

Supplementary materials

Materials

The HMEs used in this study, TATP, HMTD and MEKP, were either provided by Danish Emergency Management Agency (DEMA) or synthesized at the Technical University of Denmark (DTU) laboratories (TATP only). Two different batches of TATP and HMTD (solid HMEs) were provided by DEMA; each of the samples was synthesized in their laboratories using two different types of catalysis and following two different protocols based on their experience gained by investigations of clandestine labs and reflecting a real scenario. A batch of liquid sample MEKP was synthesized by DEMA using a protocol provided by CIA. Furthermore, we measured over two years to see the effect of ageing of the HMEs. Several batches of TATP were synthesized at DTU which were regularly destroyed after use, following safety protocols. All samples were chemically characterized by proton NMR spectroscopy.

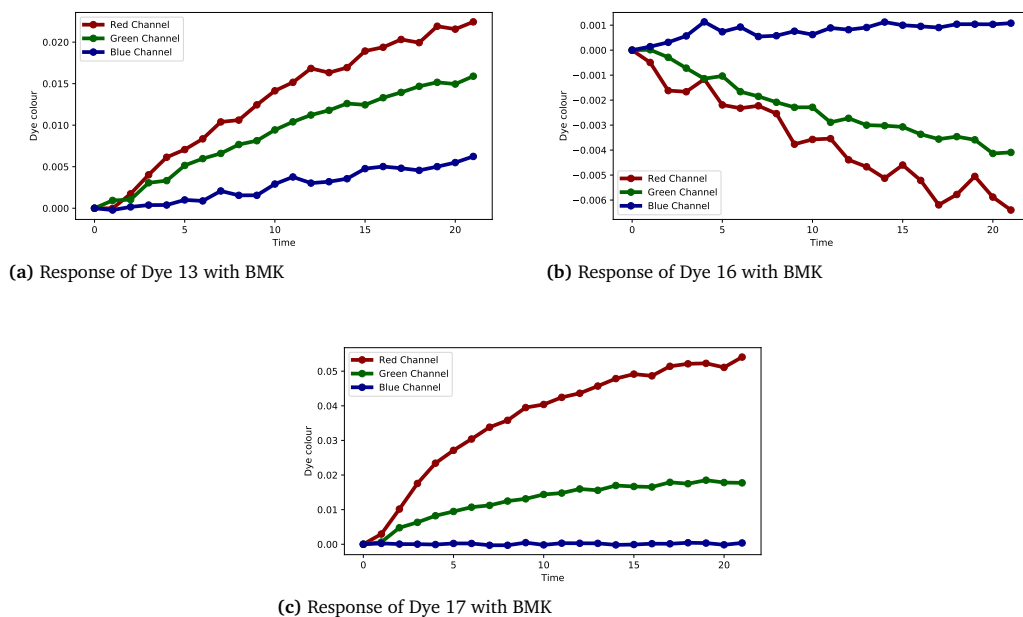


Fig. S1. Plot of time series obtained from the chip for BMK for selected dyes. The RGB channel responses of the dyes are shown as red, green, and blue lines respectively.

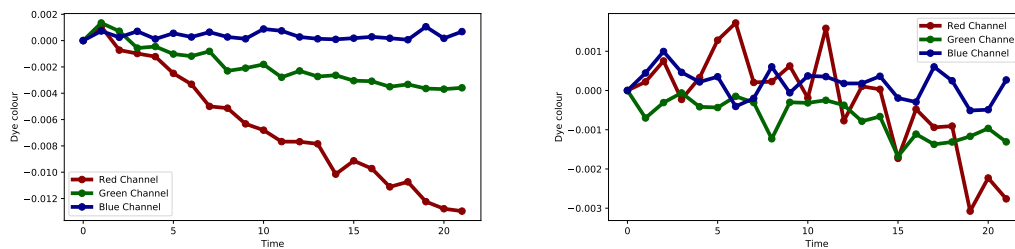


Fig. S2. An example of a normal (top) and outlier (bottom) measurement session for TATP with responses on the red channel, green channel, and blue channel.

