LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061818\
Data File : VU024704.D
Acq On : 18 Jun 2018 20:15
Operator : MD/SY
Sample : J3477-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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	1.089	144	155	175	rBV	601043	751096	17.78%	4.133%
2	1.478	269	276	287	rBV	149979	184235	4.36%	1.014%
3	2.021	435	445	462	rVB	107365	207933	4.92%	1.144%
4	2.445	568	577	594	rVB	25040	45695	1.08%	0.251%
5	2.986	735	745	758	rBV2	24113	45686	1.08%	0.251%
6	4.230	1111	1132	1158	rBV	261361	641864	15.19%	3.532%
7	4.886	1320	1336	1352	rBV	193255	433083	10.25%	2.383%
8	4.989	1352	1368	1392	rVB	259320	571613	13.53%	3.145%
9	5.313	1453	1469	1484	rBV	196087	413207	9.78%	2.273%
10	5.889	1587	1648	1673	rBV4	594665	3339183	79.03%	18.372%
11	7.567	2155	2170	2185	rBV	684211	1198801	28.37%	6.596%
12	7.850	2236	2258	2266	rBV4	78462	292957	6.93%	1.612%
13	8.985	2596	2611	2626	rBV4	21571	70784	1.68%	0.389%
14	9.095	2632	2645	2651	rBV	543588	989274	23.41%	5.443%
15	10.310	3010	3023	3042	rBV	541297	851612	20.16%	4.686%
16	11.487	3375	3389	3405	rBV	639493	1018951	24.12%	5.606%
17	12.892	3819	3826	3837	rVV	55485	88574	2.10%	0.487%
18	12.966	3838	3849	3870	rVV	480307	760358	18.00%	4.183%
19	13.320	3949	3959	3967	rBV2	596556	1225016	28.99%	6.740%
20	14.828	4415	4428	4439	rBV4	40306	81426	1.93%	0.448%
21	14.992	4470	4479	4491	rBV3	55061	96890	2.29%	0.533%
22	15.130	4512	4522	4548	rBV	236758	468049	11.08%	2.575%
23	15.689	4683	4696	4737	rBV	2308444	4225040	100.00%	23.246%
24	16.020	4792	4799	4808	rVB2	72238	99835	2.36%	0.549%
25	16.889	5061	5069	5078	rBV	54213	74155	1.76%	0.408%

