LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092618\
Data File : VU027183.D
Acq On : 26 Sep 2018 17:24
Operator : MD/SY
Sample : J5049-10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-53-SEP19

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\82U092218W.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	2.013	251	261	284	rBV	216317	345709	3.89%	1.149%
2	2.324	344	358	383	rBV	4742026	7799100	87.65%	25.912%
3	2.453	384	398	446	rVV	5090681	8897691	100.00%	29.562%
4	3.607	742	757	791	rBV	219691	521140	5.86%	1.731%
5	4.228	931	950	987	rBV2	188182	537534	6.04%	1.786%
6	4.884	1139	1154	1171	rBV	101414	224240	2.52%	0.745%
7	4.987	1171	1186	1207	rVV	139124	303997	3.42%	1.010%
8	5.350	1273	1299	1323	rBV2	523217	1419491	15.95%	4.716%
9	5.887	1453	1466	1484	rBV	218671	424836	4.77%	1.412%
10	6.170	1540	1554	1610	rBV	1089126	2224364	25.00%	7.390%
11	7.463	1946	1956	1967	rBV	155899	252183	2.83%	0.838%
12	7.565	1977	1988	2002	rBV	423491	736309	8.28%	2.446%
13	8.125	2151	2162	2176	rBV	100739	194452	2.19%	0.646%
14	8.263	2196	2205	2229	rVB	102452	177550	2.00%	0.590%
15	8.466	2258	2268	2277	rBV	330767	538498	6.05%	1.789%
16	8.546	2277	2293	2346	rVB2	368408	1182981	13.30%	3.930%
17	8.987	2416	2430	2452	rBV	203575	573550	6.45%	1.906%
18	9.089	2452	2462	2483	rVB	339718	591359	6.65%	1.965%
19	9.684	2635	2647	2664	rBV	383870	636306	7.15%	2.114%
20	9.794	2667	2681	2708	rVV3	100289	213669	2.40%	0.710%
21	9.916	2709	2719	2736	rVB2	73956	125923	1.42%	0.418%
22	10.051	2745	2761	2782	rVB	112700	210976	2.37%	0.701%
23	10.308	2827	2841	2874	rBV3	356778	678885	7.63%	2.256%
24	11.067	3068	3077	3083	rBV2	79892	121877	1.37%	0.405%
25	11.109	3083	3090	3098	rVV	200659	304977	3.43%	1.013%
26	11.154	3098	3104	3116	rVB	63475	93918	1.06%	0.312%
27	11.485	3195	3207	3221	rBV2	425115	766418	8.61%	2.546%

Sum of corrected areas: 30097933

LSC Report - Integrated Chromatogram

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Operator : MD/SY
Sample : J5049-10
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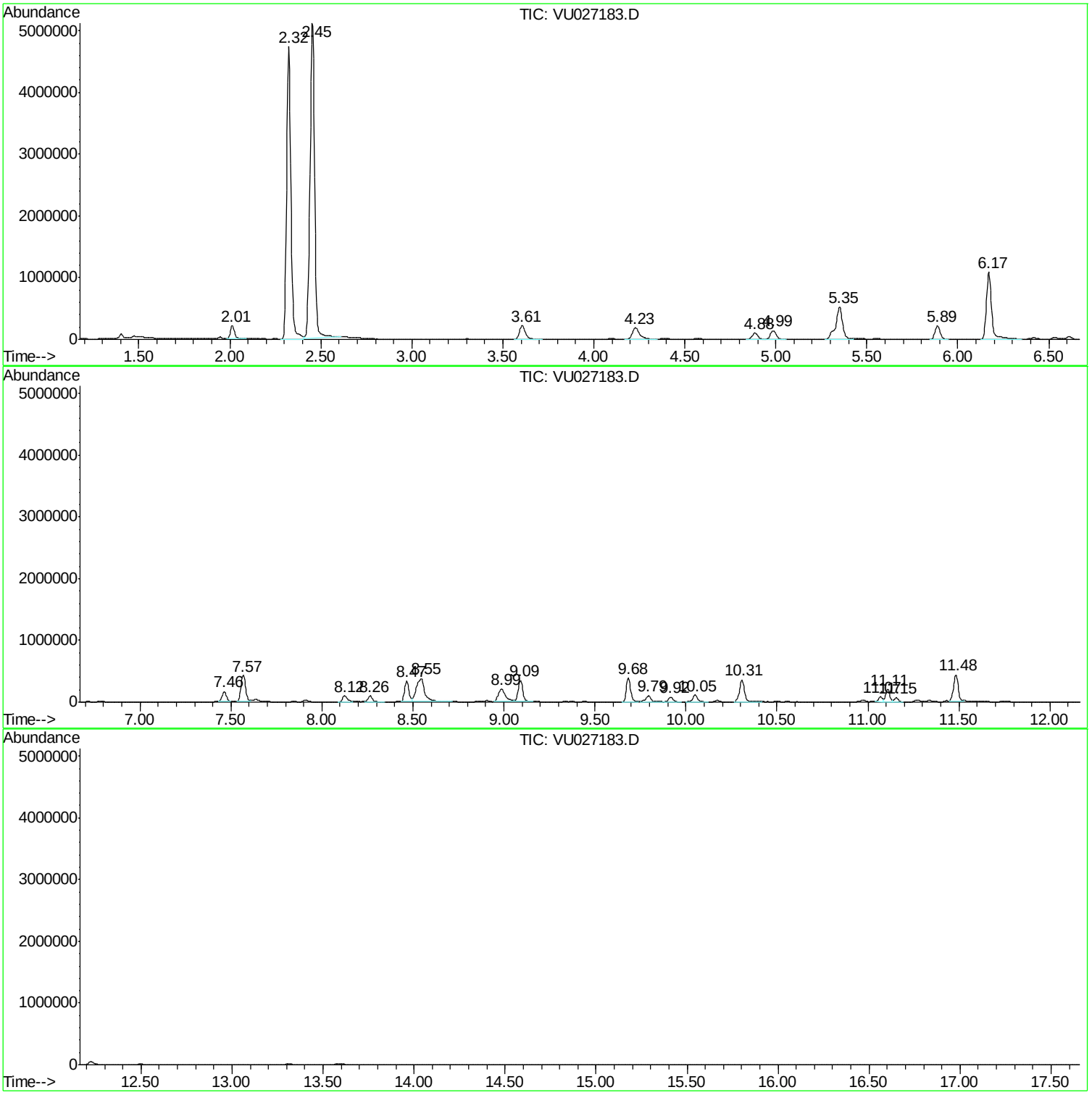
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Quant Title : SW846 8260

