Revealing the Presence of Tryptamine New Psychoactive Substances Using Fused "Neutral Loss" Spectra Derived From DART High-Resolution Mass Spectra

Supplementary material

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Contained within this supporting information document are: representative DART-high resolution mass spectra at 20 V and neutral loss mass spectra at 60 V and 90 V for the tryptamines represented in this study; a PLS-DA scores plot associated with the neutral loss data; Masses determined to be most impactful in enabling differentiation of groups; a correlation matrix and dendrogram showing the placement of the four tryptamines used for external validation; a PCA scores plot and confusion matrix showing variation between spectra analyzed by different analysts on the same day and one analyst in different days; a confusion matrix resulting from the "leave-one-structure-out" validation of the PLS-DA model; classification performance, sensitivity, specificity and precision of the "leave-one-structure-out" validation; probability prediction assignments of the PLD-DA model for the "leave-one structure out" validation; the average of ten replicates of the relative intensities for the *m/z* values in the tryptamine 60 V and 90 V neutral loss spectra ranked most important for discrimination; and the computed probabilities for assignment to each group of the tryptamines used for the external validation.

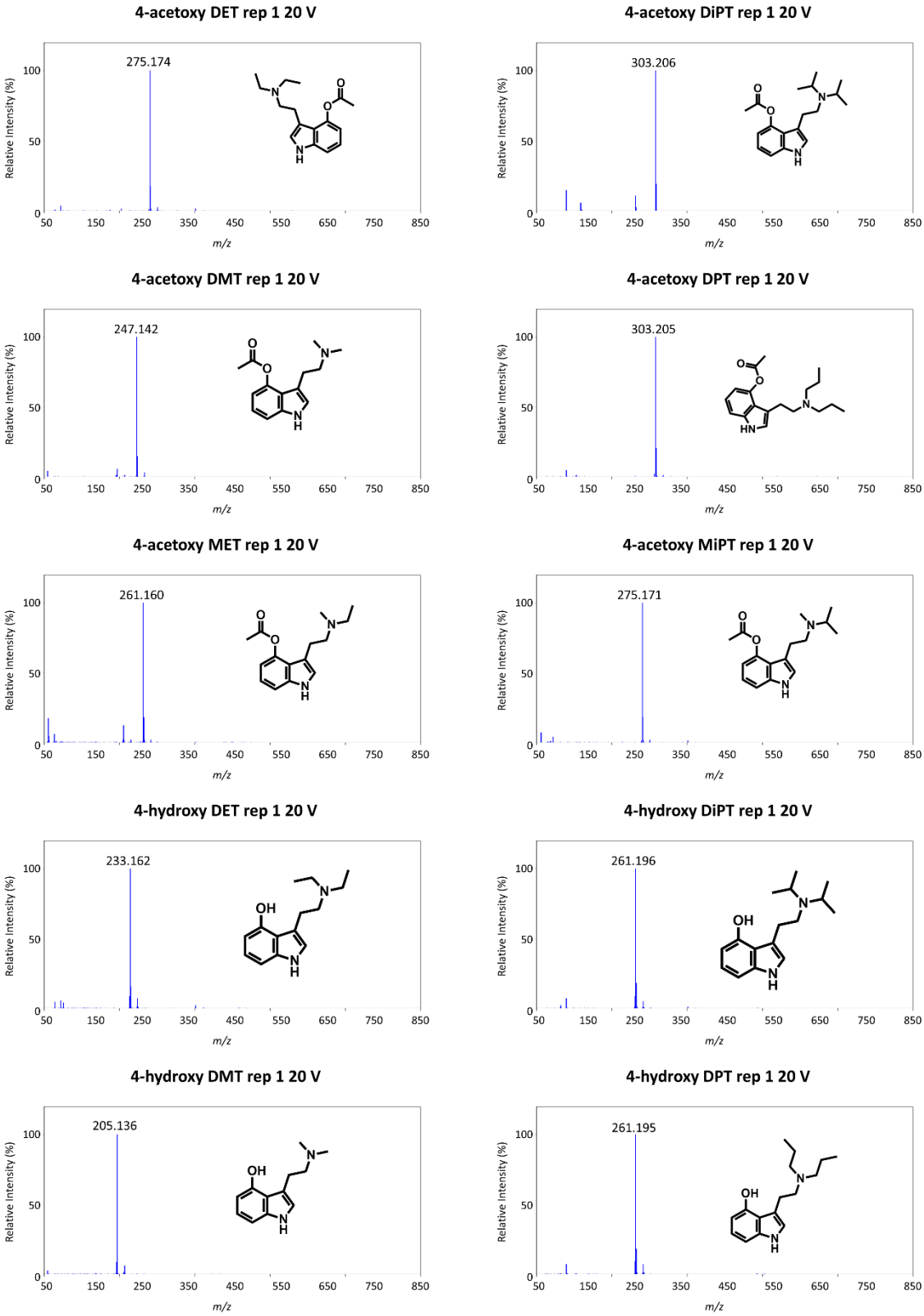


Figure S1. The 20 V soft ionization spectra and structures for the 50 tryptamines analyzed in this study.

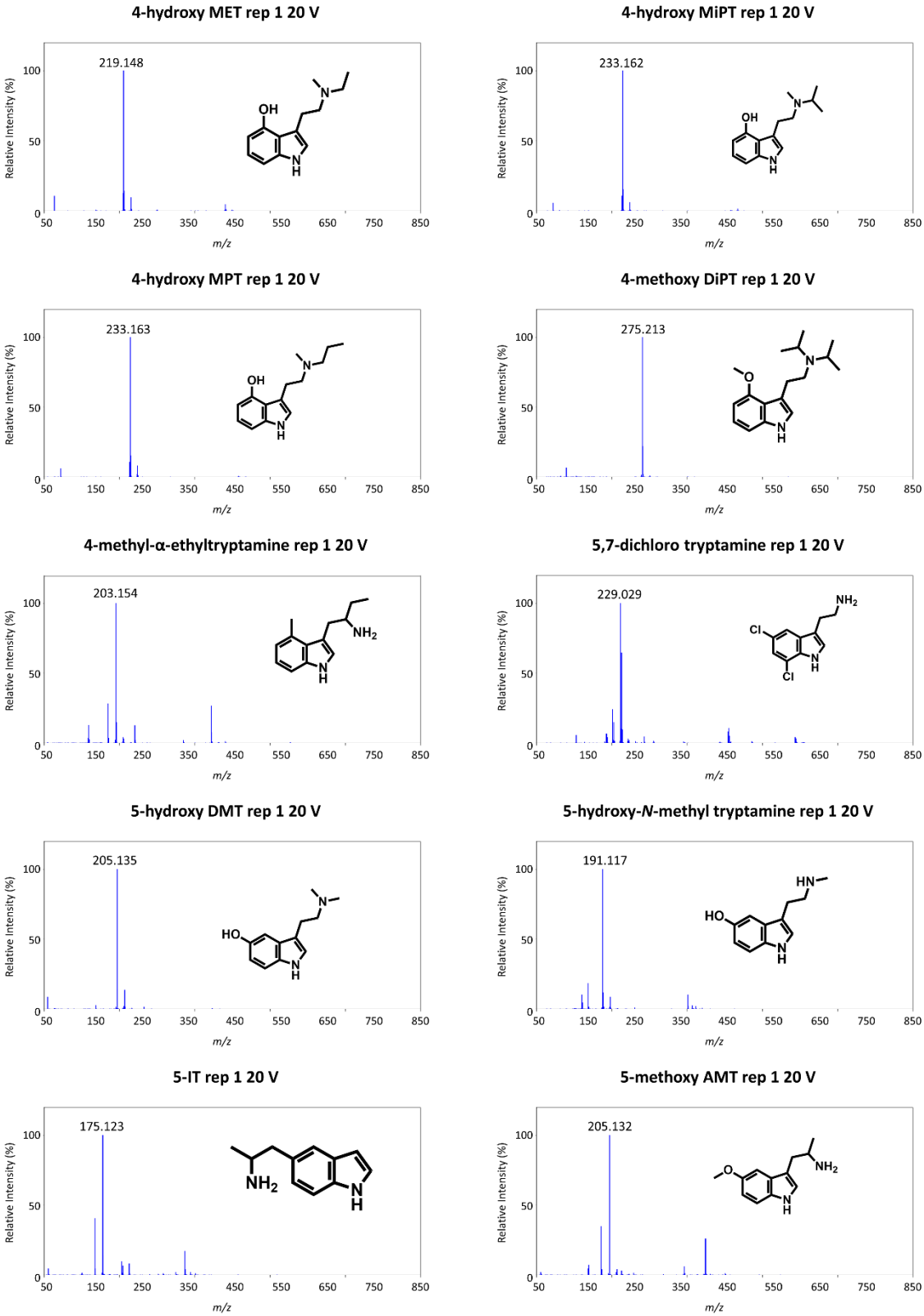
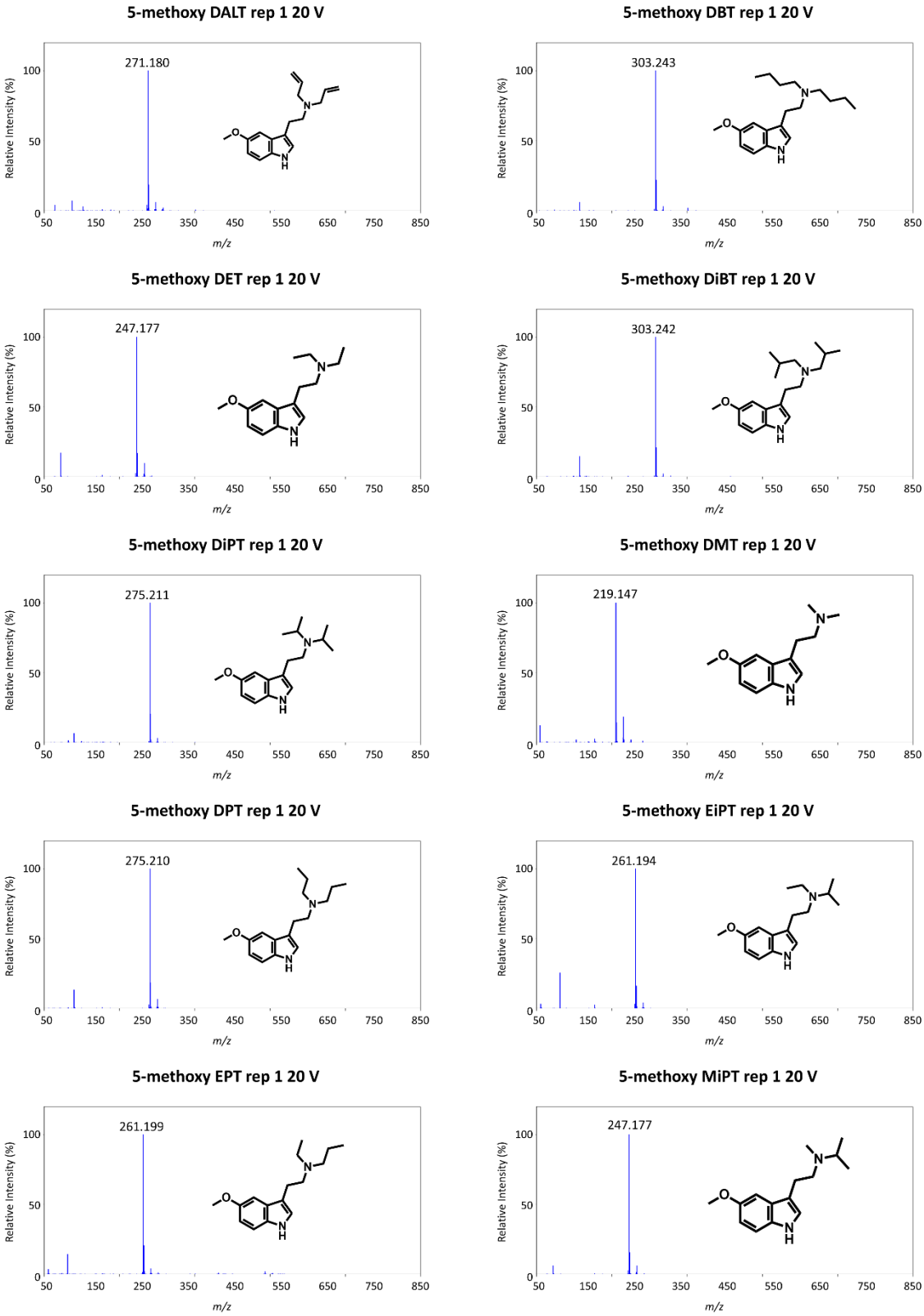


Figure S1 (continued). The 20 V soft ionization spectra and structures for the 50 tryptamines analyzed in this study.



