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Journal:	*New Journal of Chemistry*
Manuscript ID:	NJ-ART-03-2015-000516.R1
Article Type:	Paper
Date Submitted by the Author:	02-Apr-2015
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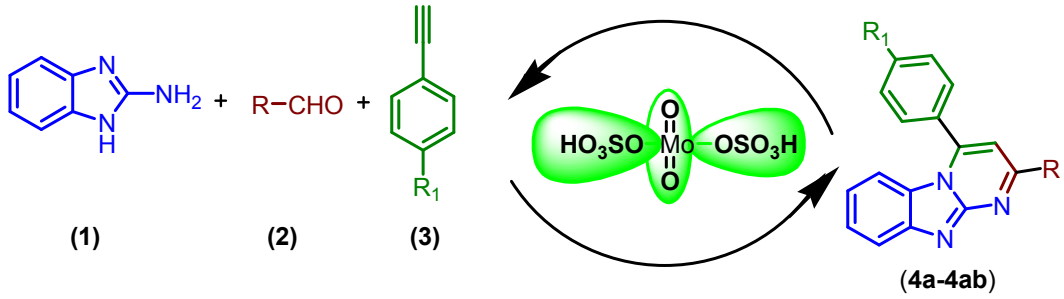

Synthesis of imidazo[1,2-*a*]pyrimidines has been accomplished for the first time under solvent-free conditions by using molybdate sulfuric acid (MSA) as a heterogeneous catalyst. The present protocol is operationally simple, green and offers several advantages over the existing methods.

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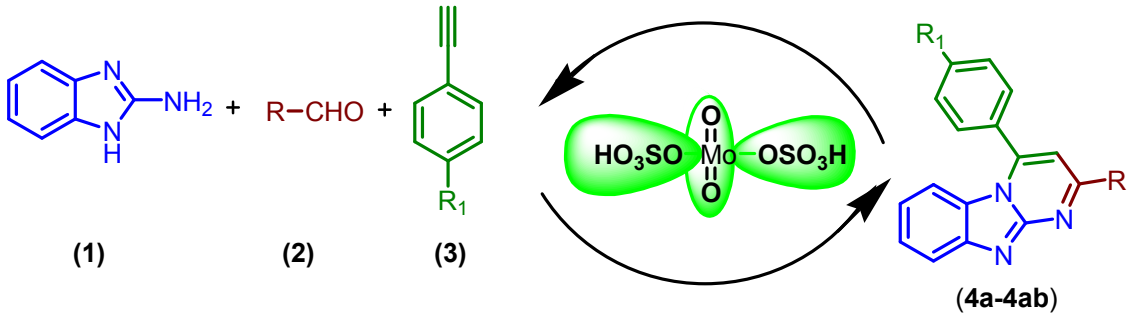
Graphical abstract



Synthesis of imidazo[1,2-*a*]pyrimidines has been accomplished for the first time under solvent-free conditions by using molybdate sulfuric acid (MSA) as a heterogeneous catalyst. The present protocol is operationally simple, green and offers several advantages over the existing methods.

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Abstract

A one-pot multi-component, green, and highly efficient protocol has been developed for the synthesis of imidazo[1,2-*a*]pyrimidines annulated heterocyclic scaffolds (**4a–4ab**) using molybdate sulfuric acid (MSA) as an eco-friendly and reusable catalyst in good to excellent yields under solvent-free conditions and efficiency of producing three new bonds (two C−N and one C−C) in a single operation. Other remarkable features of this environmentally benign protocol are short reaction time, a wide range of functional group tolerance, use of inexpensive heterogeneous catalyst, and high yield of products via a simple experimental and work-up procedure. The catalyst can be recovered and reused for at least four runs without any significant impact on product yields.

Keywords- Imidazo[1,2-*a*]pyrimidines, solid acid catalyst, *6-endo-dig* cyclization, solvent-free, MCR

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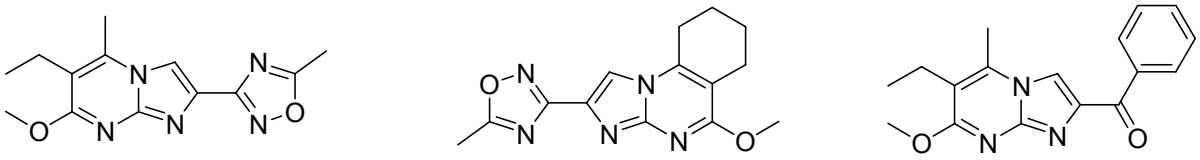
1. Introduction

There is a growing demand for complex functionalized molecules for high-throughput screening (HTS) in order to find valuable biological probes and lead molecules for drug discovery. A survey of recent literature reveals several synthesis and pharmacological properties of ring junction heterocyclic (bridge headed heterocyclic) compounds. In particular, aryl and heteroaryl imidazo[1,2-a]pyrimidines have significant importance in the pharmaceutical industry owing to their broad range of interesting pharmacological activity.[2] Contrarily, the natural abundance of nitrogen ring junction heterocycles was very less but with the available moiety many studies have been reported. Imidazo-fused heterocyclic derivatives are complex functionalized molecules, which have attracted considerable synthetic interest due to their different pharmaceutical and biomedical research. Its derivatives found in several natural and biologically active molecules and shows the remarkable biological profile such as, antimicrobial, anticancer, and antitubercular agents, benzodiazepine receptor agonists, and calcium channel blockers.[3] Currently several marketed drugs constitute the imidazo-fused fragment in the main core structure. In Fig. 1, three representative pharmacological active imidazo-fused pyrimidine derivatives are shown, namely fasiplon, taniplon, and divaplon which is used as anxiolytic drugs in many clinics.



Fasiplon Taniplon Divaplon

Figure 1 Examples of biologically active imidazo-fused pyrimidine derivatives.

So there is a strong need to develop quick and efficient synthetic methods to access a large variety of complex functionalized molecules. Multicomponent coupling reactions (MCRs) are known as a powerful tool for the construction of novel and structurally complex molecules in a single pot ensuring high atom economy, good overall yields and high selectivity, lower costs, shorter reaction times, minimizing waste, labor, energy, and avoidance of expensive purification processes.[4] Recently, a few efficient synthetic methods of imidazo-fused derivatives have been developed, including Cu-promoted synthesis of imidazopyridine via *exo-dig* cycloisomerization using aldehydes, 2-aminopyridines, and alkynes.[5] Synthesis of imidazo-fused heterocycles involving 2-aminopyridines, alkynes, and aldehydes using copper sulfate/glucose as a catalyst via *exo-dig* cyclization.[6] Synthesis of imidazopyridine compound in the presence of 2-

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aminopyridines, alkynes, and aldehydes using Cu-MOF catalysts.[7] P. Sivaramakrishna Reddy *et.al*. described $InBr_3$-catalyzed synthesis of imidazo[1,2-*a*]pyridines.[8] All these reported methodologies shows to the formation of five-membered ring systems.

To the best of our knowledge only mukesh kumar *et.al*. have reported a three-component reaction of alkyne, 2-aminobenzimidazole and aldehyde in the presence of CuI/silver carbonate as dual catalyst in acetonitrile as a solvent to give multisubstituted imidazopyrimidines via *6-endo-dig* cyclization (six-membered ring).[9] But unfortunately, they used homogenous catalyst and organic solvent are not recyclable. On the other hand, a huge amount of effort has been dedicated to the development of chemical reactions in agreement with the principles of green chemistry. Although various green solvents, such as ionic liquids and water, have been extensively studied, not using a solvent at all is definitely the best option, which makes the development of solvent-free reactions a high priority. The progress in the field of solvent and heterogenous acid catalyst[10] reactions is gaining much attention for their low cost, safety, and eco-friendliness.