Sum of corrected areas: 18175317

LSC Report - Integrated Chromatogram

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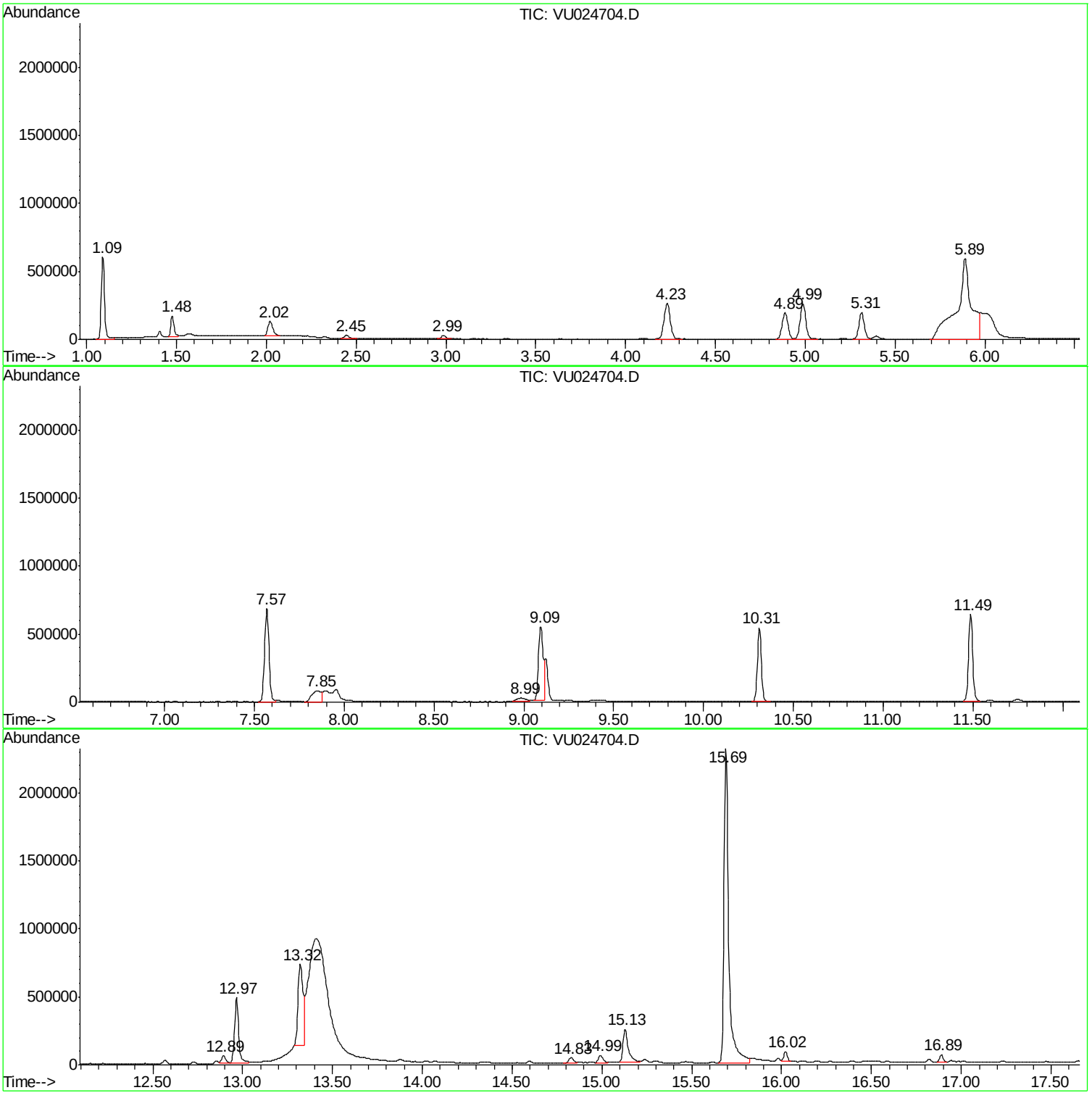
Operator : MD/SY
Sample : J3477-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061818\
Data File : VU024704.D
Acq On : 18 Jun 2018 20:15
Operator : MD/SY
Sample : J3477-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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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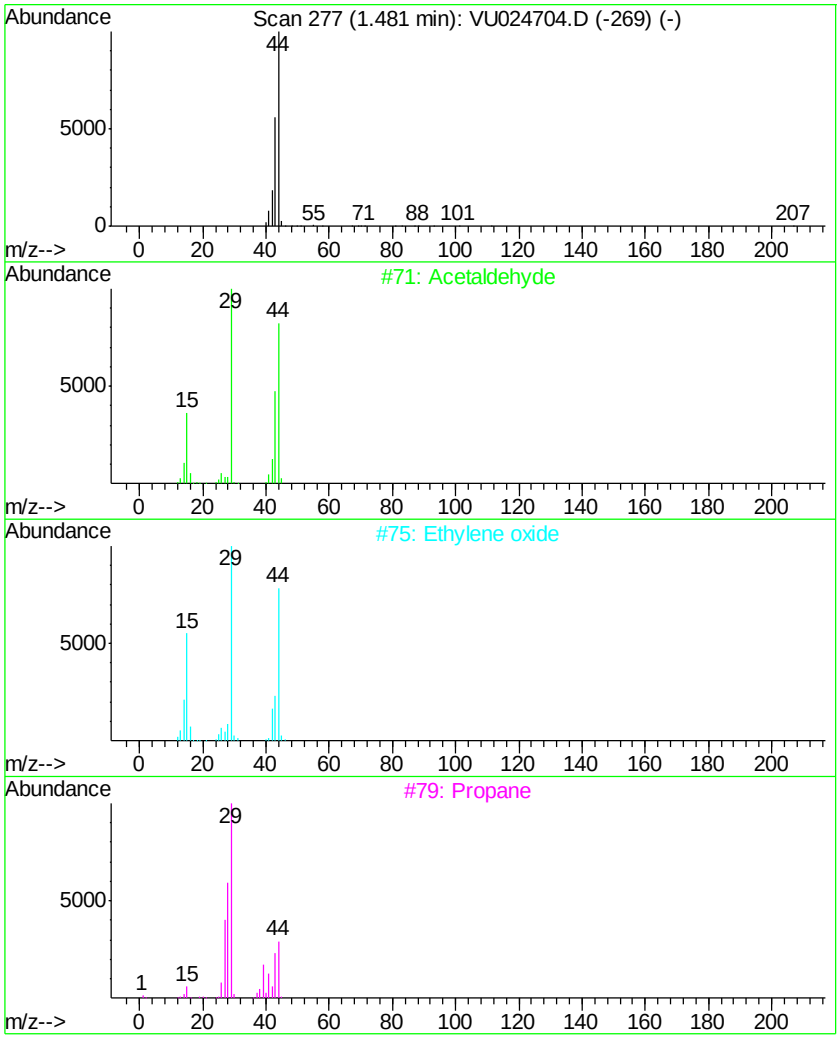
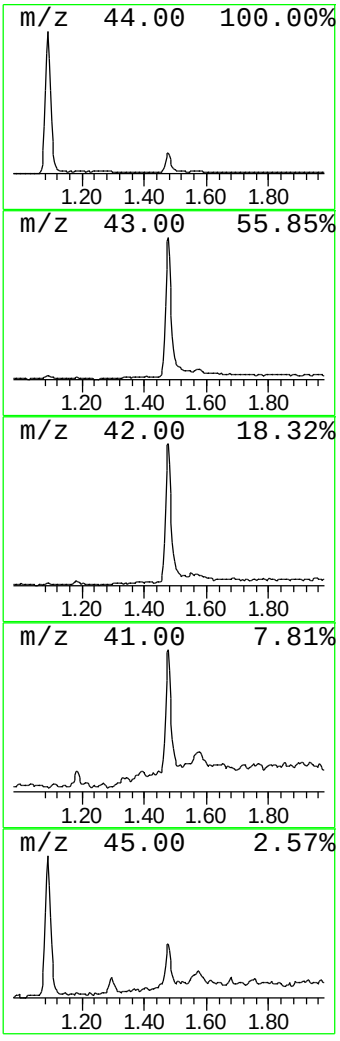
Peak Number 2 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	16.12 ug/l	184235	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Carbon dioxide	44	CO2	000124-38-9	3
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061818\
Data File : VU024704.D
Acq On : 18 Jun 2018 20:15
Operator : MD/SY
