LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092424\
Data File : VX043122.D
Acq On : 24 Sep 2024 15:03
Operator : JC/MD
Sample : P4148-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
STOCK-PILE

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\82X092324W.M
Title : SW846 8260

Signal : TIC: VX043122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	33	rBV	40961	52483	3.87%	0.612%
2	2.380	205	212	225	rBV	19283	33882	2.50%	0.395%
3	2.788	272	279	295	rBV	62761	130831	9.64%	1.524%
4	5.385	695	705	722	rBV	72836	214645	15.82%	2.501%
5	5.550	722	732	747	rVV	101051	291622	21.49%	3.398%
6	5.958	789	799	817	rBV	79441	218182	16.08%	2.542%
7	6.342	853	862	880	rBV	59975	160944	11.86%	1.875%
8	6.757	922	930	943	rBV	182622	446860	32.94%	5.207%
9	7.641	1067	1075	1080	rBV	32693	59374	4.38%	0.692%
10	7.696	1080	1084	1093	rVB	11893	23289	1.72%	0.271%
11	7.793	1094	1100	1122	rBV	761893	1356779	100.00%	15.810%
12	8.549	1217	1224	1234	rBV	188972	304787	22.46%	3.551%
13	8.647	1234	1240	1257	rVB	392779	620065	45.70%	7.225%
14	8.952	1285	1290	1301	rBV	216958	314563	23.18%	3.665%
15	9.244	1332	1338	1345	rBV	276786	384748	28.36%	4.483%
16	9.311	1345	1349	1351	rVV	20789	31290	2.31%	0.365%
17	9.342	1351	1354	1356	rVV	38019	51594	3.80%	0.601%
18	9.372	1356	1359	1367	rVB	99115	146921	10.83%	1.712%
19	9.482	1372	1377	1388	rVV	432627	558131	41.14%	6.503%
20	9.580	1388	1393	1406	rVB	254308	336667	24.81%	3.923%
21	9.909	1442	1447	1463	rBV	797017	1041031	76.73%	12.130%
22	10.055	1463	1471	1478	rBV	390218	577231	42.54%	6.726%
23	10.281	1503	1508	1516	rBV2	9185	14302	1.05%	0.167%
24	10.506	1540	1545	1552	rBV	11921	16029	1.18%	0.187%
25	10.640	1562	1567	1582	rVB	61133	81459	6.00%	0.949%
26	11.079	1634	1639	1654	rVB	355037	458493	33.79%	5.342%
27	12.018	1788	1793	1800	rBV	465845	609621	44.93%	7.103%
28	12.421	1855	1859	1864	rBV	15913	18614	1.37%	0.217%
29	13.268	1993	1998	2008	rBV2	18015	27584	2.03%	0.321%

Sum of corrected areas: 8582021

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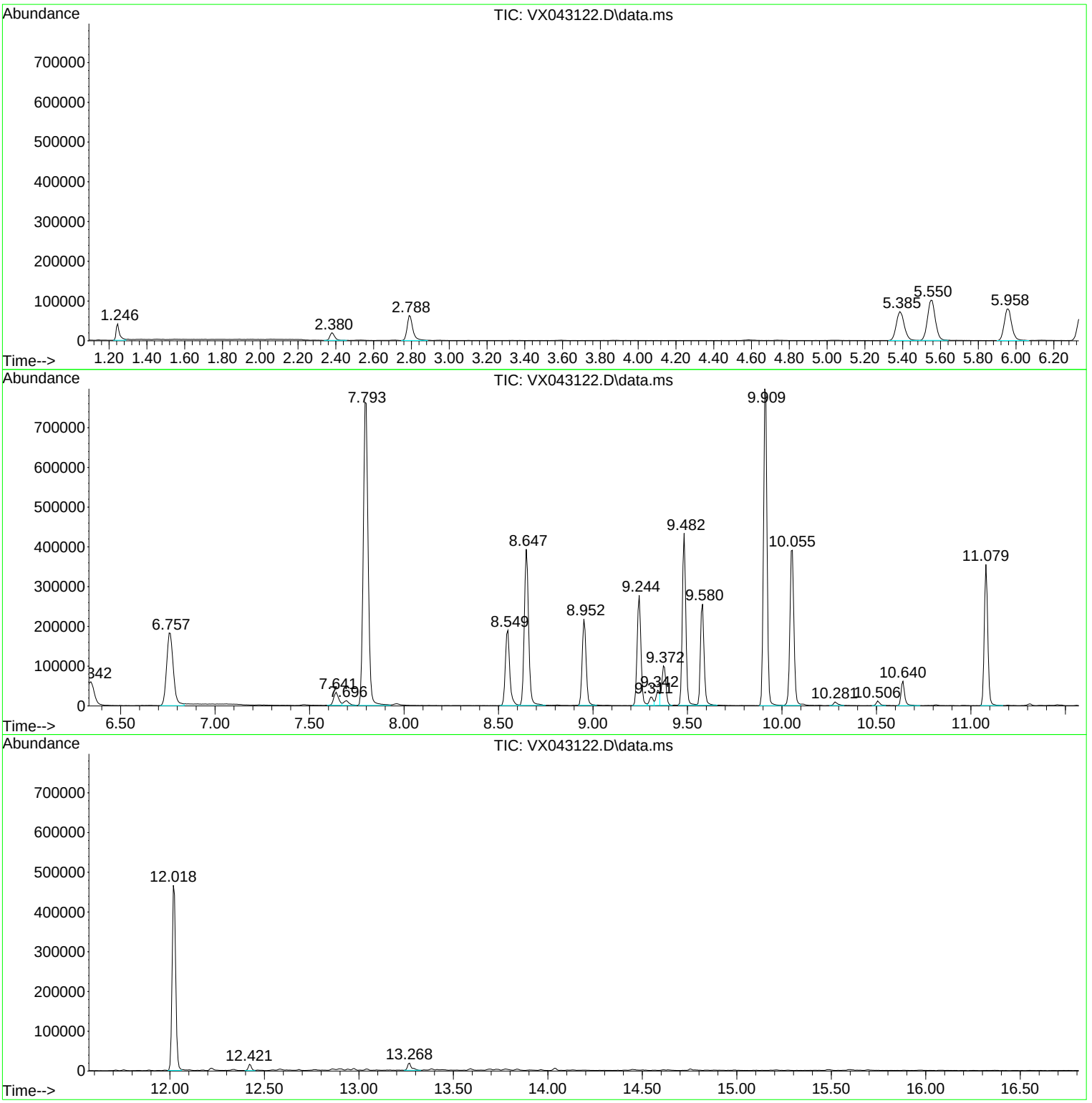
Instrument :
MSVOA_X
ClientSampleId :
STOCK-PILE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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



