

REVIEWED

By Britany Wylie at 8:06 am, Sep 22, 2018

9/21/2018

Worklist: 2703

<u>LAB CASE</u>	<u>ITEM</u>	<u>TASK ID</u>	<u>DESCRIPTION</u>
P2018-2174	1	126535	AM 28 Blood Multi-Drug Quant Panel 2 by LC-QC
P2018-2599	1	127470	AM 28 Blood Multi-Drug Quant Panel 2 by LC-QC



Toxicology AM method 28 panel 2 external prep information

working solution 14706 ng/ml in meoh Doxepin, desipramine, chlordiazepoxide, paroxetine
Stock solution 1mg/ml 150 ul each in 9700 ul meOH

Ppd 8/8/18 Exp: 8/8/19 lot 8819 by AMN

Drug	lot	expiration
Doxepine	fn01281502	2/1/2020
Desipramine	fn10231502	10/1/2020
Chlordiazepoxide	fe07241502	8/1/2020
Paroxetine	fn05111505	6/1/2020

AM 28 control 50 ul working solution lot (8819) in 9950 ul blood lot (18G207D7)

ppd 8/8/18 Exp 8/8/19 by AMN Concentration 73.53 ng/ml each

AM# 28: Multi-Drug Quantitation in Blood by LC-MS/MS

Extraction Date: 9/20/18
Plate lot#: 0530563

Analyst: Anne Nord
Plate Expiration: May 21 2019

Mobile phase A: 5mM Amm Form + 0.01% FA **Mobile phase B:** 0.01% Formic Acid in MeOH
0.5M Ammonium Hydroxide Ethyl Acetate 20% Methanol in Water

Blank Blood Lot: 18G207D7 **Column:** Agilent 120 EC-C18 (2.1x 100-4um)

LCMS-QQQ ID: 62340

Pre-Analytic:

- 1. Check levels of mobile phases and needle wash refill as needed. Ensure waste is not full.
- 2. Ensure correct column is installed and begin mobile phase flow allow to equilibrate ~ 30 minutes.
- 3. Create worklist:

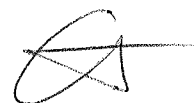
Analytic:

- 1. Remove standards, plate, controls, and samples from cold storage. Allow to reach room temperature.
- 2. Pipette **250µL blood (calibrated pipette) Pipette ID: 1926134** in wells of analytical (standards) plate.
- 3. Place on shaking incubator at ambient temp., 900rpm for 15 minutes. *Shaker ID: 66759*
- 4. Pipette **250µL 0.5M ammonium hydroxide** in wells of analytical plate.
- 5. Place on shaking incubator at ambient temp., 900rpm for 15 minutes.
- 6. Transfer **300µL of blood+base** mixture to corresponding wells of SLE+ plate.
- 7. Apply positive pressure for approx. 10-15 seconds (or until no liquid remains on top of sorbent).
(Load at 85-100 PSI- Selector to the right) Manifold ID: 66792
- 8. Wait 5 minutes.
- 9. Add **900uL ethyl acetate**.
- 10. Wait 5 minutes.
- 11. Apply positive pressure for approx. 15 seconds. *(10-15 PSI- Selector to the left).*
- 12. Add **900uL ethyl acetate**.
- 13. Wait 5 minutes.
- 14. Apply positive pressure for approx. 15 seconds. *(10-15 PSI- Selector to the left).*
- 15. Remove plate containing eluate. Place on SPE Dry and evaporate to dryness at approx. 35°C.
SPE Dry ID: 66819
- 16. Reconstitute in **100µL 20% MeOH** and heat seal plate with foil. Place in autosampler and run worklist.

Post-Analytic

- 1. Create batch and process data.
Worklist path: 092018 mdq Batch Name: p2b mdq
- 2. Make necessary changes to integration limits
- 3. Integration linear and R² values ≥0.98 for each analyte.
- 4. For unknown samples and controls: response ratio within 20% of average of controls and standards, RT within +/- 5% (tramadol RT +/-2%), S/N for primary transition >10 and secondary transitions >5.
- 5. Did all QCs pass for each analyte? Add Control data to QC tracking spreadsheet.
- 6. Central File Packet to include: LIMS Worklist, Method Checklist, Calibration and Control Reports.

COMMENTS: *Panel 2b Run MDA, MDMA and Desipramine were the only compounds evaluated.*



