LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029025.D
Acq On : 27 May 2022 15:37
Operator : JC/MD
Sample : N3028-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-1-1-5FT

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\82X051222W.M
Title : SW846 8260

Signal : TIC: VX029025.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	39	rVB	46460	74258	1.60%	0.321%
2	2.380	206	212	222	rBV	59068	98346	2.12%	0.425%
3	2.788	272	279	290	rBV	55808	100399	2.16%	0.434%
4	3.574	400	408	421	rBV	56782	134553	2.89%	0.581%
5	5.391	692	706	721	rBV3	230176	669255	14.40%	2.890%
6	5.556	721	733	750	rVB	367022	1039893	22.37%	4.490%
7	5.958	789	799	814	rBV	232970	619566	13.33%	2.675%
8	6.348	855	863	874	rBV2	19791	52595	1.13%	0.227%
9	6.763	920	931	949	rBV	596181	1452468	31.24%	6.272%
10	7.799	1094	1101	1115	rBV	1872980	3189082	68.60%	13.770%
11	8.549	1217	1224	1234	rBV	314975	484781	10.43%	2.093%
12	8.653	1234	1241	1261	rVB	1228921	1964202	42.25%	8.481%
13	9.250	1331	1339	1345	rBV	80303	118926	2.56%	0.514%
14	9.348	1350	1355	1359	rBV	211076	280155	6.03%	1.210%
15	9.488	1372	1378	1383	rBV	3500225	4648931	100.00%	20.074%
16	9.579	1389	1393	1408	rVB	368848	487278	10.48%	2.104%
17	9.915	1442	1448	1464	rBV	2193523	2661012	57.24%	11.490%
18	10.055	1464	1471	1478	rBV	1335945	1781355	38.32%	7.692%
19	10.640	1562	1567	1580	rBV	75006	101432	2.18%	0.438%
20	11.085	1634	1640	1649	rBV	1084857	1392413	29.95%	6.012%
21	12.024	1788	1794	1802	rBV	1461296	1748305	37.61%	7.549%
22	13.140	1972	1977	1987	rBV	40231	60142	1.29%	0.260%

