LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
Data File : VN084955.D
Acq On : 19 Nov 2024 18:28
Operator : JC\MD
Sample : P4849-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RR-1

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\82N103024W.M
Title : SW846 8260

Signal : TIC: VN084955.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.283	50	56	67	rBV2	43187	93749	5.67%	0.825%
2	2.659	115	120	124	rBV	14816	26988	1.63%	0.237%
3	4.436	411	422	436	rBV3	41100	119730	7.24%	1.053%
4	8.159	1045	1055	1060	rBV	138514	327920	19.83%	2.885%
5	8.224	1060	1066	1083	rVB	233435	526594	31.84%	4.633%
6	8.577	1117	1126	1133	rBV2	149719	340357	20.58%	2.994%
7	8.688	1133	1145	1154	rBV4	115267	398169	24.08%	3.503%
8	9.100	1206	1215	1225	rBV	358184	735034	44.44%	6.466%
9	9.671	1303	1312	1317	rBV	41309	91656	5.54%	0.806%
10	9.741	1317	1324	1338	rVB	919006	1653850	100.00%	14.549%
11	10.359	1419	1429	1439	rBV	181329	317593	19.20%	2.794%
12	10.565	1456	1464	1473	rBV	541791	998437	60.37%	8.783%
13	10.723	1483	1491	1507	rVB	212665	372072	22.50%	3.273%
14	10.982	1528	1535	1545	rBV	233131	398501	24.10%	3.506%
15	11.076	1545	1551	1560	rVV2	48255	91216	5.52%	0.802%
16	11.200	1560	1572	1581	rVV2	398026	798604	48.29%	7.025%
17	11.288	1581	1587	1600	rVB	266021	436327	26.38%	3.838%
18	11.600	1633	1640	1651	rBV	712395	1108076	67.00%	9.748%
19	11.770	1663	1669	1677	rVB2	11615	23344	1.41%	0.205%
20	11.865	1677	1685	1695	rVB	506794	899757	54.40%	7.915%
21	12.212	1738	1744	1749	rVB2	10469	17491	1.06%	0.154%
22	12.306	1753	1760	1768	rVB	37137	59033	3.57%	0.519%
23	12.847	1844	1852	1863	rVB	398615	682573	41.27%	6.005%
24	13.788	2005	2012	2021	rBV	485635	816779	49.39%	7.185%
25	13.876	2021	2027	2032	rVB2	10393	16588	1.00%	0.146%
26	14.553	2136	2142	2148	rVB3	11357	16786	1.01%	0.148%

