LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028484.D
Acq On : 02 May 2022 19:32
Operator : JC/MD
Sample : N2606-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-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\82X041922W.M
Title : SW846 8260

Signal : TIC: VX028484.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	694	706	720	rBV2	269784	785558	17.95%	3.347%
2	5.556	722	733	749	rVB	376977	1058496	24.19%	4.510%
3	5.958	788	799	813	rBV	278808	743985	17.00%	3.170%
4	6.348	853	863	873	rBV2	17873	49398	1.13%	0.210%
5	6.763	919	931	950	rBV	592745	1423013	32.51%	6.064%
6	7.799	1093	1101	1116	rBV	1573669	2631111	60.12%	11.211%
7	8.549	1218	1224	1234	rBV	289713	455975	10.42%	1.943%
8	8.653	1234	1241	1250	rBV	1513639	2331440	53.27%	9.934%
9	9.250	1333	1339	1345	rBV	74332	109428	2.50%	0.466%
10	9.348	1350	1355	1359	rBV	199686	266509	6.09%	1.136%
11	9.482	1372	1377	1389	rBV	3314079	4376613	100.00%	18.649%
12	9.580	1389	1393	1406	rVB	289080	382114	8.73%	1.628%
13	9.915	1442	1448	1461	rBV	2143622	2680991	61.26%	11.424%
14	10.055	1464	1471	1488	rVB	1427270	1928296	44.06%	8.217%
15	10.640	1563	1567	1572	rBV	61790	81239	1.86%	0.346%
16	11.085	1634	1640	1655	rBV	1304130	1671780	38.20%	7.124%
17	12.024	1788	1794	1803	rBV	1525849	1861434	42.53%	7.932%
18	12.616	1885	1891	1894	rBV	46455	55863	1.28%	0.238%
