

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

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Contents

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

Representative NPS of clusters in super-clusters.

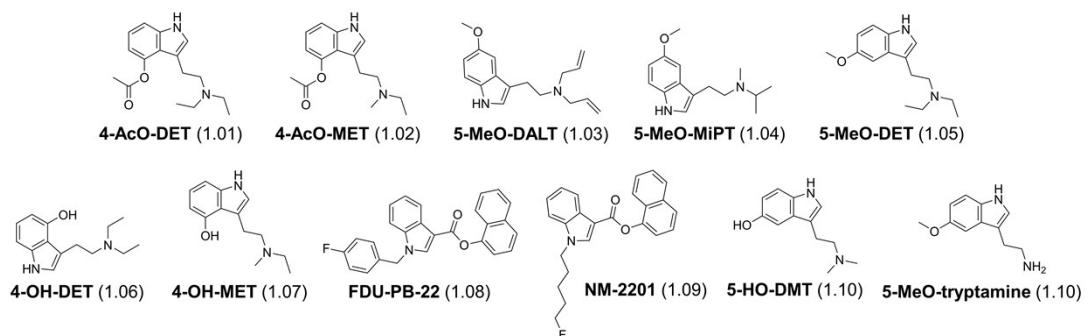


Figure S1. Representative NPs of clusters in the super-cluster 1.

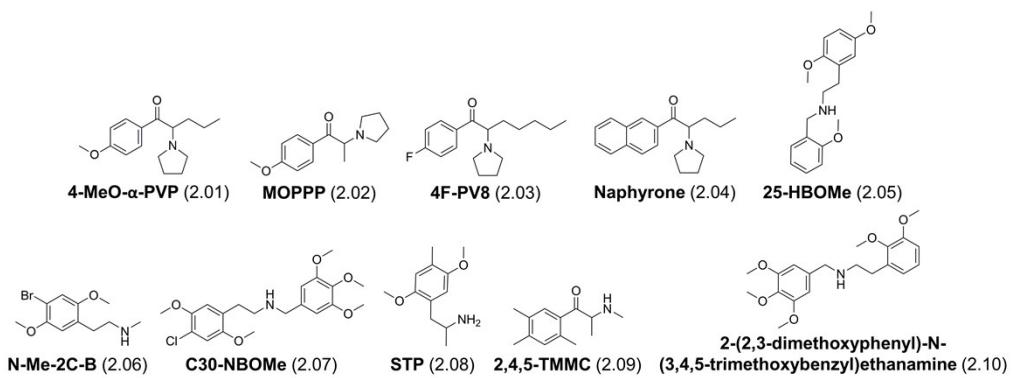


Figure S2. Representative NPs of clusters in the super-cluster 2.

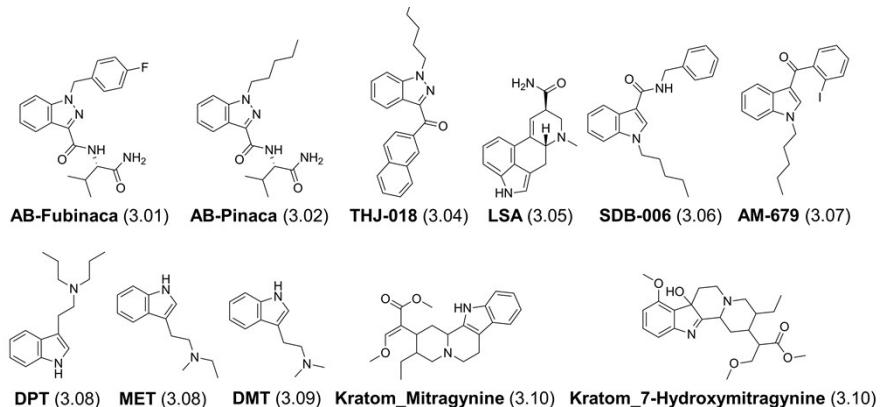


Figure S3. Representative NPs of clusters in the super-cluster 3.