Sample : J3477-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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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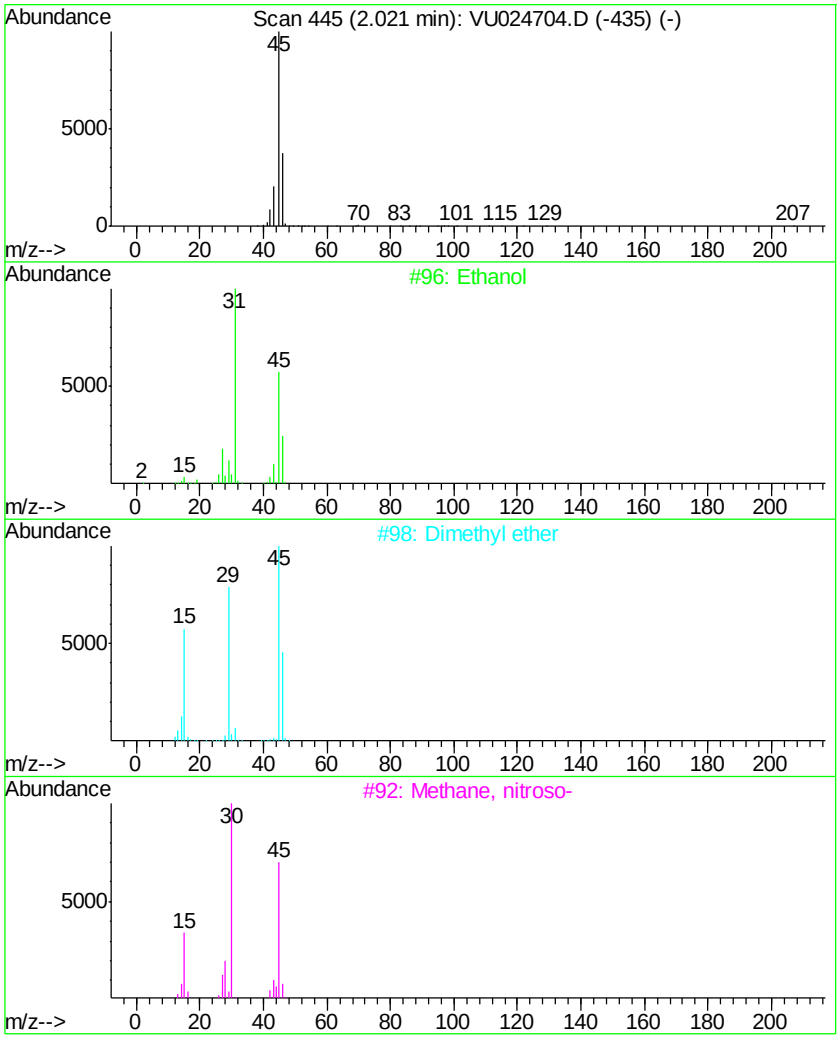
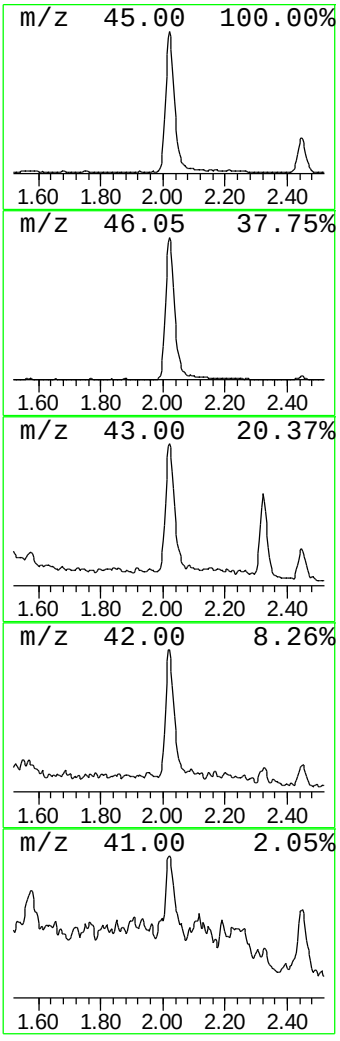
Peak Number 3 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	18.19 ug/l	207933	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	4
5	Carbazic acid, 3-(1-propylbutyli...	200	C10H20N2O2	014702-39-7	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061818\
Data File : VU024704.D
Acq On : 18 Jun 2018 20:15
Operator : MD/SY
Sample : J3477-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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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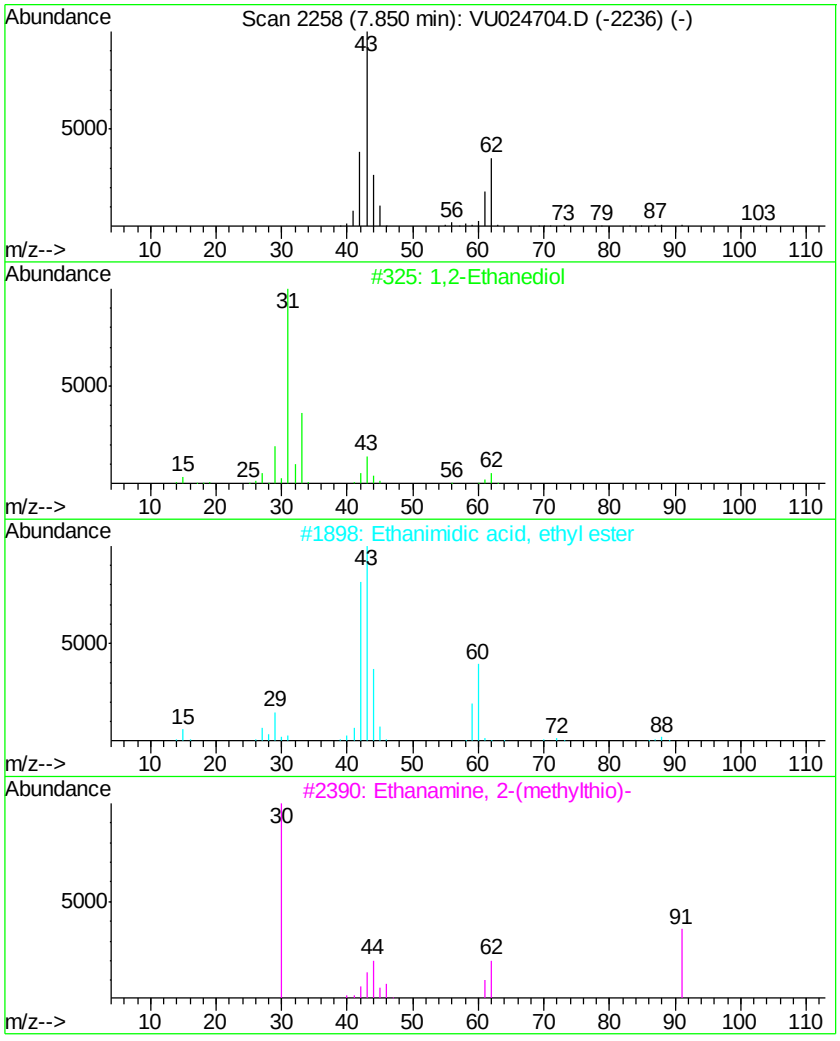
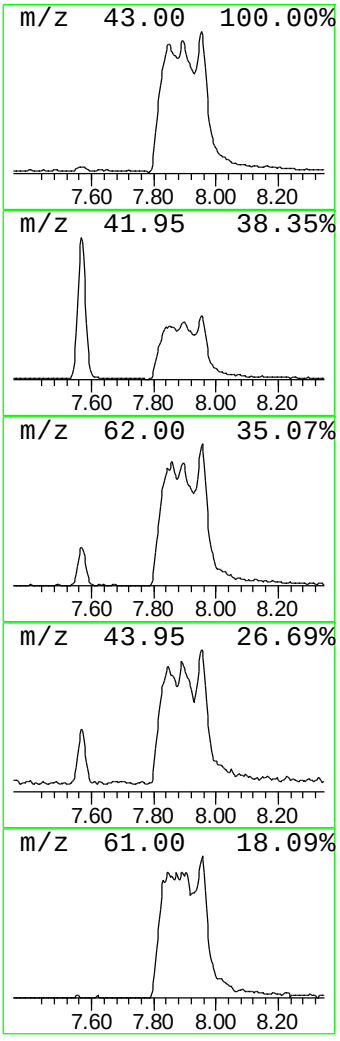
Peak Number 4 unknown7.85 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.85	14.81 ug/l	292957	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol	62	C2H6O2	000107-21-1	42