Acid-catalyzed reactions have been widely used in the production of chemicals. The homogenous mineral liquid acids, such as HCl, H_2SO_4, and HF, are efficient acid catalysts due to their uniform acid sites and strong acid strength. However, the employment of liquid acids in industry often faces problems of wastewater generation, equipment corrosion, and recycling difficulty.[11] The development of solid acids as replacements for liquid acids has received growing research attention. These considerations are currently driving our effort to develop heterogeneous organic transformations. Molybdate sulfuric acid (MSA) is an alternative to sulfuric acid that was synthesized by the reaction of anhydrous sodium molybdate with chlorosulfonic acid. This new inorganic solid acid has been applied as an efficient catalyst to a variety of organic transformations.[12] It has many advantages over conventional acid catalysts, such as ease of handling, stability, less cost, easy recyclability due to insolubility in most of the organic solvent.

In connection with our consistent interest in the development of practical strategies for the selective synthesis of various functional heterocycles, using heterogeneous acid catalysts under solvent-free conditions.[13] Herein, we communicate our discovery of a molybdate sulfuric acid (MSA) mediated synthesis of imidazo[1,2-*a*]pyrimidines (**4a-4ab**) in one pot coupling of 1*H*-benzo[*d*]imidazol-2-amine (**1**), aldehydes (**2**) and alkyne (**3**) via intramolecular C−N bond formation and 6-*endo-dig* cycloisomerization at 85 °C under solvent-free condition (Scheme 1).

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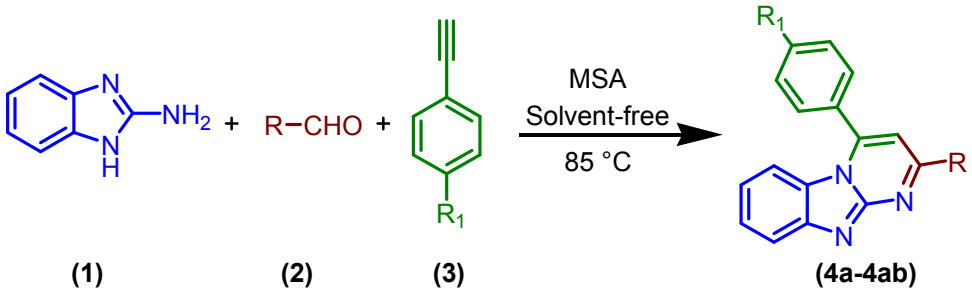

Scheme1. Synthesis of imidazo[1,2-*a*]pyrimidines derivative catalyzed by MSA under solvent-free condition.

2. Results and discussion

For our initial investigation the reaction of 1*H*-benzo[*d*]imidazol-2-amine (**1**, 1 mmol), 3,4,5-trimethoxybenzaldehyde (**2a**, 1mmol) and 1-ethynyl-4-methylbenzene (**3a**, 1.5 mmol) under neat condition at 85 °C (Scheme 1) run to standardize the experimental conditions. In the absence of catalyst we could not isolate any desired product even after 10 h stirring. After that, the same set of reaction was performed in the presence of 5 mol% of the tungstate sulfuric acid (TSA). Within 4 h the corresponding title product **4a**, was isolated in 38% product yield (Table 1, entry 2). The product **4a**, was confirmed by usual spectroscopic techniques. Encouraged by this result, we attempted to optimize the yield of the reaction by screening the same set of reaction with various sulfonic acid containing catalysts such as polystyrene supported *p*-toluenesulfonic acid (PS-PTSA), glucose sulfonic acid (GSA), phospho sulfonic acid (PSA), PEG-SO_3H and molybdate sulfuric acid (MSA) at even less than 3 h and the results are summarized in Table 1. Among all the screened catalysts MSA was found superior with respect to reaction time and product yield (Table 1, entry 7). Moreover, we found that the yields were obviously affected by the amount of MSA loaded. When 5 mol%, 10 mol%, 15 mol% and 20 mol% of MSA were used the yields were 65, 78, 87 and 87%, respectively (Table 1, entries 7-10). Therefore, 15 mol% of MSA were sufficient and no more significant improvement in the reaction rate and product yield was observed while increasing the amount of the catalyst from 5 to 15 mol% (Table 1, entry 7).

Table 1 Influence of the catalyst for the synthesis of 2-(3,4,5-Trimethoxyphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine (**4a**)[a].

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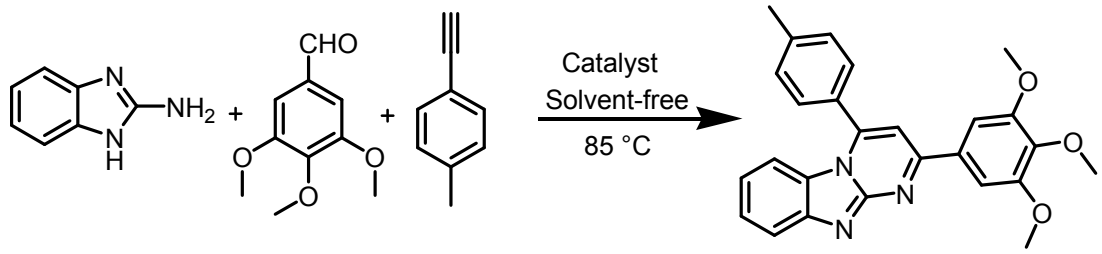

(1) **(2a)** **(3a)** **(4a)**

Entry	Catalyst (mol%)	Time (h)	Temperature (°C)	Yield[b] (%)
1[c]	Neat	10	85	NR
2	TSA (5)	4	85	38
3	GSA (5)	2.8	85	65
4	PS-PTSA (20 mg)	3.1	85	58
5	PSA (5)	2.7	85	66
6	PEG-SO_3H (30 mg)	3.5	85	54
7[d]	MSA (15)	2	85	87, 87, 82, 80
8	MSA (5)	2.5	85	65
9	MSA (10)	2.3	85	78
10	MSA (20)	2	85	87

[a]Reaction of 1*H*-benzo[*d*]imidazol-2-amine (**1**, 1 mmol), 3,4,5-trimethoxybenzaldehyde (**2a**, 1mmol) and 1-ethynyl-4-methylbenzene (**3a**, 1.5 mmol) under neat condition; [b]Isolated yield; [c]No reaction, [d] catalyst was reused four times.

