RESEARCH PAPER

Magnetic Core-Shell Fe_3O_4@Nano-Cellulose/TiCl as an Efficient and Recyclable Nano-Catalyst for the Synthesis of 2, 3-Dihydroquinazolin-4(1H)-ones

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ABSTRACT

Magnetic solid-acid catalyst Fe_3O_4@nano-cellulose/TiCl was studied for the synthesis of 2, 3-dihydroquinazolin-4(1H)-ones through two-component condensation of 2-aminobenzamide and aldehydes. This protocol offers the advantages of mild reaction conditions, easy work-up, excellent yields, simple magnetic separation of the catalyst and its recyclability up to seven cycles without any considerable loss of efficiency, which are consistent with the DFT calculation data.

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INTRODUCTION

2,3-Dihydroquinazolin-4(1*H*)-ones are an important class of fused heterocyclic compounds which have drawn much attention because of their biological potential and pharmaceutical activities such as anti-inflammatory [1], antibacterial [2], antiplasmodial [3], antitumor [4], antimicrobial and anti-oxidant [5]. Several methods have been reported for the synthesis of 2, 3-dihydroquinazolinones [6]. Among the diverse synthetic methods for the preparation of 2-aryl-2, 3-dihydroquinazolin-4(1H)-ones, the most popular method includes condensation of 2-aminobenzamide with aldehydes or ketones [7]. Various catalysts, such as Wang-OSO_3H [8], CAN.SiO_2 [9], 2-morpholinoethanesulfonic acid [10], Amberlyst-15 [11], *N*-propylsulfamic acid supported on magnetic Fe_3O_4 nanoparticles (MNPs-PSA) [12], $CuCl_2$/Fe_3O_4-TEDETA [13], $[PYC_4SO_3H][HSO_4]$/A 300 SiO_2 [14], $[Bmim]PF_6$ [15], tetrabutylammonium bromide (TBAB) [16] and NH_2SO_3H [17] have been used to promote this reaction. Some of these catalysts suffer from limitations such as high amount of catalyst, low recyclability and require tedious workup procedure for the catalyst separation. Thus, the identification of an efficient reusable heterogeneous catalytic system with numerous advantages such as cost-effectiveness, environmentally benign, easy workup and good stability for the synthesis of 2-aryl-2, 3-dihydroquinazolin-4(1H)-ones is of prime importance.

In recent decades, magnetic nanoparticles (MNPs) have appeared as an excellent type of

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catalyst support because of their good stability, easy synthesis and functionalization, high surface area and facile separation by magnetic forces, as well as low toxicity and price [18]. Other important features of these magnetic catalysts are high catalytic activity, high degree of chemical stability in various organic and inorganic solvents, reusability and benign character in the context of green chemistry. Among the various MNPs, magnetite (Fe_3O_4) is mostly used as a core magnetic support. [19] Fe_3O_4 nanoparticles have been prepared by precipitation [20], co-precipitation [21] and hydrothermal [22] methods. Surface-functionalizing of iron oxide MNPs by various materials such as surfactants [23], silica [24], carbon [25], and polymers [26] were introduced as simple approaches to stabilize and modify the as-prepared MNPs. Coating of solid surfaces by polymers imparts various desirable properties to MNPs such as excellent thermal stability, extension loading amount of immobilized catalyst, chemical inertness, improvement in catalyst leaching and ease of succedent functionalization.

Cellulose is one of the most abundant and renewable polymers in the world that has been widely studied in both academic and industrial research [27]. This biopolymer exhibits some excellent properties including mechanical

