LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036842.D
Acq On : 07 Aug 2023 17:17
Operator : JC/MD
Sample : 03891-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-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_X\Method\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036842.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	207	212	221	rBV	34610	56604	2.77%	0.464%
2	2.788	273	279	294	rBV	26828	54974	2.69%	0.451%
3	3.574	400	408	423	rBV2	20185	49435	2.42%	0.405%
4	4.568	561	571	588	rBV2	12855	40892	2.00%	0.335%
5	5.391	693	706	721	rBV2	92907	277315	13.58%	2.274%
6	5.556	722	733	749	rVB	152761	428230	20.97%	3.512%
7	5.958	787	799	818	rBV	100461	268871	13.17%	2.205%
8	6.342	851	862	877	rBV	96434	244655	11.98%	2.006%
9	6.763	921	931	946	rBV	247537	596137	29.19%	4.888%
10	7.641	1063	1075	1080	rBV	57402	107203	5.25%	0.879%
11	7.696	1080	1084	1093	rVB	18237	32885	1.61%	0.270%
12	7.799	1094	1101	1117	rBV	1193165	2041956	100.00%	16.744%
13	8.549	1214	1224	1234	rBV2	304663	591174	28.95%	4.848%
14	8.653	1234	1241	1257	rVB	505958	831134	40.70%	6.815%
15	8.958	1284	1291	1311	rVB	333548	502902	24.63%	4.124%
16	9.244	1332	1338	1345	rBV	418634	570423	27.94%	4.678%
17	9.311	1345	1349	1351	rVV	36987	50805	2.49%	0.417%
18	9.342	1351	1354	1356	rVV	58476	77908	3.82%	0.639%
19	9.378	1356	1360	1366	rVB	158824	227112	11.12%	1.862%
20	9.482	1372	1377	1383	rBV	634363	826554	40.48%	6.778%
21	9.579	1388	1393	1410	rVB	416515	527881	25.85%	4.329%
22	9.915	1442	1448	1461	rBV	1241140	1585048	77.62%	12.998%
23	10.055	1463	1471	1478	rBV	549607	758613	37.15%	6.221%
24	10.281	1503	1508	1520	rBV	16439	23112	1.13%	0.190%
25	10.506	1541	1545	1552	rVB	19346	24774	1.21%	0.203%
26	10.640	1562	1567	1573	rBV	99170	120721	5.91%	0.990%
27	11.079	1634	1639	1652	rBV	442014	559155	27.38%	4.585%
28	12.024	1788	1794	1805	rBV	512465	682202	33.41%	5.594%
29	12.219	1821	1826	1836	rBV	22795	36333	1.78%	0.298%

