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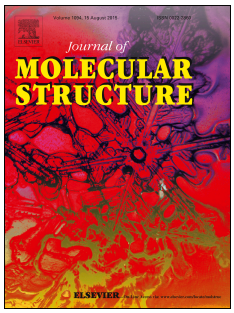

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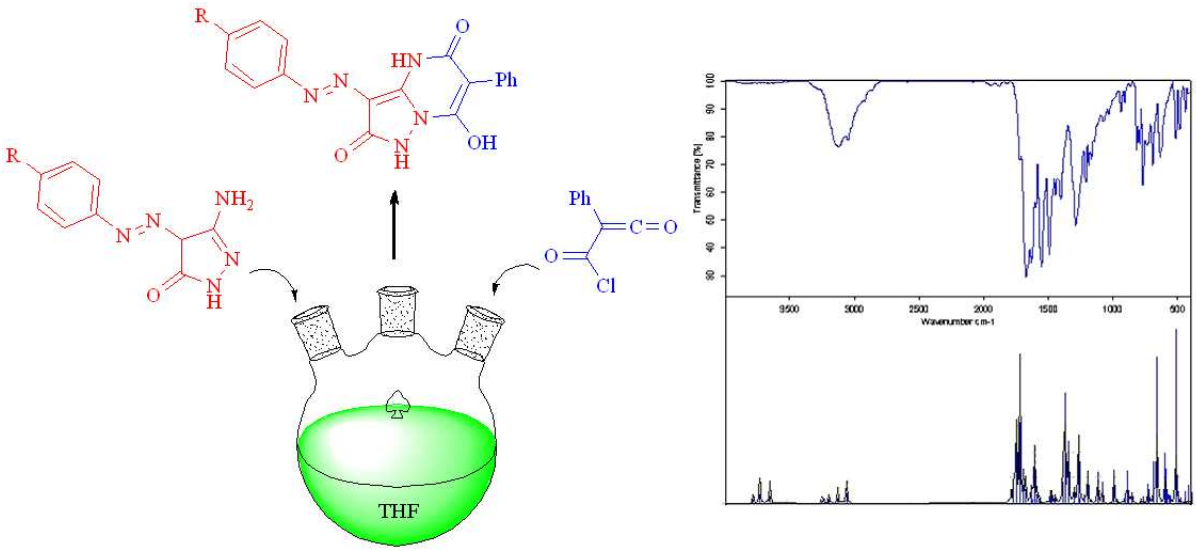

Reaction of (chloro carbonyl) phenyl ketene with 5-amino pyrazolones: synthesis, characterization and theoretical studies of 7-hydroxy-6-phenyl-3-(phenyldiazenyl)pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione derivatives

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Abstract

New 7-hydroxy-6-phenyl-3-(phenyldiazenyl)pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione derivatives were synthesized from the reaction of (chlorocarbonyl)phenyl ketene and 5-amino pyrazolones in high to excellent yields and short reaction times. Structures of the new compounds were fully characterized by their spectral data IR, ^{1}H NMR, and ^{13}C NMR and by the theoretical results. Density Functional Theory (DFT) was used to optimize the structures, compute the energies and vibrational frequencies IR and ^{1}H NMR shielding tensors of the desired products. The theoretical results excellent are compared with the experimental data.

Keywords: pyrazolo[1,5-*a*]pyrimidine; (chlorocarbonyl)phenyl ketene; Density Functional Theory; 5-amino pyrazolones

1. Introduction

(Chlorocarbonyl)ketenes are versatile bifunctional reagents for the synthesis of numerous heterocyclic compounds. The reactions of bisnucleophiles with these ketenes leads to cyclic compounds, which have been reported in several papers.[1, 2] (Chlorocarbonyl)phenyl ketene has been used mainly for the synthesis of five and six membered heterocycles functionalized with oxo and hydroxyl groups in 1,3-positions. The reactions of binucleophiles with this ketene lead to the synthesis of heterocyclic compounds.[3, 4] Structures containing such units often play

