LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036847.D
Acq On : 07 Aug 2023 19:17
Operator : JC/MD
Sample : 03887-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP9

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: VX036847.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	206	212	222	rBV	29556	49959	2.98%	0.485%
2	2.788	272	279	289	rBV	9251	18575	1.11%	0.180%
3	3.575	399	408	426	rBV3	14301	35659	2.13%	0.346%
4	4.574	562	572	585	rBV2	11176	36660	2.19%	0.356%
5	5.385	694	705	721	rBV2	91174	264694	15.79%	2.568%
6	5.550	721	732	748	rVB	144650	414021	24.70%	4.016%
7	5.958	786	799	816	rBV	95954	256538	15.31%	2.488%
8	6.342	853	862	878	rBV	71878	185384	11.06%	1.798%
9	6.763	921	931	943	rBV	242785	576347	34.39%	5.591%
10	7.641	1064	1075	1080	rBV	47908	87247	5.21%	0.846%
11	7.696	1080	1084	1093	rVB	14899	26608	1.59%	0.258%
12	7.799	1093	1101	1122	rBV	989380	1675930	100.00%	16.257%
13	8.549	1213	1224	1234	rBV2	216581	437149	26.08%	4.240%
14	8.647	1234	1240	1249	rBV	497255	797034	47.56%	7.731%
15	8.952	1284	1290	1308	rBV	260444	391874	23.38%	3.801%
16	9.244	1332	1338	1344	rBV	267849	372815	22.25%	3.616%
17	9.311	1344	1349	1351	rVV	29427	41965	2.50%	0.407%
18	9.342	1351	1354	1357	rVV	44958	71916	4.29%	0.698%
19	9.378	1357	1360	1367	rVB	113153	152949	9.13%	1.484%
20	9.482	1372	1377	1384	rVV	509450	652587	38.94%	6.330%
21	9.580	1388	1393	1411	rVB	349648	449481	26.82%	4.360%
22	9.915	1442	1448	1461	rBV	892019	1126170	67.20%	10.924%
23	10.055	1461	1471	1478	rBV	532509	747073	44.58%	7.247%
24	10.281	1503	1508	1520	rVB	12178	17757	1.06%	0.172%
25	10.506	1540	1545	1555	rVB	15182	20348	1.21%	0.197%
26	10.640	1562	1567	1573	rBV	79764	97065	5.79%	0.942%
27	11.079	1634	1639	1654	rBV	439029	561845	33.52%	5.450%
28	11.555	1712	1717	1723	rBV	12984	16921	1.01%	0.164%
29	12.018	1788	1793	1800	rBV	530776	690471	41.20%	6.698%
30	12.219	1821	1826	1837	rBV	22059	36233	2.16%	0.351%

Sum of corrected areas: 10309275

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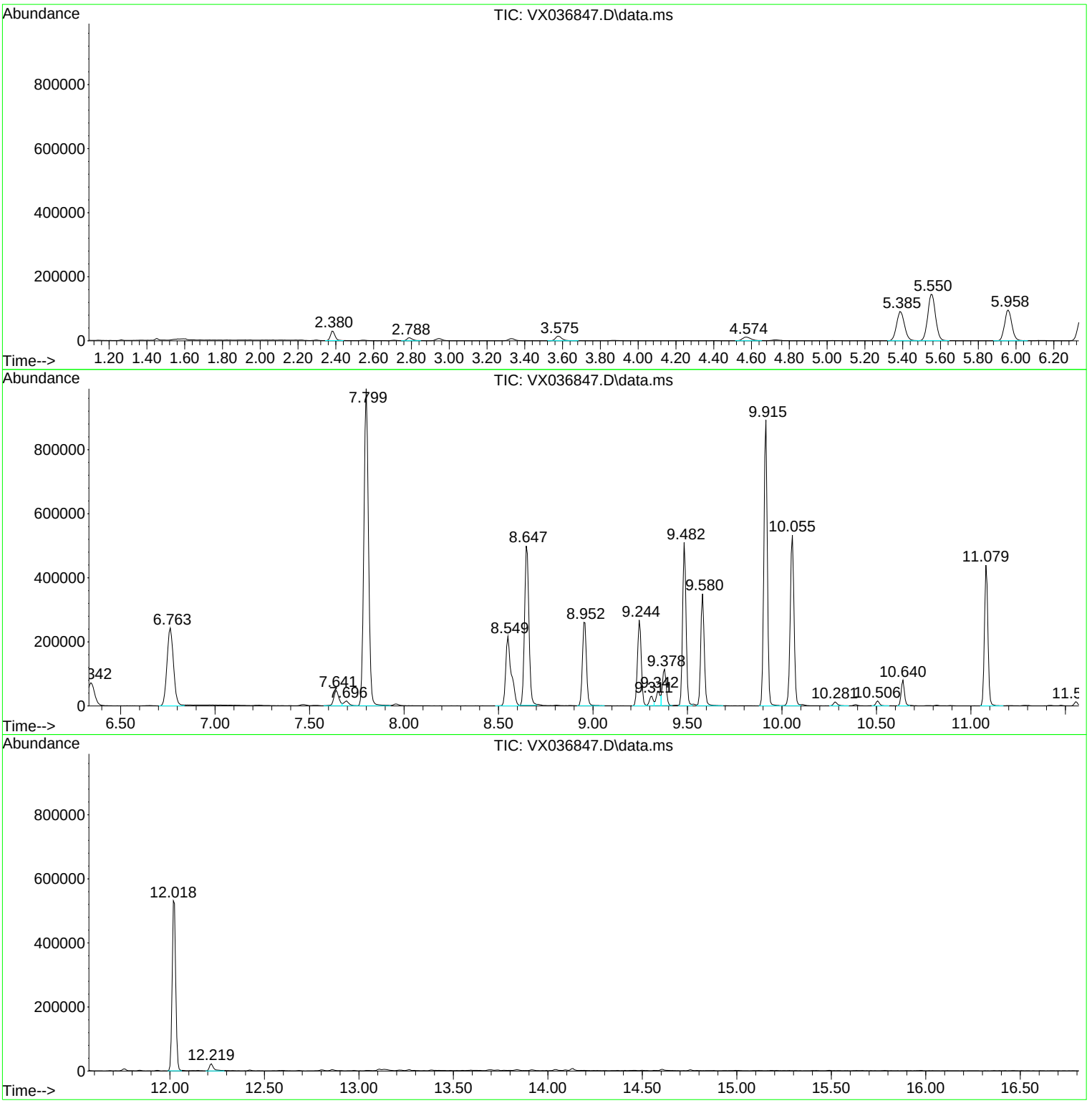
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP9

