LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045032.D
Acq On : 30 Sep 2021 07:23
Operator : SY/MD
Sample : M3971-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : KEARNY-COMP

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: VU045032.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	389	401	418	rBV	52065	88534	6.71%	0.845%
2	2.784	431	449	464	rBV	9961	22287	1.69%	0.213%
3	3.047	520	531	546	rVB	20195	38207	2.89%	0.364%
4	4.076	839	851	867	rBV6	5561	15170	1.15%	0.145%
5	5.292	1213	1229	1242	rBV	172067	364960	27.65%	3.482%
6	5.375	1242	1255	1278	rVB	299466	614682	46.57%	5.864%
7	5.706	1343	1358	1374	rBV2	212220	431586	32.70%	4.117%
8	5.919	1409	1424	1438	rBV2	13929	27675	2.10%	0.264%
9	6.253	1515	1528	1582	rVB	469207	945552	71.64%	9.020%
10	6.774	1680	1690	1707	rVB2	15953	29956	2.27%	0.286%
11	6.928	1719	1738	1761	rBV3	20030	51844	3.93%	0.495%
12	7.044	1761	1774	1800	rBV	398228	687978	52.13%	6.563%
13	7.742	1979	1991	2002	rBV	168277	278534	21.10%	2.657%
14	7.796	2002	2008	2024	rVB	12698	21869	1.66%	0.209%
15	7.902	2024	2041	2057	rBV	719198	1237503	93.76%	11.805%
16	8.468	2205	2217	2233	rBV	48090	78437	5.94%	0.748%
17	8.578	2234	2251	2261	rBV2	62874	112253	8.50%	1.071%
18	8.636	2261	2269	2282	rVB2	15548	26216	1.99%	0.250%
19	8.732	2282	2299	2315	rBV	701803	1100853	83.41%	10.502%
20	9.214	2436	2449	2481	rBV	846898	1319855	100.00%	12.591%
21	9.420	2502	2513	2538	rVB	692422	1108932	84.02%	10.579%
22	10.635	2877	2891	2915	rBV	533850	840070	63.65%	8.014%
23	11.815	3245	3258	3281	rBV	660756	1039862	78.79%	9.920%