Then we investigated the influence of various organic solvents at different reaction temperatures on the model reaction with 15 mol% of MSA. Among the various solvents such as toluene, ethanol, THF, CH_2Cl_2, and DMF rate of the reaction was sparingly slow and resulted in lower product yields (Table 2, entries 1-6). Conducting the same reaction in acetonitrile improved both the reaction rate as well as product yield (Table 2, entry 7). We also investigated different temperatures for the model reaction (Table 2, entries 8-12). It was observed that fast reaction occurred on raising the temperature from 50 °C to 85 °C and the yield of preferred product increased significantly. We were satisfied to find that the reaction proceeded smoothly and almost complete conversion of reactants was observed at 85 °C to afford the desired product (**4a**)

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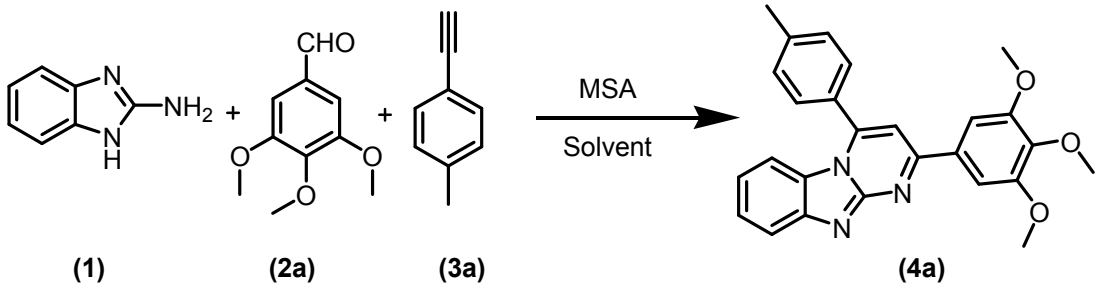
in 87% yield within 2hr under solvent-free condition (Table 2, entry 8). Further increase the temperature did not affect the product yield

However, the better the product yield was observed in solvent-free conditions (Table 2, entry 8) and could be explained by a uniform distribution of the eutectic mixture of reactants, being in closer proximity to react them. From all these establishments we concluded that 15 mol% of MSA, at 85 °C under solvent-free condition are optimized reaction.

Table 2 Optimization of reaction conditions of solvent and temperature for the synthesis of 2-(3,4,5-Trimethoxyphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine (**4a**)[a]



(1) **(2a)** **(3a)** **(4a)**

Entry	Solvent	Temperature	Time (h)	Yield (%)[b]
1	Toluene	110	3.7	48
2	Chlorobenzene	120	3.5	55
3	CH_2Cl_2	75	4.7	58
4	CCl_4	75	4.7	45
5	THF	65	3.75	54
6	Ethanol	65	4.3	55
7	Acetonitrile	85	3.53	74
8	Solvent-free	85	2	87
9	Solvent-free	50	3.2	48
10	Solvent-free	75	3	61
11	Solvent-free	90	2	87
12	Solvent-free	100	2	86

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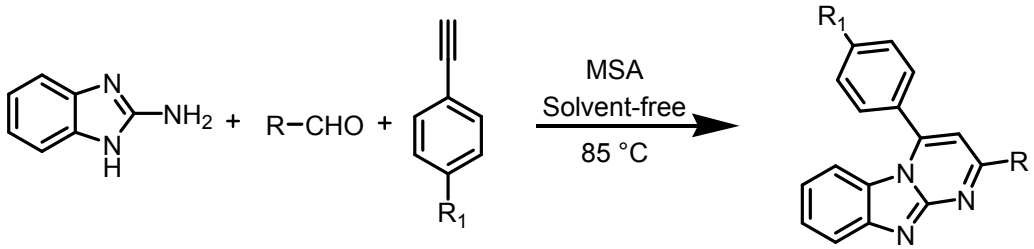
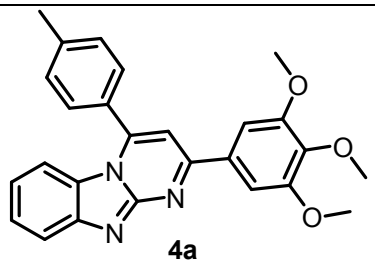
[a]Reaction of 1*H*-benzo[*d*]imidazol-2-amine (**1**, 1 mmol), 3,4,5-trimethoxybenzaldehyde (**2a**, 1mmol) and 1-ethynyl-4-methylbenzene (**3a**, 1.5 mmol), MSA (15 mol%) [b] isolated yield

Next, the generality of this novel three component reaction was examined (Table 3). To our delight, we found this transformation to be very general for a wide range of aldehydes and two different alkynes, and provided easy access to densely substituted imidazo[1,2-*a*]pyrimidines derivatives **4**. Aldehydes displayed good reactivity in this reaction. A variety of functional groups substituted at the aromatic ring of the aldehyde substrate, electron-withdrawing group such as chloro, bromo, fluoro, NO_2 (Table 3, entry 2,7,8, 10, 12, 14 and 21-24) and electron-donating groups such as OCH_3, OEt, isopropyl, Me (Table 3, entry 1, 3-6, 11, 13, 15-18, 20 and 25) were tolerated. The reaction with isopropyl aldehyde was gave lower yields (Table 3, entry 27), We also employed two different alkyne substrates, such as 1-ethynylbenzene and 1-ethynyl-4-methylbenzene, produced imidazo[1,2-*a*]pyrimidines in good to excellent yields. Therefore, the present protocol has general applicability, accommodating a variety of substitution patterns.

Table 3 MSA catalyzed multi-component synthesis of imidazo[1,2-*a*]pyrimidines derivatives[a]



(1) **(2)** **(3)** **(4a-4ab)**

Entry	R	R1	Product	Time (h)	Yield[b] (%)	M.p (°C) [ref]
1	3,4,5-$OCH_3C_6H_2$	CH_3	 **4a**	2	87	258-260

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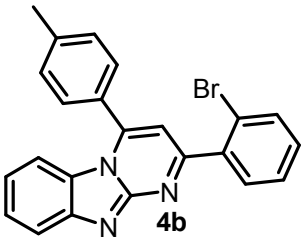
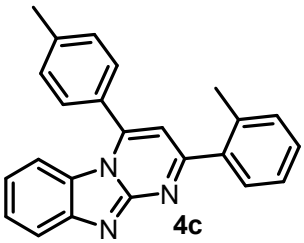
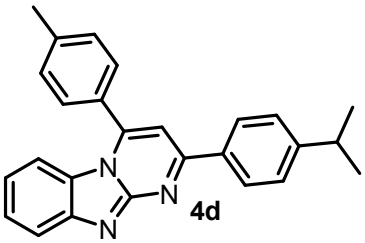
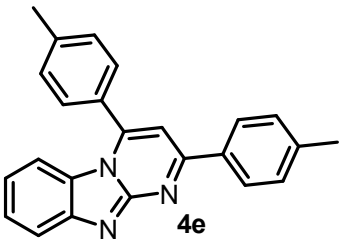
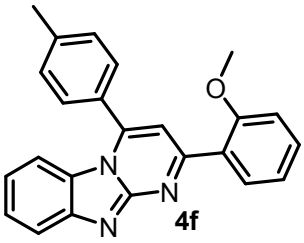
2	2-BrC_6H_4	CH_3	 4b	2.1	82	220-222
3	2-$CH_3C_6H_4$	CH_3	 4c	2.03	81	162-164
4	4-$C(CH_3)_2C_6H_4$	CH_3	 4d	2.25	86	166-168
5	4-$CH_3C_6H_4$	CH_3	 4e	2	80	238-240
6	2-$OCH_3C_6H_4$	CH_3	 4f	2.05	78	156-158