Sum of corrected areas: 23159347

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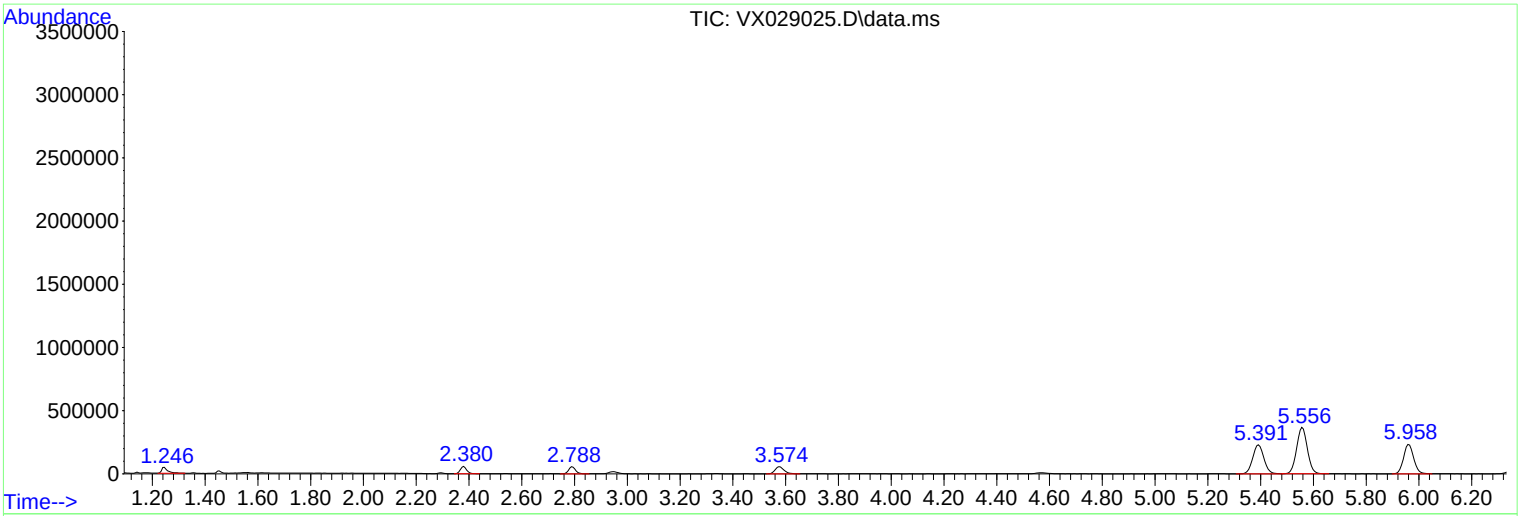
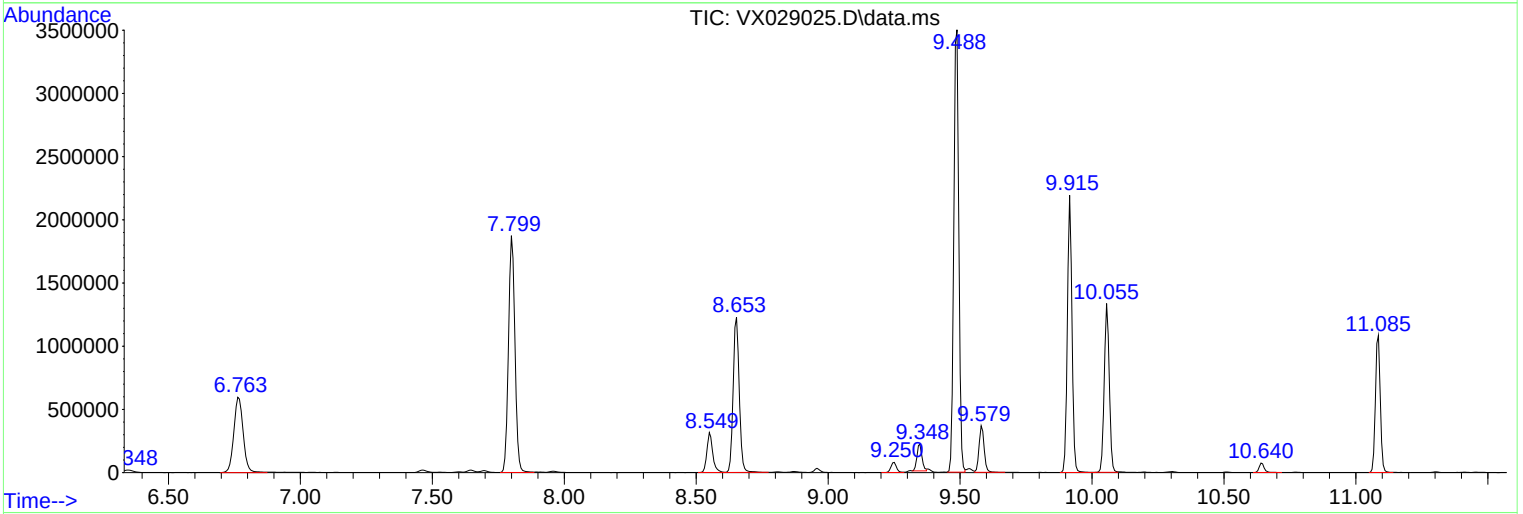
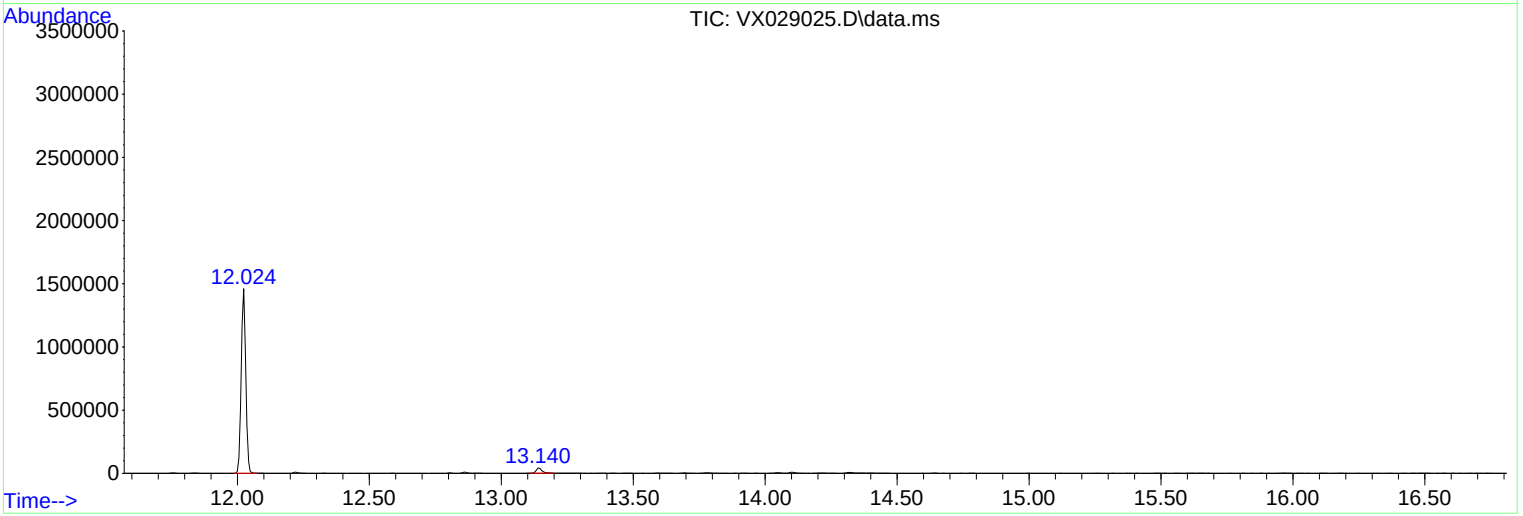
ClientSampleId :
TP-1-1-5FT

