Microwave-Assisted N,S Doped Carbon Quantum Dots as Fluorescent Nanoprobes for Vibegron Determination: Face-Centered Design Optimization, Validation, and Green Chemistry Assessment

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Table S1: Face-centered central composite design matrix showing 27 experimental runs with actual values for four independent variables (pH, buffer volume, N,S-CQD concentration, and incubation time)

		Factor 1	**Factor 2**	**Factor 3**	**Factor 4**
Std	Run	A:pH	B:Buffer Volume	C:N,S CQDs	D:Time
			mL	µg/mL	min
19	1	5.5	0.5	100	9
4	2	8	1.5	50	3
24	3	5.5	1	100	15
18	4	8	1	100	9
8	5	8	1.5	150	3
16	6	8	1.5	150	15
27	7	5.5	1	100	9
1	8	3	0.5	50	3
2	9	8	0.5	50	3
21	10	5.5	1	50	9
15	11	3	1.5	150	15
23	12	5.5	1	100	3
12	13	8	1.5	50	15
13	14	3	0.5	150	15
10	15	8	0.5	50	15
20	16	5.5	1.5	100	9
25	17	5.5	1	100	9
9	18	3	0.5	50	15
5	19	3	0.5	150	3
6	20	8	0.5	150	3
26	21	5.5	1	100	9
17	22	3	1	100	9
3	23	3	1.5	50	3
14	24	8	0.5	150	15
7	25	3	1.5	150	3
22	26	5.5	1	150	9
11	27	3	1.5	50	15

Table S2: Model adequacy statistics for the reduced quadratic model.

Std. Dev.	0.1558	**R^2**	0.9866
Mean	2.75	**Adjusted R^2**	0.9806
C.V. %	5.67	**Predicted R^2**	0.9679
		Adeq Precision	33.5350

Table S3: Effect of common pharmaceutical excipients and endogenous biological components on vibegron determination (1500 ng/mL).

Interfering Substance	**QE%**	**RSD%**	**Interference**
None (Vibegron alone)	76.90	1.54	-
Pharmaceutical Excipients			
Microcrystalline cellulose	77.15	1.68	No
Lactose monohydrate	76.73	1.82	No
Magnesium stearate	77.28	1.45	No
Polyethylene glycol	76.84	1.91	No
Hypromellose (HPMC)	77.02	1.73	No
Croscarmellose sodium	76.61	1.88	No
Colloidal silicon dioxide	77.19	1.52	No
Endogenous Biological Components			
Glucose	76.58	2.15	No
Urea	77.31	1.96	No
Uric acid	76.79	1.87	No
Creatinine	77.06	1.78	No
Albumin	76.92	2.03	No
Ascorbic acid	76.45	2.21	No
Cholesterol	77.24	1.69	No

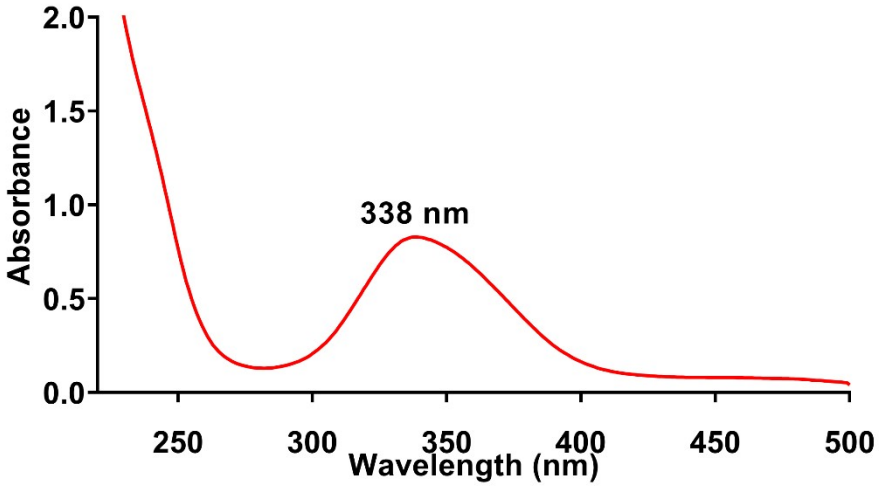

Fig. S1: Ultraviolet-visible absorption spectrum of N,S CQDs in aqueous solution showing characteristic absorption maximum at 338 nm.

