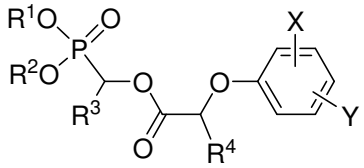
Supporting information

1. The structure of title compounds **I-1~I-71**



No.	R^1	R^2	R^3	R^4	X	Y
I-1	Me	Me	Me	H	2-Me	3-Me
I-2	Me	Me	Me	H	H	4-Br
I-3	Me	Me	Me	H	2-Br	4-Br
I-4	Me	Me	Me	H	2-NO_2	4-Cl
I-5	Me	Me	Me	H	2-Cl	4-Cl
I-6	Me	Me	Me	H	H	2-F
I-7	Me	Me	Me	H	3-Cl	4-F
I-8	Me	Me	CCl_3	H	3-Cl	4-F
I-9	Me	Me	CCl_3	H	2-Cl	4-Cl
I-10	Me	Me	Et	H	2-Cl	4-Cl
I-11	Me	Me	Ph	H	H	H
I-12	Me	Me	Ph	H	H	3-Me
I-13	Me	Me	Ph	H	H	4-Me
I-14	Me	Me	Ph	H	2-Me	3-Me
I-15	Me	Me	Ph	H	2-F	4-F
I-16	Me	Me	Ph	H	3-Cl	4-F
I-17	Me	Me	Ph	H	2-Cl	4-F
I-18	Me	Me	Ph	H	H	4-CF_3
I-19	Me	Me	Ph	H	H	2-NO_2
I-20	Me	Me	Ph	H	2-NO_2	4-CF_3
I-21	Me	Me	3-NO_2Ph	H	3- Me	4-Cl
I-22	Me	Me	3-NO_2Ph	H	2-Cl	5-Me
I-23	Me	Me	3-NO_2Ph	H	2- Me	4-Cl
I-24	Me	Me	3-NO_2Ph	H	2-Cl	3-Cl
I-25	Me	Me	3-NO_2Ph	H	2-Cl	6-Cl
I-26	Me	Me	3-NO_2Ph	H	H	4-Cl
I-27	Me	Me	3-NO_2Ph	H	2-F	4-F
I-28	Me	Me	3-NO_2Ph	H	3-Cl	4-F

I-29	Me	Me	3-NO_2Ph	H	2-Cl	4-F
I-30	Me	Me	3-NO_2Ph	H	H	3-CF_3
I-31	Me	Me	3-NO_2Ph	H	H	4-CF_3
I-32	Me	Me	3-NO_2Ph	H	2-NO_2	4-CF_3
I-33	Me	Me	3-Brph	H	2-Cl	4-Cl
I-34	Me	Me	2-OHPh	H	H	4-Cl
I-35	Me	Me	2-OHPh	H	2-Cl	4-F
I-36	Me	Me	Me	H	H	4-Me
I-37	Me	Me	Me	H	H	4-Cl
I-38	Me	Me	Me	H	2- Me	4-Cl
I-39	Me	Me	Me	H	3- Me	4-Cl
I-40	Me	Me	Me	H	2-Cl	5-Me
I-41	Me	Me	Me	H	2-Cl	3-Cl
I-42	Me	Me	Me	H	H	3-F
I-43	Me	Me	Me	H	H	4-F
I-44	Me	Me	Me	H	2-F	4-F
I-45	Me	Me	Me	H	3-F	5-F
I-46	Me	Me	Me	H	2-Cl	4-F
I-47	Me	Me	H	H	2-Cl	4-Cl
I-48	Me	Me	Me	H	H	3-CF_3
I-49	Me	Me	Me	H	H	4-CF_3
I-50	Me	Me	Me	H	H	H
I-51	Me	Me	Ph	H	2-Cl	4-Cl
I-52	Me	Me	3-NO_2Ph	H	H	2-F
I-53	Me	Me	3-NO_2Ph	H	H	3-F
I-54	Me	Me	3-NO_2Ph	H	H	4-F
I-55	Me	Me	3-NO_2Ph	H	H	2- NO_2
I-56	Me	Me	3-NO_2Ph	H	H	4- NO_2
I-57	Me	Me	3-NO_2Ph	H	2-Cl	4-Cl
I-58	Me	Me	Pr	H	2-Cl	4-Cl
I-59	Et	Et	H	H	2-Cl	4-Cl
I-60	Et	Et	Me	H	2-Cl	4-Cl
I-61	Et	Et	Et	H	2-Cl	4-Cl
I-62	Et	Et	Ph	H	2-Cl	4-Cl
I-63	Et	Et	2-ClPh	H	2-Cl	4-Cl
I-64	Me	Me	Me	Me	2-Cl	4-Cl

