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Synthesis and characterization of some novel Pyrimidines via Aldol Condensation

K. Suneel Kumar*, A. Vamsi Kanth, K. Tatendra Reddy, G. Omprakash

Pharma Zell R&D (India) Private Limited, Visakhapatnam, India

ABSTRACT

The synthesis and characterization of some novel Pyrimidine derivatives have been presented. Acylation of resorcinol followed by nuclear prenylation with isoprene gives Chroman. Chroman on treatment with p-substituted benzaldehydes affords substituted chalcones. Pyrimidines have been prepared from chalcones by condensing with Guanidine hydrochloride in alkali medium. The structure of Pyrimidines has been characterized by spectral analysis.

Keywords: Heterocyclic, Chalcones, Pyrimidines, IR, Mass and elemental spectral analysis.

INTRODUCTION

Heterocyclic compounds are very widely distributed in nature, and are essential to life in various ways. Particularly these compounds are important because of the wide variety of physiological activities associated with this class of substances. Heterocyclic rings are present in several compounds, e. g, most of the members of vitamin B complex, drugs, dye stuffs, enzymes, the genetic material DNA etc.

The paramount importance of heterocycles in nature product chemistry and pharmacology constantly drive the search for new methods for the construction of heterocyclic unit viz., Pyrimidines. These Pyrimidines were prepared from chalcones which are important intermediate products and they also possess biological and pharmacological activities [1].

Pyrimidines can be regarded as a cyclic amine and also be known as m-diazone (or) 1,3-diazine. It is the parent substance of large group of heterocyclic compounds & plays a vital role in many biological processes as found in nucleic acids, several vitamins, co-enzymes and purines.

Pyrimidine is the most important member of all the diazines as this ring occurs widely in living organisms. Pyrimidine itself is not found in nature but substituted Pyrimidines and compounds containing the Pyrimidine ring are widely distributed in nature Derivatives of barbituric acid, widely used in medicines, for eg., veronal, Pentothiol, Luminol are used as hyphotics while is used as anesthetic. Purines, Uric acid, alkoxan, barbuturic acid and a mixture of amtimalarial and antibacterial also contain the Pyrimidine ring. Substances containing un-fused Pyrimidine rings occur in free stage as in Uracil, Thymine, Orotic acid, Cytosine, the glycosides, Vitamin B (thiamine), amicetin and various others.

The chemistry of Pyrimidines [2, 3] has been widely studied. Pyrimidine was first isolated by Gabriel and Colman in 1893. Since Pyrimidine is symmetrical about the line passing C_2 and C_5, the positions of C_4 and C_6 are equivalent and so are N-1 and N-3. When a hydroxyl or amino group is present at the 2, 4 or 6 position then they are tautomeric with oxo and imino forms.

Three Pyrimidines are of considerable biological important because of their relation to the nucleic acids viz., Uracil, Thymine, Cytosine. The Purine ring system obtained from the fusion of Pyrimidine and Imidazole nucleic also is important because certain of its derivatives, in particular adenine and guanidine which are building blocks of RNA & DNA. A variety of natural products such as alkaloids also contain Pyrimidine ring system, these include Hypoxanthine, Xanthine which occurs in tea and caffeine and Theophyline are the constituents of tea leaves. Theobromine is found in cocoa beans.

Various methods employed in literature for the preparation of Pyrimidines. Uracils (or) dehydrouracils can be prepared from urea and α, β – unsaturated acids (or) their esters [4]. When S-benzyl (or) S-methyl thiourea is condensed with ethyl ψ - bromo acetoacetate, the product is a pyrimidine [5]. In the synthesis of orotic acid from urea and oxalacetic ester [6], the first formed hydantoin is rearranged to pyrimidine in presence of alkali.

Several pyrazolo[1,5,a] pyrimidine derivatives were prepared by the condensation of substituted chalcones with 5-amino pyrazole [7]. A new series of 2-[N-(Tos- or Pht-) aminoacyl-p-substituted phenylmethyleneamino]-pyrimidines was synthesized by the reaction of Schiff bases, 2-(4-substituted benzylidene)aminopyrimidines with the requisite of tosyl or phthalylaminoacy chlorides [8].

A general synthesis applicable to a wide variety of pyrimidines has been described by Whitehead [9]. Ethylorthoformate reacts with urea or thiourea to yield N, N' – dicarbamyl formamidines, which on reaction with active methylene compounds give ureidoethylenes. These ureidomethylenes undergo ready cyclization to pyrimidines in presence of a basic catalyst.

Benzamidine condenses with compounds of the type of C_6H_5 – CH = CH – COR (R does not contain α - hydrogen) to yield 2,4,6 – tri substituted Pyrimidines. The dihydropyrimidine first formed is dehydrogenated by unreacted unsaturated ketone [10]. Guanidine reacts with β-

ketoesters, diketones, cyano acetic esters and α, β – unsaturated carbonyl compounds to give 2-amino pyrimidines usually in good yields [11].

The earliest recorded pyrimidines synthesis from propionitrile and sodium is a good example [12]. But these routes of synthesis are of restricted application. The insertion of a single carbon atom between the nitrogens of a diamine to obtain a hydrogenated pyrimidine can be achieved by a number of conventional processes, treatment with diethyl carbonate [13], phosgene (or) aldehydes [14]. Rinkes synthesis of Uracil, which was brought about by treating malic diamide with sodium hypochlorite [15,16]. 2,5-Diaryl-4-(chloromethyl) imidazoline and $R'COCH_2NHCH_2Ar$ were treated with sodium hydride in DMF results the formation of 2,4,6-trisubstituted pyrimidines [17].

4-Aminopyrimidine-5carbaldehyde underwent facile condensation with various aromatic ketione derivatives in the presence of potassium carbonate and catalytic amount of KI in acetone was afforded corresponding 7-substituted pyrido[2,3-d]pyrimidine derivatives [18]. 2,4-dihydroxy substituted chalcones were synthesized via aldol condensations in the presence of $SOCl_2$/EtOH as a catalyst [19].

Wang et al [20] synthesized the 2-amino-4,6-dimethyl pyrimidines by treatment with guanidine nitrate with acetyl acetone and K_2CO_3 in H_2O at room temperature for 24 hours (97% yield). 4,6-Diaryl pyrimidines [21] were also prepared by cyclo condensation of diaryl propenones with guanidine carbonate. An improved synthesis of 5-halo pyrimidines from alkyl and aryl α-halo metyl ketones with aliphatic and aromatic nitriles in the presence O-trifluoromethane sulphonic hydride in CH_2Cl_2 was reported by Garcia Martinez et al [22].

Heterocyclization of α, β- unsaturated ketones with (E)-1-(aminomethylene) hydrazine hydrochloride results the formation of methoxy alkyl substitutd 2- amino pyrimidines [23] in 65-91% yield. Cyclo condensation of phenyl guanidine with ArCH=CHCOAr' yields (amino phenyl) pyrimidines [24]. 5-Alkyl-2,4,6-substituted pyrimidines [25] was synthesized by cyclization of alkyl malono nitriles with 2-alkyl-3-oxobutyrates.

The Bingineli reaction was first reported more than a century ago and recently reviewed [26], and involved the synthesis of 3,4-dihydrophyrimidin-2-(1H)-ones by a very simple one-pot condensation reaction of ethyl acetoacetate, benzaldehyde and urea in ethanol in the presence of lanthanum chloride as a catalyst [27]. This is a novel, one pot combination that not only preserves the simplicity of Biginelli's one pot reaction but also consistently produces excellent yields of the dihydropyrimidin -2 (1H)- ones.

