LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036844.D
Acq On : 07 Aug 2023 18:05
Operator : JC/MD
Sample : 03891-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-3

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: VX036844.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.379	207	212	223	rBV	37397	62682	3.58%	0.566%
2	2.788	272	279	290	rBV	21369	45617	2.60%	0.412%
3	3.580	400	409	421	rBV	10560	25501	1.46%	0.230%
4	4.568	561	571	585	rBV2	12208	39064	2.23%	0.352%
5	5.385	694	705	722	rBV2	92373	272318	15.55%	2.457%
6	5.556	722	733	748	rVV	147618	422353	24.11%	3.811%
7	5.958	786	799	816	rBV	99030	263930	15.07%	2.381%
8	6.342	850	862	878	rBV	83241	216984	12.39%	1.958%
9	6.763	922	931	948	rBV	245595	589954	33.68%	5.323%
10	7.641	1064	1075	1080	rBV	52193	97961	5.59%	0.884%
11	7.689	1080	1083	1093	rVB	16341	31160	1.78%	0.281%
12	7.799	1093	1101	1115	rBV	1025050	1751787	100.00%	15.807%
13	8.549	1217	1224	1234	rBV2	267630	526676	30.07%	4.752%
14	8.647	1234	1240	1249	rBV	499920	806897	46.06%	7.281%
15	8.951	1284	1290	1304	rBV	264095	395012	22.55%	3.564%
16	9.244	1332	1338	1344	rBV	360882	487087	27.81%	4.395%
17	9.305	1344	1348	1351	rVV	33190	48129	2.75%	0.434%
18	9.342	1351	1354	1356	rVV	53653	70241	4.01%	0.634%
19	9.378	1356	1360	1366	rVB	140679	204109	11.65%	1.842%
20	9.482	1372	1377	1384	rBV	563007	728157	41.57%	6.570%
21	9.579	1388	1393	1409	rVB	328232	423636	24.18%	3.823%
22	9.915	1442	1448	1463	rBV	1086638	1362436	77.77%	12.294%
23	10.055	1463	1471	1478	rBV	544368	759949	43.38%	6.857%
24	10.280	1501	1508	1516	rBV2	12622	19228	1.10%	0.173%
25	10.506	1541	1545	1553	rVB	17603	22707	1.30%	0.205%
