Supplementary Information

Colorimetric and fluorescent detection of synthetic cathinones in oral fluid with meso-aryl BODIPYs and Cu(II)

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Table S1. Comparison of the sensing properties of different optical selective probes for synthetic cathinones (SCs).

Probe	Detection technique	Selectivity	Limit of detection	Application	Reference
BODIPY derivative	Fluorescence "*turn off*"	Synthetic cathinones	0.16 µM (32 ng/mL)	Aqueous media and saliva	This study
Molecular imprinted polymer	Aggregation-induced Emission	Synthetic cathinones	0.34 µM	Urine	Shen *et al.,* 2022
BSA – Au nanoclusters	Fluorescence "*turn off*"	Synthetic cathinones	0.14 mM	Aqueous media	Yao-Te *et al.,* 2019
Carbon dots (C-dots)	Fluorescence "*turn off*"	Synthetic cathinones	1.74 mM	Aqueous media	Yao-Te *et al.,* 2019
CBS - Azyme	Fluorescence "*turn on*"	Synthetic cathinones	3 µM	Saliva (50 %) Urine (50 %)	Yingping *et al.,* 2019
-	GC-MS method	Synthetic cathinones	10 ng/mL	Saliva	Khaled *et al.,* 2016

Y. Yan, L. Jiang, S. Zhang, X. Shen, C. Huang, Specific "light-up" sensor made easy: An aggregation induced emission monomer for molecular imprinting, Biosensors and Bioelectronics 205 (**2022**) 114113. DOI: 10.1016/j.bios.2022.114113

Y.-T. Yen, T.-Y. Chen, C.-Y. Chen, C.-L. Chang, S.-C. Chyueh, H.-T. Chang, Photoluminescent Colorimetric Probe of Bovine Serum Albumin-Stabilized Gold Nanoclusters for New Psychoactive Substances: Cathinone Drugs in Seized Street Samples, Sensors 19 (**2019**) 3554. DOI: 10.3390/s19163554

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Khaled. M, Abtehaj. H, Alanoud. M, El-Said. A, A A GC–MS Method for Detection and Quantification of Cathine, Cathinone, Methcathinone and Ephedrine in Oral Fluid, J. Chromatogr. Sci., 54, 8 (**2016**) 1271-1276. DOI: 10.1093/chromsci/bmw082

