

## Appendix F.4 Turboflow Mass Spectrometer Method

LCQ Fleet Instrument Method

Creator: LCQ FLEET

Last modified: 09/10/2013 by LCQ FLEET

MS Run Time (min): 16.50

Sequence override of method parameters not enabled.

Divert Valve: not used during run

Contact Closure: not used during run

Syringe Pump: not used during run

MS Detector Settings:

Acquisition Start Delay (min): 2.45

Real-time modifications to method disabled

Stepped collision energy not enabled

Additional Microscans:

MS2	0	0
MS3	0	0
MS4	0	0
MS5	0	0
MS6	0	0
MS7	0	0
MS8	0	0
MS9	0	0
MS10	0	0

### Segment 1 Information

Duration (min): 6.61

Number of Scan Events: 5

Tune Method: AGC\_50ms\_seg1

Scan Event Details:

1: ITMS + c norm oT(125.0-800.0)

CV = 0.0V

2: ITMS + c norm Dep Wideband MS/MS Most intense ion from parent list in (1)

Activation Type: CID

Min. Signal Required: 500.0

Isolation Width: 3.00

Normalized Coll. Energy: 35.0

Default Charge State: 1

Activation Q: 0.250

Activation Time: 30.000

CV = 0.0V

3: ITMS + c norm Dep Wideband MS/MS Most intense ion from (1)

Activation Type: CID

Min. Signal Required: 500.0

Isolation Width: 3.00

Normalized Coll. Energy: 35.0

Default Charge State: 1

Activation Q: 0.250

Activation Time: 30.000

CV = 0.0V

4: ITMS + c norm Dep Wideband MS3 Neutral loss from (3)

Activation Type: CID

Min. Signal Required: 500.0

Isolation Width: 3.00

Normalized Coll. Energy: 45.0

Default Charge State: 1

Activation Q: 0.250

Activation Time: 30.000

CV = 0.0V

5: ITMS + c norm ·( 462.00)->o(125.0-300.0)

MS/MS: AT CID CE 35.0% Q 0.250 Time 30.000 IsoW 3.0

CV = 0.0V

Data Dependent Settings:

Use separate polarity settings disabled

Neutral Loss Mass List: 80.00 176.00

Product Mass List: (none)  
Neutral loss in top: 3  
Product in top: 3  
Most intense if no parent masses found not enabled  
Add/subtract mass not enabled  
Charge state screening not enabled  
Charge state rejection not enabled

### Segment 2 Information

Duration (min): 1.44  
Number of Scan Events: 5  
Tune Method: AGC\_50ms\_seg2

#### Scan Event Details:

- 1: ITMS + c norm oT(125.0-800.0)  
CV = 0.0V
- 2: ITMS + c norm Dep Wideband MS/MS Most intense ion from parent list in (1)  
Activation Type: CID Min.  
Signal Required: 500.0  
Isolation Width: 3.00  
Normalized Coll. Energy: 35.0  
Default Charge State: 1  
Activation Q: 0.250  
Activation Time: 30.000  
CV = 0.0V
- 3: ITMS + c norm Dep Wideband MS/MS Most intense ion from (1) Activation Type: CID  
Min. Signal Required: 500.0  
Isolation Width: 3.00  
Normalized Coll. Energy: 35.0  
Default Charge State: 1  
Activation Q: 0.250  
Activation Time: 30.000  
CV = 0.0V
- 4: ITMS + c norm Dep Wideband MS3 Neutral loss from (3)  
Activation Type: CID  
Min. Signal Required: 500.0  
Isolation Width: 3.00  
Normalized Coll. Energy: 45.0  
Default Charge State: 1  
Activation Q: 0.250  
Activation Time: 30.000  
CV = 0.0V
- 5: ITMS + c norm ·( 328.00)->oW(90.0-330.0)  
MS/MS: AT CID CE 35.0% Q 0.250 Time 30.000 IsoW 1.0  
CV = 0.0V

