LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045030.D
Acq On : 30 Sep 2021 06:36
Operator : SY/MD
Sample : M3971-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RO-COMP-2

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: VU045030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	2.630	387	401	420	rBV	34838	59764	2.47%	0.437%
2	2.790	435	451	465	rBV2	19170	38431	1.59%	0.281%
3	3.048	518	531	547	rVB	22118	42515	1.76%	0.311%
4	5.292	1214	1229	1242	rBV	177738	371071	15.34%	2.714%
5	5.376	1242	1255	1279	rVB	303524	624851	25.83%	4.571%
6	5.704	1342	1357	1376	rBV	216475	438212	18.11%	3.206%
7	5.919	1409	1424	1440	rBV	18317	37694	1.56%	0.276%
8	6.138	1452	1492	1494	rBV	15739	77884	3.22%	0.570%
9	6.253	1515	1528	1576	rVB	477741	980646	40.54%	7.174%
10	6.774	1680	1690	1705	rVB2	16464	30045	1.24%	0.220%
11	6.929	1716	1738	1758	rBV3	21065	61387	2.54%	0.449%
12	7.041	1759	1773	1802	rBV	988241	1693004	69.98%	12.385%
13	7.742	1977	1991	2002	rBV	205117	336437	13.91%	2.461%
14	7.900	2023	2040	2056	rBV	716208	1249185	51.64%	9.138%
15	8.469	2205	2217	2234	rBV	54144	87812	3.63%	0.642%
16	8.578	2234	2251	2261	rVV	113909	201006	8.31%	1.470%
17	8.636	2261	2269	2279	rVV2	16267	28006	1.16%	0.205%
18	8.729	2279	2298	2316	rVV	1573245	2419181	100.00%	17.697%
19	8.838	2318	2332	2358	rVB	87946	157786	6.52%	1.154%
20	9.215	2434	2449	2485	rBV	1156865	1770484	73.19%	12.951%
21	9.420	2502	2513	2535	rVB	670017	1092465	45.16%	7.992%
22	10.076	2706	2717	2733	rVB	17435	26992	1.12%	0.197%
23	10.636	2879	2891	2913	rVB	521200	823339	34.03%	6.023%
24	11.816	3245	3258	3278	rBV	649981	1022027	42.25%	7.476%

