LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN091419\
Data File : VN058025.D
Acq On : 13 Sep 2019 18:39
Operator : JC/SP
Sample : K4680-34
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : T3-2-(1.5)

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\82N091019W.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	2.423	193	202	216	rVB4	23889	44171	1.80%	0.255%
2	4.529	841	857	881	rVB3	20578	63673	2.59%	0.367%
3	7.577	1784	1805	1817	rBV	301045	754251	30.72%	4.346%
4	7.654	1817	1829	1847	rVB2	349237	830694	33.84%	4.787%
5	8.014	1922	1941	1966	rBV	372861	879366	35.82%	5.067%
6	8.152	1969	1984	1998	rBV2	75923	186945	7.62%	1.077%
7	8.577	2100	2116	2134	rBV	531693	1102401	44.91%	6.352%
8	9.178	2291	2303	2314	rBV	32709	67828	2.76%	0.391%
9	9.262	2314	2329	2355	rVV	1334814	2454852	100.00%	14.146%
10	9.902	2514	2528	2542	rBV	231307	407192	16.59%	2.346%
11	10.088	2572	2586	2606	rBV	1258398	2294637	93.47%	13.223%
12	10.281	2636	2646	2661	rVB2	54551	95603	3.89%	0.551%
13	10.541	2713	2727	2745	rBV	471202	804206	32.76%	4.634%
14	10.638	2746	2757	2770	rVV3	61543	107371	4.37%	0.619%
15	10.718	2770	2782	2788	rVV	124442	218595	8.90%	1.260%
16	10.763	2788	2796	2814	rVV	553965	914662	37.26%	5.271%
17	10.853	2814	2824	2844	rVB2	29464	54002	2.20%	0.311%
18	11.168	2907	2922	2947	rBV	929277	1463185	59.60%	8.431%
19	11.329	2964	2972	2981	rBV3	15399	25053	1.02%	0.144%
20	11.406	2982	2996	3018	rVB	785635	1377880	56.13%	7.940%
21	11.779	3101	3112	3128	rVB2	16543	28619	1.17%	0.165%
22	11.879	3131	3143	3158	rBV	77500	125476	5.11%	0.723%
23	12.406	3294	3307	3331	rBV	883010	1473363	60.02%	8.490%
24	13.348	3588	3600	3621	rVB	895517	1485387	60.51%	8.559%
25	13.889	3756	3768	3779	rVB2	14177	25042	1.02%	0.144%
26	15.136	4144	4156	4165	rBV3	23800	40526	1.65%	0.234%
27	15.271	4188	4198	4203	rBV2	16970	28892	1.18%	0.166%

