LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061818\
Data File : VU024705.D
Acq On : 18 Jun 2018 20:39
Operator : MD/SY
Sample : J3477-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0140

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_U\METHOD\82U061318W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.092	141	156	173	rBV	624543	768026	30.20%	6.715%
2	1.407	247	254	267	rVB	96129	103194	4.06%	0.902%
3	1.477	269	276	287	rBV	54915	67366	2.65%	0.589%
4	2.018	435	444	460	rVB	76800	124354	4.89%	1.087%
5	2.445	567	577	591	rVB	19303	34171	1.34%	0.299%
6	2.989	735	746	762	rVB	31963	59473	2.34%	0.520%
7	4.233	1108	1133	1155	rBV2	57068	144171	5.67%	1.261%
8	4.889	1320	1337	1353	rBV	183833	413267	16.25%	3.613%
9	4.989	1353	1368	1391	rVB	244224	536496	21.09%	4.691%
10	5.313	1453	1469	1485	rBV	184197	391240	15.38%	3.421%
11	5.394	1485	1494	1509	rVB3	18531	39913	1.57%	0.349%
12	5.889	1593	1648	1664	rBV	423894	1315966	51.74%	11.506%
13	7.570	2157	2171	2189	rBV	664999	1169168	45.97%	10.222%
14	7.853	2242	2259	2260	rBV3	44938	94338	3.71%	0.825%
15	9.091	2632	2644	2651	rBV	532070	954258	37.52%	8.343%
16	10.310	3011	3023	3040	rBV	520687	816231	32.09%	7.137%
17	11.487	3375	3389	3409	rVB	606312	959276	37.71%	8.387%
18	12.570	3718	3726	3737	rVB3	18501	28800	1.13%	0.252%
19	12.962	3837	3848	3870	rBV	232434	388593	15.28%	3.398%
20	13.323	3949	3960	3982	rBV2	99835	222901	8.76%	1.949%
21	15.130	4513	4522	4544	rBV3	51441	115421	4.54%	1.009%
22	15.689	4683	4696	4754	rBV	1298101	2543539	100.00%	22.239%
23	16.020	4792	4799	4810	rVB2	59266	82368	3.24%	0.720%
24	16.888	5061	5069	5080	rVB2	44949	64754	2.55%	0.566%