19	12.707	1901	1906	1912	rBV5	34784	64755	1.48%	0.276%
20	12.920	1934	1941	1946	rVB	40448	58526	1.34%	0.249%
21	13.286	1990	2001	2008	rBV2	140041	211786	4.84%	0.902%
22	13.664	2061	2063	2071	rVB4	32249	51636	1.18%	0.220%
23	13.926	2099	2106	2111	rBV2	31852	50801	1.16%	0.216%
24	14.231	2147	2156	2161	rBV3	35415	73512	1.68%	0.313%
25	14.481	2191	2197	2203	rBV2	47912	63860	1.46%	0.272%

Sum of corrected areas: 23468119

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ClientSampleId :
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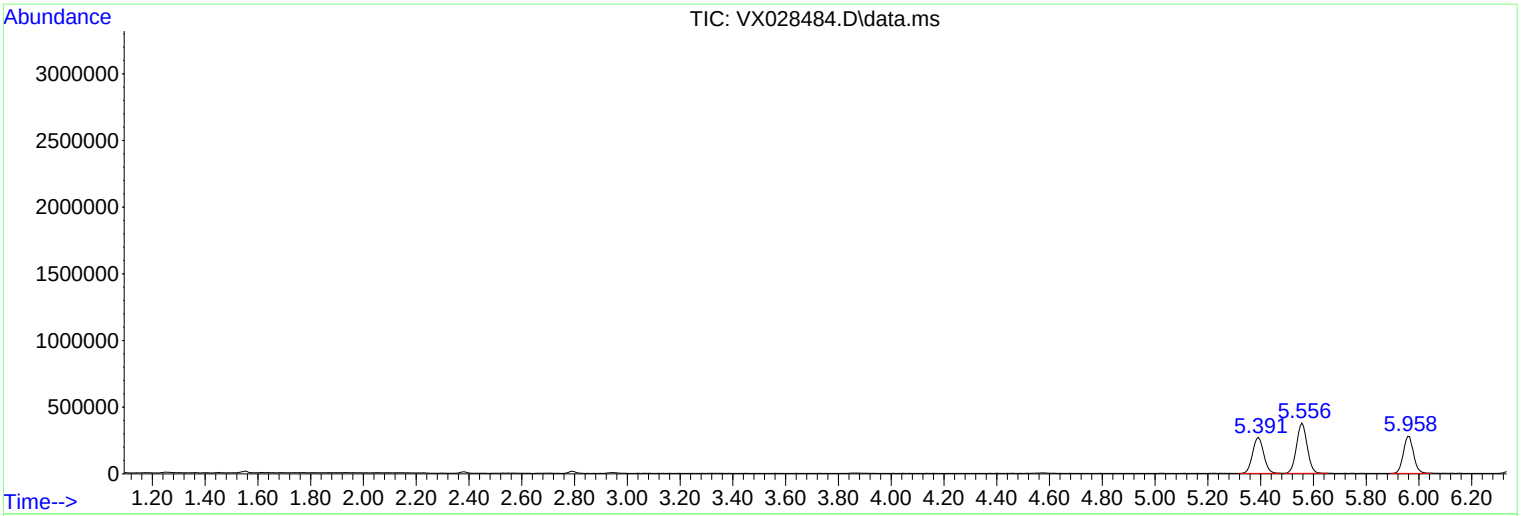
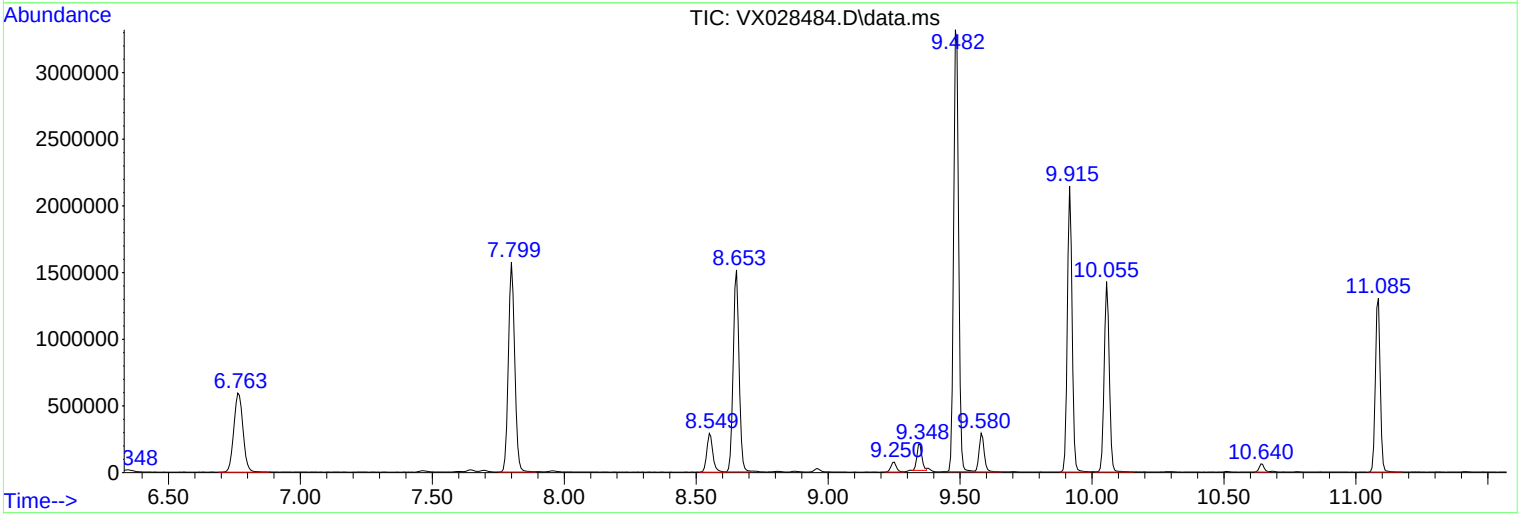
