

Figure S1. Normal UV spectra of formulation (A), first derivative spectra (B), ratio spectra of AZE (C) First derivative of ratio spectra of AZE (D)

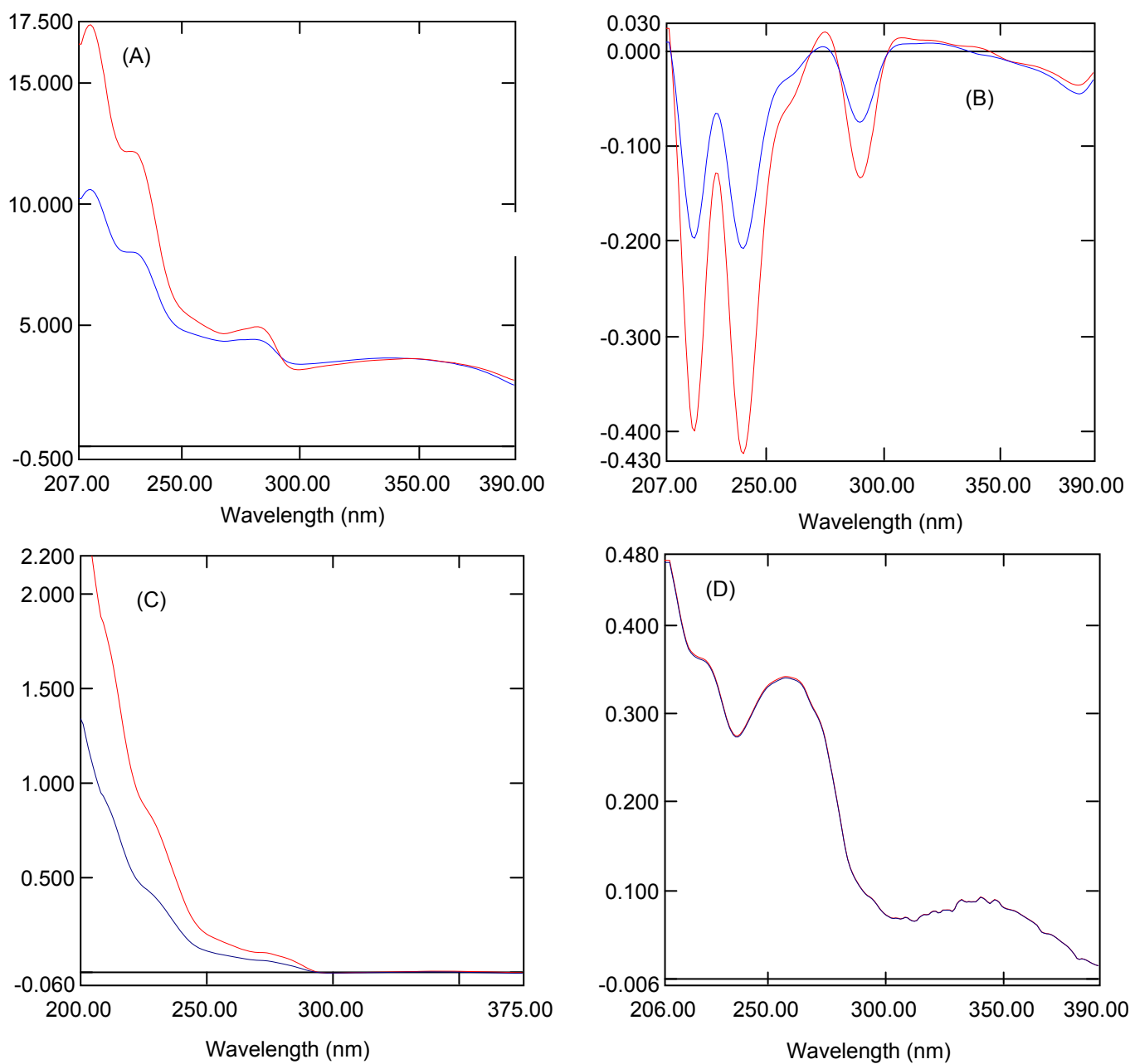
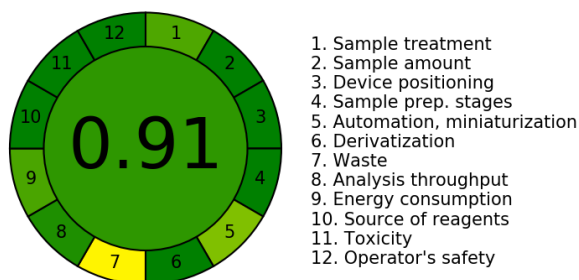