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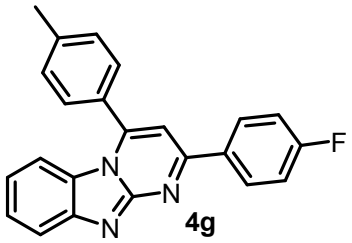
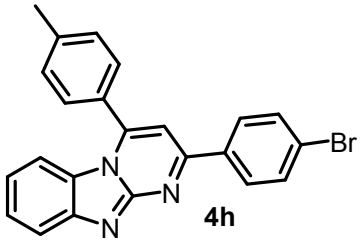
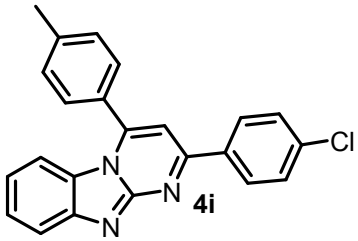
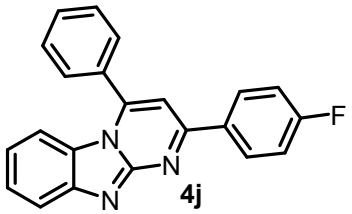
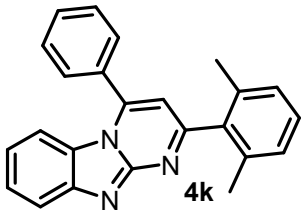
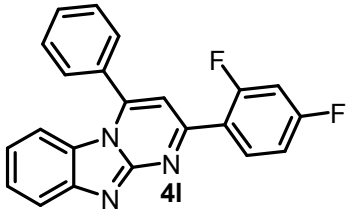
7	4-FC_6H_4	CH_3	 **4g**	2.1	81	240-242
8	4-BrC_6H_4	CH_3	 **4h**	1.9	84	240-242
9	4-ClC_6H_4		 **4i**	2.1	81	206-208[8]
10	4-FC_6H_4	H	 **4j**	2	80	197-199[8]
11	2,6-MeC_6H_3	H	 **4k**	2.3	76	190-192
12	2,4-FC_6H_3	H	 **4l**	2.6	74	252-254

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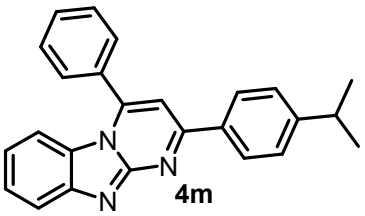
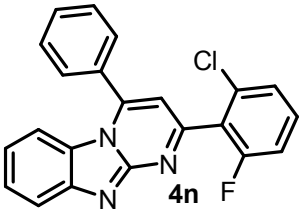
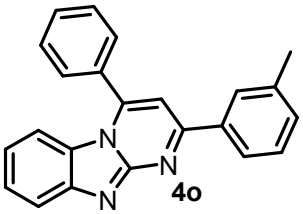
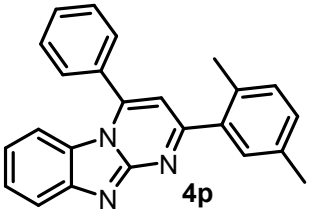
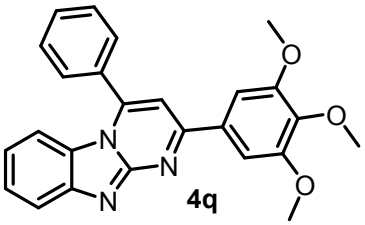
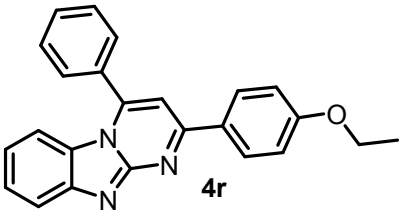
13	4-$C(CH_3)_2C_6H_4$	H	 4m	2.3	81	166-168
14	2-Cl-6-FC_6H_3	H	 4n	2.6	75	248-250
15	3-$CH_3C_6H_4$	H	 4o	2.1	82	248-250
16	2,5-$CH_3C_6H_3$	H	 4p	2.2	79	156-158
17	3,4,5-$OCH_3C_6H_2$	H	 4q	2	84	230-232
18	4-$OC_2H_5C_6H_4$	H	 4r	2.2	82	202-204

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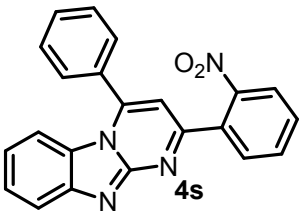
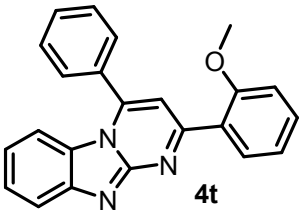
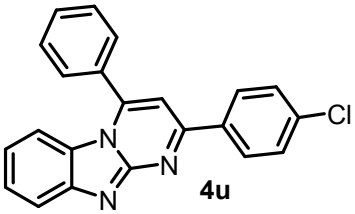
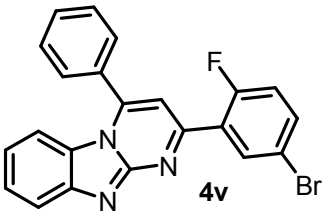
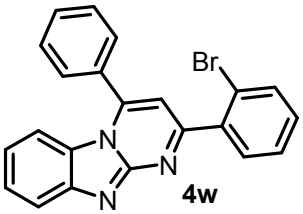
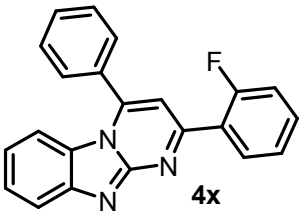
19	2-$NO_2C_6H_4$	H	 4s	2.6	71	218-220
20	2-$OCH_3C_6H_4$	H	 4t	2.2	79	160-162
21	4-ClC_6H_4	H	 4u	2	85	198-200[8]
22	2-F-5-BrC_6H_3	H	 4v	2.3	81	195-197
23	2-BrC_6H_4	H	 4w	2.1	80	188-190
24	2-FC_6H_4	H	 4x	2.1	78	172-174

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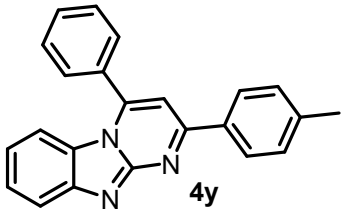
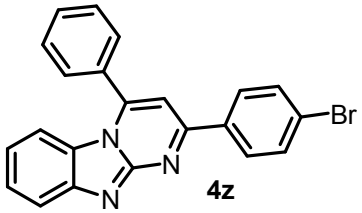
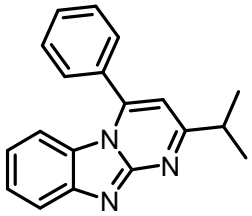
25	4-$CH_3C_6H_4$	H	 **4y**	2	83	190-192
26	4-BrC_6H_4	H	 **4z**	2	84	210-212[8]
27	-$CH(CH_3)_2$	H	 **4ab**	2.6	52	193-195[8]

[a]Reaction of 1*H*-benzo[*d*]imidazol-2-amine (**1**, 1 mmol), aldehydes (**2a**, 1mmol) and alkynes (**3a**, 1.5 mmol) catalyzed by MSA under solvent-free condition at 85 °C, [b] isolated yield

The reported as well as synthesized novel compounds (**4a-4ab**) have been ascertained on the basis of ^{1}H NMR, ^{13}C NMR and HRMS data.

In order to investigate the catalytic activity and the possibility of the catalyst recyclability and reusability, the MSA was recovered from the reaction mixture by simple filtration in ethyl acetate. The separated catalyst was dried in vacuum oven at 100 °C and was reused as such for subsequent experiments under similar reaction conditions (Table 1, entry 7). The results showed that the catalyst could be effectively reused for at least four consecutive cycles without much appreciable loss in its catalytic activity. The recyclability data demonstrate that high stability of the catalyst under the reaction conditions (See in supporting information Figure S2).