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

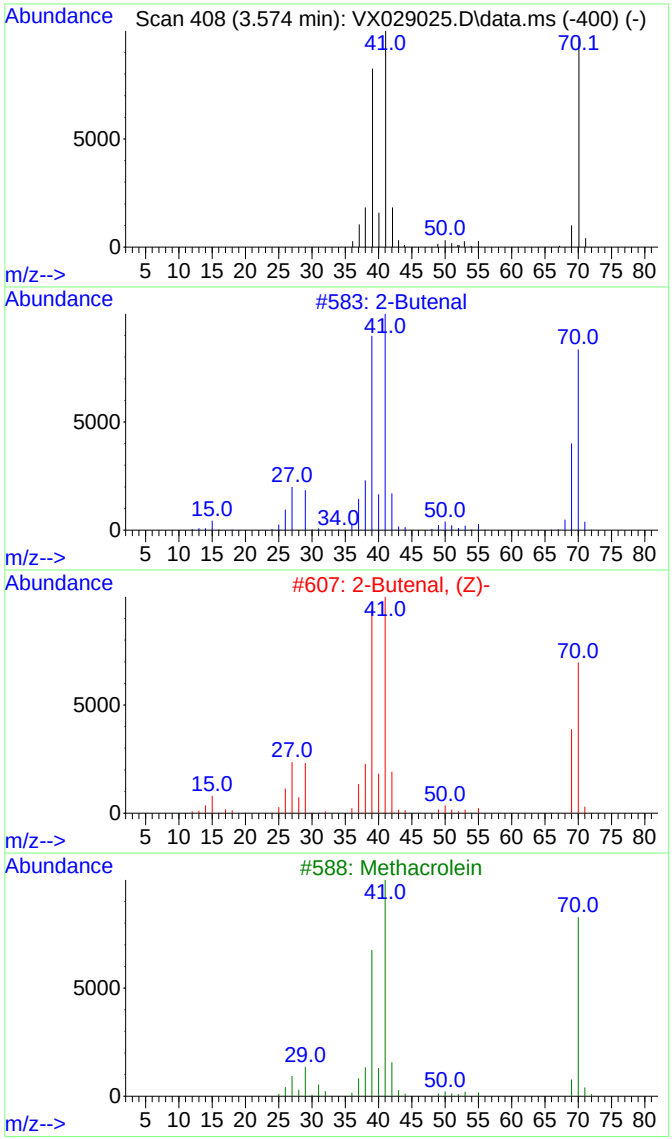
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

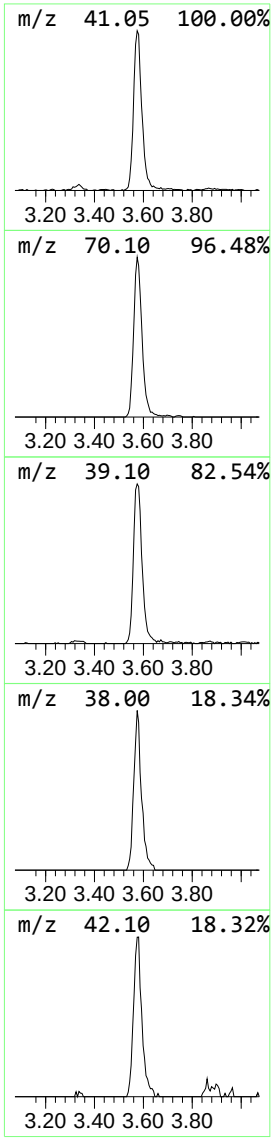
****

Peak Number 1 2-Butenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.574	6.47 ug/l	134553	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal	70	C4H6O	004170-30-3	91
2	2-Butenal, (Z)-	70	C4H6O	015798-64-8	91
3	Methacrolein	70	C4H6O	000078-85-3	91
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	91
5	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	83





