LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

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\82N062420W.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	2.416	191	200	210	rVB3	10896	19417	1.41%	0.184%
2	3.776	607	623	644	rBV2	29526	78026	5.66%	0.738%
3	4.500	831	848	872	rVB2	23264	70145	5.09%	0.664%
4	7.548	1778	1796	1808	rBV	159574	401256	29.11%	3.797%
5	7.625	1808	1820	1841	rVB	252923	602585	43.72%	5.702%
6	7.989	1916	1933	1955	rBV	187681	435045	31.56%	4.116%
7	8.127	1962	1976	1985	rBV2	37847	82581	5.99%	0.781%
8	8.220	1986	2005	2007	rBV3	25990	64998	4.72%	0.615%
9	8.551	2092	2108	2130	rVB	450165	945818	68.62%	8.949%
10	9.152	2283	2295	2307	rBV3	22589	47054	3.41%	0.445%
11	9.236	2307	2321	2344	rBV	558806	1029121	74.66%	9.738%
12	9.873	2506	2519	2534	rBV	140275	245966	17.85%	2.327%
13	9.956	2534	2545	2553	rVV3	9208	16475	1.20%	0.156%
14	10.059	2563	2577	2600	rBV	762713	1378343	100.00%	13.042%
15	10.255	2628	2638	2646	rVB3	11370	18767	1.36%	0.178%
16	10.516	2706	2719	2735	rBV	288441	479455	34.78%	4.537%
17	10.612	2738	2749	2761	rVV2	33318	61498	4.46%	0.582%
18	10.693	2761	2774	2780	rVV	80101	142387	10.33%	1.347%
19	10.738	2780	2788	2807	rVV	294801	487688	35.38%	4.615%
20	10.828	2809	2816	2831	rVB6	7893	15059	1.09%	0.142%
21	11.143	2900	2914	2934	rBV	560504	882394	64.02%	8.349%
22	11.300	2955	2963	2971	rBV3	9480	14966	1.09%	0.142%
23	11.381	2974	2988	3013	rVB	699742	1231431	89.34%	11.652%
24	11.750	3092	3103	3116	rBV4	11745	19679	1.43%	0.186%
25	11.853	3125	3135	3148	rBV2	29769	47830	3.47%	0.453%
26	12.377	3283	3298	3319	rBV	490755	819112	59.43%	7.750%
27	13.320	3578	3591	3610	rBV	559106	931454	67.58%	8.813%

