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*Research Article*

# Synthesis, Characterization, and Biological Activity of 4-(2-Hydroxy-5-(aryl-diazenyl)phenyl)-6-(aryl)pyrimidin-2-ols Derivatives

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With the aim of synthesizing new heterocyclic compounds and exploring biological potency, new series of chalcones, that is, 3-(2-hydroxy-5-(aryl-diazenyl)phenyl)-1-(aryl)prop-2-en-1-one and their pyrimidine derivatives, that is, 4-(2-hydroxy-5-(aryl-diazenyl)phenyl)-6-(aryl)pyrimidin-2-ols were synthesized using different aromatic amines and salicylaldehyde as starting moieties. The structures of newly synthesized compounds were confirmed using different spectroscopic techniques such as IR, $^1$H-NMR, $^{13}$C-NMR, and mass spectral analysis, and elemental analysis. The newly synthesized pyrimidines derivatives were screened for their in vitro antibacterial and antifungal activities. It was observed that some of the newly synthesized compounds had shown promising activity against several bacterial and fungal stains. Anti-bacterial activity and anti-fungal activity studies revealed that pyrimidine derivatives consisting of nitro group in their molecular structure possess better activity than their corresponding chalcones.

## 1. Introduction

Chalcones (1,3-diaryl-2-propen-1-ones), one of the major classes of natural products belonging to the flavonoid family, have been recently the subjects of great interest for their interesting pharmacological activities [1, 2]. In fact, the pharmacological properties of chalcones are due to the presence of both $\alpha,\beta$-unsaturation and an aromatic ring [3]. Many biological activities have been attributed to this group, such as cytotoxic [4, 5], antimalarial [6, 7], antileishmanial [8, 9], anti-inflammatory [10, 11], anti-HIV [12], antifungal [13], antioxidant [14], and as tyrosine kinase inhibitors [15]. Due to their abundance in plants and ease of synthesis, this class of compounds has generated great interest for possible therapeutic uses [16, 17]. Of the many methods available for the synthesis of chalcones, the most widely used method is the base catalyzed Claisen-Schmidt reaction [18] in which the condensation of a ketone with an aldehyde is carried out in the presence of aqueous NaOH [19], $Ba(OH)_2$ [20], KOH, and so forth. The acid catalyzed methodologies include the use of silica sulfuric acid [21], $AlCl_3$, dry HCl, and so forth [22]. Chalcone derivatives are very versatile as physiologically active compounds and substrates for the evaluation of various organic syntheses. Chalcones are valuable intermediates in the synthesis of many active pharmaceutical drugs like biosynthesis of flavonoids and Auwers synthesis of flavones [23].

Pyrimidine and its derivatives are most important nitrogen based heterocycles which play a vital role in many life processes [24]. The ring system is present in nucleic acids and

their derivatives (willardiine, tingitanine) [25] such as several vitamins (vitamin B1), antibiotics (bacimethrin, sparsomycin, bleomycin) [26], alkaloids (heteromines, crambescins, manzacidins, variolins, meridianins, psammopemmins) [27, 28], toxins [29], coenzymes, uric acid, and purines. Pyrimidine and its derivatives represents one of the important classes of heterocyclic system which is associated with the wide range of biological and pharmacological activities such as anticonvulsant [30], antimicrobial [31], anti-inflammatory [32], anti-HIV [33], antitubercular [34], antitumor [35], antineoplastic [36], antimalarial [37], diuretic [38], and cardiovascular agents. Pyrimidine compounds are also used as hypnotic drugs for the nervous system [39], calcium-sensing receptor antagonists [40], and also for antagonists of the human $A_{2A}$ adenosine receptor [41].

In view of the variety of pharmacological properties exhibited by chalcones and pyrimidines, we planned to synthesize new series of chalcones, and pyrimidine derivatives. In the present communication, we thus report here the synthesis of series of chalcones that is, 3-(2-hydroxy-5-(aryl-diazenyl)phenyl)-1-(aryl)prop-2-en-1-one following Claisen-Schmidt condensation reaction pathway and their pyrimidine derivatives that is 4-(2-hydroxy-5-(aryl-diazenyl)phenyl)-6-(aryl)pyrimidin-2-ols (Scheme 1). Different aromatic aldehydes were synthesized as depicted earlier [42]. The structures of newly synthesized chalcones and pyrimidines compounds were confirmed using spectroscopic techniques such as $^1$H-NMR, $^{13}$C-NMR, IR, and Mass spectroscopy and elemental analysis. The results of anti-bacterial and antifungal activities have also been reported here. The current investigations reveal that pyrimidine analogs exhibit better antibacterial and antifungal activities than the parent chalcone analogues.

## 2. Experimental

The chemicals and solvents were of AR grade and were used without further purification. Melting points were taken in open capillaries on TOSHNIWAL melting point apparatus and are uncorrected. IR spectra were recorded on Shimadzu Dr-8031 instrument in KBr pallets. Elemental analyses were carried out using a Perkin-Elmer, CHN elemental analyzer model 2400. $^1$H-NMR and $^{13}$C-NMR spectra of the synthesized compounds were recorded on a Bruker-Avance (300 MHz) and Varian-Gemini (200 MHz) spectrophotometer using $CDCl_3$ solvent and TMS as an internal standard. EI-MS spectra were determined on a LCQ ion trap mass spectrometer (Thermo Fisher, San Jose, C A, USA), equipped with an EI source.

*2.1. General Procedure for the synthesis of 2-Hydroxy-5-((aryl)diazenyl)benzaldehyde* ***(1a–1e)***. Aromatic amines (0.01 moL) was added in conc. HCl (5 mL) and boiled for 10 minutes. The resulting solution was then cooled to 0–5°C in ice bath. Aqueous sodium nitrite ($NaNO_2$) (0.01 moL, 10 mL) solution in the cold condition was added in dropwise manner to this solution. The reaction mixture was then vigorously stirred. The temperature of the reaction mixture was maintained within 0–5°C for at least 1 hour to obtain diazonium chloride solution.

