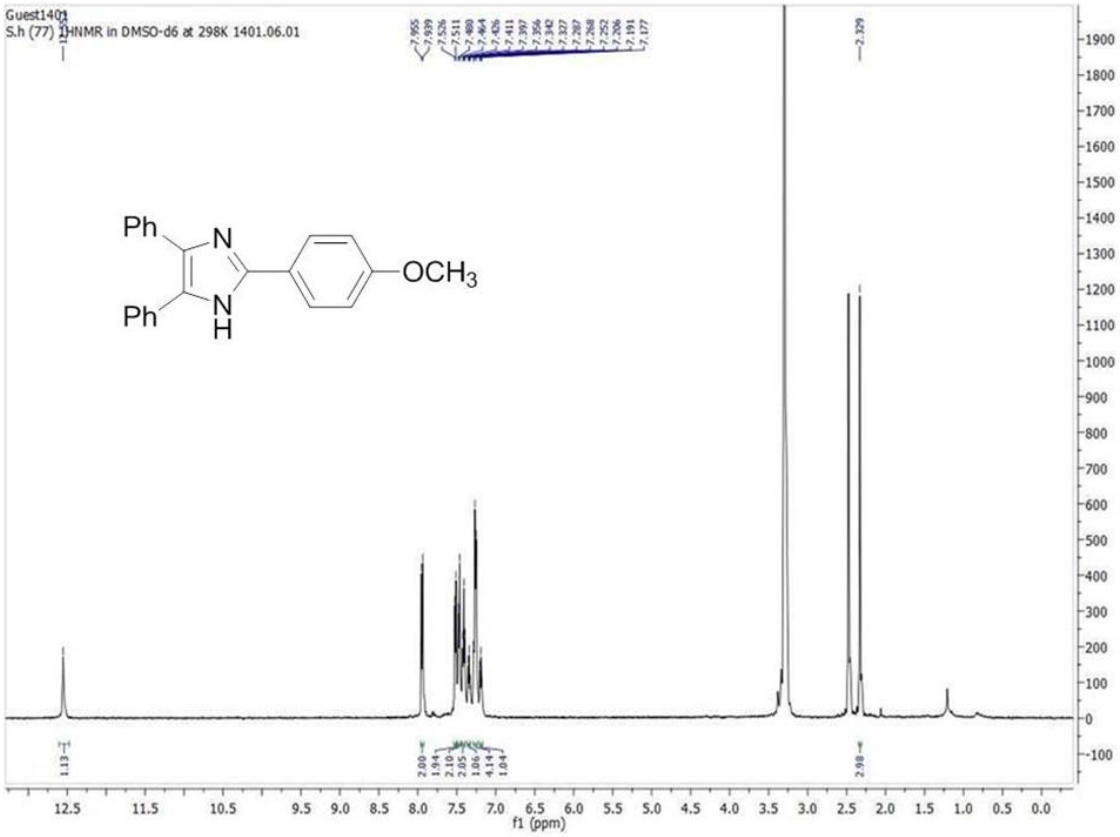


Fig. S5. ^{1}H NMR of 2-(4-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (**4k**).

2-(4-Methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (4k): White solid, M.P: 229-231 ^{o}C, ^{1}H NMR (500 MHz, DMSO-d_6, δ = ppm) δ: 3.87 (s, 3H, OCH_3), 7.24 (br, 1H, ArH), 7.30 (br, 2H, ArH), 7.40 (br, 1H, Ar-H), 7.45 (t, *J* = 6.5 Hz, 2H, Ar-H), 7.51 (d, *J* = 7.0 Hz, 2H, Ar-H), 7.55 (d, *J* = 7.0 Hz, 2H, Ar-H), 8.05 (d, *J* = 8.5 Hz, 2H, Ar-H), 8.22 (d, *J* = 8.0 Hz, 2H, Ar-H), 12.94 (s, 1H, NH).

