PeakAL: Protons I Have Known and Loved, Too — Another fifty shades of grey-market spectra

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^{1}H NMR spectra of 43 alleged psychedelic tryptamines (2-(1*H*-indol-3-yl)ethan-1-amines) and benzofuran analogues (2-(1-benzofuran-3-yl)ethan-1-amines) from grey-market internet vendors across North America and Europe were acquired and compared. Compounds having mono- or di- alkyl, cyclopropyl, or allyl amine substituents and/or substitution of the indole/benzofuran ring by acetyloxy, hydroxy, methoxy, or methyl groups were analysed. ^{1}H NMR spectra for some of these compounds have not been previously reported to my knowledge. The spectrum of each analyte is consistent with the compound as labelled and sold. None of the analytes was found to be unequivocally misrepresented. This collection of experimentally uniform spectra may help forensic and harm-reduction organizations identify these compounds, some of which appear only sporadically. The complete spectra are provided as supplementary data at https://doi.org/10.16889/isomerdesign-5-supp

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"In conclusion, a word of caution to all those youngsters who look to me as a role model. Stay off the hard stuff! Unless you know what you're doing, it can only come to grief! There is no room in the drug culture for amateurs!"

— "Uncle Duke," G. B. Trudeau

Introduction

The tryptamine (2-(1*H*-indol-3-yl)ethan-1-amine) scaffold is common to many psychedelics including natural products such as *N,N*-dimethyltryptamine (DMT), psilocin, and psilocybin, as well as scores of synthetic compounds.[1–3] Currently, after decades of widespread prohibition[4] and consequent deadening of most sanctioned research,[5] the legitimate therapeutic potential of psychedelics is being actively revisited.[6–8]

At the same time, a churning grey market in psychedelics has arisen with an unprecedented number of compounds on offer.[9,10] Psychedelic tryptamines are now often easier to source than the Bitcoins needed to pay for them. More problematic is the question of quality control in a volatile and largely self-regulated online market.[11,12] The synthetic chemistry and analytical challenges of psychedelic tryptamines has been reviewed by Brandt et al.[13,14]

The rationale and objective of this research, along with the ^{1}H NMR spectrum of 28 grey-market phenylethanamines, was reported previously.[15,16] Here, the spectra of 43 grey-market tryptamines and benzofuran analogues (2-(1-benzofuran-3-yl)ethan-1-amines) are reported.

Limitations and bias

The previously described protocol was again followed. Every tryptamine spectrum acquired has been included and reported.

Experimental

Grey-market research chemicals were purchased from internet vendors across North America and Europe, 2010–2018. Commercially available tryptamine HCl (98%) and 5-methoxy-tryptamine HCl (98%) were purchased from AK Scientific, Inc., Union City, CA. *N*-Methyltryptamine HCl (98%) was purchased from Carbosynth Limited, Compton, Berkshire, UK. Licensed software from Mestrelab Research SL, Santiago de Compostela, Spain was used for spectral analysis. Preferred IUPAC names were generated using ACD/Name 2016.1 from ACD/Labs, Toronto, Canada.

Analytical data was acquired at the University of Toronto Nuclear Magnetic Resonance facility. ^{1}H NMR spectra for analytes **T0**, **T29**, **T30**, **T41**, and **BF1** were recorded on an Agilent DD2 700 spectrometer operating at 700 MHz and equipped with an XSens Cold Probe. ^{1}H NMR spectra for analytes **T39** and **T40** were recorded on an Agilent DD2 600 spectrometer operating at 600 MHz and equipped with a OneNMR H/F{X} probe. All other analytes were recorded on an Agilent DD2 500 spectrometer operating at 500 MHz and equipped with an XSens Cold Probe. Samples were prepared for analysis in DMSO-d_6 as previously described.

Results

The analytes can be viewed as a collection of "points," a subset of the larger, multi-dimensional "chemical space" of substituted 2-arylethan-1-amines where:

- The aryl ring may be 1*H*-indol-3-yl or 1-benzofuran-3-yl (scaffolds ***T*** and ***BF*** respectively, in Table 1.)
- The ring may be variously substituted at R^2 by methyl, at R^4 by hydroxy, acetoxy, methoxy, or methyl, and at R^5 by methoxy. Seven different aryl substitution patterns are present in this subset (see Figure 1, *left.*)
- The amine ($R^{N'}$, $R^{N''}$) may be mono- or di-substituted by methyl, ethyl, isopropyl, propyl, cyclopropyl, or allyl groups, in any combination. Fifteen different amine substitution patterns are present in this subset (see Figure 1, *right.*)
- The alpha carbon (R^{α}) may be substituted by a methyl or an ethyl group (see Figure 1, *top row right.*)
- The compound may be present as a free base; as a fumarate (2:1) or hydrogen fumarate[1] (1:1) salt; or as a hydrochloride or other inorganic salt.

Analyte code names, substitution patterns, and preferred IUPAC names (PIN) are listed in Table 1. ^{1}H NMR spectral data is summarized in Table 2. Multiplets for aryl protons and substituents are listed in Table 3, grouped by ring substitution pattern. Within each group, analytes are ordered by descending shift to illustrate trends in shifts and the range of shifts observed. Multiplets for ethanamine/ethaminium and fumarate moieties are grouped together in Table 4. Multiplets for *N*- and α-substituents are grouped together in Table 5, again in descending order by shift.

Fully protonated amines arising from hydrochlorides or other inorganic salts typically have aromatic shifts slightly higher than partially protonated fumarate salts, which in turn are typically slightly higher than free base forms. Curiously, the signal arising from protonated amines and 4-hydroxy substituents is typically seen only in a fully protonated (e.g. hydrochloride) salt, not in fumarate salts. Rapid exchange of the aminium and hydroxy protons with the fumarate — facilitated by water and the polar solvent DMSO-d_6 — can lead to a broad, time-averaged signal far downfield. The signal may be so broad as to virtually disappear into the baseline.[17–19] A very broad singlet spanning 13.5–12.5 ppm can be seen in spectrum **T31:** 4-AcO-MIPT fumarate, in the supplementary data.

Counter to expectations, the signal arising from the olefinic fumarate protons *always appears as a singlet* near 6.5 ppm, regardless of the integral for the peak (1H or 2H). This suggests that in DMSO-d_6 solution these protons are equivalent, with no observable coupling, in both fumarate (2:1) and hydrogen fumarate (1:1) salts.

Spectra for each aryl substitution pattern are shown stacked in Figure 2. Parts of the stacked spectra have been cut out, leaving four regions showing (from left to right):

- indole nitrogen proton singlet peaks downfield (i.e. to the left) of 10.5 ppm, and typically broadened from presumed coupling with the adjacent aryl proton at position 2,
- other aromatic proton multiplets clustered around 7 ppm,
- methoxy substituent singlet peaks centred around 3.75 ppm, and
- acetoxy and aryl-methyl substituent singlet peaks, upfield (i.e. to the right) of 2.6 ppm.

The *idealized* splitting pattern and range of observed shifts of the six amine substituents are shown stacked in Figure 3. In some cases, the observed splitting only approximates the idealized, first-order multiplets in Figure 3. For instance, the central methylene of a propyl substituent typically does not appear as a perfect, first-order hextet—presumably the result of unequal coupling with the inner methylene group and the terminal methyl group. Similarly, the methyl groups of an isopropyl substituent are not always equivalent. Thus, twin 3H doublets are seen instead of a single 6H doublet, and the methine group exhibits a more complex splitting pattern than a first-order heptet. The correlation between substituents and observed multiplets seen in Table 5 presumes such deviations are insignificant, and to be expected.

Literature previously reporting ^{1}H NMR spectra for the analytes are cited in Table 6, grouped by analyte and solvent.

Conclusion

The spectrum of each analyte is consistent with the compound as labelled and sold. None of analytes were found to be unequivocally misrepresented. This result is in line with our previously reported analysis of 28 grey-market phenylethan-amines, which found only one case of misrepresentation.

Acknowledgements

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[1] The term *hemifumarate* is ambiguous, used by some to mean *hydrogen fumarate* and by others to mean "a half fumarate." Here, *fumarate* is used for the fully deprotonated dicarboxylate anion, and *hydrogen fumarate* for the monocarboxylate anion.

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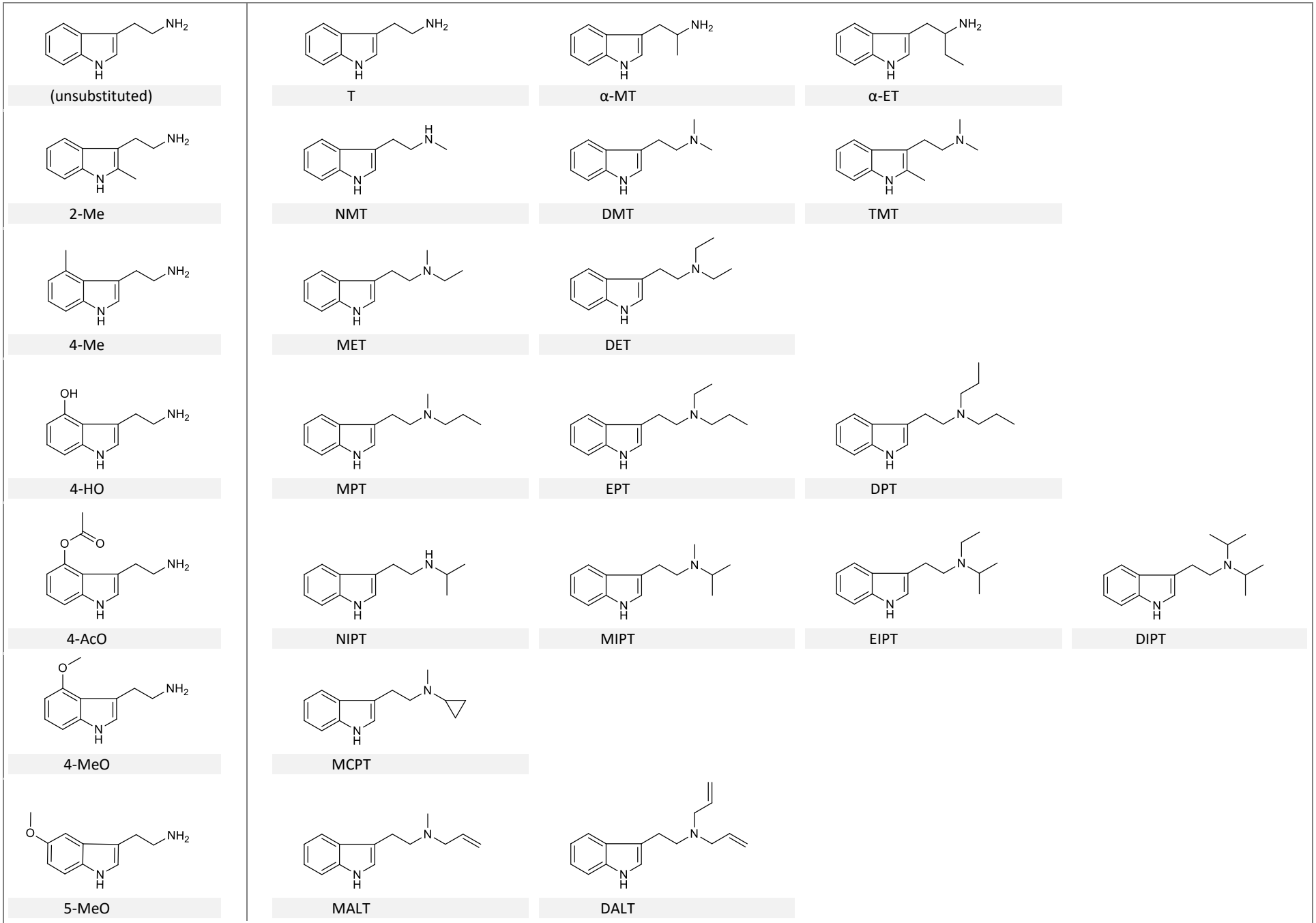


Figure 1: Structures of tryptamine analytes. *Left*: Aryl substituents and codes; *Right*: Ethanamine substituents and codes