Sum of corrected areas: 17353872

LSC Report - Integrated Chromatogram

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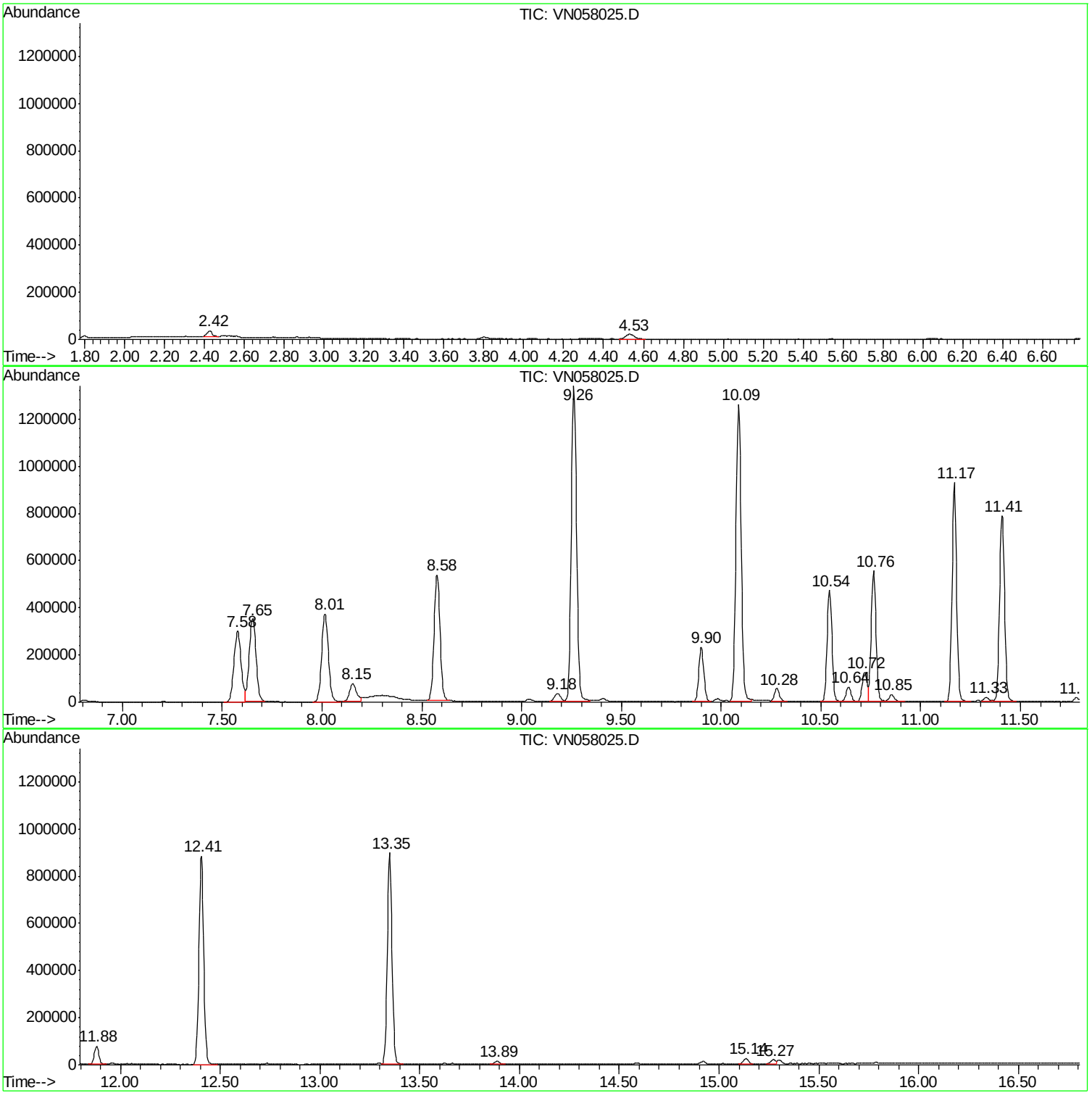
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : T3-2-(1.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.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\VN091419\
Data File : VN058025.D
Acq On : 13 Sep 2019 18:39
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Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : T3-2-(1.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

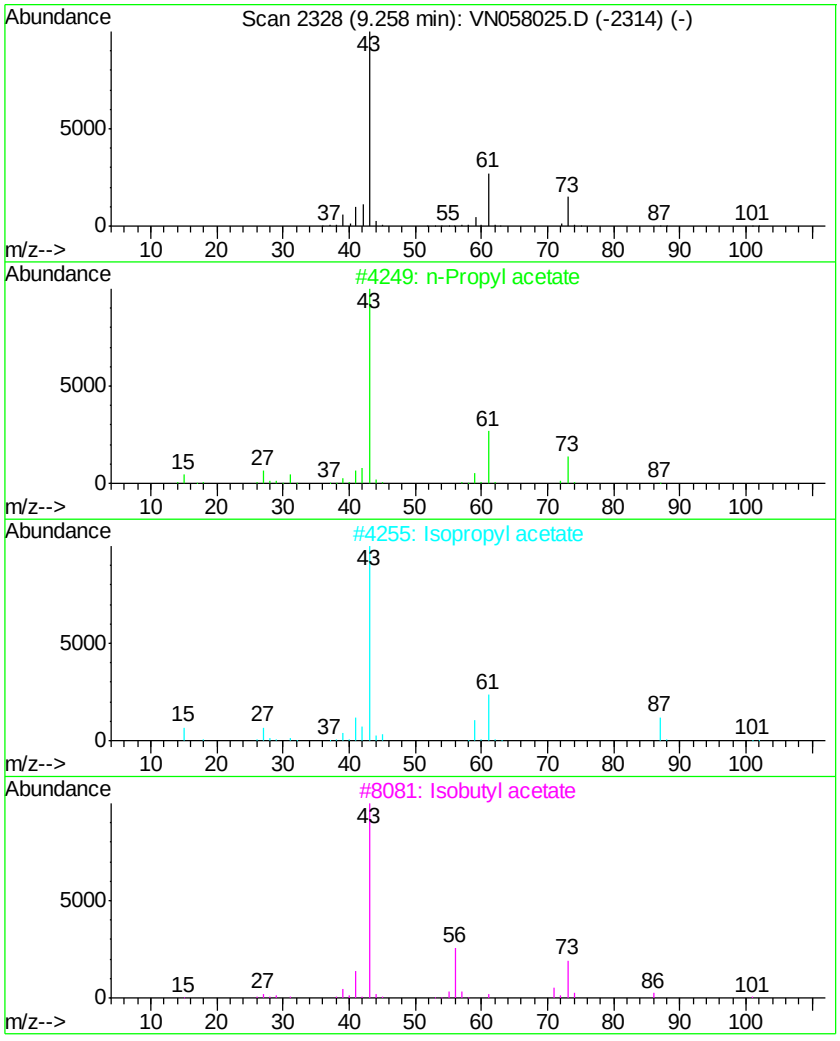
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

