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(19) **United States**(12) **Patent Application Publication**
CHADEAYNE(10) **Pub. No.: US 2025/0263371 A1**(43) **Pub. Date: Aug. 21, 2025**(54) **CRYSTALLINE**
4-(ETHYLSULFONYLOXY)-N,N-DI-N-
PROPYLTRYPTAMMONIUM CHLORIDE(52) **U.S. Cl.**
CPC **C07D 209/16** (2013.01); **A61K 45/06**
(2013.01)(71) Applicant: **CAAMTECH, INC.**, Issaquah, WA
(US)(57) **ABSTRACT**(72) Inventor: **Andrew R. CHADEAYNE**, Issaquah,
WA (US)(21) Appl. No.: **18/994,479**(22) PCT Filed: **Jul. 17, 2023**(86) PCT No.: **PCT/US2023/070309**

§ 371 (c)(1),

(2) Date: **Jan. 14, 2025****Related U.S. Application Data**(60) Provisional application No. 63/368,513, filed on Jul.
15, 2022, provisional application No. 63/368,815,
filed on Jul. 19, 2022, provisional application No.
63/368,816, filed on Jul. 19, 2022, provisional appli-
cation No. 63/368,818, filed on Jul. 19, 2022, provi-
sional application No. 63/369,294, filed on Jul. 25,
2022.**Publication Classification**(51) **Int. Cl.**
C07D 209/16 (2006.01)
A61K 45/06 (2006.01)

This disclosure relates to (2-{4-[ethanesulfonyloxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride or 4-(ethylsulfonyloxy)-DPT chloride), crystalline 4-(ethylsulfonyloxy)-DPT chloride, [2-(1H-indol-3-yl)ethyl]tripropylazanium iodide (N,N,N-tri-n-propyltryptammonium iodide or TPT iodide), crystalline TPT iodide, [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-A/,A/-di-n-isopropyltryptammonium iodide or 5-CI-DiPT iodide), crystalline 5-CI-DiPT iodide, 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate or 5-CI-T hydrogenoxalate), crystalline 5-CI-T hydrogenoxalate, bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate or 5-CI-T oxalate hydrate), crystalline 5-CI-T oxalate hydrate, and specific crystalline forms thereof, including crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form of 1 of 5-CI-DiPT iodide, crystalline form 1 of 5-CI-T hydrogenoxalate, and crystalline form 1 of 5-CI-T oxalate hydrate, to compositions containing the same, and to methods of treatment using the.

