LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027970.D
Acq On : 04 Apr 2022 20:03
Operator : JC/MD
Sample : PB143824ZHE#07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#07

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: VX027970.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	34	rBV	10498	15766	1.41%	0.278%
2	2.380	205	212	222	rVB2	7744	13245	1.18%	0.234%
3	2.788	272	279	295	rVB	150715	273257	24.39%	4.826%
4	3.575	401	408	422	rVB3	6267	14782	1.32%	0.261%
5	5.391	694	706	721	rBV	54719	157023	14.01%	2.773%
6	5.556	721	733	746	rVV	96883	271764	24.25%	4.799%
7	5.958	789	799	812	rBV2	58158	152916	13.65%	2.700%
8	6.342	854	862	872	rBV2	6223	15502	1.38%	0.274%
9	6.696	914	920	922	rBV	6739	11905	1.06%	0.210%
10	6.763	923	931	947	rVB	145763	361165	32.23%	6.378%
11	7.799	1094	1101	1116	rBV	443544	753198	67.22%	13.301%
12	8.549	1215	1224	1234	rBV	71165	110226	9.84%	1.947%
13	8.653	1234	1241	1256	rVV	256710	410507	36.64%	7.249%
14	8.958	1285	1291	1298	rBV2	7905	12427	1.11%	0.219%
15	9.250	1333	1339	1345	rBV	19246	28152	2.51%	0.497%
16	9.342	1350	1354	1359	rBV	51403	69591	6.21%	1.229%
17	9.482	1372	1377	1384	rBV	843045	1120454	100.00%	19.787%
18	9.580	1388	1393	1404	rVB	96725	122678	10.95%	2.166%
19	9.915	1442	1448	1461	rBV	547874	677649	60.48%	11.967%
20	10.055	1463	1471	1478	rBV	276943	367222	32.77%	6.485%
21	10.640	1563	1567	1575	rVB	24391	27937	2.49%	0.493%
22	11.085	1634	1640	1651	rBV	248165	327373	29.22%	5.781%
23	12.024	1789	1794	1802	rBV	284494	347909	31.05%	6.144%

