LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

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_N\METHODS\82N042220W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.503	1509	1528	1552	rBV3	10322	32143	1.91%	0.319%
2	7.313	1762	1780	1793	rBV	117115	296395	17.59%	2.946%
3	7.400	1793	1807	1833	rVB	232563	557238	33.08%	5.539%
4	7.767	1901	1921	1941	rBV	149836	346963	20.60%	3.449%
5	7.918	1951	1968	1982	rBV	45889	98731	5.86%	0.981%
6	8.349	2086	2102	2124	rBV	369356	750532	44.55%	7.460%
7	8.966	2278	2294	2307	rBV	23175	45827	2.72%	0.455%
8	9.053	2307	2321	2353	rVV	943223	1684604	100.00%	16.744%
9	9.702	2508	2523	2537	rBV	133106	224481	13.33%	2.231%
10	9.882	2565	2579	2594	rBV	617317	1076280	63.89%	10.698%
11	10.085	2630	2642	2659	rVB	42824	71092	4.22%	0.707%
12	10.352	2712	2725	2739	rBV	247939	400211	23.76%	3.978%
13	10.445	2744	2754	2766	rVV2	41605	67436	4.00%	0.670%
14	10.522	2766	2778	2785	rVV	64792	106494	6.32%	1.058%
15	10.574	2785	2794	2811	rVV	400649	619516	36.78%	6.158%
16	10.664	2811	2822	2838	rVB	24963	42736	2.54%	0.425%
17	10.982	2909	2921	2936	rBV	547087	830267	49.29%	8.252%
18	11.210	2977	2992	3010	rVB	576564	964126	57.23%	9.583%
19	11.590	3098	3110	3121	rBV	13674	21002	1.25%	0.209%
20	11.692	3128	3142	3157	rBV	70596	107529	6.38%	1.069%
21	12.210	3291	3303	3318	rBV	473737	749932	44.52%	7.454%
22	13.152	3584	3596	3614	rBV	604900	949255	56.35%	9.435%
23	13.940	3834	3841	3851	rVB4	12585	18080	1.07%	0.180%

Sum of corrected areas: 10060870

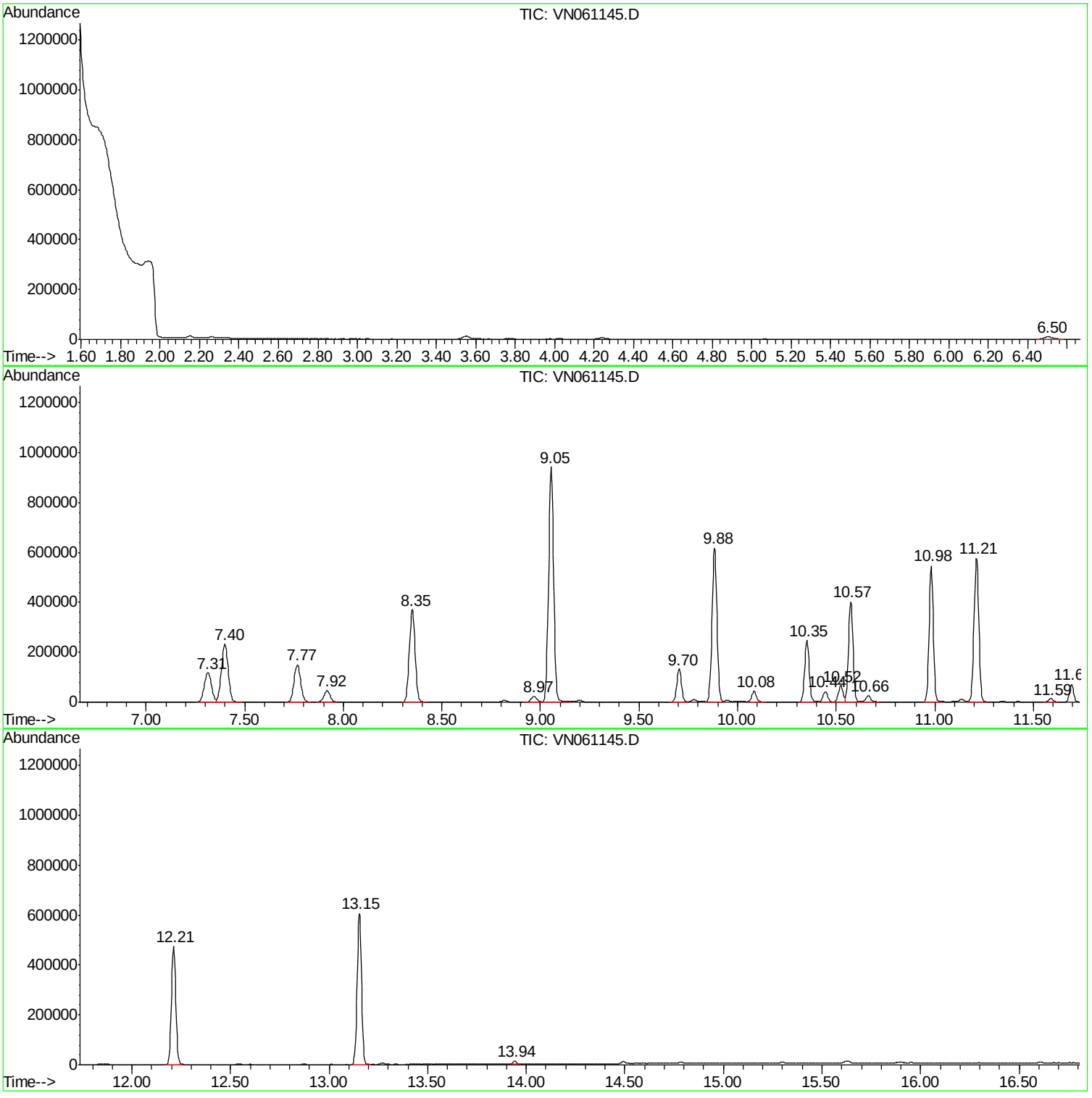
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

