LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027963.D
Acq On : 04 Apr 2022 17:21
Operator : JC/MD
Sample : PB143824TB
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824TB

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82X032922W.M
Title : SW846 8260

Signal : TIC: VX027963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% of % max.	% of total
1	1.240	22	25	37	rBV	41683	52339	3.88%	0.812%
2	2.788	271	279	291	rBV	148643	273888	20.31%	4.248%
3	3.581	401	409	420	rBV2	6442	15088	1.12%	0.234%
4	5.391	693	706	719	rBV	54282	158484	11.75%	2.458%
5	5.556	722	733	746	rVV2	100664	278896	20.68%	4.326%
6	5.958	788	799	814	rBV2	60725	158216	11.73%	2.454%
7	6.348	852	863	873	rBV2	5884	16264	1.21%	0.252%
8	6.690	914	919	923	rBV2	8084	19590	1.45%	0.304%
9	6.763	923	931	946	rVB	149427	369031	27.37%	5.724%
10	7.799	1093	1101	1115	rBV	542828	921785	68.37%	14.297%
11	8.549	1218	1224	1234	rBV	89670	139256	10.33%	2.160%
12	8.653	1234	1241	1257	rVB	295438	467017	34.64%	7.243%
13	8.958	1286	1291	1300	rVB	9966	14959	1.11%	0.232%
14	9.244	1333	1338	1345	rBV	23960	35500	2.63%	0.551%
15	9.342	1350	1354	1359	rBV	60567	81505	6.04%	1.264%
16	9.488	1372	1378	1384	rBV	991666	1348311	100.00%	20.912%
17	9.579	1388	1393	1404	rVB	119117	151113	11.21%	2.344%
