

Beyond boundaries: unveiling the art of blockchain-enshrined molecules through xSublimatio

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Supplementary Data

Table S1: Molecule description. Brief description of the 63 active ingredients found in xSublimatio, together with their chemical formula and a link to the database containing their physical and chemical characteristics. These elements have been used by AlphaFold and Avogadro to create the 3D structures of the molecules, which are encrypted by the Smart Contract. Abbreviations: CBD: Cannabidiol - CBC: Cannabichromene - CBG: Cannabigerol - CBN: Cannabinol - THC: Tetrahydrocannabinol - GHB: Gamma-Hydroxybutyrate - LSD: Lysergic Acid Diethylamide - DMT: Dimethyltryptamine - MDMA: 3,4-Methylenedioxymethamphetamine.

INDEX	Active Principle	Description	Chemical Formula	Reference
0	Water	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
1	Alcohol	Psychotropic drug used in various applications including perfumery.	CH ₃ CH ₂ OH	https://pubchem.ncbi.nlm.nih.gov/compound/702
2	Methamphetamine	Highly addictive synthetic drug producing euphoric effects.	C ₁₀ H ₁₅ N	https://pubchem.ncbi.nlm.nih.gov/compound/10836
3	Caffeine	Stimulant and mild diuretic alkaloid.	C ₈ H ₁₀ N ₄ O ₂	https://pubchem.ncbi.nlm.nih.gov/compound/2519
4	Theobromine	Stimulant and mild diuretic alkaloid, found in dark chocolate.	C ₇ H ₈ N ₄ O ₂	https://pubchem.ncbi.nlm.nih.gov/compound/5429
5	Cathine	Phenylethylamine alkaloid derived from cathinone.	C ₉ H ₁₃ NO	https://pubchem.ncbi.nlm.nih.gov/compound/441457
6	Cathinone	Alkaloid found in khat leaves with amphetamine-like effects.	C ₉ H ₁₁ NO	https://pubchem.ncbi.nlm.nih.gov/compound/62258
7	Methcathinone	Pharmacological characteristics similar to amphetamines.	C ₁₀ H ₁₃ NO	https://pubchem.ncbi.nlm.nih.gov/compound/1576
8	Cocaine	Stimulant alkaloid extracted from coca leaves.	C ₁₇ H ₂₁ NO ₄	https://pubchem.ncbi.nlm.nih.gov/compound/446220
9	CBD	active compound in hemp, similar to THC.	C ₂₁ H ₃₀ O ₂	https://pubchem.ncbi.nlm.nih.gov/compound/Cannabidiol
10	Cannabichromene	Cannabichromene is an anti-	C ₂₁ H ₃₀ O ₂	https://pubchem.ncbi.nlm.nih.gov/compound/Cannabichromene

