LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030258.D
Acq On : 28 Jul 2022 02:23
Operator : JC/MD
Sample : N3839-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ENV-DE-WC-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\82X072522W.M
Title : SW846 8260

Signal : TIC: VX030258.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	204	212	221	rBV	45385	76066	3.14%	0.539%
2	2.788	272	279	290	rVB	37843	69413	2.86%	0.492%
3	4.721	588	596	608	rBV	20163	56530	2.33%	0.400%
4	5.391	694	706	722	rBV	125685	361373	14.90%	2.560%
5	5.562	722	734	751	rVB	126024	360374	14.85%	2.553%
6	5.964	788	800	814	rBV	151265	401769	16.56%	2.846%
7	6.348	853	863	874	rBV	106883	274780	11.33%	1.947%
8	6.769	922	932	946	rBV	212745	533480	21.99%	3.779%
9	7.641	1062	1075	1081	rBV	79112	156375	6.45%	1.108%
10	7.696	1081	1084	1094	rVB	20850	34345	1.42%	0.243%
11	7.799	1094	1101	1117	rBV	1178021	2053523	84.65%	14.547%
12	8.549	1217	1224	1234	rBV	303084	484118	19.96%	3.430%
13	8.653	1234	1241	1250	rBV	666012	1039457	42.85%	7.364%
14	8.958	1284	1291	1300	rBV	249262	356241	14.68%	2.524%
15	9.250	1333	1339	1345	rBV	381303	549911	22.67%	3.896%
16	9.311	1345	1349	1352	rVV	54048	77674	3.20%	0.550%
17	9.348	1352	1355	1356	rVV	47914	56882	2.34%	0.403%
18	9.378	1356	1360	1367	rVB	212786	308745	12.73%	2.187%
19	9.488	1372	1378	1385	rBV	547870	721144	29.73%	5.109%
20	9.580	1385	1393	1421	rBV	997755	2425958	100.00%	17.186%
21	9.915	1442	1448	1456	rBV	1090750	1381464	56.95%	9.786%
22	10.055	1464	1471	1477	rBV	544194	745067	30.71%	5.278%
23	10.506	1540	1545	1554	rVB	25164	32810	1.35%	0.232%
24	10.640	1563	1567	1572	rBV2	62811	90642	3.74%	0.642%
25	11.085	1634	1640	1651	rBV	531504	680372	28.05%	4.820%
26	12.024	1789	1794	1800	rBV	652426	787629	32.47%	5.580%

Sum of corrected areas: 14116142

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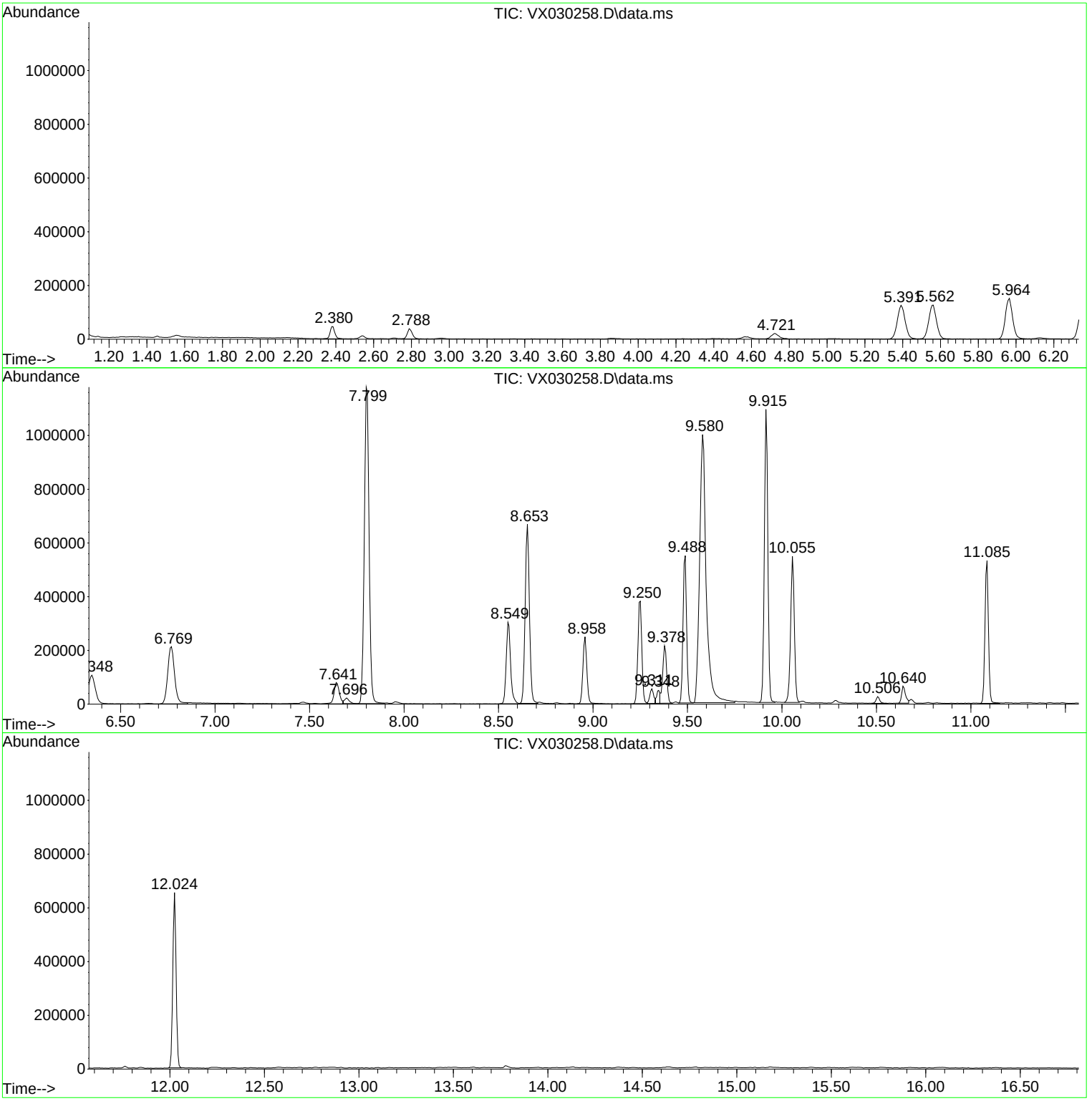
MSVOA_X
ClientSampleId :
ENV-DE-WC-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