18	9.915	1442	1448	1461	rBV	664101	810678	60.13%	12.573%
19	10.055	1465	1471	1478	rBV	307776	407614	30.23%	6.322%
20	10.640	1562	1567	1574	rBV	24289	30363	2.25%	0.471%
21	11.085	1634	1640	1650	rBV	262604	340881	25.28%	5.287%
22	12.024	1789	1794	1803	rBV	298082	356807	26.46%	5.534%

Sum of corrected areas: 6447585

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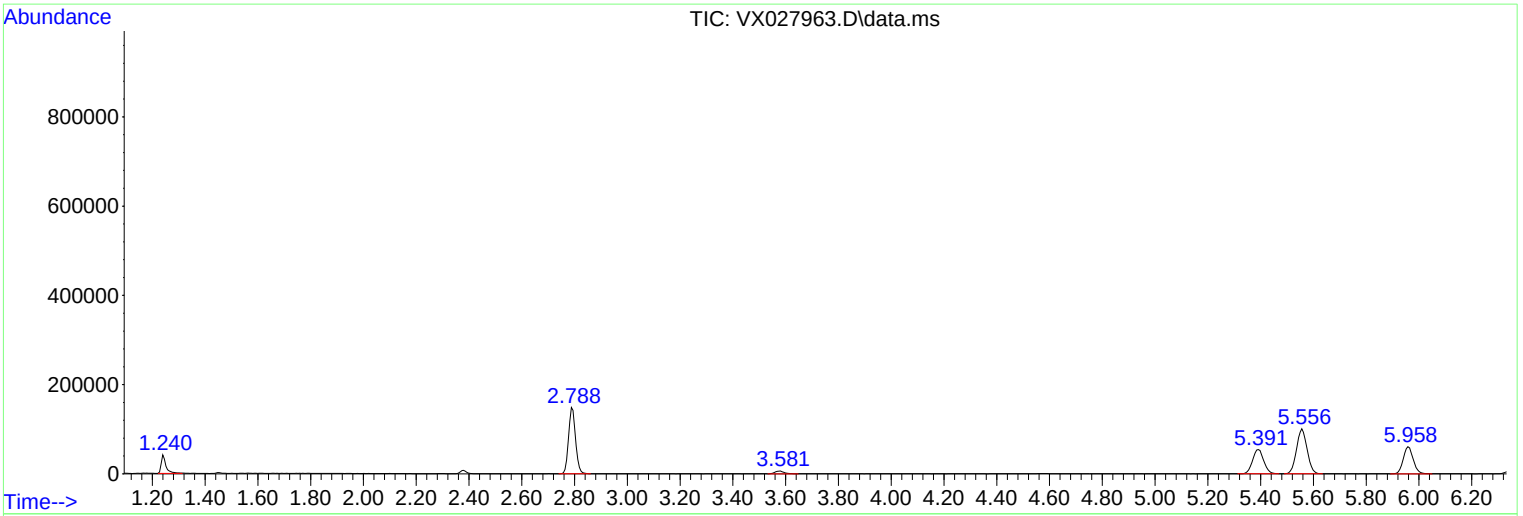
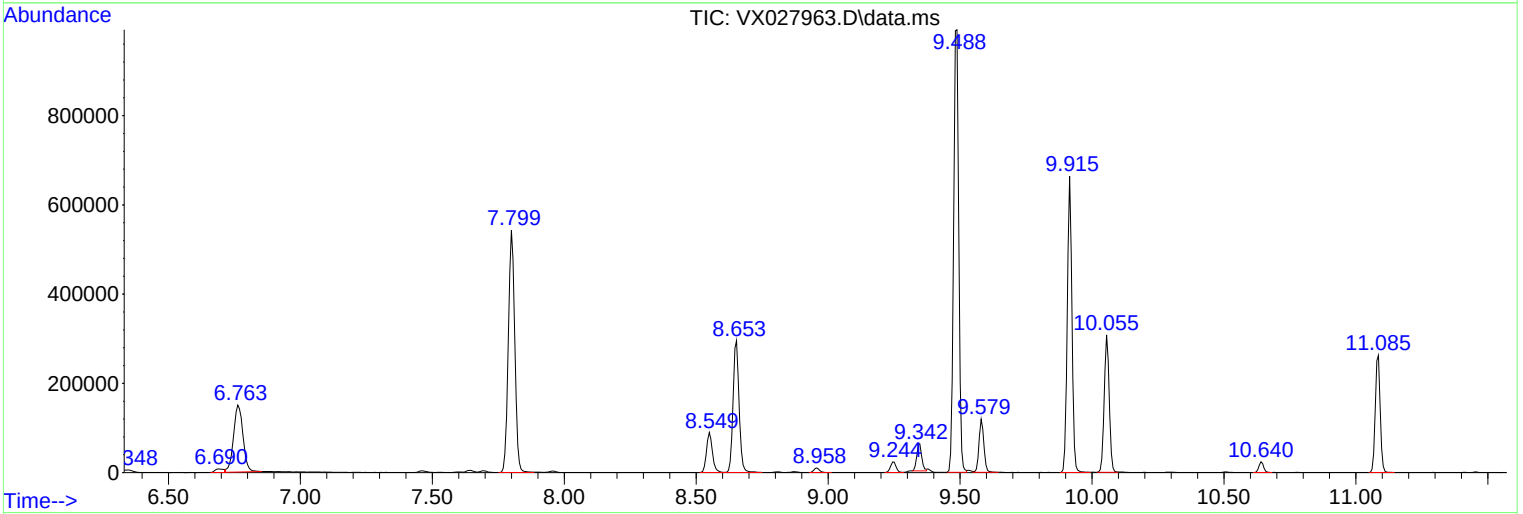
ALS Vial : 18 Sample Multiplier: 1

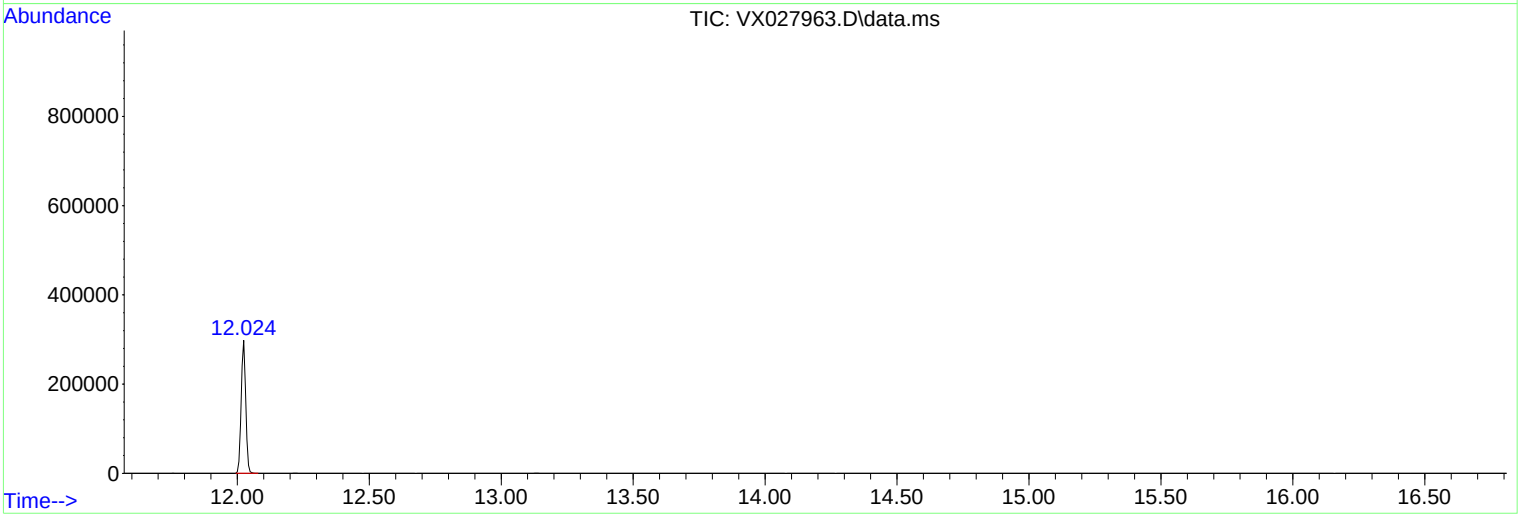
Instrument :
MSVOA_X
ClientSampleId :
PB143824TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.