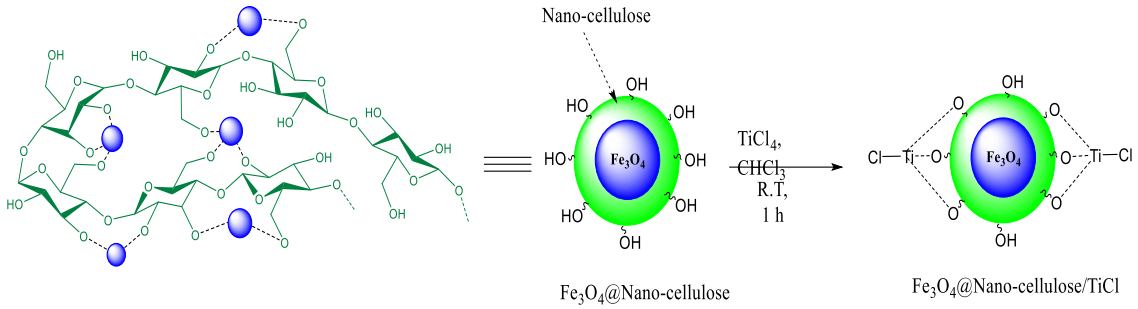
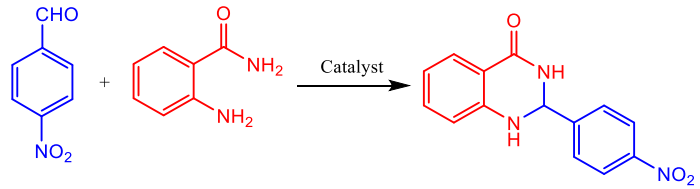


Fig. 1. Preparation of Fe_3O_4@nano-cellulose/TiCl.

Table 1. Screening of the reaction parameters for the synthesis of 2, 3-dihydroquinazolin-4(1H)-ones [a].



Entry	Solvent	Catalyst (g)	Condition	Time	Yield (%) [b]
1	THF	catalyst (0.05) [c]	R. T.	4 h	15
2	$CHCl_3$	catalyst (0.05) [c]	R. T.	4 h	30
3	CH_3CN	catalyst (0.05) [c]	R. T.	3 h	45
4	C_2H_5OH	catalyst (0.05) [c]	R. T.	15 min	88
5	CH_3OH	catalyst (0.05) [c]	R. T.	3 h	40
6	H_2O	catalyst (0.05) [c]	R. T.	3 h	41
7	-	catalyst (0.05) [c]	R. T.	3 h	50
8	C_2H_5OH	catalyst (0.04) [c]	R. T.	6 min	86
9	C_2H_5OH	catalyst (0.03) [c]	R. T.	6 min	96
10	C_2H_5OH	catalyst (0.02) [c]	R. T.	45 min	60
11	C_2H_5OH	catalyst (0.03) [c]	50 °C	3 h	45
12	C_2H_5OH	catalyst (0.03) [c]	70 °C	3 h	40
13	C_2H_5OH	catalyst (0.03) [c]	80 °C	3 h	35
14	C_2H_5OH	-	R. T.	6 h	10

[a] The amount ratio of 2-aminobenzamide (mmol) and 4-nitrobenzaldehyde (mmol) are equal to 1:1, [b] Isolated yield, and [c] Fe_3O_4@NCs/TiCl.

robustness, biodegradability, hydrophilicity, and biocompatibility [28]. Owing to these fascinating properties, cellulose has found a wide application in a variety of areas such as pharmacy, agriculture, medical science, industries, and so many other related branches [29]. Specifically, the hydroxyl groups in cellulose provide active sites for numerous attractive chemical modifications. Thus, Cellulose can be used as an efficient support for bonding several functional groups to produce impressive biopolymer-based catalysts [30].

Among cellulose derivatives, the nanostructure of the cellulose is particularly appealing due to combining important properties of cellulose with amazing features of nano-scale materials. Recently, we prepared nano-cellulose (NCs) by sulfuric acid hydrolysis of cotton [31] and we used it as a protecting shell for preparation core-shell structure Fe_3O_4@nano-cellulose (Fe_3O_4@NCs). Subsequently, we utilized Fe_3O_4@NCs as magnetic support for $TiCl_4$ lewis acid and synthesis of Fe_3O_4@nano-cellulose/TiCl (Fe_3O_4@NCs/TiCl) as a biodegradable, effective and reusable magnetic nano-catalyst (Fig. 1) [32].