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Data File : VX030258.D
Acq On : 28 Jul 2022 02:23
Operator : JC/MD
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Instrument :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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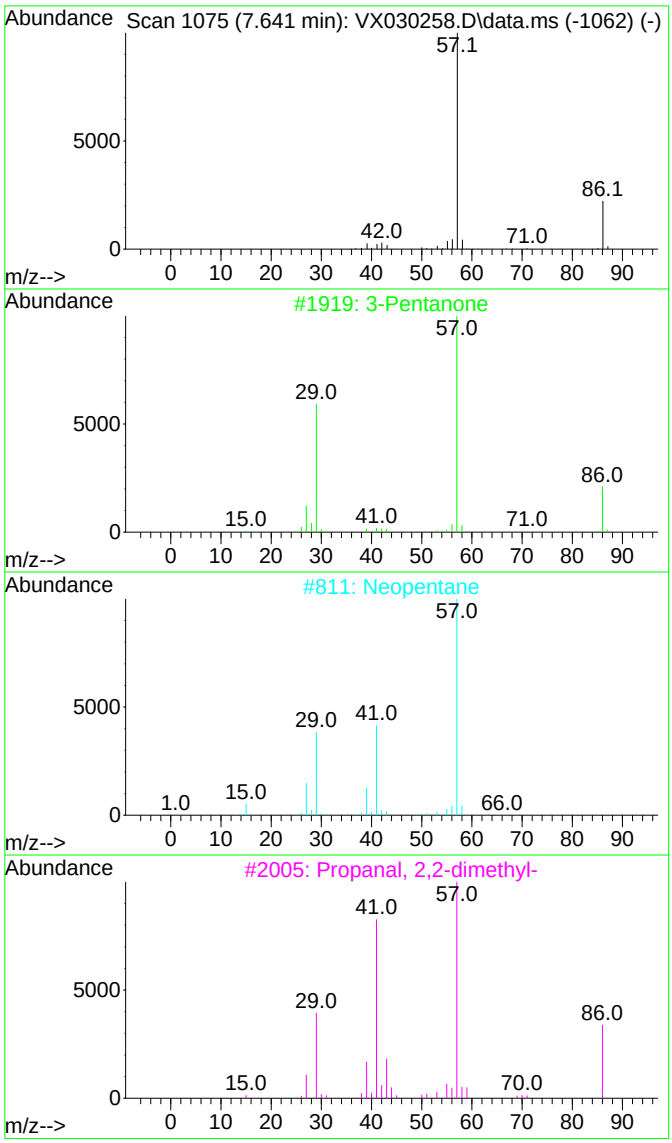
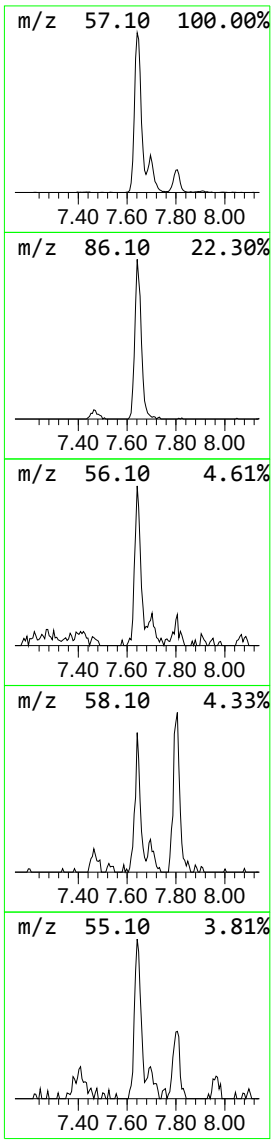
****
Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	14.66 ug/l	156375	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Neopentane	72	C5H12	000463-82-1	28
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
4	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9





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Data File : VX030258.D
Acq On : 28 Jul 2022 02:23
Operator : JC/MD
Sample : N3839-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ENV-DE-WC-1

