LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080823\
Data File : VN078798.D
Acq On : 08 Aug 2023 13:35
Operator : JC\MD
Sample : 03913-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
72-11933

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\82N080723W.M
Title : SW846 8260

Signal : TIC: VN078798.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.453	413	425	438	rBV	22314	69669	5.57%	0.711%
2	5.283	557	566	578	rBV4	23903	77114	6.17%	0.787%
3	7.500	937	943	951	rVB2	8570	19211	1.54%	0.196%
4	8.177	1048	1058	1062	rBV2	169154	407247	32.58%	4.154%
5	8.236	1062	1068	1079	rVB	275157	623154	49.85%	6.356%
6	8.588	1113	1128	1138	rBV	187021	441990	35.36%	4.508%
7	8.694	1139	1146	1155	rBV	69711	148561	11.88%	1.515%
8	9.106	1208	1216	1229	rBV	427972	885639	70.85%	9.034%
9	9.677	1305	1313	1319	rBV2	47336	98923	7.91%	1.009%
10	9.747	1319	1325	1337	rVB	363364	663041	53.04%	6.763%
11	10.365	1421	1430	1439	rBV	192852	328780	26.30%	3.354%
12	10.453	1439	1445	1457	rVB2	64745	130193	10.42%	1.328%
13	10.571	1457	1465	1476	rBV	672854	1250026	100.00%	12.751%
14	10.735	1486	1493	1502	rVB	59344	106503	8.52%	1.086%
15	10.994	1530	1537	1546	rBV	287857	482948	38.64%	4.926%
16	11.088	1546	1553	1561	rVV3	39782	73939	5.91%	0.754%
17	11.177	1561	1568	1570	rVV	123634	208940	16.71%	2.131%
18	11.206	1570	1573	1581	rVV	204229	334430	26.75%	3.411%
19	11.294	1584	1588	1596	rVB2	35700	61520	4.92%	0.628%
20	11.606	1634	1641	1652	rBV	667174	1061723	84.94%	10.830%
21	11.771	1664	1669	1678	rVB2	13006	25285	2.02%	0.258%
22	11.871	1678	1686	1697	rVB	574274	1040259	83.22%	10.611%
23	12.218	1736	1745	1750	rBV2	10156	18298	1.46%	0.187%
24	12.312	1753	1761	1766	rBV2	15645	25810	2.06%	0.263%
25	12.853	1845	1853	1863	rBV	363734	644736	51.58%	6.577%
26	13.794	2006	2013	2022	rBV	338143	575563	46.04%	5.871%

Sum of corrected areas: 9803502

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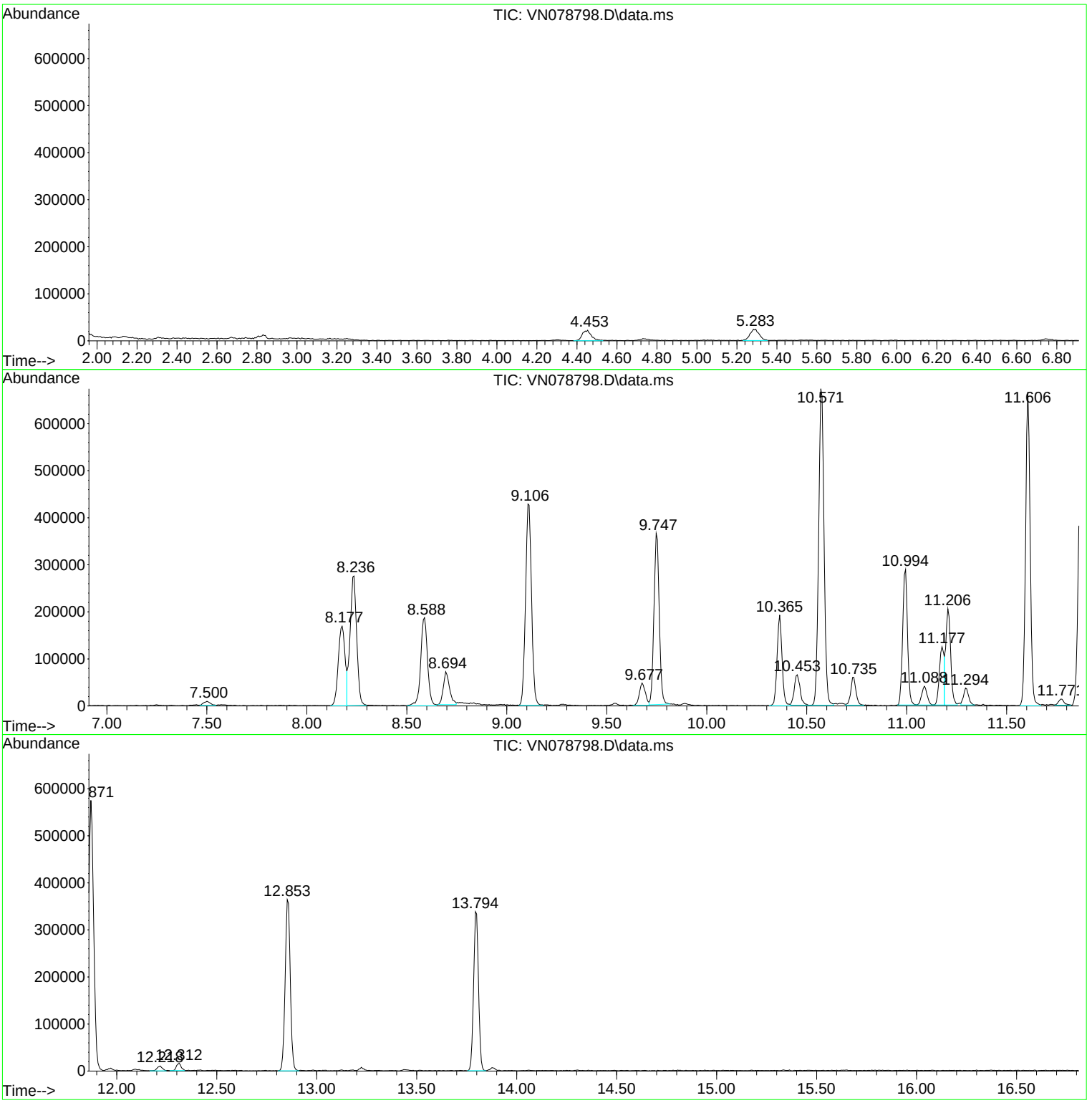
ClientSampleId :
72-11933

