Original Article

Quantitative Structure-Activity Relationships of Herbicidal *N*-Alkyl-*N*-(4-substituted benzyl)-4-chloro-2-pentenamides against *Echinochloa oryzicola*¹

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The herbicidal activity of *N*-alkyl-*N*-(4-substituted benzyl)-4-chloro-2-pentenamides against a barnyard grass species, *Echinochloa oryzicola*, was evaluated, and the potency variations were quantitatively analyzed using physicochemical parameters for the *N*-alkyl and the benzyl-benzene ring substituents in the amide moiety. The results indicated that the herbicidal potency was parabolically related with the total hydrophobicity of the amide moiety. The electron-withdrawing property of the benzene-ring substituents as well as their hydrogen-bonding accepting ability was significant in potentiating the herbicidal activity.

Key words: *N*-alkyl-*N*-(4-substituted benzyl)-4-chloro-2-pentenoic acids, *Echinochloa oryzicola*, herbicidal activity, QSAR, hydrophobicity, electron-withdrawing property, hydrogen-accepting ability.

INTRODUCTION

Our previous paper reported that certain *N*-alkyl-*N*-(4-substituted benzyl)-4-halo-2-alkenamides exhibit a potent herbicidal activity against *Echinochloa oryzicola*¹⁾ light-dependently similar to light-dependent herbicides such as oxyfluorfen.²⁾ Among a number of analogs synthesized, the 4-chloro-2-pentenoyl structure is most suitable as the acyl component. The effects of substituents in the amide moiety on the activity are not simple. That is, somewhat peculiar structure-activity patterns are observed in *N*-multi-substituted benzyl compounds as well as in *N*-branched alkyl derivatives, other things being equal.¹⁾ Because the multiple substitutions on the *N*-benzyl-benzene ring did not indicate practical advantages in potentiating the activity of already potent *para*-mono-substituted derivatives, and also because the structure of the *N*-alkyl groups was observed to be important for the activity, we synthesized and bioassayed additional 4-chloro-2-pentenamides in which a variety of substituents were introduced into the amide nitrogen directly as well as into the *para* position of the *N*-benzyl-

benzene ring.

In this paper, we analyzed the structure-activity relationships for the entire set of *N*-alkyl-*N*-(4-substituted benzyl)-4-chloro-2-pentenamides quantitatively³⁾ to disentangle the physicochemical substituent effects in the amide moiety. The structural modifications were made at the R and X positions of the skeletal structure shown in Fig. 1.

MATERIALS AND METHODS

1. Compounds

The compounds used in this paper are listed in Table 1. Compounds **1-7**, **12-14**, **18**, **20**, **21**, **27-31**, **34** and **35** were the same as used previously.¹⁾ Others were newly synthesized by the reaction of 4-chloro-2-pentenoyl chloride with the corresponding secondary amines as described previously.¹⁾ The structure of the newly synthesized compounds was confirmed by the elemental analyses and the IR and NMR spectrometric methods. Physicochemical properties are shown in Table 1. Melting points were uncorrected.

2. Bioassay

Each test compound was well mixed so that the content is 10% in a wettable powder formulation containing 0.5%

¹ Halopentenamides as Light-Dependent Herbicides (Part 2): For Part 1 see Ref. 1.

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Emalgen 810, 0.5% Demol N, 18% Kunilite 250 (diatomaceous earth), 6% Carplex No/80 (White carbon) and 65% Zeeklite (clay). The wettable powder formulation was diluted with water to give desired concentra-

Fig. 1 The general formula of herbicidal *N*-alkyl-*N*-(substituted benzyl)-4-chloro-2-pentenamides.

tions of each test compound. A 10 ml test emulsion was poured into a Petri dish (ϕ 9 cm) lined with absorbent cotton and filter paper. Ten seeds of the barnyard grass (*E. oryzicola*) were placed in each of the dishes containing various concentrations of each test compound. The dishes were kept in a greenhouse at 28°C under sunshine in the daytime and at 18°C at nights. Seven days later, the lengths of seedling shoots were measured and averaged for each of dishes. The molar concentration of each test compound to inhibit the shoot elongation to half the length of the control (I_{50}) was evaluated from the

Table 1 Physicochemical parameters and biological activity for *N*-alkyl-*N*-(4-substituted benzyl)-4-chloro-2-pentenamides.