an essential role due to their biological activity, predominantly in cancer and virus research.[5, 6] Pyrazole derivatives are one of the important class of heterocyclic compounds. This compounds can be used as the intermediate in organic synthesis and possess a range of interesting biological and antimicrobial properties.[7-10] a massive search for new anticancer agents has been fueled by various academics and industries to unveil the new molecular targets and mechanisms based on the lead candidates of different classes of compounds. A large number of pyrazolo[1,5-*a*]pyrimidine derivatives are reported to exhibit a broad spectrum of biological activities such as antitumor, [11, 12] anxiolytic [13]and antimicrobial. [14] But pyrazolo[1,5-*a*]pyrimidine derivatives are widely used as inhibitors of cyclin-dependent kinases (CDKs), that are involved in mediating the transmission of mitogenic signals and numerous other cellular events [15-18] including cell proliferation, migration, differentiation, metabolism and immune response. Some their fused pyrimidine derivatives are used as dyes.[19-23] Due to the biological activities of pyrazolo[1,5-*a*]pyrimidine derivatives new ways for the synthesis of these compounds have been of interest. So in order to access analogs of pyrimidine fused to pyrazole rings, the reaction of (chlorocarbonyl)phenyl ketene with 5-aminopyrazole-3-one derivatives was investigated in this paper.

2. Experimental

Phenyl malonic acid, aniline derivatives, ethyl cyanoacetate and hydrazine hydrate were obtained from Merck Chemical Co. and were used without further purification. (Chlorocarbonyl)phenyl ketenes **2** were prepared according to the literature procedure.[24] The 5-amino-1,2-dihydro-3*H*-pyrazol-3-one derivatives **1a-e** were known and prepared according to the general procedure reported in the literature.[25] THF was dried over sodium and distilled prior to use. Melting points were measured on an Electrothermal-9100 apparatus and are uncorrected. IR spectra were recorded on a Brucker FT-IR Tensor 27 infrared spectrophotometer. The proton and carbon NMR spectra were recorded with Bruker DRX-400 spectrometer (400 and 100 MHz, respectively) in DMSO-*d6*, internal standard TMS. Elemental analyses were carried out using a Heraeus CHN-O-Rapid analyzer.

2.1. Theoretical method:

All geometry optimizations and quantum chemical calculations were performed through Gaussian 09 software[26] using density functional theory (DFT) with B3LYP/6-311G quantum level. The B3LYP(Becke's hybrid 3-parameter functional with Lee-Yang-Parr correlation)functional was selected for the calculations. B3LYP has been introduced as one of the most accurate methods for energy calculation. Structure parameters have been calculated by optimizing type job in Gaussian package. For Thermodynamic properties (ΔG) and IR spectrum, frequency type job at Gaussian package has been done and NMR data have obtained by NMR type job with the same method.

*2.2. Typical procedure for the preparation of compounds (**3a-c**)*

To a stirred solution of corresponding 5-amino-1,2-dihydro-3*H*-pyrazol-3-one derivatives **1** (2 mmol) in 20 mL boiling dry THF was added a mixture of (chlorocarbonyl)phenyl ketene **2** (2 mmol) in 5ml dry THF dropwise over 2 min. The product was formed after 5 minutes as a colored precipitate. Stirring was then continued for an additional 15 minutes. The solid product was collected and recrystallized from dry ethyl acetate and hexane (2:3).

*2.3. 7-hydroxy-6-phenyl-3-(phenyldiazenyl)pyrazolo[1,5-a]pyrimidine-2,5(1H,4H)-dione **(3a)***

The 0.29 g (85%) red crystals, IR (KBr): 3200-2900 (NH, OH), 1657 (C=O), 1625, 1550, 1481 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-*d6*): δ (ppm): 10.01 (1H, s, NH), 9.32 (1H, s, OH), 8.17-6.97(10H, m, arom, NH)[8.16 (2H, d, $^{3}J_{H-H}$=8Hz), 8.87 (2H, d, $^{3}J_{H-H}$=8Hz), 7.46-7.43 (3H, m), 7.29-7.23 (3H, m), 7.98 (1H, t, $^{3}J_{H-H}$=8Hz)]. ^{13}C NMR (100 MHz, DMSO-*d6*): δ (ppm): 160.04, 159.80, 151.36, 145.94, 143.69, 134.35, 129.22, 127.51, 126.88, 123.31, 123.01, 117.76, 84.32, 67.93. Anal. Calcd for. $C_{17}H_{13}NO_3S$: C, 62.24; H, 3.77; N, 20.16; O, 13.82%. Found: C, 62.02; H. 3.59; N; 20.01 %.

