A Green and Sustainable UV Spectrophotometric Approach for Simultaneous Determination of Rosuvastatin, Pravastatin, and Atorvastatin in Pharmaceuticals Leveraging Firefly Algorithm-Enhanced Partial Least Squares Regression

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Table S1: The calibration set generated using a 5^3 multilevel multifactor partial design, comprising 25 synthetic mixtures with concentrations ranging from 6 to 14 µg/mL for each drug (rosuvastatin, pravastatin, and atorvastatin).

No.	Rosuvastatin (µg/mL)	Pravastatin (µg/mL)	Atorvastatin (µg/mL)
1	10	10	10
2	10	6	6
3	6	6	14
4	6	14	8
5	14	8	14
6	8	14	10
7	14	10	8
8	10	8	8
9	8	8	12
10	8	12	14
11	12	14	12
12	14	12	10
13	12	10	14
14	10	14	14
15	14	14	6
16	14	6	12
17	6	12	6
18	12	6	10
19	6	10	12
20	10	12	12
21	12	12	8
22	12	8	6
23	8	6	8
24	6	8	10
25	8	10	6

Table S2: The validation set generated using a central composite design, comprising 20 synthetic mixtures with concentrations ranging from 5.5 to 14.5 µg/mL for each drug (rosuvastatin, pravastatin, and atorvastatin).

No.	Rosuvastatin (µg/mL)	Pravastatin (µg/mL)	Atorvastatin (µg/mL)
1	13	7	7
2	7	7	13
3	7	7	7
4	13	7	13
5	7	13	13
6	10	10	10
7	10	10	10
8	10	10	10
9	13	13	13
10	13	13	7
11	7	13	7
12	10	10	10
13	10	10	14.5
14	5.5	10	10
15	10	14.5	10
16	10	10	10
17	10	10	10
18	10	5.5	10
19	10	10	5.5
20	14.5	10	10

Table S3: The optimized parameters of the Firefly algorithm as a variable selection procedure to enhance the PLS models' predictability.

Parameter	Rosuvastatin	Pravastatin	Atorvastatin
Number of fireflies	52	56	48
Maximum generations		500	
α	0.2	0.2	0.4
β_o	1.2	1.5	1.3
γ		1	

Table S4: Accuracy and precision of the developed FFA-PLS models, evaluated according to ICH guidelines.

Concentration (µg/mL)			***Accuracy (% R ± SD)*** [a]			***Precision (%RSD)*** [a]					
Rosuvastatin (µg/mL)	Pravastatin (µg/mL)	Atorvastatin (µg/mL)	Rosuvastatin	Pravastatin	Atorvastatin	Rosuvastatin		Pravastatin		Atorvastatin	
						Intra-day	*Inter-day*	*Intra-day*	*Inter-day*	*Intra-day*	*Inter-day*
8	8	8	98.65 ± 1.190	100.07 ± 1.270	100.13 ± 1.431	1.206	1.721	1.269	1.749	1.429	1.834
10	10	10	99.87 ± 1.390	99.84 ± 1.581	100.30 ± 1.197	1.392	1.541	0.996	1.251	1.194	1.504
12	12	12	100.45 ± 1.127	101.10 ± 1.007	99.25 ± 1.140	1.122	1.831	1.584	1.574	1.148	1.998

[a] Average of three determinations

Table S5: Selectivity assessment of the method through the standard addition technique, evaluating the matrix effect in the quantification of rosuvastatin, pravastatin, and atorvastatin.

Drug	Pharmaceutical taken (µg/mL)	Pharmaceutical found (µg/mL)	Pure added (µg/mL)	% Recovery ± SD
Rosuvastatin	6.0	5.999	6	98.55 ± 0.922
			7	99.48 ± 1.393
			8	100.66 ± 0.748
Pravastatin	6.0	5.954	6	100.63 ± 1.488
			7	101.89 ± 1.560
			8	100.28 ± 1.392
Atorvastatin	6.0	5.962	6	99.84 ± 0.773
			7	99.69 ± 0.829
			8	99.88 ± 1.062