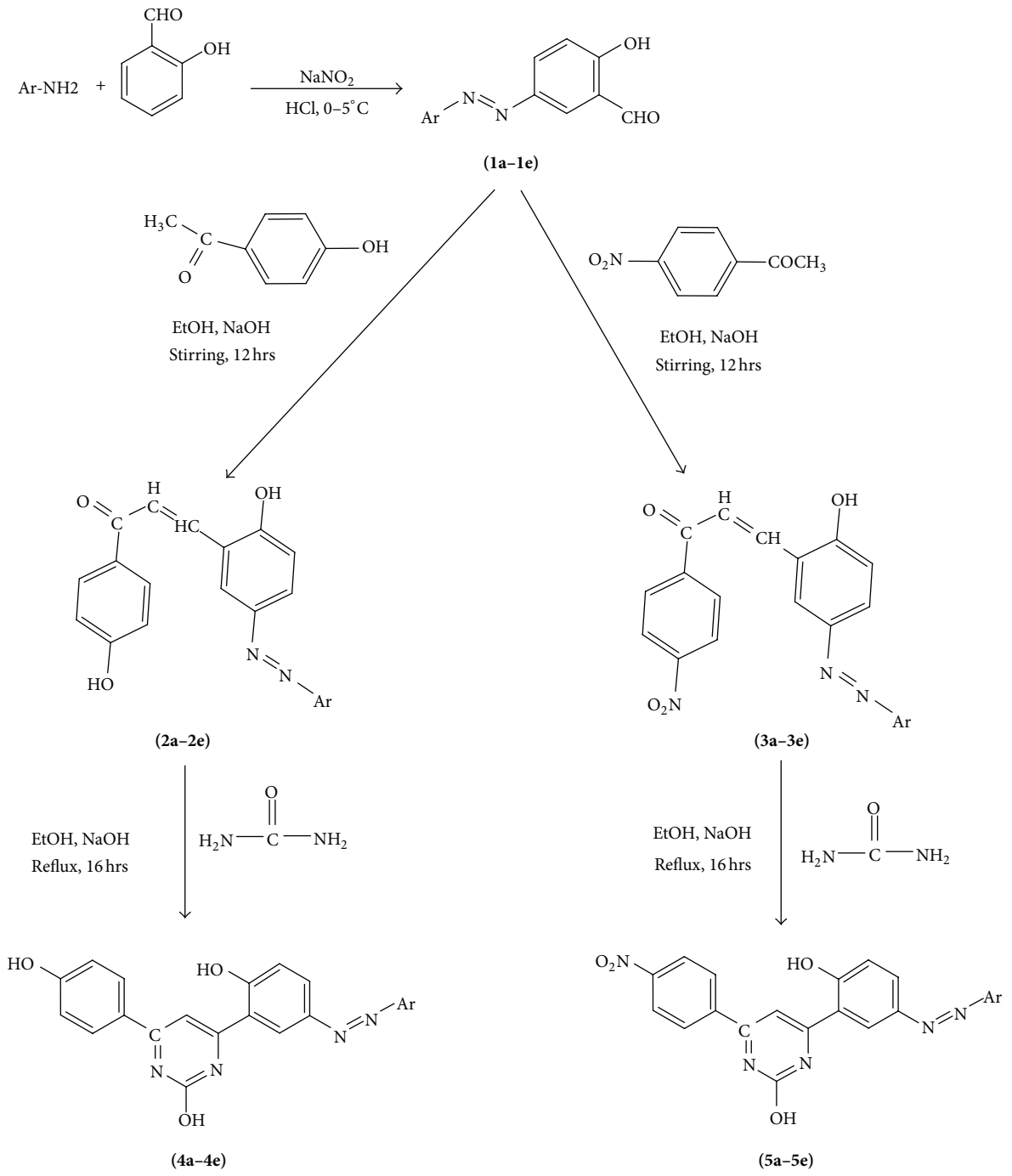
The resulting diazonium solution was then poured slowly to alkaline suspension of salicylaldehyde in water (10 mL, 0.01 moL) with continuous stirring keeping temperature within 0–5°C. The pH of the reaction mixture was maintained within 8 to 10 by simultaneous addition of 10% aqueous sodium hydroxide solution. The resulting reaction mixture was kept unstirred for overnight. The obtained solid precipitate was filtered using Whatman filter paper number 40 and recrystallized using ethanol.

*2.1.1. Characterization Data of 2-Hydroxy-5-(p-tolyldiazenyl)benzaldehyde* ***(1a)***. Brownish Powder; Yield, 87.16%; m.p., 115°C; IR (KBr) cm$^{-1}$: 1480 (N=N), 1730 (aldehydic C=O), 2850 (aldehydic H–C=), 2890 (Ar-$CH_3$), 3450 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 2.35 (s, 3H, Ar-$CH_3$), 5.10 (s, 1H, Ar-OH), 7.10 (s, 1H, Ar-CH), 7.30 (m, 2H, Ar-CH), 7.90 (d, 2H, Ar-CH), 8.10 (d, 1H, Ar-CH), 8.30 (s, 1H, Ar-CH), 10.30 (s, 1H, Ar-CHO); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 194.6, 164.0, 149.7, 145.8, 140.6, 130.2, 129.4, 129.3, 124.0, 122.9, 122.8, 118.5, 116.7 (13 aromatic carbon), 21.3 ($CH_3$); Anal. Calcd. for $C_{14}H_{12}N_2O_2$ (%): C 69.99, H 5.03, N 11.66; Found (%): C 69.60, H 4.90, N 11.40; MS: $m/z$ 240.29 (100%, $M^+$), 121.10 (50%), 119.00 (40%), 93.00 (30%), 91.10 (30%), 29.00 (10%), 28.00 (20%).

*2.1.2. Characterization Data of 2-Hydroxy-5-((2-nitrophenyl)diazenyl)benzaldehyde* ***(1b)***. Brownish Powder; Yield, 78.71%; m.p., 124°C; IR (KBr) cm$^{-1}$: 1340 (Ar-$NO_2$), 1430 (N=N), 1720 (aldehydic C=O), 2840 (aldehydic H–C=), 3030 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.20 (s, 1H, Ar-OH), 7.30 (s, 1H, Ar-CH), 7.70–8.20 (m, 6H, Ar-CH), 10.20 (s, 1H, Ar-CHO); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 194.6, 164.0, 147.6, 145.8, 143.9, 135.1, 131.8, 130.2, 124.2, 124.0, 123.9, 118.5, 116.7 (13 aromatic carbon); Anal. Calcd. for $C_{13}H_9N_3O_4$ (%): C 57.57, H 3.34, N 15.49; Found (%): C 57.40, H 3.10, N 15.20; MS: $m/z$ 271.18 (100%, $M^+$), 150.10 (40%), 122.00 (50%), 121.20 (30%), 93.10 (20%), 77.10 (30%), 45.00 (10%), 29.20 (20%), 28.10 (10%).

*2.1.3. Characterization Data of 2-Hydroxy-5-((3-nitrophenyl)diazenyl)benzaldehyde* ***(1c)***. Brownish Powder; Yield, 89.59%; m.p., 120°C; IR (KBr) cm$^{-1}$: 1320 (Ar-$NO_2$), 1420 (N=N), 1710 (aldehydic C=O), 2830 (aldehydic H–C=), 3040 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.40 (s, 1H, Ar-OH), 7.50 (s, 1H, Ar-CH), 7.90–8.30 (m, 6H, Ar-CH), 10.40 (s, 1H, Ar-CHO); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 194.6, 164.0, 152.6, 148.2, 145.8, 131.8, 130.2, 129.2, 126.7, 124.0, 118.5, 117.3, 116.5 (13 aromatic carbon); Anal. Calcd. for $C_{13}H_9N_3O_4$ (%): C 57.57, H 3.34, N 15.49; Found (%): C 57.30, H 3.20, N 15.10; MS: $m/z$ 271.20 (100%, $M^+$), 151.10 (60%), 122.10 (50%), 121.00 (40%), 93.00 (10%), 77.20 (20%), 45.10 (10%), 29.10 (10%), 28.00 (10%).

