Supplementary Data 1
Detailed Analytical Parameters

1 Cut-off and internal standards concentrations

In Table 1, [IS] is the concentration of internal standard (IS) in the IS solution added to samples, not the final concentration in the sample.

Table 1: Analyte and internal standards concentrations

Analyte	**Cut-off** (ng/mL)	**Internal Standard**	**[IS]** (ng/mL)
Alprazolam	8	Lorazepam-D_4	3300
α-Hydroxyalprazolam	20	Triazolam-D_4	1100
Amitriptyline	30	Amitriptyline-D_3	440
Amphetamine	15	Amphetamine-D_8	1100
Aripiprazole	10	Trazodone-D_6	550
Bromazepam	75	Bromazepam-D_4	4950
Buprenorphine	5	Oxycodone-D_3	1100
Bupropion	15	Ephedrine-D_3	1100
Hydroxybupropion	20	Ephedrine-D_3	1100
Chlordiazepoxide	15	Chlordiazepoxide-D_5	1100
Citalopram	30	Citalopram-D_6	440
N-Desmethylcitalopram	20	Citalopram-D_6	440
Clobazam	15	Flunitrazepam-D_7	220
N-Desmethylclobazam	20	Flunitrazepam-D_7	220
Clonazepam	8	Flunitrazepam-D_7	220

Table 1: Analyte and internal standards concentrations

Analyte	**Cut-off** (ng/mL)	**Internal Standard**	**[IS]** (ng/mL)
7-Aminoclonazepam	8	7-Aminoclonazepam-D_4	1100
Cocaethylene	8	Cocaine-D_3	550
Cocaine	8	Cocaine-D_3	550
Benzoylecgonine	8	Cocaine-D_3	550
Codeine	5	Codeine-D_3	1100
Norcodeine	20	Codeine-D_3	1100
Cyclobenzaprine	30	Amitriptyline-D_3	440
N-Desmethylcyclobenzaprine	20	Amitriptyline-D_3	440
Demoxepam	15	Demoxepam-D_5	1100
Dextromethorphane	15	Oxymorphone-D_3	1100
Dextrorphane	20	Oxycodone-D_3	1100
Diazepam	8	Diazepam-D_5	1100
Nordiazepam	8	Diazepam-D_5	1100
Diphenhydramine	30	Diphenhydramine-D_3	2200
N-Desmethyldiphenhydramine	20	Diphenhydramine-D_3	2200
Duloxetine	20	Amitriptyline-D_3	440
EDDP	30	Diphenhydramine-D_3	2200
Ephedrine	15	Ephedrine-D_3	1100
Fentanyl	0.5	Fentanyl-D_5	110
Acetyl fentanyl	1.5	Fentanyl-D_5	110
Norfentanyl	0.5	Fentanyl-D_5	110
Flunitrazepam	15	Flunitrazepam-D_7	220
7-Aminoflunitrazepam	20	7-Aminoclonazepam-D_4	1100
N-Desmethylflunitrazepam	20	Desalkylflurazepam-D_4	1100
Fluoxetine	30	Amitriptyline-D_3	440
Norfluoxetine	20	Amphetamine-D_8	1100

Table 1: Analyte and internal standards concentrations

Analyte	**Cut-off** (ng/mL)	**Internal Standard**	**[IS]** (ng/mL)
Flurazepam	6	Lorazepam-D_4	3300
Desalkylflurazepam	30	Desalkylflurazepam-D_4	1100
2-Hydroxyethylflurazepam	20	Lorazepam-D_4	3300
Hydrocodone	5	Oxycodone-D_3	1100
Hydromorphone	5	Oxymorphone-D_3	1100
Ketamine	30	Ketamine-D_4	1320
Norketamine	20	Ketamine-D_4	1320
Lorazepam	30	Lorazepam-D_4	3300
mCPP	20	Amphetamine-D_8	1100
MDA	20	Amphetamine-D_8	1100
MDEA	20	MDMA-D_5	77
MDMA	15	MDMA-D_5	77
MDPV	15	MDPV-D_8	1100
MDPV metabolite 1	20	MDPV-D_8	1100
Meperidine	15	Cocaine-D_3	550
Normeperidine	40	Codeine-D_3	1100
Methadone	10	Amitriptyline-D_3	440
Methamphetamine	15	Methamphetamine-D_5	110
Midazolam	15	Lorazepam-D_4	3300
α-Hydroxymidazolam	20	Diazepam-D_5	1100
Mirtazapine	30	Amitriptyline-D_3	440
N-Desmethylmirtazapine	20	Amitriptyline-D_3	440
Morphine	5	Morphine-D_6	1100
6-Acetylmorphine	2	Codeine-D_3	1100
Naloxone	20	Oxymorphone-D_3	1100
Naltrexone	20	Oxycodone-D_3	1100