Sum of corrected areas: 13670224

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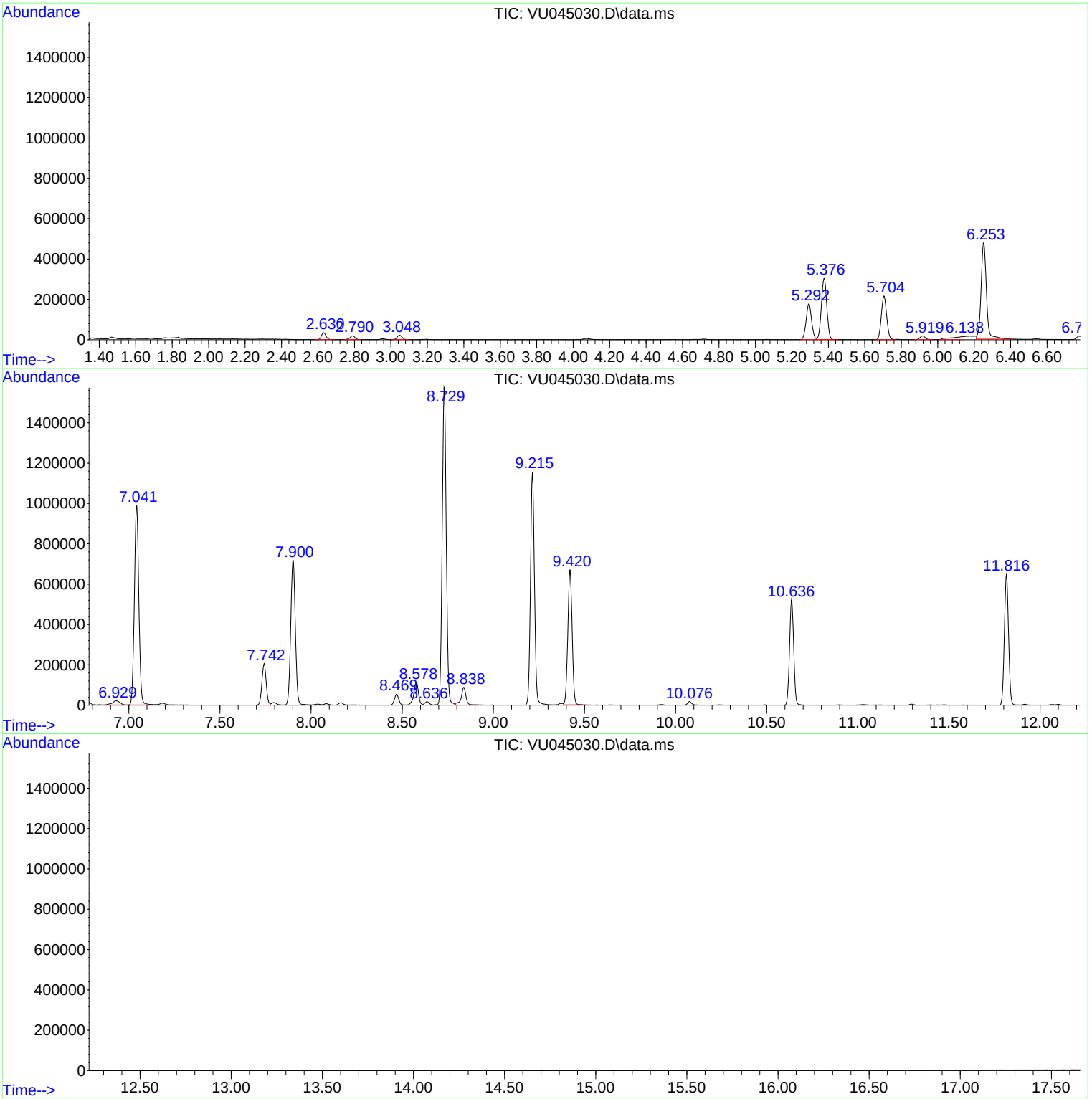
RO-COMP-2

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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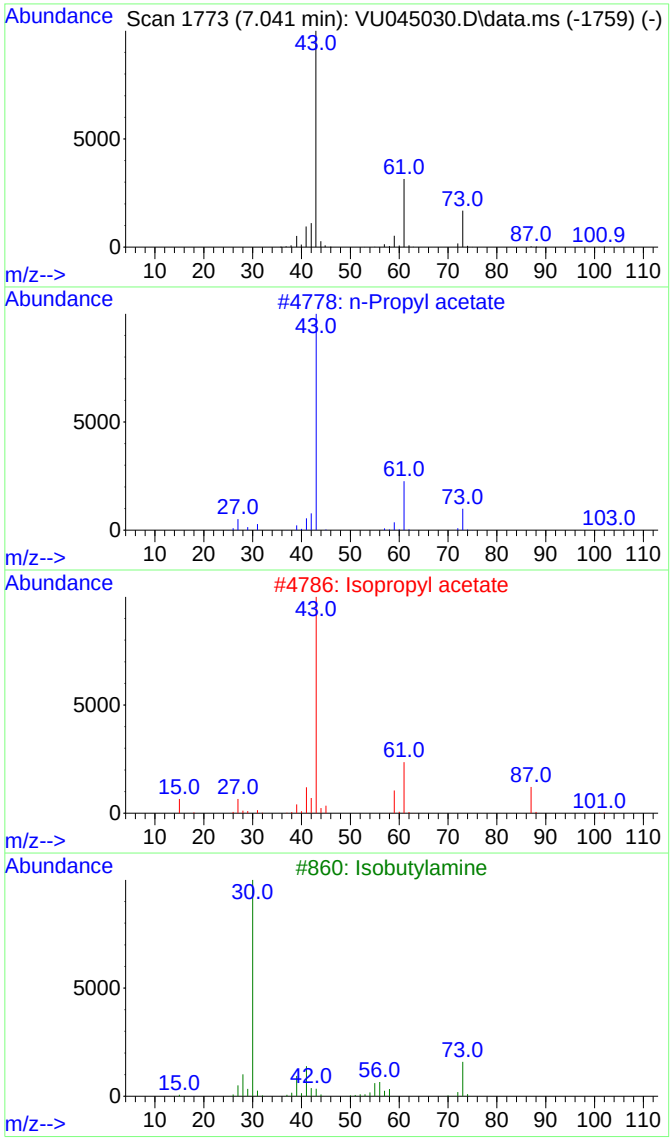
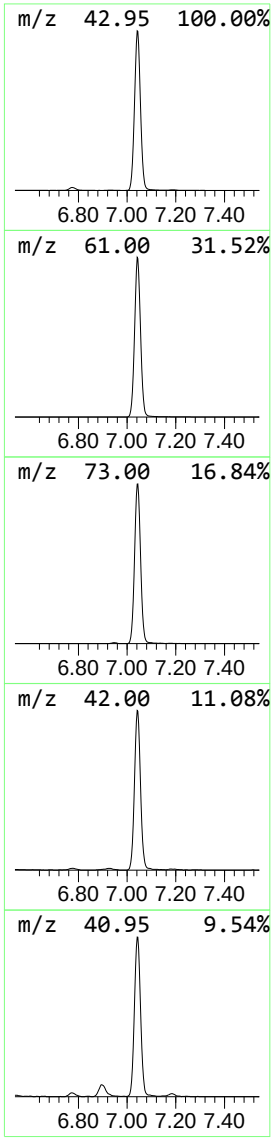
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	86.32 ug/l	1693000	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	Isobutylamine	73	C4H11N	000078-81-9	9
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9