Sum of corrected areas: 10482815

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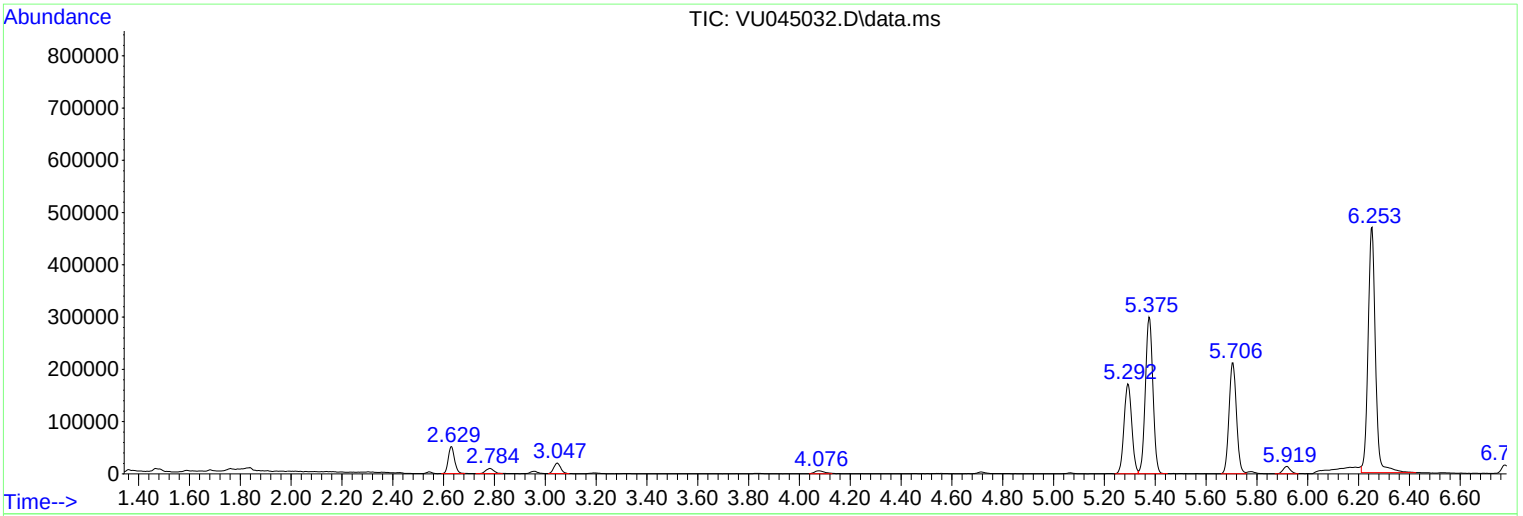
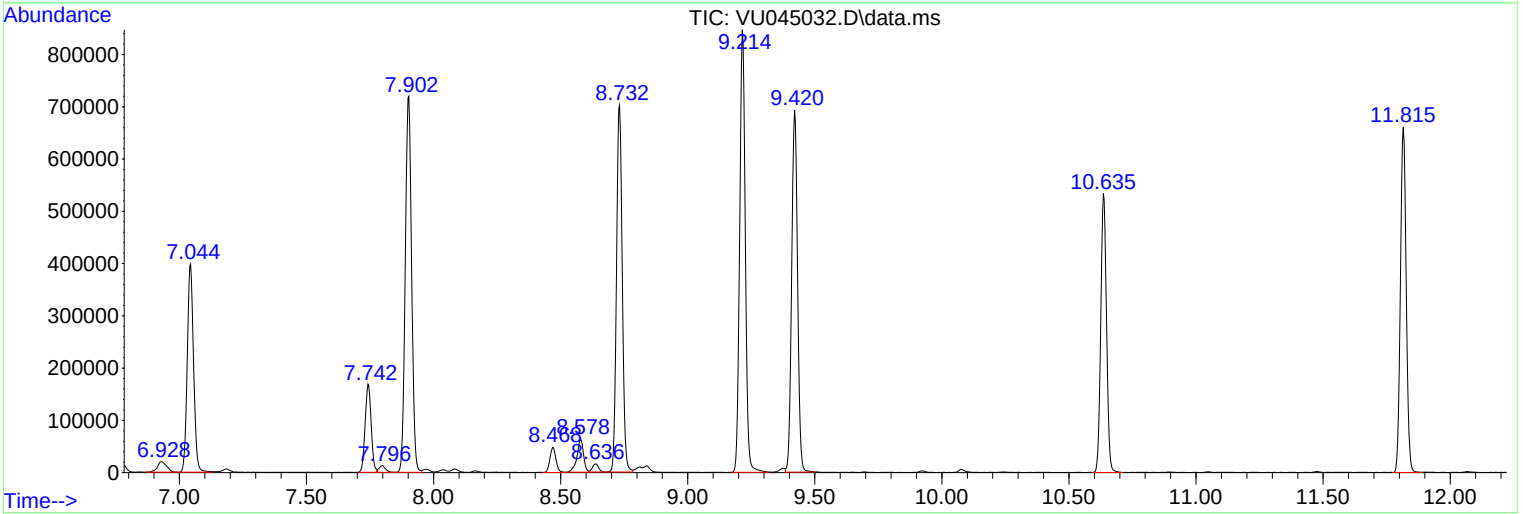
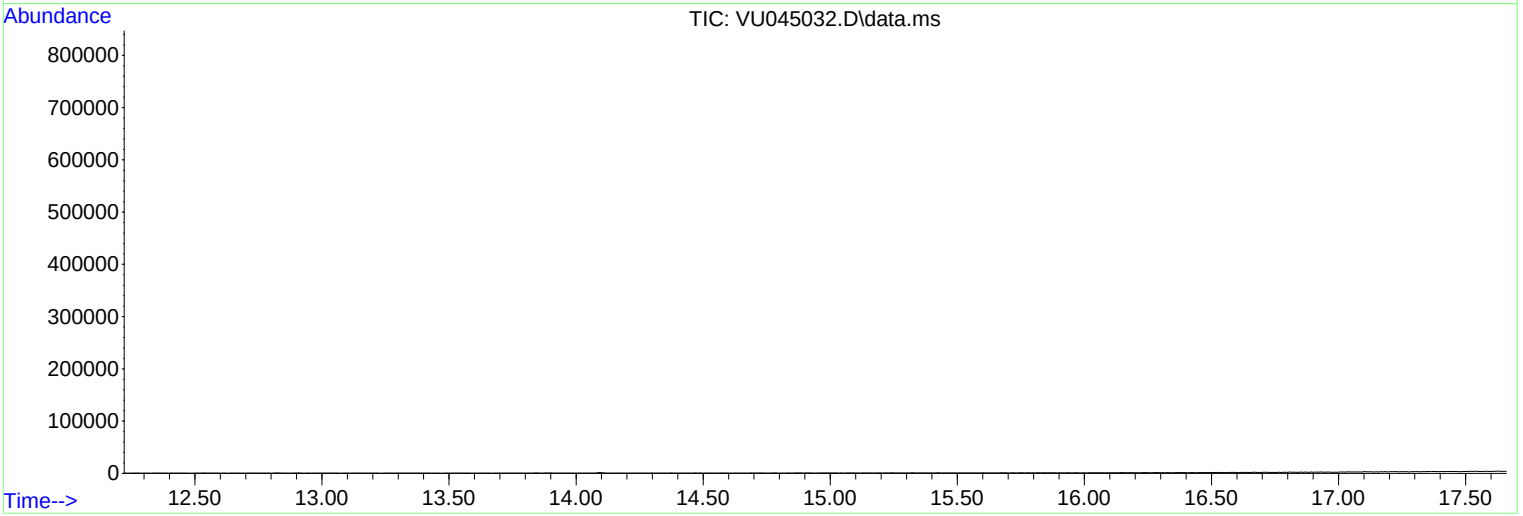
Instrument :
MSVOA_U
ClientSampleId :
KEARNY-COMP

