Supporting information

Solvent Directed Morphogenesis of Peptidic-Benzimidazolium Dipodal Receptor: Ratiometric Detection and Catalytic Degradation of Ochratoxin A

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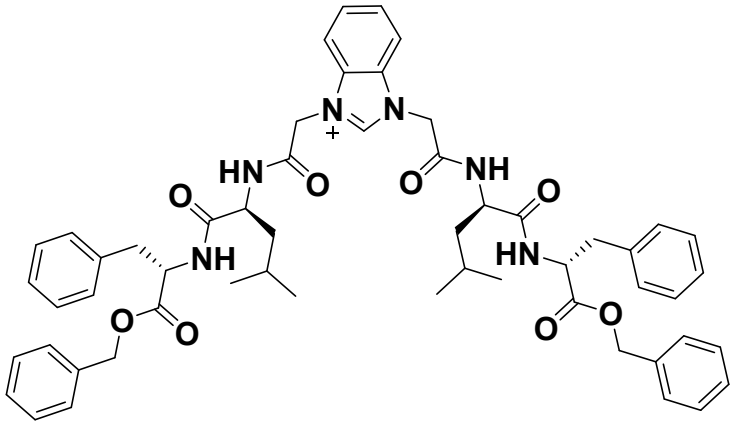
Chemical structure of Dipodal receptor (SS4)



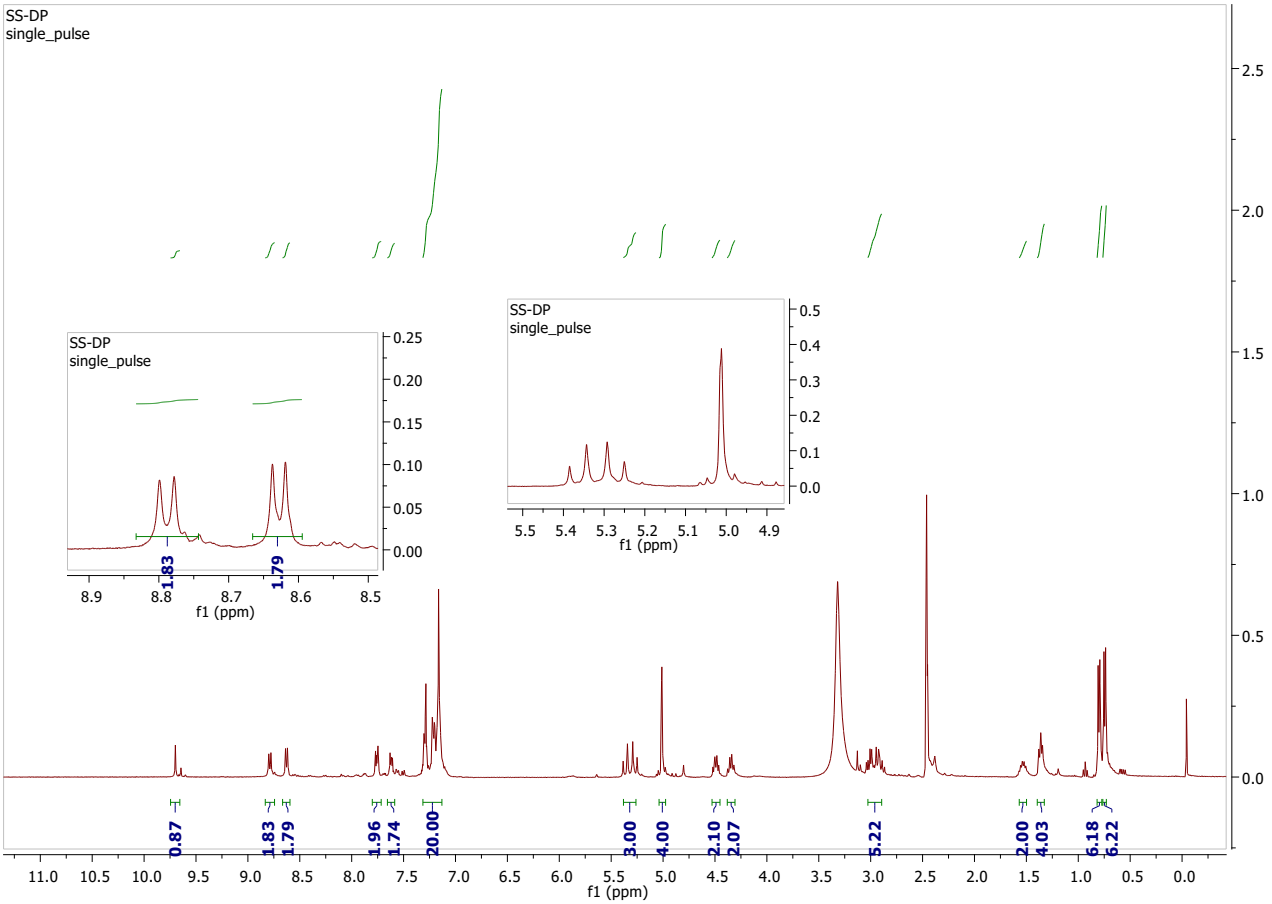


Figure SF1: ^{1}H NMR spectrum of peptidic-benzimidazole dipodal receptor (**SS4**).

