

Electronic Supplementary Information for: Detection of Newly Emerging Psychoactive Substances Using Raman Spectroscopy and Chemometrics

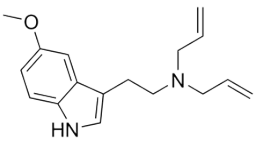
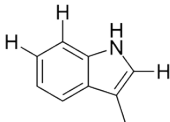
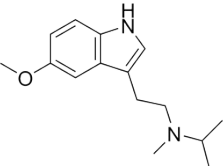
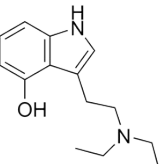
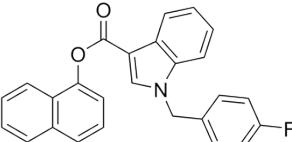
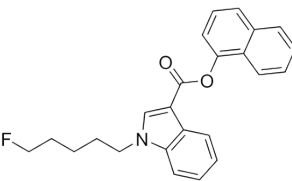
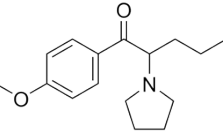
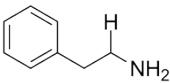
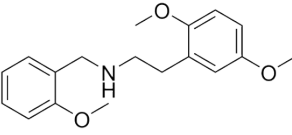
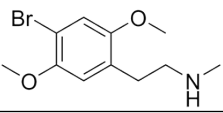
Jesus Calvo-Castro,[§] Amira Guirguis,[§] Eleftherios G. Samaras, Mire Zloh, Stewart B. Kirton and
Jacqueline L. Stair.**

Department of Pharmacy, Pharmacology and Postgraduate Medicine, School of Life and
Medical Sciences, University of Hertfordshire, Hatfield, AL10 9AB, UK.

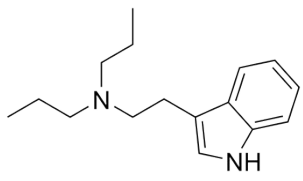
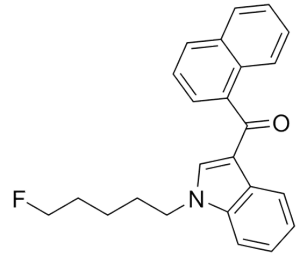
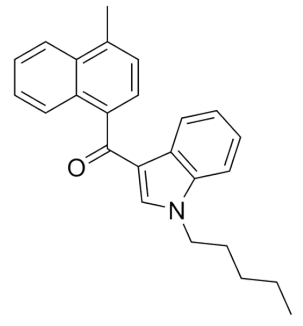
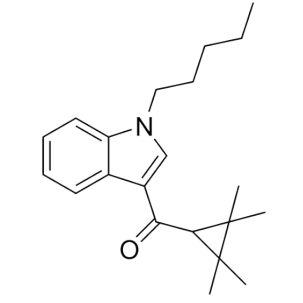
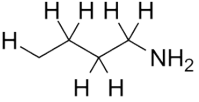
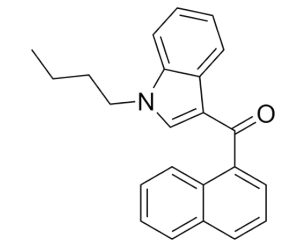
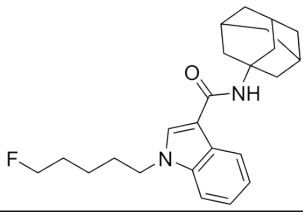
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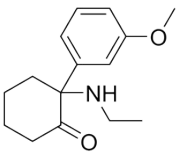
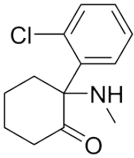
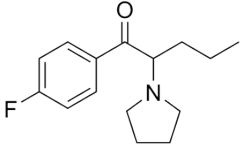
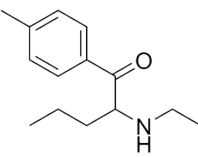
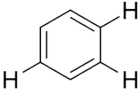
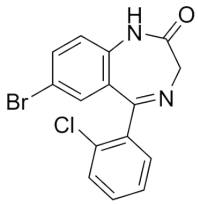
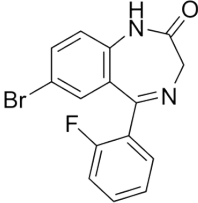
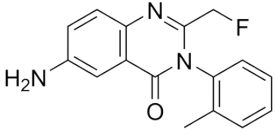
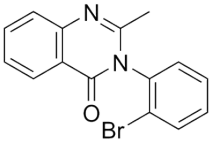
SI.1 Training set NPS