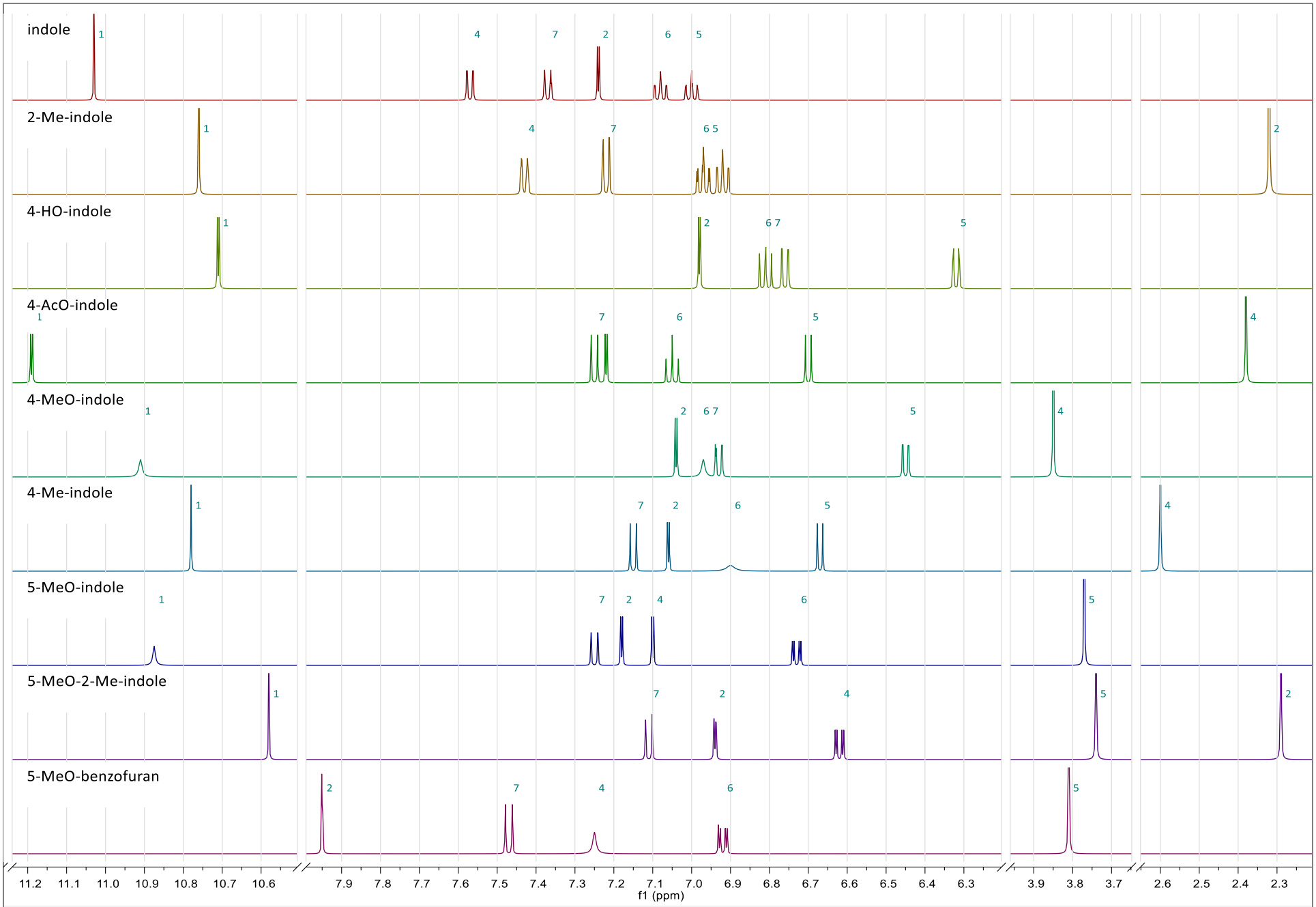


Figure 2: ^{1}H NMR spectra of aryl protons and aryl substituents.

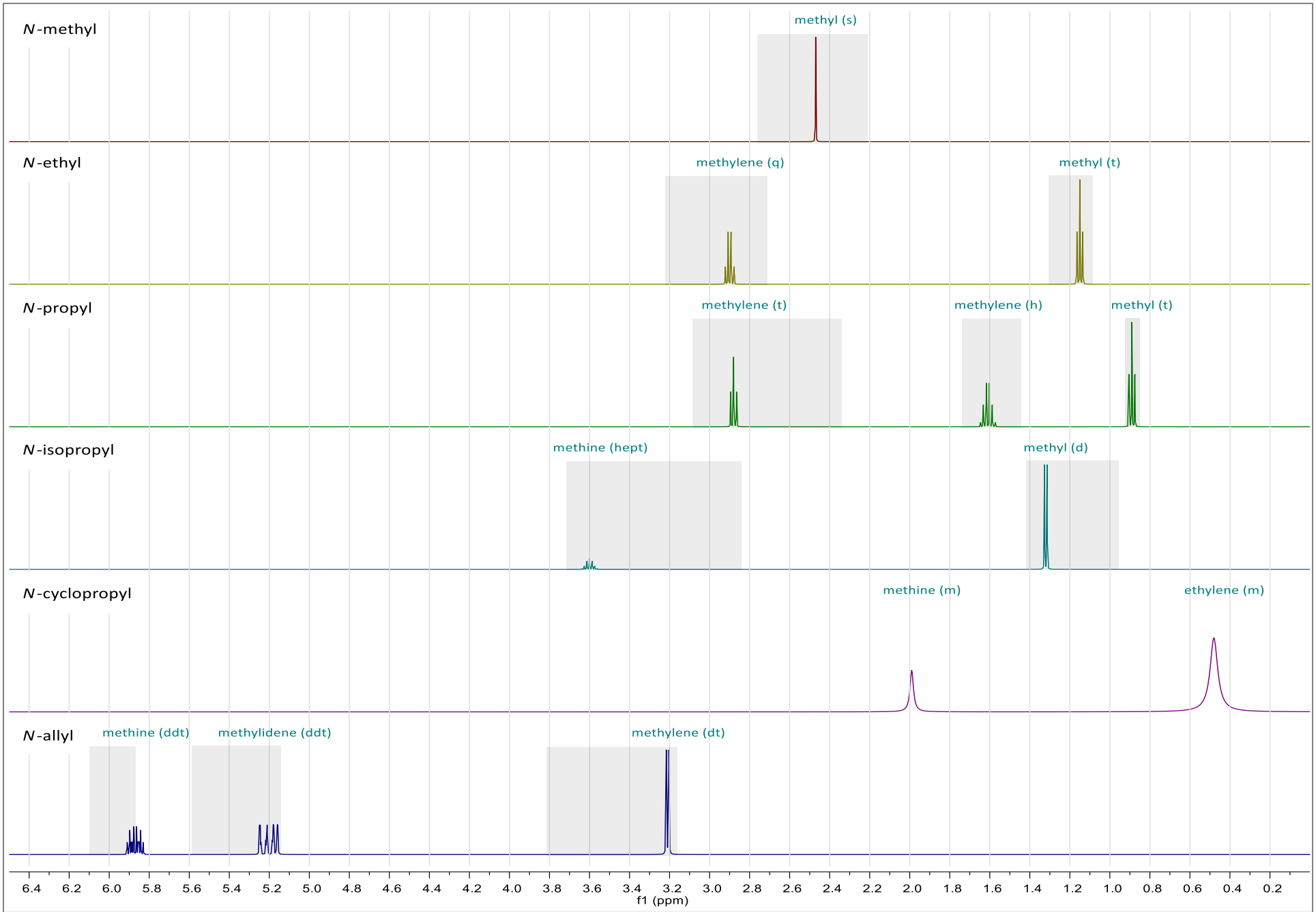
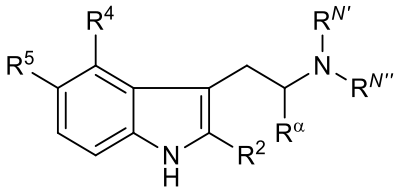


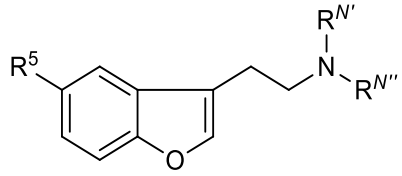
Figure 3: Representative ^{1}H NMR splitting pattern and shift range of *N*-substituents.

Table 1: Names and scaffold substitution patterns of analytes

Scaffold T



Scaffold BF

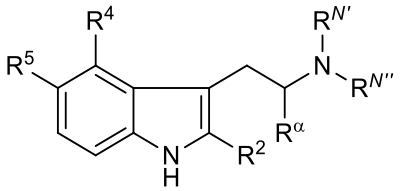


Scaffold T	R^5	R^4	R^2	R^α	$R^{N'}$	$R^{N''}$	Preferred IUPAC name (PIN)
Tryptamine	H	H	H	H	H	H	2-(1*H*-indol-3-yl)ethan-1-amine
5-MeO-T	MeO	H	H	H	H	H	2-(5-methoxy-1*H*-indol-3-yl)ethan-1-amine
α-MT	H	H	H	Me	H	H	1-(1*H*-indol-3-yl)propan-2-amine
5-MeO-α-MT	MeO	H	H	Me	H	H	1-(5-methoxy-1*H*-indol-3-yl)propan-2-amine
4-Me-α-ET	H	Me	H	Et	H	H	1-(4-methyl-1*H*-indol-3-yl)butan-2-amine
NMT	H	H	H	H	H	Me	2-(1*H*-indol-3-yl)-*N*-methylethan-1-amine
2-Me-DMT	H	H	Me	H	Me	Me	*N*,*N*-dimethyl-2-(2-methyl-1*H*-indol-3-yl)ethan-1-amine
5-MeO-TMT	MeO	H	Me	H	Me	Me	2-(5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*,*N*-dimethylethan-1-amine
4-AcO-DMT	H	AcO	H	H	Me	Me	3-[2-(dimethylamino)ethyl]-1*H*-indol-4-yl acetate
5-MeO-DMT	MeO	H	H	H	Me	Me	2-(5-methoxy-1*H*-indol-3-yl)-*N*,*N*-dimethylethan-1-amine
MET	H	H	H	H	Me	Et	*N*-ethyl-2-(1*H*-indol-3-yl)-*N*-methylethan-1-amine
4-HO-MET	H	HO	H	H	Me	Et	3-{2-[ethyl(methyl)amino]ethyl}-1*H*-indol-4-ol
4-AcO-MET	H	AcO	H	H	Me	Et	3-{2-[ethyl(methyl)amino]ethyl}-1*H*-indol-4-yl acetate
5-MeO-MET	MeO	H	H	H	Me	Et	*N*-ethyl-2-(5-methoxy-1*H*-indol-3-yl)-*N*-methylethan-1-amine
4-HO-DET	H	HO	H	H	Et	Et	3-[2-(diethylamino)ethyl]-1*H*-indol-4-ol
4-AcO-DET	H	AcO	H	H	Et	Et	3-[2-(diethylamino)ethyl]-1*H*-indol-4-yl acetate
MPT	H	H	H	H	Me	Pr	*N*-[2-(1*H*-indol-3-yl)ethyl]-*N*-methylpropan-1-amine
4-HO-MPT	H	HO	H	H	Me	Pr	3-{2-[methyl(propyl)amino]ethyl}-1*H*-indol-4-ol
4-AcO-MPT	H	AcO	H	H	Me	Pr	3-{2-[methyl(propyl)amino]ethyl}-1*H*-indol-4-yl acetate
EPT	H	H	H	H	Et	Pr	*N*-ethyl-*N*-[2-(1*H*-indol-3-yl)ethyl]propan-1-amine
4-HO-EPT	H	HO	H	H	Et	Pr	3-{2-[ethyl(propyl)amino]ethyl}-1*H*-indol-4-ol
4-AcO-EPT	H	AcO	H	H	Et	Pr	3-{2-[ethyl(propyl)amino]ethyl}-1*H*-indol-4-yl acetate
DPT	H	H	H	H	Pr	Pr	*N*-[2-(1*H*-indol-3-yl)ethyl]-*N*-propylpropan-1-amine
4-HO-DPT	H	HO	H	H	Pr	Pr	3-[2-(dipropylamino)ethyl]-1*H*-indol-4-ol
4-AcO-DPT	H	AcO	H	H	Pr	Pr	3-[2-(dipropylamino)ethyl]-1*H*-indol-4-yl acetate
5-MeO-DPT	MeO	H	H	H	Pr	Pr	*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-*N*-propylpropan-1-amine
5-MeO-NIPT	MeO	H	H	H	H	iPr	*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]propan-2-amine
MIPT	H	H	H	H	Me	iPr	*N*-[2-(1*H*-indol-3-yl)ethyl]-*N*-methylpropan-2-amine
4-HO-MIPT	H	HO	H	H	Me	iPr	3-{2-[methyl(propan-2-yl)amino]ethyl}-1*H*-indol-4-ol
4-AcO-MIPT	H	AcO	H	H	Me	iPr	3-{2-[methyl(propan-2-yl)amino]ethyl}-1*H*-indol-4-yl acetate
4-MeO-MIPT	H	MeO	H	H	Me	iPr	*N*-[2-(4-methoxy-1*H*-indol-3-yl)ethyl]-*N*-methylpropan-2-amine
5-MeO-MIPT	MeO	H	H	H	Me	iPr	*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-*N*-methylpropan-2-amine
5-MeO-EIPT	MeO	H	H	H	Et	iPr	*N*-ethyl-*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]propan-2-amine

