LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045019.D
Acq On : 30 Sep 2021 02:16
Operator : SY/MD
Sample : PB139450ZHE#02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : PB139450ZHE#02

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_U\Method\82U092821W.M
Title : SW846 8260

Signal : TIC: VU045019.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.629	384	401	422	rBV	46676	78847	1.75%	0.420%
2	3.047	518	531	548	rVB	26812	51614	1.14%	0.275%
3	5.292	1214	1229	1243	rBV	181105	383582	8.49%	2.042%
4	5.375	1243	1255	1276	rVB	319901	655590	14.51%	3.490%
5	5.703	1342	1357	1383	rBV	220879	450826	9.98%	2.400%
6	5.915	1410	1423	1439	rBV	25174	49309	1.09%	0.262%
7	6.253	1515	1528	1569	rVB	498452	1021406	22.61%	5.437%
8	6.931	1718	1739	1759	rVB3	22728	68963	1.53%	0.367%
9	7.041	1759	1773	1805	rBV	1751254	3003673	66.48%	15.989%
10	7.742	1977	1991	2002	rBV	254836	418021	9.25%	2.225%
11	7.902	2024	2041	2070	rBV	757650	1313223	29.07%	6.990%
12	8.163	2111	2122	2136	rBV	27821	46070	1.02%	0.245%
13	8.468	2205	2217	2231	rBV	65401	107985	2.39%	0.575%
14	8.578	2231	2251	2262	rVV	184287	305864	6.77%	1.628%
15	8.732	2279	2299	2318	rVV	2938334	4517875	100.00%	24.049%
16	8.838	2321	2332	2364	rVB	314650	505145	11.18%	2.689%
17	9.214	2435	2449	2484	rBV	1696613	2605226	57.66%	13.868%
18	9.420	2502	2513	2533	rVB	709486	1146645	25.38%	6.104%
19	10.076	2704	2717	2737	rBV	60969	96524	2.14%	0.514%
20	10.635	2878	2891	2916	rVB	554561	874281	19.35%	4.654%
21	11.815	3246	3258	3278	rBV	689941	1085650	24.03%	5.779%

Sum of corrected areas: 18786319

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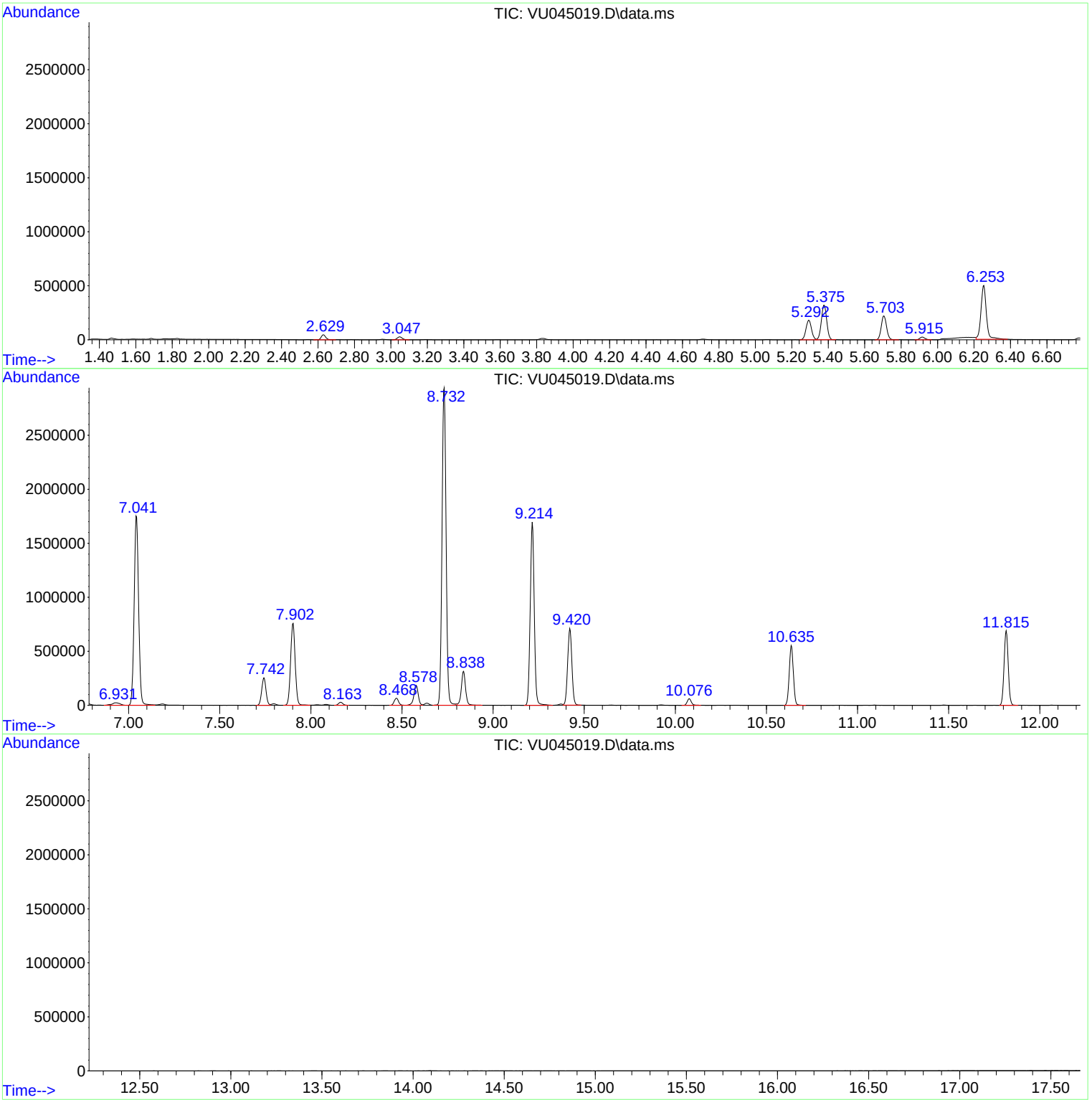
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB139450ZHE#02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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