Sum of corrected areas: 11437284

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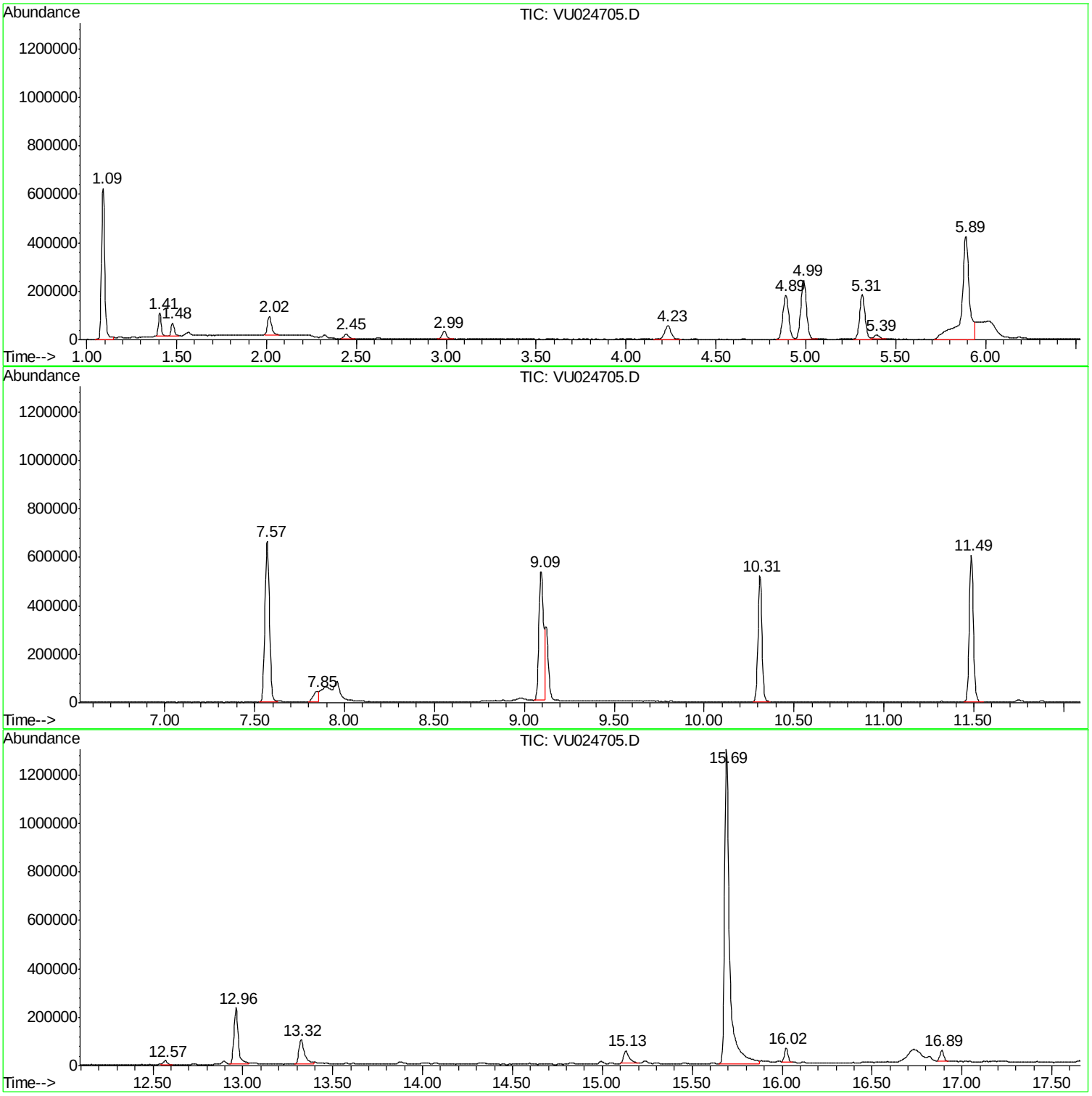
Instrument : MSVOA_U
ClientSampleId : S36-0140