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Quant Title : SW846 8260

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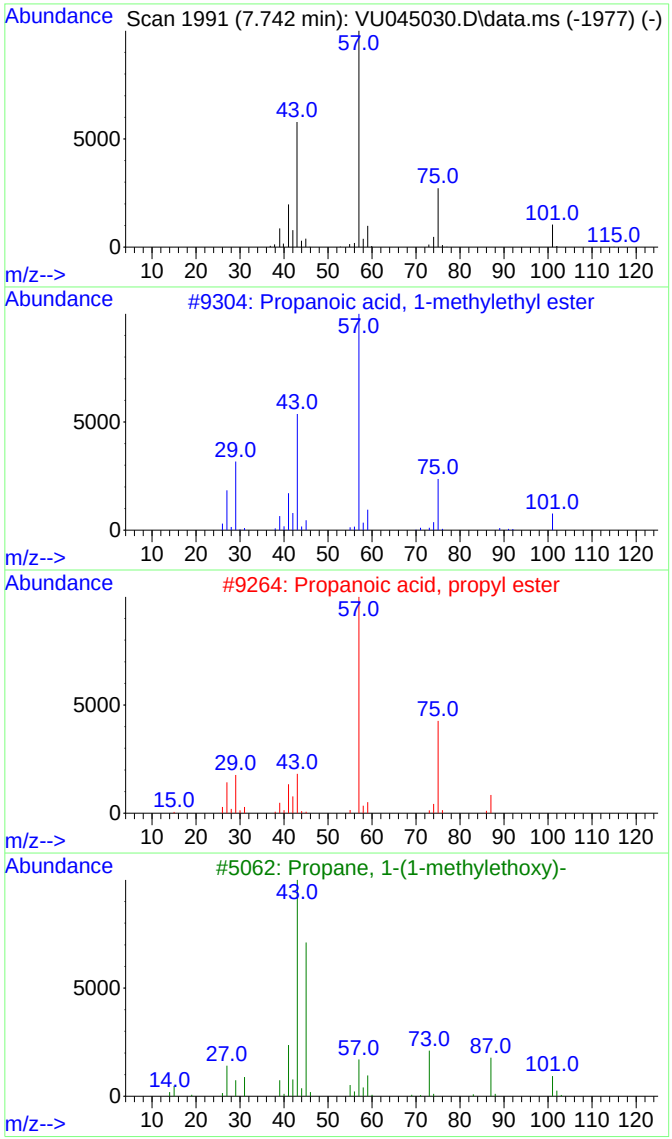
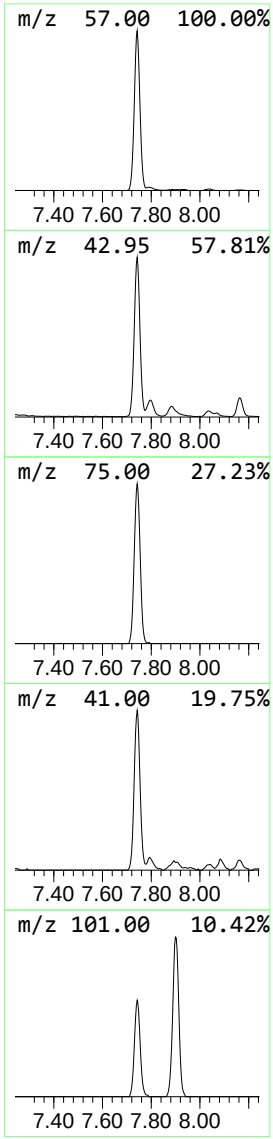
****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.742	17.15 ug/l	336437	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	42
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9