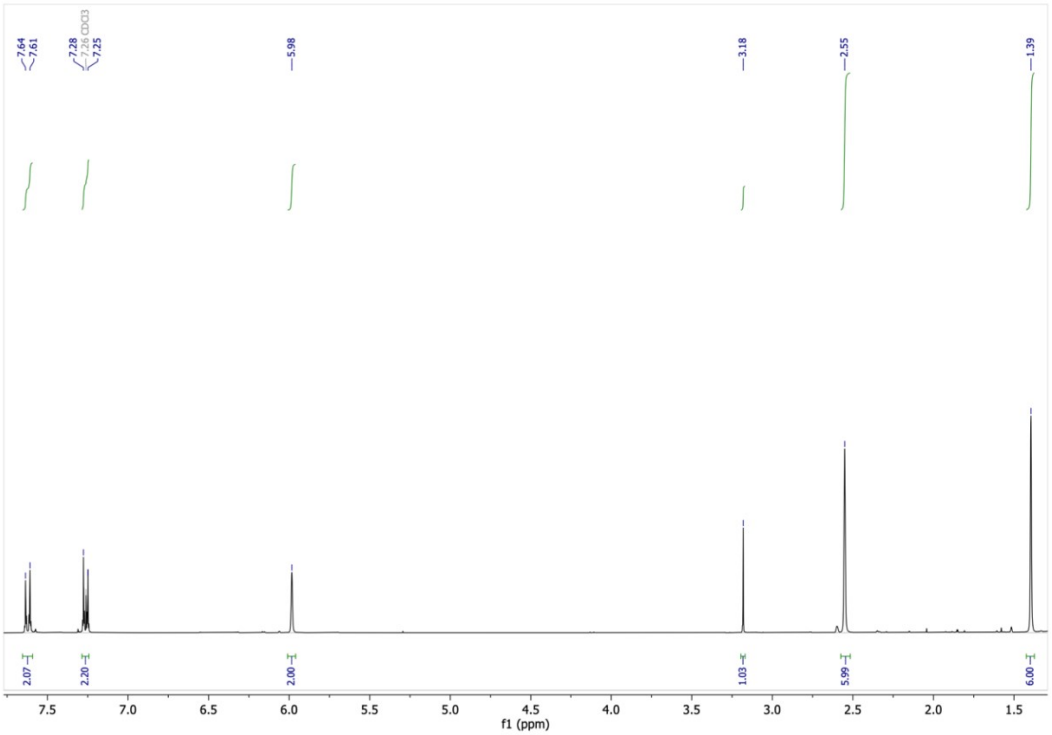


Figure S1. ^{1}H NMR of compound **1** in $CDCl_3$.

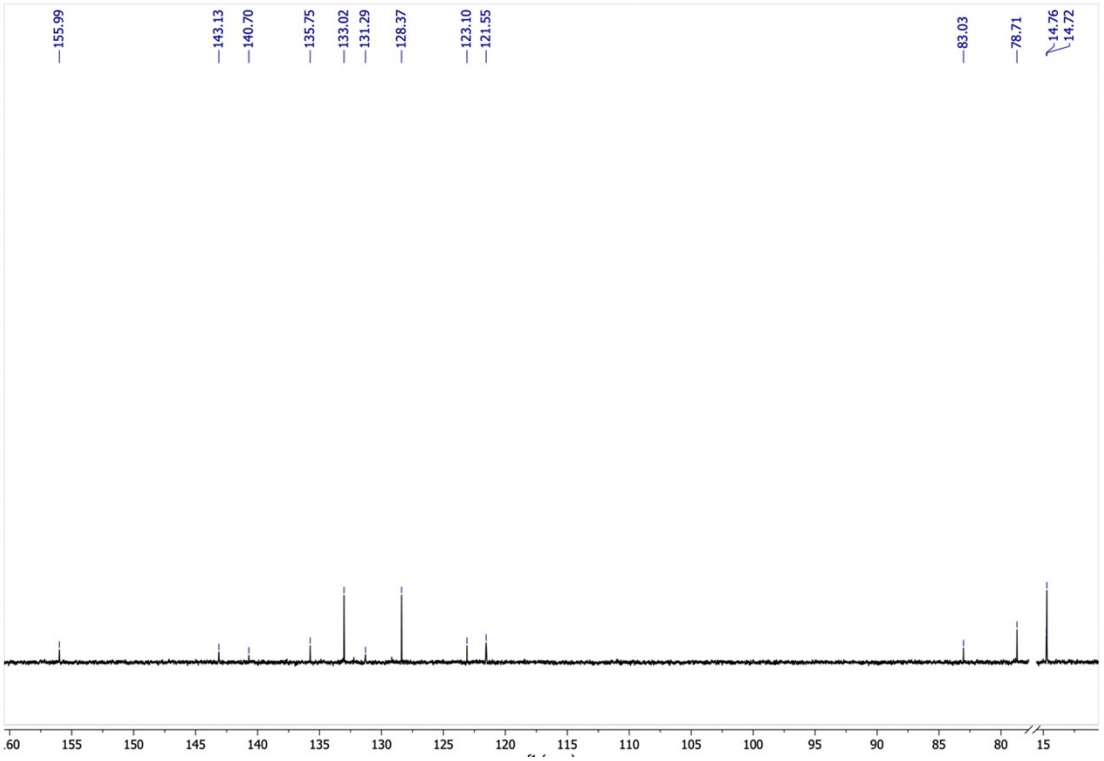


Figure S2. ^{13}C NMR of compound **1** in $CDCl_3$.

