

Supplemental Information

for

The Importance of Wavelength Selection in On-Scene Identification of Drugs of Abuse with Portable Near-Infrared Spectroscopy

Ruben F. Kranenburg^{1,2,*}, Yannick Weesepeol³, Martin Alewijn³, Sharon Sap⁴, Peter W.F. Arisz⁴, Annette van Esch⁵, Peter H.J. Keizers⁶, Arian C. van Asten^{2,7}

¹ Dutch National Police, Unit Amsterdam, Forensic Laboratory, Kabelweg 25, Amsterdam 1014 BA, The Netherlands

² Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Postbus 94157, Amsterdam 1090 GD, The Netherlands

³ Wageningen Food Safety Research part of Wageningen University and Research, Akkermaalsbos 2, Wageningen 6708 WB, The Netherlands

⁴ Dutch Customs Laboratory, Kingsfordweg 1, Amsterdam 1043 GN, The Netherlands

⁵ Netherlands Forensic Institute (NFI), Laan van Ypenburg 6, Den Haag 2497 GB, The Netherlands

⁶ National Institute of Public Health and the Environment (RIVM), Antonie van Leeuwenhoeklaan 9, Bilthoven 3721 MA, The Netherlands

⁷ Co van Ledden Hulsebosch Center (CLHC), Amsterdam Center for Forensic Science and Medicine, Postbus 94157, Amsterdam 1090 GD, The Netherlands

* Corresponding author. *E-mail address*: ruben.kranenburg@politie.nl (R.F. Kranenburg).

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Various tables. Individual sample results for all 5 sensors: see separate file '*Tables Supplemental Information.pdf*'

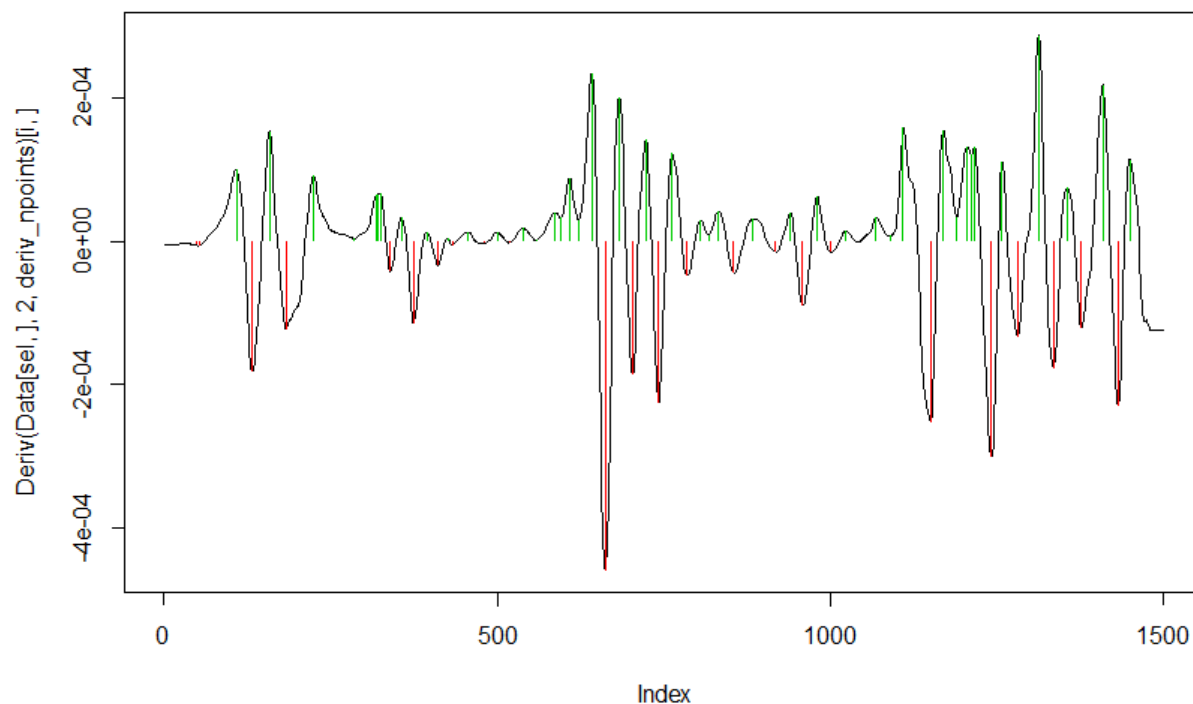


Figure S1. Example of spectral feature detection used in the statistical match score calculations. First derivative spectrum smoothed using a 43 dp filter (corresponding with a ~43 nm range) of a ketamine reference standard analyzed on the ASD LabSpec 4 sensor. Green and red lines indicate the 69 identified spectral features that were used for calculation of the Pearson’s correlation.