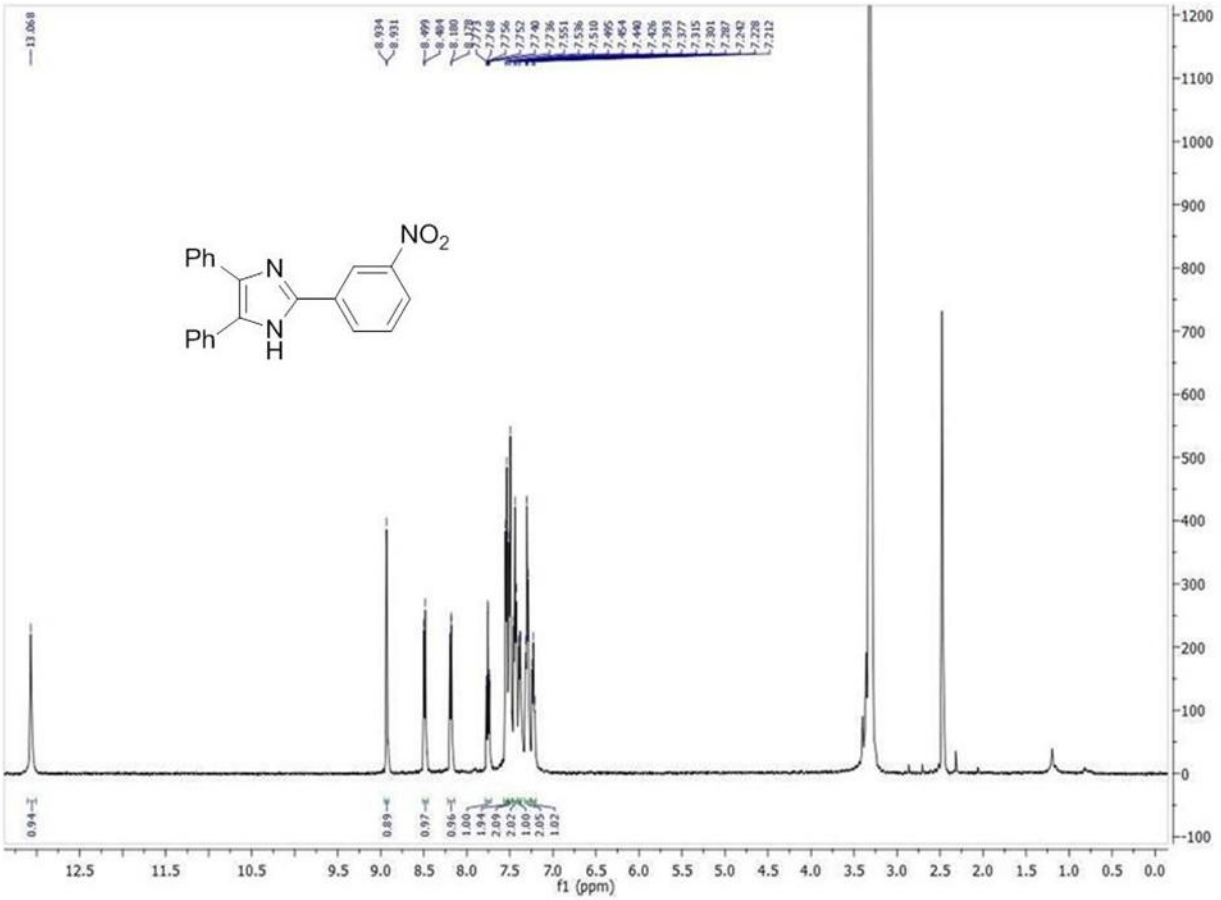


Fig. S6. ^{1}H NMR of 2-(3-nitrophenyl)-4,5-diphenyl-1*H*-imidazole (**4e**).

2-(3-Nitrophenyl)-4,5-diphenyl-1*H*-imidazole (4e): White solid, M.P: 264-266 ^{o}C , ^{1}H NMR (500 MHz, DMSO-d_6, δ = ppm) δ: 7.22 (t, *J* = 7.0 Hz, 1H, ArH), 7.30 (t, *J* = 7.0 Hz, 2H, ArH), 7.38 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.44 (t, *J* = 7.0 Hz, 2H, Ar-H), 7.50 (d, *J* = 7.5 Hz, 2H, Ar-H), 7.54 (d, *J* = 7.5 Hz, 2H, Ar-H), 7.75 (dt, *J* = 8.5 Hz, 1H, Ar-H), 8.18 (dd, *J* = 8.5 Hz, 1H, Ar-H), 8.48 (dd, *J* = 7.5 Hz, 1H, Ar-H), 8.93 (d, *J* = 1.5 Hz, 1H, Ar-H), 13.06 (s, 1H, NH).