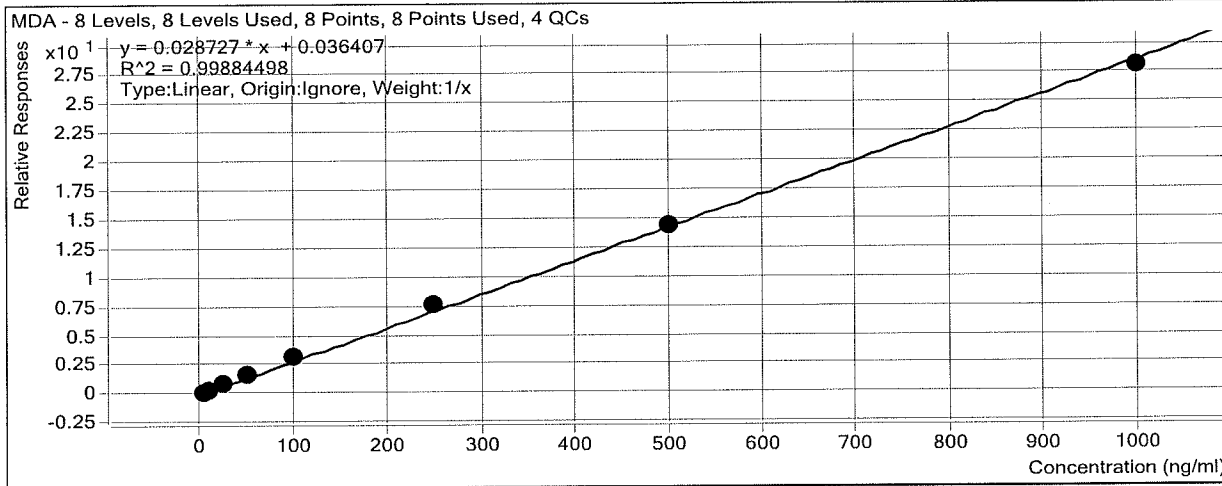
ISP Forensics Calibration Curve Report

Batch Data Path
Last Calib Update

D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
9/21/2018 8:58 AM

Analyst Name ISP TOX

Target Compound MDA
Internal Standard MDA-D5



Sample	Level	Enabled	Exp Conc	Final Conc	Accuracy
2b cal 1-5ng	1	<input checked="" type="checkbox"/>	5	4.1	82.1
2b cal 2-10ng	2	<input checked="" type="checkbox"/>	10	9.5	95.2
2b QC 10	2	<input checked="" type="checkbox"/>	10	10.9	109.5
2b cal 3-25ng	3	<input checked="" type="checkbox"/>	25	26.6	106.4
2b cal 4-50ng	4	<input checked="" type="checkbox"/>	50	53.7	107.4
2b cal 5-100ng	5	<input checked="" type="checkbox"/>	100	106.2	106.2
2b QC 100	5	<input checked="" type="checkbox"/>	100	118.5	118.5
2b cal 6-250ng	6	<input checked="" type="checkbox"/>	250	261.6	104.6
2b QC 250	6	<input checked="" type="checkbox"/>	250	281.9	112.8
2b cal 7-500ng	7	<input checked="" type="checkbox"/>	500	501.8	100.4
2b cal 8-1000ng	8	<input checked="" type="checkbox"/>	1000	976.4	97.6
2b QC 1000	8	<input checked="" type="checkbox"/>	1000	1059.5	106.0

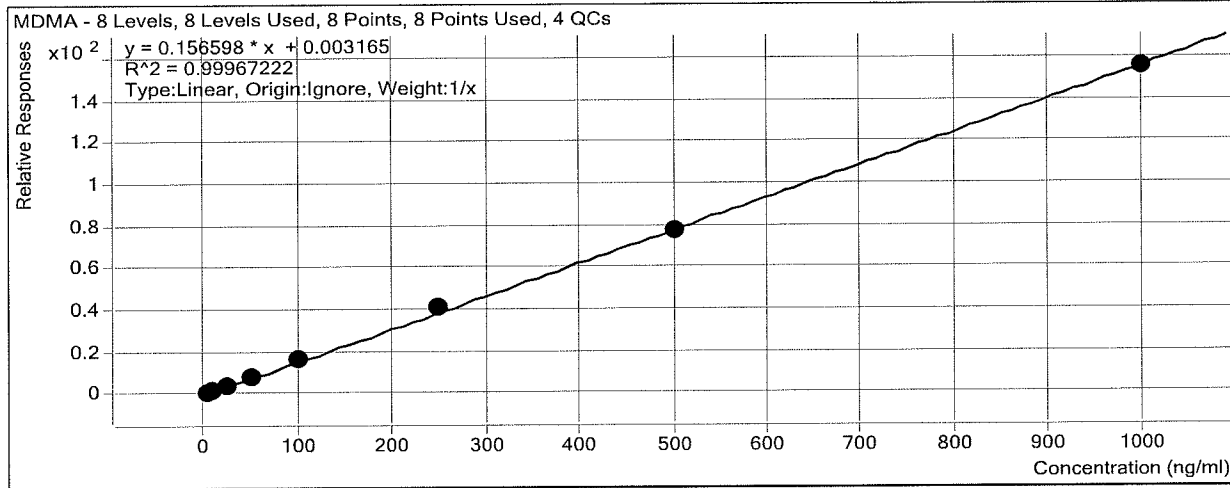
ISP Forensics Calibration Curve Report

Batch Data Path
Last Calib Update

D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
9/21/2018 8:58 AM

Analyst Name ISP TOX

Target Compound MDMA
Internal Standard MDMA-D6



Sample	Level	Enabled	Exp Conc	Final Conc	Accuracy
2b cal 1-5ng	1	<input checked="" type="checkbox"/>	5	4.7	93.9
2b cal 2-10ng	2	<input checked="" type="checkbox"/>	10	9.7	97.3
2b QC 10	2	<input checked="" type="checkbox"/>	10	10.2	102.2
2b cal 3-25ng	3	<input checked="" type="checkbox"/>	25	25.6	102.2
2b cal 4-50ng	4	<input checked="" type="checkbox"/>	50	51.2	102.4
2b cal 5-100ng	5	<input checked="" type="checkbox"/>	100	101.9	101.9
2b QC 100	5	<input checked="" type="checkbox"/>	100	108.2	108.2
2b cal 6-250ng	6	<input checked="" type="checkbox"/>	250	259.6	103.8
2b QC 250	6	<input checked="" type="checkbox"/>	250	259.8	103.9
2b cal 7-500ng	7	<input checked="" type="checkbox"/>	500	496.7	99.3
2b cal 8-1000ng	8	<input checked="" type="checkbox"/>	1000	990.6	99.1
2b QC 1000	8	<input checked="" type="checkbox"/>	1000	1027.4	102.7