	R	X	pI_{50} obs.	Calc. ^{a)}			π_R ^{b)}	π_X ^{c)}	$\sigma_p^{0d)}$	HB	n_D^{20} or mp
				(Eq. 1)	(Eq. 2)	(Eq. 4)					
1	Me	Cl	2.20	2.22	—	2.41	0.50	0.71	0.27	0	1.5527
2	Et	Cl	2.89	2.91	—	2.94	1.00	0.71	0.27	0	1.5399
3	<i>n</i> -Pr	Cl	3.49	3.27	—	3.19	1.50	0.71	0.27	0	1.5388
4	<i>i</i> -Pr	Cl	2.71	3.17	—	3.12	1.30	0.71	0.27	0	1.5387
5	<i>n</i> -Bu	Cl	3.32	3.30	—	3.16	2.00	0.71	0.27	0	1.5433
6	<i>i</i> -Bu	Cl	3.63	3.33	3.10	3.20	1.80	0.71	0.27	0	1.5455
7	<i>sec</i> -Bu	Cl	3.32	3.33	—	3.20	1.80	0.71	0.27	0	1.5433
8	<i>n</i> -Pent	Cl	2.72	3.01	—	2.84	2.50	0.71	0.27	0	1.5411
9	<i>i</i> -Pent	Cl	3.40	3.16	—	3.00	2.30	0.71	0.27	0	1.5426
10	<i>c</i> -Pent	Cl	3.59	3.33	—	3.20	1.85	0.71	0.27	0	1.5637
11	<i>n</i> -Hex	Cl	2.39	2.38	—	2.25	3.00	0.71	0.27	0	1.5400
12	<i>c</i> -Hex	Cl	3.25	3.19	—	3.03	2.26	0.71	0.27	0	1.5633
13	<i>n</i> -Oct	Cl	0.08	0.13	—	0.21	4.00	0.71	0.27	0	1.5031
14	Allyl	Cl	3.11	3.10	—	3.07	1.20	0.71	0.27	0	1.5605
15	C ₂ H ₄ OMe	Cl	2.07	2.27	—	2.45	0.53	0.71	0.27	0	1.5446
16	C ₂ H ₄ OEt	Cl	2.51	2.94	—	2.95	1.03	0.71	0.27	0	1.5361
17	C ₂ H ₄ CN	Cl	1.96	1.57	—	1.89	0.16	0.71	0.27	0	1.5498
18	<i>t</i> -Bu	Cl	1.46 ^{e)}	3.31	—	3.20	1.60	0.71	0.27	0	94–95°C
19	<i>t</i> -Pent	Cl	2.01 ^{e)}	3.27	—	3.12	2.10	0.71	0.27	0	1.5439
20	<i>i</i> -Bu	H	2.67	—	3.13	2.70	1.80	0.00	0.00	0	1.5350
21	<i>i</i> -Bu	Me	3.11	—	2.82	2.77	1.80	0.56	–0.12	0	1.5357
22	<i>i</i> -Bu	OMe	2.54	—	2.97	2.50	1.80	–0.02	–0.16	0	1.5359
23	<i>i</i> -Bu	<i>i</i> -Pr	1.60	—	1.57	2.24	1.80	1.53	–0.16	0	1.5239
24	<i>i</i> -Bu	Br	3.44	—	2.95	3.16	1.80	0.86	0.26	0	1.5568
25	<i>i</i> -Bu	I	3.49	—	2.65	3.06	1.80	1.12	0.27	0	1.5677
26	<i>i</i> -Bu	F	3.11	—	3.29	2.98	1.80	0.14	0.17	0	1.5238
27	<i>i</i> -Bu	NO ₂	3.68	—	3.91	4.23	1.80	–0.28	0.82	1	1.5529
28	<i>i</i> -Bu	CN	3.88	—	3.63	3.75	1.80	–0.57	0.69	1	1.5500
29	<i>i</i> -Bu	CF ₃	2.86	—	3.20	3.46	1.80	0.88	0.53	0	1.4944
30	<i>i</i> -Bu	SO ₂ Me	1.88	—	2.23	1.72	1.80	–1.63	0.69	1	1.5503
31	<i>i</i> -Bu	CONH ₂	1.94	—	2.16	1.68	1.80	–1.49	0.36 ^{f)}	1	138–139°C
32	<i>i</i> -Bu	Et	2.17	—	2.38	2.66	1.80	1.02	–0.13	0	1.5352
33	<i>i</i> -Bu	OH	1.29 ^{e)}	—	2.73	2.68	1.80	–0.67	–0.13	1	— ^{g)}
34	<i>i</i> -Bu	NHAc	0.41 ^{e)}	—	2.60	2.38	1.80	–0.97	0.03	1	1.5565
35	<i>i</i> -Bu	SMe	1.89 ^{e)}	—	3.01	2.99	1.80	0.61	0.08	0	1.5679