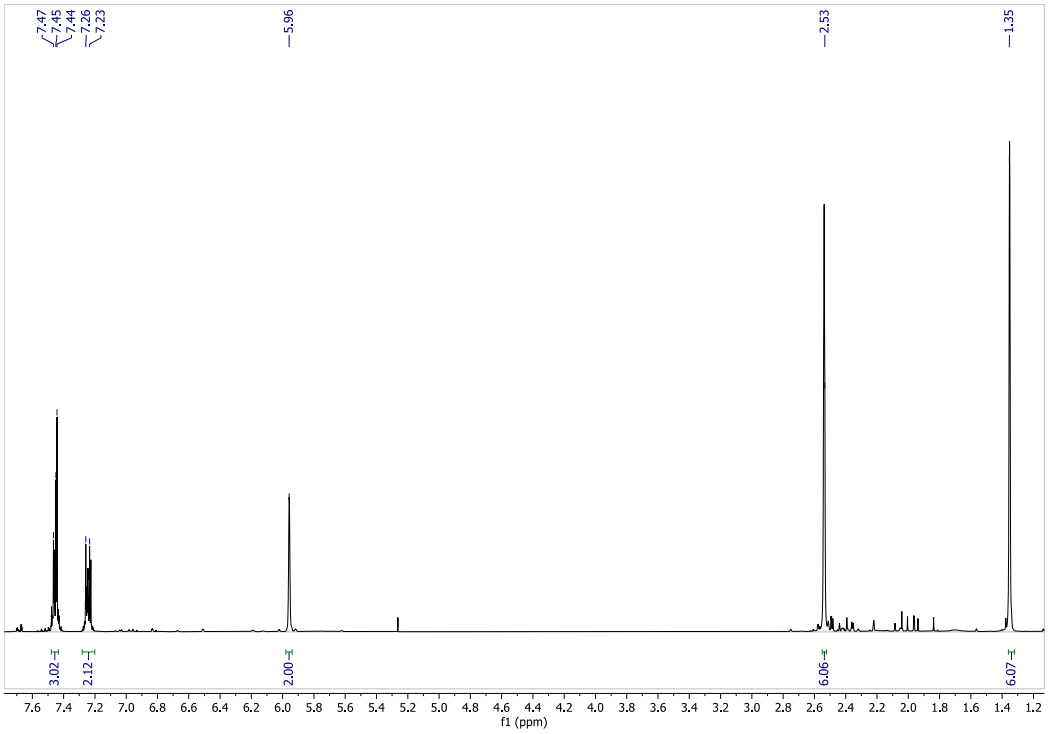


Figure S3. ^{1}H NMR of compound **2** in $CDCl_3$.