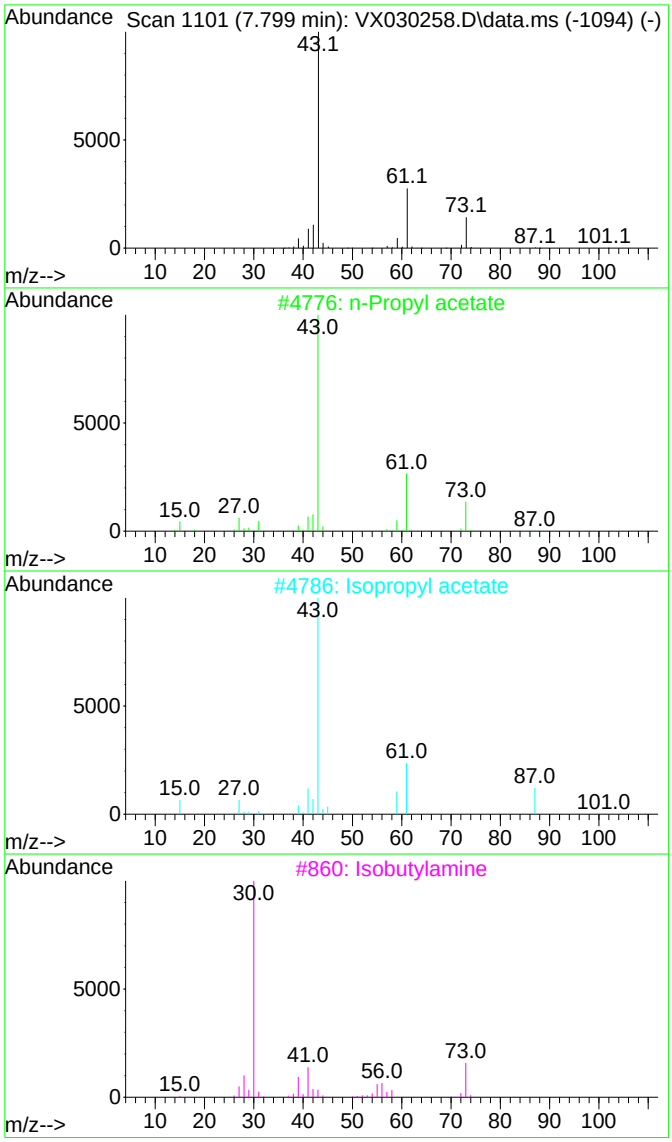
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

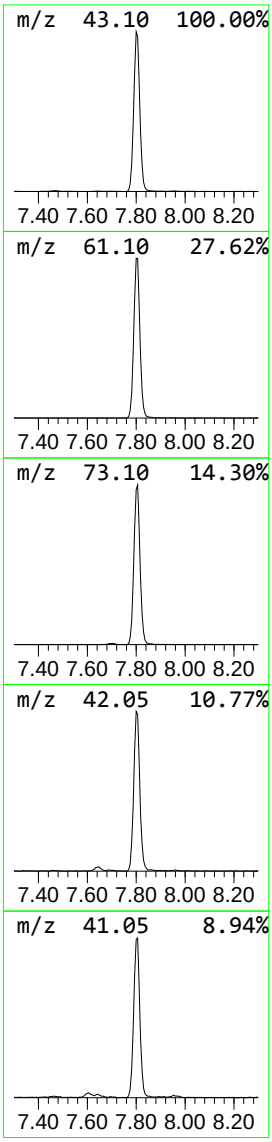
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	192.47 ug/l	2053520	1,4-Difluorobenzene	6.769

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	Isobutylamine	73	C4H11N	000078-81-9	7
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4





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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ENV-DE-WC-1

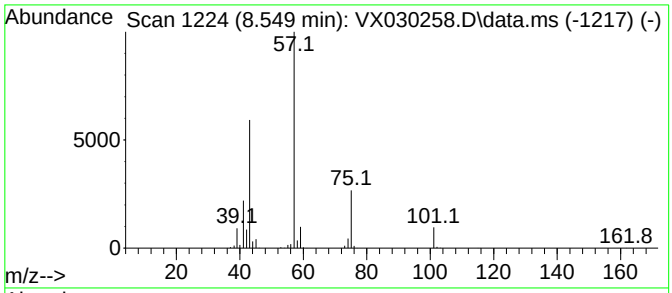
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

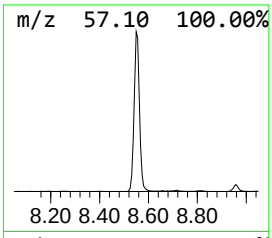
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

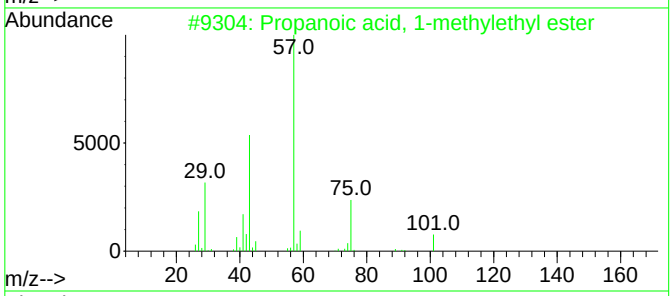
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

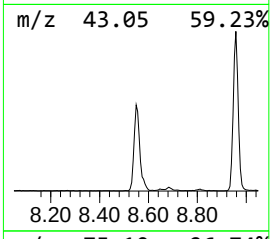
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	32.49 ug/l	484118	Chlorobenzene-d5	10.055

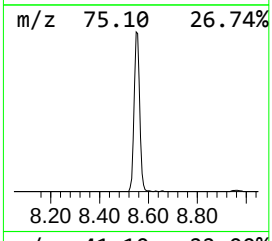
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9