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RO-COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
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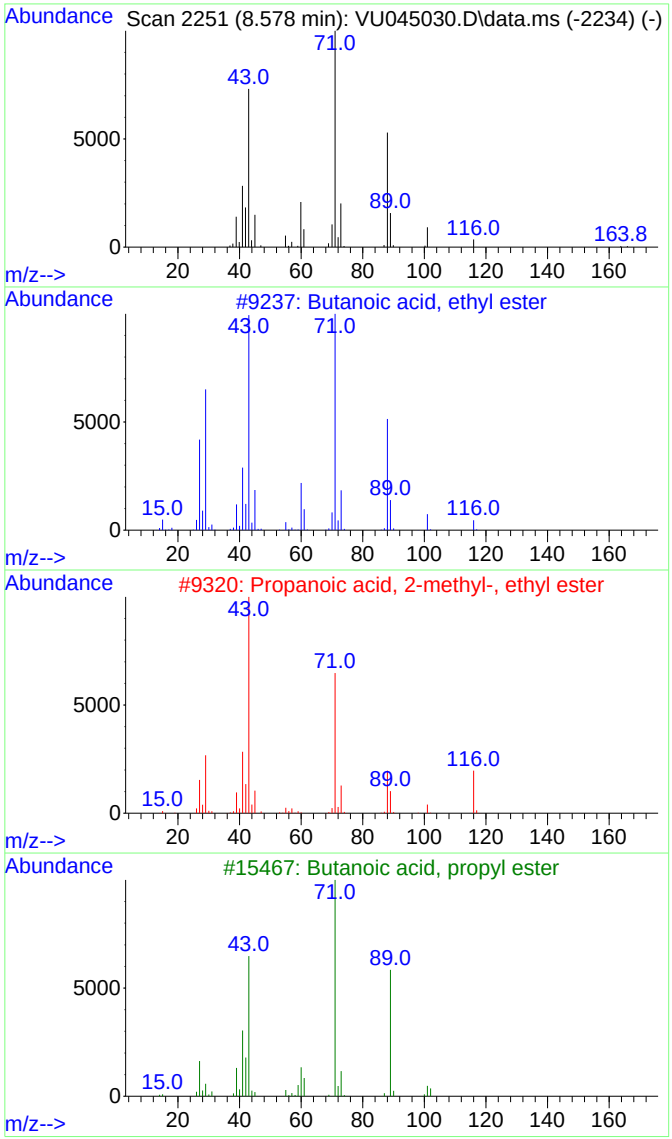
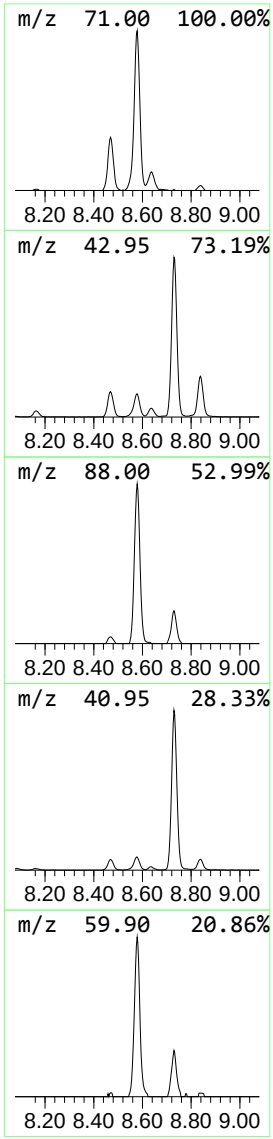
****
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.578	9.20 ug/l	201006	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	43
4	3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	42
5	4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	40