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ClientSampleId :
TP-1-1-5FT

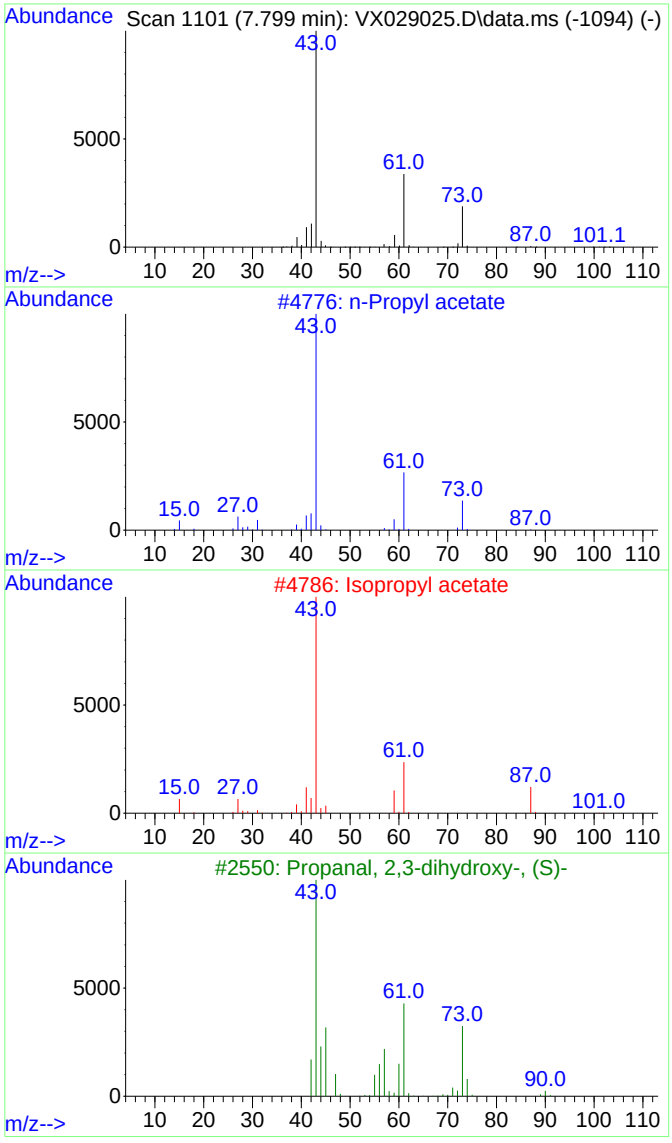
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

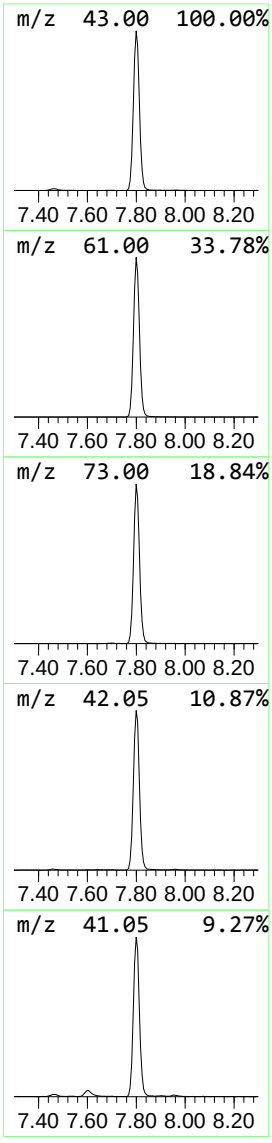
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	109.78 ug/l	3189080	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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
4	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
5	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-1-1-5FT