Sum of corrected areas: 10568550

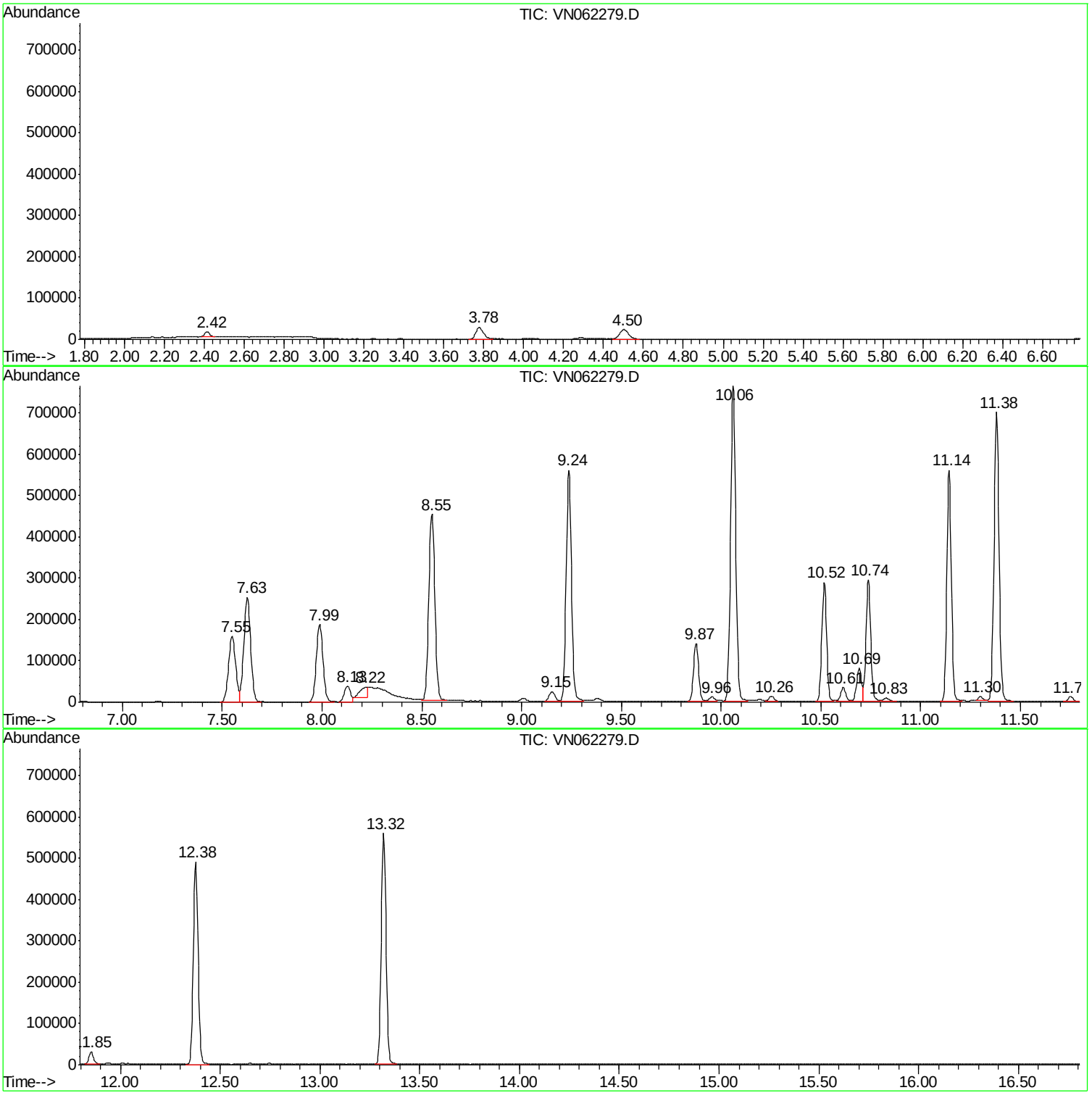
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