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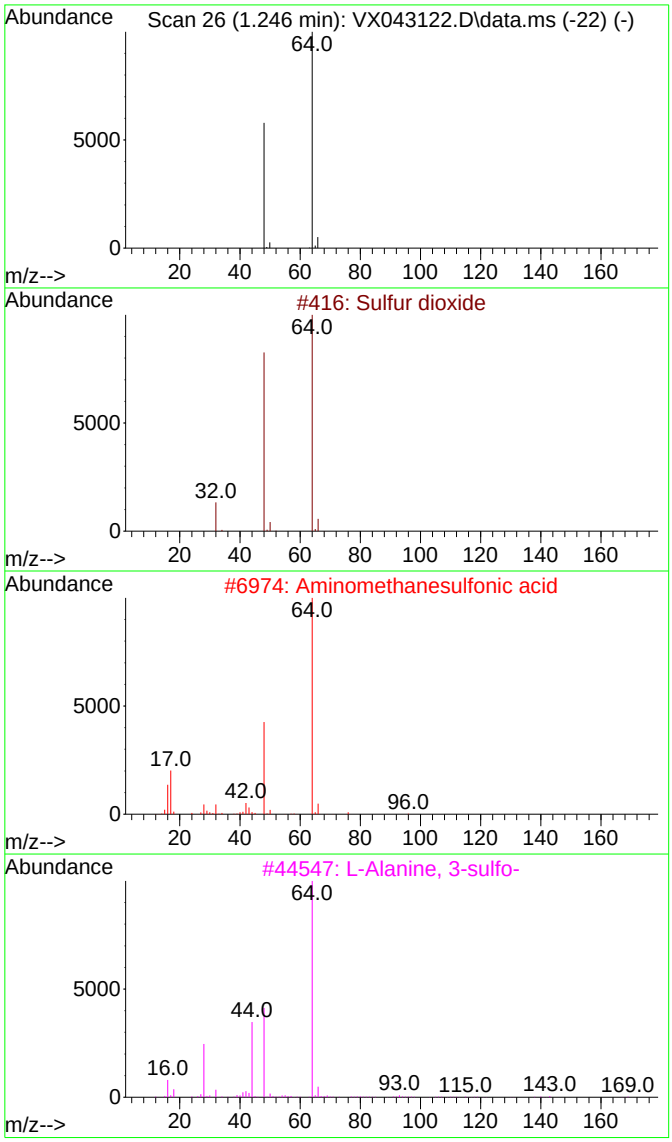
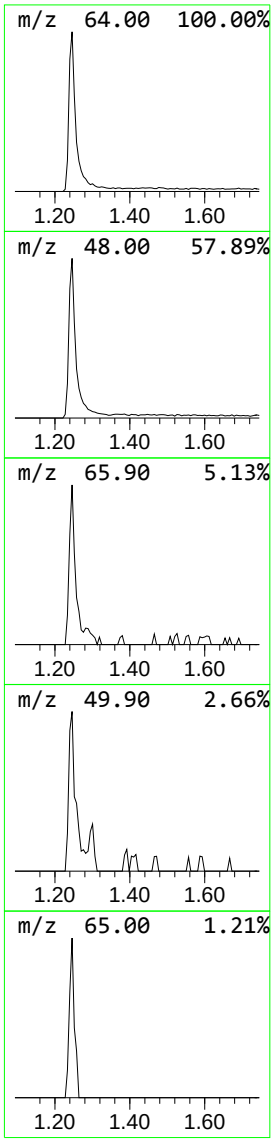
****

Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	9.00 ug/l	52483	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Instrument :
MSVOA_X
ClientSampleId :
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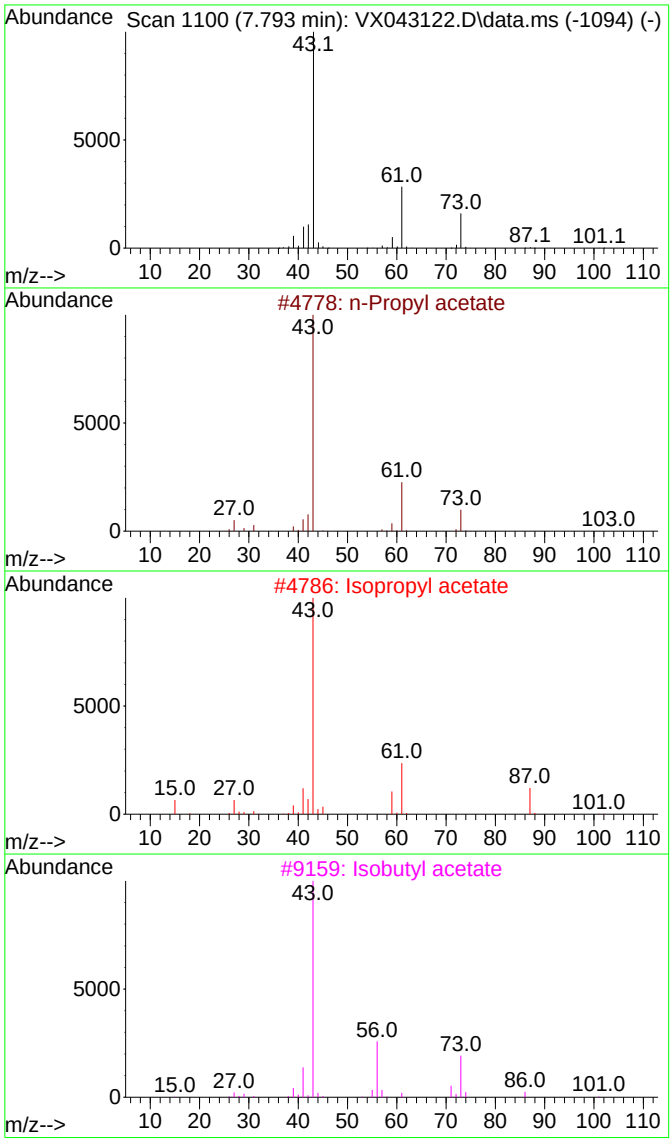
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

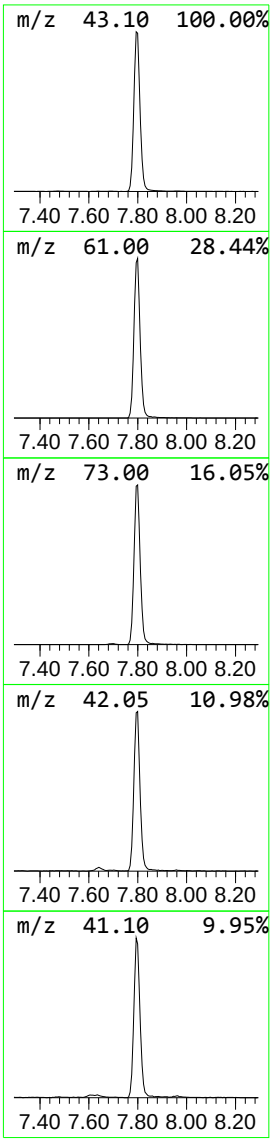
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.793	151.81 ug/l	1356780	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	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	7





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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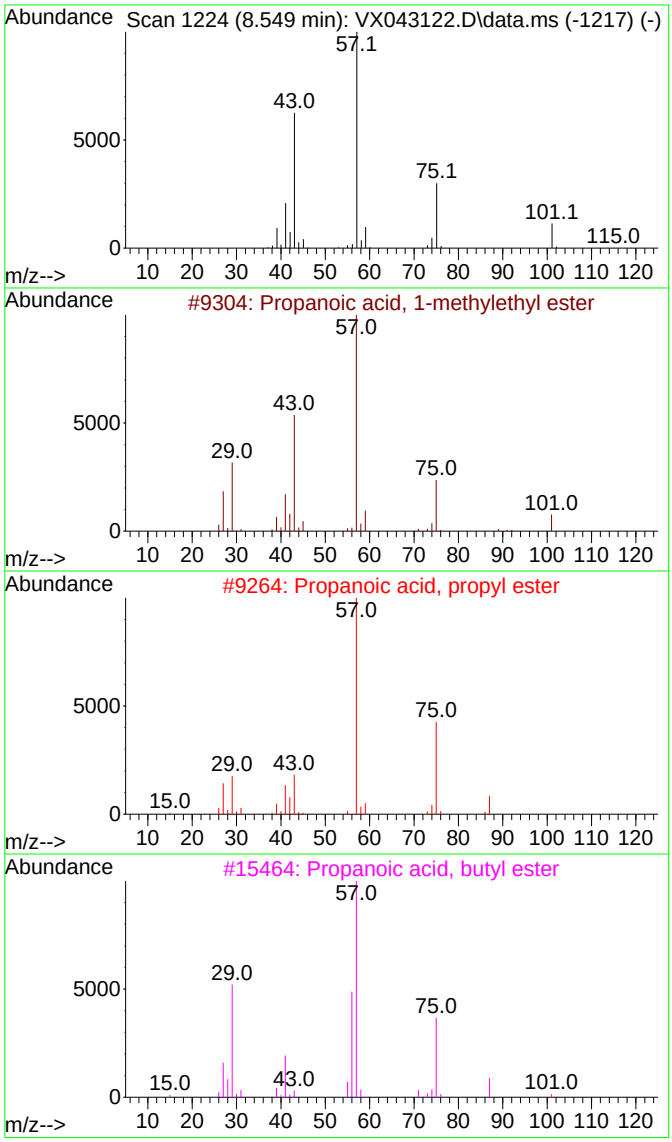
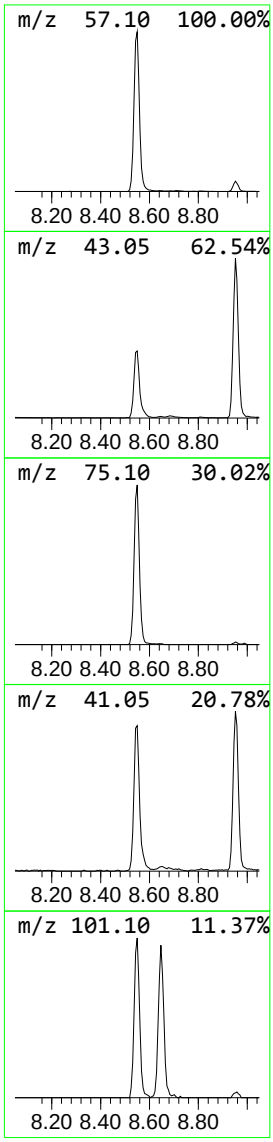
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	26.40 ug/l	304787	Chlorobenzene-d5	10.055