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Data File : VU045019.D
Acq On : 30 Sep 2021 02:16
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Quant Title : SW846 8260

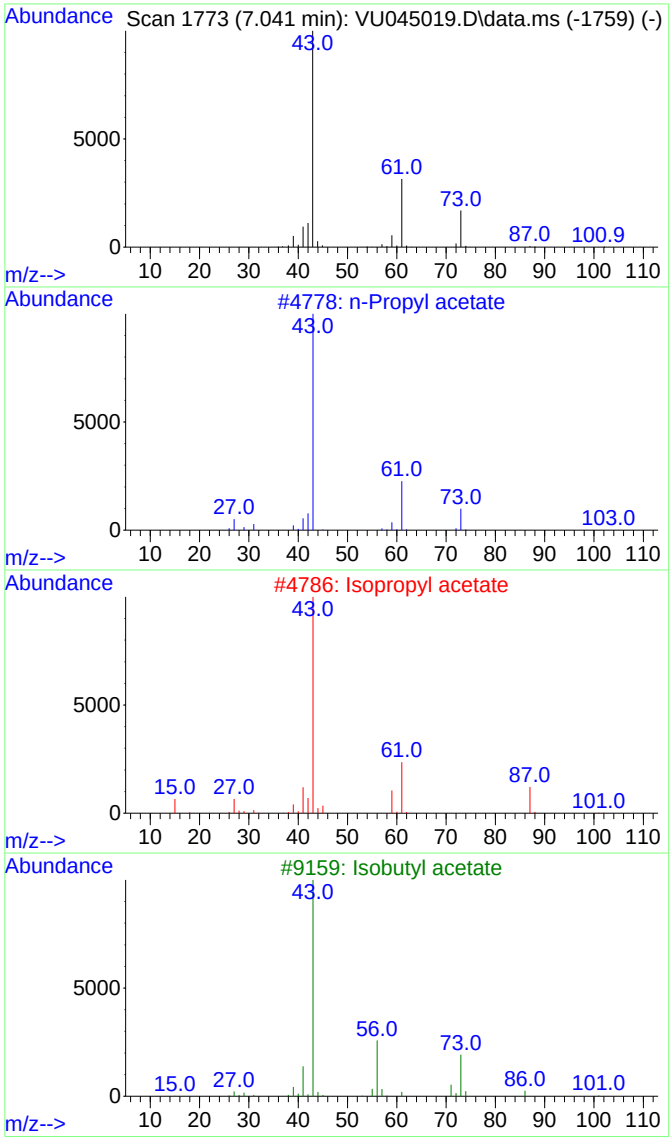
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