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

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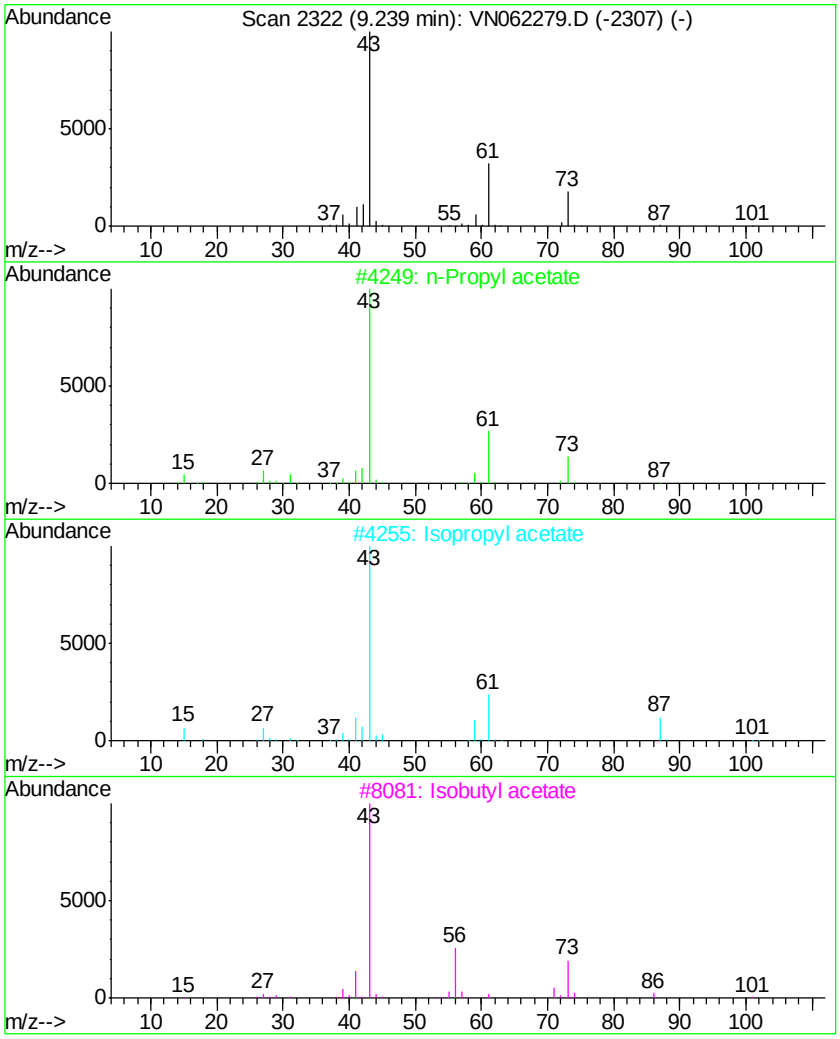
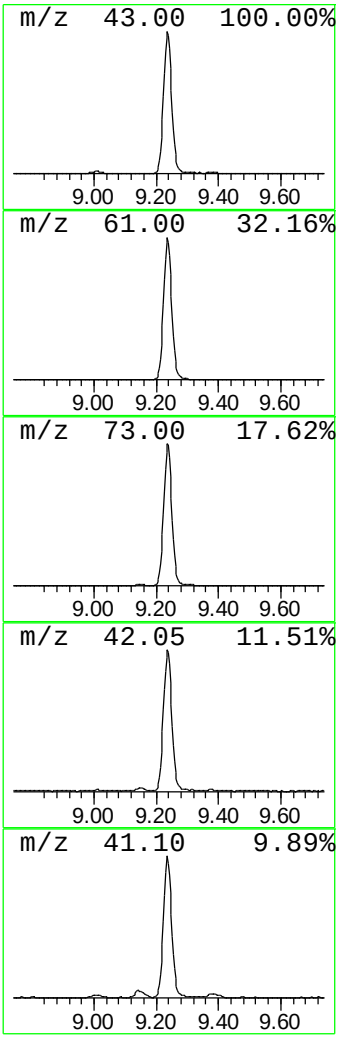
Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.24	54.40 ug/l	1029120	1,4-Difluorobenzene	8.55

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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