Table 1: Analyte and internal standards concentrations

Analyte	**Cut-off** (ng/mL)	**Internal Standard**	**[IS]** (ng/mL)
Nitrazepam	15	Nitrazepam-D_5	1100
7-Aminonitrazepam	15	7-Aminoclonazepam-D_4	1100
Nortriptyline	15	Amitriptyline-D_3	440
Olanzapine	15	Olanzapine-D_8	220
N-Desmethylolanzapine	20	Olanzapine-D_8	220
Oxazepam	8	Oxazepam-D_5	220
Oxycodone	5	Oxycodone-D_3	1100
Oxymorphone	5	Oxymorphone-D_3	1100
Paroxetine	15	Amitriptyline-D_3	440
PCP	6	PCP-D_5	220
Procyclidine	15	Citalopram-D_6	440
Pseudoephedrine	15	Ephedrine-D_3	1100
Quetiapine	30	Quetiapine-D_8	440
Norquetiapine	20	Quetiapine-D_8	440
7-Hydroxyquetiapine	20	Quetiapine-D_8	440
Risperidone	15	Trazodone-D_6	550
9-Hydroxyrisperidone	15	Trazodone-D_6	550
Rolicyclidine	9	Diphenhydramine-D_3	2200
Sertraline	9	Amitriptyline-D_3	440
Temazepam	30	Lorazepam-D_4	3300
THC	1.5	THC-D_3	110
Tramadol	10	Tramadol-D_3	2200
O-Desmethyl-cis-tramadol	10	Tramadol-D_3	2200
Trazodone	30	Trazodone-D_6	550
Triazolam	15	Triazolam-D_4	1100
α-Hydroxytriazolam	20	Triazolam-D_4	1100

Table 1: Analyte and internal standards concentrations

Analyte	**Cut-off** (ng/mL)	**Internal Standard**	**[IS]** (ng/mL)
Venlafaxine	30	Venlafaxine-D_6	2200
O-Desmethylvenlafaxine	30	Venlafaxine-D_6	2200
Zopiclone	9	Zopiclone-D_4	1100
N-Desmethylzopiclone	20	Zopiclone-D_4	1100

2 General method

2.1 Liquid chromatography

Mobile phase A: methanol : 10 mM Ammonium formate pH 3.0 (2:98 v:v)

Mobile phase B: acetonitrile (LC-MS Grade)