Sum of corrected areas: 12195008

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MSVOA_X
ClientSampleId :
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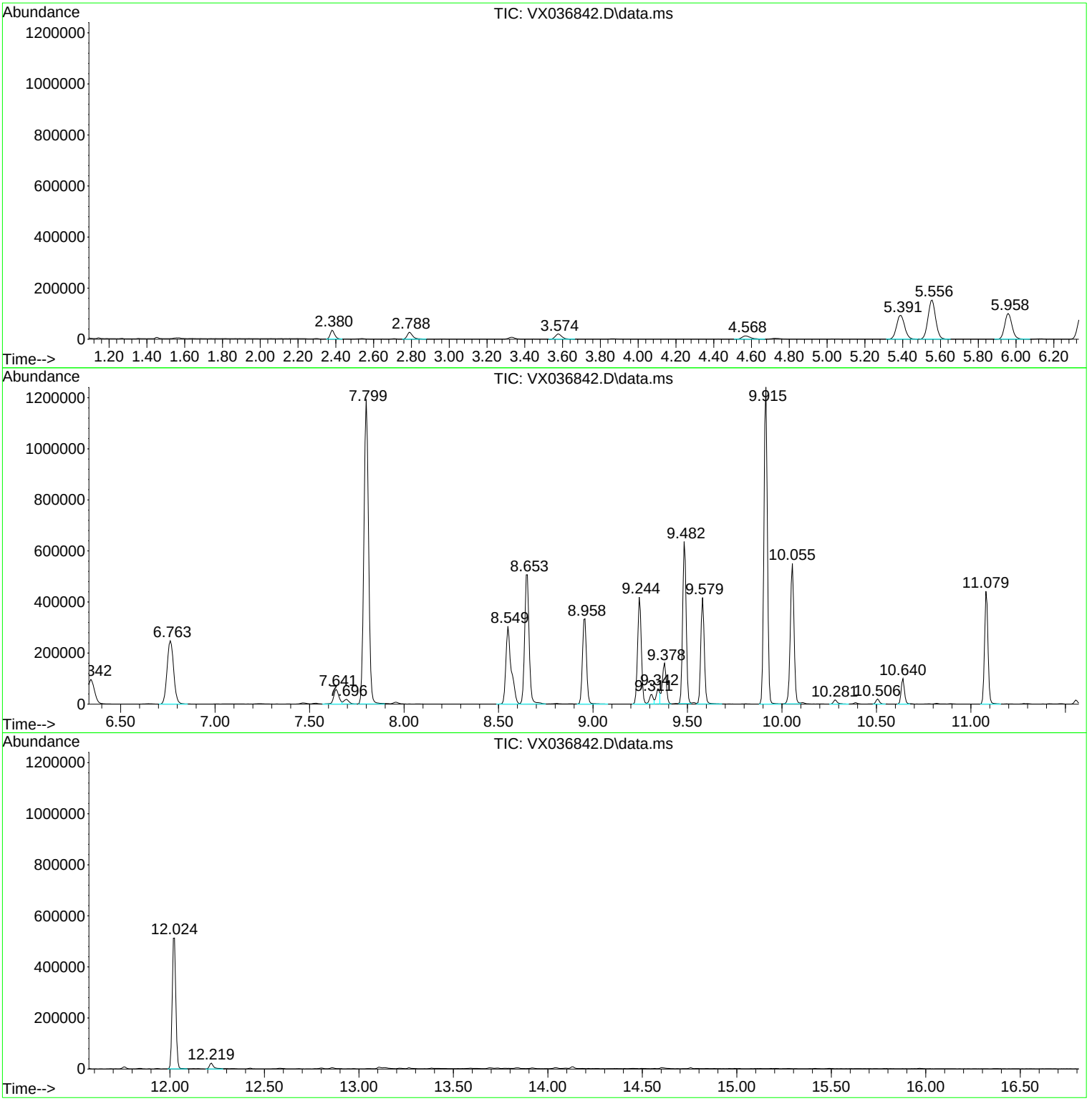
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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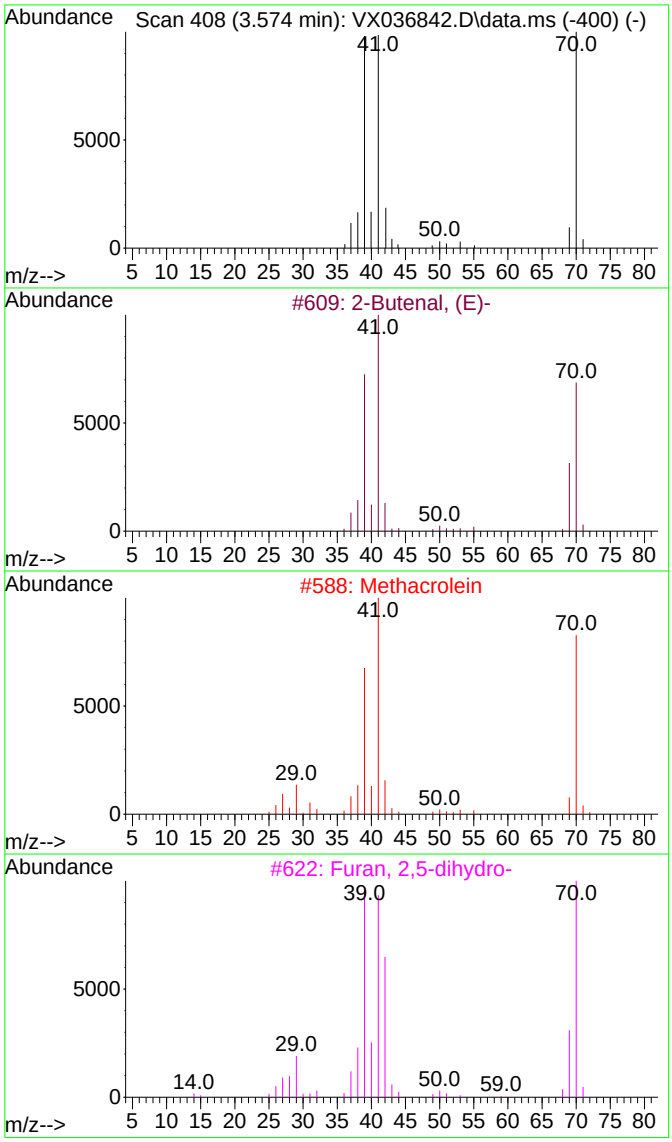
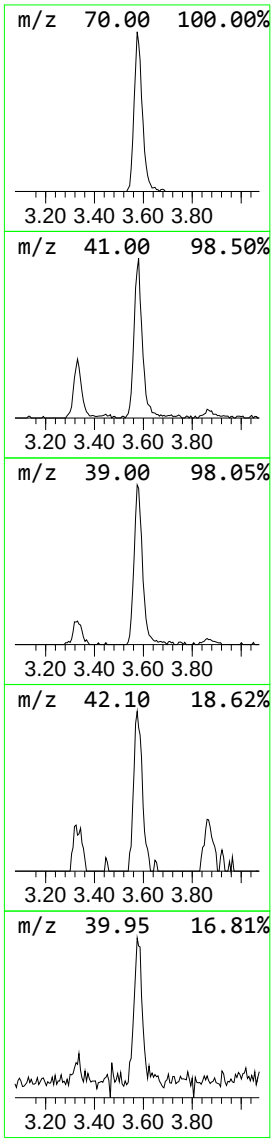
****
Peak Number 1 2-Butenal, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.574	5.77 ug/l	49435	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-	70	C4H6O	000123-73-9	91
2	Methacrolein	70	C4H6O	000078-85-3	91
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	86
4	2-Butenal, (Z)-	70	C4H6O	015798-64-8	86
5	Cyclopropanecarboxaldehyde	70	C4H6O	001489-69-6	83