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

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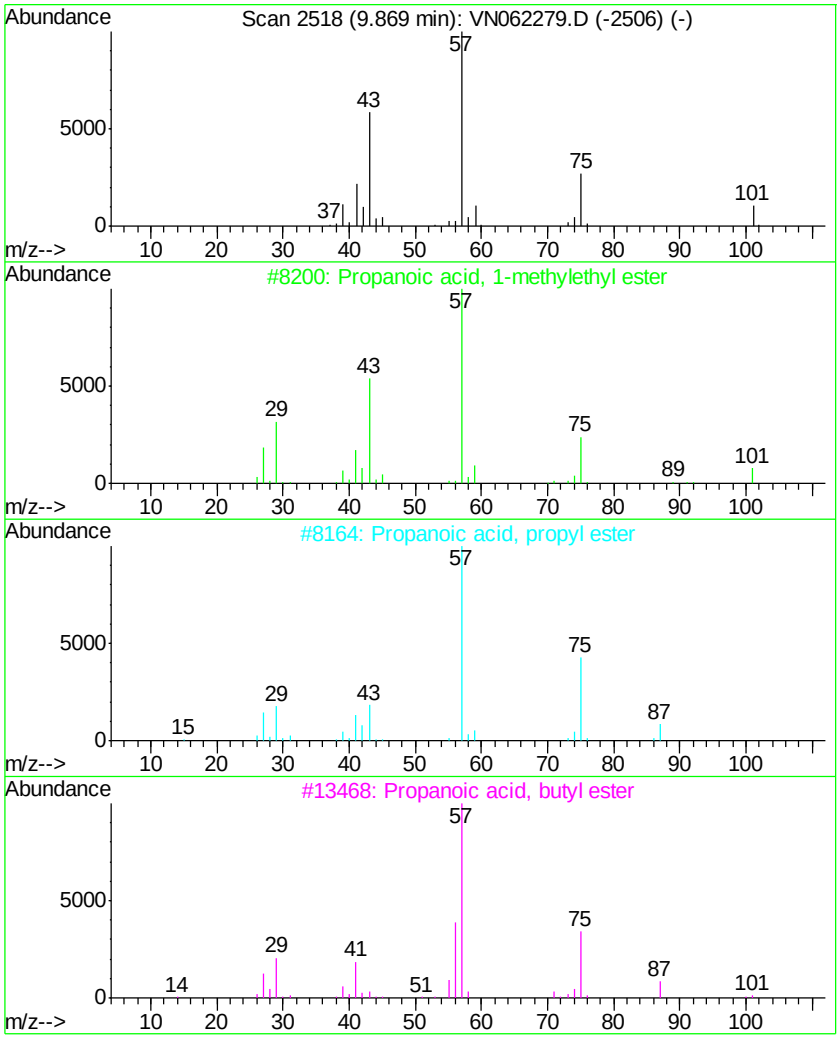
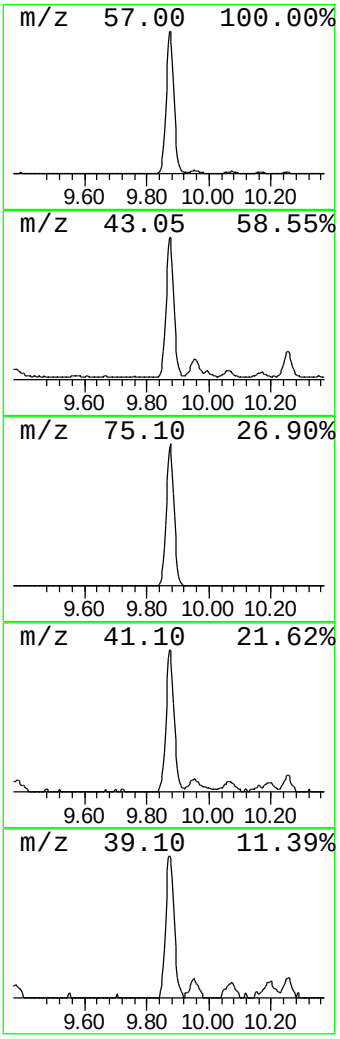
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	13.00 ug/l	245966	1,4-Difluorobenzene	8.55

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	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Azetidine	57	C3H7N	000503-29-7	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

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

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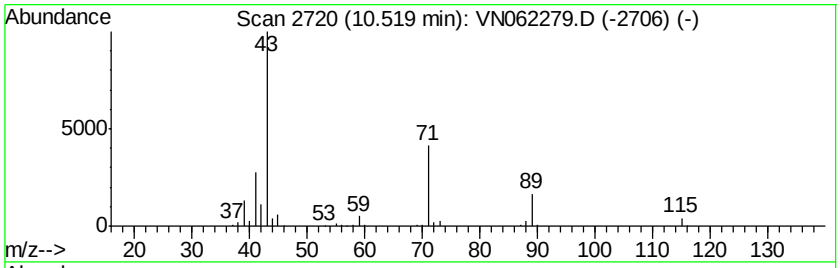
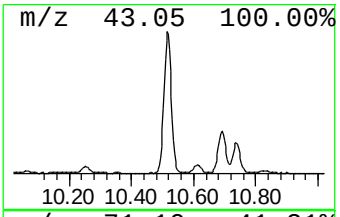
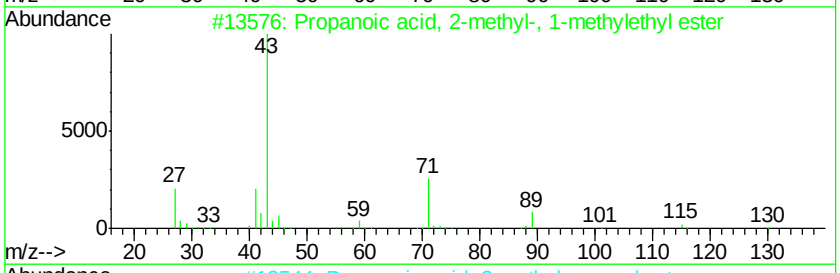
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