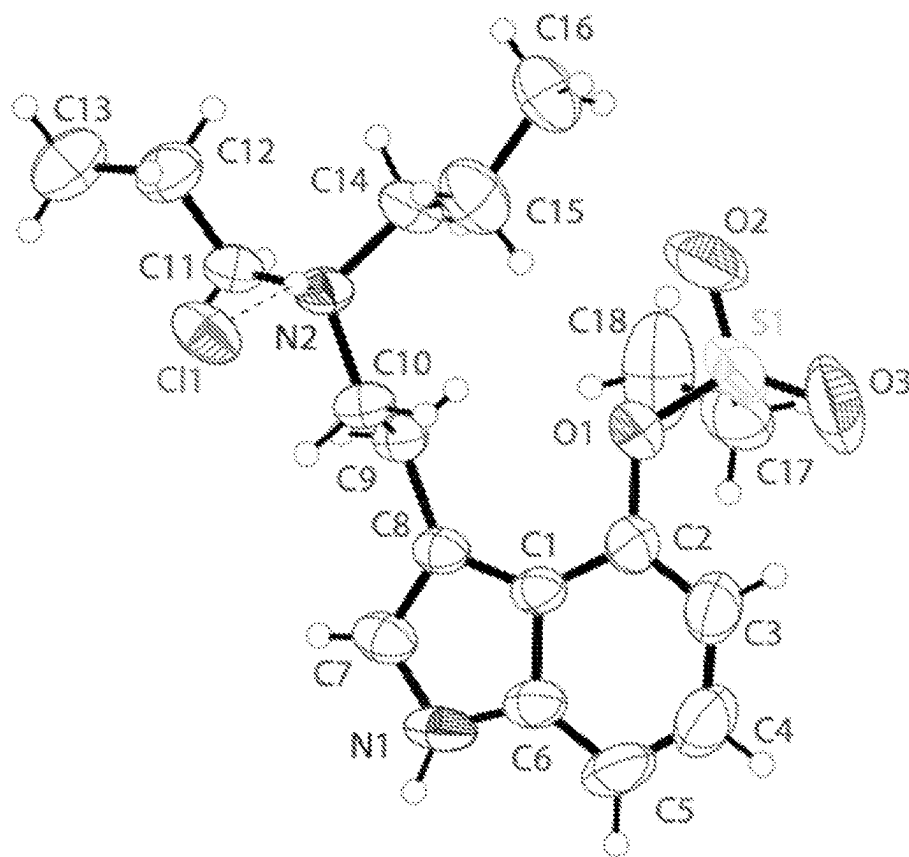


FIG. 1

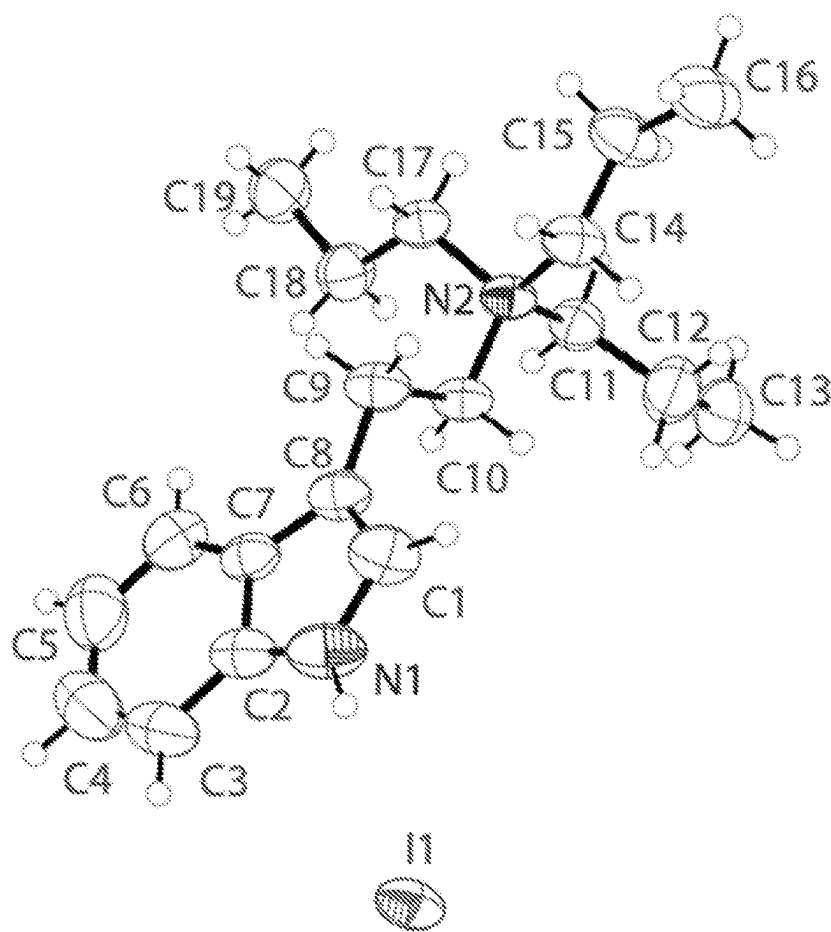


FIG. 2

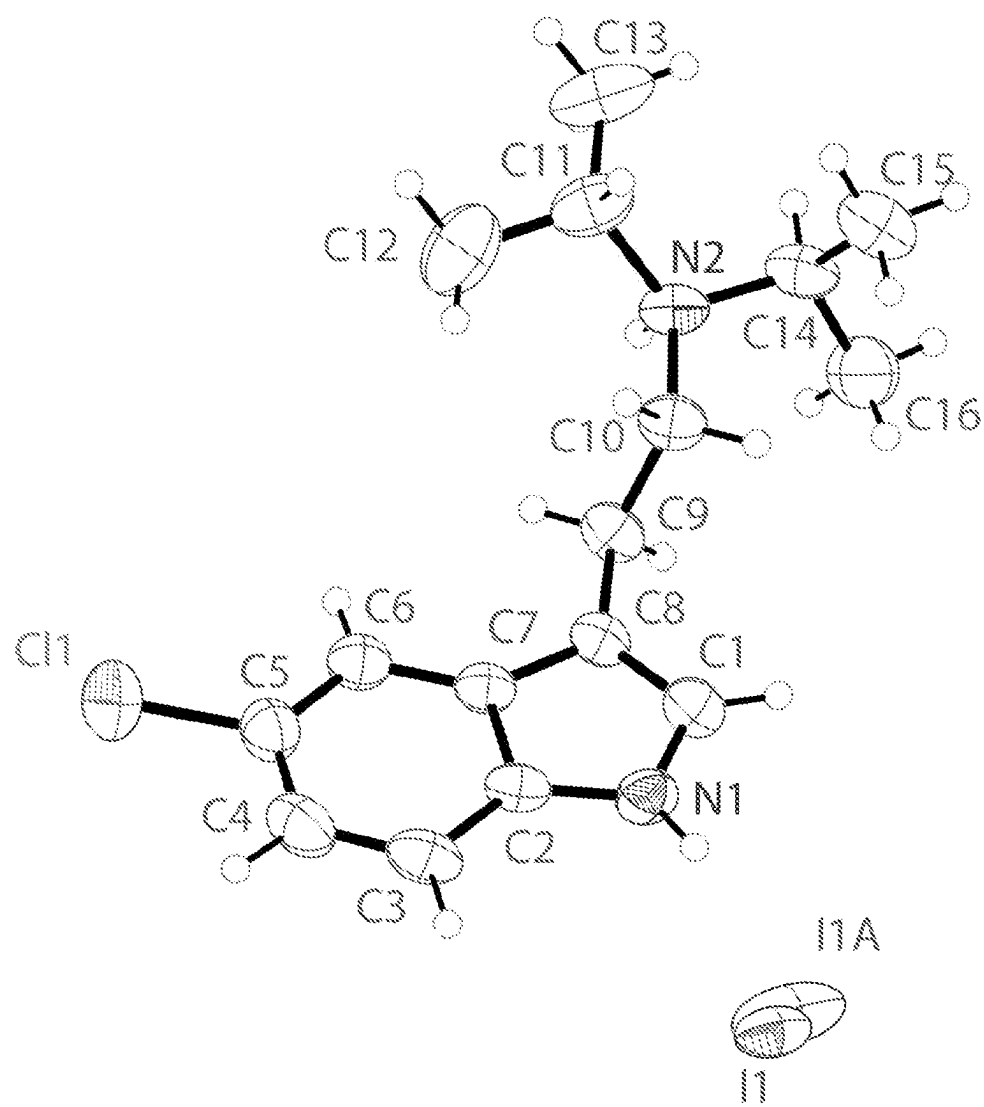


FIG. 3

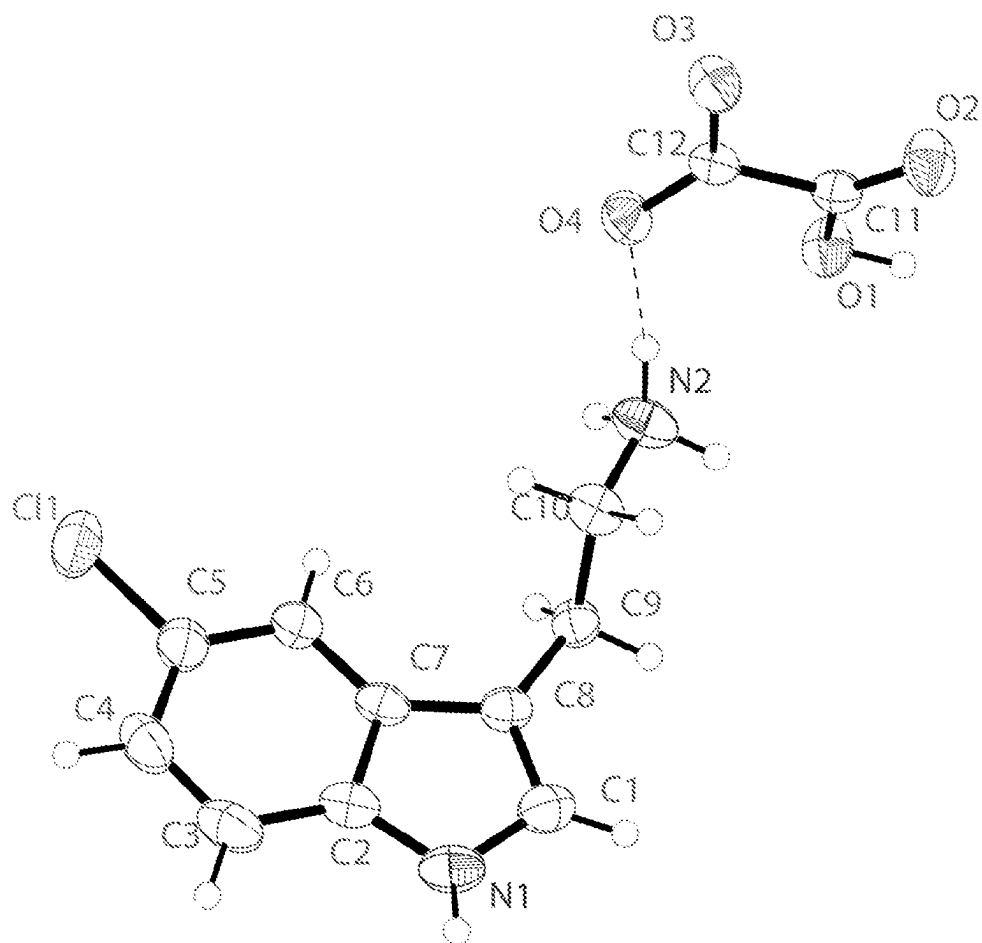


FIG. 4

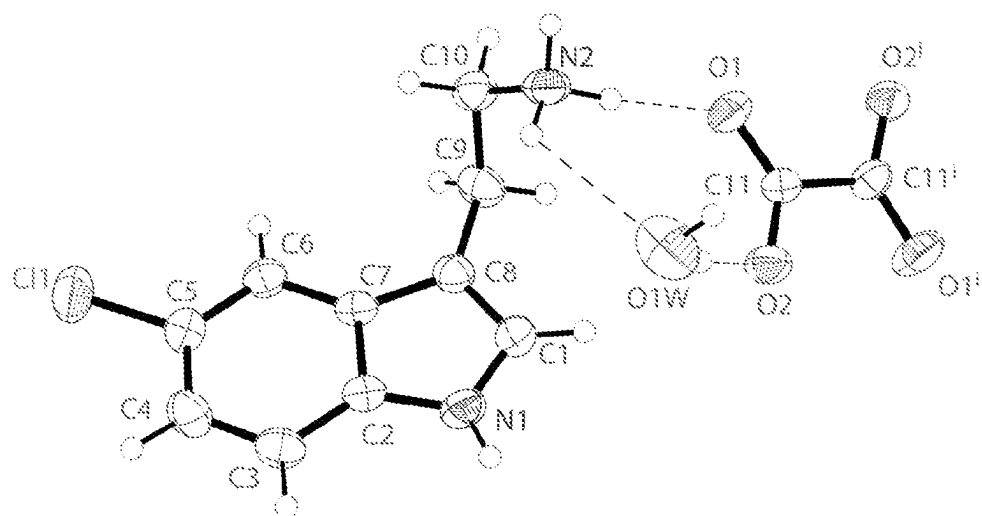


FIG. 5

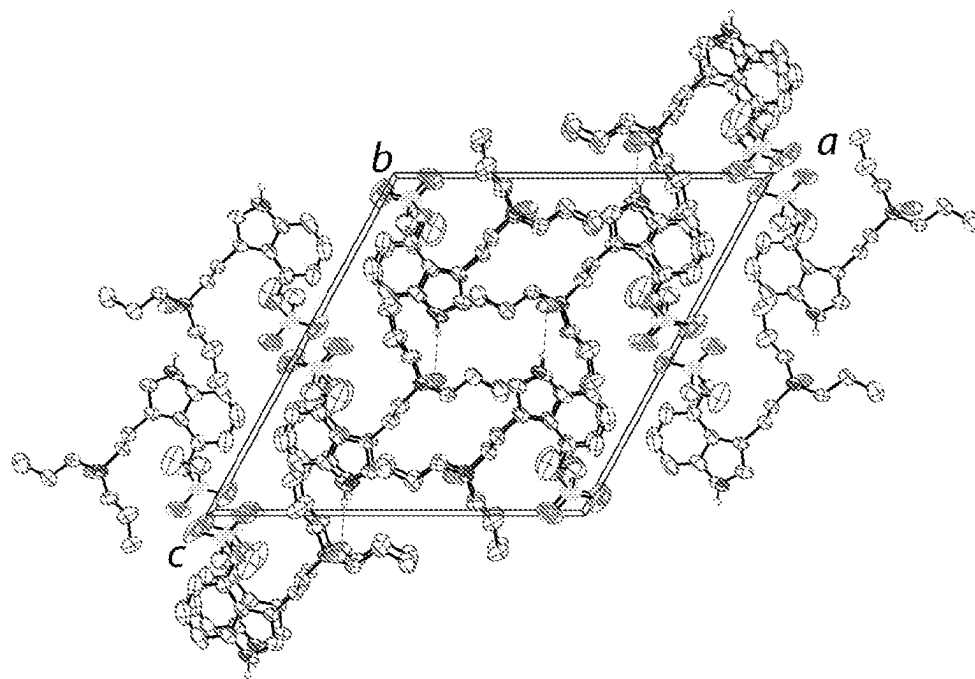


FIG. 6

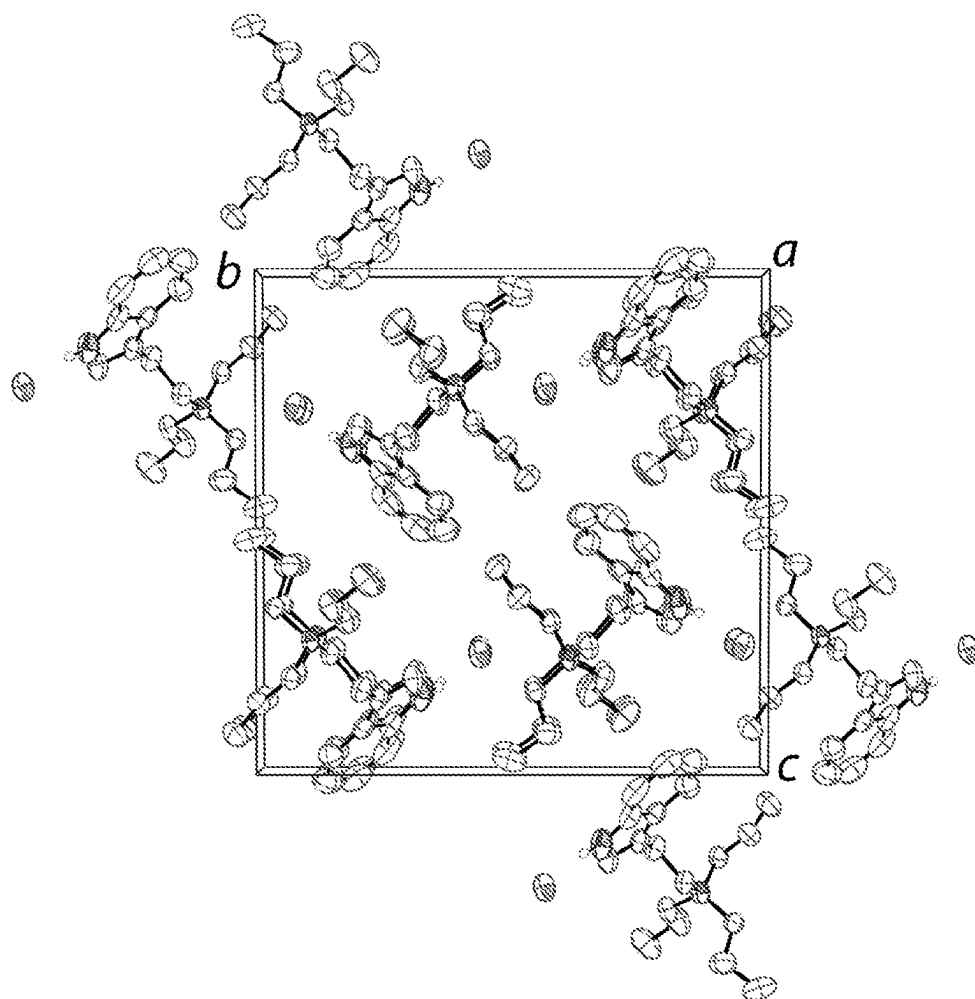


FIG. 7

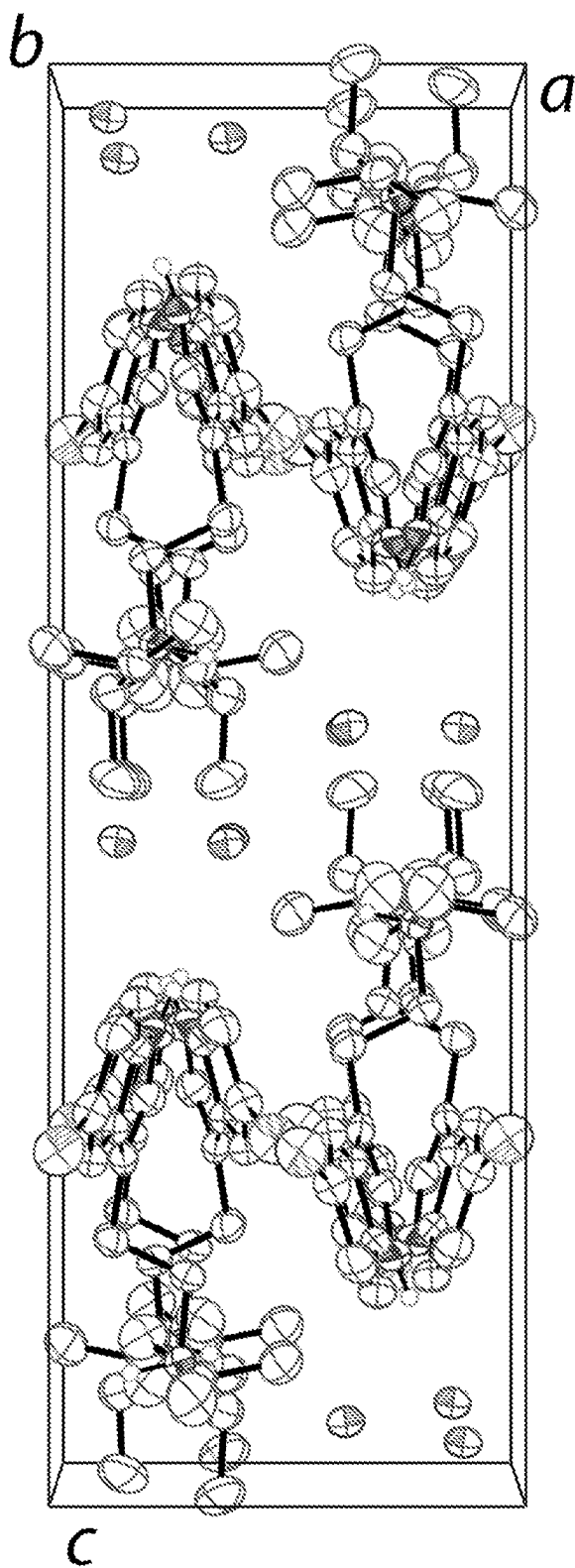


FIG. 8

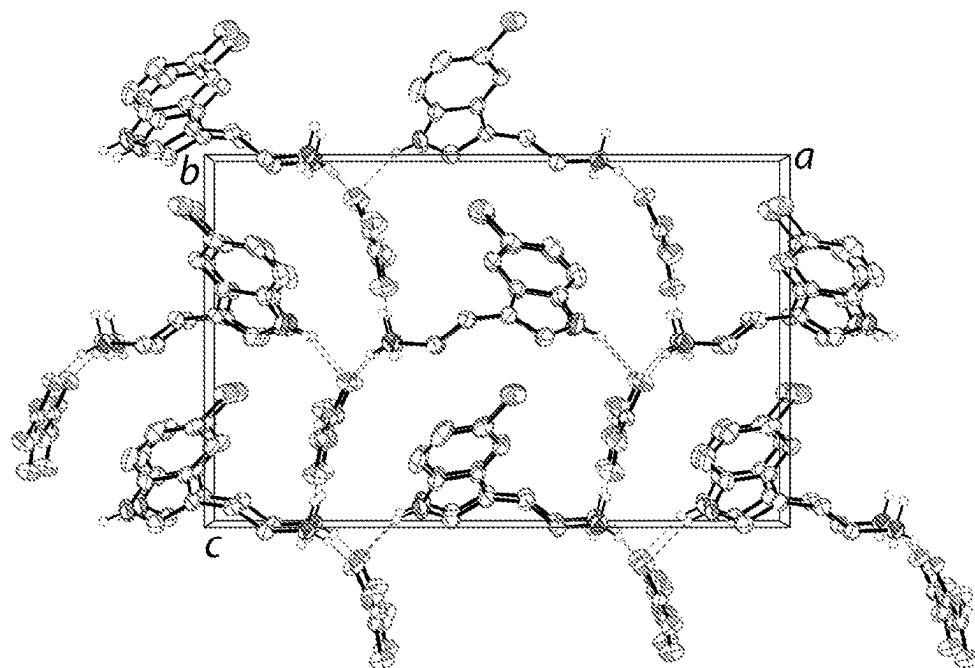


FIG. 9

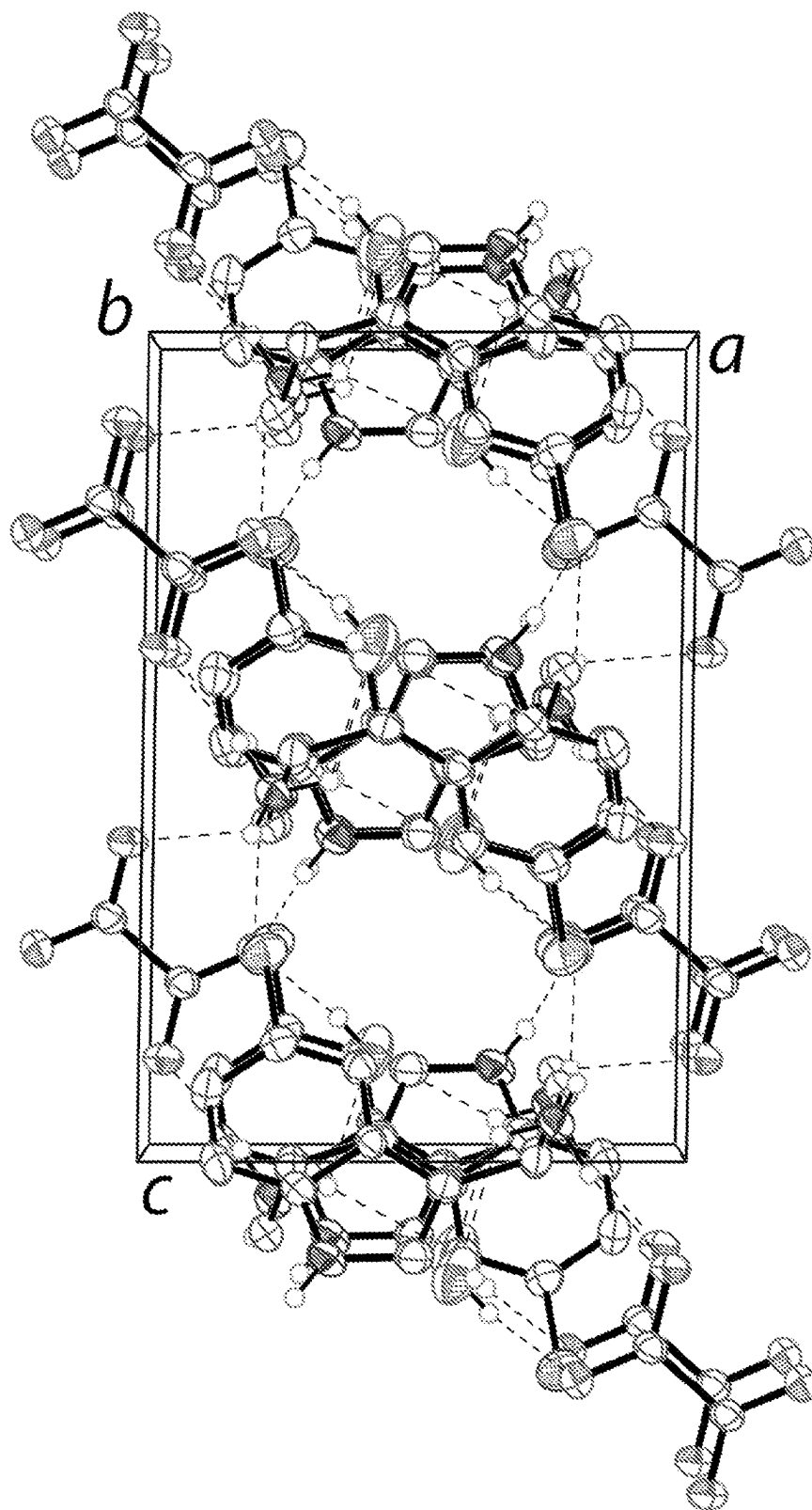


FIG. 10

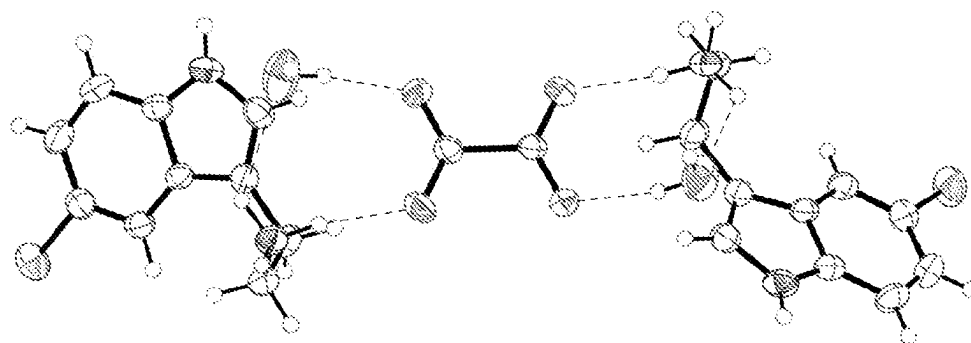


FIG. 11

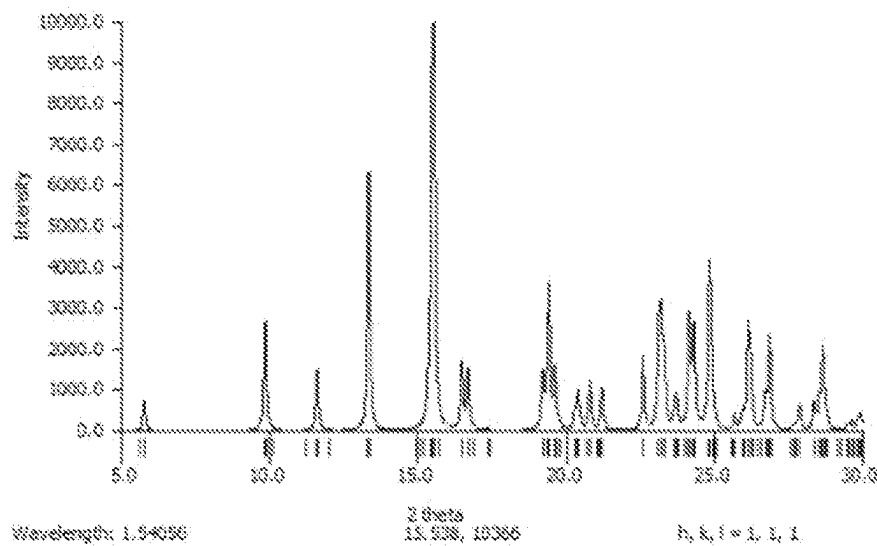


FIG. 12

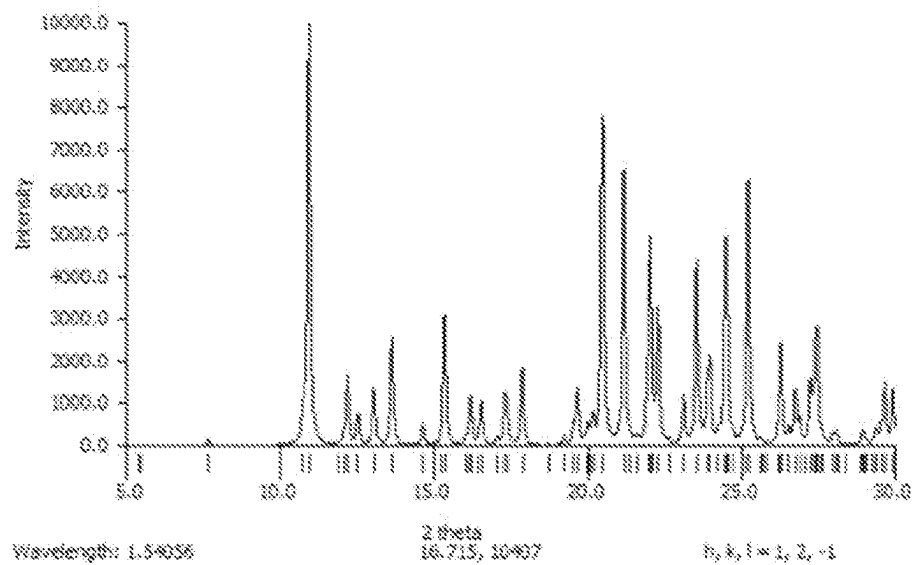


FIG. 13

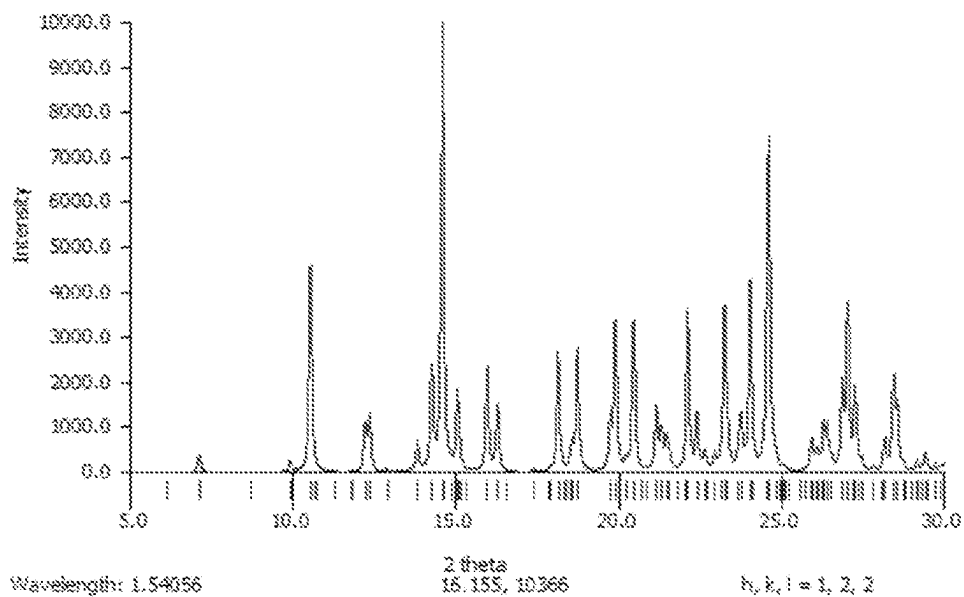


FIG. 14

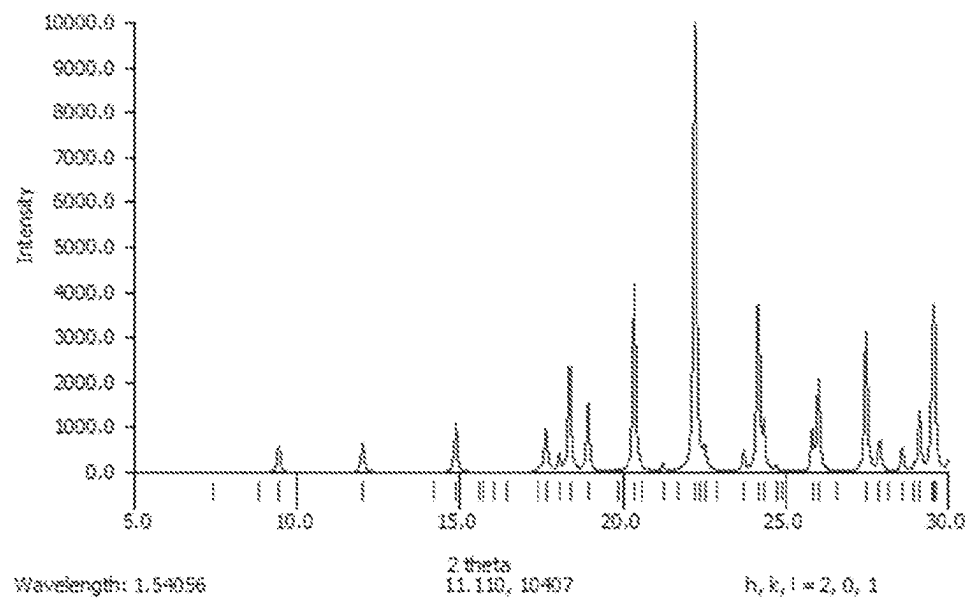


FIG. 15

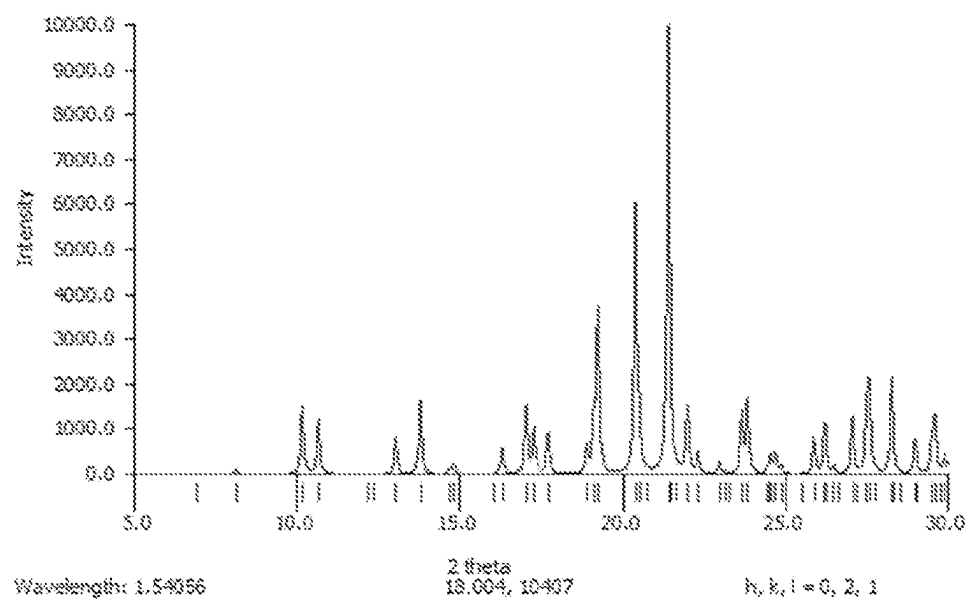


FIG. 16

**CRYSTALLINE
4-(ETHYLSULFONYLOXY)-N,N-DI-N-
PROPYLTRYPTAMMONIUM CHLORIDE**

**CROSS-REFERENCE TO RELATED
APPLICATIONS**

[0001] This application claims priority to U.S. Provisional Application No. 63/368,513, filed on Jul. 15, 2022; U.S. Provisional Application No. 63/368,815, filed on Jul. 19, 2022; U.S. Provisional Application No. 63/368,816, filed on Jul. 19, 2022; U.S. Provisional Application No. 63/368,818, filed on Jul. 19, 2022; and U.S. Provisional Application No. 63/369,294, filed on Jul. 25, 2022; the disclosures of which are all incorporated herein by reference.

TECHNICAL FIELD

[0002] This disclosure relates to (2-{4-[(ethanesulfonyl)oxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride or 4-(ethylsulfonyloxy)-DPT chloride), crystalline 4-(ethylsulfonyloxy)-DPT chloride, and specific crystalline forms thereof, including crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride; to pharmaceutical compositions containing 4-(ethylsulfonyloxy)-DPT chloride or crystalline 4-(ethylsulfonyloxy)-DPT chloride, including crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride; and to methods of treatment/therapeutic uses of 4-(ethylsulfonyloxy)-DPT chloride or crystalline 4-(ethylsulfonyloxy)-DPT chloride, including crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride.

[0003] The disclosure further relates to [2-(1H-indol-3-yl)ethyl]tripropylazanium iodide (N,N,N-tri-n-propyltryptammonium iodide or TPT iodide), crystalline TPT iodide, and specific crystalline forms thereof, including crystalline form 1 of TPT iodide; to pharmaceutical compositions containing TPT iodide or crystalline TPT iodide, including crystalline form 1 of TPT iodide; and to methods of treatment/therapeutic uses of TPT iodide or crystalline TPT iodide, including crystalline form 1 of TPT iodide.

[0004] The disclosure further relates to [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-N,N-di-n-isopropyltryptammonium iodide or 5-Cl-DiPT iodide), crystalline 5-Cl-DiPT iodide, and specific crystalline forms thereof, including crystalline form 1 of 5-Cl-DiPT iodide; to pharmaceutical compositions containing 5-Cl-DiPT iodide or crystalline 5-Cl-DiPT iodide, including crystalline form 1 of 5-Cl-DiPT iodide; and to methods of treatment/therapeutic uses of 5-Cl-DiPT iodide or crystalline 5-Cl-DiPT iodide, including crystalline form 1 of 5-Cl-DiPT iodide.

[0005] The disclosure further relates to 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate or 5-Cl-T hydrogenoxalate), crystalline 5-Cl-T hydrogenoxalate, and specific crystalline forms thereof, including crystalline form 1 of 5-Cl-T hydrogenoxalate; to pharmaceutical compositions containing 5-Cl-T hydrogenoxalate or crystalline 5-Cl-T hydrogenoxalate, including crystalline form 1 of 5-Cl-T hydrogenoxalate; and to methods of treatment/therapeutic uses of 5-Cl-T hydrogenoxalate or crystalline 5-Cl-T hydrogenoxalate, including crystalline form 1 of 5-Cl-T hydrogenoxalate.

[0006] The disclosure further relates to bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate or 5-Cl-T oxalate hydrate), crystalline 5-Cl-T oxalate hydrate, and specific crystalline forms thereof, including crystalline form 1 of 5-Cl-T oxalate hydrate; to pharmaceutical compositions containing 5-Cl-T oxalate hydrate or crystalline 5-Cl-T oxalate hydrate, including crystalline form 1 of 5-Cl-T oxalate hydrate; and to methods of treatment/therapeutic uses of 5-Cl-T oxalate hydrate or crystalline 5-Cl-T oxalate hydrate, including crystalline form 1 of 5-Cl-T oxalate hydrate.

BACKGROUND OF THE INVENTION

[0007] Obtaining specific salts or crystalline forms of an active pharmaceutical ingredient (API) is extremely useful in drug development. It permits better characterization of the drug candidate's chemical and physical properties. Crystalline forms often have better chemical and physical properties than the API in its amorphous state. Such crystalline forms may possess more favorable pharmaceutical and pharmacological properties or be easier to process. Additionally, preparing a crystalline API and solving its crystal structure provides the gold standard for chemical characterization and determining the molecular formula (and molecular weight) of the API. Accordingly, preparing a crystalline form with an accompanying crystal structure thereof prevents potential ambiguities and/or inaccuracies in the API's molecular weight. This is important because the API's molecular weight is used to calculate the concentration of compositions comprising that API. Thus, inaccuracies in molecular weight may lead to errors in the calculations pertaining to dosing, potency, toxicity, etc. in all downstream in vitro and in vivo assays that correlated the concentration of the API with a measured property. Accordingly, there remains a need to obtain and characterize crystalline forms of APIs, such as tryptamines and other psychedelic drug compounds.

SUMMARY OF THE INVENTION

[0008] This disclosure relates to (2-{4-[(ethanesulfonyl)oxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride or 4-(ethylsulfonyloxy)-DPT chloride), crystalline 4-(ethylsulfonyloxy)-DPT chloride, and specific crystalline forms thereof. In one embodiment, this disclosure pertains to particular crystalline forms of 4-(ethylsulfonyloxy)-DPT chloride, including crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride. In one embodiment, crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride is characterized by at least one of: a monoclinic, $P2_1/c$ space group at a temperature of about 297(2) K; unit cell dimensions $a=17.4829(11)$ Å, $b=7.3596(4)$ Å, $c=17.9504(11)$ Å, $\alpha=90^\circ$, $\beta=118.864(2^\circ)$, and $\gamma=90^\circ$; an X-ray powder diffraction (XRPD) pattern substantially similar to FIG. 12; and an X-ray powder diffraction pattern characterized by at least two peaks selected from 9.9, 11.6, and $13.3^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0009] This disclosure further relates to [2-(1H-indol-3-yl)ethyl]tripropylazanium iodide (N,N,N-tri-n-propyltryptammonium iodide or TPT iodide), crystalline TPT iodide, and specific crystalline forms thereof. In one embodiment, this disclosure pertains to particular crystalline forms of TPT iodide, including crystalline form 1 of TPT iodide. In one