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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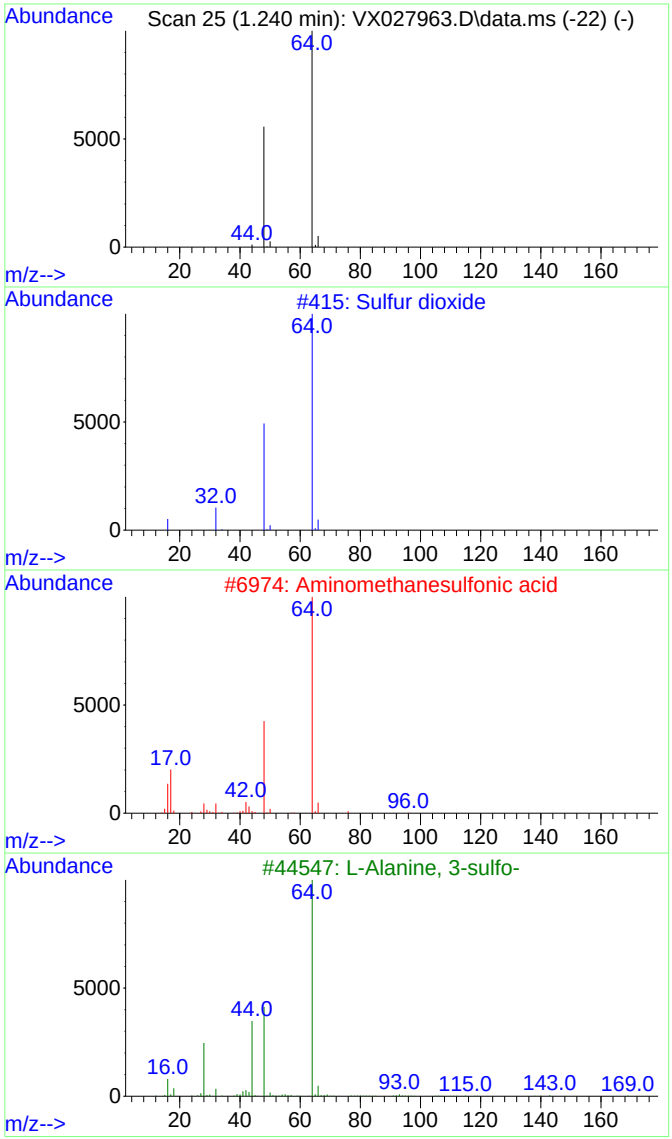
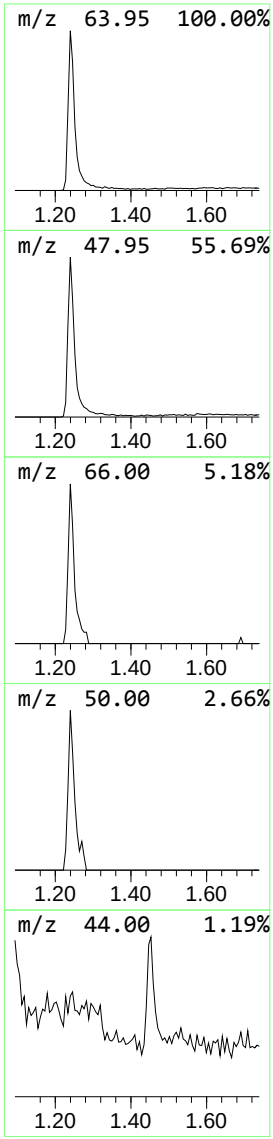
****

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	9.38 ug/l	52339	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
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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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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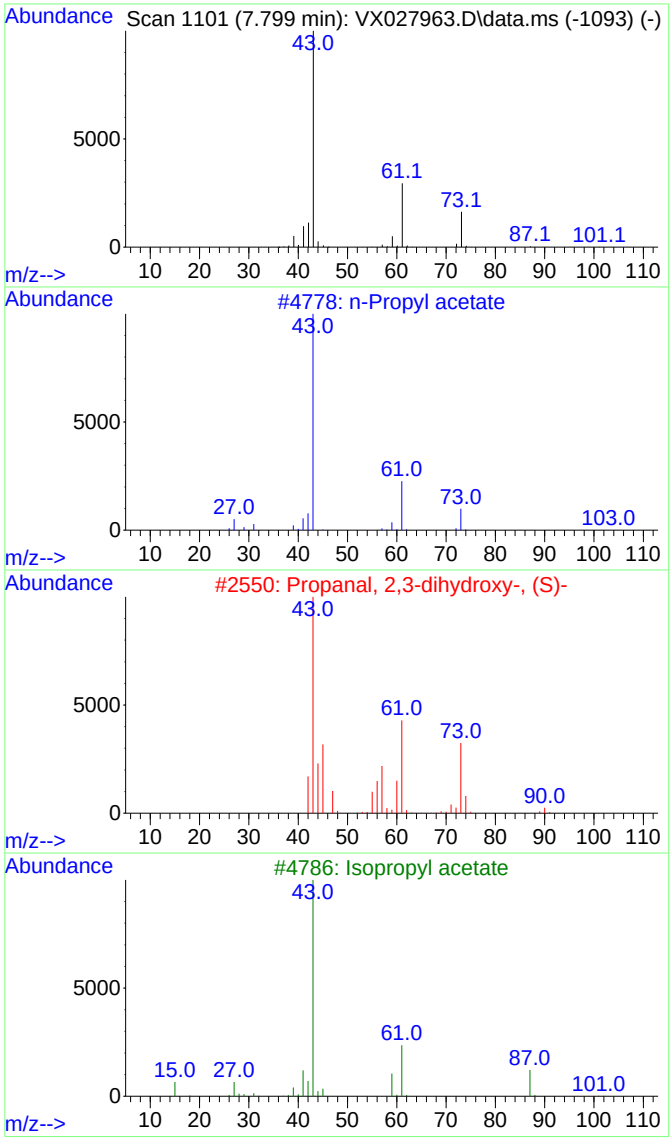
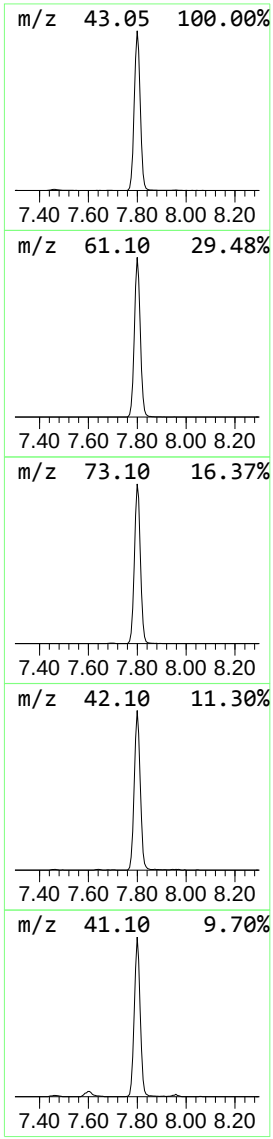
****
Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	124.89 ug/l	921785	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	9