device	wavelength range	dp (#)	filter length (dp)	Spectral features identified (#)					
				Coca HCl	Coca Base	Amph	MethAmph	Keta	MDMA
ASD LabSpec4	1000 - 2500 nm	1750	43	71	72	61	55	64	64
Si-Ware NeoSpectra	1300 - 2600 nm	160	5	71	71	61	60	62	62
Spectral Engines NIRone S2.0	1550 - 1950 nm	201	21	8	15	13	11	13	17
Viavi Solutions MicroNIR	950 - 1650 nm	125	7	24	19	19	27	24	22
Consumer Physics SCiO	740 - 1070 nm	331	43	8	10	12	13	8	9

Table S1. Overview of the number of spectral features detected in the NIR-spectra of the common drugs of abuse analyzed by the spectrometers used in this study. dp: datapoints; coca: cocaine; Amph: amphetamine sulphate; MethAmph: methamphetamine HCl; Keta: ketamine.

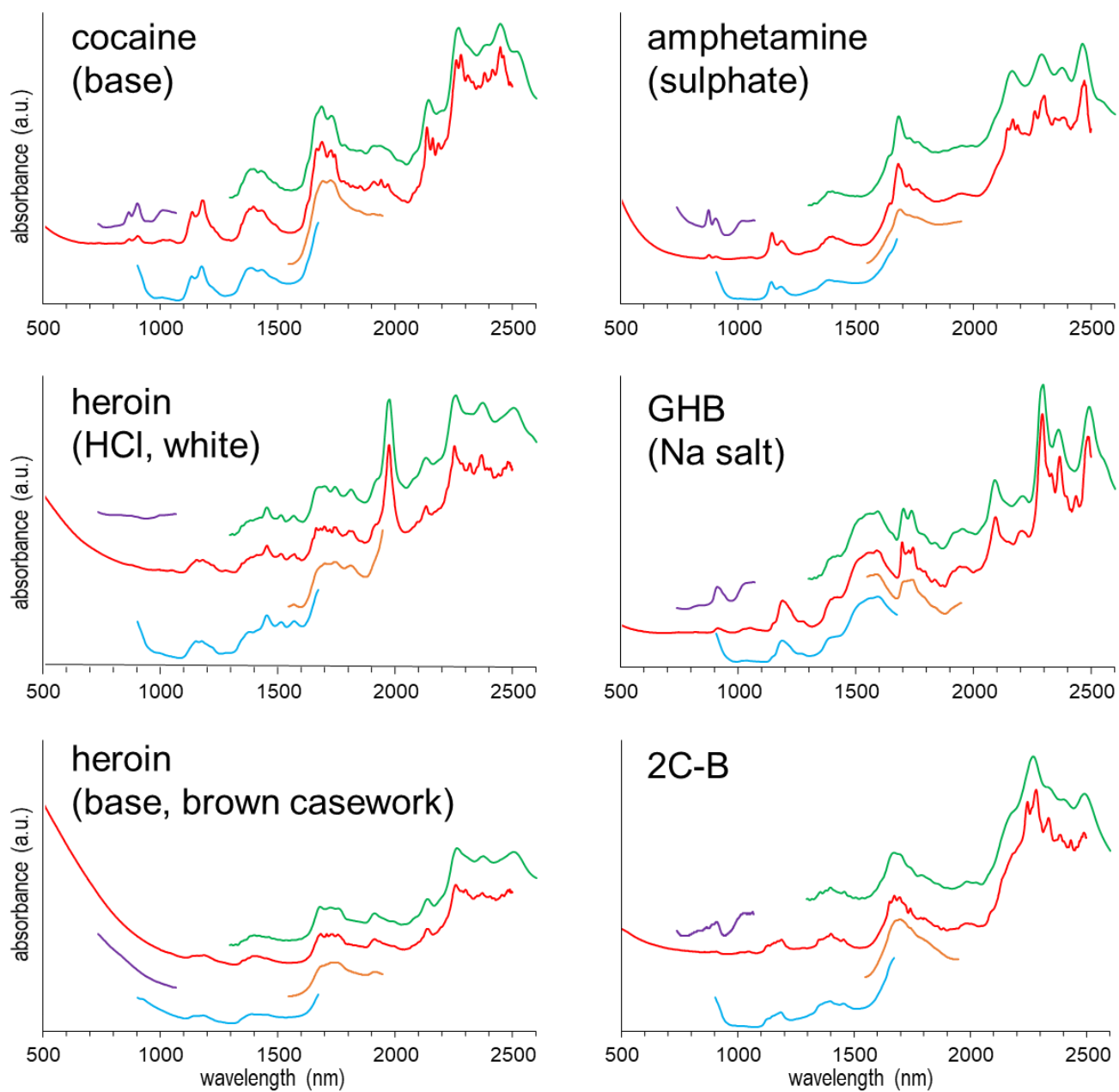


Figure S2. Comparison of the spectral output for six common illicit-drugs from the different sensors. red: ASD LabSpec4; green: NeoSpectra; orange: NIRone; blue: microNIR; purple: SCiO.