embodiment, crystalline form 1 of TPT iodide is characterized by at least one of: a monoclinic, $P2_1/n$ space group at a temperature of about 297(2) K; unit cell dimensions $a=7.4869(3)$ Å, $b=16.4570(7)$ Å, $c=16.2632(7)$ Å, $\alpha=90^\circ$, $\beta=96.2390(10^\circ)$, and $\gamma=90^\circ$; an X-ray powder diffraction (XRPD) pattern substantially similar to FIG. 13; and an X-ray powder diffraction pattern characterized by at least two peaks selected from 10.9, 15.4, and $21.2^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0010] This disclosure further relates to [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-N,N-di-n-isopropyltryptammonium iodide or 5-Cl-DiPT iodide), crystalline 5-Cl-DiPT iodide, and specific crystalline forms thereof. In one embodiment, this disclosure pertains to particular crystalline forms of 5-Cl-DiPT iodide, including crystalline form 1 of 5-Cl-DiPT iodide. In one embodiment, crystalline form 1 of 5-Cl-DiPT iodide is characterized by at least one of: an orthorhombic, $Pbca$ space group at a temperature of about 300(2) K; unit cell dimensions $a=8.2421(4)$ Å, $b=17.8313(8)$ Å, $c=24.8226(13)$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, and $\gamma=90^\circ$; an X-ray powder diffraction (XRPD) pattern substantially similar to FIG. 14; and an X-ray powder diffraction pattern characterized by at least two peaks selected from 7.1, 10.5, and $18.1^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0011] This disclosure further relates to 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate or 5-Cl-T hydrogenoxalate), crystalline 5-Cl-T hydrogenoxalate, and specific crystalline forms thereof. In one embodiment, this disclosure pertains to particular crystalline forms of 5-Cl-T hydrogenoxalate, including crystalline form 1 of 5-Cl-T hydrogenoxalate. In one embodiment, crystalline form 1 of 5-Cl-T hydrogenoxalate is characterized by at least one of: an orthorhombic, $Pna2_1$ space group at a temperature of about 300(2) K; unit cell dimensions $a=18.7293(13)$ Å, $b=5.6306(4)$ Å, $c=11.9021(6)$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, and $\gamma=90^\circ$; an X-ray powder diffraction (XRPD) pattern substantially similar to FIG. 15; and an X-ray powder diffraction pattern characterized by at least two peaks selected from 9.4, 12.0, and $14.9^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0012] This disclosure further relates to bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate or 5-Cl-T oxalate hydrate), crystalline 5-Cl-T oxalate hydrate, and specific crystalline forms thereof. In one embodiment, this disclosure pertains to particular crystalline forms of 5-Cl-T oxalate hydrate, including crystalline form 1 of 5-Cl-T oxalate hydrate. In one embodiment, crystalline form 1 of 5-Cl-T oxalate hydrate is characterized by at least one of: a monoclinic, $P2/c$ space group at a temperature of about 300(2) K; unit cell dimensions $a=8.7014(9)$ Å, $b=10.8691(11)$ Å, $c=12.8386(11)$ Å, $\alpha=90^\circ$, $\beta=90.844(3^\circ)$, and $\gamma=90^\circ$; an X-ray powder diffraction (XRPD) pattern substantially similar to FIG. 16; and an X-ray powder diffraction pattern characterized by at least two peaks selected from 10.2, 13.8, and $20.4^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0013] The disclosure further relates to a composition comprising 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, and at least one excipient.

[0014] The disclosure further relates to a composition comprising TPT iodide, crystalline TPT iodide, or specific crystalline forms thereof, such as crystalline form 1 of TPT iodide, and at least one excipient.

[0015] The disclosure further relates to a composition comprising 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, or specific crystalline forms thereof, such as crystalline form 1 of 5-Cl-DiPT iodide, and at least one excipient.

[0016] The disclosure further relates to a composition comprising 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, or specific crystalline forms thereof, such as crystalline form 1 of 5-Cl-T hydrogenoxalate, and at least one excipient.

[0017] The disclosure further relates to a composition comprising 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 5-Cl-T oxalate hydrate, and at least one excipient.

[0018] The disclosure also provides a composition comprising 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate, as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone; and at least one excipient.

[0019] The disclosure also relates to a method of preventing or treating a psychological disorder comprising the step of administering to a subject in need thereof a therapeutically effective amount of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate, or a composition according to this disclosure.

[0020] The disclosure further relates to a method of preventing or treating inflammation and/or pain, preventing or treating a neurological disorder, modulating activity of a mitogen-activated protein kinase (MAPK), modulating neurogenesis, or modulating neurite outgrowth comprising the step of administering to a subject in need thereof a therapeutically effective amount of a compound of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate, and to administering a pharmaceutical composition or a composition according to the invention.

[0021] As used herein, the term “a subject in need thereof” refers to a person requiring a composition to treat a particular disease or condition (e.g., inflammation, pain, a psychological disorder, modulating activity at a receptor, etc.). In one embodiment, the “subject in need thereof” may be identified by analyzing, diagnosing, and/or determining whether the person (or subject) requires the composition for treatment of a particular disease or condition. In one embodiment, identifying a person in need of treatment comprises diagnosing a person with a medical condition, e.g., a neurological disorder, a chemical imbalance, a hereditary condition, etc. In one embodiment, identifying a person in need of treatment comprises performing a psychiatric evaluation. In one embodiment, identifying a person in need of treatment comprises performing a blood test. In one embodiment, identifying a person in need of treatment comprises determining whether a person has a compulsive disorder. In one embodiment, identifying a person in need of treatment comprises self-identifying as having a compulsive disorder.

DESCRIPTION OF THE FIGURES

[0022] FIG. 1 shows the molecular structure of crystalline form 1 of 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride.

[0023] FIG. 2 shows the molecular structure of crystalline form 1 of N,N,N-tri-n-propyltryptammonium iodide.

[0024] FIG. 3 shows the molecular structure of crystalline form 1 of 5-chloro-N,N-di-n-isopropyltryptammonium iodide.

[0025] FIG. 4 shows the molecular structure of crystalline form 1 of 5-chlorotryptammonium hydrogenoxalate.

[0026] FIG. 5 shows the molecular structure of crystalline form 1 of 5-chlorotryptammonium oxalate hydrate.

[0027] FIG. 6 shows the unit cell of crystalline form 1 of 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium hydrochloride along the b-axis.

[0028] FIG. 7 shows the unit cell of crystalline form 1 of N,N,N-tri-n-propyltryptammonium iodide along the a-axis.

[0029] FIG. 8 shows the unit cell of crystalline form 1 of 5-chloro-N,N-di-n-isopropyltryptammonium iodide along the b-axis.

[0030] FIG. 9 shows the unit cell of crystalline form 1 of 5-chlorotryptammonium hydrogenoxalate along the b-axis.

[0031] FIG. 10 shows the unit cell of crystalline form 1 of 5-chlorotryptammonium oxalate hydrate along the b-axis.

[0032] FIG. 11 shows the 2 tryptamine: 2 water: 1 oxalate ratio of crystalline form 1 of 5-chlorotryptammonium oxalate hydrate as a dimer.

[0033] FIG. 12 shows the simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride.

[0034] FIG. 13 shows the simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of N,N,N-tri-n-propyltryptammonium iodide.