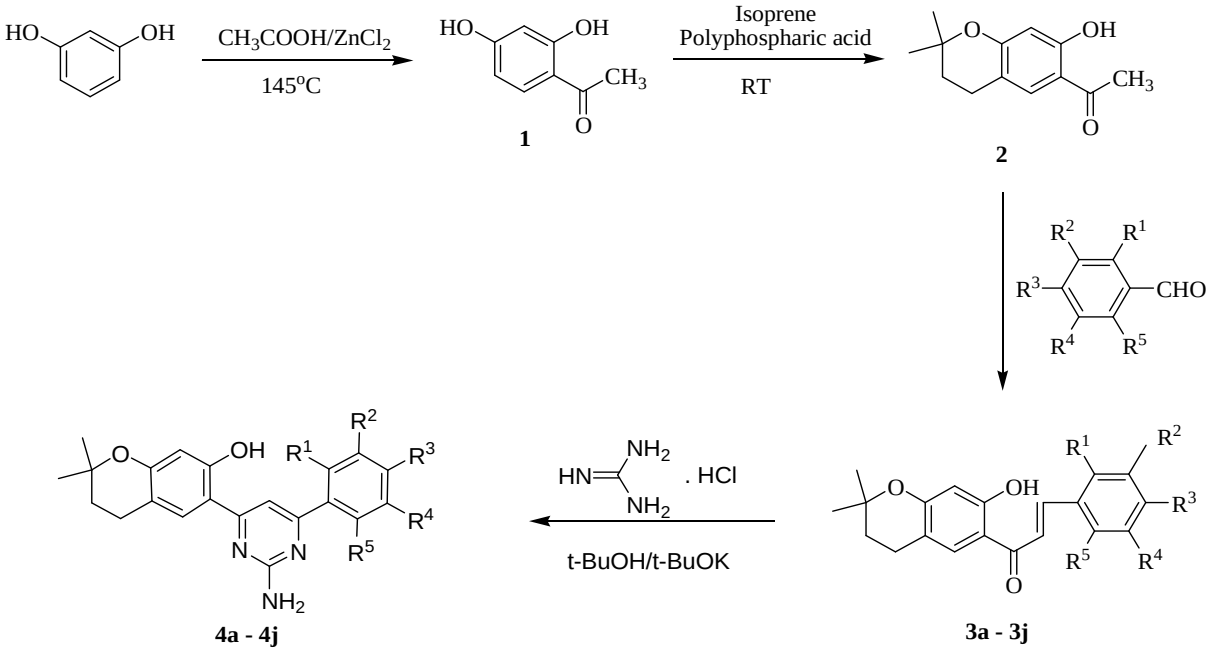
The 3,4-dihydropyrimidine-2-(1H)- one can be obtained from the reaction of benzaldehyde, ethyl acetoacetate and urea in the presence of ferric chloride hexahydrate or nickel chloride hexahydrate in 94% and 97% yield respectively [28]. Similarly, the treatment of several aromatic, aliphatic and heterocyclic aldehydes with ethyl acetoacetate and urea also gave the corresponding dihydropyrimidinone in excellent yields in this method.

Recently, researchers developed the Biginelli's one-pot condensation reaction of benzaldehyde with urea and ethylacetoaceate using bismuth triflate in acetonitrile as solvent at ambient temperature [29]. This reaction is very fast and 90% conversion was observed in one hour.

Substituted N-(5-cyanopyrimidin-4-yl)benzamide derivatives were prepared by the facile condensation of 4-aminopyrimidine-5-carbonitirle with various aromatic acid derivatives in the presence of 1-[3-(dimethylamino)propyl]-3-ethylcarbodiimidehydrochloride and catalytic amount of TEA [30]. 8-Chloro-3- cyano – 2 – methylthio - 4-oxo - 4H – pyrimido [2,1-b][1,3]benzothiazole on reaction in presence of dimethyl formamide and catalytic amount of anhydrous potassium with hydrazine hydrate / aryl hydrazine / heteryl hydrazine afforded 3-amino-8-chloro-4-oxo-(2H) / aryl/heteryl-pyrazolo [3',4':4,5] pyrimido [2,1-b] [1,3] benzothiazoles in good yield [31]. Anilines on reaction with potassium thiocyanate and bromine in acetic acid yielded substituted 2-amino[2,1-b][1,3]benzothiazoles, which on reaction with ethy acetoacetate and pheylidine acetoacetate, yielded, 2-methyl-4-H-pyrimido[2,1-b][1,3]benzothiazole-4-ones and ethyl 4-phenyl-2-methyl-4H–pyrimido[2,1-b][1,3]benzo-thiazole-3-carboxylates [32].

EXPERIMENTAL SECTION

General procedure. FT-IR spectra are recorded as KBr pellet on Nicolet 380 FT-IR Instrument (Model Thermo Electron Corporation-Spectrum One), ^{1}H NMR spectra are recorded on Varian 300 MHz spectrometer using DMSO-d6 as solvent and tetramethylsilane (TMS) as internal standard. Mass spectra are recorded on Agilent triple quadrupole mass spectrometer equipped with turboion spray interface at 375°C. All the organic extracts are dried over sodium sulfate after work up. Unless otherwise mentioned all the solvents and reagents used are of commercial grade.

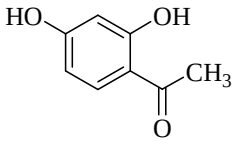


Scheme 1: Synthetic procedure of Pyrimidines

In this paper, the synthesis and characterization of some novel Pyrimidines have been presented. Synthetic scheme is described below Scheme 1. Physicochemical, spectroscopic and other related data for the synthesized compounds are given Table (1-4).

Synthesis of 1-(2,4-dihydroxyphenyl)ethanone (1):

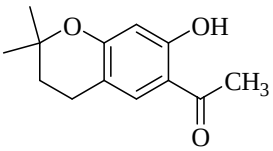
Freshly fused 33g of Zinc chloride was dissolved in 32 mL of acetic acid while heating and when all the zinc chloride is almost dissolved, 22 g of resorcinol was added and heated to 140-150^{o}C for 15 minutes with stirring. This was left for 1 hour and then 100 mL 50% aqueous HCl was added to break the zinc chloride complex. Within 5 minutes, precipitation commenced when the mixture came to room temperature. It was cooled to 5^{o}C and then filtered. The precipitate is washed with 5% dilute HCl and water. A red precipitate obtained was crystalized from 20% HCl to give 1-(2,4-dihydroxyphenyl) ethanone.



Yield 76.4%, M.F. $C_8H_8O_3$, M. Wt. 152.15. IR (ν_{max}, cm^{-1}): 2996.28 (C-H), 3395.99 (-OH), 1592.14 and 1471.71 (C-C in Ar), 1703.25 (C=O). ^{1}H-NMR (400 MHz, DMSO-d6): δ_H 2.5 (s, 3H, -CH_3), 5.5 (s, 2H, -OH), 6.3 (s, 1H, Ar-H), 6.5 (d, 1H, Ar-H), 7.4 (d, 1H, Ar-H). MS *m/z* (%) = 153.26 (M+1). Anal. Calcd for $C_8H_8O_3$: C, 63.15; H, 5.30; O, 31.55%. Found: C, 63.19; H, 5.28, O, 31.53%.

