Box-Behnken Optimized MPA-CdTe Quantum Dots as Turn-Off Fluorescent Probes for Sensitive Lurasidone Determination in Pharmaceutical, Biological, and Environmental Matrices

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Table S1: Box-Behnken experimental design matrix for optimization of sensing conditions in lurasidone determination.

		Factor 1	**Factor 2**	**Factor 3**
Std	Run	A:pH	B:MPA-CdTe QDs	C:Reaction time
			mL	min
6	1	10	1	1
16	2	7.5	1	3
2	3	10	0.5	3
5	4	5	1	1
15	5	7.5	1	3
9	6	7.5	0.5	1
1	7	5	0.5	3
12	8	7.5	1.5	5
13	9	7.5	1	3
11	10	7.5	0.5	5
17	11	7.5	1	3
10	12	7.5	1.5	1
8	13	10	1	5
7	14	5	1	5
14	15	7.5	1	3
3	16	5	1.5	3
4	17	10	1.5	3

Table S2: Analysis of variance (ANOVA) for the reduced quadratic model of fluorescence quenching response.

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	1.81	4	0.4521	63.17	< 0.0001	significant
A-pH	0.3188	1	0.3188	44.54	< 0.0001	
B-MPA-CdTe QDs	0.4408	1	0.4408	61.59	< 0.0001	
A^2	0.8461	1	0.8461	118.21	< 0.0001	
B^2	0.1589	1	0.1589	22.20	0.0005	
Residual	0.0859	12	0.0072			
Lack of Fit	0.0655	8	0.0082	1.61	0.3406	not significant
Pure Error	0.0204	4	0.0051			
Cor Total	1.89	16				

Table S3: Statistical comparison between the developed MPA-CdTe QDs fluorescence quenching method and the reported HPLC method for lurasidone determination in pharmaceutical formulations.

Method	*Mean* [a]	*SD*	*t-test (2.306)* [b]	*P value*	*F-value (6.338)* [b]	*P value*	θ_L [c]	θ_U [c]
Developed method	100.49	1.040	0.330	0.750	1.099	0.929	-1.270	1.695
Reported method	100.28	0.992						

[a] Average of five determinations

[b] The values in parenthesis are tabulated values of "t "and "F" at (P = 0.05)