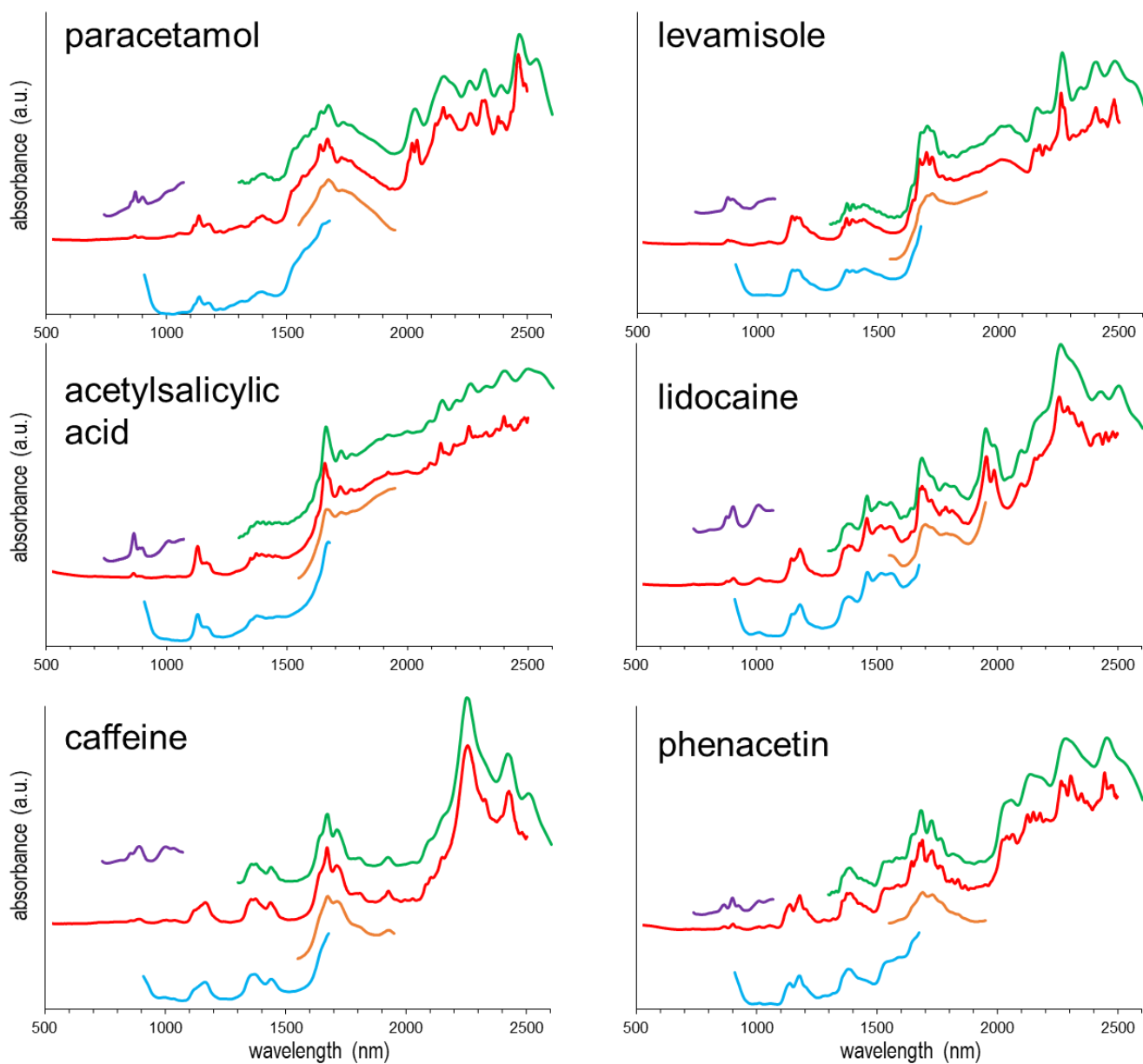


Figure S3. (part 1 of 2) - Comparison of the spectral output for ten adulterants from the different sensors. red: ASD LabSpec4; green: NeoSpectra; orange: NIRone; blue: microNIR; purple: SCiO.