Synthesis of 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone (nuclear prenylation of 1-(2,4-dihydroxyphenyl)ethanone) (2):

A solution of isoprene (1.5 mL, 0.015 mol) in Xylene (5 mL) was added drop wise over a period of 8 hours to a mixture of 1-(2,4-dihydroxyphenyl)ethanone (1.41 g, 0.0072 mol) and Polyphospharic acid (2 mL) in xylene (3 mL) with constant stirring at 30-35^{o}C. Stirring was continued for further 14 hours. The reaction mixture was extracted in chloroform (100 mL) and the chloroform solution was washed with aqueous $NaHCO_3$ (5%, 3 X 60 mL), dried over $MgSO_4$ and removed under reduced pressure to give gummy material. This on column chromatography over silica gel yielded the chroman on elution with hexane/EtOAc (96:4).



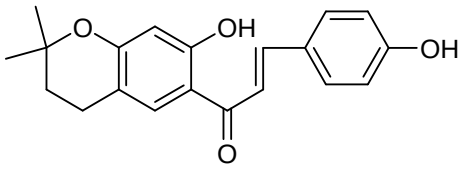
Yield 80.2%, M.F. $C_{13}H_{16}O_3$, M. Wt. 220.26. IR (ν_{max}, cm^{-1}): 2986.25 (C-H), 3378.35 (O-H), 1753.16 (C=O), 1592.18 and 1466.94 (C-C in Ar), 1174.86 (C-O-C). ^{1}H-NMR (400 MHz, DMSO-d6): δ_H 1.50 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 2.4 (s, 3H, -CH_3), 5.0 (s, 1H, -OH), 6.5 (s, 1H, Ar-H), 7.3 (s, 1H, Ar-H). MS *m/z* (%) = 221.15 (M+1). Anal. Calcd for $C_{13}H_{16}O_3$: C, 70.89; H, 7.32; O, 21.79%. Found: C, 70.88; H, 7.34; O, 21.78%.

Condensation of 1-(7-hydroxy-2,2-dimethylchroman-6-yl) ethanone with substituted benzaldehydes (3a-3j):

General procedure: A mixture of 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone (0.01 mol), substituted benzaldehyde (0.01 mol) in ethanol (30 mL) and aqueous potassium hydroxide (15 g in 15 mL of water) were stirred at room temperature for 24 hours. On acidification with hydrochloric acid an yellow (or) orange red chalcone derivatives.

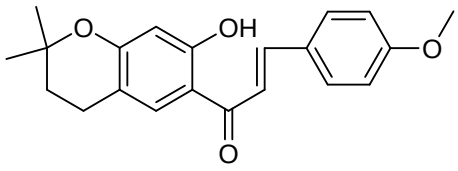
Synthesis of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-hydroxy phenyl) prop-2-en-1-one (3a):

Compound 3a was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone and 4-hydroxy benzaldehyde with the above general procedure.



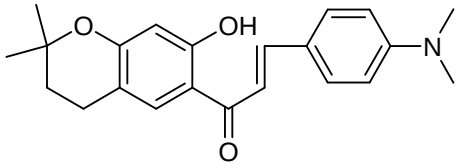
Synthesis of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-methoxy phenyl) prop-2-en-1-one (3b):

Compound 3b was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone and 4-methoxy benzaldehyde with the above general procedure.



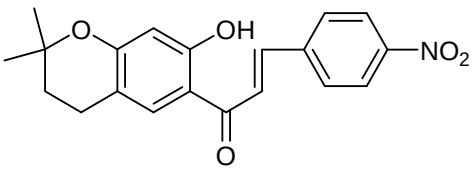
Synthesis of (E)-3-(4-(dimethylamino)phenyl)-1-(7-hydroxy-2,2-dimethyl chroman -6-yl) prop-2-en-1-one (3c):

Compound 3c was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone and 4-dimethyl amino benzaldehyde with the above general procedure.

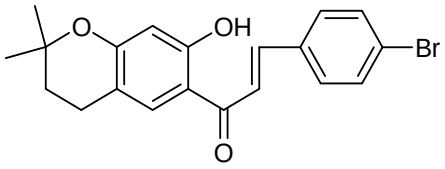


Synthesis of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-nitrophenyl) prop-2-en-1-one (3d):

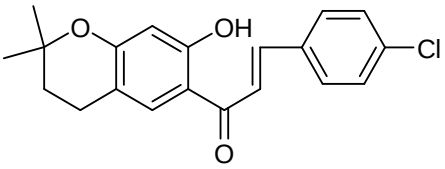
Compound 3d was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl) ethanone and 4-nitro benzaldehyde with the above general procedure.



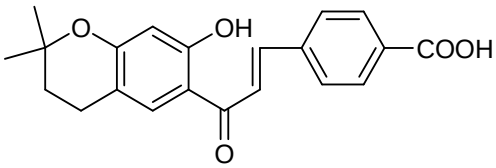
Synthesis of (E)-3-(4-bromophenyl)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)prop-2-en-1-one (3e):
Compound 3e was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl) ethanone and 4-bromo benzaldehyde with the above general procedure.



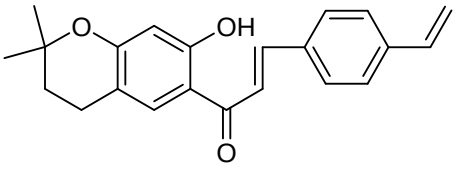
Synthesis of (E)-3-(4-chlorophenyl)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)prop-2-en-1-one (3f):
Compound 3f was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl) ethanone and 4-chloro benzaldehyde with the above general procedure.



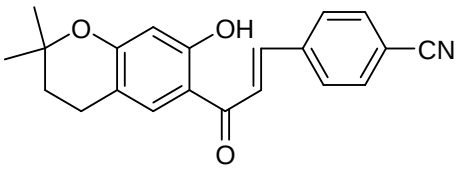
Synthesis of 4-((E)-3-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-oxoprop-1-enyl)benzoic acid (3g):
Compound 3g was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone and 4-formylbenzoic acid with the above general procedure.



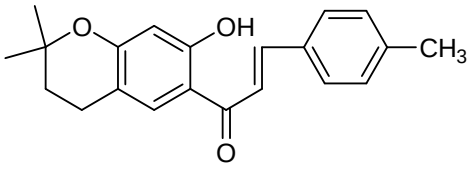
Synthesis of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-vinylphenyl) prop-2-en-1-one (3h):
Compound 3h was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone and 4-vinylbenzaldehyde with the above general procedure.



Synthesis of 4-((E)-3-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-oxoprop-1-enyl)benzonitrile (3i):
Compound 3i was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone and 4-formylbenzonitrile with the above general procedure.

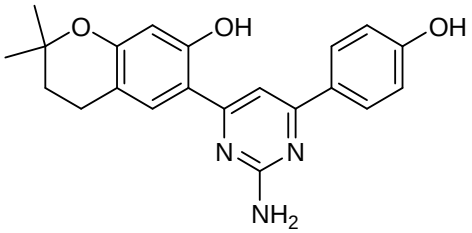


Synthesis of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-p-tolylprop-2-en-1-one (3j):
Compound 3j was prepared by using 1-(7-hydroxy-2,2-dimethylchroman-6-yl)ethanone and 4-methyl benzaldehyde with the above general procedure.

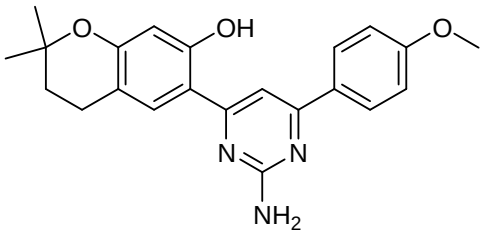


Synthesis of 6-(6-(4-substitutedphenyl)-2-aminopyrimidin-4-yl)-2,2-dimethyl chroman -7-ol (4a-4j):
General procedure:
The condensation of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-substituted-phenyl)prop-2-en-1-one with guanidine hydrochloride in the presence of potassium t-butoxide in tert-butoxide was refluxed on water bath for 4 hours. Solvent was evaporated and the residue dissolved in water and neutralized with dilute HCl, where upon a bright yellow solid separated out, which was filtered and crystallized from chloroform / methanol. The purity of these compounds were checked by HPLC.