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080723W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

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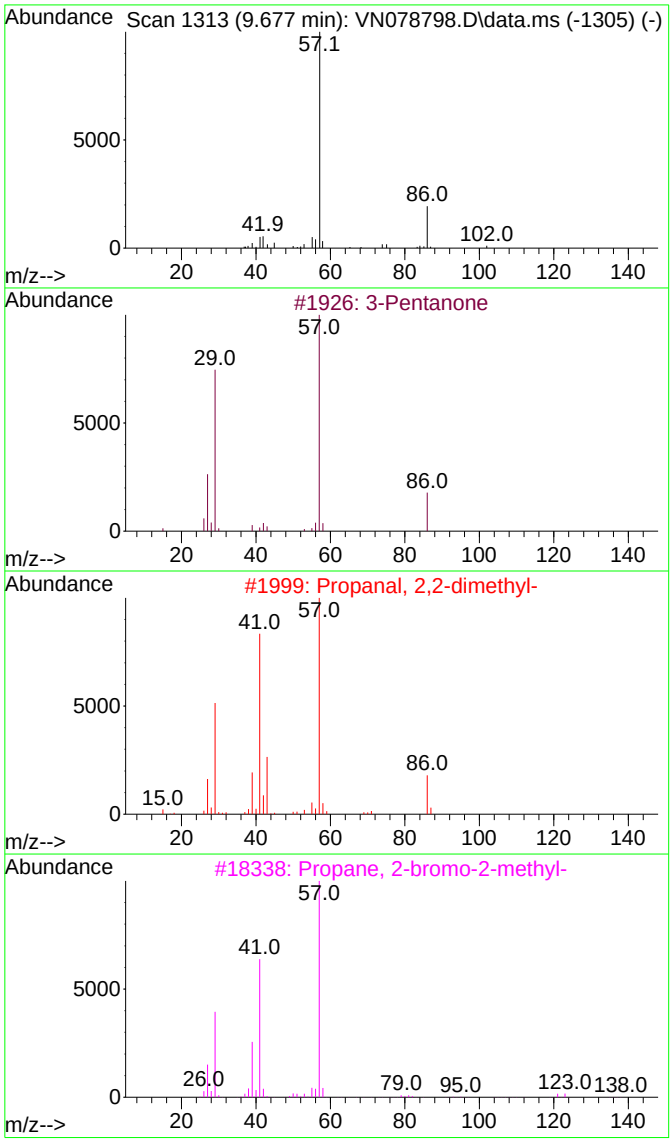
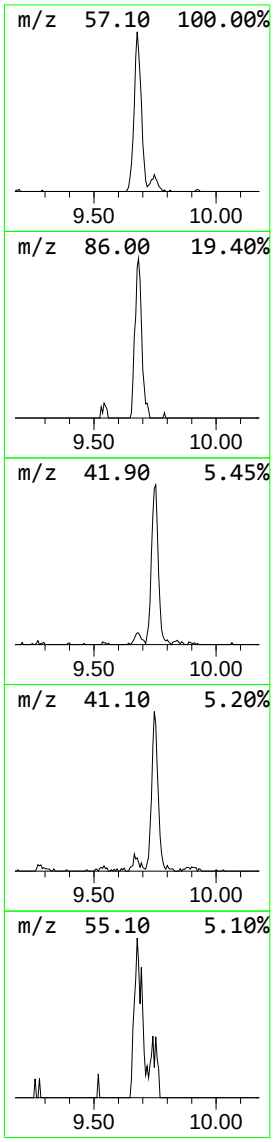
****
Peak Number 1 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	5.58 ug/l	98923	1,4-Difluorobenzene	9.112