*2.1.4. Characterization Data of 2-Hydroxy-5-((4-nitrophenyl)diazenyl)benzaldehyde* ***(1d)***. Greenish Powder; Yield,




Where, Ar- for compounds (a) -$C_6H_4$-$CH_3$; (b) 2-$NO_2$-$C_6H_4$-; (c) 3-$NO_2$-$C_6H_4$-; (d) 4-$NO_2$-$C_6H_4$-; (e) -$C_6H_5$

Scheme 1

90.32%; m.p., 146°C; IR (KBr) $cm^{-1}$: 1340 (Ar-$NO_2$), 1400 (N=N), 1700 (aldehydic C=O), 2345 (aldehydic H–C=), 2920 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.30 (s, 1H, Ar-OH), 7.60 (s, 1H, Ar-CH), 7.90–8.20 (m, 6H, Ar-CH), 10.10 (s, 1H, Ar-CHO); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 194.5, 164.2, 155.8, 150.6, 145.2, 130.4, 124.3, 124.2, 124.1, 120.8, 120.7, 118.3, 116.5 (13 aromatic carbon); Anal. Calcd. for $C_{13}H_9N_3O_4$ (%): C 57.57, H 3.34, N 15.49; Found (%): C 57.40, H 3.20, N 15.30; MS: $m/z$ 271.30 (100%, $M^+$), 150.90 (70%), 121.80 (40%), 121.10 (60%), 93.10 (30%), 77.10 (30%), 45.00 (20%), 29.20 (10%), 28.10 (20%).

*2.1.5. Characterization Data of 2-Hydroxy-5-(phenyldiazenyl)benzaldehyde* ***(1e)***. Yellowish Powder; Yield,

73.05%; m.p., 110°C; IR (KBr) $cm^{-1}$: 1440 (N=N), 1740 (aldehydic C=O), 2820 (aldehydic H–C=), 3010 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.20 (s, 1H, Ar-OH), 7.10 (d, 1H, Ar-CH), 7.50 (t, 3H, Ar-CH), 7.90–8.10 (m, 3H, Ar-CH), 8.40 (s, 1H, Ar-CH), 10.30 (s, 1H, Ar-CHO); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 194.7, 164.3, 152.6, 145.6, 130.8, 130.5, 129.6, 129.5, 124.1, 123.2, 123.1, 118.7, 116.5, (13 aromatic carbon); Anal. Calcd. for $C_{13}H_{10}N_2O_2$ (%): C 69.02, H 4.46, N 12.38; Found (%): C 69.00, H 4.30, N 12.10; MS: $m/z$ 226.20 (100, $M^+$), 121.30 (60%), 105.10 (50%), 93.20 (40%), 77.20 (30%), 29.10 (20%), 28.20 (10%).

*2.2. General Procedure for the Synthesis of Chalcones **(2a–2e, 3a–3e)**.* To synthesize the chalcone derivatives, in the first step 2-hydroxy-5-((aryl)diazenyl)benzaldehyde (0.01 moL) and *p*-acetophenone or *p*-nitroacetophenone (0.01 moL) were added to ethanol (30 mL) and then mixed thoroughly at the room temperature. In this mixture, 10 mL of 20% aqueous NaOH solution was added slowly. The reaction mixture was stirred over the magnetic stirrer for at least 12 hours. The reaction mixture was then kept for overnight. It was then poured into beaker containing crushed ice. The excess of alkali in the reaction mixture was neutralized and the reaction mixture was then slightly acidified by dropwise addition of dilute hydrochloric acid solution. The chalcone derivative, that is, 3-(2-hydroxy-5-((aryl)diazenyl)phenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (**2a**–**2e**) and 3-(2-hydroxy-5-((aryl) diazenyl)phenyl)-1-(4-nitrophenyl) prop-2-en-1-one (**3a**–**3e**) gets precipitated out and was filtered using Whatman filter paper number 40. The crude chalcone product was recrystallized using ethanol.

*2.2.1. Characterization Data of 3-(2-Hydroxy-5-(p-tolyldiazenyl)phenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(2a)**.* Yellowish Powder; Yield, 77.85%; m.p., 130°C; IR (KBr) $cm^{-1}$: 1490 (N=N), 1590 (C=C), 1680 (C=O), 2850 (Ar-$CH_3$), 3410 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 2.30 (s, 3H, Ar-$CH_3$), 4.90 (s, 2H, 2Ar-OH), 6.80–6.90 (m, 3H, Ar-CH), 7.20–7.30 (t, 3H, Ar-CH), 7.40 (d, 2H, Ar-CH), 7.60–7.80 (m, 6H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.5, 164.0, 159.2, 149.7, 145.3, 141.6, 140.5, 131.3, 131.2, 130.4, 129.3, 129.2, 123.9, 122.6, 122.9, 121.2, 120.4, 116.3, 116.1, 116.7, 116.5, 116.4 (22 aromatic carbon); 21.5 ($CH_3$); Anal. Calcd. for $C_{22}H_{18}N_2O_3$ (%): C 73.73, H 5.06, N 7.82; Found (%): C 73.20, H 4.90, N 7.70; MS: $m/z$ 358.30 (100%, $M^+$), 211.08 (54%), 147.05 (46%), 121.06 (15%), 91.10 (12%), 93 (33%), 28.06 (21%), 26.10 (10%).

*2.2.2. Characterization Data of 3-(2-Hydroxy-5-((2-nitrophenyl)diazenyl)phenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(2b)**.* Brownish Powder; Yield, 67.05%; m.p., 142°C; IR (KBr) $cm^{-1}$: 1320 (Ar-$NO_2$), 1440 (N=N), 1580 (C=C), 1680 (C=O), 3030 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.10 (s, 2H, 2Ar-OH), 6.80 (t, 3H, Ar-CH), 7.40 (d, 1H, C=CH), 7.60–7.70 (m, 7H, Ar-CH), 8.20 (d, 1H, C=CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.6, 164.2, 159.4, 147.5, 145.1, 143.9, 141.2, 135.2, 131.6, 131.2, 131.1, 130.4, 124.4, 123.8, 121.2, 123.5, 120.4, 116.6, 116.3, 116.1, 116.2 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{15}N_3O_5$ (%): C 64.73, H 3.88, N 10.79; Found (%): C 64.70, H 3.70, N 10.60; MS: $m/z$ 389.38 (100%, $M^+$), 242.10 (65%), 147.08 (40%), 121.05 (13%), 122.10 (40%), 93.10 (14%), 28.08 (21%), 26.10 (8%).