3	Isopropyl acetate	102	C5H10O2	000108-21-4	9
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824TB

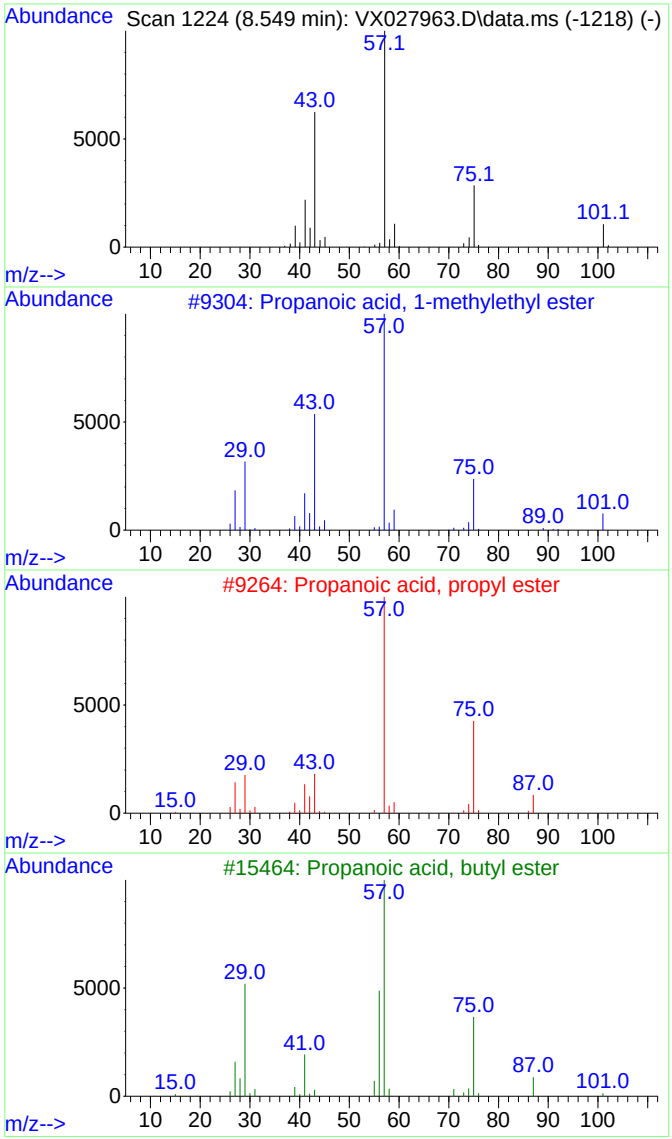
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

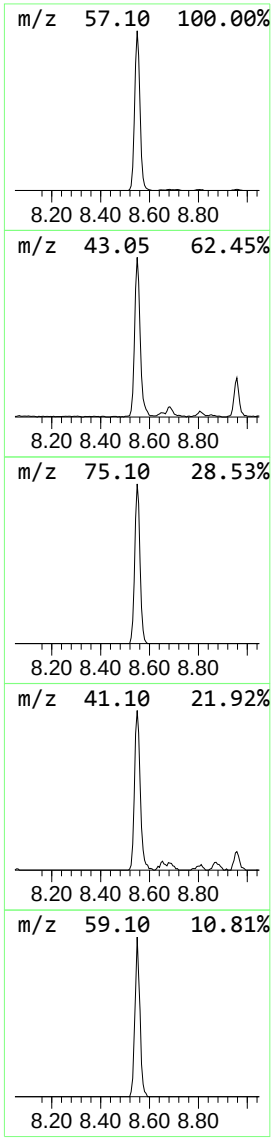
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	17.08 ug/l	139256	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	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9





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MSVOA_X
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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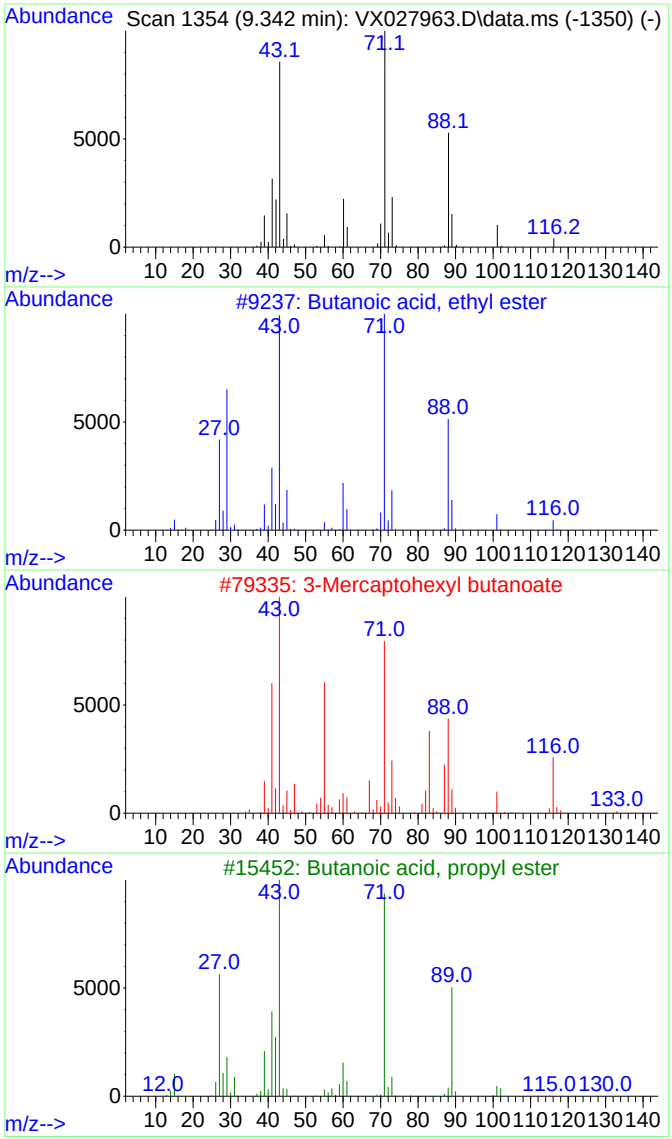