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
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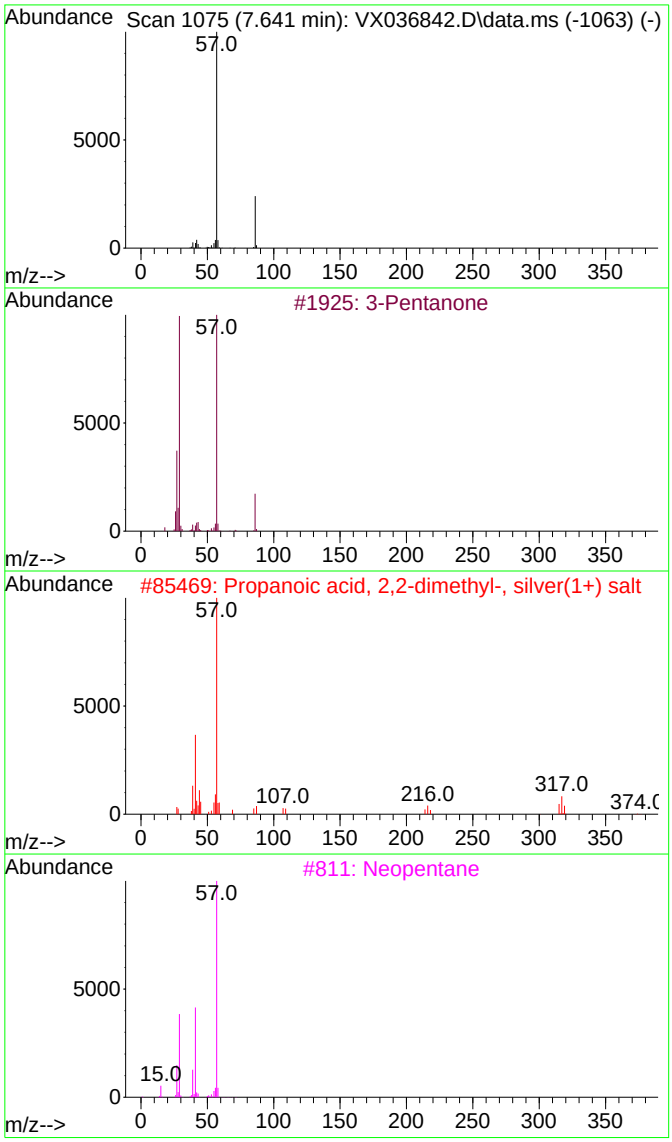
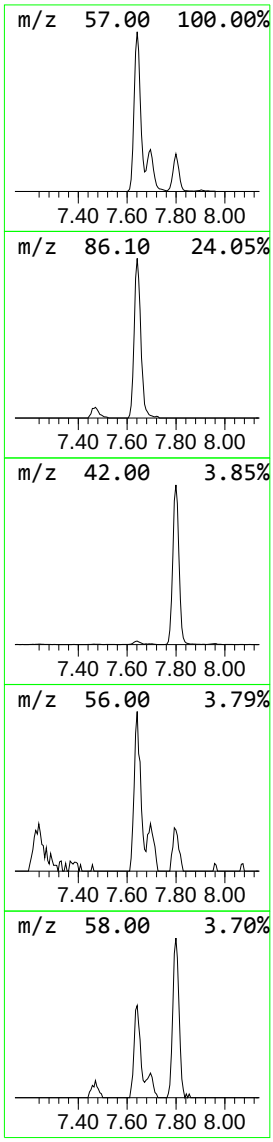
****
Peak Number 2 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	8.99 ug/l	107203	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	90
2	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
3	Neopentane	72	C5H12	000463-82-1	9
4	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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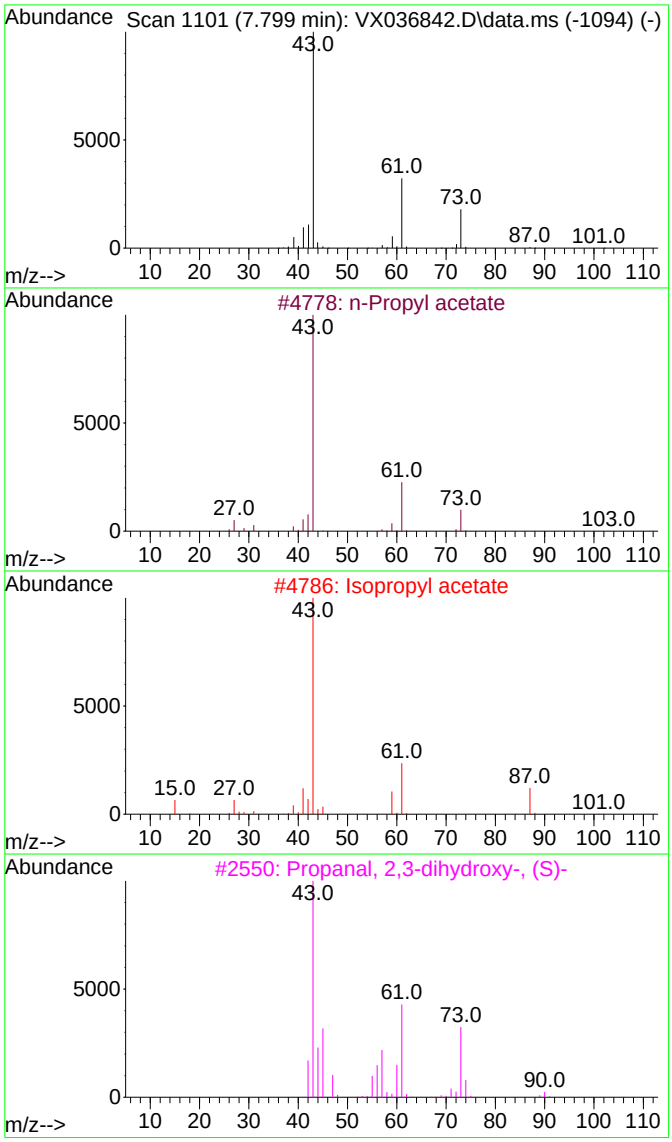
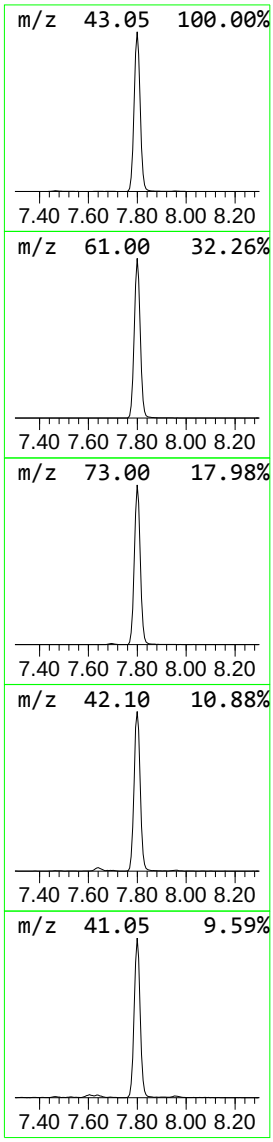
****
Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	171.27 ug/l	2041960	1,4-Difluorobenzene	6.763

