LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
Data File : VN074470.D
Acq On : 15 Sep 2022 18:47
Operator : JC\MD
Sample : N4578-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-3

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\82N091522W.M
Title : SW846 8260

Signal : TIC: VN074470.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	60	rBV	688844	1232102	14.21%	2.690%
2	4.228	389	398	408	rBV2	66157	180901	2.09%	0.395%
3	5.016	518	532	542	rBV2	35419	122083	1.41%	0.267%
4	7.333	919	926	938	rVB2	70889	191828	2.21%	0.419%
5	7.951	1021	1031	1036	rBV	370462	890148	10.27%	1.944%
6	8.016	1036	1042	1052	rVB2	619813	1401709	16.17%	3.061%
7	8.369	1092	1102	1114	rBV2	422106	979880	11.30%	2.140%
8	8.492	1115	1123	1131	rBV	423007	1025899	11.83%	2.240%
9	8.904	1183	1193	1205	rBV	1057633	2109428	24.33%	4.606%
10	9.492	1285	1293	1298	rBV2	228538	498788	5.75%	1.089%
11	9.563	1298	1305	1324	rVV	4829831	8668653	100.00%	18.929%
12	10.186	1403	1411	1420	rBV	880385	1513979	17.46%	3.306%
13	10.380	1436	1444	1455	rBV	1494341	2779380	32.06%	6.069%
14	10.557	1467	1474	1485	rVB	1193922	1974090	22.77%	4.311%
15	10.816	1511	1518	1526	rBV	1202917	1984928	22.90%	4.334%
16	10.910	1528	1534	1541	rVV2	258346	457893	5.28%	1.000%
17	10.998	1543	1549	1551	rVV	481017	785185	9.06%	1.715%
18	11.033	1551	1555	1564	rVV	1894735	3064968	35.36%	6.693%
19	11.121	1564	1570	1586	rVB	1370088	2251367	25.97%	4.916%
20	11.433	1615	1623	1633	rBV	3612232	5552459	64.05%	12.124%
21	11.598	1646	1651	1658	rVB4	54685	94531	1.09%	0.206%
22	11.686	1658	1666	1678	rVB	1657511	2882730	33.25%	6.295%
23	12.139	1737	1743	1752	rBV	267909	427250	4.93%	0.933%
24	12.674	1825	1834	1845	rBV	1276870	2123824	24.50%	4.638%
25	13.615	1983	1994	2005	rBV	1546982	2602475	30.02%	5.683%