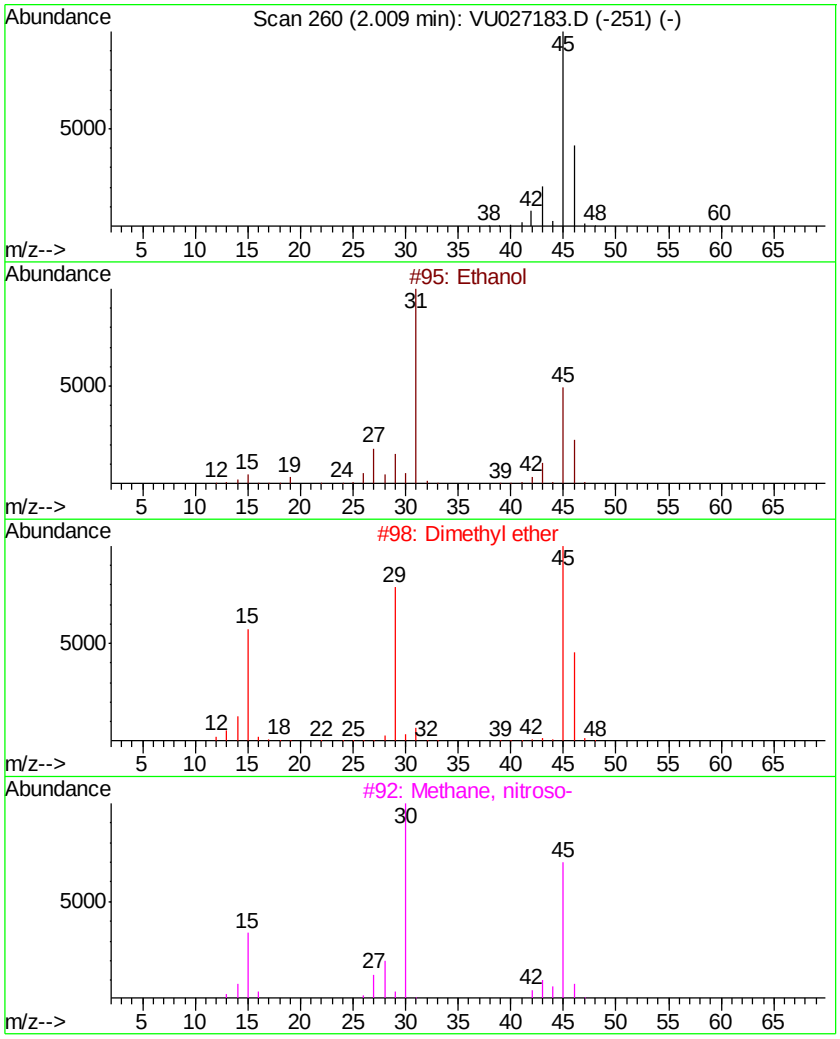
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

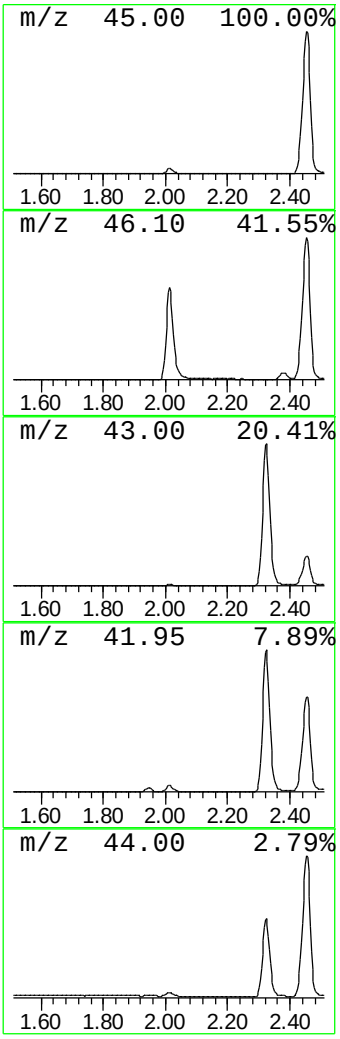
****

Peak Number 1 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	56.86 ug/l	345709	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
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	Oxalic acid	90	C2H2O4	000144-62-7	4





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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

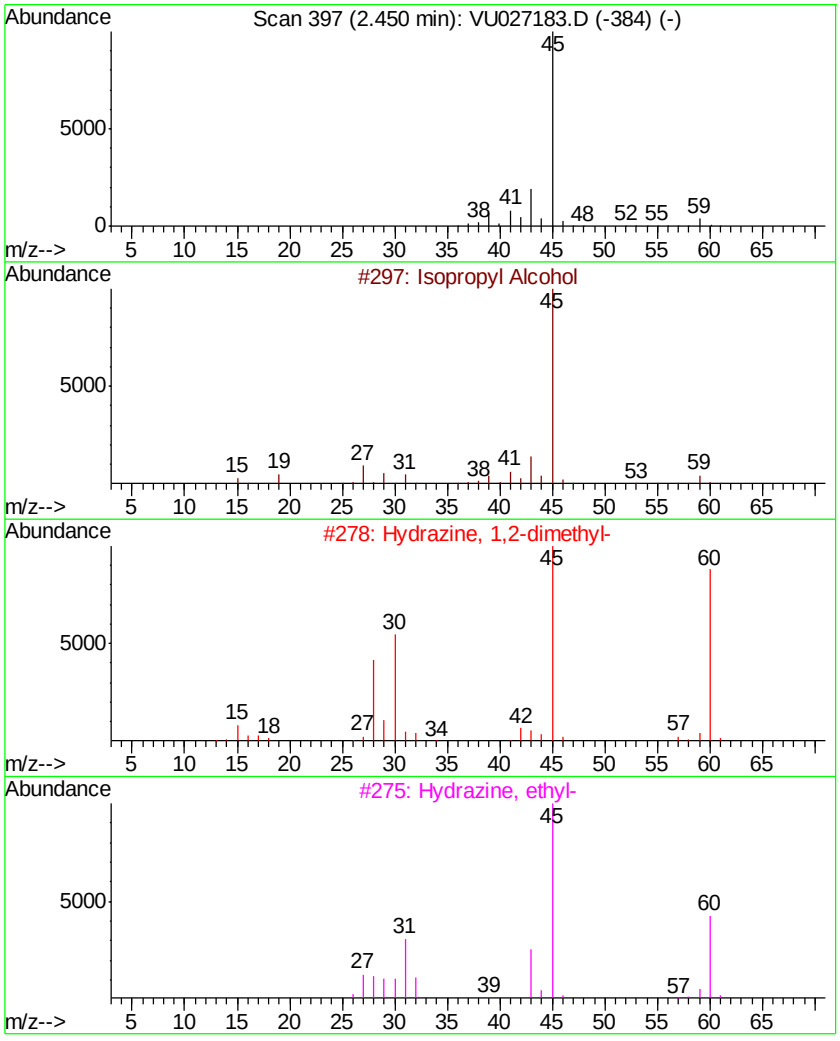
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

