

**Design of a New Glutamine–Fipronil Conjugate with α -Amino Acid
Function and Its Uptake by *A. thaliana* Lysine Histidine Transporter
1 (*AtLHT1*)**

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Author Contributions

[§]All authors conceived and designed the study. X.J. and Y.X. contributed equally to this work. X.J. designed, synthesized the compounds and wrote the manuscript. Y.X. and Z.R. performed the biology experiments and HPLC data analyses.

Supporting Information Available:

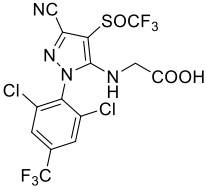
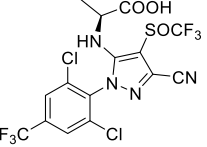
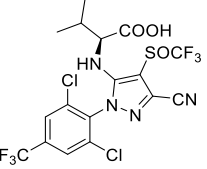
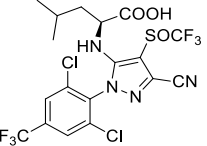
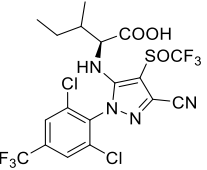
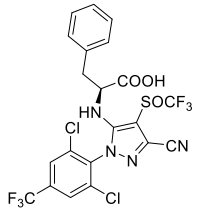
Structures and net charges of neutral amino acid-fipronil conjugates.....Table S1

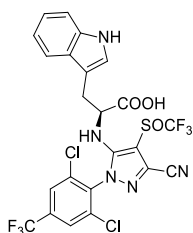
LC₅₀ values of L-GlnF, D-GlnF and fipronil against *Plutella xylostella*.....Table S2

Prediction of phloem mobility of L- /D-GlnF using a Kleier map.....Figure S1

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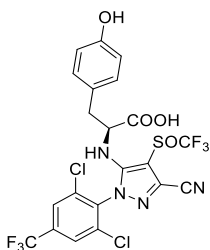
Table S1. Structures and Net Charges of Neutral Amino Acid-Fipronil Conjugates.

Structure	Conjugated Amino Acid	Net Charge ^a
	Glycine (Gly)	Electronegative
	Alanine (Ala)	Electronegative
	Valine (Val)	Electronegative
	Leucine (Leu)	Electronegative
	Isoleucine (Ile)	Electronegative
	Phenylalanine (Phe)	Electronegative



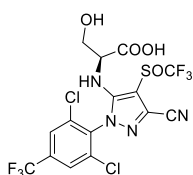
Tryptophan (Trp)

Electronegative



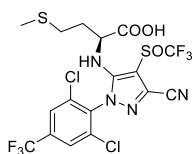
Tyrosine (Tyr)

Electronegative



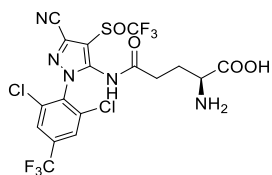
Threonine (Thr)

Electronegative



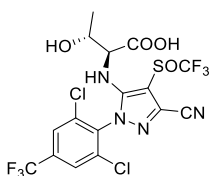
Methionine (Met)

Electronegative



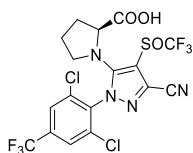
Glutamine (Gln)

Electroneutral



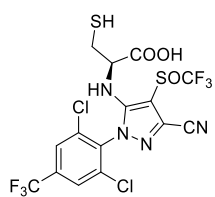
Serine (Ser)

Electronegative



Proline (Pro)

Electronegative



Cysteine (Cys)

Electronegative

^aNet charges were measured at the plant physiology pH 5.6.

Table S2. LC₅₀ values of L-GlnF, D-GlnF and fipronil against *Plutella xylostella*

Compound	$y = a + bx$	LC ₅₀ (mg L ⁻¹) ^a	R
L-GlnF	$y = 3.81 + 1.61x$	5.46	0.99
D-GlnF	$y = 2.94 + 2.38x$	7.36	0.97
fipronil	$y = 4.25 + 1.56x$	3.02	0.97

^aEvaluated by leaf disk dipping assay following procedures in literature.¹

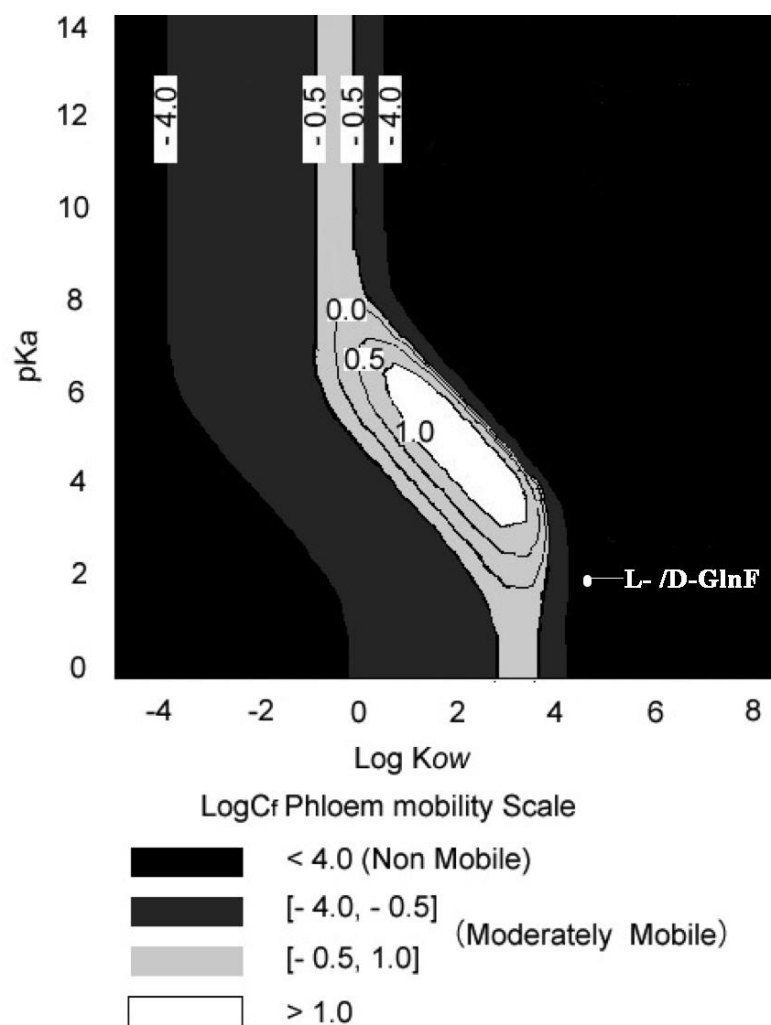


Figure S1. Prediction of phloem mobility of L-/D-GlnF using a Kleier map. L-/D-GlnF is located in the non-phloem mobile area. Log K_{ow} and pK_a were calculated by the ACD Laboratories Percepta Program, version 14.0.

References:

- (1) Xia, Q.; Wen, Y.; Hao, W.; Li, Y.; Xu, H. β -Glucosidase involvement in the bioactivation of glycosyl conjugates in plants: synthesis and metabolism of four

glycosidic bond conjugates in vitro and in vivo. *J. Agric. Food Chem.* **2014**, *62*, 11037–11046.