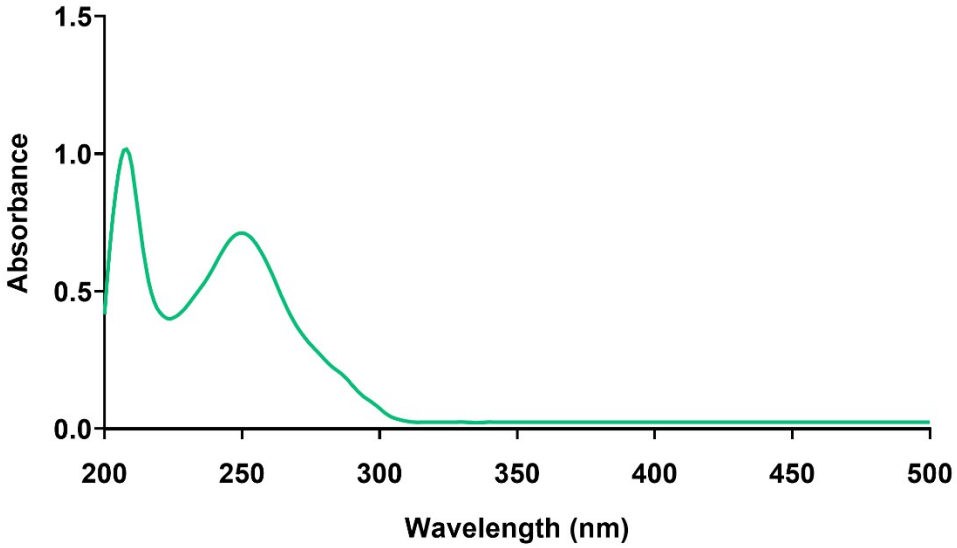

Fig. S2: Ultraviolet-visible absorption spectrum of vibegron standard solution showing absorption maxima at approximately 207 nm and 250 nm, with negligible absorption in the excitation (344 nm) and emission (418 nm) regions of N,S CQDs.