*2.4. 7-hydroxy-3-((4-methoxyphenyl)diazenyl)-6-phenylpyrazolo[1,5-a]pyrimidine-2,5(1H,4H)-dione (**3b**)*

The 034 g (90%) dark violet crystals, IR (KBr): 3200-2900 (NH, OH), 1668 (C=O), 1628, 1554, 1491 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-*d6*): δ (ppm): 9.79 (1H, s, NH), 9.09 (1H, s, OH), 8.16-6.95(10H, m, arom, NH) [8.16 (2H, d, $^{3}J_{H-H}$=4Hz), 7.83 (2H, d, $^{3}J_{H-H}$=8Hz), 7.73-7.21 (3H, m), 7.01 (2H, d, $^{3}J_{H-H}$=8Hz), 6.97 (1H, t, $^{3}J_{H-H}$=8Hz)], 3.38 (3H, s, methoxy). ^{13}C NMR (100

MHz, DMSO-*d6*): δ (ppm): 160.58, 160.48, 158.78, 150.49, 146.20, 134.59, 129.26, 126.48, 123.32, 119.88, 118.51, 114.70, 84.26, 66.30, 55.46. Anal. Calcd for. $C_{19}H_{15}N_5O_4$: C, 60.48; H, 4.01; N, 18.56; O, 16.96 %. Found: C, 60.31; H. 4.16; N; 18.39%.

*2.5. 3-((4-chlorophenyl)diazenyl)-7-hydroxy-6-phenylpyrazolo[1,5-a]pyrimidine-2,5(1H,4H)-dione (**3c**)*

The 0.34 g (90%) dark violet crystals, IR (KBr): 3200-2900 (NH, OH), 1672 (C=O), 1593, 1549, 1484 cm^{-1}. ^1H NMR (400 MHz, DMSO-*d6*): δ (ppm): 9.77 (1H, s, NH), 9.06 (1H, s, OH), 8.15-6.96(10H, m, arom, NH) [8.14 (2H, d, $^3J_{H-H}$=8Hz), 7,85 (2H, s), 7.48 (2H, d, $^3J_{H-H}$=8Hz), 7.33-7.22 (2H, m), 6.96 (2H, s)]. ^{13}C NMR (100 MHz, DMSO-*d6*): δ (ppm): 161.13, 160.35, 151.36, 145.54, 134.50, 131.10, 130.39, 129.54, 127.48, 123.26, 120.23, 116.85, 84.27, 67.64. Anal. Calcd for. $C_{18}H_{12}ClN_5O_3$: C, 56.63; H, 3.17; Cl, 9.29; N, 18.34; O, 12.57%. Found: C, 56.51; H. 3.02; N; 18.25%.

*2.6. 7-hydroxy-6-phenyl-3-(p-tolyldiazenyl)pyrazolo[1,5-a]pyrimidine-2,5(1H,4H)-dione (**3d**)*

The 0.31 g (88%) violet crystals crystals, IR (KBr): 3200-2900 (NH, OH), 1672 (C=O), 1628, 1552, 1492 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ (ppm): 9.96 (1H, s, NH), 9.25 (1H, s, OH), 8.17-6.97(10H, m, arom, NH) [7.16 (2H, d, $^3J_{H-H}$=8Hz), 7.76 (2H, d, $^3J_{H-H}$=8Hz), 7.24 (4H, t, $^3J_{H-H}$=8Hz), 6.98 (2H, t, $^3J_{H-H}$=4Hz) , 2.49 (3H, s, methyl). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm): 160.08, 159.85, 151.31, 146.12, 141.10, 136.81, 134.47, 129.80, 127.61, 123.40, 123.10, 117.77, 84.40, 64.85, 20.62. Anal. Calcd for. $C_{19}H_{15}N_5O_3$: C, 63.15; H, 4.18; N, 19.38; O, 13.28%. Found: C, 63.01; H. 4.10; N; 19.29%