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	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	9





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Instrument :
MSVOA_X
ClientSampleId :
STOCK-PILE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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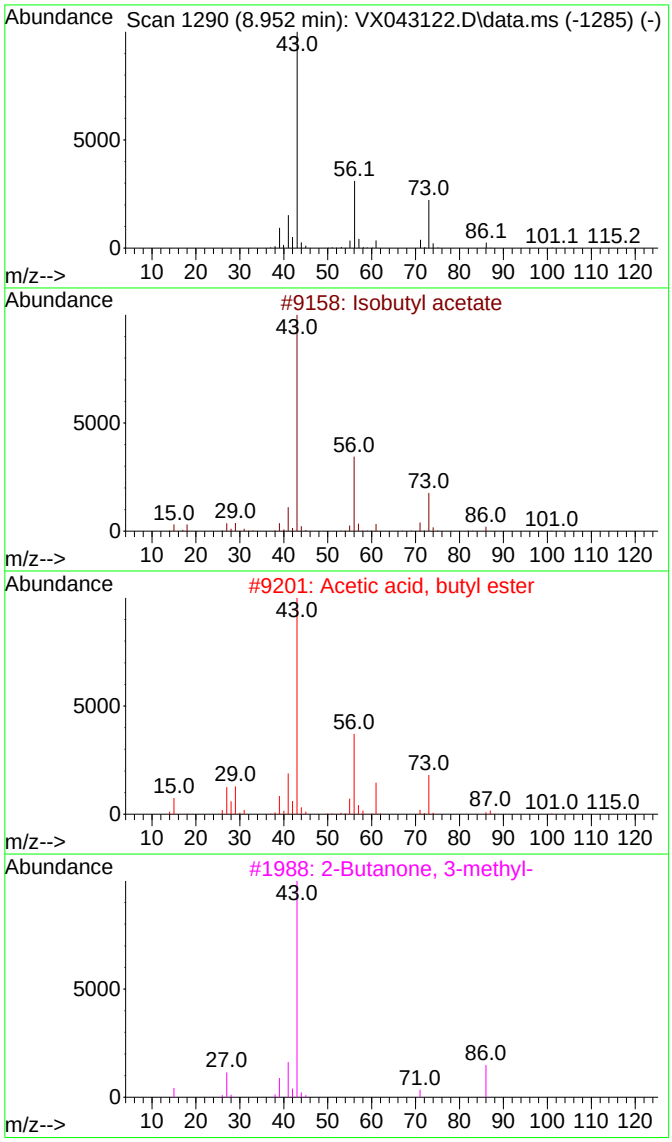
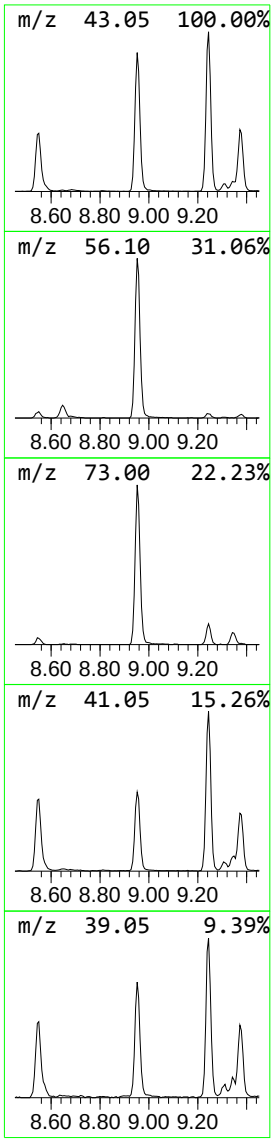
****

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	27.25 ug/l	314563	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	50
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
STOCK-PILE