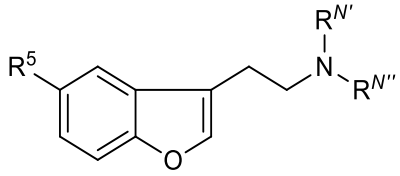
AcO: acetyloxy (acetoxy); Al: prop-2-en-1-yl (allyl); cPr: cyclopropyl; Et: ethyl; HO: hydroxy; iPr: prop-2-yl (isopropyl); Me: methyl; MeO: methoxy; Pr: propyl

Table 1: Names and scaffold substitution patterns of analytes

Scaffold T



Scaffold BF



DIPT	H	H	H	H	iPr	iPr	*N*-[2-(1*H*-indol-3-yl)ethyl]-*N*-(propan-2-yl)propan-2-amine
4-HO-DIPT	H	HO	H	H	iPr	iPr	3-{2-[di(propan-2-yl)amino]ethyl}-1*H*-indol-4-ol
4-AcO-DIPT	H	AcO	H	H	iPr	iPr	3-{2-[di(propan-2-yl)amino]ethyl}-1*H*-indol-4-yl acetate
5-MeO-DIPT	MeO	H	H	H	iPr	iPr	*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-*N*-(propan-2-yl)propan-2-amine
4-HO-MCPT	H	HO	H	H	Me	cPr	3-{2-[cyclopropyl(methyl)amino]ethyl}-1*H*-indol-4-ol
MALT	H	H	H	H	Me	Al	*N*-[2-(1*H*-Indol-3-yl)ethyl]-*N*-methylprop-2-en-1-amine
4-HO-MALT	H	HO	H	H	Me	Al	3-{2-[methyl(prop-2-en-1-yl)amino]ethyl}-1*H*-indol-4-ol
5-MeO-MALT	MeO	H	H	H	Me	Al	*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-*N*-(prop-2-en-1-yl)prop-2-en-1-amine
DALT	H	H	H	H	Al	Al	*N*-[2-(1*H*-indol-3-yl)ethyl]-*N*-(prop-2-en-1-yl)prop-2-en-1-amine
4-AcO-DALT	H	AcO	H	H	Al	Al	3-{2-[di(prop-2-en-1-yl)amino]ethyl}-1*H*-indol-4-yl acetate
5-MeO-DALT	MeO	H	H	H	Al	Al	*N*-[2-(5-methoxy-1*H*-indol-3-yl)ethyl]-*N*-(prop-2-en-1-yl)prop-2-en-1-amine

Scaffold BF	R^5	$R^{N'}$	$R^{N''}$	Preferred IUPAC name (PIN)
5-MeO-DiBF	MeO	iPr	iPr	*N*-[2-(5-methoxy-1-benzofuran-3-yl)ethyl]-*N*-(propan-2-yl)propan-2-amine

AcO: acetyloxy (acetoxy); Al: prop-2-en-1-yl (allyl); cPr: cyclopropyl; Et: ethyl; HO: hydroxy; iPr: prop-2-yl (isopropyl); Me: methyl; MeO: methoxy; Pr: propyl

Table 2: ^{1}H NMR chemical shift of analytes

Analyte		^{1}H NMR (fumarate shifts in grey)
T0	Tryptamine · HCl	700 MHz DMSO-d_6 δ 11.03 (s, 1H), 8.21 (s, 3H), 7.57 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.37 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.24 (d, *J* = 2.4 Hz, 1H), 7.08 (ddd, *J* = 8.1, 6.9, 1.1 Hz, 1H), 7.00 (ddd, *J* = 7.9, 6.9, 1.0 Hz, 1H), 3.04 (s, 4H)
T1a	4-AcO-DMT · F	500 MHz DMSO-d_6 δ 11.16 (d, *J* = 2.5 Hz, 1H), 7.25 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.20 (d, *J* = 2.4 Hz, 1H), 7.09 – 7.01 (m, 1H), 6.70 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.54 (s, 2H, fumarate), 2.95 (s, 4H), 2.56 (s, 6H), 2.37 (s, 3H)
T1b	4-AcO-DMT · F	500 MHz DMSO-d_6 δ 11.18 – 11.13 (m, 1H), 7.24 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.19 (d, *J* = 2.4 Hz, 1H), 7.09 – 7.01 (m, 1H), 6.69 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.53 (s, 2H, fumarate), 2.98 – 2.86 (m, 4H), 2.54 (s, 6H), 2.37 (s, 3H)
T2	5-MeO-DMT fb	500 MHz DMSO-d_6 δ 10.59 (s, 1H), 7.21 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.11 – 7.06 (m, 1H), 6.96 (dd, *J* = 2.4, 0.6 Hz, 1H), 6.70 (ddd, *J* = 8.8, 2.5, 0.4 Hz, 1H), 3.75 (s, 3H), 2.81 – 2.73 (m, 2H), 2.53 – 2.44 (m, 2H, obs.), 2.21 (s, 6H)
T3	2-Me-DMT · F	500 MHz DMSO-d_6 δ 10.76 (s, 1H), 7.43 (ddt, *J* = 7.8, 1.4, 0.7 Hz, 1H), 7.22 (ddd, *J* = 8.0, 0.8 Hz, 1H), 6.97 (ddd, *J* = 8.1, 7.0, 1.3 Hz, 1H), 6.92 (ddd, *J* = 7.7, 7.0, 1.1 Hz, 1H), 6.52 (s, 1H, fumarate), 2.91 – 2.83 (m, 2H), 2.73 – 2.65 (m, 2H), 2.47 (s, 6H), 2.32 (s, 3H)
T4	5-MeO-TMT · F	500 MHz DMSO-d_6 δ 10.58 (s, 1H), 7.11 (dd, *J* = 8.6, 0.5 Hz, 1H), 6.94 (dd, *J* = 2.5, 0.6 Hz, 1H), 6.62 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.51 (s, 1H), 3.74 (s, 3H), 2.87 – 2.79 (m, 2H), 2.71 – 2.64 (m, 2H), 2.47 (s, 6H), 2.29 (s, 3H)
T5	MET · F	500 MHz DMSO-d_6 δ 10.86 – 10.82 (m, 1H), 7.53 (ddd, *J* = 7.9, 1.3, 0.7 Hz, 1H), 7.33 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.19 – 7.14 (m, 1H), 7.06 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.97 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.50 (s, 1H, fumarate), 2.95 – 2.89 (m, 2H), 2.86 – 2.79 (m, 2H), 2.70 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.08 (t, *J* = 7.2 Hz, 3H).
T6	4-HO-MET · F	500 MHz DMSO-d_6 δ 10.66 (d, *J* = 2.3 Hz, 1H), 6.95 (d, *J* = 2.3 Hz, 1H), 6.81 (dd, *J* = 8.1, 7.4 Hz, 1H), 6.75 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.48 (s, 1H, fumarate), 6.30 (dd, *J* = 7.4, 1.0 Hz, 1H), 3.02 – 2.95 (m, 2H), 2.91 – 2.86 (m, 2H), 2.73 (q, *J* = 7.2 Hz, 2H), 2.45 (s, 3H), 1.08 (t, *J* = 7.2 Hz, 3H)
T7	5-MeO-MET · F	500 MHz DMSO-d_6 δ 10.70 (d, *J* = 2.5 Hz, 1H), 7.22 (dd, *J* = 8.7, 0.6 Hz, 1H), 7.15 – 7.10 (m, 1H), 7.06 – 7.02 (m, 1H), 6.71 (ddd, *J* = 8.7, 2.4, 0.4 Hz, 1H), 6.50 (s, 1H, fumarate), 3.76 (s, 3H), 2.95 – 2.82 (m, 4H), 2.75 (q, *J* = 7.2 Hz, 2H), 2.47 (s, 3H), 1.11 (t, *J* = 7.2 Hz, 3H)
T8	MIPT fb	500 MHz DMSO-d_6 δ 10.74 (s, 1H), 7.49 (ddt, *J* = 8.0, 1.4, 0.8 Hz, 1H), 7.32 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.13 (dd, *J* = 2.2, 1.1 Hz, 1H), 7.05 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 6.96 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 2.84 (hept, *J* = 6.6 Hz, 1H), 2.82 – 2.74 (m, 2H), 2.64 – 2.52 (m, 2H), 2.22 (s, 3H), 0.95 (d, *J* = 6.5 Hz, 6H)
T9	4-HO-MIPT · F	500 MHz DMSO-d_6 δ 10.65 (d, *J* = 2.4 Hz, 1H), 6.95 (d, *J* = 2.3 Hz, 1H), 6.81 (dd, *J* = 8.1, 7.5 Hz, 1H), 6.75 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.48 (s, 1H, fumarate), 6.28 (dd, *J* = 7.4, 1.0 Hz, 1H), 3.07 (hept, *J* = 6.6 Hz, 1H), 2.96 (t, *J* = 6.8 Hz, 2H), 2.84 (t, *J* = 6.8 Hz, 2H), 2.40 (s, 3H), 1.03 (d, *J* = 6.6 Hz, 6H)
T10	4-MeO-MIPT · F	500 MHz DMSO-d_6 δ 10.94 – 10.89 (m, 1H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.99 – 6.95 (m, 1H), 6.93 (dd, *J* = 8.1, 1.1 Hz, 1H), 6.51 (s, 2H, fumarate), 6.45 (dd, *J* = 7.5, 1.1 Hz, 1H), 3.85 (s, 3H), 3.38 (hept, *J* = 6.6 Hz, 1H), 3.13 – 3.05 (m, 2H), 3.08 – 2.97 (m, 2H), 2.59 (s, 3H), 1.18 (d, *J* = 6.6 Hz, 6H)
T11	5-MeO-MIPT · H^+	500 MHz DMSO-d_6 δ 10.83 (d, *J* = 2.5 Hz, 1H), 10.69 (s, 1H), 7.25 (dd, *J* = 8.8, 0.5 Hz, 1H), 7.20 (d, *J* = 2.5 Hz, 1H), 7.19 (d, *J* = 2.4 Hz, 1H), 6.73 (dd, *J* = 8.7, 2.4 Hz, 1H), 3.78 (s, 3H), 3.60 (hept, *J* = 6.7 Hz, 1H), 3.29 – 3.12 (m, 4H), 2.70 (s, 3H), 1.30 (d, *J* = 7.0 Hz, 3H), 1.24 (d, *J* = 7.0 Hz, 3H)
T12	4-HO-DET · H^+	500 MHz DMSO-d_6 δ 10.82 (d, *J* = 2.4 Hz, 1H), 10.26 (s, 1H), 9.63 (s, 1H), 7.05 (d, *J* = 2.4 Hz, 1H), 6.83 (dd, *J* = 8.1, 7.3 Hz, 1H), 6.79 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.37 (dd, *J* = 7.3, 1.0 Hz, 1H), 3.32 – 3.24 (m, 2H), 3.21 – 3.11 (m, 6H), 1.27 (t, *J* = 7.2 Hz, 6H)
T13	4-AcO-DET · F	500 MHz DMSO-d_6 δ 11.16 (d, *J* = 2.4 Hz, 1H), 7.24 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.23 (d, *J* = 2.4 Hz, 1H), 7.08 – 7.01 (m, 1H), 6.69 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.52 (s, 2H, fumarate), 3.02 – 2.93 (m, 4H), 2.90 (q, *J* = 7.2 Hz, 4H), 2.37 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 6H)
T14	5-MeO-EIPT · H^+	500 MHz DMSO-d_6 δ 10.85 (d, *J* = 2.3 Hz, 1H), 10.56 (s, 1H), 7.25 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.23 (d, *J* = 2.5 Hz, 1H), 7.18 (d, *J* = 2.4 Hz, 1H), 6.74 (ddd, *J* = 8.8, 2.5, 0.4 Hz, 1H), 3.77 (s, 3H), 3.69 (pd, *J* = 6.6, 2.6 Hz, 1H), 3.27 – 3.15 (m, 6H), 1.38 – 1.24 (m, 9H)
T15	DPT · H^+	500 MHz DMSO-d_6 δ 11.00 (s, 1H), 10.45 (s, 1H), 7.62 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.36 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.27 (d, *J* = 2.4 Hz, 1H), 7.09 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.01 (ddd, *J* = 8.0, 6.9, 1.0 Hz, 1H), 3.31 – 3.23 (m, 2H), 3.20 – 3.12 (m, 2H), 3.11 – 3.04 (m, 4H), 1.72 (h, *J* = 7.8 Hz, 4H), 0.92 (t, *J* = 7.4 Hz, 6H)