26	10.640	1562	1567	1578	rBV	86171	104043	5.94%	0.939%
27	11.079	1634	1639	1649	rBV	440653	564078	32.20%	5.090%
28	11.555	1713	1717	1723	rBV2	14173	18662	1.07%	0.168%
29	12.024	1788	1794	1805	rBV	522429	685109	39.11%	6.182%
30	12.219	1821	1826	1837	rBV	21887	37084	2.12%	0.335%

Sum of corrected areas: 11082551

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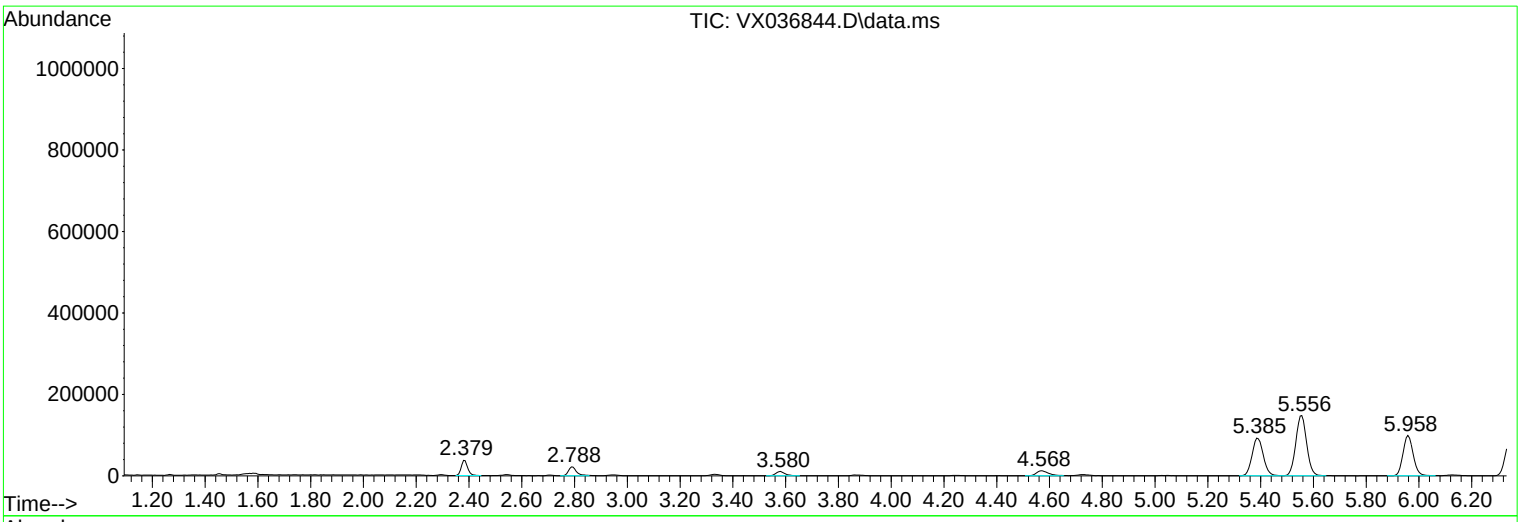
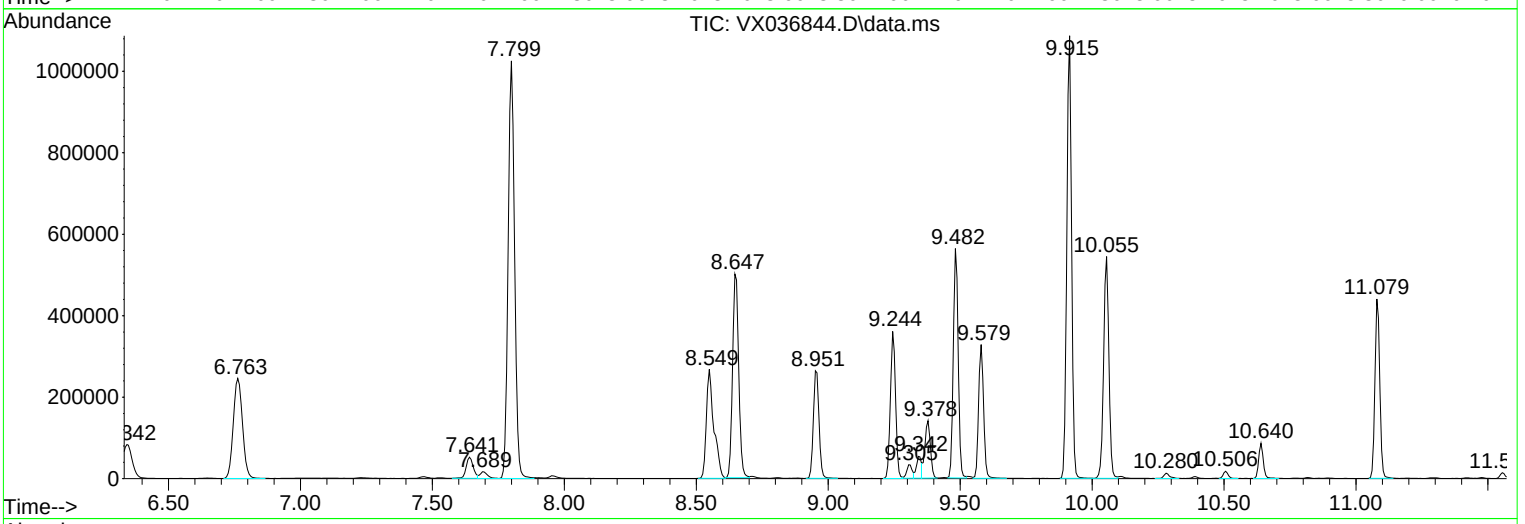
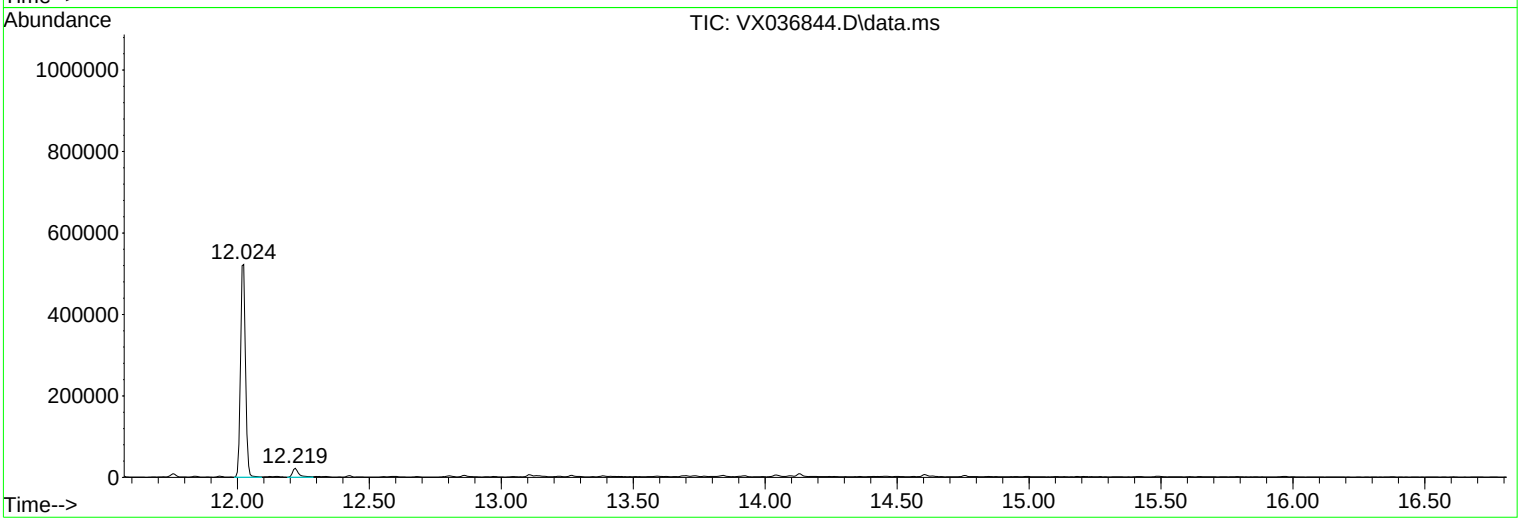
MSVOA_X
ClientSampleId :
TP-3

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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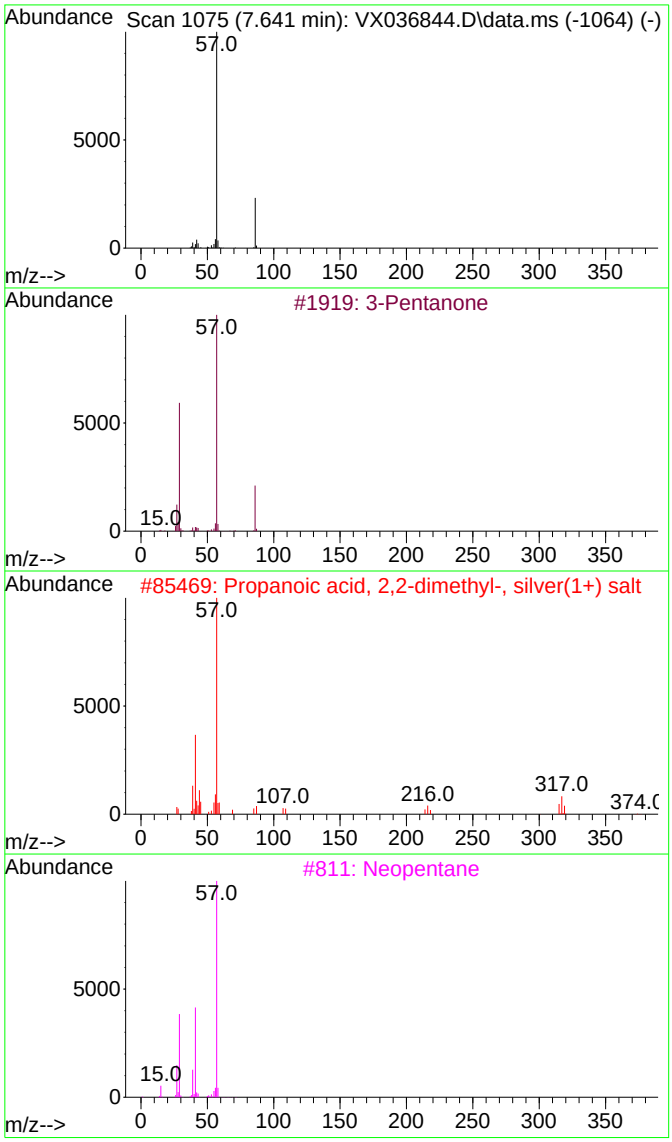
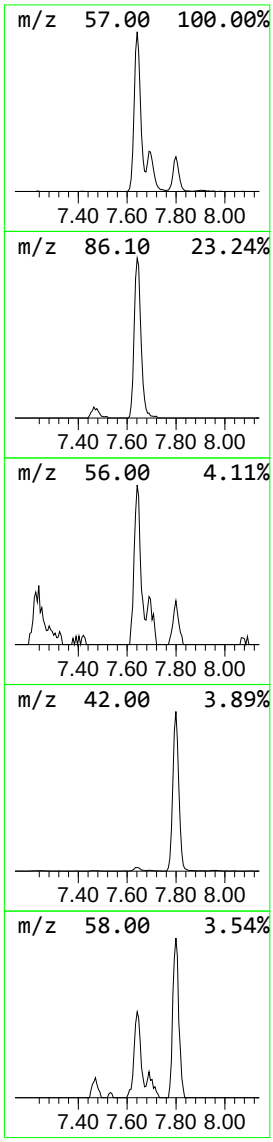
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	8.30 ug/l	97961	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
3	Neopentane	72	C5H12	000463-82-1	9