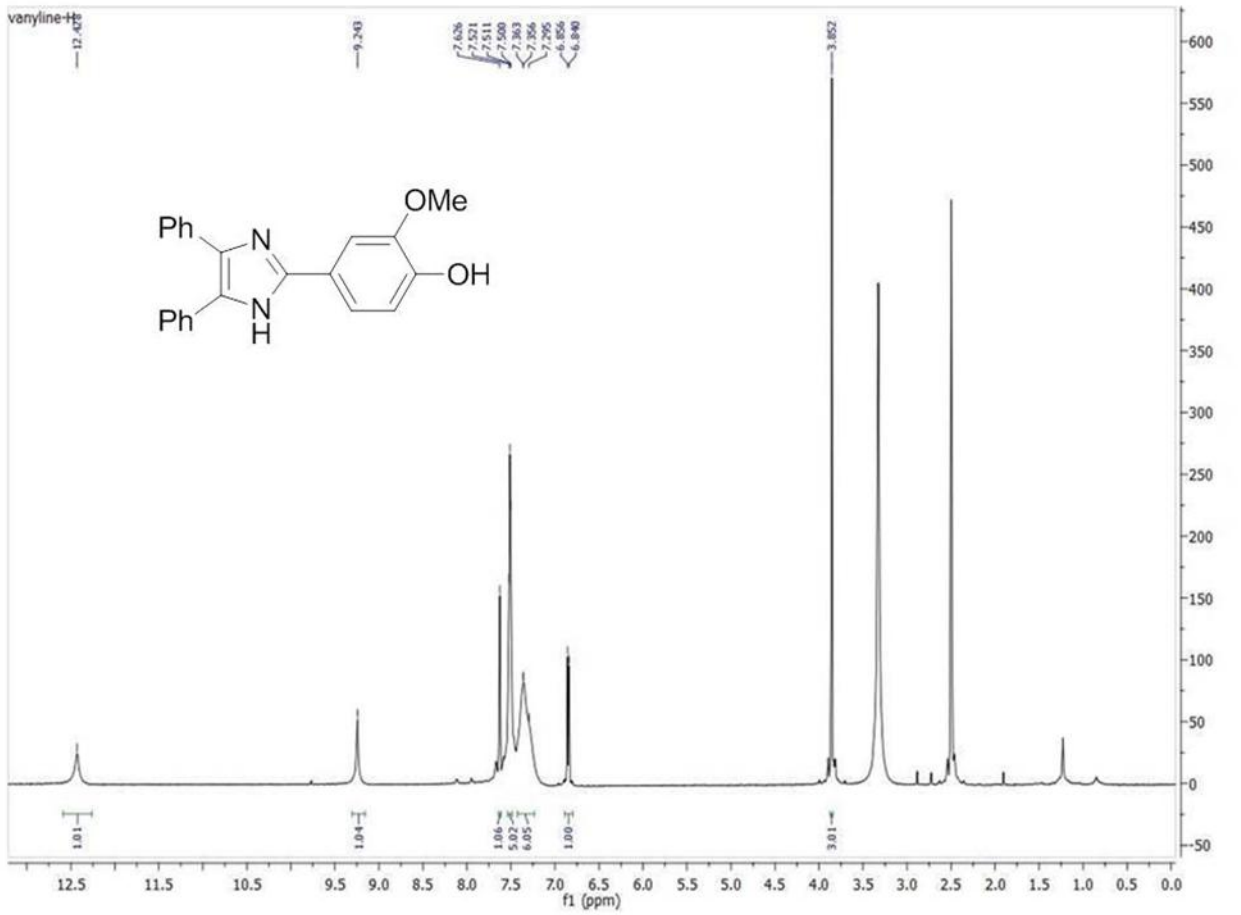


Fig. S7. ^{1}H NMR of 4-(4,5-diphenyl-1*H*-imidazol-2-yl)-2-methoxyphenol (**4l**).

4-(4,5-Diphenyl-1*H*-imidazol-2-yl)-2-Methoxyphenol (4l): White solid, M.P: 258-260 ^{o}C, ^{1}H NMR (500 MHz, DMSO-d_6, δ = ppm) δ: 3.85 (s, 3H, OCH_3), 6.85 (d, 1H, *J* = 8.0 Hz, ArH), 7.35 (m, 6H, ArH), 7.51 (m, 5H, Ar-H), 7.62 (s, 1H, Ar-H), 9.24 (s, 1H, OH), 12.42 (s, 1H, NH).

Preparation of magnetic bismuth ferrite nanoparticles (BFO MNPs)

The preparation of bismuth ferrite nanoparticles (BFO MNPs) was conducted using the solid-state thermal decomposition method. Initially, a 100 ml round-bottom flask was filled with 8.0 mmol of glycine, 4.0 mmol of $Fe(NO_3)_3$, 4.0 mmol of $Bi(NO_3)_3$, and 40.0 ml of deionized water.

This mixture was heated to 120 °C for one hour. Following this, 2.80 ml of HNO_3 was added dropwise to the reaction mixture. The mixture was then maintained at 120 °C, leading to the formation of a brown solid. Finally, the brown solid was placed in an oven, where it was heated for one hour at 350 °C, followed by an additional hour at 550 °C to synthesize the BFO MNPs.

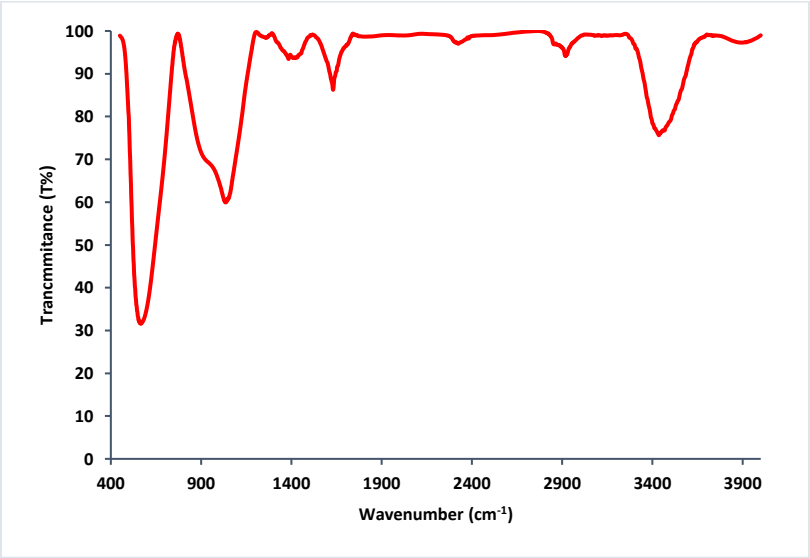


Fig. S8. Fourier-Transform infrared spectrum (FT-IR) of BFO MNPs.