HCl, hydrochloride; fb, free base; F, fumarate; H^+, aminium
br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 2: ^{1}H NMR chemical shift of analytes

Analyte		^{1}H NMR (fumarate shifts in grey)
T16	4-HO-DPT · F	500 MHz DMSO-d_6 δ 10.63 (d, *J* = 2.3 Hz, 1H), 6.94 (d, *J* = 2.3 Hz, 1H), 6.80 (dd, *J* = 8.1, 7.4 Hz, 1H), s 1H), 6.49 (s, 1H, fumarate), 6.29 (dd, *J* = 7.4, 1.0 Hz, 1H), 2.97 – 2.91 (m, 2H), 2.87 (dd, *J* = 8.4, 5.6 Hz, 2H), 2.66 – 2.58 (m, 4H), 1.58 – 1.45 (m, 4H), 0.85 (t, *J* = 7.4 Hz, 6H)
T17	5-MeO-DPT · H$^+$	500 MHz DMSO-d_6 δ 10.84 (d, *J* = 2.5 Hz, 1H), 10.77 (s, 1H), 7.25 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.21 (d, *J* = 2.4 Hz, 1H), 7.17 (d, *J* = 2.4 Hz, 1H), 6.74 (ddd, *J* = 8.7, 2.5, 0.4 Hz, 1H), 3.78 (s, 3H), 3.28 – 3.20 (m, 2H), 3.18 – 3.10 (m, 2H), 3.12 – 3.01 (m, 4H), 1.73 (h, *J* = 7.8 Hz, 4H), 0.92 (t, *J* = 7.4 Hz, 6H)
T18	DIPT · H$^+$	500 MHz DMSO-d_6 δ 11.06 (s, 1H), 9.97 (s, 1H), 7.56 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.39 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.35 (d, *J* = 2.4 Hz, 1H), 7.11 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.04 (ddd, *J* = 7.9, 7.0, 1.0 Hz, 1H), 3.77 – 3.65 (m, 2H), 3.30 – 3.17 (m, 4H), 1.41 (d, *J* = 6.6 Hz, 6H), 1.36 (d, *J* = 6.5 Hz, 6H)
T19	4-HO-DIPT · H$^+$	500 MHz DMSO-d_6 δ 10.85 (d, *J* = 2.4 Hz, 1H), 9.70 (s, 2H), 7.09 (d, *J* = 2.3 Hz, 1H), 6.83 (dd, *J* = 8.1, 7.3 Hz, 1H), 6.79 (dd, *J* = 8.1, 1.1 Hz, 1H), 6.38 (dd, *J* = 7.3, 1.1 Hz, 1H), 3.69 – 3.59 (m, 2H), 3.29 – 3.16 (m, 4H), 1.40 (d, *J* = 6.5 Hz, 6H), 1.34 (d, *J* = 6.5 Hz, 6H)
T20	4-AcO-DIPT · H$^+$	500 MHz DMSO-d_6 δ 11.33 – 11.28 (m, 1H), 10.04 (s, 1H), 7.37 (d, *J* = 2.5 Hz, 1H), 7.26 (d, *J* = 8.1 Hz, 1H), 7.06 (t, *J* = 7.9 Hz, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 3.66 (pd, *J* = 6.7, 4.0 Hz, 2H), 3.33 – 3.26 (m, 2H), 3.22 – 3.14 (m, 2H), 2.46 (s, 3H), 1.38 (d, *J* = 6.5 Hz, 6H), 1.33 (d, *J* = 6.5 Hz, 6H)
T21	5-MeO-DIPT · H$^+$	500 MHz DMSO-d_6 δ 10.87 (s, 1H), 9.97 (s, 1H), 7.28 (d, *J* = 2.5 Hz, 1H), 7.26 (dd, *J* = 8.8, 0.5 Hz, 1H), 7.05 (d, *J* = 2.4 Hz, 1H), 6.74 (dd, *J* = 8.7, 2.4 Hz, 1H), 3.77 (s, 3H), 3.70 (dp, *J* = 13.2, 6.5 Hz, 2H), 3.26 – 3.13 (m, 4H), 1.40 (d, *J* = 6.5 Hz, 6H), 1.35 (d, *J* = 6.5 Hz, 6H)
T22	DALT · H$^+$	500 MHz DMSO-d_6 δ 11.62 (s, 1H), 11.07 – 11.02 (m, 1H), 7.59 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.37 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.23 (d, *J* = 2.4 Hz, 1H), 7.09 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.00 (ddd, *J* = 7.9, 7.0, 1.0 Hz, 1H), 6.10 (ddt, *J* = 17.3, 10.3, 7.1 Hz, 2H), 5.59 (dq, *J* = 17.2, 1.4 Hz, 2H), 5.52 (dd, *J* = 10.3, 1.6 Hz, 2H), 3.81 (dd, *J* = 7.2, 4.3 Hz, 4H), 3.20 (s, 4H)
T23	4-AcO-DALT · F	500 MHz DMSO-d_6 δ 11.04 (d, *J* = 2.4 Hz, 1H), 7.23 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.16 – 7.09 (m, 1H), 7.03 (ddd, *J* = 8.1, 7.6, 0.3 Hz, 1H), 6.66 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.61 (s, 2H, fumarate), 5.87 (ddt, *J* = 17.2, 10.2, 6.4 Hz, 2H), 5.23 (ddt, *J* = 17.2, 2.1, 1.4 Hz, 2H), 5.17 (ddt, *J* = 10.2, 2.2, 1.1 Hz, 2H), 3.21 (dt, *J* = 6.5, 1.3 Hz, 4H), 2.86 – 2.77 (m, 2H), 2.76 – 2.68 (m, 2H), 2.34 (s, 3H)
T24a	5-MeO-DALT fb	500 MHz DMSO-d_6 δ 10.61 – 10.55 (m, 1H), 7.20 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.05 (d, *J* = 2.4 Hz, 1H), 6.93 (d, *J* = 2.5 Hz, 1H), 6.69 (dd, *J* = 8.7, 2.4 Hz, 1H), 5.87 (ddt, *J* = 17.3, 10.2, 6.3 Hz, 2H), 5.28 – 5.16 (m, 2H), 5.14 (ddt, *J* = 10.1, 2.3, 1.2 Hz, 2H), 3.75 (s, 3H), 3.16 (dt, *J* = 6.4, 1.4 Hz, 4H), 2.85 – 2.74 (m, 2H), 2.71 – 2.60 (m, 2H)
T24b	5-MeO-DALT fb	500 MHz DMSO-d_6 δ 10.60 – 10.56 (m, 1H), 7.21 (dd, *J* = 8.7, 0.6 Hz, 1H), 7.08 – 7.03 (m, 1H), 6.93 (dd, *J* = 2.5, 0.6 Hz, 1H), 6.70 (ddd, *J* = 8.7, 2.5, 0.4 Hz, 1H), 5.87 (ddt, *J* = 17.3, 10.2, 6.3 Hz, 2H), 5.23 (ddt, *J* = 17.2, 2.2, 1.5 Hz, 2H), 5.14 (ddt, *J* = 10.2, 2.3, 1.2 Hz, 2H), 3.75 (s, 3H), 3.16 (dt, *J* = 6.3, 1.4 Hz, 4H), 2.82 – 2.74 (m, 2H), 2.71 – 2.64 (m, 2H)
T25	4-HO-MPT · F	500 MHz DMSO-d_6 δ 10.71 (d, *J* = 2.4 Hz, 1H), 6.98 (d, *J* = 2.3 Hz, 1H), 6.81 (dd, *J* = 8.1, 7.4 Hz, 1H), 6.76 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.52 (s, 2H, fumarate), 6.32 (dd, *J* = 7.4, 1.0 Hz, 1H), 3.06 (s, 4H), 2.82 – 2.75 (m, 2H), 2.59 (s, 3H), 1.66 – 1.54 (m, 2H), 0.87 (t, *J* = 7.4 Hz, 3H)
T26	α-MT fb	500 MHz DMSO-d_6 δ 10.80 (s, 1H), 7.51 (ddt, *J* = 8.0, 1.3, 0.7 Hz, 1H), 7.33 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.14 – 7.09 (m, 1H), 7.05 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.95 (ddd, *J* = 8.0, 7.0, 1.1 Hz, 1H), 3.07 (h, *J* = 6.5 Hz, 1H), 2.63 (ddd, *J* = 6.8, 3.8, 0.8 Hz, 2H), 1.38 (s, 2H), 0.98 (d, *J* = 6.2 Hz, 3H)
T27	5-MeO-α-MT · H$^+$	500 MHz DMSO-d_6 δ 10.88 (d, *J* = 2.5 Hz, 1H), 8.17 (s, 3H), 7.25 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.18 (d, *J* = 2.3 Hz, 1H), 7.14 (dt, *J* = 2.5, 0.6 Hz, 1H), 6.73 (ddd, *J* = 8.7, 2.5, 0.4 Hz, 1H), 3.77 (s, 3H), 3.44 – 3.34 (m, 1H), 3.13 – 3.05 (m, 1H), 2.84 – 2.75 (m, 1H), 1.18 (d, *J* = 6.5 Hz, 3H)
T28	4-Me-α-ET fb	500 MHz DMSO-d_6 δ 10.78 (s, 1H), 7.15 (d, *J* = 8.1 Hz, 1H), 7.06 (d, *J* = 2.4 Hz, 1H), 6.95 – 6.85 (m, 1H), 6.67 (d, *J* = 7.0 Hz, 1H), 2.93 (dd, *J* = 14.1, 5.0 Hz, 1H), 2.75 (tt, *J* = 7.6, 4.9 Hz, 1H), 2.60 (s, 3H), 2.59 (dd, *J* = 14.2, 8.0 Hz, 1H), 1.53 – 1.41 (m, 1H), 1.30 (s, 2H), 1.26 (dq, *J* = 13.3, 7.4 Hz, 1H), 0.92 (t, *J* = 7.4 Hz, 3H)
T29	5-MeO-T · HCl	700 MHz DMSO-d_6 δ 10.89 – 10.86 (m, 1H), 8.23 (s, 3H), 7.25 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.18 (d, *J* = 2.4 Hz, 1H), 7.10 (d, *J* = 2.5 Hz, 1H), 6.73 (dd, *J* = 8.7, 2.4 Hz, 1H), 3.77 (s, 3H), 3.06 – 2.98 (m, 4H)
T30	NMT · HCl	700 MHz DMSO-d_6 δ 11.07 (s, 1H), 8.76 (s, 2H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.23 (d, *J* = 2.3 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.99 (t, *J* = 7.4 Hz, 1H), 3.10 (s, 4H), 2.54 (s, 3H)