Sum of corrected areas: 5662648

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Instrument :
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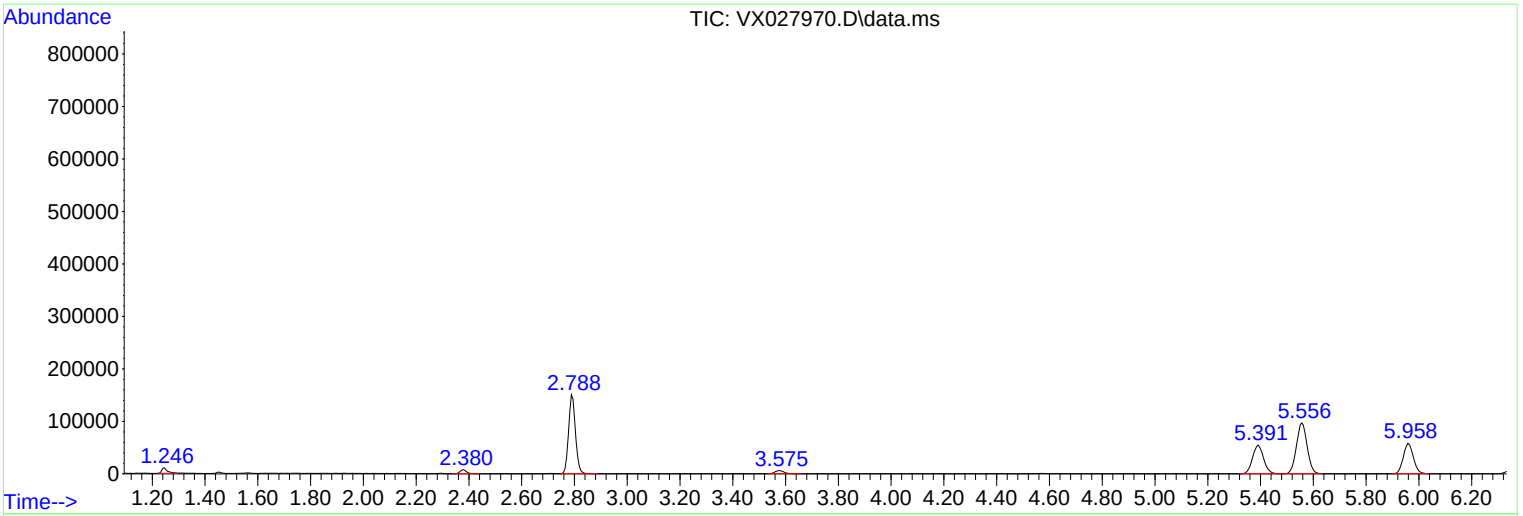
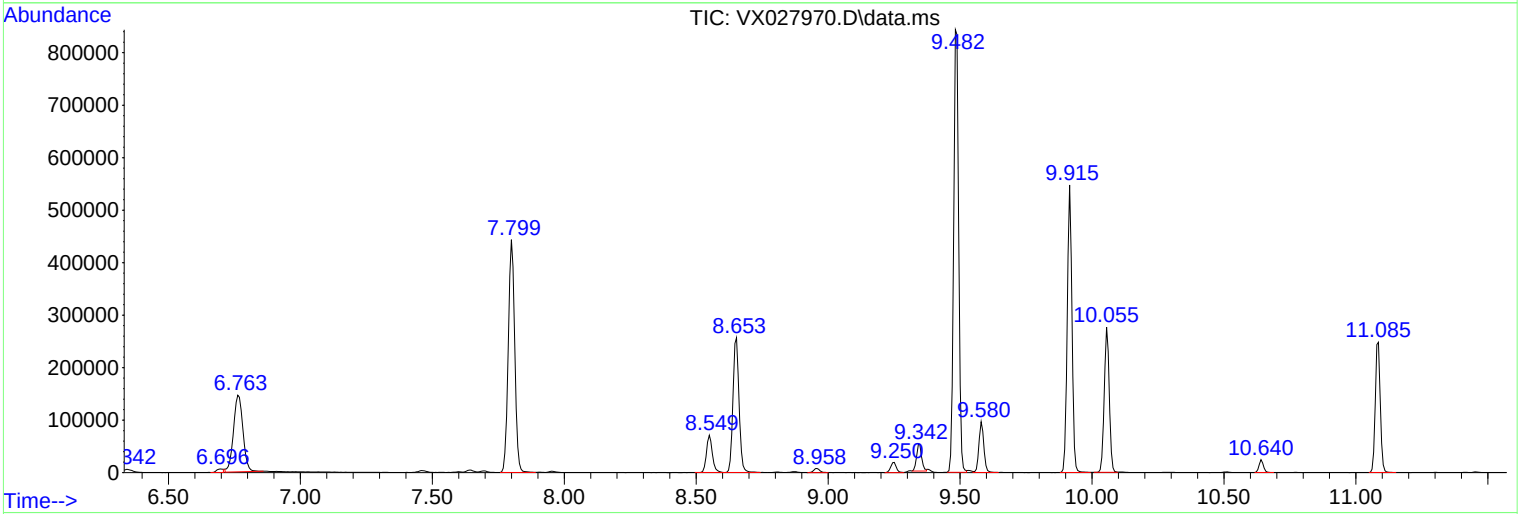
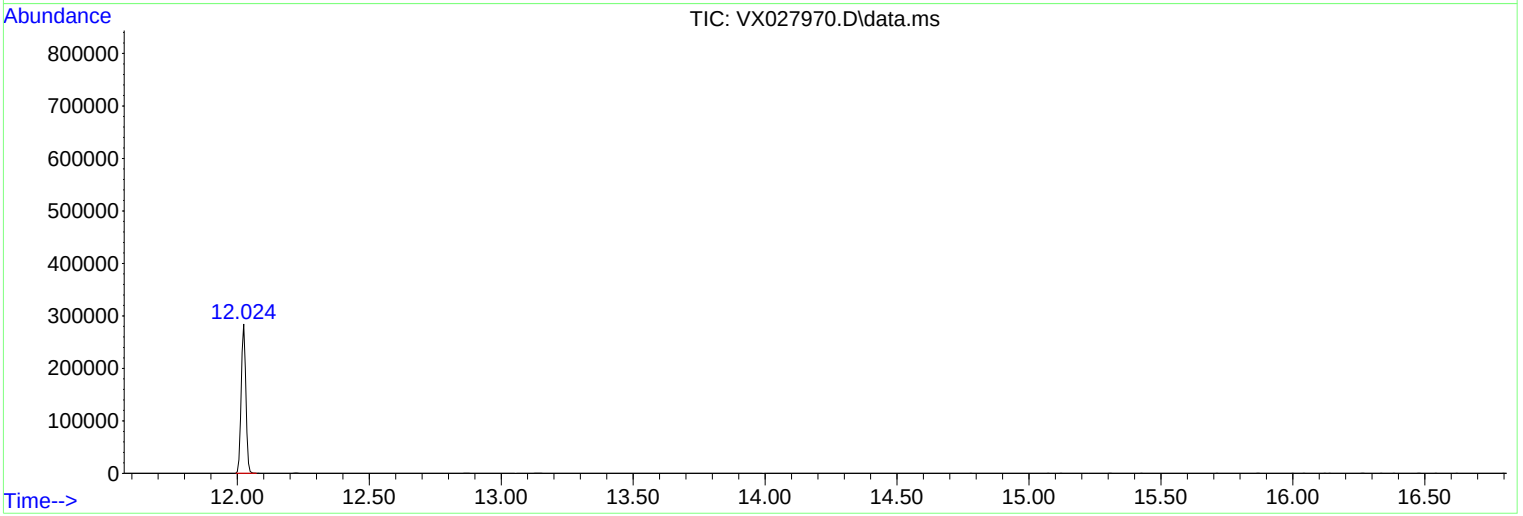
ClientSampleId :
PB143824ZHE#07