4	2,2-Dimethylpropanoic anhydride	186	C10H18O3	001538-75-6	9
5	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7





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Quant Title : SW846 8260

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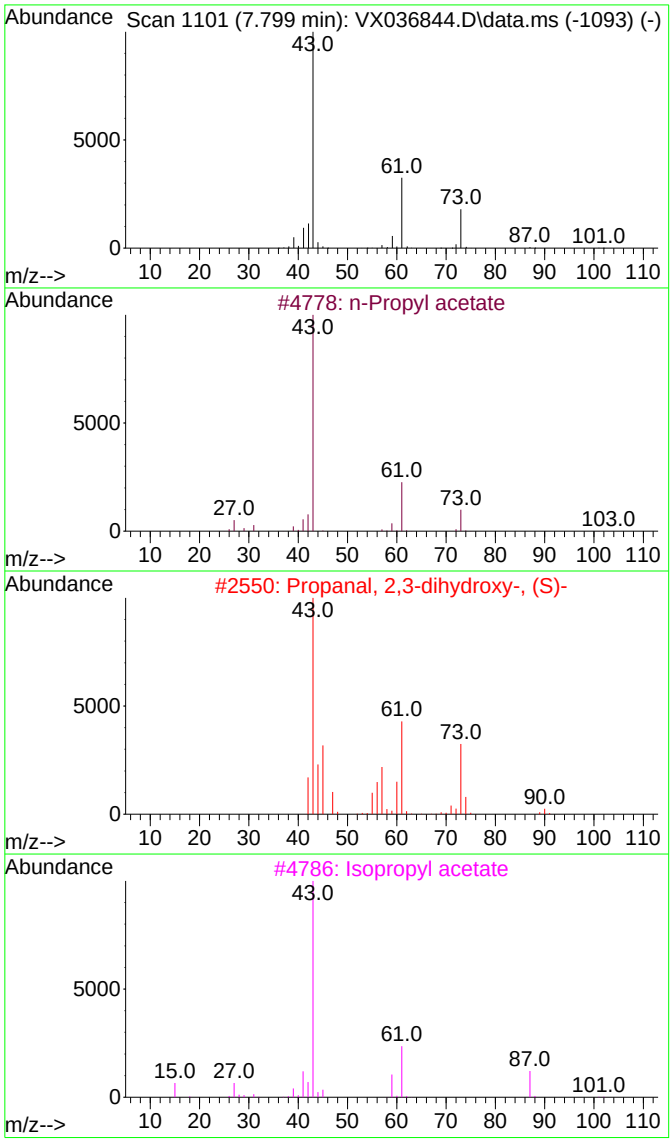
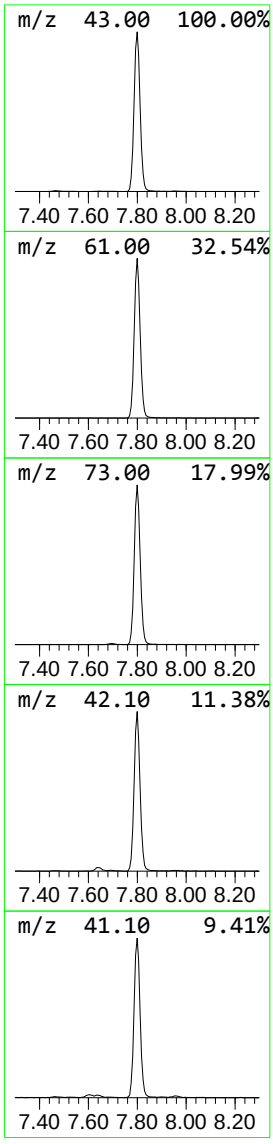
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	148.47 ug/l	1751790	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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
3	Isopropyl acetate	102	C5H10O2	000108-21-4	36
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	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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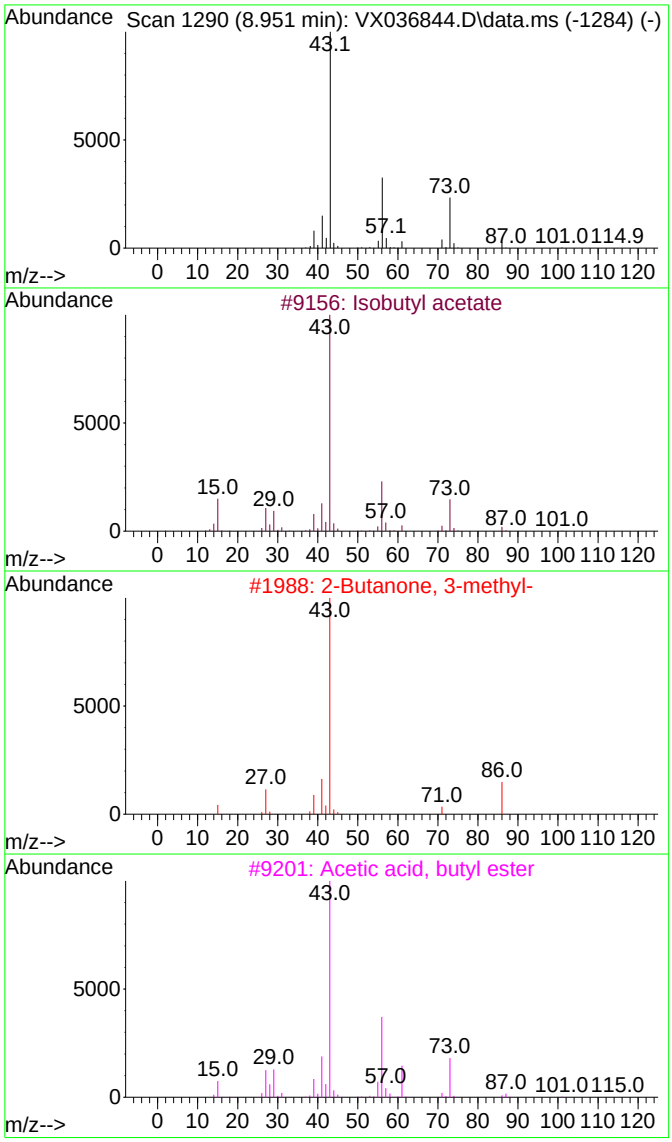
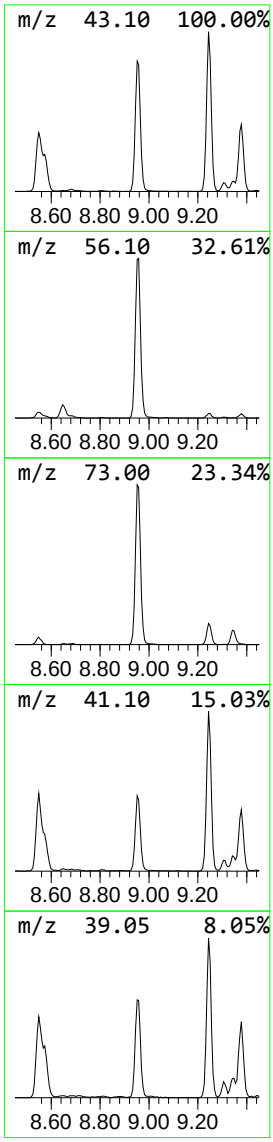