HCl, hydrochloride; fb, free base; F, fumarate; H$^+$, aminium

br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 2: ^{1}H NMR chemical shift of analytes

Analyte		^{1}H NMR (fumarate shifts in grey)
T31	4-AcO-MIPT · F	500 MHz DMSO-d_6 δ 13.01 (br s, 2H), 11.19 (d, *J* = 2.5 Hz, 1H), 7.30 – 7.21 (m, 2H), 7.05 (t, *J* = 7.9 Hz, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 6.54 (s, 2H, fumarate), 3.37 (hept, *J* = 6.6 Hz, 1H), 3.07 – 2.95 (m, 4H), 2.58 (s, 3H), 2.38 (s, 3H), 1.16 (d, *J* = 6.6 Hz, 6H)
T32	4-AcO-MET · F	500 MHz DMSO-d_6 δ 13.87 – 11.79 (m, 1H), 11.19 (d, *J* = 2.5 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 1H), 7.22 (d, *J* = 2.4 Hz, 1H), 7.05 (t, *J* = 7.9 Hz, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 6.53 (s, 2H, fumarate), 3.04 – 2.92 (m, 4H), 2.89 (q, *J* = 7.2 Hz, 2H), 2.57 (s, 3H), 2.38 (s, 3H), 1.15 (t, *J* = 7.2 Hz, 3H)
T33	5-MeO-MALT · H$^+$	500 MHz DMSO-d_6 δ 10.86 – 10.81 (m, 1H), 8.02 (s, 1H), 7.25 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.17 (d, *J* = 2.4 Hz, 1H), 7.08 (d, *J* = 2.4 Hz, 1H), 6.73 (dd, *J* = 8.7, 2.4 Hz, 1H), 5.99 (ddt, *J* = 17.2, 10.2, 7.0 Hz, 1H), 5.50 (dd, *J* = 8.7, 2.4 Hz, 2H), 3.77 (s, 3H), 3.75 (d, *J* = 7.0 Hz, 2H), 3.25 – 3.18 (m, 2H), 3.11 – 3.02 (m, 2H), 2.76 (s, 3H)
T34	5-MeO-NIPT · H$^+$	500 MHz DMSO-d_6 δ 10.84 (d, *J* = 2.4 Hz, 1H), 9.14 (s, 2H), 7.25 (dd, *J* = 8.7, 0.5 Hz, 1H), 7.21 (d, *J* = 2.5 Hz, 1H), 7.15 (d, *J* = 2.4 Hz, 1H), 6.73 (dd, *J* = 8.8, 2.5 Hz, 1H), 3.77 (s, 3H), 3.31 (hept, *J* = 6.6 Hz, 1H), 3.08 (s, 4H), 1.27 (d, *J* = 6.5 Hz, 6H)
T35	MPT fb	500 MHz DMSO-d_6 δ 10.76 (s, 1H), 7.49 (ddt, *J* = 7.9, 1.4, 0.7 Hz, 1H), 7.33 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.15 – 7.12 (m, 1H), 7.05 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 6.97 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 2.85 – 2.78 (m, 2H), 2.63 – 2.56 (m, 2H), 2.37 – 2.30 (m, 2H), 2.24 (s, 3H), 1.51 – 1.37 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 3H)
T36	4-HO-MCPT · F	500 MHz DMSO-d_6 δ 10.60 (d, *J* = 2.3 Hz, 1H), 6.92 (d, *J* = 2.3 Hz, 1H), 6.80 (dd, *J* = 8.1, 7.3 Hz, 1H), 6.75 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.58 (s, 1H, fumarate), 6.28 (dd, *J* = 7.3, 1.1 Hz, 1H), 3.03 – 2.95 (m, 2H), 2.95 – 2.88 (m, 2H), 2.47 (s, 3H), 2.03 – 1.95 (m, 1H), 0.57 – 0.39 (m, 4H)
T37	EPT · F	500 MHz DMSO-d_6 δ 10.96 – 10.92 (m, 1H), 7.57 (ddt, *J* = 7.9, 1.4, 0.7 Hz, 1H), 7.35 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.22 (d, *J* = 2.4 Hz, 1H), 7.07 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.99 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 3.13 – 3.04 (m, 2H), 3.04 – 2.96 (m, 4H), 2.94 – 2.83 (m, 2H), 1.68 – 1.54 (m, 2H), 1.16 (t, *J* = 7.2 Hz, 3H), 0.90 (t, *J* = 7.4 Hz, 3H)
T38	4-HO-EPT · F	500 MHz DMSO-d_6 δ 12.06 (s, 2H, fumarate), 10.73 (d, *J* = 2.4 Hz, 1H), 7.01 (d, *J* = 2.3 Hz, 1H), 6.82 (dd, *J* = 8.1, 7.3 Hz, 1H), 6.77 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.53 (s, 2H, fumarate), 6.33 (dd, *J* = 7.4, 1.0 Hz, 1H), 3.19 – 3.09 (m, 2H), 3.11 – 3.04 (m, 2H), 3.02 (q, *J* = 7.2 Hz, 2H), 2.93 – 2.85 (m, 2H), 1.69 – 1.57 (m, 2H), 1.18 (t, *J* = 7.2 Hz, 3H), 0.89 (t, *J* = 7.4 Hz, 3H)
T39	4-HO-MALT · F	600 MHz DMSO-d_6 δ 10.66 (d, *J* = 2.3 Hz, 1H), 6.95 (d, *J* = 2.3 Hz, 1H), 6.81 (dd, *J* = 8.1, 7.4 Hz, 1H), 6.76 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.55 (s, 2H, fumarate), 6.31 (dd, *J* = 7.4, 0.9 Hz, 1H), 5.89 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 5.33 (dq, *J* = 17.2, 1.5 Hz, 1H), 5.27 (ddt, *J* = 10.1, 1.9, 1.0 Hz, 1H), 3.37 (dt, *J* = 6.9, 1.2 Hz, 2H), 3.07 – 3.00 (m, 2H), 2.96 – 2.89 (m, 2H), 2.47 (s, 3H)
T40	4-AcO-DPT · F	600 MHz DMSO-d_6 δ 11.13 (s, 1H), 7.24 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.21 (d, *J* = 2.4 Hz, 1H), 7.07 – 7.01 (m, 1H), 6.68 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.56 (s, 2H, fumarate), 2.97 – 2.85 (m, 4H), 2.74 – 2.68 (m, 4H), 2.36 (s, 3H), 1.59 – 1.49 (m, 4H), 0.87 (t, *J* = 7.3 Hz, 6H)
T41	MALT fb	700 MHz DMSO-d_6 δ 10.76 (s, 1H), 7.49 (ddt, *J* = 7.9, 1.3, 0.8 Hz, 1H), 7.33 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.13 (dd, *J* = 2.2, 1.1 Hz, 1H), 7.05 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.96 (ddd, *J* = 7.9, 6.9, 1.0 Hz, 1H), 5.85 (ddt, *J* = 17.3, 10.2, 6.4 Hz, 1H), 5.19 (ddt, *J* = 17.2, 2.2, 1.5 Hz, 1H), 5.12 (ddt, *J* = 10.2, 2.3, 1.2 Hz, 1H), 3.04 (dt, *J* = 6.3, 1.4 Hz, 2H), 2.86 – 2.80 (m, 2H), 2.64 – 2.57 (m, 2H), 2.24 (s, 3H)
T42	4-AcO-EPT · F	500 MHz DMSO-d_6 δ 11.15 (s, 1H), 7.24 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.22 (d, *J* = 2.4 Hz, 1H), 7.04 (t, *J* = 7.9 Hz, 1H), 6.68 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.54 (s, 2H, fumarate), 3.00 – 2.92 (m, 4H), 2.88 (q, *J* = 7.1 Hz, 2H), 2.78 – 2.71 (m, 2H), 2.36 (s, 3H), 1.62 – 1.49 (m, 2H), 1.11 (t, *J* = 7.2 Hz, 3H), 0.88 (t, *J* = 7.3 Hz, 3H)
T43	4-AcO-MPT · F	500 MHz, DMSO-d_6 δ 11.16 (s, 1H), 7.24 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.20 (d, *J* = 2.4 Hz, 1H), 7.05 (t, *J* = 7.9 Hz, 1H), 6.69 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.54 (s, 2H, fumarate), 2.94 (s, 4H), 2.74 – 2.68 (m, 2H), 2.53 (s, 3H), 2.37 (s, 3H), 1.63 – 1.52 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H)
BF1	5-MeO-DIBF · H$^+$	700 MHz DMSO-d_6 δ 10.39 (s, 1H), 7.95 (d, *J* = 1.1 Hz, 1H), 7.47 (dd, *J* = 8.9, 0.5 Hz, 1H), 7.26 – 7.24 (m, 1H), 6.92 (ddd, *J* = 8.9, 2.6, 0.5 Hz, 1H), 3.81 (s, 3H), 3.72 (pd, *J* = 6.6, 3.7 Hz, 2H), 3.32 – 3.27 (m, 2H), 3.24 – 3.19 (m, 2H), 1.40 (d, *J* = 6.6 Hz, 6H), 1.35 (d, *J* = 6.6 Hz, 6H)

HCl, hydrochloride; fb, free base; F, fumarate; H$^+$, aminium

br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 3: Multiplets for aryl protons and substituents

1*H*-Indole		1-N*H*	4-*H* ↓	7-*H*	2-*H*	6-*H*	5-*H*
T15	DPT · H^+	11.00 (s)	7.62 (dd, *J* = 7.8, 1.1 Hz)	7.36 (dt, *J* = 8.1, 0.9 Hz)	7.27 (d, *J* = 2.4 Hz)	7.09 (ddd, *J* = 8.2, 6.9, 1.2 Hz)	7.01 (ddd, *J* = 8.0, 6.9, 1.0 Hz)
T30	NMT · HCl	11.07 (s)	7.60 (d, *J* = 7.8 Hz)	7.38 (d, *J* = 8.1 Hz)	7.23 (d, *J* = 2.3 Hz)	7.08 (t, *J* = 7.5 Hz)	6.99 (t, *J* = 7.4 Hz)
T22	DALT · H^+	11.07 – 11.02 (m)	7.59 (dd, *J* = 7.9, 1.0 Hz)	7.37 (dt, *J* = 8.1, 0.9 Hz)	7.23 (d, *J* = 2.4 Hz)	7.09 (ddd, *J* = 8.1, 7.0, 1.2 Hz)	7.00 (ddd, *J* = 7.9, 7.0, 1.0 Hz)
T37	EPT · F	10.96 – 10.92 (m)	7.57 (ddt, *J* = 7.9, 1.4, 0.7 Hz)	7.35 (dt, *J* = 8.1, 0.9 Hz)	7.22 (d, *J* = 2.4 Hz)	7.07 (ddd, *J* = 8.1, 7.0, 1.2 Hz)	6.99 (ddd, *J* = 8.0, 7.0, 1.0 Hz
T0	Tryptamine · HCl	11.03 (s)	7.57 (dd, *J* = 7.8, 1.1 Hz)	7.37 (dt, *J* = 8.1, 0.9 Hz)	7.24 (d, *J* = 2.4 Hz)	7.08 (ddd, *J* = 8.1, 6.9, 1.1 Hz)	7.00 (ddd, *J* = 7.9, 6.9, 1.0 Hz)
T18	DIPT · H^+	11.09 – 11.04 (m)	7.56 (dd, *J* = 7.8, 1.0 Hz	7.39 (dt, *J* = 8.1, 1.0 Hz)	7.35 (d, *J* = 2.4 Hz)	7.11 (ddd, *J* = 8.1, 7.0, 1.2 Hz)	7.04 (ddd, *J* = 7.9, 7.0, 1.0 Hz)
T5	MET · F	10.86 – 10.82 (m)	7.53 (ddd, *J* = 7.9, 1.3, 0.7 Hz)	7.33 (dt, *J* = 8.1, 0.9 Hz)	7.19 – 7.14 (m)	7.06 (ddd, *J* = 8.1, 7.0, 1.2 Hz)	6.97 (ddd, *J* = 8.0, 7.0, 1.0 Hz)
T26	α-MT fb	10.80 (s)	7.51 (ddt, *J* = 8.0, 1.3, 0.7 Hz)	7.33 (dt, *J* = 8.1, 1.0 Hz)	7.14 – 7.09 (m)	7.05 (ddd, *J* = 8.1, 7.0, 1.2 Hz)	6.95 (ddd, *J* = 8.0, 7.0, 1.1 Hz)
T8	MIPT fb	10.74 (s)	7.49 (ddt, *J* = 8.0, 1.4, 0.8 Hz)	7.32 (dt, *J* = 8.1, 0.9 Hz)	7.13 (dd, *J* = 2.2, 1.1 Hz)	7.05 (ddd, *J* = 8.2, 7.0, 1.2 Hz)	6.96 (ddd, *J* = 8.0, 7.0, 1.0 Hz)
T35	MPT fb	10.76 (s)	7.49 (ddt, *J* = 7.9, 1.4, 0.7 Hz)	7.33 (dt, *J* = 8.1, 1.0 Hz)	7.15 – 7.12 (m)	7.05 (ddd, *J* = 8.1, 7.0, 1.1 Hz)	6.97 (ddd, *J* = 8.0, 7.0, 1.0 Hz)
T41	MALT fb	10.76 (s)	7.49 (ddt, *J* = 7.9, 1.3, 0.8 Hz)	7.33 (dt, *J* = 8.1, 0.9 Hz)	7.13 (dd, *J* = 2.2, 1.1 Hz)	7.05 (ddd, *J* = 8.2, 7.0, 1.2 Hz)	6.96 (ddd, *J* = 7.9, 6.9, 1.0 Hz)