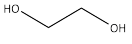
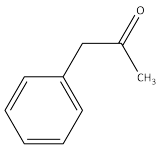
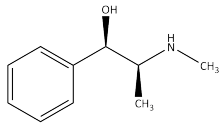
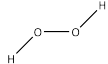
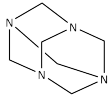
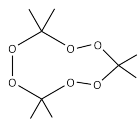
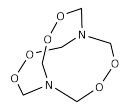
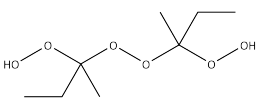
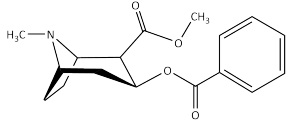
Notes and references

1 *1,2-Ethandiol*, <https://webbook.nist.gov/cgi/cbook.cgi?ID=107-21-1>, Accessed: 23-06-2022.

** Controlled chemicals, authorising licence for use needed.

†† 10-15% Aqueous solution.

§§ Nitrogen, oxygen, water vapor, argon, and carbon dioxide account for about 99% of the composition of air.

Analyte				Use	Vapor pressure at 25°C (Pa)
Name and CAS No	Acronym	Chemical structure	Physical state at 25°C		
Ethylene glycol 107-21-1	EG		Liquid	Precursor of explosive ethylene glycol dinitrate	~ 10 ¹
Benzyl methyl ketone also known as phenylacetone 103-79-7	BMK **		Liquid	Precursor of methamphetamine	21.3 ²
(1R,2S)-(-)-Ephedrine 299-42-3	EPH **		Solid	Precursor of methamphetamine	0.16 ³
Hydrogen peroxide	H ₂ O ₂		Liquid ^{††}	Precursor of TATP, 10-15% concentration	~16 ⁴
Hexamethylene-tetramine also known as hexamine 100-97-0	HEX		Solid	Precursor of HMTD	~0.1 ⁵
Triacetone triperoxide	TATP		Solid	Homemade explosive	6.2 ⁶
Hexamethylene triperoxide diamine	HMTD		Solid	Homemade explosive	~6.5e-6 Pa ⁷
Methyl ethyl ketone peroxide	MEKP		Liquid	Homemade explosive	1.3 ⁸
Cocaine free base 50-36-2	COfb **		Solid	Controlled drug	0.0003 ⁹

2 Phenylacetone, <https://pubchem.ncbi.nlm.nih.gov/compound/Phenylacetone>, Accessed: 24-06-2022.

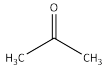
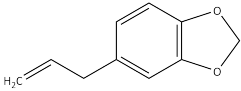
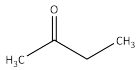
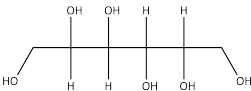
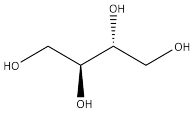
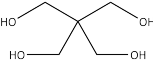
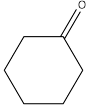
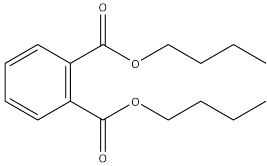
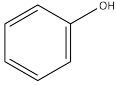
3 Ephedrine, <https://pubchem.ncbi.nlm.nih.gov/compound/Ephedrine>, Accessed: 24-06-2022.

4 H₂O₂, <http://www.h2o2.com/technical-library/physical-chemical-properties/physical-properties/default.aspx?pid=25&name=Vapor-Pressures>, Accessed: 20-06-2022.

5 I. Stranski, G. Klipping, A. Bogenschuetz, H. Heinrich and H. Maennig, in *Advances in Catalysis*, Elsevier, 1957, vol. 9, pp. 406–414.