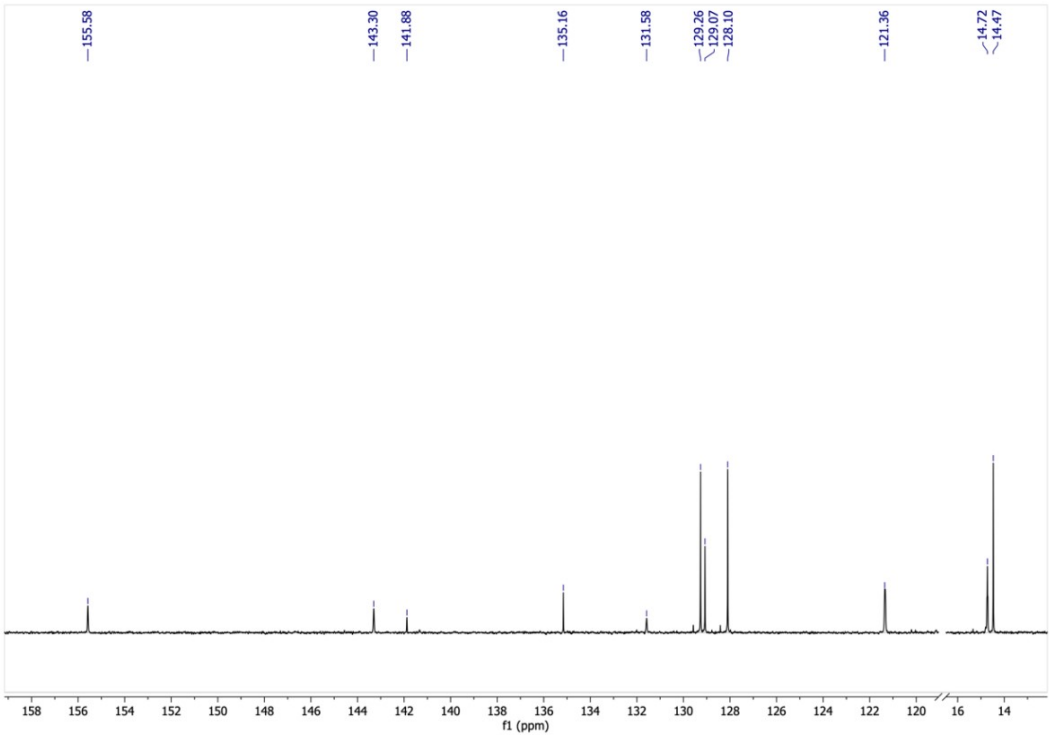


Figure S4. ^{13}C NMR of compound **2** in $CDCl_3$.

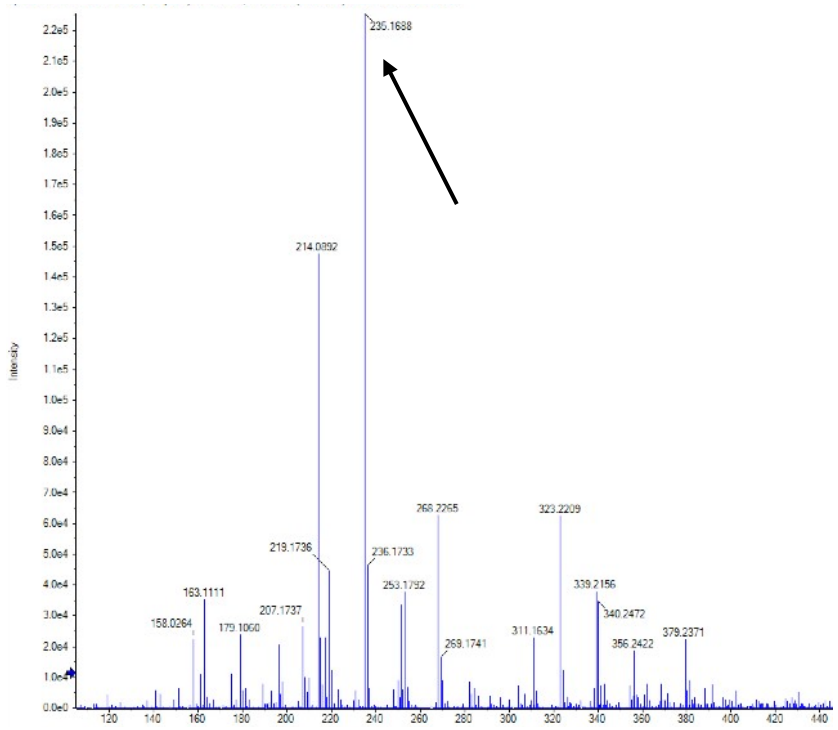


Figure S5. Mass spectroscopy data of compound **1**+Cu(I) after reflux heating for 2 minutes.