A possible mechanism of this one-pot reaction is expected on the basis of reported literature.[8] A possible mechanism for the imidazo[1,2-*a*]pyrimidines via *6-endo-dig* cyclization ring formation

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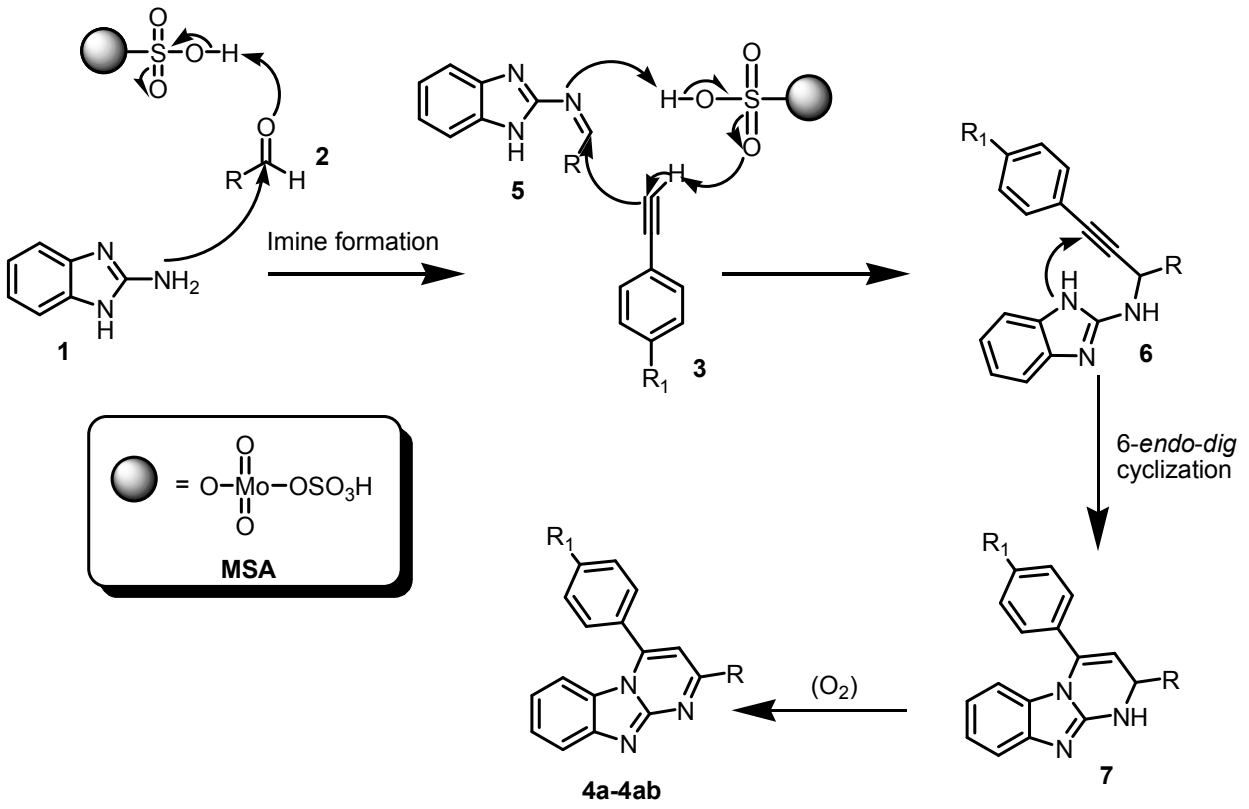
of three-component coupling reactions using molybdate sulfuric acid (MSA) as catalyst is outlined in (Scheme 2).



Scheme 2 Plausible mechanism for the formation of imidazo[1,2-*a*]pyrimidines derivatives.

The reported as well as synthesized novel compounds were further characterized by their spectral properties (^{1}H, ^{13}C NMR, and HRMS).

3. Conclusion

In conclusion, we have successfully developed a facile and highly selective synthesis of novel imidazo[1,2-*a*]pyrimidines via molybdate sulfuric acid (MSA)-mediated oxidative C-H functionalization and *6-endo-dig* cyclization from readily available starting materials. This methodology provides a simple and direct way to access derivatives of the biologically important heterocycles. These reaction conditions display a wide range of functional group tolerance. From an environmental point of view, this protocol represents good atom economy in that the expended MSA can be recycled and reused to mediate this reaction.

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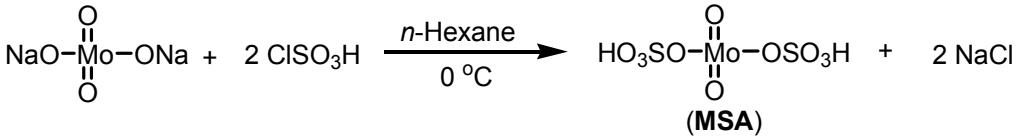
4. Experimental

4.1 Material and methods

Chemicals were purchased from Aldrich and Alfa Aesar Chemical Companies and used without further purification. NMR spectra were recorded in parts per million (ppm) in $CDCl_3$ on a Jeol JNM ECP 400 NMR instrument using TMS as internal standard. Standard abbreviations were used to denote signal multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet). Mass spectra were recorded on a Jeol JMS-700 mass spectrometer. All melting points were determined using open capillaries on an Electrothermal-9100 (Japan) instrument and are uncorrected.

4.2 Preparation of MSA

To dry n-hexane (25 mL) in a 100 mL round bottom flask equipped with overhead stirrer and kept in an ice bath was added a suspension of anhydrous sodium molybdate (20 mmol, 4.118 g). To this solution drop wise added chlorosulfonic acid (0.266 mL, 40 mmol) during 30 min and stirred for 1.5 h (Scheme 3). The reaction mixture was gradually poured into 25 mL of chilled distilled water with stirring. MSA was separated by filtration and it was washed 5-6 times with cold distilled water until its filtrate tests negative for chloride ions. It was dried at 120 °C for 5 h, and obtained in 91% yield as bluish powder.



Scheme 3: Synthesis of MSA

4.3 Synthesis of 2-(3,4,5-Trimethoxyphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine (4a).

A mixture of 1*H*-benzo[*d*]imidazol-2-amine (**1**, 1 mmol), 3,4,5-trimethoxybenzaldehyde (**2a**, 1mmol) and 1-ethynyl-4-methylbenzene (**3a**, 1.5 mmol) and MSA (15 mol %) was stirred at 85 °C under solvent-free condition for 2 h (Table 3, entry 1). The progress of the reaction was monitored by TLC. After completion of the reaction, the mixture was washed with ethyl acetate and filtered to recover the catalyst. The filtrate was evaporated, and the crude product was purified by flash column chromatography on silica gel (200−300mesh) with ethyl acetate and

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hexane as eluent to afford the product **4a** in excellent yield (87%). The MSA catalyst was reused by the way of addition of ethyl acetate to the reaction mixture and filtration followed by drying in a vacuum oven every time. Compounds **4b-4ab** were also synthesized by adopting this procedure.

4.3.1. 2-(3,4,5-Trimethoxyphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 87%; yellow solid; Mp: 258-260 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J*=8.1, 1H), 7.54-7.56 (m, 4H), 7.47 (d, *J*=8.1 Hz, 2H), 7.42 (t, *J*=7.7 Hz, 1H), 7.16 (s, 1H), 7.01 (t, *J*=7.6 Hz, 1H), 6.73 (d, *J*=8.1 Hz, 1H), 3.97 (s, 6H), 3.93 (s, 3H), 2.56 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.30, 153.53, 149.45, 145.50, 141.49, 131.97, 130.07, 128.35, 125.89, 121.08, 120.03, 114.63, 105.04, 61.04, 56.45, 21.72; HRMS (ESI, m/z): calcd for $C_{26}H_{23}N_3O_3$ ($M+H^+$) 425.1739, found: 425.1738.

