EMCDDA Framework and Practical Guidance for Naming Synthetic Cathinones

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Introduction

Synthetic cathinones (SCats), the second largest group of new psychoactive substances (NPS) monitored by the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA), are often sold as 'legal' alternatives to controlled stimulants such as amphetamine, MDMA and cocaine. Although all SCats are related to the parent compound cathinone, attributing consistent, informative and user-friendly common names to these substances is challenging. Over time different naming approaches have been applied, leading to SCats being known by several names. This work presents both a theoretical framework and practical hands-on guidance for the consistent naming of Scats. The approach is designed to be accessible and applicable for a broad audience, including the forensic community, researchers, clinical practitioners, and policy-makers. The new naming framework has been developed based on the parent structures cathinone and phenone, and considers exceptions for several SCats and their closest structural analogs, scheduled under UN and EU legislation. The proposed framework establishes clear rules to derive the EMCDDA framework names for SCats. Each name is, in turn, composed by a principal name containing a parent letter and information on the alkyl substituent of the α-amino nitrogen or the length of the keto alkyl chain. Additional substitutions are amended to the principal name.

Naming Workflow

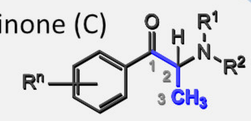
1. Identify the parent element

All SCats with a propanone (C_3) keto alkyl chain and no *N*-heterocycle are assigned the parent element cathinone.

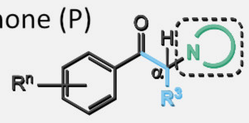
SCats that contain either a keto alkyl chain consisting of more than three carbon atoms or an *N*-heterocycle are assigned the parent element phenone.

Bicyclic or heterocyclic ring systems are additional parent elements along with the common phenyl moiety.

Cathinone (C)

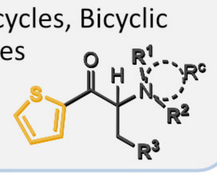


Phenone (P)



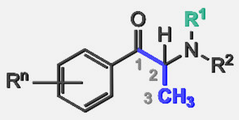
***N*-heterocycle and/or $R^3 \neq CH_3$**

Heterocycles, Bicyclic Aromates



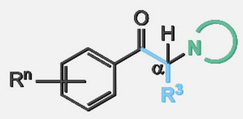
2. Concatenate to form the principal name

N-Substitution



(R^1)Alkylcathinone

Keto alkyl chain length

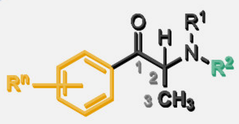


Keto alkylphenone

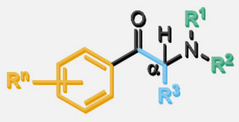
Two pieces of information are codified directly in front of the parent element's letter. In the case of a cathinone, the principal name contains information on the length of the alkyl substituent of the α-amino nitrogen. In the case of a phenone (and all other parent elements), the principal name contains information on the length of the keto alkyl chain.

Both letter codes, alkyl substituent in the case of cathinones or the keto alkyl chain length in the case of phenones, are combined with the parent element to yield the principal name, e.g., methcathinone, hexanophenone, and propiophenone.

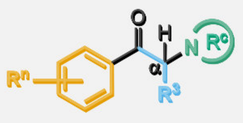
3. Amend substitutions



R^n-*N*R^2-Principal name



R^n-*N*R-Principal name



R^n-aR^c-Principal name

The principal name can be further amended with prefixes indicating the substitution type and location, e.g., 3Br, *N*Et, and αP, leading to the framework name.

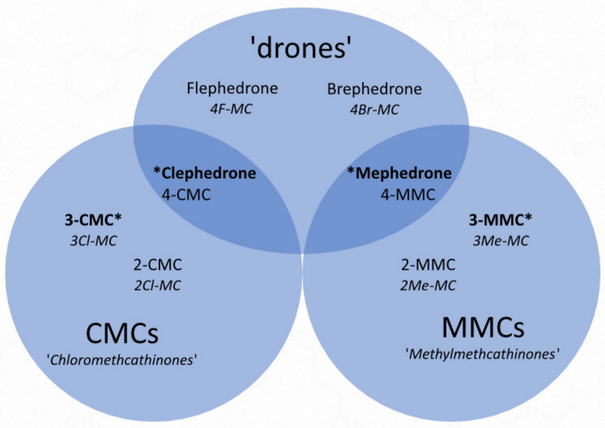
Locants are always introduced without a hyphen in front of the substitution of a structural element.