Sum of corrected areas: 11367224

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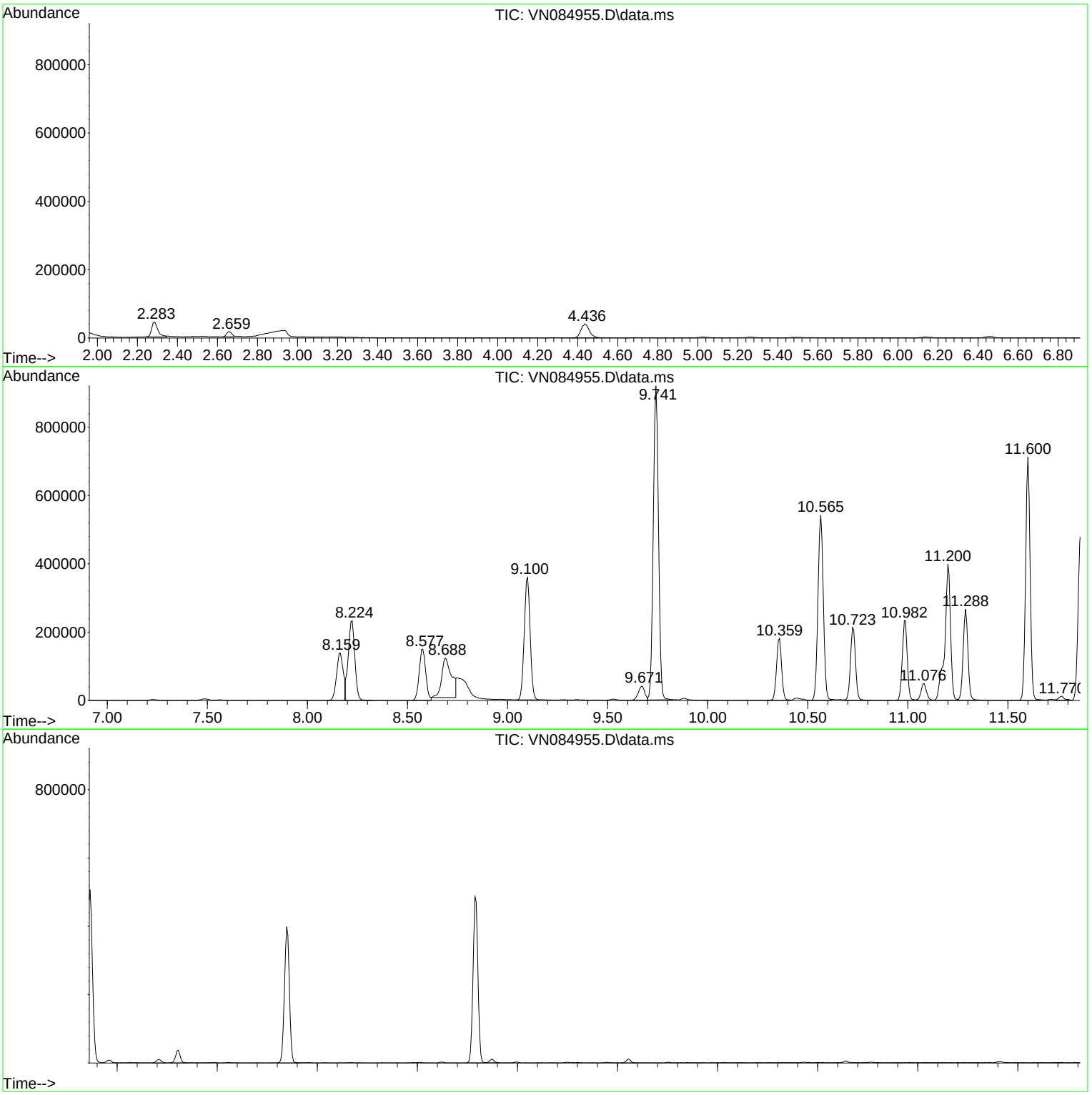
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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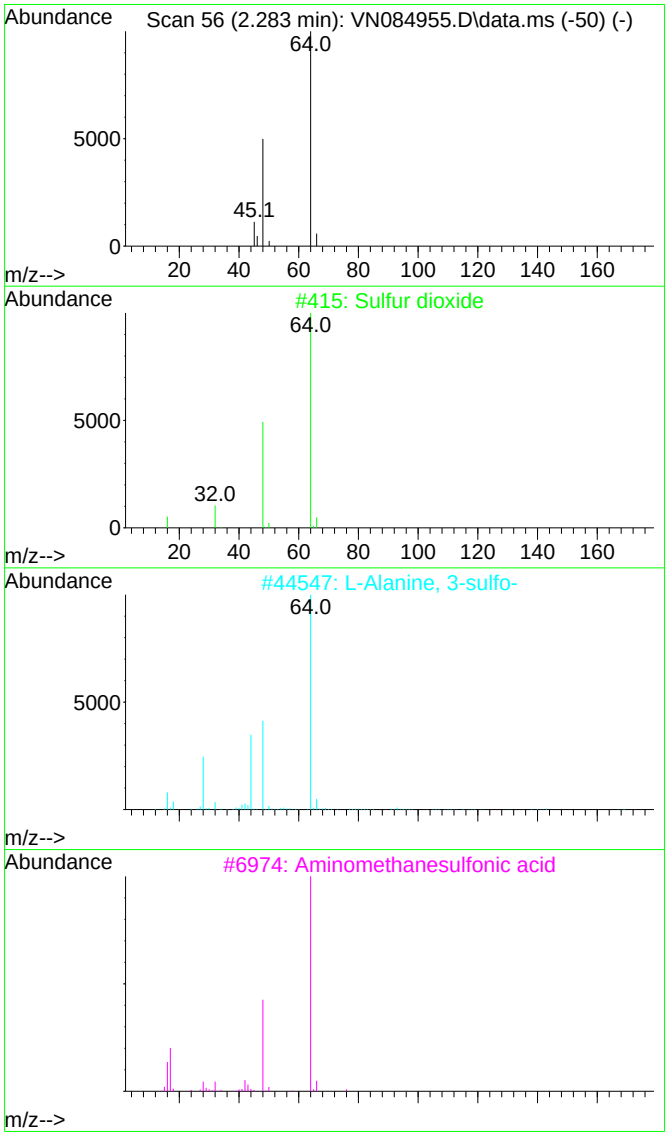
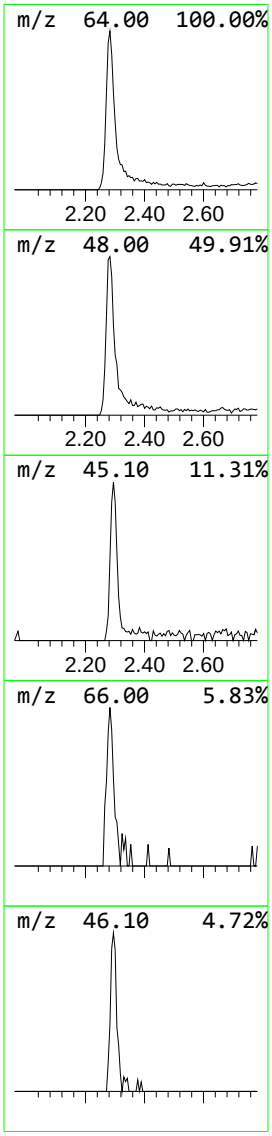
****
Peak Number 1 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.283	8.90 ug/l	93749	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	74
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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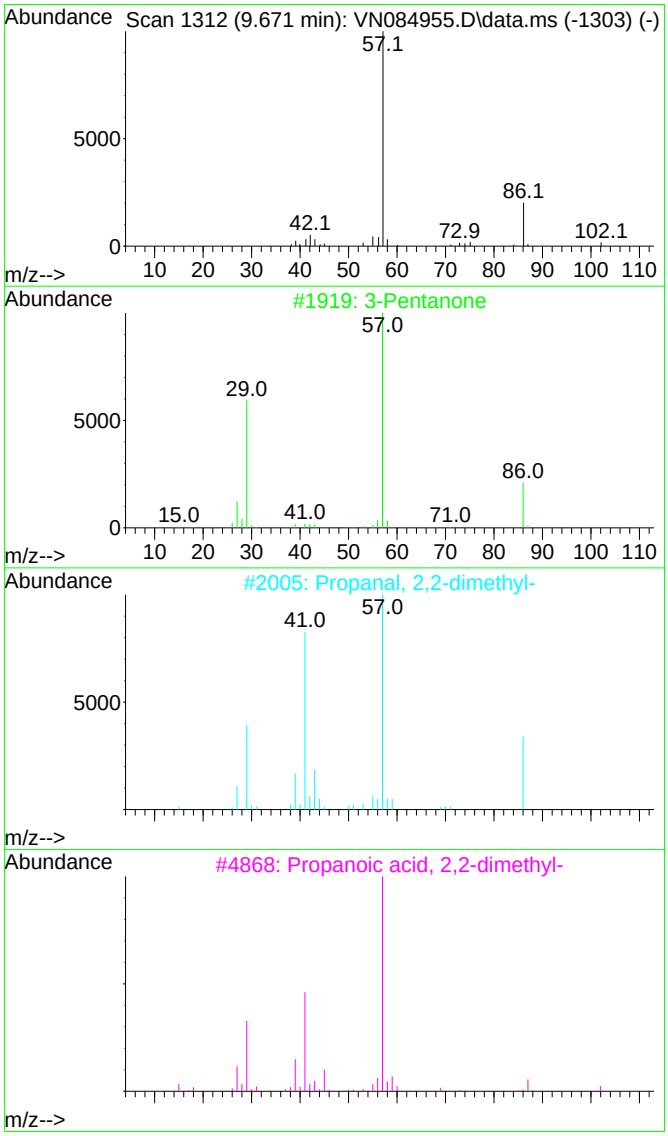
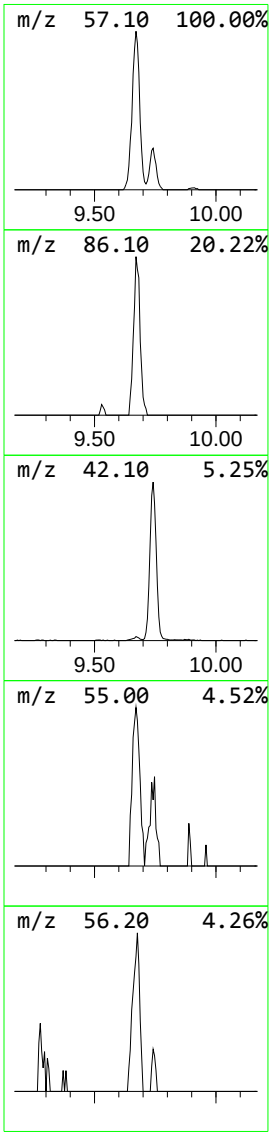
****
Peak Number 2 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.671	6.23 ug/l	91656	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	59
2	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	40
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	32
4	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9