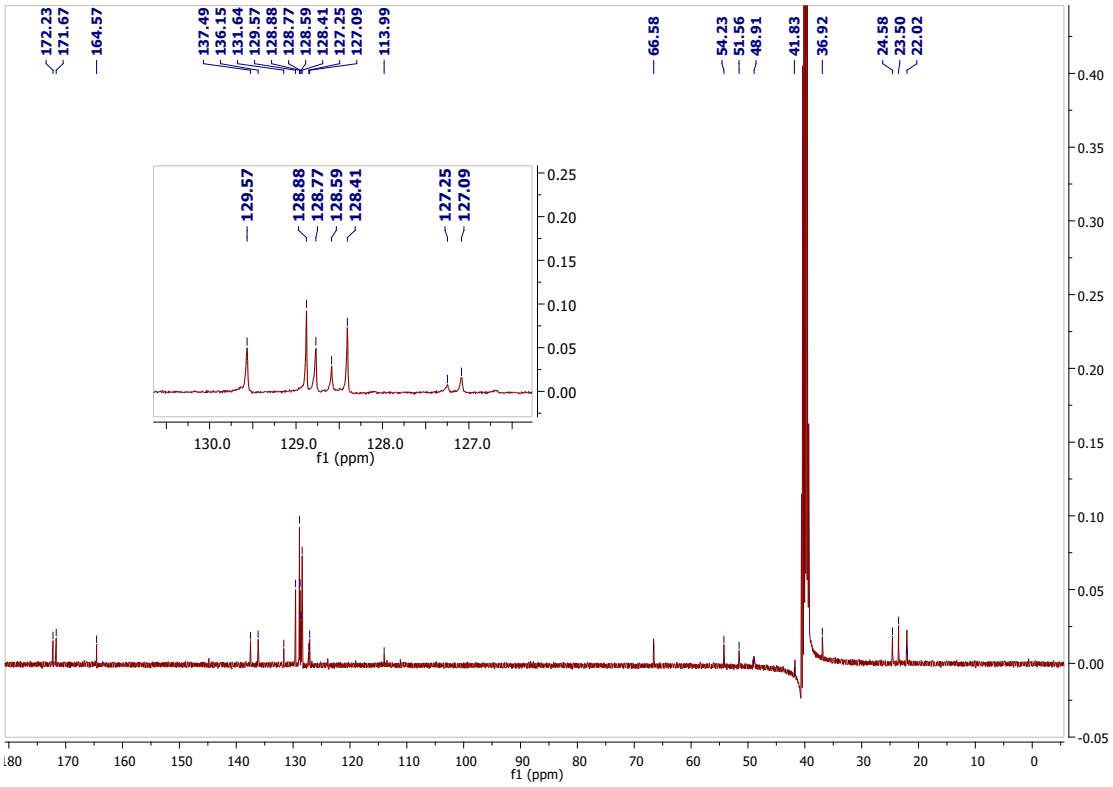


Figure SF2: ^{13}C NMR spectrum of peptidic-benzimidazole dipodal receptor (**SS4**).

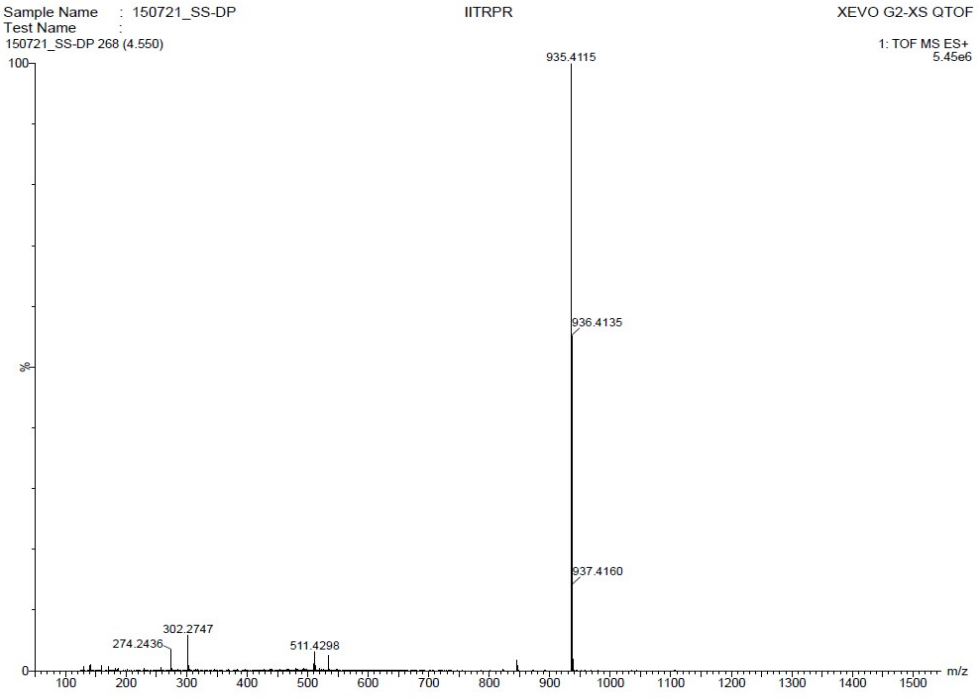


Figure SF3: Mass data of peptidic-benzimidazole dipodal receptor (**SS4**).