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	38
3	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	25
4	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	25
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	9





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
72-11933

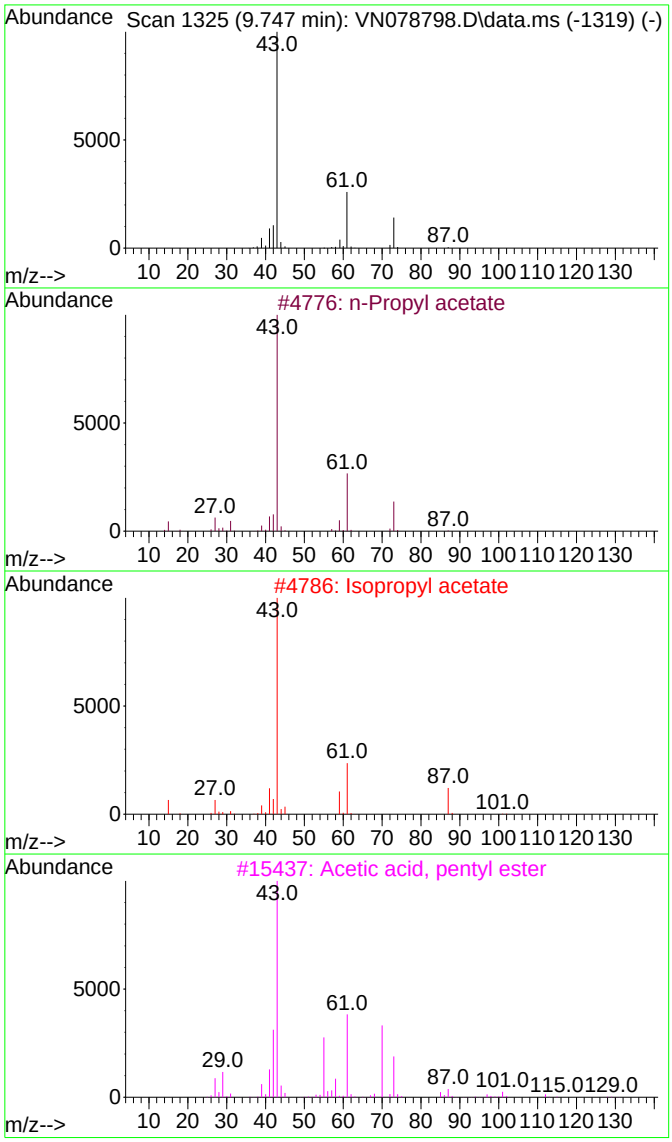
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080723W.M
Quant Title : SW846 8260

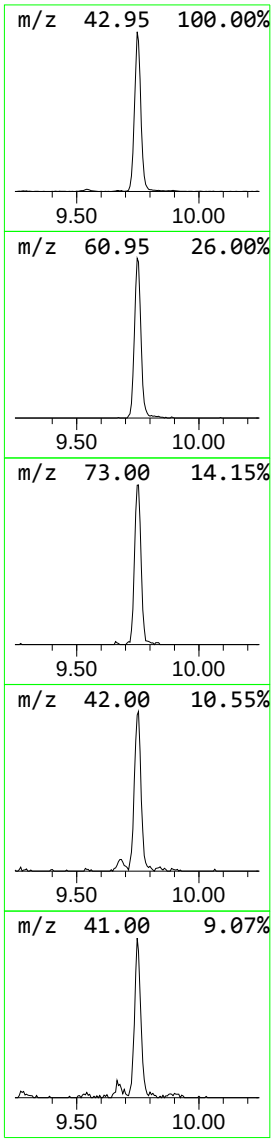
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	37.43 ug/l	663041	1,4-Difluorobenzene	9.112

