LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045368.D
Acq On : 22 Oct 2021 16:35
Operator : SY/MD
Sample : M4316-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2-IS

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Title : SW846 8260

Signal : TIC: VU045368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.636	392	403	428	rBV	24343	49068	1.04%	0.244%
2	3.044	518	530	548	rVB	35084	67188	1.43%	0.334%
3	5.292	1212	1229	1242	rBV	191308	403441	8.57%	2.004%
4	5.375	1242	1255	1280	rVB	320101	658491	13.99%	3.270%
5	5.703	1343	1357	1372	rBV	226113	461381	9.80%	2.291%
6	5.915	1410	1423	1436	rBV2	26236	55046	1.17%	0.273%
7	6.028	1447	1458	1473	rBV	66089	206362	4.38%	1.025%
8	6.250	1516	1527	1585	rVB	573559	1373076	29.17%	6.819%
9	6.941	1719	1742	1759	rVB3	25153	74089	1.57%	0.368%
10	7.044	1759	1774	1804	rBV	1734895	3250217	69.04%	16.142%
11	7.745	1975	1992	2005	rBV	265980	466166	9.90%	2.315%
12	7.899	2025	2040	2058	rBV	765786	1343054	28.53%	6.670%
13	8.166	2112	2123	2141	rBV	27171	48234	1.02%	0.240%
14	8.472	2206	2218	2228	rBV	78492	140635	2.99%	0.698%
15	8.581	2241	2252	2263	rVB	198366	356138	7.56%	1.769%
16	8.732	2282	2299	2320	rBV	2876249	4707851	100.00%	23.382%
17	8.841	2322	2333	2351	rVB	300616	498794	10.59%	2.477%
18	9.218	2435	2450	2483	rBV	1733352	2756561	58.55%	13.691%
19	9.420	2502	2513	2545	rVB	693289	1157358	24.58%	5.748%
20	10.076	2705	2717	2737	rBV3	61314	106025	2.25%	0.527%
21	10.635	2879	2891	2914	rBV	541500	867004	18.42%	4.306%
22	11.815	3245	3258	3275	rBV	696585	1088590	23.12%	5.407%

Sum of corrected areas: 20134769

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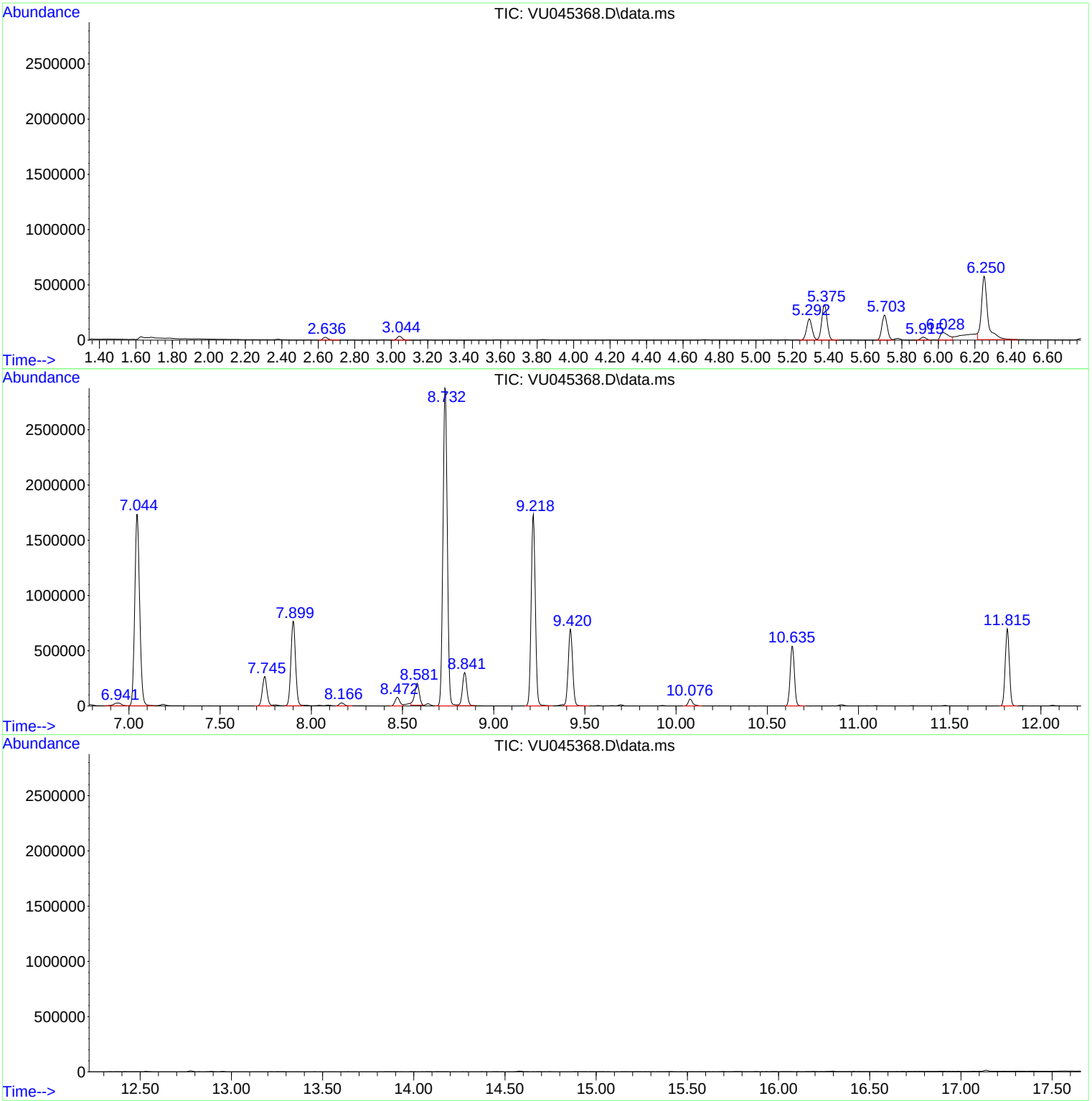
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2-IS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045368.D
Acq On : 22 Oct 2021 16:35
Operator : SY/MD
Sample : M4316-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2-IS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