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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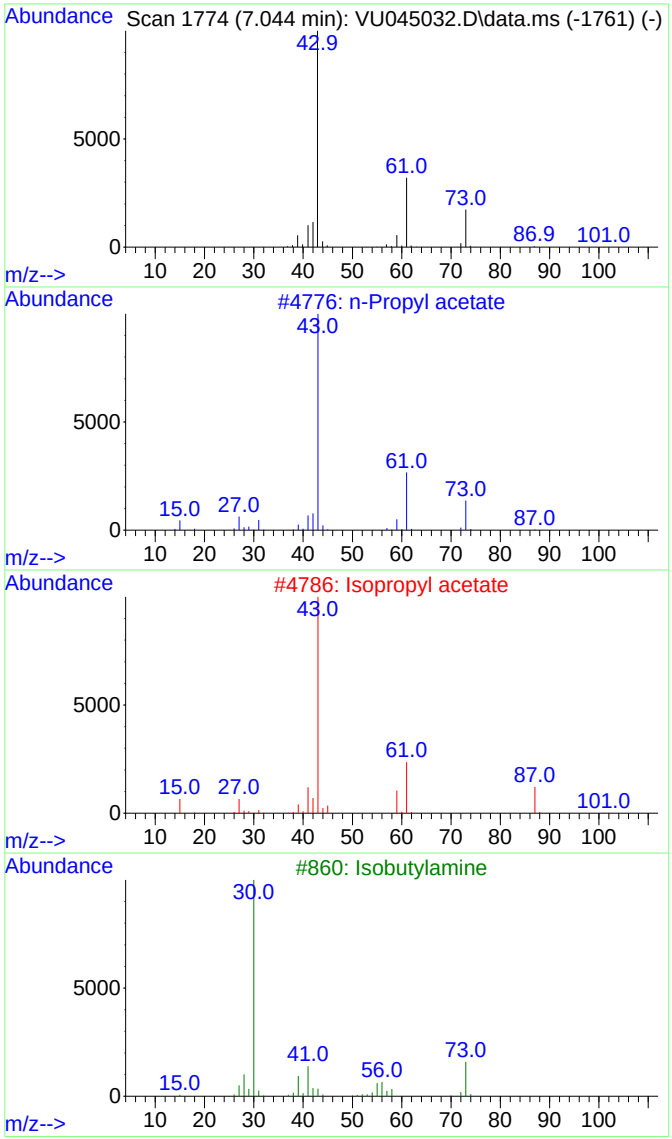
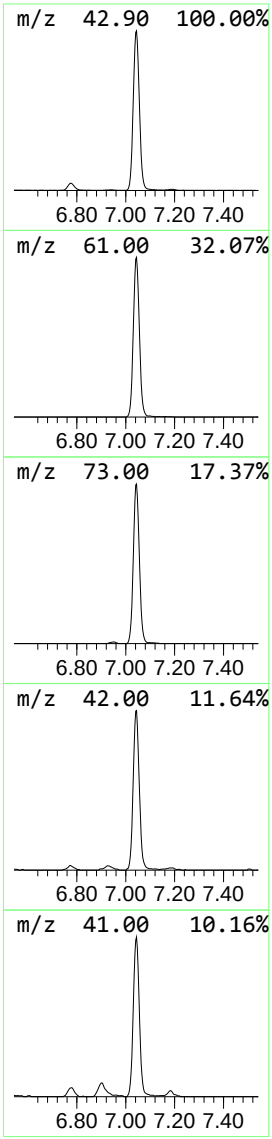
****
Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.044	36.38 ug/l	687978	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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
5	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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ALS Vial : 51 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : KEARNY-COMP