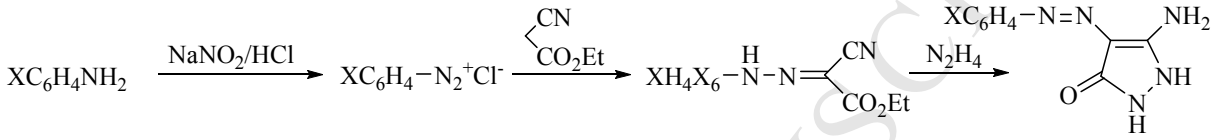
*2.7. 4-((7-hydroxy-2,5-dioxo-6-phenyl-1,2,4,5-tetrahydropyrazolo[1,5-a]pyrimidin-3-yl)diazenyl) benzenesulfonamide (**3e**)*

The 0.35 (82%) dark violet crystals, IR (KBr): 3639, 3547 (NH_2), 3300-2800 (NH, OH), 1688 (C=O), 1630, 1596, 1486 cm^{-1}. ^1H NMR (400 MHz, DMSO-*d6*): δ (ppm): 10.08 (1H, s, NH), 9.32 (1H, s, OH), 8.16-6.96 (12H, m, arom, NH, NH_2) [8.16 (2H, d, $^3J_{H-H}$=4Hz), 8.00 (2H, d, $^3J_{H-H}$=4Hz), 8.87 (2H, d, $^3J_{H-H}$=4Hz), 7.41 (2H, s, NH_2), 7.29-7.22 (3H, m), 6.98 (1H, t, $^3J_{H-H}$=8Hz). ^{13}C NMR (100 MHz, DMSO-*d6*): δ (ppm): 160.52, 160.43, 153.78, 145.48, 141.66, 134.48, 130.52, 129.82, 128.29, 127.60, 123.42, 118.41, 84.48, 67.02. Anal. Calcd for.

$C_{18}H_{14}N_6O_5S$: C, 50.70; H, 3.31; N, 19.71; O, 18.76; S, 7.52%. Found: C, 50.54; H. 3.16; N; 19.88%.

3. Result and Discussion

Synthesis of 5-aminopyrazoles **3** is readily available by diazotiazation of aniline derivatives **1a-e** followed by coupling with ethyl cyanoacetate, affording the corresponding hydrazones **2a-e**. Reaction of compounds **2** with hydrazine hydrate undergoes corresponding 5-aminopyrazoles **3a-e** [25] in good yields, scheme 1.



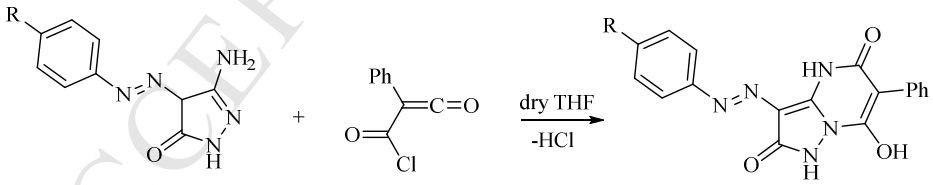
1a: X=H
1b: X=OCH_3
1c: X=Cl
1d: X=CH_3
1e: X=SO_2NH_2

2a-e

3a-e

Scheme 1. Synthesis of 5-aminopyrazoles **3a-e** from aniline derivatives.

In connection with our ongoing work on the development of new synthetic routes to heterocyclic compounds by condensation of (chlorocarbonyl)ketenes **4** with 1,3-dinucleophiles,[1, 3, 4] we report herein the reaction of (chlorocarbonyl)ketenes **4** with 5-aminopyrazoles **3** for the synthesis of 7-hydroxy-6-phenyl-3-(phenyldiazenyl)pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione derivatives **5a-e**, scheme 2.