		inflammatory cannabinoid.		mpound/30219
11	CBG	Another cannabinoid found in hemp with potential therapeutic effects.	$C_{21}H_{32}O_2$	https://pubchem.ncbi.nlm.nih.gov/compound/5315659
12	Cannabinol	Sedative cannabinoid resulting from THC oxidation.	$C_{21}H_{26}O_2$	https://pubchem.ncbi.nlm.nih.gov/compound/2543
13	THC	Main psychoactive compound in cannabis.	$C_{21}H_{30}O_2$	https://pubchem.ncbi.nlm.nih.gov/compound/12831993
14	Morphine	Potent analgesic alkaloid derived from poppy latex.	$C_{17}H_{19}NO_3$	https://pubchem.ncbi.nlm.nih.gov/compound/5288826
15	Ketamine	Psychotropic anesthetic with emerging antidepressant uses.	$C_{13}H_{16}ClNO$	https://pubchem.ncbi.nlm.nih.gov/compound/3821
16	Atropine	Tropane alkaloid with antispasmodic properties.	$C_{17}H_{23}NO_3$	https://pubchem.ncbi.nlm.nih.gov/compound/174174
17	Hyoscyamine	Blocks certain neurotransmitter actions in the nervous system.	$C_{17}H_{23}NO_3$	https://pubchem.ncbi.nlm.nih.gov/compound/154417
18	Scopolamine	Parasympatholytic agent with sedative effects.	$C_{17}H_{21}NO_4$	https://pubchem.ncbi.nlm.nih.gov/compound/3000322
19	Lactucin	Bitter compound responsible for lactucarium's properties.	$C_{15}H_{16}O_5$	https://pubchem.ncbi.nlm.nih.gov/compound/442266
20	Lactucopicrin	Bitter compound with sedative properties.	$C_{23}H_{22}O_7$	https://pubchem.ncbi.nlm.nih.gov/compound/174880
21	Lactuside A	Sesquiterpene lactone involved in plant defense.	$C_{21}H_{30}O_9$	https://pubchem.ncbi.nlm.nih.gov/compound/Lactuside-A
22	Codeine	Analgesic alkaloid found in poppy, similar to morphine.	$C_{18}H_{21}NO_3$	https://pubchem.ncbi.nlm.nih.gov/compound/5284371
23	Noscapine	Alkaloid with morphine-like properties but less addictive.	$C_{22}H_{23}NO_7$	https://pubchem.ncbi.nlm.nih.gov/compound/275196
24	Papaverine	Muscle relaxant and vasodilator alkaloid.	$C_{20}H_{22}ClNO_4$	https://pubchem.ncbi.nlm.nih.gov/compound/6084
25	Baeocystin	Psychoactive compound found in certain mushrooms.	$C_{11}H_{15}N_2O_4P$	https://pubchem.ncbi.nlm.nih.gov/compound/161359
26	Norbaeocystin	Psychoactive analog of psilocybin.	$C_{10}H_{13}N_2O_4P$	https://pubchem.ncbi.nlm.nih.gov/compound/9795063
27	Psilocin	Hallucinogenic alkaloid found in psychedelic mushrooms.	$C_{12}H_{16}N_2O$	https://pubchem.ncbi.nlm.nih.gov/compound/4980
28	Psilocybin	Hallucinogenic compound in various	$C_{12}H_{17}N_2O_4P$	https://pubchem.ncbi.nlm.nih.gov/compound/30219

		mushrooms.		mpound/10624
29	Belladonnine	Tropane alkaloid found in Solanaceae plants.	$C_{34}H_{42}N_2O_4$	https://pubchem.ncbi.nlm.nih.gov/compound/442995
30	Scopoletin	Potential anti-inflammatory and antioxidant effects.	$C_{10}H_8O_4$	https://pubchem.ncbi.nlm.nih.gov/compound/5280460
31	GHB	Endogenous sedative substance in mammals.	$C_4H_8O_3$	https://pubchem.ncbi.nlm.nih.gov/compound/10413
32	LSD	Powerful hallucinations as a lysergamide.	$C_{20}H_{25}N_3O$	https://pubchem.ncbi.nlm.nih.gov/compound/5761
33	Chloroquine	Synthetic antimalarial drug.	$C_{18}H_{26}ClN_3$	https://pubchem.ncbi.nlm.nih.gov/compound/2719
34	Mandragorin	Toxic alkaloid from mandrake roots.	$C_{13}H_{24}N_2O$	https://pubchem.ncbi.nlm.nih.gov/compound/1201543
35	Divinatorin A	Is named after constituents of Salvia divinorum.	$C_{20}H_{28}O_4$	https://pubchem.ncbi.nlm.nih.gov/compound/10882157
36	Divinatorin B	Is named after constituents of Salvia divinorum.	$C_{21}H_{30}O_5$	https://pubchem.ncbi.nlm.nih.gov/compound/11057551
37	DMT	Fast-acting hallucinogen.	$C_{12}H_{16}N_2$	https://pubchem.ncbi.nlm.nih.gov/compound/6089
38	Harmol	Natural product with β -carboline classification.	$C_{12}H_{10}N_2O$	https://pubchem.ncbi.nlm.nih.gov/compound/68094
39	Nicotine	Psychotropic alkaloid from tobacco.	$C_{10}H_{14}N_2$	https://pubchem.ncbi.nlm.nih.gov/compound/89594
40	Salvidivin B	Metabolite of the hallucinogen Salvinorin A.	$C_{23}H_{28}O_{10}$	https://pubchem.ncbi.nlm.nih.gov/compound/16099522
41	Salvinicin A	Hallucinogen in Salvia divinorum.	$C_{25}H_{36}O_{12}$	https://pubchem.ncbi.nlm.nih.gov/compound/11466688
42	Salvinorin A	Active hallucinogen in Salvia divinorum.	$C_{23}H_{28}O_8$	https://pubchem.ncbi.nlm.nih.gov/compound/128563
43	Telepathine	Plant alkaloid with hallucinogenic properties.	$C_{13}H_{12}N_2O$	https://pubchem.ncbi.nlm.nih.gov/compound/5280953
44	Tetrahydro-harmine	Fluorescent indole alkaloid with psychoactive potential.	$C_{13}H_{16}N_2O$	https://pubchem.ncbi.nlm.nih.gov/compound/159809
45	Acetylcholine	Neurotransmitter involved in memory and muscle activity.	$C_7H_{16}NO_2$	https://pubchem.ncbi.nlm.nih.gov/compound/187
46	Dopamine	Affects motivation and is known as	$C_8H_{11}NO_2$	https://pubchem.ncbi.nlm.nih.gov/compound/10624