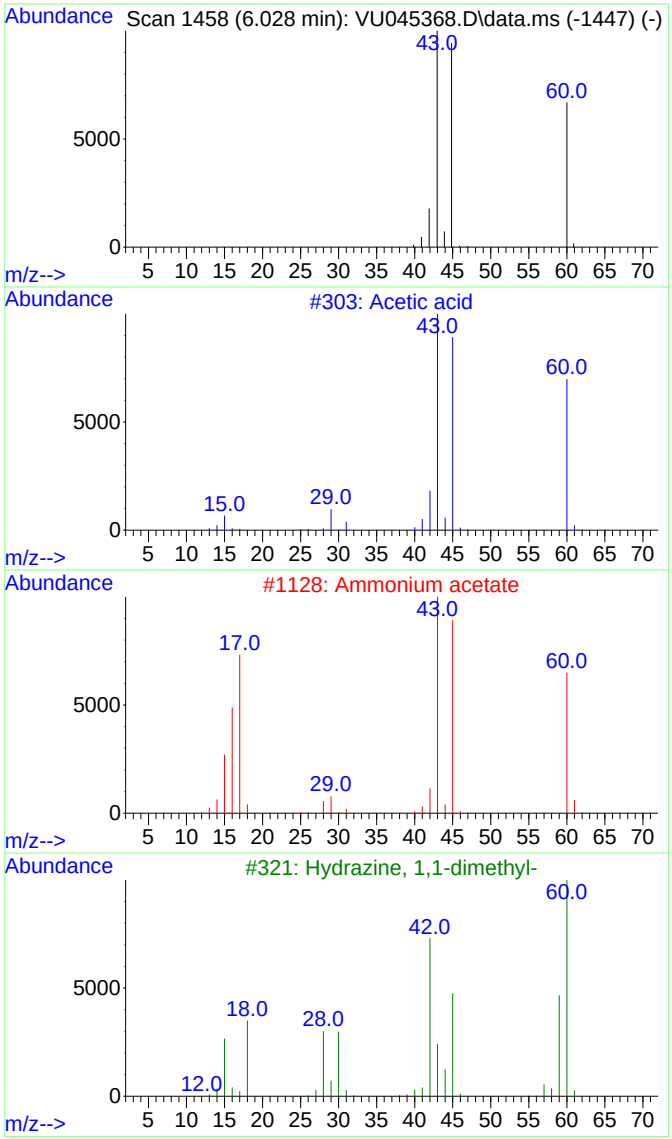
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