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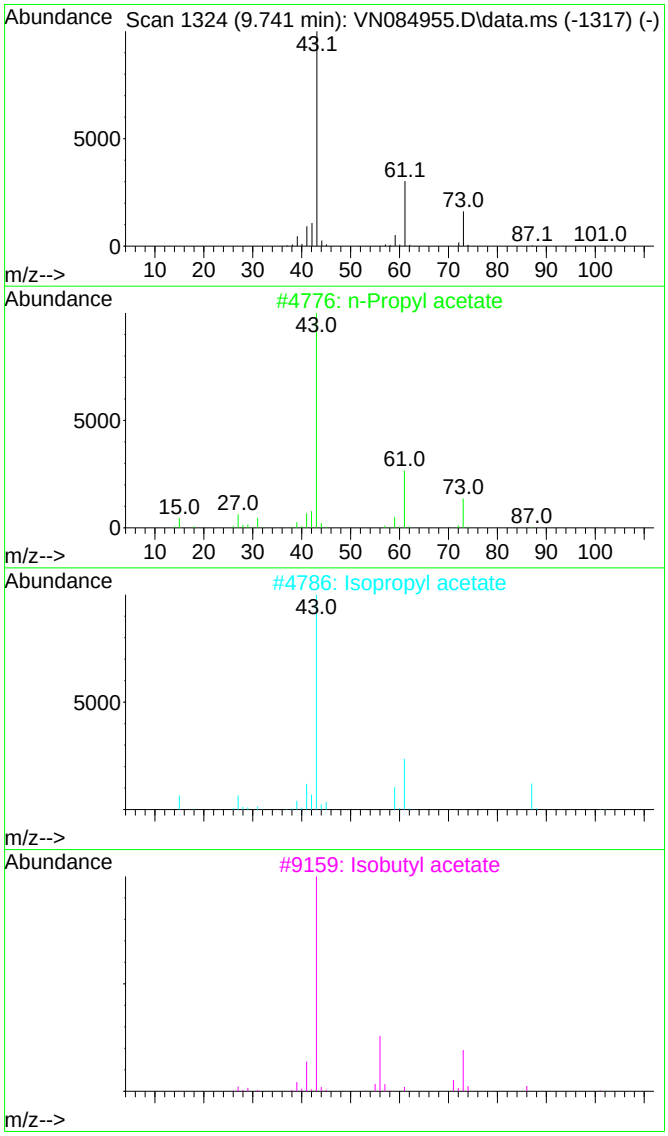
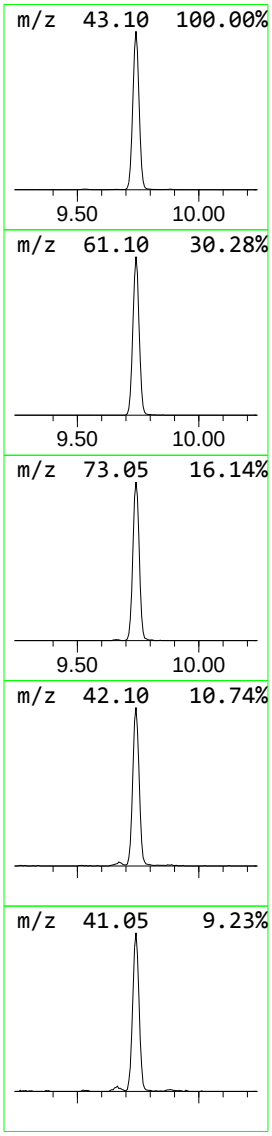
****
Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.741	112.50 ug/l	1653850	1,4-Difluorobenzene	9.100