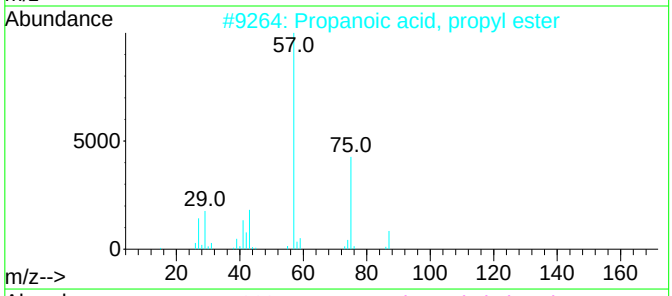


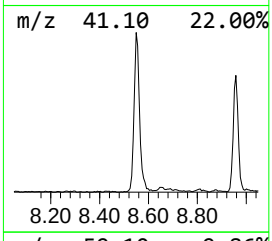


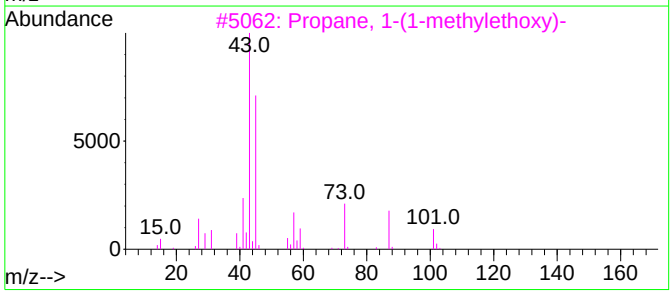


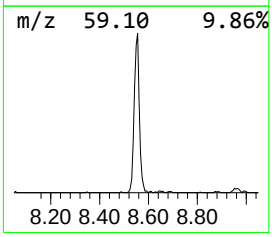












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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ENV-DE-WC-1

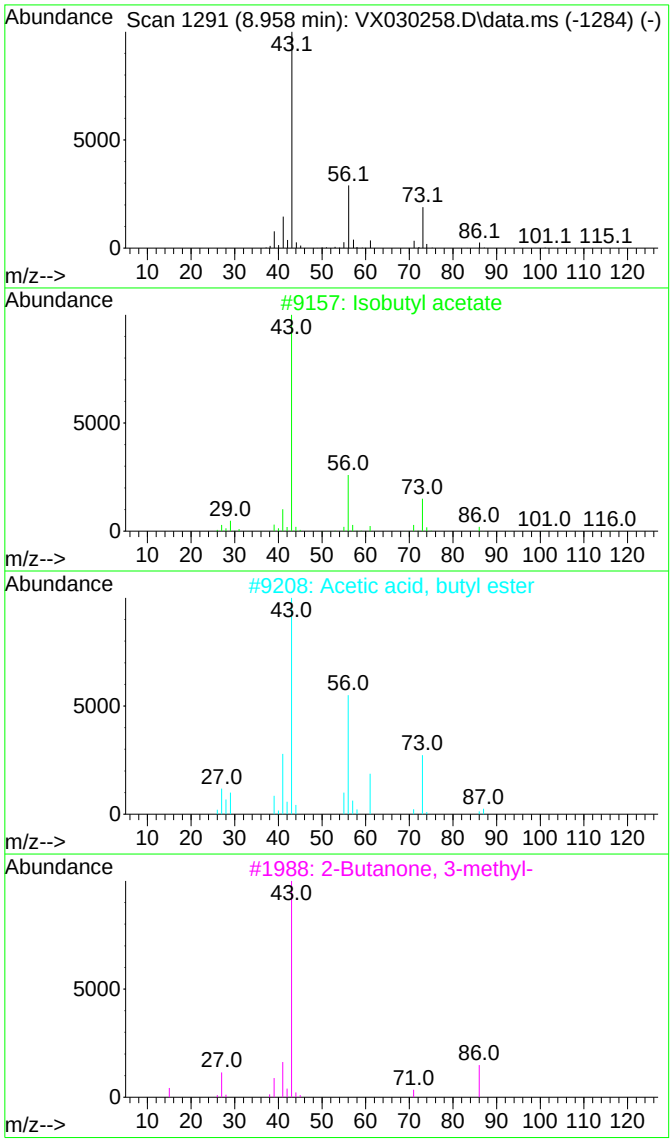
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

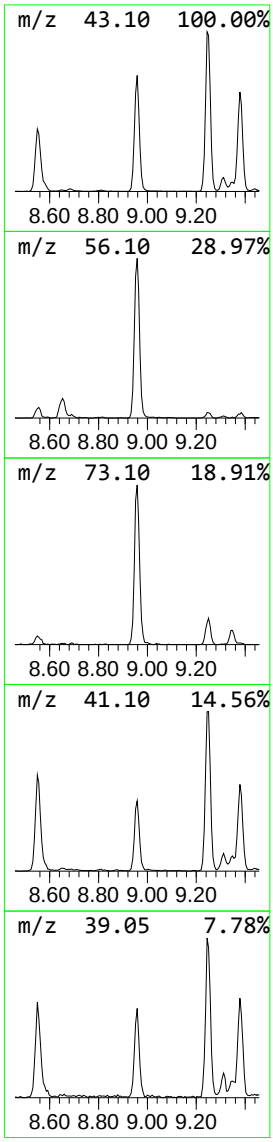
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	23.91 ug/l	356241	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	36
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	27
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9





