

The Impact of Precision Uncertainty on Predictive Accuracy Metrics of Non-Animal Testing Methods

Supplementary Data

Experimental samples of substances used in the calculation of accuracy metrics

Tab. S1: Experimental sample tested with the DPRA (borderline substances in bold)

Chemical name	CAS no	Sensitization potential in mice or humans (by conventional approach, assessed without BR)	
		LLNA	Human
Salicylic acid	69-72-7	N	N
Geraniol	106-24-1	P	-
Benzyl alcohol	100-51-6	P	P
Tween 80	9005-65-6	N	P
3-Dimethylamino propylamine	109-55-7	N	N
cis-6-Nonenal	2277-19-2	P	P
Ethyl vanillin	121-32-4	P	-
Undecylenic acid	112-38-9	N	-
2-Methoxy-4-Methylphenol	93-51-6	P	P
Ethyl benzoylacetate	94-02-0	P	-
Dihydroeugenol (2-Methoxy-4-Propyl-phenol)	2785-87-7	N	-
α -Hexyl cinnamic aldehyde	101-86-0	P	-
N,N-Diethyl-m-toluanimide	134-62-3	N	-
Penicillin G	61-33-6	P	P
d,l-Citronellol	106-22-9	P	N
Pentachlorophenol	87-86-5	P	P
p-tert-Butyl-alpha-ethyl hydrocinnamal (Lilial)	80-54-6	P	P
1-Bromobutane	109-65-9	N	-
Fumaric acid	110-17-8	N	N
Glucose	50-99-7	N	N
Propyl paraben	94-13-3	TN	TN
4-Methoxyacetophenone (Acetanisole)	100-06-1	TN	TN
6-Methylcoumarin	92-48-8	TN	TN
Nonanoic acid	112-05-0	FN	TN
Isopropanol	67-63-0	FN	TN
Methyl salicylate	119-36-8	TN	TN
Dibutyl phthalate	84-74-2	TN	inconclusive
Pyridine	110-86-1	TN	-
dl- α -Tocopherol	10191-41-0	TN	-
Clotrimazole	23593-75-1	FN	-
Methyl pyruvate	600-22-6	FN	-
1-Butanol	71-36-3	TN	TN
Xylene	1330-20-7	FN	TN
Diethyl phthalate	84-66-2	TN	TN
Vinylidene dichloride	75-35-4	TN	-
Oxalic acid anhydrous	144-62-7	FN	-
Octanoic acid (Caprylic acid)	124-07-2	TN	TN
Coumarin	91-64-5	TN	FN
Dimethyl formamide	68-12-2	TN	-
Glycerol	56-81-5	TN	TN
2,2,6,6-Tetramethyl-3,5-heptanedione	1118-71-4	FN	-
N,N-Dibutylaniline	613-29-6	FN	FN
Resorcinol	108-46-3	FN	-
Chlorobenzene	108-90-7	TN	-
Propylene glycol (1,2-Propanediol)	57-55-6	TN	TN