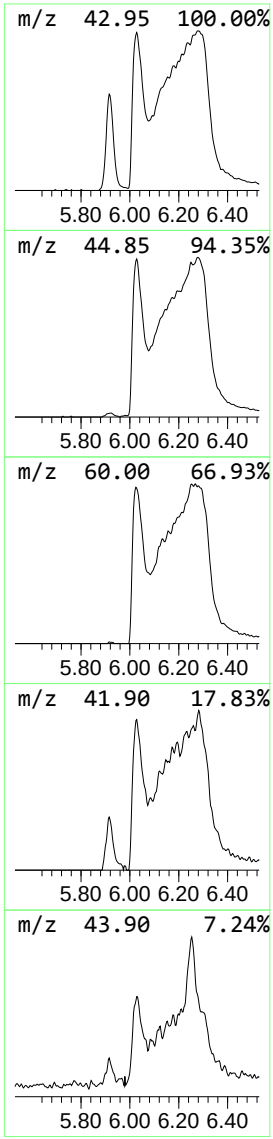
****

Peak Number 1 Acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.028	7.51 ug/l	206362	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Ammonium acetate	77	C2H7NO2	000631-61-8	64
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	16
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5	Thiirane	60	C2H4S	000420-12-2	5





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Data File : VU045368.D
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Operator : SY/MD
Sample : M4316-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2-IS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

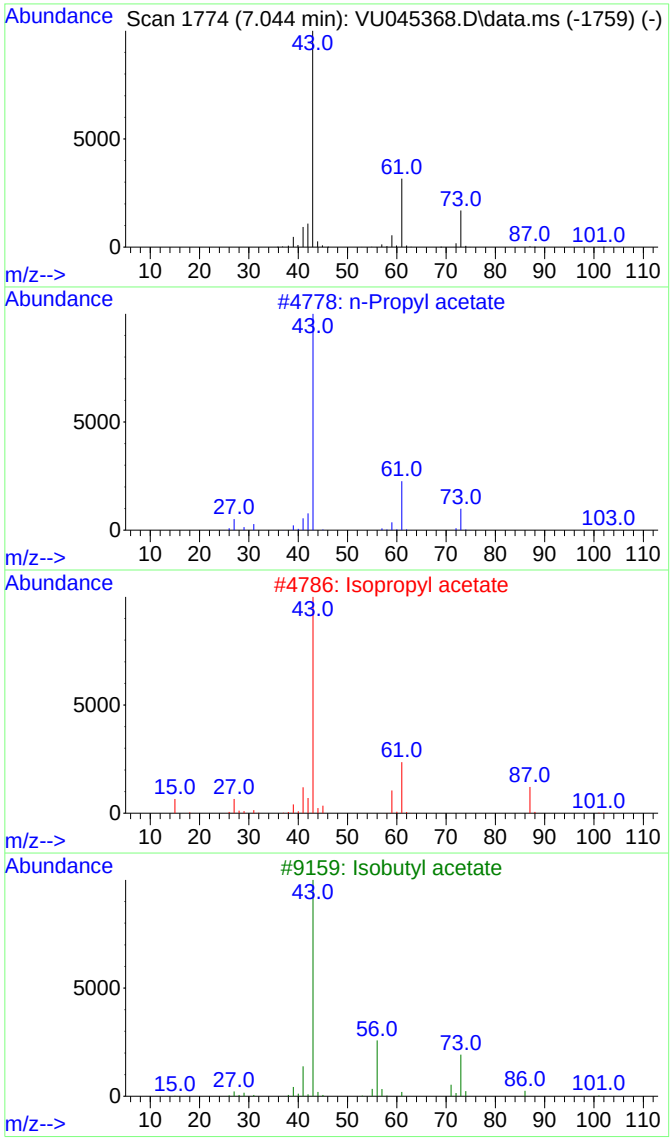
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

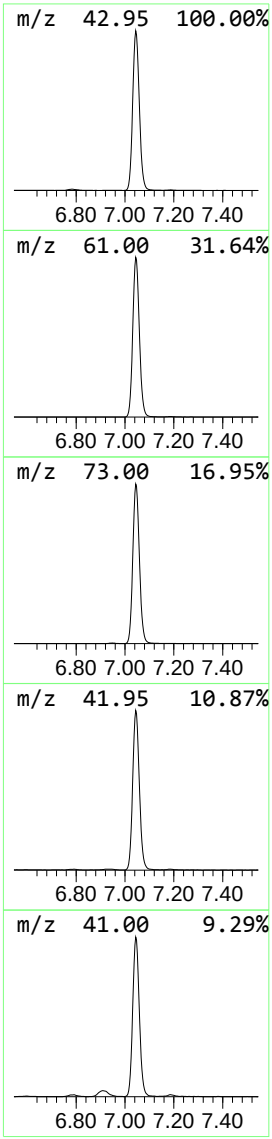
****

Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.044	118.36 ug/l	3250220	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	36
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045368.D
Acq On : 22 Oct 2021 16:35
Operator : SY/MD
Sample : M4316-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2-IS