2-Me-1*H*-indole		1-N*H*	4-*H*	7-*H*	2-CH_3	6-*H*	5-*H*
T3	2-Me-DMT · F	10.76 (s)	7.43 (ddt, *J* = 7.8, 1.4, 0.7 Hz)	7.22 (ddd, *J* = 8.0, 0.8 Hz)	2.32 (s, 3H)	6.97 (ddd, *J* = 8.1, 7.0, 1.3 Hz)	6.92 (ddd, *J* = 7.7, 7.0, 1.1 Hz)

4-HO-1*H*-indole		1-N*H*	2-*H* ↓	6-*H*	7-*H*	5-*H*	4-O*H*
T19	4-HO-DIPT · H^+	10.85 (d, *J* = 2.4 Hz)	7.09 (d, *J* = 2.3 Hz)	6.83 (dd, *J* = 8.1, 7.3 Hz)	6.79 (dd, *J* = 8.1, 1.1 Hz)	6.38 (dd, *J* = 7.3, 1.1 Hz)	9.70 (br s)
T12	4-HO-DET · H^+	10.82 (d, *J* = 2.4 Hz)	7.05 (d, *J* = 2.4 Hz)	6.83 (dd, *J* = 8.1, 7.3 Hz)	6.79 (dd, *J* = 8.1, 1.0 Hz)	6.37 (dd, *J* = 7.3, 1.0 Hz)	9.63 (br s)
T37	4-HO-EPT · F	10.73 (d, *J* = 2.4 Hz)	7.01 (d, *J* = 2.3 Hz)	6.82 (dd, *J* = 8.1, 7.3 Hz)	6.77 (dd, *J* = 8.1, 1.0 Hz)	6.33 (dd, *J* = 7.4, 1.0 Hz)	—
T25	4-HO-MPT · F	10.71 (d, *J* = 2.4 Hz)	6.98 (d, *J* = 2.3 Hz)	6.81 (dd, *J* = 8.1, 7.4 Hz)	6.76 (dd, *J* = 8.1, 1.0 Hz)	6.32 (dd, *J* = 7.4, 1.0 Hz)	—
T39	4-HO-MALT · F	10.66 (d, *J* = 2.3 Hz)	6.95 (d, *J* = 2.3 Hz)	6.81 (dd, *J* = 8.1, 7.4 Hz)	6.76 (dd, *J* = 8.1, 1.0 Hz)	6.31 (dd, *J* = 7.4, 0.9 Hz)	—
T6	4-HO-MET · F	10.66 (d, *J* = 2.3 Hz)	6.95 (d, *J* = 2.3 Hz)	6.81 (dd, *J* = 8.1, 7.4 Hz)	6.75 (dd, *J* = 8.1, 1.0 Hz)	6.30 (dd, *J* = 7.4, 1.0 Hz)	—
T9	4-HO-MIPT · F	10.65 (d, *J* = 2.4 Hz)	6.95 (d, *J* = 2.3 Hz)	6.81 (dd, *J* = 8.1, 7.5 Hz)	6.75 (dd, *J* = 8.1, 1.0 Hz)	6.28 (dd, *J* = 7.4, 1.0 Hz)	—
T16	4-HO-DPT · F	10.63 (d, *J* = 2.3 Hz)	6.94 (d, *J* = 2.3 Hz)	6.80 (dd, *J* = 8.1, 7.4 Hz)	6.75 (dd, *J* = 8.1, 1.0 Hz)	6.29 (dd, *J* = 7.4, 1.0 Hz)	—
T36	4-HO-MCPT · F	10.60 (d, *J* = 2.3 Hz)	6.92 (d, *J* = 2.3 Hz)	6.80 (dd, *J* = 8.1, 7.3 Hz)	6.75 (dd, *J* = 8.1, 1.0 Hz)	6.28 (dd, *J* = 7.3, 1.1 Hz)	—

4-MeO-1*H*-indole		1-N*H*	2-*H*	6-*H*	7-*H*	5-*H*	4-OCH_3
T10	4-MeO-MIPT · F	10.93 – 10.89 (m)	7.04 (d, *J* = 2.4 Hz)	6.99 – 6.95 (m)	6.93 (dd, *J* = 8.1, 1.1 Hz)	6.45 (dd, *J* = 7.5, 1.1 Hz)	3.85 (s, 3H)

4-Me-1*H*-indole		1-N*H*	7-*H*	2-*H*	6-*H*	5-*H*	4-CH_3
T28	4-Me-α-ET fb	10.78 (s)	7.15 (d, *J* = 8.1 Hz)	7.06 (d, *J* = 2.4 Hz)	6.95 – 6.85 (m)	6.67 (d, *J* = 7.0 Hz)	2.60 (s, 3H)

HCl, hydrochloride; fb, free base; F, fumarate; H^+, aminium; br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 3: Multiplets for aryl protons and substituents

4-AcO-1*H*-indole		1-N*H* ↓	7-*H*	2-*H*	6-*H*	5-*H*	4-OCOCH_3
T20	4-AcO-DIPT· H^+	11.33 – 11.28 (m)	7.26 (d, *J* = 8.1 Hz)	7.37 (d, *J* = 2.5 Hz)	7.06 (t, *J* = 7.9 Hz)	6.69 (d, *J* = 7.6 Hz)	2.46 (s, 3H)
T31	4-AcO-MIPT · F	11.19 (d, *J* = 2.5 Hz)	7.27 – 7.23 (m)	7.27 – 7.23 (m)	7.05 (t, *J* = 7.9 Hz)	6.69 (d, *J* = 7.6 Hz)	2.38 (s, 3H)
T32	4-AcO-MET · F	11.19 (d, *J* = 2.5 Hz)	7.25 (d, *J* = 8.1 Hz)	7.22 (d, *J* = 2.4 Hz)	7.05 (t, *J* = 7.9 Hz)	6.70 (d, *J* = 7.6 Hz)	2.38 (s, 3H)
T1a	4-AcO-DMT · F	11.16 (d, *J* = 2.5 Hz)	7.25 (dd, *J* = 8.1, 0.8 Hz)	7.20 (d, *J* = 2.4 Hz)	7.09 – 7.01 (m)	6.70 (dd, *J* = 7.6, 0.8 Hz)	2.37 (s, 3H)
T1b	4-AcO-DMT · F	11.18 – 11.13 (m)	7.24 (dd, *J* = 8.2, 0.8 Hz)	7.19 (d, *J* = 2.4 Hz)	7.09 – 7.01 (m)	6.69 (dd, *J* = 7.6, 0.8 Hz)	2.37 (s, 3H)
T13	4-AcO-DET · F	11.16 (d, *J* = 2.4 Hz)	7.24 (dd, *J* = 8.1, 0.8 Hz)	7.23 (d, *J* = 2.4 Hz)	7.08 – 7.01 (m)	6.69 (dd, *J* = 7.6, 0.8 Hz)	2.37 (s, 3H)
T40	4-AcO-DPT · F	11.13 (br s)	7.24 (dd, *J* = 8.1, 0.8 Hz)	7.21 (d, *J* = 2.4 Hz)	7.07 – 7.01 (m)	6.68 (dd, *J* = 7.6, 0.8 Hz)	2.36 (s, 3H)
T42	4-AcO-EPT · F	11.15 (br s)	7.24 (dd, *J* = 8.2, 0.8 Hz)	7.22 (d, *J* = 2.4 Hz)	7.04 (t, *J* = 7.9 Hz)	6.68 (dd, *J* = 7.6, 0.8 Hz)	2.36 (s, 3H)
T43	4-AcO-MPT · F	11.16 (br s)	7.24 (dd, *J* = 8.1, 0.8 Hz)	7.20 (d, *J* = 2.4 Hz)	7.05 (t, *J* = 7.9 Hz)	6.69 (dd, *J* = 7.6, 0.8 Hz)	2.37 (s, 3H)
T23	4-AcO-DALT · F	11.04 (d, *J* = 2.4 Hz)	7.23 (dd, *J* = 8.1, 0.8 Hz)	7.16 – 7.09 (m)	7.03 (ddd, *J* = 8.1, 7.6, 0.3 Hz)	6.66 (dd, *J* = 7.6, 0.8 Hz)	2.34 (s, 3H)

5-MeO-1*H*-indole		1-N*H*	7-*H* ↓	2-*H*	4-*H*	6-*H*	5-OCH_3
T21	5-MeO-DIPT · H^+	10.87 (s)	7.26 (dd, *J* = 8.8, 0.5 Hz)	7.28 (d, *J* = 2.5 Hz)	7.05 (d, *J* = 2.4 Hz)	6.74 (dd, *J* = 8.7, 2.4 Hz)	3.77 (s, 3H)
T11	5-MeO-MIPT · H^+	10.83 (d, *J* = 2.5 Hz)	7.25 (dd, *J* = 8.8, 0.5 Hz)	7.20 (d, *J* = 2.5 Hz)	7.19 (d, *J* = 2.4 Hz)	6.73 (dd, *J* = 8.7, 2.4 Hz)	3.78 (s, 3H)
T14	5-MeO-EIPT · H^+	10.85 (d, *J* = 2.3 Hz)	7.25 (dd, *J* = 8.7, 0.5 Hz)	7.23 (d, *J* = 2.5 Hz)	7.18 (d, *J* = 2.4 Hz)	6.74 (ddd, *J* = 8.8, 2.5, 0.4 Hz)	3.77 (s, 3H)
T17	5-MeO-DPT · H^+	10.84 (d, *J* = 2.5 Hz)	7.25 (dd, *J* = 8.7, 0.5 Hz)	7.21 (d, *J* = 2.4 Hz)	7.17 (d, *J* = 2.4 Hz)	6.74 (ddd, *J* = 8.7, 2.5, 0.4 Hz)	3.78 (s, 3H)
T27	5-MeO-α-MT · H^+	10.88 (d, *J* = 2.5 Hz)	7.25 (dd, *J* = 8.7, 0.5 Hz)	7.18 (d, *J* = 2.3 Hz)	7.14 (dt, *J* = 2.5, 0.6 Hz)	6.73 (ddd, *J* = 8.7, 2.5, 0.4 Hz)	3.77 (s, 3H)
T29	5-MeO-T · HCl	10.89 – 10.86 (m)	7.25 (dd, *J* = 8.7, 0.5 Hz)	7.18 (d, *J* = 2.4 Hz)	7.10 (d, *J* = 2.5 Hz)	6.73 (dd, *J* = 8.7, 2.4 Hz)	3.77 (s, 3H)
T33	5-MeO-MALT · H^+	10.86 – 10.81 (m)	7.25 (dd, *J* = 8.7, 0.5 Hz)	7.17 (d, *J* = 2.4 Hz)	7.08 (d, *J* = 2.4 Hz)	6.73 (dd, *J* = 8.7, 2.4 Hz)	3.77 (s, 3H)
T34	5-MeO-NIPT · H^+	10.84 (d, *J* = 2.4 Hz)	7.25 (dd, *J* = 8.7, 0.5 Hz)	7.21 (d, *J* = 2.5 Hz)	7.15 (d, *J* = 2.4 Hz)	6.73 (dd, *J* = 8.8, 2.5 Hz)	3.77 (s, 3H)
T7	5-MeO-MET · F	10.70 (d, *J* = 2.5 Hz)	7.22 (dd, *J* = 8.7, 0.6 Hz)	7.15 – 7.10 (m)	7.06 – 7.02 (m)	6.71 (ddd, *J* = 8.7, 2.4, 0.4 Hz)	3.76 (s, 3H)
T24b	5-MeO-DALT fb	10.60 – 10.56 (m)	7.21 (dd, *J* = 8.7, 0.6 Hz)	7.08 – 7.03 (m)	6.93 (dd, *J* = 2.5, 0.6 Hz)	6.70 (ddd, *J* = 8.7, 2.5, 0.4 Hz)	3.75 (s, 3H)
T2	5-MeO-DMT fb	10.59 (s)	7.21 (dd, *J* = 8.7, 0.5 Hz)	7.11 – 7.06 (m)	6.96 (dd, *J* = 2.4, 0.6 Hz)	6.70 (ddd, *J* = 8.8, 2.5, 0.4 Hz)	3.75 (s, 3H)
T24a	5-MeO-DALT fb	10.61 – 10.55 (m)	7.20 (dd, *J* = 8.7, 0.5 Hz)	7.05 (d, *J* = 2.4 Hz)	6.93 (d, *J* = 2.5 Hz)	6.69 (dd, *J* = 8.7, 2.4 Hz)	3.75 (s, 3H)