*2.2.3. Characterization Data of 3-(2-Hydroxy-5-((3-nitrophenyl)diazenyl)phenyl)-1-(4-hydroxy phenyl)prop-2-en-1-one **(2c)**.* Brownish Powder; Yield, 73.46%; m.p., 164°C; IR (KBr) $cm^{-1}$: 1310 (Ar-$NO_2$), 1460 (N=N), 1570 (C=C), 1690 (C=O), 3010 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.20 (s, 2H, 2Ar-OH), 6.90 (t, 3H, Ar-CH), 7.60 (d, 1H, C=CH), 7.80–8.10 (m, 7H, Ar-CH), 8.30 (d, 1H, C=CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.6, 164.6, 159.1, 152.3, 148.5, 145.5, 141.3, 131.4, 131.2, 131.1, 130.2, 129.5, 126.5, 123.4, 121.5, 120.3, 117.1, 116.7, 116.4, 116.3, 116.2 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{15}N_3O_5$ (%): C 64.73, H 3.88, N 10.79; Found (%): C 64.60, H 3.60, N 10.40; MS: $m/z$ 389.41 (100%, $M^+$), 242.00 (85%), 150.10 (40%), 147.10 (40%), 122.10 (40%), 121.10 (15%), 93.10 (16%), 77.00 (10%), 45.10 (20%), 28.00 (5%), 26.00 (10%).

*2.2.4. Characterization Data of 3-(2-Hydroxy-5-((4-nitrophenyl)diazenyl)phenyl)-1-(4-hydroxy phenyl)prop-2-en-1-one (2d).* Brownish Powder; Yield, 76.97%; m.p., 188°C; IR (KBr) $cm^{-1}$: 1330 (Ar-$NO_2$), 1500 (N=N), 1580 (C=C), 1660 (C=O), 3270 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.30 (s, 2H, 2Ar-OH), 6.60 (t, 3H, Ar-CH), 7.40 (d, 1H, C=CH), 7.70–8.10 (m, 7H, Ar-CH), 8.50 (d, 1H, C=CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.4, 164.4, 159.2, 155.4, 150.3, 145.3, 141.4, 131.5, 131.4, 130.4, 124.4, 124.3, 123.6, 120.8, 120.6, 120.4, 116.6, 116.5, 116.4, 116.3, 116.1 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{15}N_3O_5$ (%): C 64.73, H 3.88, N 10.79; Found (%): C 64.40, H 3.70, N 10.60; MS: $m/z$ 389.10 (100%, $M^+$), 241.90 (70%), 151.00 (40%), 147.00 (50%), 121.90 (30%), 121.00 (20%), 92.90 (20%), 77.10 (12%), 45.00 (15%), 28.10 (10%), 26.10 (13%).

*2.2.5. Characterization Data of 3-(2-Hydroxy-5-(phenyldiazenyl)phenyl)-1-(4-hydroxy phenyl)prop-2-en-1-one (2e).* Greenish Powder; Yield, 74.06%; m.p., 122°C; IR (KBr) $cm^{-1}$: 1450 (N=N), 1550 (C=C), 1680 (C=O), 3020 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.20 (s, 2H, 2Ar-OH), 6.80–7.40 (m, 10H, Ar-CH), 7.70 (s, 1H, Ar-CH), 7.90 (d, 2H, Ar-CH), 8.40 (d, 1H, C=CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.5, 164.6, 159.5, 152.3, 145.4, 141.3, 131.4, 131.6, 130.8, 130.2, 129.4, 129.3, 123.5, 123.5, 123.2, 121.1, 120.4, 116.7, 116.5, 116.4, 116.3 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{16}N_2O_3$ (%): C 73.24, H 4.68, N 8.13; Found (%): C 73.30, H 4.50, N 8.10; MS: $m/z$ 344.32 (100%, $M^+$), 147.10 (60%), 197.08 (40%), 121.10 (20%), 93.90 (50%), 77.20 (30%), 26.30 (10%).

*2.2.6. Characterization Data of 3-(2-Hydroxy-5-(p-tolyldiazenyl)phenyl)-1-(4-nitrophenyl)prop-2-en-1-one (3a).* Brownish Powder; Yield, 79.02%; m.p., 152°C; IR (KBr) $cm^{-1}$: 1350 (Ar-$NO_2$), 1510 (N=N), 1600 (C=C), 1680 (C=O), 2850 (Ar-$CH_3$), 3380 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 2.30 (s, 3H, Ar-$CH_3$), 5.10 (s, 1H, Ar-OH), 6.80–7.20 (m, 4H, Ar-CH), 7.30 (s, 1H, C=CH), 7.40 (s, 1H, C=CH), 7.70–7.80 (t, 3H, Ar-CH), 8.10 (d, 2H, Ar-CH), 8.40 (d, 2H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.5, 159.2, 153.6,

149.4, 145.2, 144.3, 141.2, 140.3, 130.7, 130.6, 129.2, 129.1, 124.3, 124.1, 123.5, 122.6, 122.2, 121.5, 120.3, 116.4, 116.3, (21 aromatic carbon), 21.5 ($CH_3$); Anal. Calcd. for $C_{22}H_{17}N_3O_4$ (%): C 68.21, H 4.42, N 10.85, Found (%): C 68.20, H 4.30, N 10.70; MS: $m/z$ 387.10 (100%, $M^+$), 211.20 (60%), 176.10 (40%), 150.00 (20%), 121.10 (40%), 93.20 (40%), 91.10 (30%), 28.00 (20%), 26.08 (10%).

*2.2.7. Characterization Data of 3-(2-Hydroxy-5-((2-nitrophenyl)diazenyl)phenyl)-1-(4-nitrophenyl)prop-2-en-1-one **(3b)**.* Brownish Powder; Yield, 73.4%; m.p., 160°C; IR (KBr) $cm^{-1}$: 1340 (Ar-$NO_2$), 1430 (N=N), 1550 (C=C), 1640 (C=O), 3140 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.10 (s, 1H, Ar-OH), 6.90 (d, 1H, Ar-CH), 7.40 (d, 1H, C=C–H), 7.60–7.80 (m, 8H, Ar-CH), 8.10 (d, 1H, C=CH), 8.40 (d, 2H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.8, 159.6, 153.5, 147.6, 145.3, 144.1, 143.7, 141.3, 135.4, 131.5, 130.6, 130.5, 124.6, 124.3, 124.2, 123.7, 123.4, 121.4, 120.3, 116.7, 116.2 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{14}N_4O_6$ (%): C 60.29, H 3.37, N 13.39; Found (%): C 60.20, H 3.30, N 13.10;; MS: $m/z$ 418.25 (100%, $M^+$), 242.10 (60%), 176.20 (50%), 150.10 (40%), 122.10 (30%), 121.00 (20%), 93.10 (10%), 77.10 (30%), 45.00 (10%), 28.10 (10%), 26.00 (10%).