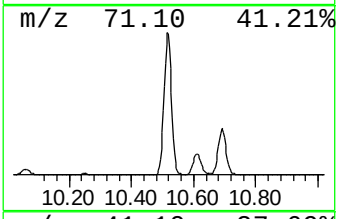
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	19.47 ug/l	479455	Chlorobenzene-d5	11.38

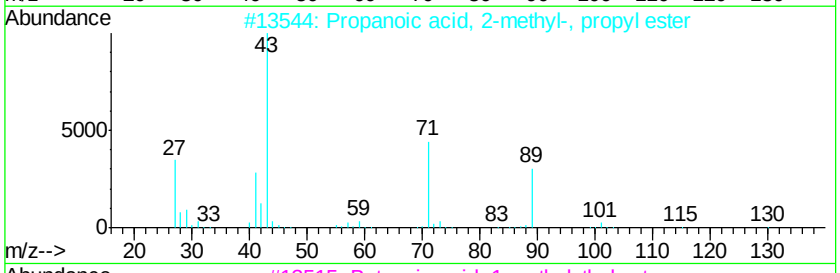
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	43
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	42

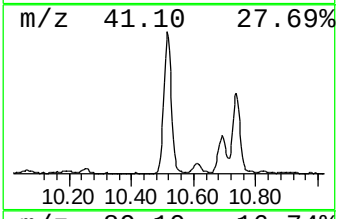


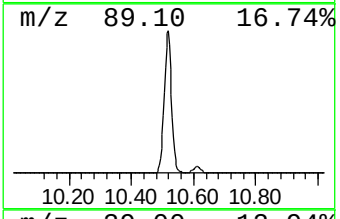


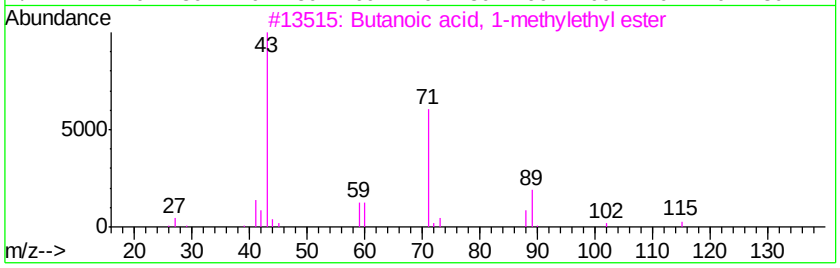


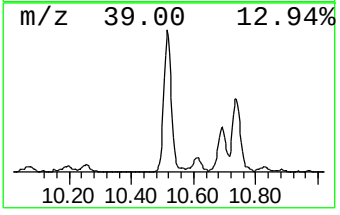












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