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ClientSampleId : RO-COMP-2

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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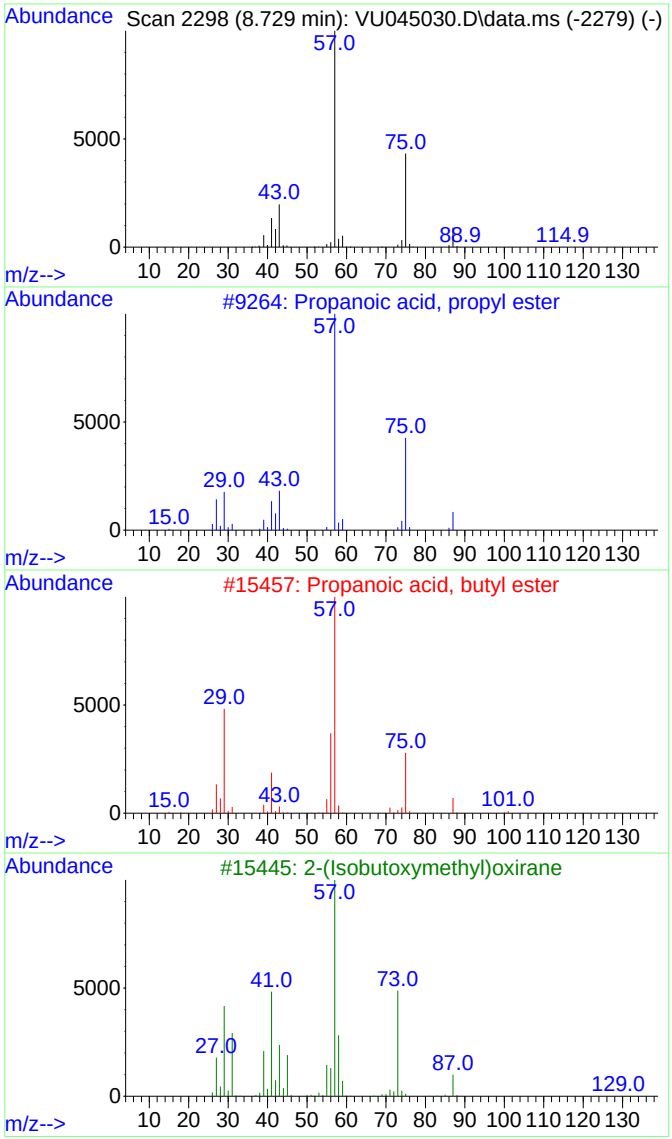
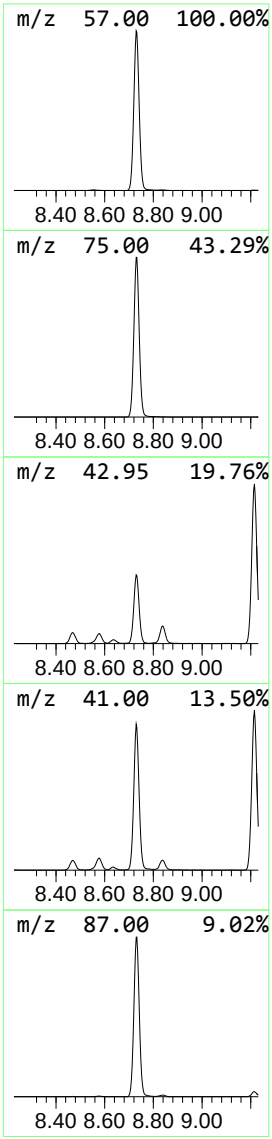
****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	110.72 ug/l	2419180	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	28
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Instrument : MSVOA_U
ClientSampleId : RO-COMP-2