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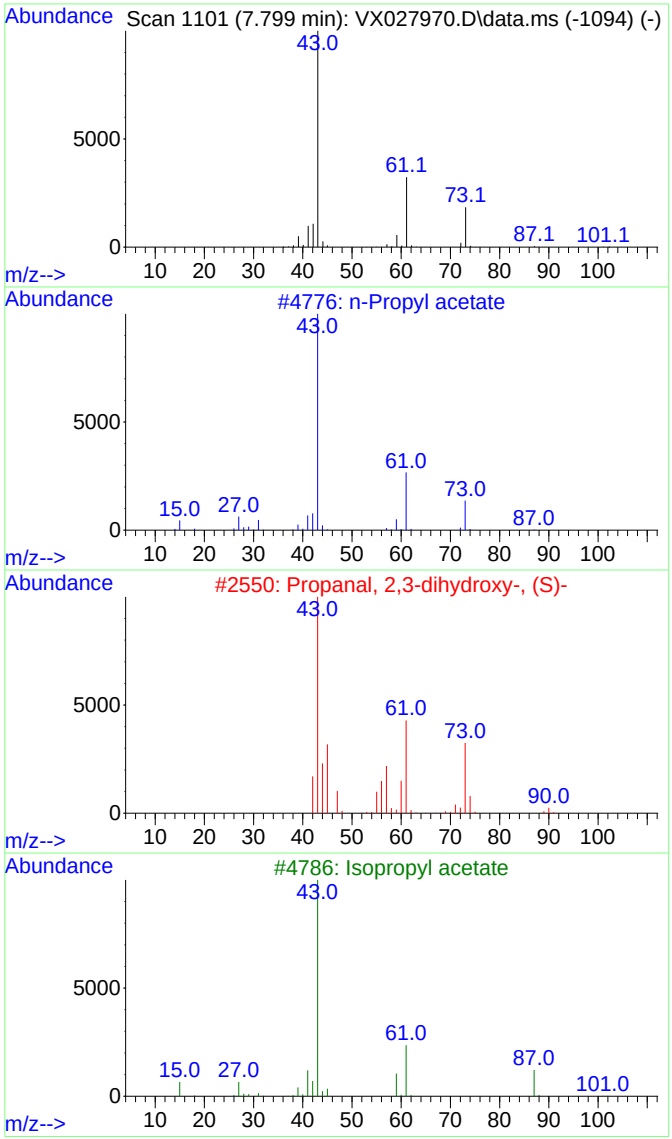
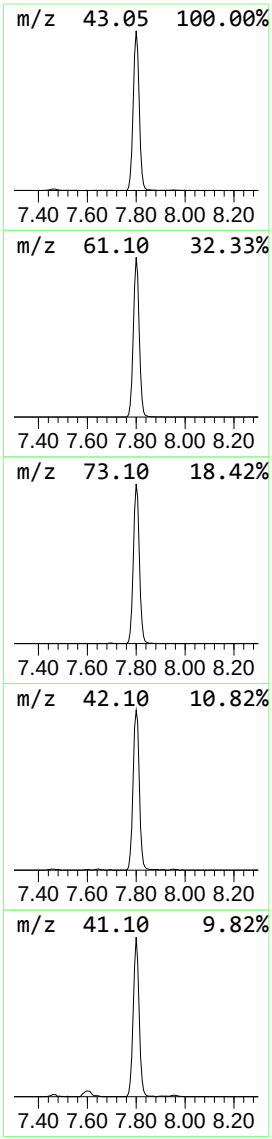
****
Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	104.27 ug/l	753198	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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Quant Title : SW846 8260