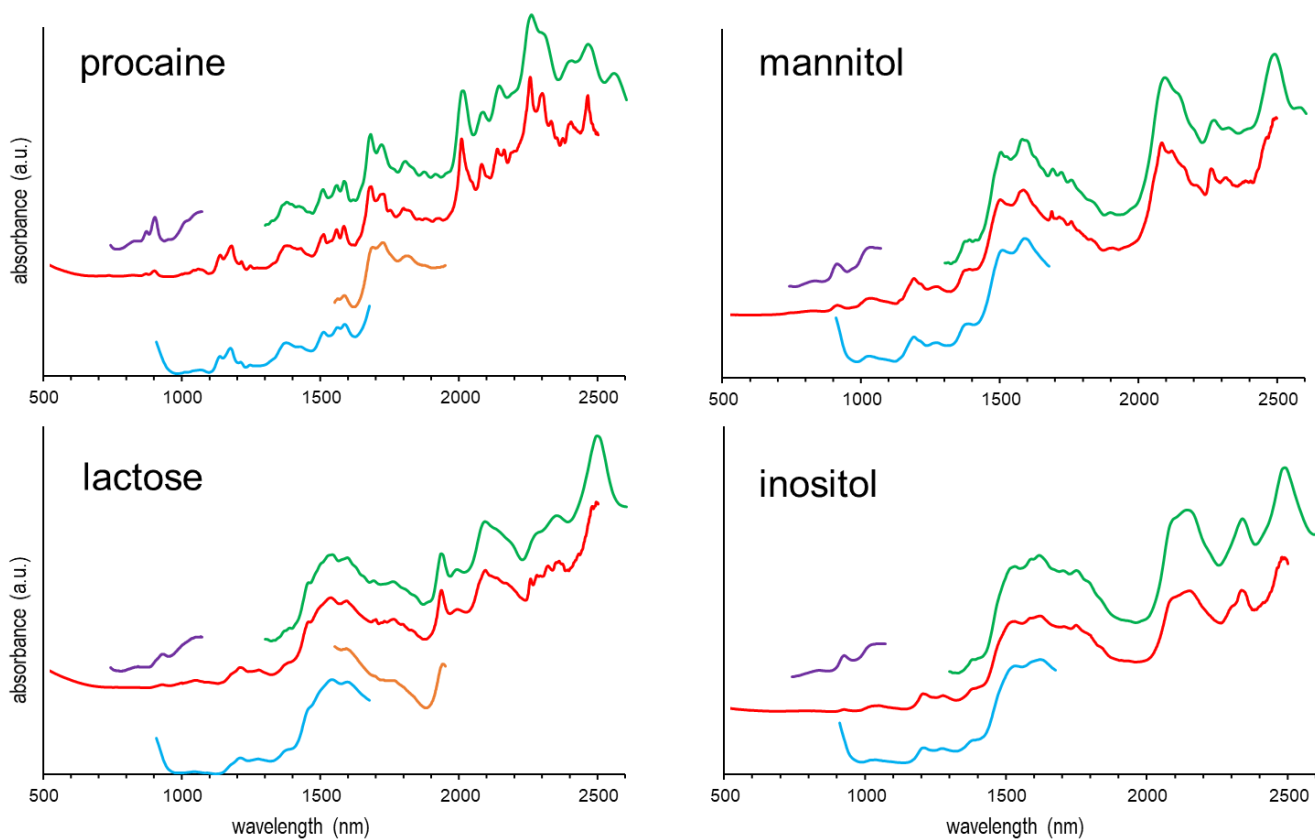


Figure S3. (part 2 of 2) - Comparison of the spectral output for ten adulterants from the different sensors. red: ASD LabSpec4; green: NeoSpectra; orange: NIRone; blue: microNIR; purple: SCiO.