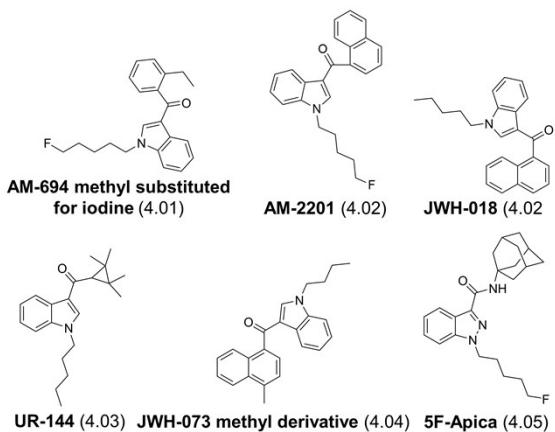


Figure S4. Representative NPS of clusters in the super-cluster 4.

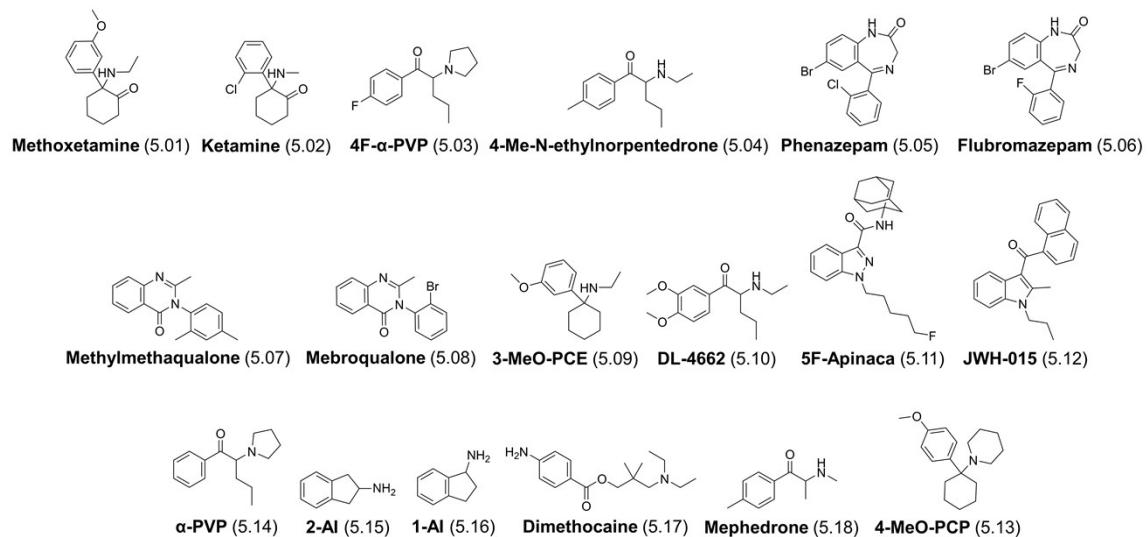


Figure S5. Representative NPS of clusters in the super-cluster 5.

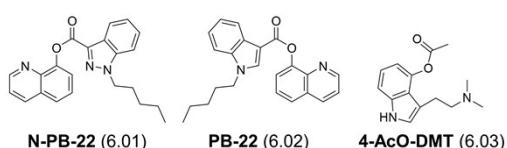


Figure S6. Representative NPS of clusters in the super-cluster 6.

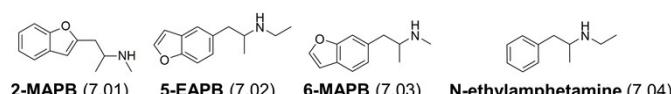
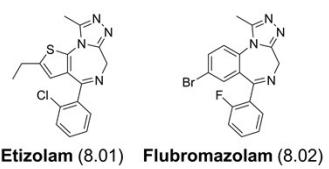


Figure S7. Representative NPS of clusters in the super-cluster 7.



Etizolam (8.01) **Flubromazolam** (8.02)

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

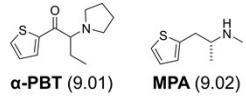


Figure S9. Representative NPS of clusters in the super-cluster 9.