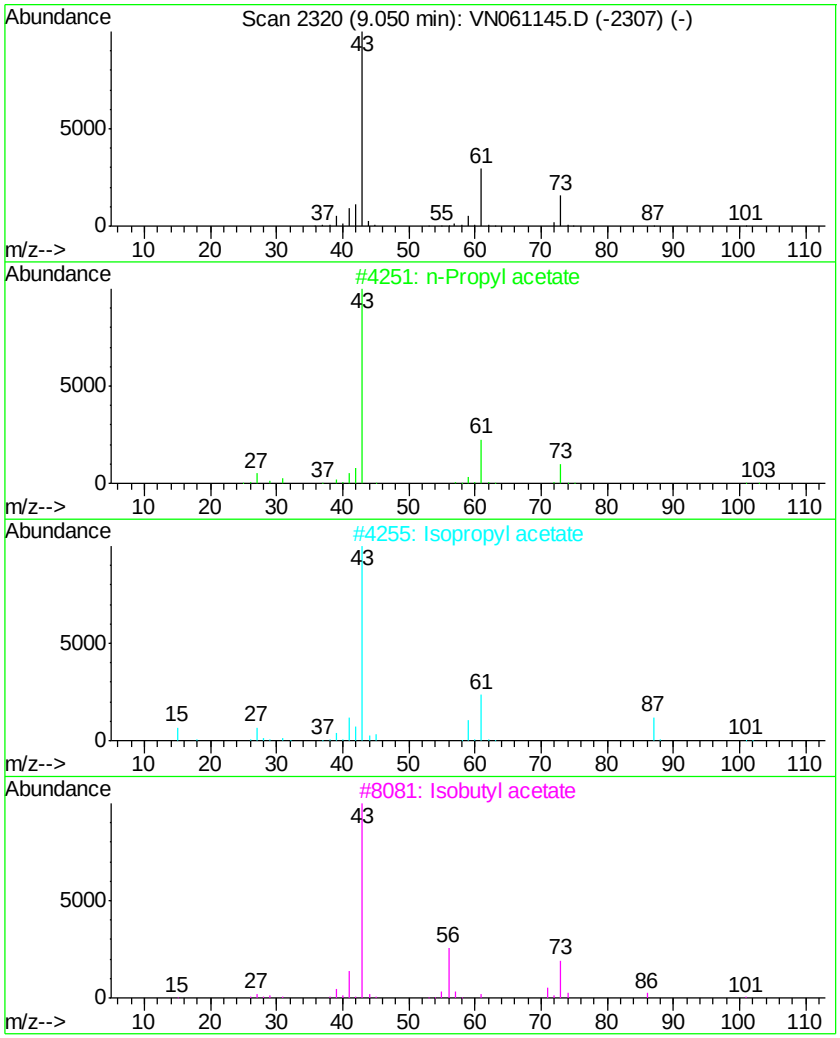
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