****
Peak Number 3 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.951	25.99 ug/l	395012	Chlorobenzene-d5	10.055

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	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
4	2-Pentanone	86	C5H10O	000107-87-9	9
5	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9





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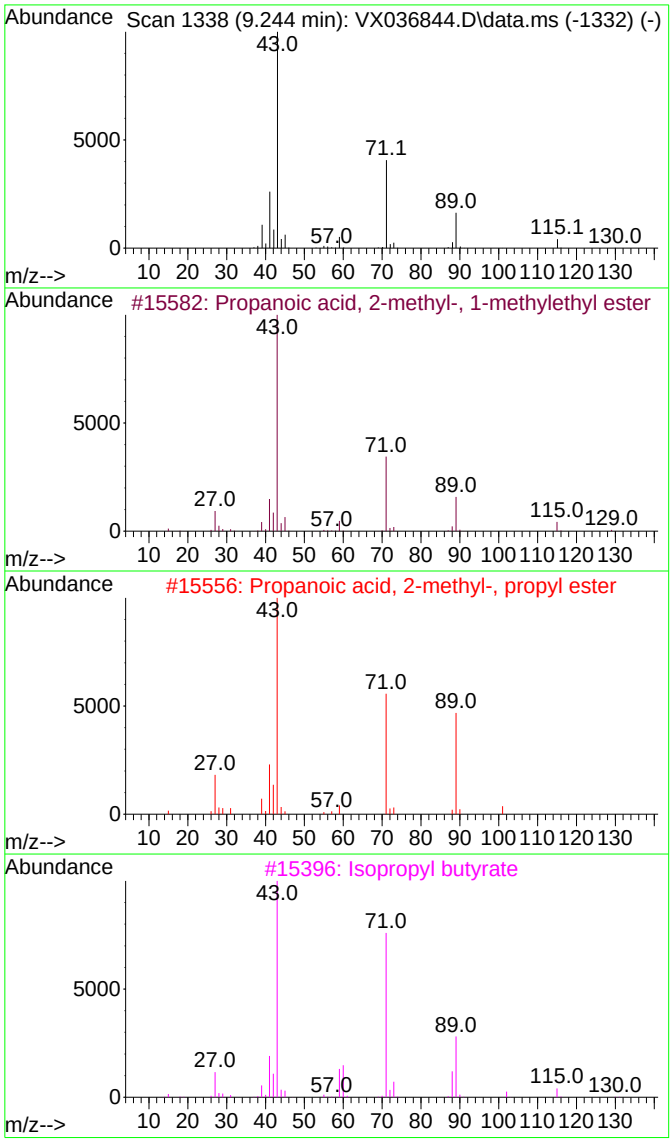
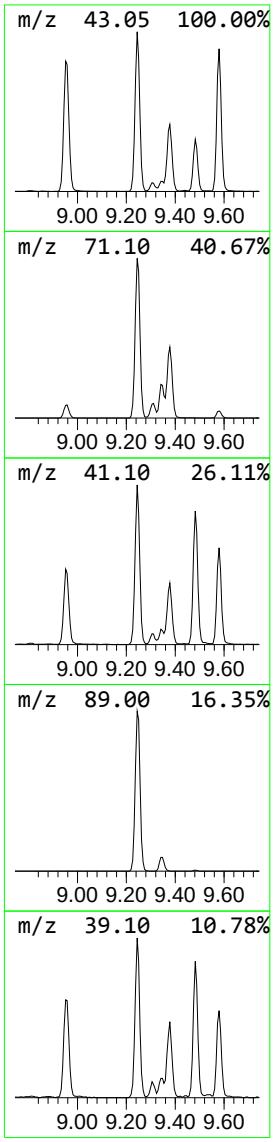
****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	32.05 ug/l	487087	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	Isopropyl butyrate	130	C7H14O2	000638-11-9	56
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	42
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	40





