LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
Data File : VN074469.D
Acq On : 15 Sep 2022 18:22
Operator : JC\MD
Sample : N4578-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-2

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: VN074469.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	46	52	61	rBV	913492	1648030	18.51%	3.458%
2	4.222	387	397	408	rBV	48088	145812	1.64%	0.306%
3	5.016	522	532	544	rVB3	35972	114034	1.28%	0.239%
4	7.339	920	927	936	rVB2	72485	168279	1.89%	0.353%
5	7.951	1020	1031	1036	rBV2	380727	906753	10.18%	1.903%
6	8.016	1036	1042	1053	rVB	641214	1428041	16.04%	2.996%
7	8.369	1093	1102	1115	rBV	426165	986998	11.09%	2.071%
8	8.492	1115	1123	1131	rBV	428203	998140	11.21%	2.094%
9	8.904	1184	1193	1203	rBV	1057256	2136015	23.99%	4.482%
10	9.492	1283	1293	1298	rBV	249338	523093	5.88%	1.098%
11	9.563	1298	1305	1324	rVV	5042584	8903286	100.00%	18.682%
12	10.186	1403	1411	1419	rBV	899475	1559431	17.52%	3.272%
13	10.380	1436	1444	1453	rBV	1591663	2852686	32.04%	5.986%
14	10.557	1466	1474	1491	rVB	1206286	2019505	22.68%	4.237%
15	10.816	1510	1518	1527	rBV	1266463	2079692	23.36%	4.364%
16	10.910	1527	1534	1542	rVV2	271211	489200	5.49%	1.026%
17	10.998	1542	1549	1551	rVV	482338	807026	9.06%	1.693%
18	11.033	1551	1555	1563	rVV	2038494	3231630	36.30%	6.781%
19	11.121	1563	1570	1582	rVB	1440037	2288734	25.71%	4.802%
20	11.433	1615	1623	1635	rBV	3681953	5747208	64.55%	12.059%
21	11.598	1646	1651	1659	rVV3	53886	98982	1.11%	0.208%
22	11.686	1659	1666	1677	rVV	1742649	2961372	33.26%	6.214%
23	12.045	1721	1727	1733	rBV2	54145	93705	1.05%	0.197%
24	12.139	1736	1743	1750	rBV	303190	486568	5.47%	1.021%