4.3.2. 2-(2-Bromophenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 82%; yellow solid; Mp: 220-222 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J*=8.1 Hz, 1H), 7.85 (d, *J*=7.7 Hz, 1H), 7.67 (d, *J*=8.1 Hz, 1H), 7.53 (d, *J*=8.1 Hz, 2H), 7.43-7.48 (m, 4H), 7.31 (t, *J*=7.5 Hz, 1H), 7.17 (s, 1H), 7.06 (t, *J*=6.9 Hz, 1H), 6.87 (d, *J*=8.4 Hz, 1H), 2.54 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.85, 148.58, 145.43, 141.55, 139.32, 133.63, 132.04, 131.15, 130.08, 129.47, 128.31, 127.88, 127.43, 126.02, 121.47, 121.32, 120.46, 114.95, 109.89, 21.74; HRMS (ESI, m/z): calcd for $C_{23}H_{16}BrN_3$ ($M+H^+$) 413.0527, found: 413.0528.

4.3.3. 2-(2-Methylphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 81%; yellow solid; Mp: 162-164 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J*=8.1 Hz, 1H), 7.62 (d, *J*=7.7 Hz, 1H), 7.50 (d, *J*=8.1 Hz, 2H), 7.42 (d, *J*=7.7 Hz, 3H), 7.23-7.35 (m, 3H), 7.02 (t, *J*=7.7 Hz, 1H), 6.92 (s, 1H), 6.82 (d, *J*=8.1 Hz, 1H), 2.63 (s, 3H), 2.52 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.57, 149.10, 145.35, 141.42, 137.87, 137.08, 131.48, 130.00, 129.78, 129.70, 129.48, 128.21, 126.02, 125.80, 121.01, 120.19, 114.78, 109.16, 21.65, 21.05; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1580.

4.3.4. 2-(4-Isopropylphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 86%; yellow solid; Mp: 166-168 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J*=8.4 Hz, 2H), 7.94 (s, 1H), 7.50 (d, *J*=8.1 Hz, 2H), 7.44 (d, *J*=7.7 Hz, 2H), 7.40 (d, *J*=7.3 Hz, 1H), 7.35 (d, *J*=8.1 Hz, 2H), 7.18 (s, 1H), 6.99 (t, *J*=7.3 Hz, 1H), 6.75 (d, *J*=8.1 Hz, 1H), 2.93-3.00 (m, 1H), 2.54 (s, 3H), 1.28 (d, *J*=7.0 Hz, 6H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.06, 152.63,

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141.37, 134.38, 130.04, 128.34, 127.94, 127.10, 125.76, 120.93, 120.08, 114.69, 105.30, 34.18, 23.86, 21.72; HRMS (ESI, m/z): calcd for $C_{26}H_{23}N_3$ ($M+H^+$) 377.1892, found: 377.1894.

4.3.5. 2-(4-Methylphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 80%; yellow solid; Mp: 238-240 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, *J*=8.1 Hz, 2H), 7.92 (d, *J*=8.1 Hz, 1H), 7.49 (d, *J*=8.1 Hz, 2H), 7.43 (d, *J*=8.1 Hz, 2H), 7.38 (d, *J*=7.7 Hz, 1H), 7.24 (d, *J*=8.1 Hz, 2H), 7.14 (s, 1H), 6.98 (t, *J*=8.1 Hz, 1H), 6.73 (d, *J*=8.1 Hz, 1H), 2.53 (s, 3H), 2.36 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.95, 149.39, 141.73, 141.33, 133.90, 129.99, 129.74, 129.63, 128.30, 127.72, 125.71, 120.86, 120.03, 114.65, 105.20, 21.69, 21.52; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1579.

4.3.6. 2-(2-Methoxyphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 78%; yellow solid; Mp: 156-158 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J*=8.1, 1H), 7.95 (d, *J* =8.1 Hz, 1H), 7.51 (d, *J*=8.1 Hz, 2H), 7.48 (s, 1H), 7.41-7.44 (m, 4H), 7.11 (t, *J*=7.3 Hz, 1H), 7.02 (d, *J*=7.7 Hz, 1H), 6.98 (d, *J*=8.1 Hz, 1H), 6.77 (d, *J*=8.1 Hz, 1H), 3.88 (s, 3H), 2.53 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.23, 158.06, 147.93, 145.36, 141.14, 132.14, 131.99, 129.95, 128.41, 126.68, 125.64, 121.32, 120.76, 120.05, 114.75, 111.53, 110.16, 55.70, 21.68; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3O$ ($M+H^+$) 365.1528, found: 365.1529.

4.3.7. 2-(4-Flurophenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 81%; yellow solid; Mp: 240-242 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.21-8.24 (m, 2H), 7.90 (d, *J*=7.3 Hz, 1H), 7.51 (d, *J*=7.7 Hz, 2H), 7.44 (d, *J*=7.7 Hz, 2H), 7.39 (t, *J*=7.7 Hz, 1H), 7.11 (t, *J*=7.3 Hz, 3H), 6.98 (t, *J*=7.3 Hz, 1H), 6.73 (d, *J*=8.4 Hz, 1H), 2.54 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.05, 163.54, 159.72, 149.77, 141.49, 132.84, 130.03, 129.90, 129.82, 129.57, 128.27, 125.87, 121.08, 120.06, 116.03, 115.82, 114.72, 104.96, 21.70; HRMS (ESI, m/z): calcd for $C_{23}H_{16}FN_3$ ($M+H^+$) 353.1328, found: 353.1330.

4.3.8. 2-(4-Bromophenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 84%; yellow solid; Mp: 240-242 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, *J*=8.4 Hz, 2H), 7.92 (s, 1H), 7.57 (d, *J*=8.1 Hz, 2H), 7.52 (d, *J*=8.1 Hz, 2H), 7.45 (d, *J*=7.7 Hz, 2H), 7.40 (t, *J*=6.4 Hz, 1H), 7.12 (s, 1H), 7.00 (t, *J*=7.3 Hz, 1H), 6.75 (d, *J*=8.4 Hz, 1H), 2.55 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.66, 149.94, 141.57, 135.55, 132.11, 130.09, 129.23, 128.30, 126.00, 121.25, 120.15, 114.80, 104.92, 21.75; HRMS (ESI, m/z): calcd for $C_{23}H_{16}BrN_3$ ($M+H^+$) 413.0527, found: 413.0526.

4.3.9. 2-(4-Chlorophenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 81%; yellow solid; Mp: 206-208 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J*=7.0 Hz, 2H), 7.91 (d, J=7.0 Hz, 1H), 7.41-7.51 (m, 8H), 7.12 (s, 1H), 7.00 (t, *J*=7.3 Hz, 1H), 6.74 (d,

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J=7.3 Hz, 1H), 2.55 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.63, 149.89, 141.56, 137.52, 130.09, 129.15, 129.03, 128.29, 125.99, 121.22, 120.18, 114.77, 104.97, 21.75; HRMS (ESI, m/z): calcd for $C_{23}H_{16}ClN_3$ ($M+H^+$) 369.1032, found: 369.1031.

