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Tab. A1 Detailed list and classification of analysed substances.

substance	drug of abuse	therapeutic drug	doping agent (WADA class)*	analytical standard supplier
(+/-)-amphetamine	✓	✓	S6 stimulants	LGC
(+/-)-methamphetamine	✓	✗	S6 stimulants	LGC
(+/-)-3,4-methylenedioxymethamphetamine (MDMA)	✓	✗	S6 stimulants	LGC
methylhexanamine (4-methylhexan-2-amine, DMAA)	✗	✗	S6 stimulants	Sigma
cocaine	✓	✓	S6 stimulants	LGC
methylphenidate	✓	✓	S6 stimulants	LGC
nikethamide (N,N-diethylnicotinamide)	✗	✓	S6 stimulants	Aldrich
strychnine	✗	✗	S6 stimulants	Sigma
(-)- Δ^9 -tetrahydrocannabinol (THC)	✓	✓	S8 cannabinoids	LGC
(-)-11-nor-9-carboxy- Δ^9 -tetrahydrocannabinol (THC-COOH)	✗	✗	S8 cannabinoids	LGC
morphine	✓	✓	S7 narcotics	LGC
heroin (diacetylmorphine)	✓	✓	S7 narcotics	LGC
hydrocodone	✓	✓	✗	Cerillant®
oxycodone	✓	✓	S7 narcotics	LGC
(+/-)-methadone	✓	✓	S7 narcotics	Cerillant®
buprenorphine	✓	✓	S7 narcotics	Cerillant®
fentanyl	✓	✓	S7 narcotics	LGC
ketamine	✓	✓	✗	LGC
phencyclidine (PCP)	✓	✗	S0 non-approved substances	LGC
lysergic acid diethylamide (LSD)	✓	✗	S0 non-approved substances	LGC
psilocybin	✓	✗	S0 non-approved substances	Cerillant®
alprazolam	✓	✓	✗	LGC
clonazepam	✓	✓	✗	Cerillant®
flunitrazepam	✓	✓	✗	LGC
zolpidem	✓	✓	✗	LGC
boldenone (Δ^1 -testosterone / 1-dehydrotestosterone)	✗	✓	S1 anabolic agents	VETRANAL™ (Sigma-Aldrich)
methandienone (methandrostenolone)	✗	✓	S1 anabolic agents	Cerillant®
nandrolone (19-nortestosterone)	✗	✓	S1 anabolic agents	LGC
stanozolol	✗	✓	S1 anabolic agents	LGC
clenbuterol	✗	✓	S1 anabolic agents	LGC
ibutamoren (MK-677)	✗	✗	S2 peptide hormones, growth factors, related substances and mimetics	Cayman Chemicals
fenoterol	✗	✓	S3 beta-2 agonists	LGC
salbutamol (albuterol)	✗	✓	S3 beta-2 agonists	LGC
terbutaline	✗	✓	S3 beta-2 agonists	LGC
anastrozole	✗	✓	S4 hormone and metabolic modulators	LGC
meldonium	✗	✓	S4 hormone and metabolic modulators	EDQM
canrenone	✗	✓	S5 diuretics and masking agents	Sigma
chlorothiazide	✗	✓	S5 diuretics and masking agents	Sigma-Aldrich
hydrochlorothiazide	✗	✓	S5 diuretics and masking agents	LGC
furosemide	✗	✓	S5 diuretics and masking agents	Sigma
betamethasone	✗	✓	S9 glucocorticoids	LGC
prednisolone	✗	✓	S9 glucocorticoids	Sigma
prednisone	✗	✓	S9 glucocorticoids	Sigma
atenolol	✗	✓	P1 beta-blockers	LGC
bisoprolol	✗	✓	P1 beta-blockers	LGC
carteolol	✗	✓	P1 beta-blockers	USP
metoprolol	✗	✓	P1 beta-blockers	LGC
nebivolol	✗	✓	P1 beta-blockers	Sigma
propranolol	✗	✓	P1 beta-blockers	LGC

*according to 2020 Prohibited List. (<https://www.wada-ama.org/en/resources/science-medicine/prohibited-list-documents>, WADA 2019)

Tab. A2 List of selected MS/MS parameters for the analytes. Substances arranged by increasing retention time.

substance	precursor ion [m/z]	product ions [m/z]			retention time [min]
		quantifier		qualifier(s)	
meldonium	147.00	58.10	59.15	-	1.499
psilocybin	284.90	58.10	205.20	240.05	2.433
morphine	286.10	152.10	201.15	165.10	2.642
salbutamol	240.00	148.10	222.25	166.20	2.913
terbutaline	226.00	152.10	107.05	125.10	3.015
atenolol	267.00	145.10	190.20	74.15	3.089
fenoterol	304.00	107.15	135.15	286.10	4.281
nikethamide	178.90	108.05	80.10	72.10	4.453
carteolol	293.00	237.15	202.15	74.10	4.548
amphetamine	135.90	91.10	119.15	65.10	4.625
oxycodone	316.10	298.20	241.20	256.10	4.629
hydrocodone	300.00	199.15	171.10	128.15	4.928
methamphetamine	150.00	91.10	65.10	119.20	5.001
chlorothiazide	294.00*	214.05	179.10	215.10	5.012
methylhexanamine	116.20	57.10	41.10	-	5.115
MDMA	194.00	163.10	105.10	133.10	5.185
strychnine	334.90	184.10	156.20	129.15	5.330
hydrochlorothiazide	296.00*	269.00	205.10	77.95	5.421
ketamine	237.90	125.05	220.10	207.15	5.665
metoprolol	267.90	116.15	74.15	72.10	6.407
clenbuterol	277.10	203.05	132.10	168.15	6.531
methylphenidate	234.00	84.15	56.10	91.10	6.650
heroin	370.10	165.15	268.20	211.10	6.866
cocaine	303.90	182.20	82.10	105.10	7.348
zolpidem	307.90	235.15	236.20	263.20	7.383
LSD	323.90	223.20	208.15	207.10	7.688
bisoprolol	326.20	116.20	74.05	72.10	7.869
phencyclidine	244.00	91.05	86.10	159.20	8.607
propranolol	260.10	116.20	183.10	155.20	8.775
fentanyl	337.00	188.20	105.15	103.10	9.114
prednisolone	361.00	147.15	325.20	307.15	9.277
prednisone	359.00	341.35	267.30	-	9.409
buprenorphine	468.10	55.15	396.25	414.25	9.672
ibutamoren	529.00	267.10	91.15	263.15	10.382
betamethasone	393.10	373.25	355.15	279.10	10.798
furosemide	329.05*	284.85	205.10	126.10	11.043
neбиволol	406.10	151.10	123.10	103.10	11.098
methadone	310.00	265.15	105.10	77.05	11.322
alprazolam	308.90	281.15	205.15	274.10	11.393
anastrozole	294.00	225.20	210.20	115.05	11.412
stanozolol	329.10	81.15	95.15	121.10	11.496
boldenone	287.00	121.20	135.20	77.15	11.942
clonazepam	316.00	270.10	214.05	207.15	11.970
nandrolone	275.10	109.10	239.10	257.30	12.320
methandienone	301.20	121.05	149.25	77.00	12.582
flunitrazepam	313.90	268.15	239.10	183.10	12.750
canrenone	341.00	107.15	187.25	235.15	15.029
THC-COOH	345.00	327.10	299.25	193.30	19.874
THC	315.00	193.10	123.10	259.15	24.788

*negative ionization mode