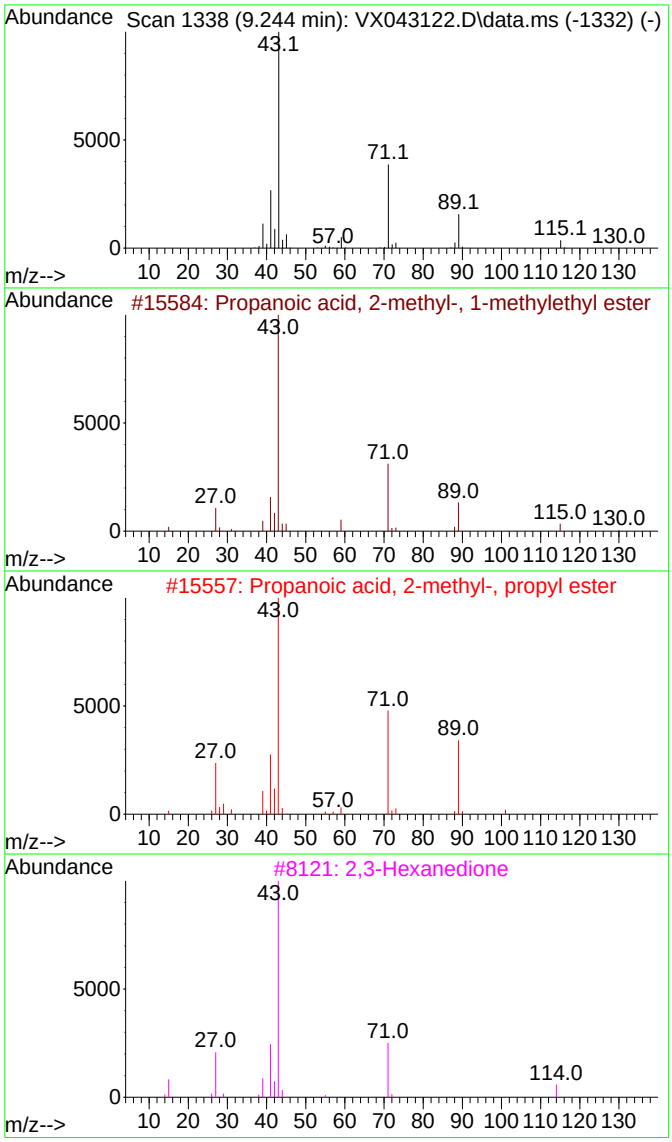
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

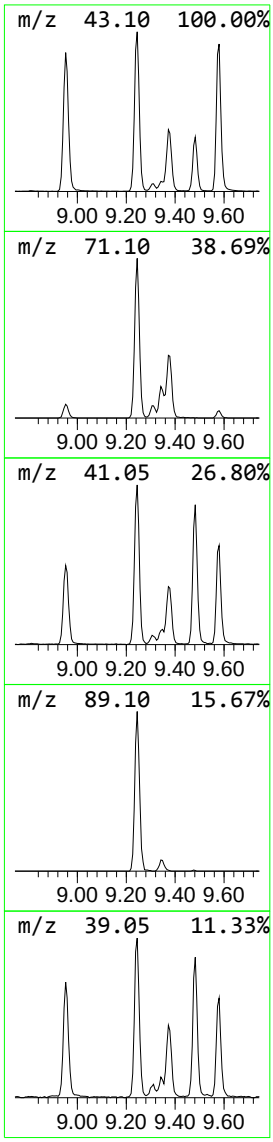
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	33.33 ug/l	384748	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	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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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
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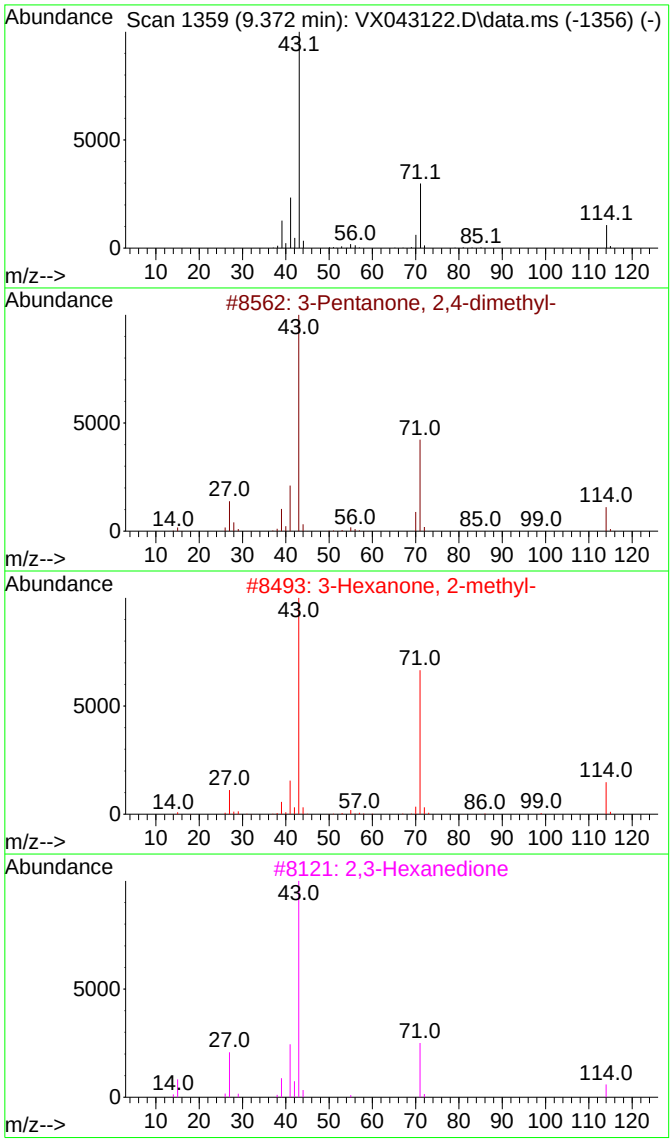
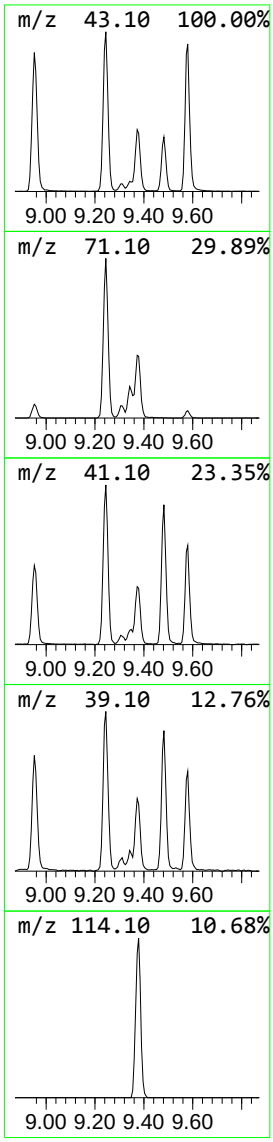
****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.372	12.73 ug/l	146921	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	2,3-Hexanedione	114	C6H10O2	003848-24-6	59
4	4-Heptanone	114	C7H14O	000123-19-3	38
5	Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	36