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





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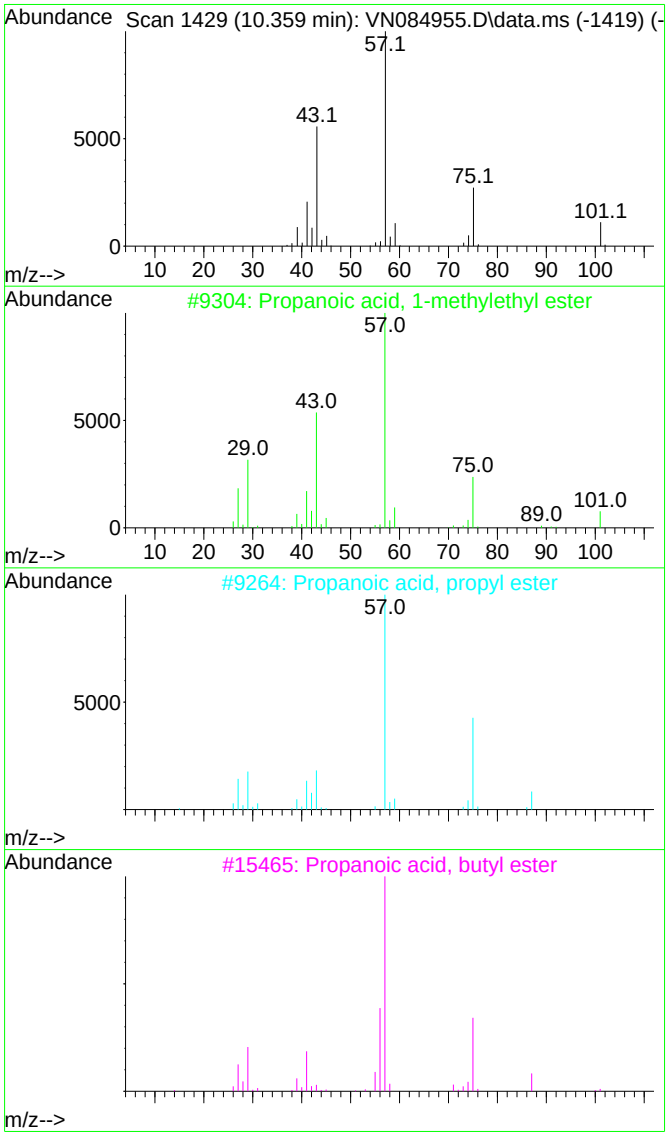
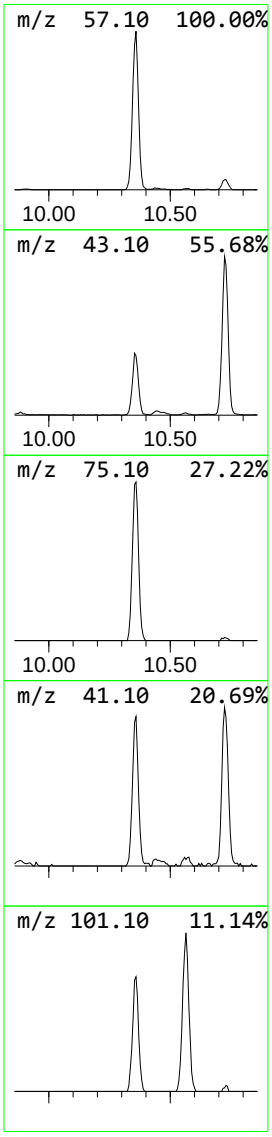
****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.359	21.60 ug/l	317593	1,4-Difluorobenzene	9.100

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	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	14