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





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
72-11933

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080723W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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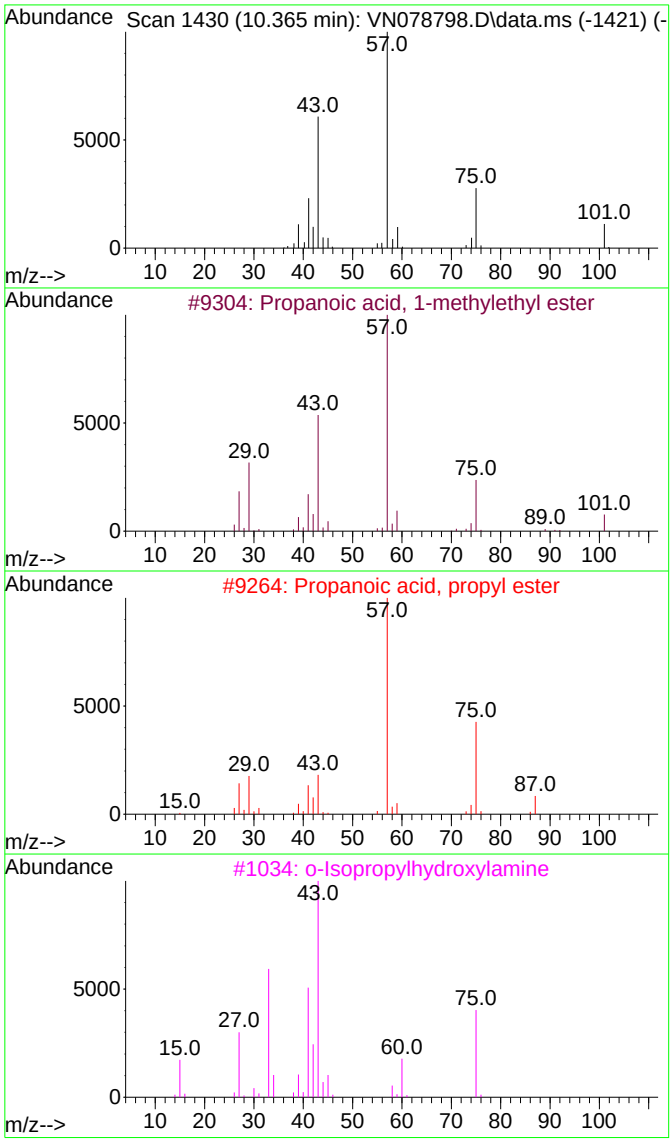
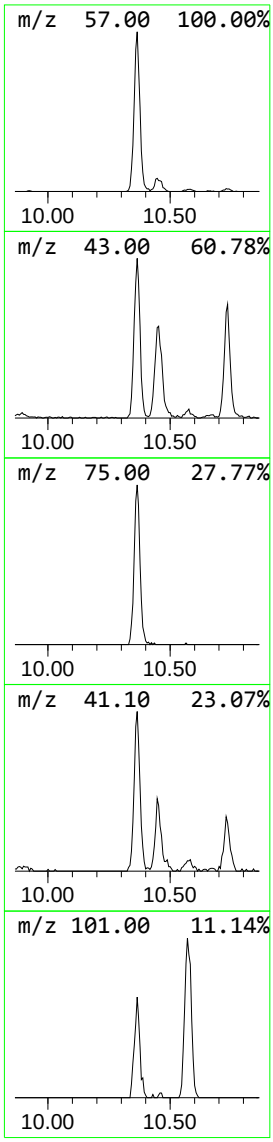
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	18.56 ug/l	328780	1,4-Difluorobenzene	9.112

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	56
3	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	35
4	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
5	Azetidine	57	C3H7N	000503-29-7	16





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Instrument :
MSVOA_N
ClientSampleId :
72-11933