Figure S2 : Ratio spectra of CTL (A), First derivative of ratio spectra of CTL (B), Zero order spectra of CTL (C) and AZE (D)


Figure S3: Analytical Greenness report sheet

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Criteria	Score	Weight
1. Direct analytical techniques should be applied to avoid sample treatment.	0.85	2
2. Minimal sample size and minimal number of samples are goals.	1.0	2
3. If possible, measurements should be performed in situ.	1.0	2
4. Integration of analytical processes and operations saves energy and reduces the use of reagents.	1.0	2
5. Automated and miniaturized methods should be selected.	0.75	2
6. Derivatization should be avoided.	1.0	2
7. Generation of a large volume of analytical waste should be avoided, and proper management of analytical waste should be provided.	0.48	2
8. Multi-analyte or multi-parameter methods are preferred versus methods using one analyte at a time.	0.94	2
9. The use of energy should be minimized.	0.86	2
10. Reagents obtained from renewable sources should be preferred.	1.0	2
11. Toxic reagents should be eliminated or replaced.	1.0	2
12. Operator's safety should be increased.	1.0	2

File


**GDANSK UNIVERSITY
OF TECHNOLOGY**

ComplexGAPI

Green Analytical
Procedure Index

SAMPLE PREPARATION AND ANALYSIS

Sample preparation

1. Collection: In-line ▼

2. Preservation: None ▼

3. Transport: None ▼

4. Storage: None ▼

5. Type of method: No sample preparation ▼

6. Scale of extraction: Nano-extraction ▼

7. Solvents/reagents used: Green solvents/reagent ▼

8. Additional treatments: None ▼

Reagents and solvents

9. Amount: < 10 mL (< 10 g) ▼

10. Health hazard: Slightly toxic, slight irri ▼

11. Safety hazard: Highest NFPA flammal ▼

instrumentation

12. Energy: <= 0.1 kWh per sample ▼

13. Occupational hazard: Hermetic sealing of th ▼

14. Waste: 1-10 mL (1-10 g) ▼

15. Waste treatment: Degradation, passivatic ▼

Method type

Type of analysis: Qualitative and quantit ▼

PRE-ANALYSIS PROCESSES

Yield and conditions

I. Yield: > 89% ▼

II. Temperature/time: Room temp., < 1 h ▼

Relation to Green Economy

III. Number of rules met: 5-6 ▼

Reagents and solvents

IVa. Health hazard: Slightly toxic, slight irri ▼

IVb. Safety hazard: Highest NFPA flammal ▼

Instrumentation

Va. Technical setup: Common setup ▼

Vb. Energy: ≤0.1 kWh per sample ▼

Vc. Occupational hazard: Hermetization of analy ▼

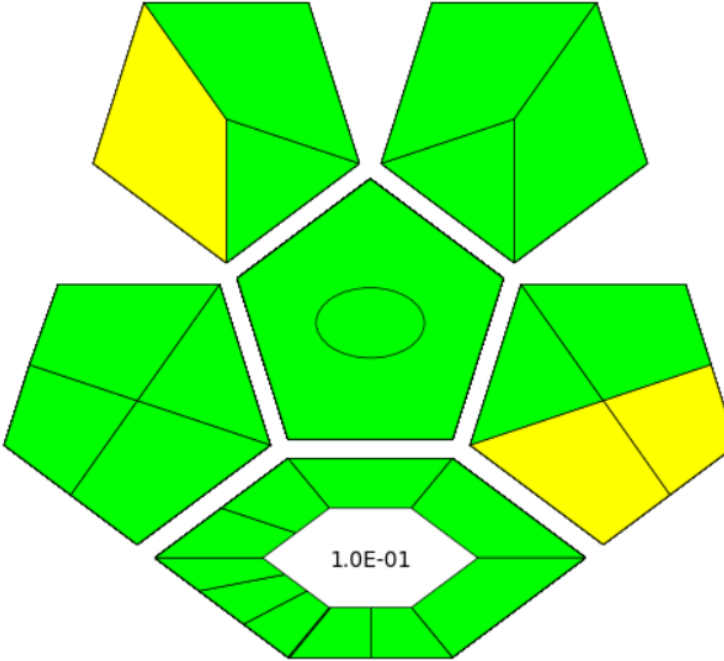