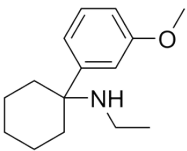
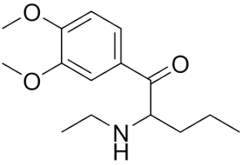
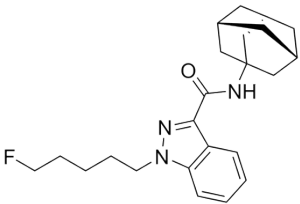
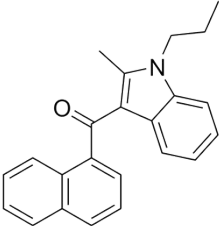
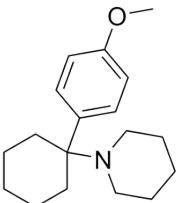
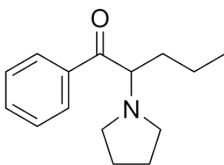
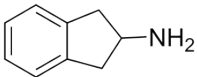
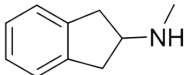
Table SI.1.1 Chemical structure, category and class of NPS reference standards belonging to the training set.

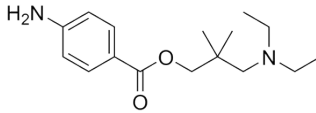
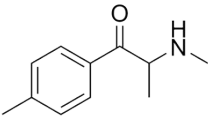
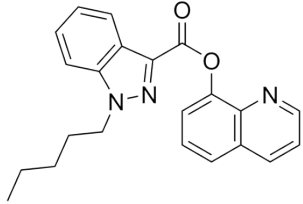
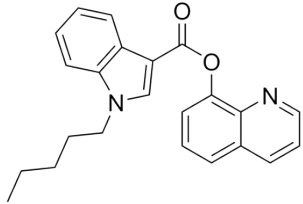
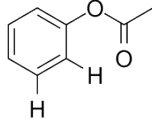
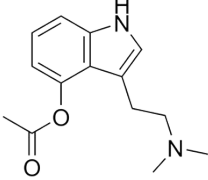
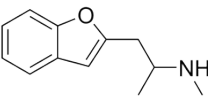
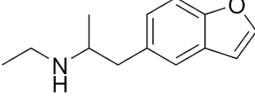
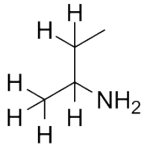
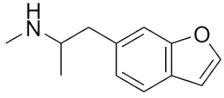
Reference Standard	Chemical Structure	Category	Common Substructure	Class
5-Meo-DALT		1		Tryptamines
5-MeO-MiPT		1		Tryptamines
4-HO-DET		1		Tryptamines
FDU-PB-22		1		Synthetic Cannabinoids
NM-2201		1		Synthetic Cannabinoids
4-MeO-α-PVP		2		
25-H-NBOMe		2	Phenethylamines	
N-Me-2C-B		2	Phenethylamines	

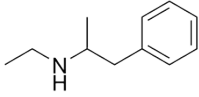
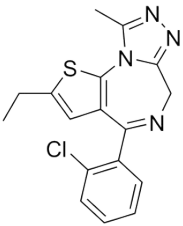
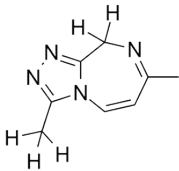
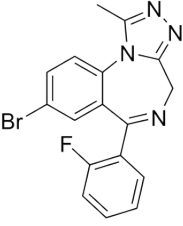
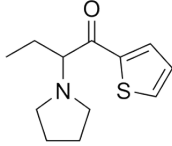
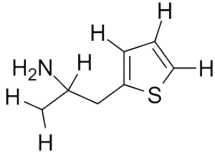
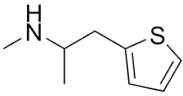
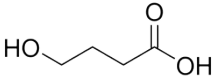
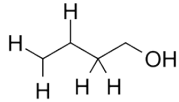
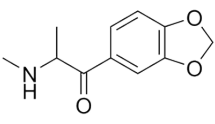
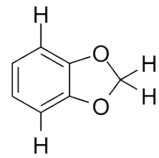
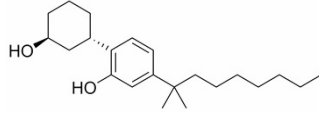
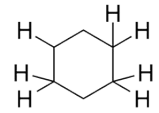
STP (DOM)		2		Phenethylamines
AB-FUBINACA		3		Synthetic Cannabinoids
AB-PINACA		3		Synthetic Cannabinoids
THJ-018 (JWH-018 indazole analogue)		3		Synthetic Cannabinoids
SDB-006		3		Synthetic Cannabinoids
AM-679		3		Synthetic Cannabinoids