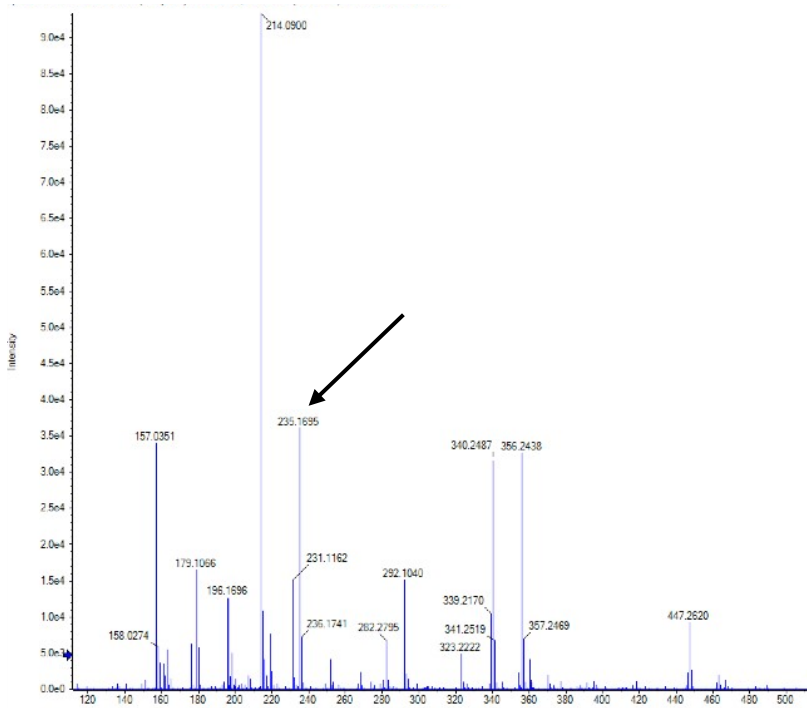


Figure S6. Mass spectroscopy data of compound **2**+Cu(I) after reflux heating for 2 minutes.

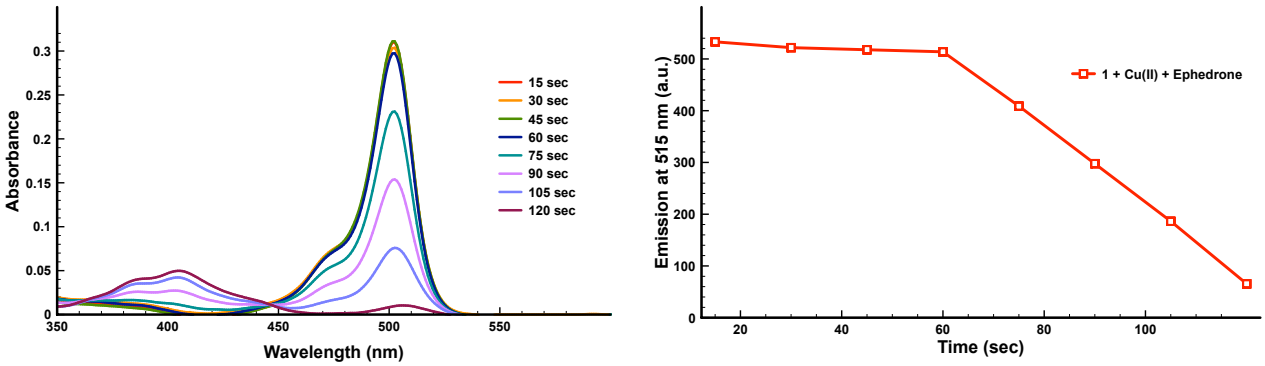


Figure S7. UV-vis (left) and fluorescence (right) emission (λ_{em} = 515 nm; λ_{exc} = 450 nm) spectra of compound **1** (50 μM in THF: water 95:5 solution) with 1 equiv. of $Cu(AcO)_2$ in presence of 2 equiv. of ephedrone after reflux heating for 2 minutes.