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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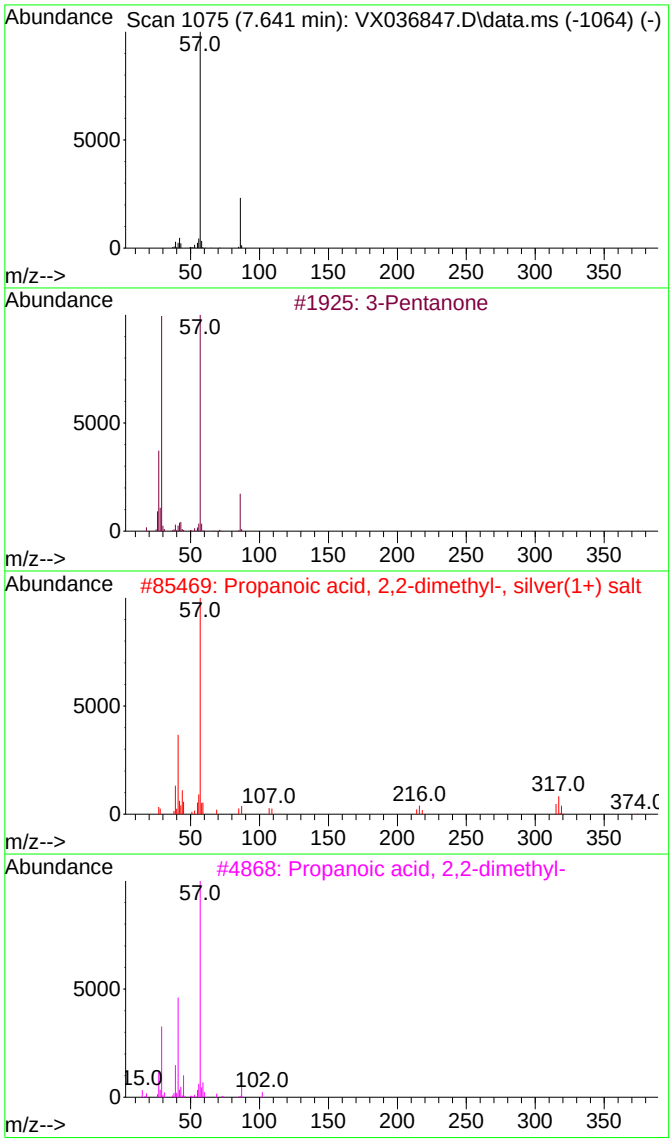
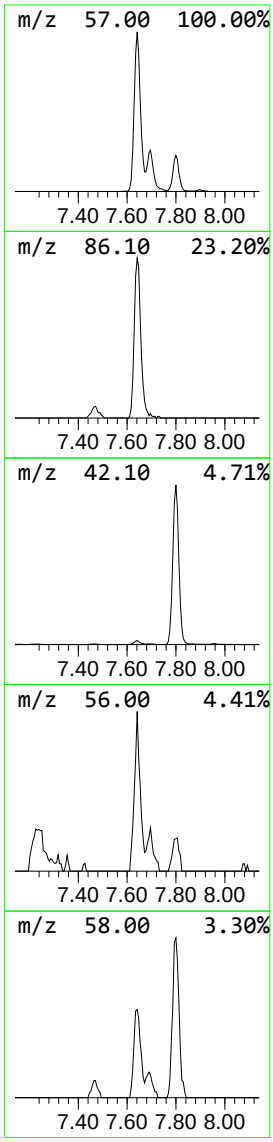
****

Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	7.57 ug/l	87247	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	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
4	Neopentane	72	C5H12	000463-82-1	9
5	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	7





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MSVOA_X
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MCLEAN-TP9

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

TIC Library : C:\Database\NIST20.L
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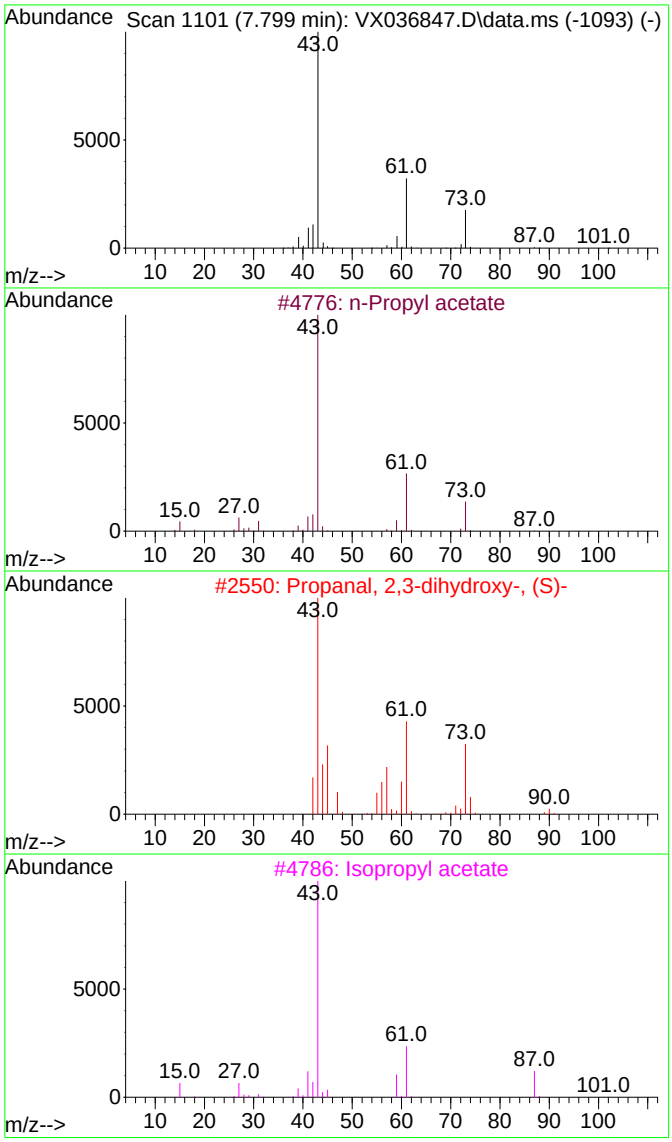
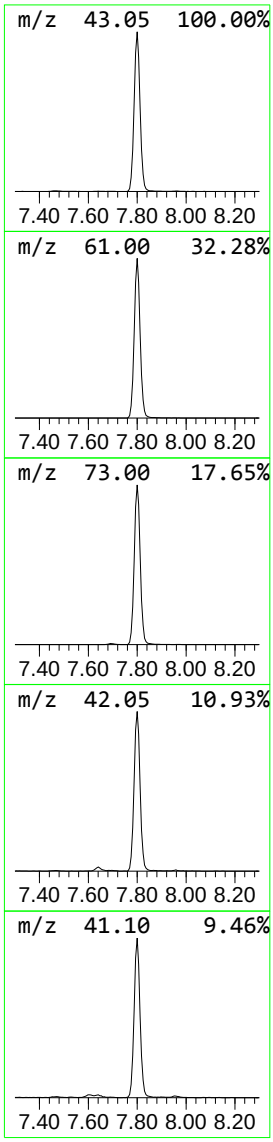
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	145.39 ug/l	1675930	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	5