I-65	Me	Me	Pr	Me	2-Cl	4-Cl
I-66	Me	Me	Ph	Me	2-Cl	4-Cl
I-67	Et	Et	Me	Me	2-Cl	4-Cl
I-68	Pr	Pr	Me	Me	2-Cl	4-Cl
I-69	Pr	Pr	Ph	Me	2-Cl	4-Cl
I-70	Pr	Pr	2-ClPh	Me	2-Cl	4-Cl

2. The source of the seeds used for bioassays

Following plants were used to test the herbicidal activity of compounds:

Amaranthus retroflexus (Common Name: amaranth pigweed)
Amaranthus spinosus (Common Name: Spiny Amaranth)
Abutilon theophrasti (Common Name: chingma abutilon)
Brassica campestris (Common Name: rape)
Brassica juncea (Common Name: leaf mustard)
Cucumis sativus (Common Name: cucumber)
Cardamine hirsuta (Common Name: pennsylvania bittercress)
Chenopodium album (Common Name: lambsquarters)
Daucus carota (Common Name: Carrot)
Digitaria sanguinalis (Common Name: ascendant crabgrass)
Echinochloa crusgalli (Common Name: barngard grass)
Eclipta prostrata (Common Name: white eclipta)
Medicago sativa (Common Name: clover)
Oryza sativa (Common Name: rice)
Phaseolus radiatus (Common Name: mung bean)
Pisum sativum (Common Name: pea)
Portulaca oleracea (Common Name: Common purslane)
Setaria viridis (Common Name: giant foxtail)
Triticum aestivum (Common Name: wheat)
Xanthium strumarium (Common Name: siberia cocklebur)
Zea mays (Common Name: Maize)

Seeds of *Triticum aestivum* (Variety is Yang Mai 1) and *Zea mays* (Variety is Gao –you 1) were come from the seed company of Jin Tu Di at Jiangsu in China.

Seeds of *Brassica campestris* (Variety is Si Yue Man) and *Medicago sativa* were purchased from the seed company, Academy of Agricultural Sciences at Tianjin.

Seeds of *Cucumis sativus* (Variety is Jin 4) was purchased from Institute of cucumber at Tianjin.

Seeds of *Phaseolus radiatus* (variety is VC2778A) were purchased from Hubei seed group company.

Seeds of *Pisum sativum* (variety is Zhongwan-2) was purchased from China

Academy of Agricultural Sciences.

Seeds of *Echinochloa crusgalli, Digitaria sanguinali, Setaria viridi, Amaranthus retroflexus*, *Abutilon theophrasti*, *Amaranthus spinosus*, *Chenopodium album*, *Brassica juncea, Eclipta prostrata, Xanthium strumarium, Cardamine hirsuta Linn., Portulaca oleracea*， *Brassica juncea* come from the storeroom of weed seed in the north at National Pesticide Engineering Research Center in Nankai University (**Table 1, 2, 3**), in the storeroom of weed seed in Hunan National Pesticide Engineering Research Center (**Table 4**，**Table 7**) and in Zhejiang National Pesticide Discovery South Center in China (**Table 5**).

3. The regression equation, and *R* values for the IC_{50} values

Table 3 The toxicity of stem length

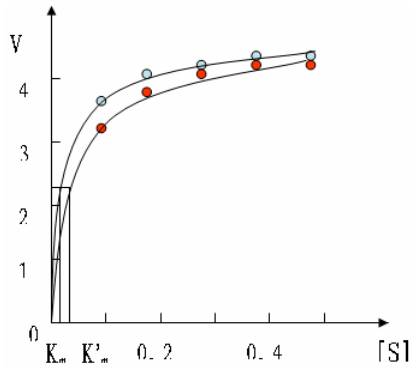
Compd.	Regression equation	IC_{50}(μM/L)	*R*
I-5	Y=3.6841+1.4977X	7.5619	*0.9989*
I-10	Y=3.3299 +1.4571 X	14.0009	*0.9855*
I-47	Y=3.6795+1.4811X	7.7910	*0.9991*
I-51	Y=3.4096 +1.6708 X	8.9515	*0.9929*
I-57	Y=3.9167+1.5459X	5.0211	*0.9962*
I-58	Y=3.5627 +1.4811 X	9.3414	*0.9628*
I-59	Y=3.5832+1.2568 X	13.4056	*0.9786*
I-61	Y=2.4626 +1.7996 X	25.7026	*0.9942*
I-62	Y=1.7430 +1.5986 X	109.0088	*0.9987*
I-64	Y=3.7036+1.5642X	6.7414	*0.9989*
I-65	Y=3.5374 +1.2873 X	13.6820	*0.9741*
I-66	Y=2.5540+1.6541 X	30.1142	*0.9908*
I-68	Y=3.1993 +1.4339 X	18.0221	*0.9863*
I-69	Y=2.2131 +1.6924 X	44.3371	*0.9988*
I-70	Y=1.1002 +1.7607 X	164.0099	*0.9967*
2,4-D	Y=3.5568 +1.4344 X	10.1428	*0.9777*