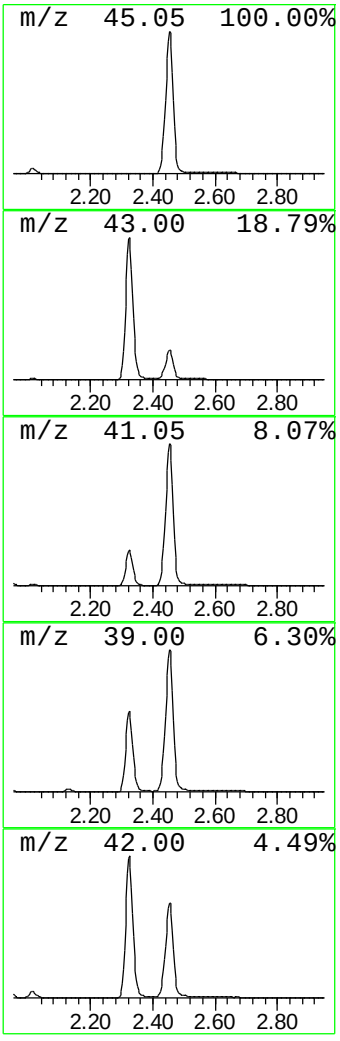
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	1463.45 ug/l	8897690	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4	Formamide	45	CH3NO	000075-12-7	5
5	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4





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Instrument : MSVOA_U
ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

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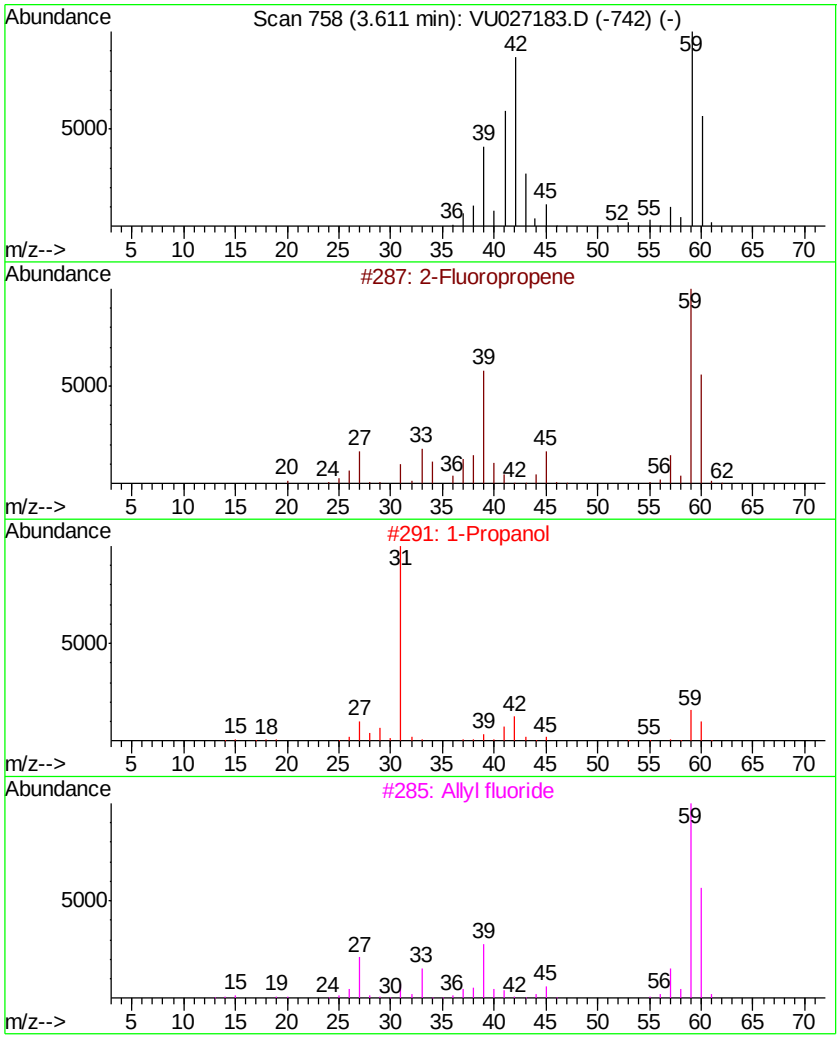
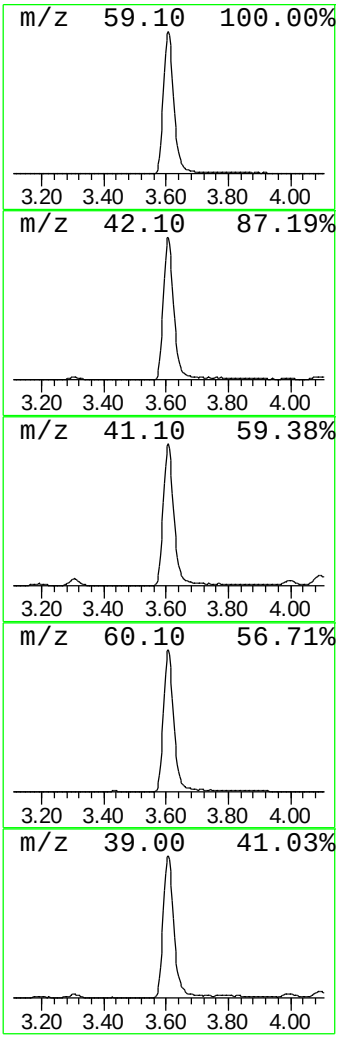
Peak Number 3 2-Fluoropropene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	85.71 ug/l	521140	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluoropropene	60	C3H5F	001184-60-7	62
2	1-Propanol	60	C3H8O	000071-23-8	59
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	25
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	10