Sum of corrected areas: 45796478

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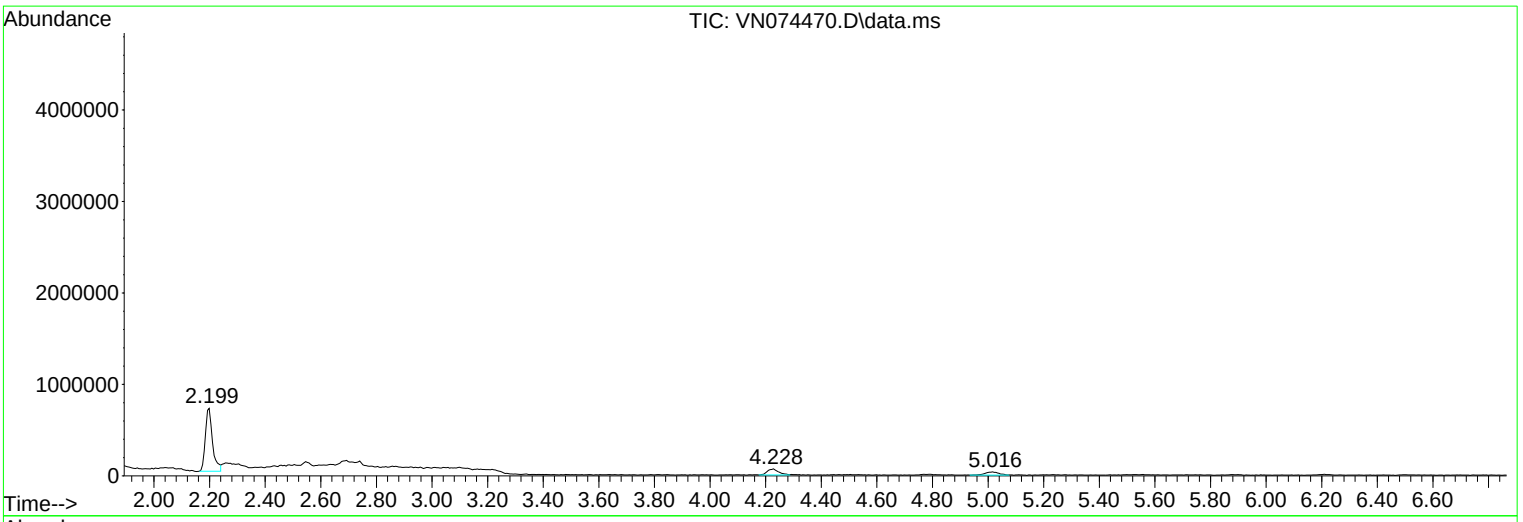
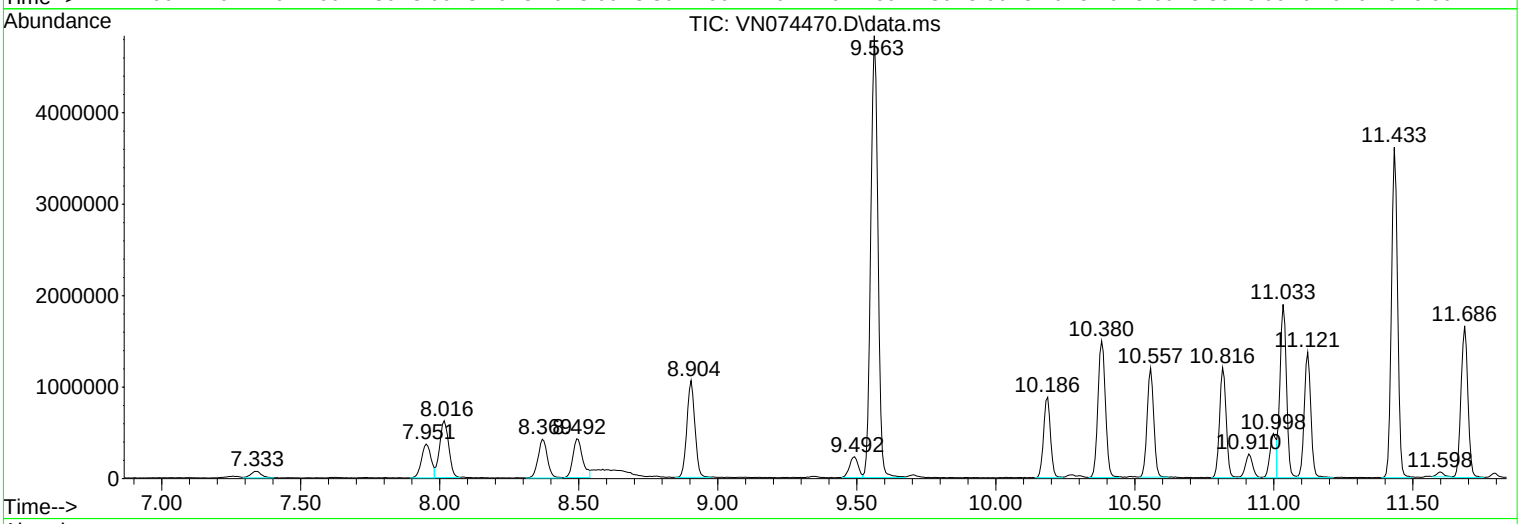
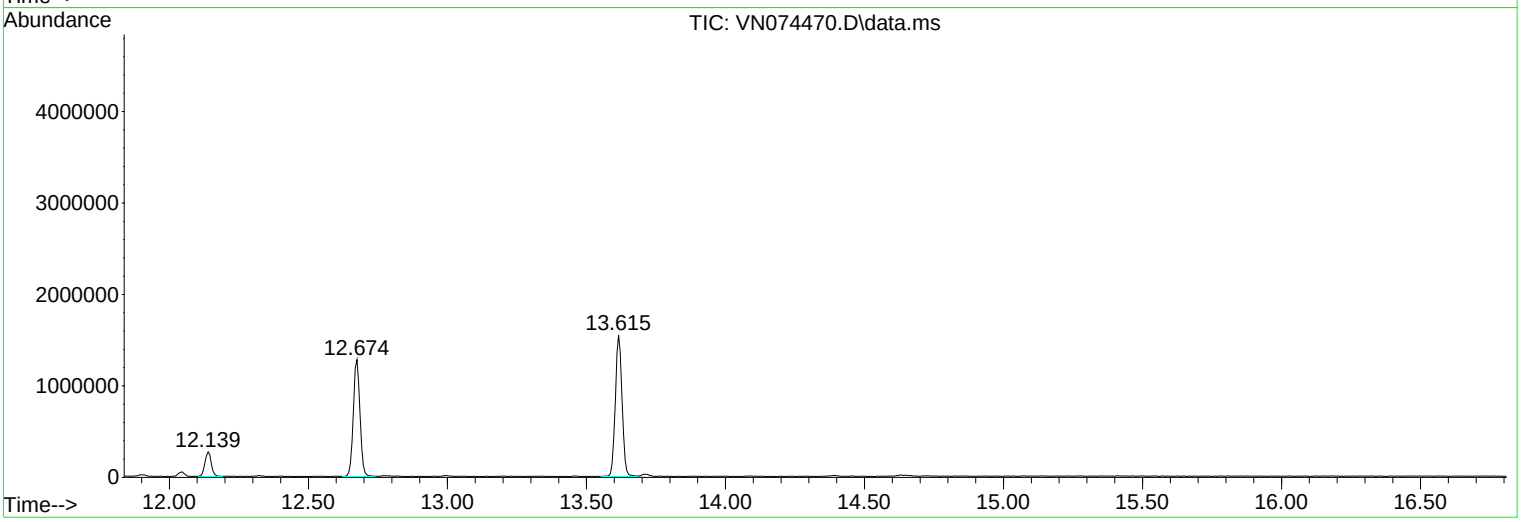
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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