2	Ethanimidic acid, ethyl ester	87	C4H9NO	001000-84-6	9
3	Ethanamine, 2-(methylthio)-	91	C3H9NS	018542-42-2	9
4	Ethanethiol	62	C2H6S	000075-08-1	5
5	Peroxide, dimethyl	62	C2H6O2	000690-02-8	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061818\
Data File : VU024704.D
Acq On : 18 Jun 2018 20:15
Operator : MD/SY
Sample : J3477-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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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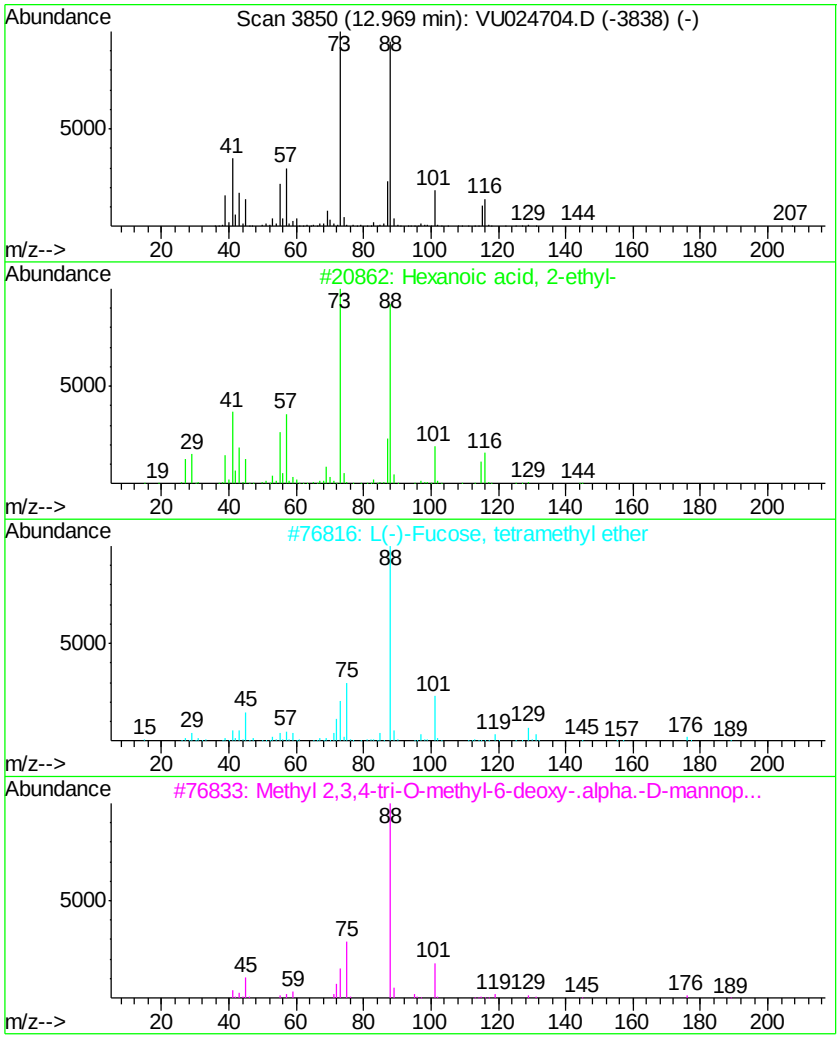
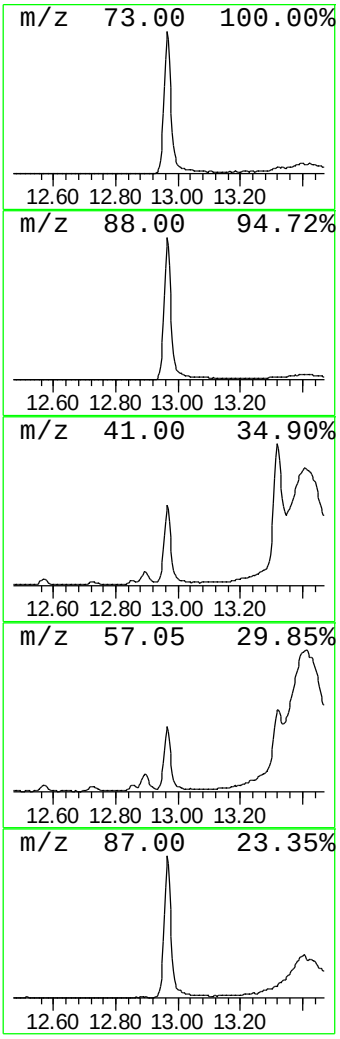
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	37.31 ug/l	760358	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	90
2	L(-)-Fucose, tetramethyl ether	220	C10H20O5	1000332-75-0	40
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
4	1,4-Dioxane	88	C4H8O2	000123-91-1	37
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	37





