Supporting Information

Mechanistic insights into stereospecific bioactivity and dissipation of chiral fungicide triticonazole in agricultural management

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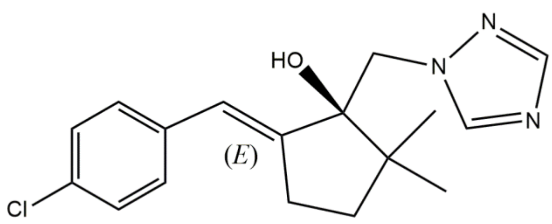
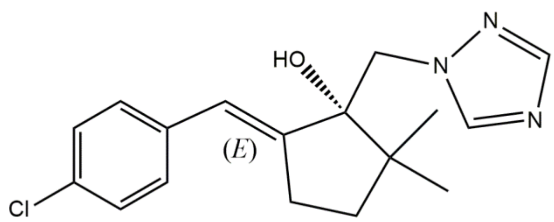


(*S*)-triticonazole



(*R*)-triticonazole

Fig. S1. Chemical structure of (*R*)-triticonazole and (*S*)-triticonazole**.**

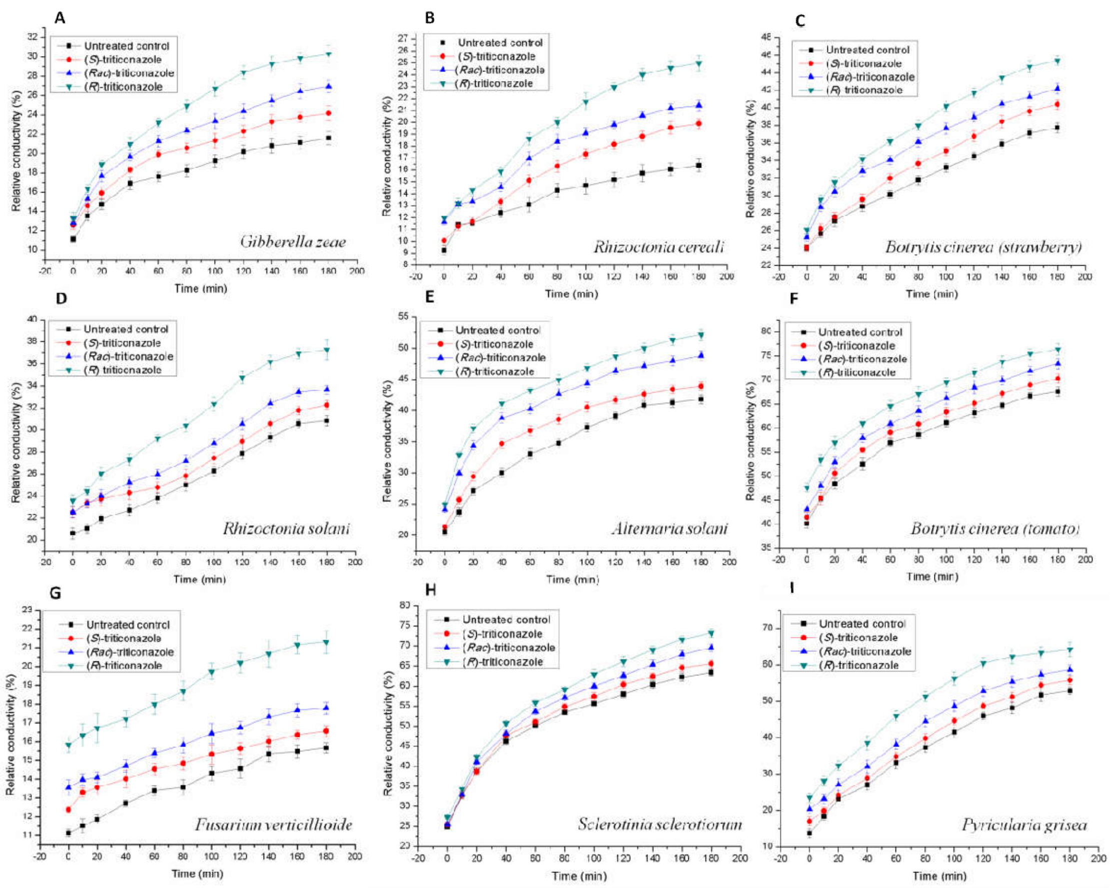


Fig. S2. Triticonazole enantioselective cell membrane permeability in nine plant pathogens (A *Gibberella zeae*, B *Rhizoctonia cereali*, C *Botrytis cinerea* (strawberry), D *Rhizoctonia solani*, E *Alternaria solani*, F *Botrytis cinerea* (tomato), G *Fusarium verticillioide*, H *Sclerotinia sclerotiorum*, I *Pyricularia grisea*).

Table S1. The spiked concentration (mg/kg) of chiral triticonazole in different kinds of plant pathogens.