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	36
3	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	5





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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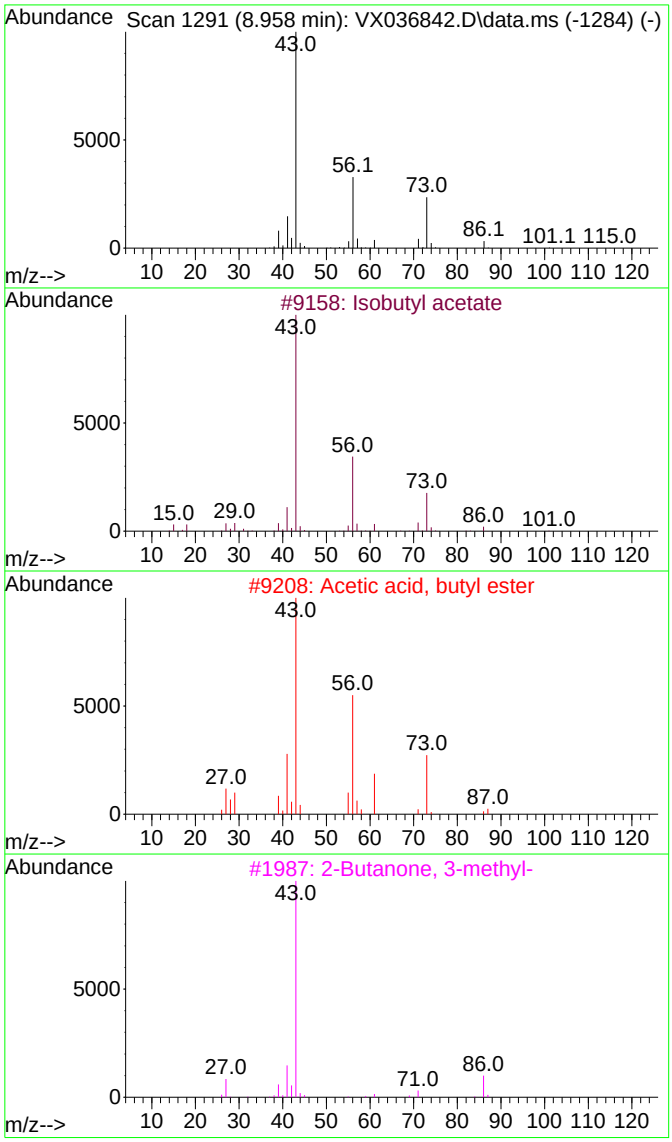
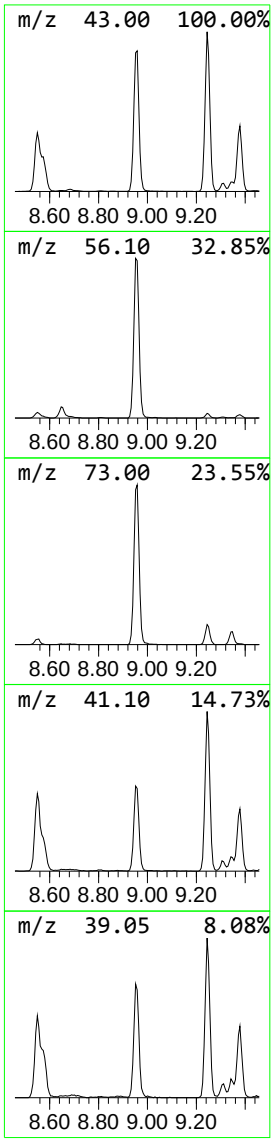
****
Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	33.15 ug/l	502902	Chlorobenzene-d5	10.055