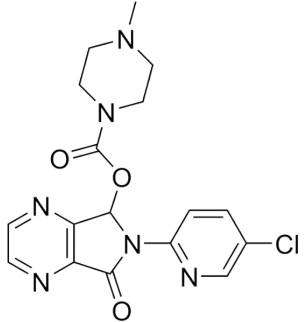
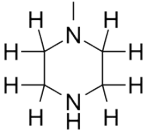
DPT		3		Tryptamines
AM-2201		4		Synthetic Cannabinoids
JWH-122		4		Synthetic Cannabinoids
UR-144		4		Synthetic Cannabinoids
JWH-073		4		Synthetic Cannabinoids
5F-APICA		4		Synthetic Cannabinoids

Methoxetamine (MXT)		5		Arylcyclohexylamines
Ketamine		5		Arylcyclohexylamines
4F-α-PVP		5		Cathinones
4-Me-N-ethylnorpentadrone		5		Cathinones
Phenazepam		5		Benzodiazepines
Flubromazepam		5		Benzodiazepines
Afloqualone		5		Quinazolines
Mebroqualone		5		Quinazolines

3-Meo-PCE		5	Arylcyclohexylamines
DL-4662		5	Cathinones
5F-APINACA		5	Synthetic Cannabinoids
JWH-015		5	Synthetic Cannabinoids
4-Meo-PCP		5	Arylcyclohexylamines
α -PVP		5	Cathinones
2-AI		5	Aminoindanes
N-Me-2-AI		5	Aminoindanes

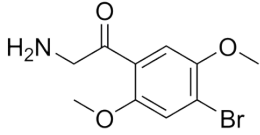
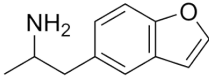
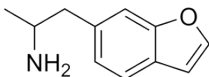
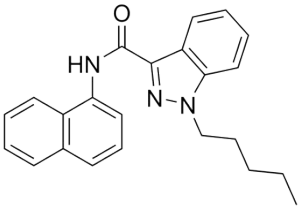
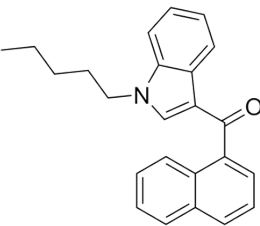
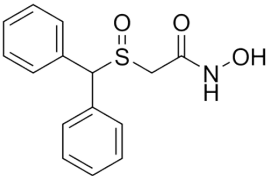
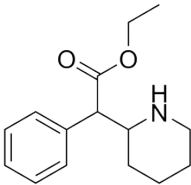
Dimethocaine		5		Anaesthetic
Mephedrone		5		Cathinones
N-PB-22 (PB-22 indazole analogue)		6		Synthetic Cannabinoids
PB-22		6		Synthetic Cannabinoids
4-acetylpsilocin fumarate (4-AcO-DMT)		6		Tryptamines
2-MAPB		7		Arylalkylamines
5-EAPB		7		Arylalkylamines
6-MAPB		7		Arylalkylamines
N-ethyl-		7		Phenethylamines

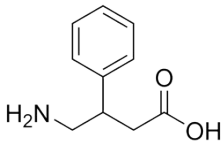
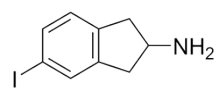
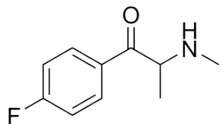
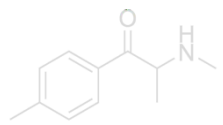
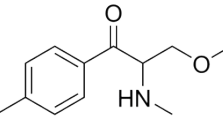
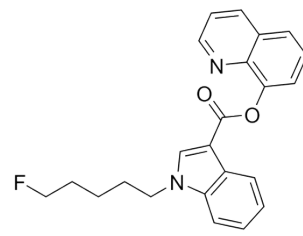
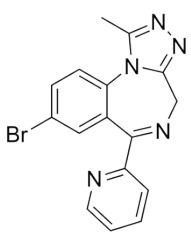
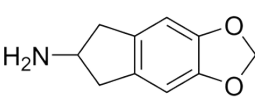
amphetamine				
Etizolam		8		Benzodiazepines
Flubromazolam		8		Benzodiazepines
α -PBT		9		Cathinones
MPA		9		Arylalkylamines
GHB		10		Hydroxybutyrate
Methylone		11		Cathinones
trans-CP 47,497-C8		12		Synthetic Cannabinoids

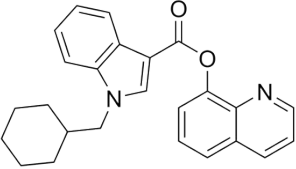
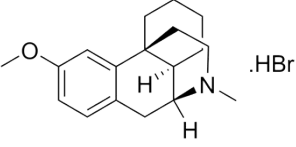
Zopiclone	 <p>The chemical structure of Zopiclone consists of a central imidazole ring. One nitrogen of the imidazole is bonded to a 4-chloropyridin-2-yl group. The other nitrogen is bonded to a 5-membered ring containing an oxygen atom and a carbonyl group. This 5-membered ring is further substituted with a 1-methylpiperazine ring.</p>	13	 <p>The chemical structure shows ethylenediamine, a six-membered ring with two nitrogen atoms and four hydrogen atoms explicitly shown on the ring carbons.</p>	Others
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SI.2 Validation set NPS

Table SI.2.1 Chemical structure, category and class of NPS reference standards belonging to the validation set.