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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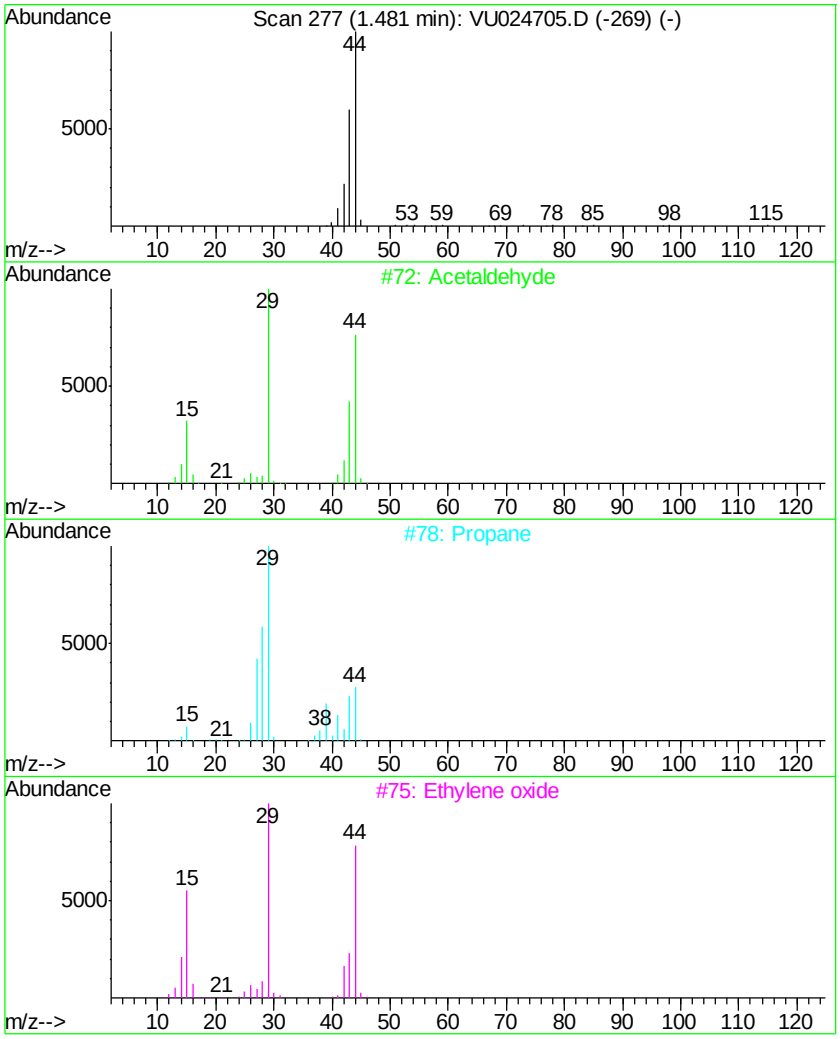
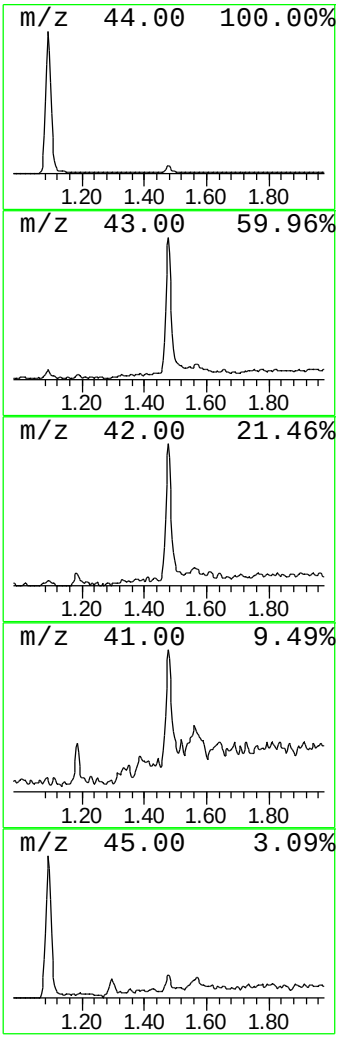
Peak Number 2 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	6.28 ug/l	67366	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	2-Hexanamine, 4-methyl-	115	C7H17N	000105-41-9	5
5	Tuaminoheptane	115	C7H17N	000123-82-0	5





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Data File : VU024705.D
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Operator : MD/SY
Sample : J3477-06
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ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0140