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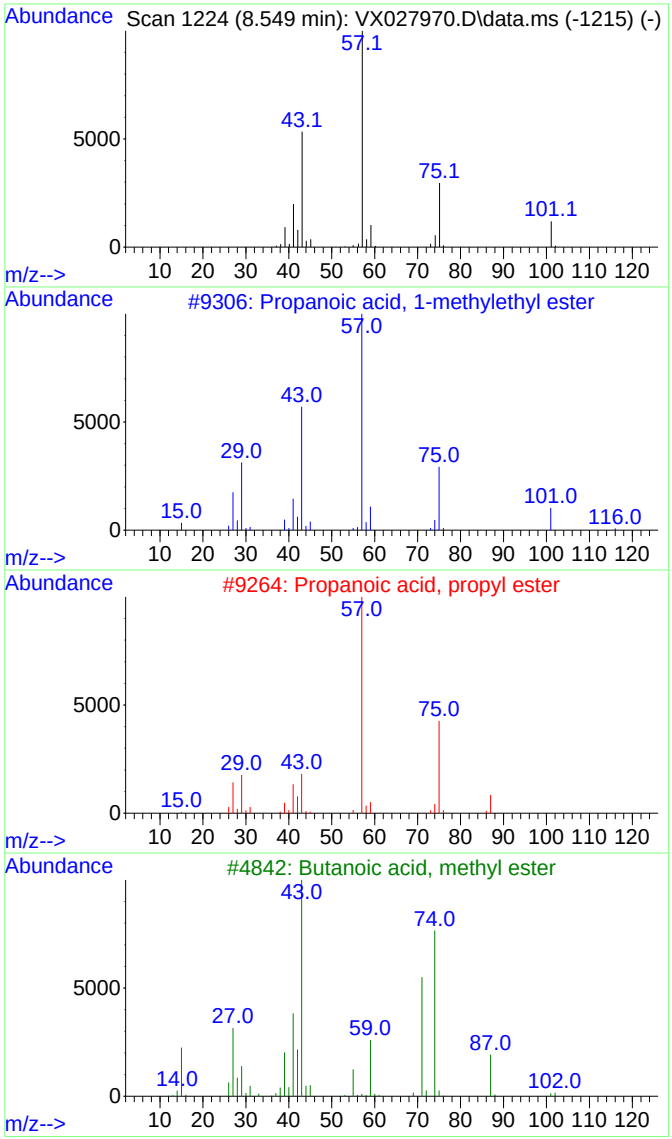
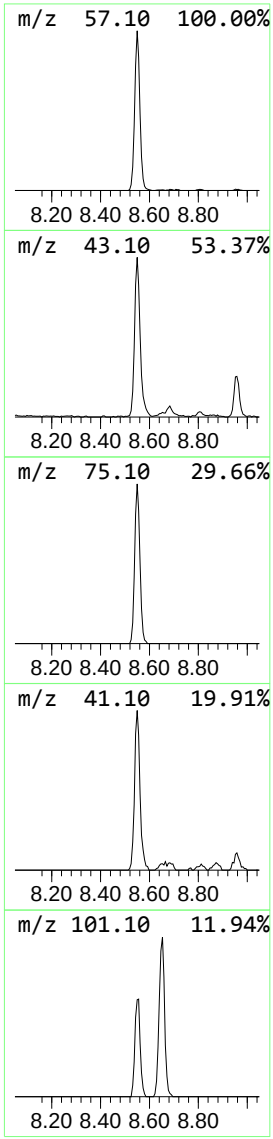
****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	15.01 ug/l	110226	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	36
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	14
4	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	9
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9