6 H. Östmark, S. Wallin and H. G. Ang, *Propellants, Explosives, Pyrotechnics*, 2012, **37**, 12–23.

7 M. J. Aernecke, T. Mendum, G. Geurtsen, A. Ostrinskaya and R. R. Kunz, *The Journal of Physical Chemistry A*, 2015, **119**, 11514–

Acetone 67-64-1	Ac		Liquid	Precursor of homemade explosive, Manufacturing solvent	30800 ¹⁰
Safrole 94-59-7	SA		Liquid	Precursor of methamphetamine	9.3 ¹¹
Methyl ethyl ketone 78-93-3	MEK		Liquid	Precursor of MEKP	12100 ¹²
Mannitol 69-65-8	MA		Solid	Precursor of homemade explosive	Data unavailable (Very low) ¹³
meso-Erythritol 149-32-6	ER		Solid	Precursor of homemade explosive	Data unavailable (Very low) ¹⁴
Pentaerythritol 115-77-5	PER		Solid	Precursor of homemade explosive	1.07e-7 ¹⁵
Cyclohexanone 108-94-1	Cy		Liquid	Manufacturing solvent	667 ¹⁶
Dibutyl phthalate 84-74-2	DP		Liquid	Additive in explosive formulations	1.9e-3 ¹⁷
Phenol 108-95-2	Ph		Solid	Toxic. Important chemical intermediate in many industrial processes	53 ¹⁸

11522.

8 *MEKP*, <https://pubchem.ncbi.nlm.nih.gov/compound/2-Butanone-peroxide#section=Vapor-Density>, Accessed: 24-06-2022.

9 A. B. Dindal, M. V. Buchanan, R. A. Jenkins and C. K. Bayne, *Analyst*, 2000, **125**, 1393–1396.

10 *Acetone*, <https://pubchem.ncbi.nlm.nih.gov/compound/acetone#section=Vapor-Pressure>, Accessed: 1-7-2022.

11 *Safrole*, <https://pubchem.ncbi.nlm.nih.gov/compound/safrole#section=Vapor-Pressure>, Accessed: 1-7-2022.

12 *MEK*, <https://pubchem.ncbi.nlm.nih.gov/compound/Methyl-ethyl-ketone#section=Vapor-Pressure>, Accessed: 1-7-2022.

Ammonium nitrate 6484-52-2	AN		Solid	Oxidizer for homemade explosive formulations	0.32 ¹⁹
2,3-Dimethyl-2,3-dinitrobutane 3964-18-9	DMNB		Solid	Additive (taggant) in explosive formulations	0.27 ²⁰
Toluene 108-88-3	Tol		Liquid	Solvent	3800 ²¹
Urea 57-13-6	Ur		Solid	Precursor of explosives	1.6e-3 ²²
Glycerin 56-81-5	Gly		Liquid	Precursor of home-made explosives	321e3 ²³
Ambient air	AA ^{§§}		Gas	Chemical	
Water	H ₂ O		Liquid	Control analyte and precursor of home-made explosives in aqueous solution	

Table S1. Analytes used for the colorimetric detection experiments with Crim-Track sniffer device. Typical quantities of 25 – 50 mg of solid analytes and 0.1 ml of liquid analytes or solution of analytes were used for the detection experiments

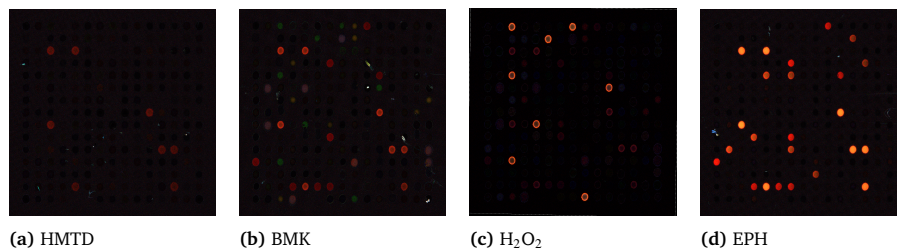


Fig. S3. Difference maps of the experiments with HMTD, BMK, H₂O₂ and EPH considered in this work.

13 *Mannitol*, <https://cameochemicals.noaa.gov/chemical/20585>, Accessed: 1-7-2022.

14 M. Bilde, K. Barsanti, M. Booth, C. D. Cappa, N. M. Donahue, E. U. Emanuelsson, G. McFiggans, U. K. Krieger, C. Marcolli, D. Topping *et al.*, *Chemical reviews*, 2015, **115**, 4115–4156.