*2.2.8. Characterization Data of 3-(2-Hydroxy-5-((3-nitrophenyl)diazenyl)phenyl)-1-(4-nitro phenyl)prop-2-en-1-one **(3c)**.* Reddish Powder; Yield, 68.01%; m.p., 200°C; IR (KBr) $cm^{-1}$: 1320 (Ar-$NO_2$), 1410 (N=N), 1570 (C=C), 1660 (C=O), 3120 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.30 (s, 1H, Ar-OH), 6.60 (d, 1H, Ar-CH), 7.20 (d, 1H, C=C–H), 7.40–7.60 (m, 8H, Ar-CH), 8.20 (d, 1H, C=CH), 8.60 (d, 2H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.5, 159.4, 153.4, 152.2, 148.4, 145.4, 144.3, 141.7, 131.8, 130.7, 130.6, 129.3, 126.5, 124.7, 124.5, 123.7, 121.8, 120.4, 117.1, 116.5, 116.4 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{14}N_4O_6$ (%): C 60.29, H 3.37, N 13.39; Found (%): C 60.10, H 3.10, N 13.20; MS: $m/z$ 418.30 (100%, $M^+$), 242.00 (70%), 176.00 (50%), 122.00 (40%), 121.10 (30%), 93.10 (10%), 28.00 (10%), 27.90 (10%).

*2.2.9. Characterization Data of 3-(2-Hydroxy-5-((4-nitrophenyl)diazenyl)phenyl)-1-(4-nitro phenyl)prop-2-en-1-one **(3d)**.* Greenish Powder; Yield, 70.81%; m.p., 245°C; IR (KBr) $cm^{-1}$: 1340 (Ar-$NO_2$), 1500 (N=N), 1590 (C=C), 1670 (C=O), 3250 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 4.90 (s, 1H, Ar-OH); 6.20 (d, 1H, Ar-CH), 7.10 (d, 1H, C=C–H), 7.30–7.50 (m, 8H, Ar-CH), 8.10 (d, 1H, C=CH), 8.30 (d, 2H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.8, 159.1, 155.7, 153.6, 150.4, 145.4, 144.5, 141.4, 130.9, 130.6, 124.7, 124.6, 124.5, 124.1, 123.7, 121.6, 120.8, 120.4, 120.3, 116.9, 116.1 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{14}N_4O_6$ (%): C 60.29, H 3.37, N 13.39; Found (%): C 60.20, H 3.20, N 13.30; MS: $m/z$ 418.40 (100%, $M^+$), 242.20 (80%), 176.10 (70%), 130 (50%), 122.20 (40%), 121.10 (30%), 105.00 (20%), 93.00 (10%), 45.00 (10%), 28.20 (10%), 27.40 (10%).

*2.2.10. Characterization Data of 3-(2-Hydroxy-5-(phenyldiazenyl)phenyl)-1-(4-nitro phenyl)prop-2-en-1-one **(3e)**.* Brownish Powder; Yield, 80.62%; m.p., 155°C; IR (KBr) $cm^{-1}$: 1310 (Ar-$NO_2$), 1450 (N=N), 1580 (C=C), 1660 (C=O), 3150 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.20 (s, 1H, Ar-OH), 6.70 (s, 1H, Ar-CH), 7.40 (t, 3H, Ar-CH), 7.60 (s, 1H, CH=CH), 7.70–7.90 (m, 6H, Ar-CH), 8.10 (s, 1H, CH=CH), 8.30 (d, 2H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 189.5, 159.5, 153.9, 152.9, 145.8, 144.7, 141.8, 130.7, 130.6, 130.5, 129.4, 129.2, 124.5, 124.4, 123.8, 123.5, 123.3, 121.9, 120.6, 116.8, 116.5 (21 aromatic carbon); Anal. Calcd. for $C_{21}H_{15}N_3O_4$ (%): C 67.56, H 4.05, N 11.25; Found (%): C 67.40, H 4.00, N 11.20; MS: $m/z$ 373.34 (100%, $M^+$), 197.10 (60%), 176.00 (50%), 150 (60%), 122.00 (50%), 121.00 (40%), 93.10 (20%), 28.10 (10%), 27.10 (10%), 26.00 (10%).

*2.3. General Procedure for the Synthesis of Pyrimidines **(4a–4e, 5a–5e)**.* A mixture of chalcone (0.01 moL) and urea (0.01 moL) was prepared in 30 mL ethanol. To this solution, 10 mL 20% aqueous NaOH solution was added. The resulting mixture was then refluxed on water bath for at least 16 hours. The mixture was then cooled to room temperature and poured into the beaker containing crushed ice. The solid product of pyrimidine derivatives, that is, 4-(2-hydroxy-5-((aryl)diazenyl)phenyl)-6-(4-hydroxy-phenyl)pyrimidin-2-ols (**4a**–**4e**) or 4-(2-hydroxy-5-((aryl)diazenyl)phenyl)-6-(4-nitrophenyl)pyrimidin-2-ols (**5a**–**5e**) gets precipitated out. The solid obtained was filtered using Whatman filter paper no. 40 and recrystallized using ethanol.

*2.3.1. Characterization Data of 4-(2-Hydroxy-5-(p-tolyldiazenyl)phenyl)-6-(4-hydroxyphenyl)-pyrimidin-2-ol **(4a)**.* Yellowish Powder; Yield, 65.18%; m.p., 174°C; IR (KBr) $cm^{-1}$: 1490 (N=N), 1610 (C=N), 2900 (Ar-$CH_3$), 3430 $cm^{-1}$ (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 2.40 (s, 3H, Ar-$CH_3$), 5.10 (s, 3H, 3Ar-OH), 6.60 (s, 1H, Ar-CH), 6.80–7.30 (m, 7H, Ar-CH), 7.70–7.90 (m, 4H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.7, 160.4, 158.5, 157.6, 154.9, 149.5, 145.6, 140.8, 129.9, 129.8, 128.9, 128.6, 128.5, 124.8, 123.8, 122.4, 122.6, 120.9, 116.8, 116.7, 116.3 (21 aromatic carbon), 95.4 (C pyrimidine), 21.6 ($CH_3$); Anal. Calcd. for $C_{23}H_{18}N_4O_3$ (%): C 69.34, H 4.55, N 14.06; Found (%): C 69.30, H 4.50, N 14.00; MS: $m/z$ 398.42 (100%, $M^+$), 279.20 (80%), 119.10 (60%), 187.00 (50%), 95.10 (30%), 93.10 (20%), 91.00 (10%), 79.00 (10%), 68.10 (20%), 28.20 (10%).