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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

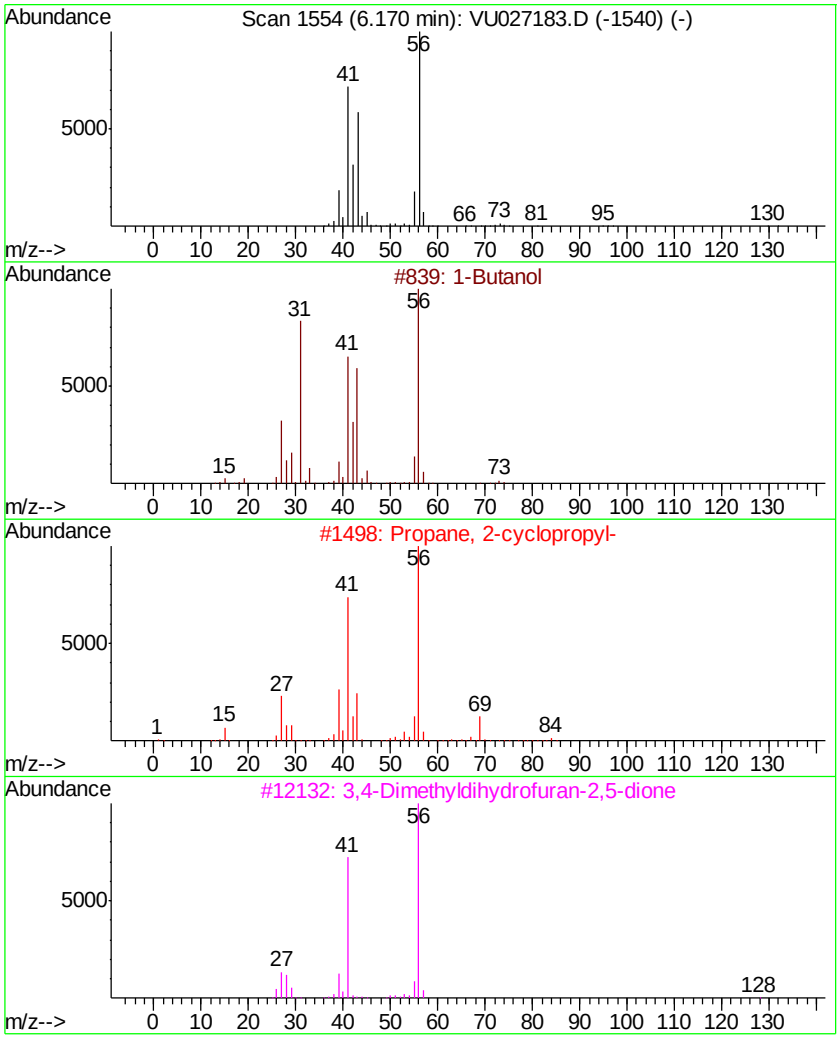
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

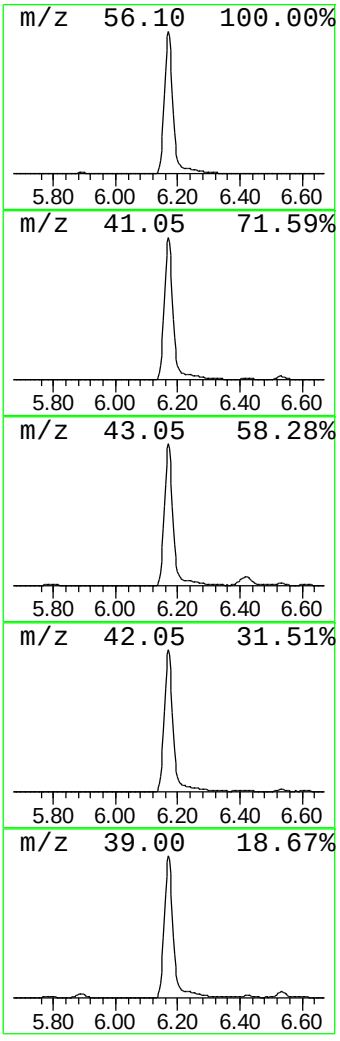
****

Peak Number 4 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.17	261.79 ug/l	2224360	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9





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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

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ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

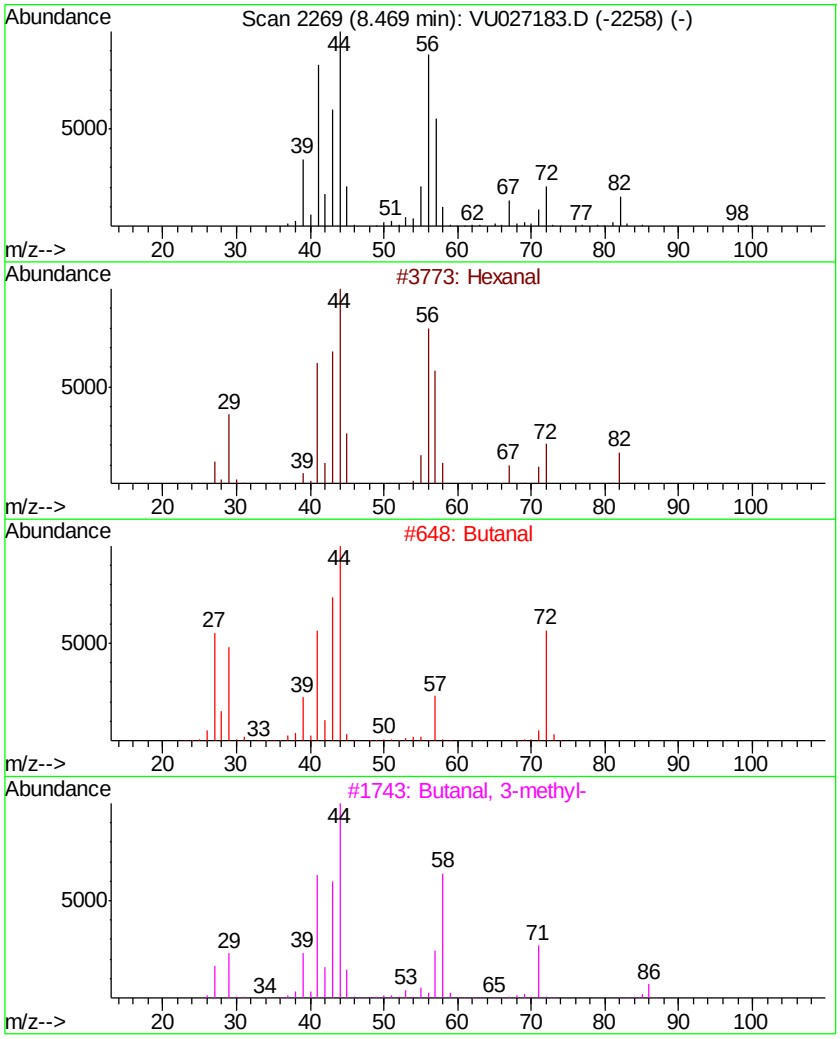
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