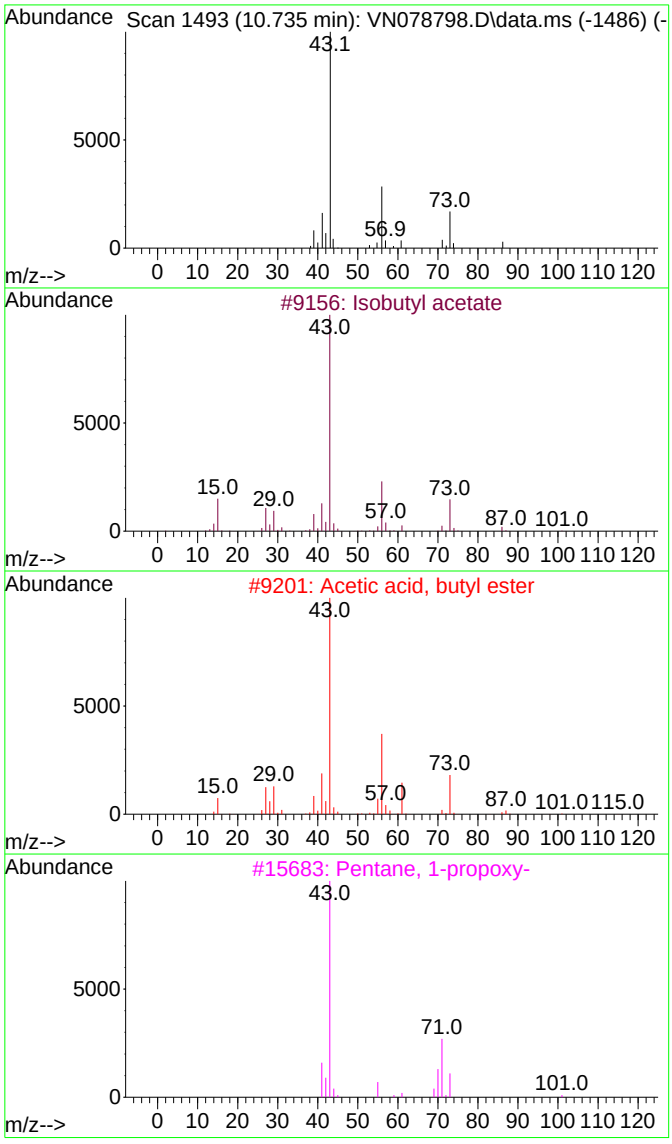
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080723W.M
Quant Title : SW846 8260

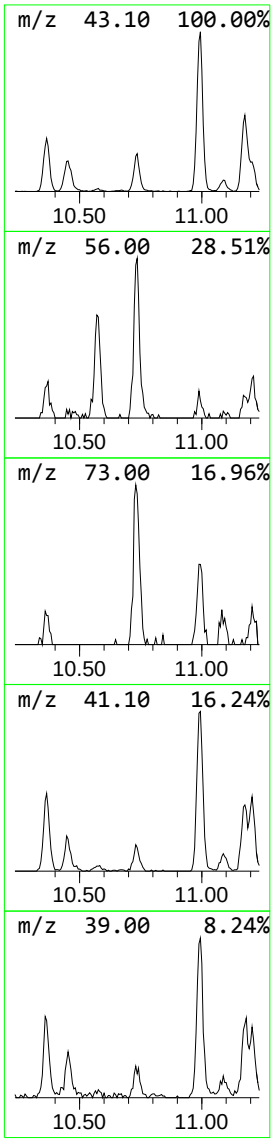
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isobutyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	5.12 ug/l	106503	Chlorobenzene-d5	11.871

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	40
3	Pentane, 1-propoxy-	130	C8H18O	018641-82-2	25
4	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9