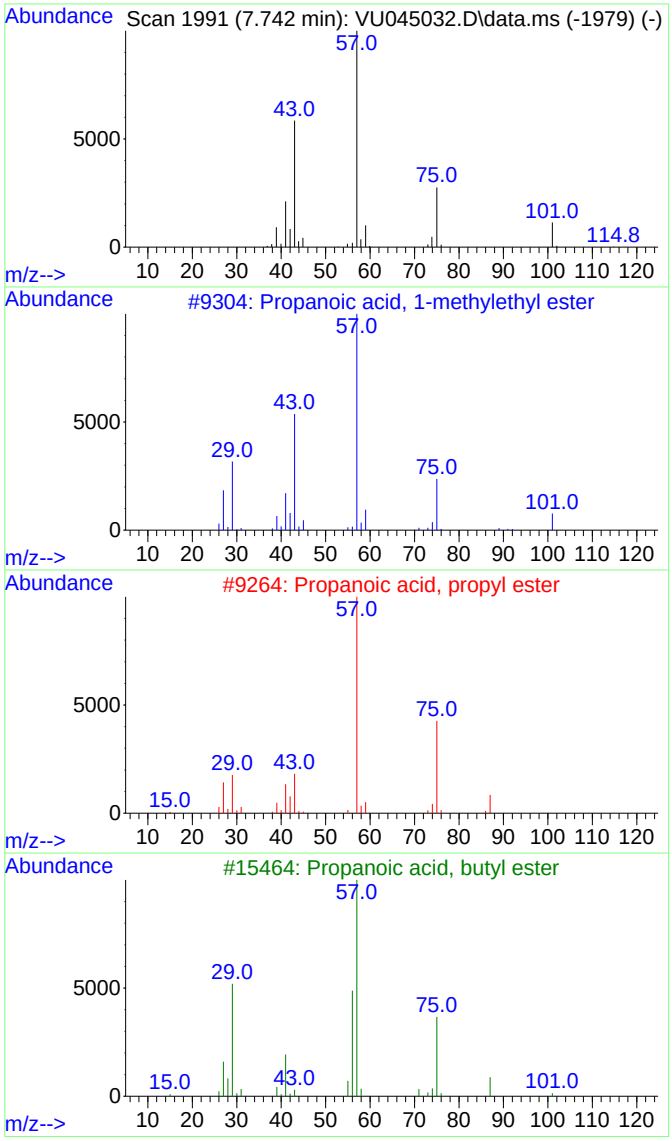
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