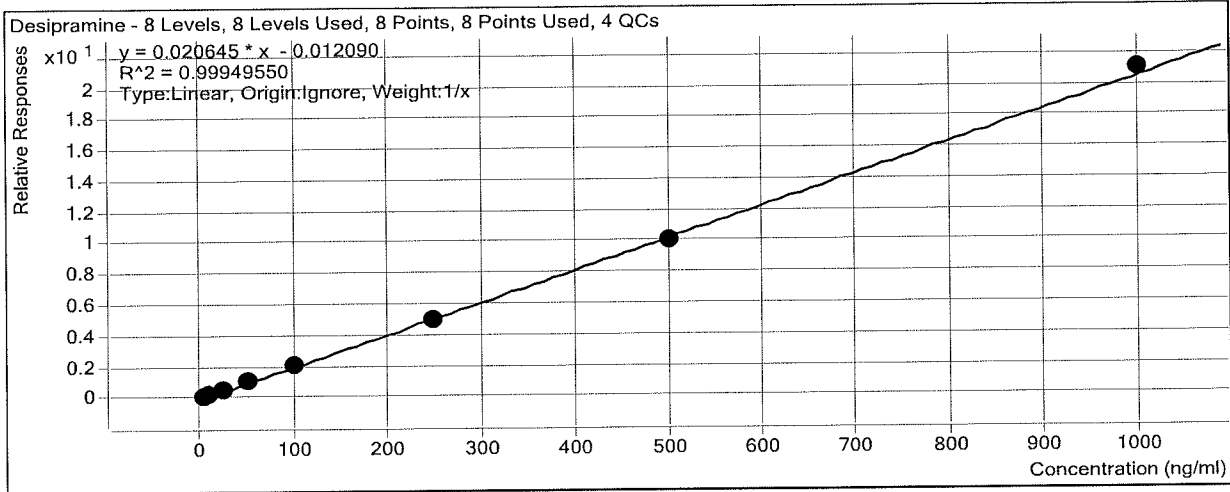
ISP Forensics Calibration Curve Report

Batch Data Path
Last Calib Update

D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
9/21/2018 8:58 AM

Analyst Name ISP TOX

Target Compound *Desipramine*
Internal Standard *Desipramine-D3*



Sample	Level	Enabled	Exp Conc	Final Conc	Accuracy
2b cal 1-5ng	1	<input checked="" type="checkbox"/>	5	5.4	107.7
2b cal 2-10ng	2	<input checked="" type="checkbox"/>	10	10.0	100.0
2b QC 10	2	<input checked="" type="checkbox"/>	10	10.1	101.2
2b cal 3-25ng	3	<input checked="" type="checkbox"/>	25	25.0	100.0
2b cal 4-50ng	4	<input checked="" type="checkbox"/>	50	48.6	97.1
2b cal 5-100ng	5	<input checked="" type="checkbox"/>	100	97.7	97.7
2b QC 100	5	<input checked="" type="checkbox"/>	100	97.9	97.9
2b cal 6-250ng	6	<input checked="" type="checkbox"/>	250	244.0	97.6
2b QC 250	6	<input checked="" type="checkbox"/>	250	239.8	95.9
2b cal 7-500ng	7	<input checked="" type="checkbox"/>	500	489.3	97.9
2b cal 8-1000ng	8	<input checked="" type="checkbox"/>	1000	1020.0	102.0
2b QC 1000	8	<input checked="" type="checkbox"/>	1000	980.0	98.0

ISP FORENSICS - Cd'A Instrument # 62340

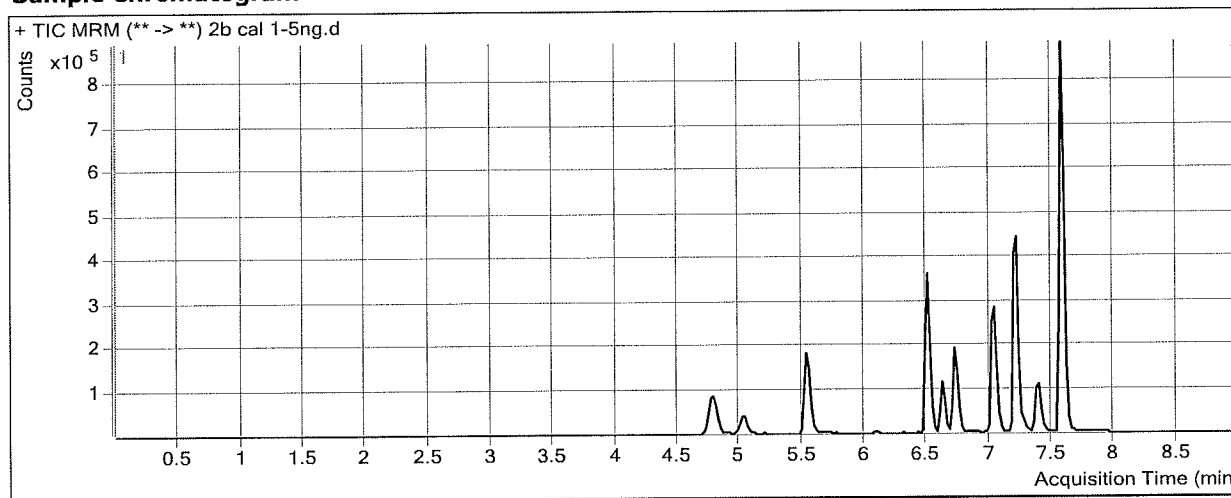
Multi-Drug Confirmatory Analysis Report

Batch Data Path	D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin		
Analysis Time	9/21/2018 8:58 AM	Analyst Name	ISP Tox
Report Time	9/21/2018 9:00 AM	Reporter Name	ISP Tox
Last Calib Update	9/21/2018 8:58 AM	Batch State	Processed

Analysis Info

Acq Time	2018-09-20 22:12	Data File	2b cal 1-5ng.d
Sample Type	Calibration	Sample Name	2b cal 1-5ng
Dilution	1	Acq Method	2b mdq 618 .m
Position	P2-A5	Sample Info	
Inj Vol	-1	Comment	AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	51374	333018	0.1543	4.1028
MDMA	MDMA-D6	5.027	55980	75785	0.7387	4.6968
Desipramine	Desipramine-D3	7.567	108972	1100083	0.0991	5.3837

ISP FORENSICS - Cd'A Instrument # 62340

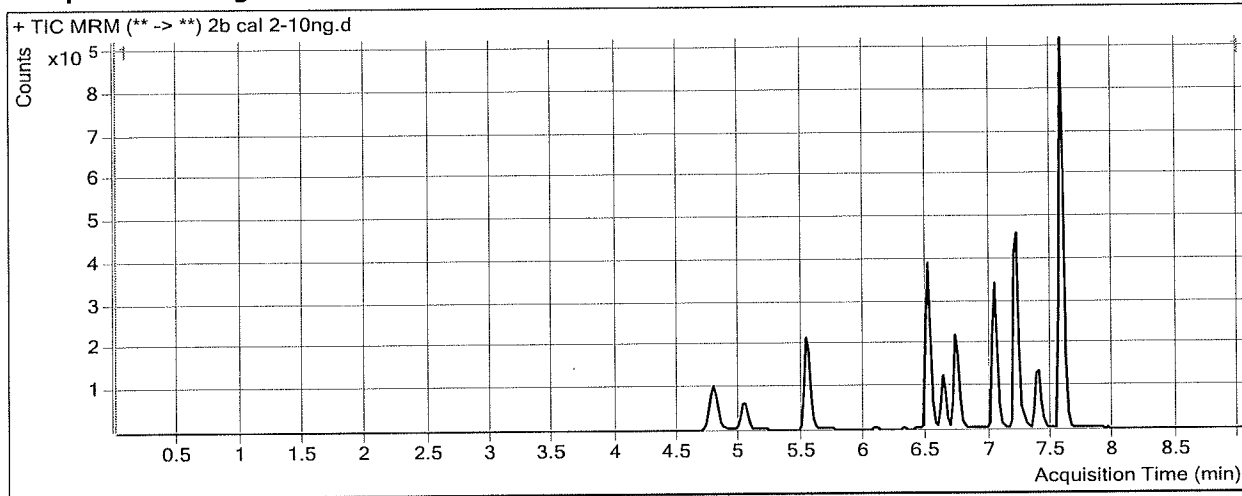
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-20 22:25 **Data File** 2b cal 2-10ng.d
Sample Type Calibration **Sample Name** 2b cal 2-10ng
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-B5 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	101250	326685	0.3099	9.5216
MDMA	MDMA-D6	5.027	112703	73842	1.5263	9.7262
Desipramine	Desipramine-D3	7.587	185510	954601	0.1943	9.9986