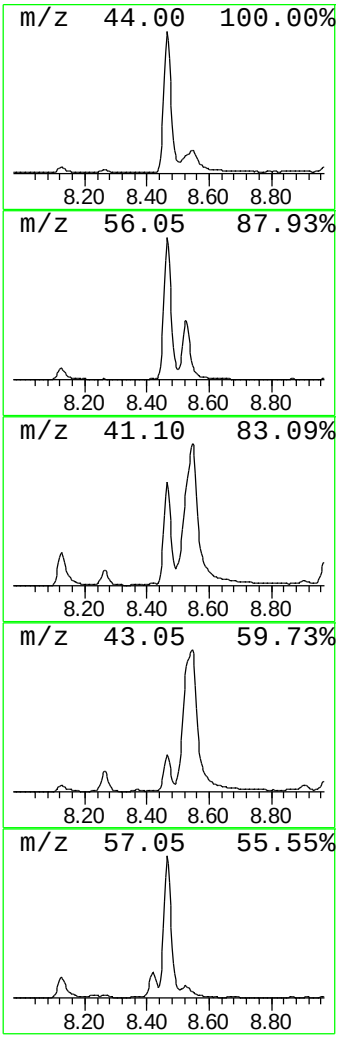
****

Peak Number 5 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	45.53 ug/l	538498	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Butanal	72	C4H8O	000123-72-8	35
3	Butanal, 3-methyl-	86	C5H10O	000590-86-3	32
4	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	27
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	22





Library Search Compound Report

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

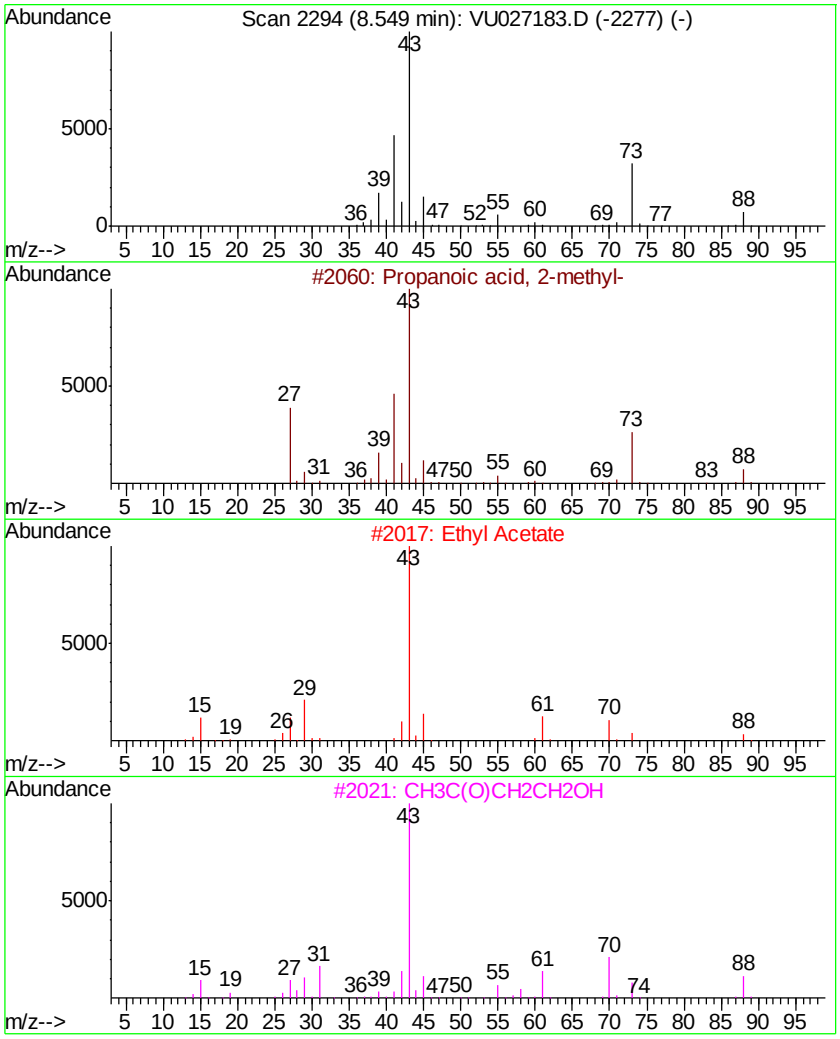
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

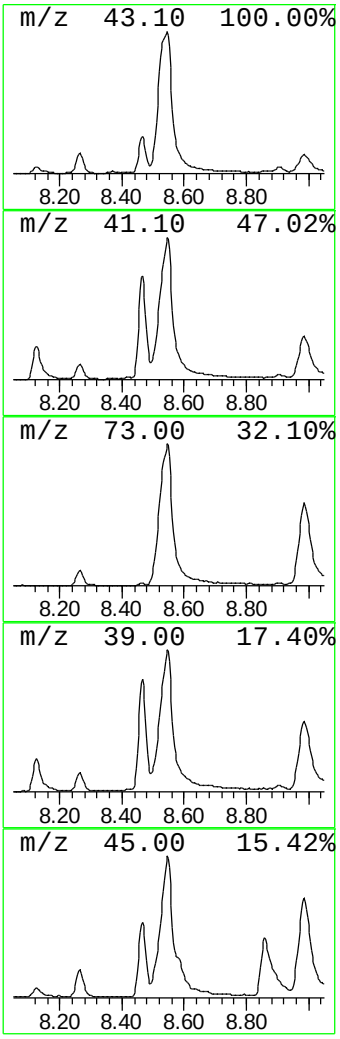
****

Peak Number 6 Propanoic acid, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.55	100.02 ug/l	1182980	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	91
2	Ethyl Acetate	88	C4H8O2	000141-78-6	50
3	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
5	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9