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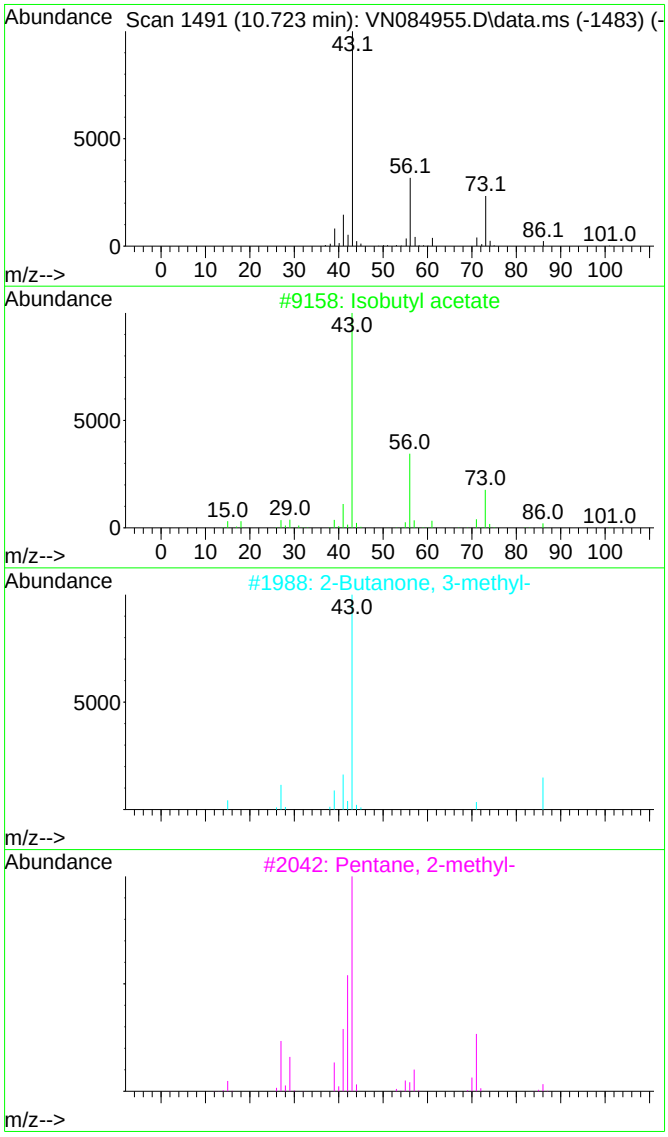
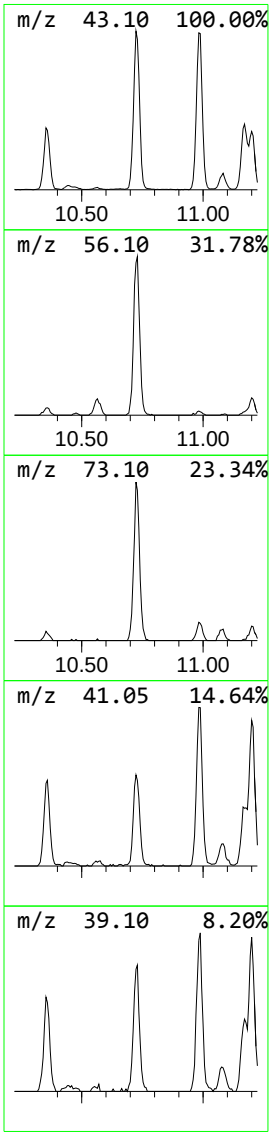
****
Peak Number 5 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.724	20.68 ug/l	372072	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4	2-Pentanone	86	C5H10O	000107-87-9	9
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9





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TIC Library : C:\Database\NIST20.L
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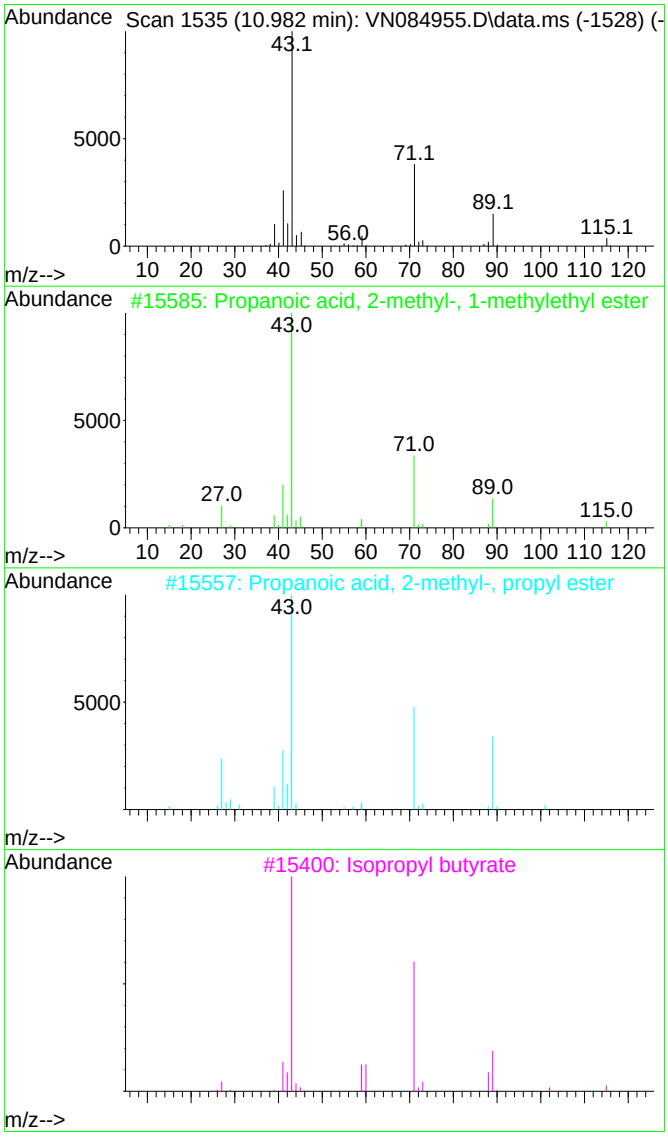
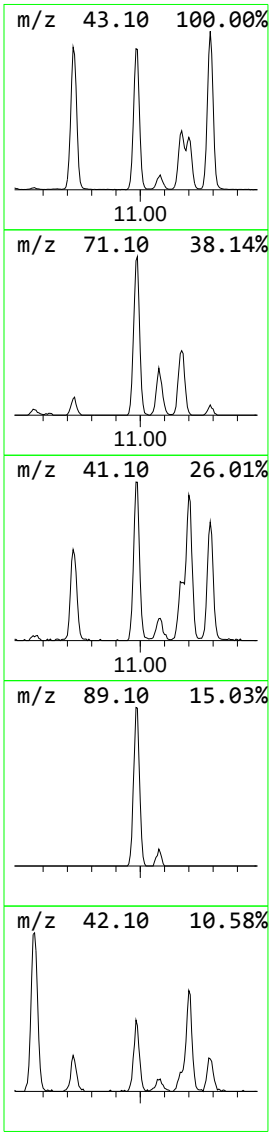
****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.982	22.14 ug/l	398501	Chlorobenzene-d5	11.865