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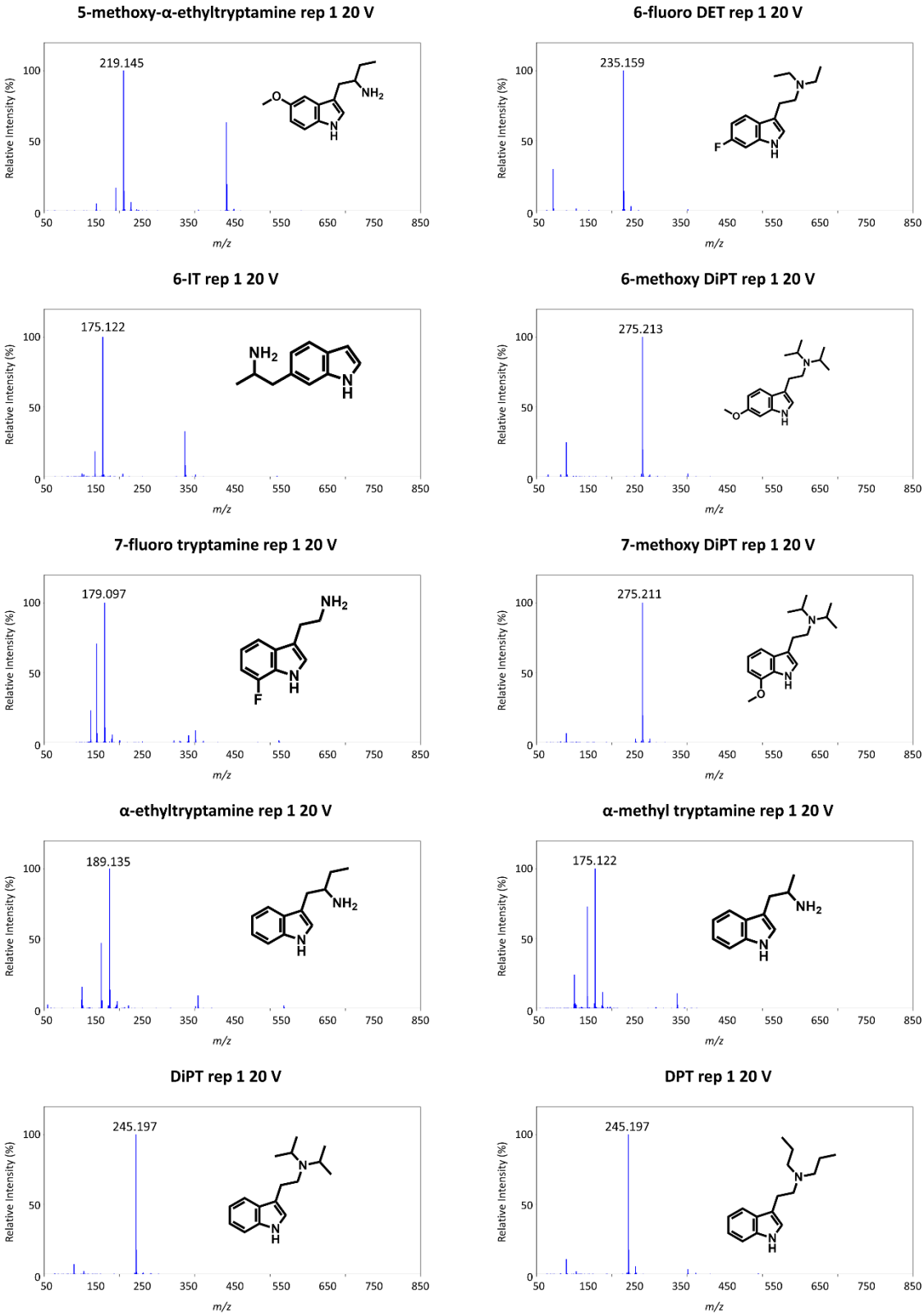

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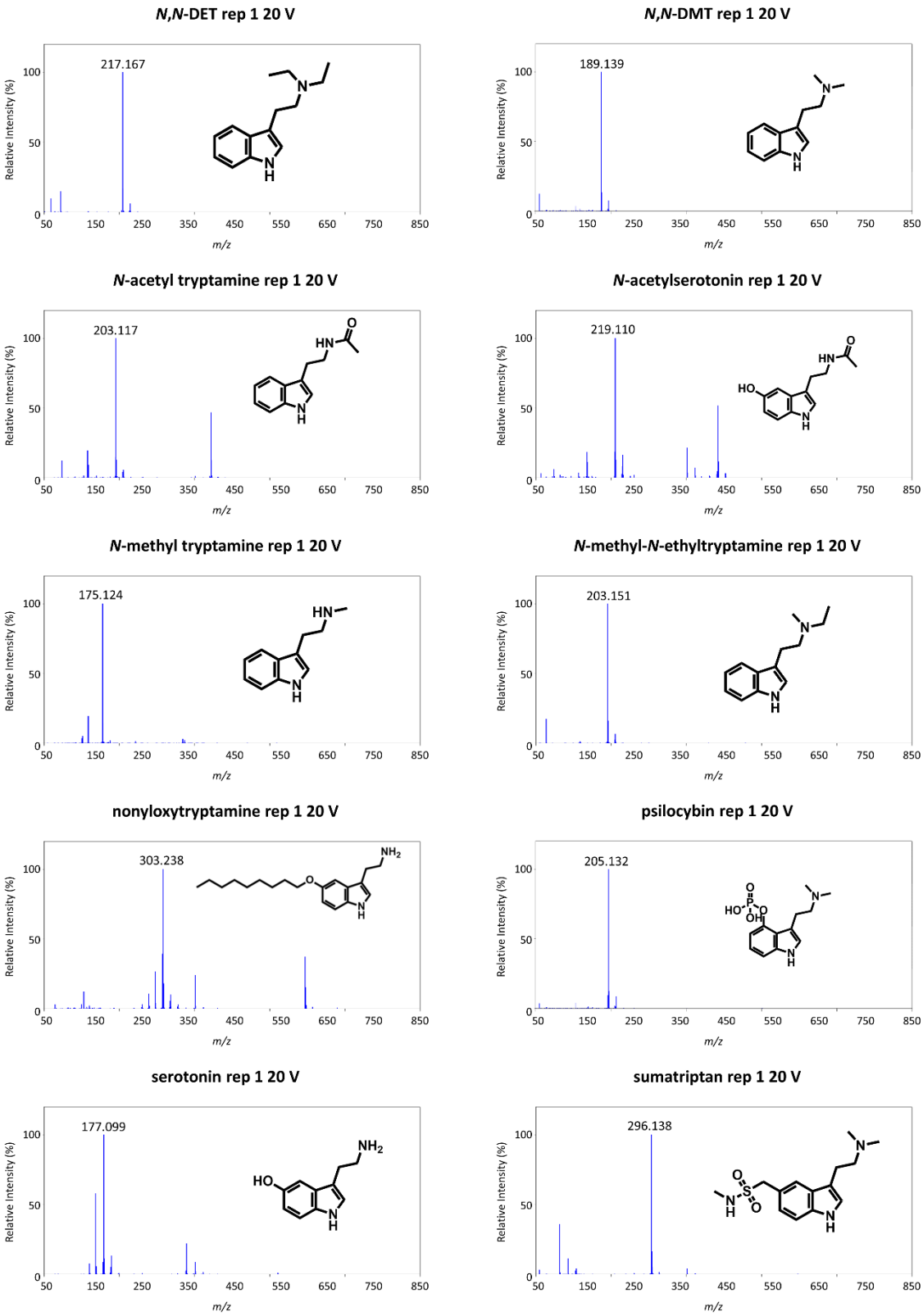