[0035] FIG. 14 shows the simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 5-chloro-N,N-di-n-isopropyltryptammonium iodide.

[0036] FIG. 15 shows the simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 5-chlorotryptammonium hydrogenoxalate.

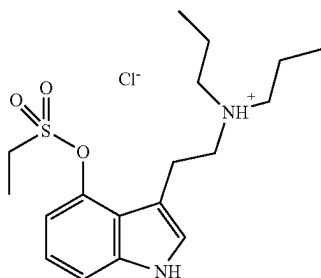
[0037] FIG. 16 shows the simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 5-chlorotryptammonium oxalate hydrate.

DETAILED DESCRIPTION

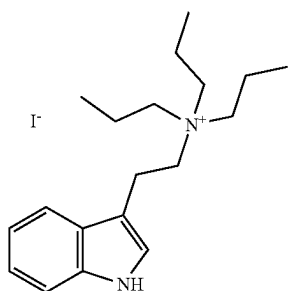
Compounds

[0038] This disclosure relates to (2-{4-[(ethanesulfonyl)oxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride or 4-(ethylsulfonyloxy)-DPT chloride), crystalline 4-(ethylsulfonyloxy)-DPT chloride, [2-(1H-indol-3-yl)ethyl]tripropylazanium iodide (N,N,N-tri-n-propyltryptammonium iodide or TPT iodide), crystalline TPT iodide, [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-N,N-di-n-isopropyltryptammonium iodide or 5-Cl-DiPT iodide), crystalline 5-Cl-DiPT iodide, 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate or 5-Cl-T hydrogenoxalate), crystalline 5-Cl-T hydrogenoxalate, bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate or 5-Cl-T oxalate hydrate), crystalline 5-Cl-T oxalate hydrate, and specific crystalline forms thereof, including crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate; to pharmaceutical compositions containing 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate according to the disclosure. The therapeutic uses of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate according to the disclosure are described below as well as compositions containing them. 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate, and some exemplary methods used to characterize them are described below.

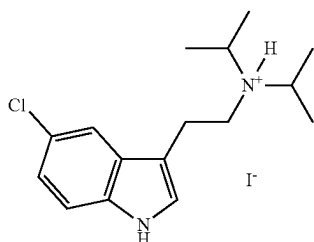
[0039] 4-(ethylsulfonyloxy)-DPT chloride has the following chemical formula:



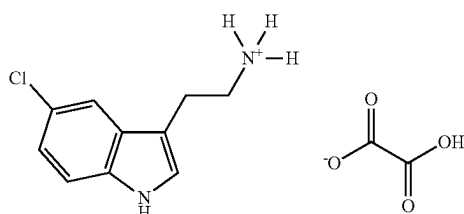
[0040] TPT iodide has the following chemical formula:



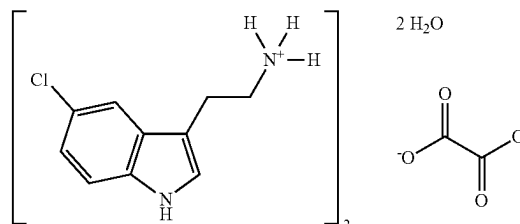
[0041] 5-Cl-DiPT iodide has the following chemical formula:



[0042] 5-Cl-T hydrogenoxalate has the following chemical formula:



[0043] 5-Cl-T oxalate hydrate has the following chemical formula:



Methods of Treatment and Therapeutic Uses

[0044] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate according to the disclosure, and the methods and the compositions (e.g., pharmaceutical compositions) are used to regulate the activity of a neurotransmitter receptor by administering a therapeutically effective dose of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate according to the disclosure, and the methods and the compositions (e.g., pharmaceutical compositions) are used to treat inflammation and/or pain by administering a therapeutically effective dose of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate according to the disclosure, and the methods and the compositions (e.g., pharmaceutical compositions) are used to treat inflammation and/or pain by administering a therapeutically effective dose of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure.

[0045] Methods of the disclosure also relate to the administration of a therapeutically effective amount of 4-(ethyl-

sulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate to prevent or treat a disease or condition, such as those discussed below for a subject in need of treatment. 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate may be administered neat or as a composition comprising 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate as discussed below.

[0046] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to prevent and/or treat a psychological disorder. The disclosure provides a method for preventing and/or treating a psychological disorder by administering to a subject in need thereof a therapeutically effective amount of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure, including the exemplary embodiments discussed herein. The psychological disorder may be chosen from: depression; psychotic disorder; schizophrenia; schizophreniform disorder (acute schizophrenic episode); schizoaffective disorder; bipolar I disorder (mania, manic disorder, manic-depressive psychosis); bipolar II disorder; major depressive disorder; major depressive disorder with psy-

chotic feature (psychotic depression); delusional disorders (paranoia); shared psychotic disorder (shared paranoia disorder); brief psychotic disorder (other and unspecified reactive psychosis); psychotic disorder not otherwise specified (unspecified psychosis); paranoid personality disorder; schizoid personality disorder; schizotypal personality disorder; anxiety disorder; social anxiety disorder; substance-induced anxiety disorder; selective mutism; panic disorder; panic attacks; agoraphobia; attention deficit syndrome; post-traumatic stress disorder (PTSD); premenstrual dysphoric disorder (PMDD); and premenstrual syndrome (PMS).

[0047] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to prevent and/or treat a brain disorder. The disclosure provides a method for preventing and/or treating a brain disorder (e.g., Huntington's disease, Alzheimer's disease, dementia, and Parkinson's disease) by administering to a subject in need thereof a therapeutically effective amount of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate.

[0048] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to prevent and/or treat developmental disorders, delirium, dementia, amnesic disorders and other cognitive disorders, psychiatric disorders due to a somatic condition, drug-related disorders, schizophrenia and other psychotic disorders, mood disorders, anxiety disorders, somatoform disorders, factitious disorders, dissociative disorders, eating disorders, sleep disorders, impulse control disorders, adjustment disorders, or personality disorders. The disclosure provides a method for preventing and/or treating these disorders by administering to a subject in need thereof a therapeutically effective amount of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1

of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate including the exemplary embodiments discussed above.

[0049] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to prevent and/or treat inflammation and/or pain, such as for example inflammation and/or pain associated with inflammatory skeletal or muscular diseases or conditions. The disclosure provides a method for preventing and/or treating an inflammation and/or pain by administering to a subject in need thereof a therapeutically effective amount of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure, including the exemplary embodiments discussed herein. Generally speaking, treatable “pain” includes nociceptive, neuropathic, and mix-type. A method of the disclosure may reduce or alleviate the symptoms associated with inflammation, including but not limited to treating localized manifestation of inflammation characterized by acute or chronic swelling, pain, redness, increased temperature, or loss of function in some cases. A method of the disclosure may reduce or alleviate the symptoms of pain regardless of the cause of the pain, including but not limited to reducing pain of varying severity, i.e., mild, moderate and severe pain, acute pain and chronic pain. A method of the disclosure is effective in treating joint pain, muscle pain, tendon pain, burn pain, and pain caused by inflammation such as rheumatoid arthritis. Skeletal or muscular diseases or conditions which may be treated include but are not limited to musculoskeletal sprains, musculoskeletal strains, tendinopathy, peripheral radiculopathy, osteoarthritis, joint degenerative disease, polymyalgia rheumatica, juvenile arthritis, gout, ankylosing spondylitis, psoriatic arthritis, systemic lupus erythematosus, costochondritis, tendonitis, bursitis, such as the common lateral epicondylitis (tennis elbow), medial epicondylitis (pitchers elbow) and trochanteric bursitis, temporomandibular joint syndrome, and fibromyalgia.

[0050] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure

may be used to modulate activity of a mitogen-activated protein kinase (MAPK), comprising administering a composition of the invention. MAPKs provide a wide-ranging signaling cascade that allow cells to quickly respond to biotic and abiotic stimuli. Exemplary MAPKs include, but are not limited to, Tropomyosin Receptor Kinase A (TrkA), P38-alpha, and c-Jun N-Terminal Kinase 3 (JNK3). TrkA is a high affinity catalytic receptor of nerve growth factor (NGF) protein. TrkA regulates NGF response, influencing neuronal differentiation and outgrowth as well as programmed cell death. p38-alpha is involved with the regulation of pro-inflammatory cytokines, including TNF- α . In the central nervous system, p38-alpha regulates neuronal death and neurite degeneration, and it is a common target of Alzheimer's disease therapies. JNK3 is a neuronal-specific protein isoform of the JNKs. It is involved with the regulation of apoptosis. JNK3 also plays a role in modulating the response of cytokines, growth factors, and oxidative stress.

[0051] As used herein, the term “modulating activity of a mitogen-activated protein kinase” refers to changing, manipulating, and/or adjusting the activity of a mitogen-activated protein kinase. In one embodiment, modulating the activity of a MAPK can influence neural health, neurogenesis, neural growth and differentiation, and neurodegenerative diseases.

[0052] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to modulate neurogenesis, comprising administering a composition of the invention. As used herein, the term “modulating neurogenesis” refers to changing, manipulating, and/or adjusting the growth and development of neural tissue. In one embodiment, neurogenesis comprises adult neurogenesis, in which new neural stem cells are generated from neural stem cells in an adult animal. In one embodiment, modulating neurogenesis comprises increasing and/or enhancing the rate at which new neural tissue is developed.

[0053] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to modulate neurite outgrowth, comprising administering a composition of the invention. As used herein, the term “modulating neurite outgrowth” refers to changing, manipulating, and/or adjusting the growth and development of neural projections, or “neurites.” In one embodiment, neurogenesis comprises modulating the growth of new neurites, the number of neurites per neuron, and/or neurite length. In one embodiment, modulating neu-

rite outgrowth comprises increasing and/or enhancing the rate and/or length at which neurites develop.

[0054] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to prevent and/or treat sexual health disorders including, but not limited to, hypoactive sexual desire disorder, hyperactive sexual desire disorder, orgasmic disorder, arousal disorder, vaginismus, and dyspareunia. In some embodiments, the disorder is a male sexual dysfunction disorder. In some embodiments, the disorder is a female sexual dysfunction disorder.

[0055] 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used to prevent and/or treat women's health disorders including, but not limited to, menstrual cramping, dysmenorrhea, post-hysterectomy pain, vaginal or vulvar vestibule mucosa disorder, menopausal-related disorders, vaginal atrophy, or vulvar vestibulitis.

Compositions

[0056] The disclosure also relates to compositions comprising an effective amount of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate and an excipient (e.g., a pharmaceutically-acceptable excipient). In another embodiment, the disclosure also relates to pharmaceutical compositions comprising a therapeutically effective amount of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate and a pharmaceutically acceptable excipient (also known as a pharmaceutically acceptable carrier). As discussed above, 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crys-

talline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be, for example, therapeutically useful to prevent and/or treat the psychological disorders, brain disorders, pain, and inflammation as well as the other disorders described herein.

[0057] A composition or a pharmaceutical composition of the disclosure may be in any form which contains 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate. The composition may be, for example, a tablet, capsule, liquid suspension, injectable, topical, or transdermal. The compositions generally contain, for example, about 1% to about 99% by weight of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure and, for example, 99% to 1% by weight of at least one suitable pharmaceutically acceptable excipient. In one embodiment, the composition may be between about 5% and about 75% by weight of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure, with the rest being at least one suitable pharmaceutically acceptable excipient or at least one other adjuvant, as discussed below.

[0058] Published US applications US 2018/0221396 A1 and US 2019/0142851 A1 disclose compositions comprising a combination of a first purified psilocybin derivative with a second purified psilocybin derivative, with one or two purified cannabinoids or with a purified terpene. Various ratios of these components in the composition are also disclosed. The disclosures of US 2018/0221396 A1 and US 2019/0142851 A1 are incorporated herein by reference. According to this disclosure, 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crys-

talline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used as the “first purified psilocybin derivative” in the compositions described in US 2018/0221396 A1 and US 2019/0142851 A1. Accordingly, this disclosure provides a composition comprising: a first component comprising 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure; at least one second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, and (d) a purified terpene; and at least one pharmaceutically-acceptable excipient or at least one other adjuvant. Such a composition may be a pharmaceutical composition wherein the components are present individually in therapeutically effective amounts or by combination in a therapeutically effective amount to treat a disease, disorder, or condition as described herein.

[0059] When used in such compositions as a first component comprising 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure with a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, and (d) a purified terpene, the compositions represent particular embodiments of the invention. Compositions having as a first component 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure with a second component selected from at least one of (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone represent additional particular embodiments of the invention represented by the compositions having 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide,

5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate according to the disclosure. In some embodiments, the first and second components can be administered at the same time (e.g., together in the same composition), or at separate times over the course of treating a patient in need thereof. Such a composition may be a pharmaceutical composition wherein the components are present individually in therapeutically effective amounts or by combination in a therapeutically effective amount to treat a disease, disorder, or condition as described herein.

[0060] Within the context of this disclosure, the term “purified” means separated from other materials, such as plant or fungal material, e.g., protein, chitin, cellulose, or water. In one embodiment, the term “purified” refers to a compound substantially free of other materials. In one embodiment, the term “purified” refers to a compound that is substantially free from a second tryptamine compound. In one embodiment, the term “purified” refers to a compound substantially free from histidine. In one embodiment, the term “purified” refers to a compound substantially free from a biological material, such as mold, fungus, plant matter, or bacteria. In one embodiment, the term “purified” refers to a compound substantially free from a paralytic.

[0061] In one embodiment, the term “purified” refers to a compound which has been separated from other compounds that are typically co-extracted when the purified compound is extracted from a naturally occurring organism. In one embodiment, a “purified” psilocybin derivative is partially or completely isolated from other psilocybin derivatives present in a source material, such as a psilocybin-containing mushroom. In one example, “purified” baeocystin is substantially free from psilocybin and/or psilocin. By contrast, traditional psilocybin mushroom extracts (aka crude extracts or fruit body extracts) would be expected to contain an unpredictable and varying amount of psilocybin, psilocin, baeocystin, norbaeocystin, salts thereof, or combinations thereof. Other examples of unpurified psilocybin derivatives would include mycelium containing psilocybin derivatives and/or naturally occurring fungal material such as biological material and/or structural material such as chitin. Similarly, the term “cannabis extracts” or “cannabinoid extracts” traditionally refers to whole plants (aka crude or full spectrum extracts) which have not been subjected to further purification to eliminate unwanted molecules that naturally occur in the cannabis plant. For example, a “cannabis extract comprising cannabidiol” could be expected to include cannabidiol (aka “CBD”) and also varying amounts of other compounds, including cannabinoids, terpenes, and other biological material.

[0062] In one embodiment, the term “purified” refers to a compound or composition that has been crystallized.

[0063] In one embodiment, the term “purified” refers to a compound or composition that has been chromatographed, for example by gas chromatography, liquid chromatography (e.g., LC, HPLC, etc.), etc.

[0064] In one embodiment, the term “purified” refers to a compound or composition that has been distilled.

[0065] In one embodiment, the term “purified” refers to a compound or composition that has been sublimed.

[0066] In one embodiment, the term “purified” refers to a compound or composition that has been subject to two or more steps chosen from crystallization, chromatography, distillation, or sublimation.

[0067] In one embodiment, the term “purified” refers to a compound that is between 80-100% pure.

[0068] In one embodiment, the term “purified” refers to a compound that is between 90-100% pure.

[0069] In one embodiment, the term “purified” refers to a compound that is between 95-100% pure.

[0070] In one embodiment, the term “purified” refers to a compound that is between 99-100% pure.

[0071] In one embodiment, the term “purified” refers to a compound that is between 99.9-100% pure.

[0072] A serotonergic drug refers to a compound that binds to, blocks, or otherwise influences (e.g., via an allosteric reaction) activity at a serotonin receptor as described in paragraphs [0245]-[0253] of US 2018/0221396 A1 and [0305]-[0311] US 2019/0142851 A1 as well as the disclosed exemplary embodiments. Exemplary psilocybin derivatives include but are not limited to psilocybin itself and the psilocybin derivatives described in paragraphs [0081]-[0109] of US 2018/0221396 A1 and [0082]-[0110] US 2019/0142851 A1 as well as the disclosed exemplary embodiments. Exemplary cannabinoids include but are not limited to the cannabinoids described in paragraphs [0111]-[0145] of US 2018/0221396 A1 and [0112]-[0146] US 2019/0142851 A1 as well as the disclosed exemplary embodiments. Exemplary terpenes include but are not limited to the terpenes described in paragraphs [0160]-[0238] of US 2018/0221396 A1 and [0161]-[0300] US 2019/0142851 A1 as well as the disclosed exemplary embodiments.

[0073] A pharmaceutical formulation of the disclosure may comprise, consist essentially of, or consist of (a) 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure and (b) at least one second active compound selected from a serotonergic drug, a purified psilocybin derivative, a purified cannabinoid, a purified terpene, an adrenergic drug, a dopaminergic drug, a monoamine oxidase inhibitor, a purified erinacine, and a purified hericenone, and (c) a pharmaceutically acceptable excipient. In some embodiments, 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate and the second active compound(s) are each present in a therapeutically effective amount using purposefully engineered and unnatu-

rally occurring molar ratios. Exemplary molar ratios of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure to the second active compound in a composition of the disclosure include but are not limited to from about 0.1:100 to about 100:0.1, from about 1:100 to about 100:1, from about 1:50 to about 50:1, from about 1:25 to about 25:1, from about 1:20 to about 20:1, from about 1:10 to about 10:1, from about 1:5 to about 5:1, from about 1:2 to about 2:1 or may be about 1:1.