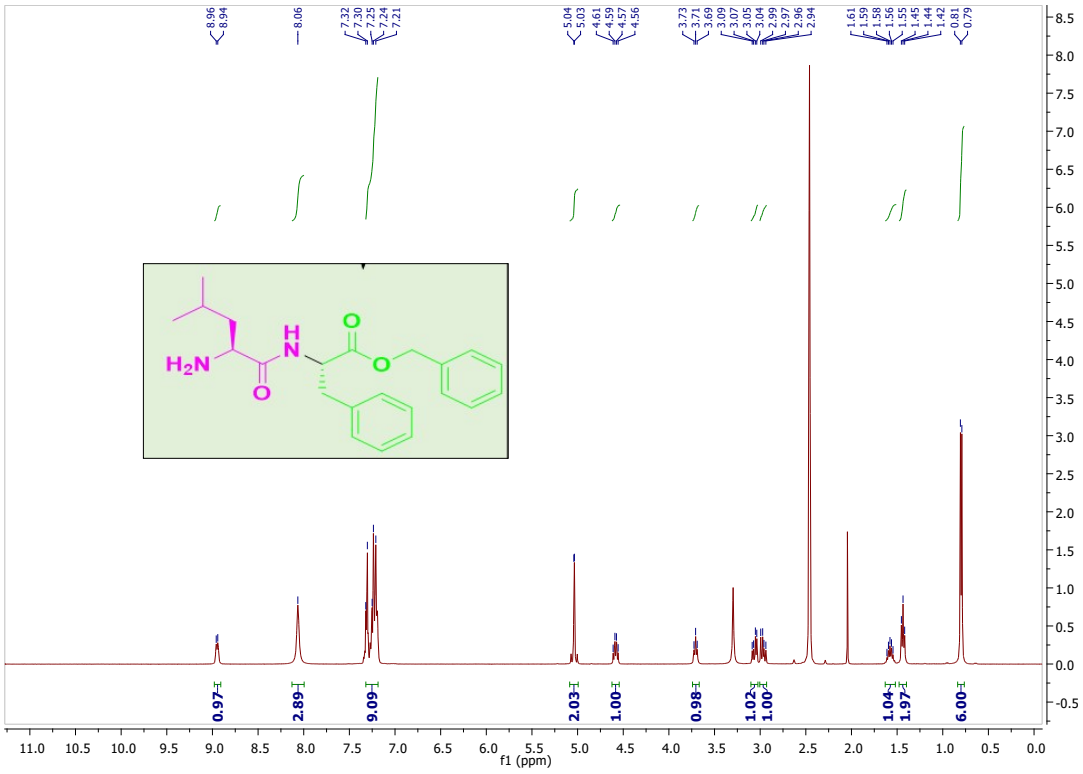


Figure SF4: [1]H NMR data of compound (2).

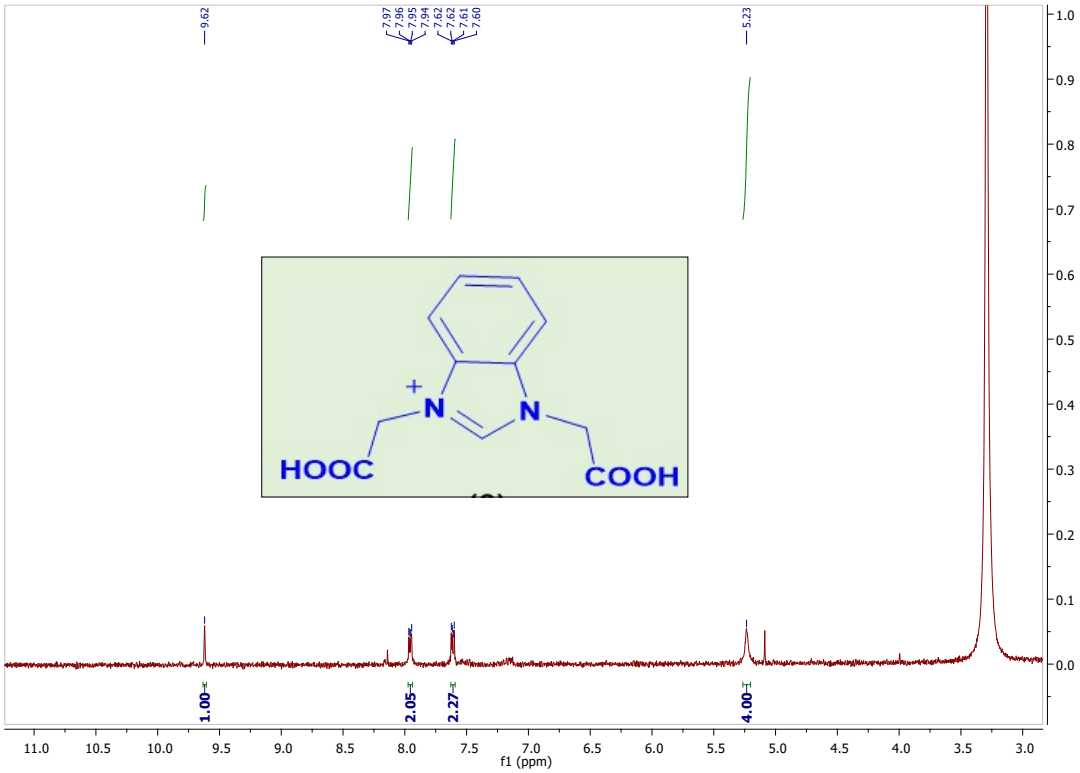
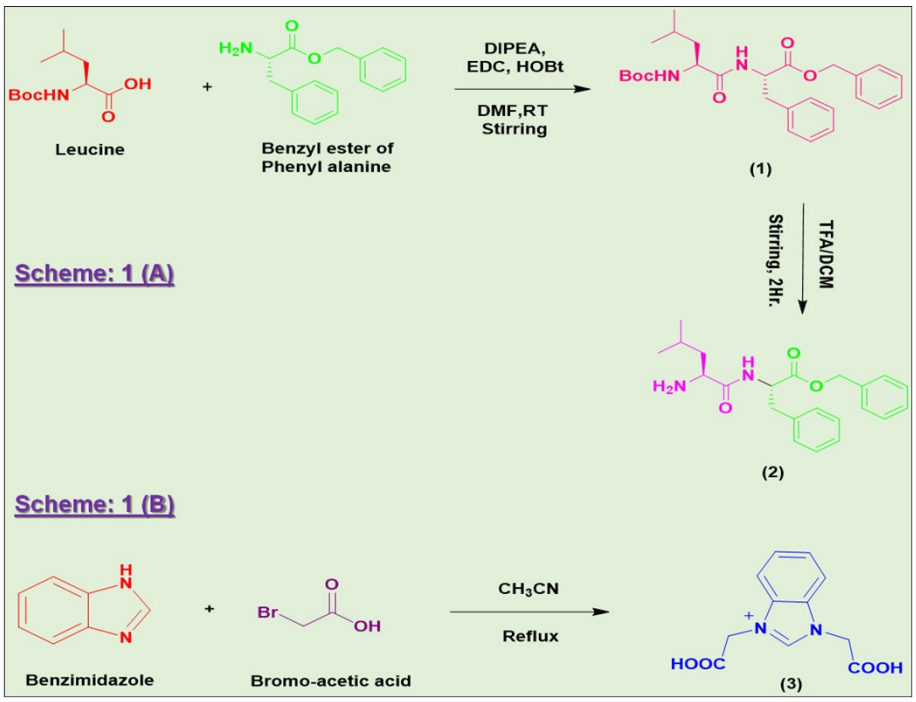