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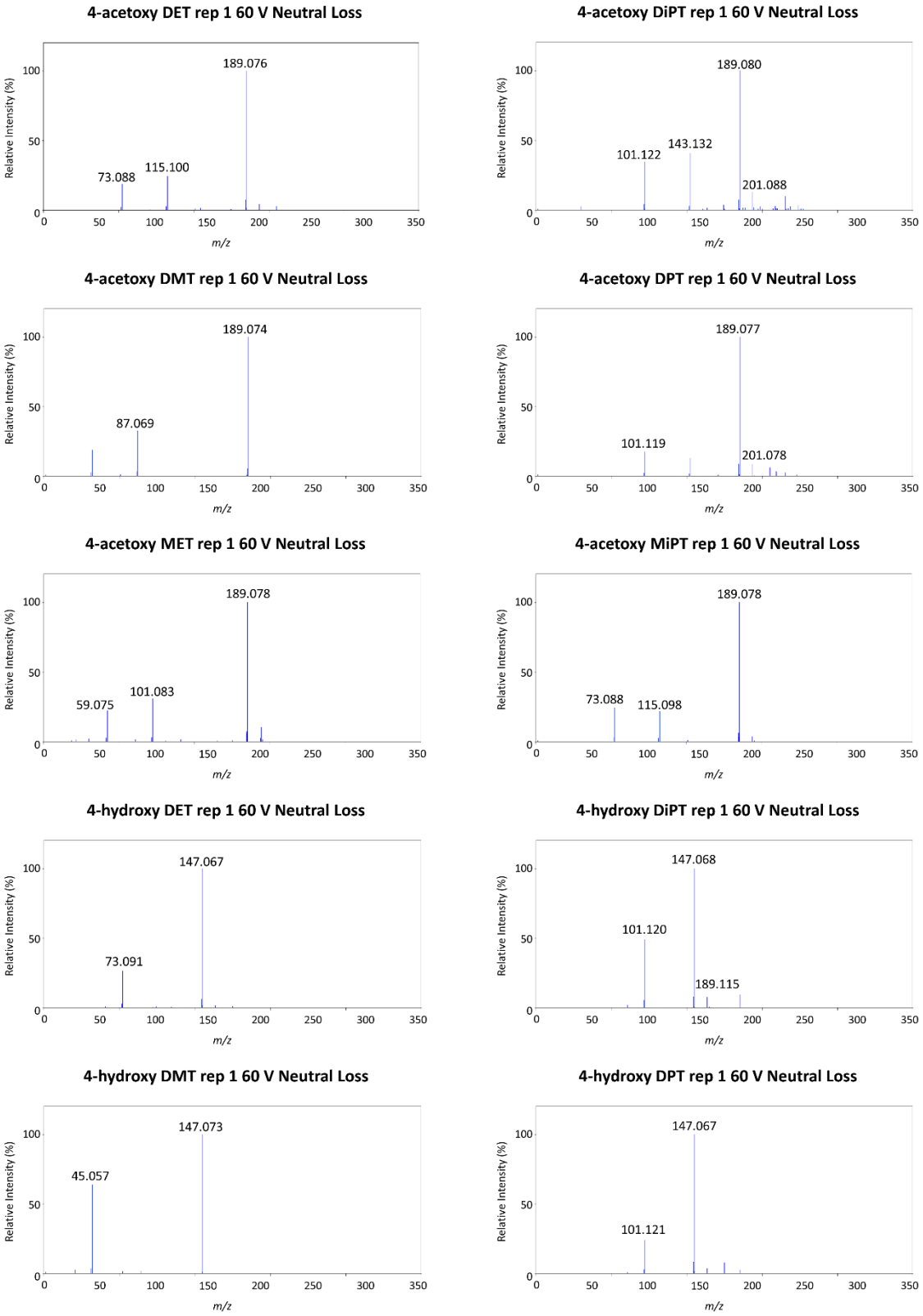
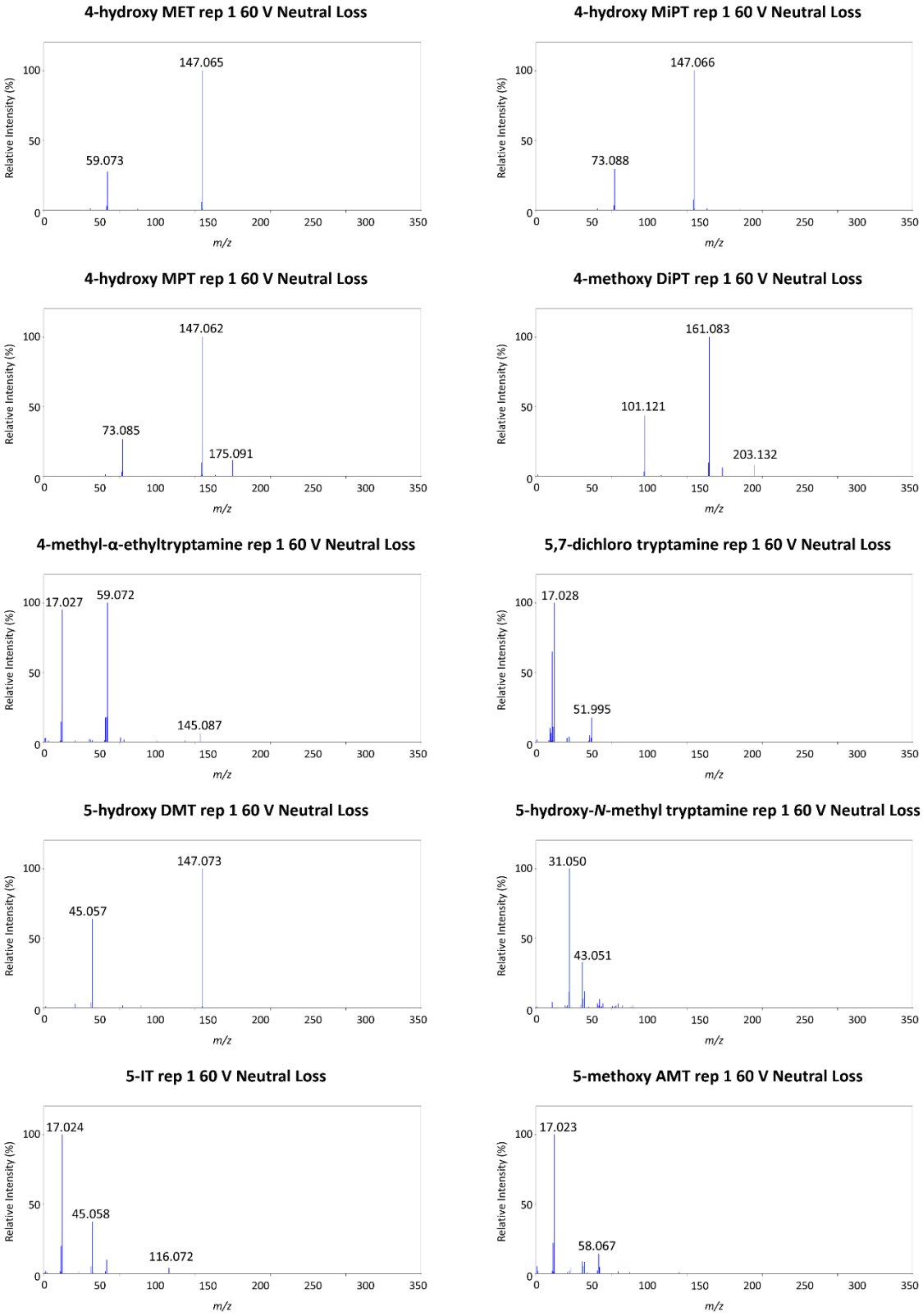


Figure S2. The 60 V neutral loss spectra for the 50 tryptamines analyzed in this study.



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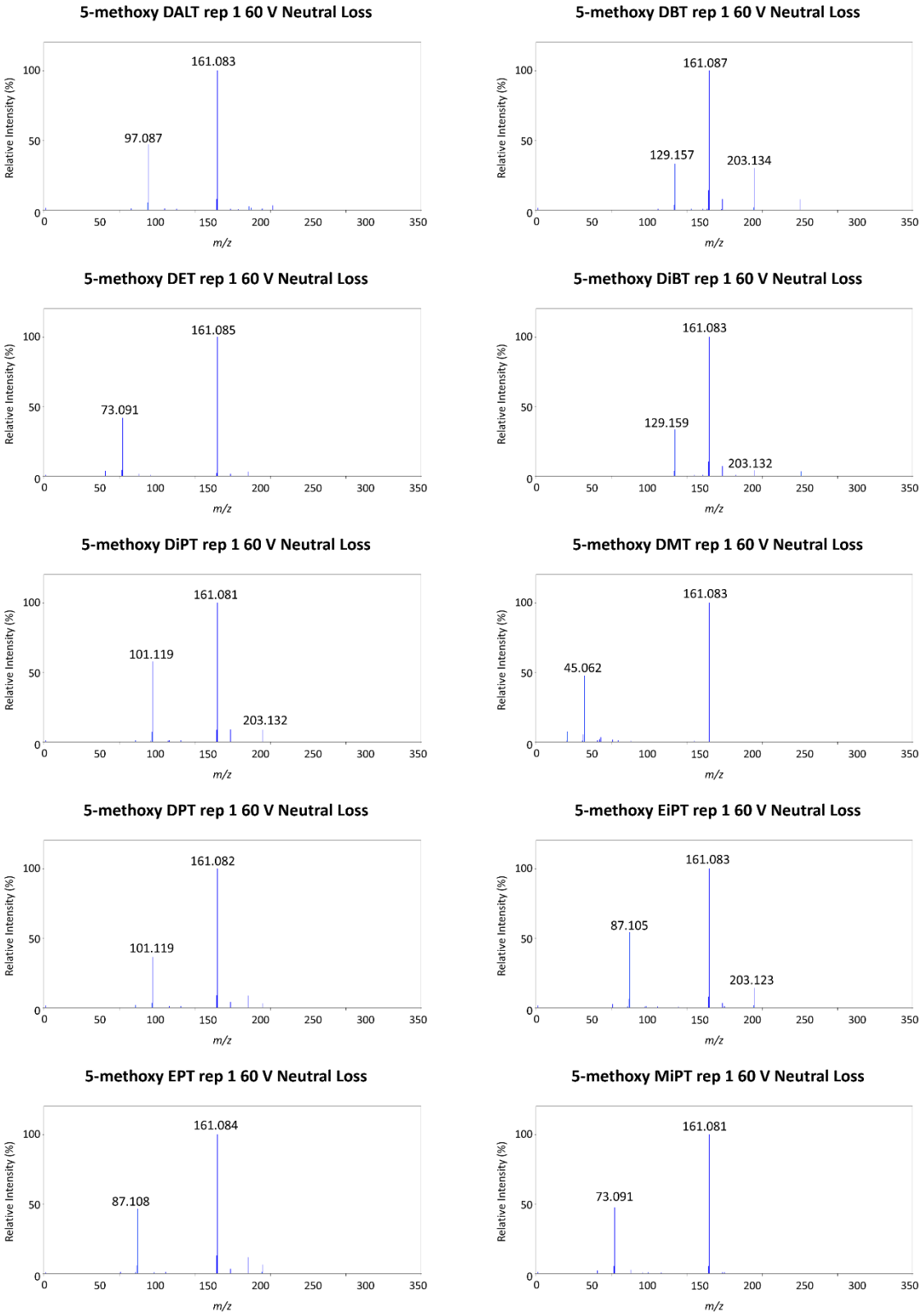

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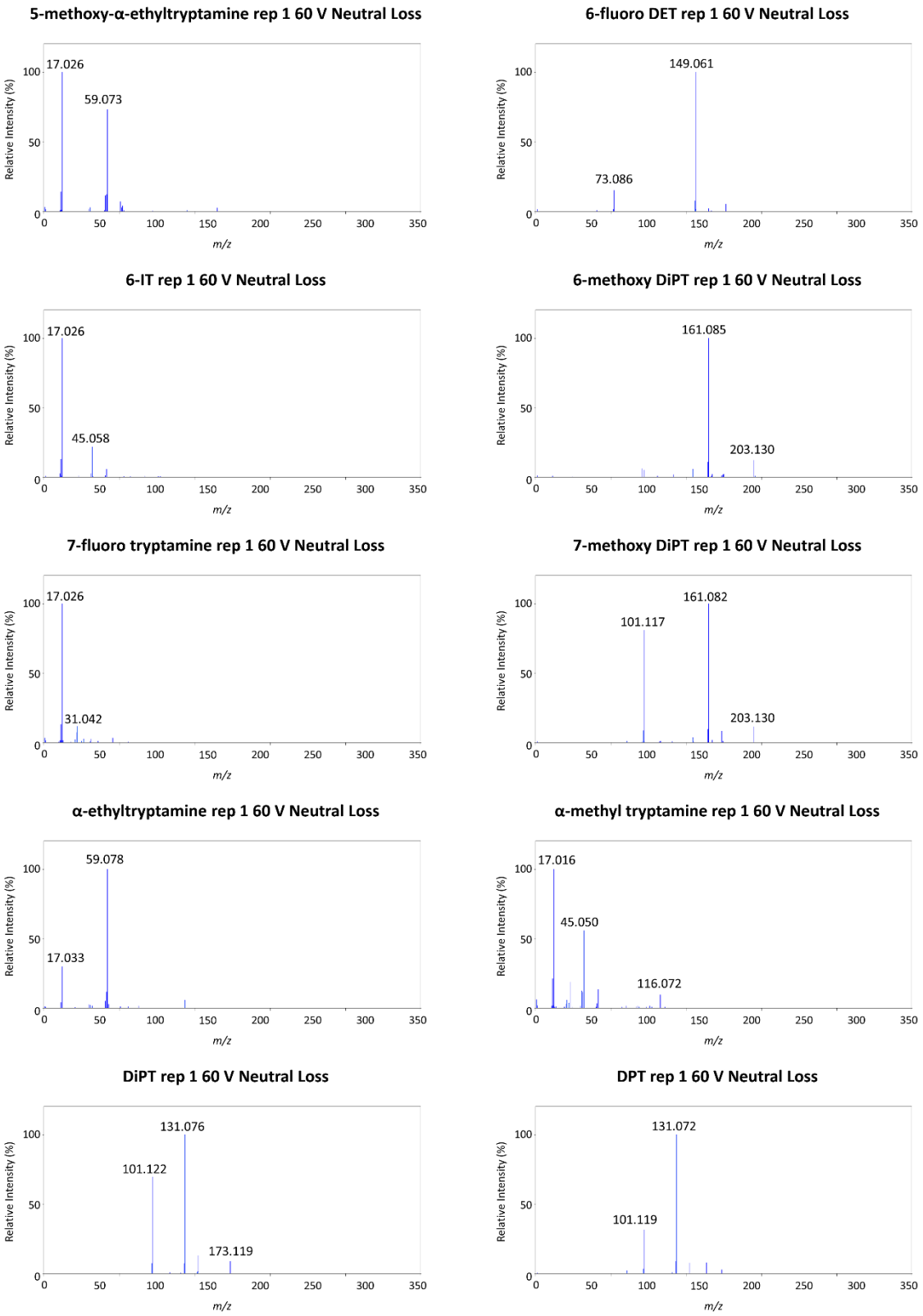