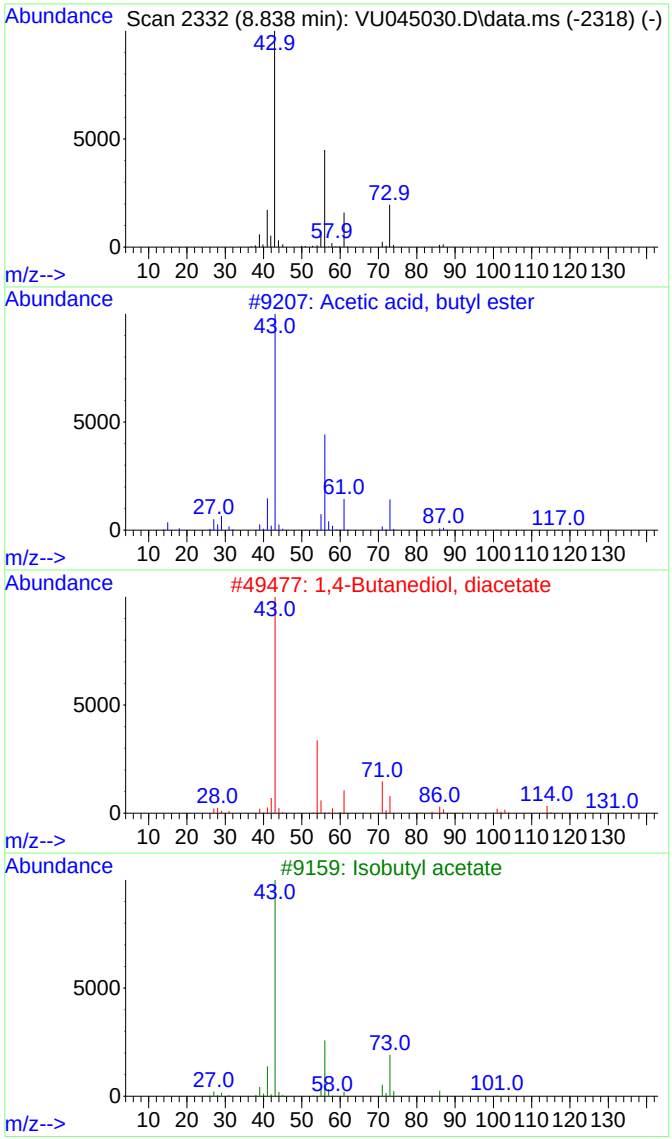
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

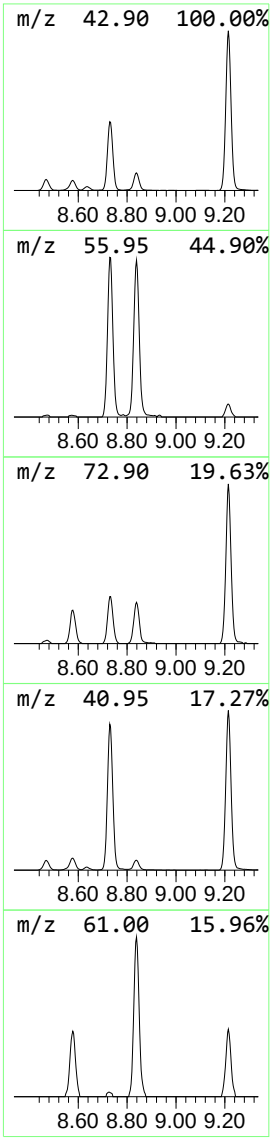
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.838	7.22 ug/l	157786	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	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9
5	n-Propyl acetate	102	C5H10O2	000109-60-4	9





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Instrument :
MSVOA_U
ClientSampleId :
RO-COMP-2