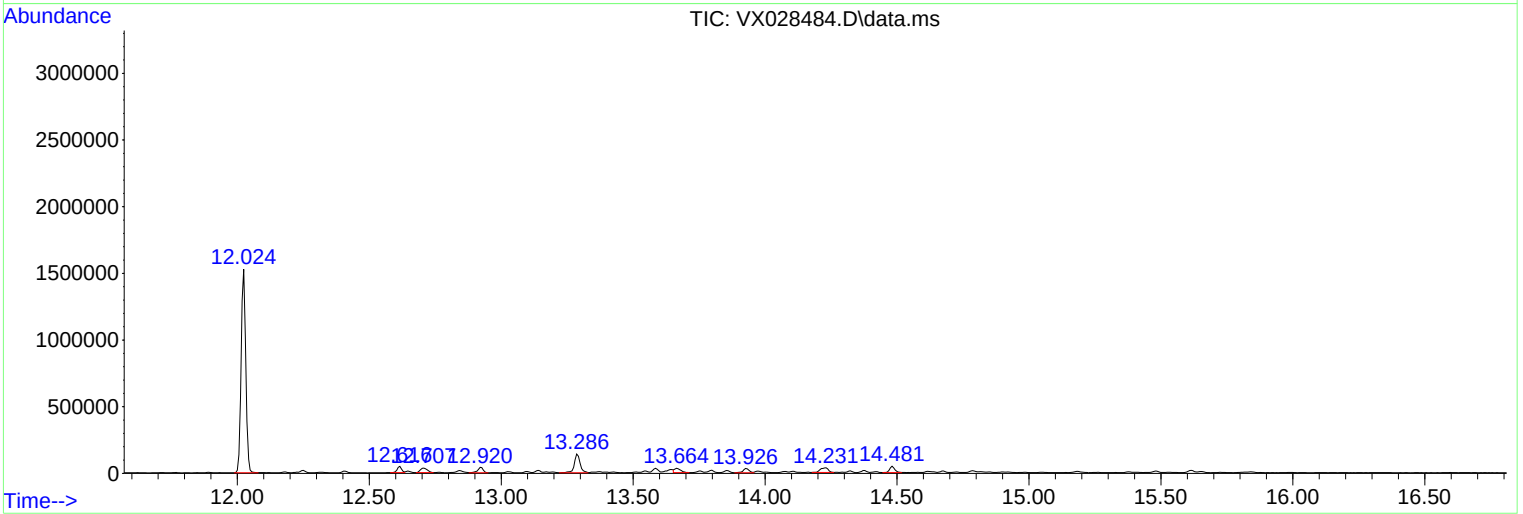
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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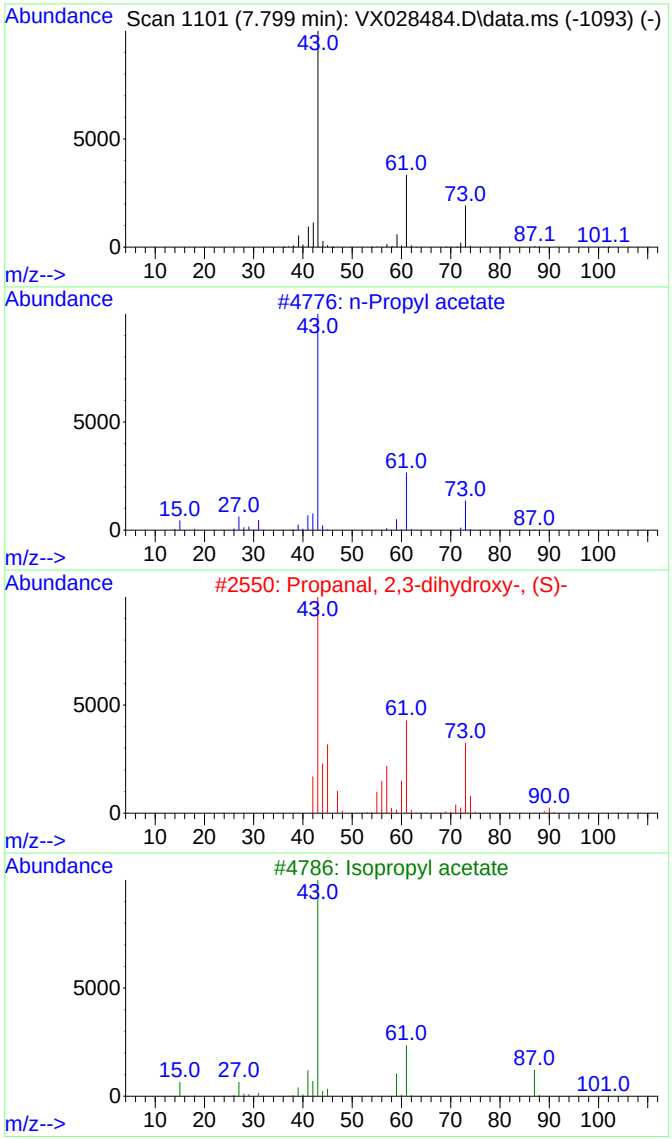
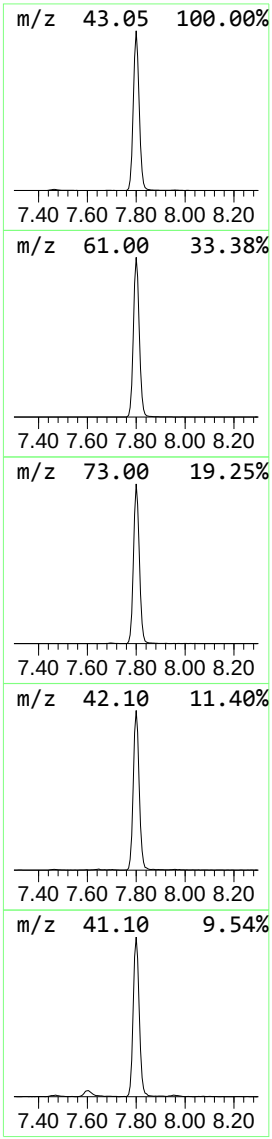
****
Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	92.45 ug/l	2631110	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	38
3	Isopropyl acetate	102	C5H10O2	000108-21-4	28
4	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9
5	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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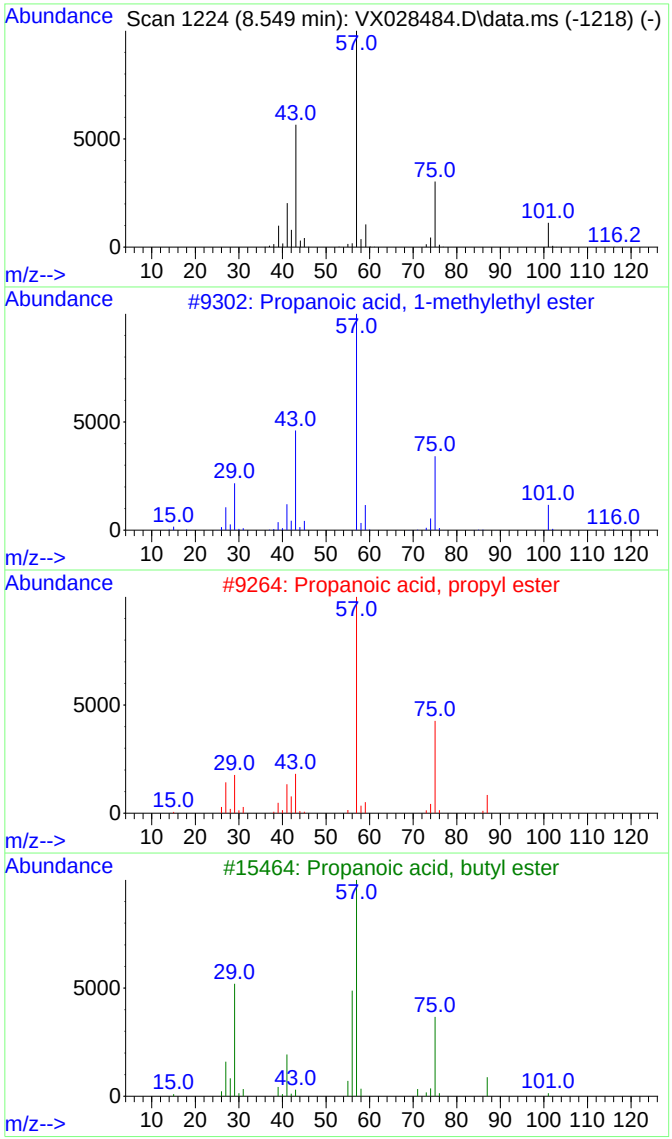
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