[0074] A pharmaceutical formulation of the disclosure may comprise a composition containing 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure and a serotonergic drug, a purified psilocybin derivative, a purified cannabinoid, or a purified terpene, each present in a therapeutically effective amount using purposefully engineered and unnaturally occurring molar ratios. Published US applications US 2018/0221396 A1 and US 2019/0142851 A1 disclose compositions comprising a combination of a purified psilocybin derivative with a second purified psilocybin derivative, with one or two purified cannabinoids or with a purified terpene. According to this disclosure composition containing 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be used in place of a “purified psilocybin derivative” in the compositions described in US 2018/0221396 A1 and US 2019/0142851 A1. Accordingly, the disclosure provides a pharmaceutical formulation comprising as (a) 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure and at least one second component selected from (a) a purified

psilocybin derivative, (b) a purified cannabinoid, and (c) a purified terpene; and at least one pharmaceutically-acceptable excipient or at least one other adjuvant, as described herein. Such a composition may be a pharmaceutical composition wherein the components are present individually in therapeutically effective amounts or by combination in a therapeutically effective amount to treat a disease, disorder, or condition as described herein.

[0075] A serotonergic drug refers to a compound that binds to, blocks, or otherwise influences (e.g., via an allosteric reaction) activity at a serotonin receptor as described in paragraphs [0245]-[0253] of US 2018/0221396 A1 and [0305]-[0311] US 2019/0142851 A1 as well as the disclosed exemplary embodiments. Some exemplary serotonergic drugs include SSRIs and SNRIs. Some examples of specific serotonergic drugs include the following molecules, including any salts, solvates, or polymorphs thereof: 6-allyl-N,N-diethyl-NL; N,N-dibutyl-T; N,N-diethyl-T; N,N-diisopropyl-T; 5-methoxy-alpha-methyl-T; N,N-dimethyl-T; 2, alpha-dimethyl-T; alpha,N-dimethyl-T; N,N-dipropyl-T; N-ethyl-N-isopropyl-T; alpha-ethyl-T; 6-N,N-Triethyl-NL; 3,4-dihydro-7-methoxy-1-methyl-C; 7-methoxy-1-methyl-C; N,N-dibutyl-4-hydroxy-T; N,N-diethyl-4-hydroxy-T; N,N-diisopropyl-4-hydroxy-T; N,N-dimethyl-4-hydroxy-T; N,N-dimethyl-5-hydroxy-T; N, N-dipropyl-4-hydroxy-T; N-ethyl-4-hydroxy-N-methyl-T; 4-hydroxy-N-isopropyl-N-methyl-T; 4-hydroxy-N-methyl-N-propyl-T; 4-hydroxy-N, N-tetramethylene-T; ibogaine; N,N-diethyl-L; N-butyl-N-methyl-T; N,N-diisopropyl-4,5-methylenedioxy-T; N,N-diisopropyl-5,6-methylenedioxy-T; N,N-dimethyl-4,5-methylenedioxy-T; N,N-dimethyl-5,6-methylenedioxy-T; N-isopropyl-N-methyl-5,6-methylenedioxy-T; N,N-diethyl-2-methyl-T; 2-N,N-trimethyl-T; N-acetyl-5-methoxy-T; N,N-diethyl-5-methoxy-T; N,N-diisopropyl-5-methoxy-T; 5-methoxy-N,N-dimethyl-T; N-isopropyl-4-methoxy-N-methyl-T; N-isopropyl-5-methoxy-N-methyl-T; 5,6-dimethoxy-N-isopropyl-N-methyl-T; 5-methoxy-N-methyl-T; 5-methoxy-N,N-tetramethylene-T; 6-methoxy-1-methyl-1, 2,3,4-tetrahydro-C; 5-methoxy-2-N,N-trimethyl-T; N,N-dimethyl-5-methylthio-T; N-isopropyl-N-methyl-T; alpha-methyl-T; N-ethyl-T; N-methyl-T; 6-propyl-N L; N,N-tetramethylene-T; tryptamine; 7-methoxy-1-methyl-1,2,3,4-tetrahydro-C; and alpha,N-dimethyl-5-methoxy-T. For additional information regarding these compounds see Shulgin, A. T., & Shulgin, A. (2016). *Tihkal: The Continuation*. Berkeley, Calif.: Transform Press. In one embodiment, a serotonergic drug is chosen from alprazolam, amphetamine, aripiprazole, azapirone, a barbiturate, bromazepam, bupropion, buspirone, a cannabinoid, chlordiazepoxide, citalopram, clonazepam, clorazepate, dextromethorphan, diazepam, duloxetine, escitalopram, fluoxetine, flurazepam, fluvoxamine, lorazepam, lysergic acid diethylamide, lysergamide, 3,4-methylenedioxymethamphetamine, milnacipran, mirtazapine, naratriptan, paroxetine, pethidine, phenethylamine, psilocaine, oxazepam, reboxetine, serenic, serotonin, sertraline, temazepam, tramadol, triazolam, a tryptamine, venlafaxine, vortioxetine, and/or derivatives thereof. In an exemplary embodiment, the serotonergic drug is 3,4-methylenedioxymethamphetamine.

[0076] Exemplary psilocybin derivatives include but are not limited to psilocybin itself and the psilocybin derivatives described in paragraphs [0081]-[0109] of US 2018/0221396 A1 and [0082]-[0110] US 2019/0142851 A1 as well as the disclosed exemplary embodiments, incorporated here by

reference. In one embodiment, the compositions disclosed herein comprise one or more purified psilocybin derivatives chosen from: [3-(2-dimethylaminoethyl)-1H-indol-4-yl]dihydrogen phosphate; 4-hydroxytryptamine; 4-hydroxy-N, N-dimethyltryptamine; [3-(2-methylaminoethyl)-1H-indol-4-yl]dihydrogen phosphate; 4-hydroxy-N-methyltryptamine; [3-(aminoethyl)-1H-indol-4-yl]dihydrogen phosphate; [3-(2-trimethylaminoethyl)-1H-indol-4-yl]dihydrogen phosphate; and 4-hydroxy-N,N,N-trimethyltryptamine.

[0077] Exemplary cannabinoids include but are not limited to the cannabinoids described in paragraphs [0111]-[0145] of US 2018/0221396 A1 and [0112]-[0146] US 2019/0142851 A1 as well as the disclosed exemplary embodiments. Examples of cannabinoids within the context of this disclosure include the following molecules: cannabichromene (CBC); cannabichromenic acid (CBCA); cannabichromevarin (CBCV); cannabichromevarinic acid (CBCVA); cannabicyclol (CBL); cannabicyclolic acid (CBLA); cannabicyclovarin (CBLV); cannabidiol (CBD); cannabidiol monomethylether (CBDM); cannabidiolic acid (CBDA); cannabidiolcol (CBD-C1); cannabidivarin (CBDV); cannabidivarinic acid (CBDVA); cannabielsoic acid B (CBEA-B); cannabielsoin (CBE); cannabielsoin acid A (CBEA-A); cannabigerol (CBG); cannabigerol monomethylether (CBGM); cannabigerolic acid (CBGA); cannabigerolic acid monomethylether (CBGAM); cannabigerovarin (CBGV); cannabigerovarinic acid (CBGVA); cannabinodiol (CBND); cannabinodivarin (CBVD); cannabinol (CBN); cannabinol methylether (CBNM); cannabinol-C2 (CBN-C2); cannabinol-C4 (CBN-C4); cannabinolic acid (CBNA); cannabiorcol (CBN-C1); cannabivarin (CBV); cannabitriol (CBT); cannabitriolvarin (CBTV); 10-ethoxy-9-hydroxy-delta-6a-tetrahydrocannabinol; cannabicitran (CBTC); cannabiripsol (CBR); 8,9-dihydroxy-delta-6a-tetrahydrocannabinol; delta-8-tetrahydrocannabinol (A8-THC); delta-8-tetrahydrocannabinolic acid (A8-THCA); delta-9-tetrahydrocannabinol (THC); delta-9-tetrahydrocannabinol-C4 (THC-C4); delta-9-tetrahydrocannabinolic acid A (THCA-A); delta-9-tetrahydrocannabinolic acid B (THCA-B); delta-9-tetrahydrocannabinolic acid-C4 (THCA-C4); delta-9-tetrahydrocannabinolcol (THC-C1); delta-9-tetrahydrocannabinolcolic acid (THCA-C1); delta-9-tetrahydrocannabivarin (THCV); delta-9-tetrahydrocannabivarinic acid (THCVA); 10-oxo-delta-6a-tetrahydrocannabinol (OTH); cannabichromanone (CBCF); cannabifuran (CBF); cannabiglendol; delta-9-cis-tetrahydrocannabinol (cis-THC); trihydroxy-delta-9-tetrahydrocannabinol (triOH-THC); dehydrocannabifuran (DCBF); and 3,4,5,6-tetrahydro-7-hydroxy-alpha-alpha-2-trimethyl-9-n-propyl-2,6-methano-2H-1-benzoxocin-5-methanol. In one embodiment, the purified cannabinoid is chosen from THC, THCA, THCV, THCVA, CBC, CBCA, CBCV, CBCVA, CBD, CBDA, CBDV, CBVD, CBDVA, CBG, CBGA, CBGV, or CBGVA.

[0078] Exemplary terpenes include but are not limited to the terpenes described in paragraphs [0160]-[0238] of US 2018/0221396 A1 and [0161]-[0300] US 2019/0142851 A1 as well as the disclosed exemplary embodiments. In one embodiment, a purified terpene is chosen from acetanilole, acetyl cedrene, anethole, anisole, benzaldehyde, bornyl acetate, borneol, cadinene, cafestol, caffeic acid, camphene, camphor, capsaicin, carene, carotene, carvacrol, carvone,

caryophyllene, caryophyllene oxide, cedrene, cedrene epoxide, cecanal, cedrol, cembrene, cinnamaldehyde, cinnamic acid, citronellal, citronellol, cymene, eicosane, elemene, estragole, ethyl acetate, ethyl cinnamate, ethyl maltol, eucalyptol/1,8-cineole, eudesmol, eugenol, euphol, farnesene, farnesol, fenchone, geraniol, geranyl acetate, guaia-1(10),11-diene, guaiacol, guaiol, guaiene, gurjunene, herniarin, hexanaldehyde, hexanoic acid, humulene, ionone, ipsdienol, isoamyl acetate, isoamyl alcohol, isoamyl formate, isoborneol, isomyrcenol, isoprene, isopulegol, isovaleric acid, lavandulol, limonene, gamma-linolenic acid, linalool, longifolene, lycopene, menthol, methyl butyrate, 3-mercapto-2-methylpentanal, beta-mercaptoethanol, mercaptoacetic acid, methyl salicylate, methylbutenol, methyl-2-methylvalerate, methyl thiobutylate, myrcene, gamma-murolene, nepetalactone, nerol, nerolidol, neryl acetate, nonanaldehyde, nonanoic acid, ocimene, octanal, octanoic acid, pentyl butyrate, phellandrene, phenylacetaldehyde, phenylacetic acid, phenylethanethiol, phytol, pinene, propanethiol, pristimerin, pulegone, retinol, rutin, sabinene, squalene, taxadiene, terpineol, terpene-4-ol, terpinolene, thujone, thymol, umbelliferone, undecanal, verdoxan, or vanillin. In one embodiment, a purified terpene is chosen from bornyl acetate, alpha-bisabolol, borneol, camphene, camphor, carene, caryophyllene, cedrene, cymene, elemene, eucalyptol, eudesmol, farnesene, fenchol, geraniol, guaiacol, humulene, isoborneol, limonene, linalool, menthol, myrcene, nerolidol, ocimene, phellandrene, phytol, pinene, pulegone, sabinene, terpineol, terpinolene, or valencene.

[0079] As used herein, the term “adrenergic drug” refers to a compound that binds, blocks, or otherwise influences (e.g., via an allosteric reaction) activity at an adrenergic receptor. In one embodiment, an adrenergic drug binds to an adrenergic receptor. In one embodiment, an adrenergic drug indirectly affects an adrenergic receptor, e.g., via interactions affecting the reactivity of other molecules at the adrenergic receptor. In one embodiment, an adrenergic drug is an agonist, e.g., a compound activating an adrenergic receptor. In one embodiment, an adrenergic drug is an antagonist, e.g., a compound binding but not activating an adrenergic receptor, e.g., blocking a receptor. In one embodiment, an adrenergic drug is an effector molecule, e.g., a compound binding to an enzyme for allosteric regulation. In one embodiment, an adrenergic drug acts (either directly or indirectly) at more than one type of receptor (e.g., 5HT, dopamine, adrenergic, acetylcholine, etc.).

[0080] In one embodiment, an adrenergic drug is an antidepressant. In one embodiment, an adrenergic drug is a norepinephrine transporter inhibitor. In one embodiment, an adrenergic drug is a vesicular monoamine transporter inhibitor. In one embodiment, an adrenergic drug is chosen from adrenalina, agmatine, amoxapine, aptazapine, atomoxetine, bupropion, clonidine, doxepin, duloxetine, esmirtazapine, mianserin, ketanserin, mirabegron, mirtazapine, norepinephrine, phentolamine, phenylephrine, piperoxan, reserpine, ritodrine, setiptiline, tesofensine, timolol, trazodone, trimipramine, or xylazine.

[0081] As used herein, the term “dopaminergic drug” refers to a compound that binds, blocks, or otherwise influences (e.g., via an allosteric reaction) activity at a dopamine receptor. In one embodiment, a dopaminergic drug binds to a dopamine receptor. In one embodiment, a dopaminergic drug indirectly affects a dopamine receptor,

e.g., via interactions affecting the reactivity of other molecules at the dopamine receptor. In one embodiment, a dopaminergic drug is an agonist, e.g., a compound activating a dopamine receptor. In one embodiment, a dopaminergic drug is an antagonist, e.g., a compound binding but not activating a dopamine receptor, e.g., blocking a receptor. In one embodiment, a dopaminergic drug is an effector molecule, e.g., a compound binding to an enzyme for allosteric regulation. In one embodiment, a dopaminergic drug acts (either directly or indirectly) at more than one type of receptor (e.g., 5HT, dopamine, adrenergic, acetylcholine, etc.).

[0082] In one embodiment, a dopaminergic drug is a dopamine transporter inhibitor. In one embodiment, a dopaminergic drug is a vesicular monoamine transporter inhibitor. In one embodiment, a dopaminergic drug is chosen from amineptine, apomorphine, benzylpiperazine, bromocriptine, cabergoline, chlorpromazine, clozapine, dihydrexidine, domperidone, dopamine, fluphenazine, haloperidol, ketamine, loxapine, methamphetamine, olanzapine, pemoline, perphenazine, pergolide, phencyclidine, phenethylamine, phenmetrazine, pimozone, piribedil, a psychostimulant, reserpine, risperidone, ropinirole, tetrabenazine, or thioridazine.

[0083] As used herein, the term “monoamine oxidase inhibitor” (MAOI) refers to a compound that blocks the actions of monoamine oxidase enzymes. In one embodiment, a MAOI inhibits the activity of one or both monoamine oxidase A and monoamine oxidase B. In one embodiment a MAOI is a reversible inhibitor of monoamine oxidase A. In one embodiment a MAOI is a drug chosen from isocarboxazid, phenelzine, or tranlycypromine. In one embodiment, a MAOI is β -carboline, pinoline, harmaline, harmine, harmaline, harmalol, tetrahydroharmine, 9-methyl- β -carboline, or 3-carboxy-tetrahydroharmine.

[0084] In one embodiment, the compositions and methods disclosed herein include one or more purified erinacine molecules. In one embodiment, the compositions and methods disclosed herein comprise purified erinacine A. In one embodiment, the compositions and methods disclosed herein comprise erinacine B. In one embodiment, the compositions and methods disclosed herein comprise erinacine C. In one embodiment, the compositions and methods disclosed herein comprise erinacine D. In one embodiment, the compositions and methods disclosed herein comprise erinacine E. In one embodiment, the compositions and methods disclosed herein comprise erinacine F. In one embodiment, the compositions and methods disclosed herein comprise erinacine G. In one embodiment, the compositions and methods disclosed herein comprise erinacine H. In one embodiment, the compositions and methods disclosed herein comprise erinacine I. In one embodiment, the compositions and methods disclosed herein comprise erinacine J. In one embodiment, the compositions and methods disclosed herein comprise erinacine K. In one embodiment, the compositions and methods disclosed herein comprise erinacine P. In one embodiment, the compositions and methods disclosed herein comprise erinacine Q. In one embodiment, the compositions and methods disclosed herein comprise erinacine R. In one embodiment, the compositions and methods disclosed herein comprise erinacine S.