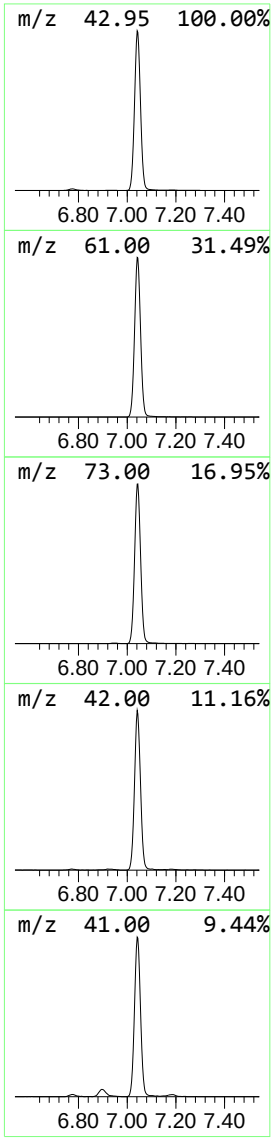
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	147.04 ug/l	3003670	1,4-Difluorobenzene	6.253

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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





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ClientSampleId :
PB139450ZHE#02

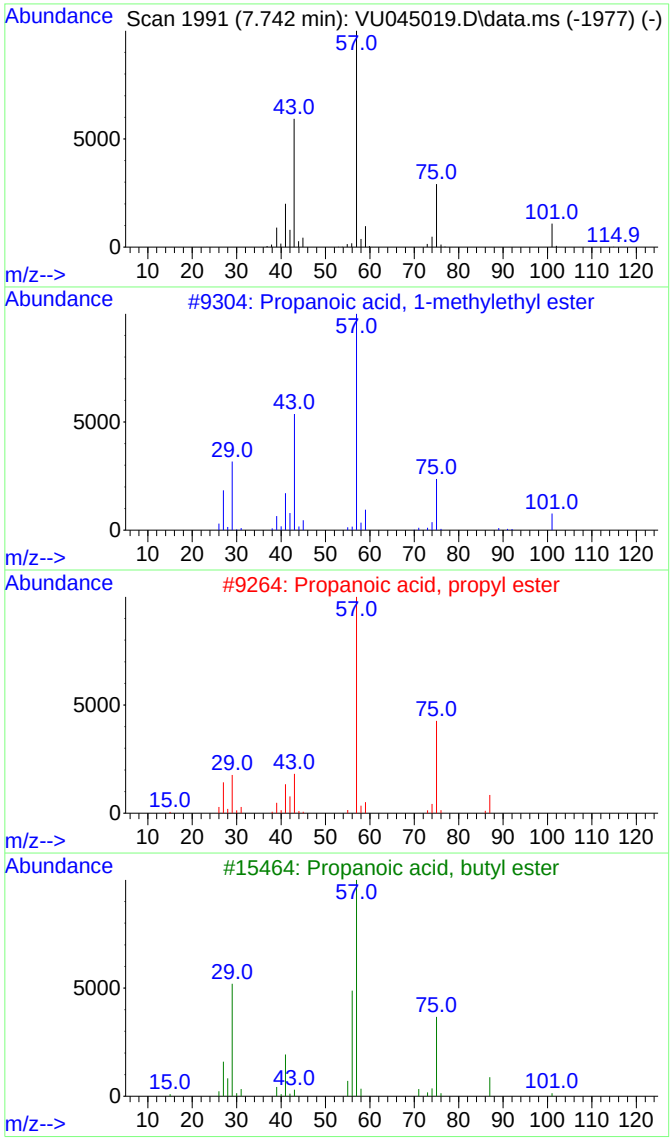
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