15 *Pentaerythritol*, <https://pubchem.ncbi.nlm.nih.gov/compound/pentaerythritol#section=Vapor-Pressure>, Accessed: 1-7-

Analyte/Dataset	Ex1	Ex2	Pc1	Pc2	Pc3	Pc4	Pc5	D1	D2
TATP	63	9							
HMTD	68								
MEKP	33								
BMK			10						
H ₂ O ₂	33	8	10	23	20	15	13	16	
HEX		9							
EG	32		10	14	18	10	12	17	
Ac			9						
H ₂ O		9							
Ur					20				
Ph				8					
MA						5			
ER						6			
PER						14			
AN							13		
Cy							12		
EPH								17	
COfb								18	24
DMNB				21					
DP							14		
SA								18	23
MEK				19					
Gly					18				
Tol					17				
AA	30	8	8	22	20	10	12	17	24

Table S2. The number of measurements of each analyte in each dataset.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Solid	HEX	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	TATP	90.00±0.20	10.00±0.20	47.00±0.12	53.00±0.12	63.00±0.11
Liquid	H ₂ O ₂	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	H ₂ O	80.00±0.24	20.00±0.24	5.00±0.10	95.00±0.10	80.00±0.16

Table S3. Classification results for Ex2 dataset obtained by using the classifier. The best classifier's results for solids (KNN) and liquid (RF) analytes are shown separately.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Liquid	Ac	70.00±0.40	30.00±0.40	8.00±0.10	92.00±0.10	-
	BMK	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	EG	90.00±0.20	10.00±0.20	3.00±0.06	97.00±0.06	90.00±0.20
	H ₂ O ₂	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00

Table S4. Classification results for Pc1 dataset obtained by using the RF classifier. This dataset only has liquid analytes.

- 2022.
- 16 Cyclohexanone, "<https://webwisser.nlm.nih.gov/WebWISER/substance?substanceId=513&identifier=Cyclohexanone&identifierType=name&catId=48>", Accessed: 1-7-2022.
- 17 Dibutyl phthalate, "<https://pubchem.ncbi.nlm.nih.gov/compound/Dibutyl-phthalate#section=InChI>", Accessed: 1-7-2022.
- 18 Phenol, <https://pubchem.ncbi.nlm.nih.gov/compound/phenol#section=Vapor-Pressure>, Accessed: 1-7-2022.
- 19 J. Brandner, N. M. Junk, J. Lawrence and J. Robins, *Journal of Chemical and Engineering Data*, 1962, 7, 227–228.
- 20 K. R. M. F. Vojtěch Štejfá, Kateřina Kadlecová, *Chemical Thermodynamics and Thermal Analysis*, 2021, 3, 100020.
- 21 Toluene, <https://pubchem.ncbi.nlm.nih.gov/compound/toluene#section=Vapor-Pressure>, Accessed: 6-7-2022.
- 22 Urea, <https://pubchem.ncbi.nlm.nih.gov/compound/urea#section=Vapor-Pressure>, Accessed: 6-7-2022.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Solid	DMNB	53.00±0.20	47.00±0.20	37.00±0.26	63.00±0.26	54.00±0.16
Liquid	EG	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	H ₂ O ₂	90.00±0.20	10.00±0.20	0.00±0.00	100.00±0.00	93.00±0.13
	MEK	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	Ph	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00

Table S5. Classification results for Pc2 dataset obtained by using the classifier. The best classifier's results for solids (KNN) and liquid (RF) analytes are shown separately.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Solid	Ur	75.00±0.27	25.00±0.27	50.00±0.35	50.00±0.35	65.00±0.17
Liquid	EG	90.00±0.12	10.00±0.12	0.00±0.00	100.00±0.00	94.00±0.07
	Gly	40.00±0.16	60.00±0.16	12.00±0.05	88.00±0.05	42.00±0.15
	H ₂ O ₂	95.00±0.10	5.00±0.10	0.00±0.00	100.00±0.00	97.00±0.06
	Tol	82.00±0.15	18.00±0.15	13.00±0.07	87.00±0.07	68.00±0.17