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	9
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
4	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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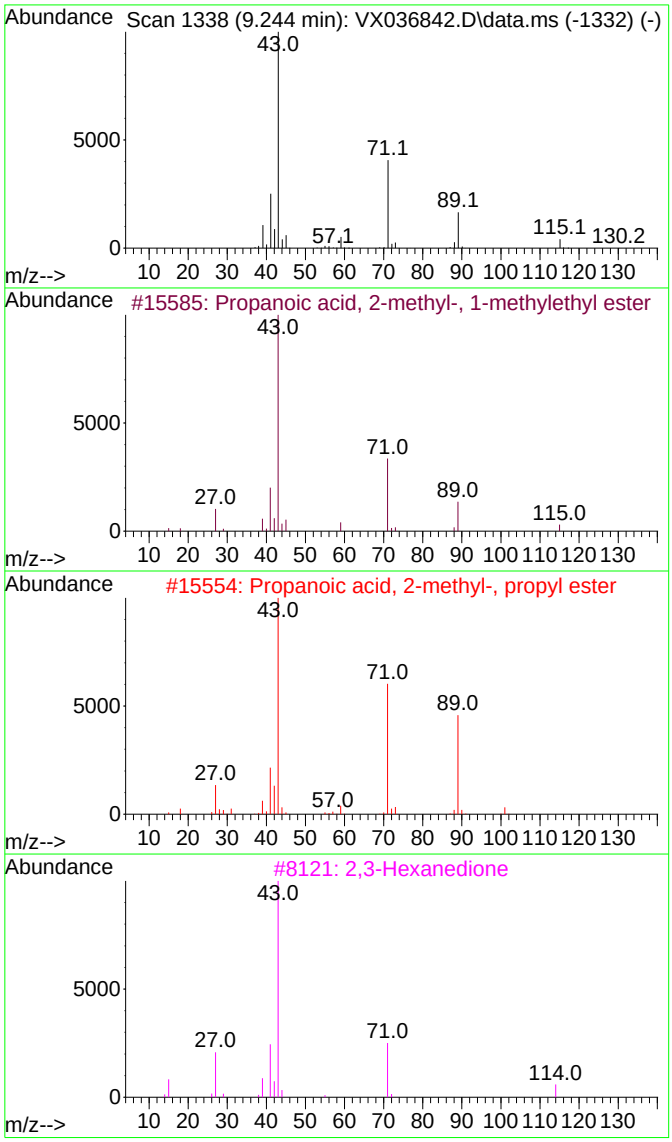
Quant Title : SW846 8260

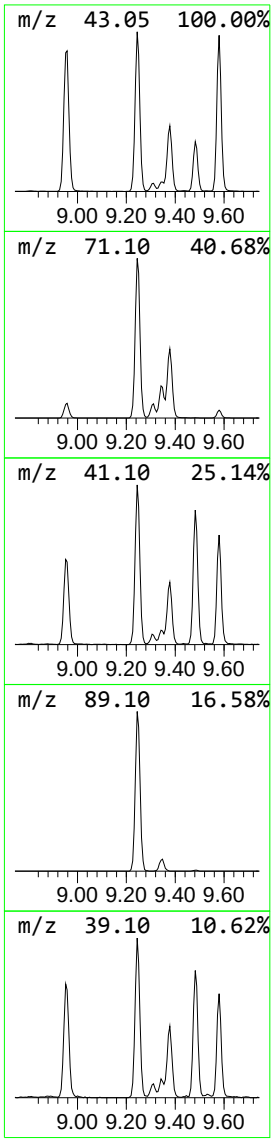
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	37.60 ug/l	570423	Chlorobenzene-d5	10.055

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	59
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	53
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	43
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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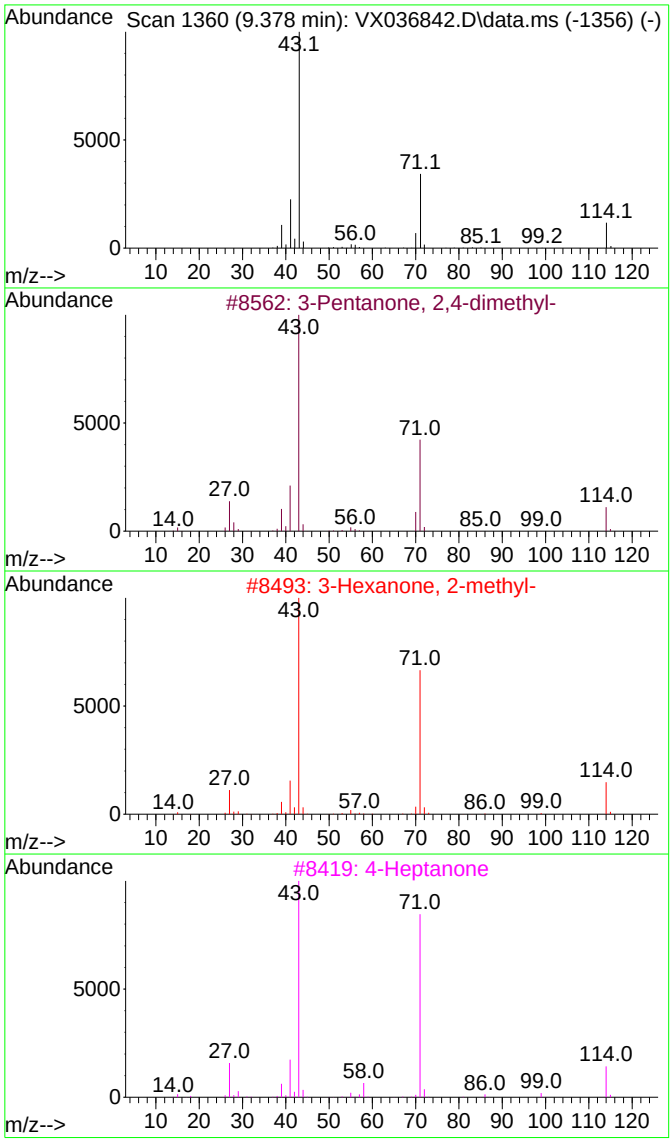
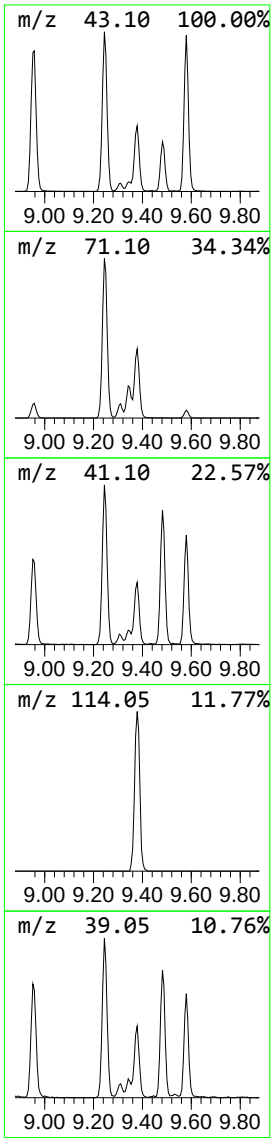
****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	14.97 ug/l	227112	Chlorobenzene-d5	10.055