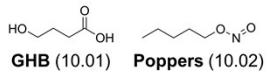


Figure S10. Representative NPS of clusters in the super-cluster 10.

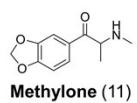


Figure S11. Representative NPS of clusters in the super-cluster 11.

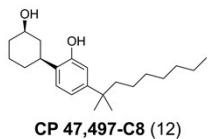


Figure S12. Representative NPS of clusters in the super-cluster 12.

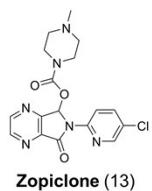


Figure S13. Representative NPS of clusters in the super-cluster 13.

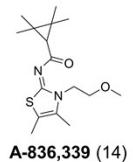


Figure S14. Singleton NPS in the super-cluster 14.

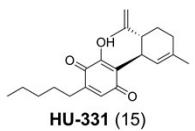


Figure S15. Singleton NPS in the super-cluster 15.

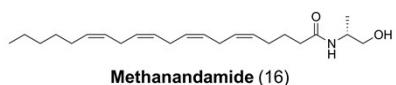


Figure S16. Singleton NPS in the super-cluster 16.

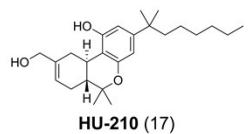


Figure S17. Singleton NPS in the super-cluster 17.



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

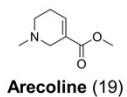
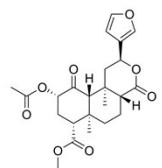
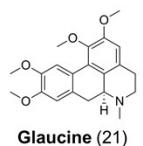


Figure S19. Singleton NPS in the super-cluster 19.



Salvia Divinorum (20)

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



Glaucine (21)

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

Full range ^1H -NMR spectra of selected NPS

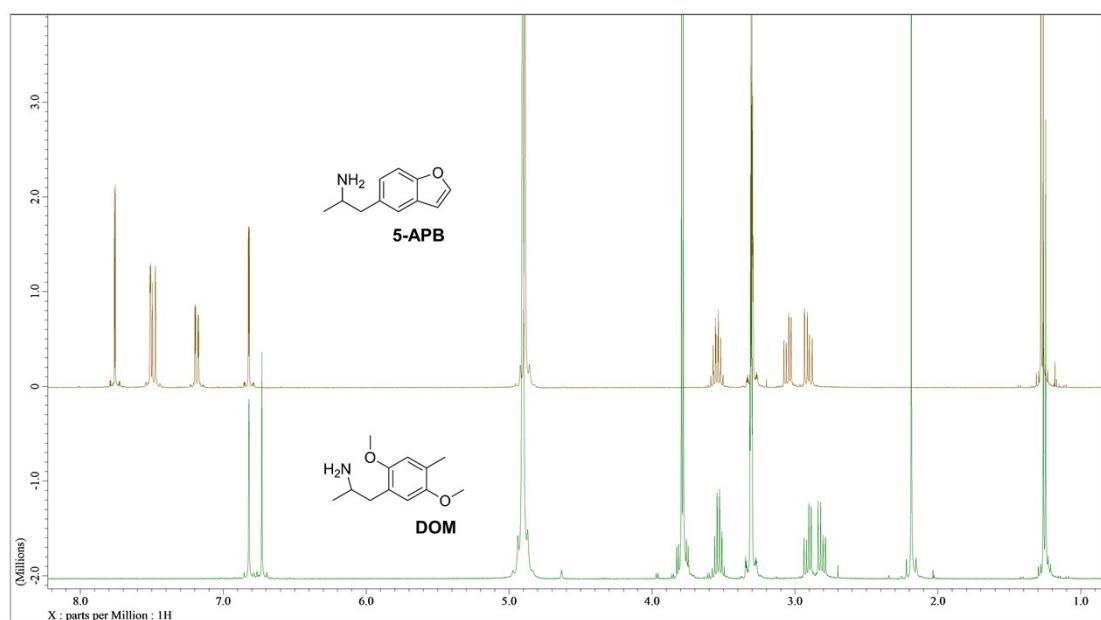


Figure S22. Full range ^1H -NMR spectra of 5-APB and DOM.