^{a)} Calculated pI_{50} values through Eqs. 1, 2 and 4. ^{b)} Taken from Ref. 5. ^{c)} Taken from Ref. 6. ^{d)} Unless noted, taken from Ref. 7. ^{e)} Omitted in the correlation calculation as an outlier. ^{f)} The σ (*para*) value is used, because it does not differ much from σ^0 for most electron-accepting substituents. ^{g)} Not measured.

plot of the inhibition percentage against the concentration on the logarithmic probability scale. The activity was expressed as pI_{50} ($=\log 1/I_{50}$) and is listed in Table 1.

3. Physicochemical Substituent Parameters

The relevant substituent parameters used for the analyses are listed in Table 1. For the hydrophobicity of the amide substituents, the π value of aliphatic substituents R and that of aromatic substituents X both in the 1-octanol/water system were used.⁴⁾ As the π value of X substituents, the one from mono-substituted benzene series was adopted.⁵⁾ The π value of R substituents was taken from that reported for aliphatic substituents.⁶⁾ For the electronic effect of aromatic substituents X, the σ^0 parameter was used.⁷⁾ It is one of various σ values which is supposed to contain no through-resonance effect between two "substituents" on the benzene ring.⁷⁾ The hydrogen-bonding accepting ability of substituents X was expressed as an indicator variable, HB.⁸⁾ It takes a value of unity for such groups as CONH_2 , NO_2 , CN , SO_2CH_3 , OH , and NHAc and of zero for other substituents. The OMe group was not classified as a hydrogen acceptor, since its hydrogen-bonding effect was not significant in a preliminary examination and it sometimes behaves as only a very weak acceptor.⁸⁾

4. Calculation

All calculations were carried out with a StatView 4.02 program, which is commercially available from Abacus Concepts Inc., on a Power Macintosh.

RESULTS

1. Effects of the Aliphatic Substituent (R) Attached to the Amide Nitrogen Atom

For compounds (1–19) in Table 1 where the X substituent is fixed as 4-Cl, the activity varied considerably with variations in the structure of the R substituent. The activity was highest when R is *n*-Pr (in 3), *i*-Bu (in 6), and *c*-Pent (in 10), but very low when R is lengthy in such substituents as *n*-Oct (in 13) and multiply branched in such substituents as *t*-Bu (in 18) and *t*-Pent (in 19). To understand factors governing the activity variations, we examined various combinations of substituent parameters. Equation 1 with the quadratic hydrophobic parameter terms, π_R and $(\pi_R)^2$, showed the best correlation after excluding the *t*-alkyl compounds (18, 19).

$$pI_{50} = 2.368(\pm 0.462)\pi_R - 0.659(\pm 0.112)(\pi_R)^2 + 1.204(\pm 0.426) \quad (1)$$

$n = 17, r = 0.961, s = 0.260, \pi_{\text{opt}}(R) = 1.80$

In this and following equations, n is the number of compounds included in the correlation, s is the standard deviation, and r is the correlation coefficient. The figures in parentheses are the 95% confidence intervals for

Fig. 2 Relationship between π_R values and herbicidal activity of *N*-alkyl-*N*-(4-chlorobenzyl)-4-chloro-2-pentenamides.

the respective regression coefficients and intercept. All parameter terms are justified at a level higher than 95%.

The use of steric parameters such as STERIMOL L^9 and B_5^{10} , did not afford significant correlations, and, in particular, they did not predict the activity of compounds with hetero-atom-containing substituents such as $\text{C}_2\text{H}_4\text{OR}$ and $\text{C}_2\text{H}_4\text{CN}$ (correlation equations not shown).

The pI_{50} values were plotted against the π value of substituents in Fig. 2. Except for the *t*-alkyl compounds, the plots relatively well fitted with a parabola. Equation 1 indicates that the optimal π for the R substituent is about 1.80 which coincides with the π_R value of *i*-Bu and *sec*-Bu.

To include *t*-alkyl groups, we tried to add terms of such steric parameters as STERIMOL B_1^9 and Taft E_s^{11} to Eq. 1. No significant improvement was observed. The low activity of *t*-alkyl compounds is presumably due to an over-crowding of branched chains at the α -position of substituents for which no relevant quantitative parameter was available.

