

A systematical methodology for finding novel NPS (New Psychoactive Substances) over the Internet

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Introduction

The market for new psychoactive substances (NPS) has evolved dramatically due to the ease of advertising and selling over the Internet, and thus today one new substance is marketed every 5-6 days. To encounter NPS, forensic chemistry and toxicology sections are often depending on seizures from police or customs, and on the availability of CRM (Certified Reference Material), meaning they are always several steps behind. Then again, as Internet plays the key role to the development of the current situation it could also be part of the solution. We here present a systematical strategy for investigating and searching for NPS over the Internet, not only NPS existing on the open market but also for NPS discussed outside those platforms.

Method

Two approaches were established: The first was to use a simple word search whereas the second was focusing on social networks related to recreational drugs. Google was chosen as the main search engine for this project.

Simple word search – The simple word search was setup by using chosen keywords that enabled to retrieve the most relevant hits concerning novel NPS. 'New stimulant', 'new research chemical', 'NPS', 'newest -', and '- 2015' were some of the keywords that were more successful than others. This approach led mostly to NPS Internet-based suppliers, also known as vendors (different countries and different size of supply), but social networks can also be discovered through this approach.

Examples of vendors:

- chemicalwire.com
- theresearchchemicalshop.net
- chemicalservices.net

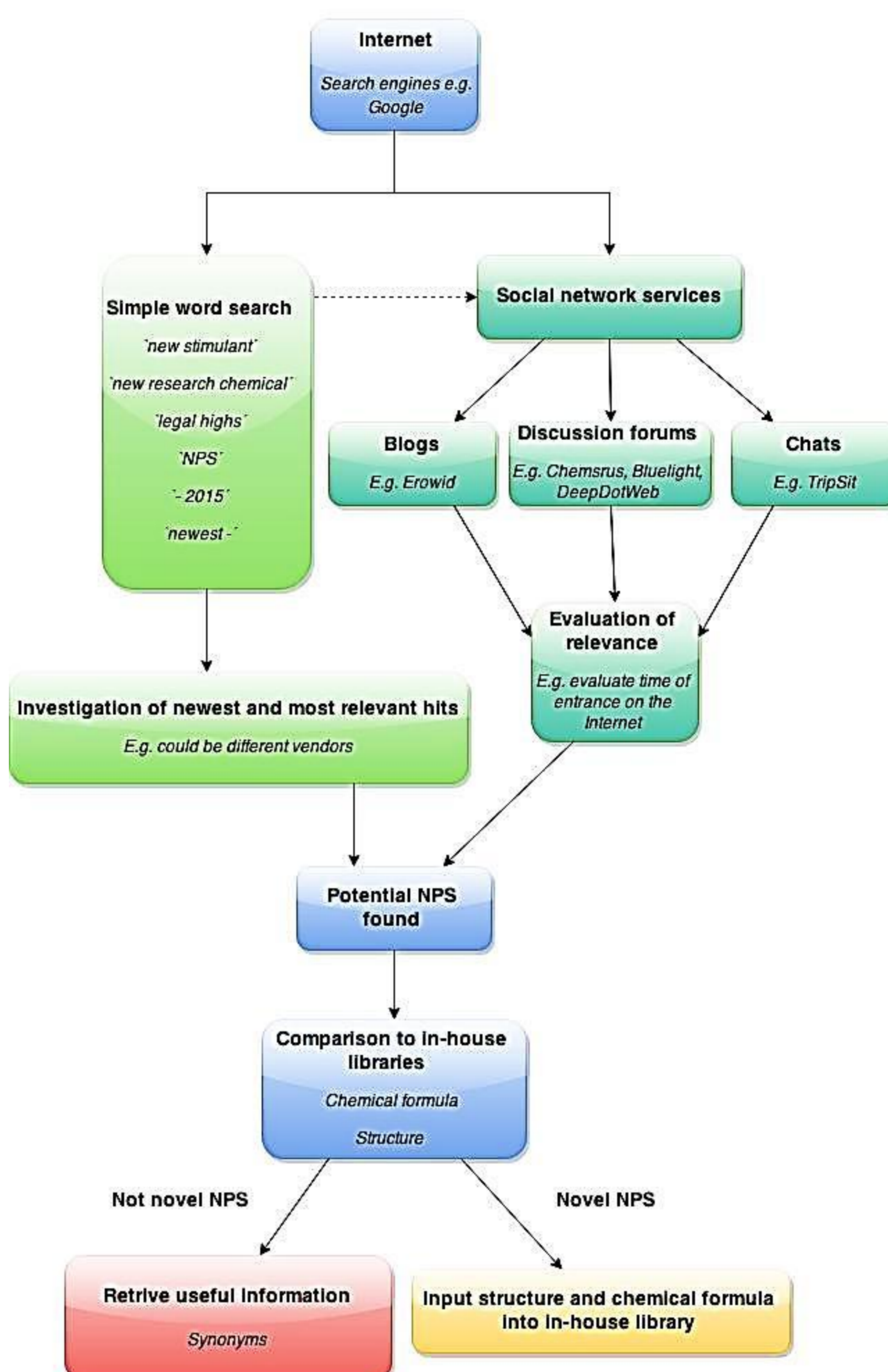
Social networks – The second approach used social networks associated with recreational drugs to monitor the introduction of novel NPS on the market. Different kinds of social networks were utilized such as blogs, discussion forums and chats. A post on a social network was only considered relevant if it had been entered during the last 6 months, and was then further investigated. Older than 6 months, gave a high probability that it was already in in-house libraries and were therefore more critically evaluated.