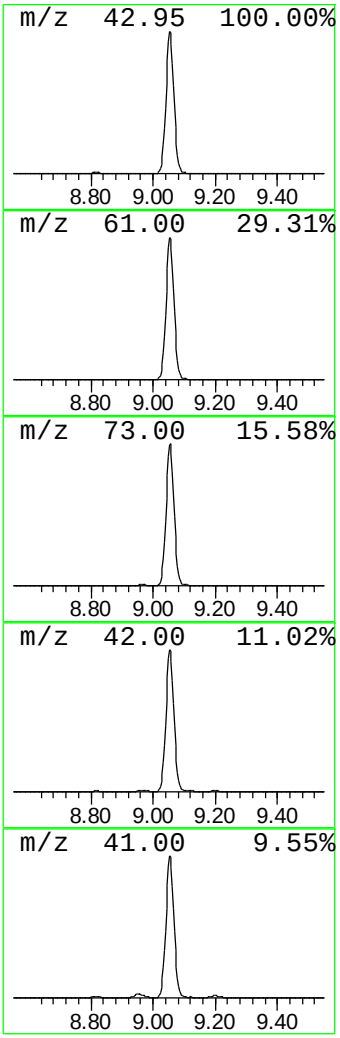
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	112.23 ug/l	1684600	1,4-Difluorobenzene	8.35

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	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	7





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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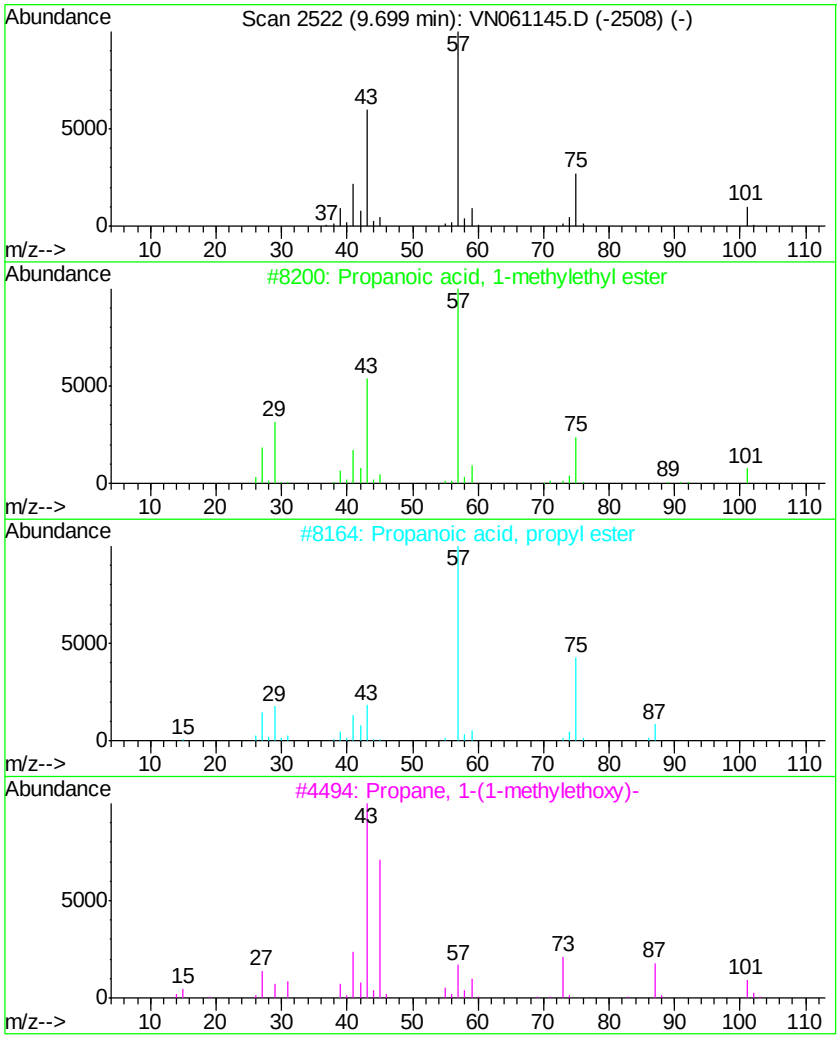
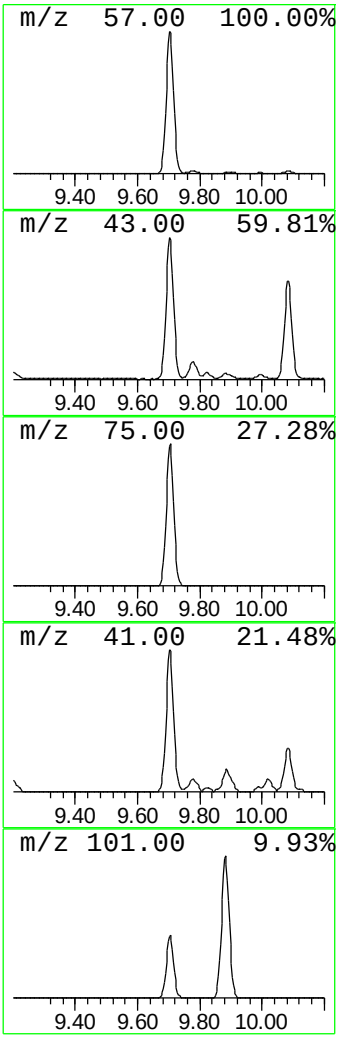
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	14.95 ug/l	224481	1,4-Difluorobenzene	8.35