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MSVOA_N
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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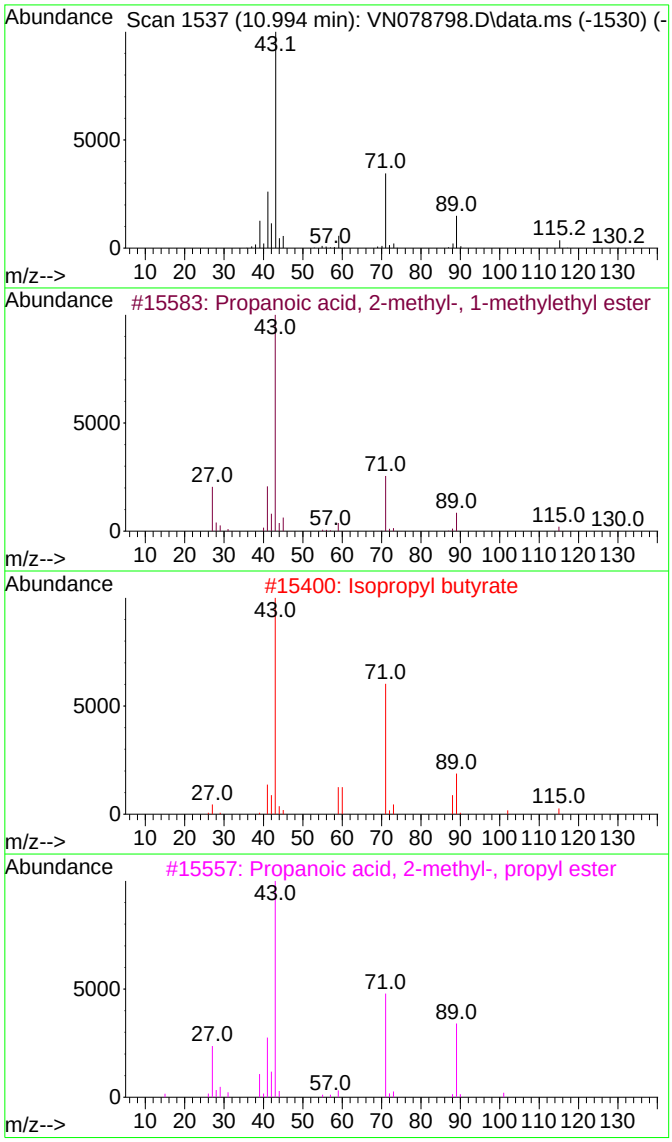
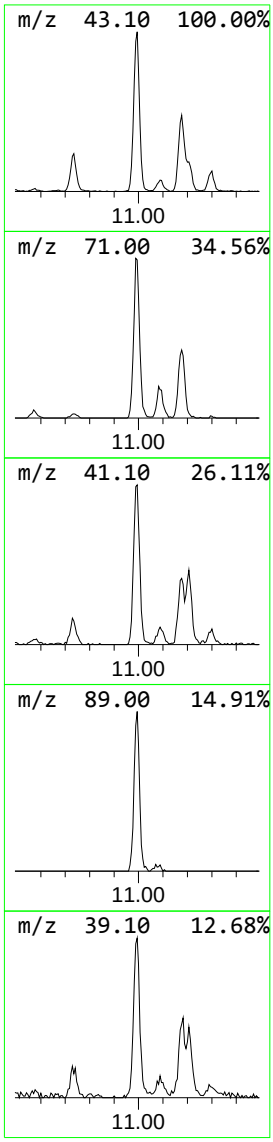
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	23.21 ug/l	482948	Chlorobenzene-d5	11.871

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	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	47





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Quant Title : SW846 8260

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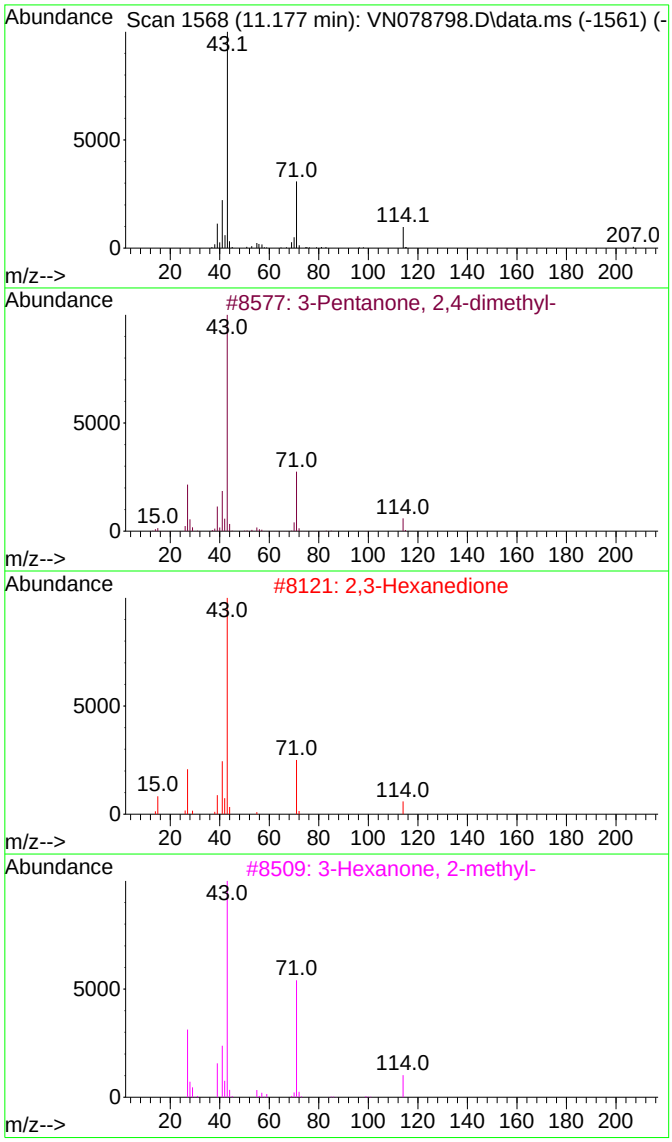
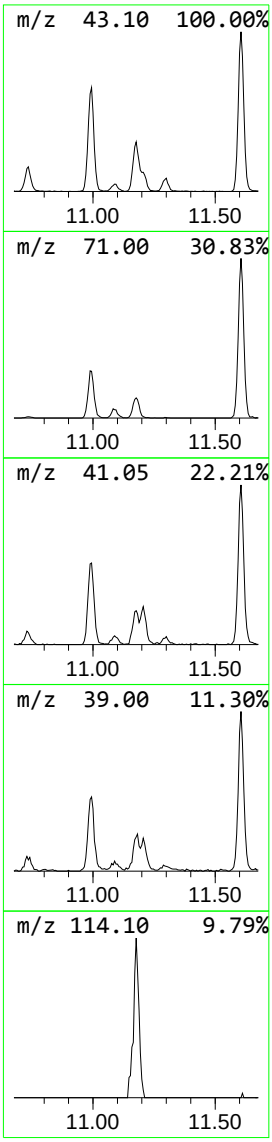
****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.177	10.04 ug/l	208940	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
3	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	50
4	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	45
5	4-Heptanone	114	C7H14O	000123-19-3	37