Chiral enanatiomers	*Gibberella zeae*	*Rhizoctonia cereali*	*Botrytiscinerea (strawberry)*	*Rhizoctonia solani*	*Alternaria solani*	*Botrytis cinerea (tomato)*	*Fusarium verticillioide*	*Sclerotiniascl erotiorum*	*Pyriculariagri sea*
(*R*)-triticonazole	5.00	8.00	2.00	1.00	4.00	5.00	0.60	4.00	6.00
(*Rac*)-triticonazole	5.00	8.00	2.00	1.00	4.00	5.00	0.60	4.00	6.00
(*S*)-triticonazole	5.00	8.00	2.00	1.00	4.00	5.00	0.60	4.00	6.00

Table S2. The primary sequences of different plant pathogens compared to the template protein (E9QY26).

Species	Identify (%)	Positives (%)	Length query|match	Start structure original sequence |temple sequence
Gibberellazeae	58.5	71.3	507|524	33|50
Fusarium verticillioide	58.6	73.1	506|524	33|50
Botrytis cinerea (tomato and strawberry)	64.6	80.8	522|524	50|50
Sclerotiniasclerotiorum	63.8	80.3	522|524	50|50
Pyriculariagrisea	61.5	79.8	608|524	132|50

Table S3. The enantioselective inhibition of ergosterol biosynthesis (%) in plant pathogens exposed to chiral triticonazole.

Chiral enantiomers	*Gibberella zeae*	*Rhizoctonia cereali*	*Botrytis cinerea (strawberry)*	*Rhizoctonia solani*	*Alternaria solani*	*Botrytis cinerea (tomato)*	*Fusarium verticillioide*	*Sclerotiniascl erotiorum*	*Pyriculariagri sea*
(*R*)-triticonazole	61.45	26.63	77.58	47.34	65.77	58.10	39.07	44.98	55.04
(*Rac*)-triticonazole	49.57	18.23	64.27	38.78	51.84	45.58	26.26	36.77	45.85
(*S*)-triticonazole	20.17	3.63	31.42	25.83	36.52	16.13	17.07	19.50	21.55
(*R*)/(*S*)[a]	3.05	7.34	2.47	1.83	1.80	3.60	2.29	2.31	2.55

a the inhibition of ergosterol biosynthesis value of *R*-triticonazole to *S*-triticonazole ratio.

Table S4. Binding affinities of chiral triticonazole enantiomers and the main interaction active site residues in plant pathogens.

Species	docking energy of (*R*)-triticonazole (kcal/mol)	active site of (*R*)-triticonazole	docking energy of (*S*)-triticonazole (kcal/mol)	active site of (*S*)-triticonazole
Gibberellazeae	-6.565	L489,T109,F212,I359,F113,T287,L288,V118,V133,Q129,I450,K130,H284,L126,Y119,H447,Y105,S295,C449,H294,A291,G292,F490,L108,HEM	-6.247	G292,A291,S295,Y119,L489,F490,I359,S358,Y51,L363,H360,S361,I362,Y105,F212,F113,T109,V118,T287,HEM
Fusarium verticillioide	-6.858	A291,S295,I362,H294,I359,T109,F490,Y105,I104,L489,S361,L108,F212,V118,M284,T287,V117,L288,V133,F113,I450,Y119,HEM	-6.043	T287,C449,S295,A291,Y105,Y119,L489,I359,F490,S358,Y51,S491,L363,H360,S361,I362,F212,T109,V118,L108,F113, HEM
Botrytis cinerea (tomato and strawberry)	-6.880	A308,S312,P373,H311,Y122,I374,F508,L125,I121,L507,S376,F229,T126,V135,M301,A304,V134,L305,M150,I468,F130,I377,Y136, HEM	-5.999	A308,C467,P373,S312,Y136,Y122,M378,I377,H375,F508,S376,I374,,L507,L125,T126,F229,V135,F130,A304,M307,HEM
Sclerotiniasclerotiorum	-7.951	T126,Y122,L507,I374,F508,F229,F130,A304,V135,L305,M150,M301,K147,I468,Y136,C467,S312,H311,P373,A308,L125, HEM	-7.386	A304,C467,S312,A308,L507,I374,F508,P373,Y68,T509,M378,H375,S376,I377,Y122,F229,F130,Y136,T126,V135,HEM
Pyriculariagrisea	-7.745	Y204,L207,L591,I455,T208,F592,F311,V217,,A385,M382,L386,M232,L225,I552,F212,K229,Y218,C551,H392,A389,S393,HEM	-7.428	A389,G390,C551,S393,Y218,Y204,R460,M459,I458,H456,F592,S457,I455,L591,L207,F311,T208,A385,F212,V217,M388,HEM

Table S5. The first-order kinetic rate constants (k), half-lives ($t_{1/2}$), and coefficient of determination (R^2) for the degradation of chiral triticonazole in fruits and vegetables.

Plant	Enantiomer	k (day^{-1})	$t_{1/2}$ (days)	R^2
spinach	*S*-(+)-triticonazoe	0.14	4.95	0.927
	R-(-)-triticonazoe	0.15	4.62	0.946
pakchoi	*S*-(+)-triticonazoe	0.24	2.89	0.950
	R-(-)-triticonazoe	0.25	2.77	0.966
Tomato	*S*-(+)-triticonazoe	0.415	1.70	0.989
	R-(-)-triticonazoe	0.431	1.61	0.989
Cucumber	*S*-(+)-triticonazoe	0.390	1.78	0.956
	R-(-)-triticonazoe	0.408	1.70	0.939