

SUPPLEMENTARY INFORMATION

Binding of mycotoxins to proteins involved in neuronal plasticity: a combined *in silico*/wet investigation.

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Running title: binding of mycotoxins to proteins

Supplementary Table 1.

Results of the blind docking simulations for mycotoxins recognizing their selected human protein targets (see Table 1).

LIGAND	BEST PREDICTED BINDING ENERGY (kcal/mol)	NUMBER OF POSES IN THE CLUSTER	CANONICAL BINDING SITE
Amine oxidase [Flavin-containing] B (2BK3)			
Ochratoxin A (deprotonated)	-10,43	3	YES
Gliotoxin	-7,79 -7,08	3 38	YES NO
Beta-zearalanol	-7,39 -6,68	1 11	NO NO
Deoxynivalenol	-7,12 -6,99	1 32	NO NO
Amino-acid oxidase (2DU8)			
Ochratoxin A (deprotonated)	-8,05	7	NO
Ochratoxin A (protonated)	-8,44	1	NO
Deoxynivalenol	-5,04 -4,27	1 10	NO NO
Gliotoxin	-5,83 -5,25	5 12	NO NO
Aldo-keto reductase family 1 member 3 (1S1P)			
Aflatoxin M1	-8,03	48	NO
Aflatoxin B2	-8,09	44	YES
Aflatoxicol	-7,95	42	YES
Alfa-zearalanol	-7,80 -6,95	2 21	YES YES
Gliotoxin	-8,23 -7,20	7 31	YES YES
Tankyrase-2 (3MHJ)			
Aflatoxin B2	-10,77	38	YES
Aflatoxin M1	-11,04	32	YES
Aflatoxin M2	-9,93	26	YES
Aflatoxicol	-10,41	25	YES
Deoxynivalenol	-7,47 -6,32	3 13	YES NO
Acetylcholinesterase (1B41)			
Aflatoxin B1	-8,37	58	YES
Aflatoxin B2	-8,95	56	NO
Aflatoxicol	-8,82 -8,22	2 21	NO NO
Ochratoxin A (protonated)	-8,33 -7,81	8 11	NO NO
Gliotoxin	-7,45	71	NO
Deoxynivalenol	-5,72	10	NO

LIGAND	BEST PREDICTED BINDING ENERGY (kcal/mol)	NUMBER OF POSES IN THE CLUSTER	CANONICAL BINDING SITE
cAMP-specif 3'-5'-cyclic phosphodiesterase 4D (1XOQ)			
Ochratoxin	-7,62	3	YES
A(deprotonated)	-6,39	14	YES
Gliotoxin	-6,78	23	YES
Beta-secretase (1FKN)			
Ochratoxin A	-9,40	19	YES
(deprotonated)	-9,13	27	YES
Gliotoxin	-6,62	8	NO
	-4,44	39	YES
5(3) deoxyribonucleotidase (1Q92)			
Aflatoxin B1	-8,70	24	YES
Alfa-zearalanol	-8,76	17	YES
	-8,37	20	YES
Aflatoxin M2	-8,51	23	YES
	-8,41	24	YES
Glutamate carboxypeptidase 2 (3D7F)			
Ochratoxin A	-9,27	2	NO
(protonated)	-8,18	6	NO
Gliotoxin	-5,34	12	NO
GMP reductase 2 (2C6Q)			
Ochratoxin A	-7,10	1	YES
(protonated)	-6,10	3	NO
Gliotoxin	-6,83	16	YES
Inositol monophosphatase (1IMB)			
Ochratoxin A	-7,05	5	NO
(protonated)	-6,51	10	YES
Gliotoxin	-7,27	4	YES
	-6,58	27	NO
Nicotinamide N-methyltransferase (2IIP)			
Ochratoxin A	-8,92	1	NO
(deprotonated)			
Alfa-zearalanol	-9,93	4	YES
	-7,16	37	NO
Beta-zearalanol	-7,12	1	NO
	-6,73	36	NO
Kynurenine-oxoglutarate transaminase 1 (3FVS)			
Ochratoxin A	-5,56	8	YES
(deprotonated)			
Gliotoxin	-5,90	3	YES
Carnitine O-Acetyltransferase (1NM8)			
Ochratoxin A	-7,91	8	NO
(protonated)			
Gliotoxin	-6,78	8	NO
	-6,30	11	NO

LIGAND	BEST PREDICTED BINDING ENERGY (kcal/mol)	NUMBER OF POSES IN THE CLUSTER	CANONICAL BINDING SITE
Neurologin-4, X-linked (3BE8)^a			
Aflatoxin B1	-7,17	27	NO
Aflatoxin B2	-6,94	36	NO
Ochratoxin A (protonated)	-6,99	19	NO
Ochratoxin A (deprotonated)	-7,49	10	YES
	-7,43	14	NO
Gliotoxin	-6,13	5	NO
	-5,43	13	NO
Deoxynivalenol	-5,05	2	NO
	-4,77	7	NO

^a: the docking were performed with the same ligands that recognize acetylcholinesterase in the inverse docking procedure

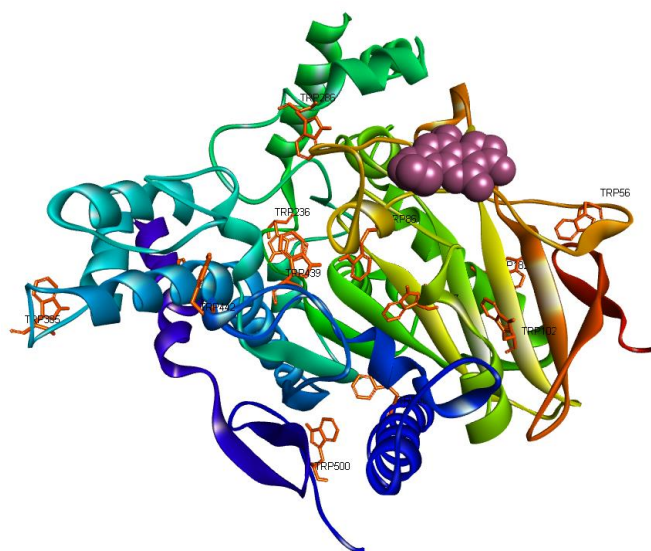
Supplementary Table 2.

Results of the docking simulations focused on the canonical binding site of AchE and NLGN4X for mycotoxins recognizing their selected human protein targets

Acetylcholinesterase (1B41)		
LIGAND	BEST PREDICTED BINDING ENERGY (kcal/mol)	NUMBER OF POSES IN THE CLUSTER
Aflatoxin B1	-4,61	100
Aflatoxin B2	-4,13 -4,10	9 83
Gliotoxin	-4,31 -4,02	40 59
Aflatoxicol	-4,60	60
Ochratoxin A (protonated)	-4,72 -3,34	8 26
Deoxynivalenol	-4,12 -3,58	6 94
Neuroigin-4, X-linked (3BE8)		
Aflatoxin B1	-7,06	51
Aflatoxin B2	-6,90 -6,49	20 62
Gliotoxin	-6,77	74
Deoxynivalenol	-6,58	89
Ochratoxin A (protonated)	-7,19 -6,62	16 18
Ochratoxin A (deprotonated)	-7,43	42

Supplementary Figure 1: Position of the Trp residues in AChE (A) and NLGN4X (B). The Trp residues are shown as sticks. The binding site of the mycotoxins is shown in CPK mode

A



B