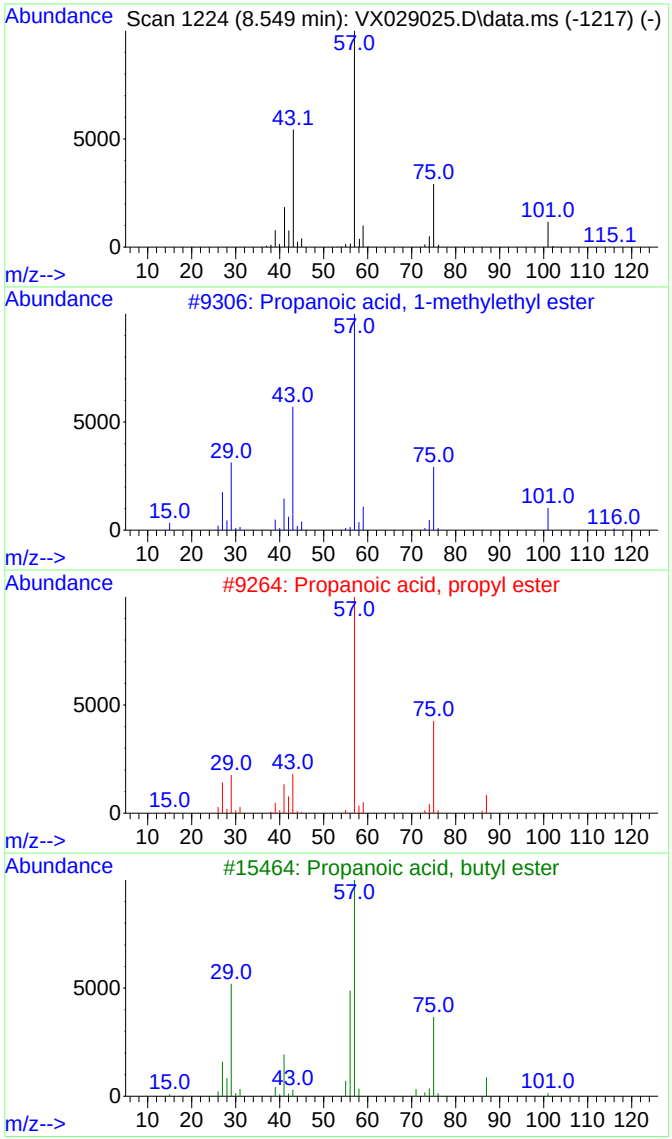
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

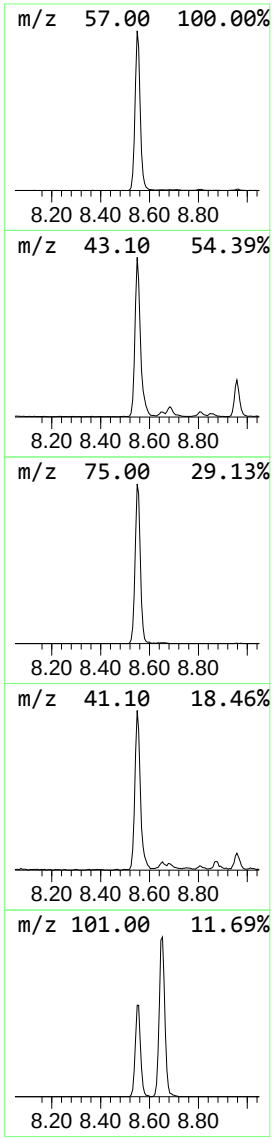
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	13.61 ug/l	484781	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	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument :
MSVOA_X
ClientSampleId :
TP-1-1-5FT

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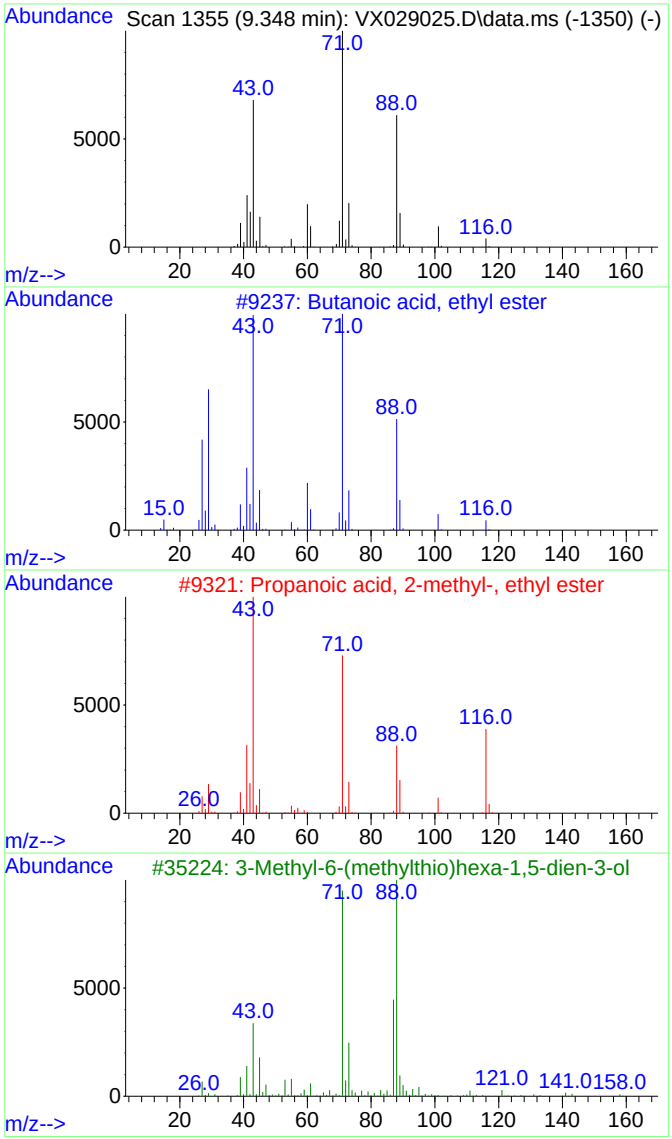
Quant Title : SW846 8260