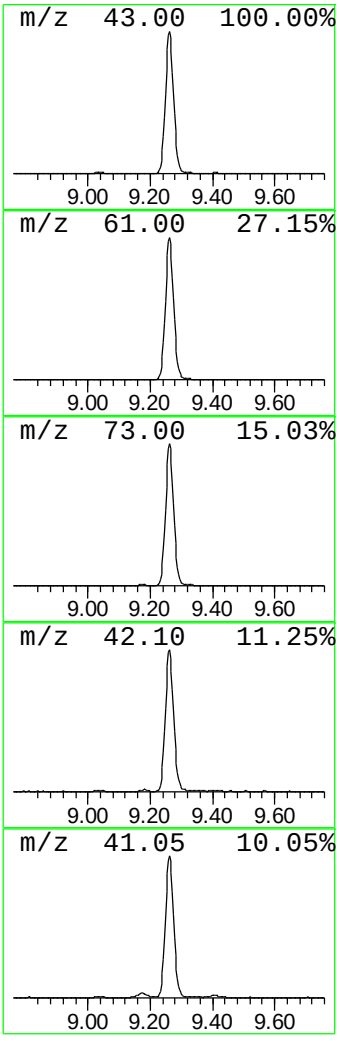
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.26	111.34 ug/l	2454850	1,4-Difluorobenzene	8.58

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	38
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	1-Butanamine	73	C4H11N	000109-73-9	5





Library Search Compound Report

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Data File : VN058025.D
Acq On : 13 Sep 2019 18:39
Operator : JC/SP
Sample : K4680-34
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : T3-2-(1.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