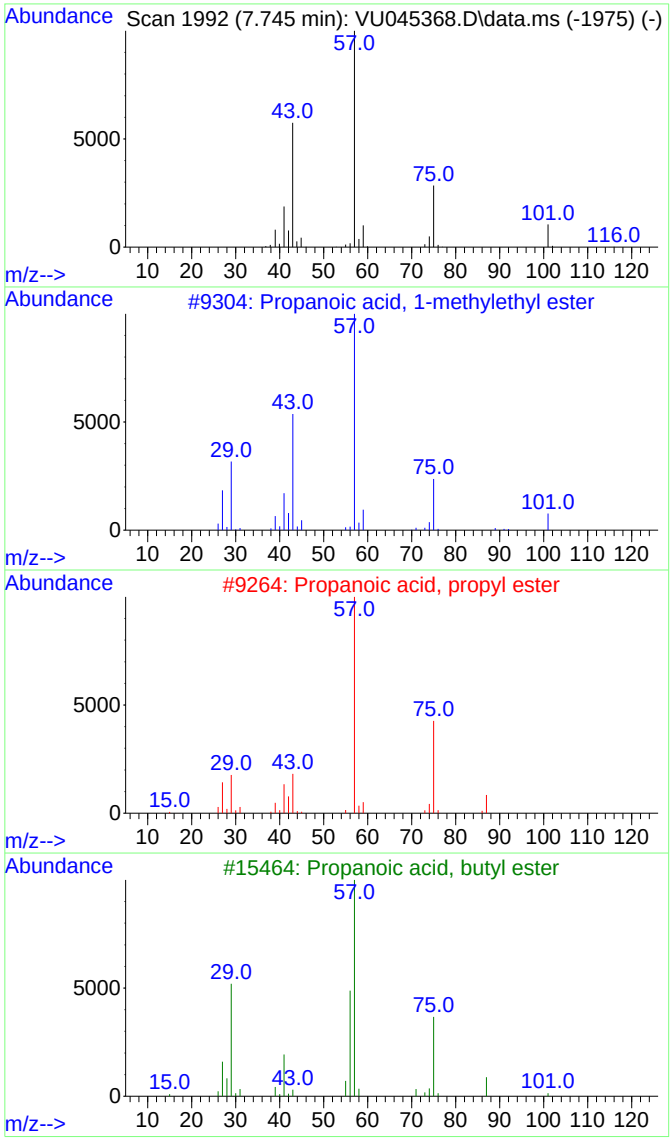
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

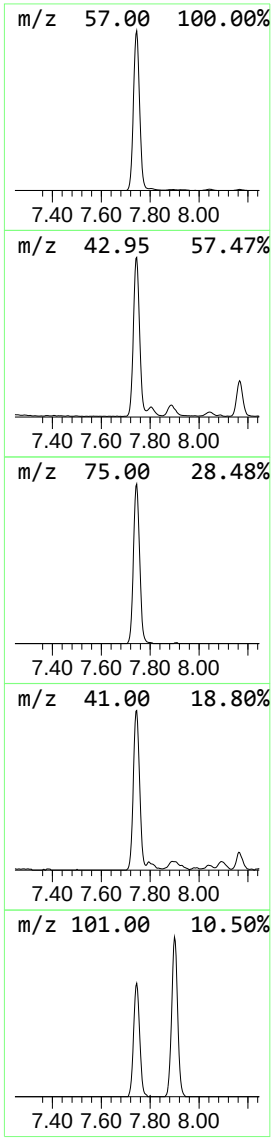
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.745	16.98 ug/l	466166	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Acq On : 22 Oct 2021 16:35
Operator : SY/MD
Sample : M4316-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2-IS