4-Chloroaniline	106-47-8	FN	-
7,12-Dimethylbenz[α]anthracene	57-97-6	FN	-
Aniline	62-53-3	FN	FN
Saccharin	81-07-2	TN	TN
Hexadecyltrimethylammonium bromide (Cetrimide)	57-09-0	TN	-
n-Hexane	110-54-3	TN	TN
Benzalkonium chloride	8001-54-5	TN	TN
Lactic acid	50-21-5	TN	TN
Octanenitrile	124-12-9	TN	-
Undec-10-enal	112-45-8	FN	-
Benzyl benzoate	120-51-4	FN	TN
Methyl 4-hydroxybenzoate (Methylparaben)	99-76-3	TN	-
Butylbenzylphthalate	85-68-7	TN	-
4-Hydroxybenzoic acid	99-96-7	TN	TN
Sulfanilamide	63-74-1	TN	TN
Cocamidopropyl betaine	61789-40-0	TN	-
Benzene,1-methoxy-4-methyl-2-nitro (4-Methyl-2-nitroanisole)	119-10-8	TN	-
Squaric acid diethyl ester	5231-87-8	FN	-
Clofibrate (Ethyl (2-(4-chlorophenoxy)-2-methylpropanoate)	637-07-0	TN	-
α-Amyl cinnamic aldehyde	122-40-7	FN	Inconclusive
Streptomycin sulfate	3810-74-0	TN	FN
α-iso-Methylionone	127-51-5	FN	TN
Carbonic acid, dioctyl ester	1680-31-5	TN	-
Hexyl salicylate	6259-76-3	FN	TN
Benzyl cinnamate	103-41-3	FN	-
Benzyl salicylate	118-58-1	FN	TN
Sulfanilic acid	121-57-3	TN	-
Isopropyl myristate a	110-27-0	FN	TN
p-Aminobenzoic acid	150-13-0	TN	TN
Tartaric acid	87-69-4	TN	TN
Zinc sulfate	7733-02-0	TN	-
Dioctyl ether	629-82-3	TN	-
2,2-Azobis phenol	2050-14-8	FN	-
Benzaldehyde	100-52-7	TN	FN
Farnesol	4602-84-0	FN	FN
3-Aminophenol	591-27-5	FN	-
(+/-) Linalool	78-70-6	FN	TN
Diethylenetriamine	111-40-0	FN	FN
Octanoic acid, 4-methyl-2-pentylbutyl ester	868839-23-0	TN	-
R(+)-Limonene	5989-27-5	TP	FP
Ethylenediamine free base	107-15-3	TP	TP
Vanillin	121-33-5	FP	FP
Cyclamen aldehyde	103-95-7	TP	-
Tropolone	533-75-5	TP	-
Cinnamyl Alcohol	104-54-1	TP	TP
R-Carvone	6485-40-1	TP	TP
Benzocaine	94-09-7	FP	TP
3-Phenoxypropionitrile	3055-86-5	FP	-
2-Acetyl-cyclohexanone	874-23-7	FP	-
Diethyl sulfate	64-67-5	TP	-
2-Phenylpropionaldehyde	93-53-8	TP	TP
5-Methyl-2,3-hexanedione	13706-86-0	TP	TP
1-Iodohexane	638-45-9	FP	-
2,2-Bis-[4-(2-hydroxy-3-methacryloxypropoxy)phenyl]-propane (Bis-GMA)	1565-94-2	TP	-
Farnesal	502-67-0	TP	-
α-Methyl-trans-Cinnamaldehyde	101-39-3	TP	-
3,4-Dihydrocoumarin	119-84-6	TP	TP
Eugenol	97-53-0	TP	TP
Lyal / 3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexene-1-carboxaldehyde	31906-04-4	TP	TP
Nickel chloride	7718-54-9	FP	TP
Bisphenol A-diglycidyl ether	1675-54-3	TP	TP
1,2,4-Benzenetricarboxylic anhydride (Trimellitic anhydride)	552-30-7	TP	-
1-(p-Methoxyphenyl)-1-penten-3-one	104-27-8	TP	-
3-Propylenephthalide	17369-59-4	TP	TP
Perillaldehyde	2111-75-3	TP	TP