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

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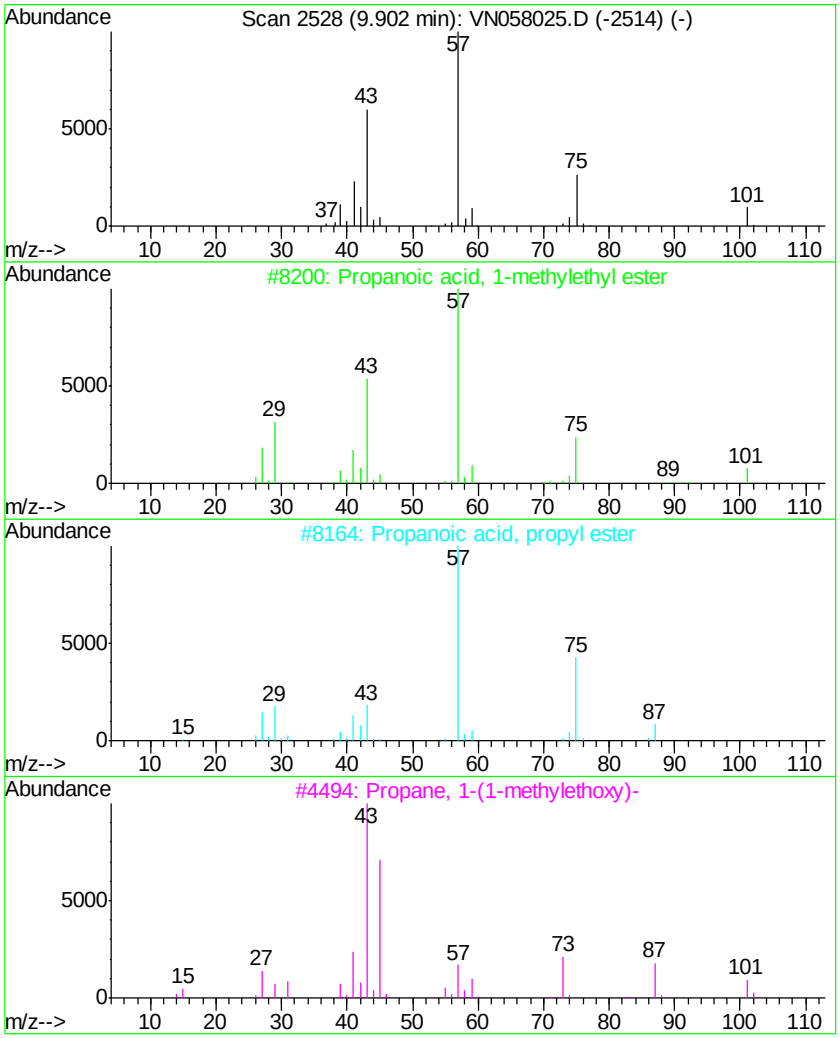
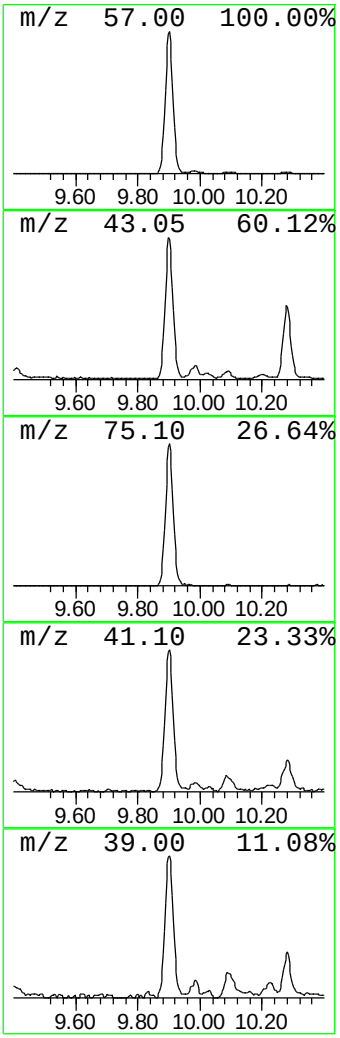
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	18.47 ug/l	407192	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
4	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	17
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10





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Data File : VN058025.D
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Operator : JC/SP
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : T3-2-(1.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