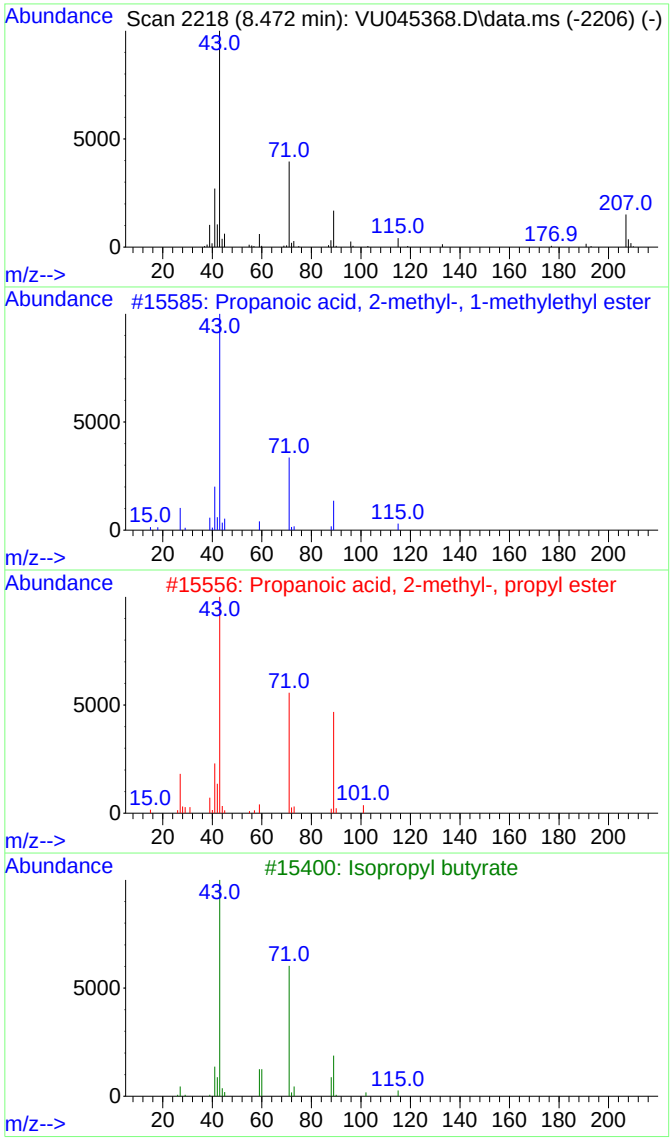
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

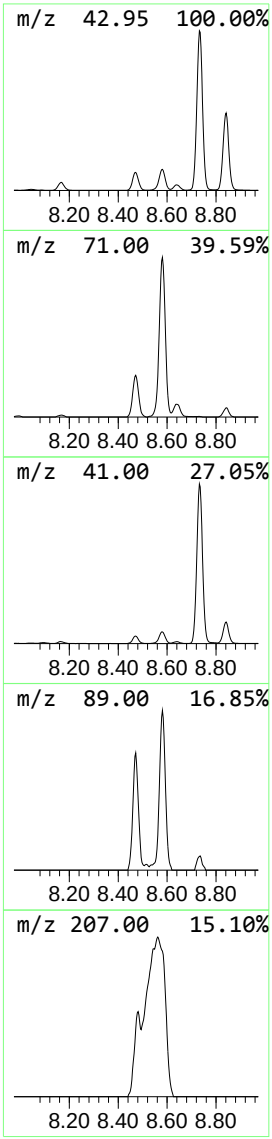
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.472	6.08 ug/l	140635	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	64
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	50
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	38





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Data File : VU045368.D
Acq On : 22 Oct 2021 16:35
Operator : SY/MD
Sample : M4316-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2-IS

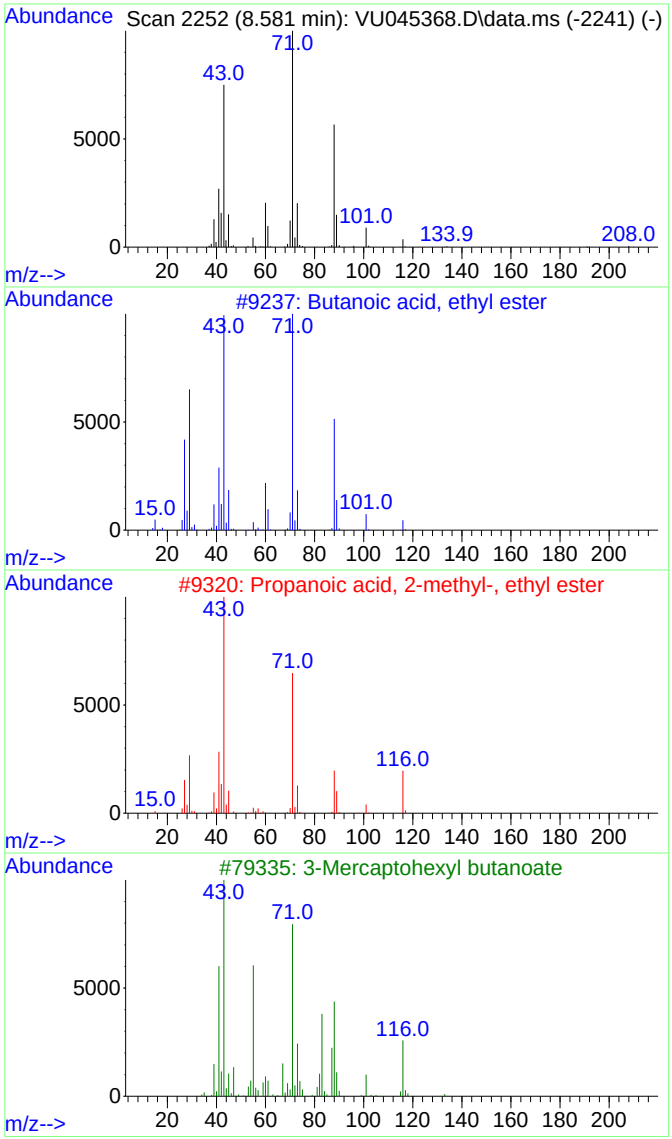
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