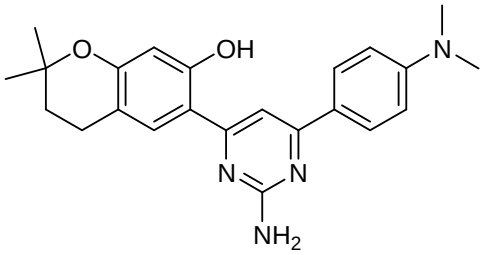
Synthesis of 6-(6-(4-hydroxyphenyl)-[2-amino]pyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4a):
Compound (4a) was prepared with (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-hydroxyphenyl)prop-2-en-1-one (3a) and Guanidine hydrochloride by using the above process.



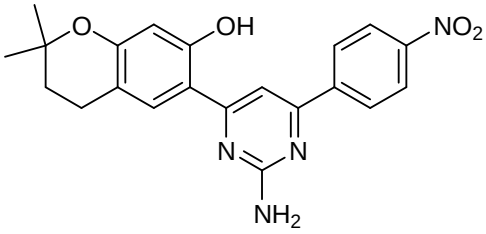
Synthesis of 6-(6-(4-hydroxyphenyl) -[2-methoxy]pyrimidin-4-yl) -2,2-dimethyl chroman-7-ol (4b):
Compound (4b) was prepared with (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (3b) and Guanidine hydrochloride by using the above process.



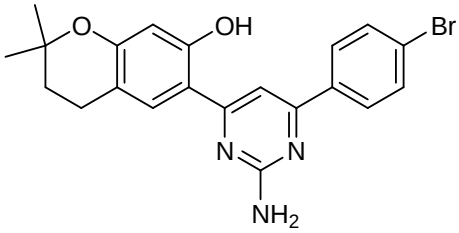
Synthesis of 6-(6-(4-hydroxyphenyl)-[2-dimethylamino] pyrimidin-4-yl)-2,2-dimethylchroman-7-ol (4c):
Compound (4c) was prepared with (E)-3-(4-(dimethylamino)phenyl)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)prop-2-en-1-one (3c) and Guanidine hydrochloride by using the above process.



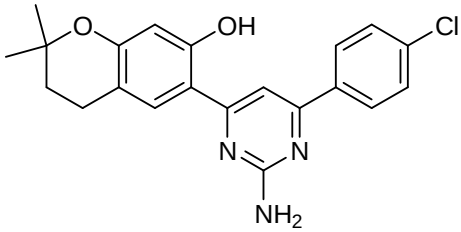
Synthesis of 6-(6-(4-hydroxyphenyl)-[2-nitro] pyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4d):
Compound (4d) was prepared with (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-nitrophenyl)prop-2-en-1-one (3d) and Guanidine hydrochloride by using the above process.



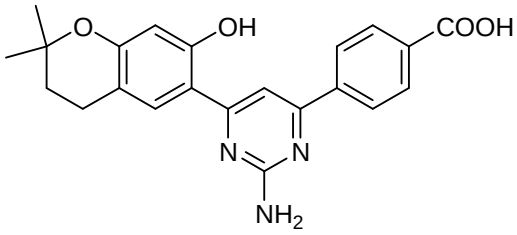
Synthesis of 6-(6-(4-Bromophenyl)-2-aminopyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4e):
Compound (4e) was prepared with (E)-3-(4-bromophenyl)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)prop-2-en-1-one (3e) and Guanidine hydrochloride by using the above process.



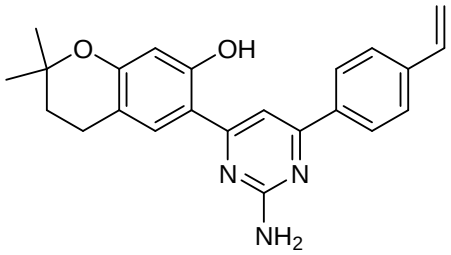
Synthesis of 6-(6-(4-Chlorophenyl)-2-aminopyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4f):
Compound (4f) was prepared with (E)-3-(4-chlorophenyl)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)prop-2-en-1-one (3f) and Guanidine hydrochloride by using the above process.



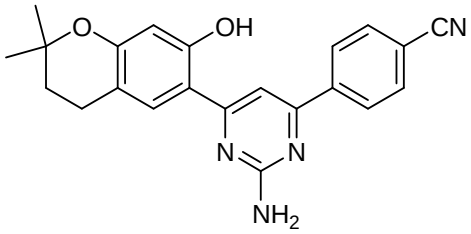
Synthesis of 4-(6-(7-hydroxy-2,2-dimethylchroman-6-yl)-2-aminopyrimidin-4-yl)benzoic acid(4g):
Compound (4g) was prepared with 4-((E)-3-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-oxoprop-1-enyl)benzoic acid (3g) and Guanidine hydrochloride by using the above process.



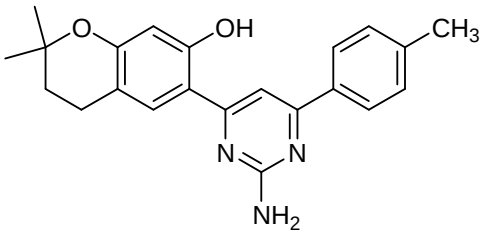
Synthesis of 2,2-dimethyl-6-(2-amino-6-(4-vinylphenyl)pyrimidin-4-yl) chroman-7-ol (4h):
Compound (4h) was prepared with (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-vinylphenyl)prop-2-en-1-one (3h) and Guanidine hydrochloride by using the above process.



Synthesis of 4-(6-(7-hydroxy- 2,2-dimethyl chroman-6-yl) -2-amino pyrimidin-4-yl) benzonitrile (4i):
Compound (4i) was prepared with 4 of 4-((E)-3-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-oxoprop-1-enyl)benzonitrile (3i) and Guanidine hydrochloride by using the above process.



Synthesis of 2,2-dimethyl-6-(2-amino-6-p-tolylpyrimidin-4-yl)chroman-7-ol (4j):
Compound (4j) was prepared with 4 of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-p-tolylprop-2-en-1-one (3j) and Guanidine hydrochloride by using the above process.



RESULTS AND DISCUSSION

This paper reports a simple and effective method for the synthesis of Pyrimidines. Our purpose was to synthesize a series of Pyrimidines derivatives through chalcones intermediates starting from substituted benzaldehyde and acetophenone.

Resorcinol was acylated using acetic acid in the presence of fused $ZnCl_2$ at 140-150^oC for 15 minutes with stirring. The reaction mixture left for 1 hour and then 100 mL of 1: 1 HCl was added to break the $ZnCl_2$ complex and within 5 minutes precipitation commenced. The precipitate was washed with very dilute HCl and water. A red precipitate was obtained; which was crystallized from 20% HCl to give resacetophenone (1) needles and characterized by comparing its spectral data with structure.