ISP FORENSICS - Cd'A Instrument # 62340

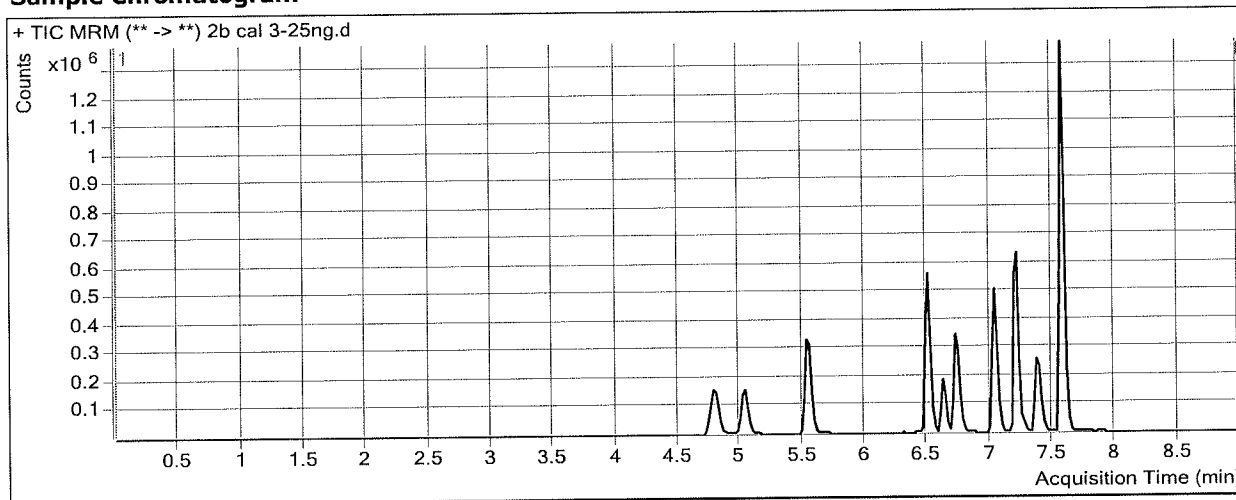
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-20 22:38 **Data File** 2b cal 3-25ng.d
Sample Type Calibration **Sample Name** 2b cal 3-25ng
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-C5 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	270604	337879	0.8009	26.6122
MDMA	MDMA-D6	5.027	314820	78591	4.0058	25.5601
Desipramine	Desipramine-D3	7.587	497516	986912	0.5041	25.0035

ISP FORENSICS - Cd'A Instrument # 62340

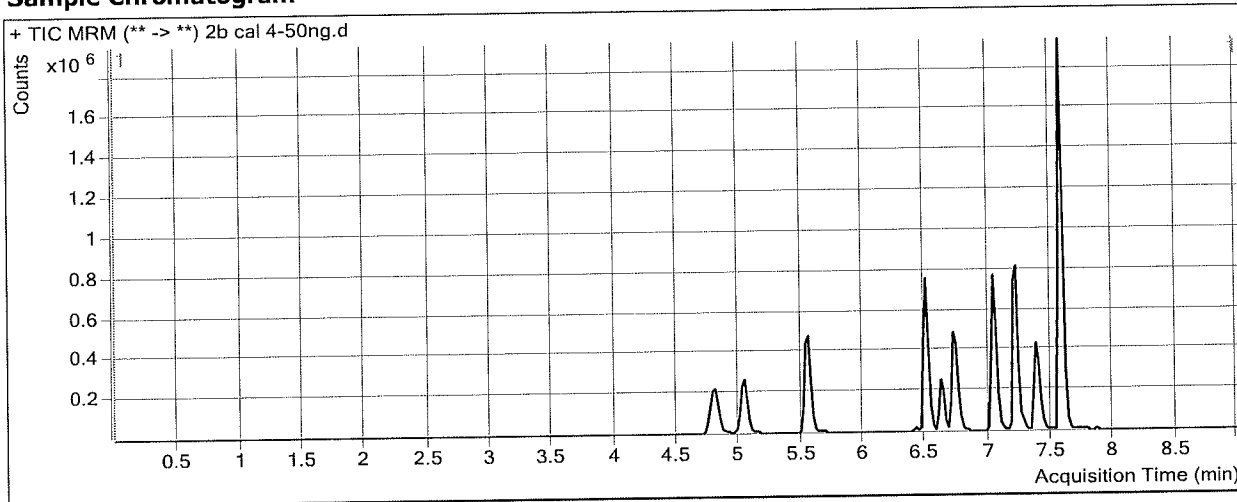
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-20 22:50 **Data File** 2b cal 4-50ng.d
Sample Type Calibration **Sample Name** 2b cal 4-50ng
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-D5 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	479021	303301	1.5794	53.7113
MDMA	MDMA-D6	5.027	575465	71711	8.0248	51.2245
Desipramine	Desipramine-D3	7.567	910320	919050	0.9905	48.5628