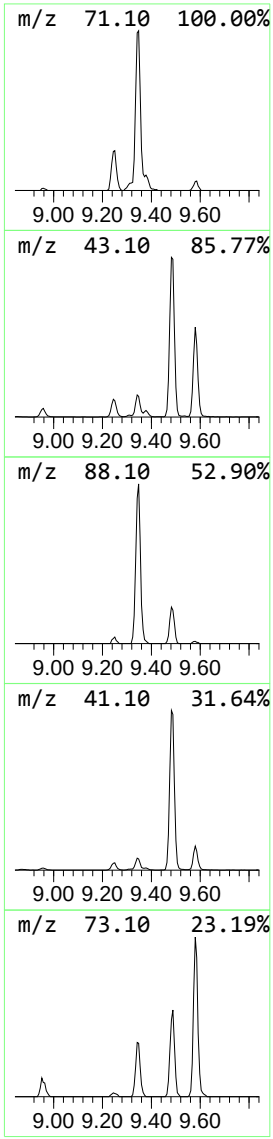
****
Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	10.00 ug/l	81505	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	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
4	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	50
5	3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	42





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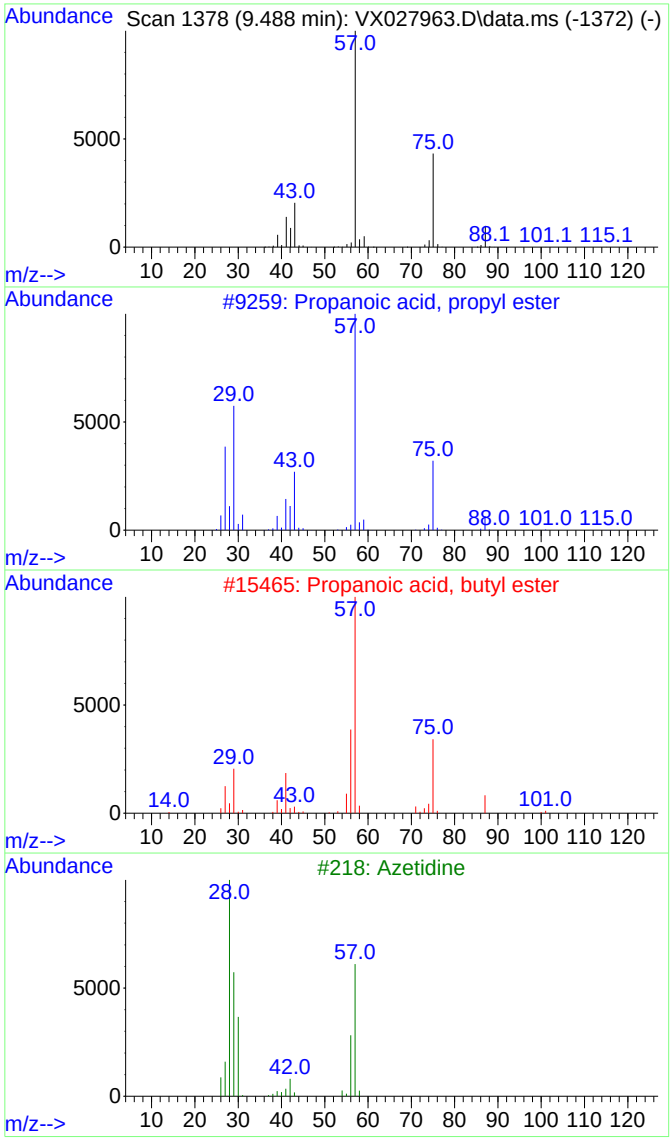
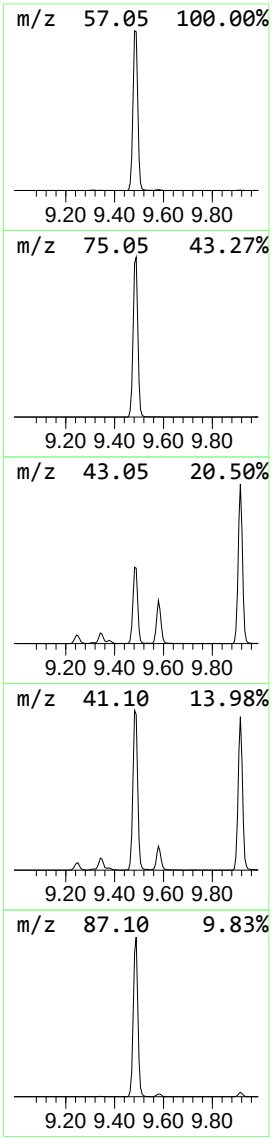
****
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	165.39 ug/l	1348310	