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	42
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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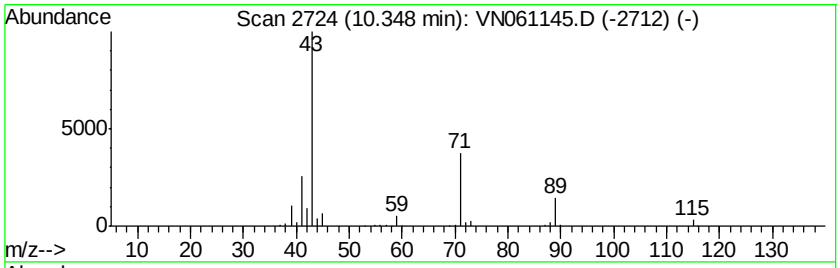
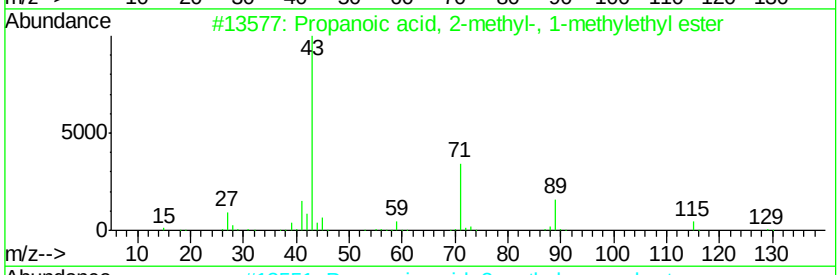
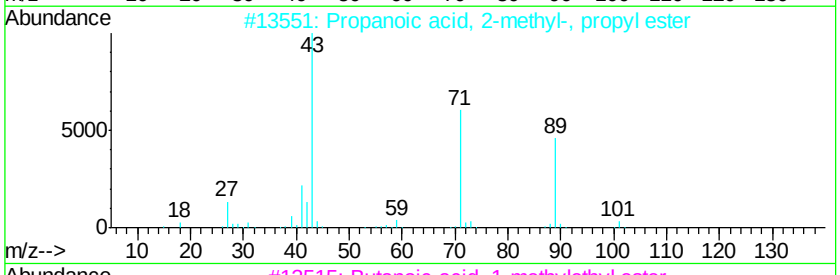
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

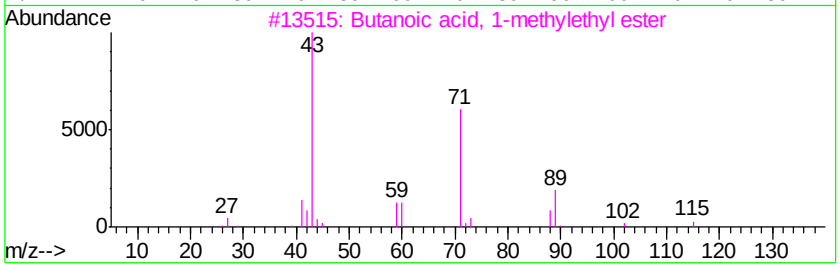
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	20.76 ug/l	400211	Chlorobenzene-d5	11.21

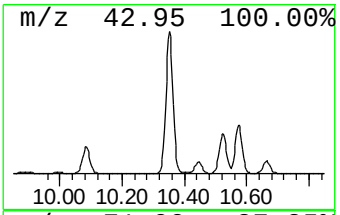
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	36