Tetrachloro-salicylanilide	1154-59-2	TP	TP
2-Fluoro-5-nitroaniline	369-36-8	FP	-
Phthalic anhydride	85-44-9	TP	FP
1,2-cyclohexane dicarboxylic anhydride	85-42-7	TP	-
Squaric acid	2892-51-5	TP	TP
Formaldehyde	50-00-0	TP	TP
2-Hydroxypropyl methacrylate	923-26-2	FP	-
1-Phenyl-1,2-propanedione	579-07-7	TP	-
Cobalt chloride	7646-79-9	TP	TP
Methylmethacrylate	80-62-6	TP	TP
Phenyl benzoate	93-99-2	TP	TP
3-Chloro-4-Methoxybenzaldehyde (3-Chloro-p-anisaldehyde)	4903-09-7	FP	-
Butyl glycidyl ether	2426-08-6	TP	TP
Imidazolidinyl urea	39236-46-9	TP	TP
1-Naphthol	90-15-3	TP	-
Ethanol-2-butoxy acetate	112-07-2	FP	-
1-Bromohexane	111-25-1	TP	-
Phenylacetaldehyde	122-78-1	TP	TP
Benzoic acid	65-85-0	FP	-
1-Iodoheptadecane	544-77-4	TP	-
Citral	5392-40-5	TP	TP
Bandrowski's Base (N,N-bis(4-aminophenyl)-2,5-diamino-1,4-quinone-diimine)	20048-27-5	TP	-
1,1,3-Trimethyl-2-Formylcyclohexa-2,4-diene (Safranal)	116-26-7	TP	TP
4-Vinyl pyridine	100-43-6	TP	-
Benzylidene acetone (4-Phenyl-3-buten-2-one)	122-57-6	TP	TP
2-Nitro-1,4-phenylenediamine	5307-14-2	TP	TP
2,5-Diaminotoluene sulfate (PTD)	615-50-9	TP	TP
Hydroxycitronellal	107-75-5	TP	TP
MCI/MI	26172-55-4 & 2682-20-4	TP	TP
Sodium lauryl sulfate / sodium dodecyl sulfate (SDS)	151-21-3	TP	FP
Methyl-2-octynoate / Methyl heptene carbonate	111-12-6	TP	TP
2-Methyl-2H-Isothiazol-3-one (MI)	2682-20-4	TP	TP
4-Allylanisole	140-67-0	TP	-
Diphenylcyclopropanone	886-38-4	TP	TP
Lauryl gallate	1166-52-5	TP	TP
Iodopropynyl butylcarbamate	55406-53-6	TP	TP
Furil	492-94-4	FP	-
2-Methylundecanal	110-41-8	TP	-
N,N-dimethyl-4-nitrosoaniline	138-89-6	TP	-
2-Propylheptyl acrylate	149021-58-9	TP	-
trans-2-Hexenal	6728-26-3	TP	TP
5-Amino-2-methylphenol	2835-95-2	TP	-
Chlorothalonil	1897-45-6	TP	-
2-Mercaptobenzothiazole	149-30-4	TP	TP
Methyl 2-nonynoate	111-80-8	TP	TP
Methyl methanesulphonate	66-27-3	TP	-
4-(N-Ethyl-N-2-methan-sulphonamido-ethyl)-2-methyl-1,4-phenylenediamine (CD3)	25646-71-3	TP	-
1,2-Dibromo-2,4-dicyanobutane (MDGN, Methylidibromo glutaronitrile)	35691-65-7	TP	TP
Trans-2-Decenal	3913-71-1	TP	-
Tetramethylthiuram disulfide	137-26-8	TP	TP
1,2-Benzisothiazolin-3-One (Proxel active)	2634-33-5	TP	TP
Propanoic acid, 3-Bromo-Mmethyl ester (Methyl-3-bromopropionate)	3395-91-3	FP	-
4-Carboxyphenylacetate	2345-34-8	TP	-
Cinnamic aldehyde	104-55-2	TP	TP
2-Aminophenol	95-55-6	TP	TP
Diethyl acetaldehyde	97-96-1	TP	-
Glutaraldehyde	111-30-8	TP	TP
Abietic acid	514-10-3	TP	TP
4-Ethoxymethylene-2-phenyl-2-oxazolin-5-one (Oxazolone)	15646-46-5	TP	TP
4-Amino-m-cresol	2835-99-6	TP	-
Isoeugenol	97-54-1	TP	TP
2-Ethylhexyl acrylate	103-11-7	TP	-

2,4-Heptadienal	5910-85-0	TP	-
2,4-Dinitrobenzenesulfonic acid, sodium salt	885-62-1	TP	-
Benzyl bromide	100-39-0	TP	-
2,4,6-Trinitrobenzenesulfonic acid	2508-19-2	TP	-
Propyl gallate	121-79-9	TP	TP
4-Nitrobenzyl bromide	100-11-8	TP	-
Glyoxal	107-22-2	TP	TP
Ethylene glycol dimethacrylate (EGDMA)	97-90-5	TP	TP
2,3-Butanedione	431-03-8	TP	-
Isophorone diisocyanate	4098-71-9	TP	-
5-Chloro-2-methyl-4-isothiazolin-3-one (MCI)	26172-55-4	TP	-
1,6-hexamethylene diisocyanate	822-06-0	TP	-
Hydroquinone	123-31-9	TP	TP
Maleic anhydride	108-31-6	TP	-
1,4-Phenylenediamine	106-50-3	TP	TP
4-(Methylamino) Phenol sulfate (Metol)	55-55-0	TP	TP
1-Chloro-2,4-Dinitrobenzene (Dinitrochlorobenzene, DNCB)	97-00-7	TP	TP
Fluorescein-5-isothiocyanate	3326-32-7	TP	-
3-Methylcatechol	488-17-5	TP	-
Diethyl maleate	141-05-9	TP	TP
Benzoyl peroxide	94-36-0	TP	TP
2-Hydroxyethyl acrylate	818-61-1	TP	TP
Ethyl acrylate	140-88-5	TP	TP
Methyl acrylate	96-33-3	TP	-
Butyl acrylate	141-32-2	TP	-
p-Benzoquinone	106-51-4	TP	TP
Tosylchloramide sodium (Chloramine T)	127-65-1	TP	-