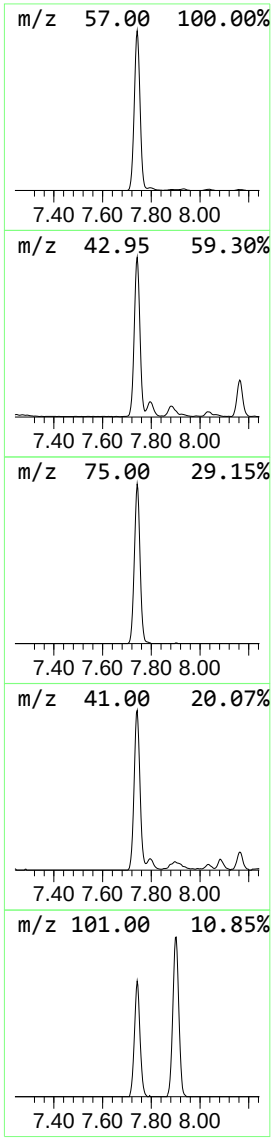
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.742	20.46 ug/l	418021	1,4-Difluorobenzene	6.253

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	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	9





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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB139450ZHE#02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

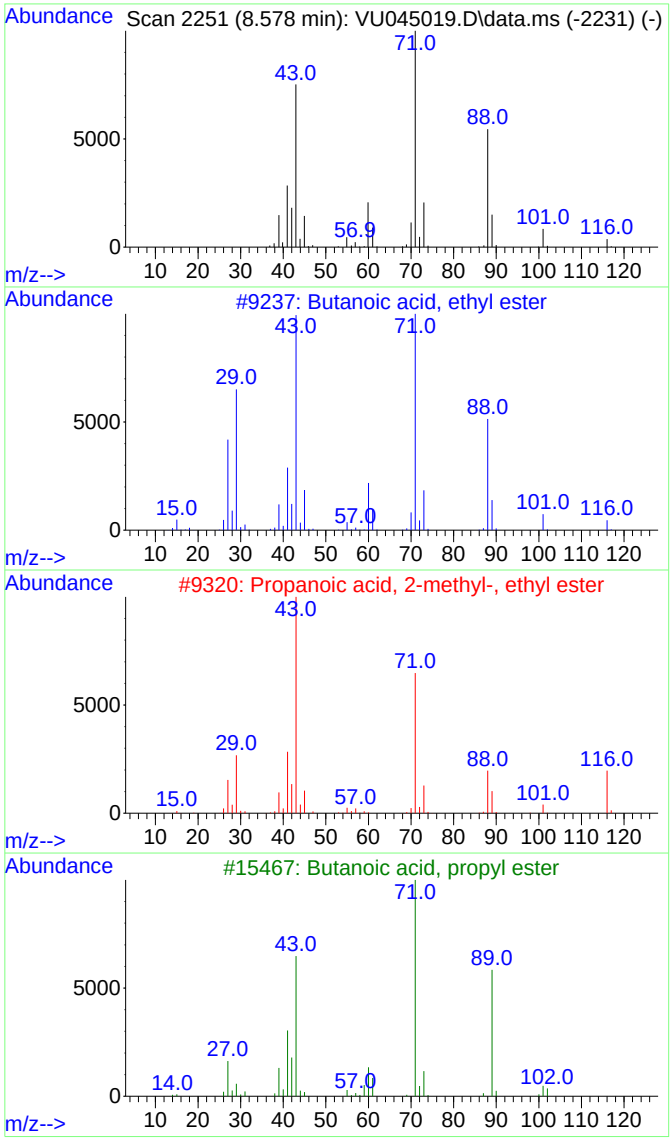
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

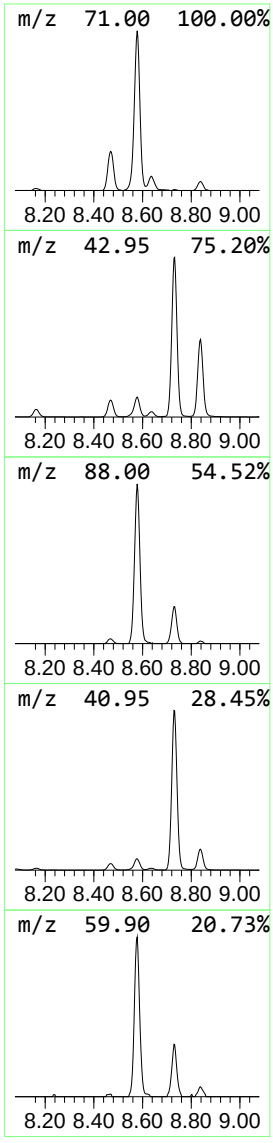
****

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.578	13.34 ug/l	305864	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
4	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
5	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38