Table S6. Classification results for Pc3 dataset obtained by using the classifier. The best classifier's results for solids (SVM) and liquid (KNN) analytes are shown separately.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Solid	ER	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-
	MA	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-
	PER	100.00±0.00	0.00±0.00	100.00±0.00	0.00±0.00	56.90±0.06
Liquid	EG	90.00±0.20	10.00±0.20	0.00±0.00	100.00±0.00	93.00±0.13
	H ₂ O ₂	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00

Table S7. Classification results for Pc4 dataset obtained by using the KNN classifier. The best classifier's results for solids (SVM) and liquid (KNN) analytes are shown separately.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Solid	AN	93.00±0.13	7.00±0.13	56.90±0.39	43.00±0.39	76.00±0.10
Liquid	EG	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	H ₂ O ₂	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00

Table S8. Classification results for Pc5 dataset obtained by using the classifier. The best classifier's results for solids (RF) and liquid (KNN) analytes are shown separately.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Solid	COfb	72.00±0.18	28.00±0.00	35.00±0.06	65.00±0.06	68.00±0.09
Liquid	SA	86.00±0.20	14.00±0.20	40.00±0.22	60.00±0.22	74.00±0.13

Table S9. Classification results for D2 dataset obtained by using the RF classifier. The best classifier's results for solids (SVM) and liquid (KNN) analytes are shown separately.

	TATP	AA	HMTD
TATP	55	13	23
AA	0	0	0
HMTD	21	23	59

Table S10. Confusion matrix of solid analyte classification of Ex1 dataset with the GPLASSO classifier.

	TATP	HEX	AA
TATP	10	0	10
HEX	0	11	0
AA	1	0	0

Table S11. Confusion matrix of solid analyte classification of Ex2 dataset with KNN classifier.

	BMK	EG	H ₂ O ₂	Ac	AA
BMK	12	0	0	0	0
EG	0	11	0	1	0
H ₂ O ₂	0	0	12	0	0
Ac	0	1	0	9	3
AA	0	0	0	1	7

Table S12. Confusion matrix of liquid analytes classification of Pc1 dataset with RF classifier.

	Gly	H ₂ O ₂	To	EG	AA
Gly	9	0	2	2	7
H ₂ O ₂	0	23	0	0	0
Tol	4	0	16	0	9
EG	0	0	0	20	0
AA	9	1	2	0	8

Table S13. Confusion matrix of liquid analytes classification of Pc3 dataset for KNN classifier.

	MA	ER	PER	AA
MA	0	0	0	0
ER	0	0	0	0
PER	6	8	16	12
AA	0	0	0	0

Table S14. Confusion matrix of solid analytes classification of Pc4 dataset with SVM classifier.

	AA	COfb
AA	14	10
COfb	10	14

Table S15. Confusion matrix of solid analytes classification of D2 dataset with SVM classifier.

	AA	E
AA	4	14
E	32	144

	AA	E	EP
AA	23	6	8
E	11	34	3
EP	2	0	67

Table S16. Confusion matrix for the Ex1 dataset in a condensed form. Left: Solid analytes, Right: Liquid analytes.

23 *Glycerin*, <https://pubchem.ncbi.nlm.nih.gov/compound/glycerol#section=Vapor-Density>, Accessed: 6-7-2022.

	AA	E	EP
AA	0	1	0
E	10	10	0
EP	0	0	11

	AA	EP
AA	7	0
EP	0	9

Table S17. Confusion matrix for the Ex2 dataset in a condensed form. Left: Solid analytes, Right: Liquid analytes.

	AA	D	DP	E	EA	EP
AA	63	30	0	24	16	59
D	5	9	0	0	0	1
DP	0	0	18	0	0	1
E	15	12	2	160	4	16
EA	8	0	0	0	6	0
EP	1	0	0	0	0	6

	AA	DP	E	EP
AA	78	35	4	39
DP	7	24	1	1
E	0	0	33	1
EP	6	2	0	199

Table S18. Confusion matrix for the combined diff dataset in a condensed form. Left: Solid analytes, Right: Liquid analytes.

