Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2017

Drowning in diversity? A systematic way of clustering and selecting a representative set of New Psychoactive Substances

Zloh, M., Samaras, E. G., Calvo-Castro, J., Guirguis, A., Stair, J. L., Kirton, S. B.* School of Life and Medical Sciences, University of Hertfordshire, College Lane, AL10 9AB, UK

*Corresponding author: Stewart B. Kirton: s.b.kirton3@herts.ac.uk

Contents

Representative NPS of clusters in super-clusters.	2
Full range ¹ H-NMR spectra of selected NPS	8

Representative NPS of clusters in super-clusters.



Figure S1. Representative NPS of clusters in the super-cluster 1.



Figure S2. Representative NPS of clusters in the super-cluster 2.



Figure S3. Representative NPS of clusters in the super-cluster 3.



UR-144 (4.03) JWH-073 methyl derivative (4.04) 5F-Apica (4.05)





Figure S5. Representative NPS of clusters in the super-cluster 5.



Figure S6. Representative NPS of clusters in the super-cluster 6.

CIP-NH CITTIN CITTI ſ 2-MAPB (7.01) 5-EAPB (7.02) 6-MAPB (7.03) N-ethylamphetamine (7.04)

Figure S7. Representative NPS of clusters in the super-cluster 7.



Figure S8. Representative NPS of clusters in the super-cluster 8.



Figure S9. Representative NPS of clusters in the super-cluster 9.

HO HO OHB (10.01) Poppers (10.02) но、



Methylone (11)

Figure S11. Representative NPS of clusters in the super-cluster 11.

CP 47,497-C8 (12)

Figure S12. Representative NPS of clusters in the super-cluster 12.



Figure S13. Representative NPS of clusters in the super-cluster 13.



Figure S14. Singleton NPS in the super-cluster 14.

Figure S15. Singleton NPS in the super-cluster 15.

~____М____ОН Methanandamide (16)

Figure S16. Singleton NPS in the super-cluster 16.

HU-210 (17)

Figure S17. Singleton NPS in the super-cluster 17.



Figure S18. Singleton NPS in the super-cluster 18.

Arecoline (19)

Figure S19. Singleton NPS in the super-cluster 19.



Salvia Divinorum (20)

Figure S20. Singleton NPS in the super-cluster 20.

Glaucine (21)

Figure S21. Singleton NPS in the super-cluster 21.

Table S1: The distribution of the NPS compounds in the dendrogram's super-clusters and number of clusters in each super-cluster. Individual clusters of super-cluster are labelled using the super-cluster number followed by full stop and sequential number.

		'Super' Cluster No.																				
	All	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
Aminoindanes	5					4						1									1	
Arylalkylamines	30		9			6		10		4		1									1	
Arylcyclohexylami	9					9																
nes																						
Benzodiazepins	11					7			4													
Canabinoids	137	4		22	57	38	4					1	7		1	1	1	1				
Cathinones	79		10			51				1		17										
Indolealkylamines	33	22		6		1	2	2														
Phenethylamines	77		48			9		13				7										
Piperazine	15					13								2								
derivatives																						
Piperidines and	6					6																
Pyrrolidines																						
Plants and	12			3		5						1								1	1	1
extracts																						
Opiods	15					13							2									
Others	49	1		1		35		1			3	0	6	1					1			
Total No.	478	27	67	32	57	197	6	26	4	5	3	28	15	3	1	1	1	1	1	1	1	1
Number of		11	10	11	5	18	3	4	2	2	2	1	1	1	1	1	1	1	1	1	1	1
clusters																						
Maximal																						
dissimilarity		0.31	0.71	0.29	0.55	0.82	0.19	0.83	0.22	0.15	0.64	0.66	0.80	0.84								
In super-clusters																						

Full range ¹H-NMR spectra of selected NPS



Figure S22. Full range ¹H-NMR spectra of 5-APB and DOM.