2. Effects of the X-Substituent at the para-Position of the N-Benzyl-benzene Ring

The effects of the X-substituent were analyzed with compounds (6, 20–32) in which the R-substituent is fixed as *i*-Bu group. The correlation with only the hydrophobic parameter terms gave no good result. The addition of a term for the electronic effect, σ^0 improved the correlation as shown by Eq. 2.

$$pI_{50} = -0.600(\pm 0.297)(\pi_X)^2 + 1.007(\pm 0.808)\sigma^0 + 3.132(\pm 0.409) \quad (2)$$

$n = 14, r = 0.834, s = 0.446, \pi_{\text{opt}}(X) = 0.00$

In this analysis, the OH (33), NHAc (34), and SMe (35) compounds were omitted as outliers. The OH compound may be conjugated readily in a metabolic process.¹²⁾ The NHAc compound may be hydrolyzed in

plants.¹³⁾ The SMe compound may be oxidized into the corresponding sulfone,¹⁴⁾ since the activity of the SMe compound was almost equivalent to that of the SO₂Me (30) compound. Equation 2 shows that electron-withdrawing substituents having an optimum hydrophobic property at about $\pi_X=0$ are favorable to the activity. No additional parameter to Eq. 2 improved the correlation.

3. Correlation Analysis for the Entire Series of *N*-Alkyl-*N*-(4-substituted benzyl)-4-chloro-2-pentenamides

Because the size of the π^2 term is not so apart between Eqs. 1 and 2, the parabolic curvature should not be much different between the two correlations. The π_{opt} value in Eqs. 1 and 2, 1.80 and 0.00, for R and X substituents, respectively, correspond with values, 2.51: $\pi_{opt}(R)+\pi_X$ (Cl) and 1.80: $\pi_{opt}(X)+\pi_R$ (*i*-Bu), on the basis of $\Sigma\pi$ (R, X). Thus, the optimal hydrophobicity in terms of $\Sigma\pi$ is also not far apart between the two correlations. Therefore, the effects of R- and X-substituents were expected to be analyzed together using the $\Sigma\pi$ (R,X) as the parameter for the hydrophobicity of the *N,N*-disubstituted amide

moiety.

As expected, Eq. 3 was formulated with the same physicochemical parameters as those included in Eqs. 1 and 2. The addition of the indicator variable for the hydrogen-bond acceptors, HB, to Eq. 3 improved the correlation as shown in Eq. 4.

$$pI_{50} = 2.309(\pm 0.527)\Sigma\pi - 0.502(\pm 0.109)(\Sigma\pi)^2 + 1.707(\pm 0.722)\sigma^0 + 0.139(\pm 0.711) \quad (3)$$

$n = 30, r = 0.889, s = 0.389, (\Sigma\pi)_{opt} = 2.30$

$$pI_{50} = 2.706(\pm 0.575)\Sigma\pi - 0.563(\pm 0.110)(\Sigma\pi)^2 + 1.131(\pm 0.804)\sigma^0 + 0.839(\pm 0.674)HB - 0.348(\pm 0.755) \quad (4)$$

$n = 30, r = 0.913, s = 0.353, (\Sigma\pi)_{opt} = 2.40$

Though the addition of the HB term was not justified at the 95% level to Eq. 2 for benzyl-benzene substituted compounds only, it is significant in Eq. 4, probably due to the increase in the number of compounds. The positive sign of HB term means that hydrogen-bond accepting property is favorable to the activity.

Table 2 log *P* values of light-dependent herbicides.

Compound	Structure	log <i>P</i>
Acifluorfen (X = COOH)		3.70 ^{a)}
Oxyfluorfen (X = OEt)		4.73 ^{a)} , 4.70 ^{b)}
Nitrofluorfen (X = H)		4.54 ^{a)}
Oxadiazon		4.78 ^{c)}
Fluthiacet-methyl		3.55 ^{d)}
Phenopylate		3.94 ^{e)}
Compound 6		4.68 ^{d)}

^{a)} Taken from Ref. 16. ^{b)} Taken from Ref. 17. ^{c)} Taken from Ref. 18. ^{d)} Experimentally measured. ^{e)} Taken from Ref. 19.