In-house library – The novel NPS would be included in in-house libraries (with both structure and chemical formula), but first it

Table 1. The compounds found by the presented methodology and included into in-house library in Copenhagen. The experience is that many of the compounds will sooner or later be identified in case samples somewhere in Europe, then reported to EMCDDA, and included in the EDND (European Database on New Drugs).

Compound	In-house library	EDND	Reported in case, DK east	Compound	In-house library	EDND	Reported in case, DK east	Compound	In-house library	EDND	Reported in case, DK east
5F-ADB-PINACA	2014-09-29	apr-15		PRO-LAD	2014-11-13			Propylphenidate (PPH)	2015-02-23	jun-15	2015-03-26
4-Fluoroethcathinone (4-FEC)	2014-10-02	feb-15		ETH-LAD	2014-11-17			Methamnetamine	2015-02-23	aug-15	03-07-2015
AL-LAD	2014-10-10	mar-15	2015-02-26	IDRA-21	2014-11-17			2-Methyl-3-phenylpropanamide	2015-03-30		
FUB AKB-48	2014-10-15	july-14		NSI-189	2014-11-17	jan-15		3-(Benzo[d][1,3]dioxol-5-yl)-2-methylpropanamide	2015-03-30		
4-Fluoro-butylfentanyl	2014-10-16	mar-15		GLYX-13	2014-11-17			3-(Benzofuran-5-yl)-2-methylpropanamide	2015-03-30		
FUB-PB-22	2014-10-16	dec-13		NESS-0327	2014-11-17			4-Chloro-alpha-PVP	2015-04-07		
Mephtramine	2014-10-16	july-13	2015-03-26	U-47700	2014-11-17	jan-15		MO-CHMINACA	2015-04-07		
MDMB-CHMICA	2014-10-28	sep-14	2015-02-26	5F-PCN	2014-11-17			IPO-33	2015-05-21		
5F-NPB22	2014-10-30	jan-14		DB-MDBP	2014-11-17	mar-15		Pyrophenidone	2015-05-21		
2-Chloro-4,5-MDMA	2014-10-30	jan-15		MDMB-FUBINACA	2014-11-18	apr-15		HDEP-28	2015-05-21		
5-Meo-NBpBrT	2014-10-30			2-Bromo-4,5-MDMA	2014-11-18			TDIQ	2015-05-21		
Isoproscaline	2014-10-30			SDB-005	2014-11-18	apr-15		3-Fluoroethamphetamine	2015-05-21		
ALD-52	2014-10-30			ALEPH-21	2014-11-20			5FCMB23	2015-05-21		
DOIP	2014-10-30	may-15		ETHYL-L	2014-11-20			24F-MeOBME	2015-05-21		
4-MeO-alpha-PV9	2014-11-05	may-15		4-CAB	2014-11-21			4-SMC	2015-05-21		
3,4-DMeO-alpha-PHP	2014-11-05	may-15		4-MAB	2014-11-21			3-CAF	2015-05-21		
Isopropylphenidate (IPH)	2014-11-05	mar-15	2015-03-26	3-Fluorophenmetrazine (3-FPM)	2014-12-01	sep-14	2015-02-26	2-BA	2015-05-21		
HDMP-28	2014-11-05	mar-15		NRG-3	2014-12-01			2-Chloro-Ephedrine	2015-05-21		
Modafinidz	2014-11-05	oct-14		5F-AMB-PICA	2014-12-01	dec-14		2-Meo-Ephedrine	2015-05-21		
Flubromazolam	2014-11-05	oct-14	15-04-2015	AZ-037	2015-01-29			5-Meo-DIBF	2015-05-21		
MDPHP	2014-11-05	nov-14		4-MPH	2015-01-29			Fluorolintane	2015-05-21		
alpha-Pyrrolidinoheptanophenone (PV-8)	2014-11-05	july-13	2014-12-23	FUB-NPB22	2015-01-29			4-Methoxybutylfentanyl	2015-05-21		
bk-IVP	2014-11-05	jan-15		4-Chloromethamphetamine (4-CMA)	2015-01-29			Cyclo-Methidrone	2015-06-08		
Clonazolam	2014-11-10	jan-15	03-07-2015	1P-LSD	2015-02-03	mar-15	2015-04-10	3-Meo-PCMo	2015-06-08	aug-15	
MDMB-CHMINACA	2014-11-10			Phenetrazine	2015-02-03			Furanylfentanyl	2015-06-08		
MA-CHMINACA	2014-11-10			MR-2096	2015-02-03			2-MPPP	2015-06-08		
FUB-AMB	2014-11-10	dec-14		TH-PVP	2015-02-03	aug-15		2-Phenyl-3,6-dimethylmorpholine	2015-06-08		
PX-2	2014-11-10	nov-14		LSM-775	2015-02-23			DMOPP	2015-06-08		
FUB-144	2014-11-10	feb-15		TH-PBP	2015-02-23						