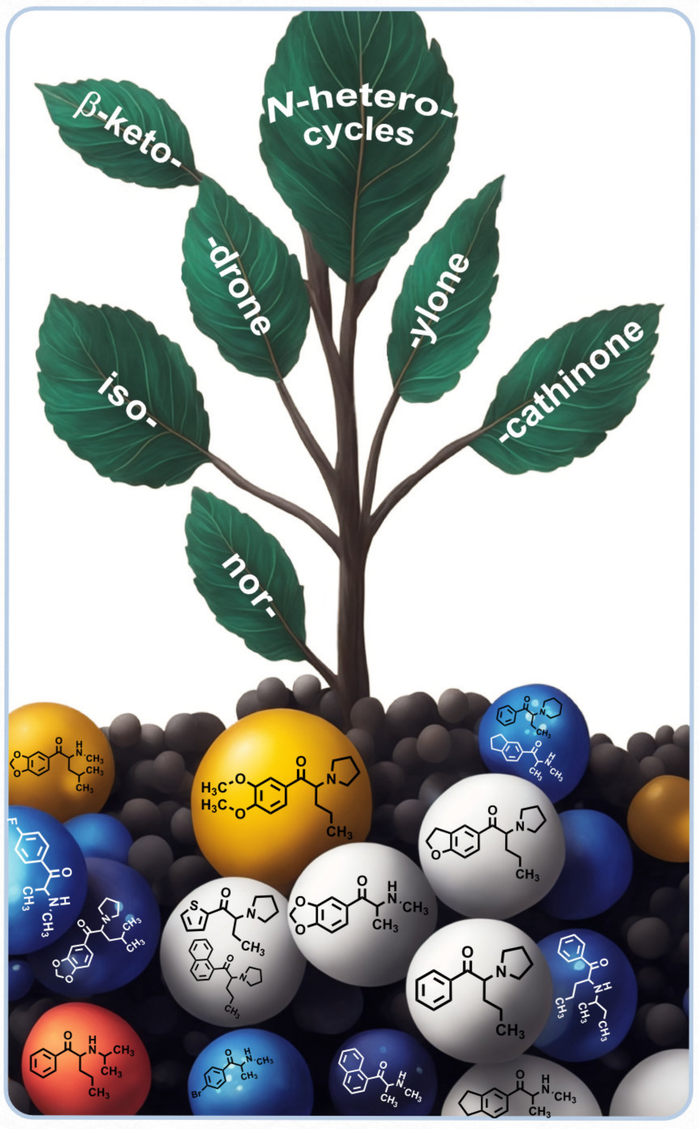
Atom numbers are assigned starting at the connection to adjacent structural elements.

Naming Approaches

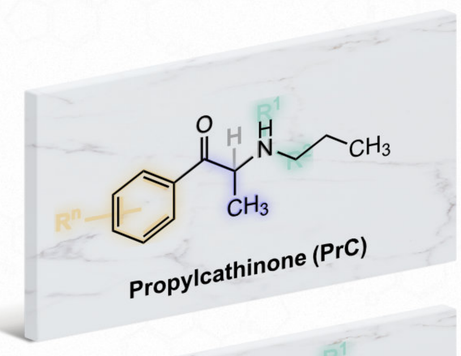
Naming approaches grew organically based on newly identified SCats and, as a results, have not always been applied consistently. Especially methcathinones are now known by several names and some names have been further established through policy efforts (asterisks):

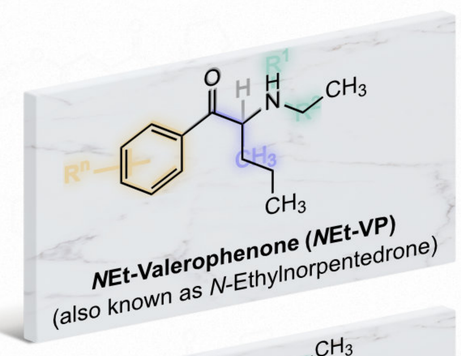
- 'cathinone' – added at the end of the name, i.e., 3-fluoromethcathinone;
- 'drone' suffix – added for SCats without a methylenedioxy group present, i.e., buphedrone;
- 'ylone' suffix – 'ylone' added for SCats with a methylenedioxy group present, i.e., butylone;
- 'iso' prefix – indicates methyl branching in contrast to the n-alkyl isomer, i.e., isohexedrone;
- 'nor' prefix – added for SCats which use 'ylone' or 'drone' suffixes to indicate an exchange of a methyl group for another one, i.e., 4-methyl-*N*-ethylnorpentedrone;
- 'bk' (β-ketone) – added for cathinones structurally similar to MDMA, i.e., bk-PBDB;
- *N*-heterocycles – added α-position of the carbonyl group, i.e., α-pyrrolidinopropiophenone (α-PPP).