DISCUSSION

The above analyses show us the most favorable physicochemical properties for light-dependent herbicidal activity of *N*-alkyl-*N*-(4-substituted benzyl)-4-chloro-2-pentenamides. The fact that the activity is parabolically related with the hydrophobic parameter for the amide moiety, $\Sigma\pi$, could mean that not only the hydrophobicity of the amide moiety but the overall molecular hydrophobicity participating in the transport process to the target site is one of the factors governing the potency of the herbicidal activity.¹⁵⁾ Based on the $(\Sigma\pi)_{\text{opt}}$ value (2.40) in Eq. 4 and $\Sigma\pi$ value (2.51) of the aliphatic *i*-Bu (1.80) and aromatic Cl (0.71) substituents, as well as the measured log *P* value (4.68) of *N*-(4-chlorobenzyl)-*N*-isobutyl-4-chloro-2-pentenamide, the optimum log *P* value is estimated as being 4.57. This optimum log *P* value for the 4-Cl-pentenamide series is close to the log *P* value of many other light-dependent herbicides shown in Table 2. These log *P* values are relatively larger than herbicides that inhibit photosystem II which are about 2.5.²⁰⁾ In the 3-dimensional CoMFA-QSAR analysis of a combined set of light-dependently herbicidal 4-pyridone-3-carboxanilides and diphenyl ethers, Osabe *et al.* suggested that the hydrophobicity of the entire molecule was significant in potentiating the herbicidal activity.¹⁷⁾ In the inhibition of protoporphyrinogen oxidase (Protox) by diphenyl ether herbicides, the molecular hydrophobicity has been considered to play an important role.¹⁶⁾

In the present series of compounds, the entire molecular hydrophobicity may be related to the binding ability toward Protox which is embedded in the cell membrane²¹⁾ besides behaviors in the transport process. In fact, we observed that certain 4-Cl-pentenamides inhibit Protox as the primary target site like other light-dependent herbicides (the result will be published elsewhere), although some pentenamides are likely to have additional targets in exhibiting the entire phytotoxicity.

The electron-withdrawing effect of the substituents on the benzyl-benzene ring was shown to contribute to potentiating the herbicidal activity, but its physicochemical significance at the molecular and/or sub-molecular levels remains to be determined. Hydrogen-bonding accepting substituents on the benzene ring increased the potency. This could indicate a specific hydrogen-bond formation of these groups with a hydrogen donor on the enzyme.

In our previous paper,¹⁾ the herbicidal activity was estimated under paddy conditions visually in terms of the ED₉₀ value required to give 90% damage to the barnyard grass seedlings. The procedure for the potency measurement in the present paper is thought to be more accurate than before, although general trends in structure-activity profile are much the same. We observed previously such

activity-potential sequences in R substituents as *n*-Pr > *i*-Pr and *i*-Bu > *n*-Bu > *sec*-Bu. We have suggested that the branching at the α -position of alkyl groups may be disadvantageous to the activity in spite of the other observations such that cyclohexyl and cycloheptyl derivatives are highly active. Apparently, not only the branching effect, but also other effect(s) may be operative at the same time. In the present work, substituents at the R position were shown to contribute to the potency variations mostly with their hydrophobic effect. The activity-potentiating sequence of R substituents is mostly rationalized by their π value as shown in Eq. 1, although exceptionally high activity of the *i*-Bu compound is still left to be rationalized.

Under the paddy conditions, 4-Cl and 4-CN substituents were best as the X substituent almost equivalently. The activity of the 4-NO₂ compound was much lower in the previous work. In the present study, the most potent compound has the substituent combination of R = *i*-Bu and X = 4-CN. Those in which X = 4-NO₂ and Cl with R = *i*-Bu come next. Under paddy conditions where rice plants are growing simultaneously, some amount of the aromatic NO₂ group may be reductively metabolized before exerting the activity against barnyard grass seedlings.²²⁾ The 4-Cl substituent seems to be stable enough against the metabolic detoxification.

The selection of compound 6 as the candidate for detailed field trial as indicated previously was supported by a present analyses as well as the comparison with the previous results.

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要 約

N-アルキル-*N*-(4-置換ベンジル)-4-クロロ-2-ペンテンアミドの *Echinochloa oryzicola* に対する除草活性の定量的構造活性相関

松成健二, 吉田文隆, 中村安夫, 藤田稔夫
タイヌビエ, *Echinochloa oryzicola* に対する *N*-アルキル-*N*-(4-置換ベンジル)-4-クロロ-2-ペンテンアミドの除草活性を評価し, アミド部位に於ける *N*-アルキル基及びベンジル基のベンゼン環置換基と除草活性との関係を物理化学パラメーターを用い定量的に解析した。除草活性はアミド部位に於けるトータルな疎水性とパラボリックな関係であることが示された。また, ベンゼン環上置換基の電子吸引性及び水素結合受容性が除草活性に重要であることが判明した。