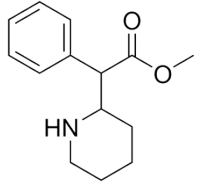
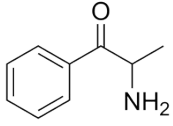
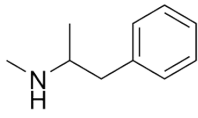
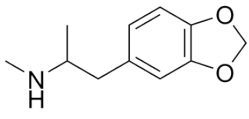
NPS	Chemical Structure	Category	Class
β k-2C-B		2	Cathinones
5-APB		2	Alkylarylamines
6-APB		2	Alkylarylamines
MN-18		3	Synthetic Cannabinoids
JWH-018		4	Synthetic Cannabinoids
Adrafinil		5	Others
Ethylphenidate (EPD)		5	Piperidine

Phenibut		5	Others
5-IAI		5	Aminoindanes
Flephedrone (4-FMC) ¹		5	Cathinones
Mephedrone (4-MMC) ¹		5	Cathinones
Mexedrone		5	Cathinones
5F-PB-22		6	Synthetic Cannabinoids
Pyrazolam		8	Benzodiazepines
5,6-MDAI		11	Aminoindanes

BB-22	 <p>The structure shows a cyclohexane ring attached to the nitrogen of an indazole ring. The 3-position of the indazole ring is substituted with a carbonyl group, which is further linked to an oxygen atom. This oxygen atom is part of an ester linkage to a quinoline ring system.</p>	12	Synthetic Cannabinoids
Dextromethorphan HBr (DXM)	 <p>The structure shows the dextromethorphan cation, a pentacyclic tropane alkaloid with a methoxy group on the benzene ring. The nitrogen atom is shown with a methyl group and a hydrogen atom, and is associated with a bromide counterion (.HBr).</p>	12	Others

SI.3 Test set NPS

Table SI.3.1 Chemical structure and class of NPS reference standards belonging to the test set.

NPS	Chemical Structure	Class
Methylphenidate (MPD)		Piperidine
S-Cathinone		Cathinones
Methamphetamine		Phenethylamines
MDMA		Phenethylamines

SI.4 Line loading plot PC1-3

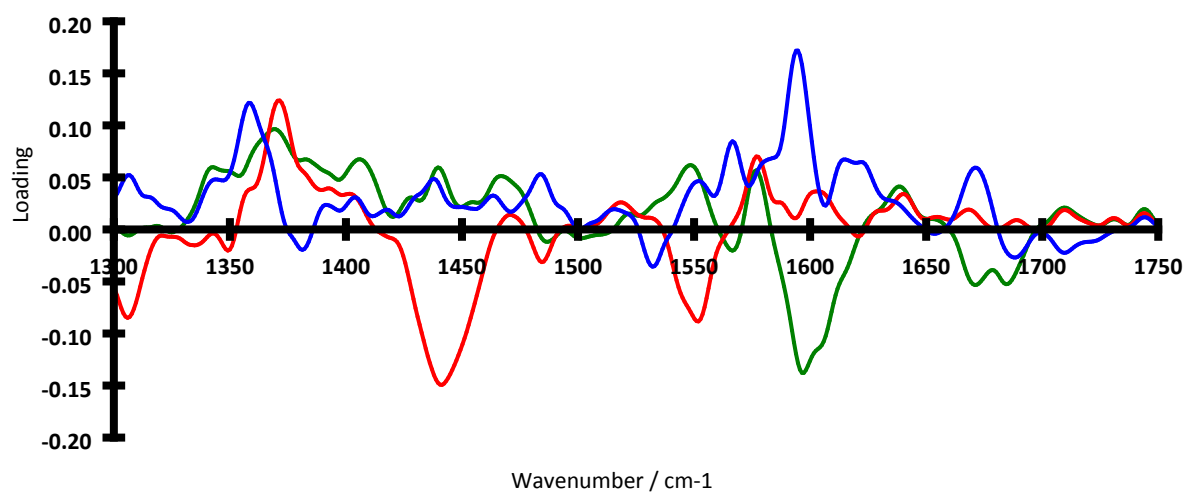


Figure SI.4.1 PC1 (blue solid line), PC2 (red solid line) and PC3 (green solid line) loadings from the generated three dimensional model system.