4.3.10. 2-(4-Fluorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 80%; yellow solid; Mp: 197-199 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21-8.24 (m, 2H), 7.89 (d, *J* =8.1 Hz, 1H), 7.64-7.71 (m, 5H), 7.39 (t, *J*=7.5 Hz, 1H), 7.11 (t, *J*=8.4 Hz, 3H), 6.97 (t, *J*=7.7 Hz, 1H), 6.62 (d, *J*=8.4 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.73, 151.96, 149.47, 145.47, 136.93, 132.47, 131.13, 129.93, 129.83, 129.41, 128.40, 127.38, 125.91, 121.20, 120.12, 116.05, 115.83, 114.56, 104.90; HRMS (ESI, m/z): calcd for $C_{22}H_{14}FN_3$ ($M+H^+$) 339.1171, found: 339.1172.

4.3.11. 2-(2,6-Dimethylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 76%; yellow solid; Mp: 190-192 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J*=8.4, 1H), 7.63-7.70 (m, 5H), 7.47 (t, *J* =7.3 Hz, 1H), 7.22 (d, *J*=7.3 Hz, 1H), 7.12 (d, *J*=7.7 Hz, 2H), 7.06 (t, *J*=8.1 Hz, 1H), 6.80 (d, *J*=8.1 Hz, 1H), 6.74 (s, 1H), 2.25 (s, 6H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.98, 154.59, 147.80, 138.65, 135.43, 132.24, 131.22, 129.44, 128.79, 128.39, 127.92, 126.03, 121.33, 120.47, 114.82, 109.92, 20.42; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1580.

4.3.12. 2-(2,4-diluorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 74%; yellow solid; Mp: 252-254 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49-8.55 (m, 1H), 8.96 (d, *J*=8.1 Hz, 1H), 7.62-7.73 (m, 5H), 7.45 (t, *J*=8.1 Hz, 1H), 7.34 (s, 1H), 7.08 (t, *J*=8.4 Hz, 1H), 7.03 (t, *J*=8.5 Hz, 1H), 6.90-6.95 (m, 1H), 6.71 (d, *J*=8.4, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.46, 156.92, 151.67, 149.24, 145.41, 133.23, 133.13, 132.42, 131.16, 129.44, 128.43, 126.12, 121.35, 120.27, 114.73, 112.48, 108.52, 108.39, 104.66 ; HRMS (ESI, m/z): calcd for $C_{22}H_{13}F_2N_3$ ($M+H^+$) 357.1077, found: 357.1075.

4.3.13. 2-(4-Isopropylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 81%; yellow solid; Mp: 166-168 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J*=8.4 Hz, 2H), 7.93 (d, *J* =7.7, Hz, 1H), 7.61-7.71 (m, 5H), 7.40 (t, *J*=7.7 Hz, 1H), 7.35 (d, *J*=8.1 Hz, 2H), 7.20 (s, 1H), 6.98 (t, *J*=7.7 Hz, 1H), 6.65 (d, *J*=8.4 Hz, 1H), 2.93-3.0 (m, 1H), 1.28 (d, *J*=6.6 Hz, 6H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.06, 152.69, 149.18, 134.30, 132.69, 131.04, 129.42, 128.47, 127.95, 127.11, 125.80, 121.04, 120.13, 114.54, 105.23, 34.17, 23.85; HRMS (ESI, m/z): calcd for $C_{25}H_{21}N_3$ (M+H+) 363.1735, found: 363.1736.

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4.3.14. 2-(2-chloro-6-fluorolphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 75%; yellow solid; Mp: 248-250 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J*=7.3, 1H), 7.64-7.71 (m, 5H), 7.47 (t, *J*=7.3, 1H), 7.34-7.40 (m, 1H), 7.31 (d, *J* =8.1 Hz, 1H), 7.13 (t, *J* =8.1 Hz, 1H), 7.06 (t, *J*=8.4 Hz, 1H), 6.88 (s, 1H), 6.78 (d, *J*=8.4 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.77, 159.26, 157.27, 151.50, 149.23, 145.43, 133.96, 132.08, 131.26, 131.17, 129.45, 128.40, 126.23, 125.90, 121.61, 120.67, 114.91, 114.83, 114.61, 110.11; HRMS (ESI, m/z): calcd for $C_{22}H_{13}ClFN_3$ ($M+H^+$) 373.0782, found: 373.0784.

4.3.15. 2-(3-Methylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 82%; yellow solid; Mp: 248-250 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (s, 1H), 8.03 (d, *J*=7.7, 1H), 7.94 (d, *J*=8.1, 1H), 7.62-7.72 (m, 5H), 7.42 (t, *J* =7.7 Hz, 1H), 7.37 (t, *J* =7.7 Hz, 1H), 7.30 (d, *J*=7.7 Hz, 1H), 7.22 (s, 1H), 6.99 (t, *J*=7.7 Hz, 1H), 6.66 (d, *J*=8.4 Hz, 1H), 2.44 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.21, 149.27, 145.60, 138.73, 136.61, 132.67, 132.14, 131.09, 129.44, 128.83, 128.57, 128.47, 125.88, 124.97, 121.13, 120.23, 114.59, 105.42, 21.57; HRMS (ESI, m/z): calcd for $C_{23}H_{17}N_3$ ($M+H^+$) 335.1422, found: 335.1421.

4.3.16. 2-(2,5-Dimethylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 79%; yellow solid; Mp: 156-158 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J*=8.1, 1H), 7.62-7.72 (m, 5H), 7.49 (s, 1H), 7.45 (t, *J* =8.2 Hz, 1H), 7.21 (d, *J*=8.1 Hz, 1H), 7.18 (d, *J*=7.7 Hz, 1H), 7.03 (t, *J*=8.4 Hz, 1H), 6.97 (s, 1H), 6.72 (d, *J*=8.4 Hz, 1H), 2.60 (s, 3H), 2.37 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.87, 151.87, 148.76, 145.44, 137.72, 135.67, 134.01, 132.54, 131.56, 131.13, 130.65, 130.54, 129.48, 128.96, 128.45, 127.42, 125.93, 121.19, 120.39, 114.68, 109.24, 21.02, 20.67; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1579.

4.3.17. 2-(3,4,5-Trimethoxyphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 84%; yellow solid; Mp: 230-232 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J*=8.4 Hz, 1H), 7.67-7.71 (m, 5H), 7.53 (s, 2H), 7.39 (t, *J*=7.3 Hz, 1H), 7.16 (s, 1H), 6.97 (t, *J*=7.7 Hz, 1H), 6.62 (d, *J*=8.4 Hz, 1H), 3.95 (s, 6H), 3.93 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ; 160.15, 153.40, 149.08, 145.33, 140.98, 132.45, 131.75, 129.34, 128.70, 128.40, 127.38, 125.80, 121.08, 119.89, 114.42, 104.92, 60.94, 56.33; HRMS (ESI, m/z): calcd for $C_{25}H_{21}N_3O_3$ (M+H+) 411.1582, found: 411.1581.

4.3.18. 2-(4-Ethoxyphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 82%; yellow solid; Mp: 202-204 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J*=7.7, 2H), 7.90 (s, 1H), 7.61-7.65 (m, 5H), 7.37 (s, 1H), 7.10 (s, 1H), 6.89-6.96 (m, 3H), 6.61 (d, *J*=7.7 Hz, 1H), 4.0 (q, *J*=7.0 Hz, 2H), 1.39 (t, *J*=7.0 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.71, 160.49, 148.90, 145.44, 132.63, 130.93, 129.42, 129.31, 128.78, 128.42, 125.59, 120.78, 119.87,

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114.61, 114.41, 104.84, 63.61, 14.74; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3O$ ($M+H^+$) 365.1528, found: 365.1529.