Table 3 The toxicity of root length

Compd.	Regression equation	IC_{50}(mM/L)	*R*

I-5	Y=7.4735 +0.9509 X	0.0025	*0.9901*
I-10	Y=5.6556+1.3520X	0.3273	*0.9764*
I-18	Y=6.0788 +1.1688X	0.1194	*0.9927*
I-47	Y=6.6761+1.3531X	0.0577	*0.9818*
I-51	Y=6.8465 +1.0001 X	0.0142	*0.9915*
I-57	Y=7.4990 +1.0127 X	0.0034	*0.9944*
I-58	Y=7.4990 +1.0127 X	0.0075	*0.9953*
I-59	Y=5.5056+1.1939X	0.3772	*0.9864*
I-60	Y=5.6967+1.37949X	0.3125	*0.9865*
I-61	Y=5.6909+1.3745X	0.3142	*0.9833*
I-62	Y=6.6796 +1.2802 X	0.0488	*0.9394*
I-63	Y=4.7880 +1.2236 X	1.4902	*0.9992*
I-64	Y=4.7714 +1.5069 X	1.4182	*0.9987*
I-65	Y=4.4383 +1.1843 X	2.9805	*0.9997*
I-67	Y=4.9548+1.2927 X	1.0839	*0.9687*
I-68	Y=4.5248 +1.2253 X	2.4427	*0.9976*
I-69	Y=4.0697 +1.4201 X	4.5194	*0.9874*
I-70	Y=3.4774 +1.4061 X	12.1026	*0.9892*
2,4-D	Y=5.8601+1.3379X	0.2276	*0.9877*

4. Enzyme kinetic experiment data of **I-5** against PDHc from *Phaseolus radiatus*[a,b]



K_m no inhibitor **K'_m** inhibitor present

[S]: The concentration of substrate (sodium pyruvate)

Substrate concentration (mM) Sodium pyruvate	Inhibitor concentration (mM)	Velocity (V) NADH（μM/ per minute）
0.1	0	3.86
0.2	0	4.10
0.3	0	4.16
0.4	0	4.20
0.5	0	4.22
0.1	0.028	3.28
0.2	0.028	3.74
0.3	0.028	4.08
0.4	0.028	4.14
0.5	0.028	4.16

a) 0.028 mM = 10^{-5}(g/ml)

b) The values are the average of >3 experiments.

According to $V=\frac{\overline{V}_{max}[S]}{K_m+[S]}$, V_{max} and K_m could be obtained.

5. The regression equation, and *R* values for the IC_{50} values in **Table 7**

1) IC_{50} values against PDHc from *Phaseolus radiatus in vitro*

NO.	Cocentration μg/g	Inhibitory rate %	Regression	IC_{50} μM	R
I-5 (HW02)	1000 100 10 1.0 0.1	77.78 55.56 48.89 43.70 39.26	Y=8.89X+44.148	12.75	0.9305
I-47	1000 100 10 1.0 0.1	75.65 53.42 46.90 42.68 38.57	Y=8.49X+42.954	19.70	0.9192
I-51	1000 100 10 1.0 0.1	60.27 51.28 44.42 39.78 36.46	Y=5.912X+40.53	95.38	0.9816
	1000	73.68	Y=8.308X+42.11	23.12	0.9276

I-60	100 10 1.0 0.1	52.76 46.24 41.78 37.63			

2) IC_{50} values against PDHc from *Oryza sativa in vitro*

NO.	Cocentration µg/g	Inhibitory rate %	Regression	IC_{50} µM	R
I-5 (HW02)	1000 100 10 1.0 0.1	55.1 21.3 16.9 8.2 3.4	Y=11.65X+9.33	**867.33.**	0.906

3) IC_{50} values against PDHc from *Pisum sativum in vitro*

NO.	Cocentration µg/g	Inhibitory rate %	Regression	IC_{50} µM	R
I-5 (HW02)	1000 100 10 1.0 0.1	73.77 59.02 50.80 44.26 31.15	Y= 6.24663 + 0.263 x	18.195	0.98903
I-48	1000 100 10 1.0 0.1	60.66 49.18 31.15 22.95 11.48	Y= 6.23006 + 0.36666 x	442	0.99584
2,4-D	1000 100 10 1.0 0.1	48.15 27.80 18.48 12.91 8.8		> 4530	