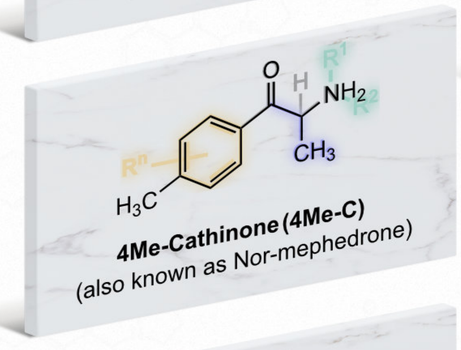


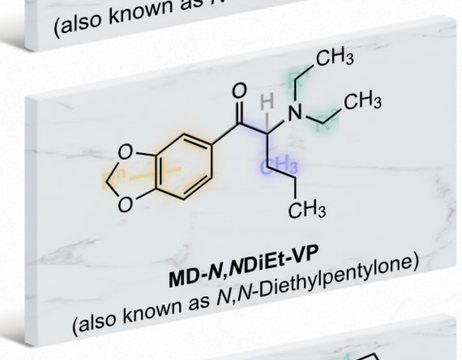


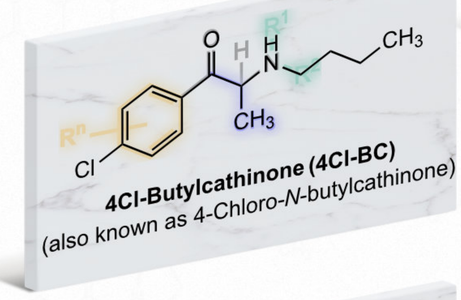
Practical Guidance

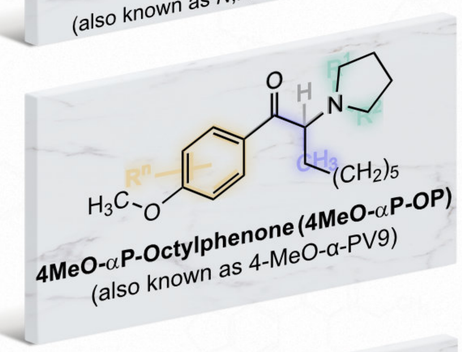


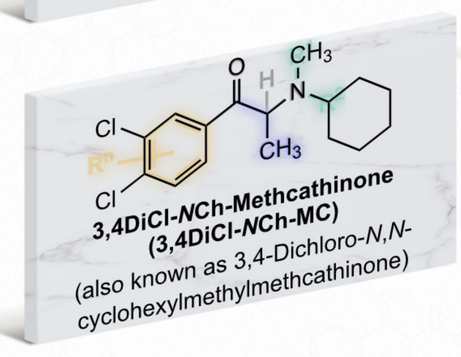


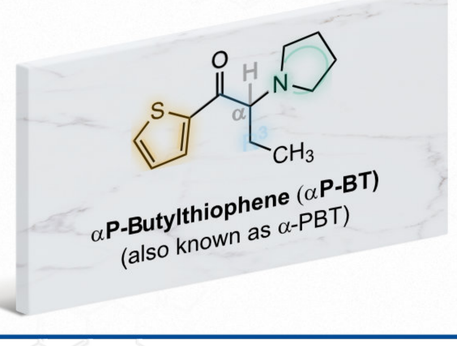












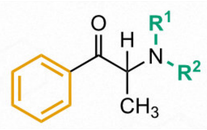
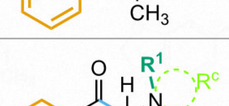
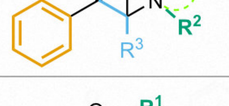
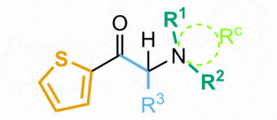
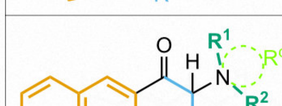
- Most alkyl chains are represented by single letters in the principal name:

M - methyl, **E** - ethyl, **Pr** - propyl, **B** - butyl, and **V** - valero.

- Alkyl chains as substituents are codified using an additional letter:

Me - methyl, **Et** - ethyl, **Pro** - propyl, and **Bu**-butyl.

- Substitutions at the amino nitrogen and *N*-heterocycles are indicated through '*N*' and 'α', respectively.
- Multiple substituents of the same kind are indicated through multiplicative prefixes, i.e., di- and tri-.

General scheme	Parent Element	
	**C**	Cathinone
	**P**	Phenone
	**T**	Thiophene
	**Na**	Naphthyl
	**1Na**	1-Naphthyl

Conclusion

Given the structural diversity of NPS, ensuring precise and unambiguous naming in legislative texts and scientific dialog is required. The EMCDDA naming framework for SCats is based on the parent elements cathinone, phenone, and a third group of other parent elements. Earlier naming approaches using cathinone as a suffix and the naming approach applied to *N*-heterocyclic SCats were incorporated and the possibility to modify the parent elements via substitutions at the benzene ring, amino, and keto alkyl functions are included. For SCats already referred to in policy making documents and their closest structural isomers and analogs, the historical names represent exceptions considered within the proposed framework. The framework on naming SCats is combined with practical guidance and explanations of the rationale on how consistent semi-systematic names for SCats can be derived, to facilitate its application by the forensic community, researchers, clinical practitioners, and policy-makers.