Figure SF5: [1]H NMR data of compound (3).



Scheme S1 (A) and (B): Reaction scheme for the preparation of dipeptide (2) and di-acid (3), respectively.

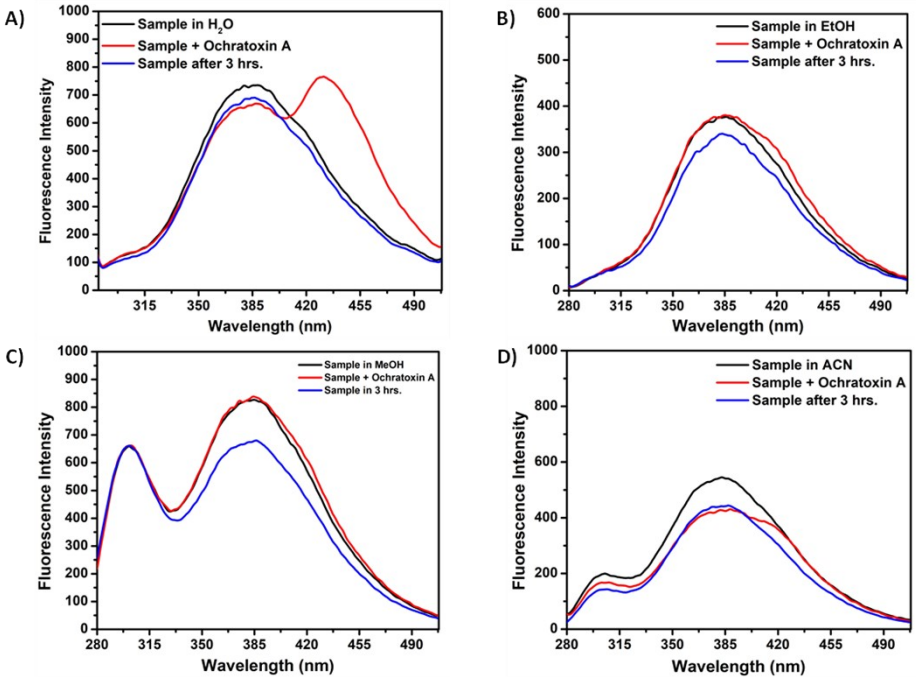


Figure SF6: A) Fluorescence emission profile of sample 4 on addition of Ochratoxin A. **B)** Fluorescence emission profile of sample 2 on addition of Ochratoxin A. **C)** Fluorescence emission profile of sample 1 on addition of Ochratoxin A. **D)** Fluorescence emission profile of sample 3 on addition of Ochratoxin A.