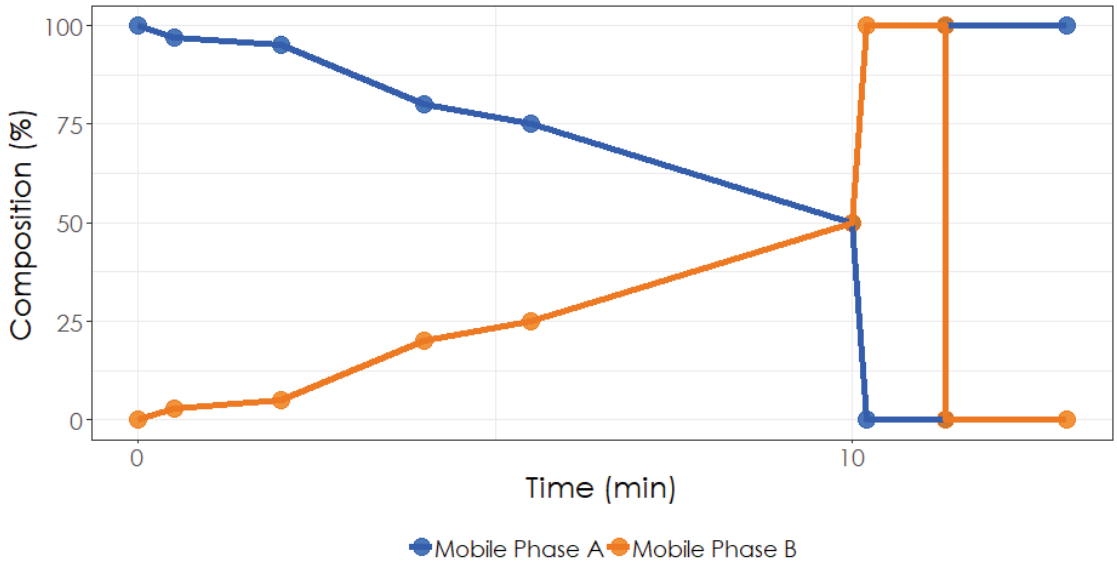
Rinsing solution: methanol : 1% formic acid in water : isopropanol (50:25:25 v:v:v)

Analytical column: Zorbax Eclipse Plus C18, 2.1 $\times$ 100 mm, 3.5 μm (Agilent)

Flow rate: 650 $\mu L/min$

Table 2: LC Pump Gradient

Time (min)	A (%)	B (%)
0.00	100	0
0.50	97	3
2.00	95	5
4.00	80	20
5.50	75	25
10.00	50	50
10.20	0	100
11.30	0	100
11.31	100	0
13.00	100	0



2.2 Autosampler and thermostat Settings

- Injection volume: 5 μL
- Wash time: 10 *sec*
- Autosampler temperature: 4 °C
- Column oven temperature: 50 °C

Table 3: Divert Valve Program

Time (min)	Position
0.0	MS
0.1	Waste
1.5	MS
10.5	Waste
12.5	MS

2.3 Mass spectrometry method

- Scan type: scheduled multiple reaction monitoring (MRM)
- Polarity: positive
- MRM detection window: 45 *sec*
- Target scan time: 0.6 *sec*
- Break: 3.00 *msec*
- Acquisition time: 13 minutes
- Ion source: Turbo Spray
- Curtain Gas (CUR): 30.0
- Collision Gas (CAD): 10.0
- Ion Spray Voltage (IS): 3000.0 *V*
- Source temperature (TEM): 700.0 °C
- Ion Source Gas 1 (GS1): 60.0
- Ion Source Gas (GS2): 65.0

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
309.1	205.0	8.6	Alprazolam 1	140	10	50	15
311.1	283.1	8.6	Alprazolam 2	140	10	37	12
325.1	297.2	8.0	α-Hydroxyalprazolam 1	110	10	38	11
325.1	216.1	8.0	α-Hydroxyalprazolam 2	110	10	56	18
279.2	118.0	8.3	Amitriptyline 1	76	10	32	11
279.2	106.0	8.3	Amitriptyline 2	76	10	30	11
136.1	119.0	3.5	Amphetamine 1	40	10	13	10
136.1	91.1	3.5	Amphetamine 2	40	10	28	10
448.1	285.1	8.3	Aripiprazole 1	80	10	37	10
448.1	176.1	8.3	Aripiprazole 2	80	10	42	11
290.1	105.0	4.5	Benzoylecgonine 1	70	10	26	10
290.1	82.0	4.5	Benzoylecgonine 2	70	10	25	10
316.0	182.2	7.0	Bromazepam 1	100	10	45	18
316.0	209.1	7.0	Bromazepam 2	100	10	38	18
240.1	139.0	5.7	Bupropion 1	55	10	29	10
240.1	103.0	5.7	Bupropion 2	55	10	45	10
256.1	130.1	5.0	Hydroxybupropion 1	50	10	48	12
256.1	103.1	5.0	Hydroxybupropion 2	50	10	49	18
300.1	227.1	6.5	Chlordiazepoxide 1	65	10	35	20
300.1	165.1	6.5	Chlordiazepoxide 2	65	10	70	13
326.2	235.0	7.2	Citalopram 1	85	10	40	15
326.2	263.1	7.2	Citalopram 2	85	10	22	15
312.2	110.1	7.1	N-Desmethylcitalopram 1	70	10	30	15
312.2	263.1	7.1	N-Desmethylcitalopram 2	70	10	24	25
301.1	224.1	9.1	Clobazam 1	100	10	47	15
301.1	259.0	9.1	Clobazam 2	100	10	20	15