Ahluwalia et at[33] reported the synthesis of 2,2-dimethyl chromans in very good yield by condensing polyphenol derivatives with isoprene in presence of orthophosphoric acid as catalyst. PPA was found to be a better condensing agent compared to orthophosphoric acid to result in a more or less homogeneous reaction mixture leading to the cyclic chroman derivatives in very good yields. A solution of isoprene in xylene was added dropwise during 8 hours to a mixture of resacetophenone and PPA in xylene with constant stirring at 30-35^oC. Stirring was continued for further 1 hour. The reaction mixture was taken into reduced pressure to give a yellow gummy material. This on column chromatography over silica gel yielded the chroman in hexane / EA elutes (96:4) and the unreacted resactophenone from hexane / EA elutes.

The resacetophenene (1) on nuclear prenylation [34] with isoprene in the presence of PPA at room temperature resulted the formation of 2,2-dimethyl-6-acetyl-7-hydroxy chroman (2) in 63% yield and it is crystallized as colourless needles.

The chroman (2) on condensation with different substituted benzaldehydes in the presence of 30% alcoholic alkali at room temperature resulted the formation of chalcone derivatives in good yield. The thin layer chromatography (TLC) of these chalcones showed characteristic colors with methanol – H_2SO_4 (9:1) as a spraying reagent. They also exhibited the characteristic color test with antionyl trioxide. With the above procedure, compounds (3a-3j) were synthesized.

The chalcones (3a-3j) which were synthesized have now have been taken for the preparation of corresponding new Pyrimidine derivatives (4a-4b). The condensation above chalcone with guanidine hydrochloride in alkalinemedium viz., in potassium tertiary butoxide in presence of tert-butanol at reflux temperatures resulted the formation of corresponding Pyrimidine derivatives.

The synthesized chalcone derivatives were undergone physicochemical characterization and the obtained results are given in Table.1. The yields of the synthesized compounds were found to be significant. The structure of the synthesized compounds was confirmed by IR, Mass and elemental analysis. Elemental analysis showed that the percentage of the nitrogen, hydrogen and carbon was found experimentally is equivalent to the calculated values in all compounds.

All the compounds give the characteristic IR peak that proved that the presence of particular functional group (Table 3 and 4) and mass spectroscopy helps to find the molecular weight of the synthesized compounds (Table3 and 4). The Pyrimidines derivatives showed that the molecular ion peak that equivalent to the molecular weight of proposed compound. Hence m/z value confirms the molecular weight of the respective synthesized compound.

Table 1: Physicochemical characterization data for synthesized compounds 3a – 3j

Compound ID	Molecular formula	Molecular weight	Yield (%)	Elemental analysis			
				C	H	N	O
3a	$C_{20}H_{20}O_4$	324.37	74.2	74.06 (74.00)	6.21(6.23)	--	19.73(19.77)
3b	$C_{21}H_{22}O_4$	338.4	70.9	74.54(74.52)	6.55(6.56)	--	18.91(18.92)
3c	$C_{22}H_{25}NO_3$	351.44	77.5	75.19(75.22)	7.17(7.14)	3.99(4.00)	13.66(13.64)
3d	$C_{20}H_{19}NO_5$	353.37	78.2	67.98(67.96)	5.42(5.43)	3.96(3.99)	22.64(22.62)
3e	$C_{20}H_{19}BrO_3$	387.27	68.2	62.03(62.05)	4.95(4.94)	--	12.39(12.40)
3f	$C_{20}H_{19}ClO_3$	342.82	73.5	70.07(70.10)	5.59(5.58)	--	14.00(14.02)
3g	$C_{21}H_{20}O_5$	352.38	80.1	71.58(71.60)	5.72(5.73)	--	22.70(22.67)
3h	$C_{22}H_{22}O_3$	334.41	84.1	79.02(79.04)	6.63(6.65)	--	14.35(14.31)
3i	$C_{21}H_{19}NO_3$	333.38	78.1	75.66(75.68)	5.74(5.75)	4.20(4.21)	14.40(14.36)
3j	$C_{21}H_{22}O_3$	322.4	86.1	78.23(78.25)	6.88(6.89)	--	14.89(14.86)

Table 2: Physicochemical characterization data for synthesized compounds 4a – 4j

Compound ID	Molecular formula	Molecular weight	Yield (%)	HPLC Purity (%)	Elemental analysis			
					C	H	N	O
4a	$C_{21}H_{21}N_3O_3$	363.41	73.85	99.02	69.41(69.45)	5.82(5.80)	11.56(11.55)	13.21(13.20)
4b	$C_{22}H_{23}N_3O_3$	377.44	84.26	99.55	70.01(70.05)	6.14(6.15)	11.13(11.15)	12.72(12.65)
4c	$C_{23}H_{26}N_4O_2$	390.48	80.26	98.94	70.75(70.78)	6.71(6.70)	14.35(14.34)	8.19(8.18)
4d	$C_{21}H_{20}N_4O_4$	392.41	74.26	99.65	64.28(64.30)	5.14(5.15)	14.28(14.25)	16.31(16.30)
4e	$C_{21}H_{20}BrN_3O_2$	426.31	77.54	99.24	59.17(59.18)	4.73(4.72)	9.86(9.90)	7.51(7.50)
4f	$C_{21}H_{20}ClN_3O_2$	381.86	79.54	97.06	66.05(66.04)	5.28(5.30)	11.00(11.01)	8.38(8.37)
4g	$C_{22}H_{21}N_3O_4$	391.42	86.25	99.96	67.51(67.50)	5.41(5.42)	10.74(10.76)	16.35(16.32)
4h	$C_{23}H_{23}N_3O_2$	373.45	88.25	99.82	73.97(74.0)	6.21(6.23)	11.25(11.26)	8.57(8.51)
4i	$C_{22}H_{20}N_4O_2$	372.42	86.75	99.87	70.95(70.98)	5.41(5.40)	15.04(15.07)	8.59(8.55)
4j	$C_{22}H_{23}N_3O_2$	361.44	86.75	99.31	73.11(73.10)	6.41(6.42)	11.63(11.65)	8.85(8.83)

Table 3: Spectral data of synthesized compounds 3a – 3j

Compound ID	IR (v_{max}, cm^{-1})	HNMR (400 MHz, DMSO-d6)	Mass (*m/z*)
3a	2954.19 (C-H), 3351.49 (O-H), 1728.32 (C=O), 3159.54 (C-H in Ar-H), 772.22 (C-H in Ar-H), 1601.38 and 1436.22 (C-C in Ar), 1146.67 (C-O-C).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 4.9 (s, 2H, -OH), 6.2 (s, 1H, Ar-H), 6.5 (d, 1H, -CH=CH-), 6.6 (d, 2H, Ar-H), 7.1 (d, 2H, Ar-H), 7.6 (d, 1H, -CH=CH-), 7.9 (d, 1H, Ar-H).	325.38
3b	2953.98 (C-H), 3352.18 (O-H), 1728.57 (C=O), 3159.65 (C-H in Ar-H), 772.31 (C-H in Ar-H), 1601.71 and 1436.22 (C-C in Ar), 1146.82 (C-O-C), 2889.80 (C-H in –OCH_3).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 3.7 (s, 3H, -OCH_3), 4.9 (s, 2H, -OH), 6.2 (s, 1H, Ar-H), 6.5 (d, 1H, -CH=CH-), 6.7 (d, 2H, Ar-H), 7.1 (d, 2H, Ar-H), 7.6 (d, 1H, -CH=CH-), 7.9 (d, 1H, Ar-H).	339.38
3c	2953.98 (C-H), 3159.65 (C-H in Ar-H), 3385.49 (O-H), 1601.71, 1574.61 and 1458.83 (C-C in Ar), 1707.64 (C=O), 1213.39 (Ar-O-C), 1349.45 (C-N).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 2.9 (s, 6H, -$N(CH_3)_2$), 4.9 (s, 1H, -OH), 6.3 (s, 1H, Ar-H), 6.5 (d, 1H, Ar-H), 6.7 (d, 2H, Ar-H), 7.1 (d, 2H, Ar-H),	352.40

