

Tab 1 S: Summary of parameters required for system suitability testing of the proposed HPLC method

Parameters	CHP	BZP	CIN	DIP	DPP	Reference values⁶⁰
t_R	0.86	1.84	3.42	5.80	13.06	-
Tailing factor (T)	1.02	1.03	1.05	1.25	1.42	<2
N	525.93	442.20	1169.64	538.24	3369.15	Increase with increase in column efficiency
Resolution (Rs)		3.92	4.16	3.66	5.00	>2
Selectivity (α)		3.38	2.14	4.24	2.35	>1
K capacity (K')	0.91	3.08	6.60	11.88	28.02	<10
HETP (cm)	0.48	0.57	0.21	0.46	0.07	The smaller the value, the higher the column efficiency

Tab 2 S: Results of testing method robustness

Parameter	t_R				Parameter	t_R			
SLS conc. (± 0.01)	CHP	BZP	CIN	DPP	% acetonitrile (± 1)	CHP	BZP	CIN	DPP
0.09	0.88	1.84	3.53	13.29	89	0.85	1.86	3.8	12.98
0.10	0.86	1.84	3.42	13.06	90	0.86	1.84	3.42	13.06
0.11	0.84	1.83	3.39	12.99	91	0.82	1.79	3.38	13.2
SD	0.02	0.01	0.07	0.16	SD	0.02	0.04	0.23	0.11

Tab 3 S: The penalty points for determination of Analytical Eco-scale score of the developed and reported methods.

Parameters	Developed HPLC method	Penalty points (PP)	Reported TLC-densitometric²²	Penalty points (PP)
Reagents (PP of solvent = subtotal PP × number of pictograms × signal word)	Acetonitrile Consumed volume/sample =26. 1mL <u>Subtotal PP = 2</u> [solvent 10-100 mL]. <u>Signal word = 2</u> Danger. <u>No. of pictograms = 2</u>	8	Hexane Consumed volume/sample = 1.94mL <u>Subtotal PP = 1</u> [solvent <10 mL]. <u>Signal word = 2</u> Danger. <u>No. of pictograms = 4</u>	8
	0.1% SLS Consumed volume/sample = 2.9 mL <u>Subtotal PP = 1</u> [solvent <10 mL]. <u>Signal word = 2</u> Danger. <u>No. of pictograms = 2</u>	4	Ethanol Consumed volume/sample = 0.83mL <u>Subtotal PP = 1</u> [solvent <10 mL]. <u>Signal word = 2</u> Danger. <u>No. of pictograms = 2</u>	4
				Acetone Consumed volume/sample = 0.19mL <u>Subtotal PP = 1</u> [solvent <10 mL]. <u>Signal word = 2</u>

			Danger. <u>No. of pictogram</u> <u>=2</u>	
			Glacial acetic acid Consumed volume = 0.14 mL <u>Subtotal PP = 1</u> [solvent <10 mL]. <u>Signal word = 2</u> Danger <u>No. of pictogram =2</u>	4
Instruments	≤1.5 kWh per sample	1	≤1.5 kWh per sample	1
	Analytical process hermitization	0	Analytical process hermitization	0
	Waste >10 mL	5	1-10 mL Waste	3
Total penalty points	18		24	
Analytical Eco-Scale total score	88		76	

Tab 4 S: Green Analytical Procedure Index parameters for the developed and reported methods

Parameters	Developed HPLC method	Reported TLC-densitometric method²²
Sample preparation		
Collection (1)	Off-line	Off-line
Preservation (2)	None	None
Transport (3)	None	None
Storage (4)	Under normal conditions	Under normal conditions
Type of method: direct or indirect (5)	Filtration	Filtration
Scale of extraction (6)	Microextraction	Microextraction
Solvents/reagents used (7)	Green	Non green
Additional treatments (8)	None	-
Reagents and solvents		
Amount (9)	10-100 g	1-10 g
Health hazards (10)	2 or 3	1 or 2 or 3
Safety hazards (11)	1 or 3	0 or 1 or 3
Instrumentation		
Energy (12)	≤1.5 kWh per sample	≤1.5 kWh per sample
Occupational hazard (13)	Hermetic sealing	-
Waste (14)	>10	1-10 mL
Waste treatment (15)	Recycling possible	Recycling possible
Quantification	Yes	Yes