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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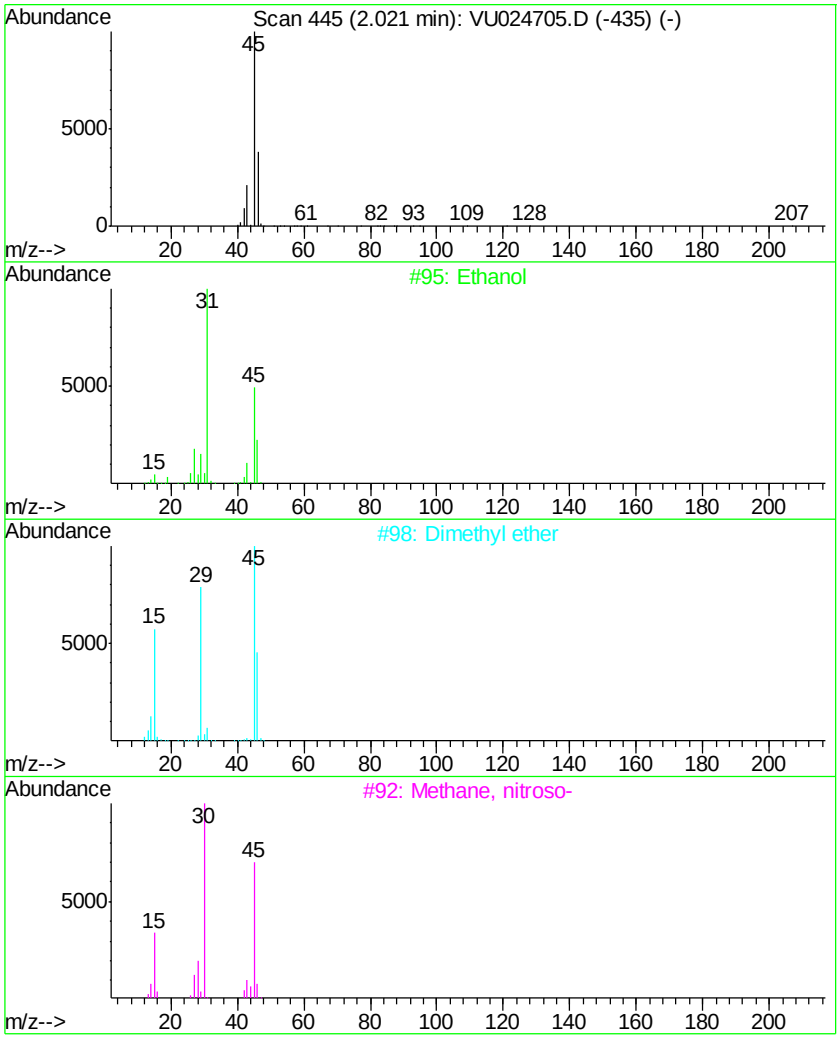
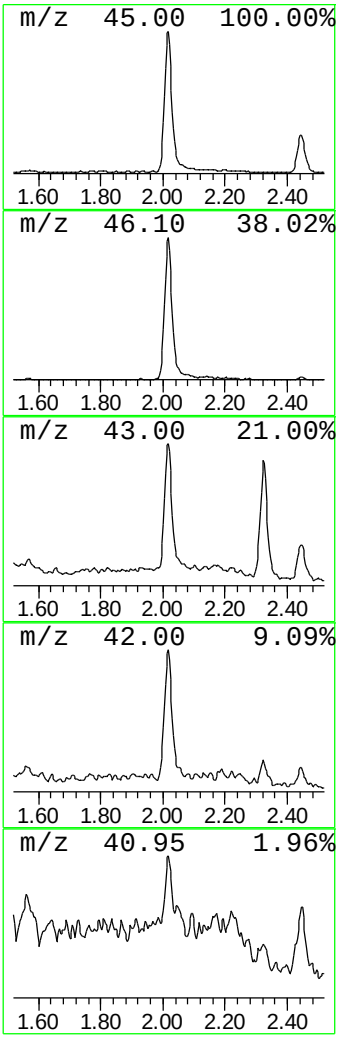
Peak Number 3 unknown2.02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	11.59 ug/l	124354	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	40
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Fluoroacetic acid	78	C2H3FO2	000144-49-0	2





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Operator : MD/SY
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ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0140