#### Data Dependent Settings:

Use separate polarity settings disabled  
Neutral Loss Mass List: 80.00 176.00  
Product Mass List: (none)  
Neutral loss in top: 3  
Product in top: 3  
Most intense if no parent masses found not enabled  
Add/subtract mass not enabled  
Charge state screening not enabled  
Charge state rejection not enabled

### Segment 3 Information

Duration (min): 8.45  
Number of Scan Events: 5  
Tune Method: AGC\_50ms\_seg3

#### Scan Event Details:

- 1: ITMS + c norm oT(125.0-800.0)  
CV = 0.0V
- 2: ITMS + c norm Dep Wideband  
MS/MS Most intense ion from parent list in (1)  
Activation Type: CID  
Min. Signal Required: 500.0

- Isolation Width: 3.00  
Normalized Coll. Energy: 35.0  
Default Charge State: 1  
Activation Q: 0.250  
Activation Time: 30.000  
CV = 0.0V
- 3: ITMS + c norm Dep Wideband MS/MS Most intense ion from (1)  
Activation Type: CID  
Min. Signal Required: 500.0  
Isolation Width: 3.00  
Normalized Coll. Energy: 35.0  
Default Charge State: 1  
Activation Q: 0.250  
Activation Time: 30.000  
CV = 0.0V
- 4: ITMS + c norm Dep Wideband MS3 Neutral loss from (3)  
Activation Type: CID  
Min. Signal Required: 500.0  
Isolation Width: 3.00  
Normalized Coll. Energy: 45.0  
Default Charge State: 1  
Activation Q: 0.250  
Activation Time: 30.000  
CV = 0.0V
- 5: ITMS + c norm ·( 342.00)->oW(90.0-350.0)  
MS/MS: AT CID CE 35.0% Q 0.250 Time 30.000 IsoW 3.0  
CV = 0.0V

Data Dependent Settings:

Use separate polarity settings disabled  
Neutral Loss Mass List: 80.00 176.00  
Product Mass List: (none)  
Neutral loss in top: 3  
Product in top: 3  
Most intense if no parent masses found not enabled  
Add/subtract mass not enabled  
Charge state screening not enabled  
Charge state rejection not enabled  
Global Data Dependent Settings:  
Use global parent and reject mass lists enabled  
Exclude parent mass from data dependent selection not enabled  
Exclusion mass width by mass  
Exclusion mass width low: 1.50  
Exclusion mass width high: 1.50  
Parent mass width by mass  
Parent mass width low: 0.50  
Parent mass width high: 0.50  
Reject mass width by mass  
Reject mass width low: 0.80  
Reject mass width high: 0.80  
Zoom/UltraZoom scan mass width by mass  
Zoom/UltraZoom scan mass width low: 5.00  
Zoom/UltraZoom scan mass width high: 5.00  
Neutral Loss candidates processed by decreasing intensity  
Neutral Loss mass width by mass  
Neutral Loss mass width low: 0.50  
Neutral Loss mass width high: 0.50  
Product candidates processed by decreasing intensity  
Product mass width by mass  
Product mass width low: 0.50  
Product mass width high: 0.50  
MS mass range: 0.00-1000000.00  
MSn mass range by mass  
MSn mass range: 0.00-1000000.00  
Analog UV data dep. not enabled  
Dynamic exclusion enabled  
Repeat Count: 1 Repeat  
Duration: 30.00

Exclusion List Size: 50  
 Exclusion Duration: 2.50  
 Exclusion mass width by mass  
 Exclusion mass width low: 1.50  
 Exclusion mass width high: 1.50  
 Expiration: disabled  
 Isotopic data dependence not enabled  
 Mass Tags data dependence not enabled