		7.6 (d, 1H, -CH=CH-), 7.9 (d, 1H, -CH=CH).	
3d	2967.56 (C-H), 3164.18 (C-H in Ar-H), 3296.49 (O-H), 1594.44, 1563.19 and 1445.77 (C-C in Ar), 1709.37 (C=O), 1212.80 (Ar-O-C), 1462.46 (N-O).	1.5 (d, 6H, $-CH_3$), 2.0 (m, 4H, $-CH_2$-), 4.9 (s, 1H, -OH), 6.8 (s, 1H, Ar-H), 7.4 (d, 1H, Ar-H), 7.6 (d, 2H, Ar-H), 8.1 (d, 2H, Ar-H), 8.5 (d, 1H, -CH=CH-), 8.7 (d, 1H, -CH=CH).	354.21
3e	2954.09 (C-H), 3158.81 (C-H in Ar-H), 3385.87 (O-H), 1602.18, 1575.86 and 1459.26 (C-C in Ar), 1708.51 (C=O), 1213.26 (Ar-O-C), 772.45 (C-Br).	1.5 (d, 6H, $-CH_3$), 2.0 (m, 4H, $-CH_2$-), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (d, 2H, Ar-H), 8.1 (d, 2H, Ar-H), 8.5 (d, 1H, -CH=CH-), 8.7 (d, 1H, -CH=CH).	388.33
3f	2954.35 (C-H), 3353.45 (O-H), 1602.22, 1574.32 and 1458.91 (C-C in Ar), 1707.40 (C=O), 1213.15 (Ar-O-C), 694.76 (C-Cl).	1.5 (d, 6H, $-CH_3$), 2.0 (m, 4H, $-CH_2$-), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (d, 2H, Ar-H), 8.1 (d, 2H, Ar-H), 8.5 (d, 1H, -CH=CH-), 8.7 (d, 1H, -CH=CH).	343.88
3g	2954.18 (C-H), 3159.00 (C-H in Ar-H), 3385.27 (O-H), 1602.51, 1575.96 and 1446.18 (C-C in Ar), 1708.83 (C=O), 1213.29 (Ar-O-C).	1.5 (d, 6H, $-CH_3$), 2.0 (m, 4H, $-CH_2$-), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (d, 2H, Ar-H), 8.1 (d, 2H, Ar-H), 8.5 (d, 1H, -CH=CH-), 8.7 (d, 1H, -CH=CH), 10.1 (bs, 1H, -COOH).	353.61
3h	2955.68 (C-H), 3163.10 (C-H in Ar-H), 3383.72 (O-H), 1598.70, 1564.30 and 1522.94 (C-C in Ar), 1708.98 (C=O), 1212.83 (Ar-O-C).	1.5 (d, 6H, $-CH_3$), 2.2 (m, 4H, $-CH_2$-), 4.9 (s, 1H, -OH), 5.1 – 5.3 (dd, $-CH=CH_2$), 6.4 (s, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (d, 2H, Ar-H), 8.1 (d, 2H, Ar-H), 8.5 (d, 1H, -CH=CH-), 8.7 (d, 1H, -CH=CH).	335.61
3i	2954.62 (C-H), 3167.29 (C-H in Ar-H), 3349.75 (O-H), 1599.65, 1575.18 and 1445.85 (C-C in Ar), 1707.88 (C=O), 1212.54 (Ar-O-C), 2349.06 (CN).	1.5 (d, 6H, $-CH_3$), 2.2 (m, 4H, $-CH_2$-), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (d, 2H, Ar-H), 8.1 (d, 2H, Ar-H), 8.5 (d, 1H, -CH=CH-), 8.7 (d, 1H, -CH=CH).	334.34
3j	2922.76 (C-H), 3155.57 (C-H in Ar-H), 3385.05 (O-H), 1601.71, 1575.22 and 1459.12 (C-C in Ar), 1707.91 (C=O), 1213.27 (Ar-O-C).	1.5 (d, 6H, $-CH_3$), 2.0 (m, 4H, $-CH_2$-), 2.5 (s, 3H, $-CH_3$), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (d, 2H, Ar-H), 8.1 (d, 2H, Ar-H), 8.5 (d, 1H, -CH=CH-), 8.7 (d, 1H, -CH=CH).	323.88

Table 4: Spectral data of synthesized compounds 4a – 4j

Compound ID	IR (ν_{max}, cm^{-1})	HNMR (400 MHz, DMSO-d6): δH	Mass *m/z*
4a	2952.45 (C-H), 3116.43 (C-H in Ar-H), 3369.73 (O-H), 1581.29 and 1459.07 (C-C in Ar), 1240.95 (Ar-O-C), 1647.82 (C=N-O), 3583.44 (N-H).	1.5 (d, 6H, -CH3), 2.0 (m, 4H, -CH2-), 3.9 (bs, 2H, -NH2), 4.9 (s, 2H, -OH), 6.2 (s, 1H, Ar-H), 6.3 – 6.4 (m, 3H, Ar-H), 6.8 (d, 1H, Ar-H), 7.1 (d, 2H, Ar-H).	364.25
4b	2993.58 (C-H), 3116.65 (C-H in Ar-H), 3245.61 (O-H), 1610.32, 1580.61 and 1459.62 (C-C in Ar), 1240.86 (Ar-O-C), 1647.37 (C=N-O), 3473.62 (N-H).	1.5 (d, 6H, $-CH_3$), 2.0 (m, 4H, $-CH_2$-), 3.7 (s, 3H, $-CH_3$), 4.0 (bs, 2H, $-NH_2$), 4.9 (s, 1H, -OH), 6.2 (s, 1H, Ar-H), 6.5 (d, 1H, Ar-H), 6.7 (d, 2H, Ar-H), 6.9 (s, 1H, Ar-H), 7.1 (d, 2H, Ar-H).	378.38
4c	2950.80 (C-H), 3058.39(C-H in Ar-H),	1.5 (d, 6H, $-CH_3$), 2.0 (m, 4H, $-CH_2$-),	391.40