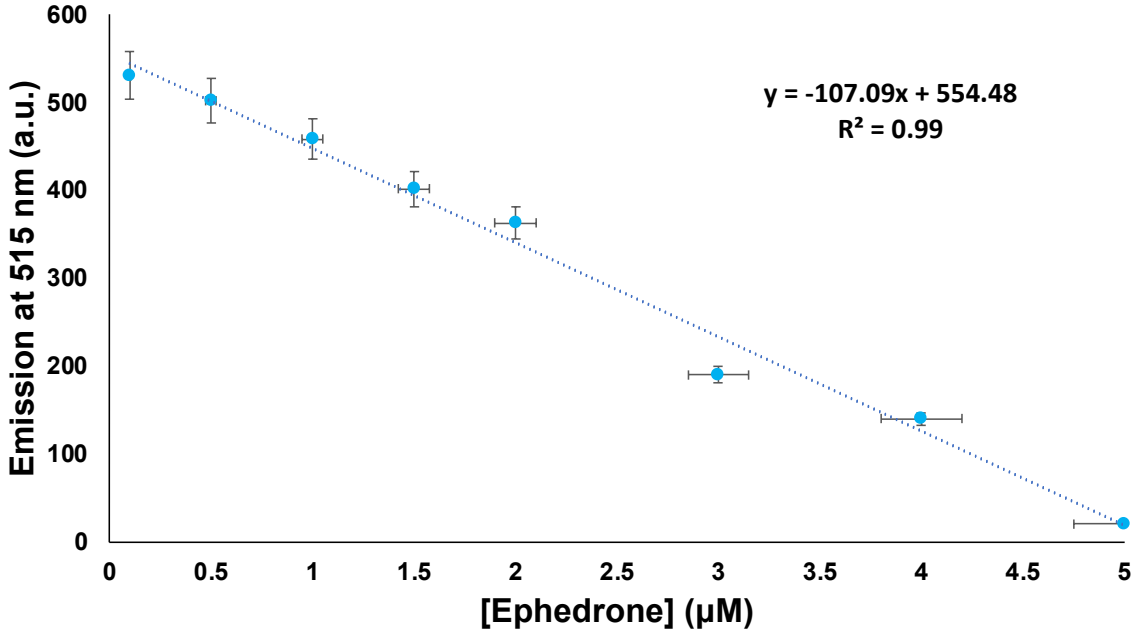


Figure S8. Fluorescence emission calibration curve at 515 nm (λ_{exc} = 450 nm) of water samples spiked with cathinone (0.15 to 5 μM).

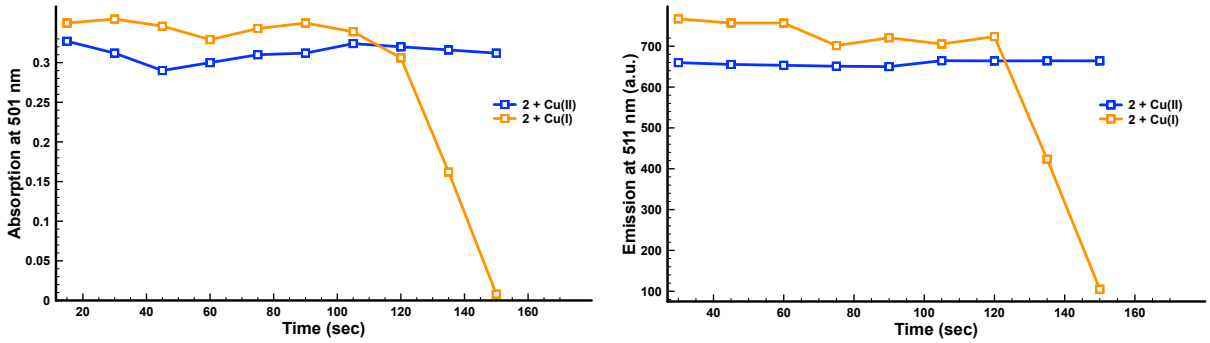
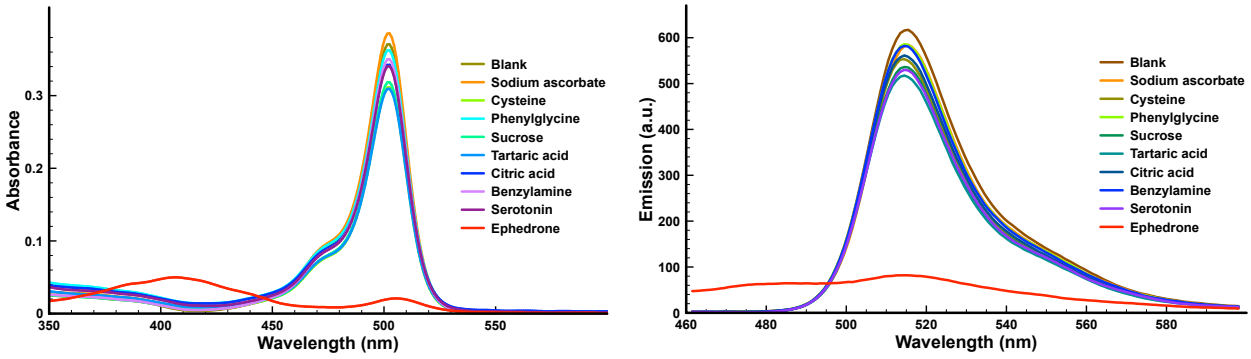