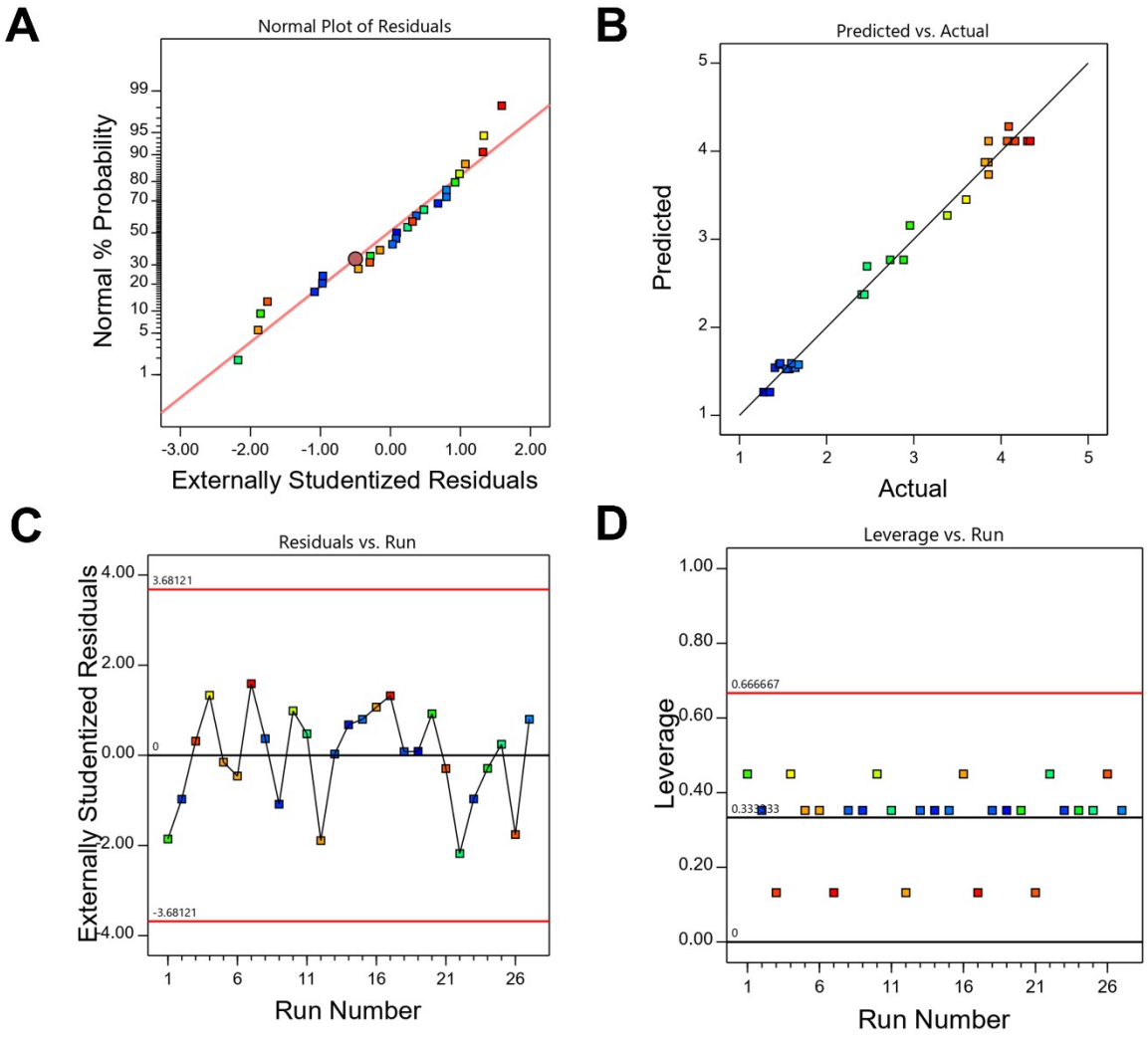

Fig. S3: (A) Normal probability plot of externally studentized residuals showing approximate linearity; (B) Predicted versus actual values plot demonstrating strong correlation along the 45° line; (C) Residuals versus run number plot showing random scatter without systematic patterns; (D) Leverage versus run number plot indicating absence of influential outliers.