4.3.19. 2-(2-Nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 71%; yellow solid; Mp: 218-220 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J*=7.7, 2H), 7.19 (d, *J* =6.2 Hz, 1H), 7.61-7.68 (m, 4H), 7.55 (t, *J*=7.3 Hz, 1H), 7.45 (t, *J*=6.6 Hz, 2H), 7.05 (t, *J*=7.7 Hz, 2H), 6.79 (s, 1H), 6.75 (d, *J*=7.7 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.59, 149.57, 148.42, 145.24, 133.62, 133.24, 131.89, 131.56, 131.37, 130.68, 129.48, 128.36, 126.32, 124.74, 121.83, 120.38, 114.93, 107.89; HRMS (ESI, m/z): calcd for $C_{22}H_{14}N_4O_2$ ($M+H^+$) 366.1116, found: 366.1117.

4.3.20. 2-(2-Methoxyphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 79%; yellow solid; Mp: 160-162 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, *J*=8.1, 1H), 7.95 (d, *J* =8.4 Hz, 1H), 7.62-7.70 (m, 5H), 7.50 (s, 1H), 7.40-7.45 (m, 2H), 7.12 (t, *J*=7.7 Hz, 1H), 6.98 (d, *J*=8.4 Hz, 2H), 6.68 (d, *J*=8.4 Hz, 1H), 3.87 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.26, 158.07, 152.28, 147.64, 145.37, 132.88, 132.20, 131.98, 130.85, 129.32, 128.53, 127.41, 126.62, 125.68, 121.33, 120.87, 120.12, 114.59, 111.54, 110.10, 55.71; HRMS (ESI, m/z): calcd for $C_{23}H_{17}N_3O$ ($M+H^+$) 351.13716, found: 351.13716.

4.3.21. 2-(4-Chlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 85%; yellow solid; Mp: 198-200 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, *J*=8.8 Hz, 2H), 7.90 (d, *J* =8.1 Hz, 1H), 7.63-7.73 (m, 5H), 7.42 (d, *J*=8.8 Hz, 3H), 7.14 (s, 1H), 6.98 (t, *J*=8.1 Hz, 1H), 6.64 (d, *J*=8.4 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.66, 151.93, 149.62, 145.57, 137.61, 135.07, 132.49, 131.20, 129.48, 129.18, 129.06, 128.44, 127.44, 126.05, 121.35, 120.25, 114.63, 104.92; HRMS (ESI, m/z): calcd for $C_{22}H_{14}ClN_3$ ($M+H^+$) 355.0876, found: 355.0877.

4.3.22. 2-(2-Fluoro,5-bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 81%; yellow solid; Mp: 195-197 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.64 (d, *J*=6.6, 1H), 7.97 (d, *J*=6.6, 1H), 7.64-7.72 (m, 5H), 7.54-7.57 (m, 1H), 7.46 (t, *J*=7.3, 1H), 7.36 (s, 1H), 7.02-7.09 (m, 2H), 6.73 (d, *J*=7.7 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.71, 156.25, 149.49, 145.56, 135.42, 134.25, 131.27, 129.52, 128.46, 126.30, 121.59, 118.52, 118.26, 114.86, 108.59, 108.45; HRMS (ESI, m/z): calcd for $C_{22}H_{13}BrFN_3$ ($M+H^+$) 417.0276, found: 417.0278.

4.3.23. 2-(2-Bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 80%; yellow solid; Mp: 188-190 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 7.98 (s, 1H), 7.83 (d, *J* =7.3 Hz, 1H), 7.61-7.65 (m, 6H), 7.43 (t, *J*=7.0 Hz, 2H), 7.28 (t, *J*=7.7 Hz, 1H), 7.17 (s, 1H), 7.01 (t, *J*=7.3 Hz, 1H), 6.75 (d, *J*=7.7 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.75, 148.32,

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139.18, 133.58, 132.35, 131.95, 131.15, 129.39, 128.33, 127.84, 125.95, 121.42, 121.37, 114.85, 109.83; HRMS (ESI, m/z): calcd for $C_{22}H_{14}BrN_3$ ($M+H^+$) 399.0371, found: 399.0373.

4.3.24. 2-(2-Fluorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 78%; yellow solid; Mp: 172-174 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 8.00 (s, 1H), 7.63-7.69 (m, 5H), 7.45-7.50 (m, 2H), 7.39 (s, 1H), 7.33 (t, *J*=7.7 Hz, 1H), 7.14-7.19 (m, 1H), 7.01 (t, *J*=7.7 Hz, 1H), 6.76 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.05, 157.68, 149.23, 147.32, 145.79, 132.69, 132.60, 131.52, 131.01, 129.28, 128.31, 125.80, 124.79, 121.26, 116.48, 116.25, 108.95, 108.82; HRMS (ESI, m/z): calcd for $C_{22}H_{14}FN_3$ ($M+H^+$) 339.1171, found: 339.1172.

4.3.25. 2-(4-Methylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 83%; yellow solid; Mp: 190-192 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J*=8.4 Hz, 2H), 7.93 (d, *J* =8.4 Hz, 1H), 7.61-7.66 (m, 3H), 7.38-7.41 (m, 1H), 7.33 (d, *J*=8.1 Hz, 1H), 7.27 (d, *J*=8.1 Hz, 2H), 7.19 (s, 1H), 7.16 (d, *J*=8.1 Hz, 1H), 6.98 (t, *J*=7.7 Hz, 1H), 6.64 (d, *J*=8.4 Hz, 1H), 2.39 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.09, 152.29, 149.19, 145.52, 141.88, 133.92, 132.69, 131.06, 129.71, 128.42, 128.99, 128.47, 127.80, 127.53, 126.67, 125.84, 121.06, 120.14, 114.53, 105.23, 21.55; HRMS (ESI, m/z): calcd for $C_{23}H_{17}N_3$ ($M+H^+$) 335.1422, found: 335.1421.

4.3.26. 2-(4-Bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine

Yield 84%; yellow solid; Mp: 210-212 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 8.12 (d, *J*=6.6 Hz, 2H), 7.96 (s, 1H), 7.65-7.72 (m, 5H), 7.59 (d, *J*=7.3 Hz, 2H), 7.42 (s, 1H), 7.17 (s, 1H), 7.00 (t, *J*=7.7 Hz, 1H), 3.69 (d, *J*=7.0 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.61, 152.40, 151.45, 138.47, 136.25, 135.58, 133.78, 132.25, 129.68, 128.18, 127.88, 125.71, 122.62, 116.54, 114.68, 103.02; HRMS (ESI, m/z): calcd for $C_{22}H_{14}BrN_3$ ($M+H^+$) 399.0371, found: 399.0372.

4.3.27. 2-Isopropyl-4-phenylbenzo[4,5]imidazo[1,2-*a*]pyrimidine

Yield 52%; yellow solid; Mp: 193-195 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 7.98 (br, 1H), 7.66−7.60 (m, 5H), 7.43 (s, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.69 (s, 2H), 3.23 (m, 1H), 1.43 (d, *J* = 6.2 Hz, 6H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.49, 148.88, 132.67, 130.89, 129.26, 128.81, 128.13, 127.78, 125.46, 120.67, 120.09, 114.39, 106.88, 37.13, 21.52; HRMS (ESI, m/z): calcd for $C_{19}H_{17}N_3$ ($M+H^+$) 287.1422, found: 287.1424.

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