25	12.674	1826	1834	1846	rBV	1317359	2214076	24.87%	4.646%
26	13.615	1985	1994	2005	rBV	1640560	2769691	31.11%	5.812%

Sum of corrected areas: 47657987

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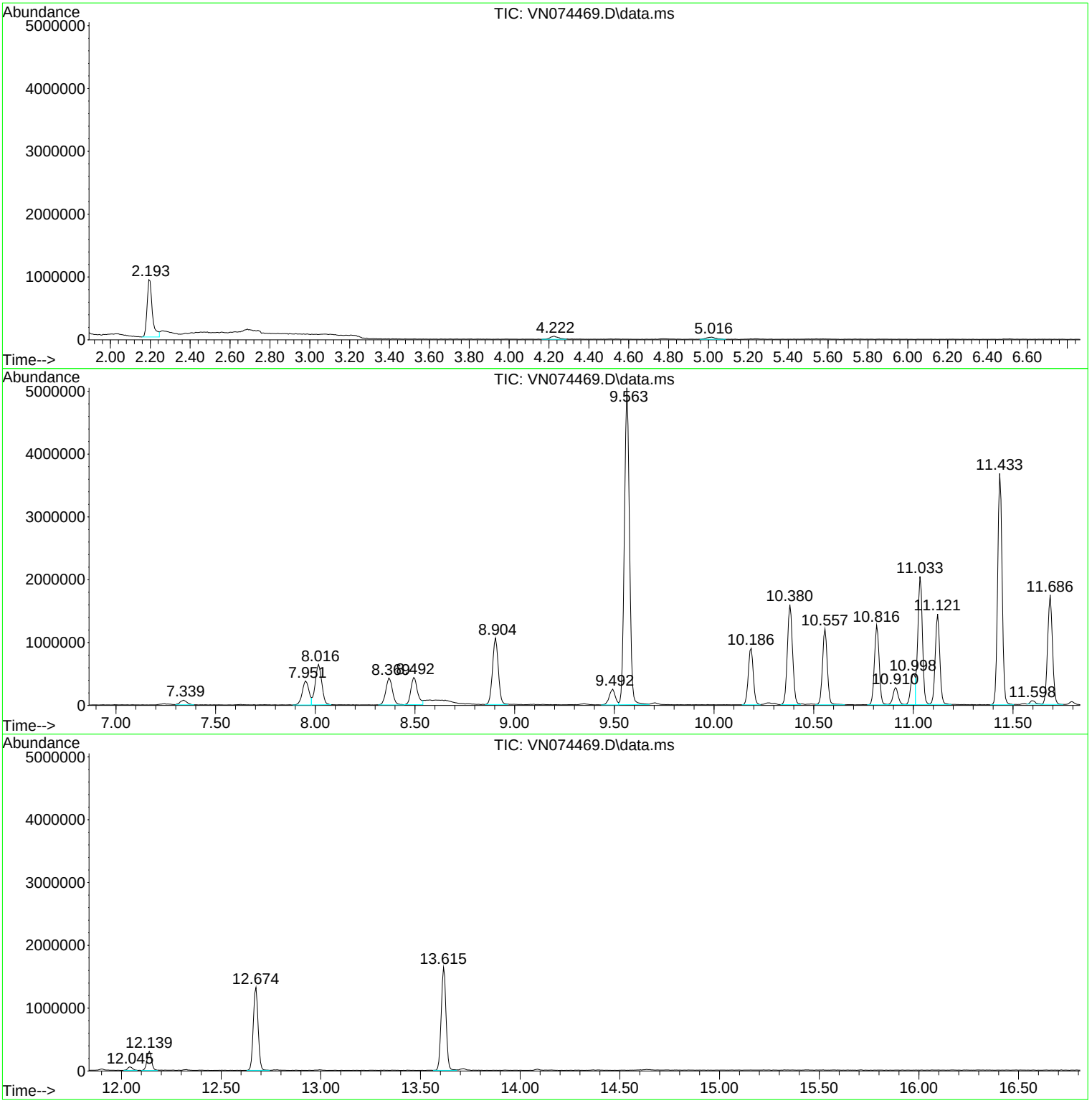
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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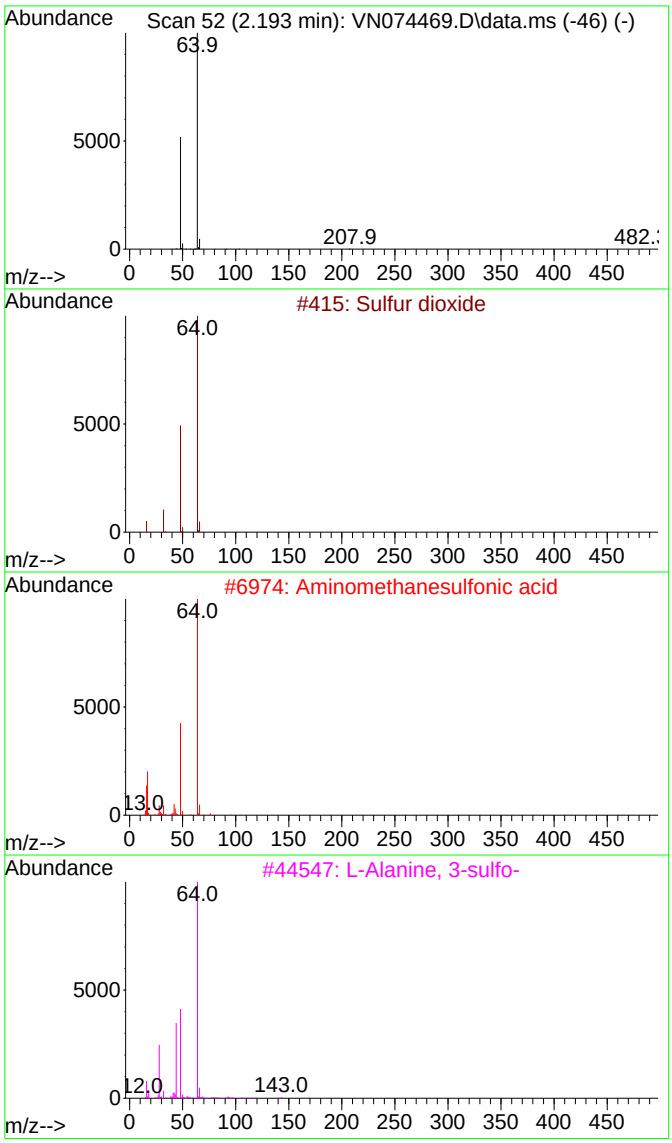
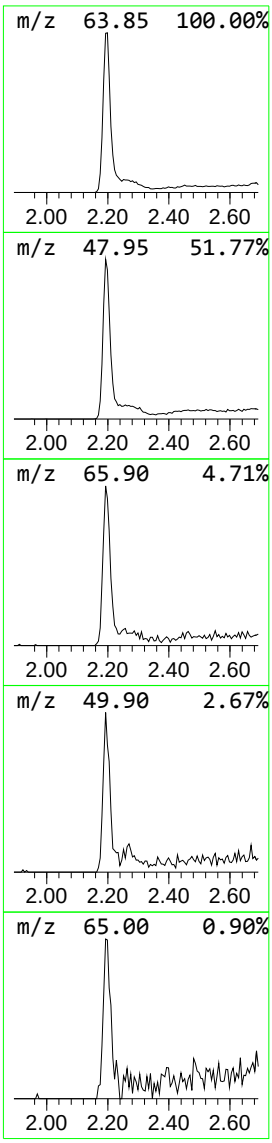
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	57.70 ug/l	1648030	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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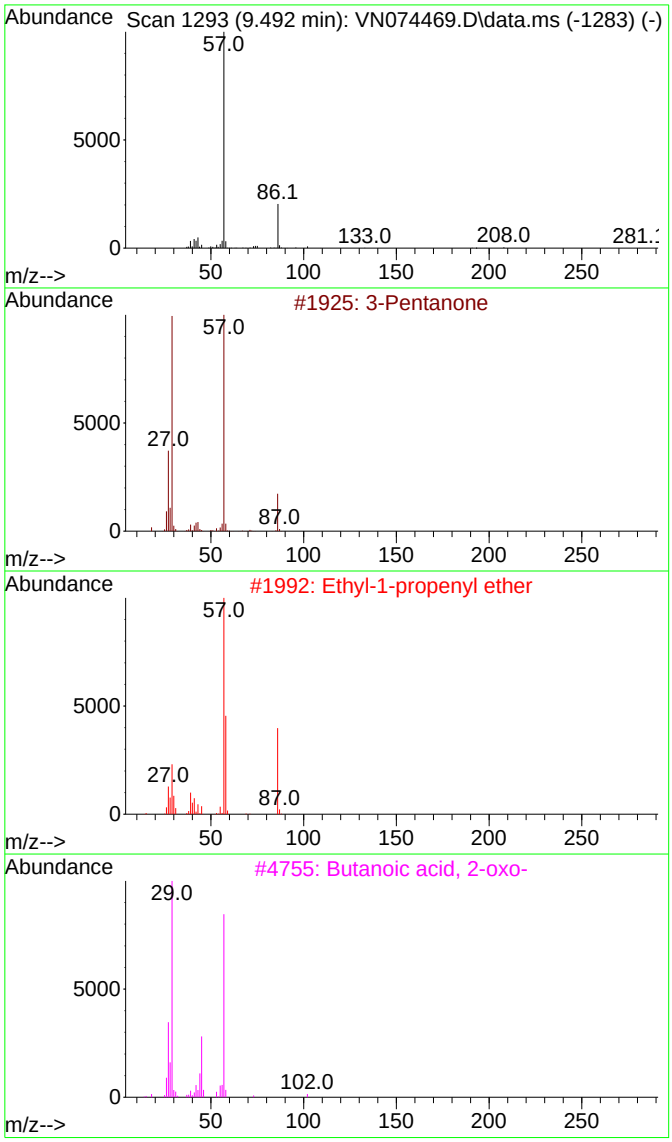
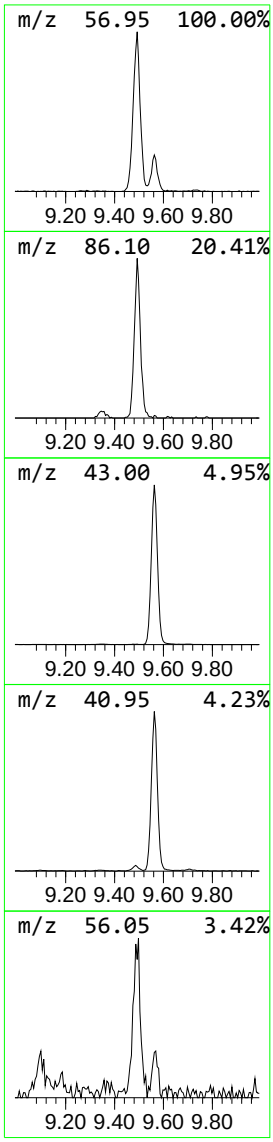
****
Peak Number 2 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.492	12.24 ug/l	523093	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	64