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

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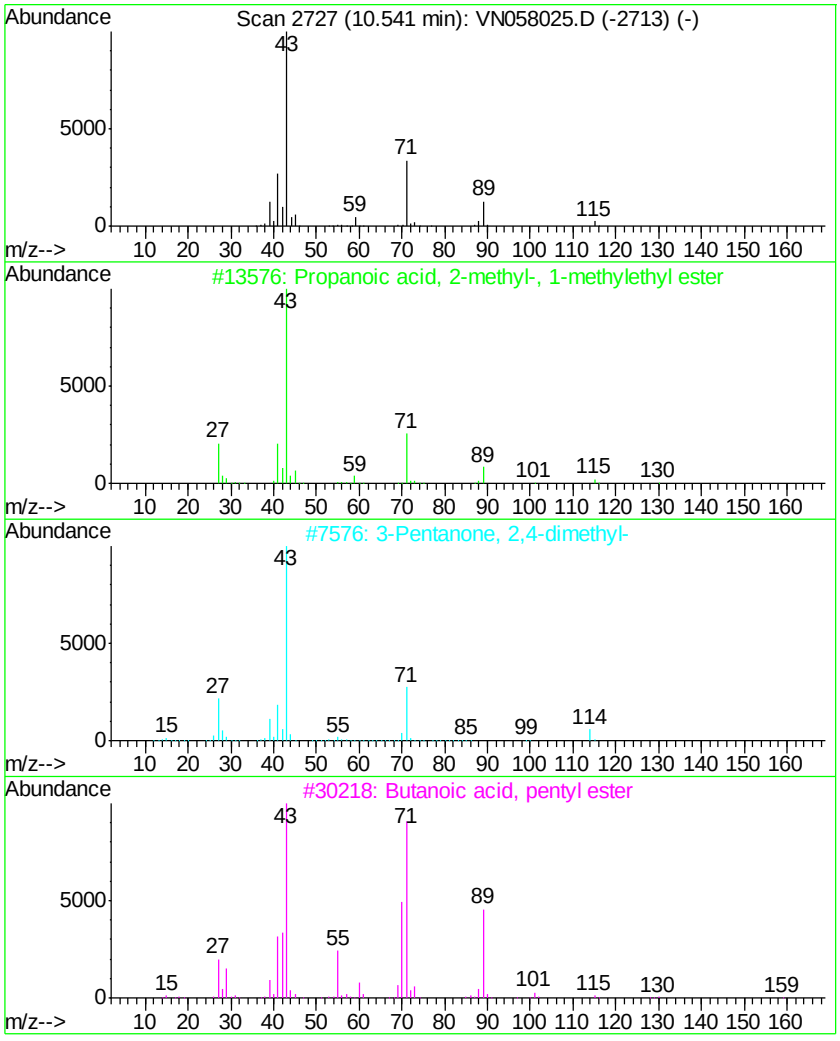
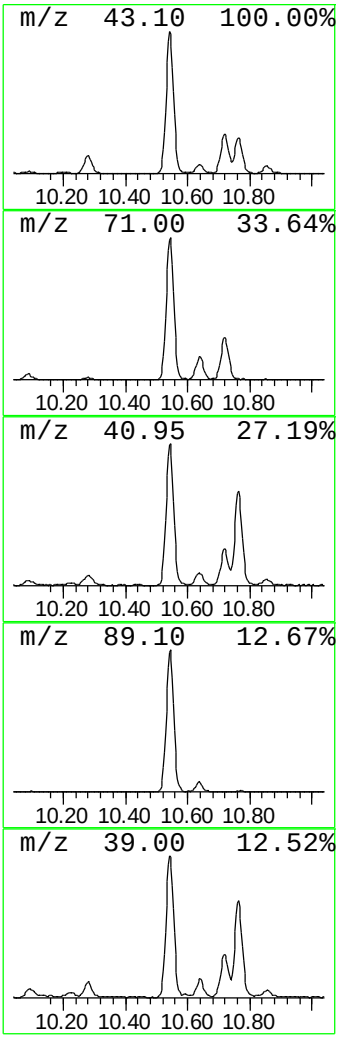
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	29.18 ug/l	804206	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38
4	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	36
5	Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	28





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Data File : VN058025.D
Acq On : 13 Sep 2019 18:39
Operator : JC/SP
Sample : K4680-34
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : T3-2-(1.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