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
287.1	245.0	8.3	N-Desmethylclobazam 1	100	10	28	15
287.1	210.0	8.3	N-Desmethylclobazam 2	100	10	42	13
316.1	270.0	8.3	Clonazepam 1	90	10	36	15
316.1	214.0	8.3	Clonazepam 2	90	10	53	19
286.1	250.1	4.9	7-Aminoclonazepam 1	80	10	30	18
286.1	94.1	4.9	7-Aminoclonazepam 2	80	10	56	13
305.2	183.1	5.3	Cocaine 1	30	10	21	15
304.2	91.0	5.3	Cocaine 2	30	10	38	12
319.2	197.1	6.1	Cocaethylene 1	100	10	20	15
318.2	150.0	6.1	Cocaethylene 2	100	10	28	15
300.2	215.0	3.4	Codeine 1	110	10	36	18
300.2	152.0	3.4	Codeine 2	110	10	91	18
286.1	115.0	3.3	Norcodeine 1	100	10	90	15
286.1	128.0	3.3	Norcodeine 2	100	10	80	15
277.2	232.1	8.0	Cyclobenzaprine 1	85	10	19	15
276.1	115.1	8.0	Cyclobenzaprine 2	85	10	33	12
263.2	216.0	8.0	N-Desmethylcyclobenzaprine 1	60	10	51	17
263.2	232.0	8.0	N-Desmethylcyclobenzaprine 2	60	10	22	21
287.1	241.0	7.4	Demoxepam 1	100	10	50	15
287.1	115.1	7.4	Demoxepam 2	100	10	33	15
273.2	216.1	6.7	Dextromethorphane 1	120	10	35	20
273.2	172.0	6.7	Dextromethorphane 2	120	10	52	15
259.2	158.1	4.8	Dextrorphan 1	85	10	53	17
259.8	115.0	4.8	Dextrorphan 2	85	10	83	15
285.1	89.0	9.8	Diazepam 1	45	10	70	15
285.1	223.1	9.8	Diazepam 2	45	10	37	12

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
298.1	154.0	8.2	Duloxetine 1	60	10	9	9
298.1	44.0	8.2	Duloxetine 2	60	10	50	10
271.1	140.0	8.9	Nordiazepam 1	95	10	42	13
271.1	165.1	8.9	Nordiazepam 2	95	10	39	15
256.2	115.0	7.0	Diphenhydramine 1	55	10	70	10
256.2	128.1	7.0	Diphenhydramine 2	55	10	70	10
243.1	168.1	6.9	N-Desmethyldiphenhydramine 1	40	10	20	15
243.1	153.1	6.9	N-Desmethyldiphenhydramine 2	40	10	50	15
279.2	250.1	7.5	EDDP 1	100	10	26	15
279.2	116.0	7.5	EDDP 2	100	10	95	13
166.1	133.0	2.9	Ephedrine 1	40	10	29	12
166.1	117.0	2.9	Ephedrine 2	40	10	29	10
337.2	188.2	6.8	Fentanyl 1	110	10	34	17
337.2	105.1	6.8	Fentanyl 2	110	10	55	14
233.2	84.1	4.6	Norfentanyl 1	60	10	26	10
233.2	150.1	4.6	Norfentanyl 2	60	10	25	13
323.2	188.2	5.9	Acetyl fentanyl 1	100	10	33	14
323.2	105.0	5.9	Acetyl fentanyl 2	100	10	55	12
314.1	268.1	8.8	Flunitrazepam 1	100	10	36	12
314.1	183.0	8.8	Flunitrazepam 2	100	10	75	15
284.1	240.0	5.5	7-Aminoflunitrazepam 1	120	10	51	20
284.1	226.1	5.5	7-Aminoflunitrazepam 2	120	10	40	20
300.1	254.0	7.9	N-Desmethylflunitrazepam 1	85	10	36	15
300.1	198.1	7.9	N-Desmethylflunitrazepam 2	85	10	55	15
310.1	148.0	8.6	Fluoxetine 1	40	10	10	15
310.1	44.0	8.6	Fluoxetine 2	130	10	23	10