ISP FORENSICS - Cd'A Instrument # 62340

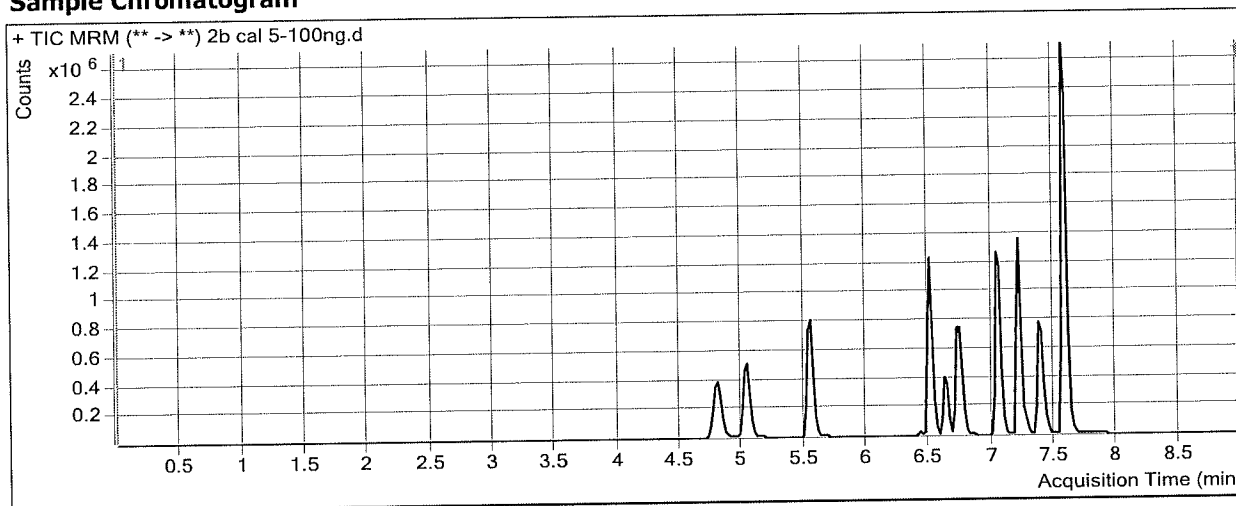
Multi-Drug Confirmatory Analysis Report

Batch Data Path	D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin		
Analysis Time	9/21/2018 8:58 AM	Analyst Name	ISP Tox
Report Time	9/21/2018 9:00 AM	Reporter Name	ISP Tox
Last Calib Update	9/21/2018 8:58 AM	Batch State	Processed

Analysis Info

Acq Time	2018-09-20 23:03	Data File	2b cal 5-100ng.d
Sample Type	Calibration	Sample Name	2b cal 5-100ng
Dilution	1	Acq Method	2b mdq 618 .m
Position	P2-E5	Sample Info	
Inj Vol	-1	Comment	AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	923243	298992	3.0878	106.2229
MDMA	MDMA-D6	5.027	1159680	72680	15.9560	101.8714
Desipramine	Desipramine-D3	7.587	1679599	837474	2.0056	97.7293

ISP FORENSICS - Cd'A Instrument # 62340

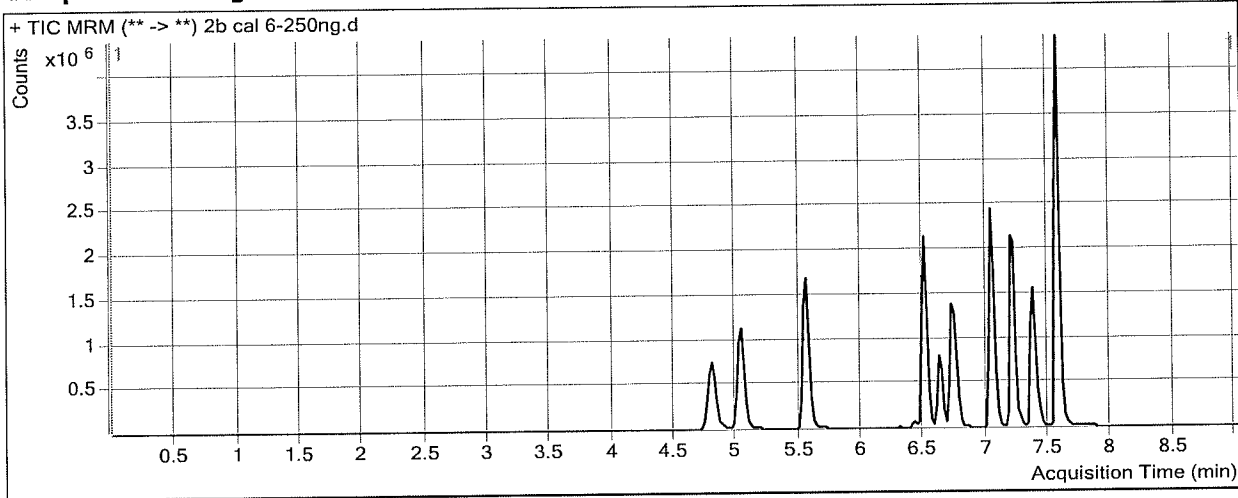
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-20 23:16 **Data File** 2b cal 6-250ng.d
Sample Type Calibration **Sample Name** 2b cal 6-250ng
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-F5 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	1905730	252405	7.5503	261.5640
MDMA	MDMA-D6	5.027	2593216	63788	40.6534	259.5829
Desipramine	Desipramine-D3	7.567	2741527	545471	5.0260	244.0307

ISP FORENSICS - Cd'A Instrument # 62340

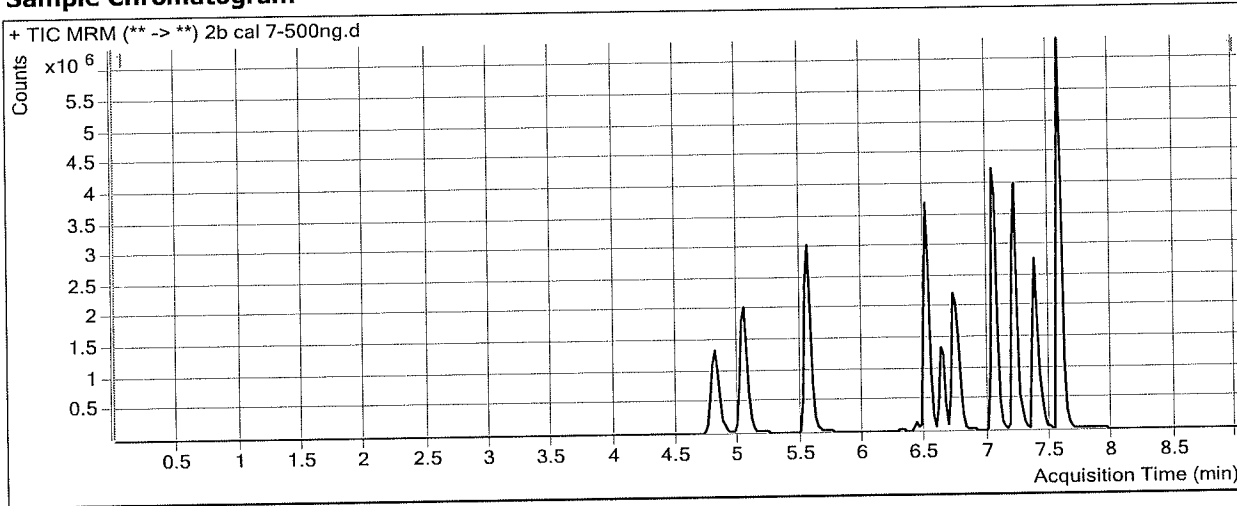
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-20 23:28 **Data File** 2b cal 7-500ng.d
Sample Type Calibration **Sample Name** 2b cal 7-500ng
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-G5 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	3535242	244617	14.4521	501.8219
MDMA	MDMA-D6	5.027	5029252	64650	77.7921	496.7423
Desipramine	Desipramine-D3	7.587	4071543	403538	10.0896	489.2993