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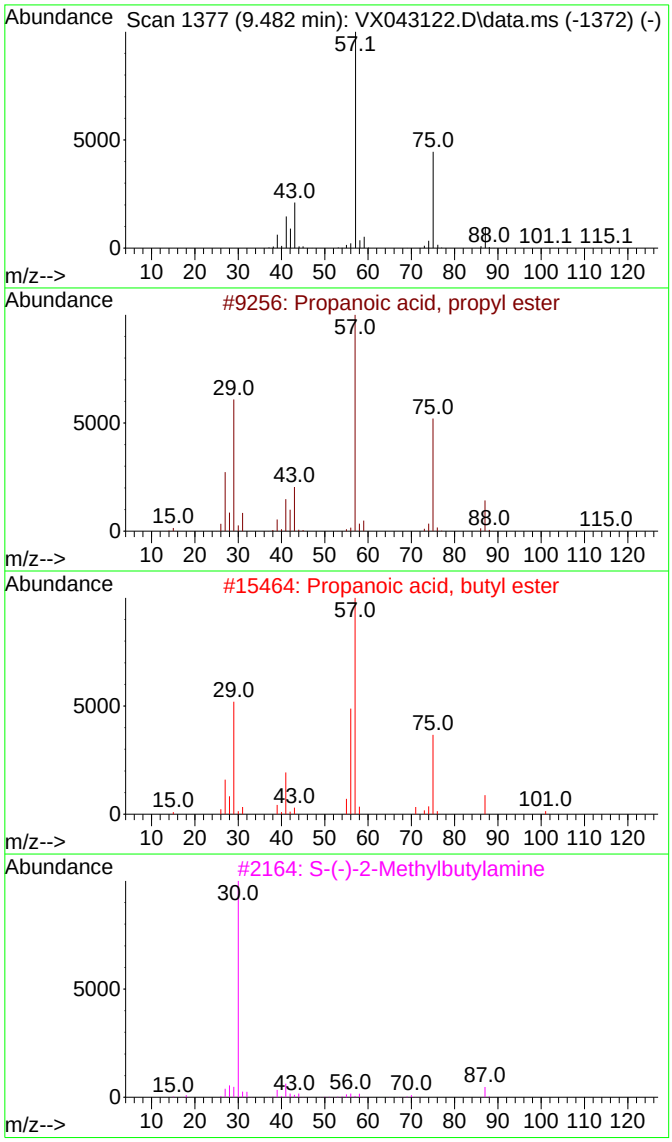
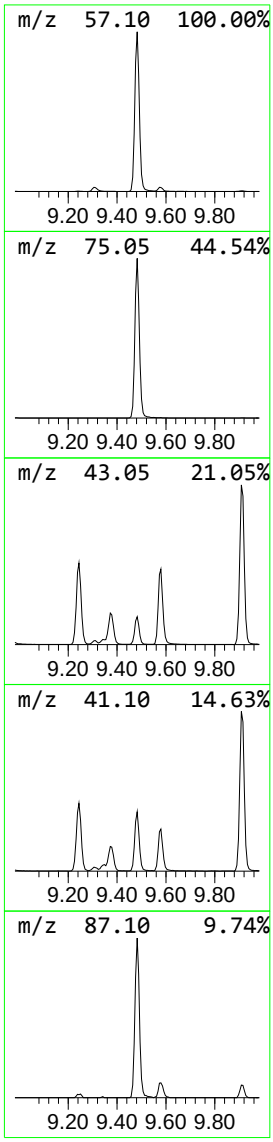
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	48.35 ug/l	558131	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	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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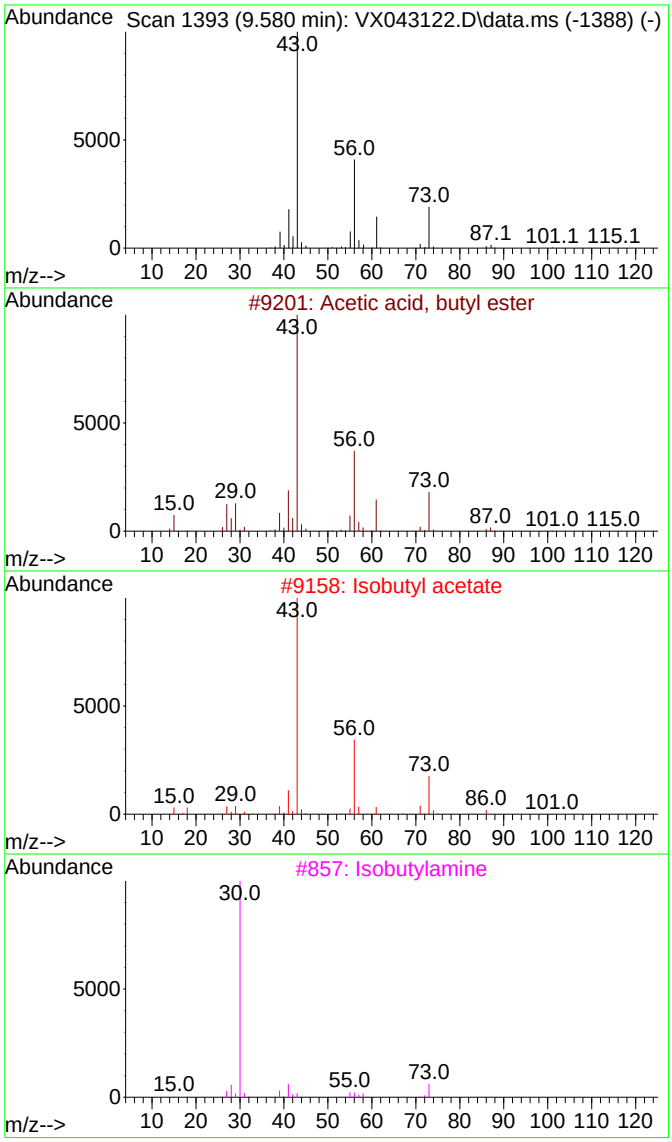
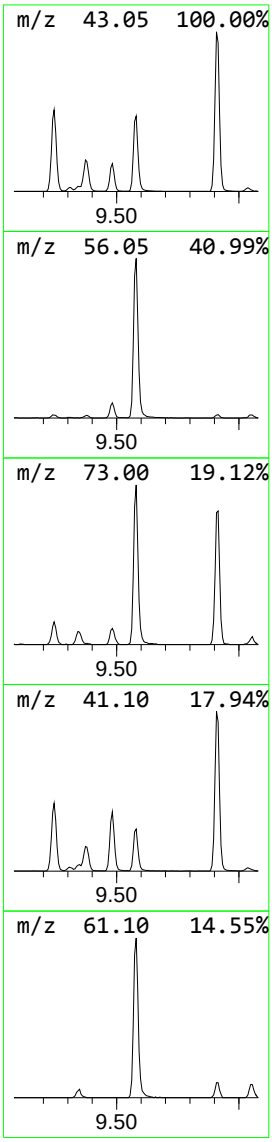
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	29.16 ug/l	336667	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	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Pentanone	86	C5H10O	000107-87-9	9
5	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9