*2.3.2. Characterization Data of 4-(2-Hydroxy-5-((2-nitrophenyl)diazenyl)phenyl)-6-(4-hydroxy-phenyl)pyrimidin-2-ol (4b).* Brownish Powder; Yield, 54.58%; m.p., 210°C; IR (KBr) $cm^{-1}$: 1310 (Ar-$NO_2$), 1420 (N=N), 1670 (C=N), 3030 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 4.90 (s, 3H, 3Ar-OH), 6.60–6.90 (m, 4H, Ar-CH), 7.30 (d, 2H, Ar-CH), 7.70–8.40 (m, 6H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 160.7, 162.4, 158.2, 157.9, 154.6, 147.7, 145.6, 143.8, 135.7 131.9, 128.8, 128.3, 128.1, 124.7, 124.6, 123.6, 123.4, 120.6, 116.6, 116.5, 116.2 (21 aromatic carbon), 95.2 (C pyrimidine); Anal. Calcd. for $C_{22}H_{15}N_5O_5$ (%): C 61.54, H 3.52, N 16.31; Found (%): C 61.40, H 3.30, N 16.10; MS: $m/z$ 429.34 (100%, $M^+$), 307.20 (70%), 187.00 (50%), 122.10 (50%), 120.00 (40%), 95.20 (30%), 93.00 (20%), 79.10 (10%), 77.20 (20%), 45.10 (10%), 68.00 (10%), 28.10 (10%).

*2.3.3. Characterization Data of 4-(2-Hydroxy-5-((3-nitrophenyl)diazenyl)phenyl)-6-(4-hydroxy-phenyl)pyrimidin-2-ol* ***(4c)***. Brownish Powder; Yield, 59.62%; m.p., 224°C; IR (KBr) $cm^{-1}$: 1320 (Ar-$NO_2$), 1430 (N=N), 1640 (C=N), 3010 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 4.70 (s, 3H, 3Ar-OH), 6.40–6.60 (m, 4H, Ar-CH), 7.40 (d, 2H, Ar-CH), 7.60–8.20 (m, 6H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.8, 160.9, 158.3, 157.1, 154.4, 152.9, 148.1, 145.7, 131.2, 129.4, 128.8, 128.7, 128.4, 126.4, 124.2, 123.8, 120.3, 117.9, 116.5, 116.1, 116.3 (21 aromatic carbon), 95.9 (C pyrimidine); Anal. Calcd. for $C_{22}H_{15}N_5O_5$ (%): C 61.54, H 3.52, N 16.31; Found (%): C 61.30, H 3.20, N 16.20; MS: $m/z$ 429.28 (100%, $M^+$), 279.10 (60%), 187.20 (40%), 150.10 (30%), 122.20 (50%), 95.10 (30%), 93.20 (10%), 79.20 (20%), 77.10 (10%), 45.00 (10%), 68.10 (10%), 28.10 (10%).

*2.3.4. Characterization Data of 4-(2-Hydroxy-5-((4-nitrophenyl)diazenyl)phenyl)-6-(4-hydroxy-phenyl)pyrimidin-2-ol* ***(4d)***. Brownish Powder; Yield, 63.87%; m.p., 240°C; IR (KBr) $cm^{-1}$: 1340 (Ar-$NO_2$), 1450 (N=N), 1650 (C=N), 3400 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 4.80 (s, 3H, 3Ar-OH), 6.30–6.50 (m, 4H, Ar-CH), 7.20 (d, 2H, Ar-CH), 7.50–7.90 (m, 6H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.2, 160.4, 158.4, 157.3, 155.4, 154.6, 150.2, 145.7, 128.9, 128.8, 128.3, 124.3, 124.2, 124.1, 123.2, 120.9, 120.8, 120.7, 116.6, 116.3, 116.2 (21 aromatic carbon), 95.1 (C pyrimidine); Anal. Calcd. for $C_{22}H_{15}N_5O_5$ (%): C 61.54, H 3.52, N 16.31; Found (%): C 61.50, H 3.40, N 16.30; MS: $m/z$ 429.41 (100%, $M^+$), 279.20 (70%), 187.10 (50%), 150.00 (40%), 122.10 (40%), 95.00 (20%), 93.10 (20%), 79.10 (10%), 77.00 (10%), 45.10 (10%), 68.20 (20%), 28.00 (10%).

*2.3.5. Characterization Data of 4-(2-Hydroxy-5-(phenyldiazenyl)phenyl)-6-(4-hydroxy-phenyl)pyrimidin-2-ol* ***(4e)***. Yellowish Powder; Yield, 60.49%; m.p., 170°C; IR (KBr) $cm^{-1}$: 1330 (Ar-$NO_2$), 1440 (N=N), 1650 (C=N), 3070 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 4.50 (s, 3H, 3Ar-OH), 6.60–6.80 (m, 4H, Ar-CH), 7.30 (d, 2H, Ar-CH), 7.40–7.90 (m, 7H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.6, 160.1, 158.9, 157.7, 154.8, 152.3, 145.4, 130.8, 129.7, 129.4, 128.6, 128.5, 128.1, 124.7, 123.9, 123.7, 123.4, 120.1, 116.8, 116.7, 116.2, (21 aromatic carbon), 95.6 (C pyrimidine); Anal. Calcd. for $C_{22}H_{16}N_4O_3$ (%): C 68.74, H 4.20, N 14.58; Found (%): C 68.60, H 4.10, N 14.30; MS: $m/z$ 384.32 (100%, $M^+$), 279.10 (70%), 187.10 (60%), 105.10 (40%), 95.20 (20%), 93.10 (10%), 79.00 (10%), 77.20 (10%), 45.10 (10%), 68.10 (20%), 28.10 (10%).

*2.3.6. Characterization Data of 4-(2-Hydroxy-5-(p-tolyldiazenyl)phenyl)-6-(4-nitrophenyl)-pyrimidin-2-ol* ***(5a)***. Brownish Powder; Yield, 70.26%; m.p., 165°C; IR (KBr) $cm^{-1}$: 1350 (Ar-$NO_2$), 1490 (N=N), 1600 (C=N), 2900 (Ar-$CH_3$), 3390 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 2.40 (s, 3H, Ar-$CH_3$), 5.20 (s, 2H, 2Ar-OH), 6.70 (s, 1H, Ar-CH), 6.80 (d, 2H, Ar-CH), 7.30 (d, 2H, Ar-CH), 7.50–7.70 (m, 8H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.5, 160.4, 157.3, 154.6, 149.6, 147.8, 145.7, 141.8, 140.5, 129.4, 129.2, 126.2, 126.1, 124.3, 124.2, 123.2, 123.1, 122.9, 122.8, 120.7, 116.6 (21 aromatic carbon), 95.9 (C pyrimidine), 21.2 ($CH_3$); Anal. Calcd. for $C_{23}H_{17}N_5O_4$ (%): C 64.63, H 4.01, N 16.39; Found (%): C 64.40, H 4.00, N 16.20; MS: $m/z$ 427.10 (100%, $M^+$), 308.10 (80%), 187.00 (60%), 122.10 (50%), 119.00 (40%), 95.10 (30%), 93.00 (10%), 91.10 (20%), 79.10 (10%), 77.10 (10%), 45.90 (30%), 68.00 (10%), 28.00 (20%).