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Instrument :
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ClientSampleId :
ENV-DE-WC-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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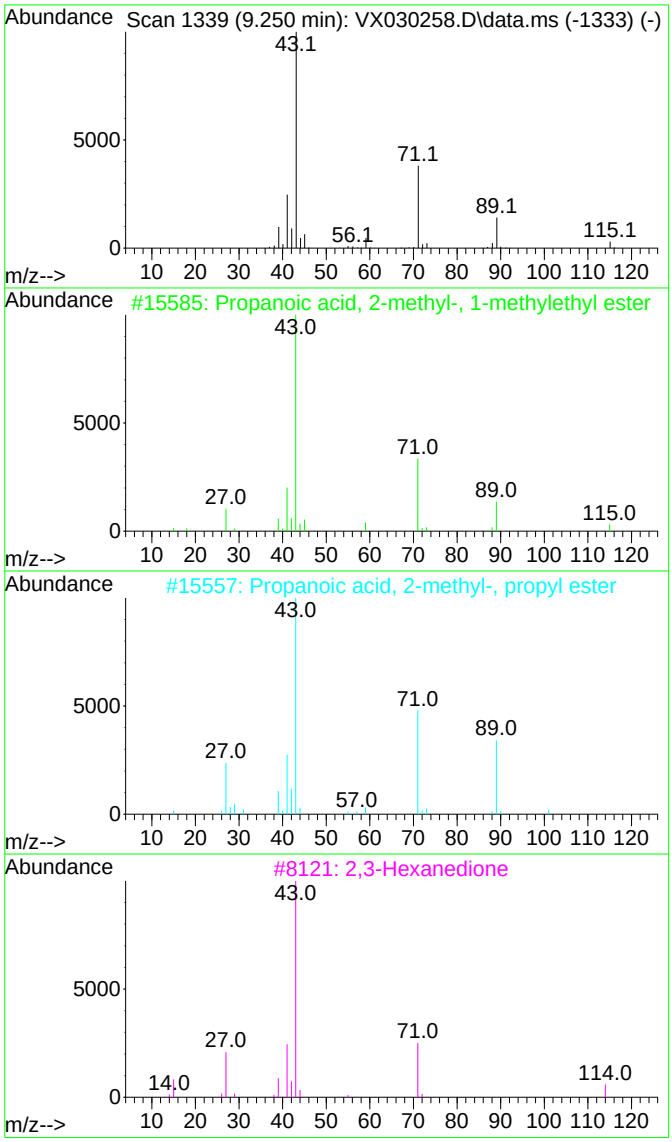
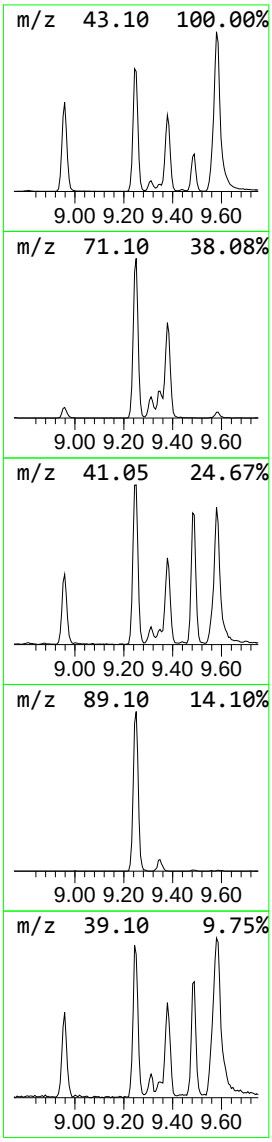
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.250	36.90 ug/l	549911	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	78
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	59
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	45
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	45





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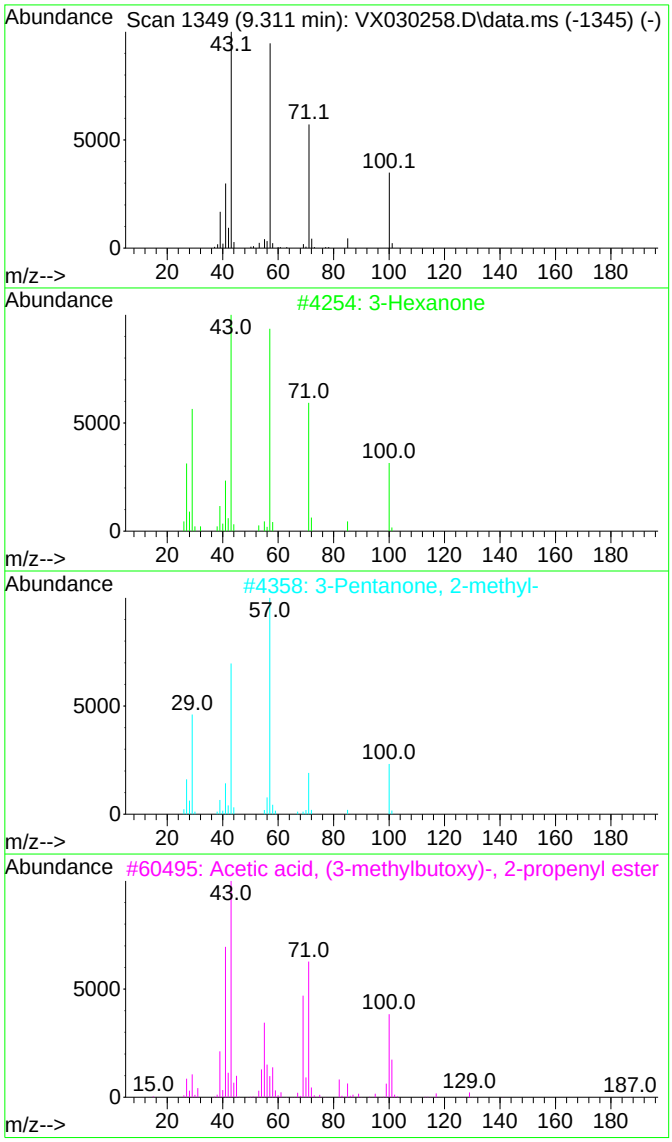
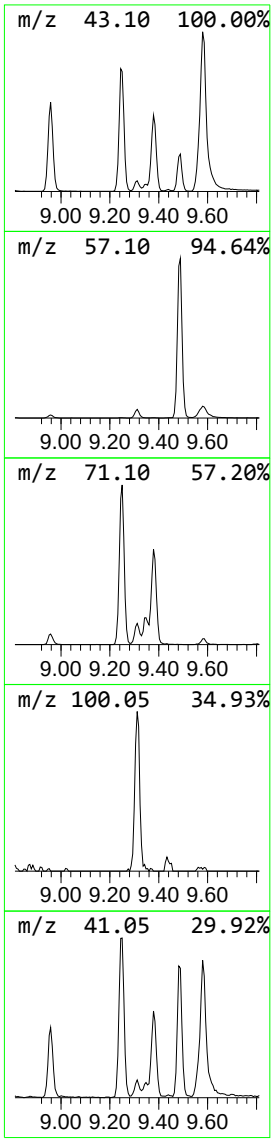
****