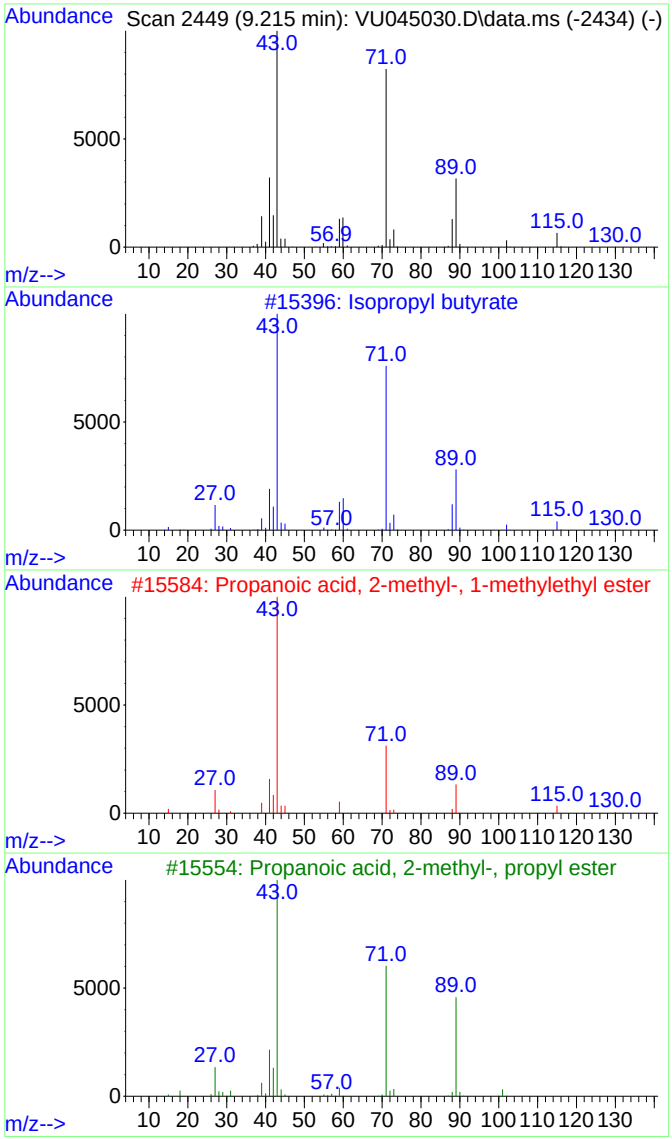
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

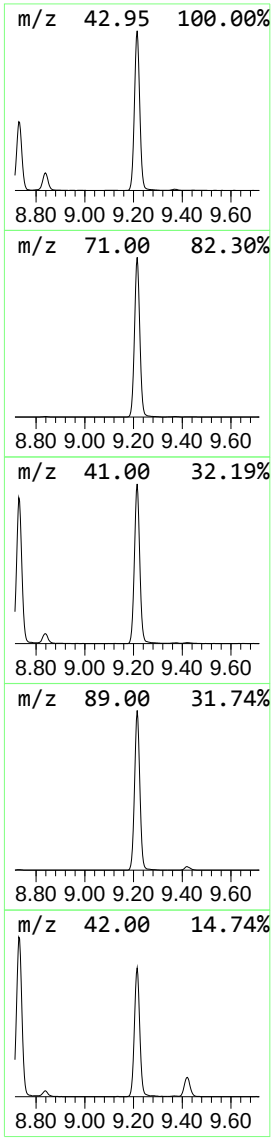
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.215	81.03 ug/l	1770480	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	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64





Tentatively Identified Compound (LSC) summary

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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	86.3	ug/l	1693000	2	6.253	980646	50.0
Propanoic acid,...	7.742	17.2	ug/l	336437	2	6.253	980646	50.0
Butanoic acid, ...	8.578	9.2	ug/l	201006	3	9.420	1092470	50.0
Propanoic acid,...	8.729	110.7	ug/l	2419180	3	9.420	1092470	50.0
Acetic acid, bu...	8.838	7.2	ug/l	157786	3	9.420	1092470	50.0
Isopropyl butyrate	9.215	81.0	ug/l	1770480	3	9.420	1092470	50.0