		the happiness hormone.		mpound/681
47	Dynorphin	Opioid peptides from prodynorphin, influencing pain, addiction, and mood.	C ₉₉ H ₁₅₅ N ₃₁ O ₂₃	https://pubchem.ncbi.nlm.nih.gov/compound/16129685
48	Met- enkephalin	Endogenous opioid neurotransmitter released during intense pain.	C ₂₇ H ₃₅ N ₅ O ₇ S	https://pubchem.ncbi.nlm.nih.gov/compound/443363
49	MDMA	Or ecstasy. Stimulates the CNS with mild hallucinogenic effects.	C ₁₁ H ₁₆ ClNO ₂	https://pubchem.ncbi.nlm.nih.gov/compound/71285
50	Oxytocin	Neuropeptide, affects trust, empathy, and sexuality.	C ₄₃ H ₆₆ N ₁₂ O ₁₂ S ₂	https://pubchem.ncbi.nlm.nih.gov/compound/439302
51	Phenethylamine	Monoamine alkaloid, acts as a neurotransmitter and is found in some foods.	C ₈ H ₁₁ N	https://pubchem.ncbi.nlm.nih.gov/compound/1001
52	Water (Ayahuasca)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
53	Water (Belladonna)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
54	Water (Cannabis)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
55	Water (Khat)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
56	Water (Lactuca Virosa)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
57	Water (Love Elixir)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
58	Water (Magic Truffle)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
59	Water (Mandrake)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
60	Water (Mate)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
61	Water (Opium)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962
62	Water (Salvia Divinorum)	Stable solvent.	H ₂ O	https://pubchem.ncbi.nlm.nih.gov/compound/962

Table S2: Molecule classification. The list of active ingredients by drug is not exhaustive. Here, we have selected active principles with evocative names that are familiar to the public because of their roots in pop culture. For example, to represent seer's sage (*Salvia Divinorum*), Divinatorin has been chosen, as has Lactucine for opium lettuce (*Lactuca Virosa*), Belladonnine for belladonna, mandragorin (=cuscohygrin) for mandrake, telepathine (=harmine) in the Ayawaska hallucinogenic plant mix and so on. LOVE elixir is the drug developed by Pierre Pauze for the Please Love Party project (2019) and contains the following active principles: cannabidiol, acetylcholine, dopamine, dynorphin, met-enkephalin, MDMA, oxytocin, phenylethylamine and water. Abbreviations: CBD: Cannabidiol - CBC: Cannabichromene - CBG: Cannabigerol - CBN: Cannabinol - THC: Tetrahydrocannabinol - GHB: Gamma-Hydroxybutyrate - LSD: Lysergic Acid Diethylamide - DMT: Dimethyltryptamine - MDMA: 3,4-Methylenedioxymethamphetamine.