2	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
3	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9
4	Propanoic acid, anhydride	130	C6H10O3	000123-62-6	9
5	Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	9





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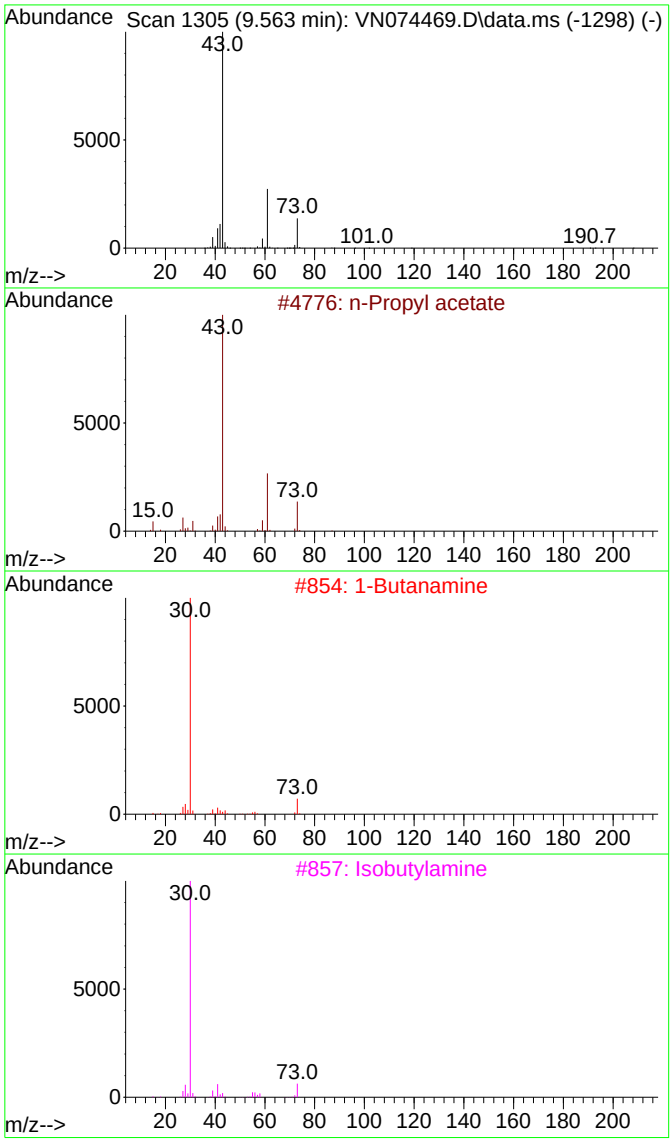
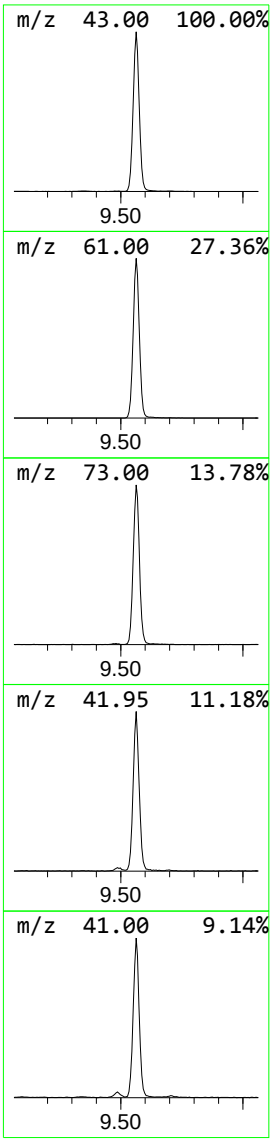
****
Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.563	208.41 ug/l	8903290	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	1-Butanamine	73	C4H11N	000109-73-9	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
5	Isobutyl acetate	116	C6H12O2	000110-19-0	4





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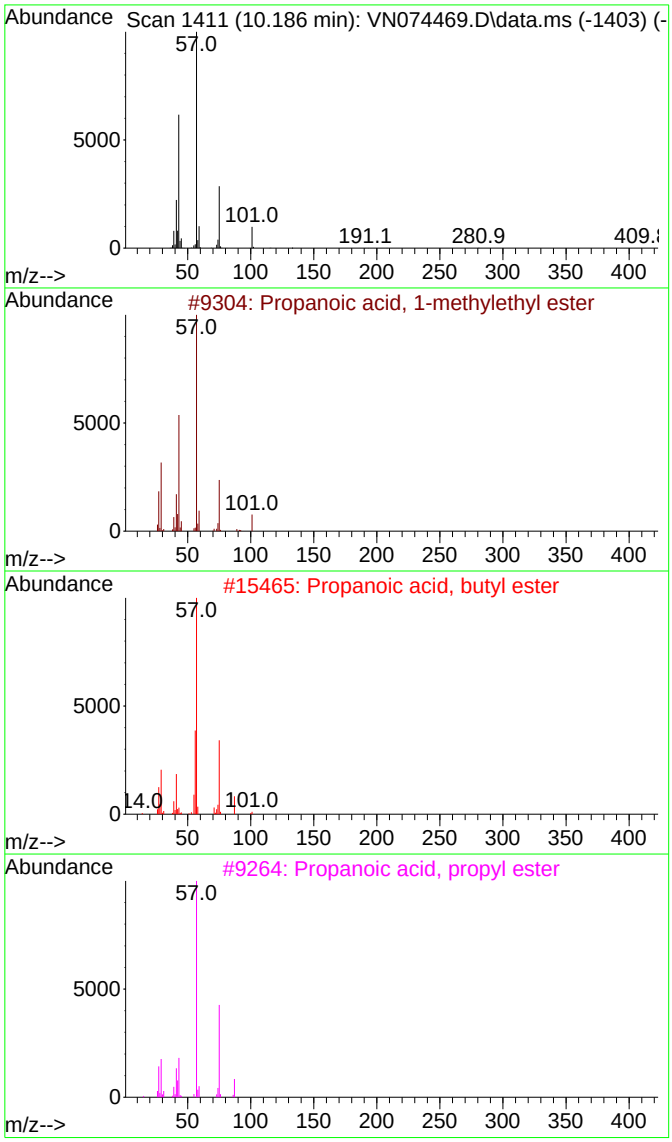
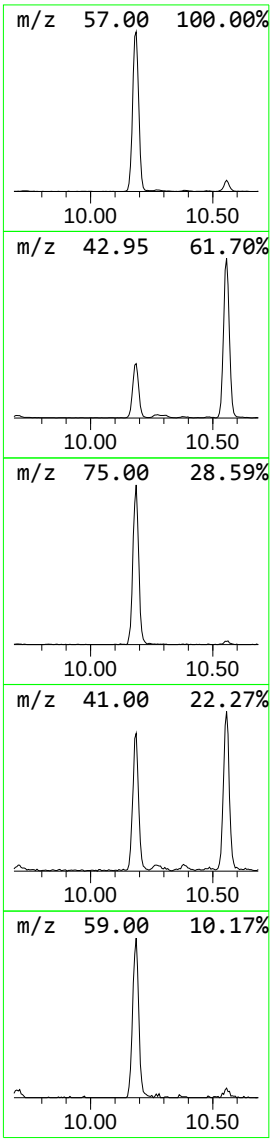
