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Synthesis and Biological Activity of N-[N'-(4,5,6-Trisubstitued pyrimidin-2-yl)acetylureido] Benzoic Sulfimide Derivatives

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Abstract: Fourteen N'- (4,5,6-Trisubstitued pyrimidin-2-yl) -2-chloroacetylureas and fourteen N-[N'- (4,5,6-trisubstitued pyrimidin-2-yl) acetylureido] benzoic sulfimide derivatives were synthesized. Among them twenty-seven are new compounds and their structures have been confirmed by ^{1}HNMR, IR, MS and elemental analysis. The preliminary biological tests showed that some of the target compounds have excellent inhibitory activities against barnyard grass and rape, and the others have a good regulating activity for plant growth.

Keywords: Benzoic sulfimide, 2-amino-pyrimidine, biological activity, synthesis.

In the molecular design of pesticides "Substructure Link Way" plays an important role in inventing new kind of lead compounds. We have found that benzisothiazole is the bioisosterism of sulfonylurea herbicides (such as DPX-T6376)[1]. It has been reported that acyl urea derivatives with multisubstituted pyrimidine ring had potent biological activity[2]. In order to search for new kind of medicines with excellent efficiency, lower poison and less side-effect, we devised and synthesized fourteen α-chloroacetylureas containing 4,5,6-trisubstituted pyrimidin ring **5a~n** and used "substructure link way" to obtain fourteen N-[N'-(4,5,6-trisubstitued pyrimidin-2-yl)acetylureido] benzoic sulfimide derivatives **6a~n**. Among them twenty-seven are new compounds and their structures have been confirmed by ^{1}HNMR, IR, MS and elemental analysis. The preliminary biological tests showed that most of the target compounds **5** have excellent inhibitory activities against barnyard grass and rape, and some have obviously selective activity and are safe against barnyard grass. The target compounds **6** showed good promoter action for plant growth .The property of substituting groups on pyrimidine ring has a great effect on the biological activity of the compounds **5a~n** and **6a~n**.

The title compounds were prepared by the method shown is **scheme 1**.

Scheme 1

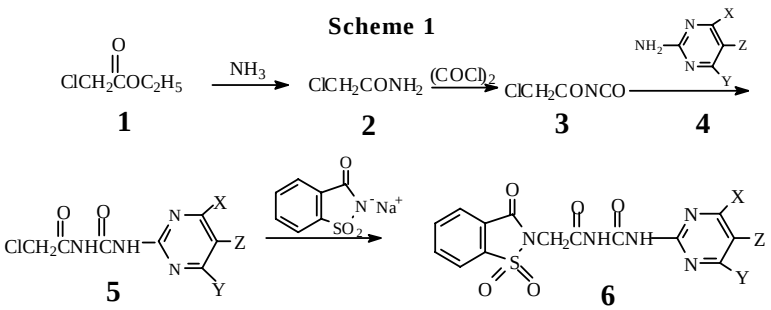

Table 1. Compounds **5a** ~ **n** and **6a** ~ **n**

5/6	a	b	c	d	e	f	g	h	i	J	k	l	m	n
X	OH	OH	OH	OH	OH	OH	Cl	Cl	Cl	Cl	Cl	Cl	CH_3	CH_3
Y	CH_3	CH_3	C_2H_5	$C_3H_7^n$	$C_4H_9^n$	$PhCH_2$	CH_3	CH_3	C_2H_5	$C_3H_7^n$	$C_4H_9^n$	$PhCH_2$	CH_3	C_2H_5
Z	CH_3	C_2H_5	CH_3	CH_3	CH_3	CH_3	CH_3	C_2H_5	CH_3	CH_3	CH_3	CH_3	CH_3	CH_3

Compounds **2, 3** and **4** were prepared according to the literature[3,4,5].

General procedure for preparation of compounds **5a~n** and **6a~n**: A solution of equimolar quantity of α-chloroacetyl isocyanate **3** and 2-amino-4,5,6-trisubstituted pyrimidine **4** in CH_3CN, $(CH_2Cl)_2$ or $C_6H_5CH_3$ is stirred at room temperature for 3 to 24 hrs. The resulting deposit was collected by filtration wash with CH_3CN, and recrystallized from CH_3CN to yield compounds **5a~n** with 78~92% yields. A solution of equimolar quantity of sodium saccharin and α-chloroacetylurea **5a~n** in DMF was heated at 120°C with stirring for 2 hrs, then all stirred at room temperature for 16 hrs, poured into ice water or trichloromethane. The resulting precipitate was collected and recrystallized from methanol to give **6a~n** with 72~84% yield.

Table 2. The inhibition percentage of some compounds (**5, 6**) to barnyard grass and rape*

Compd	Barnyard grass				Rape			
	Stalk		Root		Stalk		Root	
	10ppm	100ppm	10ppm	100ppm	10ppm	100ppm	10ppm	100ppm
5e	-0.56	58.18	26.67	84.85	3.23	100	-24.49	100
5f	-16.98	72.72	6.67	96.97	6.45	100	-26.53	100
5g	-1.89	69.09	30.00	93.94	-0.97	-100	-18.37	100
5j	-18.87	10.91	-13.33	12.12	12.90	0.36	-40.82	-52.27
5l	-33.96	-9.09	-16.67	3.03	9.68	10.71	-53.06	-43.18
6a	-22.64	16.36	-50.00	9.09	16.13	17.86	-44.90	-65.91
6l	30.19	9.09	23.33	21.21	16.13	14.29	-34.69	-65.91
DPX-63 76	-4.00	-18.50	88.50	93.33	41.89	56.46	74.60	86.96

*Negative inhibition percentage shows promotive action for plant growth

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