[0085] In one embodiment, the compositions and methods disclosed herein include one or more purified hericenone

Second Compound	Molar ratio of 4-(ethylsulfonyloxy)-DPT chloride or crystalline 4-(ethylsulfonyloxy)-DPT chloride, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride:second compound	Molar ratio of TPT iodide or crystalline TPT iodide, such as crystalline form 1 of TPT iodide:second compound	Molar ratio of 5-Cl-DiPT iodide or crystalline 5-Cl-DiPT iodide, such as crystalline form 1 of 5-Cl-DiPT iodide:second compound	Molar ratio of 5-Cl-T hydroge-noxalate or crystalline 5-Cl-T hydroge-noxalate, such as crystalline form 1 of 5-Cl-T hydroge-noxalate:second compound	Molar ratio of 5-Cl-T oxalate hydrate or crystalline 5-Cl-T oxalate hydrate, such as crystalline form 1 of 5-Cl-T oxalate hydrate:second compound
Duloxetine	About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1
[3-(2-dimethylaminoethyl)-1H-indol-4-yl] dihydrogen phosphate 4-hydroxytryptamine	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1 About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1
4-hydroxy-N,N-dimethyltryptamine	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1
[3-(2-methylaminoethyl)-1H-indol-4-yl] dihydrogen phosphate 4-hydroxy-N-methyltryptamine	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1
[3-(aminoethyl)-1H-indol-4-yl] dihydrogen phosphate	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1
[3-(2-trimethylaminoethyl)-1H-indol-4-yl] dihydrogen phosphate 4-hydroxy-N,N,N-trimethyltryptamine	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1	About 1:100 to about 100:1 About 1:25 to about 25:1 About 1:5 to about 5:1
THC	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1

TABLE 1-continued

[illegible]

TABLE 1-continued

Second Compound	Molar ratio of 4-(ethylsulfonyloxy)-DPT chloride or crystalline 4-(ethylsulfonyloxy)-DPT chloride, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride:second compound		Molar ratio of 5-Cl-DiPT iodide or crystalline 5-Cl-DiPT iodide, such as crystalline form 1 of 5-Cl-DiPT iodide:second compound		Molar ratio of 5-Cl-T hydrogene-oxalate or crystalline 5-Cl-T hydrogene-oxalate, such as crystalline form 1 of 5-Cl-T hydrogene-oxalate:second compound	
	Molar ratio of 4-(ethylsulfonyloxy)-DPT chloride, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride:second compound	Molar ratio of TPT iodide or crystalline TPT iodide, such as crystalline form 1 of TPT iodide:second compound	Molar ratio of 5-Cl-DiPT iodide, such as crystalline form 1 of 5-Cl-DiPT iodide:second compound	Molar ratio of 5-Cl-T hydrogene-oxalate, such as crystalline form 1 of 5-Cl-T hydrogene-oxalate:second compound	Molar ratio of 5-Cl-T oxalate hydrate or crystalline 5-Cl-T oxalate hydrate, such as crystalline form 1 of 5-Cl-T oxalate hydrate:second compound	Molar ratio of 5-Cl-T oxalate hydrate or crystalline 5-Cl-T oxalate hydrate, such as crystalline form 1 of 5-Cl-T oxalate hydrate:second compound
Amineptine	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1
	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1
	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1
	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1
Erinacine A	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1
	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1
	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1
	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1
Hericenone A	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1
	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1
	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1
	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1
Phenelzine	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1
	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1	About 1:5 to about 5:1
	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1	About 1:100 to about 100:1
	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1	About 1:25 to about 25:1

[0087] Exemplary pharmaceutical compositions of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure and a second compound selected from a serotonergic drug, a purified psilocybin derivative, a purified cannabinoid, a purified terpene, an adrenergic drug, a dopaminergic drug, a monoamine oxidase inhibitor, a purified erinacine, and a purified hericenone and an excipient with exemplary molar ratios of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide,

5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate to the second compound are shown in Table 2. 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be any one of the exemplary embodiments described above including the crystalline forms as disclosed herein.

TABLE 2

[illegible]

TABLE 2-continued

[illegible]

TABLE 2-continued

[illegible]

[0088] An “effective amount” or a “therapeutically effective amount” of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure is generally in the range of about 0.1 to about 100 mg daily (oral dose), of about 0.1 to about 50 mg daily (oral dose), of about 0.25 to about 25 mg daily (oral dose), of about 0.1 to about 5 mg daily (oral dose), or of about 0.5 to about 2.5 mg daily (oral dose). The actual amount required for treatment of any particular patient may depend upon a variety of factors including, for example, the disease being treated and its severity; the specific pharmaceutical composition employed; the age, body weight, general health, sex, and diet of the patient; the mode of administration; the time of administration; the route of administration; and the rate of excretion; the duration of the treatment; any drugs used in combination or coincidental with the specific compound employed; and other such factors well known in the medical arts. These factors are discussed in Goodman and Gilman’s “The Pharmacological Basis of Therapeutics,” Tenth Edition, A. Gilman, J. Hardman and L. Limbird, eds., McGraw-Hill Press, 155-173 (2001), which is incorporated herein by reference. 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure and pharmaceutical compositions containing it may be used in combination with other agents that are generally administered to a patient being treated for psychological and other disorders discussed above. They may also be co-formulated with one or more of such agents in a single pharmaceutical composition.

[0089] Depending on the type of pharmaceutical composition, the pharmaceutically acceptable carrier may be chosen from any one or a combination of carriers known in the art. The choice of the pharmaceutically acceptable carrier depends upon the pharmaceutical form and the desired method of administration to be used. Exemplary carriers include those that do not substantially alter the structure or activity of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure, or produce undesirable biological effects or otherwise

interact in a deleterious manner with any other component(s) of the pharmaceutical composition.

[0090] The pharmaceutical compositions of the disclosure may be prepared by methods known in the pharmaceutical formulation art, for example, see Remington’s Pharmaceutical Sciences, 18th Ed., (Mack Publishing Company, Easton, Pa., 1990), which is incorporated herein by reference. In a solid dosage form, 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure may be admixed with at least one pharmaceutically acceptable excipient such as, for example, sodium citrate or dicalcium phosphate or (a) fillers or extenders, such as, for example, starches, lactose, sucrose, glucose, mannitol, and silicic acid, (b) binders, such as, for example, cellulose derivatives, starch, alginates, gelatin, polyvinylpyrrolidone, sucrose, and gum acacia, (c) humectants, such as, for example, glycerol, (d) disintegrating agents, such as, for example, agar-agar, calcium carbonate, potato or tapioca starch, alginic acid, croscarmellose sodium, complex silicates, and sodium carbonate, (e) solution retarders, such as, for example, paraffin, (f) absorption accelerators, such as, for example, quaternary ammonium compounds, (g) wetting agents, such as, for example, cetyl alcohol, and glycerol monostearate, magnesium stearate and the like, (h) adsorbents, such as, for example, kaolin and bentonite, and (i) lubricants, such as, for example, talc, calcium stearate, magnesium stearate, solid polyethylene glycols, sodium lauryl sulfate, or mixtures thereof. In the case of capsules, tablets, and pills, the dosage forms may also comprise buffering agents. In some embodiments, the excipient is not water. In some embodiments, the excipient is not a solvent (e.g., EtOH, diethyl ether, ethyl acetate, or hydrocarbon-based solvents (e.g., hexanes)). In some embodiments, the dosage form is substantially free of water and/or solvents, for example less than about 5% water by mass, less than 2% water by mass, less than 1% water by mass, less than 0.5% water by mass, or less than 0.1% water by mass.

[0091] Excipients or pharmaceutically acceptable adjuvants known in the pharmaceutical formulation art may also be used in the pharmaceutical compositions of the disclosure. These include, but are not limited to, preserving, wetting, suspending, sweetening, flavoring, perfuming, emulsifying, and dispensing agents. Prevention of the action of microorganisms may be ensured by inclusion of various antibacterial and antifungal agents, for example, parabens, chlorobutanol, phenol, sorbic acid, and the like. It may also be desirable to include isotonic agents, for example, sugars, sodium chloride, and the like. If desired, a pharmaceutical composition of the disclosure may also contain minor amounts of auxiliary substances such as wetting or emulsifying agents, pH buffering agents, antioxidants, and the like, such as, for example, citric acid, sorbitan monolaurate, triethanolamine oleate, butylated hydroxytoluene, etc.

[0092] Solid dosage forms as described above may be prepared with coatings and shells, such as enteric coatings and others well known in the art. They may contain paci-

fying agents and can also be of such composition that they release the active compound or compounds in a certain part of the intestinal tract in a delayed manner. Non-limiting examples of embedded compositions that may be used are polymeric substances and waxes. The active compounds may also be in microencapsulated form, if appropriate, with one or more of the above-mentioned excipients.

[0093] Suspensions, in addition to the active compounds, may contain suspending agents, such as, for example, ethoxylated isostearyl alcohols, polyoxyethylene sorbitol and sorbitan esters, microcrystalline cellulose, aluminum metahydroxide, bentonite, agar-agar and tragacanth, or mixtures of these substances, and the like.

[0094] Solid dosage forms for oral administration, which includes capsules, tablets, pills, powders, and granules, may be used. In such solid dosage forms, the active compound may be mixed with at least one inert, pharmaceutically acceptable excipient (also known as a pharmaceutically acceptable carrier).

[0095] Administration of 4-(ethylsulfonyloxy)-DPT chloride, crystalline 4-(ethylsulfonyloxy)-DPT chloride, TPT iodide, crystalline TPT iodide, 5-Cl-DiPT iodide, crystalline 5-Cl-DiPT iodide, 5-Cl-T hydrogenoxalate, crystalline 5-Cl-T hydrogenoxalate, 5-Cl-T oxalate hydrate, crystalline 5-Cl-T oxalate hydrate, or specific crystalline forms thereof, such as crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, crystalline form 1 of TPT iodide, crystalline form 1 of 5-Cl-DiPT iodide, crystalline form 1 of 5-Cl-T hydrogenoxalate, and crystalline form 1 of 5-Cl-T oxalate hydrate of the disclosure in pure form or in an appropriate pharmaceutical composition may be carried out via any of the accepted modes of administration or agents for serving similar utilities. Thus, administration may be, for example, orally, buccally, nasally, parenterally (intravenous, intramuscular, or subcutaneous), topically, transdermally, intravaginally, intravesically, or intrasystemically, in the form of solid, semi-solid, lyophilized powder, or liquid dosage forms, such as, for example, tablets, suppositories, pills, soft elastic and hard gelatin capsules, powders, solutions, suspensions, or aerosols, or the like, such as, for example, in unit dosage forms suitable for simple administration of precise dosages. One route of administration may be oral administration, using a convenient daily dosage regimen that can be adjusted according to the degree of severity of the disease-state to be treated.

EXEMPLARY EMBODIMENTS

[0096] E1. Crystalline (2-{4-[(ethanesulfonyl)oxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride).

[0097] E2. Crystalline form 1 of (2-{4-[(ethanesulfonyl)oxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride).

[0098] E3. Crystalline form 1 of 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to E2, characterized by at least one of:

[0099] a monoclinic crystal system at a temperature of about 297 K;

[0100] a $P2_{1/c}$ space group at a temperature of about 297 K;

[0101] unit cell dimensions $a=17.4829(11)$ Å, $b=7.3596(4)$ Å, $c=17.9504(11)$ Å, $\alpha=90^\circ$, $\beta=118.864(2^\circ)$, and $\gamma=90^\circ$;

[0102] an X-ray powder diffraction pattern substantially similar to FIG. 12; or

[0103] an X-ray powder diffraction pattern characterized by at least two peaks selected from 9.9, 11.6, and $13.3^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0104] E4. A composition comprising crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to any one of E1-E3 and an excipient.

[0105] E5. A composition comprising crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to any one of E1-E3 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.

[0106] E6. A method of preventing or treating a psychological disorder comprising the step of:

[0107] administering to a subject in need thereof a therapeutically effective amount of crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to any one of E1-E3.

[0108] E7. A method of preventing or treating a psychological disorder comprising the step of:

[0109] administering to a subject in need thereof a composition according to E4 or E5.

[0110] E8. A method of preventing or treating inflammation and/or pain comprising the step of:

[0111] administering to a subject in need thereof a therapeutically effective amount of crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to any one of E1-E3.

[0112] E9. A method of preventing or treating inflammation and/or pain comprising the step of:

[0113] administering to a subject in need thereof a composition according to E4 or E5.

[0114] E10. Crystalline [2-(1H-indol-3-yl)ethyl]tripropylazanium iodide (N,N,N-tri-n-propyltryptammonium iodide).

[0115] E11. Crystalline form 1 of [2-(1H-indol-3-yl)ethyl]tripropylazanium iodide (N,N,N-tri-n-propyltryptammonium iodide).

[0116] E12. Crystalline form 1 of N,N,N-tri-n-propyltryptammonium iodide according to E11, characterized by at least one of:

[0117] a monoclinic crystal system at a temperature of about 297 K;

[0118] a $P2_{1/n}$ space group at a temperature of about 297 K;

[0119] unit cell dimensions $a=7.4869(3)$ Å, $b=16.4570(7)$ Å, $c=16.2632(7)$ Å, $\alpha=90^\circ$, $\beta=96.2390(10^\circ)$, and $\gamma=90^\circ$;

[0120] an X-ray powder diffraction pattern substantially similar to FIG. 13; or

[0121] an X-ray powder diffraction pattern characterized by at least two peaks selected from 10.9, 15.4, and $21.2^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0122] E13. A composition comprising crystalline N,N,N-tri-n-propyltryptammonium iodide according to any one of E10-E12 and an excipient.

[0123] E14. A composition comprising crystalline N,N,N-tri-n-propyltryptammonium iodide according to any one of E10-E12 as a first component and a second component

selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.

[0124] E15. A method of preventing or treating a psychological disorder comprising the step of:

[0125] administering to a subject in need thereof a therapeutically effective amount of crystalline N,N,N-tri-n-propyltryptammonium iodide according to any one of E10-E12.

[0126] E16. A method of preventing or treating a psychological disorder comprising the step of:

[0127] administering to a subject in need thereof a composition according to E13 or E14.

[0128] E17. A method of preventing or treating inflammation and/or pain comprising the step of:

[0129] administering to a subject in need thereof a therapeutically effective amount of crystalline N,N,N-tri-n-propyltryptammonium iodide according to any one of E10-E12.

[0130] E18. A method of preventing or treating inflammation and/or pain comprising the step of:

[0131] administering to a subject in need thereof a composition according to E13 or E14.

[0132] E19. [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-N,N-di-n-isopropyltryptammonium iodide).

[0133] E20. Crystalline [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-N,N-di-n-isopropyltryptammonium iodide).

[0134] E21. Crystalline form 1 of [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-N,N-di-n-isopropyltryptammonium iodide).

[0135] E22. Crystalline form 1 of 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to E21, characterized by at least one of:

[0136] an orthorhombic crystal system at a temperature of about 300 K;

[0137] a Pbc_a space group at a temperature of about 300 K;

[0138] unit cell dimensions $a=8.2421(4)$ Å, $b=17.8313(8)$ Å, $c=24.8226(13)$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, and $\gamma=90^\circ$;

[0139] an X-ray powder diffraction pattern substantially similar to FIG. 14; or

[0140] an X-ray powder diffraction pattern characterized by at least two peaks selected from 7.1, 10.5, and $18.1^\circ 2\theta \pm 0.2^\circ 2\theta$.

[0141] E23. A composition comprising 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to E19 and an excipient.

[0142] E24. A composition comprising crystalline 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to any one of E20-E22 and an excipient.

[0143] E25. A composition comprising 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to E19 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.

[0144] E26. A composition comprising crystalline 5-chloro-N,N-di-n-isopropyltryptammonium iodide accord-

ing to any one of E20-E22 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.

[0145] E27. A method of preventing or treating a psychological disorder comprising the step of:

[0146] administering to a subject in need thereof a therapeutically effective amount of 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to E19.

[0147] E28. A method of preventing or treating a psychological disorder comprising the step of:

[0148] administering to a subject in need thereof a therapeutically effective amount of crystalline 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to any one of E20-E22.

[0149] E29. A method of preventing or treating a psychological disorder comprising the step of:

[0150] administering to a subject in need thereof a composition according to E23 or E25.

[0151] E30. A method of preventing or treating a psychological disorder comprising the step of:

[0152] administering to a subject in need thereof a composition according to E24 or E26.

[0153] E31. A method of preventing or treating inflammation and/or pain comprising the step of:

[0154] administering to a subject in need thereof a therapeutically effective amount of 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to E19.

[0155] E32. A method of preventing or treating inflammation and/or pain comprising the step of:

[0156] administering to a subject in need thereof a therapeutically effective amount of crystalline 5-chloro-N,N-di-n-isopropyltryptammonium iodide according to any one of E20-E22.

[0157] E33. A method of preventing or treating inflammation and/or pain comprising the step of:

[0158] administering to a subject in need thereof a composition according to E23 or E25.

[0159] E34. A method of preventing or treating inflammation and/or pain comprising the step of:

[0160] administering to a subject in need thereof a composition according to E24 or E26.

[0161] E35. 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate).

[0162] E36. Crystalline 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate).

[0163] E37. Crystalline form 1 of 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate).