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061818\
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Acq On : 18 Jun 2018 20:15
Operator : MD/SY
Sample : J3477-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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

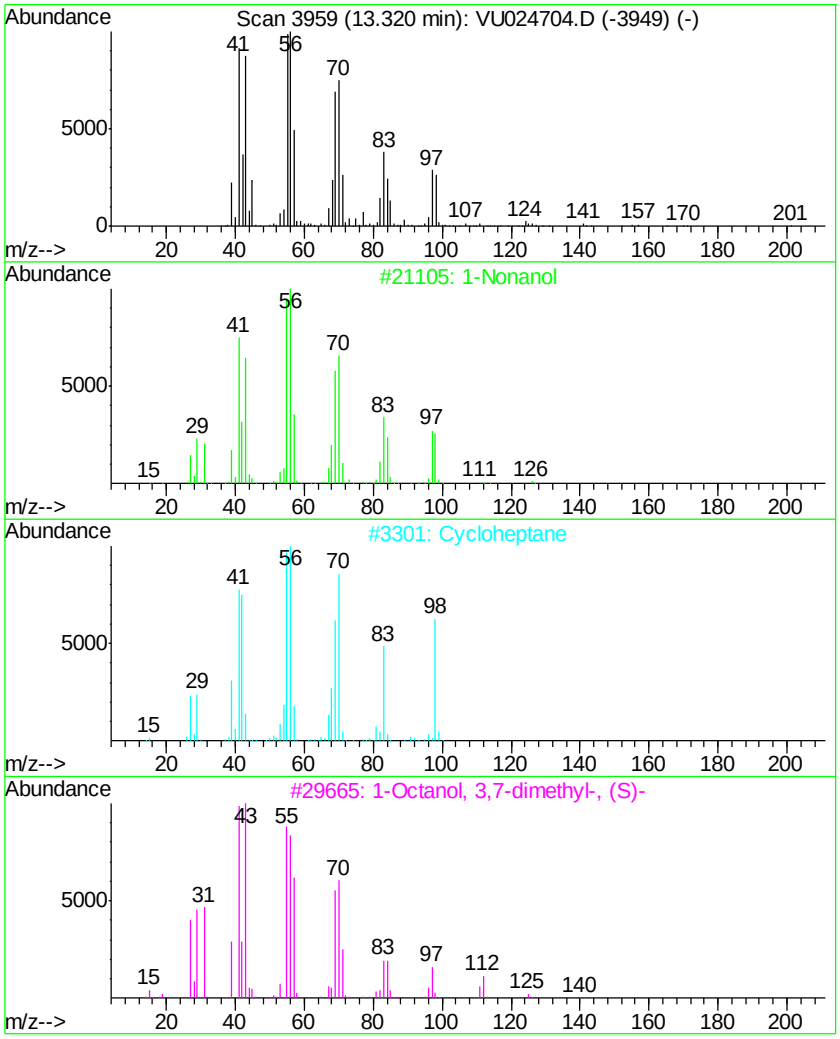
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