3a: R=H
3b: R=OCH_3
3c: R=Cl
3d: R=CH_3
3e: R=SO_2NH_2

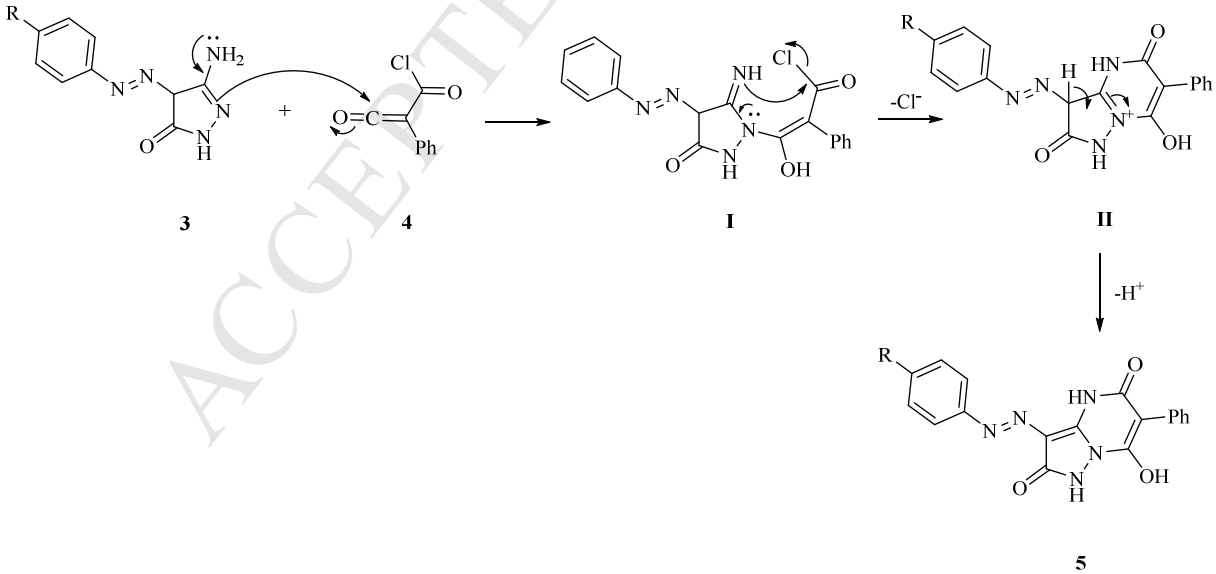
4

5a-e

Scheme 2. Synthesis of 7-hydroxy-6-phenyl-3-(aryldiazenyl)pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione derivatives **5** from the reaction of (chlorocarbonyl)phenyl ketene **4** and 5-amino-4-(aryldiazenyl)-1,2-dihydro-3*H*-pyrazol-3-one derivatives **3**

A literature survey indicates that only a few references are available on the synthesis and chemistry of pyrazolo[1,5-a]pyrimidine derivatives[27]. In this method, 7-hydroxy-6-phenyl-3-(aryldiazenyl)pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione derivatives **5a-e** have been produced from the one-pot cyclocondensation of (chlorocarbonyl)phenyl ketene **4** and 5-amino-4-(aryldiazenyl)-1,2-dihydro-3*H*-pyrazol-3-one derivatives **3**. The simplicity and efficient one-pot procedure is one aspect of particular interest, in comparison to the other multi-step methods. On the other hand, readily available starting materials such as (chlorocarbonyl)phenyl ketene, shorten experimental time, and high yield of the final products are the other advantages of this method. When (chlorocarbonyl)phenyl ketenes **4** were added to a solution of the 5-aminopyrazolone derivatives **3** at boiling solvent, precipitate of the product was formed immediately.

A plausible mechanism for the formation of the product **5** is outlined in scheme 3. 5-aminopyrazolones have three sites of electron rich positions, at the nitrogen atoms. Nucleophilic reactions on these compounds can take place on either of the exocyclic or the endocyclic nitrogen atoms. Here, the endocyclic nitrogen atom will attack the central carbon atom of the ketene group, which possesses a low-lying LUMO. Subsequent cyclization affords compound II. H^+ elimination gives compound **5**.