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
296.1	134.2	8.5	Norfluoxetine 1	65	10	10	10
296.1	296.1	8.5	Norfluoxetine 2	65	10	5	10
389.2	316.0	7.1	Flurazepam 1	100	10	35	20
389.2	134.0	7.1	Flurazepam 2	100	10	75	16
289.1	140.0	8.8	Desalkylflurazepam 1	110	10	40	15
289.1	226.1	8.8	Desalkylflurazepam 2	110	10	40	12
333.1	211.1	8.5	2-Hydroxyethylflurazepam 1	120	10	51	15
333.1	109.1	8.5	2-Hydroxyethylflurazepam 2	120	10	40	14
300.2	128.2	3.9	Hydrocodone 1	90	10	78	15
300.2	115.0	3.9	Hydrocodone 2	90	10	85	14
286.1	185.1	2.2	Hydromorphone 1	120	10	40	15
286.1	157.0	2.2	Hydromorphone 2	120	10	58	20
239.1	126.0	4.6	Ketamine 1	64	10	43	12
239.1	208.1	4.6	Ketamine 2	64	10	21	16
224.1	179.3	4.5	Norketamine 1	70	10	20	15
224.1	126.0	4.5	Norketamine 2	70	10	35	20
321.0	275.0	8.3	Lorazepam 1	70	10	31	15
321.0	229.1	8.3	Lorazepam 2	70	10	72	15
197.1	154.1	4.9	mCPP 1	75	10	20	13
197.1	118.0	4.9	mCPP 2	75	10	29	14
180.1	79.0	3.7	MDA 1	50	10	40	12
180.1	135.0	3.7	MDA 2	50	10	26	12
209.1	164.0	4.4	MDEA 1	60	10	14	15
209.1	136.1	4.4	MDEA 2	601	10	30	15
195.1	164.1	4.0	MDMA 1	60	10	20	15
195.1	106.1	4.0	MDMA 2	60	10	35	10

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
277.2	176.1	5.3	MDPV 1	75	10	31	15
277.2	127.1	5.3	MDPV 2	75	10	35	15
279.2	176.1	4.6	MDPV metabolite 1	50	10	23	20
279.2	127.2	4.6	MDPV metabolite 2	50	10	23	15
249.2	22.1	5.4	Meperidine 1	80	10	31	20
249.2	175.2	5.4	Meperidine 2	80	10	27	13
235.1	161.1	5.5	Normeperidine 1	60	10	22	15
234.1	115.1	5.5	Normeperidine 2	60	10	85	11
311.2	266.0	8.4	Methadone 1	80	10	15	10
311.2	224.2	8.4	Methadone 2	80	10	31	20
151.1	120.1	3.8	Methamphetamine 1	65	10	15	10
150.1	91.0	3.8	Methamphetamine 2	40	10	15	10
326.1	291.0	7.0	Midazolam 1	85	10	30	12
326.1	249.0	7.0	Midazolam 2	85	10	53	12
342.1	168.1	7.3	α-Hydroxymidazolam 1	110	10	55	15
342.1	140.0	7.3	α-Hydroxymidazolam 2	110	10	84	12
267.2	210.1	5.2	Mirtazapine 1	90	10	33	10
266.2	115.0	5.2	Mirtazapine 2	90	10	50	15
253.2	196.2	5.0	N-Desmethylmirtazapine 1	70	10	31	15
252.2	209.2	5.0	N-Desmethylmirtazapine 2	70	10	22	20
286.1	152.1	1.7	Morphine 1	100	10	79	14
286.1	165.0	1.7	Morphine 2	100	10	60	15
328.2	165.0	4.0	6-Acetylmorphine 1	80	10	55	10
328.2	211.0	4.0	6-Acetylmorphine 2	80	10	37	10
328.2	212.2	3.4	Naloxone 1	100	10	55	15
328.2	253.2	3.4	Naloxone 2	100	10	38	15