Figure 1. A flow chart over the systematical approach for finding NPS on Internet.



would be compared to existing entries to avoid duplication. The comparison was first based on chemical formula and secondly based on structure to evaluate possible isomers. Even though the conclusion is that it was not a novel NPS, valuable information could still be retrieved. Synonyms would be such valuable information which would make the identification process much faster and simpler in the future.

Implementation in Forensic Toxicology

The method has been used since mid-2014 in forensic toxicology at the University of Copenhagen for building and continuously updating MS-QTOF libraries for blood screening.

Figure 2. An example of a post that resulted in the finding of a novel NPS. The substance was included into in-house libraries with chemical formula, structure and potential synonyms.

Methamnetamine (N-methyl-PAL-287) thread

Category: Stimulants

Topic started 2 days 12 hours ago by Sandbwoy

ISEC project "RESPONSE"

The methodology is included as one of several approaches in the newly started ISEC project "RESPONSE", in which one of the goals is to enhance the NPS identification capability and efficiency of forensic laboratories.

Shared samples (Slovenian seizures) – Within the frame of the RESPONSE project, Slovenian samples of fully structure-elucidated NPS were shared between partner laboratories in March/April 2015. The compounds had not been seen in DK east, and we did not have reference standards. However, because the QTOF library was updated according to the presented methodology, we had a library match for 16 out of 17 samples.

This demonstrates how the methodology works in practice.

Purchasing NPS – It is the intention in the project to retrieve about 200 – 300 NET-NPS (i.e. from Internet vendors), supplemented by CRM (Certified Reference Material; from ordinary suppliers). The compounds will be fully identified in the Slovenian forensic laboratory, and EI-MS and IR libraries updated. The libraries are to be shared within the forensic community.

Purchasing from Internet vendors is not a routine matter. Additional selection criteria has to be applied, and several challenges are faced.

Criteria:

- Preferably "pure", powdered form theresearchchemicalshop.net
- Small amounts (some only sell bulk amounts at the 100 g or kilo-level)
- Acceptable payment options

Challenges:

- Public procurement procedures do not fit. The forensic lab cannot purchase directly, but need to go through a company
- Information exchange system needed between the forensic lab, customs, and the Ministry of health to prevent that the importing company becomes blacklisted in any official systems in EU or worldwide
- Finding a vendor, when compounds are only known from blogs or forums
- Slow delivery
- Received substance differs from ordered substance

Conclusion

A systematical methodology for search of novel NPS through Internet is here presented. Two different approaches were established: Simple word search together with investigation of social networks. The methodology has been implemented for library-building within forensic toxicology at the University of Copenhagen and has given rise to more than 80 internet-findings of novel NPS in the time frame of Sep-2014 up to June-2015.

In the ISIS project "RESPONSE" the same approach was applied for creating a gross list of compounds. The purpose was to purchase NPS as reference compounds, either as NET-NPS (from Internet vendors) or as CRM (Certified Reference Material; from ordinary suppliers). Purchasing NET-NPS for use as reference material is a relatively unexplored field, and it has proved to be difficult and time-consuming. However, with the massive effort laid down on the task by the RESPONSE project, valuable experiences are being collected for the possible future benefit of the forensic community in general.