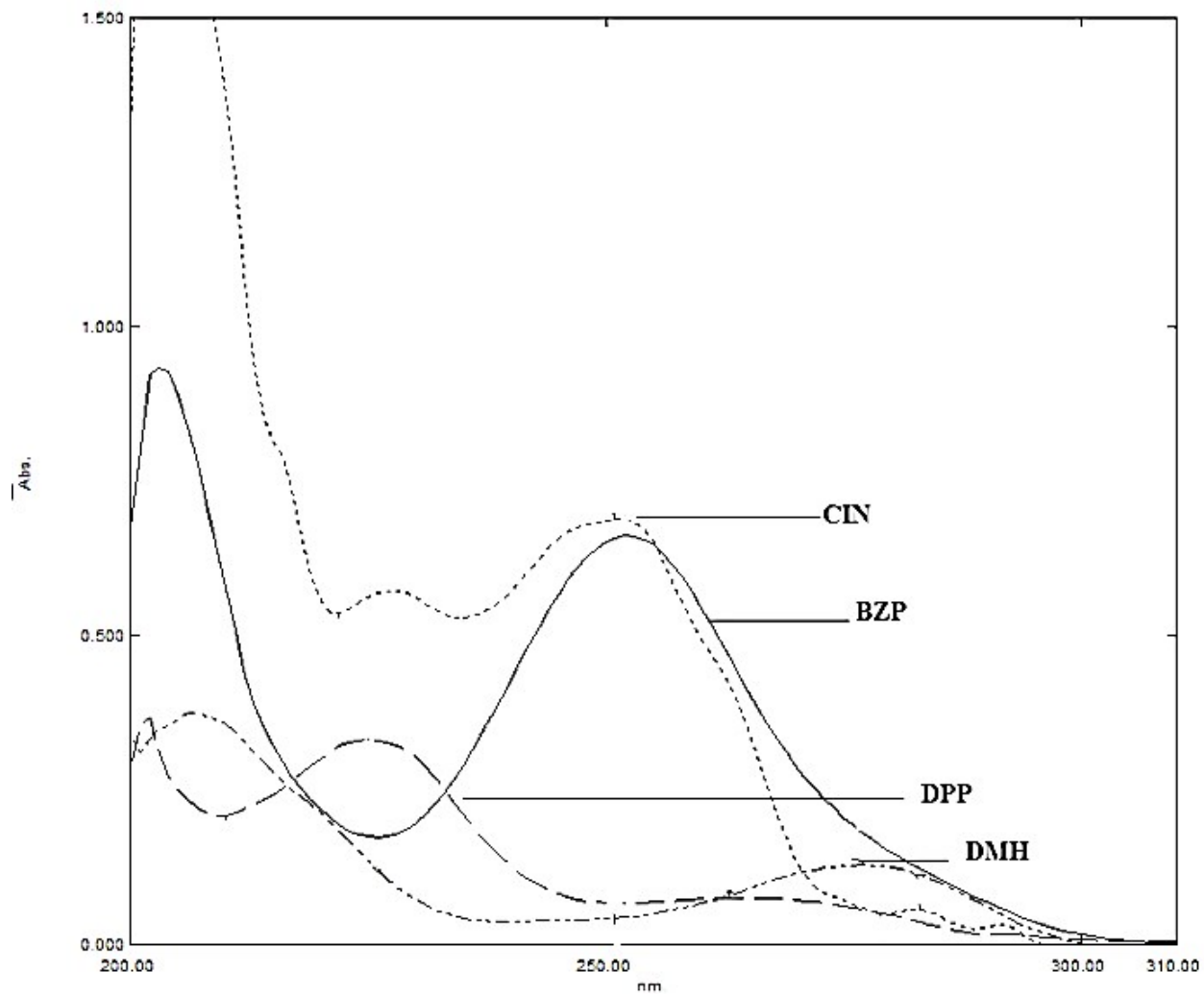


Fig. 1 S: UV spectra of 10 $\mu\text{g/mL}$ of the studied compounds in methanol

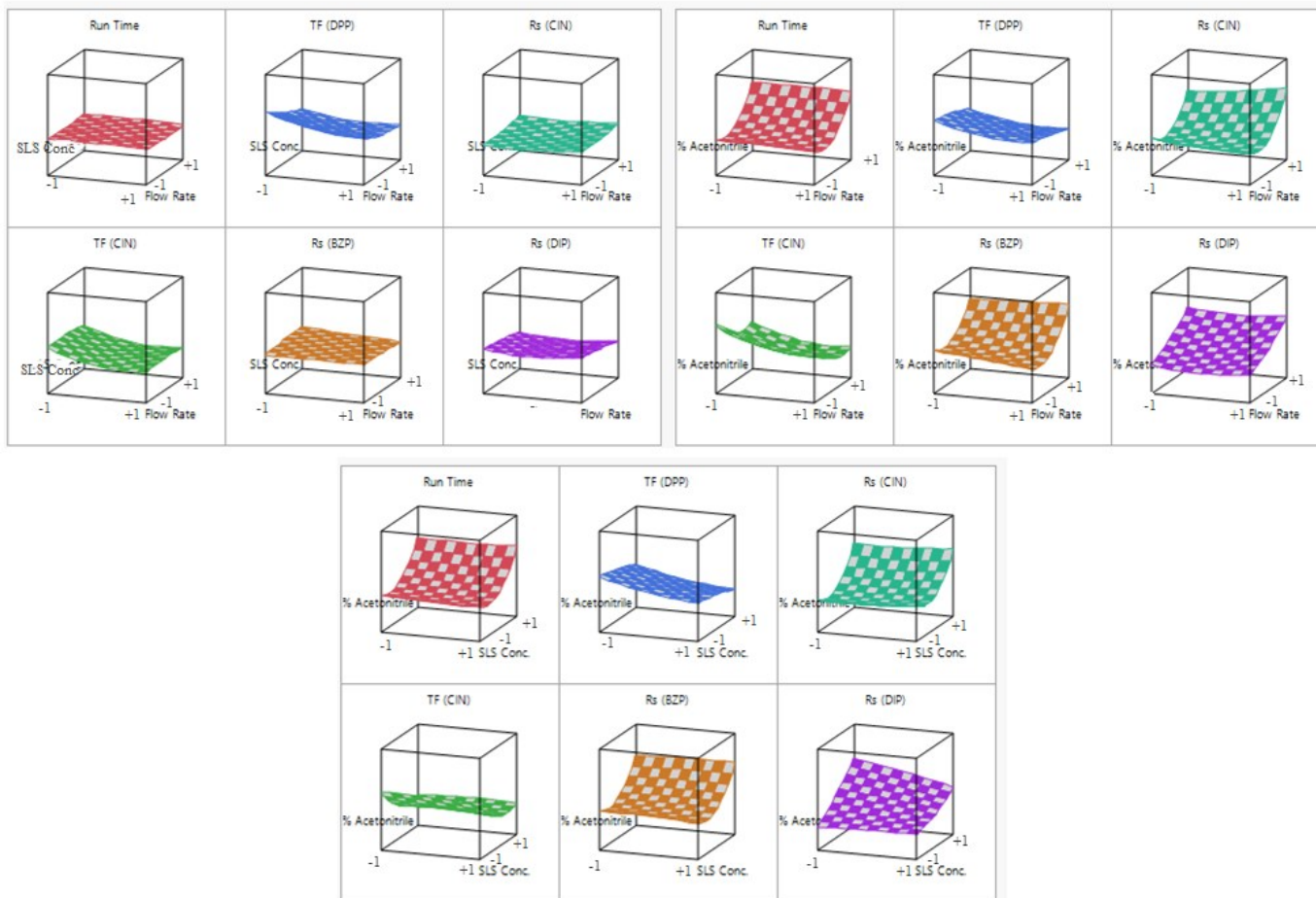