INDEX	ACTIVE PRINCIPLE	ORIGIN	DRUG	CLASSIFICATION	"
0	Water		None	Natural	None
1	Alcohol	Alcoholic fermentation	Ethanol	Natural	Depressant
2	Methamphetamine	Synthetic drug	Crystal meth	Synthetic	Stimulant
3	Caffeine	<i>Ilex paraguariensis</i>	Mate	Natural	Stimulant
4	Theobromine	<i>Ilex paraguariensis</i>	Mate	Natural	Stimulant
5	Cathine	<i>Catha edulis</i>	Khat	Natural	Stimulant
6	Cathinone	<i>Catha edulis</i>	Khat	Natural	Stimulant
7	Methcathinone	Pseudoephedrine	Pseudoephedrine	Synthetic	Stimulant
8	Cocaine	<i>Erythroxylum coca</i>	Cocaine	Natural	Stimulant
9	CBD	<i>Cannabis sativa</i>	Cannabis	Natural	Neuroleptic
10	CBC	<i>Cannabis sativa</i>	Cannabis	Natural	Depressant, stimulant, hallucinogenic, neuroleptic
11	CBG	<i>Cannabis sativa</i>	Cannabis	Natural	None
12	CBN	<i>Cannabis sativa</i>	Cannabis	Natural	None
13	THC	<i>Cannabis sativa</i>	Cannabis	Natural	Depressant, stimulant, hallucinogenic

14	Morphine	<i>Papaver somniferum L.</i>	Opium poppy	Natural	Depressant
15	Ketamine	Synthetic drug	Ketamine	Synthetic	Depressant, hallucinogenic
16	Atropine	<i>Atropa belladonna L. and Mandragora officinarum</i>	Belladonna	Natural	Depressant, stimulant, hallucinogenic
17	Hyoscyamine	<i>Atropa belladonna L. and Mandragora officinarum</i>	Belladonna	Natural	Hallucinogenic
18	Scopolamine	<i>Atropa belladonna L. and Mandragora officinarum</i>	Belladonna	Natural	Depressant, hallucinogenic
19	Lactucin	<i>Lactuca Virosa</i>	Lactucarium or Lettuce opium	Natural	Depressant
20	Lactucopicrin	<i>Lactuca Virosa</i>	Lactucarium or Lettuce opium	Natural	Depressant
21	Lactuside A	<i>Lactuca Virosa</i>	Lactucarium or Lettuce opium	Natural	Depressant
22	Codeine	<i>Papaver somniferum</i>	Opium poppy	Natural	Depressant
23	Noscapine	<i>Papaver somniferum</i>	Opium poppy	Natural	Depressant
24	Papaverine	<i>Papaver somniferum</i>	Opium poppy	Natural	Depressant
25	Baeocystin	<i>Psilocybe Valhalla, Norwegian Psilocybe semilanceata</i>	Magic truffle	Natural	Stimulant, hallucinogenic
26	Norbaeocystin	<i>Psilocybe Valhalla, Norwegian Psilocybe semilanceata</i>	Magic truffle	Natural	Stimulant, hallucinogenic
27	Psilocin	<i>Psilocybe Valhalla, Norwegian Psilocybe semilanceata</i>	Magic truffle	Natural	Stimulant, hallucinogenic
28	Psilocybin	<i>Psilocybe Valhalla, Norwegian Psilocybe semilanceata</i>	Magic truffle	Natural	Stimulant, hallucinogenic
29	Belladonnine	<i>Atropa belladonna L. and Mandragora officinarum</i>	Belladonna	Natural	Hallucinogenic
30	Scopoletin	<i>Atropa belladonna L. and Mandragora officinarum</i>	Belladonna	Natural	Hallucinogenic
31	GHB	Neurotransmitter gamma-Hydroxybutyric acid	GHB	Natural and synthetic	Depressant, hallucinogenic, neuroleptic
32	LSD	Semi-synthetic drug (synthesized from lysergic acid: Rye ergot (ascomycete))	LSD or lysergide	Natural and synthetic	Stimulant, hallucinogenic
33	Chloroquine	Quinine synthetic substitute	None	Synthetic	None
34	Mandragorin	<i>Mandragora officinarum</i>	Mandragora	Natural	Stimulant
35	Divinatorin A	<i>Salvia Divinorum</i>	Seer's sage	Natural	None