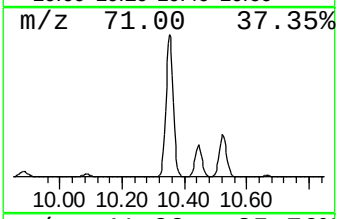


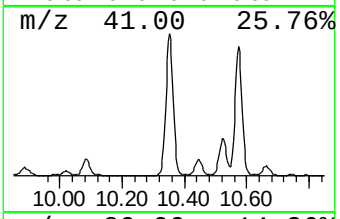


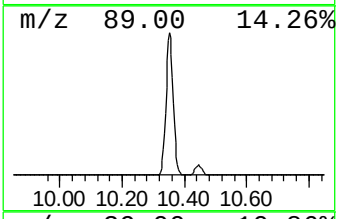


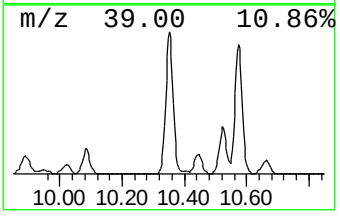












Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

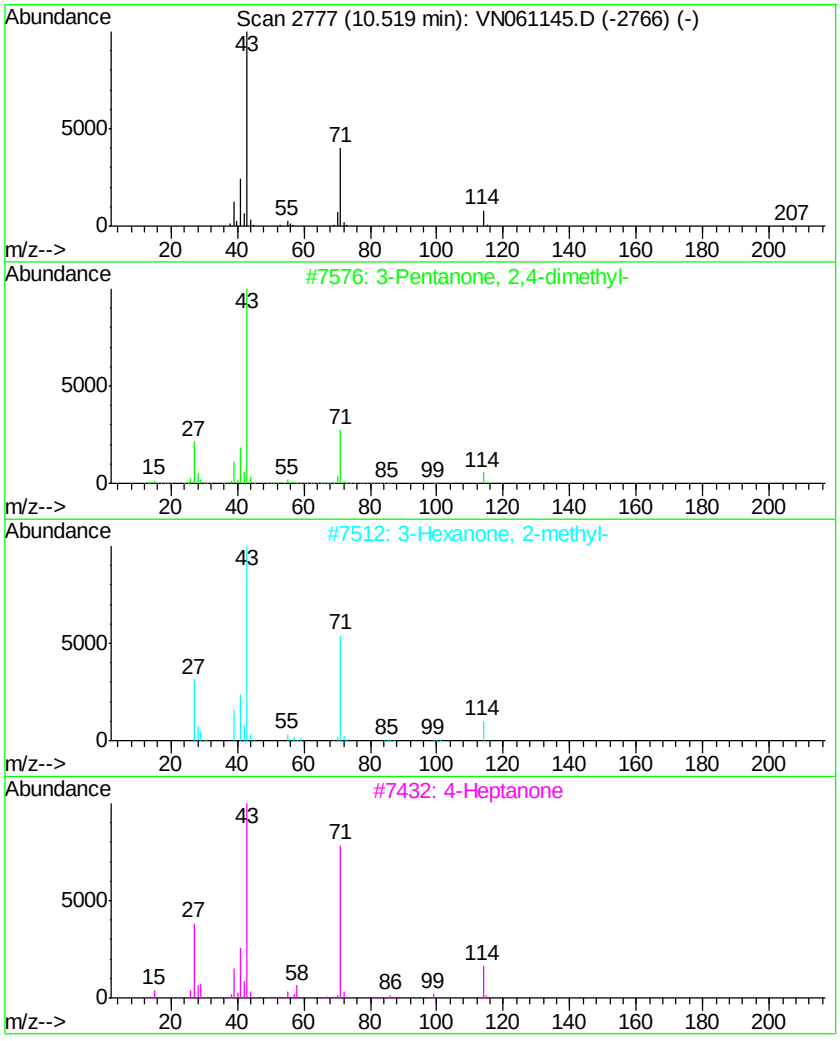
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

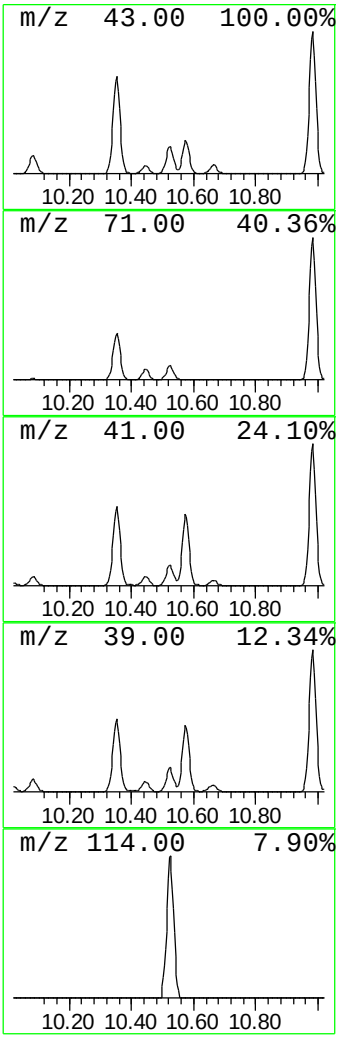
****

Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	5.52 ug/l	106494	Chlorobenzene-d5	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
3	4-Heptanone	114	C7H14O	000123-19-3	59
4	Pyrrolidine	71	C4H9N	000123-75-1	42
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