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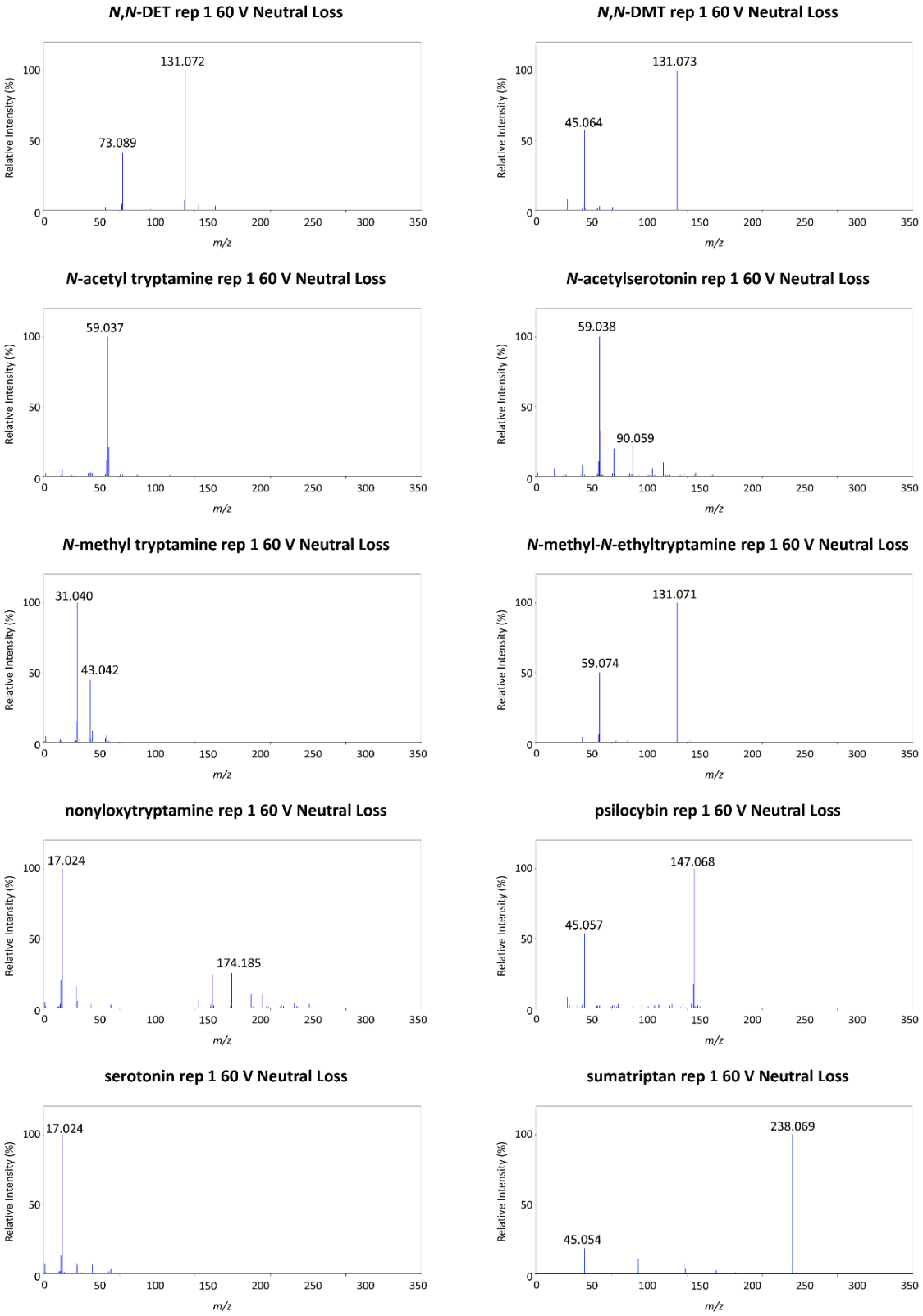

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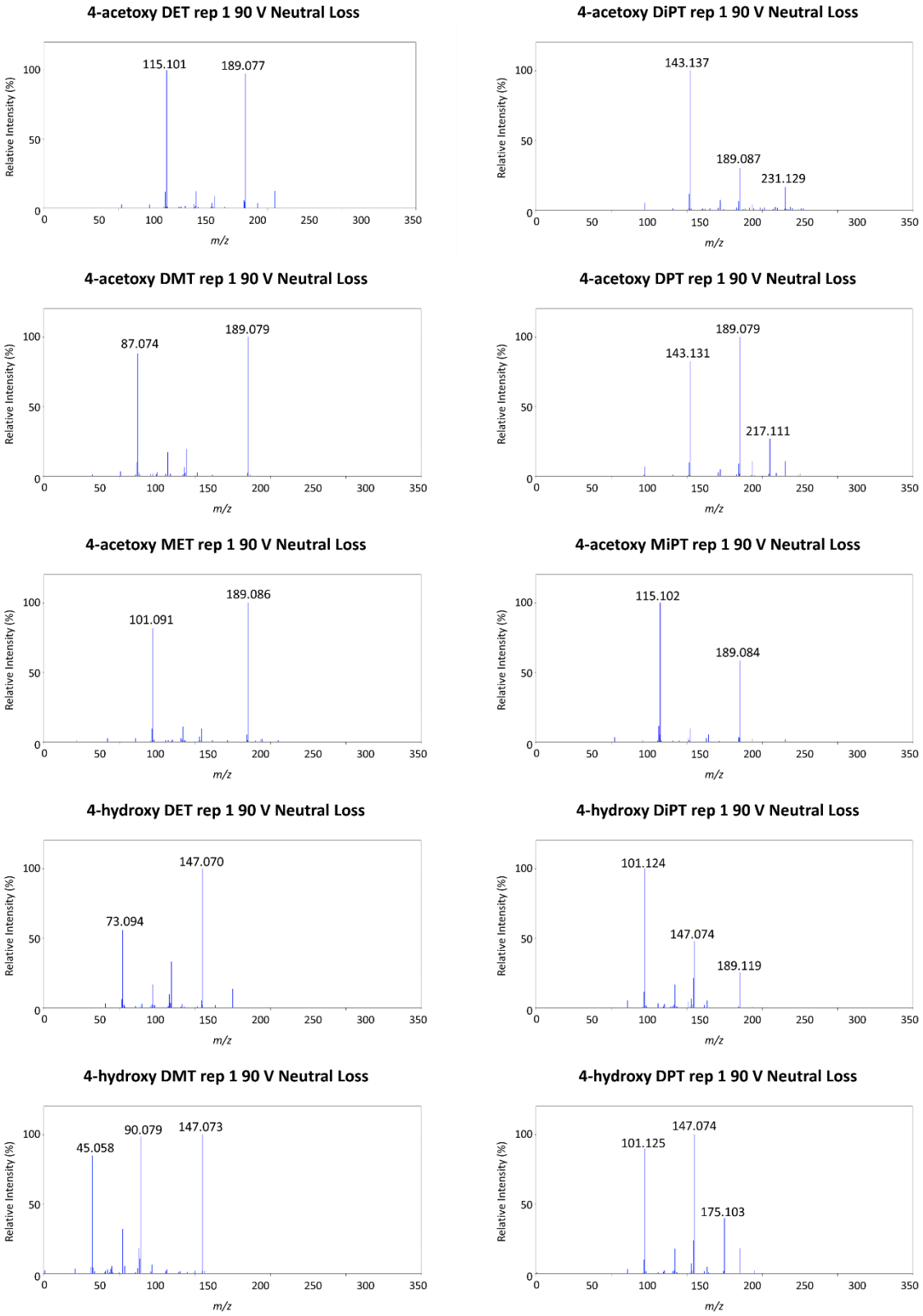


Figure S3. The 90 V neutral loss spectra for the 50 tryptamines analyzed in this study.

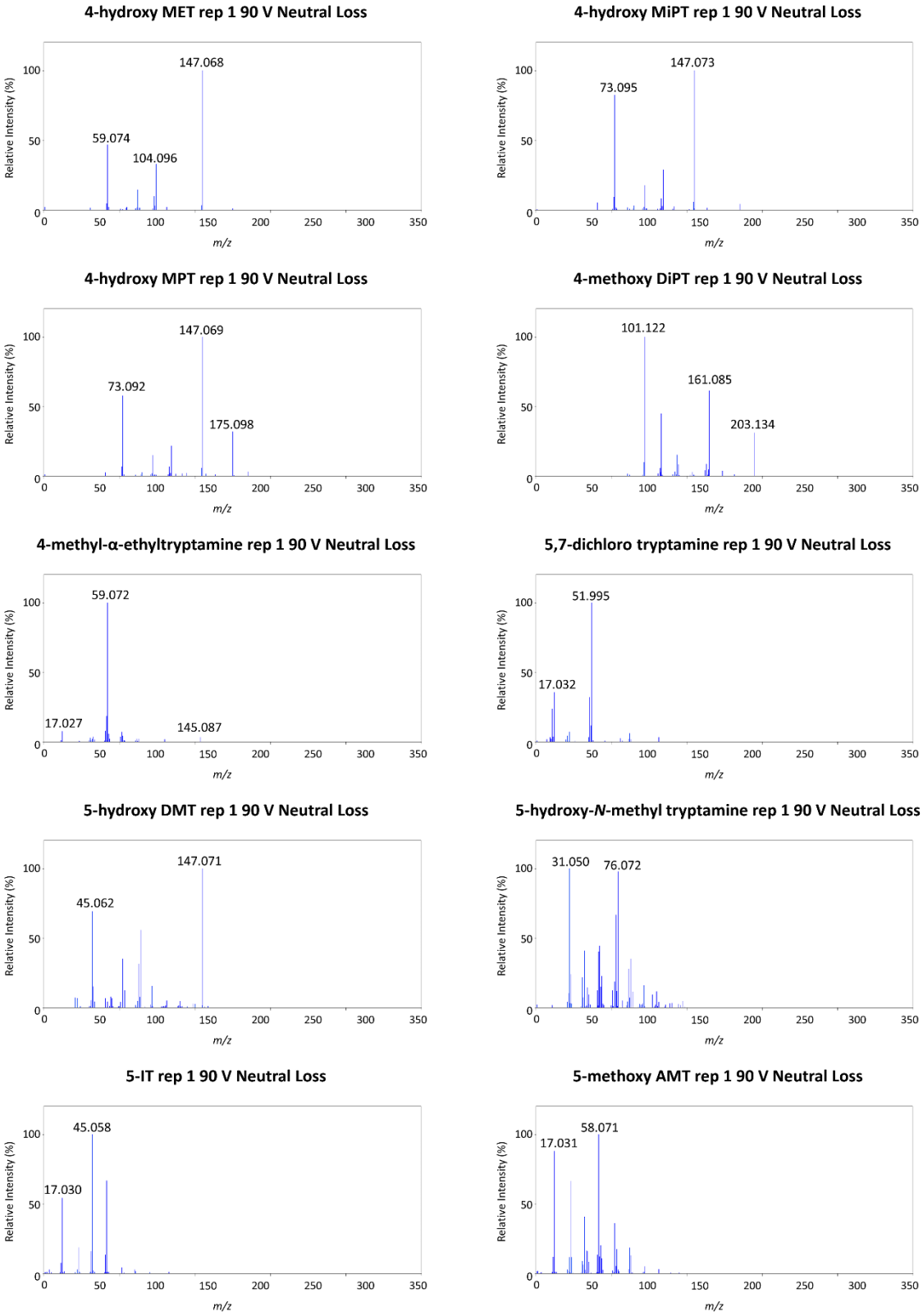
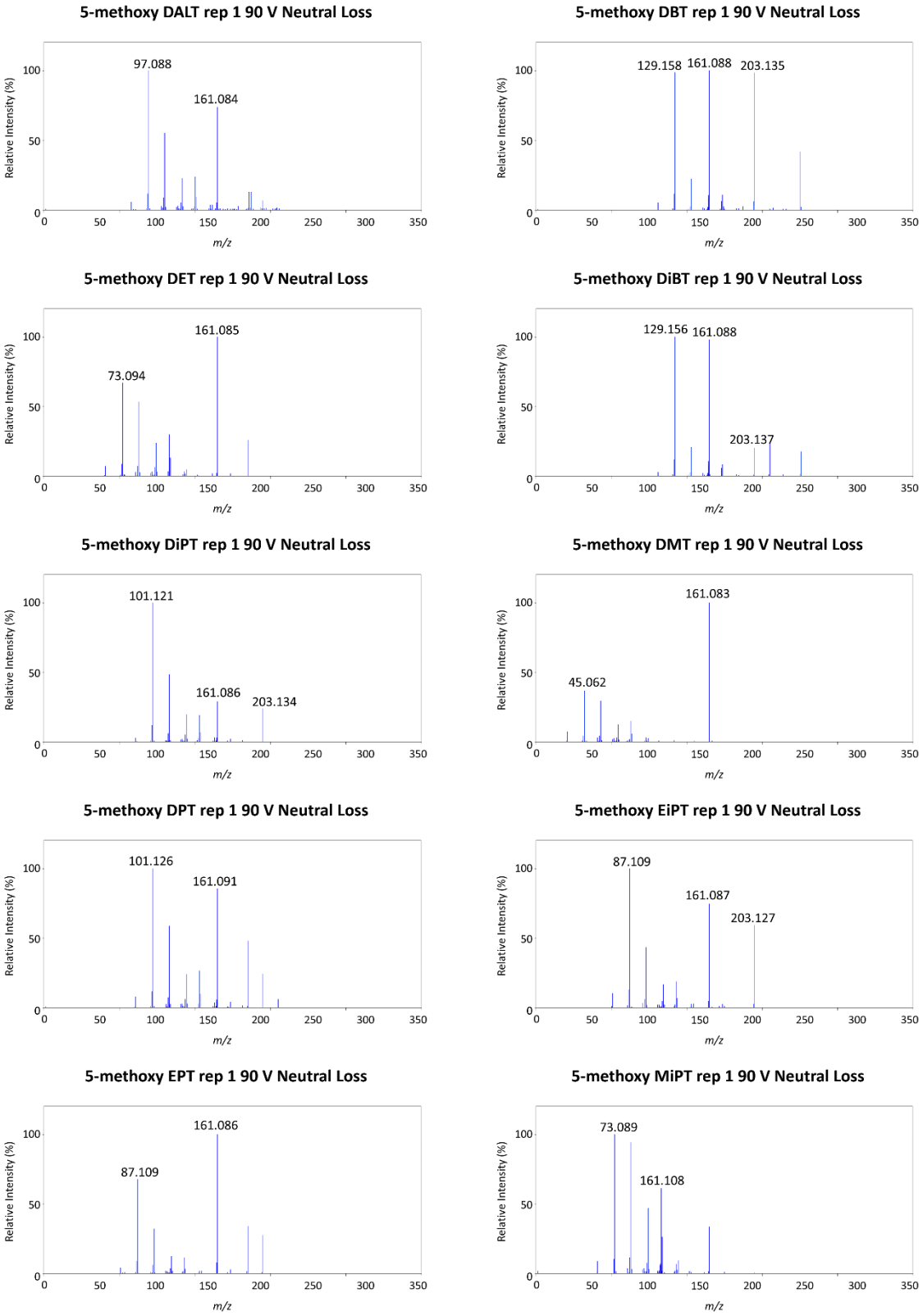