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	78
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	64
4	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	56
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	53





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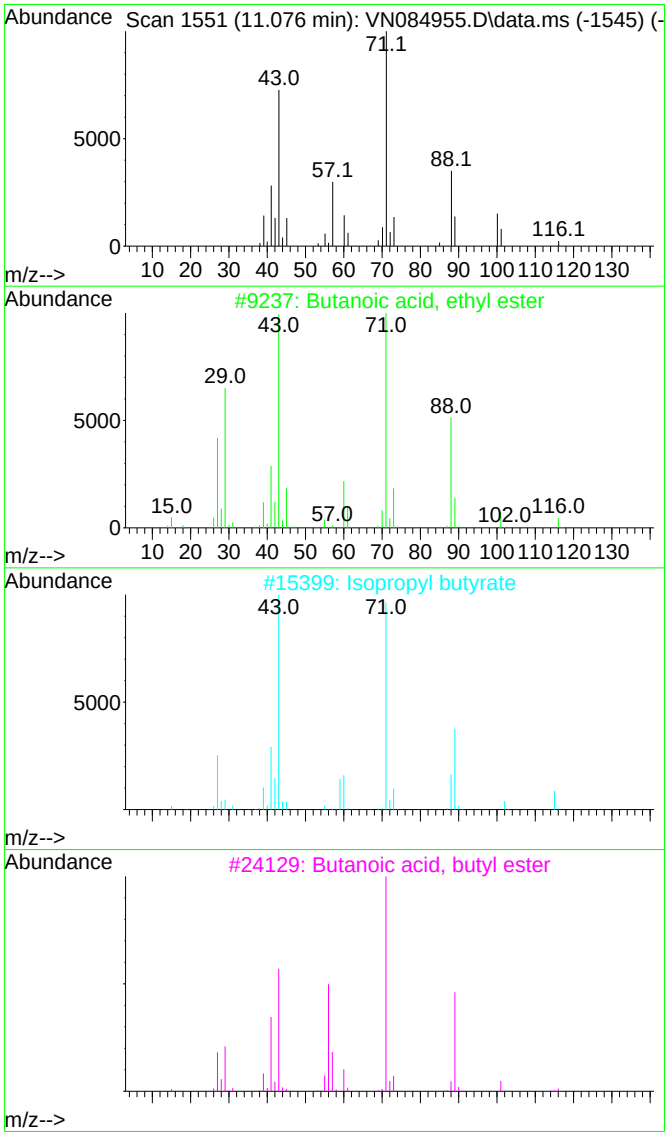
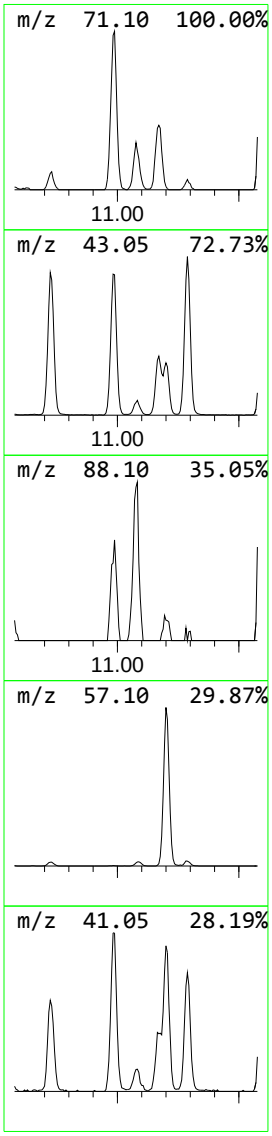
****
Peak Number 7 Butanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.076	5.07 ug/l	91216	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	53
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	53
4	3-Methoxy-1-pentene	100	C6H12O	014092-18-3	47
5	2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	47