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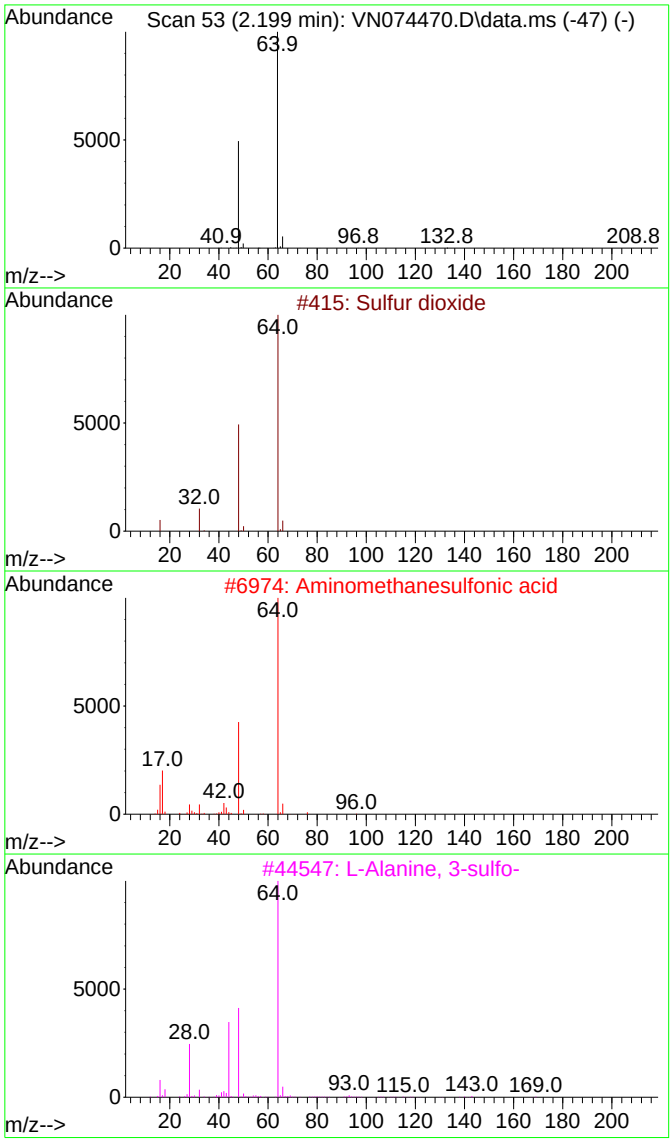
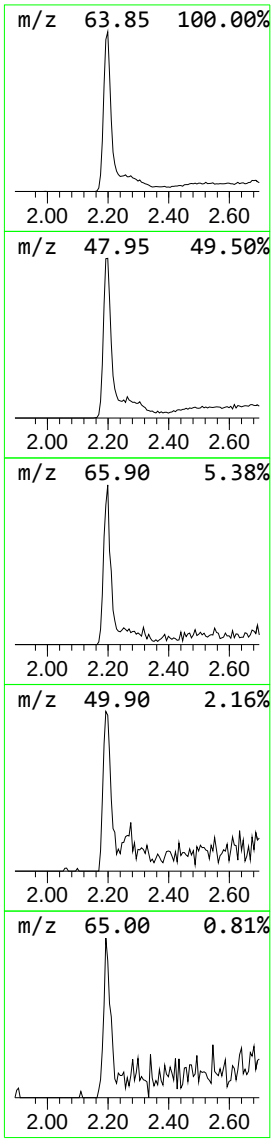
****

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	43.95 ug/l	1232100	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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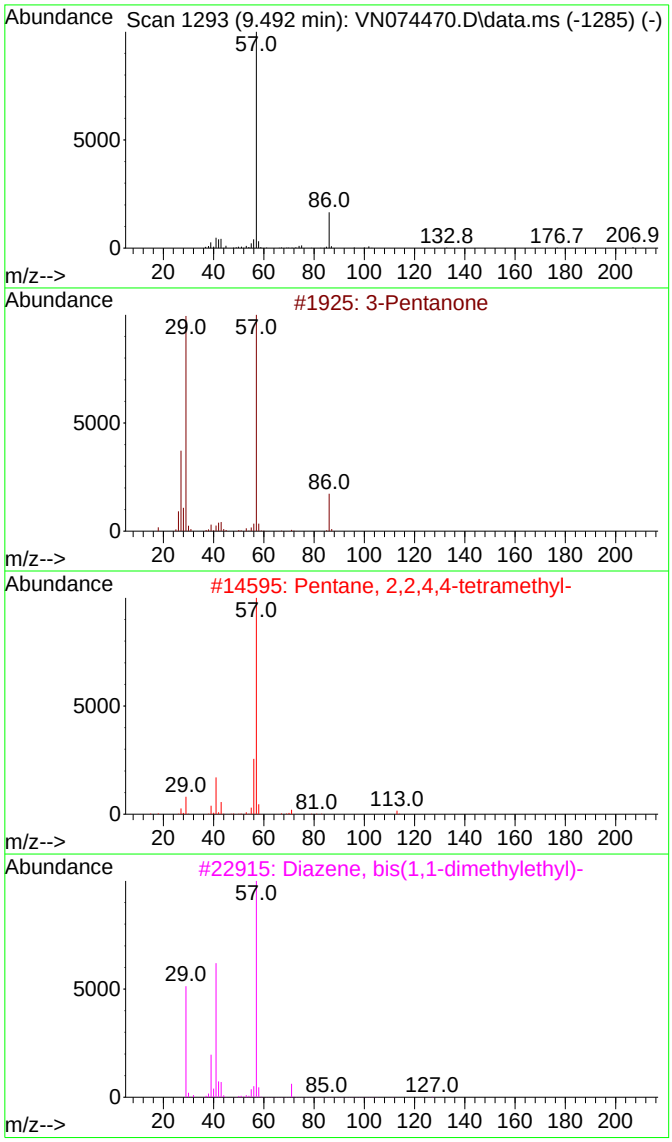
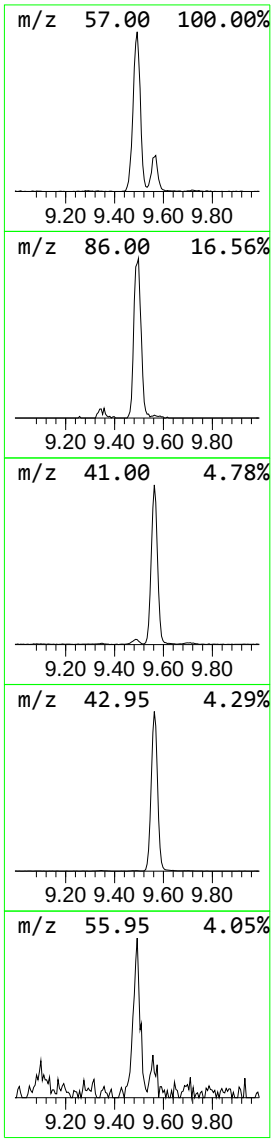
****
Peak Number 2 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.492	11.82 ug/l	498788	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	64
2	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	9
3	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	9
4	Sulfurous acid, butyl isobutyl e...	194	C8H18O3S	1010309-17-0	9
5	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	9