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Instrument :
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ClientSampleId :
PB143824ZHE#07

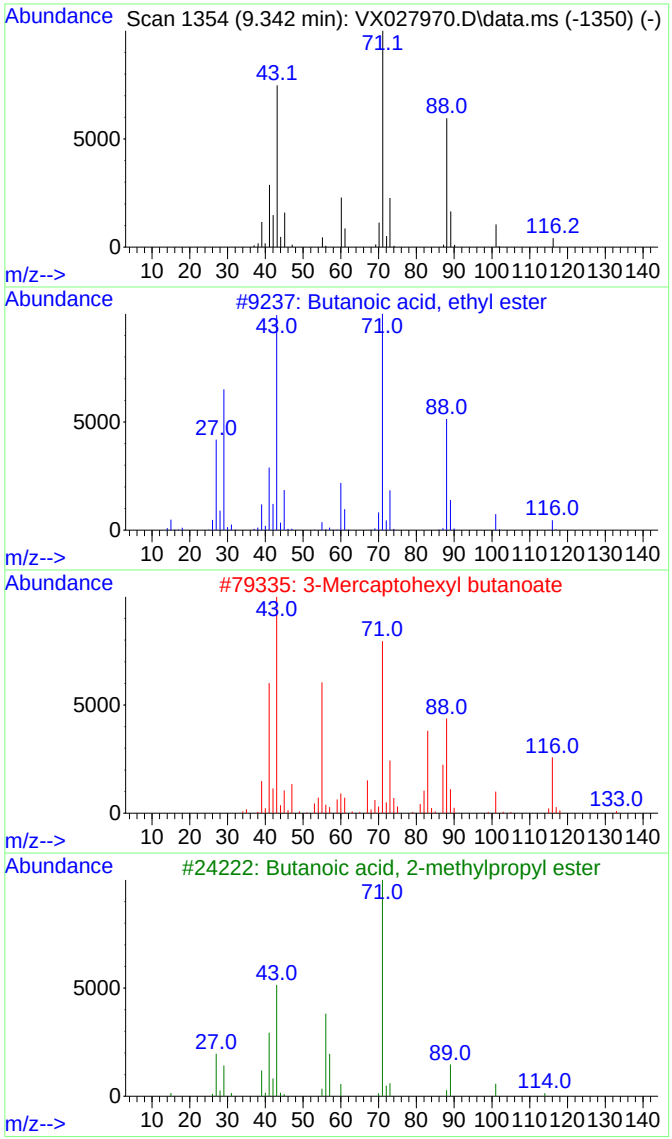
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

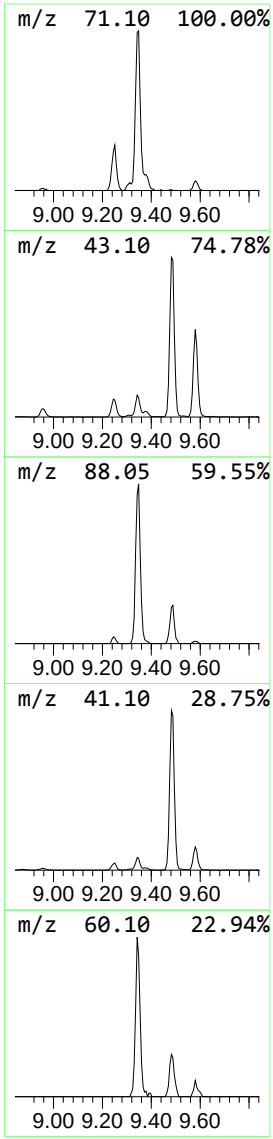
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	9.48 ug/l	69591	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	56
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	43
4	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	40
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	37