Herein we wish to report Fe_3O_4@nano-cellulose/TiC as a green, magnetic and effective heterogeneous nano-catalyst for the synthesis of 2-aryl-2, 3-dihydroquinazolin-4(1H)-ones *via* two-component condensation reaction of 2-aminobenzamide and aldehydes in EtOH at

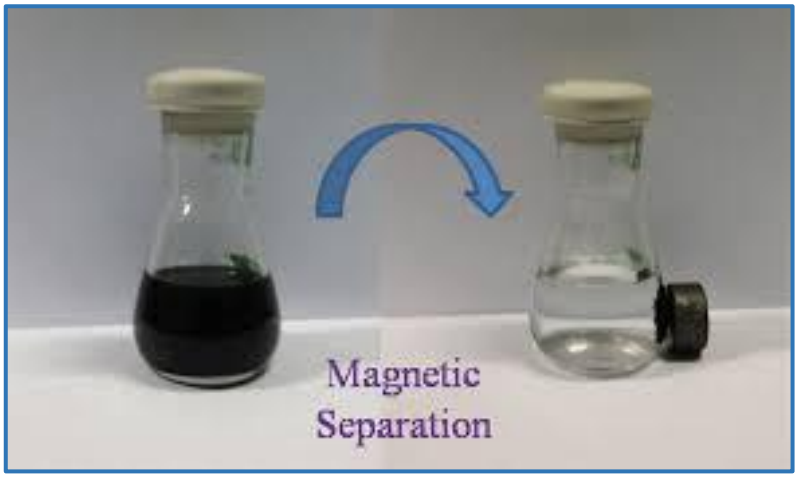


Fig. 2. Magnetic separation of Fe_3O_4@NCs/TiCl.

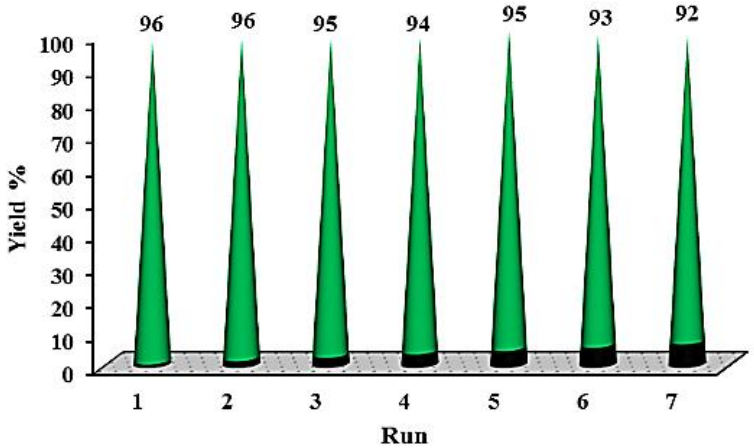


Fig. 3. Recycling experiment.

room temperature.

MATERIALS AND METHODS

General

All compounds were purchased from Merck, Aldrich and Fluka chemical companies and used without any additional purification. FT-IR spectra were run on a Bruker, Equinox 55 spectrometer. A Bruker (DRX-400 Avance) NMR was used to record the ^{1}H-NMR spectra. Melting points were determined by a Buchi melting point B-540 B.V.CHI apparatus and were uncorrected.

General procedure for synthesis of 2, 3-dihydroquinazolin-4(1H)-ones

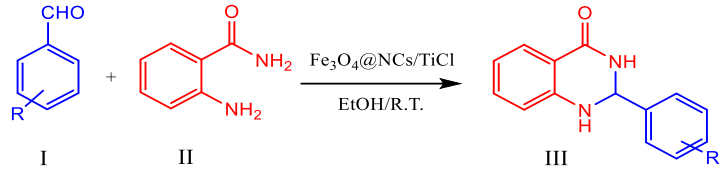
Fe_3O_4@NCs/TiCl (0.03 g) was added to a solution of 2-aminobezamide (1 mmol) and aldehyde (1 mmol) in EtOH (3 mL). The mixture was stirred at room temperature for an appropriate time as indicated in Table 3. After completion of the reaction (monitored by TLC), the catalyst was separated by using an external magnet and the reaction mixture was decanted. Subsequently, by adding water to the decanted solution, the product appeared as a pure solid in high yields.