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ClientSampleId :
MCLEAN-TP9

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

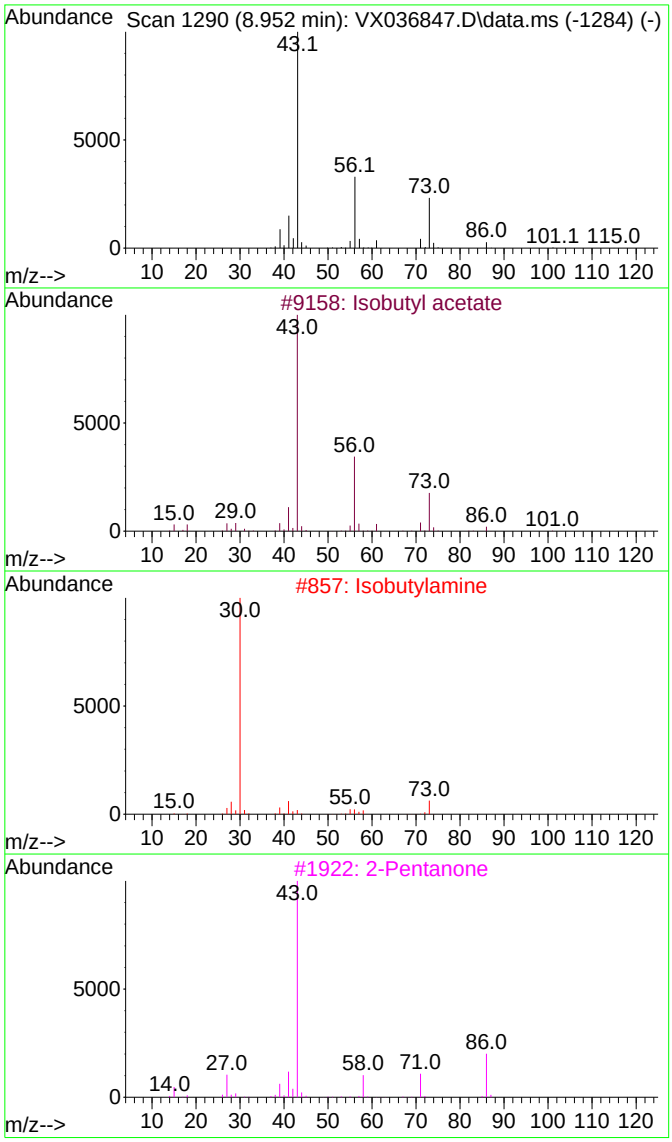
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

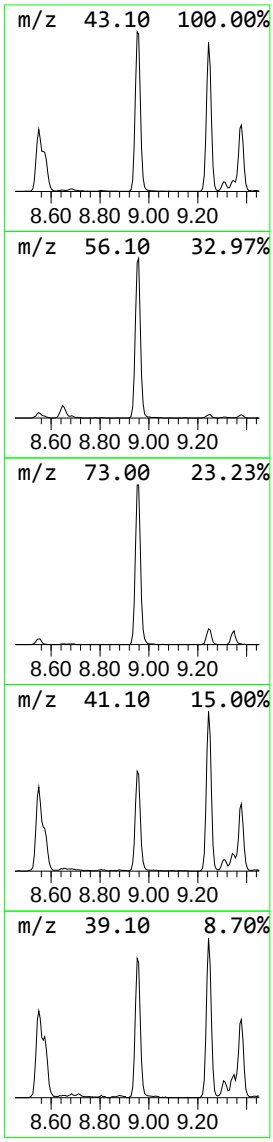
****

Peak Number 3 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	26.23 ug/l	391874	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Isobutylamine	73	C4H11N	000078-81-9	9
3	2-Pentanone	86	C5H10O	000107-87-9	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9





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Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP9

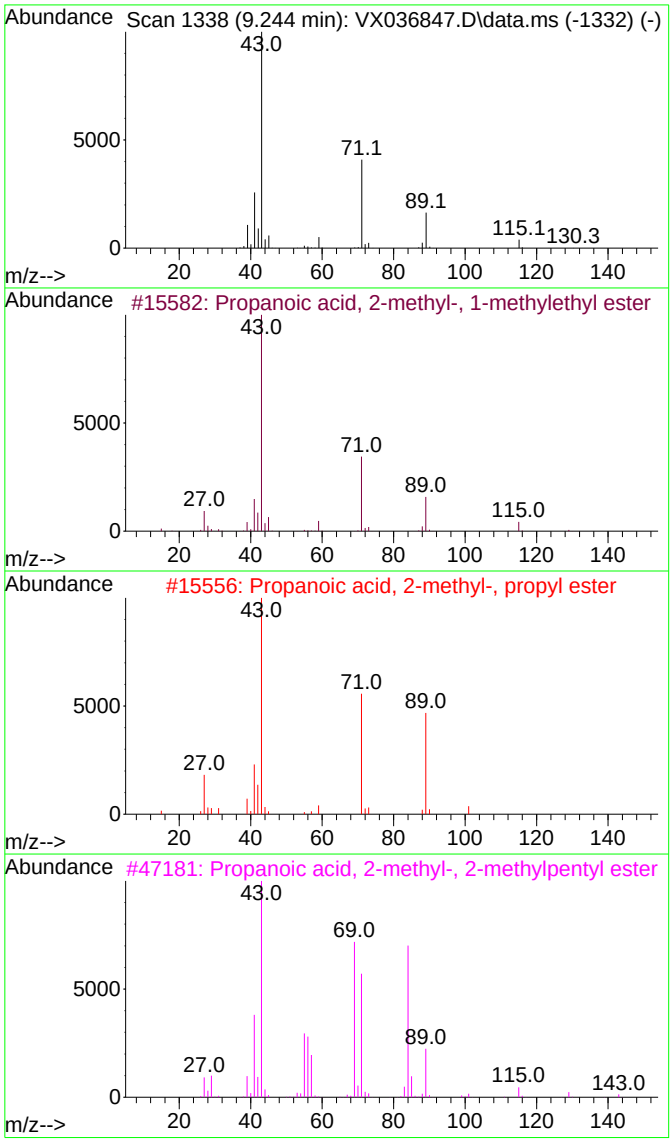
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