Tab. S2: Experimental sample tested with LuSens (borderline substances in bold)

Chemical name	CAS no	Sensitization potential in mice or humans (by conventional approach, assessed without BR)	
		LLNA	Human
1-Butanol	71-36-3	N	N
Benzoyl peroxide	94-36-0	P	P
4-Allylanisole	140-67-0	P	-
Methyldibromo glutaronitrile (MDGN)	35691-65-7	P	P
Phthalic anhydride	85-44-9	FN	TN
Resorcinol	108-46-3	FN	FN
Sodium lauryl sulfate / sodium dodecyl sulfate (SDS)	151-21-3	FN	TN
Nickel chloride	7718-54-9	TN	FN
Salicylic acid	69-72-7	TN	TN
Farnesal	502-67-0	FN	-
Propyl gallate	121-79-9	FN	FN
Hexadecyltrimethylammonium bromide (Cetrimide)	57-09-0	TN	TN
Lactic acid	50-21-5	TN	TN
Aniline	62-53-3	FN	FN
4-Hydroxybenzoic acid	99-96-7	TN	TN
Glucose	50-99-7	TN	TN
Sulfanilamide	63-74-1	TN	TN
Penicillin G	61-33-6	FN	FN
p-Aminobenzoic acid	150-13-0	TN	TN
Ethylenediamine free base	107-15-3	FN	FN
Phenyl benzoate	93-99-2	FN	FN
Glycerol	56-81-5	TN	TN
Cocamidopropyl betaine	61789-40-0	TN	-
Propylene glycol (1,2-Propanediol)	57-55-6	TN	TN
n-Hexane	110-54-3	TN	TN
Isopropanol	67-63-0	TN	TN
Fumaric acid	110-17-8	TN	TN
Tartaric acid	87-69-4	TN	TN
Xylene	1330-20-7	FN	TN
Pyridine	110-86-1	FN	TN
Vanillin	121-33-5	TN	TN
Octanoic acid, 4-methyl-2-pentylbutyl ester	868839-23-0	TN	-
Benzyl alcohol	100-51-6	FP	TP
Diethyl ether	629-82-3	FP	-
Hydroxycitronellal	107-75-5	TP	TP
Methyl salicylate	119-36-8	FP	FP
1,6-hexamethylene diisocyanate	822-06-0	TP	-
p-Benzoquinone	106-51-4	TP	TP
Potassium dichromate	7778-50-9	TP	TP
4-Nitrobenzyl bromide	100-11-8	TP	-
α -Hexyl cinnamic aldehyde	101-86-0	TP	inconclusive
1-Chloro-2,4-dinitrobenzene (Dinitrochlorobenzene, DNCB)	97-00-7	TP	TP
Diethyl phthalate	84-66-2	TN	TN
2-Ethylhexyl acrylate	103-11-7	TP	-
2-Phenylpropionaldehyde	93-53-8	TP	TP
6-Methylcoumarin	92-48-8	FP	inconclusive
Tween 80	9005-65-6	FP	FP
Propyl paraben (propyl-4-hydroxybenzoate)	94-13-3	FP	FP
Formaldehyde	50-00-0	TP	TP
Isophorone diisocyanate	4098-71-9	TP	-
2-Propylheptyl acrylate	149021-58-9	TP	-
Glyoxal	107-22-2	TP	TP
Ethyl acrylate	140-88-5	TP	TP
Imidazolidinyl urea	39236-46-9	TP	TP
Butyl glycidyl ether	2426-08-6	TP	TP
Tetramethylthiuram disulfide	137-26-8	TP	TP
Eugenol	97-53-0	TP	TP
2,4,6-Trinitrobenzenesulfonic acid	2508-19-2	TP	-
Glutaraldehyde	111-30-8	TP	TP
Methyl 4-hydroxybenzoate (Methylparaben)	99-76-3	FP	-
MCI/MI	26172-55-4 & 2682-20-4	TP	TP
Cinnamyl Alcohol	104-54-1	TP	TP
Methylmethacrylate	80-62-6	TP	TP