Scheme 3. Proposed mechanism for the formation of 7-hydroxy-6-phenyl-3-(aryldiazenyl) pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione **5**

The structures of compounds **5a**–**e** were determined on the basis of their elemental analyses, ^{1}H- and ^{13}C-NMR and IR spectral data. Only one product was obtained in each case. The ^{1}H NMR spectrum of **5a-e** indicated two signal at low field (10-9 ppm) attributed to the OH and NH groups.

In the present work, DFT/B3LYP approach was employed by using Gaussian 09 software. At first, the different possible conformers was considered and optimized for the synthesized products and then stable conformer was employed to calculate the vibrational frequencies and NMR spectrum to confirm that the reported structures are true minima. Obtained positive first frequency for each compound in frequency type job output data confirmed accurately true minima .[28] To predict the spectroscopic properties of the most stable structure, DFT approach was used in the Gaussian software. The computed wavenumbers were scaled with the scaling factor in order to figure out how the predicted vibrational spectra are in agreement with experimental ones. Vibrational analysis of molecule was computed by using B3LYP level with basis set 6-311 G. The detected and predicted vibrational spectrum with results of fundamental vibrational modes were given in table 1 and figure 1.

As shown in table 1, the experimental N-H and O-H stretching frequencies appeared in the range of 3300-2800 cm^{-1} for compound **5a-e**, the theoretically predicted IR for N-H and O-H stretching frequencies also were observed in the same range ~ 3199-2902 cm^{-1} by B3LYP/6-311 G. The frequencies characteristics of the C=O stretching modes were observed in the range of 1690-1650 cm^{-1} in the experimental part which is in good correlation with B3LYP/6-311 G studies, 1690-1650 cm^{-1}. For example, in the case of compound **5d**, the experimental C=O stretching frequencies appeared in 1672 cm^{-1} and the theoretically C=O stretching frequencies was appeared in 1669 cm^{-1} (figure 1). The strongly intense peaks from B3LYP/6-311+G(d,p) agree well to the intensities obtained experimentally. In this calculations, chemical shifts value were predicted by ‘‘Gauge-Independent Atomic Orbital’’ (GIAO).

Compound	Experimental IR(cm^{-1})	Theoretical IR(cm^{-1}) B3LYP/6-311G
5a	(NH,OH) 3200-2900,(C=O) 1657, 1625, 1481, 1550	(NH,OH) 3209-2902, (C=O) 1651, 1660, 1624, 1633, 1543, 1552, 1480, 1489
5b	(NH,OH) 3200-2900, (C=O) 1668, 1628, 1554, 1491	(NH,OH) 3199-2893, (C=O) 1669, 1624, 1633, 1552, 1489,1498
5c	(NH,OH)3200-2900, (C=O) 1672, 1593, 1549, 1484	(NH,OH) 3208-2902, (C=O) 1670, 1679, 1588, 1597, 1543, 1480, 1489
5d	(NH,OH) 3200-2900, (C=O) 1672, 1628, 1552, 1492	(NH,OH) 3207-2902, (C=O) 1669,1678, 1624, 1633, 1552, 1561, 1489, 1498
5e	(NH_2) 3639, 3547, (NH, OH) 3300-2800, (C=O) 1688, 1630, 1596, 1486	(NH,OH) 3325-2803, (C=O) 1687, 1624, 1633, 1642, 1588, 1597, 1480,1489