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	78
3	4-Heptanone	114	C7H14O	000123-19-3	72
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	72
5	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50





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TIC Library : C:\Database\NIST20.L
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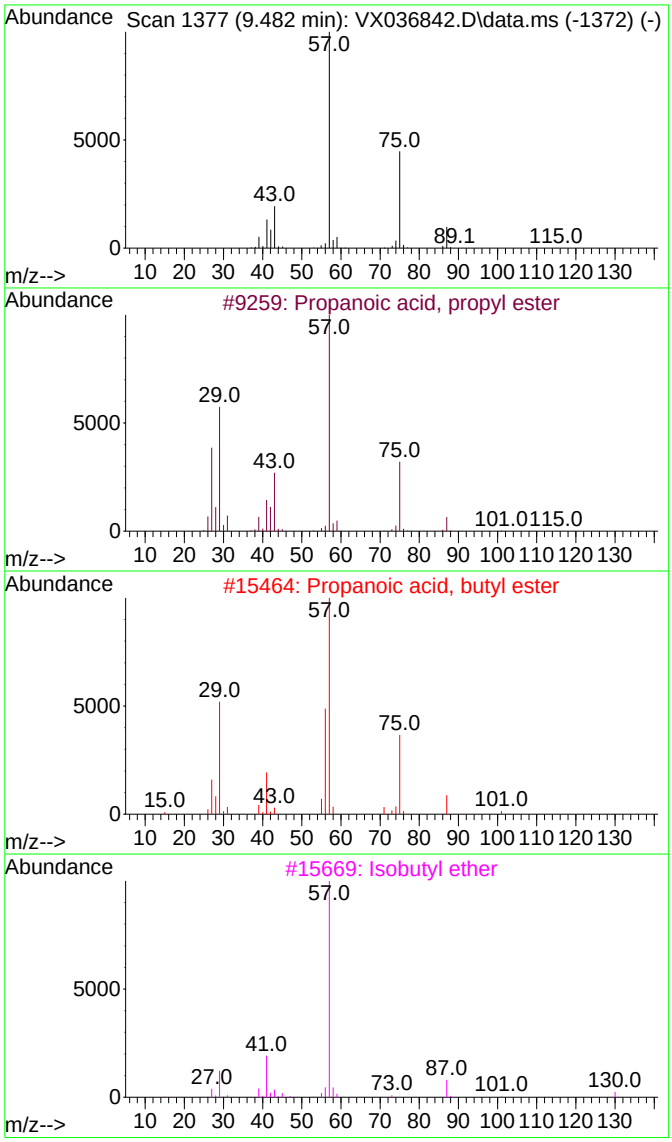
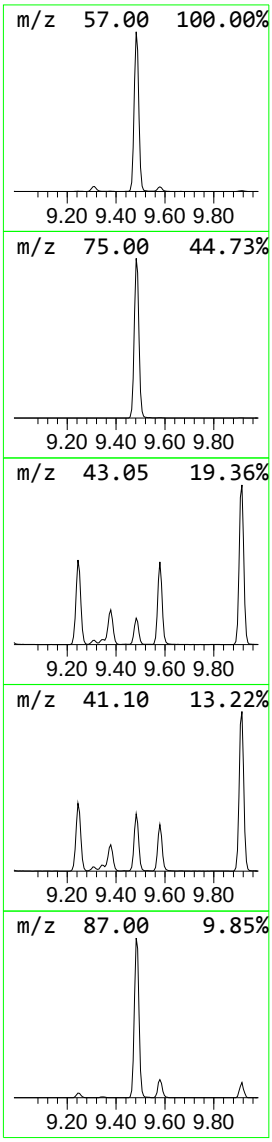
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	54.48 ug/l	826554	Chlorobenzene-d5	10.055

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	12
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