Peak Number 6 3-Hexanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.311	5.21 ug/l	77674	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone	100	C6H12O	000589-38-8	90
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	40
3	Acetic acid, (3-methylbutoxy)-, ...	186	C10H18O3	067634-00-8	39
4	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	37
5	Acetylacetone	100	C5H8O2	000123-54-6	35





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TIC Library : C:\Database\NIST20.L
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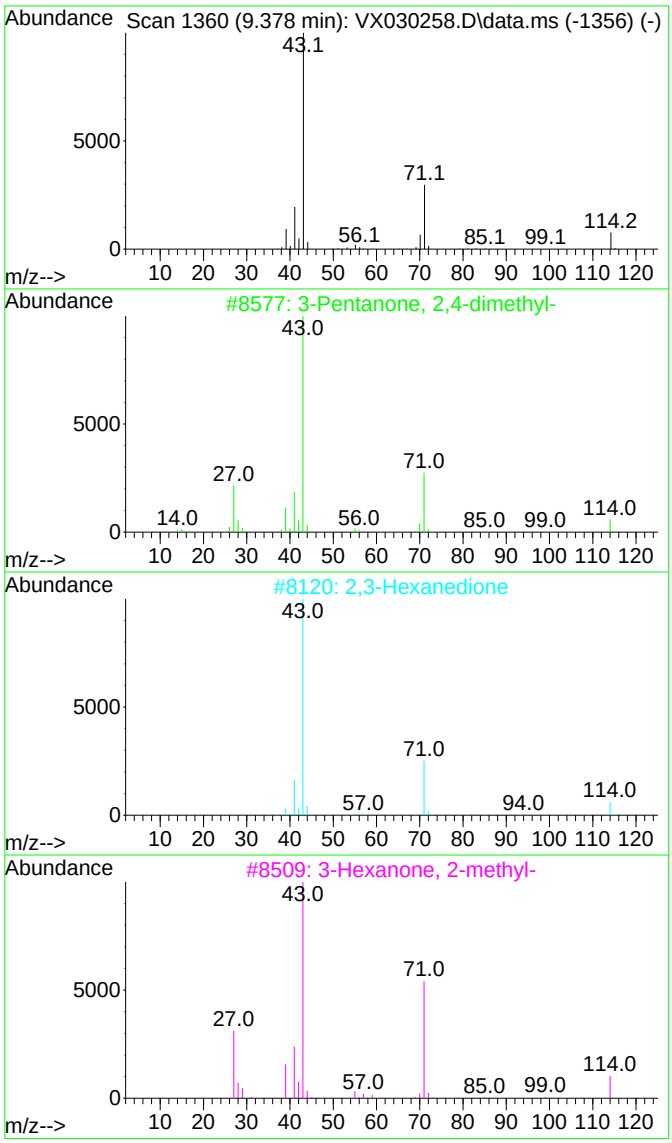
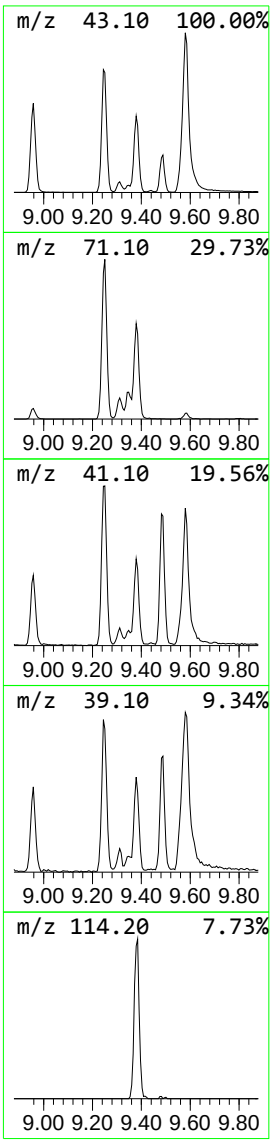
****
Peak Number 7 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	20.72 ug/l	308745	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	80
3	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	59
4	2,5-Hexanedione	114	C6H10O2	000110-13-4	42
5	4-Heptanone	114	C7H14O	000123-19-3	42





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MSVOA_X
ClientSampleId :
ENV-DE-WC-1