Cobalt chloride	7646-79-9	TP	TP
4-Ethoxymethylene-2-phenyl-2-oxazolin-5-one (Oxazolone)	15646-46-5	TP	TP
4-(Methylamino)phenol sulfate (Metol)	55-55-0	TP	TP
Undecylenic acid	112-38-9	TP	TP
2,3-Butanedione	431-03-8	TP	-
4-Methoxyacetophenone (Acetanisole)	100-06-1	FP	FP
Butyl acrylate	141-32-2	TP	-
1,4-Phenylenediamine	106-50-3	TP	TP
Methyl acrylate	96-33-3	TP	
Diethyl maleate	141-05-9	TP	TP
Benzylidene acetone (4-Phenyl-3-buten-2-one)	122-57-6	TP	TP
Cinnamic aldehyde	104-55-2	TP	TP
2-Mercaptobenzothiazole	149-30-4	TP	TP
Isoeugenol	97-54-1	TP	TP
Ethylene glycol dimethacrylate (EGDMA)	97-90-5	TP	TP
Citral	5392-40-5	TP	TP

Tab. S3: Experimental sample tested with the h-CLAT (borderline substances in bold)

Chemical name	CAS no	Sensitization potential in mice or humans (by conventional approach, assessed without <i>BR</i>)	
		LLNA	Human
4-phenylenediamine	106-50-3	P	P
Phenyl benzoate	93-99-2	P	P
Ethylene diamine	107-15-3	P	P
Aniline	62-53-3	P	P
Farnesal	502-67-0	P	-
Methyldibromo Glutaronitrile (MDGN)	35691-65-7	P	P
p-Benzoquinone	106-51-4	P	P
Propyl gallate	121-79-9	P	P
MCI/MI	26172-55-4 & 2682-20-4	TP	TP
1-chloro-2,4-dinitrobenzene	97-00-7	TP	-
Cobalt chloride	7646-79-9	TP	TP
Citral	5392-40-5	TP	TP
Cinnamic alcohol	104-54-1	TP	TP
Methylmethacrylate	80-62-6	TP	TP
Isopropanol	67-63-0	TN	TN
DL-lactic acid	50-21-5	TN	TN
Methyl salicylate	119-36-8	TN	TN
Sodium lauryl sulfate	151-21-3	FP	TN
Ethylene glycol dimethacrylate (EDGMA)	97-90-5	TP	TP
Xylene	1330-20-7	FN	TN
Sulfanilamide	63-74-1	TN	TN
2,4,6-trinitrobenzenesulfonic acid	2508-19-2	FN	-
2,3-butanedione	431-03-8	TP	-
2-phenylpropionaldehyde	93-53-8	TP	TP
4-allylanisole	140-67-0	TP	-
Benzylidene acetone	122-57-6	TP	TP
Diethyl maleate	141-05-9	TP	TP
Fumaric acid	110-17-8	TN	TN
Glucose	50-99-7	TN	TN
Hydroxycitronellal	107-75-5	TP	TP
p-aminobenzoic acid	150-13-0	TN	TN
Phthalic anhydride	85-44-9	FN	TP
Undecylenic acid	112-38-9	TP	TP
Vanillin	121-33-5	TN	TN
Propyl-4-hydroxybenzoate	99-76-3	FP	FP
Tartaric acid	87-69-4	TN	TN
n-hexane	110-54-3	TN	TN
Hexadecyltrimethylammonium bromid	57-09-0	TN	TN
Glycerol	56-81-5	TN	TN
Propylene glycol (1,2-Propanediol)	57-55-6	TN	TN

Tab. S4: Experimental sample tested with the “2 out of 3” WoE approach (borderline substances in bold)