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TIC Library : C:\Database\NIST20.L
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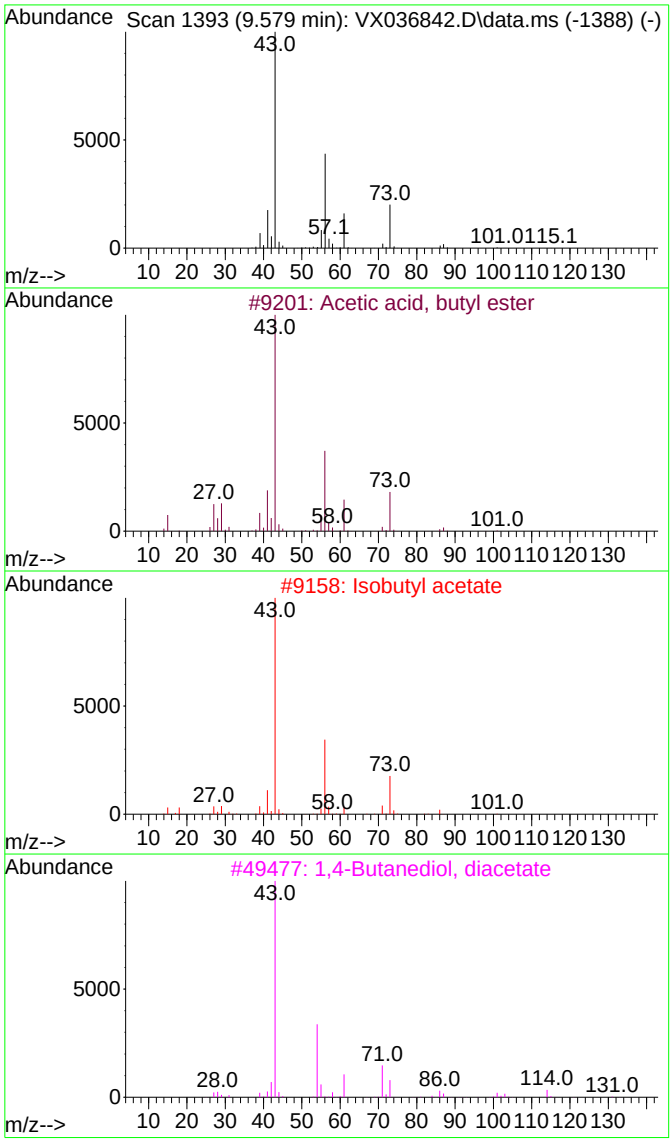
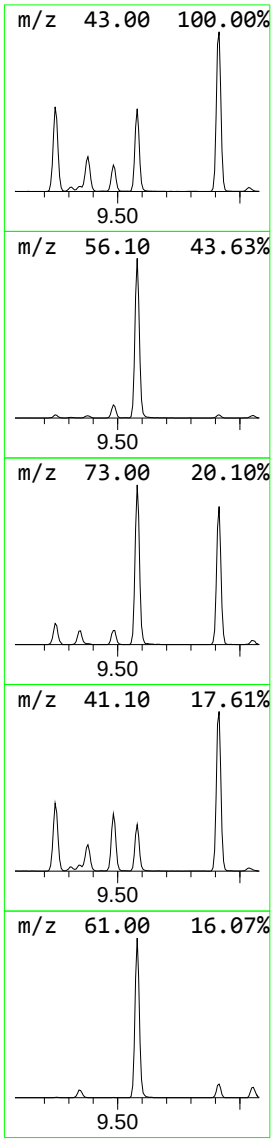
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	34.79 ug/l	527881	Chlorobenzene-d5	10.055

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	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9





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ClientSampleId :
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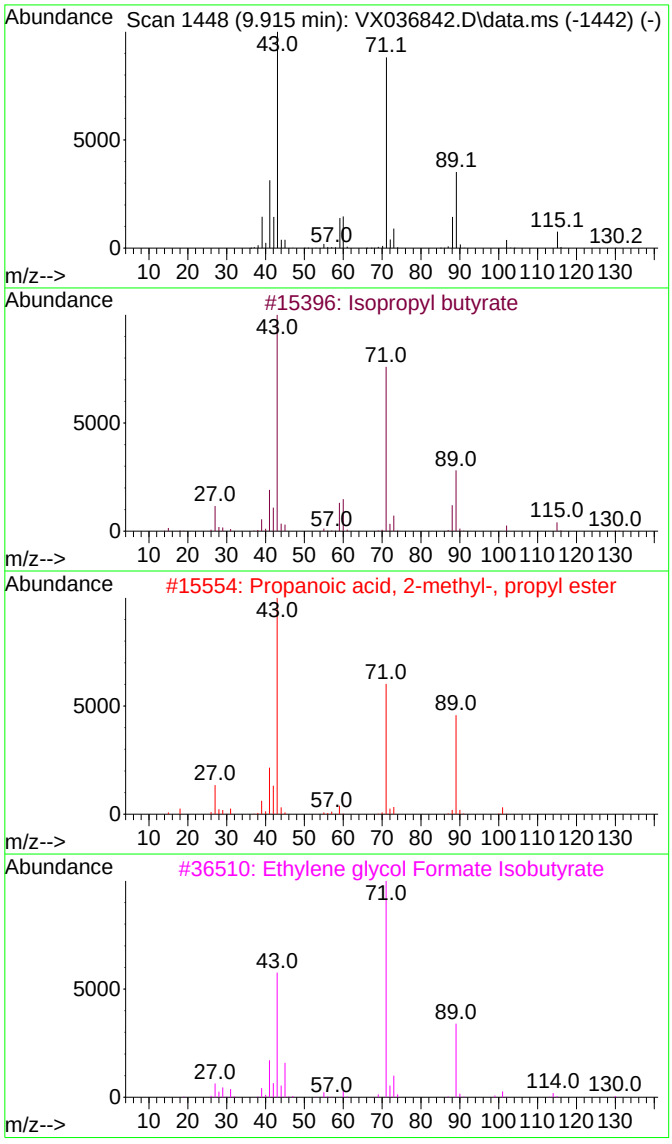
Quant Title : SW846 8260