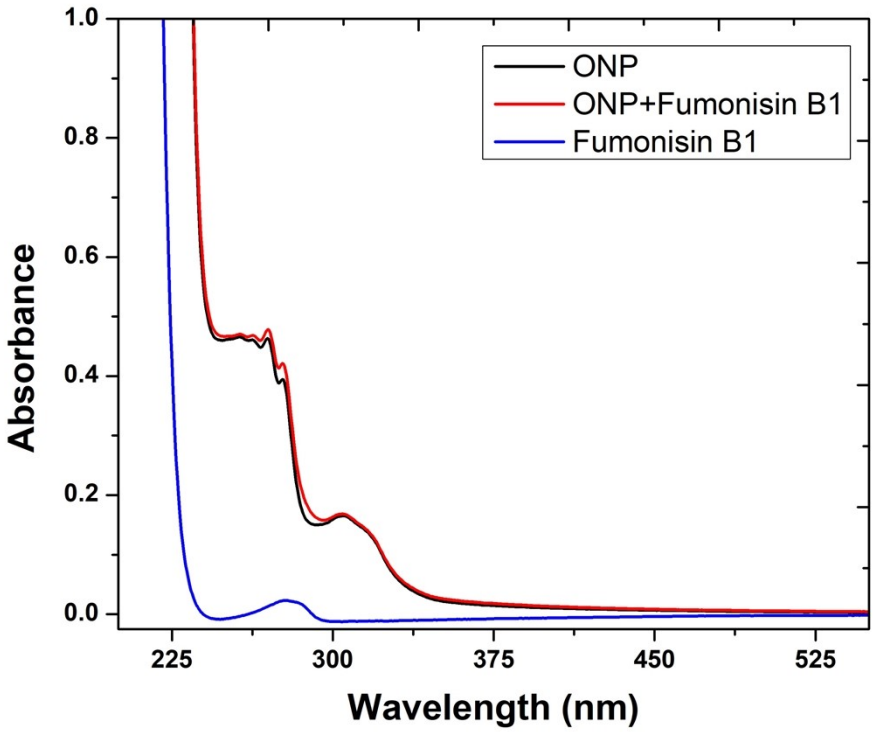


Figure SF7: UV-Visible absorption study of **SS4** (ONPs) with Fumonisin B1.

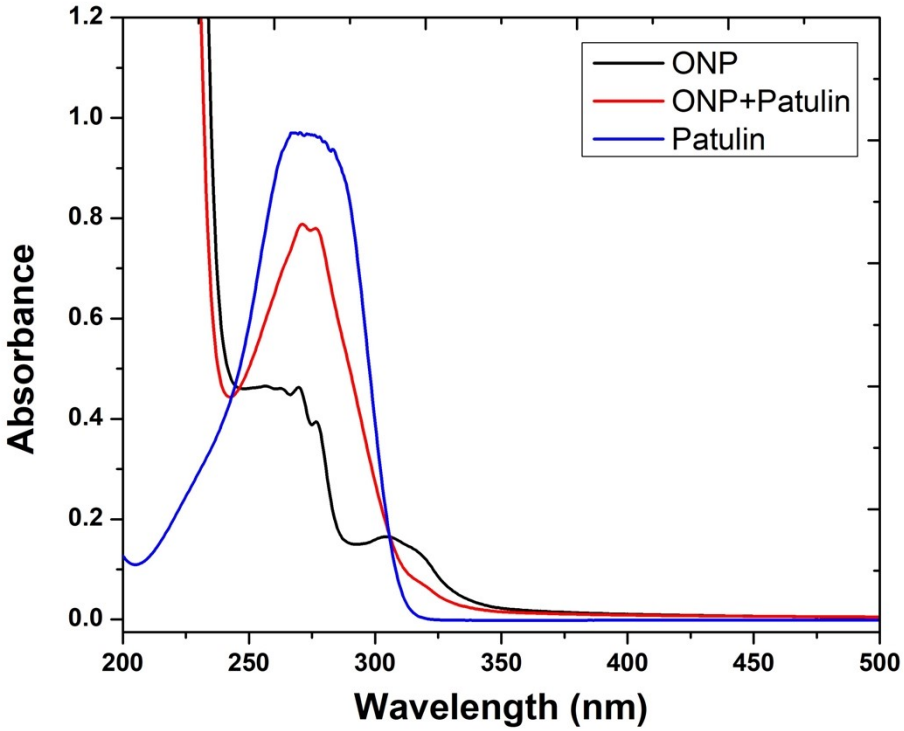


Figure SF8: UV-Visible absorption study of **SS4** (ONPs) with Patulin.

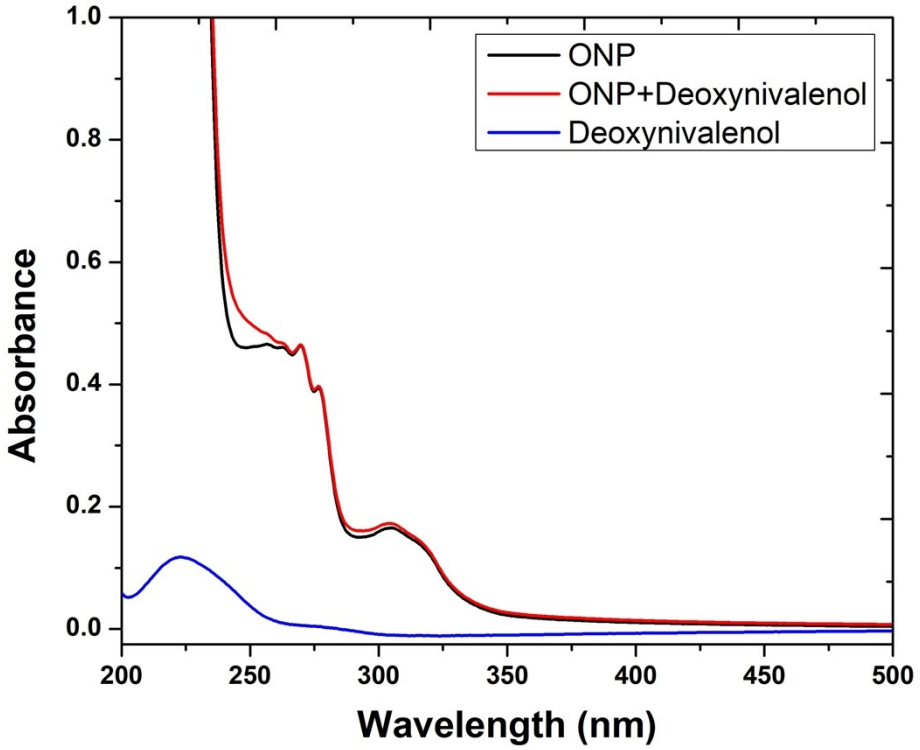


Figure SF9: UV-Visible absorption study of **SS4** (ONPs) with Deoxynivalenol.