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ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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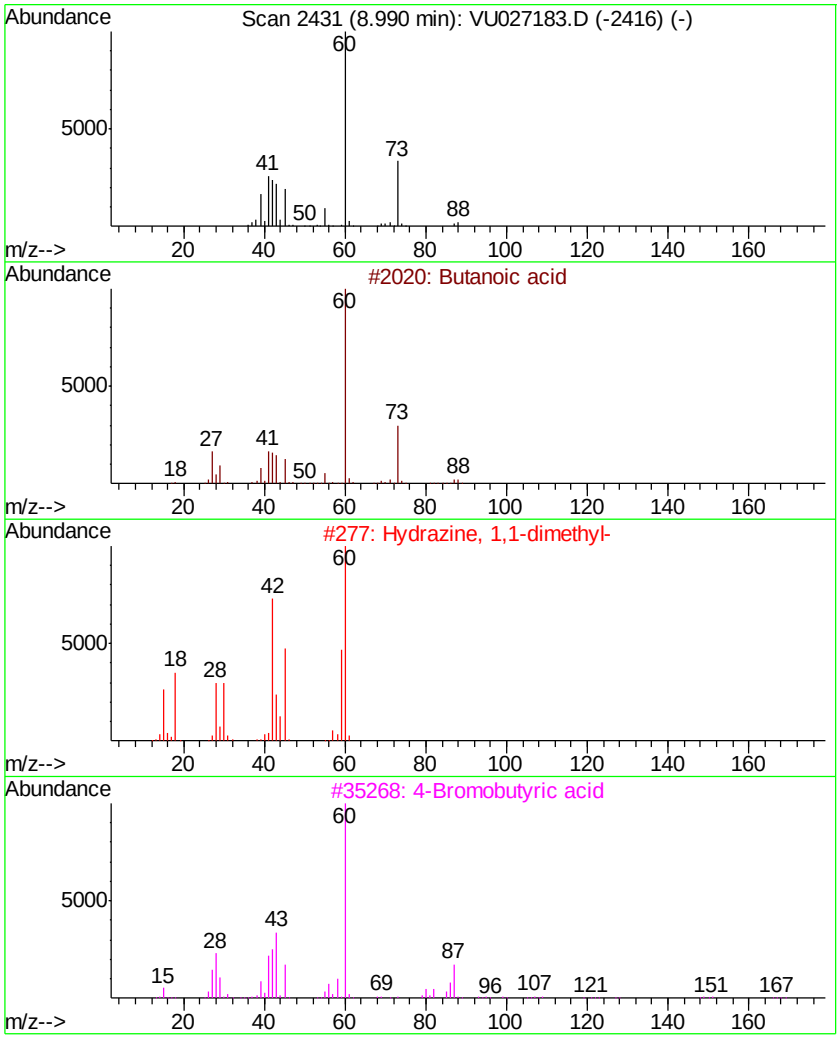
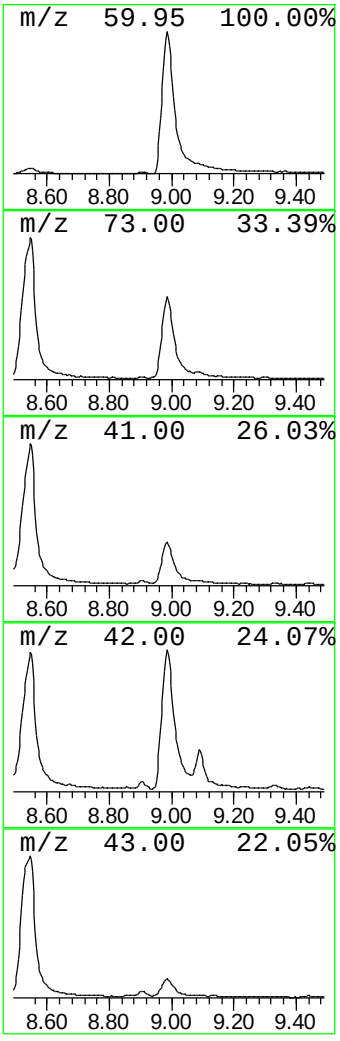
****

Peak Number 7 Butanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.99	48.49 ug/l	573550	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	83
2	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
3	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
4	Benserazide	257	C10H15N3O5	000322-35-0	9
5	Hexanoic acid	116	C6H12O2	000142-62-1	9