*2.3.7. Characterization Data of 4-(2-Hydroxy-5-((2-nitrophenyl)diazenyl)phenyl)-6-(4-nitrophenyl)pyrimidin-2-ol* ***(5b)***. Reddish Powder; Yield, 65.18%; m.p., 214°C; IR (KBr) $cm^{-1}$: 1320 (Ar-$NO_2$), 1430 (N=N), 1630 (C=N), 3130 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.30 (s, 2H, 2Ar-OH), 6.50 (s, 1H, Ar-CH), 6.80 (d, 1H, Ar-CH), 7.70–7.90 (m, 10H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.4, 160.3, 157.5, 154.3, 147.9, 147.5, 145.7, 143.7, 141.5, 135.3 131.7, 126.5, 126.4, 124.6, 124.8, 124.7, 124.3, 123.9, 123.8, 120.6, 116.3 (21 aromatic carbon), 95.4 (C pyrimidine), Anal. Calcd. for $C_{22}H_{14}N_6O_6$ (%): C 57.65, H 3.08, N 18.33; Found (%): C 57.40, H 3.00, N 18.20; MS: $m/z$ 458.10 (100%, $M^+$), 308.20 (70%), 216.10 (40%), 222.00 (50%), 150.00 (60%), 122.00 (30%), 95.00 (20%), 93.10 (20%), 79.00 (10%), 68.20 (20%).

*2.3.8. Characterization Data of 4-(2-Hydroxy-5-((3-nitrophenyl)diazenyl)phenyl)-6-(4-nitrophenyl)pyrimidin-2-ol* ***(5c)***. Brownish Powder; Yield, 54.33%; m.p., 239°C; IR (KBr) $cm^{-1}$: 1330 (Ar-$NO_2$), 1410 (N=N), 1650 (C=N), 3030 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.20 (s, 2H, 2Ar-OH), 6.40 (s, 1H, Ar-CH), 6.90 (d, 1H, Ar-CH), 7.60–7.90 (m, 10H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.2, 160.6, 157.3, 154.6, 152.5, 148.8, 147.4, 145.6, 141.9, 131.9, 129.9, 126.7, 126.6, 126.1, 124.8, 124.7, 124.5, 123.4, 120.7, 117.4, 116.8 (21 aromatic carbon), 95.1 (C pyrimidine), Anal. Calcd. for $C_{22}H_{14}N_6O_6$ (%): C 57.65, H 3.08, N 18.33; Found (%): C 57.50, H 2.90, N 18.10; MS: $m/z$ 458.38 (100%, $M^+$), 242.10 (60%), 216.20 (50%), 122.10 (40%), 121.20 (20%), 95.10 (20%), 93.00 (10%), 79.10 (20%), 68.10 (10%).

*2.3.9. Characterization Data of 4-(2-Hydroxy-5-((4-nitrophenyl)diazenyl)phenyl)-6-(4-nitrophenyl)pyrimidin-2-ol* ***(5d)***. Brownish Powder; Yield, 61.87%; m.p., 250°C; IR (KBr) $cm^{-1}$: 1320 (Ar-$NO_2$), 1450 (N=N), 1670 (C=N), 3420 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 5.40 (s, 2H, 2Ar-OH), 6.20 (s, 1H, Ar-CH), 6.70 (d, 1H, Ar-CH), 7.50–7.80 (m, 10H, Ar-CH); $^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.1, 160.7, 155.7, 157.5, 154.6, 150.8, 147.7, 145.6, 141.8, 126.9, 126.8, 124.9, 124.8, 124.4, 124.3, 124.2, 123.5, 120.9, 120.7, 120.6, 116.9, (21 aromatic carbon), 95.7 (C pyrimidine), Anal. Calcd. for $C_{22}H_{14}N_6O_6$ (%): C 57.65, H 3.08, N 18.33; Found (%): C 57.30, H 3.10, N 18.30; MS: $m/z$ 458.46 (100%, $M^+$), 242.20 (80%), 216.10 (60%), 122.20 (50%), 121.10 (10%), 95.20 (10%), 93.20 (10%), 79.20 (10%), 77.10 (20%), 68.20 (20%).

*2.3.10. Characterization Data of 4-(2-Hydroxy-5-(phenyldiazenyl)phenyl)-6-(4-nitrophenyl)pyrimidin-2-ol* ***(5e)***. Yellowish Powder; Yield, 74.22%; m.p., 160°C; IR (KBr) $cm^{-1}$: 1310 (Ar-$NO_2$), 1420 (N=N), 1670 (C=N), 3080 (Ar-OH); $^1$H-NMR ($CDCl_3$) $\delta$: 4.90 (s, 2H, 2Ar-OH), 6.70 (s, 1H, Ar-CH), 7.10 (d, 1H, Ar-CH), 7.50–7.80 (m, 11H, Ar-CH);

Table 1: Antibacterial and anti-fungal activity of newly synthesized chalcone derivatives (**2a**–**2e**, **3a**–**3e**) and pyrimidine derivatives (**4a**–**4e**, **5a**–**5e**).

| Compound (500 $\mu$g/disk) | Average value of zone of inhibition in mm | | | | | |
|---|---|---|---|---|---|---|
| | Antimicrobial Activity | | | | | |
| | Gram Positive | | Gram Negative | | Antifungal activity | |
| | *S. aureus* | *B. subtilis* | *P. vulgaris* | *E. coli* | *C. albicans* | *A. niger* |
| **2a** | — | — | — | — | — | — |
| **2b** | 10 | 08 | 13 | 12 | 11 | 13 |
| **2c** | 11 | 06 | 16 | 14 | 12 | 16 |
| **2d** | 6 | 8 | 10 | 08 | 08 | 10 |
| **2e** | — | 4 | — | — | — | — |
| **3a** | — | — | 5 | 4 | — | — |
| **3b** | 13 | 10 | 14 | 14 | 16 | 15 |
| **3c** | 12 | 13 | 16 | 15 | 17 | 18 |
| **3d** | 8 | 14 | 12 | 10 | 12 | 13 |
| **3e** | — | 5 | — | 4 | 5 | 4 |
| **4a** | 4 | 3 | 6 | 8 | 8 | 10 |
| **4b** | 14 | 13 | 17 | 14 | 16 | 17 |
| **4c** | 15 | 08 | 19 | 18 | 18 | 20 |
| **4d** | 10 | 12 | 12 | 14 | 16 | 20 |
| **4e** | 7 | 6 | 8 | 10 | 14 | 12 |
| **5a** | 5 | 6 | 9 | 8 | 12 | 14 |
| **5b** | 29 | 18 | 24 | 26 | 22 | 25 |
| **5c** | 22 | 24 | 26 | 24 | 20 | 27 |
| **5d** | 13 | 15 | 16 | 12 | 24 | 21 |
| **5e** | 12 | 10 | 15 | 16 | 16 | 15 |
| Ciprofloxacin | 30 | 26 | 32 | 31 | — | — |
| Fluconazole | — | — | — | — | 24 | 26 |

"—" represent "inactive".

