

An *in-silico* pipeline for rapid screening of DNA aptamers against mycotoxins: the case-study of fumonisin B1, aflatoxin B1 and ochratoxin A

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Programs, configuration files and actual input and outputs can be found at:
https://github.com/oivulf/dna_toxin_binding

Table S1. *In-silico* selectivity tests for aflatoxin B1 (AFB1) aptamers towards ochratoxin A (OTA) and comparison with docking calculations for the target AFB1.

Aptamer name	Docking energy (kcal/mol)	
	AFB1	OTA
AF_AB3	-9.2	-9.1
AF_APT1	-10.66	-12.6

Table S2. *In-silico* selectivity tests for ochratoxin A (OTA) aptamers towards aflatoxin B1 (AFB1) and comparison with docking calculations for the target OTA.

Aptamer name	Docking energy (kcal/mol)	
	OTA	AFB1
1.12.2	-10.38	-8.2
A08	-17.08	-12.8
A08min	-12.05	-5.1
H8	-12.91	-10.5
H12	-9.98	-8.9

Table S3. Timings (s)

Aptamer name	Annealing	Dynamics	Docking: grid generation (20 core)	Docking: space sampling, single pose, mean
Fumonisin B1				
FB1_39	41358	109729	720	6325
FB1_39T3	39000	78500	835	5131
FB1_10	49698	81250	735	1500
Aflatoxin B1				
AF_AB3	43272	69537	360	93
AF_APT1	49345	78681	280	105
Ochratoxin A				
1.12.2	17567	27912	481	123
A08	45211	71216	475	74
A08min	20900	34216	417	55
H8	38385	61370	312	55
H12	37150	60121	312	53