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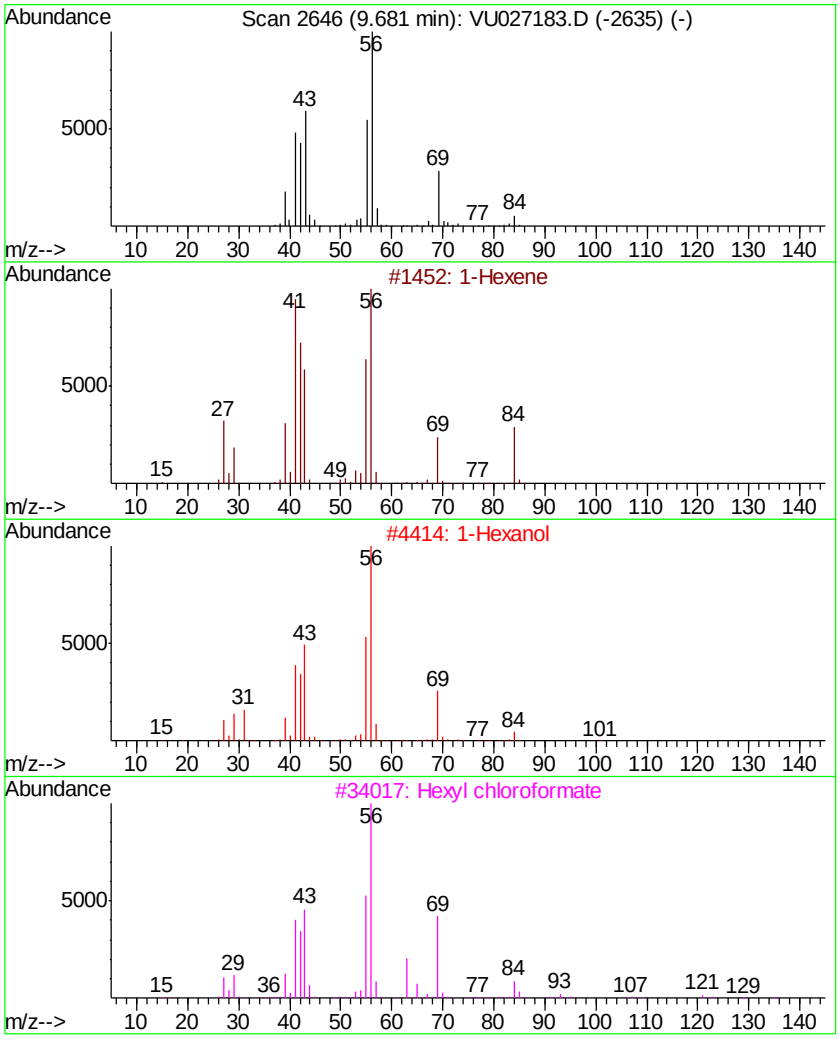
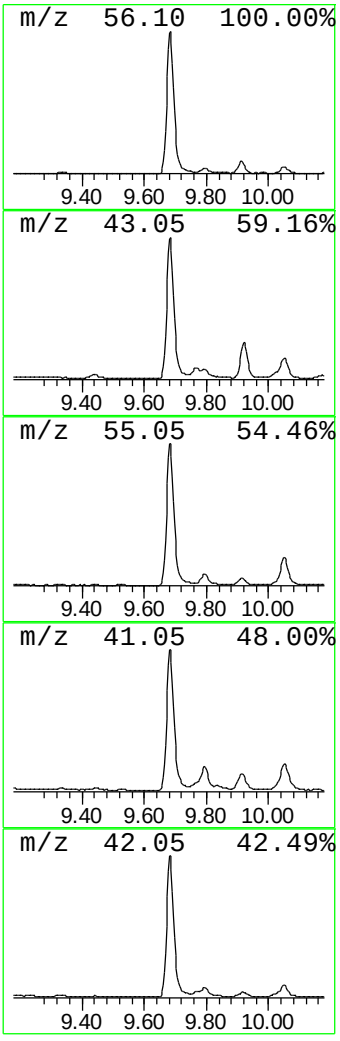
****

Peak Number 8 1-Hexene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.68	53.80 ug/l	636306	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene	84	C6H12	000592-41-6	83
2	1-Hexanol	102	C6H14O	000111-27-3	78
3	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
4	2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	64
5	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64





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Quant Title : SW846 8260

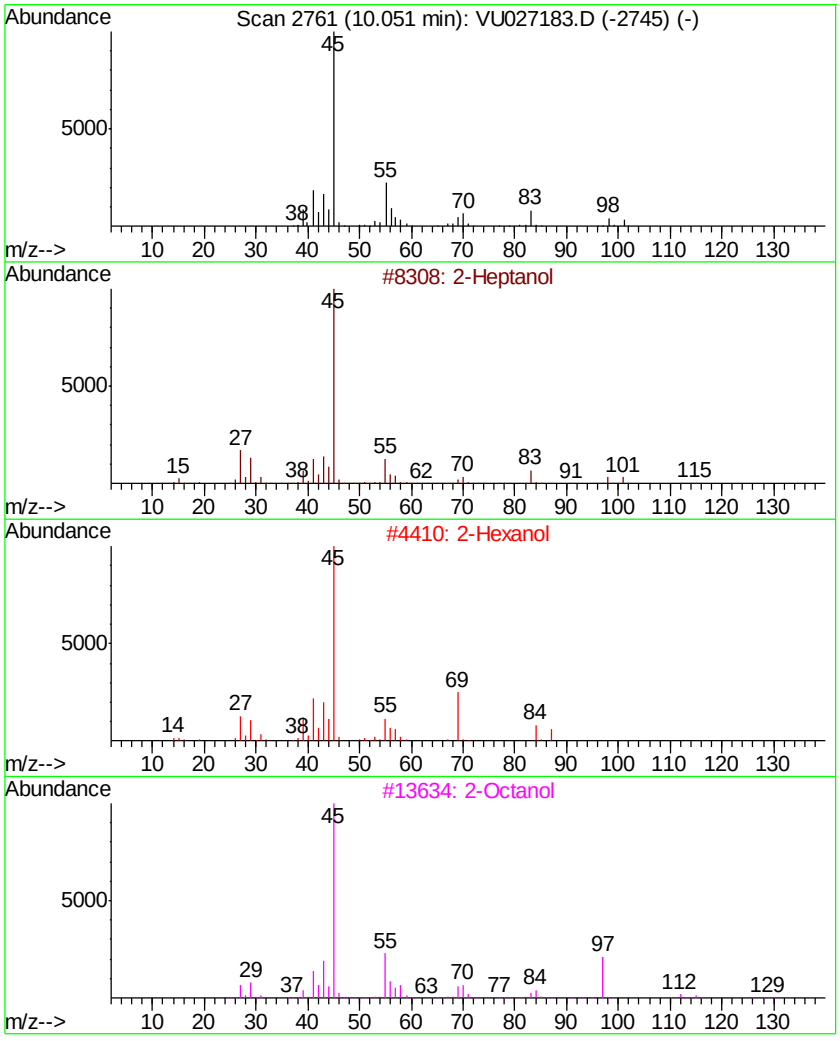
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

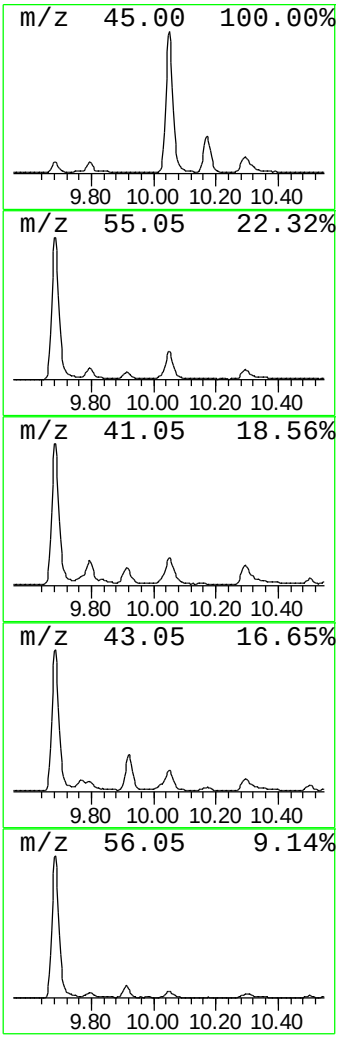
****

Peak Number 9 2-Heptanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	17.84 ug/l	210976	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanol	116	C7H16O	000543-49-7	78
2	2-Hexanol	102	C6H14O	000626-93-7	64
3	2-Octanol	130	C8H18O	000123-96-6	64
4	2-Heptanol, (S)-	116	C7H16O	006033-23-4	64
5	(+-)-5-Methyl-2-hexanol	116	C7H16O	111768-09-3	56