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB143824ZHE#07

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
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TIC Library : C:\Database\NIST20.L
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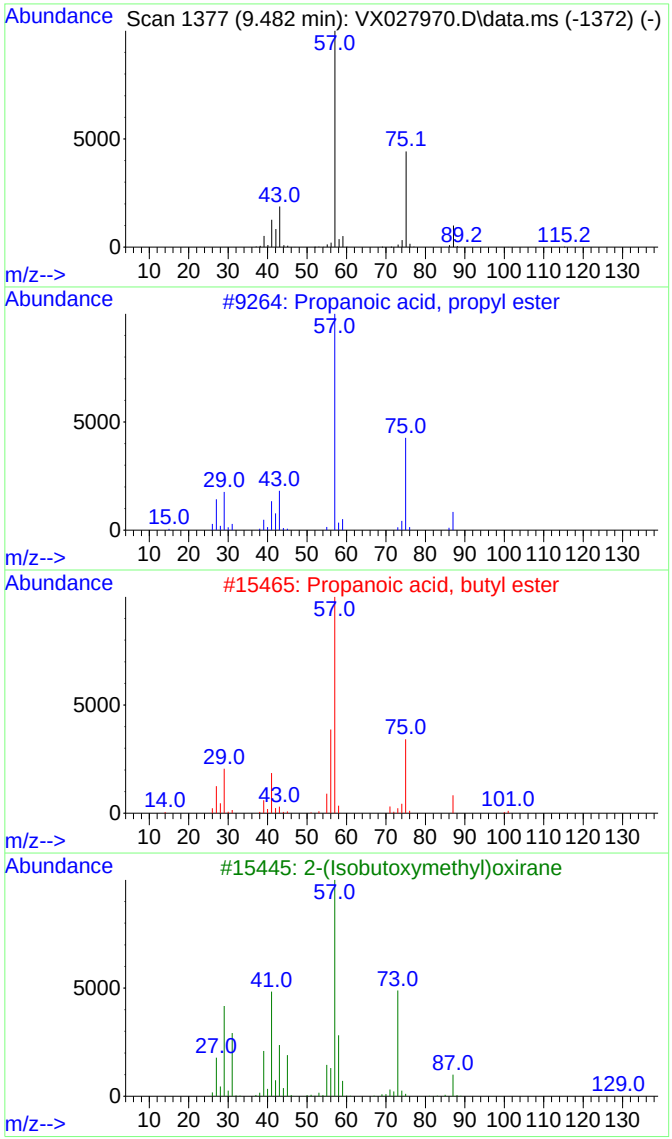
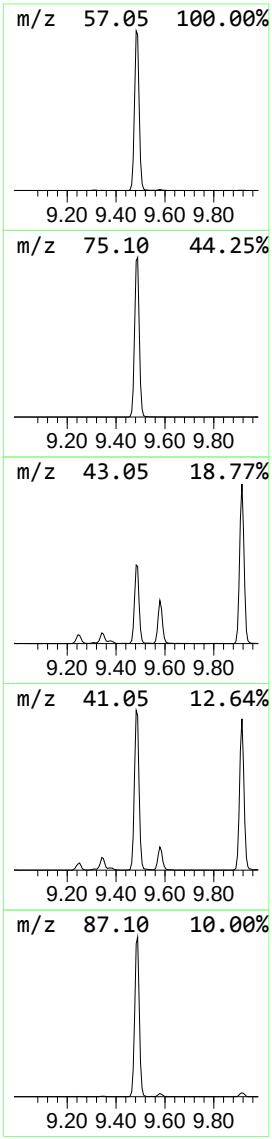
****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	152.56 ug/l	1120450	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	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	7