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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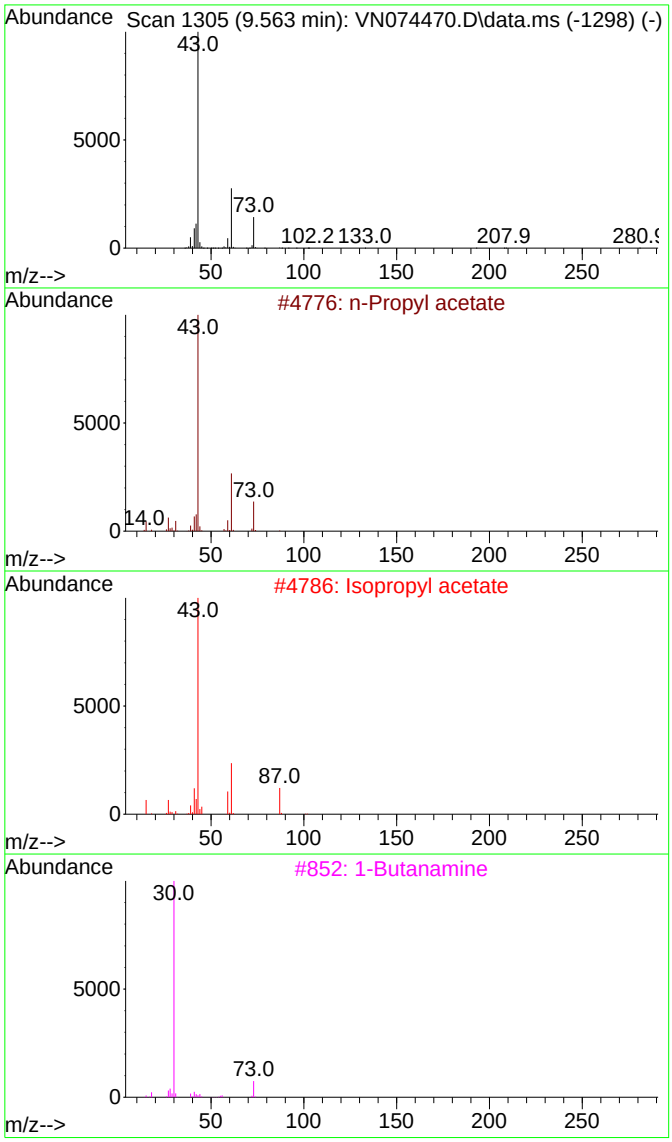
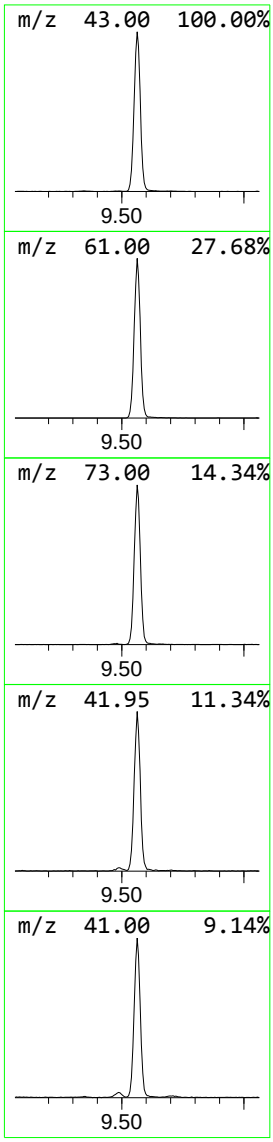
****

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.563	205.47 ug/l	8668650	1,4-Difluorobenzene	8.904

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	9
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4





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Instrument :
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ClientSampleId :
CHERRY-HILL-COMP-3

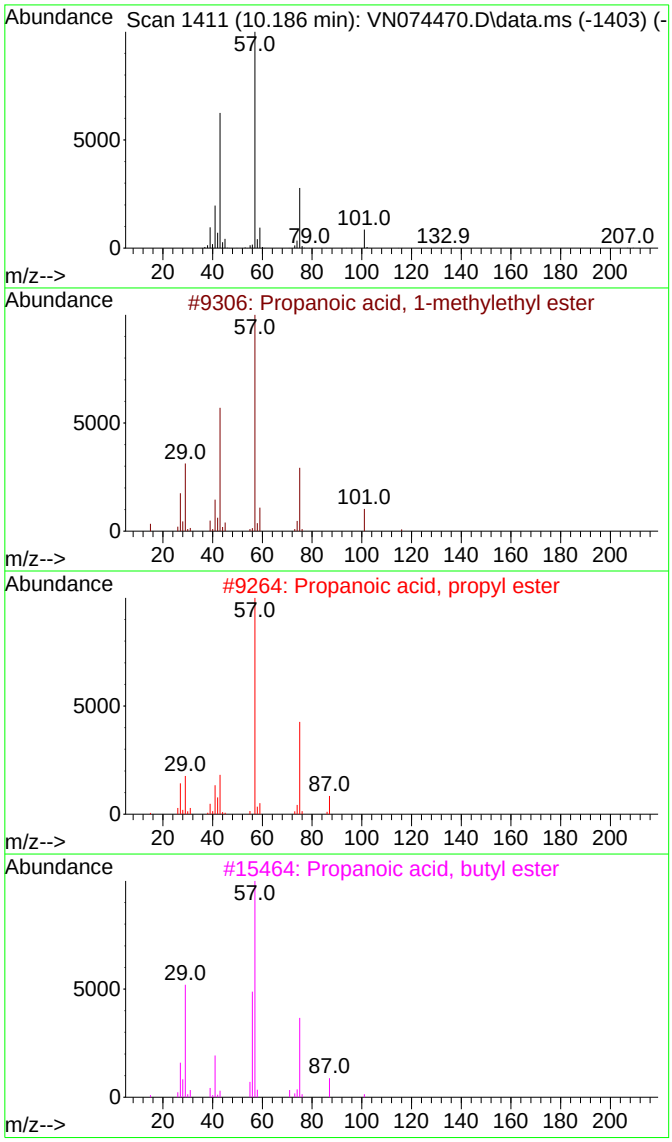
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