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Sample : PB139450ZHE#02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB139450ZHE#02

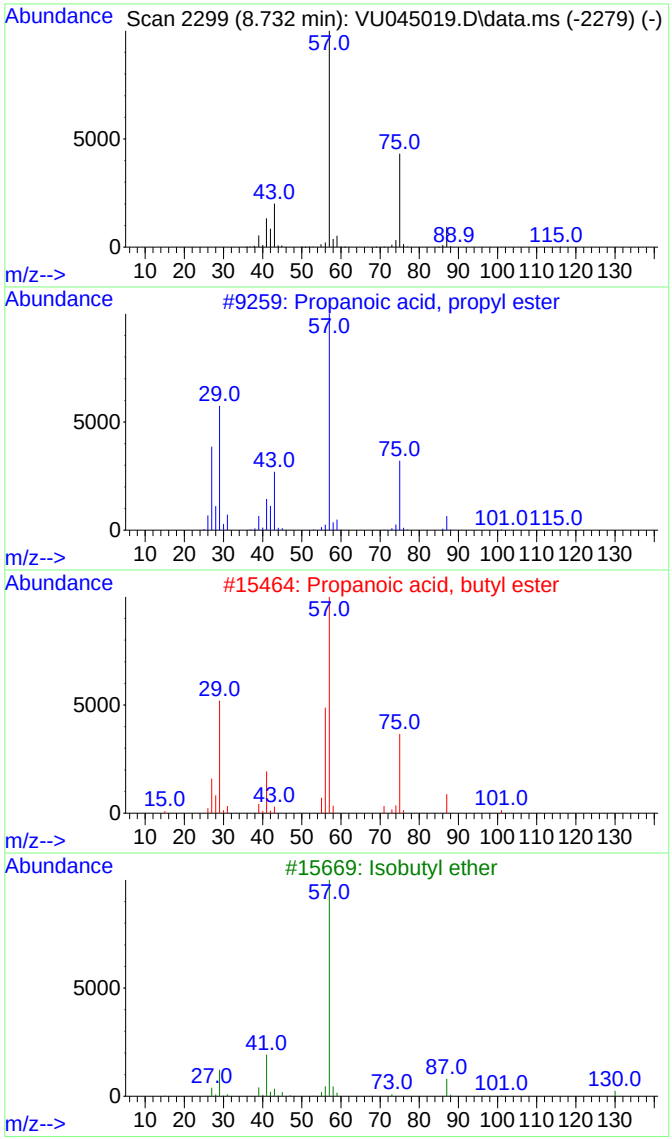
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

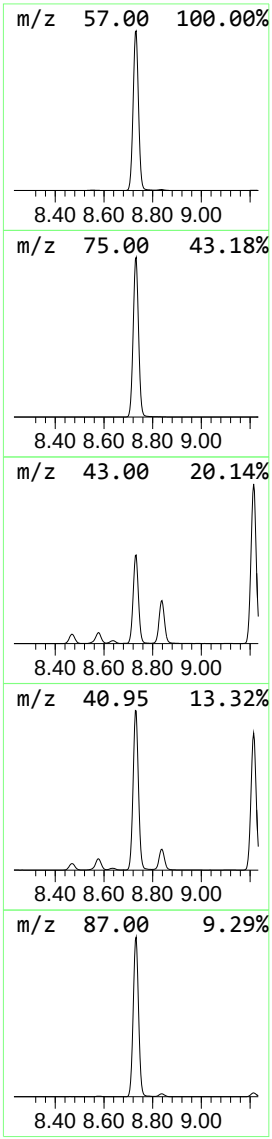
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.732	197.00 ug/l	4517880	Chlorobenzene-d5	9.420