Table 2. Comparative study of the present method and some other reported methods for synthesis of 2, 3-dihydroquinazolin-4(1H)-ones.

Entry	Catalyst	Condition	Time	Yield (%) [a] [Ref]
1 [b]	Wang-OSO_3H (10% w/w)	H_2O /100 °C	30 min	85 [8]
2 [b]	Y (10 mol %) [e]	Aq.EtOH/60 °C	2 h	91 [10]
3 [b]	Amberlyst-15 (50% w/w)	CH_3CN/80 °C	1 h	75 [11]
4 [c]	MNPs-PSA (10 mg) [f]	H_2O/70 °C	25 min	90 [12]
5 [d]	$CuCl_2$/Fe_3O_4-TEDETA (5mg)	EtOH/ Reflux	20 min	96 [13]
6 [c]	X (0.03 g) [g]	-/ 110 °C	10 min	90 [14]
7 [b]	[Bmim]PF_6 (3 mL)	-/75 °C	45 min	82 [15]
8 [b]	TBAB (1.6 mmol) [h]	-/100 °C	90 min	80 [16]
9 [c]	NH_2SO_3H (10 mol %)	H_2O/70 °C	35 min	89 [17]
10 [b]	Fe_3O_4@NCs/TiCl (0.03 g)	EtOH/R.T.	6 min	96 [18]

[a] Isolated yield, [b] 2-aminobenzamide, and 4-nitrobenzaldehyde, [c] 2-aminobenzamide, and 4-Chlorobenzaldehyde, [d] 2-aminobenzamide, and 4-Fluorobenzaldehyde, [e] 2-morpholinoethanesulfonic, [f] N-propylsulfamic acid supported onto magnetic Fe_3O_4 nanoparticles, [g] [PYC_4SO_3H][HSO_4]/A 300 SiO_2., [h] tetrabutylammonium bromide were used, and [i] This work.

Table 3. Fe_3O_4@NCs/TiCl-catalyzed synthesis of 2, 3-dihydroquinazolin-4(1H)-ones (IIIa-k) [a].



Entry	R	Product	Time (min)	Yield (%) [b]	M.P. [Ref]
1	H	III_a	10	92	219-220 [9]
2	4-NO_2-	III_b	6	96	309-312 [16]
3	4-Cl-	III_c	6	97	193-194 [8]
4	4-Br	III_d	6	95	199-200 [13]
5	4-$(CH_3)_2CH$-	III_e	10	85	158-161 [9]
6	2-NO_2-	III_f	10	90	191-192 [10]
7	2-Cl-	III_g	9	95	206-208 [8]
8	3-NO_2-	III_h	10	90	193-195 [10]
9	3-Br-	III_i	10	93	223-224 [14]
10	2, 4-$(Cl)_2$-	III_j	12	89	166-169 [33]
11	2, 4-$(MeO)_2$-	III_k	12	85	185-187 [17]

[a] Reaction conditions: 2-aminobenzamide (1.0 mmol), aldehyde (1.0 mmol) and Fe_3O_4@NCs-TiCl (0.03 g) were used in EtOH at room temperature. [b] Isolated yield.

The recovered catalyst was washed 3 times with ethanol, dried and reused for subsequent runs under the same reaction conditions.

^{1}H-NMR data for selected compounds

2-(4-Nitrophenyl)-2, 3-dihydroquinazolin-4(1H)-one

Yellow solid. ^{1}H NMR (Acetone-d_6, 400 MHz): δ 8.26(d, J=8 Hz, 2H), 7.87 (d, J=8 Hz, 2H), 7.78 (m, 1H), 7.52 (brs, 1H), 7.30 (m, 1H), 6.84 (d, J=8 Hz, 1H), 6.79 (d, J=6.8 Hz, 1H), 6.51 (brs, 1H), 6.11 (s, 1H). IR (KBr): 3283, 3172, 1641, 1606, 1515, 1460, 1346 cm^{-1}. mp: 309-312 ˚C.

