SYNTHESIS & SPECTOSCOPIC STUDIES OF SOME NEW 2-AMINO-6-ALKYL (PERFLUOROALKYL) -4-ARYLPYRIMIDINES

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ABSTRACT

The reaction of guanidine carbonate & fluorinated 1,3-diketones [**1]** in alcoholic media have been investigated. Six new 2-amino-4-(4`-Fluorophenyl)-6-alkyl(perfluoroalkyl) trisubstituted pyrimidines have been prepared from the same diketones and guanidine carbonate in the presence of Hydrochloric acid using absolute alcohol as a solvent, viz.;

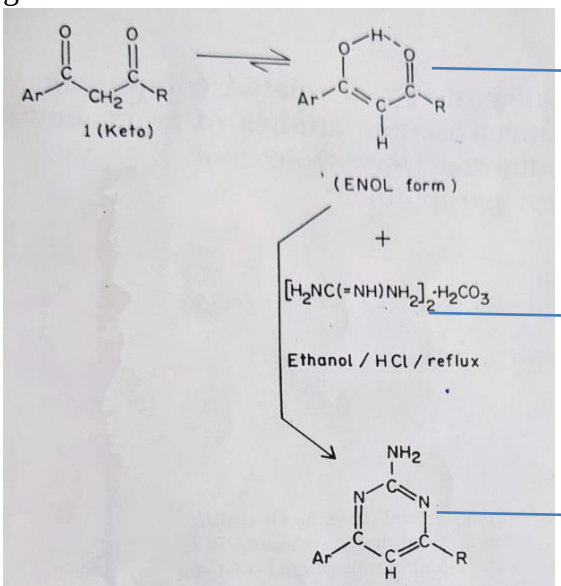
- ☒ 2-amino-4(4`-fluorophenyl)-6-methyl pyrimidine
- ☒ 2-amino-4(4`-fluorophenyl)-6-trifluoromethyl pyrimidine
- ☒ 2-amino-6-ethyl-4(4`-fluorophenyl) pyrimidine
- ☒ 2-amino-6-pentafluoroethyl-4-(4`-fluorophenyl) pyrimidine
- ☒ 2-amino-4-(4`-fluorophenyl)-6-n-propylpyrimidine
- ☒ 2-amino-6-(heptafluoropropyl)-4-(4`-fluorophenyl) pyrimidine

All new fluorinated pyrimidines have been characterized by elemental and spectral studies.

INTRODUCTION

The use of 1,3-diketones and related compounds is well recognized. Pyrimidine derivatives are well known for various biological activities; e.g., hypotensive [1], hypoglycimic [2], cytostatic [3], psychotropic [4] and as coronary vasodilators [5].

In continuation to our previous study [6], we synthesised and characterisation of new fluorinated pyrimidines using guanidine carbonate.



3a-f	Ar=4-F-C_6H_4
3a;	R=CH_3
3b;	R=CF_3
3c;	R=C_2H_5
3d;	R=C_2F_5
3e;	R=n-C_3H_7
3f;	R=n-C_3F_7

RESULT & DISCUSSION

The IR spectra of the substituted fluorinated pyrimidines **[3]** showed very strong absorption band at the reason 1180-1010 cm^{-1} due to C--F stretching vibrations also C--N was found in the region 1240-1220 cm^{-1} while C--N stretching vibrations were observed in the region 1680-1470 cm^{-1}.

In the ^{1}HNMR spectra, the methine —CH resonance signal was observed for compound **[3]** in the region δ 6.5-7.4 ppm, methyl (--CH_3) while methylene (--CH_2) signals were noted in the region δ 1.0-1.5 ppm respectively. Ar—H protons were observed in the region δ 6.5-8.5 ppm. In addition to these, 6-alkyl (perfluoroalkyl)-2-amino-5-arylpyrimidines (3) showed amino, --NH_2 proton signal at δ 4.0 ppm as confirmed by deuterium exchange studies. The structure was further confirmed by mass spectral analysis, 3d $[M]^+$ at *m/z* 307.

Table 1:

Analytical & characteristic data of 2-amino-6-alkyl/perfluoroalkyl-4-arylpyridines

				C(%)		H(%)		N(%)		F(%)	
Compound No.	Moelcular Formula	M.P. (°C)	Yield (%)	Calc.	Found	Calc.	Found	Calc.	Found	Calc.	Found
3a	$C_{11}H_{10}FN_3$	153	75	65.02	65	4.92	4,92	20.69	20.68	9.35	9.3
3b	$C_{11}H_7F_4N_3$	158	78	51.36	51.36	2.72	2.71	16.34	16.35	29.57	29.5
3c	$C_{12}H_{12}FN_3$	148	80	66.36	66.35	5.52	5.51	19.35	19.35	8.75	8.74
3d	$C_{12}H_7F_6N_3$	168	82	46.9	46.89	2.28	2.27	13.68	13.65	37.13	37.1
3e	$C_{13}H_{14}FN_3$	172	76	67.53	67.52	6.06	6.05	18.18	18.17	8.22	8.2
3f	$C_{13}H_7F_8N_3$	182	73	43.69	43.68	1.96	1.95	11.76	11.74	42.58	42.56

Table 2: Spectroscopic data for fluorinated pyrimidines

Compound No.	IR (cm^{-1})			^{1}H NMR δ (ppm)			Mass Spectrum $[M]^+$
	C=N	C--N	C—F	R	=CH	Ar	
3a	1600	1235	1175	1.3 (s)	7.3 (s)	6.5-8.5 (m)	
3b	1610	1220	1160	-	7.45 (s)	6.5-8.5 (m)	
3c	1590	1238	1130	1.0 (t); 1.4 (q)	7.2 (s)	6.5-8.5 (m)	
3d	1510	1230	1070	-	7.1 (s)	6.5-8.5 (m)	307
3e	1575	1240	1060	1.05 (t); 1.20 (m); 1.45 (m)	7.0 (s)	6.5-8.5 (m)	
3f	1560	1236	1010	-	7.25 (s)	6.5-8.5 (m)	

EXPERMIMENTAL

IR Spectra were recoded on a Perkin-Elmer 337 spectrometer using Nujol mulls while ^{1}HNMR spectra were measured by means of a Perkin-Elmer RB-12 spectrometer in $CDCl_3$ solution with TMS as the internal standard. The purity of all the compounds were checked by TLC on silica gel plates.

Synthesis of fluorinated 1,3-diketones

These were prepared by Claisen condensation of the fluorinated acetophenones with the appropriate esters in the presence of sodamine [7].

Synthesis of 2,4,6-trisubstitutes pyrimidines

These were prepared by refluxing a mixture of fluorinated 1,3-diketones with guanidine carbonate for 10-14 h in absolute ethanol containing a few drops of hydrochloric acid. Excess ethanol was then distilled off and the residue poured into ice cold water. All these compounds were recrystallized from ethanol until they gave single spots on TLC analysis. All are recoded along with their analytical data in Table 1 and Table 2.

REFERENCES

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