

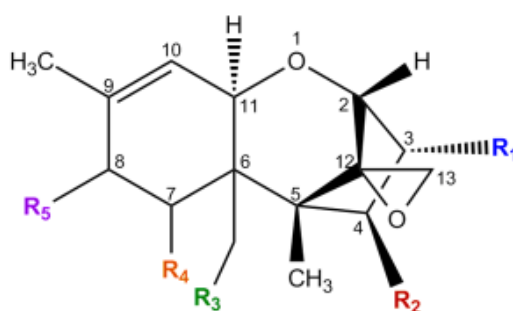
Signatures of *TRI5*, *TRI8* and *TRI11* Protein Sequences of *Fusarium incarnatum-equiseti* Species Complex (FIESC) Indicate Differential Trichothecene Analogue Production

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Table S1. Reference strains included in the study.

Gene	Species	GenBank Accession No.	Strain	Host	Country	Reference	Trichothecene toxin
<i>TRI5</i>	FIESC	LN995579	ITEM 15511	cereals	USA	Villani et al. 2016,	DAS, FUS-X
	FIESC	LN995580	ITEM 11348	oat	Canada	Villani et al. 2016	DAS, FUS-X
	FIESC	LN995581	ITEM 11401	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO, NIV
	FIESC	LN995582	ITEM 10395	wheat	Italy	Villani et al. 2016	DAS, FUS-X, NEO, NIV
	FIESC	LN995583	ITEM 11294	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995584	ITEM 11345	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995585	ITEM 11363	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995586	ITEM 10392	wheat	Italy	Villani et al. 2016	DAS
	FIESC	GQ915545	NRRL 13381	unknown	unknown	Proctor et al. 2009	NA
	FIESC	GQ915550	NRRL 31160	lung of patient with adenocarcinoma	USA	Proctor et al. 2009	NA
<i>TRI8</i>	<i>Fusarium</i> sp.	GQ915553	FRC R-06979	unknown	unknown	Proctor et al. 2009	NA
	<i>Myrothecium roridum</i>	DQ676576 (outgroup)	UAM H 1369	root	Canada	Koster et al. 2006	NA
	FIESC	LN995587	ITEM 15511	cereals	USA	Villani et al. 2016	DAS, FUS-X
	FIESC	LN995588	ITEM 11348	oat	Canada	Villani et al. 2016	DAS, FUS-X
	FIESC	LN995589	ITEM 11401	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO, NIV
	FIESC	LN995590	ITEM 11407	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO, NIV
	FIESC	LN995591	ITEM 10395	wheat	Italy	Villani et al. 2016	NA
	FIESC	LN995592	ITEM 11294	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995593	ITEM 11345	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995594	ITEM 11363	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995595	ITEM 10392	wheat	Italy	Villani et al. 2016	DAS

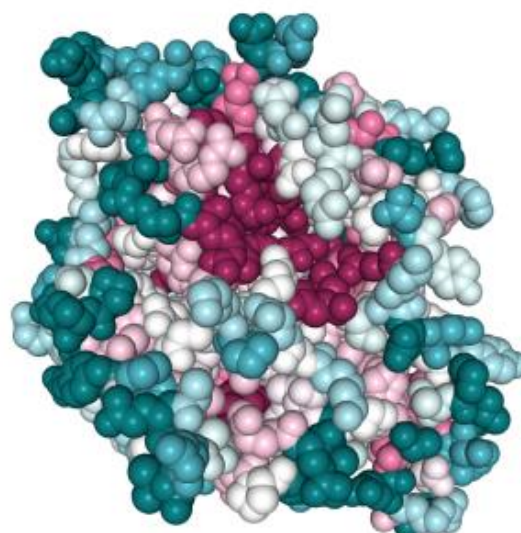
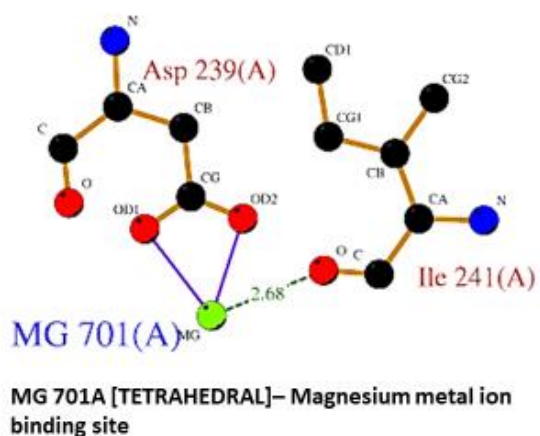
TR 111	<i>Fusarium</i> sp.	GQ865563	NRRL 13405	sweet corn	USA	Proctor et al. 2009	NA
	<i>F. sambucinum</i>	KT597832 (outgroup)	FRC R-07843	barley	USA	Rocha et al. 2015	NA
	FIESC	LN995596	ITEM 15511	cereals	USA	Villani et al. 2016	DAS, FUS-X
	FIESC	LN995597	ITEM 11348	oat	Canada	Villani et al. 2016	DAS, FUS-X
	FIESC	LN995598	ITEM 11401	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO, NIV
	FIESC	LN995599	ITEM 11407	oat	Canada	Villani et al. 2016	NA
	FIESC	LN995600	ITEM 10395	wheat	Italy	Villani et al. 2016	DAS, FUS-X, NEO, NIV
	FIESC	LN995601	ITEM 11294	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995602	ITEM 11345	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995603	ITEM 11363	oat	Canada	Villani et al. 2016	DAS, FUS-X, NEO
	FIESC	LN995604	ITEM 10392	wheat	Italy	Villani et al. 2016	DAS
	FIESC	GQ915563	NRRL 31160	lung of patient with adenocarcinoma	USA	Proctor et al 2009	NA
	<i>Fusarium</i> sp.	GQ915566	FRC R-06979	unknown	unknown	Proctor et al 2009	NA
	FIESC	GQ915558	NRRL 13381	unknown	unknown	Proctor et al 2009	NA
	<i>Trichoderma hypoxylon</i>	MF600470 (outgroup)	N/A	stroma of <i>Hypoxylon anthochroum</i>	China	Liu et al. 2018	NA