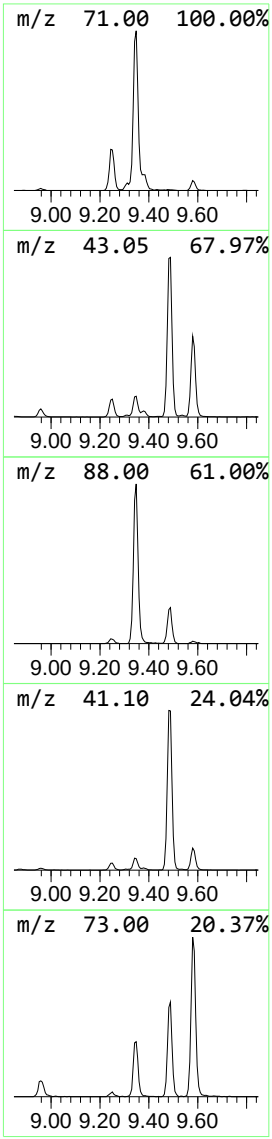
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.348	7.86 ug/l	280155	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	58
3	3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	42
4	4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	33
5	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	27





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Quant Title : SW846 8260

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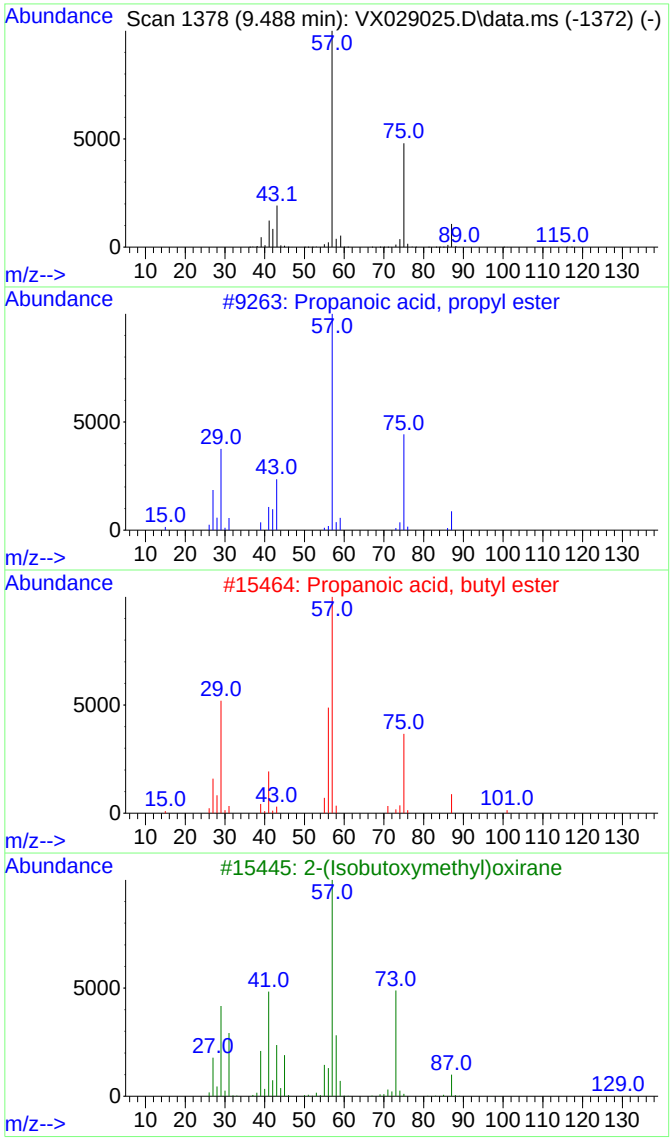
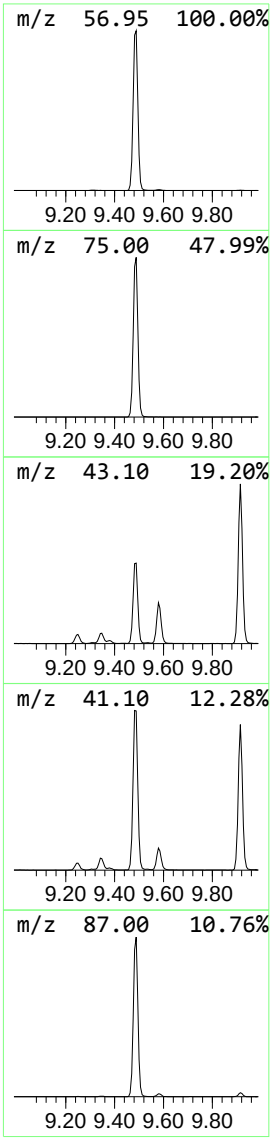
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	130.49 ug/l	4648930	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	1-Penten-3-ol	86	C5H10O	000616-25-1	7