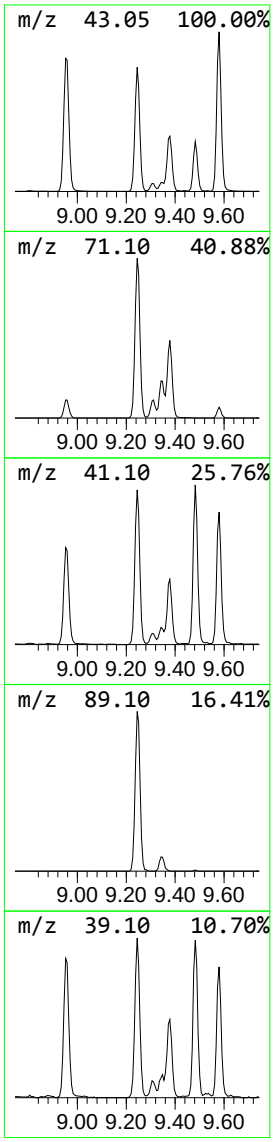
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	24.95 ug/l	372815	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	72
3	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	56
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	56
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	53





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP9

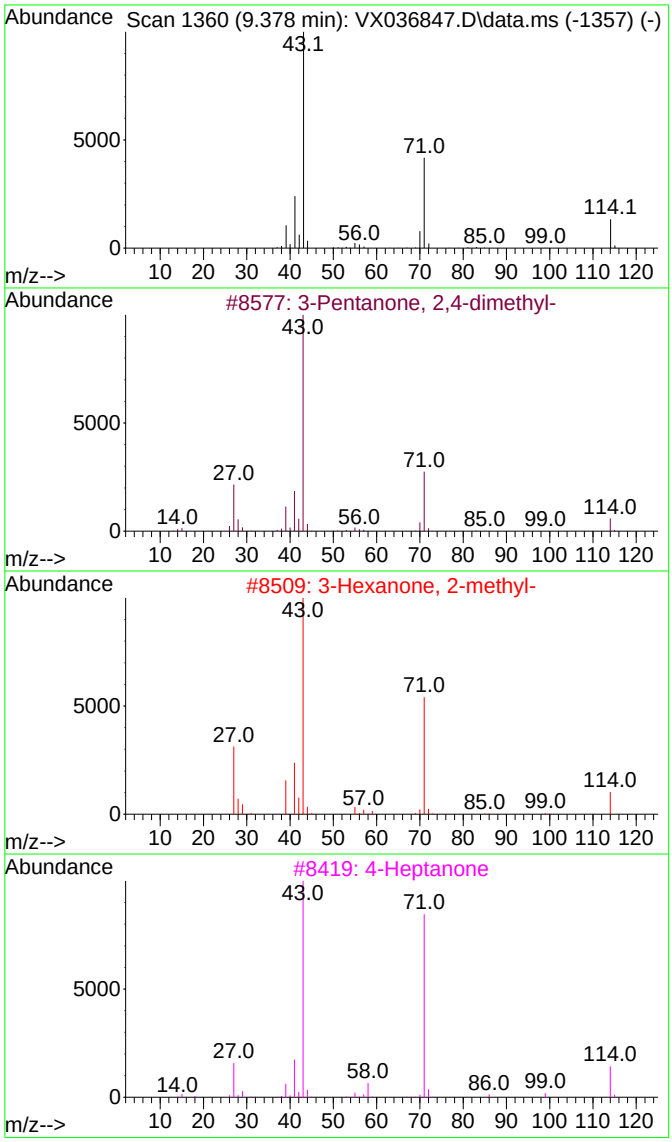
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

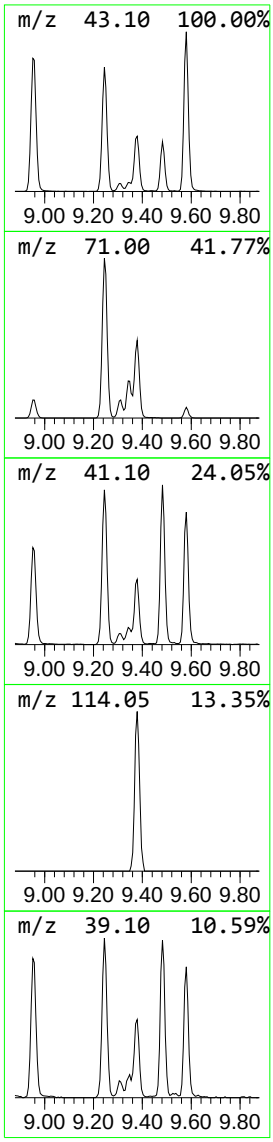
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	10.24 ug/l	152949	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3	4-Heptanone	114	C7H14O	000123-19-3	72
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
5	Pyrrolidine	71	C4H9N	000123-75-1	42