ISP FORENSICS - Cd'A Instrument # 62340

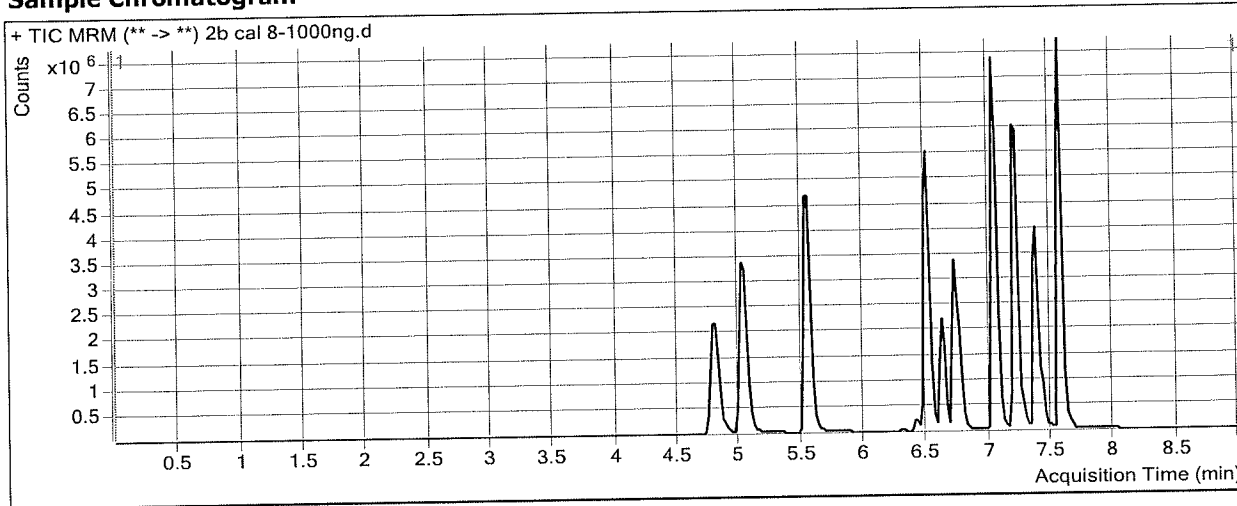
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-20 23:41 **Data File** 2b cal 8-1000ng.d
Sample Type Calibration **Sample Name** 2b cal 8-1000ng
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-H5 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	6318770	224976	28.0865	976.4434
MDMA	MDMA-D6	5.007	8973965	57849	155.1286	990.5958
Desipramine	Desipramine-D3	7.567	4767670	226537	21.0459	1019.9921

ISP FORENSICS - Cd'A Instrument # 62340

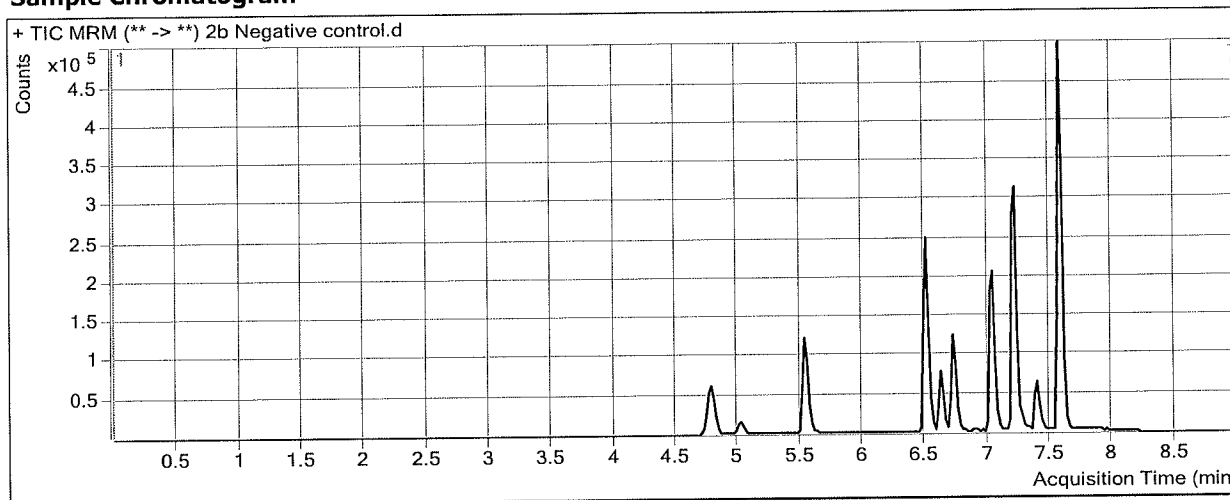
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-21 00:07 **Data File** 2b Negative control.d
Sample Type Sample **Sample Name** 2b Negative control
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-E6 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
Desipramine	Desipramine-D3	7.587	17726	692204	0.0256	1.8260 <i>LS</i>