Type A							
R groups	Verrucarol (VER)	Diacetoxyscirpenol (DAS)	T-2	T-2 tetraol	T-2 triol	HT-2	Neosolaniol (NEO)
1	H	OH	OH	OH	OH	OH	OH
2	OH	OAc	OAc	OH	OH	OH	OAc
3	OH	OAc	OAc	OH	OH	OH	OAc
4	H	H	H	H	H	H	H
5	H	H	OCO=CH ₂ CH(CH ₃) ₂	OH	OCO=CH ₂ CH(CH ₃) ₂	OCO=CH ₂ CH(CH ₃) ₂	OH
Type B							
R groups	Nivalenol (NIV)	Deoxynivalenol (DON)	3-Acetyldeoxynivalenol (3-ADON)	15-Acetyldeoxynivalenol (15-ADON)	Fusarenon X (FUS-X)		
1	OH	OH	OAc	OH	OH		
2	OH	H	H	H	OAc		
3	OH	OH	OH	OAc	OH		
4	OH	OH	OH	OH	OH		
5	=O	=O	=O	=O	=O		

Figure S1. R group substitutes in the 2-ring trichothecene core structure.

Protein: Trichodiene synthase
 PDB ID: 2PS5; Chain: A
 Ligand interaction: MG701A: Magnesium



Variable				Conserved				
1	2	3	4	5	6	7	8	9
1	2	3	4	5	6	7	8	9

Figure S2. Conserved ligand-binding region of trichodiene synthase (PDB model 2PS5 Chain A).

Protein: Trichodiene synthase
 PDB ID: 2PS5; Chain: A and B
 Ligand interaction: Pyrophosphate-2 and Magnesium in Chain B

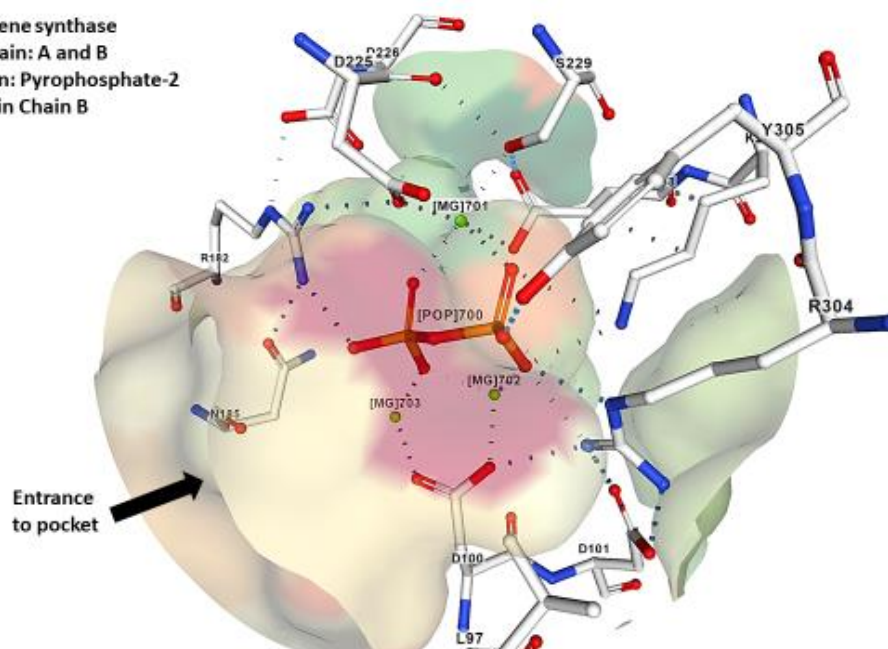


Figure S3. Ligand-binding sites of the tertiary conformation of trichodiene synthase (PDB model 2PS5 Chains A and B).