	3372.62 (O-H), 1583.54 and 1477.80 (C-C in Ar), 1263.82 (Ar-O-C), 3578.82 (N-H), 1306.85 (-N(CH_3)$_2$).	3.0 (s, 6H, -N(CH_3)$_2$), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 6.3 (s, 1H, Ar-H), 6.5 (d, 1H, Ar-H), 6.7 (d, 2H, Ar-H), 6.9 (s, 1H, Ar-H), 7.1 (d, 2H, Ar-H).	
4d	2951.38 (C-H), 3058.53 (C-H in Ar-H), 3372.07 (O-H), 1583.57 and 1454.65 (C-C in Ar), 1264.07 (Ar-O-C), 3578.92 (N-H).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 6.9 (s, 1H, Ar-H), 7.4 (d, 1H, Ar-H), 7.6 (d, 2H, Ar-H), 7.8 (s, 1H, Ar-H), 8.1 (d, 2H, Ar-H).	393.21
4e	2951.23 (C-H), 3058.62 (C-H in Ar-H), 3372.52 (O-H), 1619.11, 1583.52 and 1445.68 (C-C in Ar), 1239.08 (Ar-O-C), 3579.16 (N-H), 727.60 (C-Br).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 6.7 (d, 1H, Ar-H), 7.1 (d, 2H, Ar-H), 7.5 (s, 1H, Ar-H), 8.1 (d, 2H, Ar-H).	427.42
4f	2951.81 (C-H), 3080.12 (C-H in Ar-H), 3371.89 (O-H), 1445.06 (C-C in Ar), 1265.19 (Ar-O-C), 3579.21 (N-H), 728.14 (C-Cl).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 6.9 (d, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (s, 2H, Ar-H), 8.1 (d, 2H, Ar-H).	382.88
4g	2951.20 (C-H), 3058.67 (C-H in Ar-H), 3372.22 (O-H), 1619.16, 1445.79 (C-C in Ar), 1238.85 (Ar-O-C), 3578.35 (N-H).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 6.9 (d, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (s, 2H, Ar-H), 8.1 (d, 2H, Ar-H).	392.61
4h	2951.12 (C-H), 3058.78 (C-H in Ar-H), 3371.87 (O-H), 1445.77 (C-C in Ar), 1239.03 (Ar-O-C), 3578.66 (N-H).	1.5 (d, 6H, -CH_3), 2.2 (m, 4H, -CH_2-), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 5.1 – 5.3 (d, 3H, -CH=CH2), 6.4 (s, 1H, Ar-H), 6.8 (d, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (s, 2H, Ar-H), 8.1 (d, 2H, Ar-H).	373.61
4i	2951.13 (C-H), 3058.33 (C-H in Ar-H), 3378.99 (O-H), 1619.16, 1583.44 and 1446.67 (C-C in Ar), 1238.95 (Ar-O-C), 3578.99 (N-H), 1984.59(CN).	1.5 (d, 6H, -CH_3), 2.2 (m, 4H, -CH_2-), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 6.8 (d, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (s, 2H, Ar-H), 8.1 (d, 2H, Ar-H).	374.34
4j	2953.73 (C-H), 3038.32 (C-H in Ar-H), 3246.76 (O-H), 1610.96, 1581.02 and 1444.67 (C-C in Ar), 1241.06 (Ar-O-C), 3474.29 (N-H).	1.5 (d, 6H, -CH_3), 2.0 (m, 4H, -CH_2-), 2.5 (s, 3H, -CH3), 4.0 (bs, 2H, -NH_2), 4.9 (s, 1H, -OH), 6.4 (s, 1H, Ar-H), 6.8 (d, 1H, Ar-H), 7.1 (d, 1H, Ar-H), 7.5 (s, 2H, Ar-H), 8.1 (d, 2H, Ar-H).	362.88

(E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-hydroxy phenyl) prop-2-en-1-one (3a) of $C_{20}H_{20}O_4$ with molecular ion peak at (M+1) showed that m/z is equivalent to molecular weight (324.37) of proposed compound. Hence m/z value confirms the molecular weight of the compound. The IR peak at 1728 cm^{-1} suggesting the presence of C=O group. The IR peaks at 1601 cm^{-1} and 1436 cm^{-1} indicates that the presence of C=C group. IR peak at 3351 cm^{-1} indicates presence of O-H group. The HNMR peak at δ 4.9 (s, 2H) indicates the presence of two O-H groups and δ 6.5 and 7.6 suggests α, β-unsaturated ethylene group.

(E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-methoxy phenyl) prop-2-en-1-one (3b) has molecular formula $C_{21}H_{22}O_4$ and the molecular weight of the compound is equivalent to the molecular ion peak at (M+H) of the compound. Hence m/z value confirms the molecular weight (338.4) of compound. The IR peak at 1728 cm^{-1} suggesting the presence of C=O group. The IR peak at 1601 cm^{-1} and 1436 cm^{-1} indicates C=C group. The IR peak at 3352 cm^{-1} indicates

presence of O-H group. The HNMR peak at δ 4.9 indicates the presence of O-H group and δ 3.7 indicates methoxy group. The HNMR peaks at δ 6.5 and 7.6 suggest α, β-unsaturated ethylene group.

The molecular formula of Synthesis of (E)-3-(4-(dimethylamino)phenyl)-1-(7-hydroxy-2,2-dimethyl chroman -6-yl) prop-2-en-1-one (3c) is $C_{22}H_{25}NO_3$ and the molecular weight of the compound is equivalent to the molecular ion peak at (M+H) of the compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 1707 cm^{-1} suggesting the presence of C=O group and 3385 cm^{-1} indicates the presence of O-H group. The IR peak at 1581 cm^{-1} indicates that the presence of C=C group. IR peak at 1349 cm^{-1} indicates presence of C-N group. The HNMR peak at δ 4.9 indicates the presence of O-H group and δ 2.9 represents the presence of dimethyl amine group. The HNMR peaks at δ 6.5 and 7.6 suggest α, β-unsaturated ethylene group.

The obtained molecular ion peak of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-nitrophenyl) prop-2-en-1-one (3d) (molecular formula, ($C_{20}H_{19}NO_5$) at 354.21 (M+1) that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 3296 cm^{-1} suggesting the presence of O-H group and 1709 cm^{-1} indicates the presence of C=O group. The IR peak at 1462 cm^{-1} indicates that the presence of Nitro group. The HNMR peak at δ 4.9 and the HNMR peaks at δ 8.5 and 8.7 suggest α, β-unsaturated ethylene group.

(E)-3-(4-bromophenyl)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)prop-2-en-1-one (3e) of $C_{20}H_{19}BrO_3$ with molecular ion peak at (388.33, M+1) showed that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of the compound. The IR peak at 3385 cm^{-1} suggesting the presence of O-H group and 1708 cm^{-1} indicates the presence of C=O group. The IR peak at 772 cm^{-1} indicates that the presence of C-Br group. The HNMR peak at δ 4.9 indicates the presence of O-H group and the HNMR peaks at δ 8.5 and 8.7 suggests α, β-unsaturated ethylene group.

Synthesis of (E)-3-(4-chlorophenyl)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)prop-2-en-1-one (3f) has molecular formula $C_{20}H_{19}ClO_3$ and the molecular weight of the compound is equivalent to the molecular ion peak at (343.88, M+H) of the compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 1707 cm^{-1} suggesting the presence of C=O group and 3553 indicates O-H group. The IR peak at 694 cm^{-1} indicates that the presence of C-Cl group. The HNMR peak at δ 4.9 indicates the presence of O-H group and the HNMR peaks at δ 8.5 and 8.7 suggests α, β-unsaturated ethylene group.

The molecular formula of 4-((E)-3-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-oxoprop-1-enyl)benzoic acid (3g) is $C_{21}H_{20}O_5$ molecular ion peak at (353.61, M+H) that m/z is equivalent to molecular weight of proposed compound Hence m/z value confirms the molecular weight of compound. The IR peak at 1708 cm^{-1} suggesting the presence of C=O group and 3385 cm^{-1} indicates the presence of O-H group. The HNMR peak at δ 4.9 indicates the presence of O-H group and the HNMR peaks at δ 8.5 and 8.7 suggests α, β-unsaturated ethylene group. The HNMR peak at δ 10.1 indicates the presence of carboxylic acid group.

The obtained molecular ion peak of (E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-(4-vinylphenyl) prop-2-en-1-one (3h) (molecular formula, $C_{22}H_{22}O_3$) at 335.61 (M+1) that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 1708 cm^{-1} suggesting the presence of C=O group. The IR peak at 3383 cm^{-1} indicates that the presence of O-H group. The HNMR peak at δ 4.9 indicates the presence of O-H group and the HNMR peaks at δ 8.5 and 8.7 suggests α, β-unsaturated ethylene group. The HNMR peak at δ 5.1-5.3 indicates the presence of ethylene group.

