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PRESUMPTIVE COLOR TESTS -

DATABASE DESCRIPTION and GUIDELINES FOR USE

Dr. Sonja Klemenc, Denis Saboti, Brigita Nemec

R Slovenia Ministry of the Interior, General Police Directorate
National Forensic Laboratory,



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1. Foreword

Simple color test reactions (presumptive test) may be important element of the harm reduction among NPS users. They can use such test (at home or at NGO points) and this way to a certain degree confirm or reject the identity of the compound in their possession. It is important to emphasize that presumptive color tests can only give an indication of which type of substance could be present - but they can't specifically identify the substance.

The identities of all compound presented in this database have been chemically confirmed by instrumental analyses performed in the framework of the project RESPONSE. Characterizations strategies are presented at the RESPONSE project WEB site:

<http://www.policija.si/eng/index.php/generalpolicedirectorate/1669-nfl-page-response> (English)

Important notice: A positive test result for a particular substance does not mean that the sample really contains this particular compound or that it is completely pure and safe!

Disclaimer: We do not encourage drug use. RESPONSE presumptive color tests database shall be regarded as supporting tool only! We are not responsible for your use of this database, testing practices and your interpretation of the results. Anything you do is at your own risk.

Dr. Sonja Klemenc
RESPONSE
project manager



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2. Testing procedures

The testing has been conducted by applying a drop of reagent on a white ceramic testing plate, adding a small amount of NPS sample and observing any potential coloration of the sample. Since some of NPS samples were highly potent and all reagents were containing concentrated acid, standard laboratory safety procedures like wearing laboratory gloves and coats were followed.

2.1 Reagents applied

Several commercially available and laboratory made testing kits have been tested. Finally, a commercial testing kit which includes Marquis¹, Mandelin¹, Mecke¹, Libermann¹, Froehde² and Gallic¹ acid reagent was applied to establish the database. Test kits applied for taking the photos presented in this database were purchased from a UK based company SafeTest 4³:<https://www.safetest4.co.uk/>.

2.2 Data acquisition

The observations from presumptive color test reactions were documented by an analyst (observation by eye) and photographs were taken simultaneously with a Canon 5D Mark II camera at the following time intervals: 0s (blank) 2s, 10s, 20s, 60s and 120s, respectively. Two Leica flexible lamps have been used as a light source in a dark room in order to assure constant and relatively repeatable lighting conditions. The improvised laboratory setup can be seen from Figure 1.



Figure 1: Experimental photographic setup for presumptive color test reactions

2.3 Description of results

Results given in the database include a text color description observed by applying particular presumptive test reagent on a particular substance and picture of the results where one can get more visual information from reactions (see in the next section).

Text description refers to a color observed at the reaction time of 20 s. This time has been selected as the most representative based on empirical observations. Text descriptions of colors done by an analyst during the experiment were afterwards cross checked by images taken with a camera. In the case of serious inconsistencies the experiments were repeated.






Text description of the exact color, taking into account hue, saturation, intensity and subjective perceptions was very challenging. Therefore, with regard to intended purpose of database use, we tried to keep descriptions simple, which was also not an easy task. To achieve at least a minimum consistency of our own descriptions, we applied a very simplified variation of the system described by Society of Dyers and Colourists & AATCC (see at: <https://colour-index.com/technical-info>). In addition we also used a color sphere: <https://galactic.ink/sphere/#>

It has to be stressed that color of the test reaction depends also on sample amount, sample purity and the “freshness” of reagents. It is also important to know that colors observed on monitor or printer may not be correctly reproduced. The type and/or calibration of the monitor or printer are important. Anyhow, discussion of these factors is beyond the scope this work.

3. Database description and use

Database is structured as a table as shown in the Figure 2 and on line it is accessible here: http://www.policija.si/apps/nfl_response_web/seznamColors.php?lang=eng. Each field has a sort button which enables sorting of entries (alphabetically or ascending/descending order).