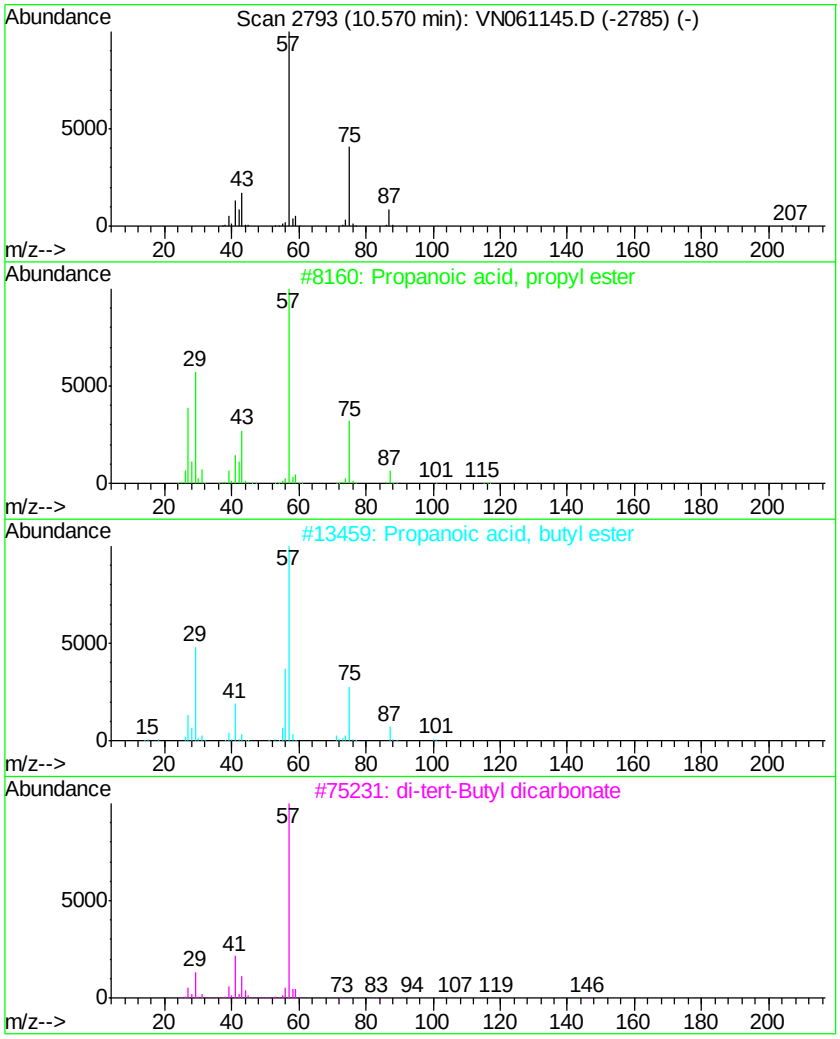
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

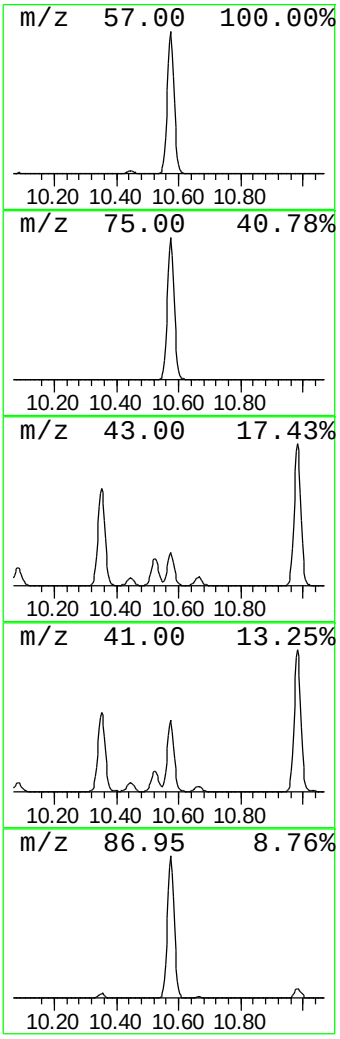
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	32.13 ug/l	619516	Chlorobenzene-d5	11.21

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	28
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	12
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