[c] Bias of ± 2% is acceptable

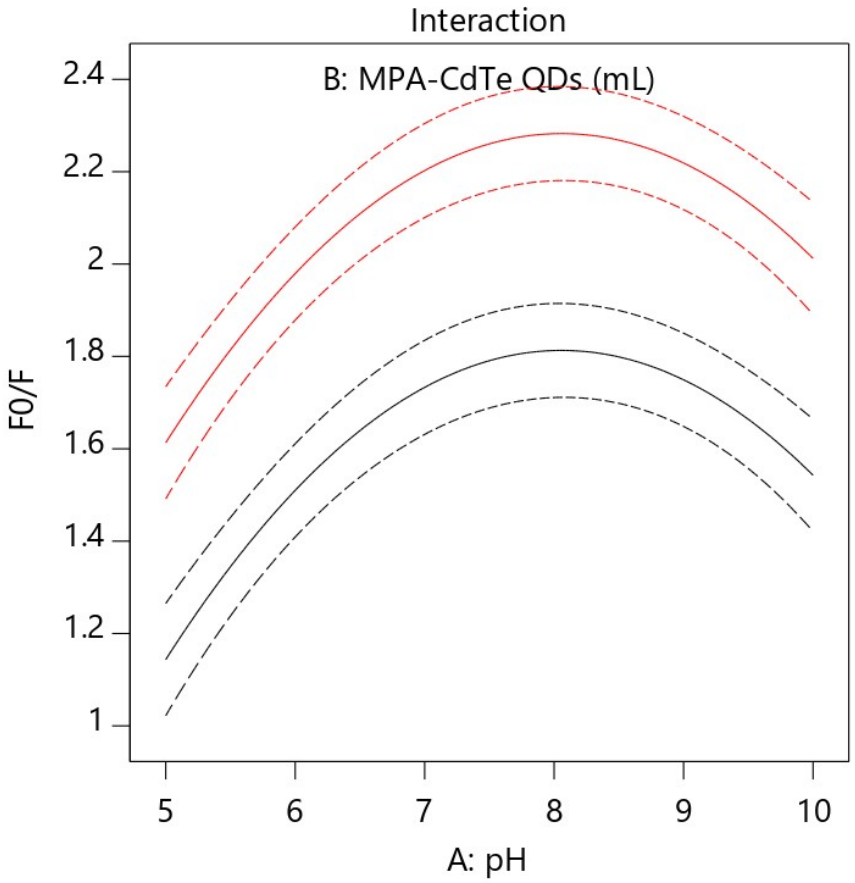

Fig. S1: Interaction plot showing the effect of pH (Factor A) and MPA-CdTe QDs volume (Factor B) on the fluorescence quenching response (F0/F) for lurasidone determination.

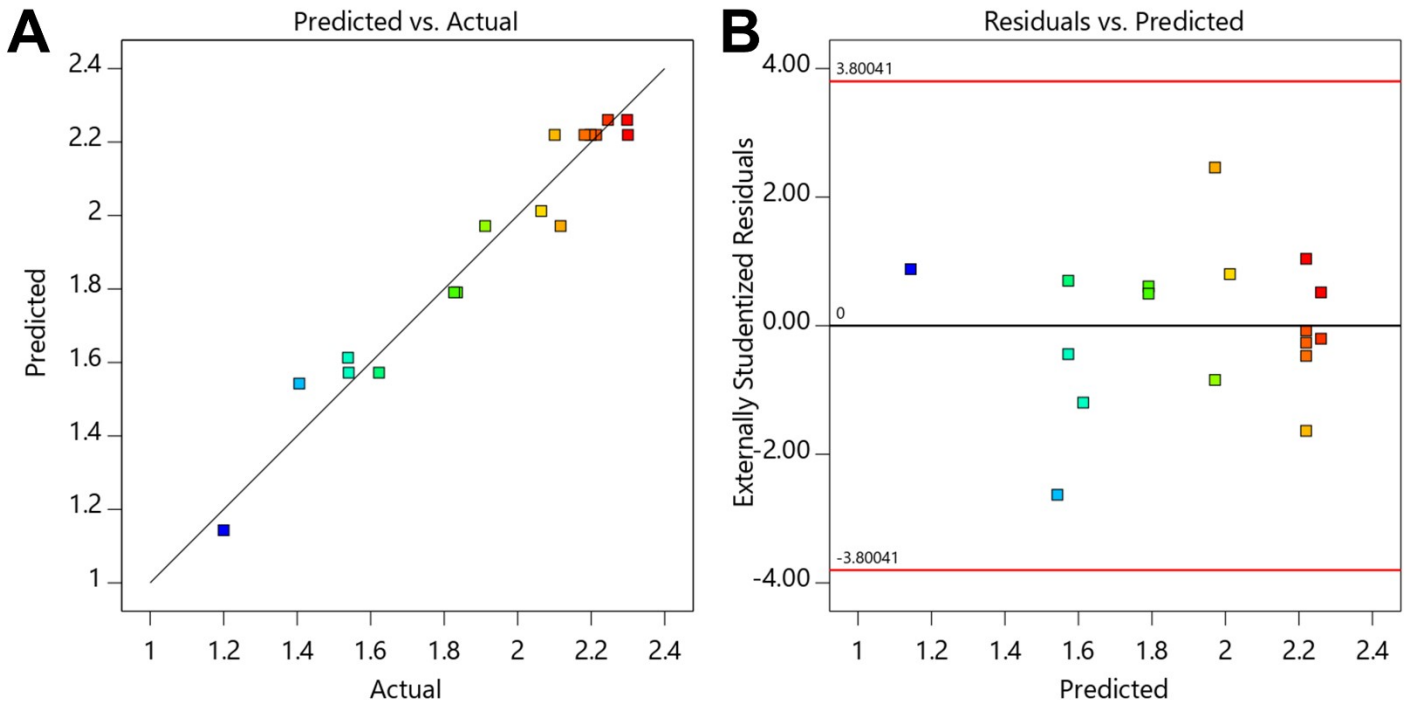

Fig. S2: Model validation plots for the fluorescence quenching response. (A) Predicted versus actual values plot showing good agreement between experimental and model-predicted responses. (B) Residuals versus predicted values plot demonstrating random distribution of residuals within acceptable limits (±3.80), indicating absence of systematic bias in the model.