Figure S3 continued. The 90 V neutral loss spectra for the 50 tryptamines analyzed in this study.



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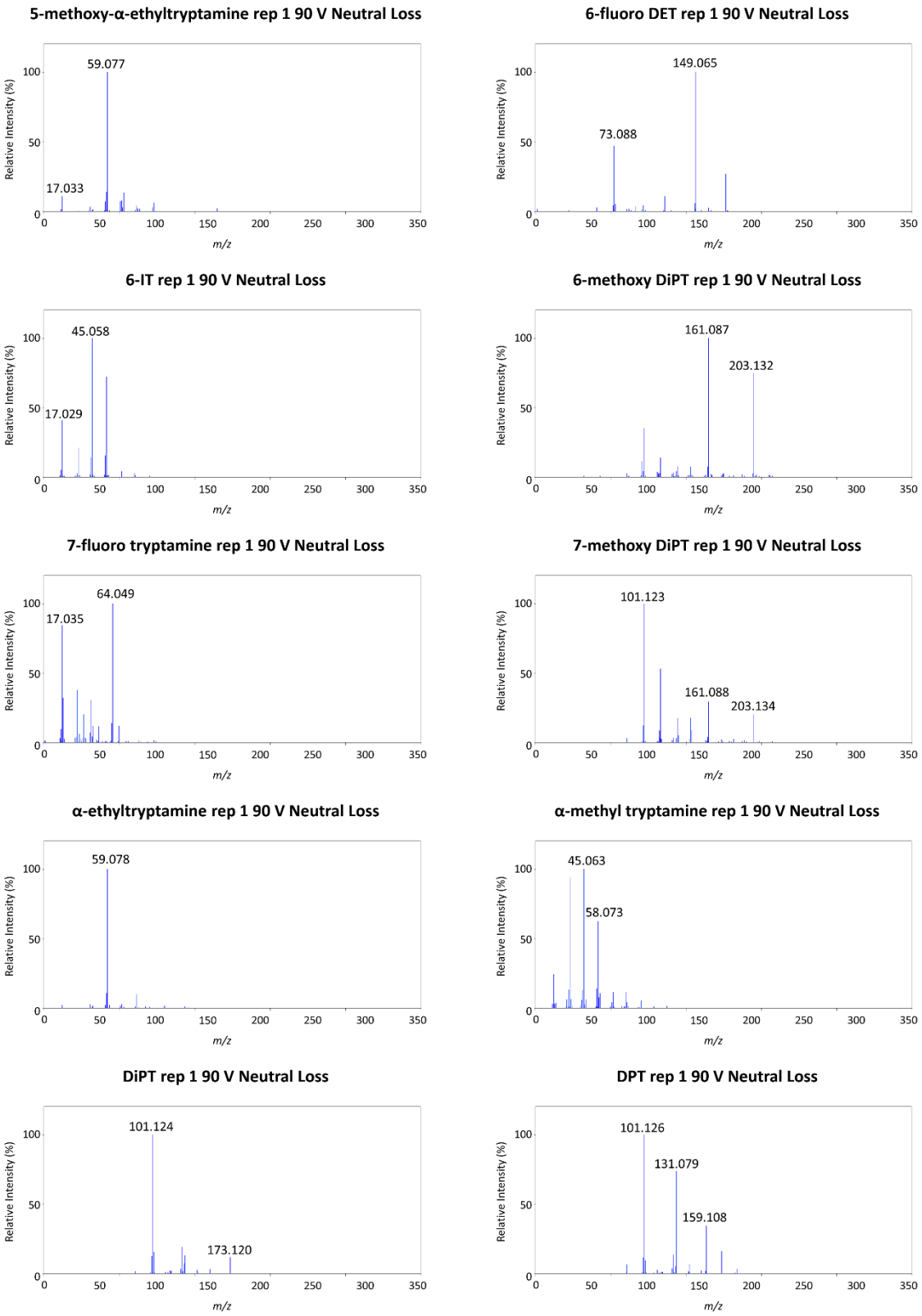

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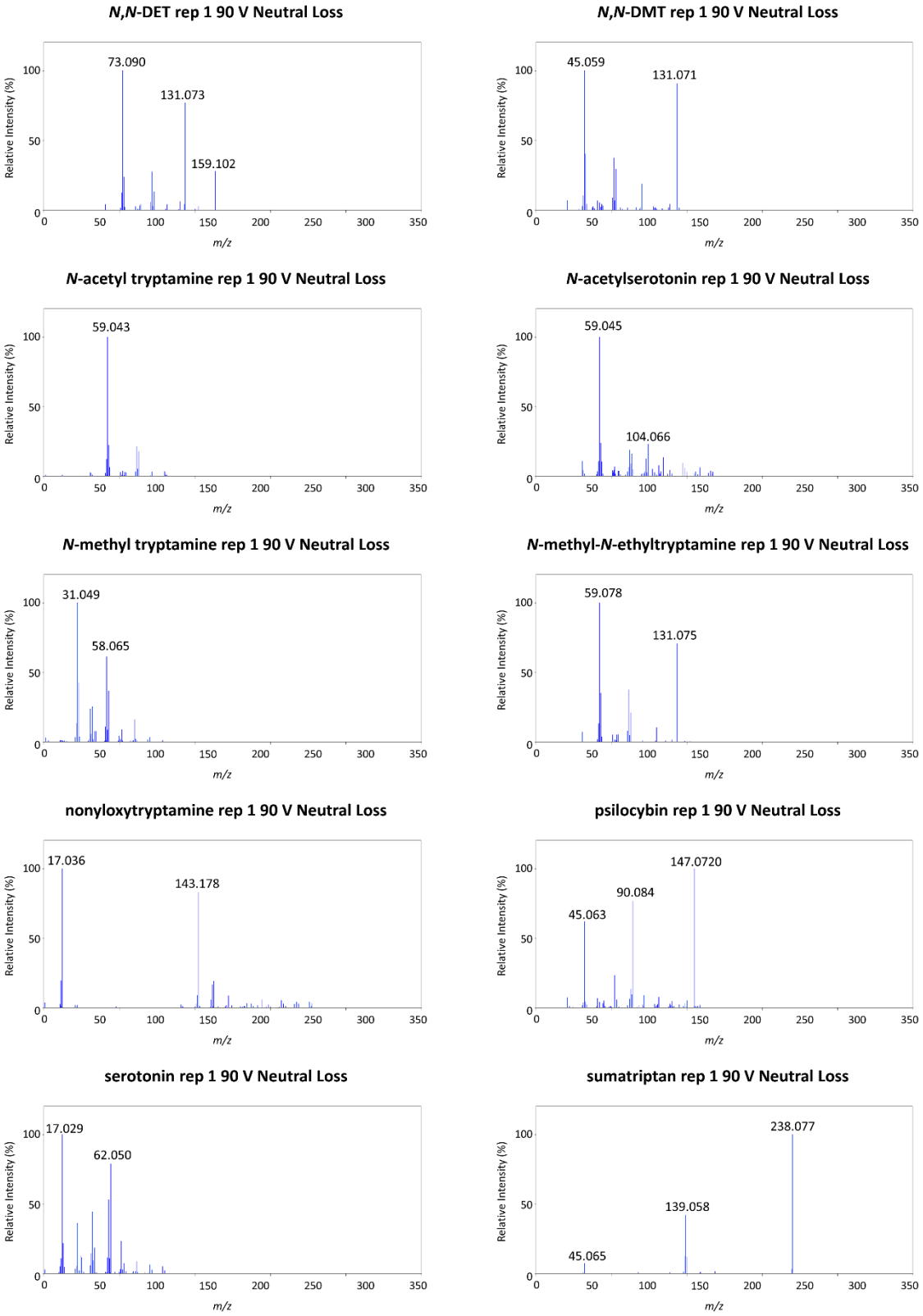