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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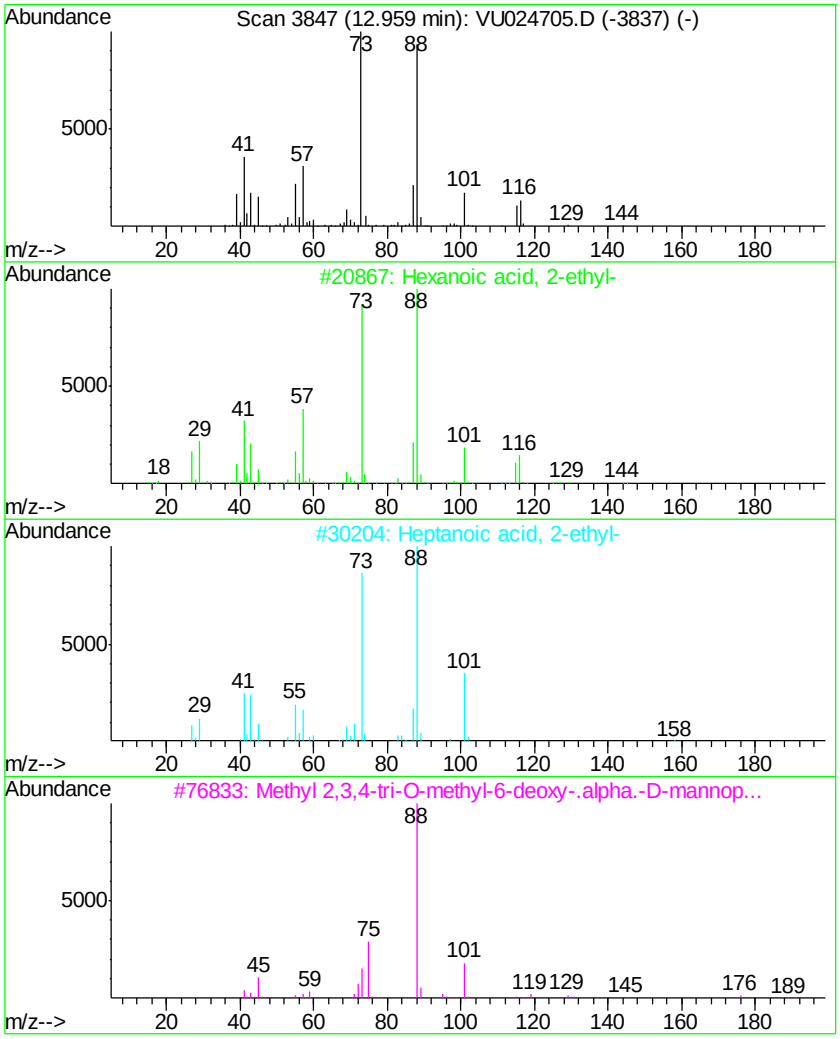
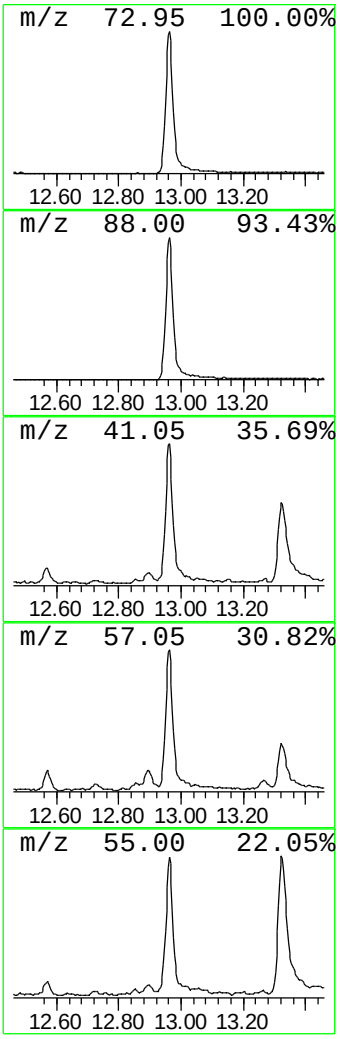
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	20.25 ug/l	388593	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	94
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
4	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	40
5	Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	38





Library Search Compound Report

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ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0140