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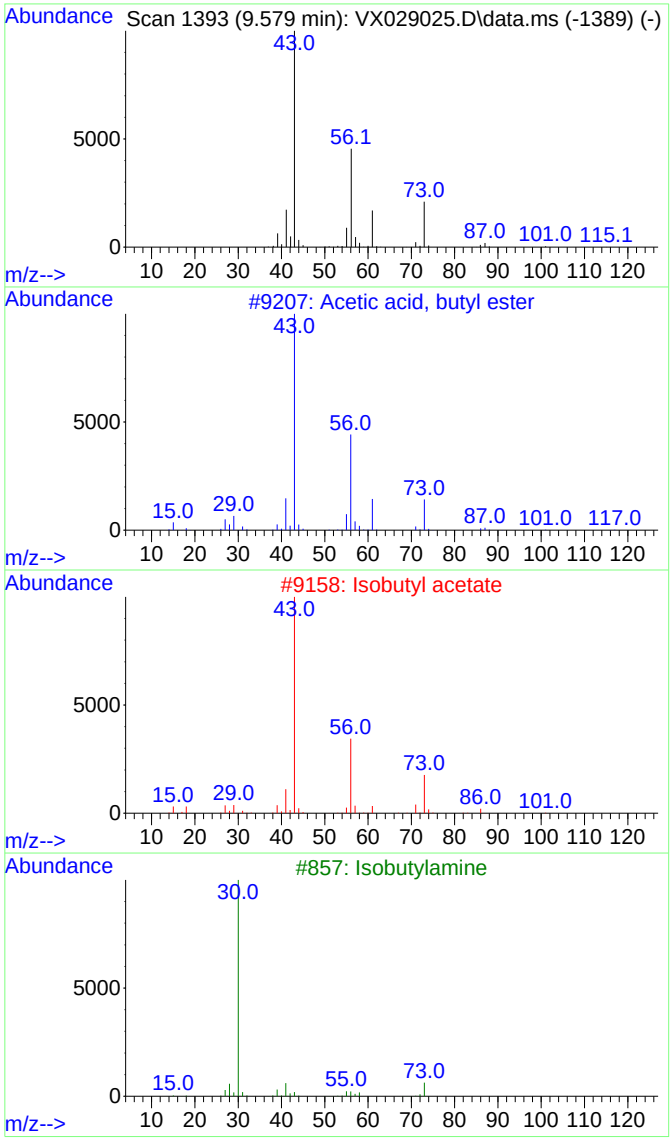
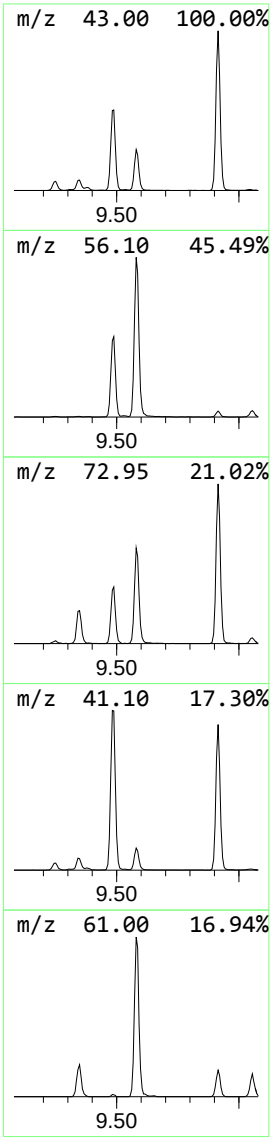
****
Peak Number 6 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	13.68 ug/l	487278	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	Isopropyl acetate	102	C5H10O2	000108-21-4	9
5	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9