Chemical name	CAS no	Sensitization potential in mice or humans (by conventional approach, assessed without <i>BR</i>)	
		LLNA	Human
Phenyl benzoate	93-99-2	P	P
Ethylene diamine	107-15-3	P	P
Methyldibromo glutaronitrile (MDGN)	35691-65-7	P	P
Propyl gallate	121-79-9	P	P
Propylene glycol (1,2-Propanediol)	57-55-6	TN	TN
Tartaric acid	87-69-4	TN	TN
Glycerol	56-81-5	TN	TN
n-Hexane	110-54-3	TN	TN
Propyl paraben (Propyl-4-Hydroxybenzoate)	99-76-3	FP	FP
Sulfanilamide	63-74-1	TN	TN
Vanillin	121-33-5	TN	TN
Isopropanol	67-63-0	TN	TN
Lactic acid	50-21-5	TN	TN
Methyl salicylate	119-36-8	TN	TN
Fumaric acid	110-17-8	TN	TN
Glucose	50-99-7	TN	TN
p-Aminobenzoic acid	150-13-0	TN	TN
Hexadecyltrimethylammonium bromide (Cetrimide)	57-09-0	TN	TN
Xylene	1330-20-7	FN	TN
Methylmethacrylate	80-62-6	TP	TP
Aniline	62-53-3	FN	FN
Ethylene glycol dimethacrylate (EGDMA)	97-90-5	TP	TP
Undecylenic acid	112-38-9	TP	TP
Hydroxycitronellal	107-75-5	TP	TP
Cinnamyl Alcohol	104-54-1	TP	TP
4-Allylanisole	140-67-0	TP	
Sodium lauryl sulfate / sodium dodecyl sulfate (SDS)	151-21-3	FN	TN
Farnesal	502-67-0	TP	
2,3-Butanedione	431-03-8	TP	
Citral	5392-40-5	TP	TP
2-Phenylpropionaldehyde	93-53-8	TP	TP
Benzylidene acetone (4-Phenyl-3-buten-2-one)	122-57-6	TP	TP
Diethyl maleate	141-05-9	TP	TP
Cobalt chloride	7646-79-9	TP	TP
2,4,6-Trinitrobenzenesulfonic acid	2508-19-2	TP	
Phthalic anhydride	85-44-9	FN	TN
1,4-Phenylenediamine	106-50-3	TP	TP
1-Chloro-2,4-dinitrobenzene (Dinitrochlorobenzene, DNCB)	97-00-7	TP	TP
p-Benzoquinone	106-51-4	TP	TP
MCI/MI	26172-55-4 & 2682-20-4	TP	TP

Accuracy metrics of testing methods when compared to human reference data

Tab. S5: Number of substances in the experimental samples (*k*) used for calculating accuracy metrics of non-animal testing methods and the “2 out of 3” ITS approach
(test results compared to human data)

	Including borderline substances	Excluding borderline substance
DPRA	107	95
LuSens	62	59
h-CLAT	35	28
“2 out of 3”ITS approach	35	32

Tab. S6: Minimum and maximum number of substances in randomized samples resulting from bootstrap resampling, after excluding borderline substances
(test results compared to human data)

Randomized sample size (<i>k</i>)	DPRA	LuSens	h-CLAT	“2 out of 3” ITS approach
Min	80	52	19	24
Max	105	62	35	36

Source: Own calculations

Tab. S7: Accuracy metrics of DPRA, LuSens, h-CLAT and the “2 out of 3” ITS approach derived from experimental test results and randomized samples using bootstrap resampling
(test results compared to human data)

		Experimental set of substances	Randomized samples from bootstrap resampling	
			Mean ± SD	95%CI
DPRA		k=107		
Entire sample (including borderline substances)	Sensitivity [%]	85	85±4	(76;93)
	Specificity [%]	80	80±7	(66;93)
	Concordance [%]	83	83±4	(76;90)
		k=95		
Adapted sample (excluding borderline substances)	Sensitivity [%]	89	89±4	(81;96)
	Specificity [%]	87	87±6	(73;97)
	Concordance [%]	88	88±4	(82;95)
LuSens		k=62		
Entire sample (including borderline substances)	Sensitivity [%]	79	79±7	(65;91)
	Specificity [%]	83	83±8	(67;96)
	Concordance [%]	81	81±5	(69;90)
		k=59		
Adapted sample (excluding borderline substances)	Sensitivity [%]	81	81±7	(67;93)
	Specificity [%]	83	83±8	(65;96)
	Concordance [%]	81	81±5	(71;91)
h-CLAT		k=35		
Entire sample (including borderline substances)	Sensitivity [%]	100	100±0	(100;100)
	Specificity [%]	94	94±6	(80;100)
	Concordance [%]	97	97±3	(91;100)
		k=28		
Adapted sample (excluding borderline substances)	Sensitivity [%]	100	100±0	(100;100)
	Specificity [%]	94	94±6	(80;100)
	Concordance [%]	96	96±4	(88;100)
“2 out of 3” ITS approach		k=35		
Entire sample (including borderline substances)	Sensitivity [%]	95	95±5	(82;100)
	Specificity [%]	94	94± 8	(80;100)
	Concordance [%]	94	94±4	(86;100)
		k=32		
Adapted sample (excluding borderline substances)	Sensitivity [%]	93	93±7	(78;100)
	Specificity [%]	94	94±6	(80;100)
	Concordance [%]	94	94±4	(84;100)

Source: Own calculations