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
342.2	270.1	3.9	Naltrexone 1	100	10	38	15
342.2	212.0	3.9	Naltrexone 2	100	10	60	20
282.2	236.0	8.0	Nitrazepam 1	100	10	36	15
282.2	207.0	8.0	Nitrazepam 2	100	10	50	11
252.1	146.0	3.6	7-Aminonitrazepam 1	100	10	40	14
253.1	122.1	3.6	7-Aminonitrazepam 2	100	10	37	15
265.2	234.2	8.1	Nortriptyline 1	80	10	20	10
265.2	192.0	8.1	Nortriptyline 2	80	10	35	10
314.1	257.0	4.0	Olanzapine 1	40	10	26	25
313.1	282.0	4.0	Olanzapine 2	40	10	38	10
299.1	213.1	3.9	N-Desmethylolanzapine 1	140	10	30	11
299.1	198.1	3.9	N-Desmethylolanzapine 2	140	10	42	12
287.1	241.1	8.1	Oxazepam 1	60	10	30	20
287.1	104.1	8.1	Oxazepam 2	60	10	45	12
316.2	256.1	3.7	Oxycodone 1	95	10	35	15
316.2	241.0	3.7	Oxycodone 2	95	10	42	15
302.1	284.0	1.9	Oxymorphone 1	90	10	22	16
302.1	227.0	1.9	Oxymorphone 2	90	10	41	12
330.2	70.0	7.8	Paroxetine 1	100	10	45	10
330.2	109.0	7.8	Paroxetine 2	100	10	75	10
244.2	159.1	6.3	PCP 1	50	10	20	20
244.2	91.0	6.3	PCP 2	50	10	35	10
152.1	117.1	2.3	Phenylpropanolamine 1	40	10	23	12
152.1	91.0	2.3	Phenylpropanolamine 2	40	10	47	16
288.2	42.0	7.7	Procyclidine 1	90	10	75	10
289.2	85.2	7.7	Procyclidine 2	90	10	30	10

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
166.1	133.0	3.1	Pseudoephedrine 1	45	10	29	12
166.1	117.0	3.1	Pseudoephedrine 2	45	10	28	11
385.2	248.1	7.1	Quetiapine 1	70	10	55	15
385.2	280.1	7.1	Quetiapine 2	70	10	40	20
297.1	140.1	6.9	Norquetiapine 1	70	10	80	15
297.1	184.0	6.9	Norquetiapine 2	70	10	53	15
401.1	270.0	4.7	7-Hydroxyquetiapine 1	30	10	35	18
401.1	209.1	4.7	7-Hydroxyquetiapine 2	30	10	60	20
411.2	110.0	6.1	Risperidone 1	90	10	56	15
411.2	163.0	6.1	Risperidone 2	90	10	68	15
427.2	179.2	5.7	9-Hydroxyrisperidone 1	110	10	60	15
427.2	165.2	5.7	9-Hydroxyrisperidone 2	110	10	60	15
230.2	72.0	6.0	Rolicyclidine 1	50	10	18	10
230.2	159.0	6.0	Rolicyclidine 2	50	10	18	12
306.1	123.1	8.7	Sertraline 1	50	10	75	15
306.1	275.1	8.7	Sertraline 2	50	10	12	15
301.1	177.0	9.0	Temazepam 1	65	10	43	17
302.1	256.1	9.0	Temazepam 2	65	10	23	15
264.2	42.0	5.0	Tramadol 1	80	10	75	10
265.2	59.0	5.0	Tramadol 2	80	10	45	10
250.2	58.0	4.0	O-Desmethyl-cis-tramadol 1	150	10	90	10
250.2	42.0	4.0	O-Desmethyl-cis-tramadol 2	70	10	105	14
373.2	177.1	6.2	Trazodone 1	50	10	25	14
373.2	149.1	6.2	Trazodone 2	90	10	37	15
343.1	204.2	8.7	Triazolam 1	100	10	70	18
343.1	177.2	8.7	Triazolam 2	100	10	90	15