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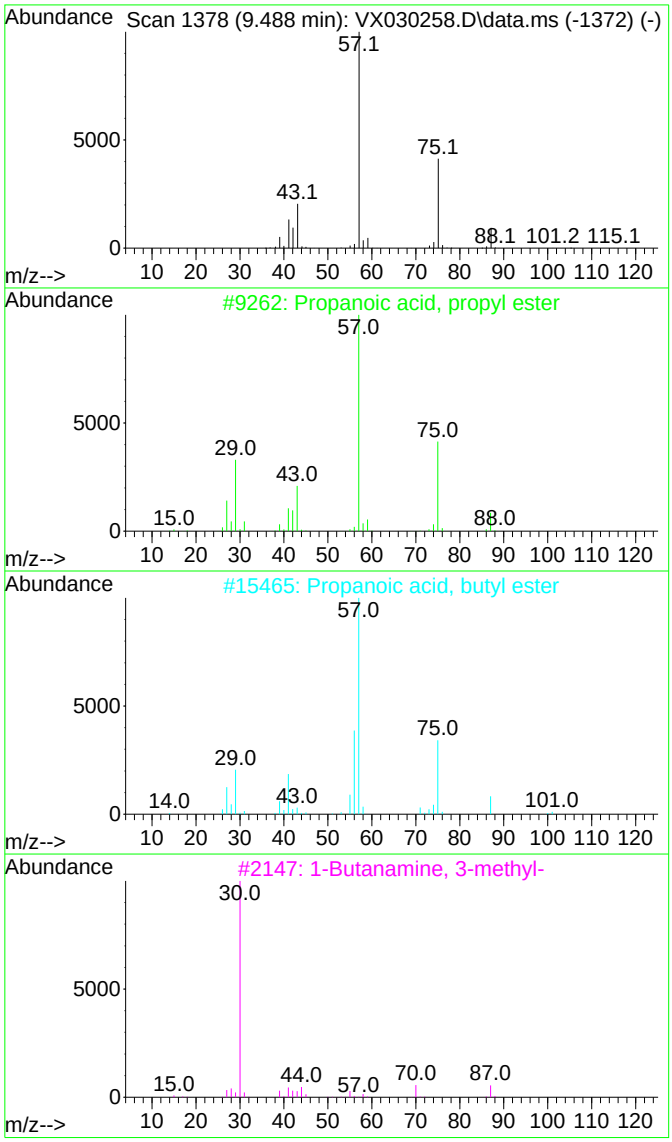
Quant Title : SW846 8260

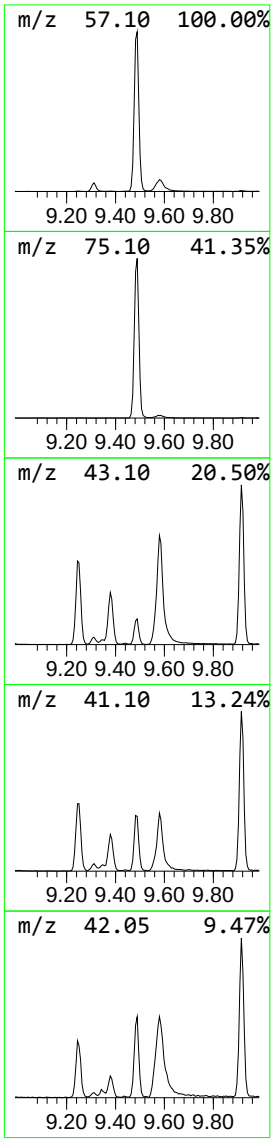
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	48.39 ug/l	721144	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	39
3	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
4	1-Penten-3-ol	86	C5H10O	000616-25-1	7
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030258.D
Acq On : 28 Jul 2022 02:23
Operator : JC/MD
Sample : N3839-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ENV-DE-WC-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

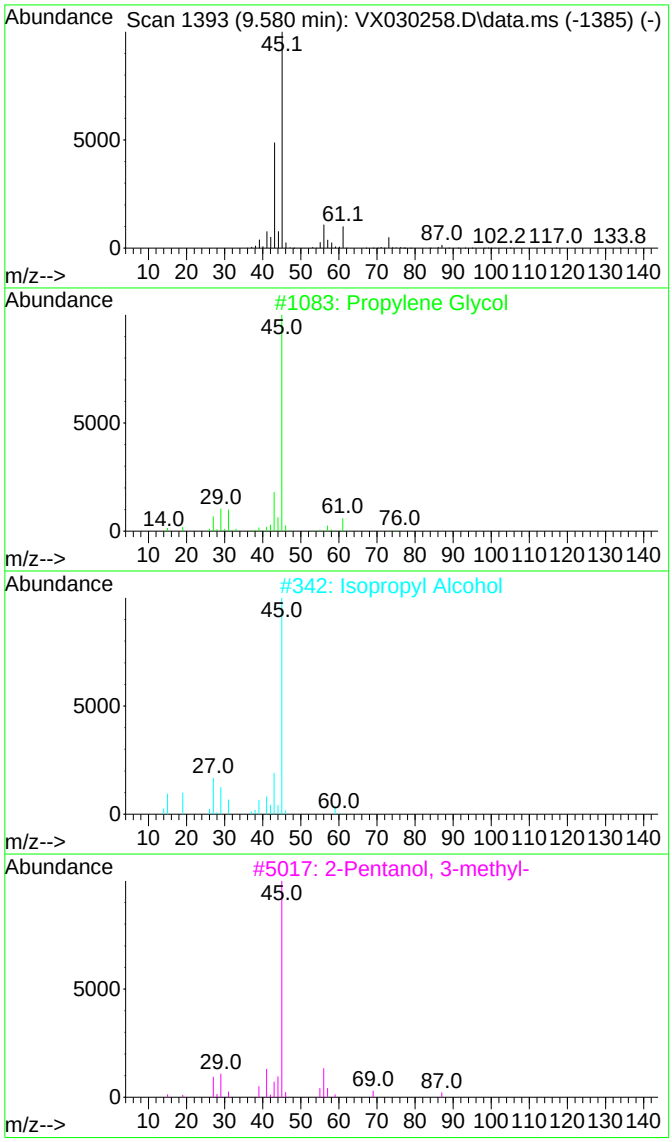
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