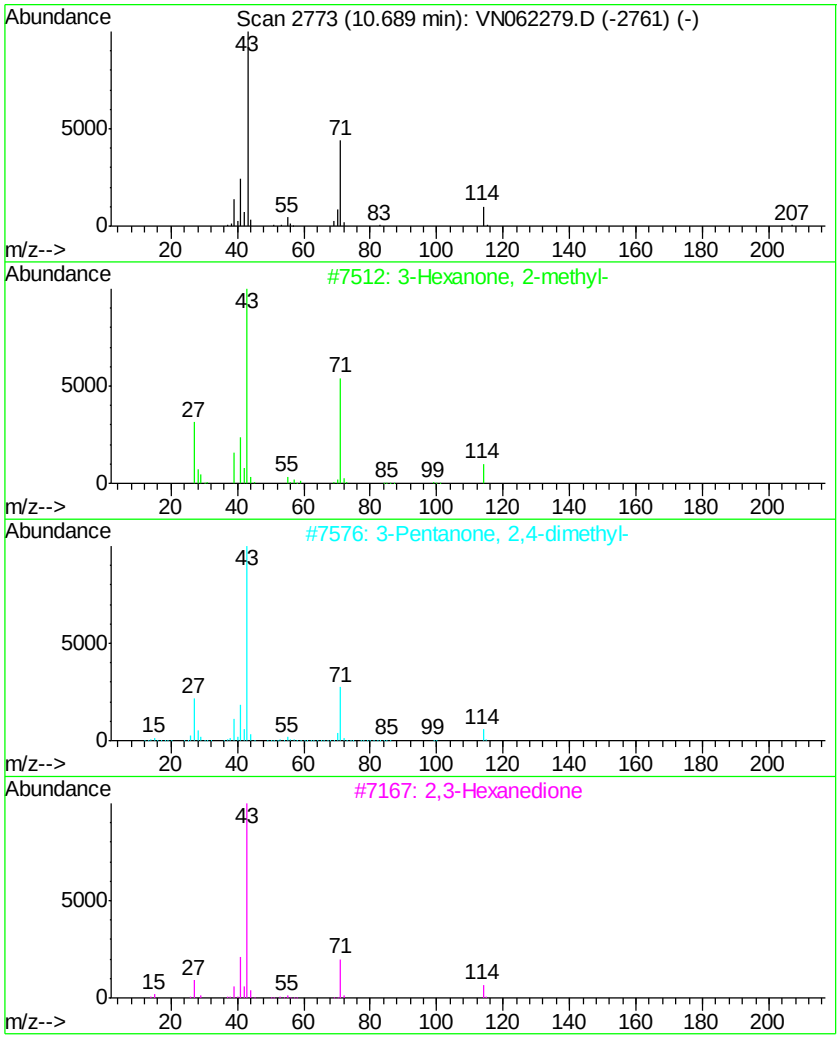
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

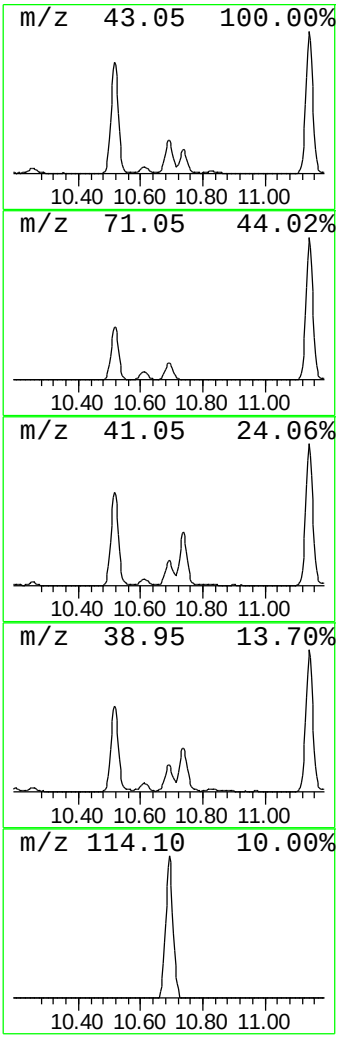
****

Peak Number 4 3-Hexanone, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	5.78 ug/l	142387	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
2	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	72
4	4-Heptanone	114	C7H14O	000123-19-3	59
5	Pyrrolidine	71	C4H9N	000123-75-1	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