[0164] E38. Crystalline form 1 of 5-chlorotryptammonium hydrogenoxalate according to E37, characterized by at least one of:

[0165] an orthorhombic crystal system at a temperature of about 300 K;

[0166] a Pna2₁ space group at a temperature of about 300 K;

[0167] unit cell dimensions $a=18.7293(13)$ Å, $b=5.6306(4)$ Å, $c=11.9021(6)$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, and $\gamma=90^\circ$;

[0168] an X-ray powder diffraction pattern substantially similar to FIG. 15; or

- [0169] an X-ray powder diffraction pattern characterized by at least two peaks selected from 9.4, 12.0, and $14.9^{\circ}2\theta \pm 0.2^{\circ}2\theta$.
- [0170] E39. A composition comprising 5-chlorotryptammonium hydrogenoxalate according to E35 and an excipient.
- [0171] E40. A composition comprising crystalline 5-chlorotryptammonium hydrogenoxalate according to any one of E36-E38 and an excipient.
- [0172] E41. A composition comprising 5-chlorotryptammonium hydrogenoxalate according to E35 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.
- [0173] E42. A composition comprising crystalline 5-chlorotryptammonium hydrogenoxalate according to any one of E36-E38 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.
- [0174] E43. A method of preventing or treating a psychological disorder comprising the step of:
- [0175] administering to a subject in need thereof a therapeutically effective amount of 5-chlorotryptammonium hydrogenoxalate according to E35.
- [0176] E44. A method of preventing or treating a psychological disorder comprising the step of:
- [0177] administering to a subject in need thereof a therapeutically effective amount of crystalline 5-chlorotryptammonium hydrogenoxalate according to any one of E36-E38.
- [0178] E45. A method of preventing or treating a psychological disorder comprising the step of:
- [0179] administering to a subject in need thereof a composition according to E39 or E41.
- [0180] E46. A method of preventing or treating a psychological disorder comprising the step of:
- [0181] administering to a subject in need thereof a composition according to E40 or E42.
- [0182] E47. A method of preventing or treating inflammation and/or pain comprising the step of:
- [0183] administering to a subject in need thereof a therapeutically effective amount of 5-chlorotryptammonium hydrogenoxalate according to E35.
- [0184] E48. A method of preventing or treating inflammation and/or pain comprising the step of:
- [0185] administering to a subject in need thereof a therapeutically effective amount of crystalline 5-chlorotryptammonium hydrogenoxalate according to any one of E36-E38.
- [0186] E49. A method of preventing or treating inflammation and/or pain comprising the step of:
- [0187] administering to a subject in need thereof a composition according to E39 or E41.
- [0188] E50. A method of preventing or treating inflammation and/or pain comprising the step of:
- [0189] administering to a subject in need thereof a composition according to E40 or E42.
- [0190] E51. Bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate).
- [0191] E52. Crystalline bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate).
- [0192] E53. Crystalline form 1 of bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate).
- [0193] E54. Crystalline form 1 of 5-chlorotryptammonium oxalate hydrate according to E53, characterized by at least one of:
- [0194] a monoclinic crystal system at a temperature of about 300 K;
- [0195] a P2/c space group at a temperature of about 300 K;
- [0196] unit cell dimensions $a=8.7014(9)$ Å, $b=10.8691(11)$ Å, $c=12.8386(11)$ Å, $\alpha=90^{\circ}$, $\beta=90.844(3)^{\circ}$, and $\gamma=90^{\circ}$;
- [0197] an X-ray powder diffraction pattern substantially similar to FIG. 16; or
- [0198] an X-ray powder diffraction pattern characterized by at least two peaks selected from 10.2, 13.8, and $20.4^{\circ}2\theta \pm 0.2^{\circ}2\theta$.
- [0199] E55. A composition comprising 5-chlorotryptammonium oxalate hydrate according to E51 and an excipient.
- [0200] E56. A composition comprising crystalline 5-chlorotryptammonium oxalate hydrate according to any one of E52-E54 and an excipient.
- [0201] E57. A composition comprising 5-chlorotryptammonium oxalate hydrate according to E51 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.
- [0202] E58. A composition comprising crystalline 5-chlorotryptammonium oxalate hydrate according to any one of E52-E54 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.
- [0203] E59. A method of preventing or treating a psychological disorder comprising the step of:
- [0204] administering to a subject in need thereof a therapeutically effective amount of 5-chlorotryptammonium oxalate hydrate according to E51.
- [0205] E60. A method of preventing or treating a psychological disorder comprising the step of:
- [0206] administering to a subject in need thereof a therapeutically effective amount of crystalline 5-chlorotryptammonium oxalate hydrate according to any one of E52-E54.
- [0207] E61. A method of preventing or treating a psychological disorder comprising the step of:
- [0208] administering to a subject in need thereof a composition according to E55 or E57.
- [0209] E62. A method of preventing or treating a psychological disorder comprising the step of:
- [0210] administering to a subject in need thereof a composition according to E56 or E58.

[0211] E63. A method of preventing or treating inflammation and/or pain comprising the step of:

[0212] administering to a subject in need thereof a therapeutically effective amount of 5-chlorotryptammonium oxalate hydrate according to E51.

[0213] E64. A method of preventing or treating inflammation and/or pain comprising the step of:

[0214] administering to a subject in need thereof a therapeutically effective amount of crystalline 5-chlorotryptammonium oxalate hydrate according to any one of E52-E54.

[0215] E65. A method of preventing or treating inflammation and/or pain comprising the step of:

[0216] administering to a subject in need thereof a composition according to E55 or E57.

[0217] E66. A method of preventing or treating inflammation and/or pain comprising the step of:

[0218] administering to a subject in need thereof a composition according to E56 or E58.

EXAMPLES

[0219] The preparation and characterization of each of crystalline form 1 of (2-{4-[(ethanesulfonyl)oxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride or 4-(ethylsulfonyloxy)-DPT chloride), crystalline form 1 of [2-(1H-indol-3-yl)ethyl]tripropylazanium iodide (N,N,N-tri-n-propyltryptammonium iodide or TPT iodide), crystalline form 1 of [2-(5-chloro-1H-indol-3-yl)ethyl]bis(propan-2-yl)azanium iodide (5-chloro-N,N-di-n-isopropyltryptammonium iodide or 5-Cl-DiPT iodide), crystalline form 1 of 2-(5-chloro-1H-indol-3-yl)ethan-1-aminium hydrogen oxalate (5-chlorotryptammonium hydrogenoxalate or 5-Cl-T hydrogenoxalate), and crystalline form 1 of bis(2-(5-chloro-1H-indol-3-yl)ethan-1-aminium) dihydrate oxalate (5-chlorotryptammonium oxalate hydrate or 5-Cl-T oxalate hydrate) are described below.

[0220] Single Crystal X-Ray Diffraction (SCXRD) Characterization: Data were collected on a Bruker D8 Venture CMOS Diffractometer equipped with an Oxford Cryosystems Cryostream cooling device and using Mo K α radiation. Structures were solved using the Bruker SHELXTL program and refined with the SHELXTL program as part of the Bruker SHELXTL suite, or OLEX2 software. Unless otherwise stated, hydrogen atoms attached to carbon were placed geometrically and allowed to refine with a riding isotropic displacement parameter. Hydrogen atoms attached to a heteroatom were located in a difference Fourier synthesis and were allowed to refine freely with an isotropic displacement parameter.

Preparation and Characterization of Crystalline Form 1 of 4-(Ethylsulfonyloxy)-DPT Chloride

Synthesis

[0221] At 0° C. to a reaction vial containing 3-(2-(dipropylamino)ethyl)-1H-indol-4-ol (0.4 mmol, 1 equiv) in anhydrous DCM (8 mL) was added triethylamine (2 equiv) followed by corresponding acid chloride (1.5 equiv) in a dropwise manner. The resulting contents were then stirred at room temperature under nitrogen until the disappearance of the starting material (per TLC). The typical reaction times were between 1.5 to 2 h. The reaction contents were then

diluted with DCM (20 mL) and washed twice with cold water followed by brine. The resulting organic layer was dried using sodium sulfate and reduced under pressure to afford a residue which was dissolved in toluene (10 mL). To the resulting solution was added HCl in ether (2M, 1.1 equiv) dropwise and stirred at room temperature for 15 min. In the case of sulfonates the residue after salt formation in toluene was subjected to column chromatography (DCM: MeOH) to obtain the desired compound. Off white solid, Yield 46%.

NMR

[0222] ¹H NMR (400 MHz, Deuterium Oxide) δ 7.45 (d, J=8.2 Hz, 1H), 7.30 (s, 1H), 7.19 (t, J=8.0 Hz, 1H), 7.03 (d, J=7.8 Hz, 1H), 3.60 (q, J=7.4 Hz, 2H), 3.48-3.34 (m, 2H), 3.34-3.19 (m, 2H), 3.07 (dd, J=10.4, 5.6 Hz, 4H), 1.62 (p, J=7.8 Hz, 4H), 1.48 (t, J=7.4 Hz, 3H), 0.85 (t, J=7.4 Hz, 6H).

[0223] ¹³C NMR (101 MHz, Chloroform-d) δ 142.7, 139.1, 125.0, 122.0, 119.6, 111.6, 110.9, 108.2, 54.5, 54.3, 45.2, 20.8, 17.1, 11.2, 8.2.

[0224] HRMS (ES+) m/z calc. for [C₁₈H₂₉N₂O₃S]⁺: 353.1893; found: 353.1900.

Crystallization

[0225] Single crystals suitable for X-ray diffraction studies were grown from the slow evaporation of an aqueous solution.

Single Crystal Characterization

[0226] The single crystal data and structure refinement parameters for the crystalline form 1 structure of 4-(ethylsulfonyloxy)-DPT chloride are reported in Table 3, below.

Preparation and Characterization of Crystalline Form 1 of TPT Iodide

Synthesis

[0227] 159 mg of tryptamine, 316 mg of sodium carbonate, and 1.5 mL of 1-iodopropane were dissolved in 10 mL of isopropanol. The solution was heated at reflux under nitrogen for twelve hours. The solvent was removed in vacuo to yield a yellow powder. The powder was triturated with diethyl ether to yield a pure yellow powder.

Crystallization

[0228] Single crystals suitable for X-ray diffraction studies were grown from a slow evaporation of an acetone/water solution of this solid.

Single Crystal Characterization

[0229] The single crystal data and structure refinement parameters for the crystalline form 1 structure of TPT iodide are reported in Table 3, below.

Preparation and Characterization of Crystalline Form 1 of 5-Cl-DiPT Iodide

Synthesis

[0230] 1.009 g (1 mmol) of 5-chlorotryptamine hydrochloride was dissolved in 50 mL of isopropyl alcohol, and 6.112 mL (14 mmol) of iodopropane, and 1.388 mg (3 mmol) of sodium carbonate were added. The mixture was

refluxed in air, showing a color change from off-white to orange after 36 hours of refluxing. The reaction mixture was filtered, to obtain off-white powder (72.6% yield).

NMR

[0231] ^1H NMR (400 MHz, D_2O): δ 7.67 (d, $J=2.0$ Hz, 1H, ArH), 7.50 (d, $J=8.6$ Hz, 1H, ArH), 7.26 (dd, $J=8.7$, 2.0 Hz, 1H, ArH), 3.81 (m, $J=6.6$ Hz, 2H, CH), 3.44-3.37 (m, 2H, CH_2), 3.25-3.19 (m, 2H, CH_2), 1.39 (d, $J=6.6$ Hz, 12H, CH_3).

Crystallization

[0232] Single crystals suitable for X-ray diffraction studies were grown from the slow evaporation of an acetone/water solution.

Single Crystal Characterization

[0233] The single crystal data and structure refinement parameters for the crystalline form 1 structure of 5-Cl-DiPT iodide are reported in Table 3, below.

Preparation and Characterization of Crystalline Form 1 of 5-Cl-T Oxalate Hydrate

Synthesis

[0234] 77 mg of free base 5-chlorotryptamine and 50 mg of oxalic acid dihydrate were dissolved in 12 mL of methanol. The solution was stirred and heated at reflux for 48 hours. The solution was cooled and solvent was removed in vacuo to yield the product as a powder.

Crystallization

[0235] Single crystals suitable for X-ray diffraction studies were grown from the slow evaporation of a methanol solution.

Single Crystal Characterization

[0236] The single crystal data and structure refinement parameters for the crystalline form 1 structure of 5-Cl-T hydrogenoxalate are reported in Table 3, below.

Preparation and Characterization of Crystalline Form 1 of 5-Cl-T Oxalate Hydrate

Synthesis

[0237] 76 mg of free base 5-chlorotryptamine and 25 mg of oxalic acid dihydrate were dissolved in 12 mL of methanol. The solution was stirred and heated at reflux for 48 hours. The solution was cooled and solvent was removed in vacuo to yield the product as a powder.

Crystallization

[0238] Single crystals suitable for X-ray diffraction studies were grown from the slow evaporation of a methanol solution.

Single Crystal Characterization

[0239] The single crystal data and structure refinement parameters for the crystalline form 1 structure of 5-Cl-T oxalate hydrate are reported in Table 3, below. The data for crystalline form 1 of 5-Cl-T oxalate hydrate in Table 3 relates to the asymmetric unit.

TABLE 3

Crystal data	Crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride	Crystalline form 1 of TPT iodide	Crystalline form 1 of 5-Cl-DiPT iodide	Crystalline form 1 of 5-Cl-T hydrogenoxalate	Crystalline form 1 of 5-Cl-T oxalate hydrate
Chemical formula	$\text{C}_{18}\text{H}_{29}\text{N}_2\text{O}_3\text{S}\cdot\text{Cl}$	$\text{I}\cdot\text{C}_{19}\text{H}_{31}\text{N}_2$	$\text{I}\cdot\text{C}_{16}\text{H}_{24}\text{ClN}_2$	$\text{C}_{10}\text{H}_{12}\text{ClN}_2\cdot\text{C}_2\text{HO}_4$	$\text{C}_{10}\text{H}_{12}\text{ClN}_2\cdot\text{CO}_2\cdot\text{H}_2\text{O}$
M_r	388.94	414.36	406.72	284.69	257.69
Crystal system, space group	monoclinic, $\text{P2}_1/c$	monoclinic, $\text{P2}_1/n$	orthorhombic, Pbca	orthorhombic, Pna2_1	monoclinic, $\text{P2}/c$
Temperature (K)	297 (2)	297 (2)	300 (2)	300 (2)	300 (2)
a, b, c (Å)	17.4829 (11), 7.3596 (4), 17.9504 (11)	7.4869 (3), 16.4570 (7), 16.2632 (7)	8.2421 (4), 17.8313 (8), 24.8226 (13)	18.7293 (13), 5.6306 (4), 11.9021 (6)	8.7014 (9), 10.8691 (11), 12.8386 (11)
α (°)	90	90	90	90	90
β (°)	118.864 (2)	96.2390 (10)	90	90	90.844 (3)
γ (°)	90	90	90	90	90
V (Å ³)	2022.7 (2)	1991.95 (14)	3648.1 (3)	1255.16 (14)	1214.1 (2)
Z	4	4	8	4	4
F(000)	832	848	1632	592	540
D_x (Mg m ⁻³)	1.277	1.382	1.481	1.507	1.410
Radiation type	Mo K α	Mo K α	Mo K α	Mo K α	Mo K α
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
θ (°)	2.67-25.51	2.78-26.39	2.81-26.04	2.77-26.31	3.00-25.65
μ (mm ⁻¹)	0.311	1.608	1.896	0.317	0.313
Crystal size (mm)	0.38 ×	0.27 ×	0.22 ×	0.3 ×	0.18 ×
Crystal description	BLOCK	BLOCK	block	block	block
Crystal color	colourless	colourless	colourless	colourless	colourless

TABLE 3-continued

Crystal data	Crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride	Crystalline form 1 of TPT iodide	Crystalline form 1 of 5-Cl-DiPT iodide	Crystalline form 1 of 5-Cl-T hydrogenoxalate	Crystalline form 1 of 5-Cl-T oxalate hydrate
Data collection					
Diffractionmeter	Bruker APEX-II CCD	Bruker APEX-II CCD	Bruker APEX-II CCD	Bruker APEX-II CCD	Bruker APEX-II CCD
Absorption correction	Multi-scan SADABS (Bruker, 2016) was used. wR2(int) was 0.0735 before and 0.0670 after correction. The Ratio of minimum to maximum transmission is 0.9207. The $\lambda/2$ correction factor is not present.	Multi-scan SADABS (Bruker, 2016) was used. wR2(int) was 0.0596 before and 0.0455 after correction. The Ratio of minimum to maximum transmission is 0.9112. The $\lambda/2$ correction factor is not present.	Multi-scan SADABS (Bruker, 2016) was used. wR2(int) was 0.0643 before and 0.0541 after correction. The Ratio of minimum to maximum transmission is 0.8607. The $\lambda/2$ correction factor is not present.	Multi-scan SADABS (Bruker, 2016) was used. wR2(int) was 0.0591 before and 0.0541 after correction. The Ratio of minimum to maximum transmission is 0.9453. The $\lambda/2$ correction factor is not present.	Multi-scan SADABS (Bruker, 2016) was used. wR2(int) was 0.0577 before and 0.0517 after correction. The Ratio of minimum to maximum transmission is 0.9628. The $\lambda/2$ correction factor is not present.
T_{min} , T_{max}	0.6862, 0.7453	0.6792, 0.7454	0.6416, 0.7454	0.7046, 0.7454	0.7176, 0.7453
No. of measured, independent, and observed [$I > 2\sigma(I)$] reflections	41583, 3842, 3060	55412, 4056, 3612	49055, 3742, 2750	39843, 2553, 2497	37212, 2311, 2033
R_{int}	0.0593	0.0286	0.0573	0.0354	0.0377
θ_{max} , θ_{min} (°)	25.754, 2.591	26.406, 3.004	26.398, 2.813	26.386, 2.768	25.707, 2.999
h, k, l	-21 \rightarrow 21, -8 \rightarrow 8, -21 \rightarrow 21	-9 \rightarrow 9, -20 \rightarrow 20, -20 \rightarrow 20	-10 \rightarrow 10, -22 \rightarrow 22, -31 \rightarrow 31	-23 \rightarrow 23, -7 \rightarrow 7, -14 \rightarrow 14	-10 \rightarrow 10, -13 \rightarrow 13, -15 \rightarrow 14
Refinement					
$R[F^2 > 2\sigma(F^2)]$, wR(F ²), S	0.0610, 0.1606, 1.054	0.0206, 0.0502, 1.064	0.0425, 0.0991, 1.109	0.0258, 0.0639, 1.082	0.0362, 0.0963, 1.030
No. of reflections	3842	4056	3742	2553	2311
No. of parameters	234	206	203	192	178
No. of restraints	2	1	14	6	7
Absolute structure	—	—	—	Flack x determined using 1133 quotients [(I+) - (I-)]/[(I+) + (I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	—
Absolute structure parameter	—	—	—	0.010 (13)	—
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
w	$w = 1/[\sigma^2(F_o^2) + (0.0570P)^2 + 2.3852P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0202P)^2 + 0.7301P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 5.8047P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 0.3076P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.6638P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	0.000	0.002	0.000	0.000	0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.708, -0.366	0.397, -0.305	0.393, -0.626	0.148, -0.151	0.273, -0.291

TABLE 3-continued

Crystal data	Crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride	Crystalline form 1 of TPT iodide	Crystalline form 1 of 5-Cl-DiPT iodide	Crystalline form 1 of 5-Cl-T hydrogenoxalate	Crystalline form 1 of 5-Cl-T oxalate hydrate
Software					
Data collection	Bruker APEX3	Bruker APEX3	Bruker APEX4	Bruker APEX4	Bruker APEX4
Cell	Bruker SAINT	Bruker SAINT	Bruker SAINT	Bruker SAINT	Bruker SAINT
refinement					
Data reduction	Bruker SAINT	Bruker SAINT	Bruker SAINT	Bruker SAINT	Bruker SAINT
Structure	SHELXS	SHELXS-97	SHELXS-97	SHELXS-97	SHELXS-97
solution	(Sheldrick, 2008)	(Sheldrick, 2008)	(Sheldrick, 2008)	(Sheldrick, 2008)	(Sheldrick, 2008)
Structure refinement	SHELXL 2018/3 (Sheldrick, 2015)	SHELXL 2018/3 (Sheldrick, 2015)	SHELXL 2018/3 (Sheldrick, 2015)	SHELXL 2018/3 (Sheldrick, 2015)	SHELXL 2018/3 (Sheldrick, 2015)
Molecular graphics	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)
Publication material preparation	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)	Olex2 1.3 (Dolomanov et al., 2009)

[0240] FIG. 1 shows the molecular structure of crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride, showing the atomic labeling.