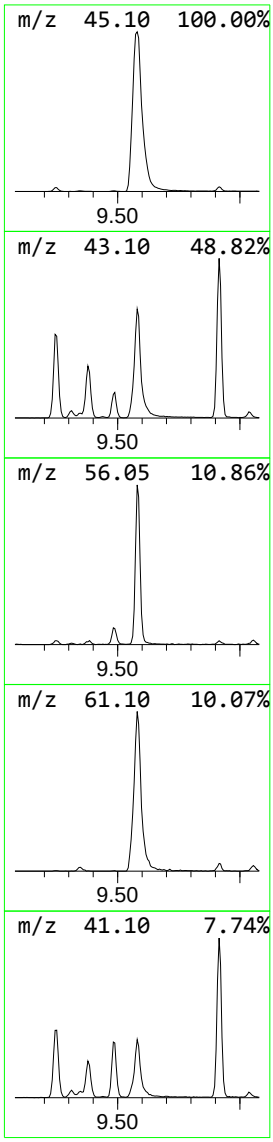
****

Peak Number 9 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	162.80 ug/l	2425960	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	64
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	50
4	(+-)-5-Methyl-2-hexanol	116	C7H16O	111768-09-3	38
5	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030258.D
Acq On : 28 Jul 2022 02:23
Operator : JC/MD
Sample : N3839-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ENV-DE-WC-1

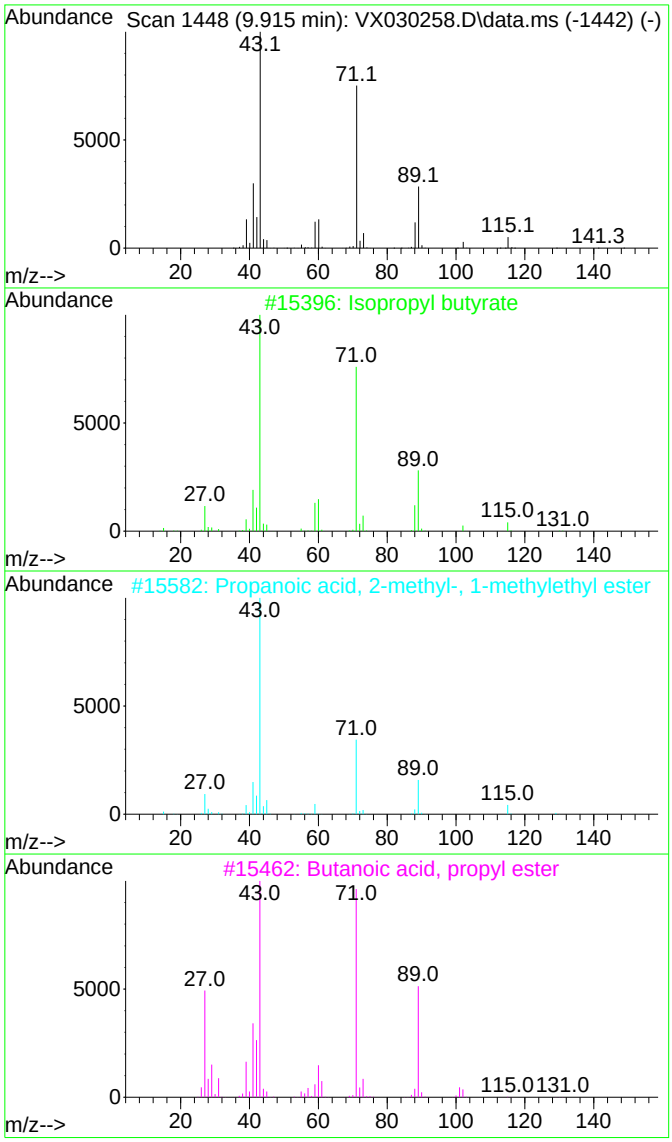
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

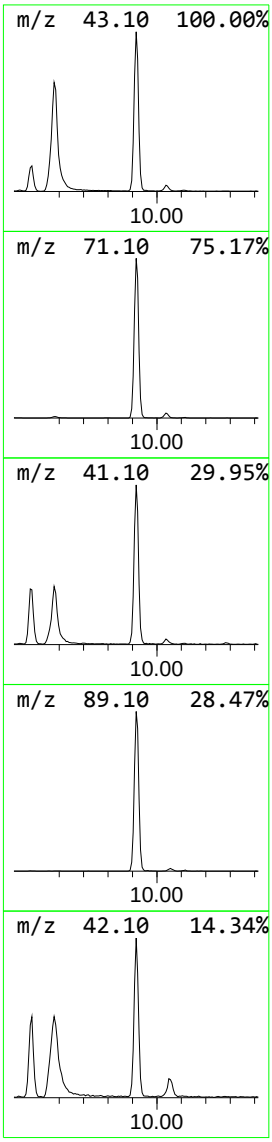
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	92.71 ug/l	1381460	Chlorobenzene-d5	10.055

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	78
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030258.D
Acq On : 28 Jul 2022 02:23
Operator : JC/MD
Sample : N3839-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ENV-DE-WC-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.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
3-Pentanone	7.641	14.7	ug/l	156375	2	6.769	533480	50.0
n-Propyl acetate	7.799	192.5	ug/l	2053520	2	6.769	533480	50.0
Propanoic acid,...	8.549	32.5	ug/l	484118	3	10.055	745067	50.0
Isobutyl acetate	8.958	23.9	ug/l	356241	3	10.055	745067	50.0
Propanoic acid,...	9.250	36.9	ug/l	549911	3	10.055	745067	50.0
3-Hexanone	9.311	5.2	ug/l	77674	3	10.055	745067	50.0
3-Pentanone, 2,...	9.378	20.7	ug/l	308745	3	10.055	745067	50.0
Propanoic acid,...	9.488	48.4	ug/l	721144	3	10.055	745067	50.0
Propylene Glycol	9.580	162.8	ug/l	2425960	3	10.055	745067	50.0
Isopropyl butyrate	9.915	92.7	ug/l	1381460	3	10.055	745067	50.0