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	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Sample : PB139450ZHE#02
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ALS Vial : 38 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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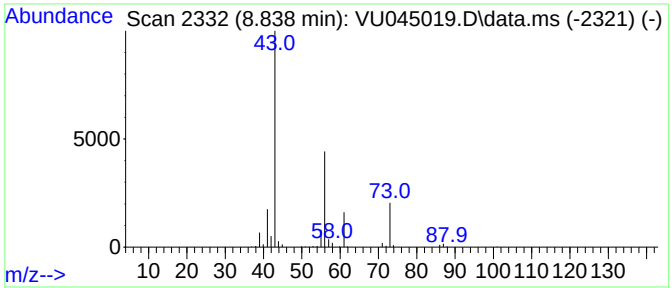
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

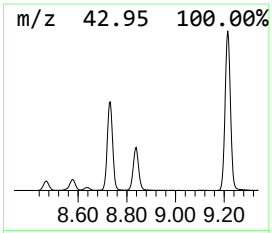
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

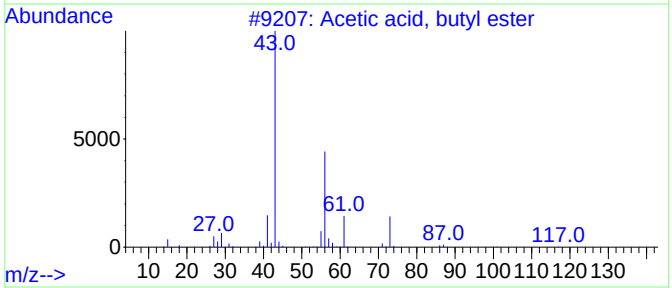
****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

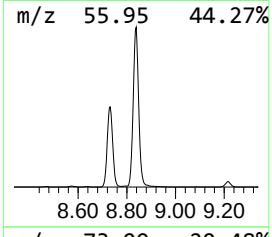
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.838	22.03 ug/l	505145	Chlorobenzene-d5	9.420

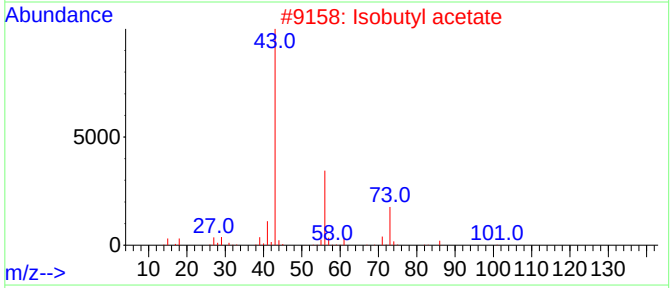
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9

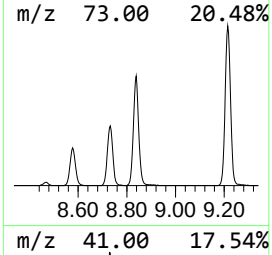


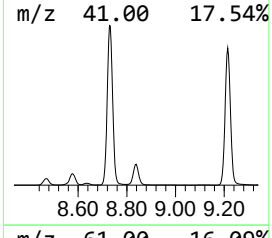


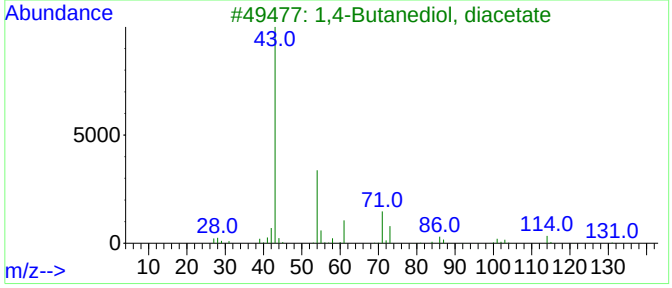


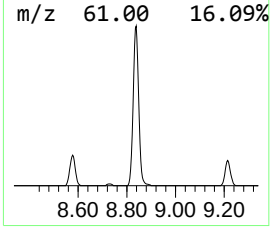












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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