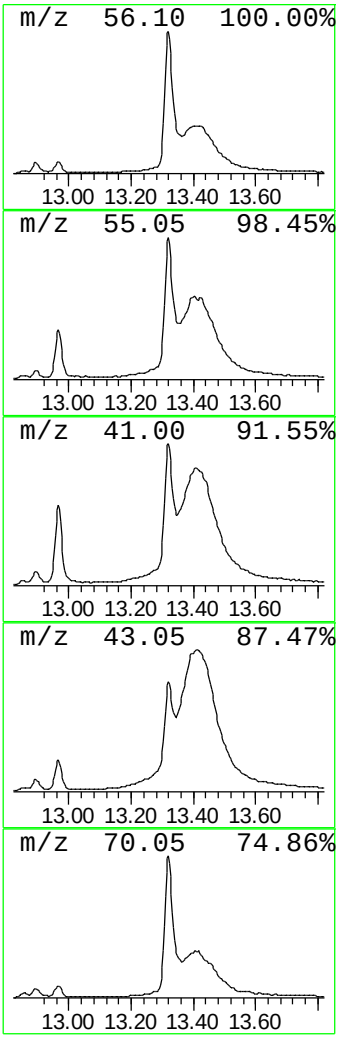
****

Peak Number 6 1-Nonanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	60.11 ug/l	1225020	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	Cycloheptane	98	C7H14	000291-64-5	68
3	1-Octanol, 3,7-dimethyl-, (S)-	158	C10H22O	068680-98-8	64
4	Isopropylcyclobutane	98	C7H14	000872-56-0	62
5	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	58