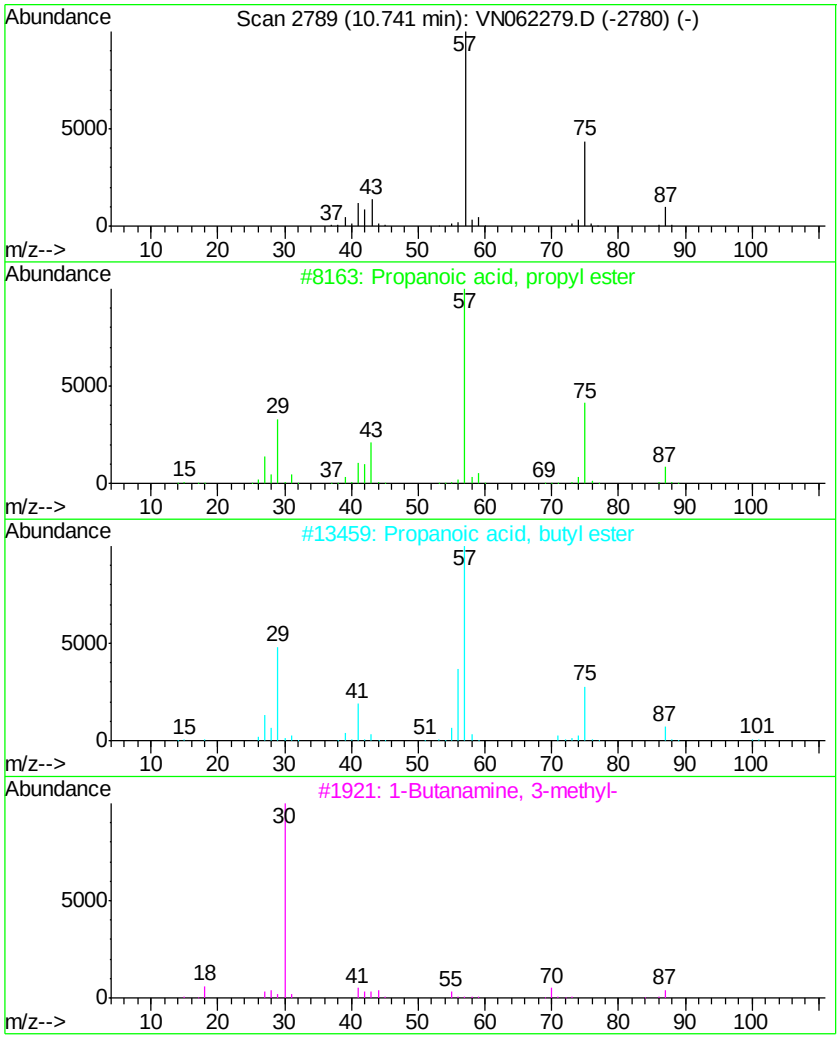
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

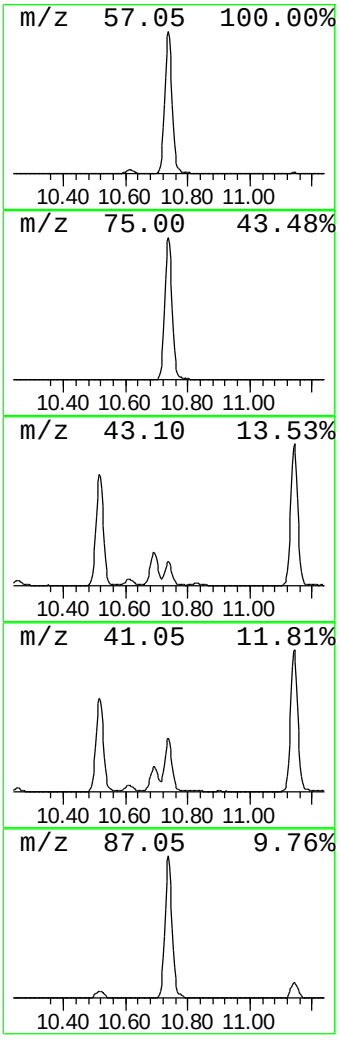
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	19.80 ug/l	487688	Chlorobenzene-d5	11.38

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	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
Acq On : 1 Jul 2020 8:20
Operator : JC/MD
Sample : L3153-38
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