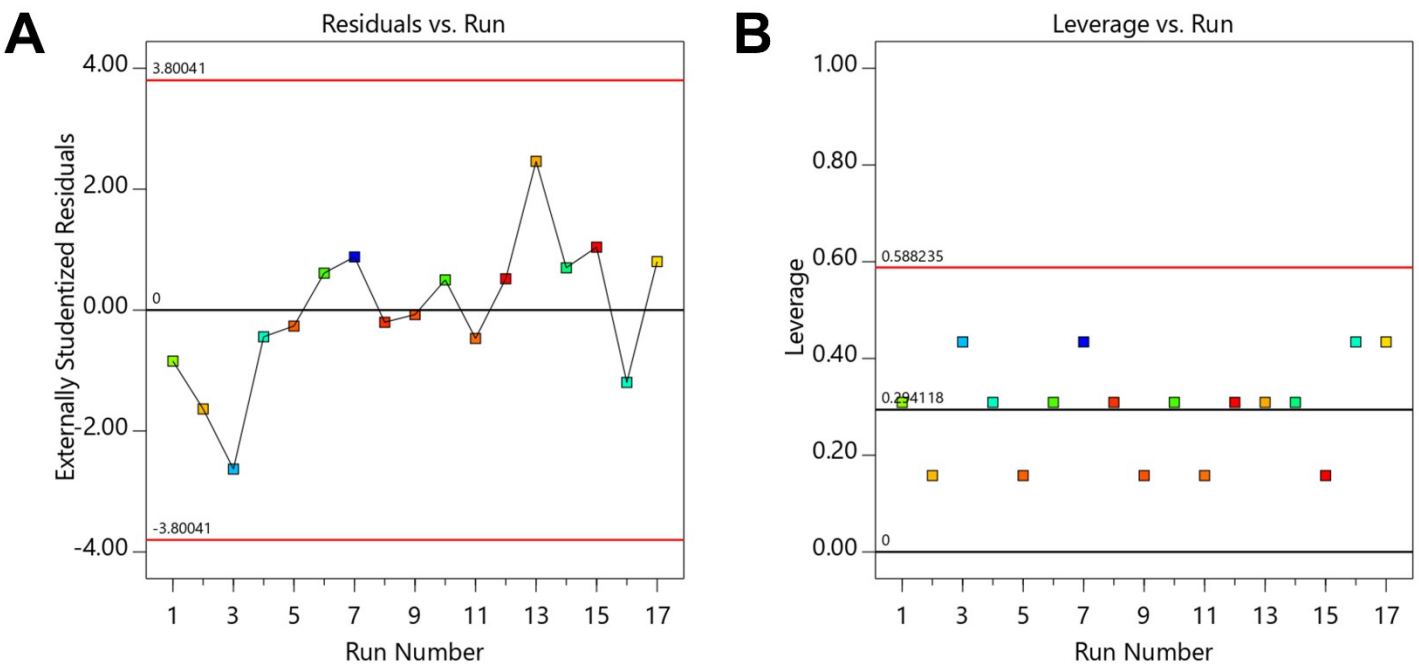

Fig. S3: Model diagnostic plots for experimental run sequence. (A) Externally studentized residuals versus run number plot showing all points within control limits (±3.80), confirming absence of outliers. (B) Leverage versus run number plot with all points below the critical value (0.588), indicating no influential experimental runs.