****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.186	36.50 ug/l	1559430	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	90
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	33
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	9





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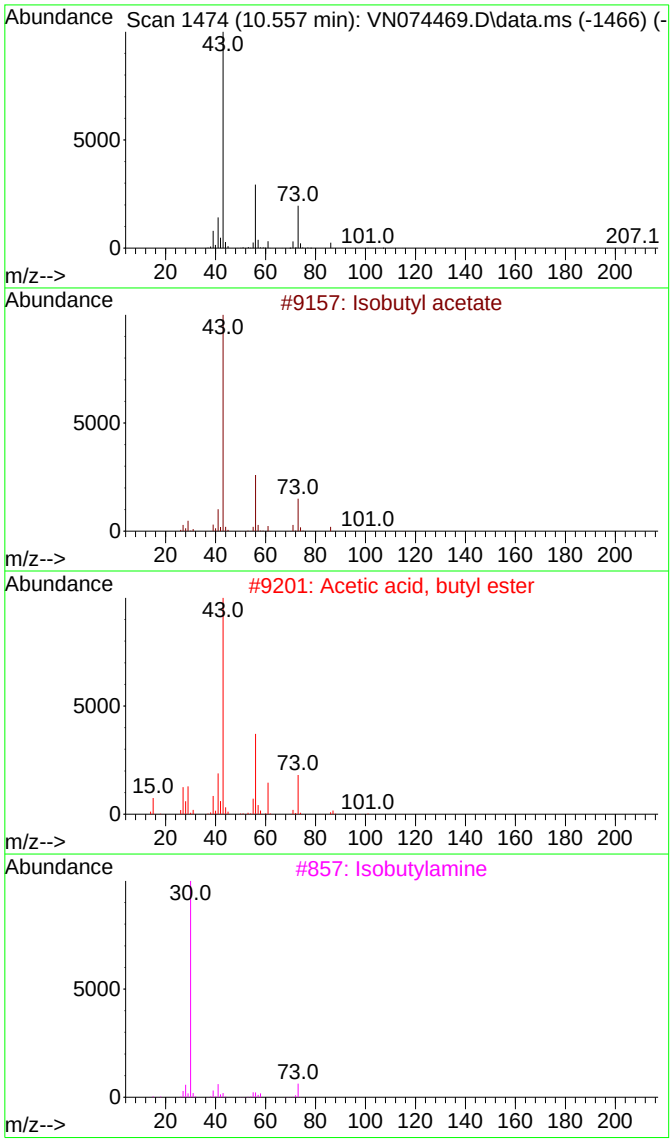
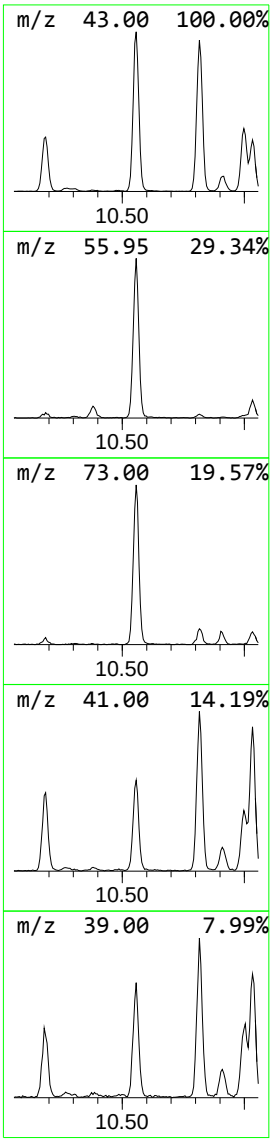
****
Peak Number 5 Isobutyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	34.10 ug/l	2019510	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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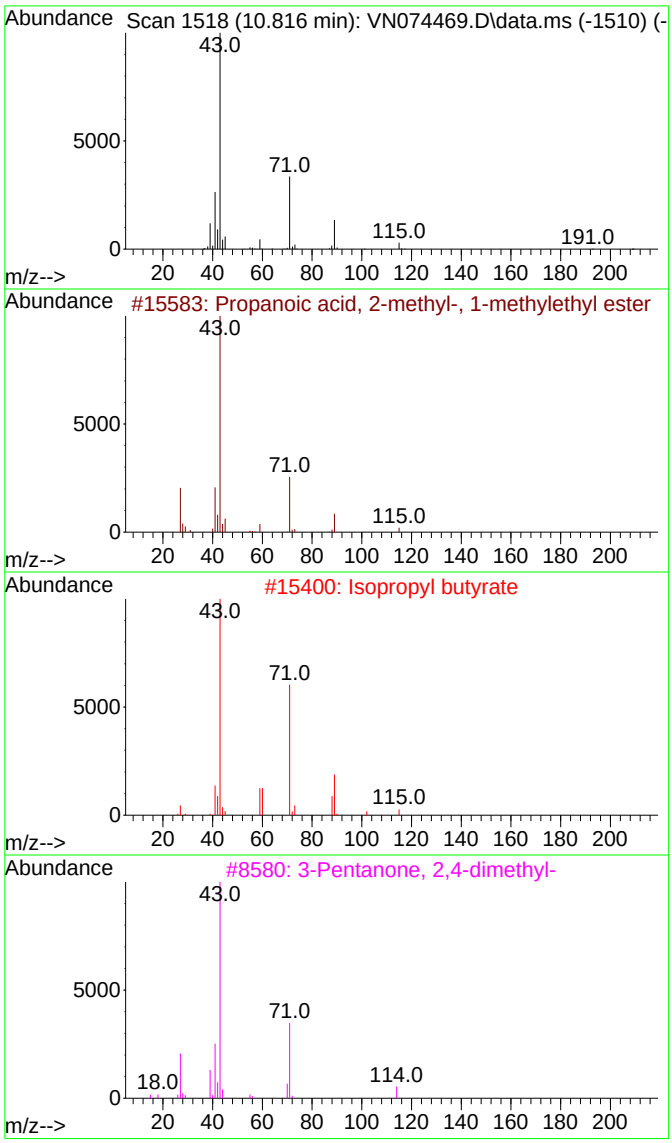
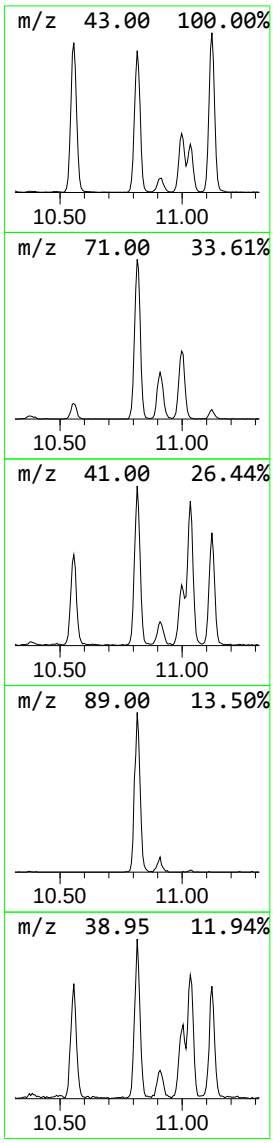
****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	35.11 ug/l	2079690	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	Isopropyl butyrate	130	C7H14O2	000638-11-9	56
3	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	38