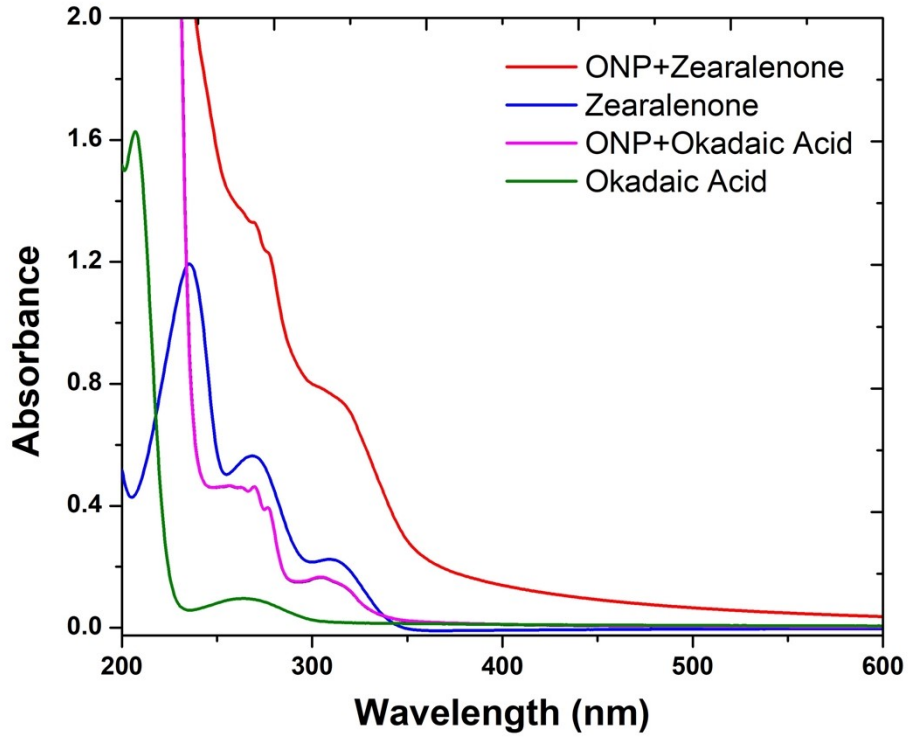


Figure SF10: UV-Visible absorption study of **SS4** (ONPs) with Zearalenone and Okadaic acid.

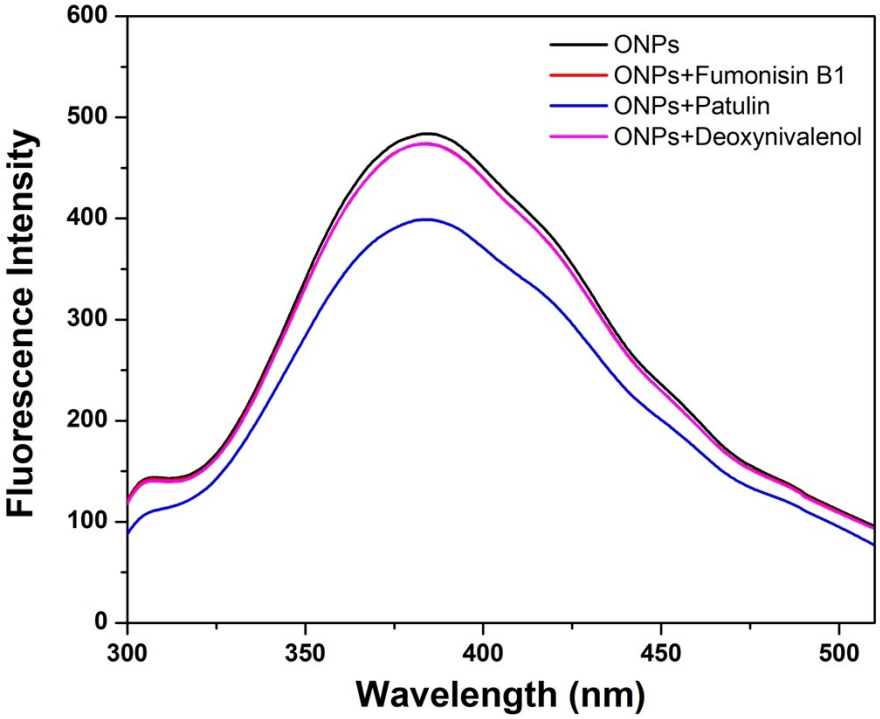


Figure SF11: Fluorescence emission profile of **SS4** (ONPs) on addition of various toxins.