ISP FORENSICS - Cd'A Instrument # 62340

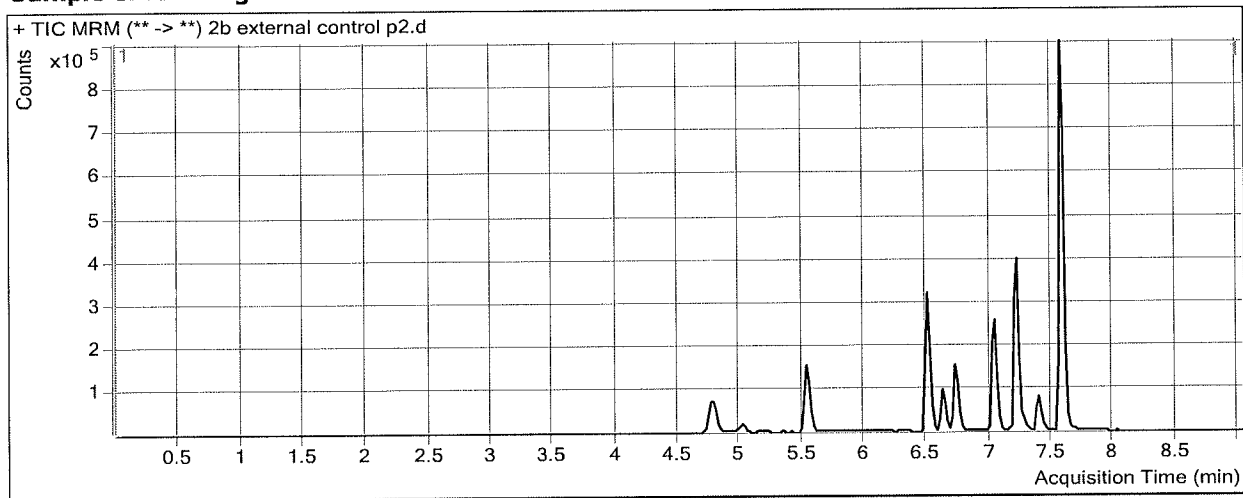
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-21 00:19 **Data File** 2b external control p2.d
Sample Type Sample **Sample Name** 2b external control p2
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-F6 **Sample Info**
Inj Vol -1 **Comment** AM 28 meperidine 50ng

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
Desipramine	Desipramine-D3	7.567	768797	645363	1.1913	58.2871

ISP FORENSICS - Cd'A Instrument # 62340

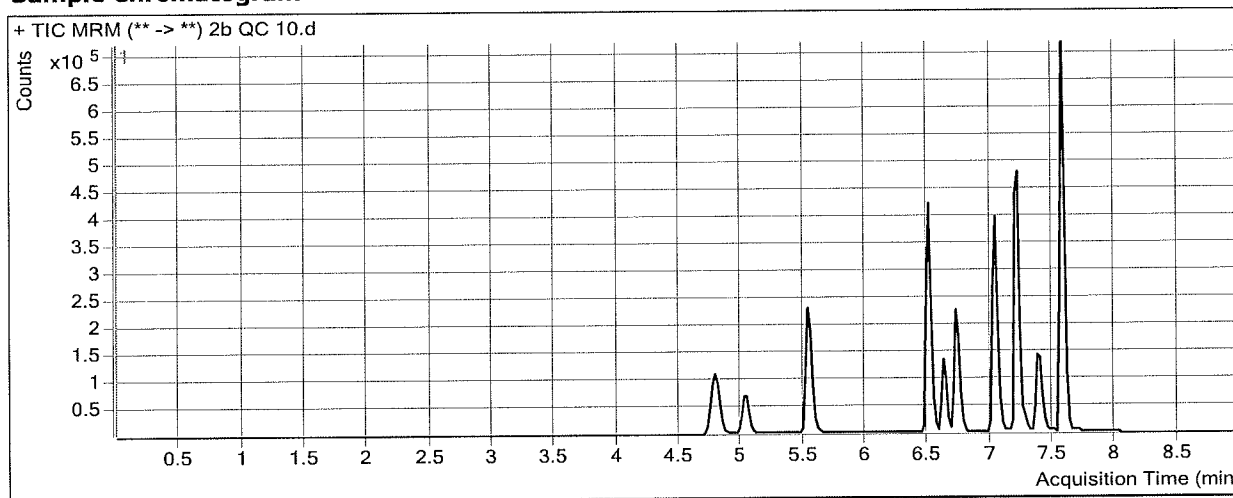
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-21 00:32 **Data File** 2b QC 10.d
Sample Type QC **Sample Name** 2b QC 10
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-A6 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	120276	342800	0.3509	10.9465
MDMA	MDMA-D6	5.027	125621	78327	1.6038	10.2213
Desipramine	Desipramine-D3	7.567	133606	678847	0.1968	10.1187

ISP FORENSICS - Cd'A Instrument # 62340

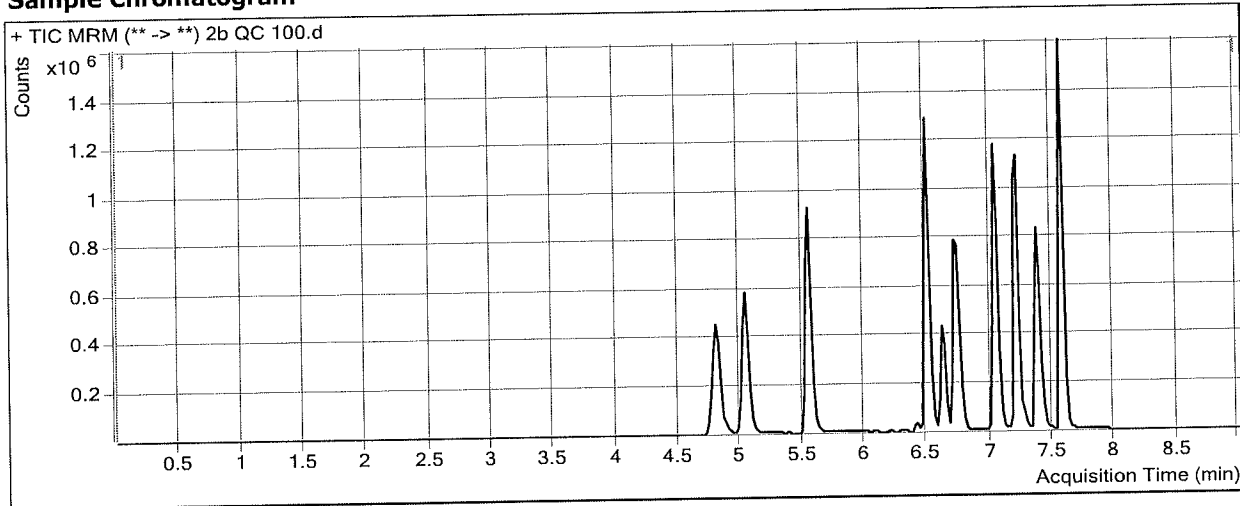
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-21 01:35 **Data File** 2b QC 100.d
Sample Type QC **Sample Name** 2b QC 100
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-B6 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	1070840	311326	3.4396	118.4679
MDMA	MDMA-D6	5.027	1280517	75544	16.9507	108.2230
Desipramine	Desipramine-D3	7.567	722289	359488	2.0092	97.9066