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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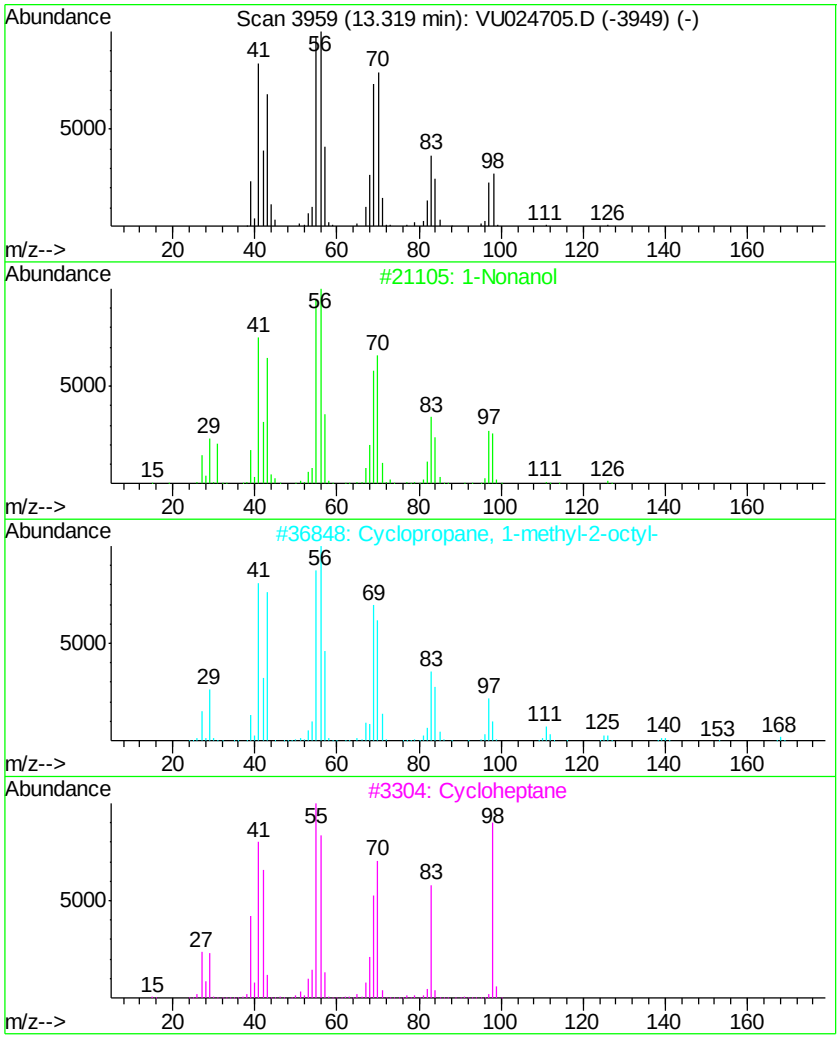
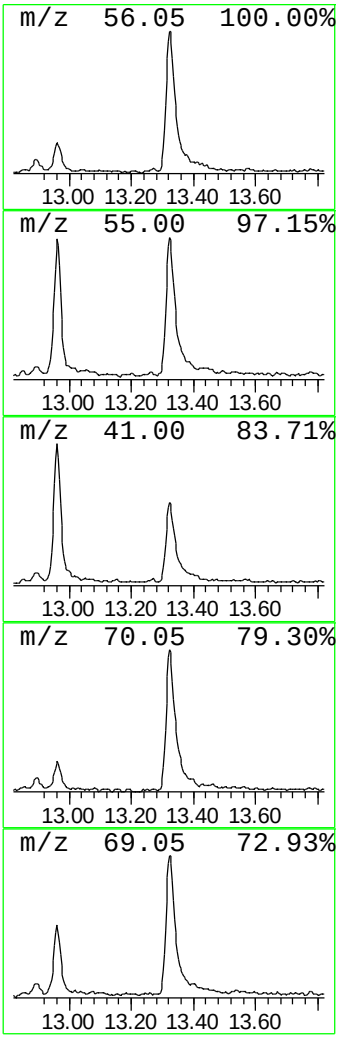
Peak Number 5 1-Nonanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	11.62 ug/l	222901	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
3	Cycloheptane	98	C7H14	000291-64-5	74
4	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	64
5	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	64





Library Search Compound Report

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Sample : J3477-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0140