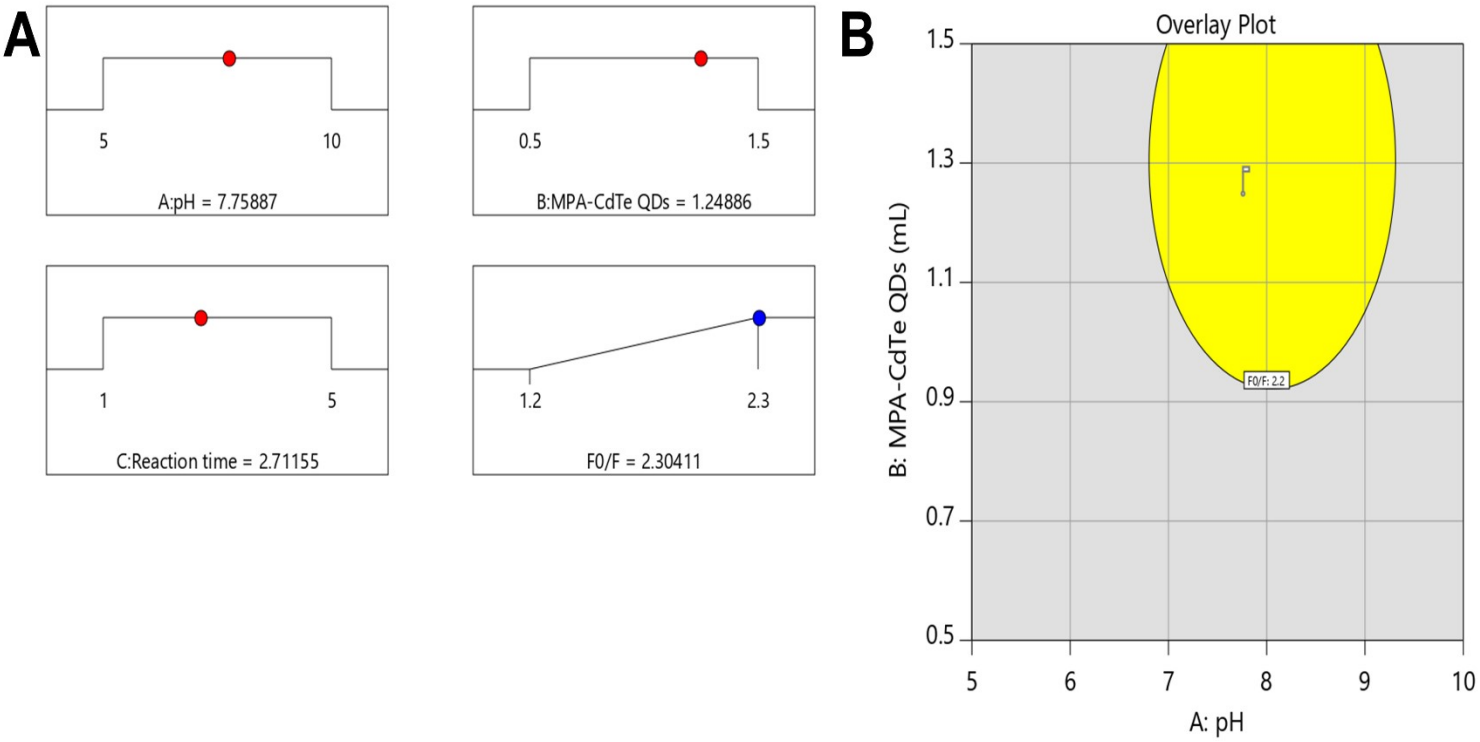

Fig. S4: Optimization of experimental conditions for maximum fluorescence quenching of MPA-CdTe QDs by lurasidone. (A) Individual desirability ramps showing optimal values for pH (7.8), MPA-CdTe QDs volume (1.25 mL), reaction time (2.71 min), and predicted maximum fluorescence quenching response (F0/F = 2.30). (B) Overlay plot displaying the optimal region (yellow) where all constraints for pH and MPA-CdTe QDs volume are satisfied to achieve maximum quenching response.