	AA	D	DP	E	EA	EP
AA	60	28	0	26	5	49
D	3	15	0	4	0	2
DP	0	0	18	0	0	0
E	22	7	0	152	0	23
EA	6	0	0	1	19	0
EP	1	1	2	1	2	9

	AA	DP	E	EP
AA	73	33	4	25
DP	6	20	4	6
E	4	4	23	7
EP	6	2	0	202

Table S19. Confusion matrix for the combined time series dataset in a condensed form. Left: Solid analytes, Right: Liquid analytes.

Phase	Analyte name	TPR	FNR	FPR	TNR	F1 SCORE
Solid	AN	0.00±0.00	100.00±0.00	0.26±0.52	99.74±0.52	-
	COfb	22.50±20.00	77.50±20.00	1.41±2.18	98.59±2.18	-
	MA	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-
	DMNB	24.00±15.94	76.00±15.94	2.13±4.27	97.87±4.27	-
	EPH	90.00±20.00	10.00±20.00	0.26±0.52	99.74±0.52	90.48±13.13
	ER	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-
	HEX	70.00±40.00	30.00±40.00	0.00±0.00	100.00±0.00	-
	HMTD	75.60±30.11	24.40±30.11	9.05±3.61	90.95±3.61	65.06±17.78
	PER	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-
	TATP	48.86±14.55	51.14±14.55	15.95±6.05	84.05±6.05	43.17±5.44
Ur	0.00±0.00	100.00±0.00	0.26±0.53	99.74±0.53	-	
Liquid	Ac	10.00±20.00	90.00±20.00	1.15±2.31	98.85±2.31	-
	BMK	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	Cy	0.00±0.00	100.00±0.00	0.19±0.38	99.81±0.38	-
	DP	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-
	EG	84.27±15.51	15.73±15.51	2.93±2.26	97.07±2.26	86.26±11.32
	Gly	0.00±0.00	100.00±0.00	0.20±0.39	99.80±0.39	-
	H ₂ O ₂	95.84±6.68	4.16±6.68	1.55±1.91	98.45±1.91	95.79±5.83
	H ₂ O	80.00±40.00	20.00±40.00	0.00±0.00	100.00±0.00	-
	MEK	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00
	MEKP	82.38±10.61	17.62±10.61	0.80±0.75	99.20±0.75	84.80±10.30
Ph	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00	
SA	26.67±8.58	73.33±8.58	2.23±2.44	97.77±2.44	34.77±10.16	
To	6.67±13.33	93.33±13.33	0.00±0.00	100.00±0.00	-	

Table S20. Classification results for the combined dataset consisting of all analytes obtained by using the RF classifier. The best classifier's results for solids and liquid analytes are shown separately.

	MA	HMTD	AA	TATP	PER	ER	EPH	COfb	DMNB	AN	Ur	HEX
MA	0	0	0	0	0	0	0	0	0	0	0	0
HMTD	0	64	1	27	0	0	2	0	0	2	2	4
AA	24	2	63	17	23	20	0	30	16	5	12	0
TATP	0	15	14	43	1	2	0	11	4	9	9	0
PER	0	0	0	0	0	0	0	0	0	0	0	0
ER	0	0	0	0	0	0	0	0	0	0	0	0
EPH	0	0	0	0	0	0	18	0	0	0	0	1
COfb	0	0	5	0	0	0	0	9	0	0	1	0
DMNB	0	0	8	0	0	0	0	0	6	0	0	0
AN	0	0	0	0	0	0	0	1	0	0	0	0
Ur	0	0	1	0	0	0	0	0	0	0	0	0
HEX	0	0	0	0	0	0	0	0	0	0	0	6

Table S21. Confusion matrix of solid analytes classification of the combined dataset with RF classifier.