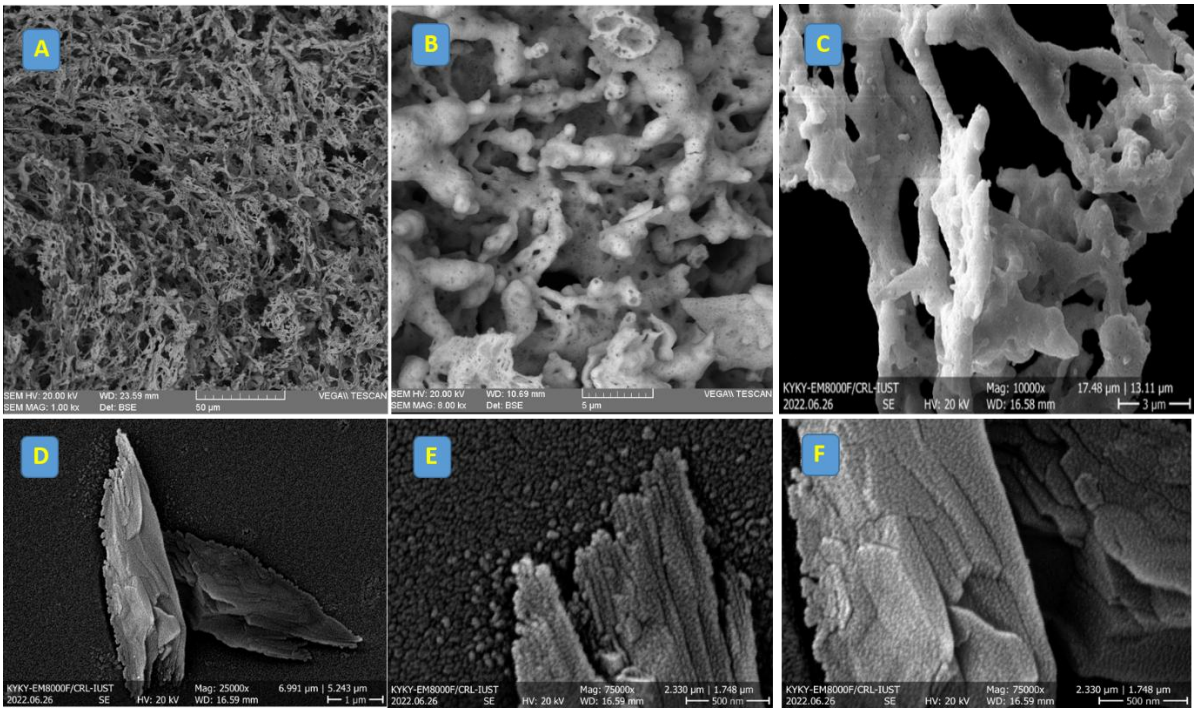


Fig S9. FESEM images of $BiFeO_3$ nanoparticles; **a**) 50 µm, **b**) 5 µm, **c**) 3 µm, **d**) 1 µm, **e** and **f**) 500 nm.

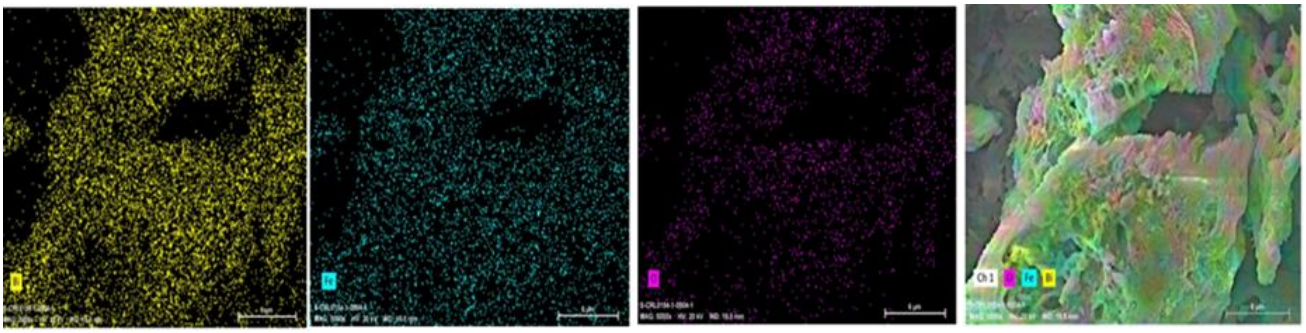


Fig. S10. EDS elemental mapping analysis of BFO MNPs.

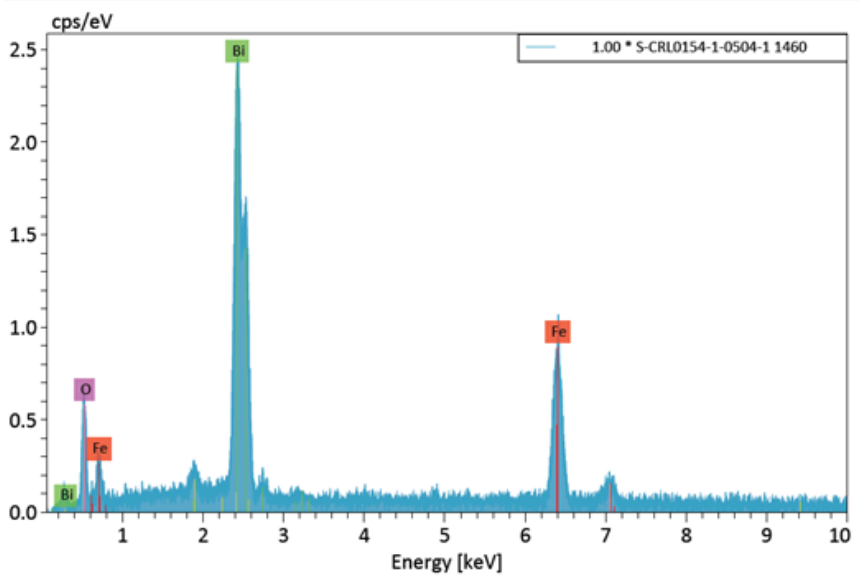


Fig. S11. Elemental analysis by energy-dispersive X-ray spectroscopy (EDS) of the BFO MNPs.