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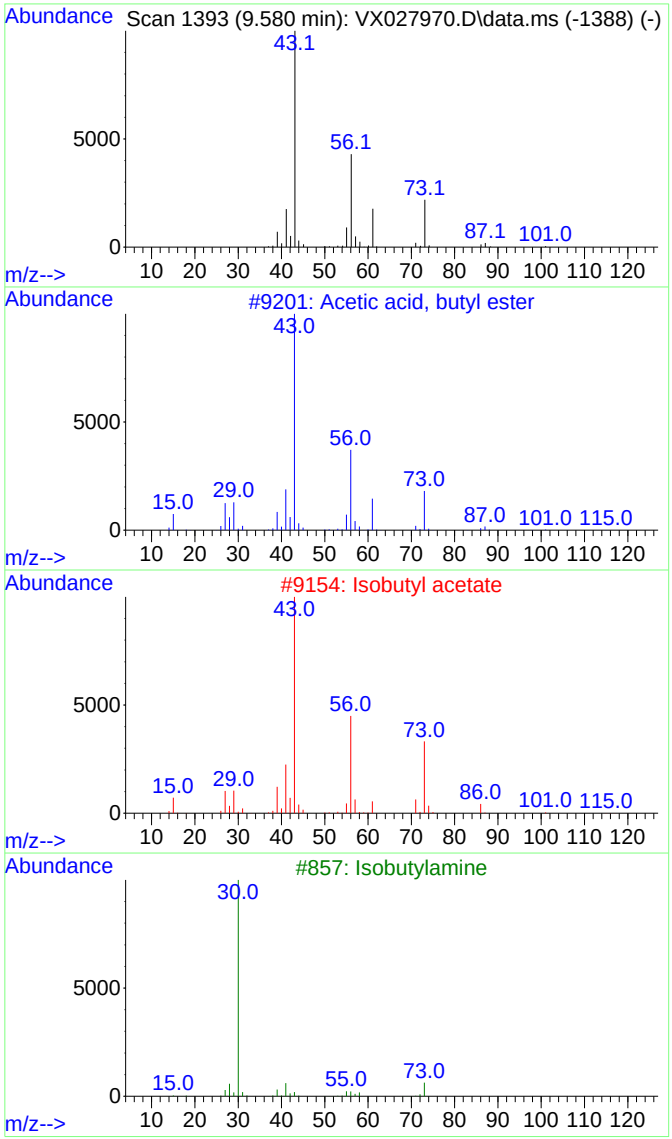
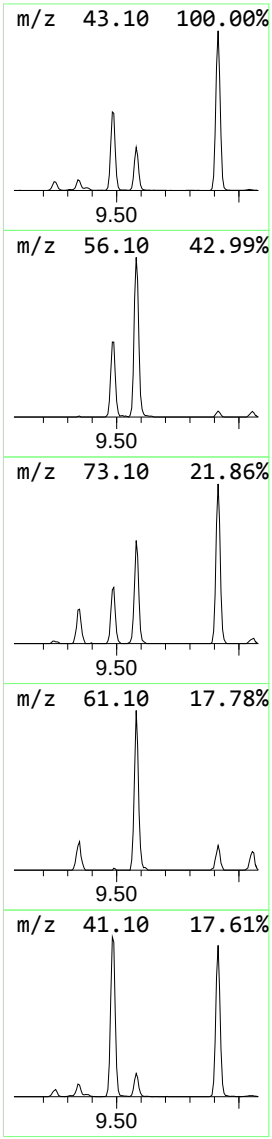
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	16.70 ug/l	122678	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	56
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Pentanone	86	C5H10O	000107-87-9	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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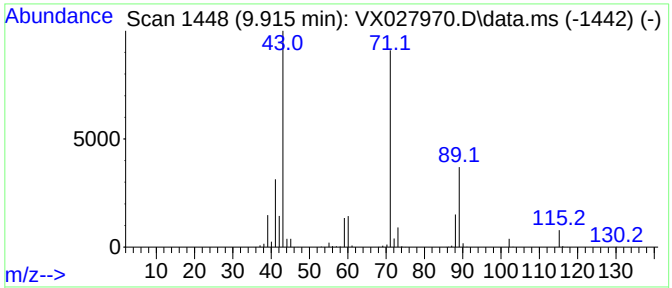
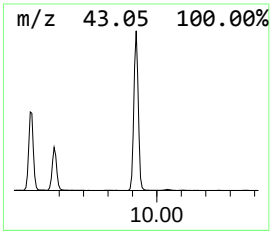
****