Fig. 2 S: Surface plots for the measured responses

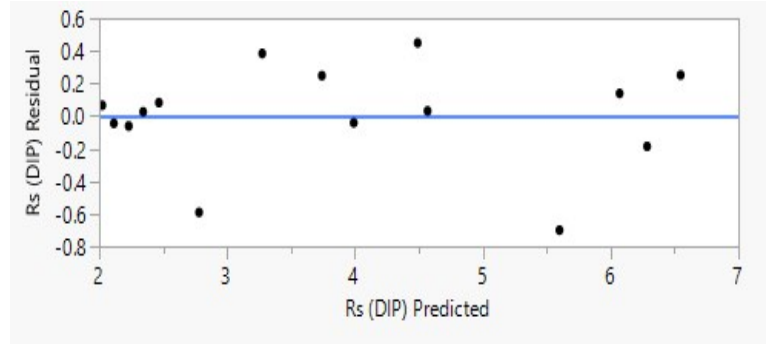
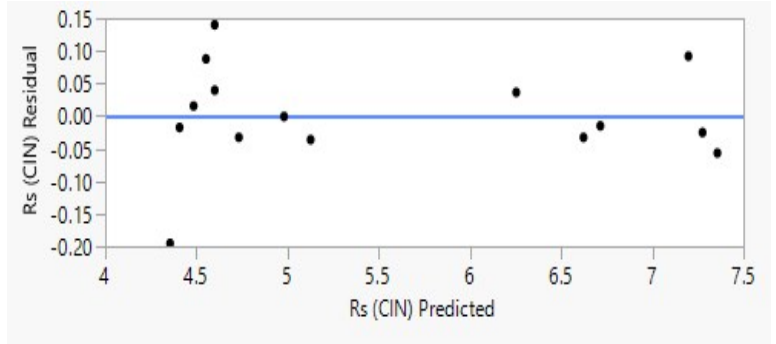
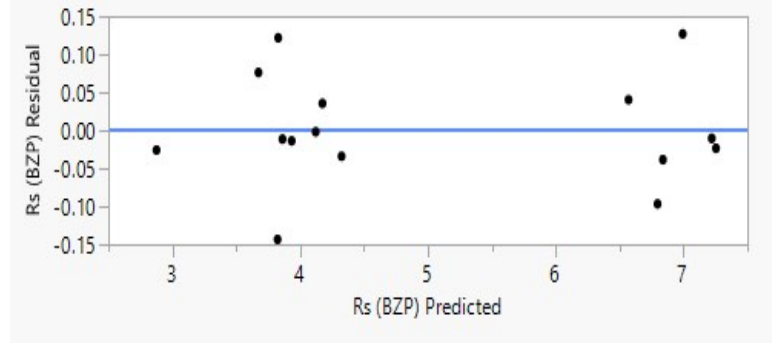