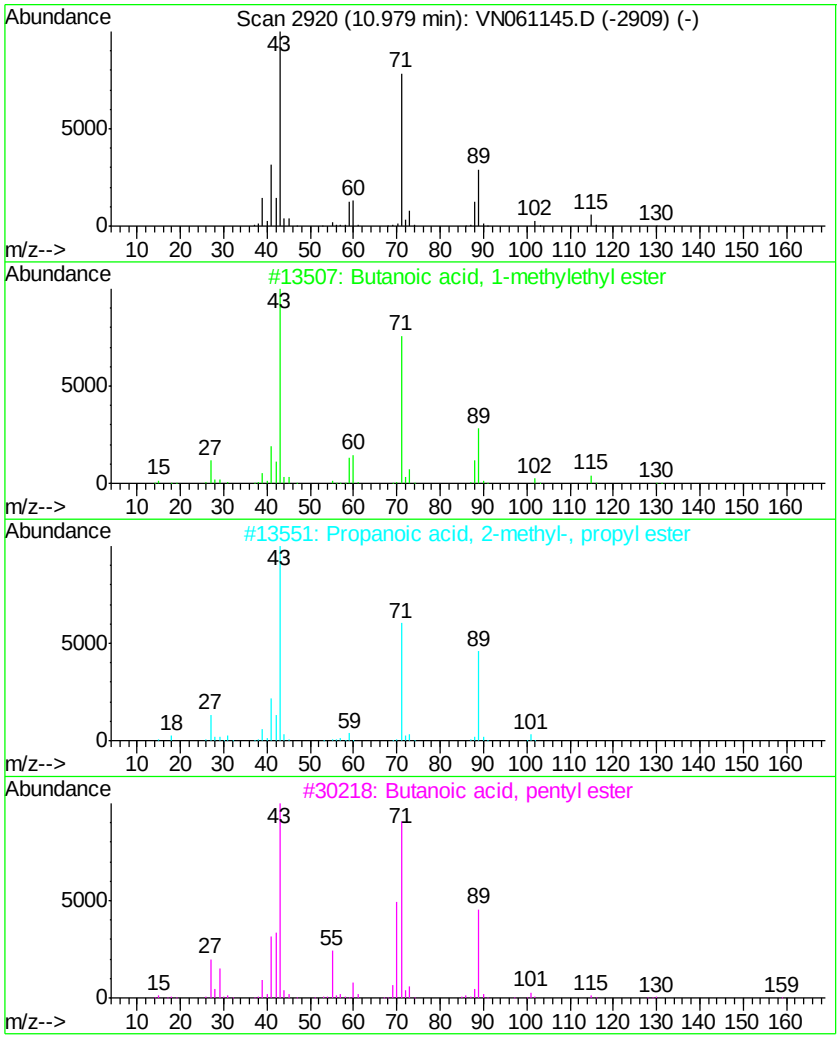
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

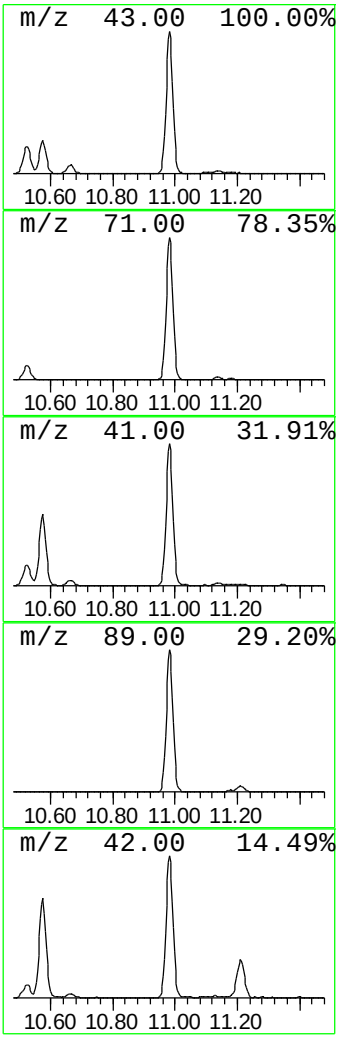
****

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	43.06 ug/l	830267	Chlorobenzene-d5	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	94
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