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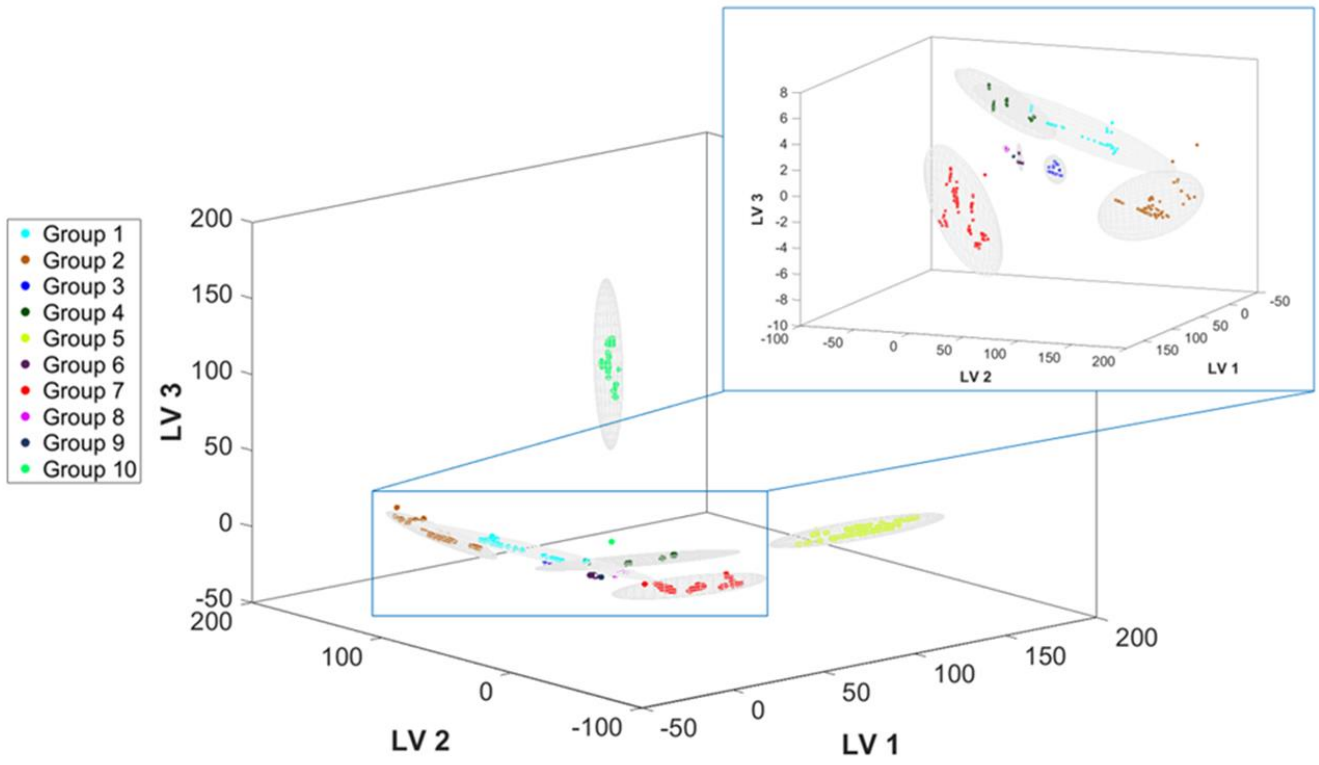


Figure S4. PLS-DA scores plot based on DART-HRMS neutral loss data. Class distinctions are indicated with color coding.

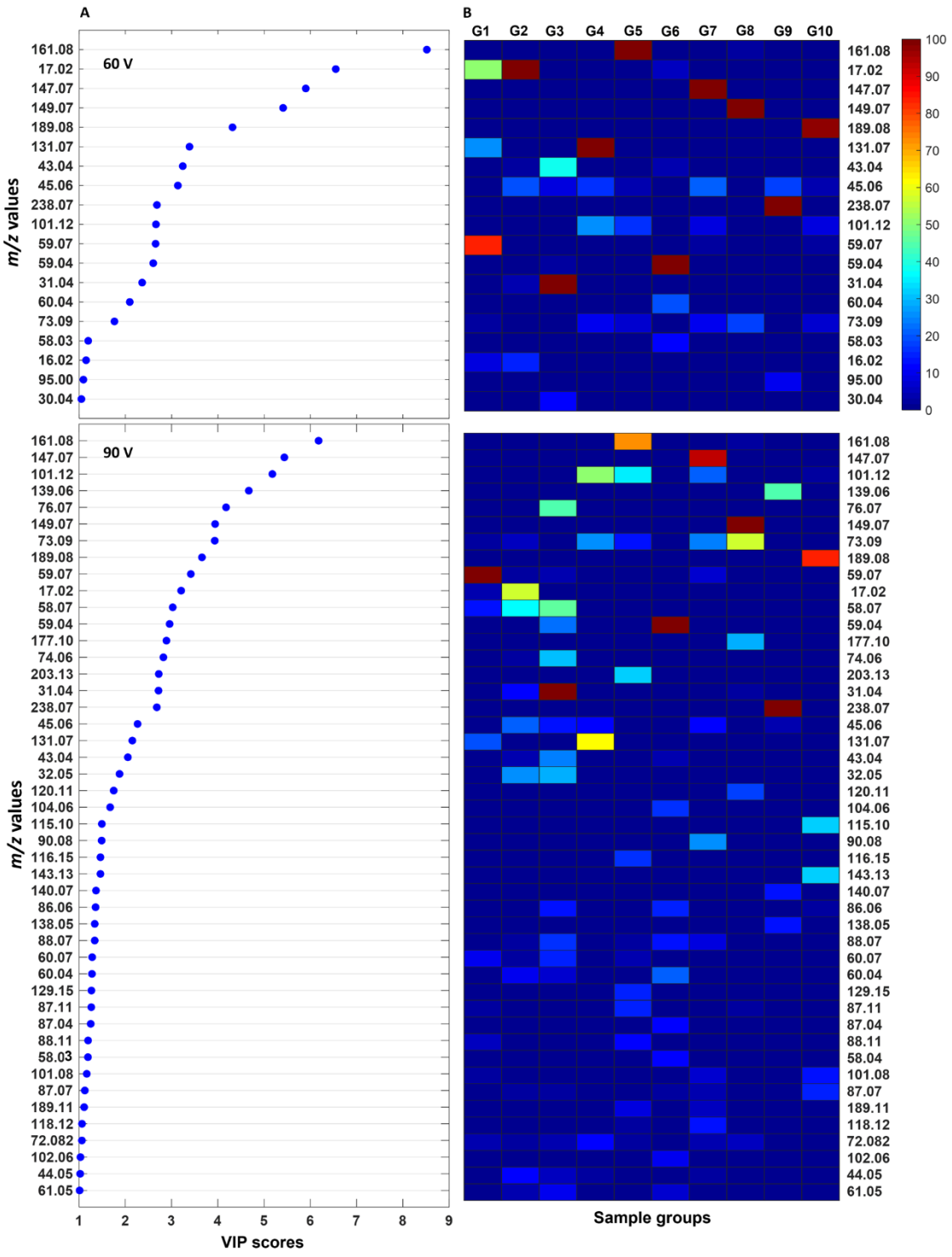


Figure S5. Masses determined to be most impactful in enabling differentiation of groups, based on differences in the fragmentation patterns of the represented compounds under CID conditions. Panel A: variable importance in projection (VIP) scores >1 revealed by the one-vs-all PLS-DA models for data collected at 60 V and 90 V; Panel B: neutral loss data corresponding with the indicated *m/z* values, averaged for each class and displayed as heatmaps for 60 V and 90 V spectral data.

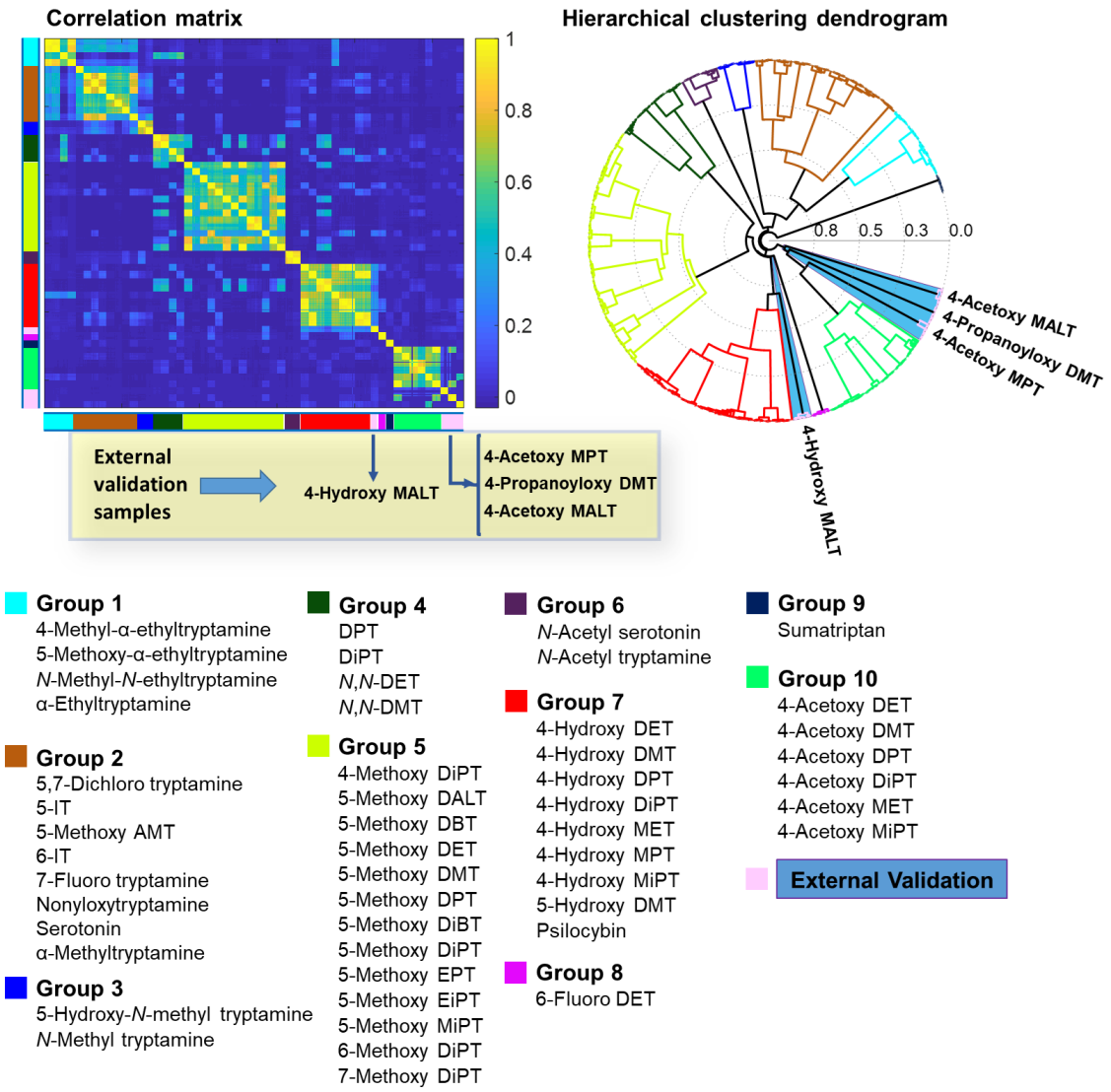
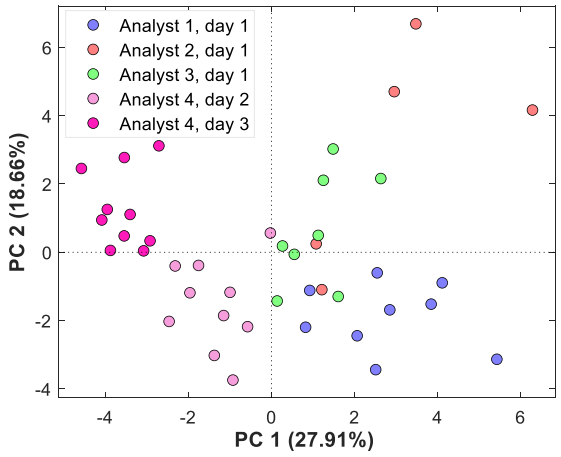


Figure S6. Correlation matrix and dendrogram showing the placement of the four tryptamines used for external validation. The four tryptamine external validation sample "unknowns" were: 4-Hydroxy MALT, 4-acetoxy MALT, 4-propanoyloxy DMT, and 4-acetoxy MPT. These are highlighted in the yellow box to show their placement in the correlation matrix (indicated in pink). Their placement in the dendrogram is indicated with blue shading. 4-Hydroxy MALT was correctly placed into group 7; and 4-acetoxy MALT, 4-propanoyloxy DMT, and 4-acetoxy MPT were correctly placed into group 10.