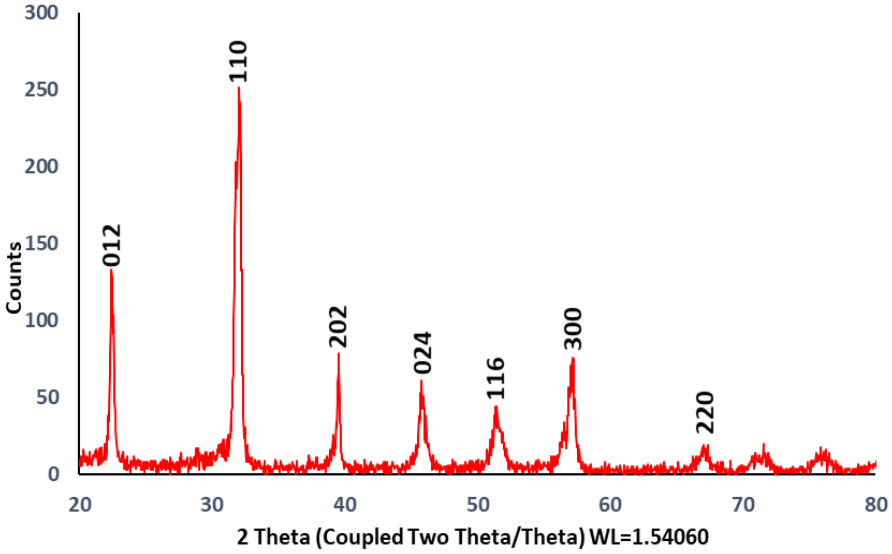


Fig. S12. X-Ray diffraction pattern of BFO MNPs.

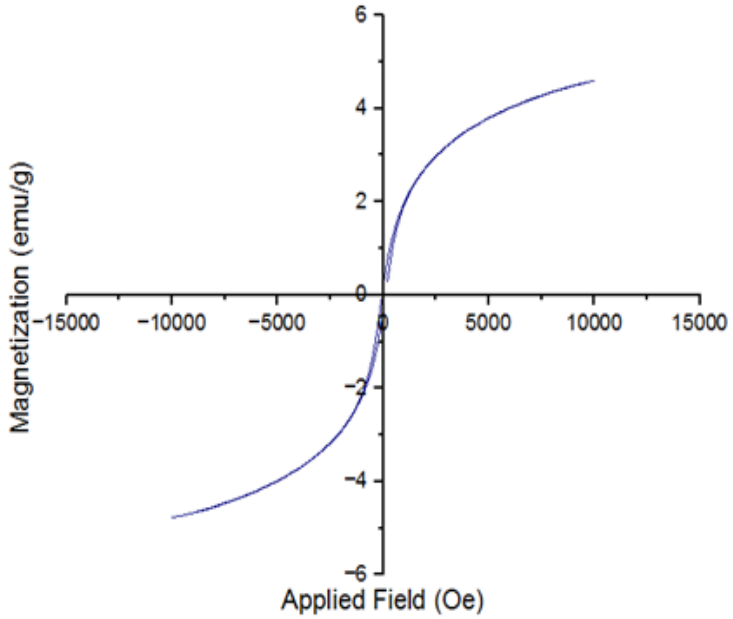


Fig. S13. Hysteresis diagram of BFO MNPs.

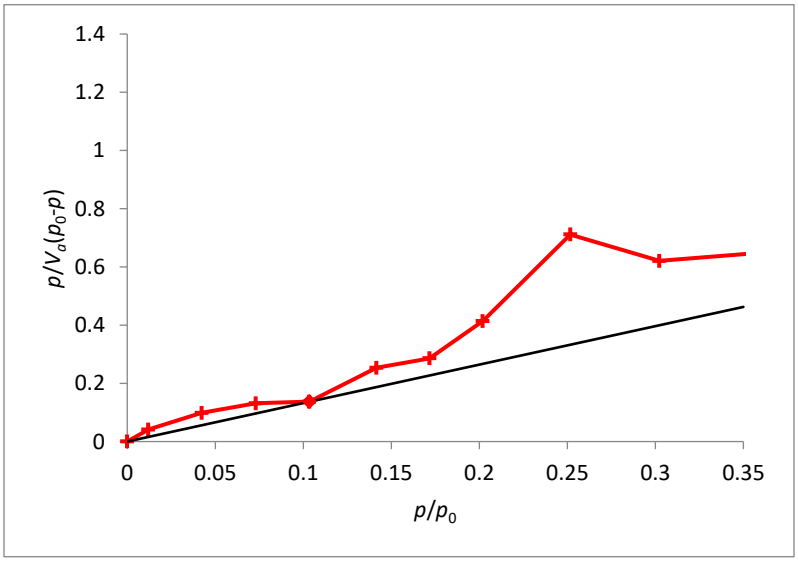


Fig. 14. Brunauer-Emmett-Teller (BET) surface area analysis of the BFO MNPs.

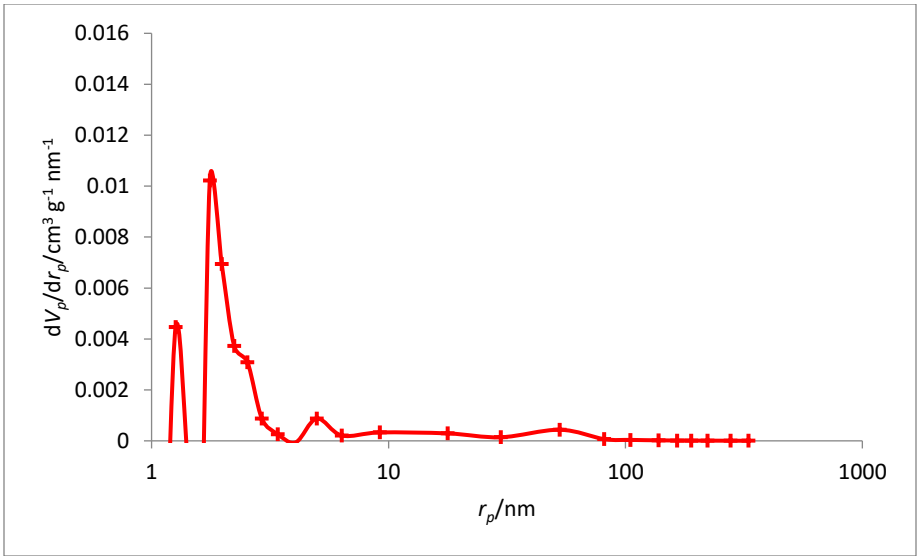


Fig. 15. Barrett-Joyner-Halenda (BJH) analysis of the BFO MNPs.