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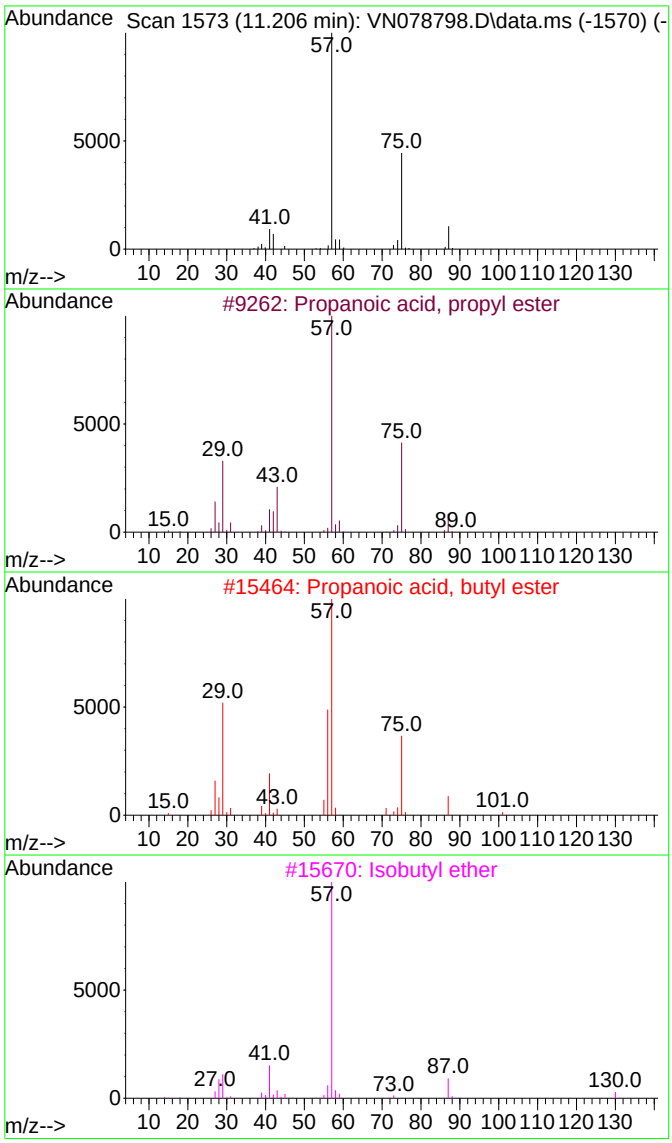
Quant Title : SW846 8260

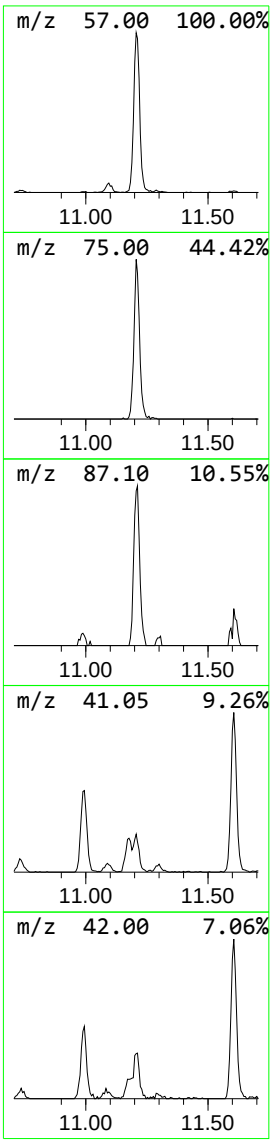
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	16.07 ug/l	334430	Chlorobenzene-d5	11.871