Figure S9. Evolution of the absorption at 501 nm (left) and fluorescence emission (right) at 515 nm (λ_{exc} = 450 nm) over time of a mixture of compound **2** (50 μM in THF: water 95:5 solution) and 1 equiv. of $Cu(AcO)_2$ or 1 equiv. of CuBr. In each case, the solution was refluxed for 2.5 minutes.



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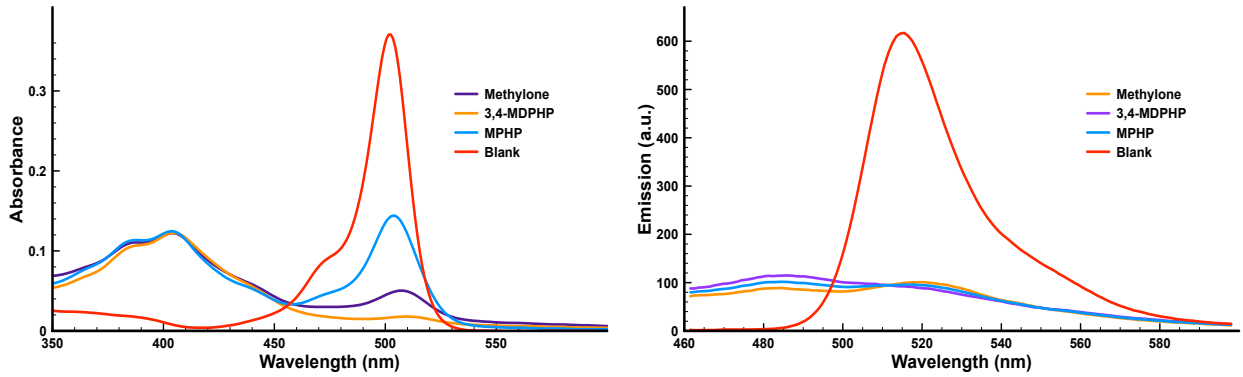

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Table S2. Recovery and accuracy of the method[1] to detect cathinones in saliva samples.

Analite	**Known concentration** (μM)	**Found concentration** (μM)	**Recovery** (%)[a]	**Accuracy** (%)[b]
Cathinone (Ephedrone)	0.75	0.67	89	-11

[a] recovery % (found concentration/known concentration) x 100

[b] accuracy % (found concentration – known concentration/known concentration) x 100

[1] K. A. Rawat, R. K. Singhal, S. K. Kailasa, *RSC Adv.* 6 (2016) 32025-32036.