5-MeO-2-Me-1*H*-indole		1-N*H*	7-*H*	4-*H*	6-*H*	5-OCH_3	2-CH_3
T4	5-MeO-TMT · F	10.58 (s)	7.11 (dd, *J* = 8.6, 0.5 Hz)	6.94 (dd, *J* = 2.5, 0.6 Hz)	6.62 (dd, *J* = 8.6, 2.4 Hz)	3.74 (s, 3H)	2.29 (s, 3H)

5-MeO-1-benzofuran			2-*H*	7-*H*	4-*H*	6-*H*	5-OCH_3
BF1	5-MeO-DIBF · H^+	—	7.95 (d, *J* = 1.1 Hz)	7.47 (dd, *J* = 8.9, 0.5 Hz)	7.27 – 7.23 (m)	6.92 (ddd, *J* = 8.9, 2.6, 0.5 Hz)	3.81 (s, 3H)

HCl, hydrochloride; fb, free base; F, fumarate; H^+, aminium; br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 4: Multiplets for ethanamine/ethaminium and fumarate moieties

		NH^+ | NH_2^+ | NH_3^+	Fumarate	α - C*H*	α - CH_2 | β - CH_2	NH_2
T0	Tryptamine · HCl	8.21 (s, 3H)			3.04 (s, 4H)	
T1a	4-AcO-DMT · F		6.54 (s, 2H)		2.95 (s, 4H)	
T1b	4-AcO-DMT · F		6.53 (s, 2H)		2.98 – 2.86 (m, 4H)	
T2	5-MeO-DMT fb				2.81 – 2.73 (m, 2H) 2.53 – 2.44 (m, 2H)	
T3	2-Me-DMT · F		6.52 (s, 1H)		2.91 – 2.83 (m, 2H) 2.73 – 2.65 (m, 2H)	
T4	5-MeO-TMT · F		6.51 (s, 1H)		2.87 – 2.79 (m, 2H) 2.71 – 2.64 (m, 2H)	
T5	MET · F		6.50 (s, 1H)		2.95 – 2.89 (m, 2H) 2.86 – 2.79 (m, 2H)	
T6	4-HO-MET · F		6.48 (s, 1H)		3.02 – 2.95 (m, 2H) 2.91 – 2.86 (m, 2H)	
T7	5-MeO-MET · F		6.50 (s, 1H)		2.95 – 2.82 (m, 4H)	
T8	MIPT fb				2.82 – 2.74 (m, 2H) 2.64 – 2.52 (m, 2H)	
T9	4-HO-MIPT · F		6.48 (s, 1H)		2.96 (t, *J* = 6.8 Hz, 2H) 2.84 (t, *J* = 6.8 Hz, 2H)	
T10	4-MeO-MIPT · F		6.51 (s, 2H)		3.13 – 3.05 (m, 2H) 3.08 – 2.97 (m, 2H)	
T11	5-MeO-MIPT · H^+	10.69 (s, 1H)			3.30 – 3.07 (m, 4H)	
T12	4-HO-DET · H^+	10.26 (s, 1H)			3.32 – 3.24 (m, 2H) 3.21 – 3.11 (m, 2H)[1]	
T13	4-AcO-DET · F		6.52 (s, 2H)		3.02 – 2.93 (m, 4H)	
T14	5-MeO-EIPT · H^+	10.56 (s, 1H)			3.27 – 3.15 (m, 4H)[2]	
T15	DPT · H^+	10.45 (s, 1H)			3.31 – 3.23 (m, 2H) 3.20 – 3.12 (m, 2H)	
T16	4-HO-DPT · F		6.49 (s, 1H)		2.97 – 2.91 (m, 2H) 2.87 (dd, *J* = 8.4, 5.6 Hz, 2H)	
T17	5-MeO-DPT · H^+	10.77 (s, 1H)			3.28 – 3.20 (m, 2H) 3.18 – 3.10 (m, 2H)	
T18	DIPT · H^+	9.97 (s, 1H)			3.30 – 3.17 (m, 4H)	
T19	4-HO-DIPT · H^+	9.70 (s, 2H)[2]			3.29 – 3.16 (m, 4H)	
T20	4-AcO-DIPT · H^+	10.04 (s, 1H)			3.33 – 3.26 (m, 2H) 3.18 (dd, *J* = 11.1, 5.9 Hz, 2H)	
T21	5-MeO-DIPT · H^+	9.97 (s, 1H)			3.26 – 3.13 (m, 4H)	
T22	DALT · H^+	11.62 (s, 1H))			3.20 (s, 4H)	
T23	4-AcO-DALT · F		6.61 (s, 2H)		2.86 – 2.77 (m, 2H) 2.76 – 2.68 (m, 2H)	
T24a	5-MeO-DALT fb				2.85 – 2.74 (m, 2H) 2.71 – 2.60 (m, 2H)	
T24b	5-MeO-DALT fb				2.82 – 2.74 (m, 2H) 2.71 – 2.64 (m, 2H)	

[1] Overlaps with *N,N*-dimethylene multiplet.
[2] Overlaps with indol-4-ol peak.

HCl, hydrochloride; fb, free base; F, fumarate; H^+, aminium
br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 4: Multiplets for ethanamine/ethaminium and fumarate moieties

		NH^+ | NH_2^+ | NH_3^+	Fumarate	α - CH	α - CH_2 | β - CH_2	NH_2
T25	4-HO-MPT · F		6.52 (s, 2H)		3.06 (s, 4H)	
T26	α-MT fb			3.07 (h, *J* = 6.5 Hz, 1H)	2.63 (ddd, *J* = 6.8, 3.8, 0.8 Hz, 2H)	1.38 (br s, 2H)
T27	5-MeO-α-MT · H^+	8.17 (s, 3H)		3.44 – 3.34 (m, 1H)	3.13 – 3.05 (m, 1H) 2.84 – 2.75 (m, 1H)	
T28	4-Me-α-ET fb			2.75 (tt, *J* = 7.6, 4.9 Hz, 1H)	2.93 (dd, *J* = 14.1, 5.0 Hz, 1H) 2.59 (dd, *J* = 14.2, 8.0 Hz, 1H)	1.30 (br s, 2H)
T29	5-MeO-T · HCl	8.23 (s, 3H)			3.06 – 2.98 (m, 4H)	
T30	NMT · HCl	8.76 (br s, 2H)			3.10 (s, 4H)	
T31	4-AcO-MIPT · F		6.54 (s, 2H)		3.07 – 2.95 (m, 4H)	
T32	4-AcO-MET · F		6.53 (s, 2H)		3.04 – 2.92 (m, 4H)	
T33	5-MeO-MALT · H^+	8.02 (br s, 1H)			3.25 – 3.18 (m, 2H) 3.11 – 3.02 (m, 2H)	
T34	5-MeO-NIPT · H^+	9.14 (br s, 2H)			3.08 (s, 4H)	
T35	MPT fb				2.85 – 2.78 (m, 2H) 2.63 – 2.56 (m, 2H)	
T36	4-HO-MCPT · F		6.58 (s, 1H)		3.03 – 2.95 (m, 2H) 2.95 – 2.88 (m, 2H)	
T37	EPT · F		6.54 (s, 2H)		3.13 – 3.04 (m, 2H) 3.04 – 2.96 (m, 2H)	
T38	4-HO-EPT · F		6.53 (s, 3H)		3.19 – 3.09 (m, 2H) 3.11 – 3.04 (m, 2H)	
T39	4-HO-MALT · F		6.55 (s, 2H)		3.07 – 3.00 (m, 2H) 2.96 – 2.89 (m, 2H)	
T40	4-AcO-DPT · F		6.56 (s, 2H)		3.32 – 3.27 (m, 2H) 3.24 – 3.19 (m, 2H)	
T41	MALT fb				3.32 – 3.27 (m, 2H) 3.24 – 3.19 (m, 2H)	
T42	4-AcO-EPT · F		6.54 (s, 2H)		3.00 – 2.92 (m, 4H)	
T43	4-AcO-MPT · F		6.54 (s, 2H)		2.94 (s, 4H)	
BF1	5-MeO-DIBF · H^+	10.39 (s, 1H)			3.32 – 3.27 (m, 1H) 3.24 – 3.19 (m, 2H)	

HCl, hydrochloride; fb, free base; F, fumarate; H^+, aminium

br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 5: Multiplets for N- and α-substituents, in descending order by shift

N-methyl		N - C*H*$_3$ ↓
T33	5-MeO-MALT · H$^+$	2.76 (s, 3H)
T11	5-MeO-MIPT · H$^+$	2.70 (s, 3H)
T10	4-MeO-MIPT · F	2.59 (s, 3H)
T25	4-HO-MPT · F	2.59 (s, 3H)
T31	4-AcO-MIPT · F	2.58 (s, 3H)
T32	4-AcO-MET · F	2.57 (s, 3H)
T1a	4-AcO-DMT · F	2.56 (s, 6H)
T1b	4-AcO-DMT · F	2.54 (s, 6H)
T30	NMT · HCl	2.54 (s, 3H)
T3	2-Me-DMT · F	2.47 (s, 6H)
T4	5-MeO-TMT · F	2.47 (s, 6H)
T7	5-MeO-MET · F	2.47 (s, 3H)
T39	4-HO-MALT · F	2.47 (s, 3H)
T6	4-HO-MET · F	2.45 (s, 3H)
T5	MET · F	2.43 (s, 3H)
T9	4-HO-MIPT · F	2.40 (s, 3H)
T43	4-AcO-MPT · F	2.37 (s, 3H)
T36	4-HO-MCPT · F	2.24 (s, 3H)
T35	MPT fb	2.24 (s, 3H)
T41	MALT fb	2.24 (s, 3H)
T8	MIPT fb	2.22 (s, 3H)
T2	5-MeO-DMT fb	2.21 (s, 6H)