4-((E)-3-(7-hydroxy- 2,2-dimethylchroman- 6-yl)-3-oxoprop-1- enyl) benzonitrile (3i) of $C_{21}H_{19}NO_3$ with molecular ion peak at (334.34, M+1) showed that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of the compound. The IR peak at 3349 cm^{-1} suggesting the presence of O-H group and 1707 cm^{-1} indicates the presence of C=O group. The IR peak at 2349 cm^{-1} indicates that the presence of Nitrile group. The HNMR peak at δ 4.9 indicates the presence of O-H group and the HNMR peaks at δ 8.5 and 8.7 suggests α, β-unsaturated ethylene group.

(E)-1-(7-hydroxy-2,2-dimethylchroman-6-yl)-3-p-tolylprop-2-en-1-one (3j) have molecular formula $C_{21}H_{22}O_3$and the molecular weight of the compound is equivalent to the molecular ion peak at (323.88, M+H) of the compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 3385 cm^{-1} suggesting the presence of O-H group and 1707 cm^{-1} indicates the presence of C=O. The HNMR peak at δ 4.9 indicates the presence of O-H group and the HNMR peaks at δ 8.5 and 8.7 suggests α, β-unsaturated ethylene group.

The molecular formula of 6-(6-(4-hydroxyphenyl)-[2-amino]pyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4a) is $C_{21}H_{21}N_3O_3$ molecular ion peak at (364.25, M+H) that m/z is equivalent to molecular weight of proposed compound Hence m/z value confirms the molecular weight of compound. The IR peak at 3369 cm^{-1} suggesting the presence of O-H group and 3583 cm^{-1} indicates the presence of N-H group. The HNMR peak at δ 3.9 (bs, 2H) indicates $–NH_2$ group and 4.9 (s, 1H) indicates –OH group.

The obtained molecular ion peak of 6-(6-(4-hydroxyphenyl) -[2-methoxy]pyrimidin-4-yl) -2,2-dimethyl chroman-7-ol (4b) (molecular formula, $C_{22}H_{23}N_3O_3$) at 378.38 (M+H) that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 3245 cm^{-1} suggests the presence of O-H group and the IR peak at 3473 cm^{-1} indicates that the presence of N-H group. The HNMR peak at δ 4.0 (bs, 2H) indicates the presence of $–NH_2$ group and δ 4.9 represents –OH group.

6-(6-(4-hydroxyphenyl)-[2-dimethylamino] pyrimidin-4-yl)-2,2-dimethylchroman-7-ol (4c) of $C_{23}H_{26}N_4O_2$ with molecular ion peak at (391.40, M+1) showed that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of the compound. The IR peak at 3372 cm^{-1} suggesting the presence of O-H group and the IR peak at 3578 cm^{-1} indicates that the presence of N-H group. The IR peak at 1306 cm^{-1} indicates the presence of dimethyl amine group. The HNMR peak at δ 3.0 (s, 6H) indicates the presence of dimethyl amine group and δ 4.0 (bs, 2H) represents the presence of $–NH_2$ group.

6-(6-(4-hydroxyphenyl)-[2-nitro] pyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4d) have molecular formula $C_{21}H_{20}N_4O_4$ and the molecular weight of the compound is equivalent to the molecular ion peak at (393.21, M+H) of the compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 3372 cm^{-1} suggests the presence of O-H group and the IR peak at 3578 cm^{-1} indicates that the presence of N-H group. The HNMR peak at δ 4.0 (s, 1H) indicates the presence of -OH group and δ 4.0 (bs, 2H) represents the presence of $–NH_2$ group.

The molecular formula of 6-(6-(4-Bromophenyl)-2-aminopyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4e) is $C_{21}H_{20}BrN_3O_2$ molecular ion peak at (427.42, M+H) that m/z is equivalent to molecular weight of proposed compound Hence m/z value confirms the molecular weight of compound. The IR peak at 3372 cm^{-1} suggesting the presence of O-H group and 3579 cm^{-1} indicates that the presence of N-H group. The IR peak at 727 cm^{-1} indicates presence of –Br group. The HNMR peak at δ 4.0 (bs, 2H) indicates $–NH_2$ group and δ 4.9 (s, 1H) represents the presence of –OH group.

The obtained molecular ion peak of 6-(6-(4-Chlorophenyl)-2-aminopyrimidin-4-yl)-2,2-dimethyl chroman-7-ol (4f) (molecular formula, ($C_{21}H_{20}ClN_3O_2$) at 382.88 (M+H) that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 3371 cm^{-1} suggesting the presence of O-H group and 728 cm^{-1} indicates that the presence of -Cl group. The IR peak at 3579 cm^{-1} indicates presence of N-H group. The HNMR peak at δ 4.0 (bs, 2H) indicates $–NH_2$ group and δ 4.9 (s, 1H) represents the presence of –OH group.

4-(6-(7-hydroxy-2,2-dimethylchroman-6-yl)-2-aminopyrimidin-4-yl)benzoic acid (4g) of $C_{22}H_{21}N_3O_4$ with molecular ion peak at (392.61, M+1) showed that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of the compound. The IR peak at 3372 cm^{-1} suggesting the presence of O-H group and the IR peak at 3578 cm^{-1} indicates that the presence of N-H group. The HNMR peak at δ 4.0 (bs, 2H) indicates $–NH_2$ group and δ 4.9 (s, 1H) represents the presence of –OH group.

2,2-dimethyl-6-(2-amino-6-(4-vinylphenyl)pyrimidin-4-yl) chroman-7-ol (4h) have molecular formula $C_{23}H_{23}N_3O_2$ and the molecular weight of the compound is equivalent to the molecular ion peak at (373.61, M+H) of the compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 3371 cm^{-1} suggesting the presence of O-H group and the IR peak at 3578 cm^{-1} indicates that the presence of N-H group. The HNMR peak at δ 4.0 (bs, 2H) indicates $–NH_2$ group and δ 4.9 (s, 1H) represents the presence of –OH group. The HNMR peaks at δ 5.1-5.3 represents methylene group.

The molecular formula of 4-(6-(7-hydroxy-2,2-dimethylchroman-6-yl)-2-aminopyrimidin-4-yl)benzonitrile (4i) is $C_{22}H_{20}N_4O_2$ molecular ion peak at (374.34, M+H) that m/z is equivalent to molecular weight of proposed compound Hence m/z value confirms the molecular weight of compound. The IR peak at 3378 cm^{-1} suggesting the presence of O-H group and the IR peak at 3578 cm^{-1} indicates that the presence of N-H group. The IR peak at 1984 cm^{-1} indicates presence

of Nitrile group. The HNMR peak at δ 4.0 (bs, 2H) indicates $–NH_2$ group and δ 4.9 (s, 1H) represents the presence of –OH group.

The obtained molecular ion peak of 2,2-dimethyl-6-(2-amino-6-p-tolylpyrimidin-4-yl)chroman-7-ol (4j) (molecular formula, ($C_{22}H_{23}N_3O_2$) at 362.88 (M+1) that m/z is equivalent to molecular weight of proposed compound. Hence m/z value confirms the molecular weight of compound. The IR peak at 3246 cm^{-1} suggesting the presence of O-H group and the IR peak at 3474 cm^{-1} indicates that the presence of N-H group. The HNMR peak at δ 4.0 (bs, 2H) indicates $–NH_2$ group and δ 4.9 (s, 1H) represents the presence of –OH group. The HNMR peak at δ 2.5 (s, 3H) confirms the presence of methyl group.

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