Workup and purification

VIa. End products workup, purification: None or simple proces ▼

VIb. Purity: > 98% ▼

E-factor

VII. E-factor input: 0.1



1.0E-01

Figure S4: ComplexGAPI for spectroscopic method

Reference

1. J. Płotka-Wasyłka, and W. Wojnowski, “Complementary green analytical procedure index (ComplexGAPI) and software,” *Green Chemistry*, vol. 23, pp. 8657-8665, 2021. (A compiled, stand-alone version is currently available for Windows and can be downloaded from <http://mostwiedzy.pl/complexgapi>)

RED PRINCIPLES (analytical performance)			R1: Scope of application	R2: LOD and LOQ			R3: Precision			R4: Accuracy		
	Method number	Method name	0-100	LOD	LOQ	0-100	RSD% (repeatability)	RSD% (reproducibility)	0-100	Relative error (%)	Recovery (%)	0-100
	1	UV spectroscopic method	95	0.128- 0.328	0.38- 0.997	95	0.397-1.803	0.893-1.758	100	0.924-1.607	98.37%10.38%	100

GREEN PRINCIPLES (green chemistry)			G1: Toxicity of reagents (impact and biodegradation)		G2: Amount of reagents and waste			G3: Consumption of energy and other media	G4: Direct impacts (safety, use of animals and GMOs)			
	Method number	Method name	Total number of pictograms	0-100	Reagent consumpt ion	Waste production	0-100	1-100	Occupational hazards	Safety of users (0-100)	Use of animals (0 if no, 1 if yes)	Use of GMO (0 if no, 1 if yes)
	1	UV spectroscopic method	Safe and biodegradable	95	less than 10ml	Less than 10 ml	95	95	Not Hazardus	100	0	0

BLUE PRINCIPLES (practical side)			B1: Cost-efficiency		B2: Time-efficiency		B3: Requirements			B4: Operational simplicity		
	Method number	Method name	Total cost	0-100	Speed of analysis	0-100	Sample consumption	Sample consumption (0- 100)	Other needs: advanced instruments, skills, facilities (0-100)	Miniaturizati on (0-100)	Integration and automation (0- 100)	Portability (0- 100)
	1	UV spectroscopic method	5 USD per sample	100	50 samples /hour	100	in micrograms	100	100	95	95	95

Method number	Method name	R (%)	G (%)	B (%)	Whiteness (%)
1	UV spectroscopic method	97.5	96.3	98.8	97.5

Table S1. White analytical chemistry Evaluation

Reference: P. M. Nowa, and P. Kościelniak, “What Color Is Your Method? Adaptation of the RGB Additive Color Model to Analytical Method Evaluation,” *Analytical Chemistry*, vol. 91, no. 16, pp. 10343-10352, 2019. DOI: 10.1021/acs.analchem.9b01872. The excel is available for download from the <https://pubs.acs.org/doi/pdf/10.1021/acs.analchem.9b01872>