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
359.0	331.0	8.0	α-Hydroxytriazolam 1	100	10	40	10
359.0	176.0	8.0	α-Hydroxytriazolam 2	100	10	38	16
278.2	147.1	6.0	Venlafaxine 1	60	10	25	13
279.2	216.2	6.0	Venlafaxine 2	60	10	24	16
264.2	201.2	4.6	O-Desmethylvenlafaxine 1	60	10	25	20
264.2	107.0	4.6	O-Desmethylvenlafaxine 2	60	10	27	15
389.1	245.0	4.9	Zopiclone 1	60	10	26	10
389.1	217.0	4.9	Zopiclone 2	60	10	47	16
375.1	245.1	4.9	N-Desmethylzopiclone 1	70	10	25	10
375.1	217.0	4.9	N-Desmethylzopiclone 2	70	10	50	10
281.2	117.0	8.3	Amitriptyline-D_3	76	10	32	11
144.1	127.0	3.4	Amphetamine-D_8	40	10	13	10
320.0	186.2	6.9	Bromazepam-D_4	100	10	45	18
305.1	232.2	6.4	Chlordiazepoxide-D_5	65	10	35	20
331.2	234.0	7.2	Citalopram-D_6	85	10	40	15
209.1	254.0	4.8	7-Aminoclonazepam-D_4	80	10	30	18
308.2	185.0	5.3	Cocaine-D_3	30	10	21	15
303.3	215.0	3.5	Codeine-D_3	110	10	36	18
292.1	246.2	7.3	Demoxepam-D_5	100	10	50	15
290.1	89.0	9.8	Diazepam-D_5	45	10	70	15
259.2	115.0	7.0	Diphenhydramine-D_3	55	10	80	10
169.1	136.0	2.9	Ephedrine-D_3	40	10	29	12
342.2	188.2	6.8	Fentanyl-D_5	110	10	34	17
321.1	275.1	8.7	Flunitrazepam-D_7	100	10	36	12
293.1	140.0	8.8	Desalkylflurazepam-D_4	110	10	40	15
244.1	131.0	4.6	Ketamine-D_4	64	10	43	12

Table 4: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
327.1	281.0	8.3	Lorazepam-D_4	70	10	33	15
199.1	165.1	4.0	MDMA-D_5	60	10	20	15
285.2	175.1	5.3	MDPV-D_8	75	10	31	15
155.1	121.1	3.8	Methamphetamine-D_5	65	10	15	10
292.1	152.1	1.7	Morphine-D_6	100	10	79	14
287.1	185.1	8.0	Nitrazepam-D_5	100	10	50	10
321.1	261.1	4.0	Olanzapine-D_8	40	10	26	25
292.1	246.1	8.1	Oxazepam-D_5	60	10	30	14
319.2	259.0	3.8	Oxycodone-D_3	95	10	35	15
305.2	287.0	1.9	Oxymorphone-D_3	90	10	22	16
249.2	164.2	6.3	PCP-D_5	50	10	20	20
392.2	254.0	7.0	Quetiapine-D_8	70	10	55	15
268.2	42.0	5.0	Tramadol-D_3	80	10	75	10
379.2	182.1	6.2	Trazodone-D_6	90	10	35	14
347.1	208.0	8.7	Triazolam-D_4	100	10	70	18
284.2	147.0	6.0	Venlafaxine-D_6	60	10	34	13
393.1	245.0	4.9	Zopiclone-D_4	60	10	26	10

Q1: parent mass; Q3: fragment mass; DP: declustering potential; EP: entrance potential; CE: collision energy; CXP: collision cell exit potential. Transition 1 is the "identification transition", transition 2 is the "confirmation transition".