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

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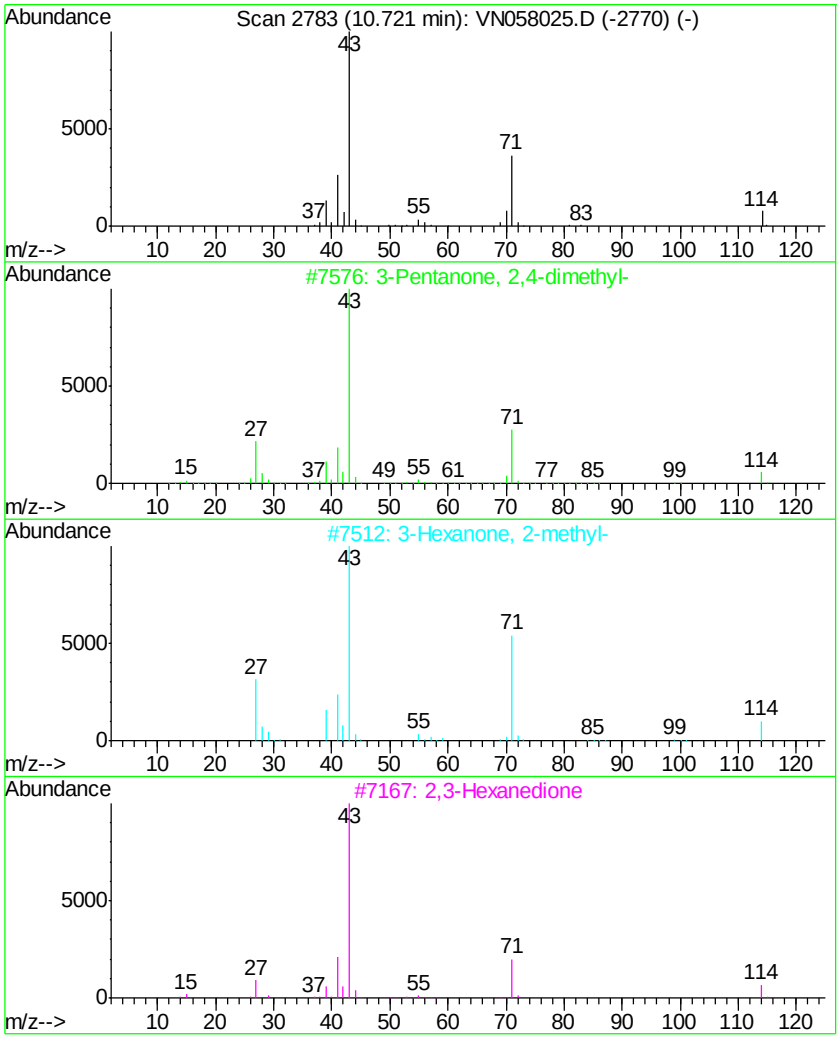
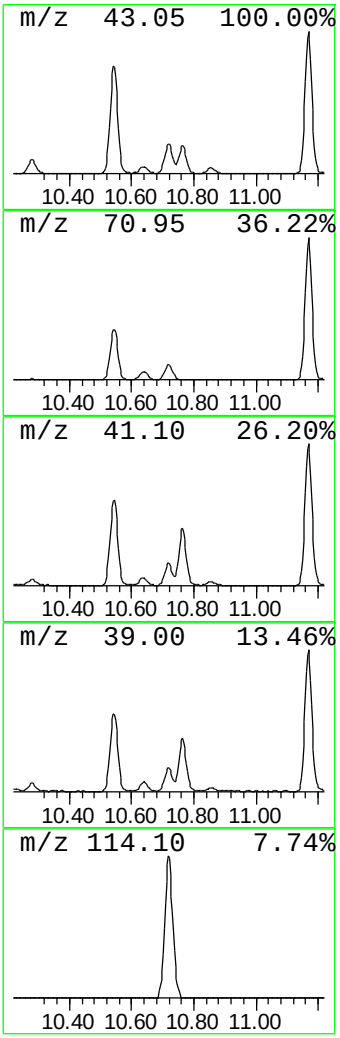
Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	7.93 ug/l	218595	Chlorobenzene-d5	11.41

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	78
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	59
4	Pyrrolidine	71	C4H9N	000123-75-1	59
5	4-Heptanone	114	C7H14O	000123-19-3	53





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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : T3-2-(1.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