N-ethyl		N - C*H*$_2$ - CH$_3$ ↓	N - CH$_2$ - C*H*$_3$
T14	5-MeO-EIPT · H$^+$	3.27 – 3.15 (m, 2H)	1.38 – 1.24 (m, 3H)
T12	4-HO-DET · H$^+$	3.21 – 3.11 (m, 4H)	1.27 (t, *J* = 7.2 Hz, 6H)
T37	EPT · F	3.04 – 2.96 (m, 2H)	1.16 (t, *J* = 7.2 Hz, 3H)
T38	4-HO-EPT · F	3.02 (q, *J* = 7.2 Hz, 2H)	1.18 (t, *J* = 7.2 Hz, 3H)
T13	4-AcO-DET · F	2.90 (q, *J* = 7.2 Hz, 4H)	1.12 (t, *J* = 7.2 Hz, 6H)
T32	4-AcO-MET · F	2.89 (q, *J* = 7.2 Hz)	1.15 (t, *J* = 7.2 Hz, 3H)
T42	4-AcO-EPT · F	2.88 (q, *J* = 7.1 Hz, 2H)	1.11 (t, *J* = 7.2 Hz, 3H)
T7	5-MeO-MET · F	2.75 (q, *J* = 7.2 Hz, 2H)	1.11 (t, *J* = 7.2 Hz, 3H)
T6	4-HO-MET · F	2.73 (q, *J* = 7.2 Hz, 2H)	1.08 (t, *J* = 7.2 Hz, 3H)
T5	MET · F	2.70 (q, *J* = 7.2 Hz, 2H)	1.08 (t, *J* = 7.2 Hz, 3H)

N-cyclopropyl		N - C*H* - (- CH$_2$ - CH$_2$ -)	N - CH - (- C*H*$_2$ - C*H*$_2$ -)
T36	4-HO-MCPT · F	2.03 – 1.95 (m, 1H)	0.57 – 0.39 (m, 4H)

α-methyl		α - *H* ↓	α - C*H3*
T27	5-MeO-α-MT · H$^+$	3.44 – 3.34 (m, 1H)	1.18 (d, *J* = 6.5 Hz, 3H)
T26	α-MT fb	3.07 (h, *J* = 6.5 Hz, 1H)	0.98 (d, *J* = 6.2 Hz, 3H)

N-propyl		N - C*H*$_2$ - CH$_2$ - CH$_3$ ↓	N - CH$_2$ - C*H*$_2$ - CH$_3$	N - CH$_2$ - CH$_2$ - C*H*$_3$
T17	5-MeO-DPT · H$^+$	3.12 – 3.01 (m, 4H)	1.73 (h, *J* = 7.8 Hz, 4H)	0.92 (t, *J* = 7.4 Hz, 6H)
T15	DPT · H$^+$	3.11 – 3.04 (m, 4H)	1.72 (h, *J* = 7.8 Hz, 4H)	0.92 (t, *J* = 7.4 Hz, 6H)
T37	EPT · F	2.94 – 2.83 (m, 2H)	1.68 – 1.54 (m, 2H)	0.90 (t, *J* = 7.4 Hz, 3H)
T38	4-HO-EPT · F	2.93 – 2.85 (m, 2H)	1.69 – 1.57 (m, 2H)	0.89 (t, *J* = 7.4 Hz, 3H)
T25	4-HO-MPT · F	2.82 – 2.75 (m, 2H)	1.66 – 1.54 (m, 2H)	0.87 (t, *J* = 7.4 Hz, 3H)
T42	4-AcO-EPT · F	2.78 – 2.71 (m, 2H)	1.62 – 1.49 (m, 2H)	0.87 (t, J = 7.4 Hz, 3H)
T43	4-AcO-MPT · F	2.74 – 2.68 (m, 2H)	1.63 – 1.52 (m, 2H)	0.88 (t, *J* = 7.4 Hz, 3H)
T40	4-AcO-DPT · F	2.74 – 2.68 (m, 4H)	1.59 – 1.49 (m, 4H)	0.87 (t, *J* = 7.3 Hz, 6H)
T16	4-HO-DPT · F	2.66 – 2.58 (m, 4H)	1.58 – 1.45 (m, 4H)	0.85 (t, *J* = 7.4 Hz, 6H)
T35	MPT fb	2.37 – 2.30 (m, 2H)	1.51 – 1.37 (m, 2H)	0.86 (t, *J* = 7.4 Hz, 3H)

α-ethyl		α - *H*	α - C*H*$_2$ - CH$_3$	α - C*H*$_3$
T28	4-Me-α-ET fb	2.75 (tt, *J* = 7.6, 4.9 Hz, 1H)	1.53 – 1.41 (m, 1H) 1.26 (dq, J = 13.3, 7.4 Hz, 1H)	0.92 (t, *J* = 7.4 Hz, 3H)

HCl, hydrochloride; fb, free base; F, fumarate; H$^+$, aminium

br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 5: Multiplets for N- and α-substituents, in descending order by shift

N-propan-2-yl · isopropyl		N - C*H* - $(CH_3)_2$ ↓	N - C*H* - $(CH_3)_2$	N - C*H* - $(CH_3)_2$
T18	DIPT · H^+	3.77 – 3.65 (m, 2H)	1.41 (d, *J* = 6.6 Hz, 6H)	1.36 (d, *J* = 6.5 Hz, 6H)
BF1	5-MeO-DiBF · H^+	3.72 (pd, *J* = 6.6, 3.7 Hz, 2H)	1.40 (d, *J* = 6.6 Hz, 6H)	1.35 (d, *J* = 6.6 Hz, 6H)
T21	5-MeO-DIPT · H^+	3.70 (dp, *J* = 13.2, 6.5 Hz, 2H)	1.40 (d, *J* = 6.5 Hz, 6H)	1.35 (d, *J* = 6.5 Hz, 6H)
T14	5-MeO-EIPT · H^+	3.69 (pd, *J* = 6.6, 2.6 Hz, 1H)	1.38 – 1.24 (m, 6H)	
T20	4-AcO-DIPT · H^+	3.66 (pd, *J* = 6.7, 4.0 Hz, 2H)	1.38 (d, *J* = 6.5 Hz, 6H)	1.33 (d, *J* = 6.5 Hz, 6H)
T19	4-HO-DIPT · H^+	3.69 – 3.59 (m, 2H)	1.40 (d, *J* = 6.5 Hz, 6H)	1.34 (d, *J* = 6.5 Hz, 6H)
T11	5-MeO-MIPT · H^+	3.60 (hept, *J* = 6.7 Hz, 1H)	1.30 (d, *J* = 7.0 Hz, 3H)	1.24 (d, *J* = 7.0 Hz, 3H)
T10	4-MeO-MIPT · F	3.38 (hept, *J* = 6.6 Hz, 1H)	1.18 (d, *J* = 6.6 Hz, 6H)	
T31	4-AcO-MIPT · F	3.37 (hept, *J* = 6.6 Hz, 1H)	1.16 (d, *J* = 6.6 Hz, 6H)	
T34	5-MeO-NIPT · H^+	3.31 (hept, *J* = 6.6 Hz, 1H)	1.27 (d, *J* = 6.5 Hz, 6H)	
T9	4-HO-MIPT · F	3.07 (hept, *J* = 6.6 Hz, 1H)	1.03 (d, *J* = 6.6 Hz, 6H)	
T8	MIPT fb	2.84 (hept, *J* = 6.6 Hz, 1H)	0.95 (d, *J* = 6.5 Hz, 6H)	

N-prop-2-en-1-yl · allyl		N - C*H*$_2$ - CH = CH_2 ↓	N - CH_2 - C*H* = CH_2	N - CH_2 - CH = C*H*$_2$
T22	DALT · H^+	3.81 (dd, *J* = 7.2, 4.3 Hz, 4H)	6.10 (ddt, *J* = 17.3, 10.3, 7.1 Hz, 2H)	5.59 (dq, *J* = 17.2, 1.4 Hz, 2H) 5.52 (dd, *J* = 10.3, 1.6 Hz, 2H)
T33	5-MeO-MALT · H^+	3.75 (d, *J* = 7.0 Hz, 2H)	5.99 (ddt, *J* = 17.2, 10.2, 7.0 Hz, 1H)	5.50 (dd, *J* = 8.7, 2.4 Hz, 2H)
T39	4-HO-MALT · F	3.37 (dt, *J* = 6.9, 1.2 Hz, 2H)	5.89 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H)	5.33 (dq, *J* = 17.2, 1.5 Hz, 1H) 5.27 (ddt, *J* = 10.1, 1.9, 1.0 Hz, 1H)
T23	4-AcO-DALT · F	3.21 (dt, *J* = 6.5, 1.3 Hz, 4H)	5.87 (ddt, *J* = 17.2, 10.2, 6.4 Hz, 2H)	5.23 (ddt, *J* = 17.2, 2.1, 1.4 Hz, 2H) 5.17 (ddt, *J* = 10.2, 2.2, 1.1 Hz, 2H)
T24a	5-MeO-DALT fb	3.16 (dt, *J* = 6.4, 1.4 Hz, 4H)	5.87 (ddt, *J* = 17.3, 10.2, 6.3 Hz, 2H)	5.28 – 5.16 (m, 2H) 5.14 (ddt, *J* = 10.1, 2.3, 1.2 Hz, 2H)
T24b	5-MeO-DALT fb	3.16 (dt, *J* = 6.3, 1.4 Hz, 4H)	5.87 (ddt, *J* = 17.3, 10.2, 6.3 Hz, 2H)	5.23 (ddt, *J* = 17.2, 2.2, 1.5 Hz, 2H) 5.14 (ddt, *J* = 10.2, 2.3, 1.2 Hz, 2H)
T41	MALT fb	3.04 (dt, *J* = 6.3, 1.4 Hz, 2H)	5.85 (ddt, *J* = 17.3, 10.2, 6.4 Hz, 1H)	5.19 (ddt, *J* = 17.2, 2.2, 1.5 Hz, 1H) 5.12 (ddt, *J* = 10.2, 2.3, 1.2 Hz, 1H)

HCl, hydrochloride; fb, free base; F, fumarate; H^+, aminium
br, broad; d, doublet; h, hextet; hept, heptet; obs, partially obscured; m, multiplet; q, quartet; s, singlet; t, triplet; vb, very broad; *J*, coupling constant

Table 6: Literature reporting ^{1}H NMR spectra for analytes, by solvent

	Substance	$CDCl_3$	CD_2Cl_2	CD_3OD	D_2O	DMSO-d_6
T0	Tryptamine	[20]				[21] [22]
T1	4-AcO-DMT	[23]		[24]		
T2	5-MeO-DMT	[25]		[26] [27]	[28] [29]	[30]
T2	5-MeO-DMT-d_4	[31]				
T4	5-MeO-TMT	[32]				
T5	MET					[30]
T5	MET-d_4	[31]				
T6	4-HO-MET					[33]
T7	5-MeO-MET					[30]
T7	5-MeO-MET-d_4	[31]				
T8	MIPT					[30]
T8	MIPT-d_4	[31]				
T9	4-HO-MIPT	[29]	[34]			[35]
T11	5-MeO-MIPT	[25] [36]			[28] [37]	[30]
T12	4-HO-DET	[29] [38]				
T13	4-AcO-DET					[39]
T14	5-MeO-EIPT			[40]		[30]
T14	5-MeO-EIPT-d_4	[31]				
T15	DPT	[29] [41]		[26]	[28] [42]	[30]
T15	DPT-d_4	[31]				
T16	4-HO-DPT	[38]				
T17	5-MeO-DPT	[29]		[27]	[43]	[30] [31]
T17	5-MeO-DPT-d_4	[31]				
T18	DIPT	[29]			[44]	[30]
T18	DIPT-d_4	[31]				
T19	4-HO-DIPT		[45]			[38]
T20	4-AcO-DIPT				[29]	[46]
T21	5-MeO-DIPT	[25] [29] [47]		[26] [27] [48]	[28]	[30] [49]
T21	5-MeO-DIPT-d_4	[31]				
T22	DALT	[50]		[51]		
T22	DALT-d_4	[28]				
T26	α-MT	[52] [53] [54]		[26] [27] [55]		[56]
T27	5-MeO-α-MT		[53]	[27] [57]	[28]	
T29	5-MeO-T	[47]				[58]
T30	NMT		[20]	[27]		[56] [59] [60] [61]
T32	4-AcO-MET					[62]
T34	5-MeO-NIPT					[30]
T35	MPT					[30]
T35	MPT-d_4	[31]				
T37	EPT					[30]
T37	EPT-d_4	[31]				
BF1	5-MeO-DIBF					[63]