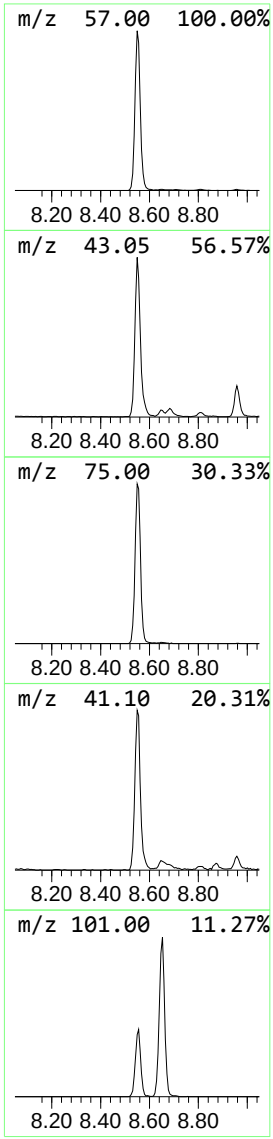
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	11.82 ug/l	455975	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	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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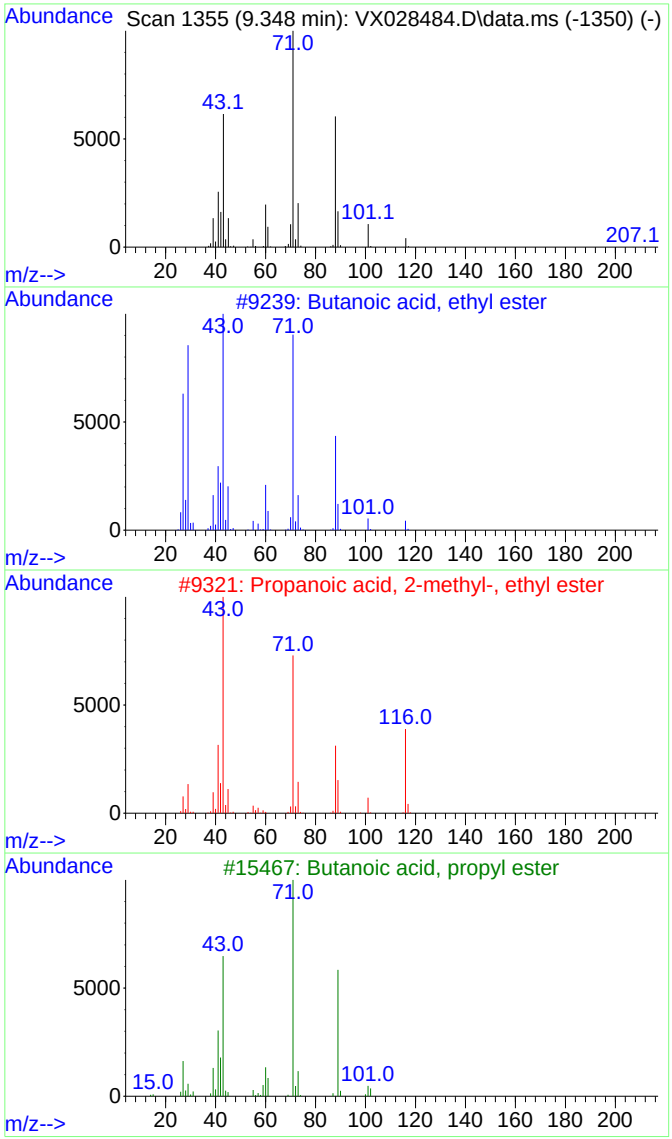
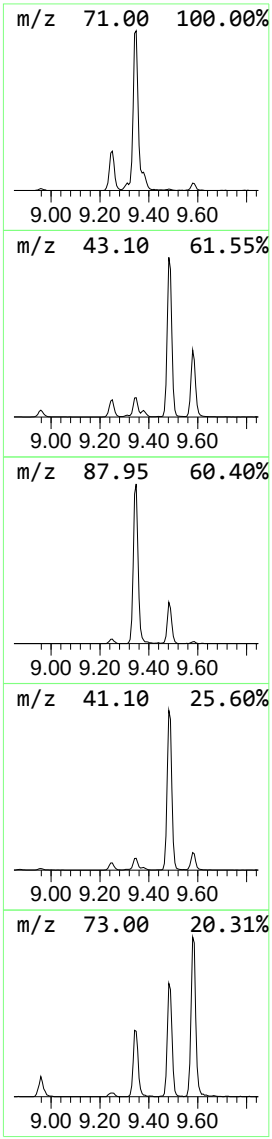
****
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.348	6.91 ug/l	266509	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
4	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	38
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	37





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-3