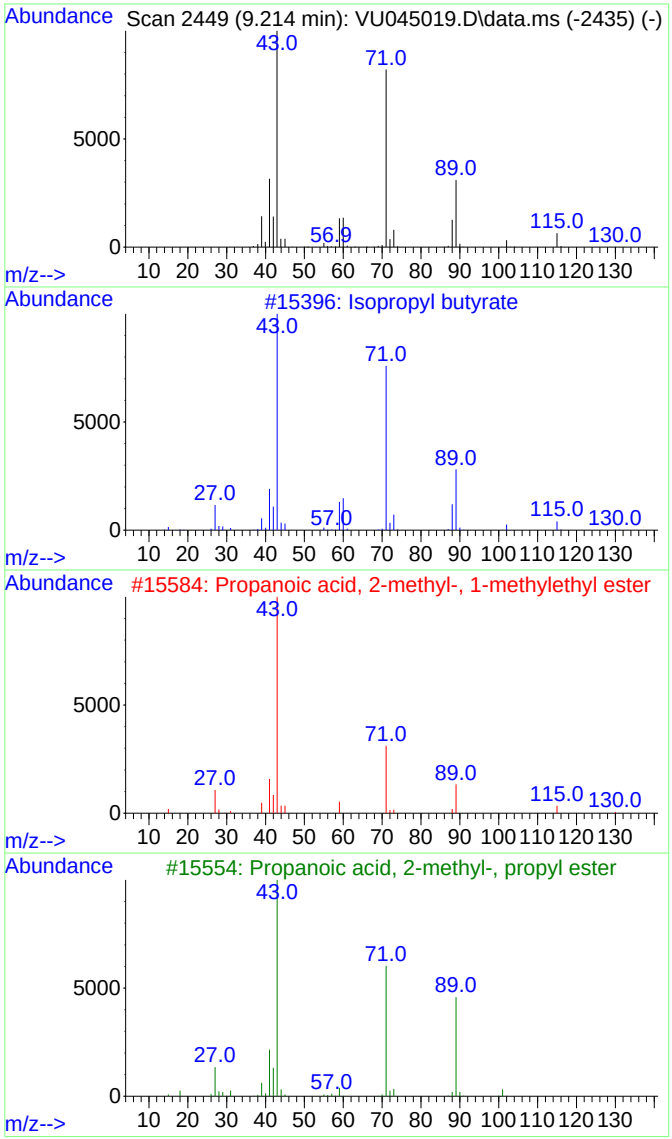
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

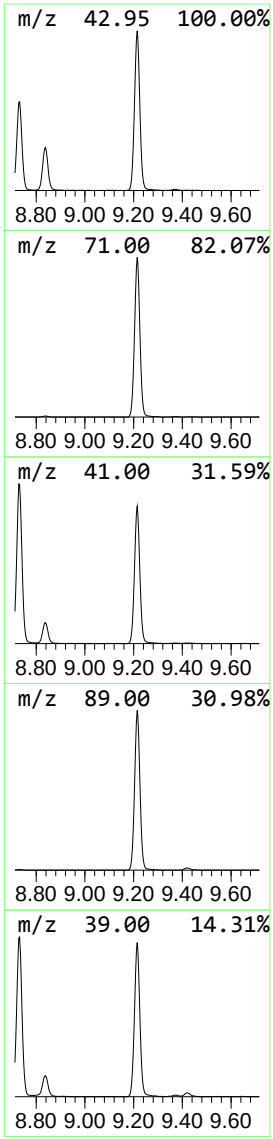
****

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.214	113.60 ug/l	2605230	Chlorobenzene-d5	9.420

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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	53





Tentatively Identified Compound (LSC) summary

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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
n-Propyl acetate	7.041	147.0	ug/l	3003670	2	6.253	1021410	50.0
Propanoic acid,...	7.742	20.5	ug/l	418021	2	6.253	1021410	50.0
Butanoic acid, ...	8.578	13.3	ug/l	305864	3	9.420	1146650	50.0
Propanoic acid,...	8.732	197.0	ug/l	4517880	3	9.420	1146650	50.0
Acetic acid, bu...	8.838	22.0	ug/l	505145	3	9.420	1146650	50.0
Isopropyl butyrate	9.214	113.6	ug/l	2605230	3	9.420	1146650	50.0