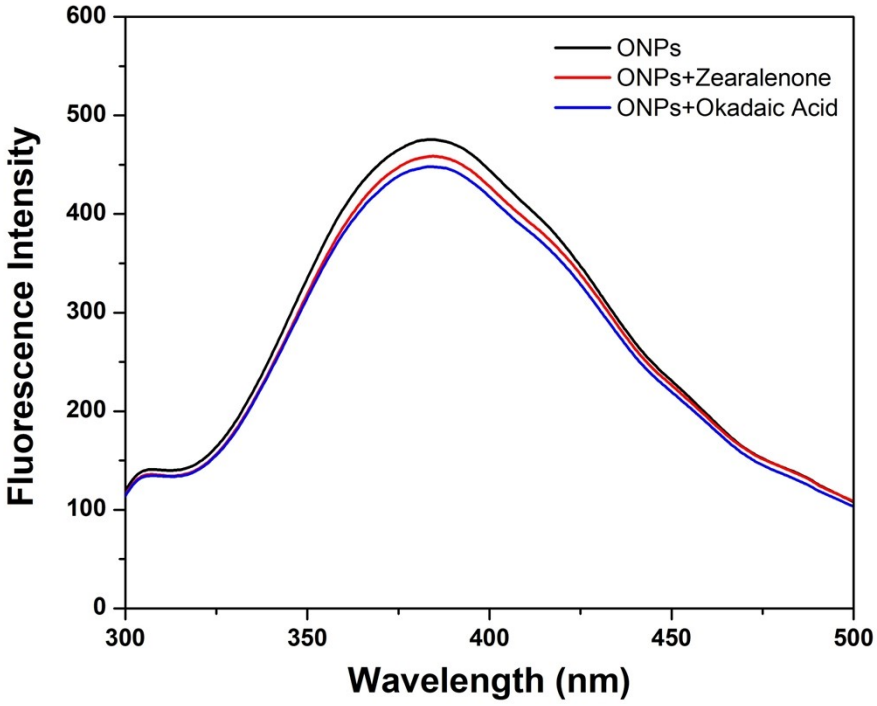


Figure SF12: Fluorescence emission profile of **SS4** (ONPs) on addition of Zearalenone and Okadaic acid.

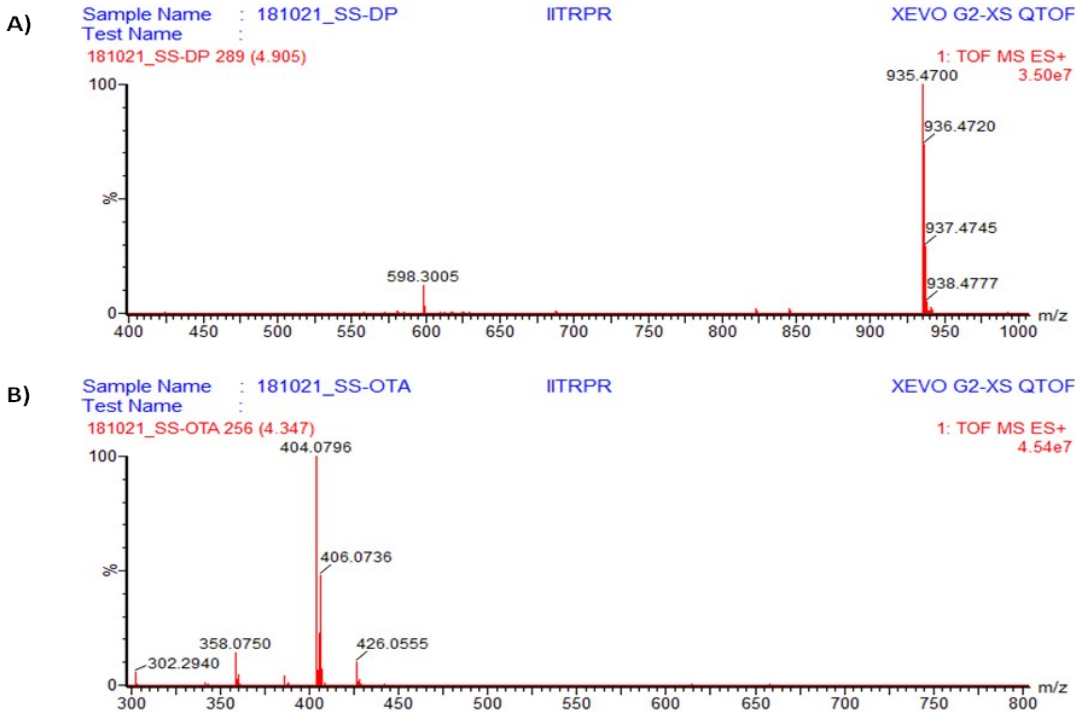


Figure SF13: LCMS data showing m/z value of dipodal receptor (**SS4**) and ochratoxin A.

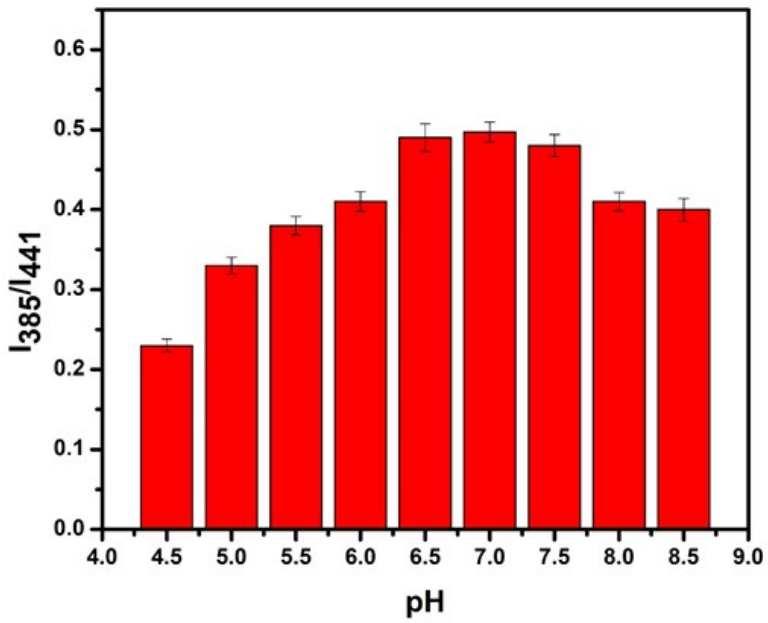


Figure SF14: Relative fluorescence intensity of sensing probe at different pH

The binding constant was calculated using Benesi-Hildebrand Equation stated below.