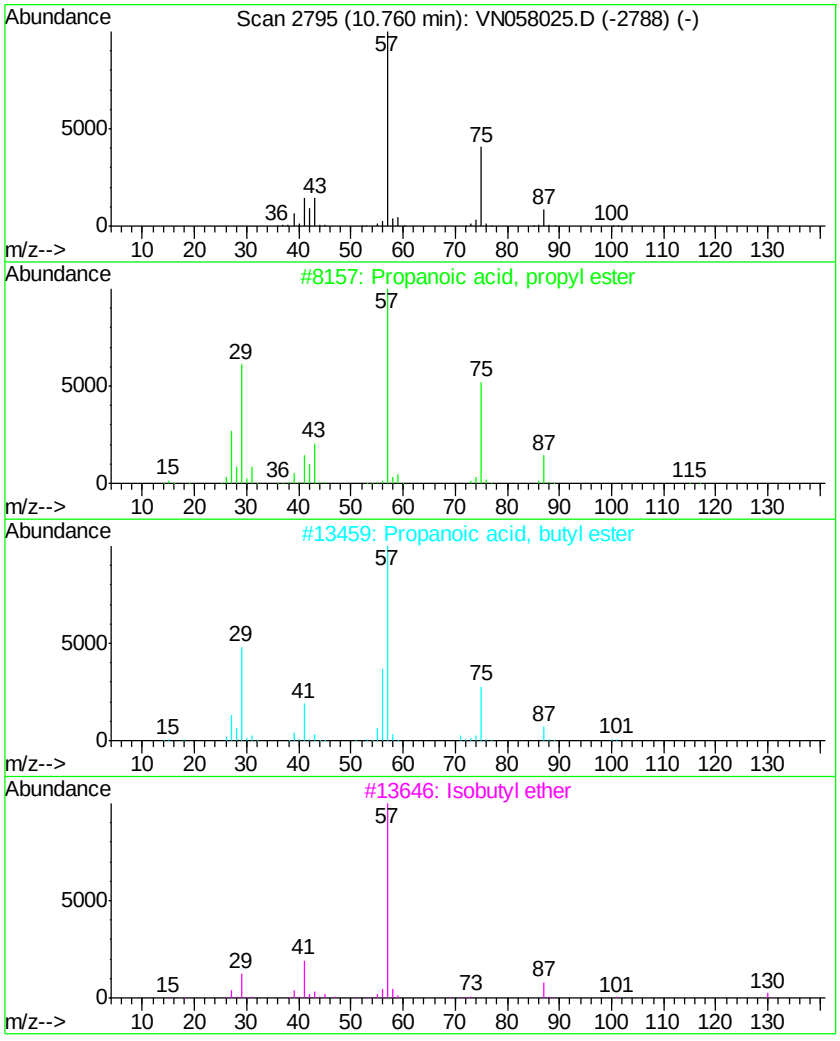
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

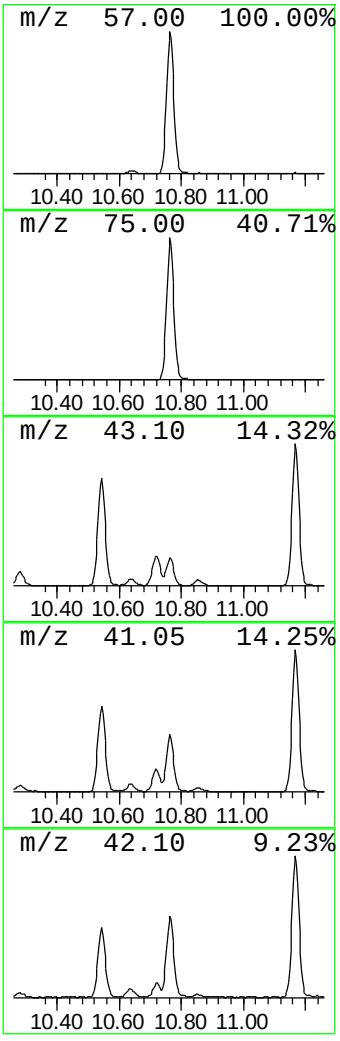
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	33.19 ug/l	914662	Chlorobenzene-d5	11.41

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	38
3	Isobutyl ether	130	C8H18O	000628-55-7	12
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	Trimethylaluminum	72	C3H9Al	000075-24-1	9