Presumptive color tests

Substance class [▲]	Substance common name [▲]	Systematic name [▲]	structure (created by OPSIN free tool)	StdInChIKey (click and search)	Marquis[1]	Mandelin[2]	Mecke[3]	Libermann[4]	Froehde[5]	Galic Acid[6]	Show reactions [1-6] (picture)
Aminoindanes	5-IAI	5-Iodo-2,3-dihydro-1H-inden-2-amine		BIHPYCDDPGNWQO = UHFFFAOYSA -N	brown	green (L)	orange	brown (D)	green (L)	NR	show
Aminoindanes	N-methyl-2AI	N-methyl-2,3-dihydro-1H-inden-2-amine		SKWZQUCTTQBHJT = UHFFFAOYSA -N	orange	brown (D)	brown (D)	brown (D)	brown (D)	orange	show
Aminoindanes	MDAI	2H,5H,6H,7H-indeno[5,6-d][1,3]dioxol-6-amine		FQDRMHHCWZAXJM = UHFFFAOYSA -N	orange	brown (D)	brown (D)	brown (D)	brown (D)	orange	show
Aminoindanes	2-AI	2,3-dihydro-1H-inden-2-amine		LMHHFZAXSANGGM = UHFFFAOYSA -N	red	green	brown (L)	red	NR	NR	show
Arylalkylamines	5-EAPB	1-(Benzofuran-5-yl)-N-ethylpropan-2-amine		ZBZDDOARNPAMSP = UHFFFAOYSA -N	black	black	black	black	violet (D)	black	show

Showing 1 to 5 of 310 entries
Table updated 22.06.2017

Presumptive color tests

Marquis[1]	Mandelin[2]	Mecke[3]	Libermann[4]	Froehde[5]	Galic Acid[6]	Show reactions [1-6] (picture)	Analytical comments (colour change)	date of entry	entry updated	Chem-ID or Report-ID
brown	green (L)	orange	brown (D)	green (L)	NR	show		2017-01-31	-	1599-16
orange	brown (D)	brown (D)	brown (D)	brown (D)	orange	show		2017-01-31	-	1348-15
orange	brown (D)	brown (D)	brown (D)	brown (D)	orange	show		2017-01-31	-	1347-15
red	green	brown (L)	red	NR	NR	show	[2]: light green -- > blue	2017-01-31	-	1598-16
black	black	black	black	violet (D)	black	show		2017-01-31	-	1111-14A

Search:

Previous ... Next

Figure 2: Database caption (print screen in two parts)

On the top left side of the window there is a field “show” (Figure 2). It serves for the adjustments of database window, i.e. how many records one wish to see per page. Given options are: 5, 10, 25, 50 and All.

At the bottom (left corner) there is information of what you see on the screen (example on Figure 3: Showing 1 to 5 of 310 entries), a date of the last database update is given bellow and a database view counter is at the bottom.

Buttons on the bottom right side of the window enable movements between the pages. Scroll bar enables left – right movements along the database window. Vertical scroll bar will appear on as needed basis.

On the top right side of the window there is a “search” field that functions as a filter.

Each row of the database table describes a single compound, containing 16 fields (columns) – further described in Table 2.

Table 2: List and description of columns in the database

No	Field	Description	Comments
1	Substance class	Substances are classified into several classes along their physicochemical characteristics. This classification was adopted from EMCDDA ⁴ .	Click the sort button – records will be sorted from A-Z or in opposite direction;
2	Substance common name	Be aware that this is not a unique name (for the same substance we can find more than one common name). Basically we (NFL) follow EMCDDA naming or apply other names available over the internet or we create the name in the NFL if the compound is reported for the first time.	Click the sort button – records will be sorted from A-Z or in opposite direction;
3	NPS systematic name	Systematic name – IUPAC based name which describes compound structure.	Click the sort button to sort records ascending/descending order. Apply the search field to search for the whole name or only a part of the name (for example indole or indazole or carboxylate..)
4	Structure	Picture of structure (in .png format).	Click or double click to enlarge – structure opens in new window.
5	StdInChIKey	Standard InChI Key = standardized International Chemical Identifier is a textual identifier for small organic molecules. The condensed, 27 characters standard InChIKey is a hashed version of the full standard InChI string, designed to allow for easy web searches of chemical compounds. ⁵	Click the link and search the internet for information on particular compound.

No	Field	Description	Comments
6-11	Reagents: Marquis, Mandelin, Mecke, Libermann, Froehde, Gallic Acid	Gives description of colors at 20 s interval	Click the sort button – records will be sorted from A-Z or in opposite direction;
12	Show reactions	Picture of reactions	Click or double click “show” to enlarge – picture opens in new window, showing colors of blank, at 2s, at 10s, at 20s, at 60s and at 120s
13	Analytical comments (color change)	Comments about the analytical findings	Click the sort button to sort ascending/descending.
14	Date of entry	Date when the compound was entered into database	Click the sort button to sort ascending/descending
15	Entry updated	Date when database entry was updated	Click the sort button to sort ascending/descending
16	Chem-ID	Chem-ID is the unique label of particular sample in the NFL chemicals database.	Click the sort button to sort ascending/descending

Columns 6-11 include color developed at the reaction time of 20s. In addition to basic color, some additional indicators are given: light (L), dark (D), No reaction (NR). Color descriptions ending with “ish” describe colors with very low intensity.