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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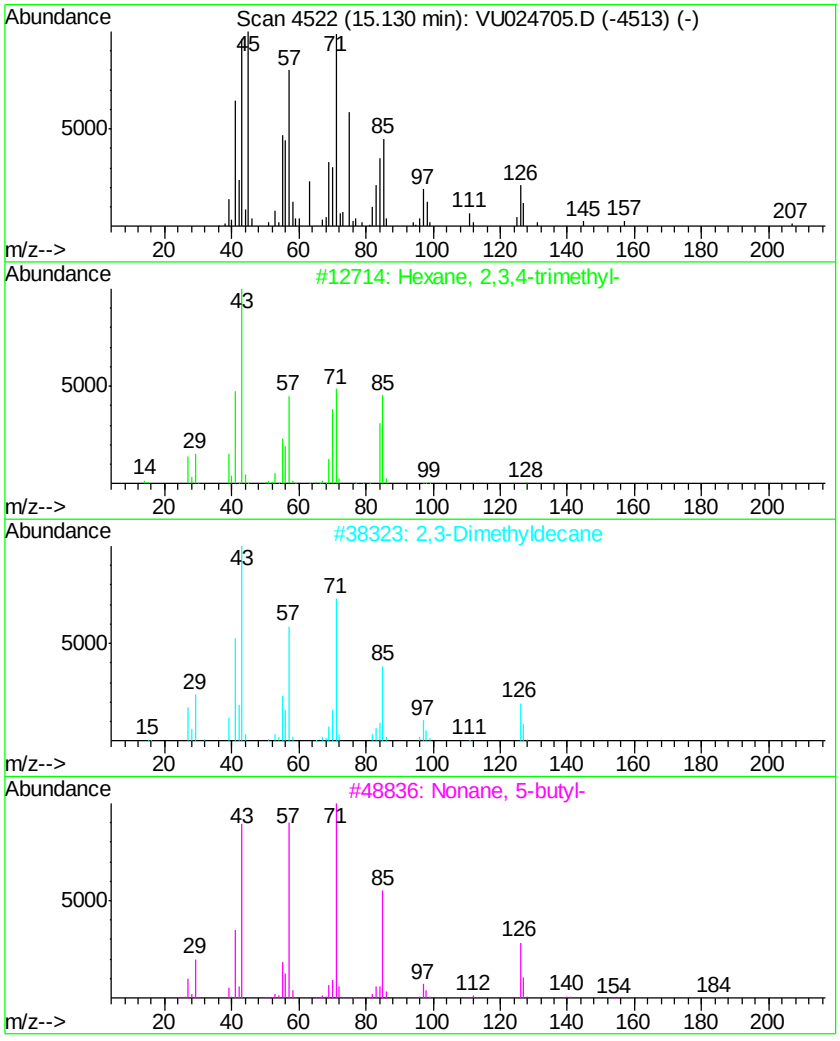
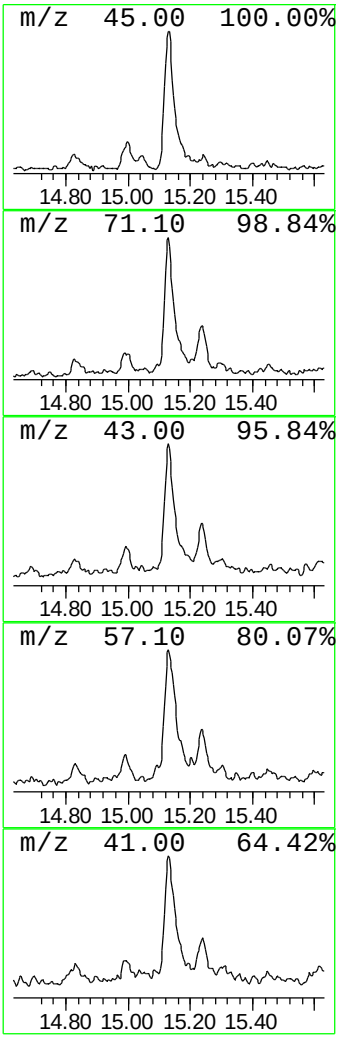
****

Peak Number 6 unknown15.13 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	6.02 ug/l	115421	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	43
2	2,3-Dimethyldecane	170	C12H26	017312-44-6	38
3	Nonane, 5-butyl-	184	C13H28	017312-63-9	35
4	Ether, hexyl pentyl	172	C11H24O	032357-83-8	35
5	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	35





Library Search Compound Report

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ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0140

