Article

Targeted UHPLC-ESI-MS/MS Analysis of Selected Neurotransmitters, Tryptophan and Its Metabolite Kynurenine in Tau Transgenic Rat Brain Tissue: A Pivotal Study

Juraj Piestansky [1,2], Andrea Forgacsova [1], Dominika Olesova [3], Jaroslav Galba [4], Peter Mikus [1,2], Petra Majerova [3] and Andrej Kovac [3,*]

[1] Department of Pharmaceutical Analysis and Nuclear Pharmacy, Faculty of Pharmacy, Comenius University in Bratislava, Odbojarov 10, SK-832 32 Bratislava, Slovakia; piestansky@fpharm.uniba.sk (J.P.); andreaforgacsova@gmail.com (A.F.); mikus@fpharm.uniba.sk (P.M.)

[2] Toxicological and Antidoping Center, Faculty of Pharmacy, Comenius University in Bratislava, Odbojárov 10, SK-832 32 Bratislava, Slovakia

[3] Institute of Neuroimmunology, Slovak Academy of Science, Dubravska Cesta 9, SK-845 10 Bratislava, Slovakia; petra.majerova@savba.sk (P.M.); dominika.olesova@savba.sk (D.O.)

[4] Institute of Virology, Biomedical Research Center Slovak Academy of Science, Dubravska Cesta 9, SK-845 05 Bratislava, Slovakia; jaroslav.galba@gmail.com

* Correspondence: andrej.kovac@savba.sk; Tel.: +421-2-54788100

1. Evaluation of the LC-MS/MS Method with the Use of RGB Additive Color Model

The developed LC-MS/MS method for simultaneous determination of 11 substances in rat brain tissue was evaluated in a global manner with the use of the RGB Additive Color Model which was described by Nowak and Kościelniak [42]. The model uses three primary colors that represent three main attributes of the evaluated method: analytical performance—Red, compliance with the "green" chemistry principles—Green, and productivity/practical effectiveness—Blue. A final color of the method results from the additive synthesis of the primary colors. The model provides also a quantitative parameter (method brilliance) that integrates all primary colours and treats them with varying importance. The results of the evaluation are summarized in Figure S1.

			w=3	w=3		w=2	w=2
REDNESS (analytical performance)		W=4	Accuracy	Precision (RSD%)		Linearity range	LOD
CS: 77.0%		LAV=33.3	85%	15%		one decadic order	5 µg/mL
		LSV=66.6	90%	5%		two decadic orders	1 µg/mL
		Result	89.5	4.5		three decadic orders	0.64 µg/mL
		Score (0-100)	65 · 65 · 65	70 · 70 · 70		100 · 100	88 · 88

			w=3	w=3		w=3	w=1
GREENNESS (safety and eco-friendliness)		W=2	Chemical consumption	Chemical safety/hazards		Additional risk factors	Energy
CS: 69.6%		LAV=33.3	2L/100 samples	15 hazard pictograms in total		10 independent hazards	>1.5 kWh
		LSV=66.6	1L/100 samples	5 hazard pictograms in total		3 independent hazards	0.5 kWh
		Result	0.63 L/100 samples	6 hazard pictograms in total		1 independent hazard	>1.5 kWh
		Score (0-100)	80 · 80 · 80	60 · 60 · 60		90 · 90 · 90	33.3

			w=3	w=3		w=2	w=2
BLUENESS (productivity / practical effectiveness)		W=3	Cost-effectiveness	Time-effectiveness		Sample destruction	Service
CS: 85.2%		LAV=33.3	30 euro/sample	30 samples/hour		20 mL/100 runs	2/100 samples
		LSV=66.6	10 euro/sample	10 samples/hour		10 mL/100 runs	1/100 samples
		Result	10 euro/sample	6.7 samples/hour		1 mL/100 runs	0/100 samples
		Score (0-100)	66.6 · 66.6 · 66.6	90 · 90 · 90		97 · 97	100 · 100

FINAL COLOR:			REDNESS		GREENNESS		BLUENESS		BRILLIANCE (MB):	77.0%
WHITE			≥33.3%	≥66.6%	≥33.3%	≥66.6%	≥33.3%	≥66.6%		
			yes	yes	yes	yes	yes	yes		
Short annotation: 77.0white			Long annotation: 77.0white(77.0/4red-69.6/2green-85.2/3blue)							

Figure S1. Evaluation of the LC-MS/MS method with the use of RGB Additive Color Model.