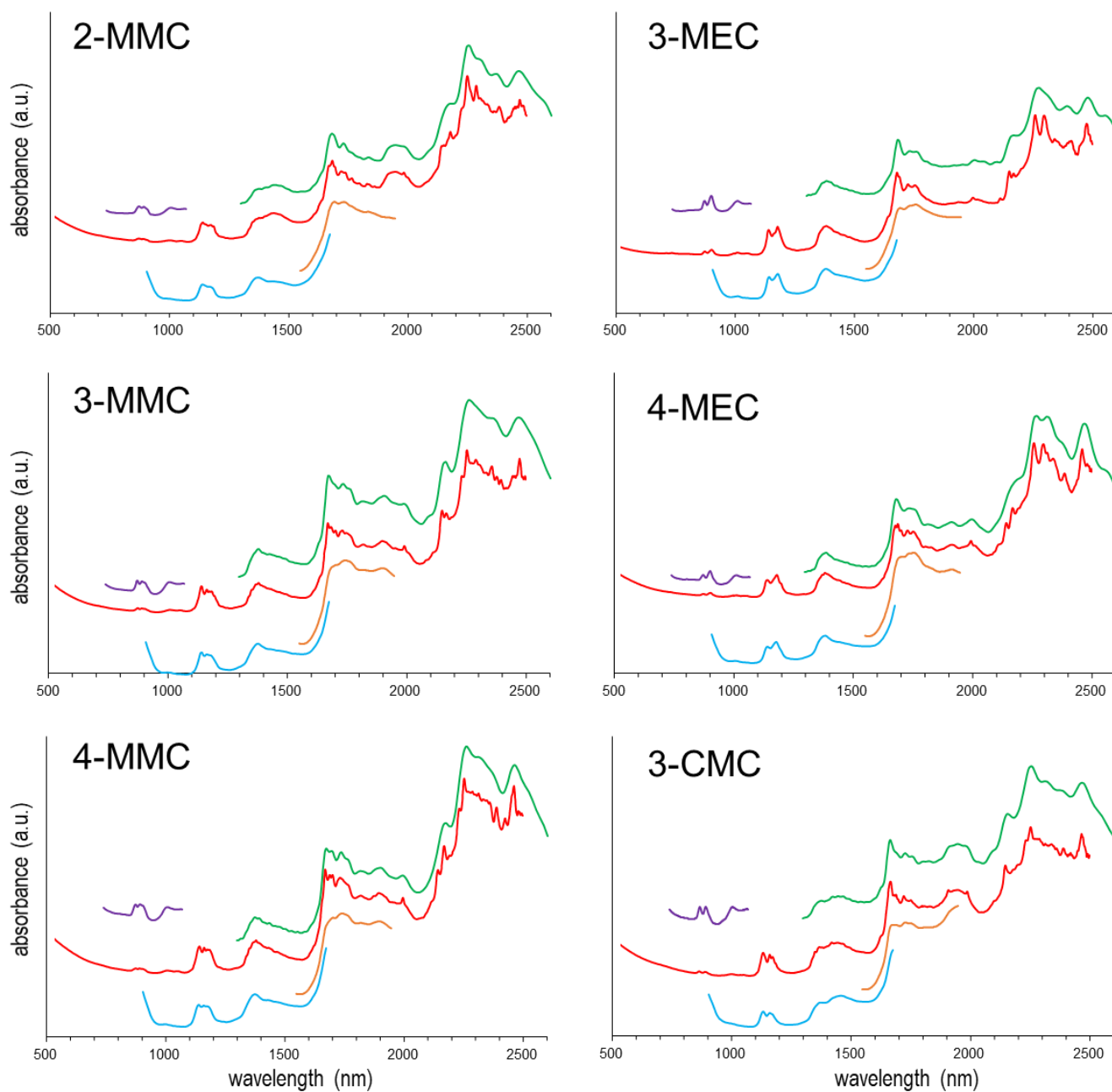


Figure S4. Comparison of the spectral output for six new psychoactive substances from the different sensors. red: ASD LabSpec4; green: NeoSpectra; orange: NIRone; blue: microNIR; purple: SCiO.