2-Phenyl-2, 3-dihydroquinazolin-4(1H)-one

White solid. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.45 (brs, 1H), 8.16 (m, 1H), 8.02 (m, 2H), 7.83 (d, J=7.6 Hz, 3H), 7.69 (brs, 1H), 7.37 (brs, 1H), 7.26 (d, J=6.4 Hz, 1H), 7.15 (brs, 1H), 6.27 (s, 1H). IR (KBr): 3303, 3176, 3060, 1652, 1610, 1507, 1481 cm^{-1}. mp: 219-220 ˚C.

RESULTS AND DISCUSSION

To optimize the reaction conditions, initially, the reaction of 2-aminobenzamide and 4-nitrobenzaldehyde was selected as the

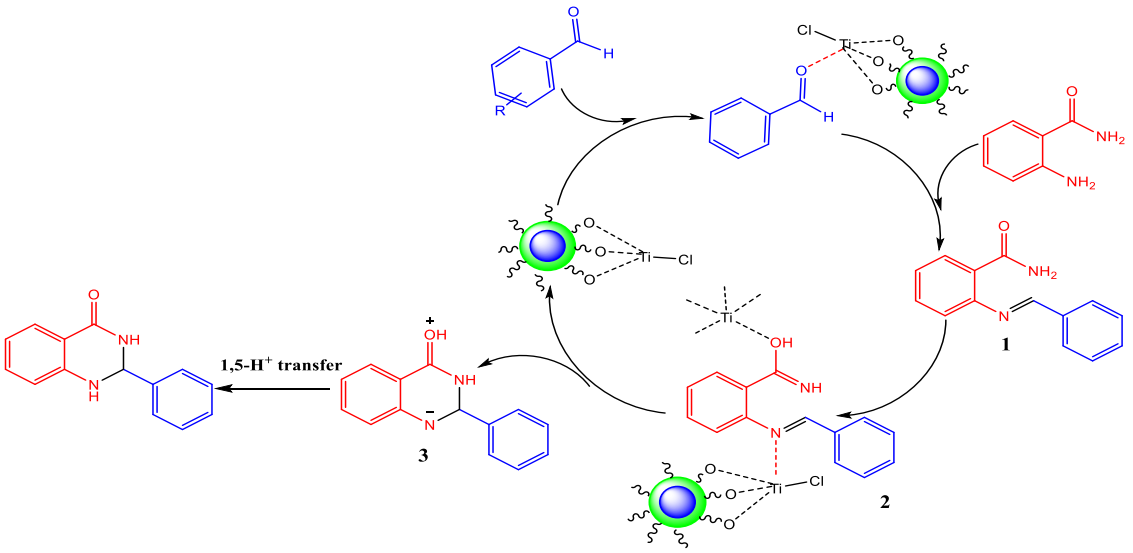


Fig. 4. Proposed mechanism for the synthesis of 2, 3-dihydroquinazolin-4(1H)-ones.

Table 4. The electronic band gap (E_g=E_{HOMO}-E_{LUMO}) and total energy computations for all 2, 3-dihydroquinazolin-4(1H)-ones derivatives.

Entry	R	E_{tot} (a.u)	E_g=E_{HOMO}-E_{LUMO}
1	H	-720.85527	0.0878
2	4-NO_2-	-3282.06230	0.09436
3	4-Cl-	-3282.06232	0.09638
4	4-Br-	-3178.24761	0.09055
5	4-$(CH_3)_2$CH-	-835.63981	0.05385
6	2-NO_2-	-924.20942	0.08615
7	2-Cl-	-3178.24079	0.09027
8	3-NO_2-	-924.19831	0.08625
9	3-Br-	-2948.65271	0.08853
10	2, 4-$(Cl)_2$-	-838.16266	0.07661
11	2, 4-$(MeO)_2$-	-834.20644	0.05328

model reaction. The reaction was optimized for various parameters such as solvent, temperature and catalyst loading. The effect of solvent was investigated by performing the model reaction in the presence of 0.05 g catalyst in various solvents such as THF, $CHCl_3$, CH_3CN, EtOH, MeOH, H_2O and also in solvent-free conditions at room temperature (Table 1, entries 1-7). Among all the screened solvents, EtOH was found to be the best solvent (Table 1, entry 4) in terms of the reaction time and yield of the desired product and work-up procedure.