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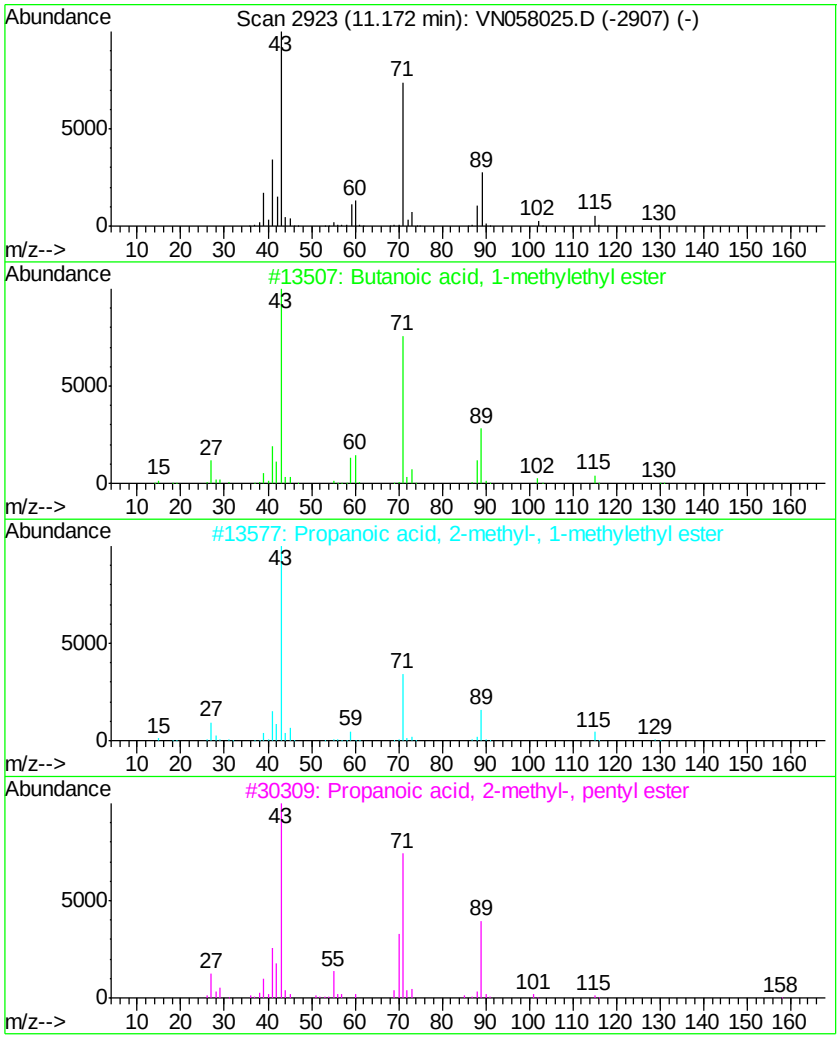
Quant Title : SW846 8260

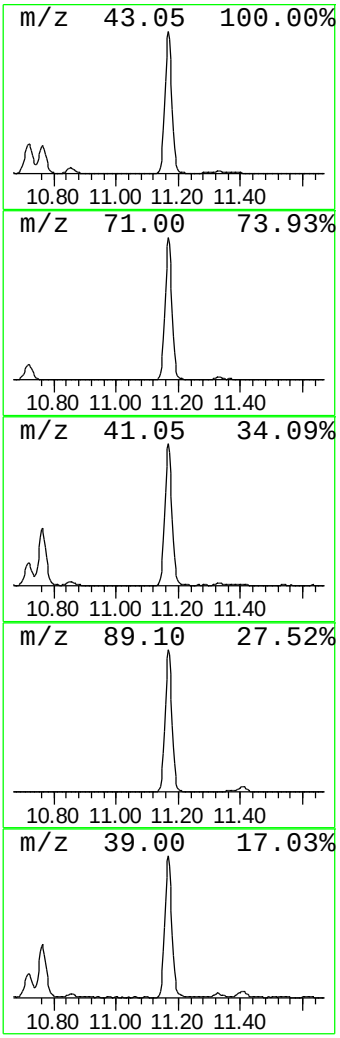
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	53.10 ug/l	1463190	Chlorobenzene-d5	11.41

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-, 1-met...	130	C7H14O2	000617-50-5	78
3	Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64
4	Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN091419\
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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	9.26	111.3	ug/l	2454850	2	8.58	1102400	50.0
Propanoic acid, 1...	9.90	18.5	ug/l	407192	2	8.58	1102400	50.0
Propanoic acid, 2...	10.54	29.2	ug/l	804206	3	11.41	1377880	50.0
3-Pentanone, 2,4-...	10.72	7.9	ug/l	218595	3	11.41	1377880	50.0
Propanoic acid, p...	10.76	33.2	ug/l	914662	3	11.41	1377880	50.0
Butanoic acid, 1-...	11.17	53.1	ug/l	1463190	3	11.41	1377880	50.0