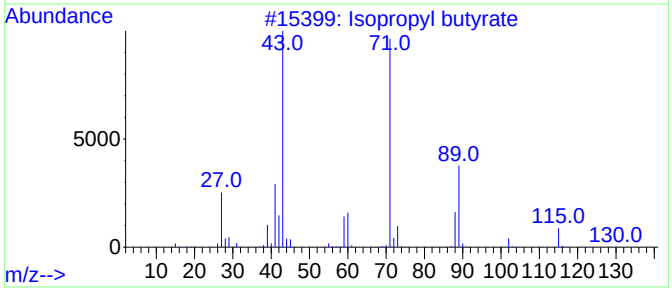
Peak Number 6 Isopropyl butyrate Concentration Rank 3

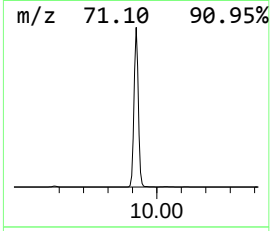
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	92.27 ug/l	677649	Chlorobenzene-d5	10.055

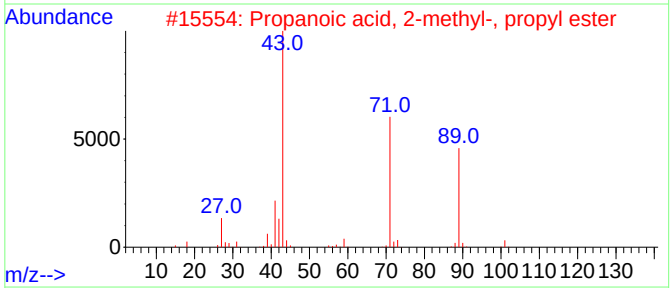
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64

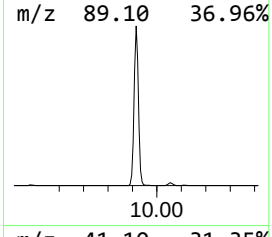


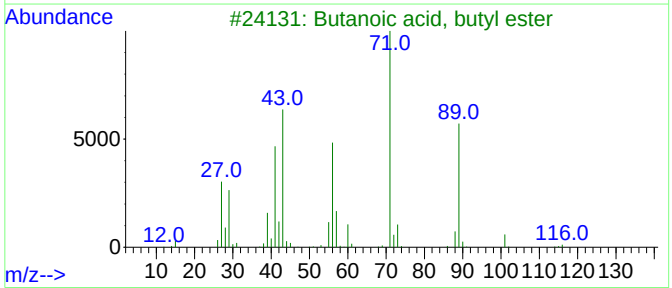


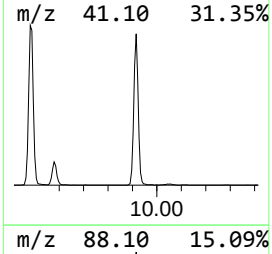


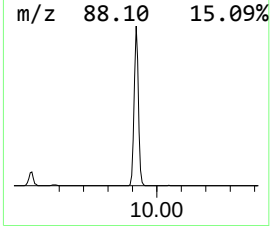












Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.799	104.3	ug/l	753198	2	6.763	361165	50.0
Propanoic acid,...	8.549	15.0	ug/l	110226	3	10.055	367222	50.0
Butanoic acid, ...	9.342	9.5	ug/l	69591	3	10.055	367222	50.0
Propanoic acid,...	9.482	152.6	ug/l	1120450	3	10.055	367222	50.0
Acetic acid, bu...	9.580	16.7	ug/l	122678	3	10.055	367222	50.0
Isopropyl butyrate	9.915	92.3	ug/l	677649	3	10.055	367222	50.0