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP9

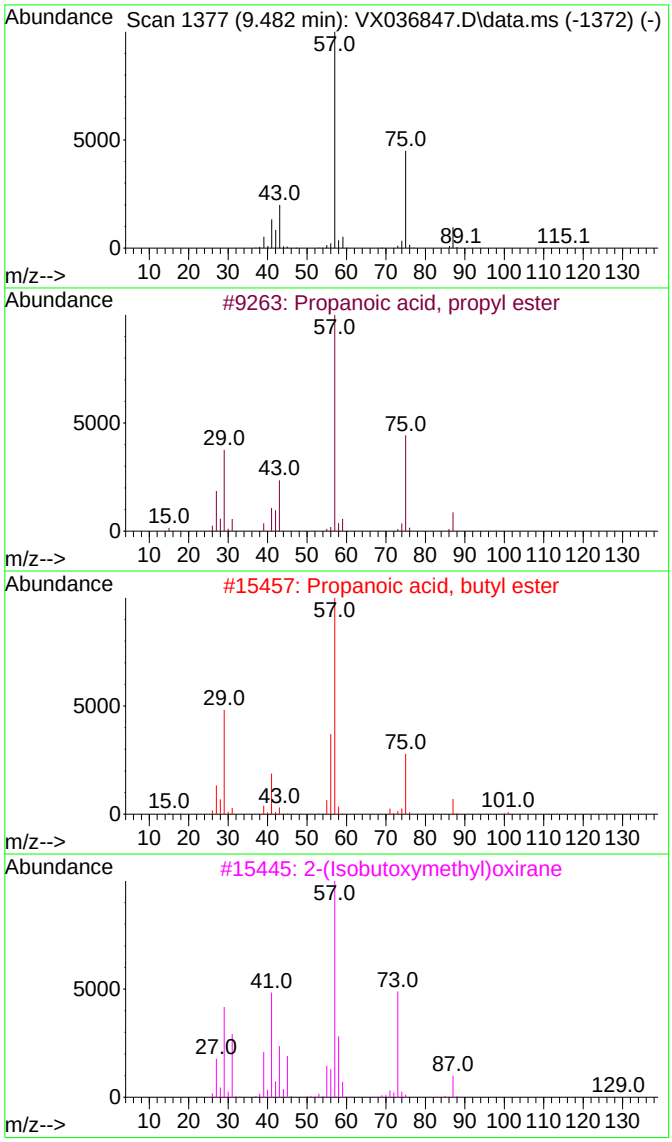
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

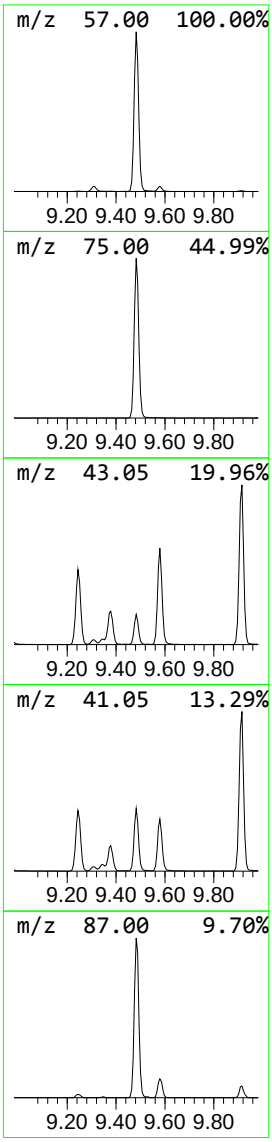
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	43.68 ug/l	652587	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	28
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	Isobutyl ether	130	C8H18O	000628-55-7	9