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MSVOA_X
ClientSampleId :
STOCK-PILE

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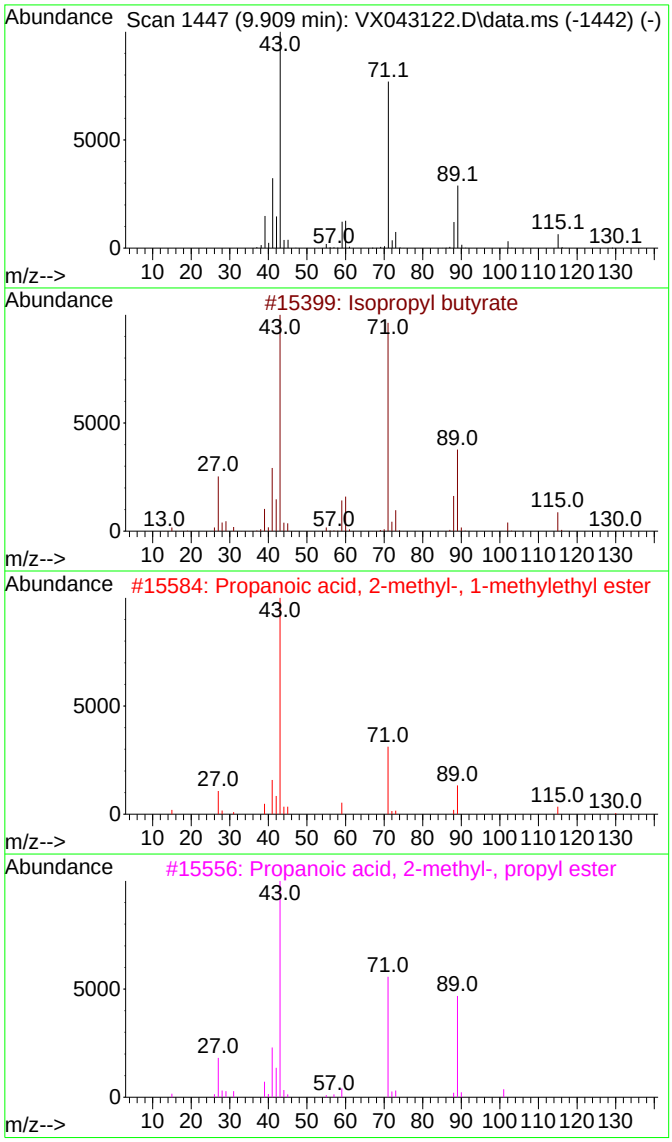
Quant Title : SW846 8260