Analyte name	TPR	FNR	FPR	TNR	F1 SCORE	
AN	0.00±0.00	100.00±0.00	0.26±0.52	99.74±0.52	-	
COfb	37.22±28.75	62.78±28.75	2.25±1.69	97.75±1.69	-	
DMNB	77.00±20.40	23.00±20.40	2.13±3.64	97.87±3.64	74.48±16.41	
EPH	93.33±13.33	6.67±13.33	0.00±0.00	100.00±0.00	96.00±8.00	
ER	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-	
Solid	HEX	80.00±40.00	20.00±40.00	0.26±0.51	99.74±0.51	-
HMTD	70.66±22.50	29.34±22.50	9.07±3.92	90.93±3.92	63.83±13.38	
MA	0.00±0.00	100.00±0.00	1.32±2.04	98.68±2.04	-	
PER	0.00±0.00	100.00±0.00	0.26±0.53	99.74±0.53	-	
TATP	47.14±10.90	52.86±10.90	17.51±4.02	82.49±4.02	41.31±5.98	
Ur	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-	
Ac	70.00±24.49	30.00±24.49	4.01±5.92	95.99±5.92	53.89±31.99	
BMK	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00	
Cy	26.67±38.87	73.33±38.87	0.58±0.77	99.42±0.77	-	
DP	0.00±0.00	100.00±0.00	0.00±0.00	100.00±0.00	-	
EG	77.57±24.42	22.43±24.42	3.66±2.18	96.34±2.18	79.74±15.98	
Gly	0.00±0.00	100.00±0.00	0.19±0.38	99.81±0.38	-	
Liquid	H ₂ O ₂	86.87±16.07	13.13±16.07	1.03±1.51	98.97±1.51	90.80±10.31
H ₂ O	90.00±20.00	10.00±20.00	0.19±0.38	99.81±0.38	89.33±13.73	
MEK	100.00±0.00	0.00±0.00	0.00±0.00	100.00±0.00	100.00±0.00	
MEKP	60.48±14.88	39.52±14.88	3.63±3.42	96.37±3.42	58.51±11.88	
Ph	90.00±20.00	10.00±20.00	0.00±0.00	100.00±0.00	93.33±13.33	
SA	14.44±8.81	85.56±8.81	3.48±2.40	96.52±2.40	-	
Tol	0.00±0.00	100.00±0.00	0.19±0.39	99.81±0.39	-	

Table S22. Time series classification results for combined dataset obtained by using the CNN classifier. The best classifier's results for solids and liquid analytes are shown separately.

Analyte	Varying dyes
Ac	4, 5, 8, 10, 13, 14, 15, 16, 17, 19, 20, 22, 25, 26
AN	10, 13, 14, 16, 18, 20, 21
BMK	4, 5, 8, 10, 13, 14, 15, 16, 17, 19, 20, 22, 24
COfb	9, 13, 16, 18, 20, 21
Cy	13, 14, 16, 18, 20
DMNB	6, 13, 14, 16, 17, 18, 19, 20, 22, 25
DP	13, 14, 16, 18, 20, 21
EG	4, 5, 6, 8, 10, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 25, 26, 27
EPH	6, 7, 10, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 27
ER	13, 16
Gly	13, 14, 16, 18, 21
H ₂ O	4, 5, 14, 15, 16, 17, 18, 19, 21, 22, 25
H ₂ O ₂	4, 5, 8, 9, 10, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27
HEX	5, 6, 8, 14, 15, 16, 17, 18, 19, 20, 21, 22, 27
HMTD	4, 5, 10, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 26
MA	13, 14, 16
MEK	4, 5, 7, 13, 16, 20, 25
MEKP	2, 4, 5, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22
PER	13, 14, 16
Ph	9, 11, 13, 14, 16, 18, 20, 21, 23, 25, 26, 28
SA	13, 16, 18, 21
TATP	4, 5, 8, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 25, 26
To	10, 16, 18, 20, 21
Ur	14, 16, 20, 21

Table S23. List of dyes that vary when exposed to an analyte. A simple linear regression model is fitted to the data and the dyes for which we get a fit with $R^2 \geq 0.8$ are shown.