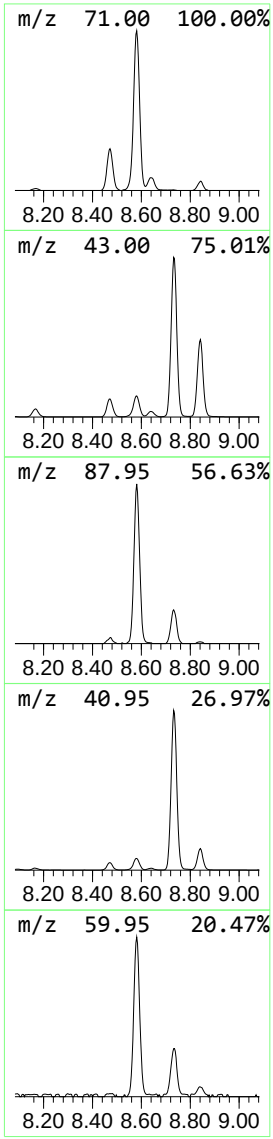
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.581	15.39 ug/l	356138	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	50
3	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	38
5	Ethyl hydrogen suberate	202	C10H18O4	1000342-39-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
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Acq On : 22 Oct 2021 16:35
Operator : SY/MD
Sample : M4316-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2-IS

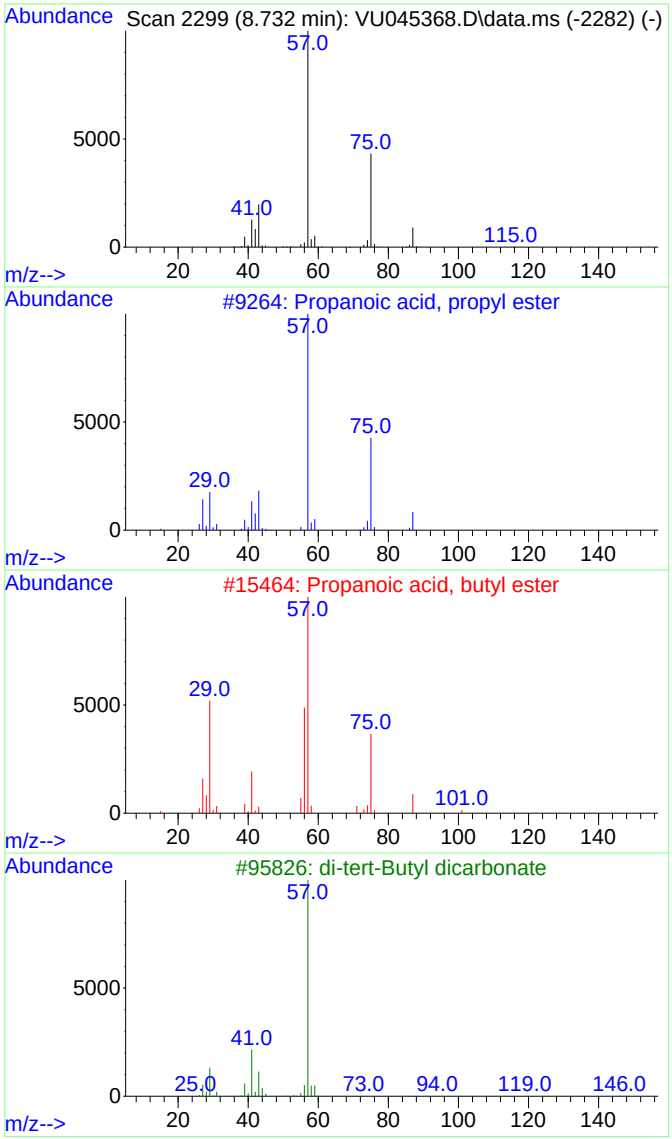
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