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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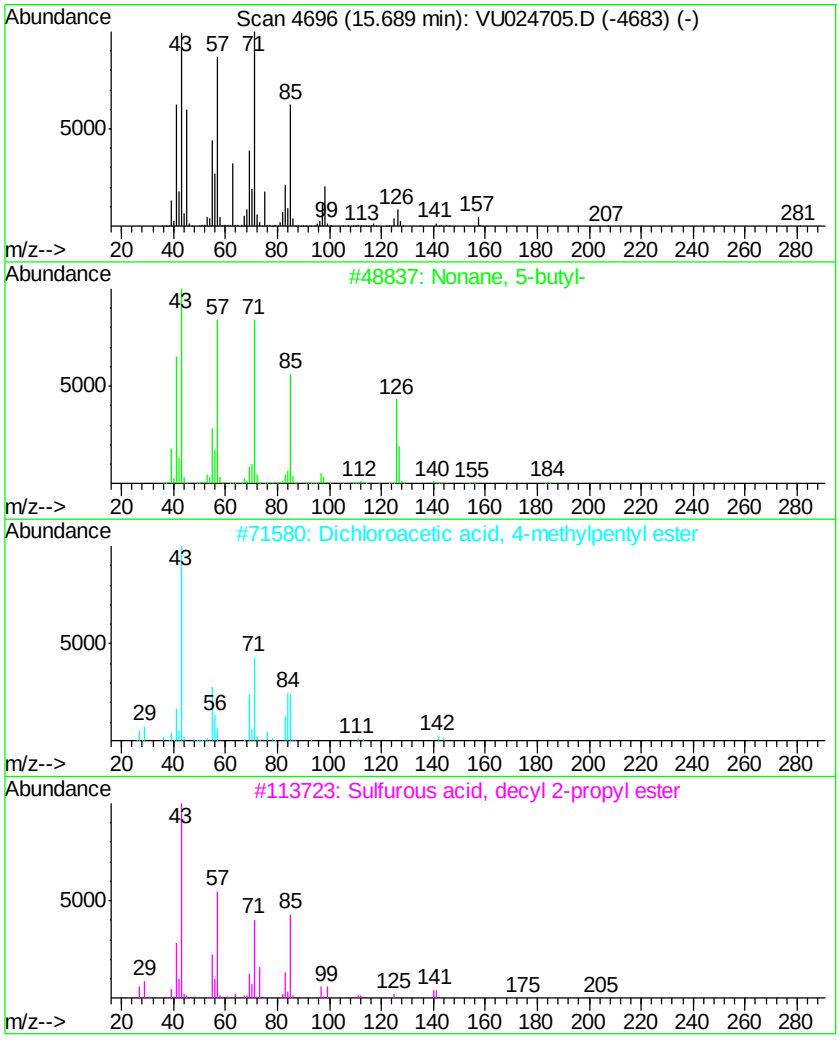
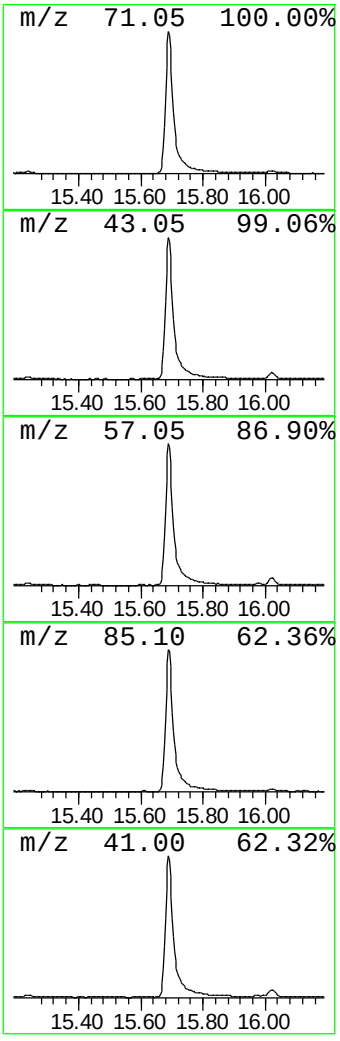
Peak Number 7 unknown15.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	132.58 ug/l	2543540	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 5-butyl-	184	C13H28	017312-63-9	47
2	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	38
3	Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	38
4	10-Methylnonadecane	282	C20H42	056862-62-5	38
5	Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	35





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
Acetaldehyde	1.48	6.3	ug/l	67366	1	4.99	536496	50.0
unknown2.02	2.02	11.6	ug/l	124354	1	4.99	536496	50.0
Hexanoic acid, 2-...	12.96	20.3	ug/l	388593	4	11.49	959276	50.0
1-Nonanol	13.32	11.6	ug/l	222901	4	11.49	959276	50.0
unknown15.13	15.13	6.0	ug/l	115421	4	11.49	959276	50.0
unknown15.69	15.69	132.6	ug/l	2543540	4	11.49	959276	50.0