A



B

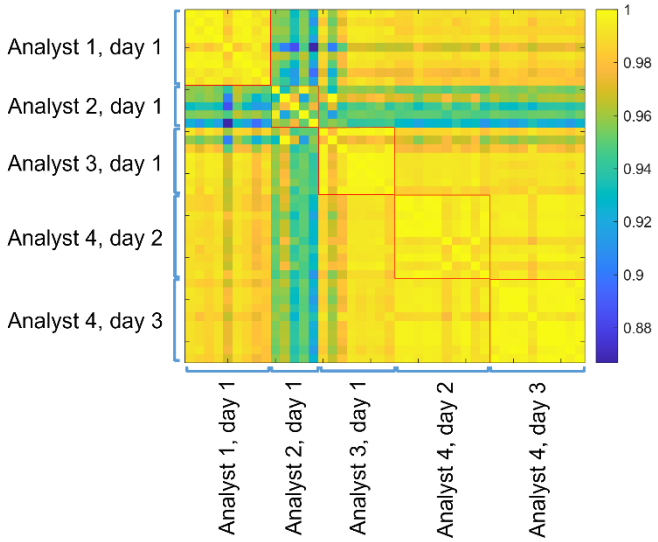


Figure S7. Results of the analysis of variation between DART-HRMS-derived neutral loss spectra collected by different individuals on the same day and one individual on different days. A: PCA scores plot of the collected data. B: Correlation matrix, where yellow shows the highest inter-spectral correlation and blue shows the lowest.

Table S1. Confusion matrix resulting from the "leave-one-structure-out" validation of the PLS-DA model.

Confusion matrix		Predicted											
		G 1	G 2	G 3	G 4	G 5	G 6	G 7	G 8	G 9	G 10	Not assigned	Multi-label assignment
True	G 1 (40)	24	0	0	0	0	0	0	0	0	0	0	16
	G 2 (80)	0	80	0	0	0	0	0	0	0	0	0	0
	G 3 (20)	0	0	20	0	0	0	0	0	0	0	0	0
	G 4 (40)	0	0	0	40	0	0	0	0	0	0	0	0
	G 5 (130)	0	0	0	0	130	0	0	0	0	0	0	0
	G 6 (20)	0	0	0	0	0	20	0	0	0	0	0	0
	G 7 (90)	0	0	0	0	0	0	80	0	0	0	0	10
	G 8 (10)	0	0	0	0	0	0	0	0	0	0	10	0
	G 9 (10)	0	0	0	0	0	0	0	0	0	0	10	0
	G 10 (60)	0	0	0	0	0	0	0	0	0	60	0	0

G 1: Group 1; G 2: Group 2; G 3: Group 3; G 4: Group 4; G 5: Group 5; G 6: Group 6; G 7: Group 7; G 8: Group 8; G 9: Group 9; G 10: Group 10

Table S2. Classification performance, sensitivity, specificity and precision of the "leave-one-structure-out" validation for tryptamine discrimination using the PLS-DA model.

	G 1	G 2	G 3	G 4	G 5	G 6	G 7	G 8	G 9	G 10
Sensitivity	1.00	1.00	1.00	1.00	1.00	1.00	1.00	Not assigned	Not assigned	1.00
Specificity	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Precision	1.00	1.00	1.00	1.00	1.00	1.00	1.00	Not assigned	Not assigned	1.00

Table S3. Probability prediction assignments of the PLD-DA model for the "leave-one structure out" validation when screened against the ten groups that were identified in the cluster analysis. The correctly classified tryptamines with a probability of one are shown in blue, whereas the red numbers show the probabilities for tryptamines with multilabel assignments.

Compound	G 1	G 2	G 3	G 4	G 5	G 6	G 7	G 8	G 9	G 10
4-Methyl-α-ethyl tryptamine	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5-Methoxy-α-ethyl tryptamine	**1.00**	**0.52**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
***N*-Methyl-*N*-ethyltryptamine**	**1.00**	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00
α-Ethyltryptamine	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5,7-Dichloro tryptamine	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5-IT	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5-Methoxy AMT	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6-IT	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7-Fluoro tryptamine	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nonyloxytryptamine	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Serotonin	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
α-Methyl tryptamine	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5-Hydroxy-*N*-methyl tryptamine	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
***N*-Methyl tryptamine**	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DPT	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00
DiPT	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00
***N*, *N*-DET**	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00
***N*, *N*-DMT**	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00	0.00
4-Methoxy DiPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy DALT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy DBT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy DET	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy DMT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy DPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy DiBT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy DiPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy EPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy EiPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
5-Methoxy MiPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
6-Methoxy DiPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
7-Methoxy DiPT	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	0.00
***N*-Acetyl serotonin**	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00
***N*-Acetyl tryptamine**	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00
4-Hydroxy DET	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy DPT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy DiPT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MET	**1.00**	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MiPT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
5-Hydroxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
Psilocybin	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
6-Fluoro DET	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Sumatriptan	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4-Acetoxy DET	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy DPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy DiPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MET	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MiPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**

Table S4. The relative intensities for the *m/z* values in the tryptamine 60 V neutral loss spectra ranked most important in discrimination of the ten tryptamine clusters, from the average of ten replicates.

		Neutral loss 60																		
Group	**Compound**	**16.02**	**17.03**	**30.04**	**31.04**	**43.04**	**45.06**	**58.03**	**59.04**	**59.07**	**60.04**	**73.09**	**95.00**	**101.12**	**131.07**	**147.07**	**149.07**	**161.08**	**189.08**	**238.07**
G 1	**4-Methyl-α-ethyl tryptamine**	13.3	80.6	0.0	0.0	0.0	0.8	0.0	0.0	100.0	0.0	0.1	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0
	5-Methoxy-α-ethyl tryptamine	14.8	98.2	0.0	0.0	0.0	0.0	0.0	0.0	83.6	0.0	6.8	0.0	0.0	0.0	0.0	0.0	2.7	0.0	0.0
	***N*-Methyl-*N*-ethyltryptamine**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	48.7	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0	0.0
	α-Ethyltryptamine	3.5	27.4	0.0	0.0	0.0	0.8	0.0	0.0	100.0	0.0	0.0	0.0	0.0	5.7	0.0	0.0	0.0	0.0	0.0
G 2	**5,7-Dichloro tryptamine**	11.2	100.0	4.4	4.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-IT	19.8	100.0	0.0	0.0	0.0	53.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy AMT	16.4	100.0	0.0	1.2	6.7	8.2	0.0	0.0	3.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	6-IT	15.5	100.0	0.0	0.0	0.1	43.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	7-Fluoro tryptamine	12.3	100.0	6.0	10.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Nonyloxytryptamine	20.0	100.0	1.3	3.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Serotonin	13.3	100.0	0.0	5.2	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	α -Methyl tryptamine	16.3	100.0	0.0	3.7	10.0	51.5	1.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 3	**5-Hydroxy-*N*-methyl tryptamine**	0.0	0.0	11.2	100.0	32.8	9.1	0.0	5.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	***N*-Methyl tryptamine**	0.3	0.0	13.1	100.0	42.3	7.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 4	**DPT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	29.9	100.0	0.0	0.0	0.0	0.0	0.0
	DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	71.9	100.0	0.0	0.0	0.0	0.0	0.0
	***N,N*-DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	37.5	0.0	0.0	100.0	0.0	0.0	0.0	0.0	0.0
	***N,N*-DMT**	0.0	0.0	0.0	0.0	0.0	63.2	0.0	0.0	2.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0	0.0
G 5	**4-Methoxy DiPT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	44.4	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy DALT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy DBT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy DET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	46.7	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy DMT	0.0	0.0	0.0	0.0	0.0	48.2	0.0	0.0	1.2	0.0	0.0	0.0	0.0	0.0	0.5	0.0	100.0	0.0	0.0
	5-Methoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	38.0	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy DiBT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	59.3	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy EPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0
	5-Methoxy EiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	0.0	100.0	0.0	0.0
	5-Methoxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	48.8	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0
	6-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.4	0.0	0.0	0.0	100.0	0.0	0.0
	7-Methoxy DiPT	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	75.7	0.0	0.0	0.0	100.0	0.0	0.0
G 6	***N*-Acetylserotonin**	0.0	5.5	0.0	0.0	4.6	0.1	11.0	100.0	0.0	20.5	0.0	0.0	0.0	0.0	0.4	0.0	0.0	0.0	0.0
	***N*-Acetyl tryptamine**	0.0	4.5	0.0	0.0	2.3	1.1	11.8	100.0	0.0	19.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 7	**4-Hydroxy DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	30.5	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	4-Hydroxy DMT	0.0	0.0	0.0	0.0	0.0	57.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	4-Hydroxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24.8	0.0	100.0	0.0	0.0	0.0	0.0
	4-Hydroxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	46.6	0.0	100.0	0.0	0.0	0.0	0.0
	4-Hydroxy MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	25.5	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	4-Hydroxy MPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	25.7	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	4-Hydroxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	28.8	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	5-Hydroxy DMT	0.0	0.0	0.0	4.7	0.0	82.8	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	Psilocybin	0.0	0.0	0.0	0.1	0.0	53.4	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.1	100.0	0.0	0.0	0.0	0.0
G 8	**6-Fluoro DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.6	0.0	0.0	0.0	0.0	100.0	2.1	0.0	0.0
G 9	**Sumatriptan**	0.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0	0.0	0.0	10.2	0.0	0.0	0.0	0.3	0.0	0.0	100.0
G 10	**4-Acetoxy DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	23.2	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0
	4-Acetoxy DMT	0.0	0.0	0.0	0.0	0.0	20.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0
	4-Acetoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	18.7	0.0	0.0	0.0	0.0	90.0	0.0
	4-Acetoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	31.2	0.0	0.0	0.0	0.0	100.0	0.0
	4-Acetoxy MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0
	4-Acetoxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	22.3	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0

Table S5. The relative intensities for the *m/z* values in the tryptamine 90 V neutral loss spectra ranked most important in discrimination of the ten tryptamine clusters, from the average of ten replicates.