To optimize the catalyst amount, the model reaction was performed in the presence of various amounts of the catalyst and according to the obtained results (Table 1, entries 8–10) 0.03 g of the catalyst was chosen as the best catalyst amount. The effect of reaction temperature was also examined (Table 1, Entry 11-13). Increasing the reaction temperature up to 80 °C led to a decrease in the yield of desired product due to the increase in by-products. In a blank reaction, without a catalyst, low yield of the product was achieved after a prolonged reaction time (Table 1, entry 14). This shows that the catalyst has an important role in the completion of this reaction. In conclusion, the best reaction condition for this transformation is the use of 0.03 g of the catalyst in EtOH at room temperature (Table 1, Entry 9).

The reusability of the catalyst was also investigated in the model reaction under the optimized reaction conditions. The magnetic nature of the catalyst allowed its facile recovery by simple separation by an external magnet (Fig. 2), washing with ethanol and drying at room temperature to provide an opportunity for recycling experiments. The separated nano-catalyst was reused in the mentioned reaction

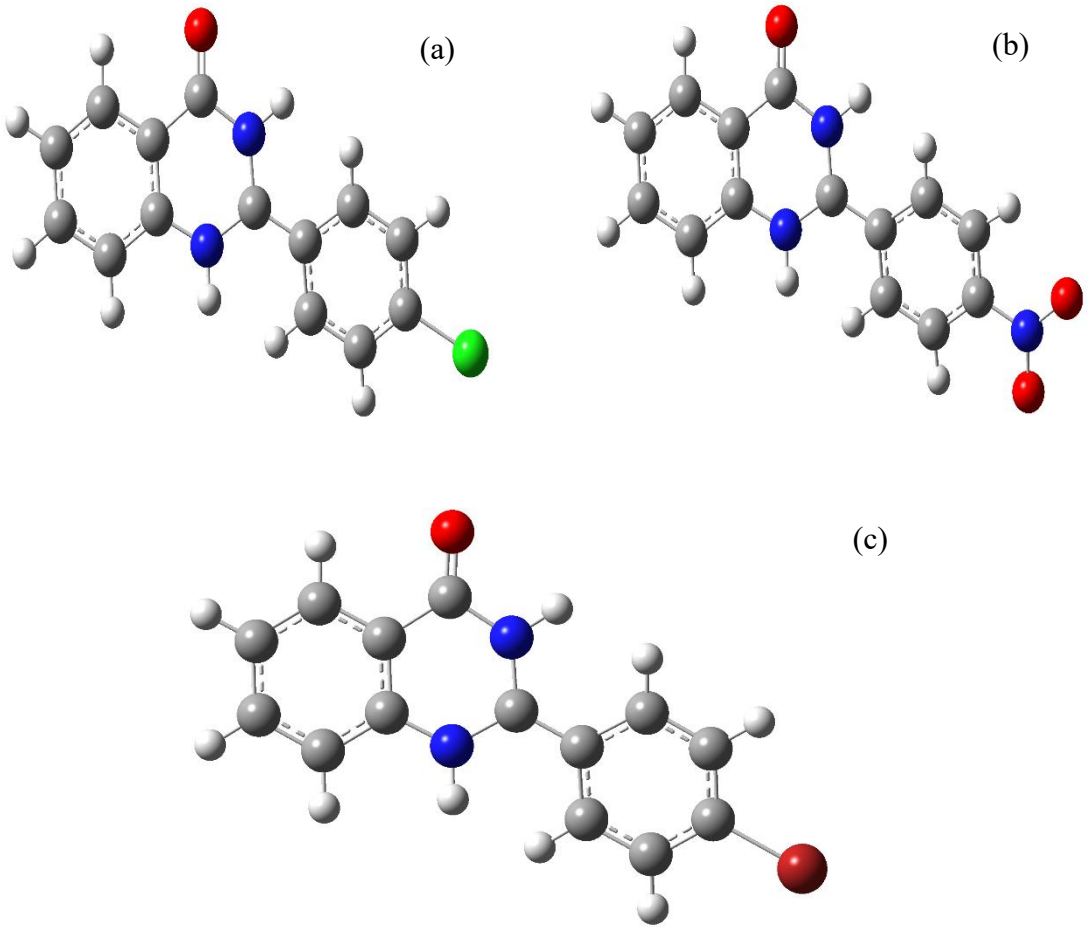


Fig. 5. The optimized structures for (a) 4-Cl-, (b) 4-NO_2-, and (c) 4-Br- compounds.

seven times without considerable loss of its catalytic activity (Fig. 3). Partial loss of activity may be due to blockage of some active sites of the catalyst.