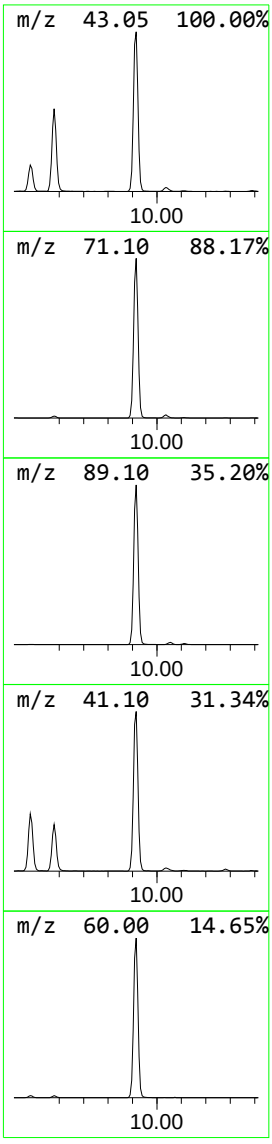
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	104.47 ug/l	1585050	Chlorobenzene-d5	10.055

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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59





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Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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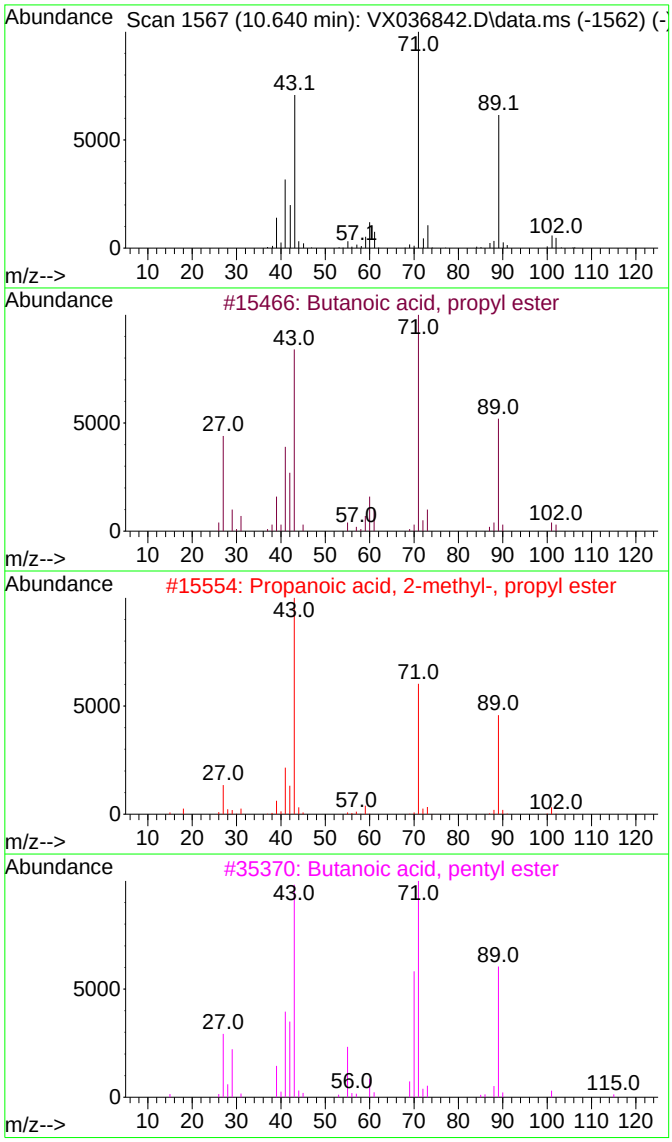
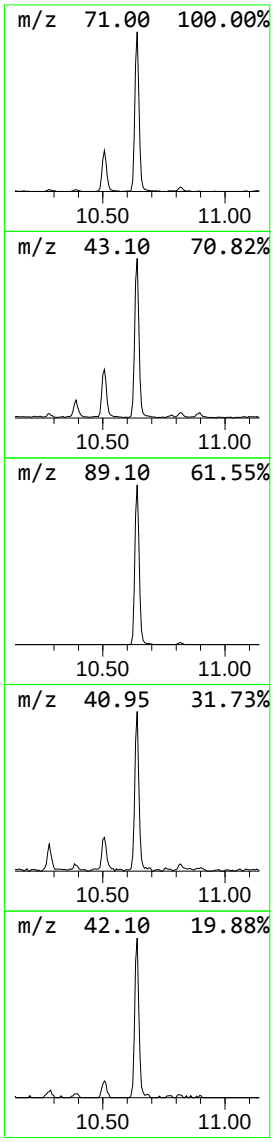
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.96 ug/l	120721	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5	Malic Acid	134	C4H6O5	006915-15-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036842.D
Acq On : 07 Aug 2023 17:17
Operator : JC/MD
Sample : 03891-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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
2-Butenal, (E)-	3.574	5.8	ug/l	49435	1	5.556	428230	50.0
3-Pentanone	7.641	9.0	ug/l	107203	2	6.763	596137	50.0
n-Propyl acetate	7.799	171.3	ug/l	2041960	2	6.763	596137	50.0
Isobutyl acetate	8.958	33.1	ug/l	502902	3	10.055	758613	50.0
Propanoic acid,...	9.244	37.6	ug/l	570423	3	10.055	758613	50.0
3-Pentanone, 2,...	9.378	15.0	ug/l	227112	3	10.055	758613	50.0
Propanoic acid,...	9.482	54.5	ug/l	826554	3	10.055	758613	50.0
Acetic acid, bu...	9.579	34.8	ug/l	527881	3	10.055	758613	50.0
Isopropyl butyrate	9.915	104.5	ug/l	1585050	3	10.055	758613	50.0
Butanoic acid, ...	10.640	8.0	ug/l	120721	3	10.055	758613	50.0