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ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S36-0141

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

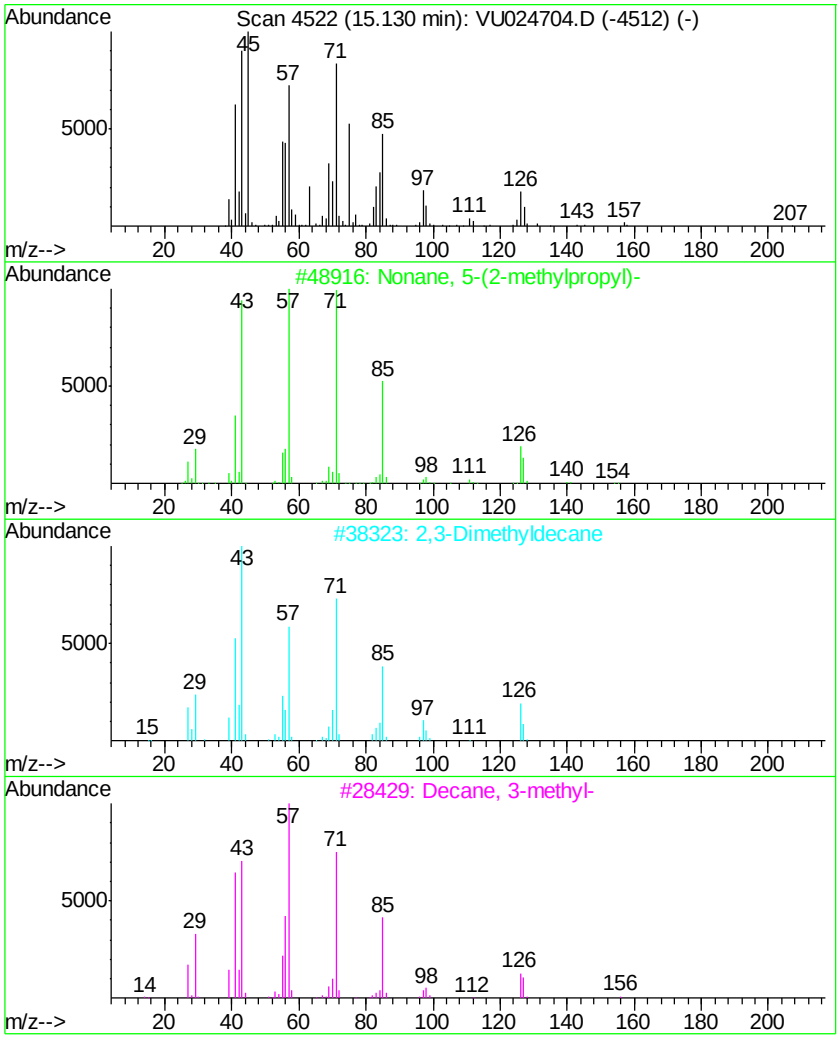
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

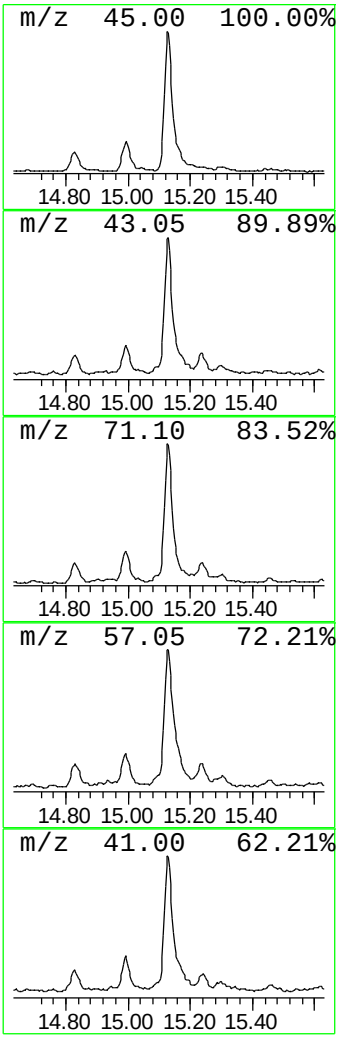
****

Peak Number 7 unknown15.13 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	22.97 ug/l	468049	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	38
2	2,3-Dimethyldecane	170	C12H26	017312-44-6	38
3	Decane, 3-methyl-	156	C11H24	013151-34-3	38
4	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	35
5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	35