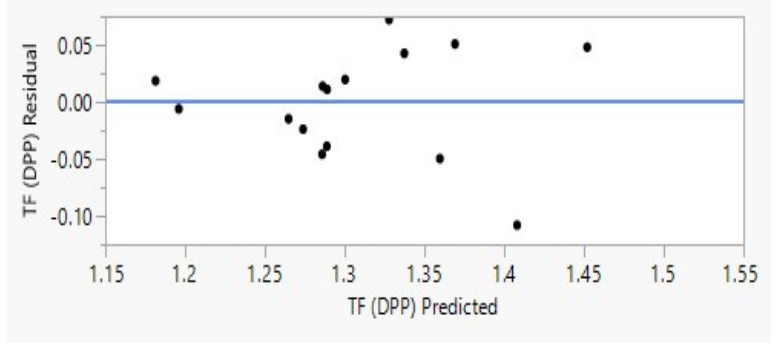
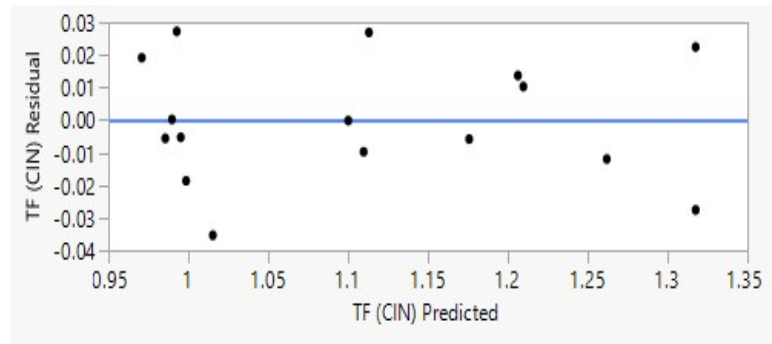
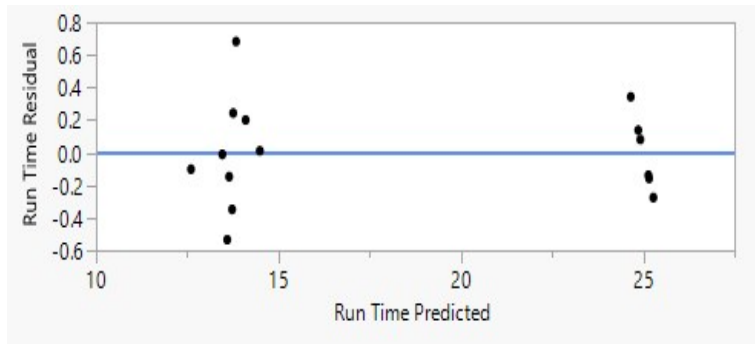


Fig 3 S: Residuals by predicted plots