$^{13}$C-NMR (100 MHz, $CDCl_3$-$d_6$, $\delta$, ppm): 162.4, 160.9, 157.7, 154.8, 152.5, 147.6, 145.7, 141.5, 130.8, 129.8, 129.5, 126.9, 126.7, 124.4, 124.3, 124.1, 123.8, 123.5, 123.4, 120.9, 116.8 (21 aromatic carbon), 95.3 (C pyrimidine), Anal. Calcd. for $C_{22}H_{15}N_5O_4$ (%): C 63.92, H 3.66, N 16.94; Found (%): C 63.80, H 3.50, N 16.80; MS: $m/z$ 413.36 (100%, $M^+$), 216.20 (70%), 197.10 (40%), 122.10 (60%), 121.00 (30%), 95.00 (20%), 93.10 (30%), 77.20 (20%), 68.10 (10%).

*2.4. Biological Activity.* The newly synthesized compounds were examined for antibacterial and antifungal activity using well diffusion method against the panel of different gram positive and gram negative bacterial stains and fungi stains. Different bacterial stains used for the screening were *S. aureus* (gram Positive), *B. subtilis* (gram Positive), *P. vulgaris* (gram Negative), and *E. coli* (gram Negative). Antifungal activities of these compounds were also tested against *C. albicans* and *A. niger*. The stains for antibacterial and antifungal activities were obtained from Department of Microbiology, S. F. S. College, Nagpur. The stock solutions of pyrimidine derivatives or standard drug in dimethyl sulfoxide (100 $\mu$g/mL) were prepared for the study. The sterilized petri dishes and agar medium were used in the present work. The antibacterial activities of compounds were evaluated by measuring the zone of inhibition on nutrient agar plate. Muller Hinton agar was used in the anti-bacterial study whereas Sabouraud's Dextrose agar was used for the anti-fungal activity study. The composition of nutrient agar medium to culture the bacterial strains used in the present study was as follows: Peptone (10 gm), agar powder (20 gm), sodium chloride powder (10 gm), beaf extract (5 gm), and distilled water (1000 mL). The pH of the nutrient agar medium was adjusted to 7.2. The nutrient agar medium was mixed well and was autoclaved at 15 lbs pressure at 120°C for at least 15 minutes.

In the sterilized agar medium, 10 mL of one-day-old bacterial/fungal cultures were added. Bacterial or fungal culture were inoculated into nutrient broth and incubated at 37 ± 2°C on rotary shaker at 100 rpm. After 36-hour incubation, bacterial suspensions were used for further tests. This media were poured in petri dishes and allowed to set. Two wells were created using a 5 mm cork borer. In this well 0.1 mL of test sample/standards were filled. All the nutrient agar plates were incubated at 37°C for 24 hours in

anti-bacterial study and at 37°C for 48 hours in anti-fungal activity study. The plates were observed for clear zone of inhibition. Then diameters of the zone of inhibition for these compounds were measured. The biological activities were tested for at least three times for all the compounds against all microorganisms and average value has been reported here. The results of antimicrobial activity and antifungal activity of the test compounds have been collected in Table 1.

## 3. Results and Discussion

A new series of chalcones, that is, 3-(2-hydroxy-5-(aryl-diazenyl)phenyl)-1-(aryl)prop-2-en-1-one (**2a**–**2e**, **3a**–**3e**) and pyrimidines derivatives 4-(2-hydroxy-5-(aryl-diazenyl)phenyl)-6-(aryl)pyrimidin-2-ols (**4a**–**4e**, **5a**–**5e**), were synthesized as depicted in Scheme 1. In the first step, different azo-aldehydes (**1a**–**1e**) were prepared by the reaction of aromatic amines with salicylaldehyde in equimolar condition. Typical procedure of synthesis of chalcones (**2a**–**2e**, **3a**–**3e**) in the present work involves the reaction of equimolar quantities of various substituted azo-aldehydes with either 4-nitroacetophenone or *p*-acetophenone in ethanolic alkaline medium. Pyrimidine derivatives (**4a**–**4e**, **5a**–**5e**) were obtained by refluxing newly synthesized substituted chalcones and urea in ethanol in presence of aqueous NaOH solution and then cooling the reaction mixture in crushed ice. The newly synthesized compounds were characterized on the basis of their spectroscopic data ($^1$H-NMR, $^{13}$C-NMR, IR, and Mass) and elemental analysis. In elemental analysis, the percentage of the nitrogen, hydrogen, and carbon was found to be experimentally equivalent to the calculated values in all compounds. In general, compounds **1a**–**1e** have shown aldehydic C=O peak within the range of 1700-1700 $cm^{-1}$ whereas aldehydic H–C= peaks approximately within 2820 up to 2850 $cm^{-1}$. The $^1$H-NMR spectra have shown the peaks of protons present in the compounds at their appropriate $\delta$ values whereas $^{13}$C-NMR confirmed the numbers of C atoms in the newly synthesized compounds. In the LCMS of the synthesized compounds, peaks for molecular ion peak were observed at its respective molecular mass. The newly synthesized chalcones and pyrimidines were evaluated for in vitro antibacterial and antifungal activities against various gram positive, gram negative bacteria, and fungal species. The results have been collected in Table 1. Ciprofloxacin as the standard drug was tested against bacterial strains whereas Fluconazole as the standard drug was tested against fungal strains for comparison with newly synthesized compounds. The close survey of values indicates that the chalcones compound (**2a**–**2e**, **3a**–**3e**) exhibited varied range zone of inhibition depending upon the substituent on the ring structure. Most of the compounds have shown moderate to good biological activity against the bacterial and fungal strains. Compounds **5a** and **5b** have shown excellent activity against both gram positive and gram negative bacterial strains as compared to standard drug Ciprofloxacin. Compounds **5b**, **5c**, and **5d** have shown excellent activity against as compared to standard drug Fluconazole.

## 4. Conclusion

A series of chalcones, that is, 3-(2-hydroxy-5-(aryl-diazenyl)phenyl)-1-(aryl)prop-2-en-1-one and pyrimidines derivatives 4-(2-hydroxy-5-(aryl-diazenyl)phenyl)-6-(aryl) pyrimidin-2-ols, were successfully synthesized. All the newly synthesized compounds were characterized spectroscopically and using analytical techniques such as $^1$H-NMR, $^{13}$C-NMR, IR and mass, and elemental analysis. Anti-bacterial activity studies reveal that compounds **5b** and **5c** have shown the highest activity among all newly synthesized compounds as compared to standard drug, whereas compounds **5b**, **5c**, and **5d** have shown the highest antifungal activity among all newly synthesized compounds as compared to standard drug.

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