3 Cannabinoid method

3.1 Liquid chromatography

Mobile phase A: methanol : 10 mM Ammonium formate pH 3.0 (2:98 v:v)

Mobile phase B: acetonitrile (LC-MS Grade)

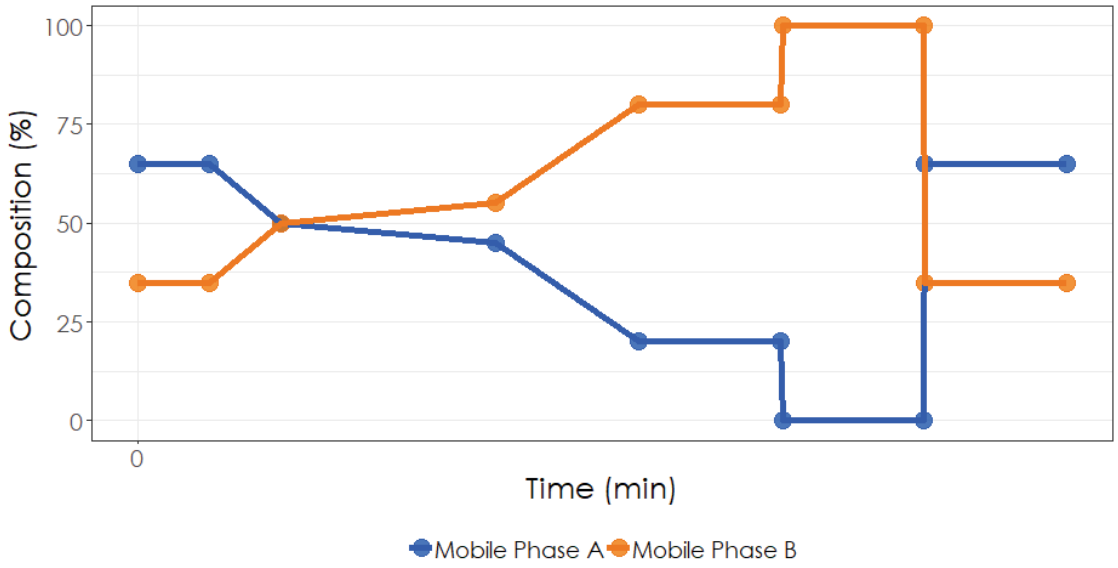
Rinsing solution: methanol : 1% formic acid in water : isopropanol (50:25:25 v:v:v)

Analytical column: Zorbax Eclipse Plus C18, 2.1 × 50 mm, 3.5 μm (Agilent)

Flow rate: 550 $\mu L/min$

Table 5: LC Pump Gradient

Time (min)	A (%)	B (%)
0.00	65	35
0.50	65	35
1.00	50	50
2.50	45	55
3.50	20	80
4.50	20	80
4.51	0	100
5.50	0	100
5.51	65	35
6.50	65	35



3.2 Autosampler and thermostat Settings

- Injection volume: 10 μL
- Wash time: 10 *sec*
- Autosampler temperature: 4 °C
- Column oven temperature: 50 °C

3.3 Mass spectrometry method

Table 6: Divert Valve Program

Time (min)	Position
0	MS
0.1	Waste
4.2	MS
5.3	Waste
6.5	MS

- Scan type: scheduled multiple reaction monitoring (MRM)
- Polarity: positive
- MRM detection window: 60 *sec*
- Target scan time: 0.6 *sec*
- Break: 3.00 $msec$
- Acquisition time: 6 minutes 30 seconds
- Ion source: Turbo Spray
- Curtain Gas (CUR): 30.0
- Collision Gas (CAD): 10.0
- Ion Spray Voltage (IS): 5500.0 V

- Source temperature (TEM): 700.0 °C
- Ion Source Gas 1 (GS1): 60.0
- Ion Source Gas (GS2): 65.0

Table 7: Monitored MRM transitions

Q1 (Da)	Q3 (Da)	Time (min)	Analyte	DP (V)	EP (V)	CE (V)	CXP (V)
315.2	193.1	4.8	THC 1	100	10	30	15
315.2	123.1	4.8	THC 2	100	10	47	10
318.3	196.1	4.8	THC-D_3	100	10	30	15

The method is validated on the following systems: HPLC Agilent 1200 series and 1260 Infinity, LC-MS/MS 5500 QTRAP Sciex.

The data acquisition software used is Analyst® 1.6.2 build 8489 and the data analysis software used is Multiquant® 3.0.1 (Version 3.0.6256.0)