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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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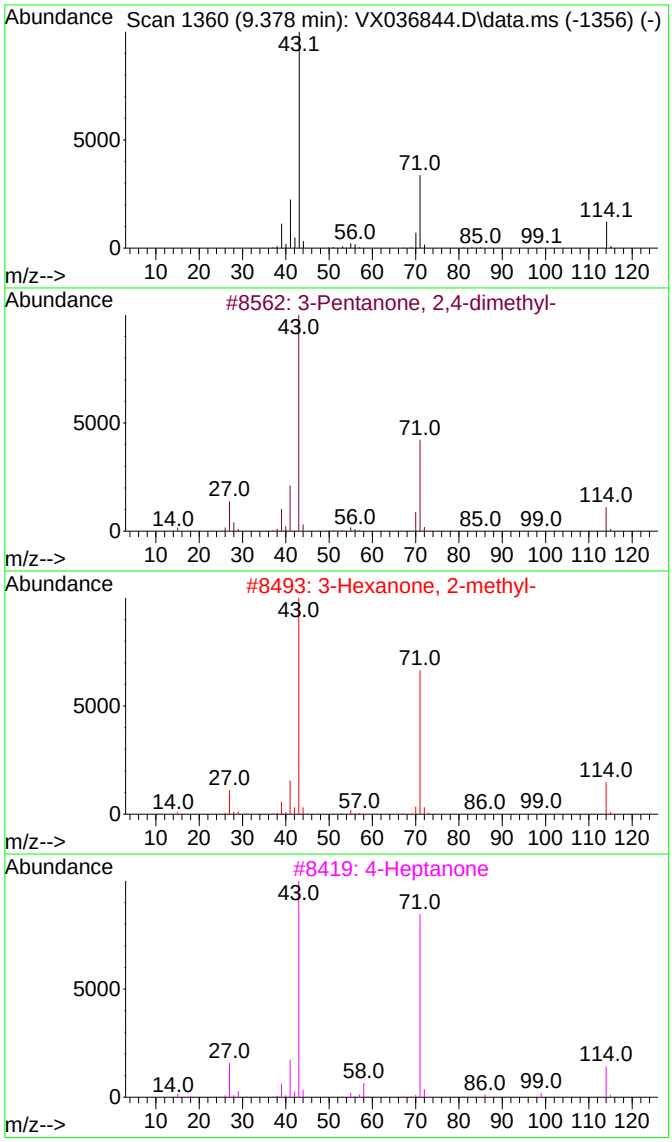
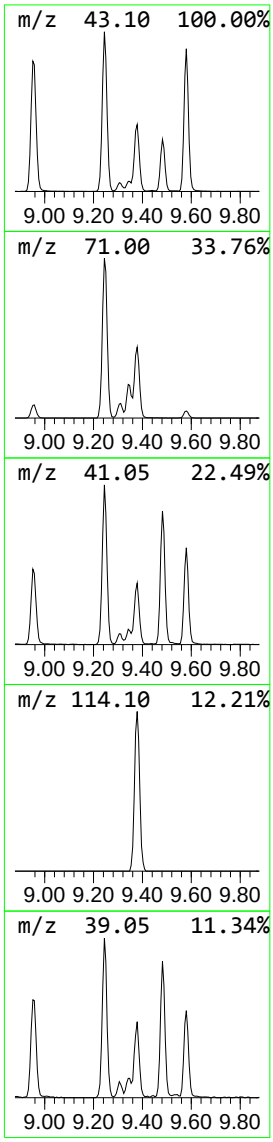
****
Peak Number 5 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	13.43 ug/l	204109	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	64
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	59
5	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50





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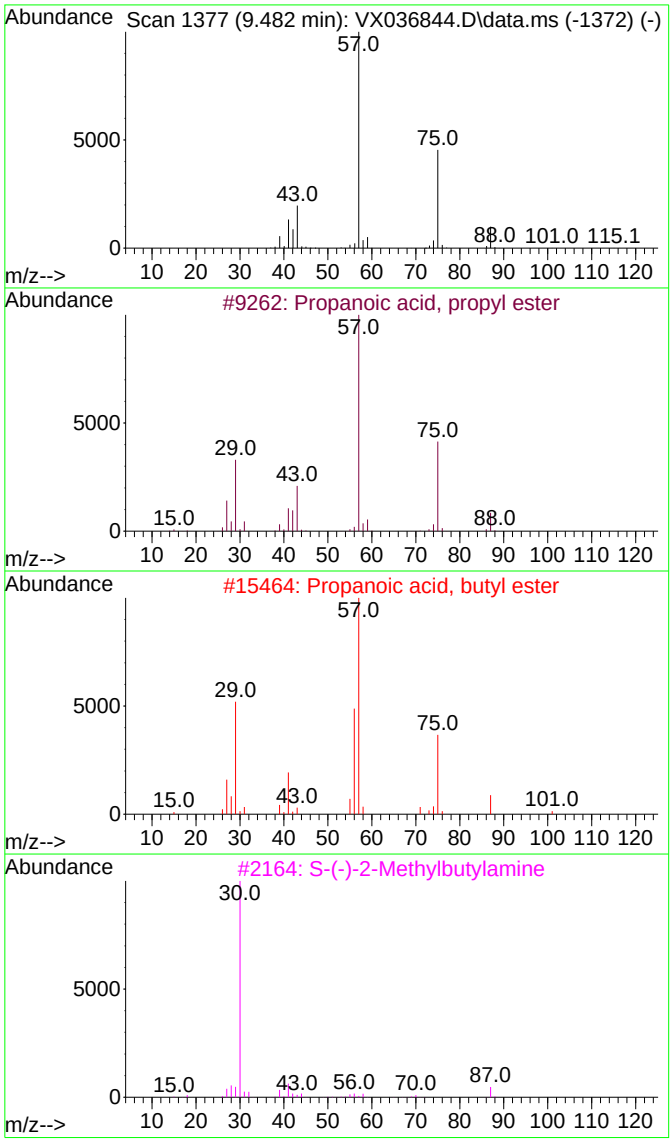
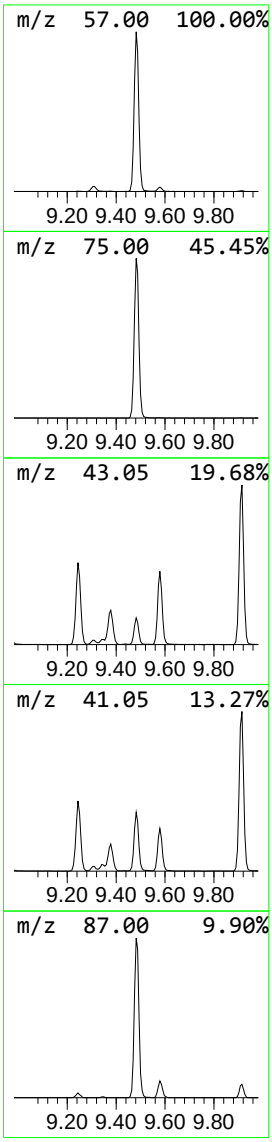
****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	47.91 ug/l	728157	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	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
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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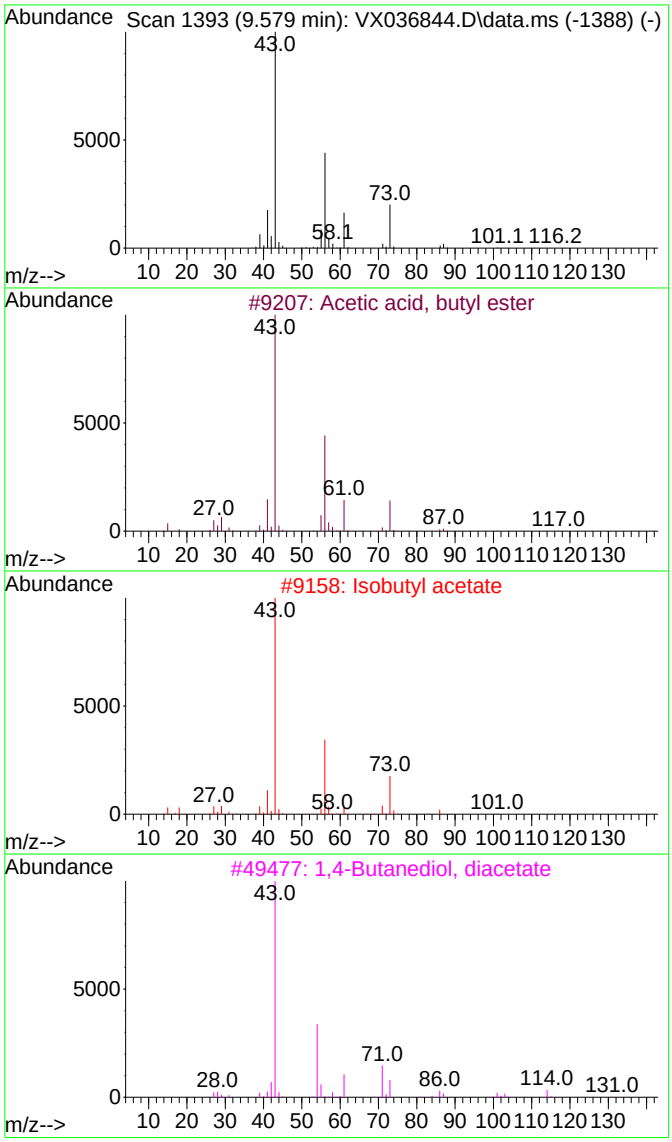