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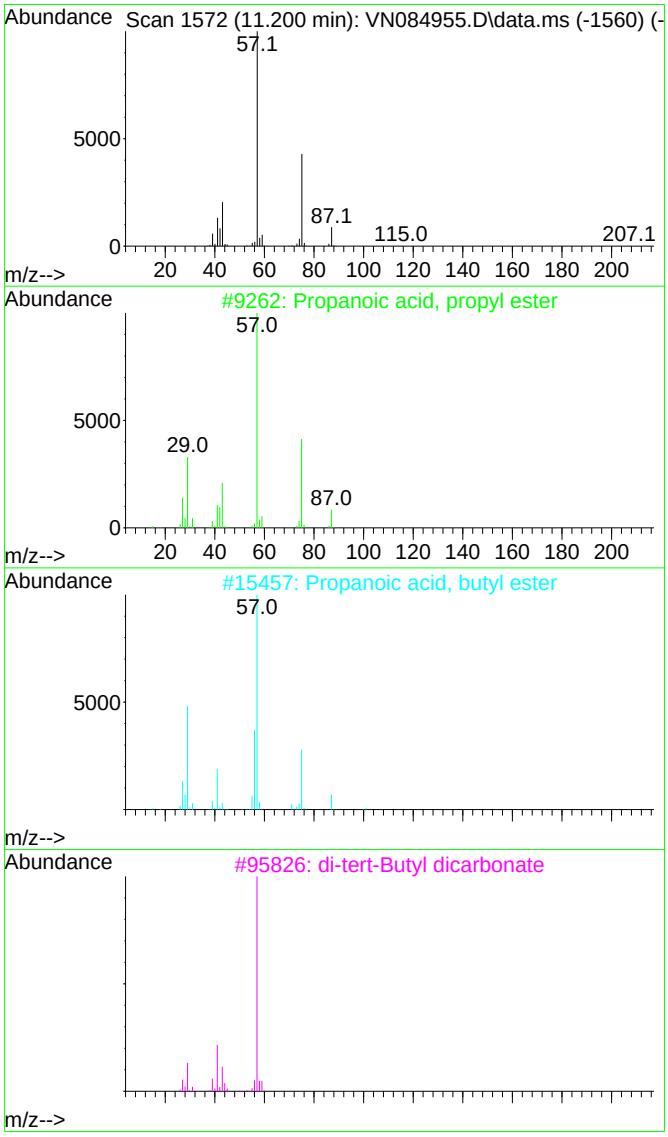
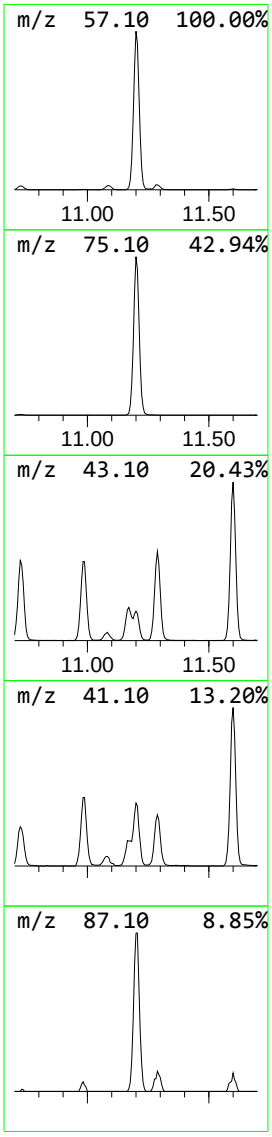
****
Peak Number 8 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.200	44.38 ug/l	798604	Chlorobenzene-d5	11.865

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	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7





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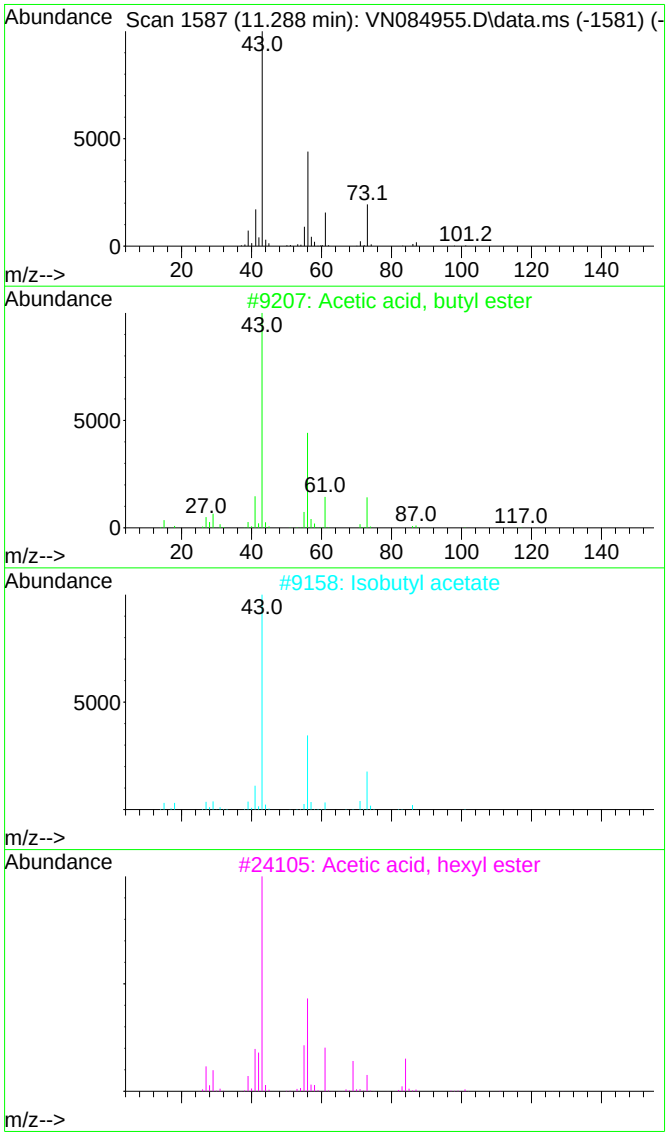
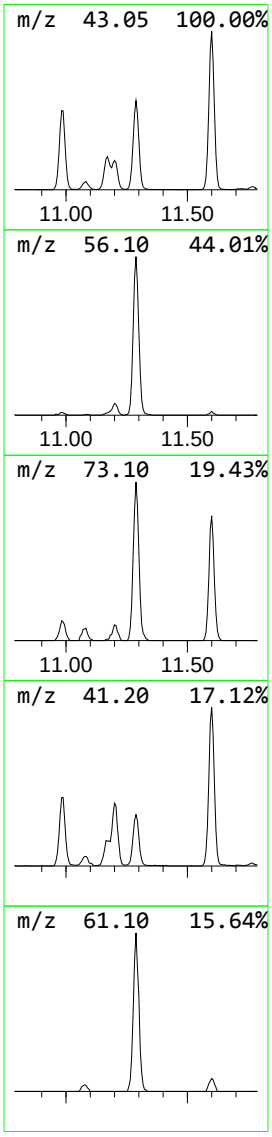
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.288	24.25 ug/l	436327	Chlorobenzene-d5	11.865