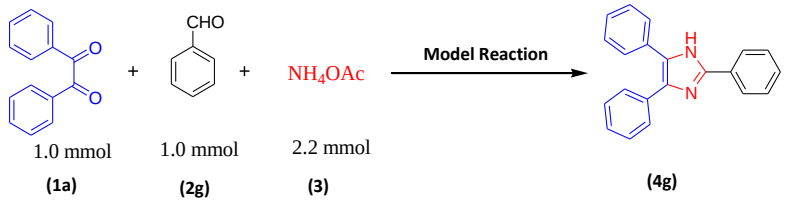


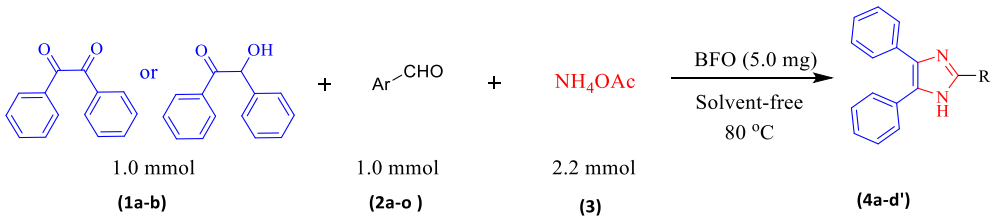
Table S1: Optimizing the preparation of imidazole derivatives using the three-component reaction between benzoin (1a), benzaldehyde (2g), and ammonium acetate (3) [a]

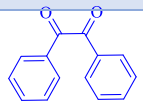
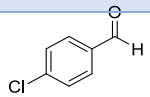
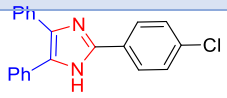
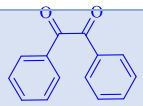
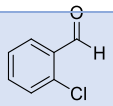
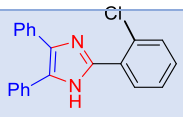
Entry.	Catalyst(mg)	Solvent (ml)	Temperature (^{0}C)	Time (min)	Yield (%)[b]	TON	TOF
1	-	Solvent Free	25	45	-		
2	-	H_2O(2.0)	25	45	low interest		
3	$BiFeO_3$ (2.0)	H_2O(2.0)	25	45	28	41666.66	1037.03
4	$BiFeO_3$ (2.0)	MeOH(2.0)	25	45	25	41666.66	925.92
5	$BiFeO_3$ (2.0)	EtOH(2.0)	25	45	32	53333.33	1185.18
6	$BiFeO_3$ (2.0)	EtOAc(2.0)	25	45	28	41666.66	1037.03
7	$BiFeO_3$ (2.0)	CH_2Cl_2(2.0)	25	45	23	38333.33	851.85

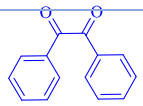
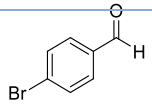
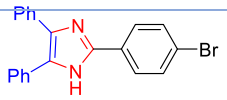
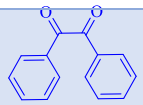
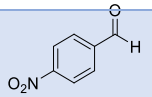
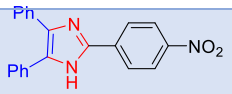
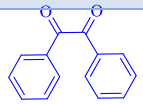
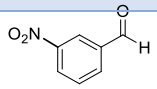
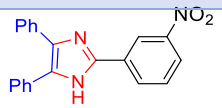
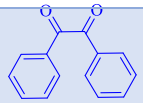
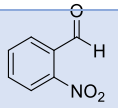
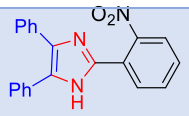
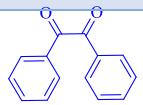
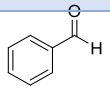
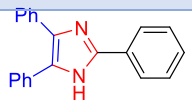
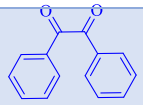
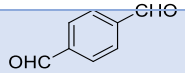
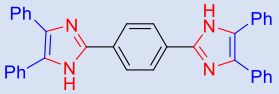
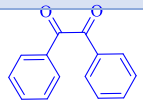
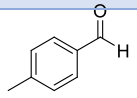
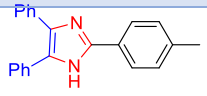
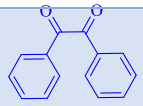
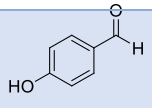
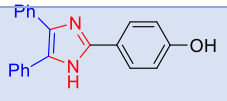
8	$BiFeO_3$ (2.0)	H_2O/EtOH(2.0)	25	45	41	68333.33	1518.51
9	$BiFeO_3$ (2.0)	Solvent Free	25	45	48	80000	1777.77
10	$BiFeO_3$ (2.0)	Solvent Free	80	30	68	113333.33	3777.77
11	**$BiFeO_3$ (5.0)**	**Solvent Free**	**80**	**15**	**91**	**60666.66**	**4044.44**
12	$BiFeO_3$ (7.5)	Solvent Free	80	15	92	40000	2666.66
13	Fe_3O_4(5.0)	Solvent Free	80	15	92	20666.66	1377.77
14	-	Solvent Free	80	15	low interest		