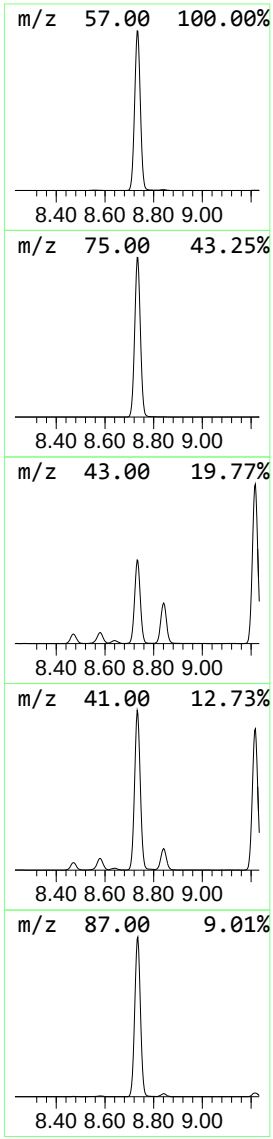
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.732	203.39 ug/l	4707850	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2-IS

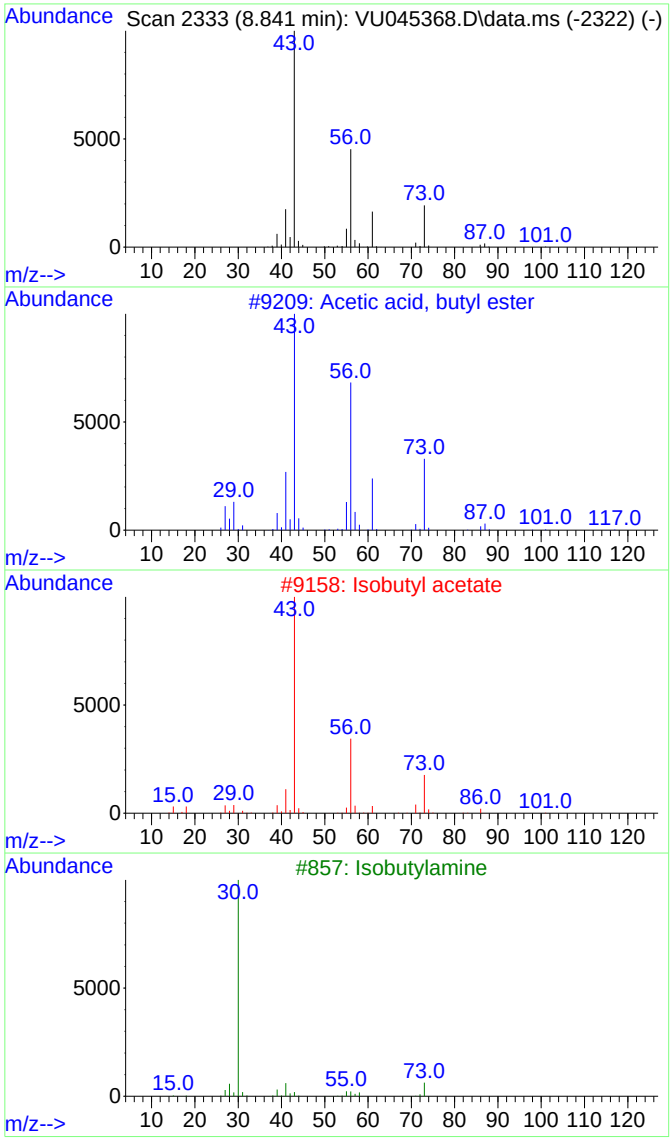
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

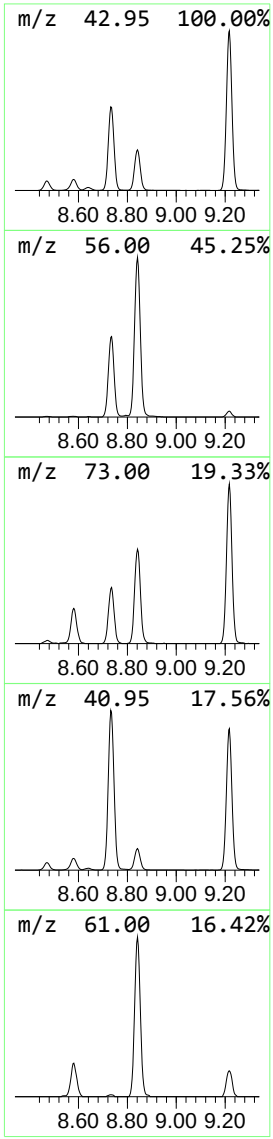
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.841	21.55 ug/l	498794	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
5	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9