36	Divinatorin B	<i>Salvia Divinorum</i>	Seer's sage	Natural	None
37	DMT	<i>Psychotria viridis</i> or Derivate of L -tryptophan or synthetic drug	DMT	Natural and synthetic	Stimulant, hallucinogenic
38	Harmol	<i>Banisteriopsis caapi</i> or <i>Festuca ovina</i> or <i>Passiflora foetida</i>	Ayahuasca	Natural	Stimulant, neuroleptic
39	Nicotine	<i>Nicotiana tabacum</i>	Tobacco	Natural	Depressant, stimulant, neuroleptic
40	Salvidivin B	<i>Salvia Divinorum</i>	Seer's sage	Natural	Hallucinogenic
41	Salvinicin A	<i>Salvia Divinorum</i>	Seer's sage	Natural	Hallucinogenic
42	Salvinorin A	<i>Salvia Divinorum</i>	Seer's sage	Natural	Depressant, hallucinogenic
43	Telepathine	<i>Banisteriopsis caapi</i>	Ayahuasca	Natural	Stimulant, neuroleptic
44	Tetrahydroharmine	<i>Banisteriopsis caapi</i>	Ayahuasca	Natural	Stimulant, hallucinogenic
45	Acetylcholine	Human neurotransmitter	LOVE Elixir	Natural	None
46	Dopamine	Human neurotransmitter	LOVE Elixir	Natural	Stimulant
47	Dynorphin	Human peptide	LOVE Elixir	Natural	Hallucinogenic
48	Met-enkephalin	Human peptide	LOVE Elixir	Natural	Depressant
49	MDMA	Synthetic drug	MDMA or ecstasy	Synthetic	Stimulant, hallucinogenic, neuroleptic
50	Oxytocin	Human peptide	LOVE Elixir	Natural	None
51	Phenethylamine	Human neurotransmitter	MDxx derivatives	Natural and synthetic	Stimulant
52	Water (Ayahuasca)		Joker	Artistic drug	
53	Water (Belladonna)		Joker	Artistic drug	
54	Water (Cannabis)		Joker	Artistic drug	
55	Water (Khat)		Joker	Artistic drug	
56	Water (Lactuca Virosa)		Joker	Artistic drug	
57	Water (Love Elixir)		Joker	Artistic drug	
58	Water (Magic Truffle)		Joker	Artistic drug	
59	Water (Mandrake)		Joker	Artistic drug	
60	Water (Mate)		Joker	Artistic drug	
61	Water (Opium)		Joker	Artistic drug	
62	Water (Salvia Divinorum)		Joker	Artistic drug	

Table S3: Smart Contract Recipes. This table shows the recipes for the drugs that can be formed using xSublimatio (vertical entries) and the finite quantity of NFTs that can be generated for each of them. All are the result of the combination of a water molecule and at least one of the molecules described in the horizontal entries. The presence of a molecule in the composition of a drug is indicated by "1". The Probability column indicates the proportion of these molecules among the 5748 generatable NFTs. In all, 1134 drug NFTs can be generated. The unalterable Smart Contract incorporates this data to authorize or refuse the fusion of molecules by a buyer/cook. Abbreviations: CBD: Cannabidiol - CBC: Cannabichromene - CBG: Cannabigerol - CBN: Cannabinol - THC: Tetrahydrocannabinol - GHB: Gamma-Hydroxybutyrate - LSD: Lysergic Acid Diethylamide - DMT: Dimethyltryptamine - MDMA: 3,4-Methylenedioxymethamphetamine.