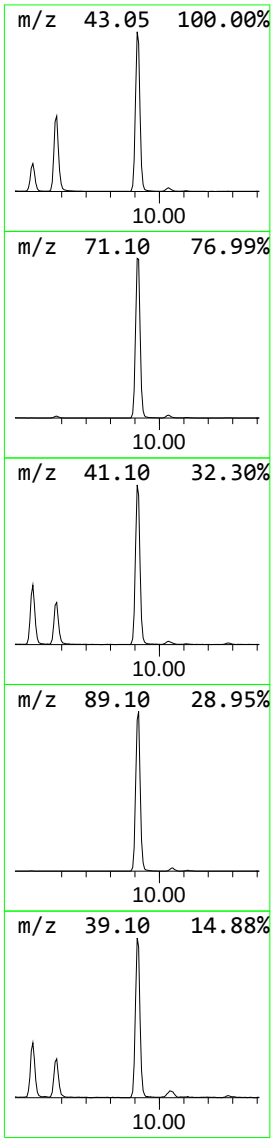
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.909	90.17 ug/l	1041030	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-, 1-met...	130	C7H14O2	000617-50-5	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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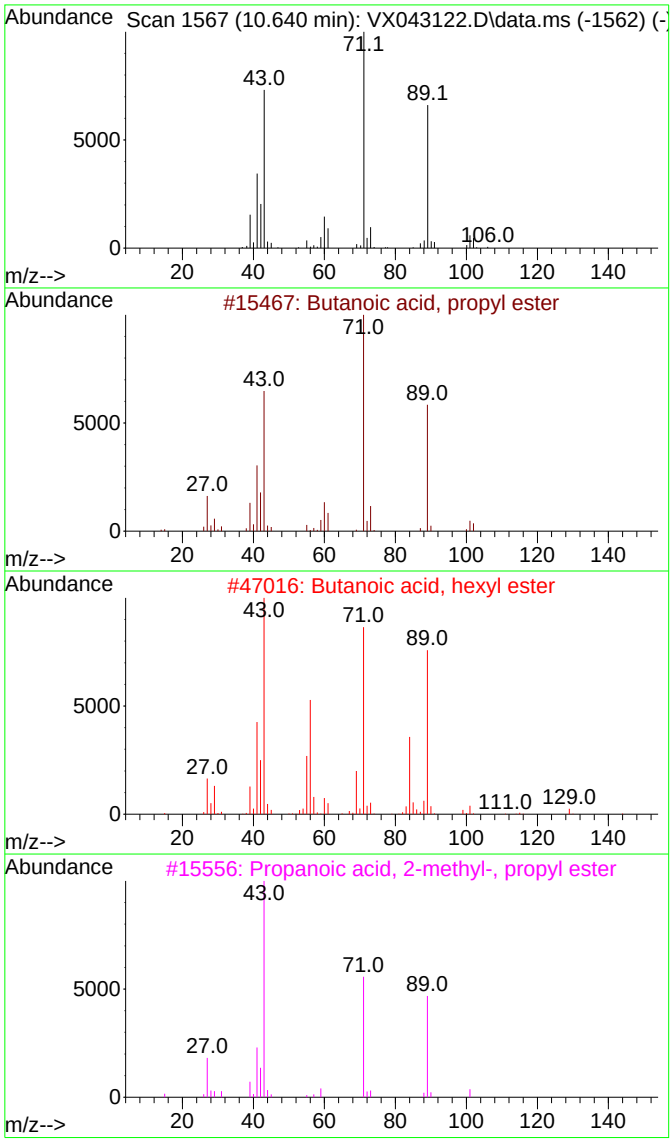
Quant Title : SW846 8260

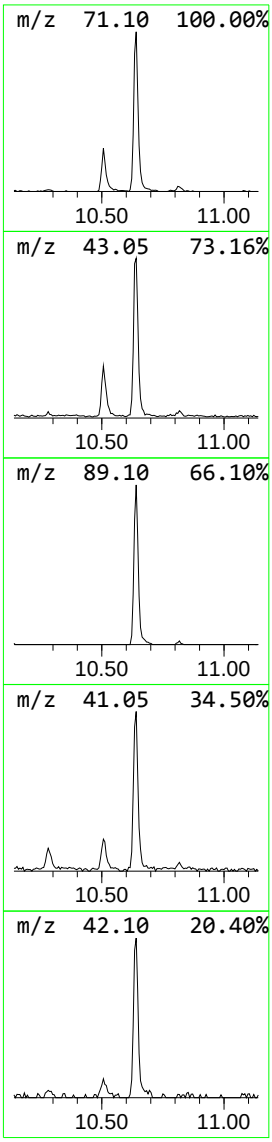
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.06 ug/l	81459	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	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	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\VX092424\
Data File : VX043122.D
Acq On : 24 Sep 2024 15:03
Operator : JC/MD
Sample : P4148-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
STOCK-PILE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.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
Sulfur dioxide	1.246	9.0	ug/l	52483	1	5.550	291622	50.0
n-Propyl acetate	7.793	151.8	ug/l	1356780	2	6.763	446860	50.0
Propanoic acid,...	8.549	26.4	ug/l	304787	3	10.055	577231	50.0
Isobutyl acetate	8.952	27.3	ug/l	314563	3	10.055	577231	50.0
Propanoic acid,...	9.244	33.3	ug/l	384748	3	10.055	577231	50.0
3-Pentanone, 2,...	9.372	12.7	ug/l	146921	3	10.055	577231	50.0
Propanoic acid,...	9.482	48.4	ug/l	558131	3	10.055	577231	50.0
Acetic acid, bu...	9.580	29.2	ug/l	336667	3	10.055	577231	50.0
Isopropyl butyrate	9.909	90.2	ug/l	1041030	3	10.055	577231	50.0
Butanoic acid, ...	10.640	7.1	ug/l	81459	3	10.055	577231	50.0