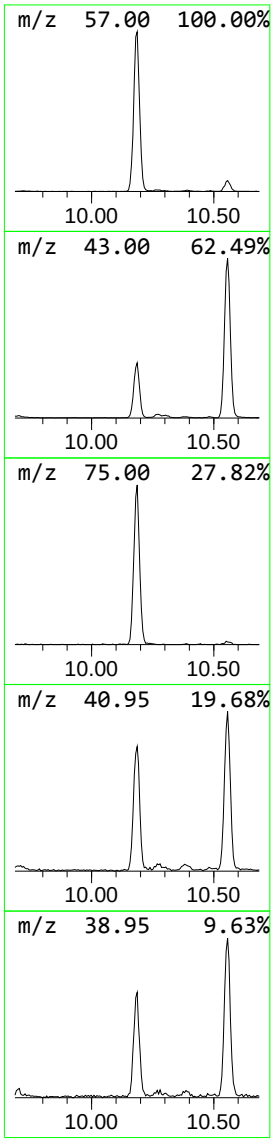
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.186	35.89 ug/l	1513980	1,4-Difluorobenzene	8.904

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	59
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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ALS Vial : 20 Sample Multiplier: 1

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TIC Library : C:\Database\NIST20.L
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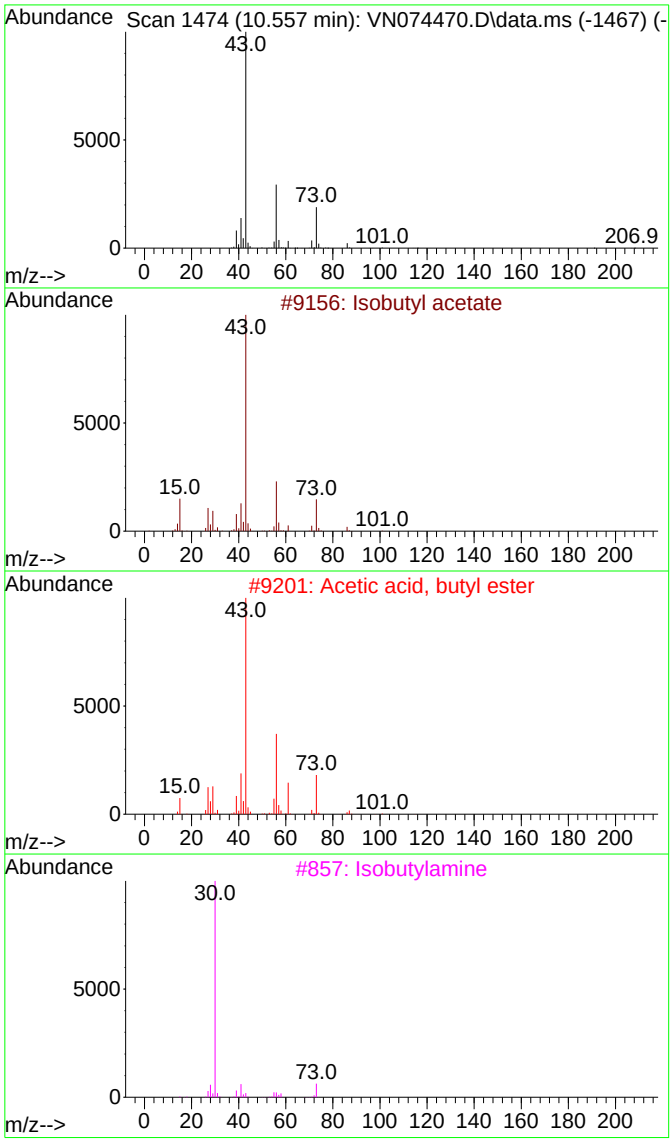
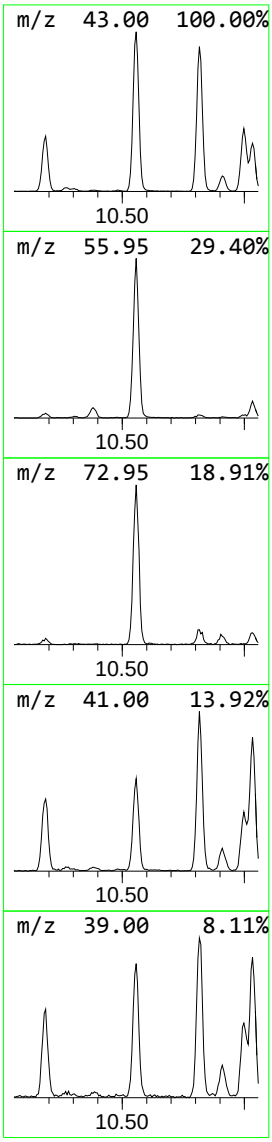
****

Peak Number 5 Isobutyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	34.24 ug/l	1974090	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9