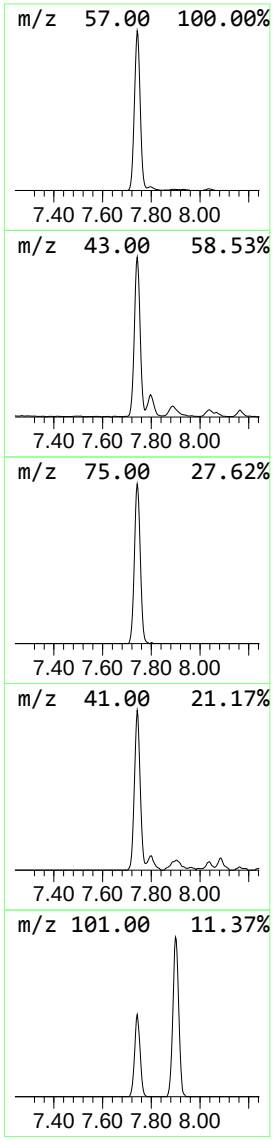
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.742	14.73 ug/l	278534	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	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
KEARNY-COMP

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

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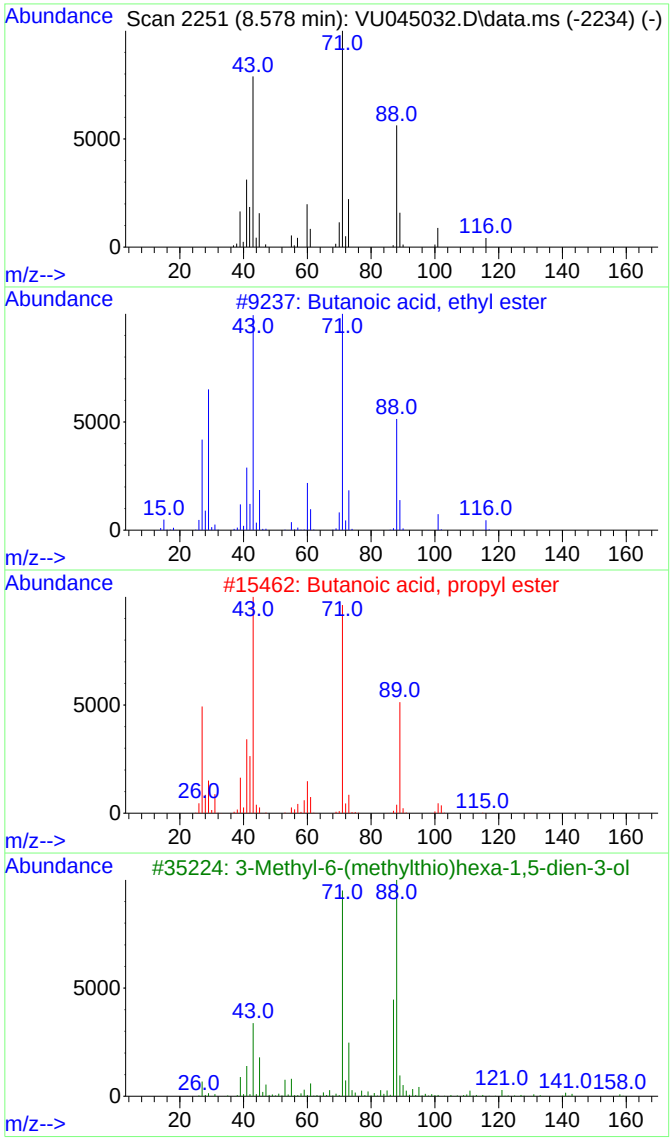
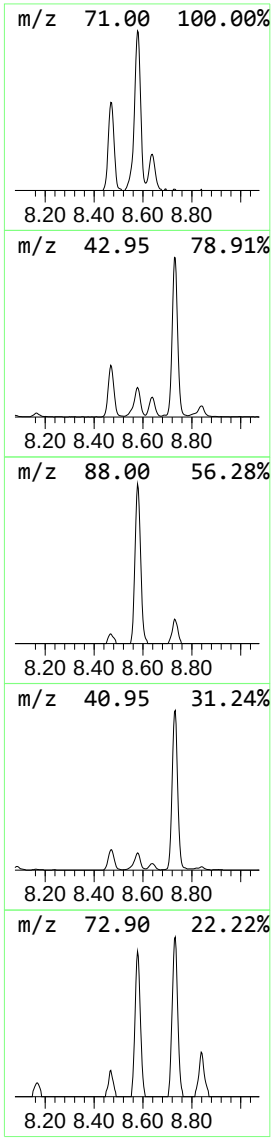
****
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.578	5.06 ug/l	112253	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	95
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
3	3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	45
4	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
5	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42