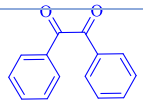
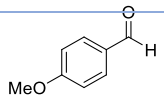
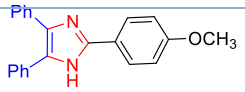
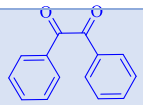
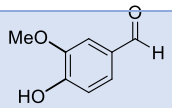
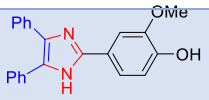
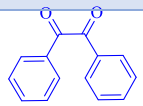
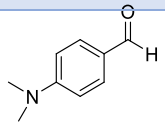
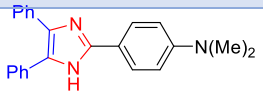
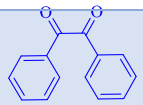
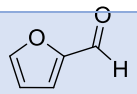
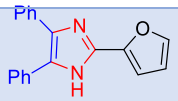
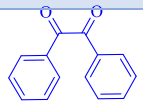
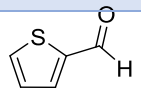
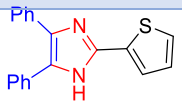
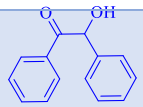
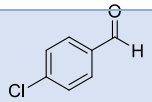
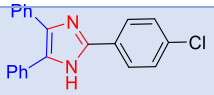
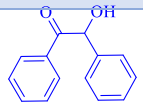
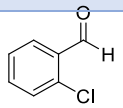
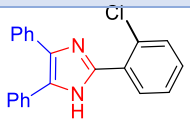
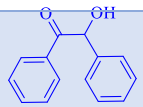
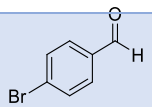
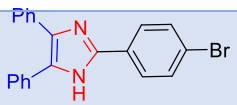
[a] Reaction conditions: Three-component reaction between benzyl (1.0 mmol), benzaldehyde (1.0 mmol) and 2.20 mmol of ammonium acetate. [b] The yield of purified products is reported. Recrystallization in ethyl acetate or chloroform was used for purification.

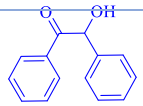
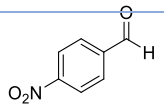
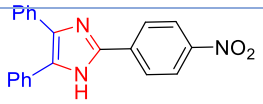
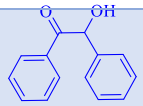
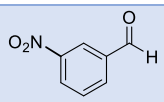
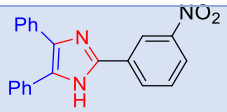
Table 2: Development of imidazole reaction using 2,1-dicarbonyl compounds and various aromatic and heteroaromatic aldehydes in the presence of bismuth ferrite magnetic nanoparticles.



Entry	Dicarbonyls (1a-b)	Aldehyde (2a-o)	Product (4a-d')	Time (min)	Yield[b] (%)	M.p (^{0}C)
1	 **1a**	 **2a**	 **4a**	10	96	263-265[34]
2	 **1a**	 **2b**	 **4b**	15	90	197-199[35]

3	 **1a**	 **2c**	 **4c**	10	95	250-252[36]
4	 **1a**	 **2d**	 **4d**	10	98	199-201[37]
5	 **1a**	 **2e**	 **4e**	10	91	264-266[38]
6	 **1a**	 **2f**	 **4f**	15	90	233-235[39]
7	 **1a**	 **2g**	 **4g**	15	91	270-272[40]
8	 **1a**	 **2h**	 **4h**	20	89	286-289[41]
9	 **1a**	 **2i**	 **4i**	15	88	230-232[42]
10	 **1a**	 **2j**	 **4j**	20	92	259-261[43]

11	 **1a**	 **2k**	 **4k**	20	90	229-231[44]
12	 **1a**	 **2l**	 **4l**	15	89	258-260[45]
13	 **1a**	 **2m**	 **4m**	25	93	256-258[46]
14	 **1a**	 **2n**	 **4n**	20	91	230-233[47]
15	 **1a**	 **2o**	 **4o**	20	95	255-256[36]
16	 **1b**	 **2a**	 **4p**	15	91	263-265[34]
17	 **1b**	 **2q**	 **4q**	20	93	197-199[35]
18	 **1b**	 **2c**	 **4r**	15	93	250-252[36]

						
19	**1b**	**2d**	**4s**	15	96	199-201[37]
						
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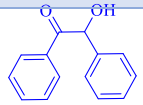
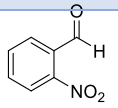
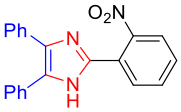
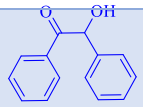
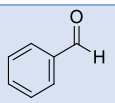
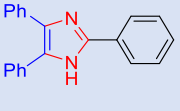
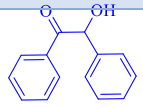
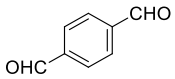
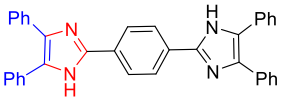
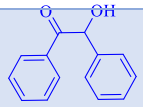
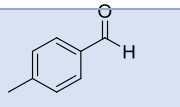
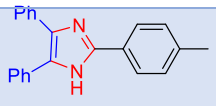
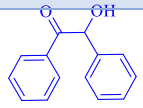
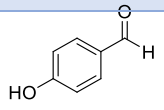
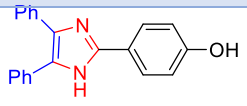
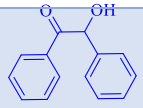
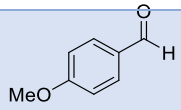
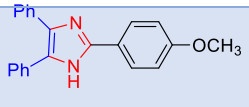
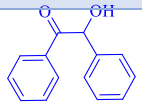
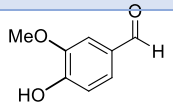
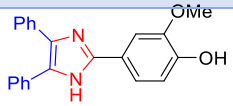
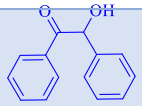
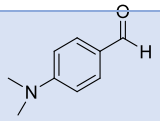
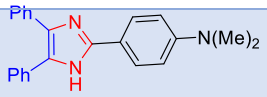
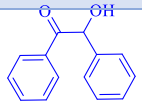
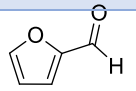
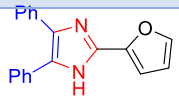
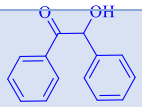
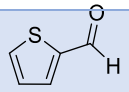
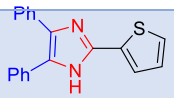
						