MS Mass	Start (min)	End (min)	MS Normalized Collision Energy	Name
136.00	6.000	9.000	30.0	Amphetamine
150.10	6.700	9.000	30.0	Methamphetamine/phentermine
152.00	1.400	2.000	35.0	Norephidrine
163.20	4.200	5.500		Nicotine?
168.10	8.000	10.000		anhydroecgonine
177.20	6.600	7.500		Cotinine?
180.00	6.200	7.500	25.0	MDA
182.10	2.000	6.000	40.0	desmethylmeconine
186.00	0.800	1.500	40.0	Ecgonine
194.10	7.200	8.500	25.0	MDMA
195.10	9.000	9.500	40.0	Caffeine/Meconine
200.20	7.000	9.000	45.0	Ecgonine Methyl Esther
205.00	1.000	5.000	35.0	dihydrocotarnine
208.10	7.600	8.500		MDEA
220.00	3.000	9.000	35.0	Hydrocotarnine
224.00	7.000	8.500	35.0	NORKETAMINE
238.70	6.000	9.500		Ketamine
250.10	6.500	8.000		nortramadol
251.00	10.500	13.000	50.0	Methaqualone
264.30	8.500	13.500	50.0	Nortriptyline / tramadol
267.00	12.000	13.500	30.0	Cyclizine
271.10	11.800	12.300	45.0	?Nordiazepam
272.20	6.500	7.500		Normorphine?
272.20	12.000	13.500		Dextromethorphan
278.20	12.000	14.000	50.0	EDDP/Amitriptyline
281.10	10.000	11.500		Imipramine
284.10	10.000	14.000		7-amino-flunitrazepam
285.10	12.500	14.000	50.0	Diazepam
286.15	5.000	8.500	40.0	Morphine
286.20	10.000	14.000		7-Amino-Clonazepam
287.00	11.400	12.000	45.0	Oxazepam?
287.40	10.500	12.000		?demoxepam
289.00	12.000	15.000		desmethylclobazam

290.20	7.300	8.500	30.0	benzoylecgonine
292.00	5.000	8.500	40.0	Morphine-D6
293.20	7.500	8.300	30.0	Benzoylecgonine-D3
296.00	7.500	8.500		Diclofenac?
300.15	6.700	7.600	40.0	Codeine
300.80	11.000	12.000		Chlordiazepoxide?
301.10	12.500	14.000		?Temazepam
301.30	12.500	13.500		Norclomipramine
302.30	6.400	7.500	40.0	DHC
304.15	9.500	11.000	30.0	Cocaine
308.00	11.000	13.000		Norpropoxyphene?
309.00	10.000	14.000	45.0	ALPRAZOLAM
310.15	12.000	15.000	26.0	Methadone
312.00	1.500	7.000	45.0	DiHydroxypapaverine
313.00	12.000	15.000	26.0	Methadone-D3
316.00	12.000	14.000		?Clonazepam
318.20	10.000	12.400		cocaethylene
325.00	8.500	14.000	40.0	a-hydroxyAlprazolam/quinine
326.00	6.500	8.500	45.0	Hydroxypapaverine
337.20	12.500	14.000		Fentanyl
340.00	4.000	10.000	35.0	papaverine
340.25	12.200	14.000	25.0	Propoxyphene
342.10	10.000	15.000		alpha-hydroxymidazolam
342.20	7.500	9.000		Naltrexone
370.00	7.300	8.300	28.0	Heroin
388.00	12.300	13.000		Trazodone
399.00	6.500	8.000	40.0	Pholcodine
414.00	8.500	9.500	45.0	Norbuprenorphine/noscapine
429.60	9.500	10.500		mebeverine

Global Reject Masses:

Mass	Start (min)	End (min)	Mass	Start (min)	End (min)
453.30	0.000	17.000	454.20	7.000	9.000
460.00	3.000	5.000	475.00	7.000	9.000
498.00	7.000	9.000	498.60	3.000	5.000
550.70	6.000	7.000	561.80	6.000	7.000
562.70	6.000	7.000	566.60	3.000	5.000
634.50	3.000	5.000	679.00	9.000	14.000