[0241] FIG. 2 shows the molecular structure of crystalline form 1 of TPT iodide, showing the atomic labeling.

[0242] FIG. 3 shows the molecular structure of crystalline form 1 of 5-Cl-DiPT iodide, showing the atomic labeling.

[0243] FIG. 4 shows the molecular structure of crystalline form 1 of 5-Cl-T hydrogenoxalate, showing the atomic labeling.

[0244] FIG. 5 shows the molecular structure of crystalline form 1 of 5-Cl-T oxalate hydrate, showing the atomic labeling.

[0245] FIG. 6 shows the unit cell of crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride along the b-axis.

[0246] FIG. 7 shows the unit cell of crystalline form 1 of TPT iodide along the a-axis.

[0247] FIG. 8 shows the unit cell of crystalline form 1 of 5-Cl-DiPT iodide along the b-axis.

[0248] FIG. 9 shows the unit cell of crystalline form 1 of 5-Cl-T hydrogenoxalate along the b-axis.

[0249] FIG. 10 shows the unit cell of crystalline form 1 of 5-Cl-T oxalate hydrate along the b-axis.

[0250] FIG. 11 shows the 2 tryptamine: 2 water: 1 oxalate ratio of crystalline form 1 of 5-Cl-T oxalate hydrate as a dimer.

Simulated Powder X-ray Diffraction (PXRD) Pattern

[0251] FIG. 12 shows a simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride generated from its single crystal data. Table 4 lists the angles, $^{\circ}2\theta \pm 0.2^{\circ}2\theta$, and d-spacing of the peaks identified in the experimental XRPD pattern of FIG. 12. The entire list of peaks, or a subset thereof, may be sufficient to characterize the cocrystal. For example, the cocrystal may be characterized by at least two peaks selected from the peaks at 9.9, 11.6, and $13.3^{\circ}2\theta \pm 0.2^{\circ}2\theta$ or their corresponding d-spacing as well as by an XRPD pattern substantially similar to FIG. 12.

Simulated Powder X-Ray Diffraction (PXRD) Pattern

[0252] FIG. 13 shows a simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of TPT iodide generated from its single crystal data. Table 5 lists the angles, $^{\circ}2\theta \pm 0.2^{\circ}2\theta$, and d-spacing of the peaks identified in the experimental XRPD pattern of FIG. 13. The entire list of peaks, or a subset thereof, may be sufficient to characterize the cocrystal. For example, the cocrystal may be characterized by at least two peaks selected from the peaks at 10.9, 15.4, and $21.2^{\circ}2\theta \pm 0.2^{\circ}2\theta$ or their corresponding d-spacing as well as by an XRPD pattern substantially similar to FIG. 13.

Simulated Powder X-Ray Diffraction (PXRD) Pattern

[0253] FIG. 14 shows a simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 5-Cl-DiPT iodide generated from its single crystal data. Table 6 lists the angles, $^{\circ}2\theta \pm 0.2^{\circ}2\theta$, and d-spacing of the peaks identified in the experimental XRPD pattern of FIG. 14. The entire list of peaks, or a subset thereof, may be sufficient to characterize the cocrystal. For example, the cocrystal may be characterized by at least two peaks selected from the peaks at 7.1, 10.5, and $18.1^{\circ}2\theta \pm 0.2^{\circ}2\theta$ or their corresponding d-spacing as well as by an XRPD pattern substantially similar to FIG. 14.

Simulated Powder X-ray Diffraction (PXRD) Pattern

[0254] FIG. 15 shows a simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 5-Cl-T hydrogenoxalate generated from its single crystal data. Table 7 lists the angles, $^{\circ}2\theta \pm 0.2^{\circ}2\theta$, and d-spacing of the peaks identified in the experimental XRPD pattern of FIG. 15. The entire list of peaks, or a subset thereof, may be sufficient to characterize the cocrystal. For example, the cocrystal may be characterized by at least two peaks selected from the peaks at 9.4, 12.0, and $14.9^{\circ}2\theta \pm 0.2^{\circ}2\theta$ or their corresponding d-spacing as well as by an XRPD pattern substantially similar to FIG. 15.

Simulated Powder X-ray Diffraction (PXRD) Pattern

[0255] FIG. 16 shows a simulated X-ray powder diffraction pattern (XRPD) for crystalline form 1 of 5-Cl-T oxalate

hydrate generated from its single crystal data. Table 8 lists the angles, $^{\circ} 2\theta \pm 0.2^{\circ} 2\theta$, and d-spacing of the peaks identified in the experimental XRPD pattern of FIG. 16. The entire list of peaks, or a subset thereof, may be sufficient to characterize the cocrystal. For example, the cocrystal may be characterized by at least two peaks selected from the peaks at 10.2, 13.8, and $20.4^{\circ} 2\theta \pm 0.2^{\circ} 2\theta$ or their corresponding d-spacing as well as by an XRPD pattern substantially similar to FIG. 16.

TABLE 4

Crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride		
d-spacing (Å)	$^{\circ} 2\theta \pm 0.2^{\circ} 2\theta$	Intensity
15.31	5.77	1000
8.97	9.85	10895
7.86	11.25	17
7.66	11.55	21
7.62	11.60	8291
6.67	13.27	137
6.63	13.34	27707
6.63	13.35	19348
5.93	14.94	151
5.73	15.46	67807
5.70	15.53	62661
5.69	15.56	19859
5.63	15.73	552
5.37	16.49	18498
5.31	16.70	16971
5.30	16.73	27
5.10	17.36	864
4.62	19.21	19599
4.61	19.25	1304
4.58	19.35	251
4.57	19.41	55522
4.52	19.61	4544
4.52	19.63	19339
4.50	19.69	1092
4.48	19.78	2189
4.37	20.30	8120
4.35	20.42	16019
4.27	20.79	3496
4.26	20.82	19342
4.19	21.17	5351
4.18	21.23	17694
3.93	22.61	39290
3.84	23.13	47787
3.83	23.21	18944
3.83	23.22	37467
3.81	23.32	36991
3.76	23.66	5253
3.75	23.72	14637
3.74	23.76	6215
3.70	24.01	989
3.69	24.10	516
3.68	24.17	67587
3.66	24.31	51236
3.65	24.36	17353
3.58	24.83	63382
3.58	24.86	22960
3.58	24.87	36162
3.57	24.95	27970
3.48	25.60	10
3.47	25.68	10734
3.43	25.96	11329
3.41	26.14	17163
3.40	26.15	52667
3.40	26.22	30946
3.39	26.25	274
3.38	26.31	5713
3.33	26.73	23444
3.32	26.86	30348
3.31	26.88	44058
3.31	26.90	1571
3.23	27.62	2874

TABLE 4-continued

Crystalline form 1 of 4-(ethylsulfonyloxy)-DPT chloride		
d-spacing (Å)	$^{\circ} 2\theta \pm 0.2^{\circ} 2\theta$	Intensity
3.22	27.70	1804
3.21	27.78	3864
3.20	27.89	20727
3.14	28.37	21150
3.14	28.39	1020
3.13	28.53	19479
3.12	28.55	5202
3.12	28.62	3982
3.11	28.66	45572
3.11	28.70	31847
3.10	28.74	1230
3.10	28.80	66
3.10	28.82	9368
3.06	29.14	18
3.06	29.16	832
3.05	29.28	697
3.03	29.48	4615
3.02	29.55	1239
3.01	29.64	8777
2.99	29.86	9404
2.98	29.91	5901
2.98	29.95	9999

TABLE 5

Crystalline Form 1 of TPT iodide		
d-spacing (Å)	$^{\circ} 2\theta \pm 0.2^{\circ} 2\theta$	Intensity
11.53	7.66	623
8.23	10.74	4876
8.08	10.94	89090
7.33	12.06	2339
7.26	12.19	18145
7.06	12.53	8287
6.78	13.04	17550
6.50	13.62	4580
6.49	13.64	31576
6.04	14.64	8337
5.77	15.35	55244
5.52	16.04	3310
5.47	16.19	22408
5.36	16.53	21343
5.19	17.05	3663
5.12	17.30	23082
5.10	17.38	17548
4.96	17.87	45435
4.74	18.71	289
4.61	19.24	5232
4.54	19.54	13592
4.51	19.68	38414
4.44	19.99	12306
4.42	20.09	6282
4.40	20.18	16951
4.33	20.49	254228
4.19	21.18	223050
4.16	21.36	192
4.11	21.58	3668
4.04	21.97	36417
4.03	22.04	166952
4.02	22.09	783
3.99	22.28	110600
3.98	22.29	7742
3.93	22.64	3568
3.84	23.12	46250
3.77	23.55	188162
3.72	23.89	51553
3.71	23.97	76272
3.67	24.25	10769
3.63	24.48	176761

TABLE 5-continued

Crystalline Form 1 of TPT iodide		
d-spacing (Å)	$2\theta \pm 0.2^\circ 2\theta$	Intensity
3.63	24.50	2793
3.63	24.52	64074
3.62	24.54	17601
3.60	24.70	7330
3.55	25.03	3166
3.53	25.21	141511
3.53	25.22	171439
3.48	25.61	5043
3.46	25.70	10
3.45	25.80	1235
3.39	26.24	879
3.39	26.26	81189
3.39	26.29	60440
3.36	26.54	18124
3.33	26.75	70855
3.31	26.89	28776
3.27	27.25	77893
3.25	27.38	68609
3.25	27.39	16032
3.25	27.43	53073
3.24	27.48	109806
3.23	27.62	3199
3.23	27.63	1
3.19	27.97	15171
3.17	28.10	19247
3.17	28.12	114
3.14	28.38	257
3.09	28.86	4891
3.08	28.95	20268
3.08	28.97	487
3.08	29.00	4379
3.07	29.07	53
3.05	29.27	5848
3.04	29.38	23963
3.02	29.54	25328
3.01	29.65	40602
3.01	29.66	29209
3.01	29.68	34326
2.98	29.93	93009
2.98	30.00	722

TABLE 6

Crystalline form 1 of 5-Cl-DiPT iodide		
d-spacing (Å)	$2\theta \pm 0.2^\circ 2\theta$	Intensity
12.41	7.12	5245
8.92	9.91	5955
8.39	10.53	141789
7.24	12.21	42001
7.16	12.35	49929
6.87	12.88	3495
6.41	13.81	33677
6.21	14.26	125410
6.06	14.59	598740
5.88	15.05	112375
5.55	15.96	164366
5.44	16.28	112105
5.09	17.40	4400
4.96	17.88	4552
4.88	18.15	247292
4.78	18.56	55143
4.73	18.73	269241
4.49	19.74	116800
4.46	19.90	367110
4.39	20.22	22153
4.34	20.46	339478
4.33	20.48	63197
4.20	21.16	175080

TABLE 6-continued

Crystalline form 1 of 5-Cl-DiPT iodide		
d-spacing (Å)	$2\theta \pm 0.2^\circ 2\theta$	Intensity
4.17	21.31	113247
4.14	21.46	78231
4.14	21.46	3113
4.12	21.55	53189
4.02	22.12	498176
3.96	22.41	180294
3.92	22.64	58879
3.91	22.72	11578
3.87	22.94	54433
3.84	23.15	34424
3.82	23.26	546461
3.81	23.35	64284
3.75	23.69	84700
3.74	23.77	56309
3.74	23.78	118118
3.70	24.04	315726
3.70	24.05	381442
3.62	24.57	190553
3.62	24.57	291426
3.61	24.62	1071160
3.58	24.84	33684
3.54	25.11	15090
3.46	25.74	7268
3.43	25.93	136000
3.42	26.07	53137
3.41	26.12	57848
3.39	26.29	203848
3.37	26.42	186654
3.36	26.54	50107
3.32	26.86	5327
3.31	26.87	373553
3.30	27.04	761668
3.27	27.27	391239
3.24	27.46	39393
3.20	27.82	14913
3.20	27.82	10930
3.16	28.17	153660
3.14	28.40	115306
3.13	28.45	419668
3.12	28.57	311606
3.10	28.75	27170
3.08	28.99	1584
3.06	29.16	64001
3.04	29.32	19469
3.03	29.43	97962
3.03	29.49	19108
3.00	29.72	37663
2.99	29.88	34669

TABLE 7

Crystalline form 1 of 5-Cl-T hydrogenoxalate		
d-spacing (Å)	$2\theta \pm 0.2^\circ 2\theta$	Intensity
9.36	9.44	1251
7.36	12.02	2354
5.95	14.87	6064
5.39	16.43	26
5.09	17.41	738
5.02	17.64	7572
4.91	18.05	3123
4.83	18.37	20507
4.68	18.94	13785
4.47	19.84	339
4.36	20.36	44063
4.18	21.23	1856
4.00	22.23	128658
3.94	22.52	4661
3.75	23.72	6557

TABLE 7-continued

Crystalline form 1 of 5-Cl-T hydrogenoxalate		
d-spacing (Å)	$2\theta \pm 0.2^\circ 2\theta$	Intensity
3.68	24.17	55354
3.65	24.35	14764
3.60	24.71	1689
3.45	25.83	15191
3.42	26.02	35056
3.24	27.48	60688
3.20	27.90	14377
3.12	28.57	960
3.12	28.60	11065
3.08	28.96	2042
3.06	29.11	29220
3.03	29.49	14842
3.02	29.56	75440
3.02	29.59	6796

TABLE 8

Crystalline form 1 of 5-Cl-T oxalate hydrate		
d-spacing (Å)	$2\theta \pm 0.2^\circ 2\theta$	Intensity
10.87	8.13	122
8.70	10.16	2709
8.30	10.66	2388
6.79	13.02	2377
6.42	13.79	5623
6.03	14.67	391
5.98	14.81	950
5.53	16.02	0
5.43	16.30	2788
5.20	17.03	7998
5.13	17.27	5255
5.00	17.71	5236
4.69	18.90	3679
4.64	19.12	7986
4.61	19.24	23610
4.35	20.40	15525
4.35	20.40	28988
4.33	20.51	5294
4.15	21.41	83776
4.04	21.99	13386
3.98	22.31	4515
3.87	22.97	2732
3.84	23.16	272
3.76	23.66	13379
3.73	23.83	17044
3.64	24.44	993
3.63	24.53	1623
3.62	24.55	2901
3.60	24.70	4889
3.58	24.87	1867
3.49	25.53	103
3.44	25.88	9921
3.40	26.21	10803
3.40	26.22	3815
3.36	26.49	1876
3.34	26.63	82
3.29	27.06	17130
3.27	27.22	63
3.24	27.50	17016
3.23	27.57	25739
3.21	27.77	533
3.16	28.26	31399
3.15	28.32	336

TABLE 8-continued

Crystalline form 1 of 5-Cl-T oxalate hydrate		
d-spacing (Å)	$2\theta \pm 0.2^\circ 2\theta$	Intensity
3.12	28.55	29
3.08	28.99	11730
3.03	29.50	10696
3.02	29.59	20011
3.00	29.79	210
2.99	29.88	6001

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- [0257] Sheldrick, G. M. (2015). *Acta Cryst. C* 71, 3-8.
- (canceled)
 - Crystalline form 1 of (2-{4-[(ethanesulfonyl)oxy]-1H-indol-3-yl}ethyl)dipropylazanium chloride (4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride).
 - Crystalline form 1 of 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to claim 2, characterized by at least one of:
 - a monoclinic crystal system at a temperature of about 297 K;
 - a $P2_{1/c}$ space group at a temperature of about 297 K;
 - unit cell dimensions $a=17.4829(11)$ Å, $b=7.3596(4)$ Å, $c=17.9504(11)$ Å, $\alpha=90^\circ$, $\beta=118.864(2^\circ)$, and $\gamma=90^\circ$;
 - an X-ray powder diffraction pattern substantially similar to FIG. 12; or
 - an X-ray powder diffraction pattern characterized by at least two peaks selected from 9.9, 11.6, and $13.3^\circ 2\theta \pm 0.2^\circ 2\theta$.
 - A composition comprising crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to claim 2 and an excipient.
 - A composition comprising crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to claim 2 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.
 - (canceled)
 - A composition comprising crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to claim 3 and an excipient.
 - A composition comprising crystalline 4-(ethylsulfonyloxy)-N,N-di-n-propyltryptammonium chloride according to claim 3 as a first component and a second component selected from at least one of (a) a serotonergic drug, (b) a purified psilocybin derivative, (c) a purified cannabinoid, (d) a purified terpene, (e) an adrenergic drug, (f) a dopaminergic drug, (g) a monoamine oxidase inhibitor, (h) a purified erinacine, and (i) a purified hericenone.

* * * * *