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Instrument : MSVOA_U
ClientSampleId : KEARNY-COMP

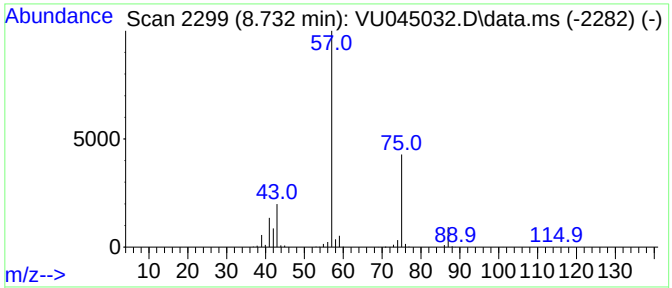
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

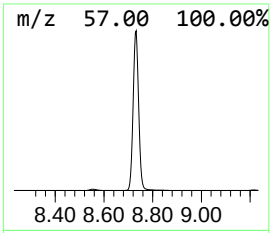
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

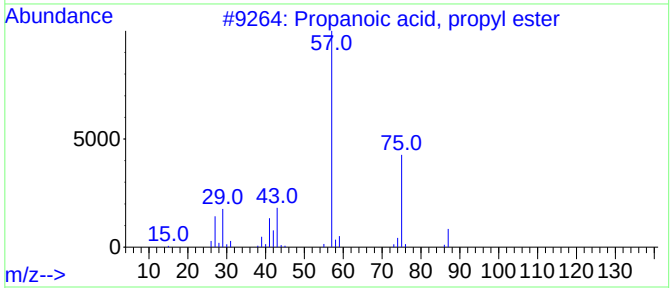
****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

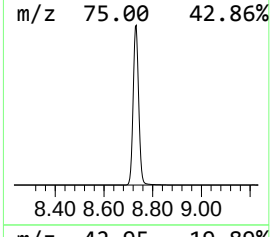
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.732	49.64 ug/l	1100850	Chlorobenzene-d5	9.420

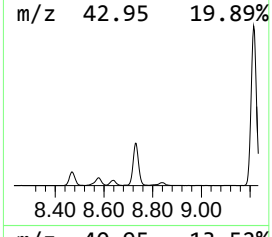
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3	Isobutyl ether	130	C8H18O	000628-55-7	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9