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Quant Title : SW846 8260

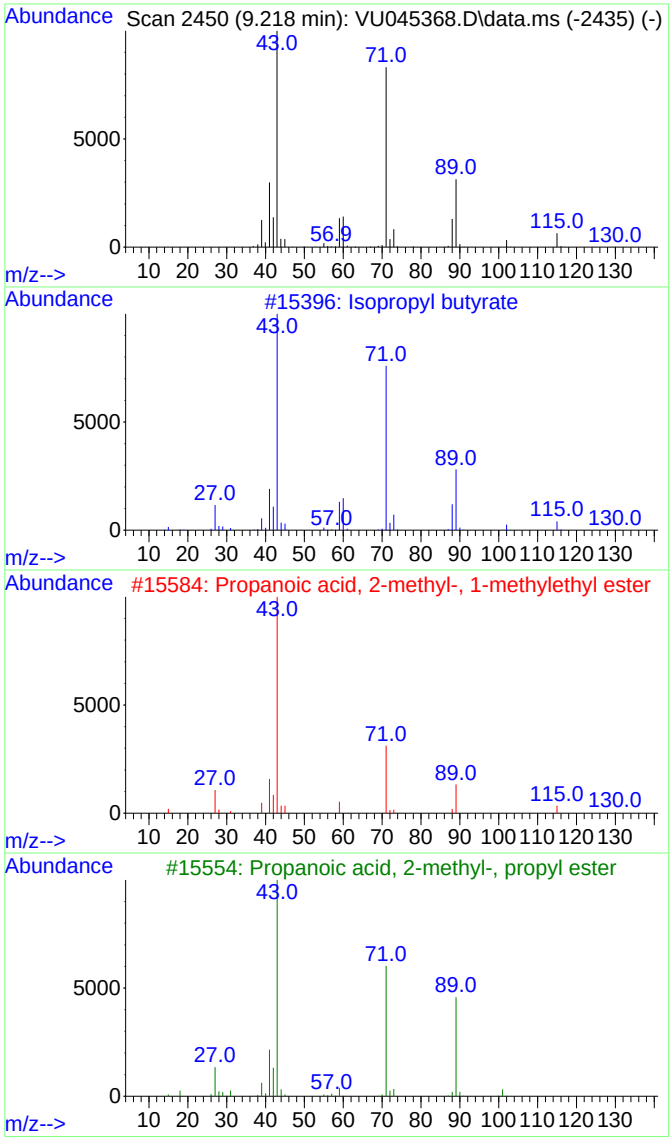
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

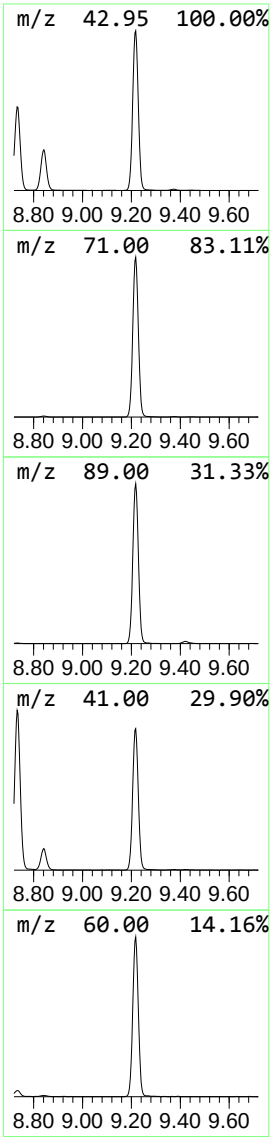
****

Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.218	119.09 ug/l	2756560	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64





Tentatively Identified Compound (LSC) summary

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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : WC-2-IS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetic acid	6.028	7.5	ug/l	206362	2	6.250	1373080	50.0
n-Propyl acetate	7.044	118.4	ug/l	3250220	2	6.250	1373080	50.0
Propanoic acid,...	7.745	17.0	ug/l	466166	2	6.250	1373080	50.0
Propanoic acid,...	8.472	6.1	ug/l	140635	3	9.420	1157360	50.0
Butanoic acid, ...	8.581	15.4	ug/l	356138	3	9.420	1157360	50.0
Propanoic acid,...	8.732	203.4	ug/l	4707850	3	9.420	1157360	50.0
Acetic acid, bu...	8.841	21.6	ug/l	498794	3	9.420	1157360	50.0
Isopropyl butyrate	9.218	119.1	ug/l	2756560	3	9.420	1157360	50.0