Comparison of the results of the Fe_3O_4@NCs/TiCl-catalyzed reaction of 2-aminobenzamide (1 mmol) and aldehydes (1 mmol) with previously reported methods shows the merit of the present protocol (Table 2).

Based on the optimized reaction conditions, a range of 2, 3-dihydroquinazolin-4(1*H*)-one derivatives were synthesized by the reaction of 2-aminobenzamide (1 mmol) and various aromatic aldehydes (1 mmol) (Table 3).

All compounds were identified by physical and spectroscopic data (mp, FT-IR and ^{1}H NMR). Aldehydes with both electron-donating and electron-withdrawing substituents were reacted with 2-aminobenzamide at the same reaction conditions and the corresponding 2-aryl-2,3-dihydroquinazolin-4(1H)-ones were obtained in the 85–97% yields (Table 2, entries 2–11).

It is noteworthy that the reaction procedure is very clean without any undesirable side reactions. The workup and purification procedure was also very simple. After completion of the reaction (monitored by TLC), the catalyst was separated by magnetic decantation. Subsequently, cold water was added to the reaction mixture and the precipitate was filtered. The crude products were obtained with very high purity.

The suggested mechanism for this reaction is shown in Fig. 4. The reaction proceeds with the formation of imine through the nucleophilic attack of the amino group in 2-aminobenzamide at the activated carbonyl group of the aldehyde by titanium in Fe_3O_4@NCs/TiCl. The part of amide in the imine intermediate 1 is converted into its tautomer in the presence of a catalyst to give intermediate 2. The formed intermediate 2 could be activated by Fe_3O_4@NCs/TiCl, which will be further converted into intermediate 3 by intramolecular nucleophile attack of the nitrogen on the imine carbon. Finally, we obtained the desired product 2, 3-dihydroquinazolin- 4(1H)-ones by a simple 1, 5-proton transfer (Fig. 4).

Computational details

The density functional theory (DFT) computations were carried out using the Gaussian g09 program package [34-36], with the B3LYP exchange-correlation functional (Beck, 3-parameter, Lee-Yang-Parr) [37, 38] and 6-311G (d, p) basis set [39, 40] in order to determine the most stable combination of 2, 3-dihydroquinazolin-4(1H)-ones derivatives. The total energy and electronic band gap (E_g=E_{HOMO}-E_{LUMO}) computations for all 2, 3-dihydroquinazolin-4(1H)-ones derivatives are given in Table 4. From this figure, it is found that the stability of 4-Cl- compound is more than that of the other reported compounds, according to stability statistics and total energy.

In addition, the optimized structures of 4-Cl-, 4-NO_2-, and 4-Br- compounds with the E_{tot} of -3282.06232, -3282.06230, and -3178.24761 a.u, respectively, are shown in Fig. 5.

As a result, from the amount of electronic band gap and total energy, and also the relaxed structures, we conclude that the 4-Cl- compound is more stable in comparison with the other reported compounds, which is in good accordance with the experimental reported data.

CONCLUSION

In summary, a very simple, highly efficient and eco-friendly synthetic method has been developed for the synthesis of 2, 3-dihydroquinazolin-4(1H)-ones through direct cyclocondensation of 2-aminobenzamide and aryl aldehydes in the presence catalytic amount of Fe_3O_4@NCs/TiCl in ethanol at room temperature. This protocol offers the advantages of mild reaction conditions, excellent yields, short reaction time, easy work-up procedure, product purity, magnetic separation and reusability of nano-catalyst. The calculation outcomes revealed that the DFT simulation results validated the experimental reported data.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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