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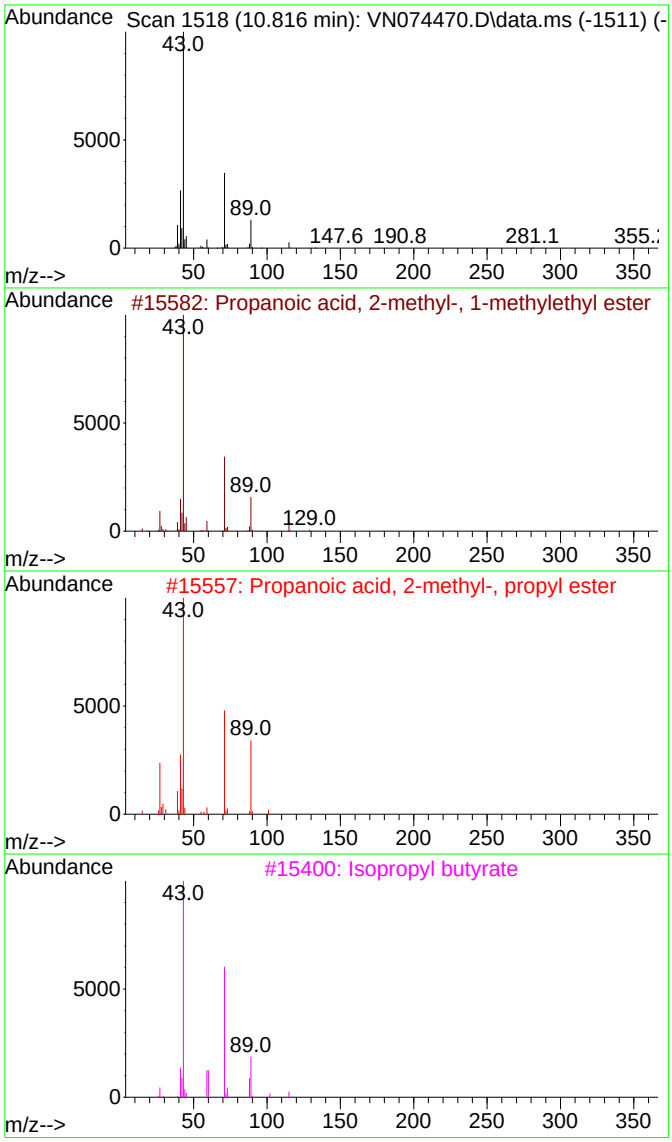
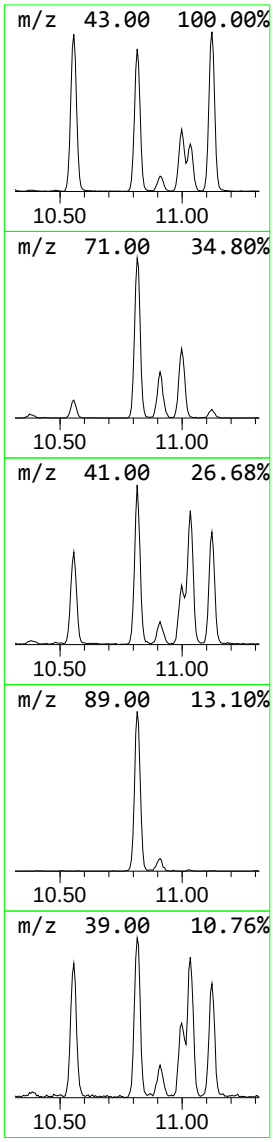
****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	34.43 ug/l	1984930	Chlorobenzene-d5	11.686

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	Isopropyl butyrate	130	C7H14O2	000638-11-9	56
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	42
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	42





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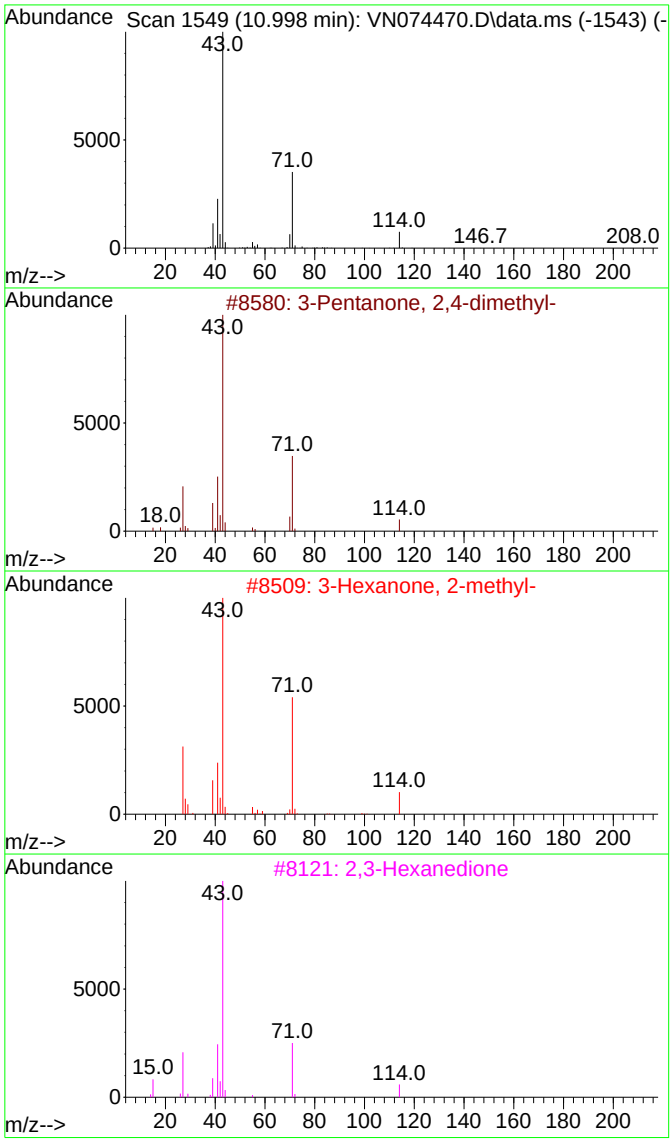
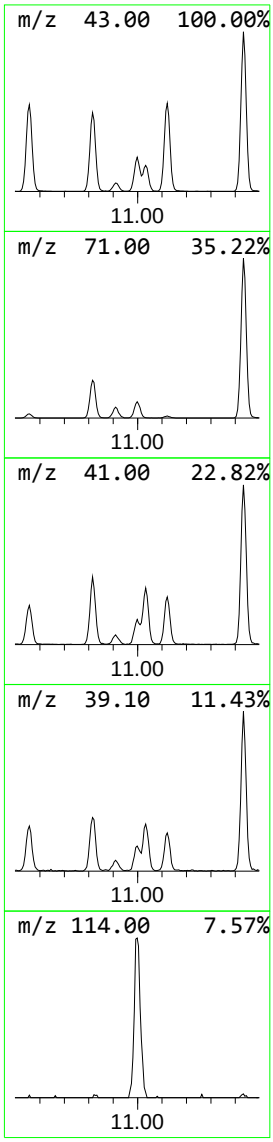
****
Peak Number 7 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.998	13.62 ug/l	785185	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	59
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	47
4	4-Heptanone	114	C7H14O	000123-19-3	9
5	2,4-Pentanedione, 3-methyl-	114	C6H10O2	000815-57-6	9