Table 1
Calculated IR frequency of synthesized compound by B3LYP/6-311G

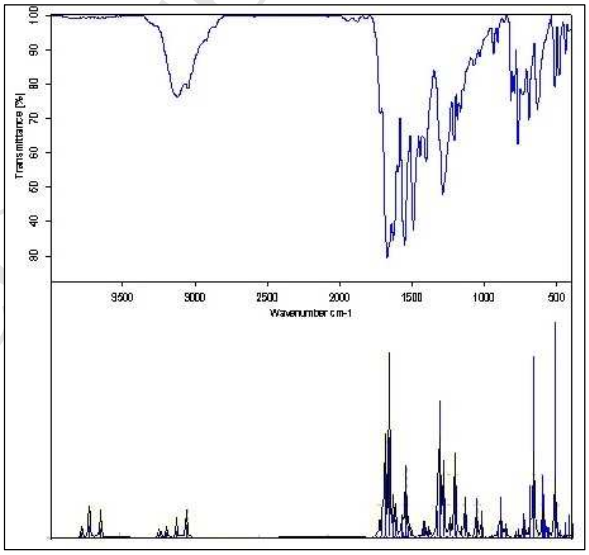


Figure 1. The calculated and the experimental IR spectra of compound **5d**

The Nuclear Magnetic Resonance spectra of the ground state geometry of molecule have been obtained by DFT/GIAO method. The GIAO method is one of the most common methods for calculating isotropic nuclear magnetic. The predicted and measured NMR values were listed in table 2.

The investigated compounds contain C=O and C=C-OH group, the oxygen atom causes an increase in the chemical shift of the carbon atom band. This is evidence for a decrease in the electron density around this atom. So, C-2, C-5, and C-7 appeared around 160-150 ppm in experimental CNMR data. The theoretical CNMR data for C-2, C-5 and C-7 also appeared around 160-150 ppm. The aromatic carbon atoms both for experimental and theoretical studies appeared in 150-100 area. Because of resonance effect, the electron densities around the C-3 and C-6 atom are higher than for other carbon double bonds, affording the lower chemical shift values for these atoms, 84 ppm for C-3 and 64-68 ppm for C-6 in experimental data. The experimental reaction was done in the solution but the theoretical method has been done in the gas phase and caused to small differences between the calculated and experimentally obtained chemical shift values in the last. Experimental NMR spectra of molecules are in excellent agreement with theoretical ones.

Table2

NMR calculated chemical shift by B3LYP/6-311G

Experimental NMR(ppm)					Theoretical NMR(ppm) B3LYP/6-311G				
^{13}C NMR					^{13}C NMR				
5a	**5b**	**5c**	**5d**	**5e**	**5a**	**5b**	**5c**	**5d**	**5e**
160.04	160.58	161.13	160.08	160.52	159.71	159.06	159.51	159.83	159.00
159.80	160.48	160.35	159.85	160.43	154.94	157.75	152.63	153.00	156.16
151.36	158.78	151.36	151.31	153.78	149.63	149.75	149.28	149.69	155.05
145.94	150.49	145.54	146.12	145.48	145.92	149.24	146.56	145.66	148.70
143.69	146.20	134.50	141.10	141.66	130.44	140.89	146.12	136.29	147.12
134.35	134.59	131.10	136.81	134.48	129.65	132.99	130.44	130.45	130.50
129.22	129.26	130.39	134.47	130.52	128.24	129.31	130.05	129.96	127.93
127.51	126.48	129.54	129.80	129.82	127.96	128.17	129.69	128.73	126.36
126.88	123.32	127.48	127.61	128.29	126.29	127.62	127.68	128.15	125.68
123.31	119.88	123.26	123.40	127.60	125.97	123.34	126.08	126.90	122.12
123.01	118.51	120.23	123.10	123.42	124.19	118.31	125.51	125.90	120.93
117.76	114.70	116.85	117.77	118.41	115.81	116.19	115.83	115.76	115.94

84.32	84.26	84.27	84.40	84.48	110.77	104.55	110.85	110.29	108.90
67.93	66.30	67.64	64.85	67.02	100.40	96.46	101.71	100.34	103.17
	55.46		20.62			50.13		15.37	

The optimized geometries of the desired products are depicted in figure 2.