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	Azetidine	57	C3H7N	000503-29-7	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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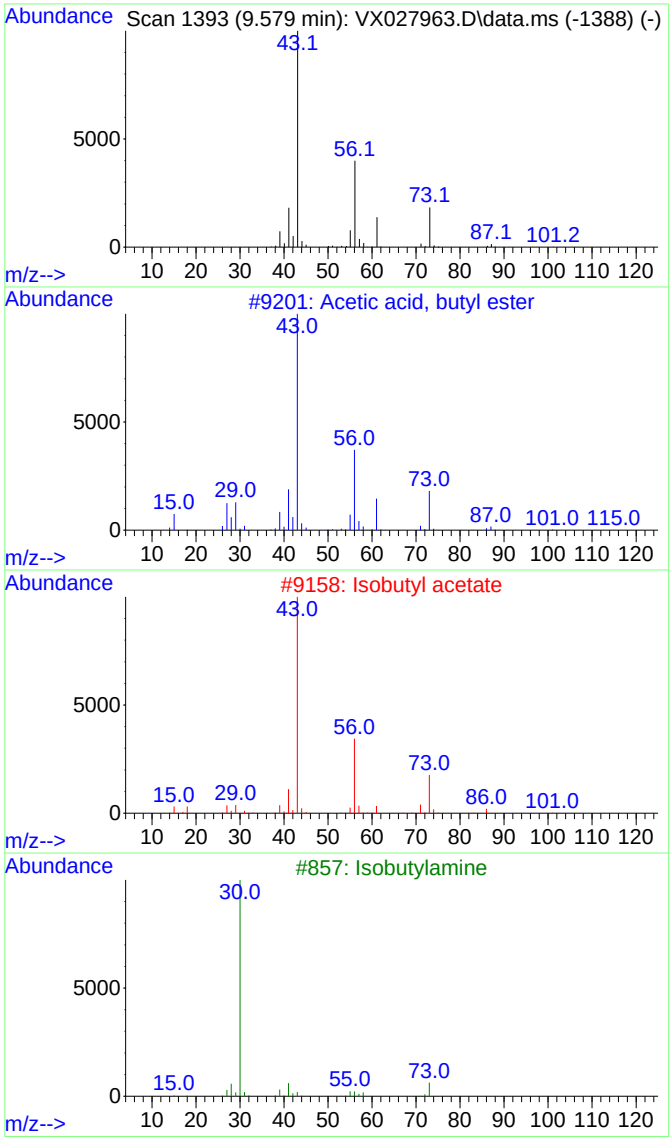
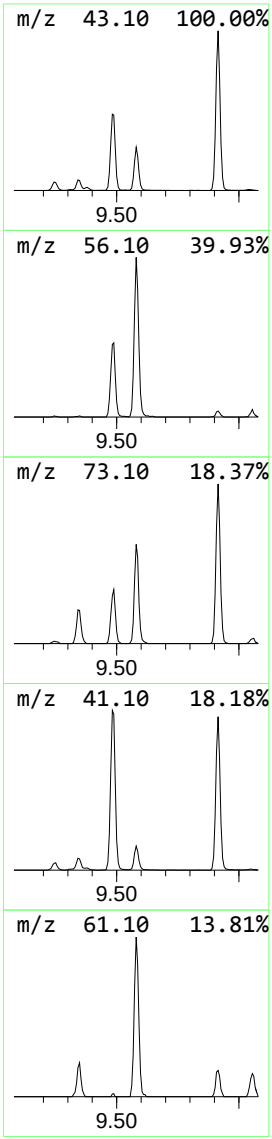
****
Peak Number 6 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	18.54 ug/l	151113	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
2	Isobutyl acetate	116	C6H12O2	000110-19-0	39
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9





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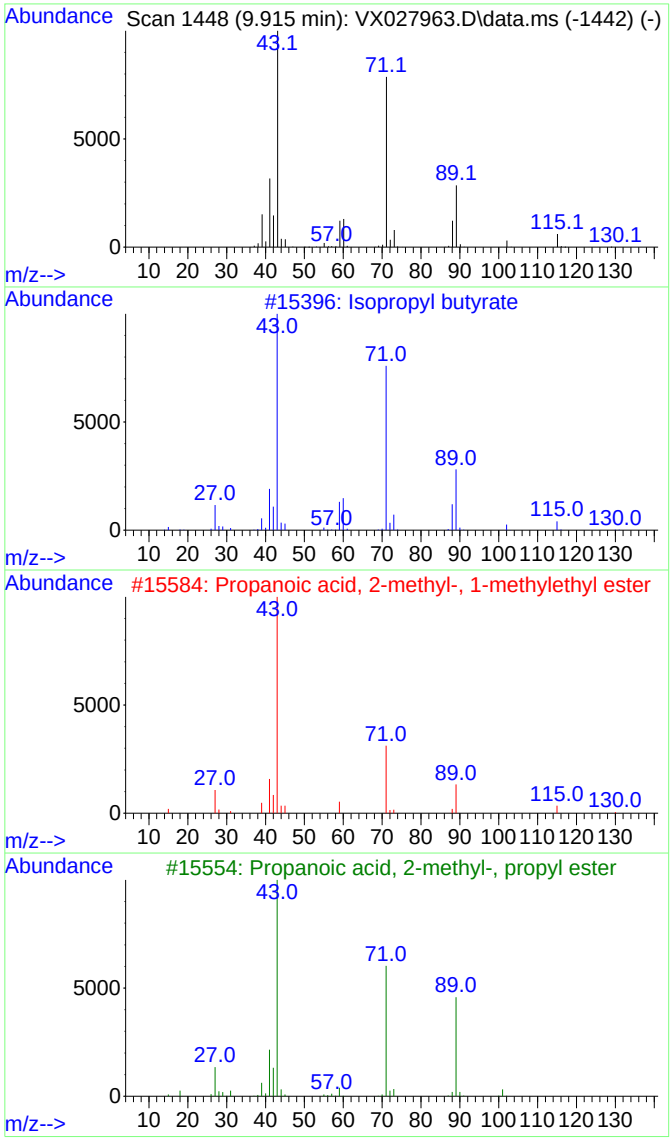
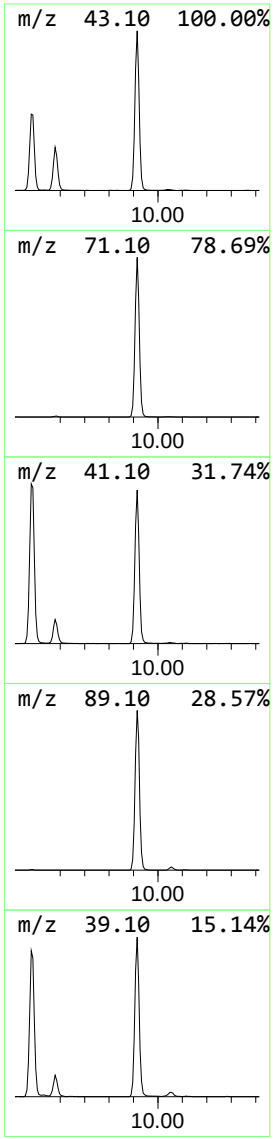
****
Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	99.44 ug/l	810678	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	94
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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.240	9.4	ug/l	52339	1	5.562	278896	50.0
n-Propyl acetate	7.799	124.9	ug/l	921785	2	6.763	369031	50.0
Propanoic acid,...	8.549	17.1	ug/l	139256	3	10.055	407614	50.0
Butanoic acid, ...	9.342	10.0	ug/l	81505	3	10.055	407614	50.0
Propanoic acid,...	9.488	165.4	ug/l	1348310	3	10.055	407614	50.0
Acetic acid, bu...	9.579	18.5	ug/l	151113	3	10.055	407614	50.0
Isopropyl butyrate	9.915	99.4	ug/l	810678	3	10.055	407614	50.0