$$1/(A\text{-}A_o) = 1/\{K(A_{max} - A_o)[OTA]\} + 1/[A_{max} - A_o]$$

Here Ao is the absorbance of receptor (SS4) in the absence of OTA, A is the absorbance recorded in the presence of OTA, A_{max} is absorbance in presence of added $OTA]_{max}$ and K_a is the association constant. The association constant (K_a) could be determined from the slope of the straight line of the plot of 1/(A-Ao) against 1/[OTA] and is found to be $8.59 \times 10^4\ M^{-1}$

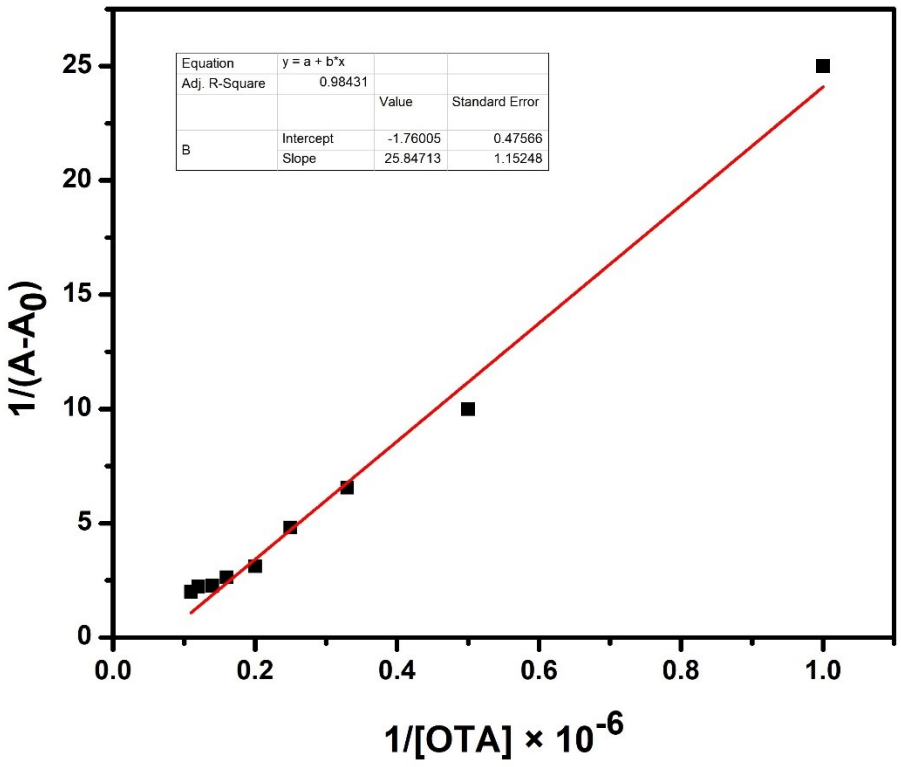


Figure SF15: Benesi–Hildebrand plot from UV/vis titration data of SS4 (50 μM) with OTA.

The following equation was used to calculate the quantum yields by comparison with fluorescein (Φs = 0.97 in basic ethanol) as a reference.

$$\Phi X = \Phi S \times \left(\frac{Ix}{Is}\right) \times \left(\frac{As}{Ax}\right) \times \left(\frac{nx}{ns}\right)^2$$

where A is the absorbance, n is the solvent's refractive index, Φ is the quantum yield, I is the integrated area under the fluorescence emission curve, and x and s, respectively, denote the unknown and standard solution.

Using the aforementioned equation, we were able to compute the quantum yields of SS4 and SS4-OTA, which come out to be 0.51 and 0.53 respectively.

Table S1: Ochratoxin A recovery experiment in spiked samples.

S. No.	Sample	Spiked concentration	Found concentration	Recovery (%)	RSD
1.		1.5 µM	1.54 µM	102.6	3.21
		2.0 µM	1.96 µM	98	2.75
		2.5 µM	2.47µM	98.8	1.86
2.		1.5 µM	1.48 µM	98.6	2.38
		2.0 µM	1.97 µM	98.5	3.54
		2.5 µM	2.54 µM	101.6	1.73

Table S2: Literature comparison with present work.

S. No.	Type of Method		Medium	LOD	References
	Detection	**Degradation**			
1.	Fluorescence based	✕	Binding buffer (pH – 8.5)	17.2 nM	Food Control 60 (2016) 296-301.
2.	Colorimetric method	✕	Buffer solution	5.0 nM	Journal of Hazardous Materials 388 (2020) 1217583
3.	Colorimetric ELISA	✕	Bicarbonate buffer pH (8.6) & PBS buffer (7.4)	40 pg/mL	Sensors and Actuators B 262 (2018) 102–109
4.	Fluorescence based ratiometric detection	Catalytic degradation by peptidic-benzimidazole dipodal receptor	Aqueous medium	2.1×10^{-7} M	Present work
5.	HPLC	By hydrolytic action of Alcaligenes faecalis	LB medium	NA	Journal of Applied Microbiology 123, 661 – 668
6.	LCMS	By lactic acid bacteria	MRS medium	NA	Food and Chemical Toxicology 112 (2018) 60 - 66
7.	HPLC	commercial peroxidase (POD) enzyme (Armoracia rusticana)	Potassium phosphate buffer, water, H_2O_2	NA	Food research international 131 (2020) 109039