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

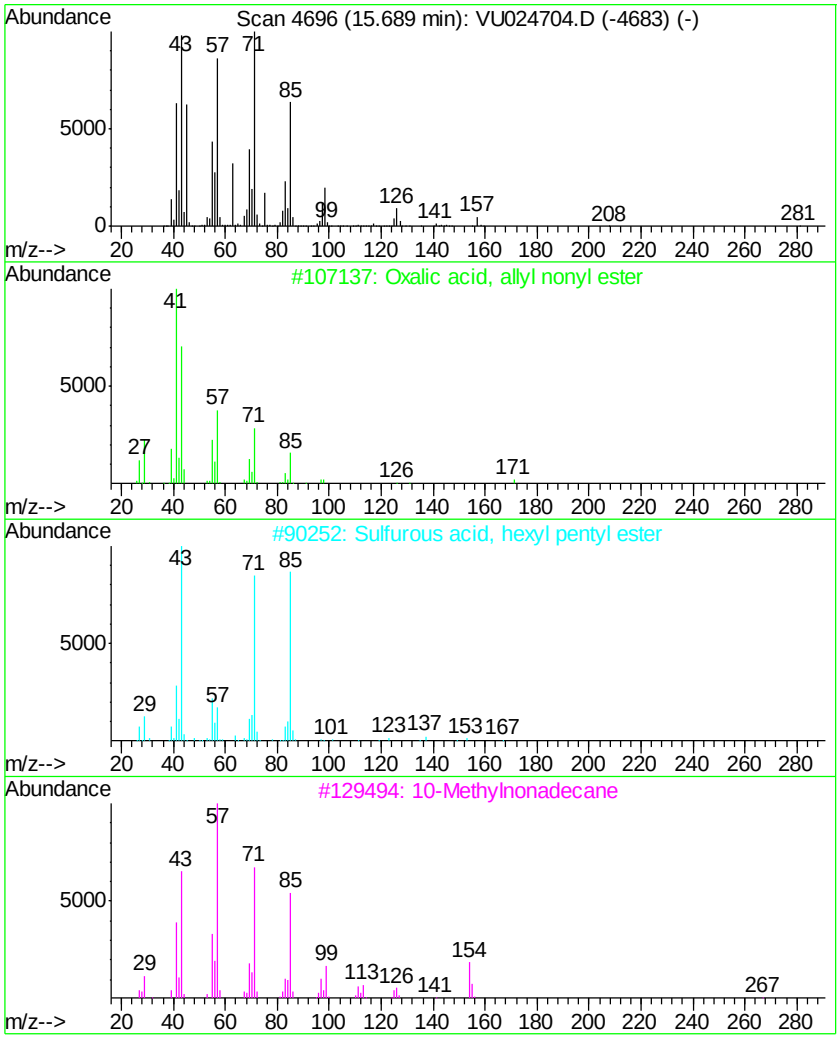
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

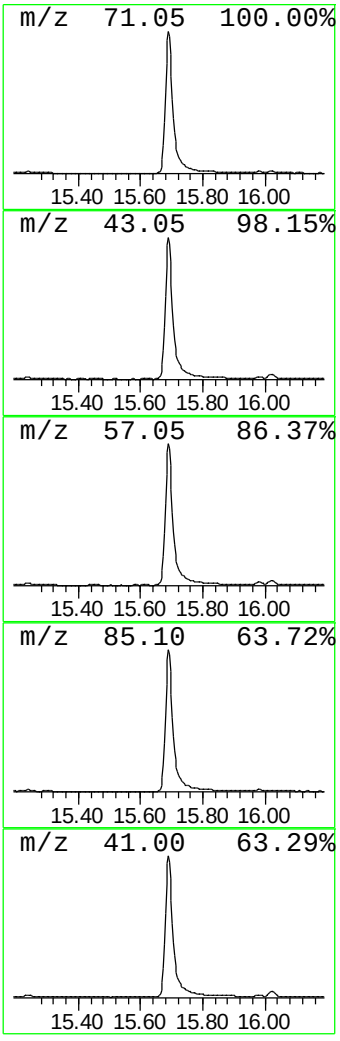
****

Peak Number 8 Oxalic acid, allyl nonyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	207.32 ug/l	4225040	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	52
2	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	43
3	10-Methylnonadecane	282	C20H42	056862-62-5	38
4	Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	35
5	Undecane	156	C11H24	001120-21-4	35





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.48	16.1	ug/l	184235	1	4.99	571613	50.0
Ethanol	2.02	18.2	ug/l	207933	1	4.99	571613	50.0
unknown7.85	7.85	14.8	ug/l	292957	3	9.09	989274	50.0
Hexanoic acid, 2-...	12.97	37.3	ug/l	760358	4	11.49	1018950	50.0
1-Nonanol	13.32	60.1	ug/l	1225020	4	11.49	1018950	50.0
unknown15.13	15.13	23.0	ug/l	468049	4	11.49	1018950	50.0
Oxalic acid, ally...	15.69	207.3	ug/l	4225040	4	11.49	1018950	50.0