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38





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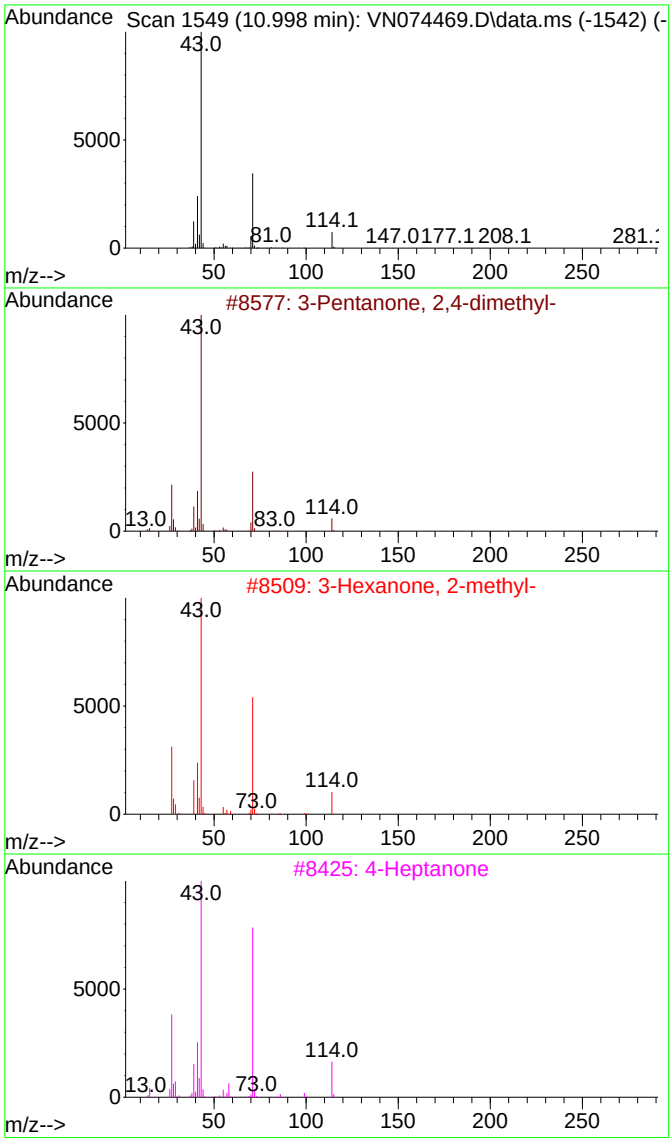
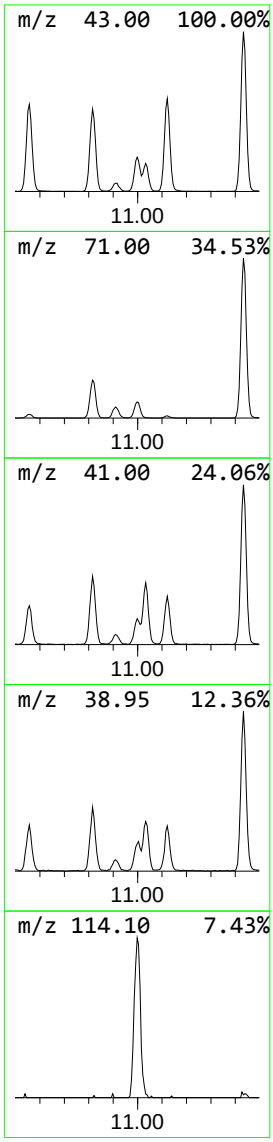
****
Peak Number 7 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.998	13.63 ug/l	807026	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	4-Heptanone	114	C7H14O	000123-19-3	47
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	47
5	2,5-Hexanedione	114	C6H10O2	000110-13-4	38





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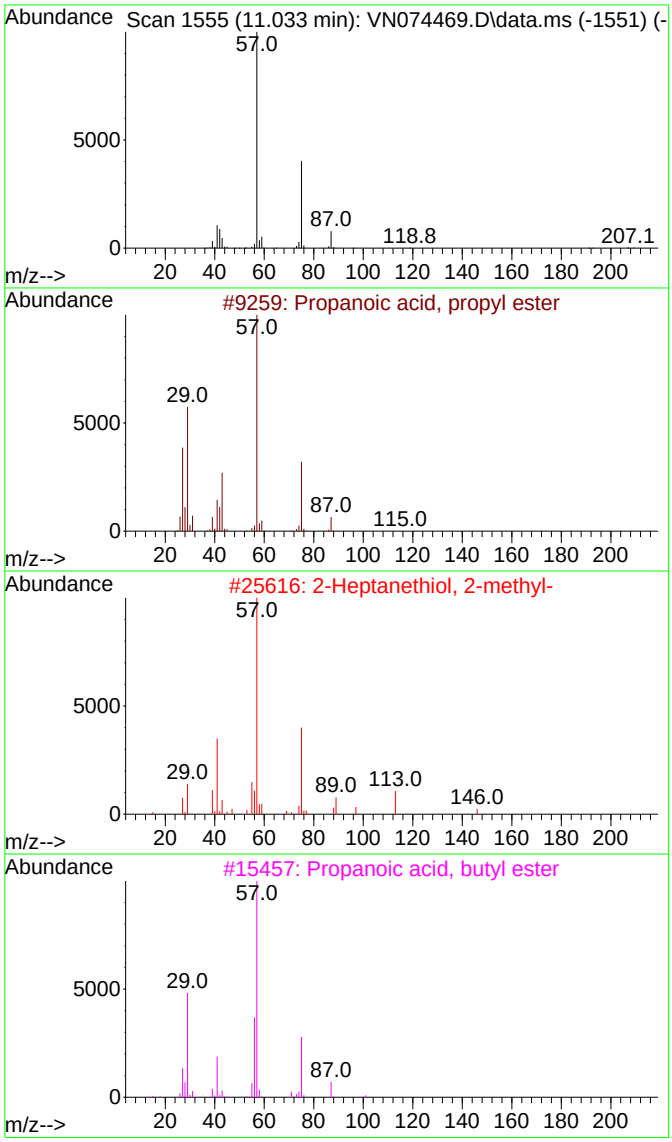
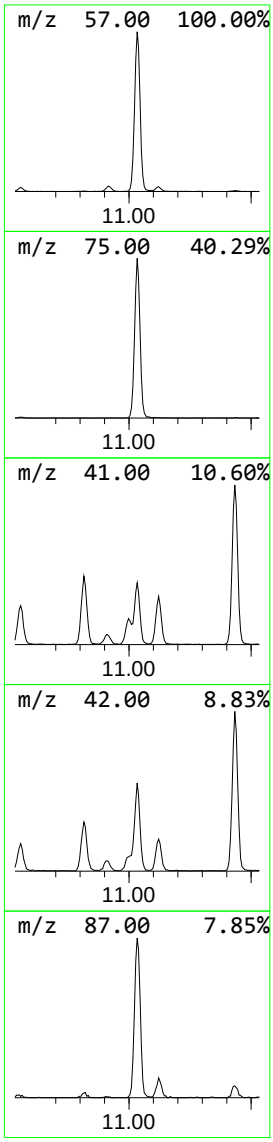
****
Peak Number 8 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.033	54.56 ug/l	3231630	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	2-Heptanethiol, 2-methyl-	146	C8H18S	000763-20-2	39