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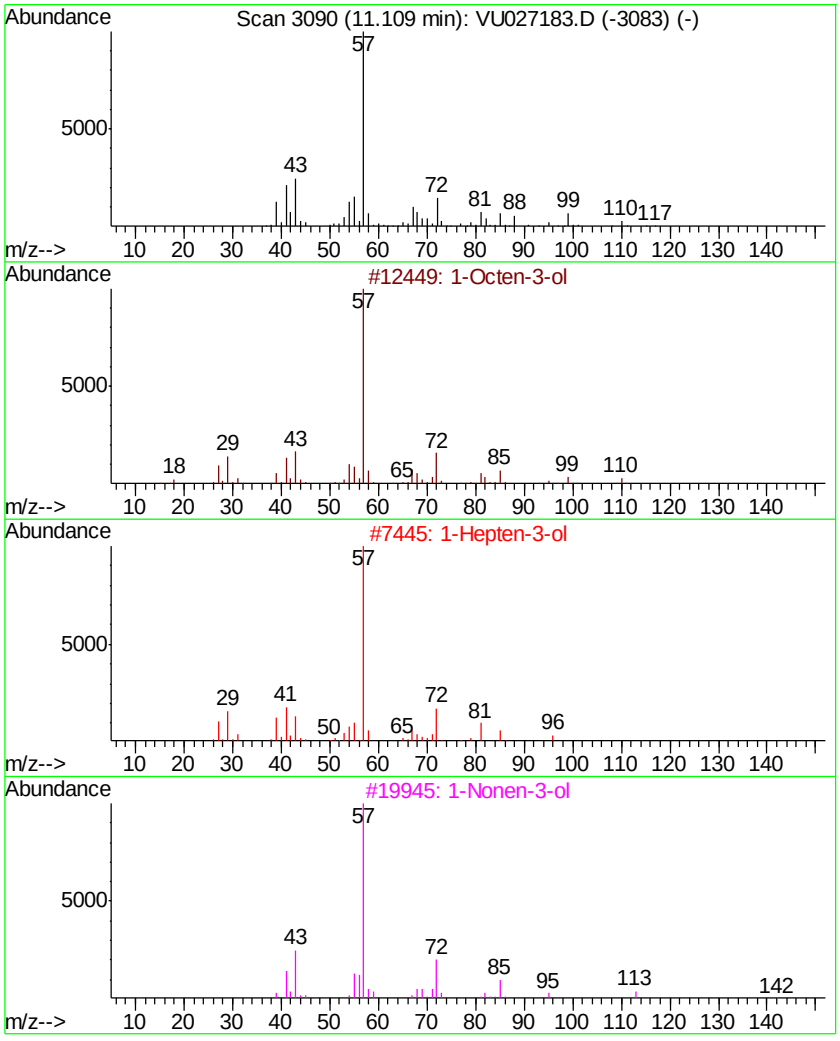
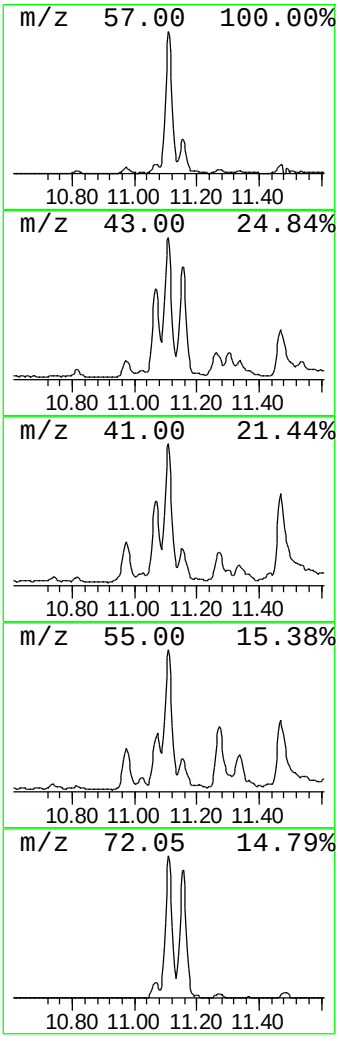
****

Peak Number 10 1-Octen-3-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.11	19.90 ug/l	304977	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octen-3-ol	128	C8H16O	003391-86-4	78
2	1-Hepten-3-ol	114	C7H14O	004938-52-7	59
3	1-Nonen-3-ol	142	C9H18O	021964-44-3	38
4	6-Oxa-bicyclo[3.1.0]hexan-3-ol	100	C5H8O2	025494-14-8	27
5	1-Hexen-3-ol	100	C6H12O	004798-44-1	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092618\
Data File : VU027183.D
Acq On : 26 Sep 2018 17:24
Operator : MD/SY
Sample : J5049-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-53-SEP19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
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
Ethanol	2.01	56.9	ug/l	345709	1	4.99	303997	50.0
Isopropyl Alcohol	2.45	1463.5	ug/l	8897690	1	4.99	303997	50.0
2-Fluoropropene	3.61	85.7	ug/l	521140	1	4.99	303997	50.0
1-Butanol	6.17	261.8	ug/l	2224360	2	5.89	424836	50.0
Hexanal	8.47	45.5	ug/l	538498	3	9.09	591359	50.0
Propanoic acid, 2...	8.55	100.0	ug/l	1182980	3	9.09	591359	50.0
Butanoic acid	8.99	48.5	ug/l	573550	3	9.09	591359	50.0
1-Hexene	9.68	53.8	ug/l	636306	3	9.09	591359	50.0
2-Heptanol	10.05	17.8	ug/l	210976	3	9.09	591359	50.0
1-Octen-3-ol	11.11	19.9	ug/l	304977	4	11.48	766418	50.0