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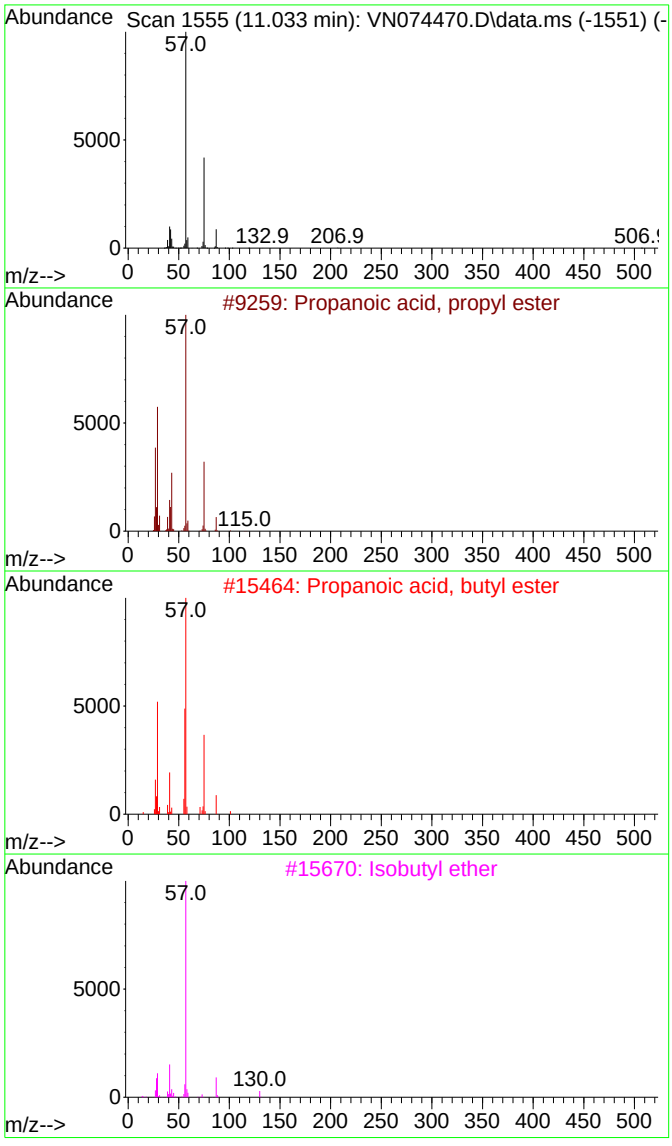
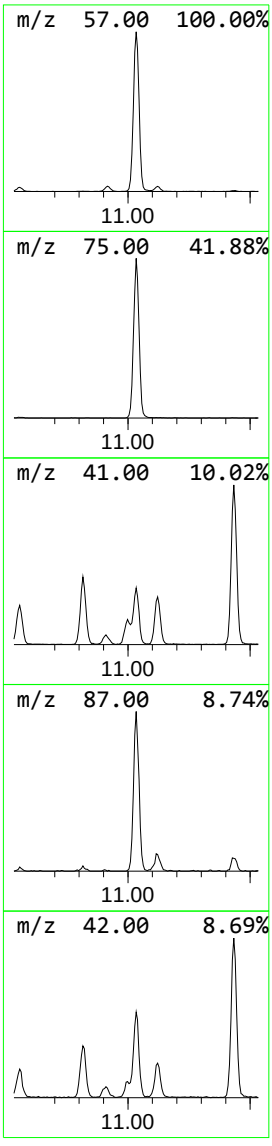
****
Peak Number 8 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.033	53.16 ug/l	3064970	Chlorobenzene-d5	11.686

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	39
3	Isobutyl ether	130	C8H18O	000628-55-7	9
4	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
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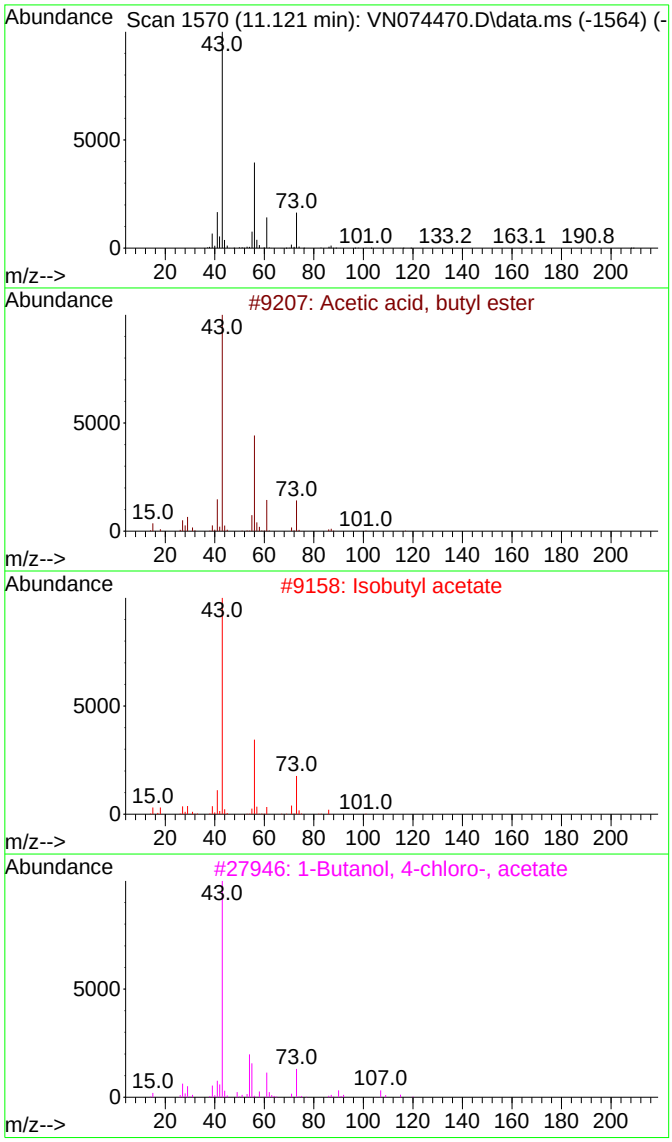
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