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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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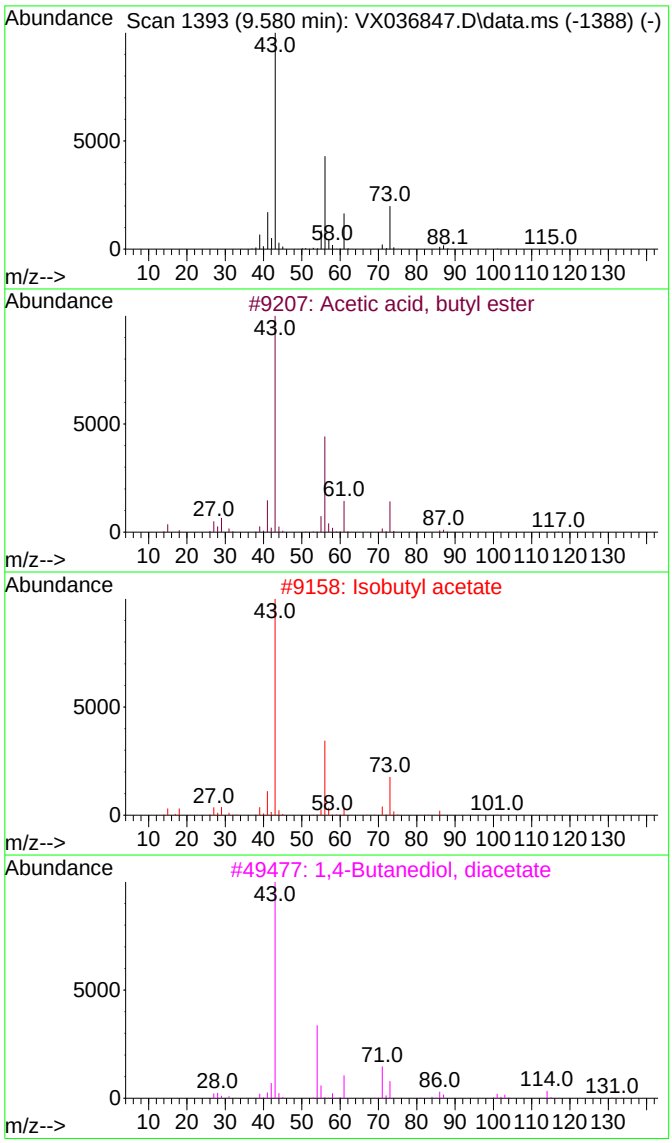
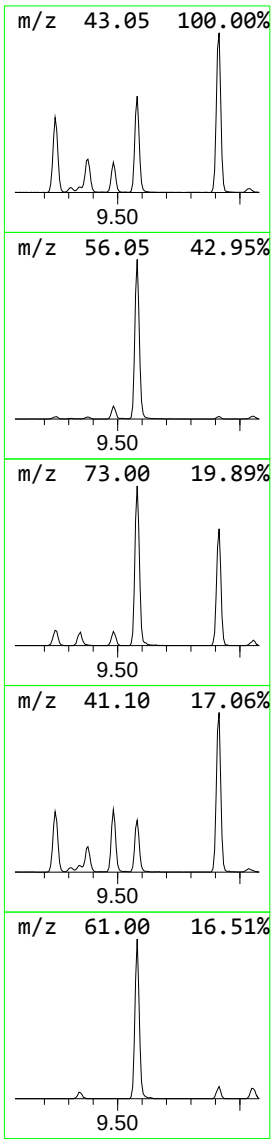
****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	30.08 ug/l	449481	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	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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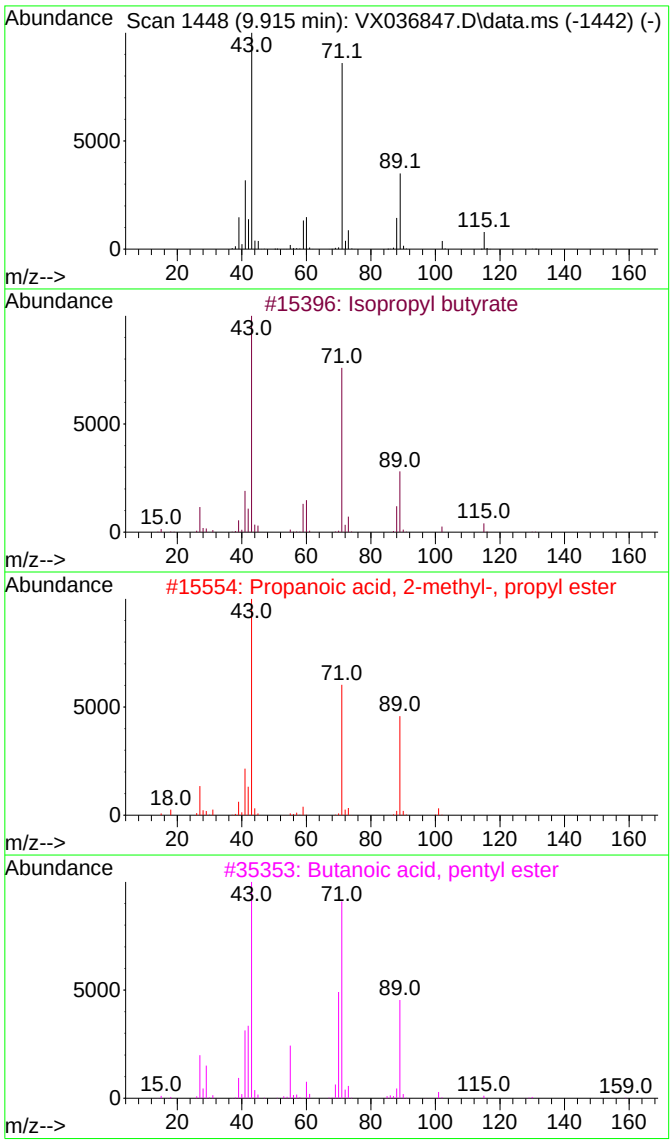
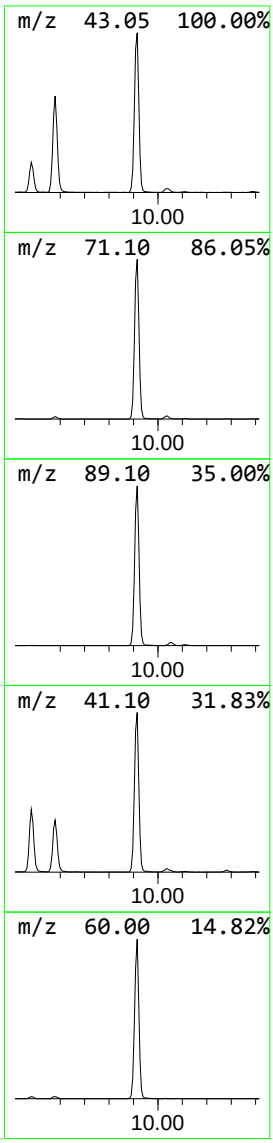
****

Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	75.37 ug/l	1126170	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	95
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, butyl ester	144	C8H16O2	000109-21-7	64
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64





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MSVOA_X
ClientSampleId :
MCLEAN-TP9

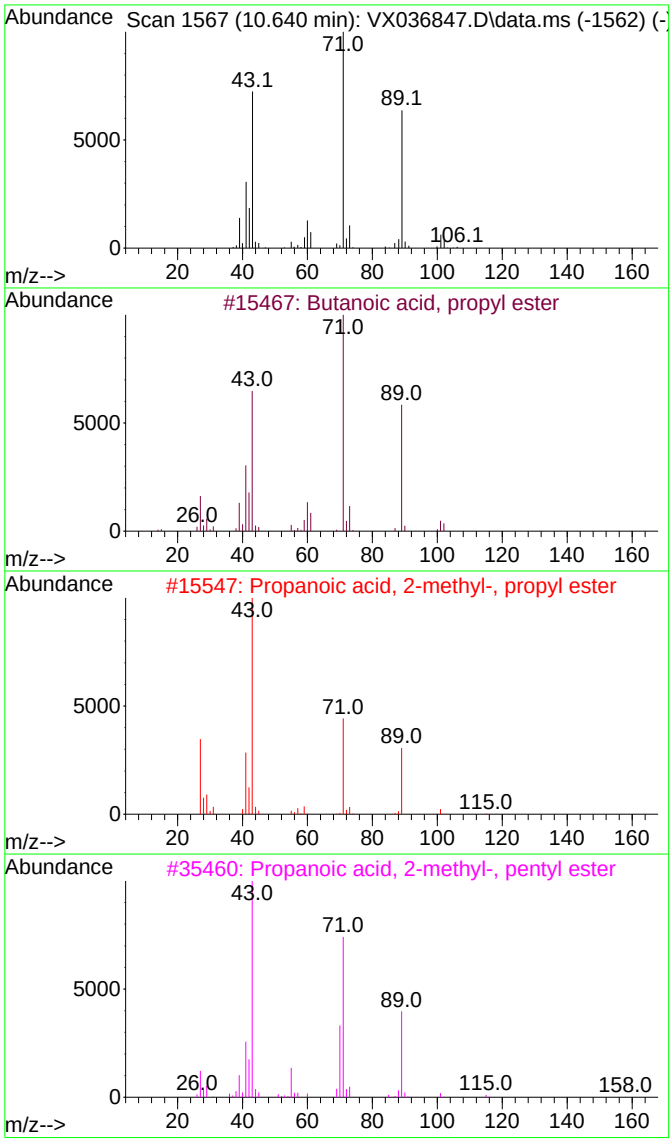
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

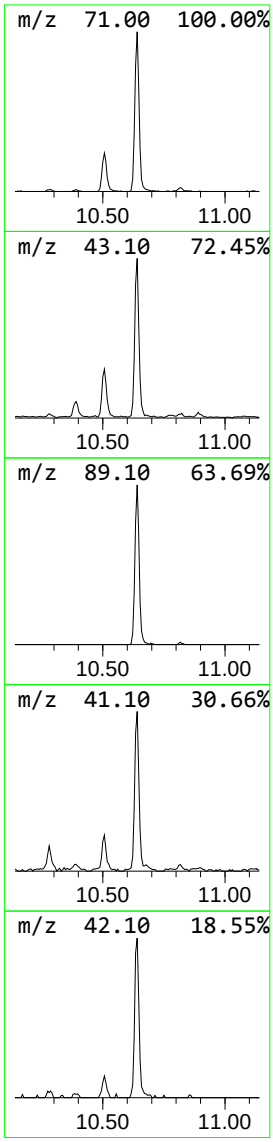
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	6.50 ug/l	97065	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	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72
4	Malic Acid	134	C4H6O5	006915-15-7	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





Tentatively Identified Compound (LSC) summary

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ClientSampleId :
MCLEAN-TP9

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	7.6	ug/l	87247	2	6.763	576347	50.0
n-Propyl acetate	7.799	145.4	ug/l	1675930	2	6.763	576347	50.0
Isobutyl acetate	8.952	26.2	ug/l	391874	3	10.055	747073	50.0
Propanoic acid,...	9.244	24.9	ug/l	372815	3	10.055	747073	50.0
3-Pentanone, 2,...	9.378	10.2	ug/l	152949	3	10.055	747073	50.0
Propanoic acid,...	9.482	43.7	ug/l	652587	3	10.055	747073	50.0
Acetic acid, bu...	9.580	30.1	ug/l	449481	3	10.055	747073	50.0
Isopropyl butyrate	9.915	75.4	ug/l	1126170	3	10.055	747073	50.0
Butanoic acid, ...	10.640	6.5	ug/l	97065	3	10.055	747073	50.0