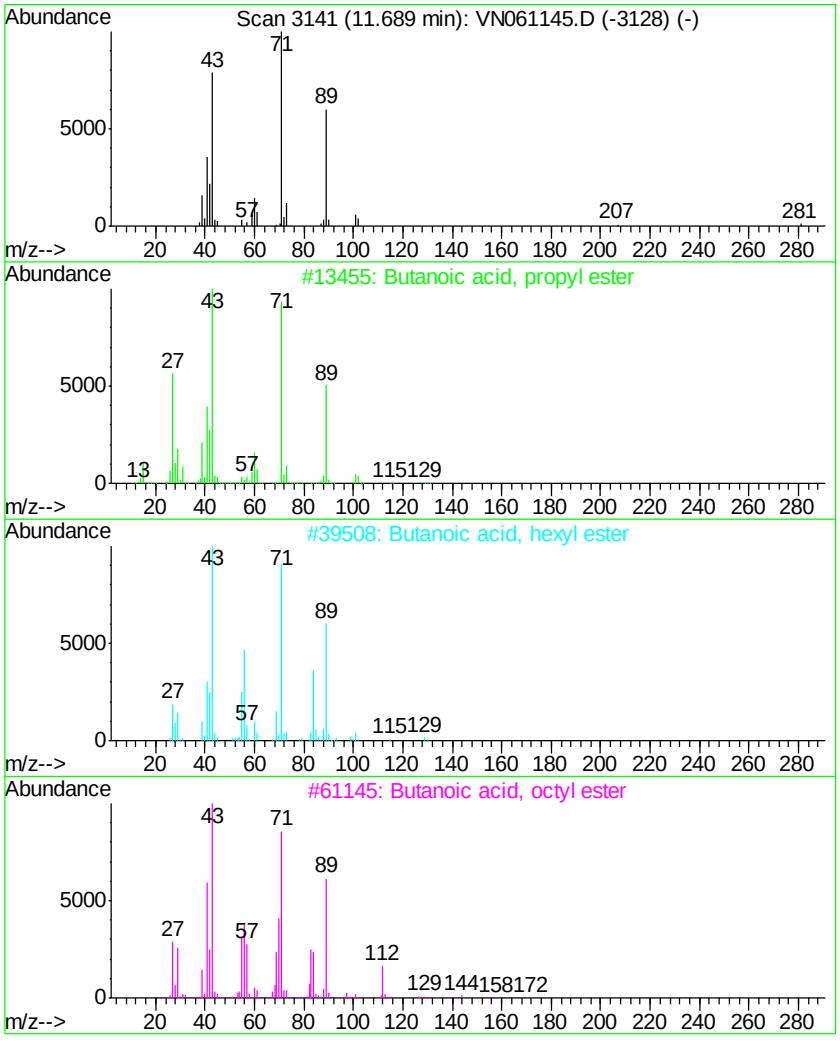
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

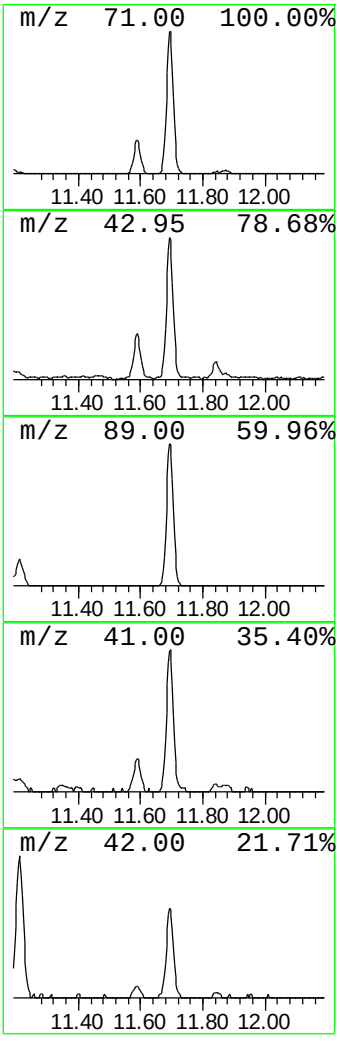
****

Peak Number 7 Butanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	5.58 ug/l	107529	Chlorobenzene-d5	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
3	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN042220\
Data File : VN061145.D
Acq On : 22 Apr 2020 22:10
Operator : JC/MD
Sample : L2359-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-1B-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	9.05	112.2	ug/l	1684600	2	8.35	750532	50.0
Propanoic acid, 1...	9.70	14.9	ug/l	224481	2	8.35	750532	50.0
Propanoic acid, 2...	10.35	20.8	ug/l	400211	3	11.21	964126	50.0
3-Pentanone, 2,4-...	10.52	5.5	ug/l	106494	3	11.21	964126	50.0
Propanoic acid, p...	10.57	32.1	ug/l	619516	3	11.21	964126	50.0
Butanoic acid, 1-...	10.98	43.1	ug/l	830267	3	11.21	964126	50.0
Butanoic acid, pr...	11.69	5.6	ug/l	107529	3	11.21	964126	50.0