21	**1b**	**2f**	**4u**	20	89	233-235[39]
						
22	**1b**	**2g**	**4v**	15	89	270-272[41]
						
23	**1b**	**2h**	**4w**	20	92	286-289[41]
						
24	**1b**	**2i**	**4x**	15	90	230-232[42]
						
25	**1b**	**2j**	**4y**	20	92	259-261[43]
						

26	**1b**	**2k**	**4z**	20	89	229-231[44]
						
27	**1b**	**2l**	**4a'**	15	87	258-260[45]
						
28	**1b**	**2m**	**4b'**	15	88	256-258[46]
						
29	**1b**	**2n**	**4c'**	20	88	230-233[47]
						
30	**1b**	**2o**	**4d'**	20	91	255-256[44]

[a]Reaction conditions: benzyl/benzoin (1, 1.0 mmol), aldehyde (2, 1.0 mmol), 2.2 mmol of ammonium acetate 3, and 5.0 mg of BFO MNPs, and solvent-free conditions and a temperature of 80 °C. The yield of the reaction is related to the purified product.[b]

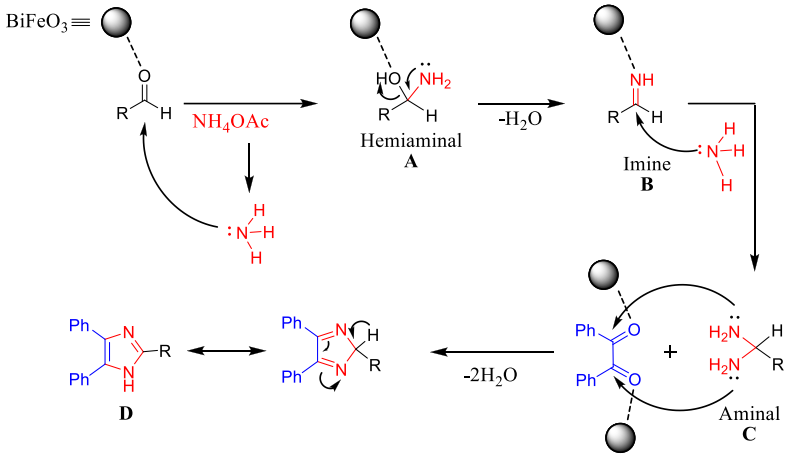


Fig. S16. Proposed mechanism for the synthesis of Imidazole derivatives in the presence of magnetic BFO MNPs nanocatalyst.

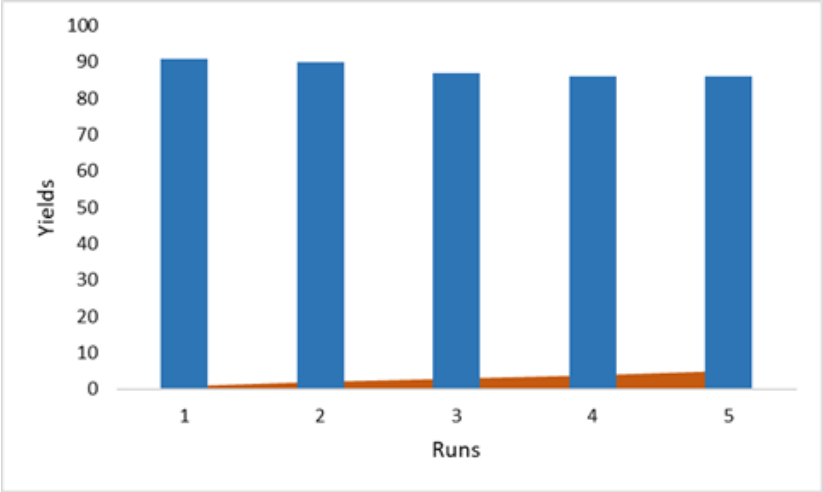


Fig. S17. The results of recyclability and reusability of the BFO MNPs nanoparticles in the model reaction.

Table 4: Comparing the response of the model in terms of time and product yield with recent reports.

En.	Catalyst (loading)	Solvent	Temperature (^{0}C)	Time (min)	Yield (%)	Ref.
1	20 mol%, MoO_3/SiO_2	CH_3CN	80	132	95	[48]
2	0.1 mmol, ZnO	-	110	15	99	[49]
3	0.8 g, of urea/zinc-chloride(3.5:1)	DES	110	15	99	[41]

4	10.0 mol, $Mn(MCG)(H_2O)_3$	EtOH	Reflux	40	89	[43]
5	30.0 mg Fe_3O_4-DOPA-Cu	EtOH	M.W, 100-W	15	95	[50]
6	20.0 mg, $[P_4$-VP$]$-$TiCl_4$	-	80	20	97	[51]
7	10.0 mg, $BiFeO_3$	-	80	15	91	This work