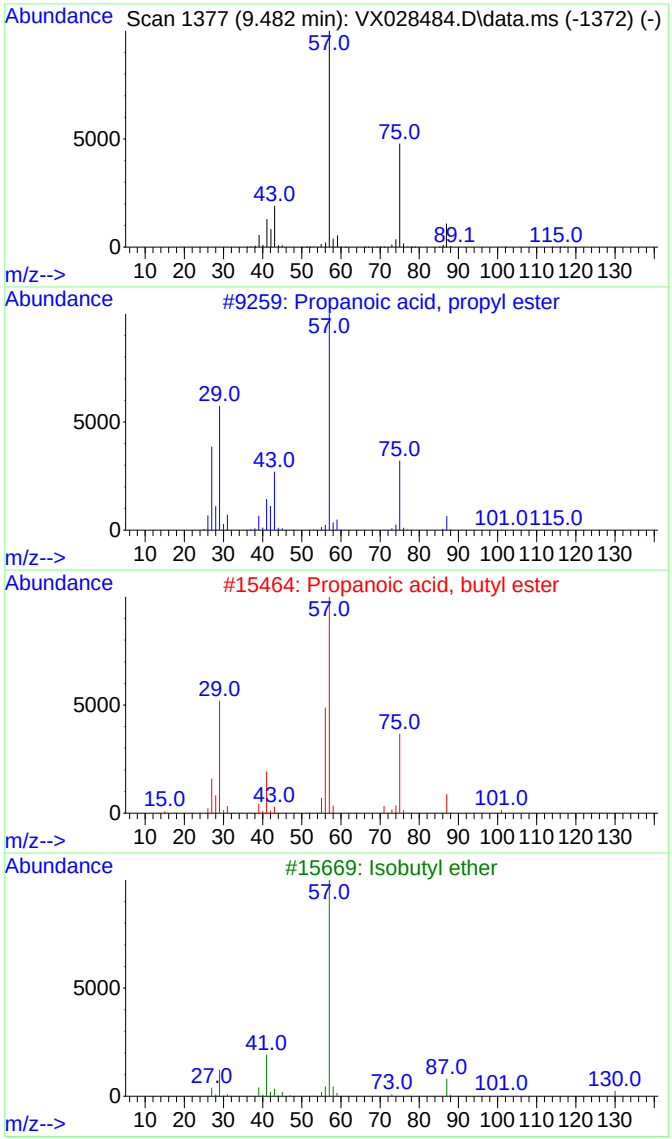
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

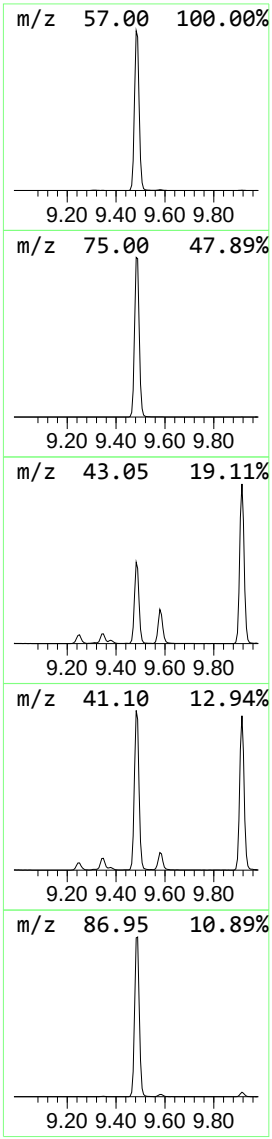
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	113.48 ug/l	4376610	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	8





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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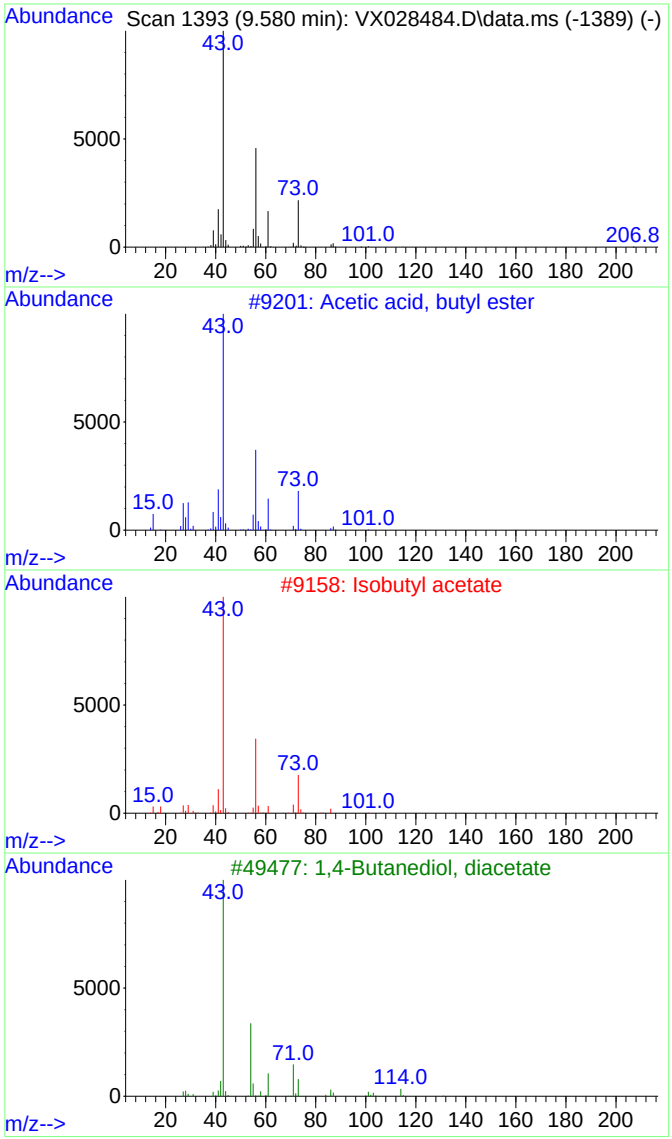
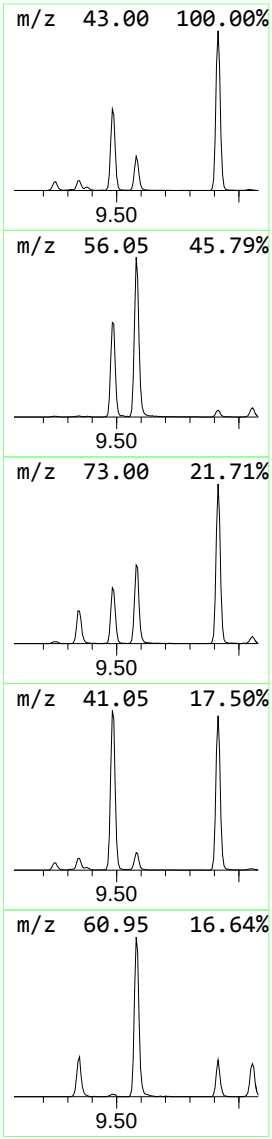
****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	9.91 ug/l	382114	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	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9





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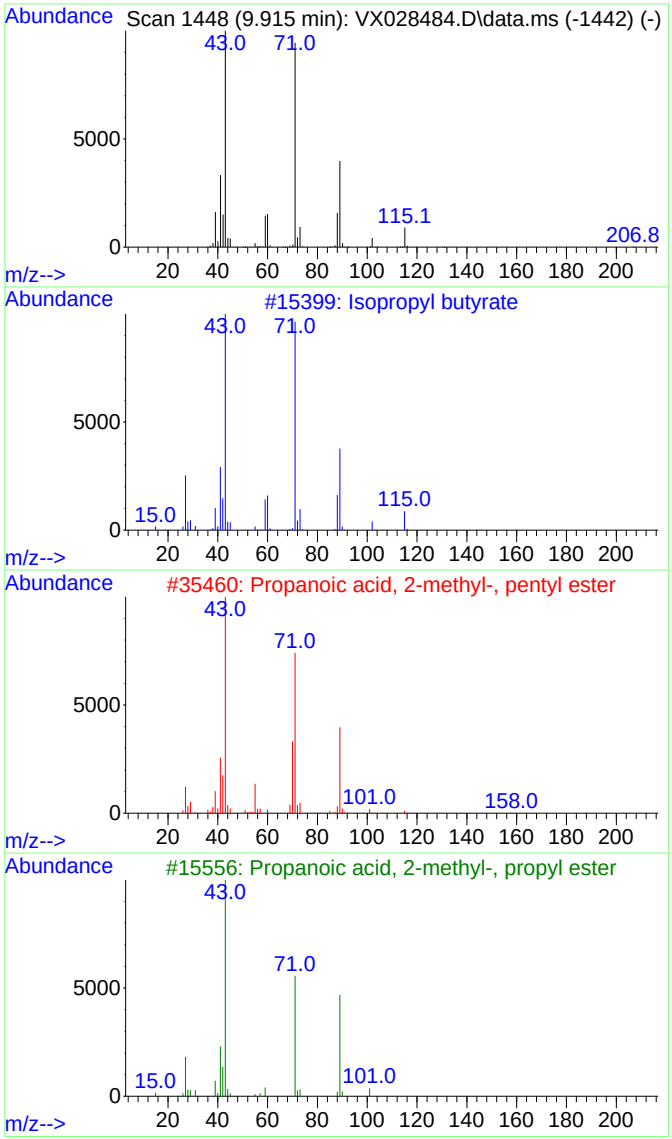