Protein: Trichodiene synthase

PDB ID: 2PS5

Chain: B

Ligand interaction: MG: Magnesium ion;

POP: Pyrophosphate-2

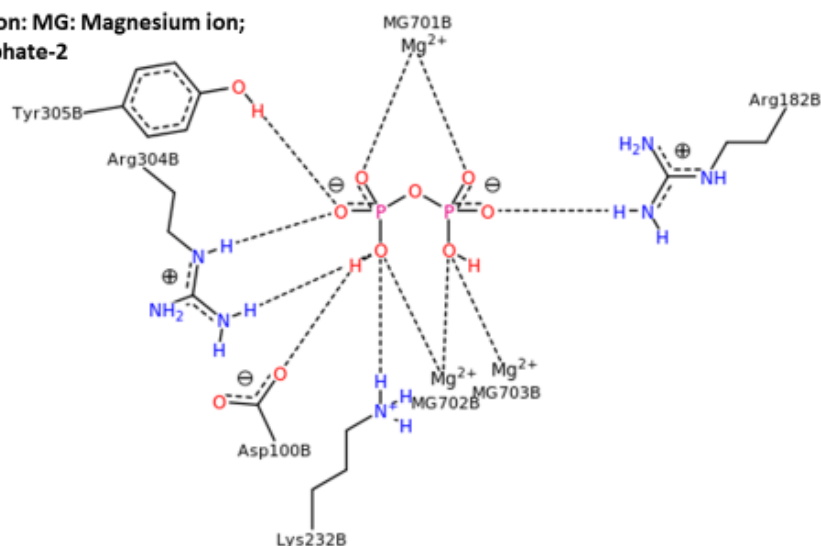
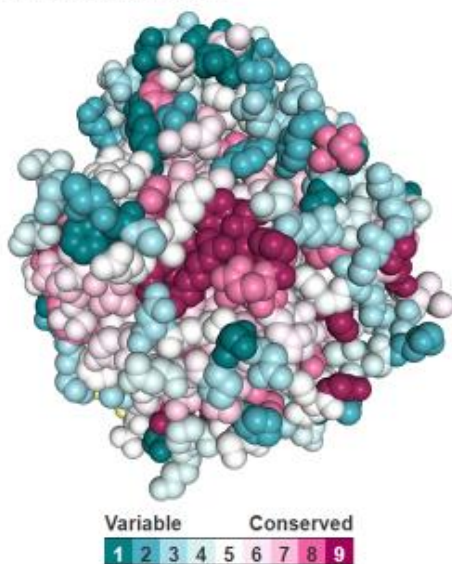


Figure S4. Interaction sites of Mg²⁺ and pyrophosphate-2 of trichodiene synthase (PDB model 2PS5 Chain B).

Protein: Lipase A

PDB ID: 3GUU; Chain: A

Ligand interaction: None



Protein: Lipase A

PDB ID: 3GUU; Chain: A

Ligand interaction: EDO802:A; 1,2-Ethanediol

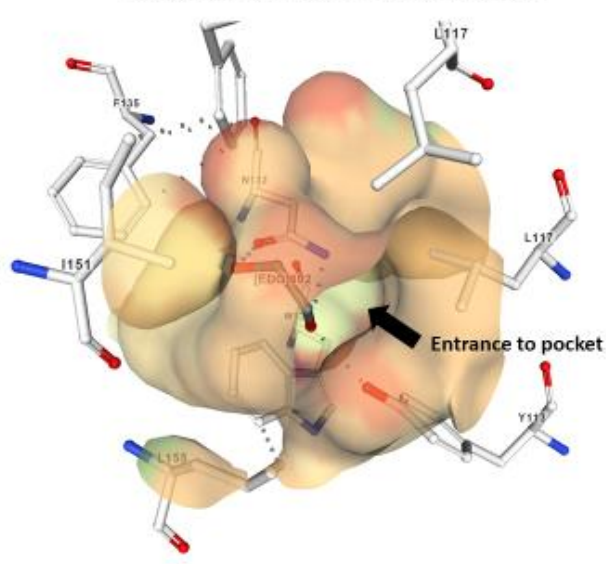


Figure S5. Ligand-binding sites of the tertiary conformation of trichothecene C-3 esterase (PDB model 3GUU Chains A).