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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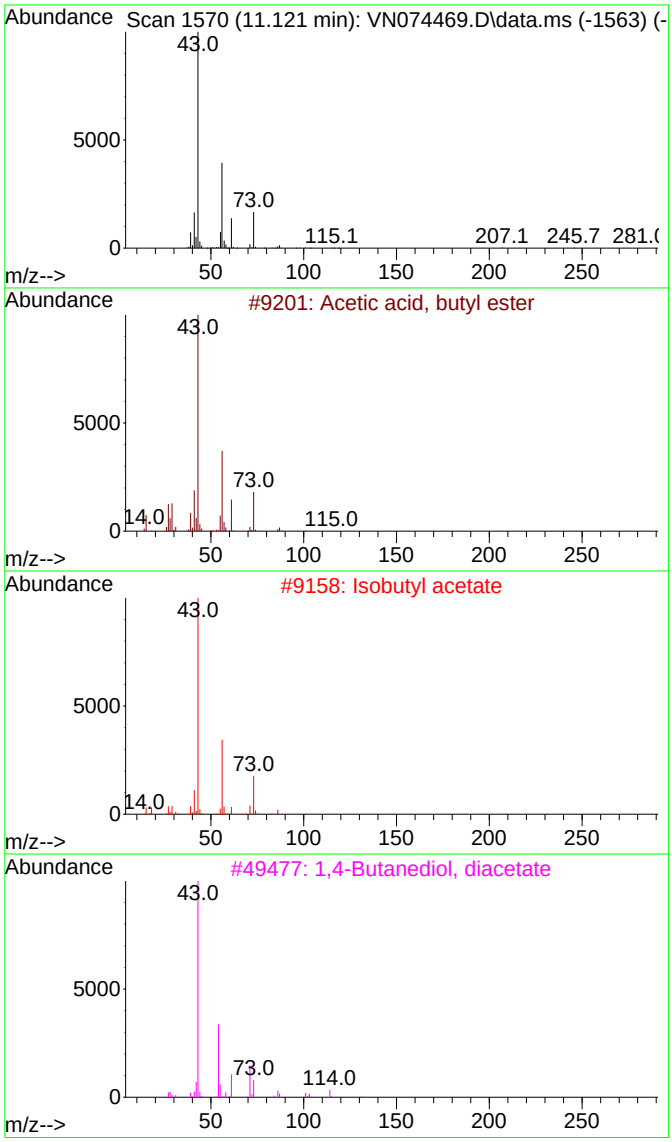
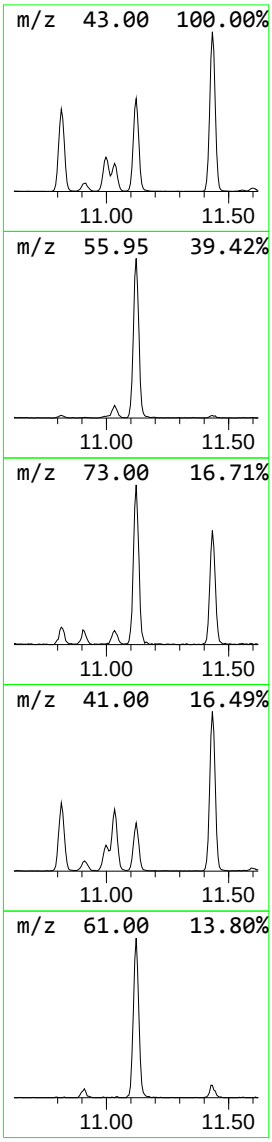
****
Peak Number 9 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.121	38.64 ug/l	2288730	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	39
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
4	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
5	Isobutylamine	73	C4H11N	000078-81-9	9





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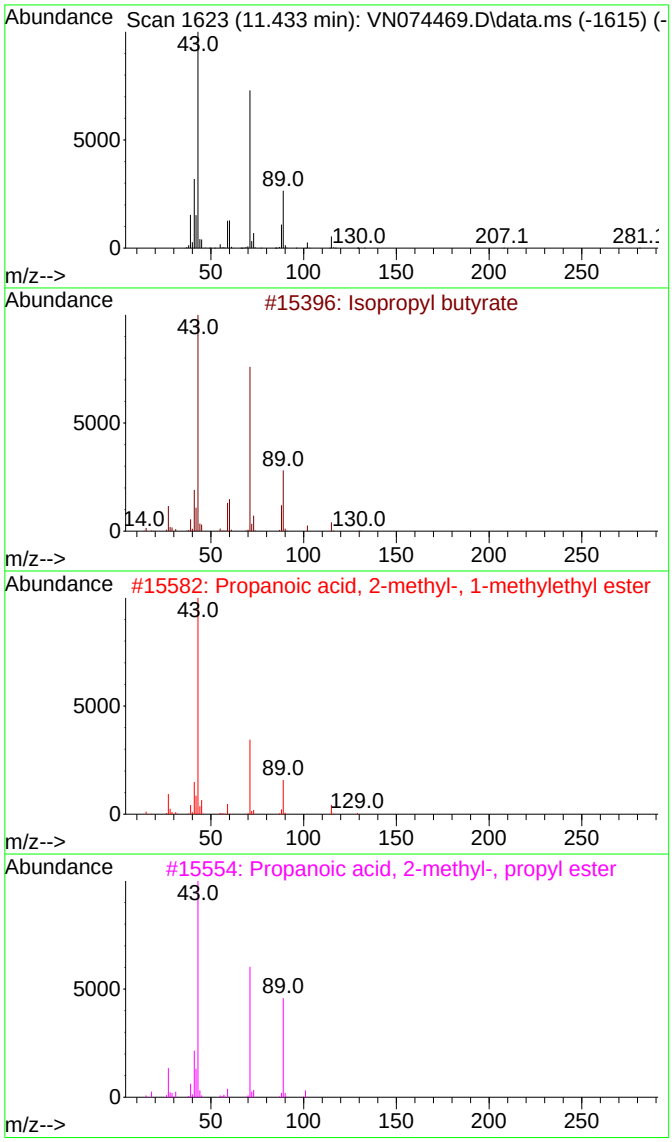
Quant Title : SW846 8260

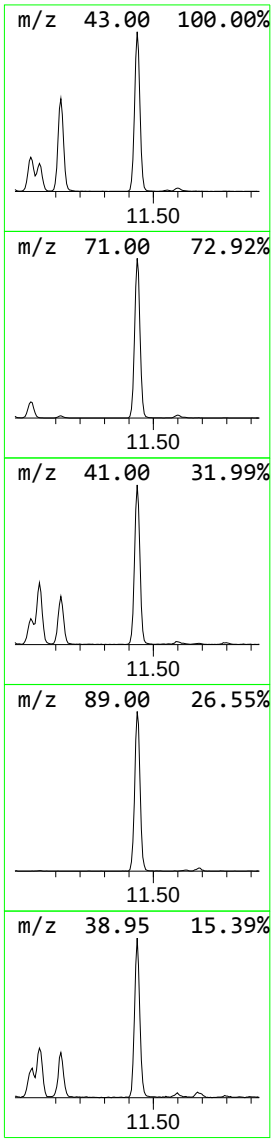
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.433	97.04 ug/l	5747210	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	59
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
Data File : VN074469.D
Acq On : 15 Sep 2022 18:22
Operator : JC\MD
Sample : N4578-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-2

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	2.193	57.7	ug/l	1648030	1	8.016	1428040	50.0
3-Pentanone	9.492	12.2	ug/l	523093	2	8.904	2136020	50.0
n-Propyl acetate	9.563	208.4	ug/l	8903290	2	8.904	2136020	50.0
Propanoic acid,...	10.186	36.5	ug/l	1559430	2	8.904	2136020	50.0
Isobutyl acetate	10.557	34.1	ug/l	2019510	3	11.686	2961370	50.0
Propanoic acid,...	10.816	35.1	ug/l	2079690	3	11.686	2961370	50.0
3-Pentanone, 2,...	10.998	13.6	ug/l	807026	3	11.686	2961370	50.0
Propanoic acid,...	11.033	54.6	ug/l	3231630	3	11.686	2961370	50.0
Acetic acid, bu...	11.121	38.6	ug/l	2288730	3	11.686	2961370	50.0
Isopropyl butyrate	11.433	97.0	ug/l	5747210	3	11.686	2961370	50.0