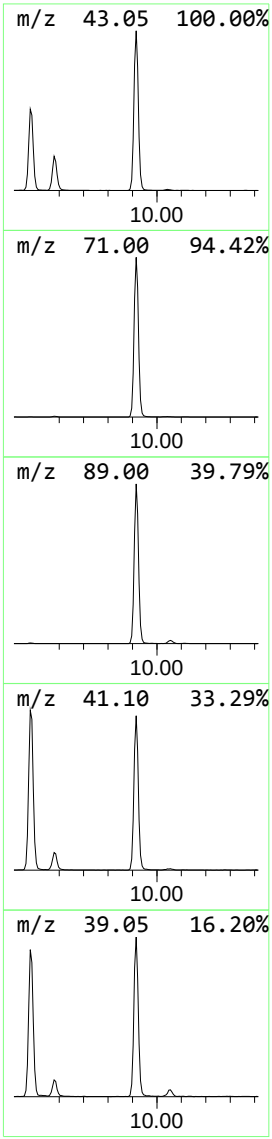
****
Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	69.52 ug/l	2680990	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-, penty...	158	C9H18O2	002445-72-9	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





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TIC Library : C:\Database\NIST20.L
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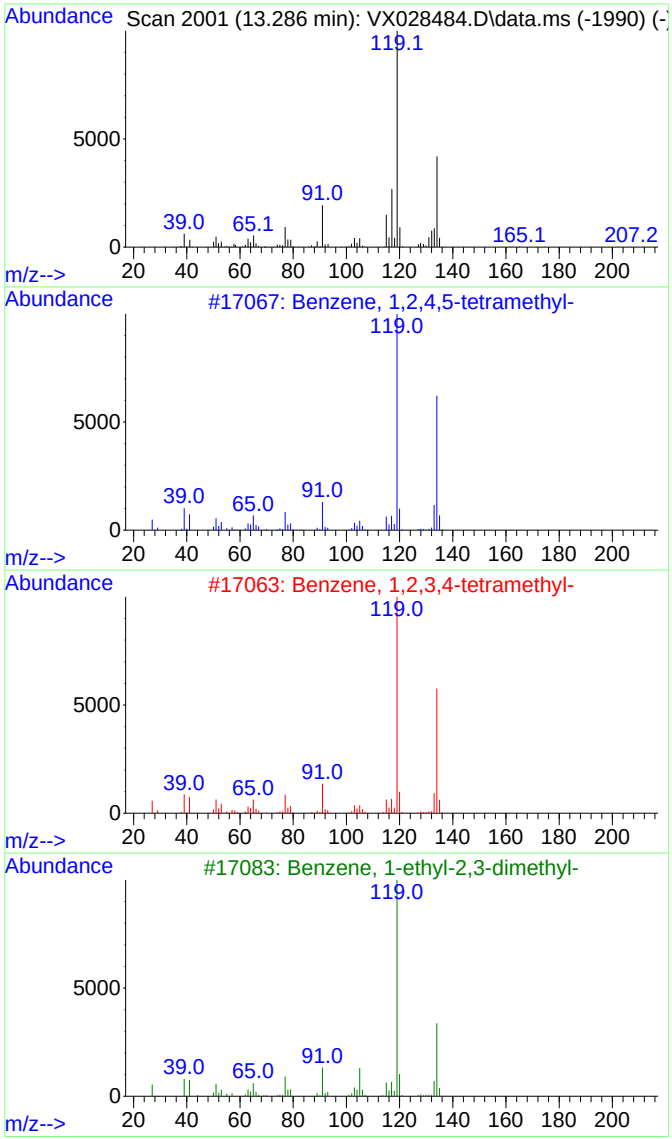
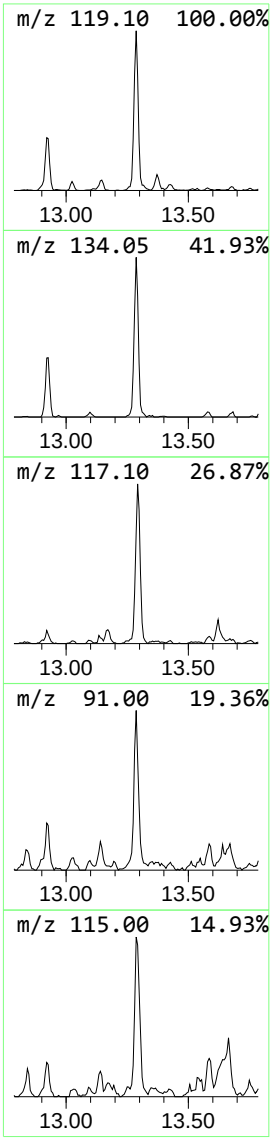
****
Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	5.69 ug/l	211786	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	83
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	83
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	83
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.799	92.5	ug/l	2631110	2	6.763	1423010	50.0
Propanoic acid,...	8.549	11.8	ug/l	455975	3	10.055	1928300	50.0
Butanoic acid, ...	9.348	6.9	ug/l	266509	3	10.055	1928300	50.0
Propanoic acid,...	9.482	113.5	ug/l	4376610	3	10.055	1928300	50.0
Acetic acid, bu...	9.580	9.9	ug/l	382114	3	10.055	1928300	50.0
Isopropyl butyrate	9.915	69.5	ug/l	2680990	3	10.055	1928300	50.0
Benzene, 1,2,4,...	13.286	5.7	ug/l	211786	4	12.024	1861430	50.0