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	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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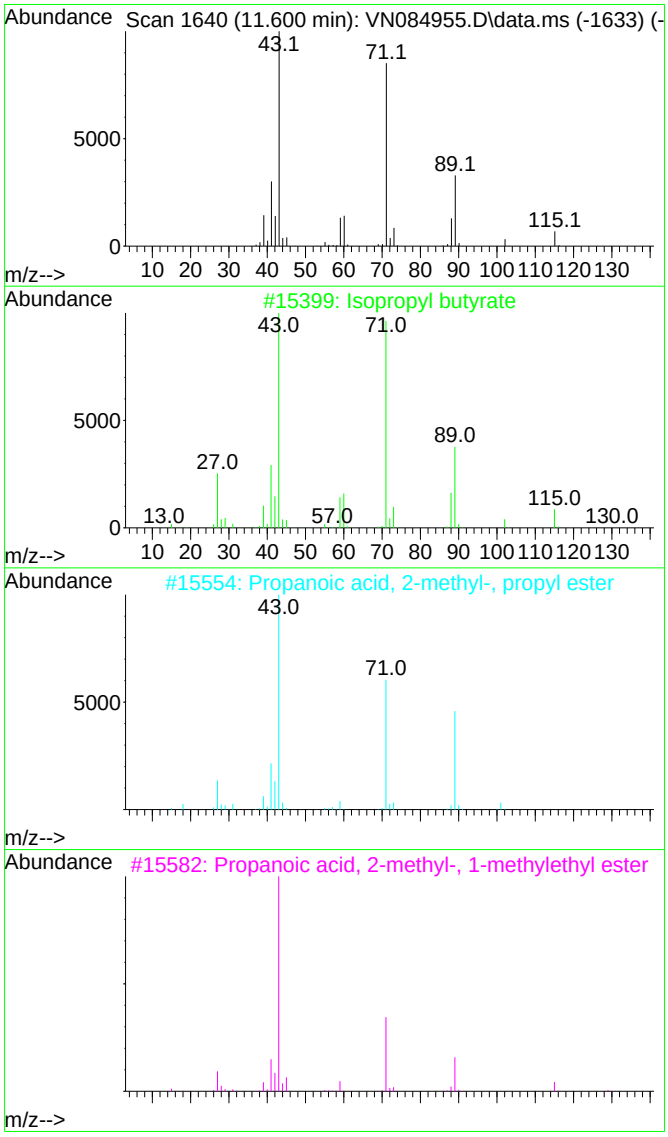
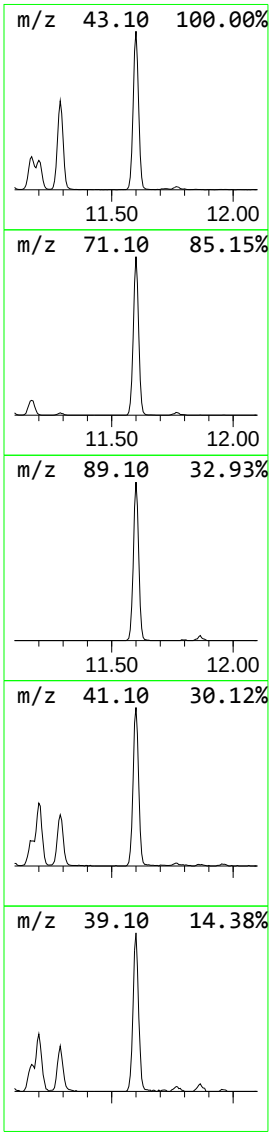
****
Peak Number 10 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.600	61.58 ug/l	1108080	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	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\VN111924\
Data File : VN084955.D
Acq On : 19 Nov 2024 18:28
Operator : JC\MD
Sample : P4849-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RR-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.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	2.283	8.9	ug/l	93749	1	8.224	526594	50.0
3-Pentanone	9.671	6.2	ug/l	91656	2	9.100	735034	50.0
n-Propyl acetate	9.741	112.5	ug/l	1653850	2	9.100	735034	50.0
Propanoic acid,...	10.359	21.6	ug/l	317593	2	9.100	735034	50.0
Isobutyl acetate	10.724	20.7	ug/l	372072	3	11.865	899757	50.0
Propanoic acid,...	10.982	22.1	ug/l	398501	3	11.865	899757	50.0
Butanoic acid, ...	11.076	5.1	ug/l	91216	3	11.865	899757	50.0
Propanoic acid,...	11.200	44.4	ug/l	798604	3	11.865	899757	50.0
Acetic acid, bu...	11.288	24.3	ug/l	436327	3	11.865	899757	50.0
Isopropyl butyrate	11.600	61.6	ug/l	1108080	3	11.865	899757	50.0