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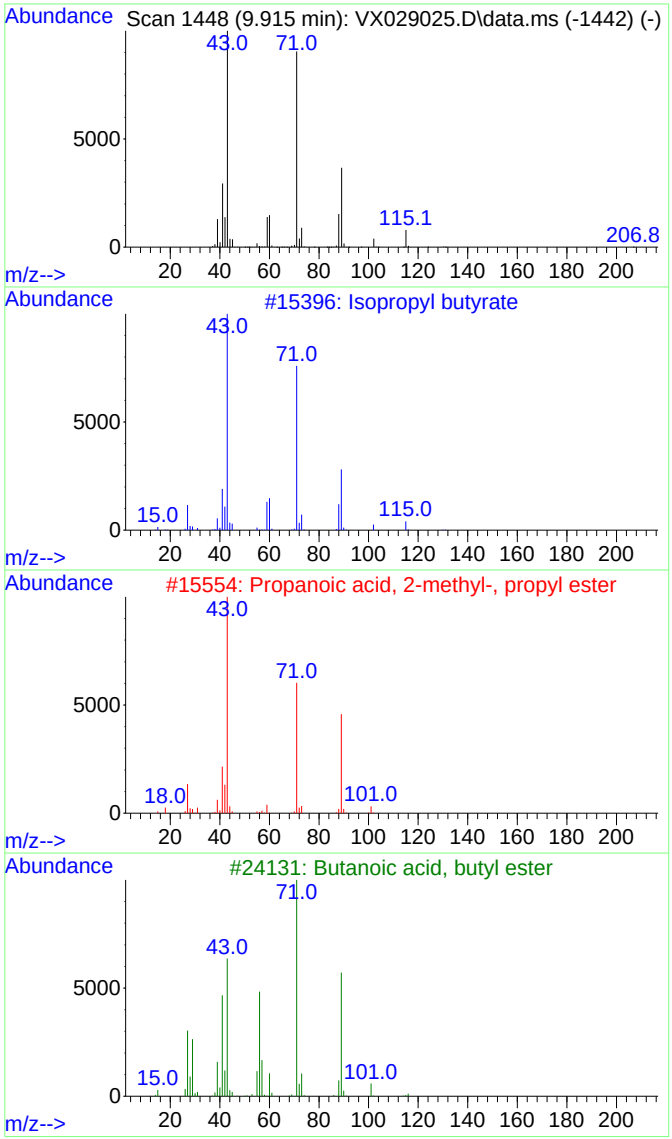
Quant Title : SW846 8260

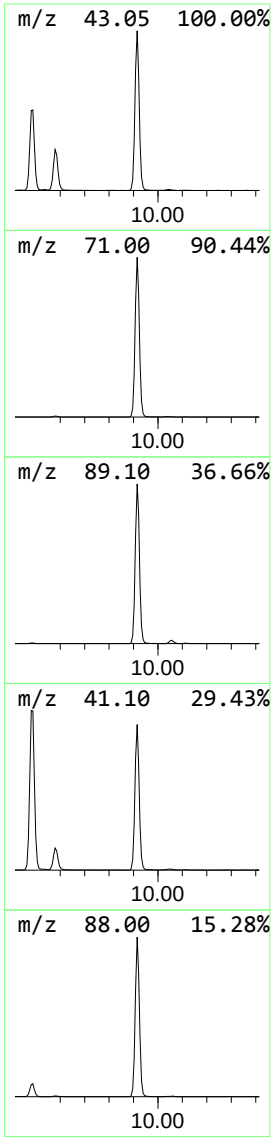
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	74.69 ug/l	2661010	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	97
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Butenal	3.574	6.5	ug/l	134553	1	5.556	1039890	50.0
n-Propyl acetate	7.799	109.8	ug/l	3189080	2	6.763	1452470	50.0
Propanoic acid,...	8.549	13.6	ug/l	484781	3	10.055	1781360	50.0
Butanoic acid, ...	9.348	7.9	ug/l	280155	3	10.055	1781360	50.0
Propanoic acid,...	9.488	130.5	ug/l	4648930	3	10.055	1781360	50.0
Acetic acid, bu...	9.579	13.7	ug/l	487278	3	10.055	1781360	50.0
Isopropyl butyrate	9.915	74.7	ug/l	2661010	3	10.055	1781360	50.0