Due to their own coloration some samples can give a false positive “reaction”. In such cases samples are adequately described as NR.

Clicking on “show” link in the “Show reaction” column opens up a separate window containing a picture of presumptive color test for a single NPS (Figure 3). At the top of the image there is a rectangle with a name of the NPS. Below there is a row with the names of reagents that correspond to individual columns. On the left side there are numbers indicating time intervals in seconds, starting with Blank (no NPS added) for better comparison of any color change.

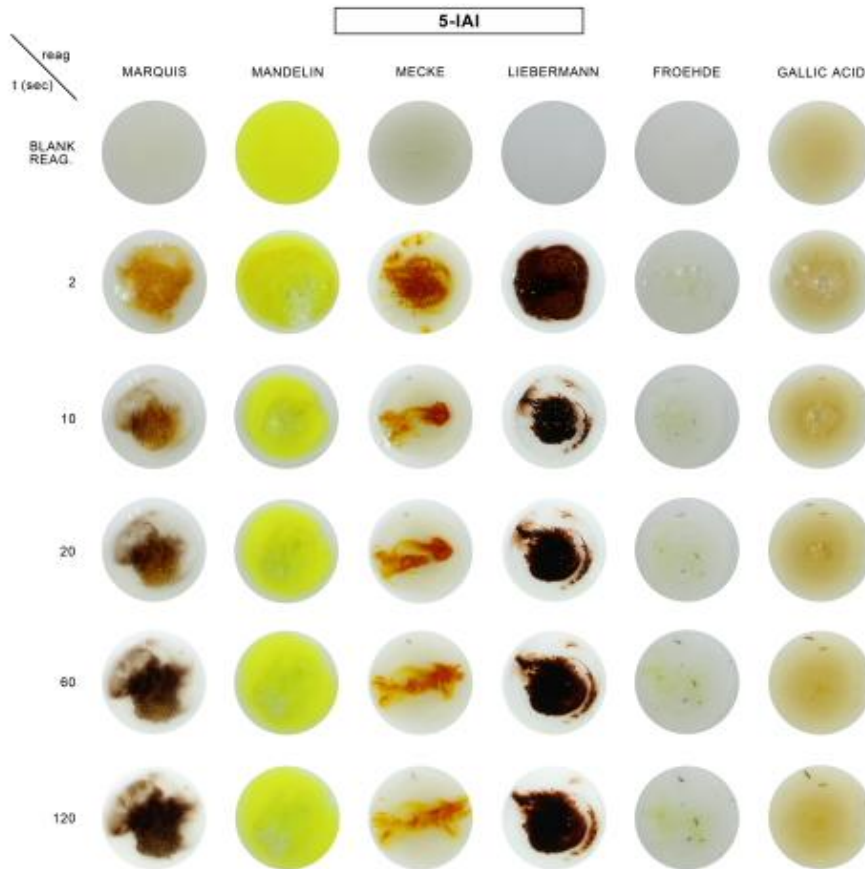


Figure 3: Presumptive color test picture (example)

4. Conclusions

We hope that this database will be helpful for professionals and for harm reduction purposes among users.

If you have found this database useful in your work citing our database would be very much appreciated.

5. References

¹ Rapid Testing Methods of Drugs of Abuse. Manual for use by national law enforcement and narcotics laboratory personnel (ST/NAR/13/REV.1), United Nations, New York, 1994; https://www.unodc.org/documents/scientific/Rapid_Testing_Methods_of_Drugs_of_Abuse_E.pdf

² Color Test Reagents/Kits for Preliminary Identification of Drugs of Abuse". Law Enforcement and Corrections Standards and Testing Program. July 2000. <https://www.ncjrs.gov/pdffiles1/nij/183258.pdf>

³ <https://www.safetest4.co.uk/>

⁴ <http://www.emcdda.europa.eu/>

⁵ https://en.wikipedia.org/wiki/International_Chemical_Identifier