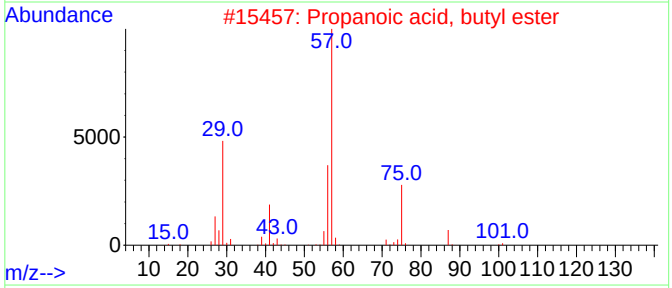


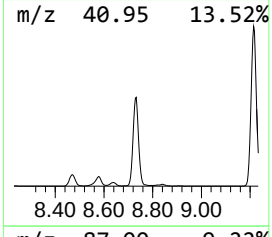


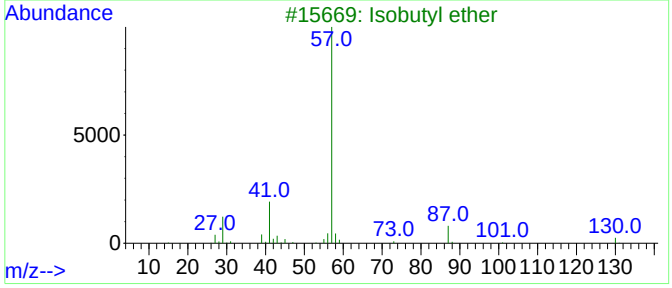


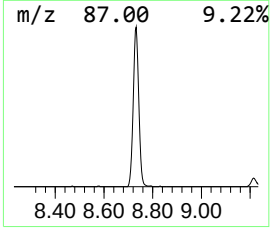












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Quant Title : SW846 8260

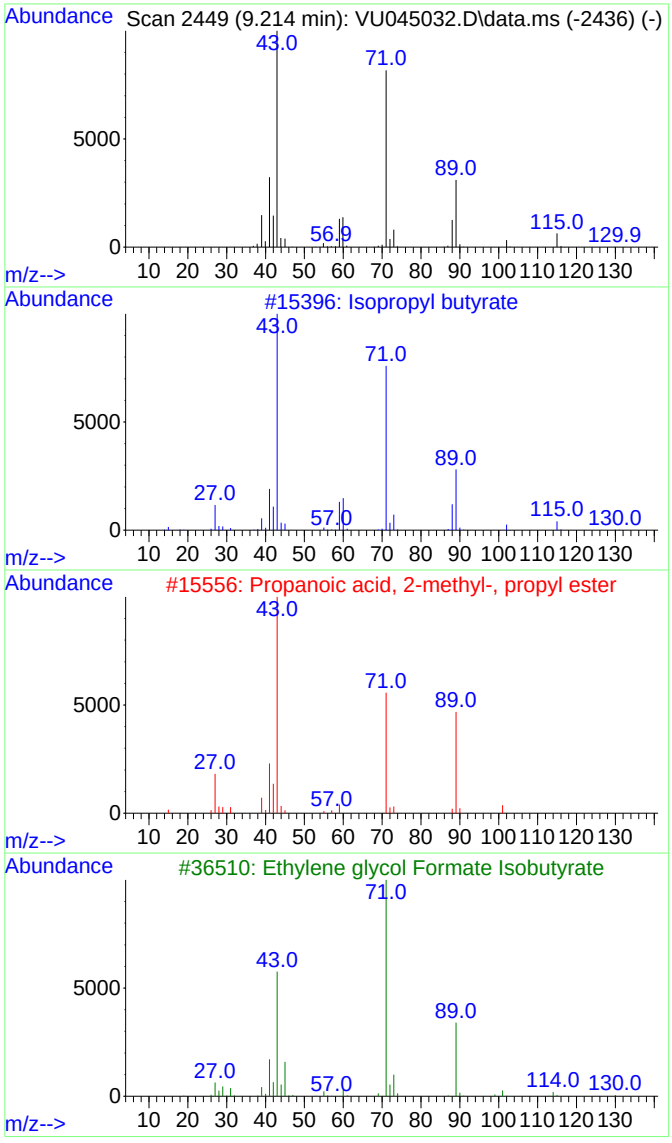
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

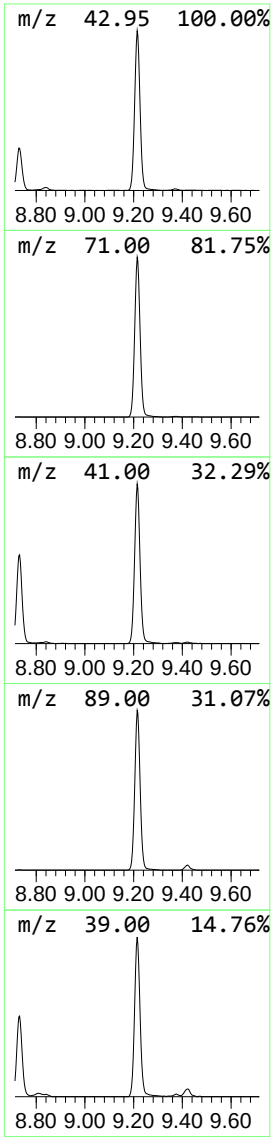
****

Peak Number 5 Isopropyl butyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.214	59.51 ug/l	1319860	Chlorobenzene-d5	9.420

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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.044	36.4	ug/l	687978	2	6.253	945552	50.0
Propanoic acid,...	7.742	14.7	ug/l	278534	2	6.253	945552	50.0
Butanoic acid, ...	8.578	5.1	ug/l	112253	3	9.420	1108930	50.0
Propanoic acid,...	8.732	49.6	ug/l	1100850	3	9.420	1108930	50.0
Isopropyl butyrate	9.214	59.5	ug/l	1319860	3	9.420	1108930	50.0