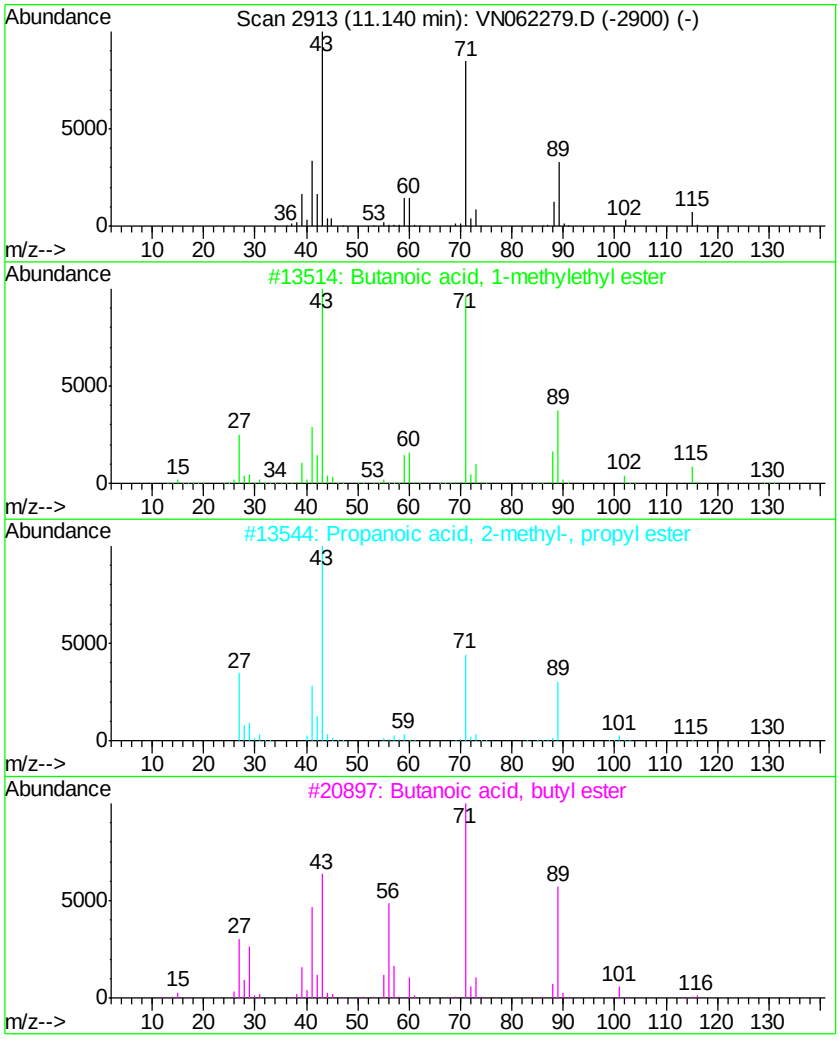
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

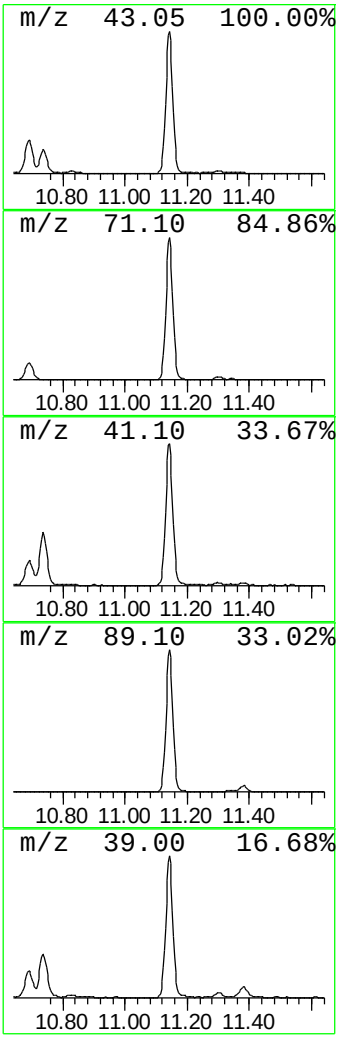
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	35.83 ug/l	882394	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
Data File : VN062279.D
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Operator : JC/MD
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ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SP2-J

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.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	9.24	54.4	ug/l	1029120	2	8.55	945818	50.0
Propanoic acid, 1...	9.87	13.0	ug/l	245966	2	8.55	945818	50.0
Propanoic acid, 2...	10.52	19.5	ug/l	479455	3	11.38	1231430	50.0
3-Hexanone, 2-met...	10.69	5.8	ug/l	142387	3	11.38	1231430	50.0
Propanoic acid, p...	10.74	19.8	ug/l	487688	3	11.38	1231430	50.0
Butanoic acid, 1-...	11.14	35.8	ug/l	882394	3	11.38	1231430	50.0