ISP FORENSICS - Cd'A Instrument # 62340

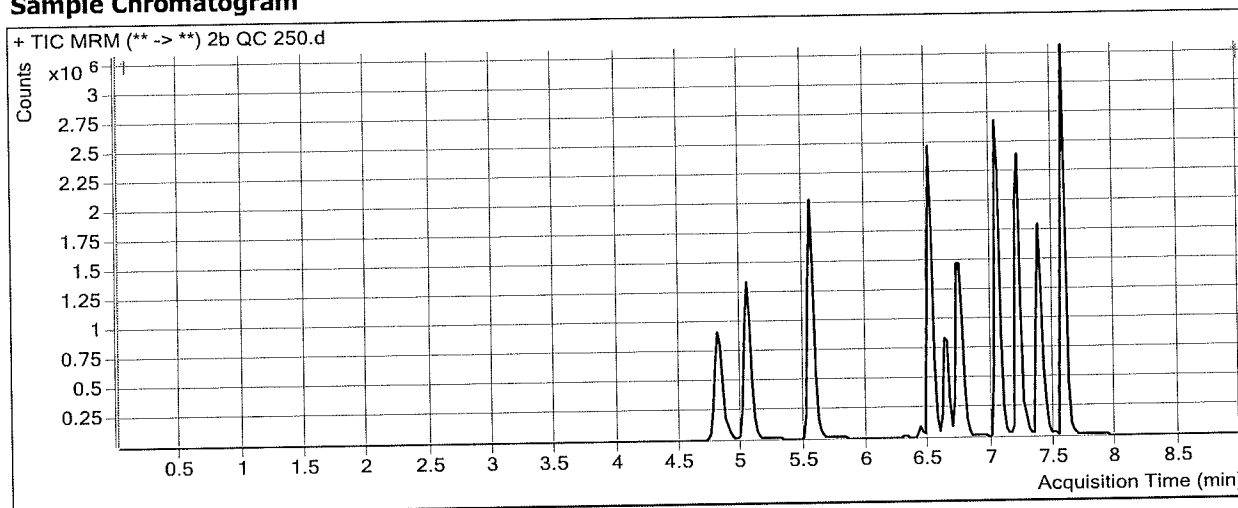
Multi-Drug Confirmatory Analysis Report

Batch Data Path D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin
Analysis Time 9/21/2018 8:58 AM **Analyst Name** ISP Tox
Report Time 9/21/2018 9:00 AM **Reporter Name** ISP Tox
Last Calib Update 9/21/2018 8:58 AM **Batch State** Processed

Analysis Info

Acq Time 2018-09-21 01:48 **Data File** 2b QC 250.d
Sample Type QC **Sample Name** 2b QC 250
Dilution 1 **Acq Method** 2b mdq 618 .m
Position P2-C6 **Sample Info**
Inj Vol -1 **Comment** AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	2368411	291122	8.1355	281.9342
MDMA	MDMA-D6	5.027	3088965	75915	40.6898	259.8159
Desipramine	Desipramine-D3	7.567	1777988	359956	4.9395	239.8399

ISP FORENSICS - Cd'A Instrument # 62340

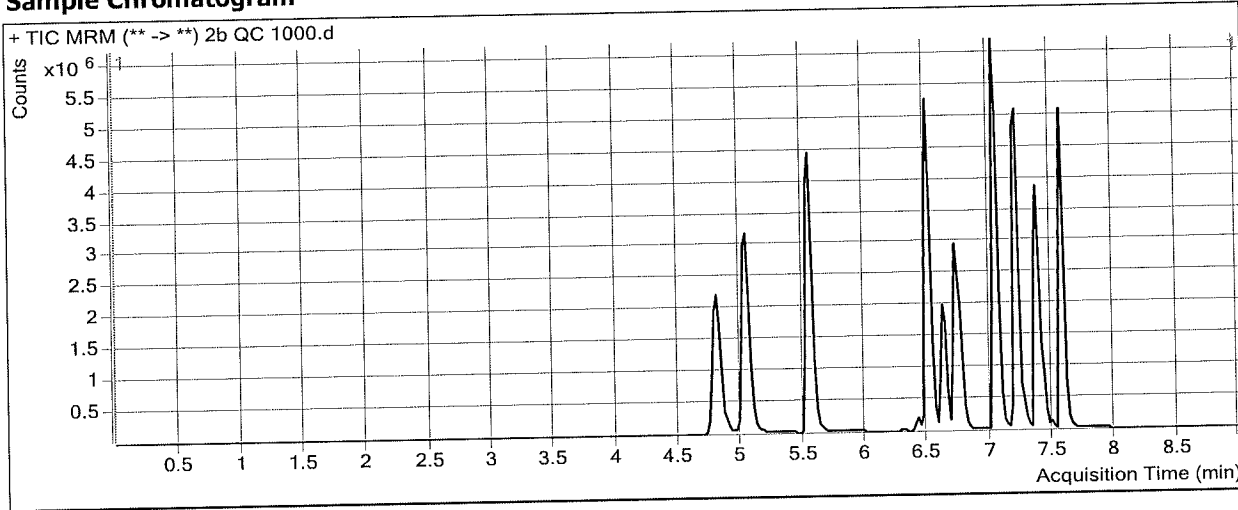
Multi-Drug Confirmatory Analysis Report

Batch Data Path	D:\2018 Data\092018 mdq\QuantResults\mdq p2b.batch.bin		
Analysis Time	9/21/2018 8:58 AM	Analyst Name	ISP Tox
Report Time	9/21/2018 9:00 AM	Reporter Name	ISP Tox
Last Calib Update	9/21/2018 8:58 AM	Batch State	Processed

Analysis Info

Acq Time	2018-09-21 02:01	Data File	2b QC 1000.d
Sample Type	QC	Sample Name	2b QC 1000
Dilution	1	Acq Method	2b mdq 618 .m
Position	P2-D6	Sample Info	
Inj Vol	-1	Comment	AM 28 Panel 2

Sample Chromatogram



Results

Compound	ISTD Compound	RT	Response	ISTD Resp	Resp Ratio	Final Conc
MDA	MDA-D5	4.809	6081069	199558	30.4727	1059.5107
MDMA	MDMA-D6	5.027	8228821	51146	160.8879	1027.3730
Desipramine	Desipramine-D3	7.587	2751952	136100	20.2201	979.9933