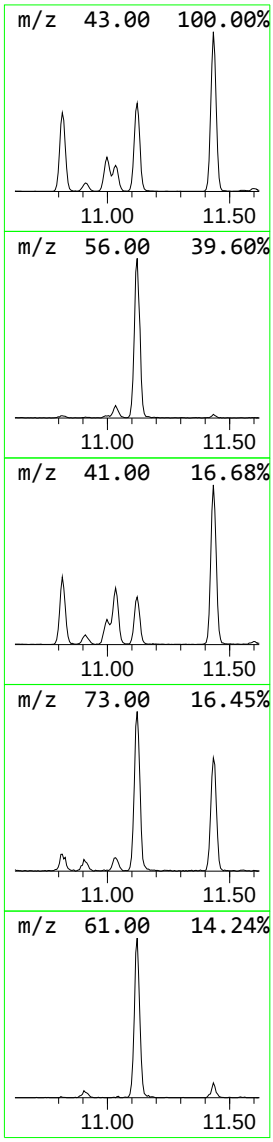
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.121	39.05 ug/l	2251370	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	Guanidine, methyl-	73	C2H7N3	000471-29-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
Data File : VN074470.D
Acq On : 15 Sep 2022 18:47
Operator : JC\MD
Sample : N4578-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-3

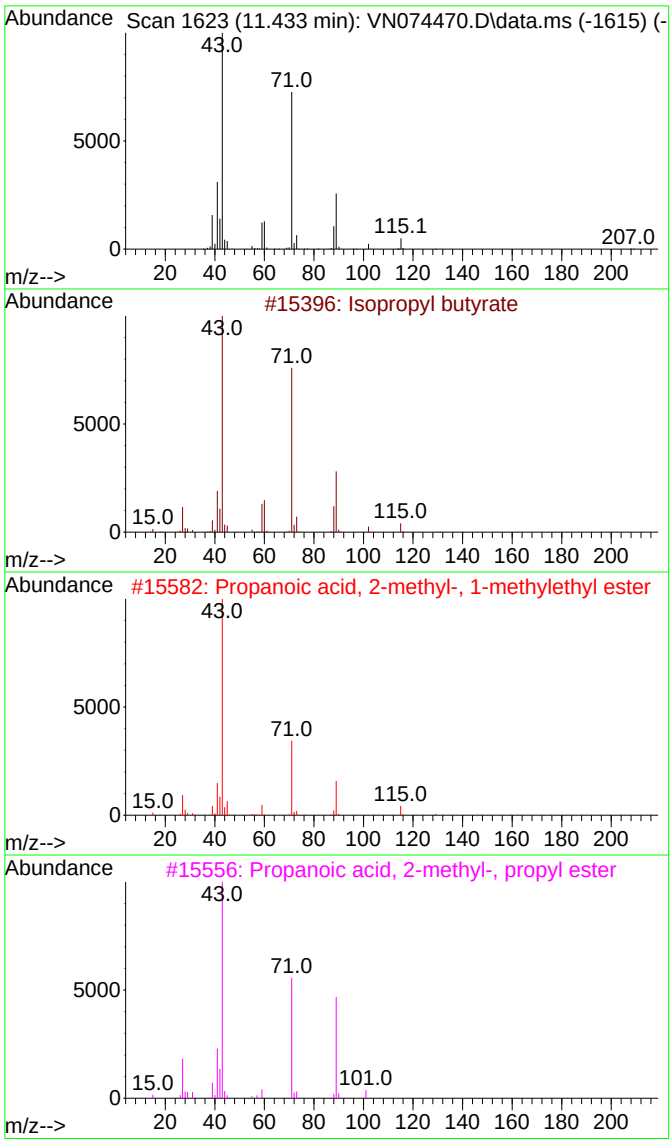
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

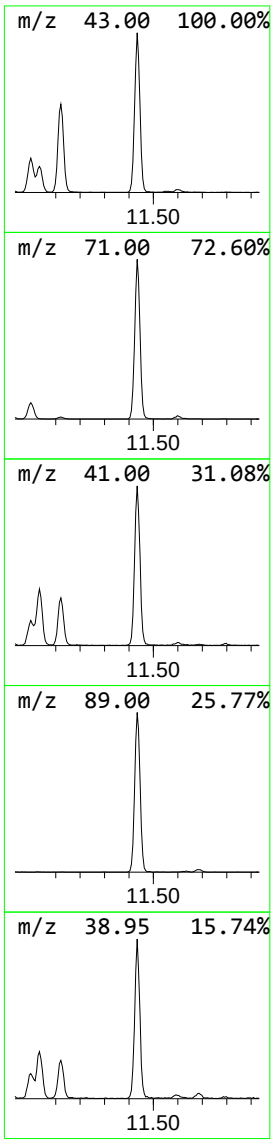
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.433	96.31 ug/l	5552460	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
Data File : VN074470.D
Acq On : 15 Sep 2022 18:47
Operator : JC\MD
Sample : N4578-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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
Sulfur dioxide	2.199	44.0	ug/l	1232100	1	8.016	1401710	50.0
3-Pentanone	9.492	11.8	ug/l	498788	2	8.904	2109430	50.0
n-Propyl acetate	9.563	205.5	ug/l	8668650	2	8.904	2109430	50.0
Propanoic acid,...	10.186	35.9	ug/l	1513980	2	8.904	2109430	50.0
Isobutyl acetate	10.557	34.2	ug/l	1974090	3	11.686	2882730	50.0
Propanoic acid,...	10.816	34.4	ug/l	1984930	3	11.686	2882730	50.0
3-Pentanone, 2,...	10.998	13.6	ug/l	785185	3	11.686	2882730	50.0
Propanoic acid,...	11.033	53.2	ug/l	3064970	3	11.686	2882730	50.0
Acetic acid, bu...	11.121	39.0	ug/l	2251370	3	11.686	2882730	50.0
Isopropyl butyrate	11.433	96.3	ug/l	5552460	3	11.686	2882730	50.0