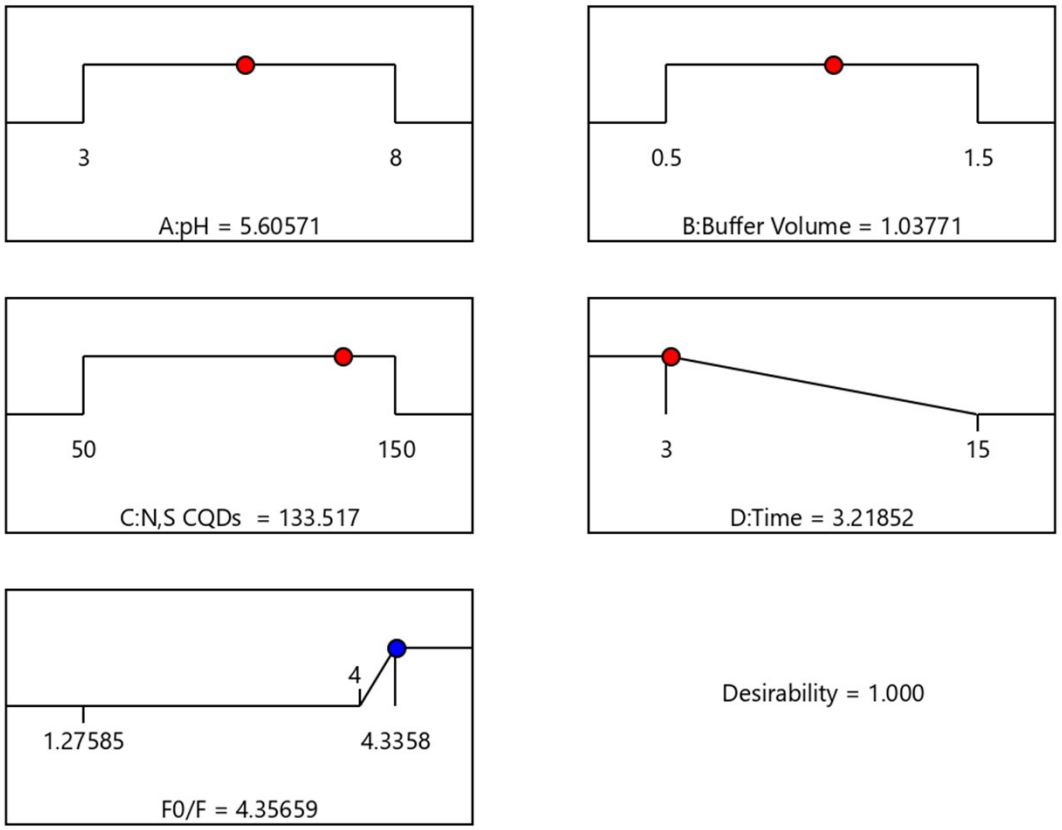

Fig. S4: Optimization ramp display showing individual desirability functions for each factor (pH, buffer volume, N,S-CQD concentration, and incubation time) with optimal settings identified yielding predicted maximum F0/F value of 4.36 with overall desirability of 1.000.

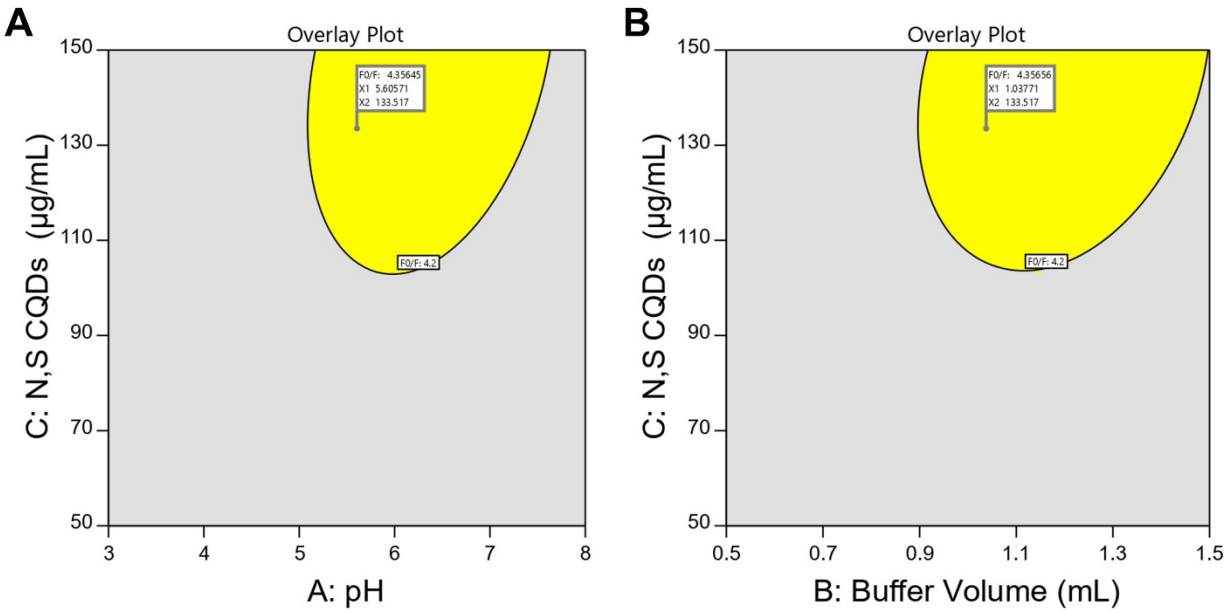

Fig. S5: Overlay plot displaying the feasible design space region (yellow area) where all optimization criteria are satisfied, showing the interaction between (A) pH and N,S CQDs concentration, and (B) buffer volume and N,S CQDs concentration.