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	40
3	Isobutyl ether	130	C8H18O	000628-55-7	9
4	Oxalic acid, ethyl isobutyl ester	174	C8H14O4	1000309-36-7	9
5	n-Butyl ether	130	C8H18O	000142-96-1	9





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MSVOA_N
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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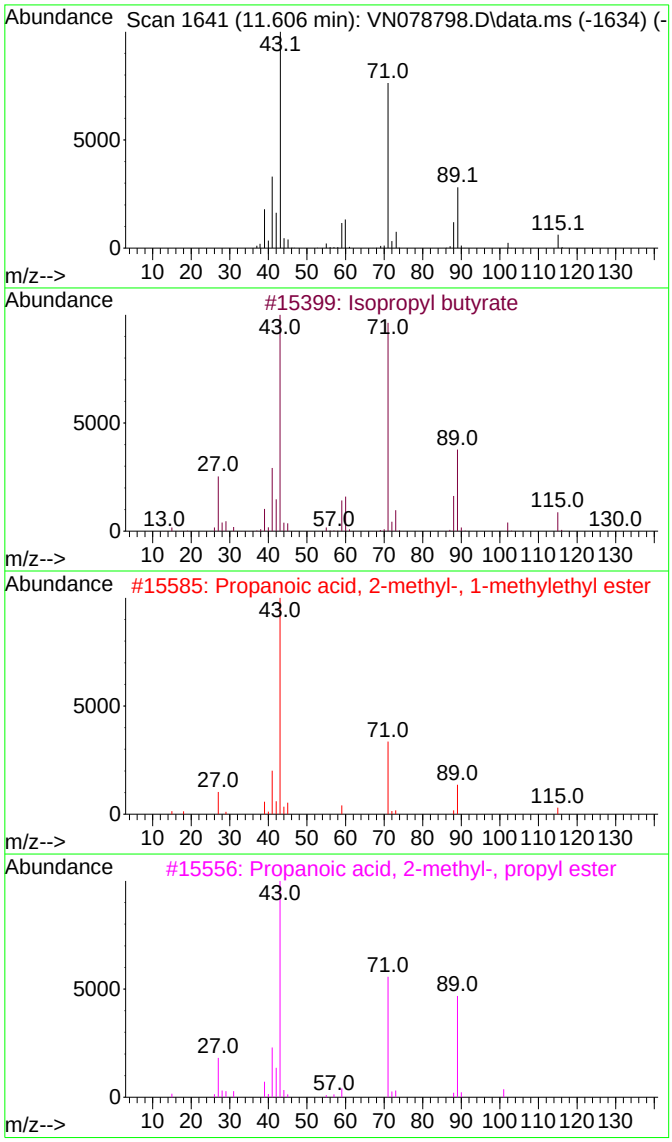
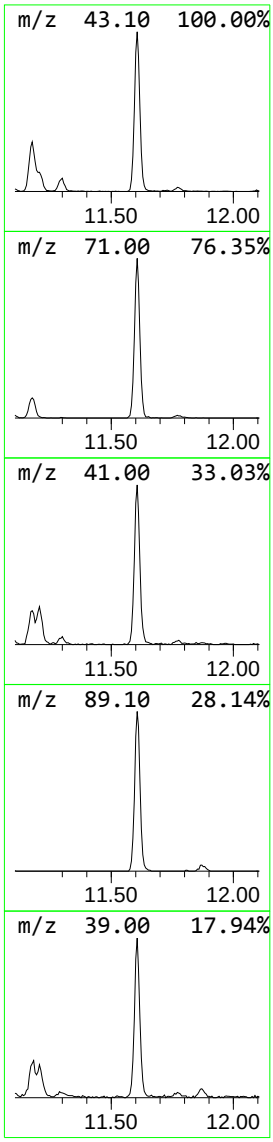
****
Peak Number 8 Isopropyl butyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	51.03 ug/l	1061720	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





Tentatively Identified Compound (LSC) summary

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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
3-Pentanone	9.677	5.6	ug/l	98923	2	9.112	885639	50.0
n-Propyl acetate	9.747	37.4	ug/l	663041	2	9.112	885639	50.0
Propanoic acid,...	10.365	18.6	ug/l	328780	2	9.112	885639	50.0
Isobutyl acetate	10.735	5.1	ug/l	106503	3	11.871	1040260	50.0
Propanoic acid,...	10.994	23.2	ug/l	482948	3	11.871	1040260	50.0
3-Pentanone, 2,...	11.177	10.0	ug/l	208940	3	11.871	1040260	50.0
Propanoic acid,...	11.206	16.1	ug/l	334430	3	11.871	1040260	50.0
Isopropyl butyrate	11.606	51.0	ug/l	1061720	3	11.871	1040260	50.0