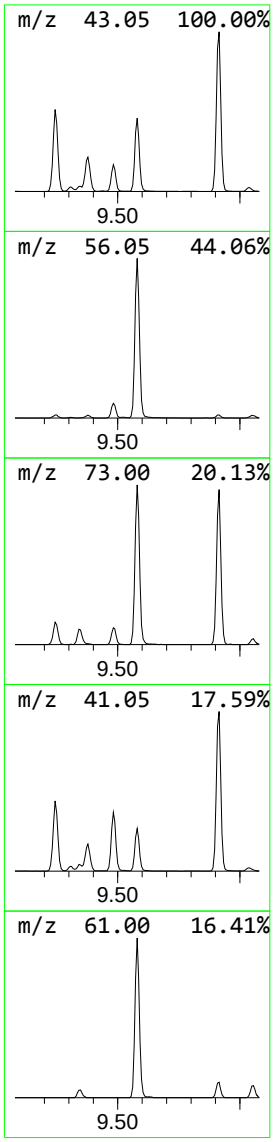
****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	27.87 ug/l	423636	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	Isopropyl acetate	102	C5H10O2	000108-21-4	9





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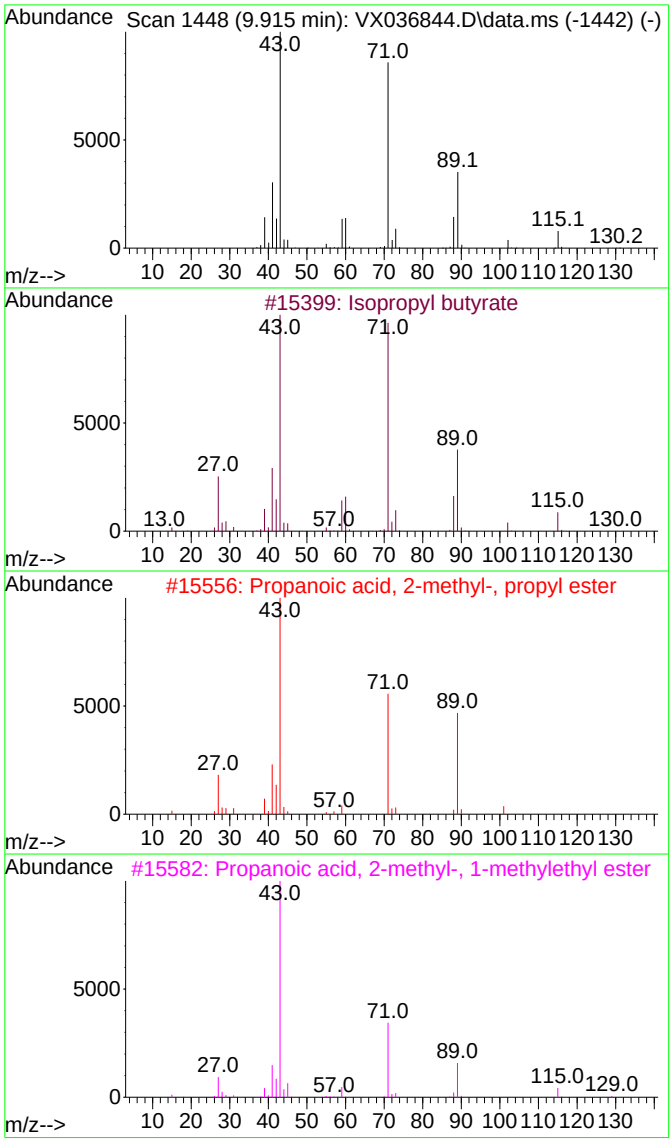
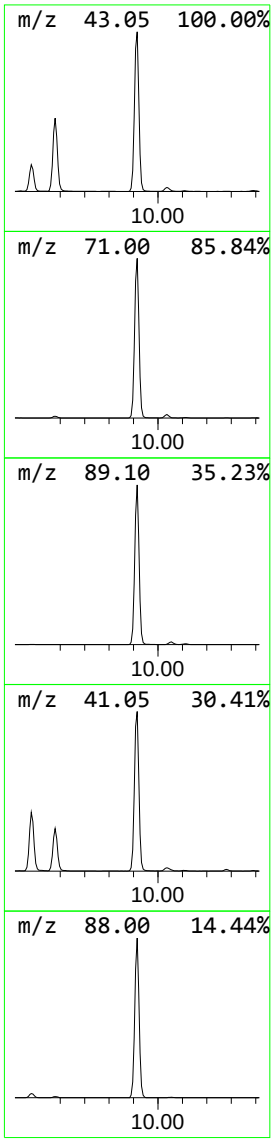
****
Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	89.64 ug/l	1362440	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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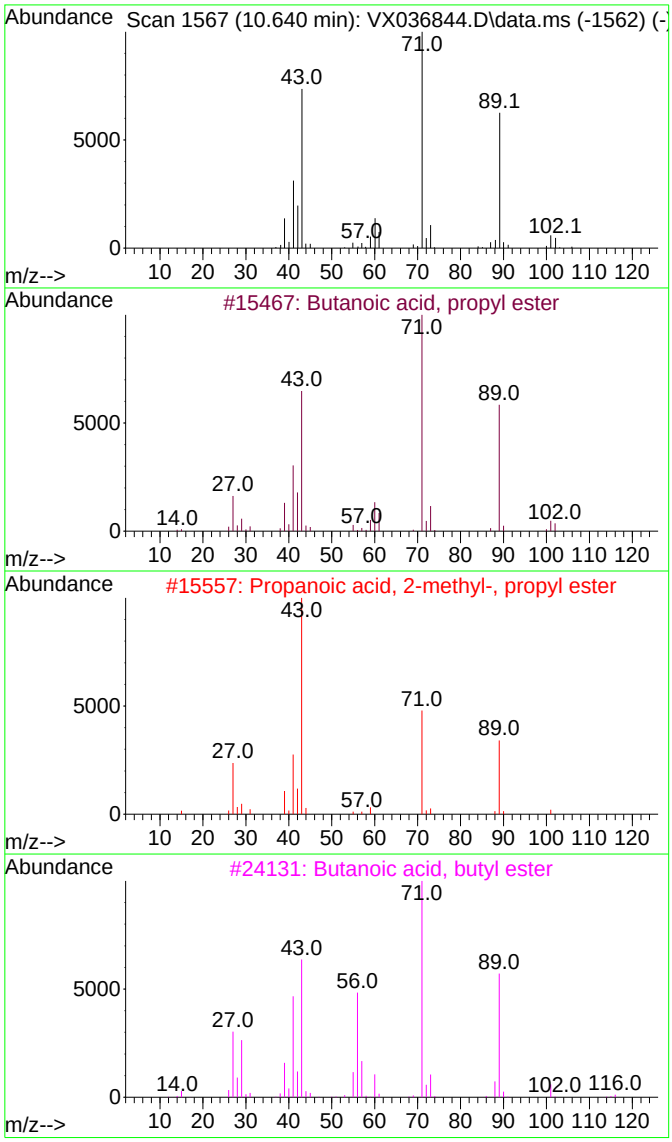
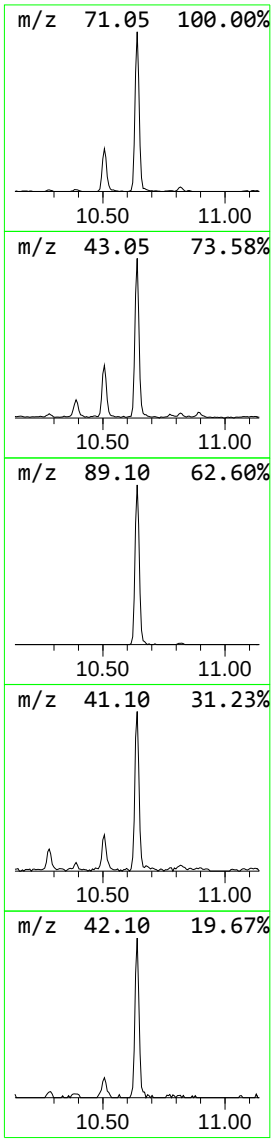
****
Peak Number 9 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	6.85 ug/l	104043	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, butyl ester	144	C8H16O2	000109-21-7	72
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036844.D
Acq On : 07 Aug 2023 18:05
Operator : JC/MD
Sample : 03891-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-3

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
3-Pentanone	7.641	8.3	ug/l	97961	2	6.763	589954	50.0
n-Propyl acetate	7.799	148.5	ug/l	1751790	2	6.763	589954	50.0
Isobutyl acetate	8.951	26.0	ug/l	395012	3	10.055	759949	50.0
Propanoic acid,...	9.244	32.0	ug/l	487087	3	10.055	759949	50.0
3-Pentanone, 2,...	9.378	13.4	ug/l	204109	3	10.055	759949	50.0
Propanoic acid,...	9.482	47.9	ug/l	728157	3	10.055	759949	50.0
Acetic acid, bu...	9.579	27.9	ug/l	423636	3	10.055	759949	50.0
Isopropyl butyrate	9.915	89.6	ug/l	1362440	3	10.055	759949	50.0
Butanoic acid, ...	10.640	6.8	ug/l	104043	3	10.055	759949	50.0