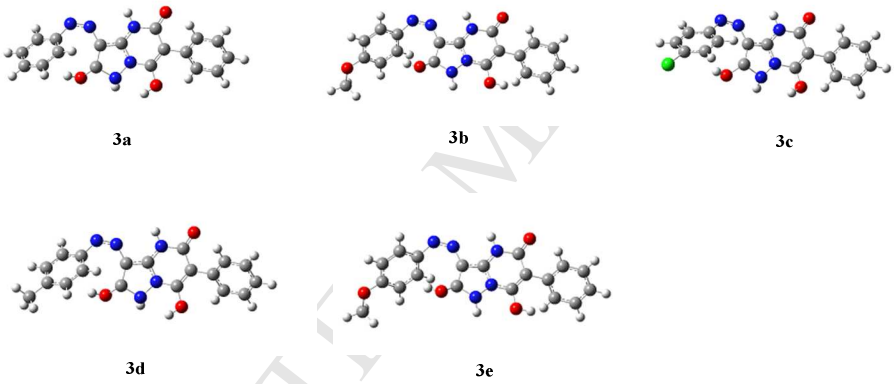


Figure 2. The optimized geometries of the compounds **5a-e**

Table 3 indicated Gibbs free energy for each compound at 298K. According to these data of this table, Fig 2 was shown the activity energy surface of doing the reaction .Energy surface of the product is higher than the reactant energy surface at room temperature. This happen obtained the reaction will be done by external energy. Therefore for the experimental process must use boiling point of THF used for synthesis reaction.

Table 3

Gibbs free energy of all compound calculated by B3LYP/6-311G at 298K in gas phase

Comp	**4**	**3a**	**3b**	**3c**	**3d**	**3e**	**5a**	**5b**	**5c**	**5d**	**5e**	**THF**	**HCl**

ΔG°_{f} (j)×10^{4}	-2.51	-1.83	-6.70	-4.86	-6.53	-1.04	-3.13	-3.43	-4.34	-6.67	-4.72	-6.10	-1.21

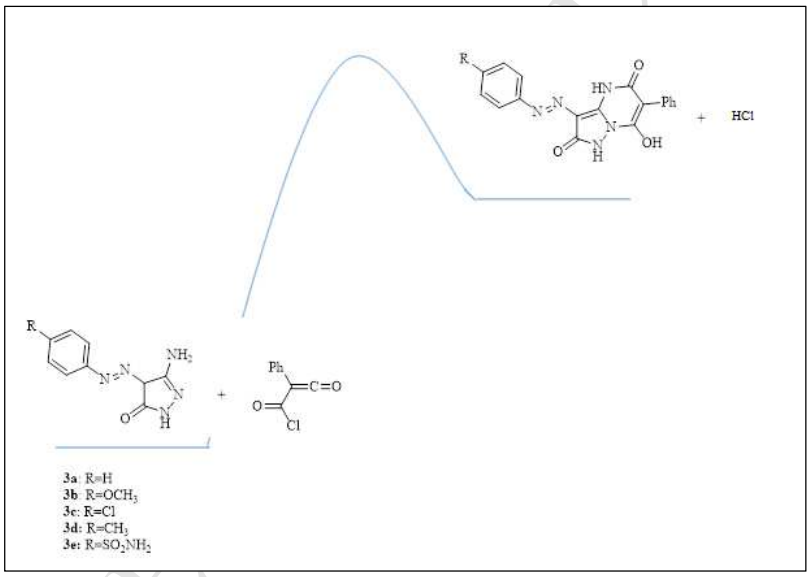


Figure 3. Activity energy surface of reactant and product in THF

4. Conclusion

In conclusion, we have presented the condensation of (chlorocarbonyl)phenyl ketene **4** with 1,2-bisnucleophilic 5-amino pyrazolone compounds **3**, affording a convenient and rapid synthesis of pharmacologically interesting 7-hydroxy-6-phenyl-3-(phenyldiazenyl)pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione derivatives **5** in excellent yields. Also, no cumbersome apparatus is needed and the desired product precipitated from the reaction mixtures and their purification is straightforward. Furthermore, Calculated Gibbs free energy accordance with experimental

process showed this reaction can be done at the boiling point of THF. Additionally, Vibration frequencies recognized the experimental products of this reaction with different substitutes can be produced and has the best accordance with empirical spectrum. NMR data also showed the products in the experimental method are correct products of this reaction. Calculated parameters predicted that this reaction theoretically suitable for experimental synthesis.

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Highlights

- Highly efficient synthesis of pharmacologically interesting 7-hydroxy-6-phenyl-3-(phenyldiazenyl)pyrazolo[1,5-*a*]pyrimidine-2,5(1*H*,4*H*)-dione derivatives
- Easy product separation and purification.
- Excellent yields and short reaction time.
- Excellent agreement of experimental results with theoretical ones.