		Neutral loss 90														
Group	**Compound**	**17.03**	**31.05**	**32.05**	**43.05**	**44.05**	**45.06**	**58.03**	**58.07**	**59.04**	**59.07**	**60.05**	**60.08**	**61.06**	**72.08**	**73.09**
G 1	**4-Methyl-α-ethyl tryptamine**	7.0	0.0	0.2	0.0	0.8	1.1	0.0	17.6	0.0	100.0	0.0	6.5	0.0	6.3	5.0
	5-Methoxy-α-ethyl tryptamine	7.5	0.0	0.0	0.0	0.0	0.5	0.0	13.6	0.0	100.0	0.0	0.0	0.0	8.3	4.7
	***N*-Methyl-*N*-ethyltryptamine**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	12.7	0.0	100.0	0.0	32.1	0.0	0.0	1.1
	α-Ethyltryptamine	1.4	0.0	0.0	0.0	0.0	0.4	0.0	11.7	0.0	100.0	0.0	0.0	0.0	3.0	0.0
G 2	**5,7-Dichloro tryptamine**	25.1	6.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-IT	45.9	2.8	17.8	1.0	14.8	50.0	0.0	63.9	0.0	0.5	0.0	1.1	0.0	5.2	0.0
	5-Methoxy AMT	77.1	11.2	72.5	7.6	5.9	20.5	0.0	100.0	0.0	13.4	25.0	0.0	15.7	2.2	48.8
	6-IT	20.7	2.3	21.9	1.1	12.1	50.0	0.0	65.8	0.0	1.7	0.0	1.9	0.0	5.4	0.0
	7-Fluoro tryptamine	91.6	29.0	0.0	6.1	29.4	1.8	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Nonyloxytryptamine	98.6	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Serotonin	99.8	29.7	1.8	5.5	15.7	0.0	0.2	0.0	10.7	0.0	54.0	0.0	11.8	0.0	0.0
	α-Methyl tryptamine	2.4	13.5	98.0	5.3	12.6	49.3	0.0	67.1	0.9	8.5	1.1	11.6	0.0	10.7	0.0
G 3	**5-Hydroxy-*N*-methyl tryptamine**	0.0	97.6	22.7	22.2	5.7	17.1	0.0	38.3	44.6	0.0	13.5	0.0	21.6	0.0	0.0
	***N*-Methyl tryptamine**	0.3	100.0	35.2	25.7	4.2	10.3	0.0	53.1	0.0	6.5	0.0	29.2	0.0	6.6	0.0
G 4	**DPT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	***N*,*N*-DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.7	100.0
	***N*,*N*-DMT**	0.0	0.0	0.0	0.2	10.7	47.1	0.0	0.0	0.0	5.2	0.0	0.6	0.0	34.3	5.9
G 5	**4-Methoxy DiPT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DALT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DBT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.0	66.9
	5-Methoxy DMT	0.0	0.0	0.0	0.0	4.4	17.5	0.0	0.0	0.0	6.0	0.0	41.7	0.0	3.9	0.4
	5-Methoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DiBT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy EPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy EiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10.6	95.7
	6-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	7-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 6	***N*-Acetylserotonin**	0.6	0.0	0.0	5.4	1.5	0.1	10.4	0.0	100.0	0.0	19.4	0.0	7.6	0.0	0.0
	***N*-Acetyl tryptamine**	0.1	0.0	0.0	2.3	0.0	0.0	12.4	0.0	100.0	0.0	22.5	0.0	5.9	0.0	0.0
G 7	**4-Hydroxy DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	62.3
	4-Hydroxy DMT	0.0	0.0	0.0	0.0	5.6	36.3	0.0	0.0	0.0	2.6	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.5	0.0	54.4	0.0	2.3	0.0	0.0	0.0
	4-Hydroxy MPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7.6	78.0
	4-Hydroxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.9	83.0
	5-Hydroxy DMT	0.0	7.6	0.0	0.0	8.1	38.0	0.0	0.2	0.0	4.2	0.0	0.0	0.8	9.2	0.0
	Psilocybin	0.0	0.1	0.0	0.0	3.9	29.1	0.0	0.1	0.0	4.6	0.0	0.0	0.0	2.8	0.0
G 8	**6-Fluoro DET**	0.0	2.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	5.7	56.9
G 9	**Sumatriptan**	0.0	0.0	0.0	0.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 10	**4-Acetoxy DET**	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	3.9
	4-Acetoxy DMT	0.0	0.0	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	4-Acetoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	4-Acetoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	4-Acetoxy MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.2	0.0	0.0	0.0	0.0	0.0
	4-Acetoxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.8

Table S5 (continued). The relative intensities for the *m/z* values in the tryptamine 90 V neutral loss spectra ranked most important in discrimination of the ten tryptamine clusters, from the average of ten replicates.

		Neutral loss 90														
Group	**Compound**	**74.06**	**76.07**	**86.06**	**87.04**	**87.07**	**87.11**	**88.07**	**88.11**	**90.08**	**101.09**	**101.12**	**102.06**	**104.06**	**115.10**	**116.15**
G 1	**4-Methyl-α-ethyl tryptamine**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy-α-ethyl tryptamine	0.0	0.0	0.0	0.0	0.1	3.1	1.7	0.0	0.0	8.0	0.0	0.0	0.0	0.1	0.0
	***N*-Methyl-*N*-ethyltryptamine**	0.0	0.0	0.0	0.0	0.0	4.3	0.0	19.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	α-Ethyltryptamine	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 2	**5,7-Dichloro tryptamine**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-IT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy AMT	5.2	2.7	3.3	0.0	21.8	0.0	13.6	0.0	0.1	9.9	0.0	0.0	0.0	0.0	0.0
	6-IT	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	7-Fluoro tryptamine	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.2	0.0	0.0	0.0
	Nonyloxytryptamine	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Serotonin	7.8	0.0	8.0	0.0	1.0	0.0	1.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	α-Methyl tryptamine	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 3	**5-Hydroxy-*N*-methyl tryptamine**	60.3	89.4	26.0	0.0	6.3	0.0	32.6	0.0	1.1	0.5	0.0	0.0	0.0	0.0	0.0
	***N*-Methyl tryptamine**	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 4	**DPT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.1
	DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	***N,N*-DET**	0.0	0.0	0.0	0.0	0.0	1.2	0.0	0.0	0.0	0.0	2.8	0.0	0.0	0.0	0.0
	***N,N*-DMT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 5	**4-Methoxy DiPT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	42.9
	5-Methoxy DALT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DBT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DET	0.0	0.0	0.0	0.0	0.0	6.5	0.0	50.8	0.0	0.1	0.0	0.0	0.0	3.0	0.0
	5-Methoxy DMT	0.1	20.2	0.0	0.0	3.4	0.0	30.3	0.0	0.0	1.2	0.0	0.0	0.0	0.8	0.0
	5-Methoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	52.0
	5-Methoxy DiBT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	50.0
	5-Methoxy EPT	0.0	0.0	0.0	0.0	0.0	67.6	0.0	0.0	0.0	0.0	5.4	1.8	0.0	0.0	0.0
	5-Methoxy EiPT	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.4	0.0	0.0	7.1	0.0	0.0	0.0	0.0
	5-Methoxy MiPT	0.1	0.0	0.0	0.4	0.0	12.2	0.0	97.9	0.0	0.4	0.8	0.4	1.2	6.8	0.0
	6-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	41.5	0.0	0.0	0.0	19.5
	7-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	51.1
G 6	***N*-Acetylserotonin**	0.0	0.0	6.8	23.6	0.0	0.0	7.7	0.0	0.0	0.0	0.0	19.4	31.4	0.0	0.0
	***N*-Acetyl tryptamine**	0.0	2.6	21.6	0.0	5.1	0.0	17.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 7	**4-Hydroxy DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	17.7	0.0	0.0	0.0	1.1	0.0
	4-Hydroxy DMT	0.1	0.0	0.0	0.0	3.5	0.0	17.5	0.0	75.9	0.0	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	87.3	0.0	0.0	0.0	0.0
	4-Hydroxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0
	4-Hydroxy MET	0.0	1.4	2.0	0.0	16.5	0.0	1.3	0.0	0.0	1.2	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy MPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.6	21.2	0.0	0.0	0.0	1.2	0.0
	4-Hydroxy MiPT	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	1.4	19.3	0.0	0.0	0.0	1.3	0.0
	5-Hydroxy DMT	5.1	0.2	0.0	0.0	4.5	0.0	35.8	0.0	58.5	1.7	0.0	0.0	0.0	0.0	0.0
	Psilocybin	2.5	0.1	0.0	0.0	7.5	0.0	20.5	0.0	87.2	1.1	0.0	0.0	0.0	0.0	0.0
G 8	**6-Fluoro DET**	0.0	0.0	0.0	0.0	0.0	2.6	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0
G 9	**Sumatriptan**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 10	**4-Acetoxy DET**	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	96.1	0.0
	4-Acetoxy DMT	0.0	0.0	9.6	0.0	84.6	0.0	1.6	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0
	4-Acetoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.5	0.0	0.0	0.0	0.0
	4-Acetoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.2	0.0	0.0	0.0	0.0
	4-Acetoxy MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	82.6	0.0	0.0	0.0	0.3	0.0
	4-Acetoxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	99.4	0.0

Table S5 (continued). The relative intensities for the *m/z* values in the tryptamine 90 V neutral loss spectra ranked most important in discrimination of the ten tryptamine clusters, from the average of ten replicates.

		Neutral loss 90															
Group	**Compound**	**118.12**	**120.11**	**129.15**	**131.08**	**138.05**	**139.06**	**140.07**	**143.13**	**147.07**	**149.07**	**161.08**	**177.10**	**189.08**	**189.12**	**203.13**	**238.08**
G 1	**4-Methyl-α-ethyl tryptamine**	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy-α-ethyl tryptamine	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0
	***N*-Methyl-*N*-ethyltryptamine**	0.0	0.8	0.0	75.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	α-Ethyltryptamine	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 2	**5,7-Dichloro tryptamine**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-IT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy AMT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	6-IT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	7-Fluoro tryptamine	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Nonyloxytryptamine	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Serotonin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	α-Methyl tryptamine	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 3	**5-Hydroxy-*N*-methyl tryptamine**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	***N*-Methyl tryptamine**	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 4	**DPT**	0.0	0.0	0.3	69.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	DiPT	0.0	0.0	1.2	16.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	***N*,*N*-DET**	0.0	0.0	0.0	67.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	***N*,*N*-DMT**	0.0	0.0	0.0	93.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 5	**4-Methoxy DiPT**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	67.8	0.0	0.0	0.0	33.0	0.0
	5-Methoxy DALT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	58.6	0.0	0.0	1.5	7.0	0.0
	5-Methoxy DBT	0.0	0.0	94.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	80.6	0.0	0.0	0.0	98.7	0.0
	5-Methoxy DET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	1.2	23.9	0.0	0.0
	5-Methoxy DMT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.6	0.0	100.0	0.0	0.0	0.0	0.0	0.0
	5-Methoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.2	0.0	0.0	90.3	0.0	2.9	45.5	21.3	0.0
	5-Methoxy DiBT	0.0	0.0	100.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	81.1	0.0	0.0	0.0	20.0	0.0
	5-Methoxy DiPT	0.0	0.0	0.1	0.0	0.0	0.0	0.0	2.3	0.0	0.0	37.2	0.0	0.0	0.0	26.3	0.0
	5-Methoxy EPT	13.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.8	34.0	27.6	0.0
	5-Methoxy EiPT	21.9	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.3	0.0	67.4	0.0	0.0	0.0	66.7	0.0
	5-Methoxy MiPT	0.1	0.0	0.0	0.0	0.0	0.0	0.0	1.6	0.0	0.0	33.9	0.0	0.0	0.0	0.0	0.0
	6-Methoxy DiPT	0.0	0.0	0.1	0.0	0.0	0.0	0.0	2.9	0.0	0.0	91.4	0.0	0.0	0.0	91.3	0.0
	7-Methoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.4	0.0	0.0	34.1	0.0	0.0	0.0	21.1	0.0
G 6	***N*-Acetylserotonin**	0.0	0.0	0.0	0.0	0.8	0.3	2.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	***N*-Acetyl tryptamine**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
G 7	**4-Hydroxy DET**	37.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy DMT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy DPT	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.7	94.1	0.0	0.0	0.0	0.0	16.5	2.2	0.0
	4-Hydroxy DiPT	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1	53.7	0.0	0.0	0.0	1.7	25.3	0.0	0.0
	4-Hydroxy MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	4-Hydroxy MPT	42.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	99.3	0.0	0.0	0.0	0.0	2.2	0.0	0.0
	4-Hydroxy MiPT	35.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	87.7	0.0	0.0	0.0	0.0	1.7	0.0	0.0
	5-Hydroxy DMT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	99.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Psilocybin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	95.2	0.8	0.0	0.0	0.0	0.0	0.0	0.0
G 8	**6-Fluoro DET**	0.0	17.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	1.7	29.4	0.0	0.0	0.0	0.0
G 9	**Sumatriptan**	0.0	0.0	0.0	0.0	12.5	43.9	12.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0
G 10	**4-Acetoxy DET**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	96.5	0.0	0.0	0.0
	4-Acetoxy DMT	0.0	0.0	0.0	1.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0
	4-Acetoxy DPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	91.3	0.0	0.0	0.0	0.0	89.1	0.0	0.0	0.0
	4-Acetoxy DiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0	0.0	37.8	0.0	0.0	0.0
	4-Acetoxy MET	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0.0	0.0
	4-Acetoxy MiPT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	74.0	0.0	0.0	0.0

Table S6. Probabilities of the external validation tryptamines being assigned to each group.

	G 1	G 2	G 3	G 4	G 5	G 6	G 7	G 8	G 9	G 10
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Acetoxy MPT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Hydroxy MALT	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**	0.00	0.00	0.00
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**
4-Propanoyloxy DMT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**1.00**