LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092618\
Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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	2.135	249	299	306	rBV2	19913794	117329962	100.00%	23.390%
2	2.338	352	362	389	rVB	1981311	3881473	3.31%	0.774%
3	2.534	390	423	523	rVB2	25074223	88940414	75.80%	17.730%
4	3.807	745	819	869	rBV	7834495	57244065	48.79%	11.412%
5	4.235	934	952	987	rBV	536878	1465408	1.25%	0.292%
6	4.399	988	1003	1036	rVB	563008	1276155	1.09%	0.254%
7	5.399	1294	1314	1355	rVB	3485031	9383855	8.00%	1.871%
8	6.296	1535	1593	1626	rBV	18641963	88762701	75.65%	17.695%
9	6.620	1681	1694	1714	rVB	721118	1338973	1.14%	0.267%
10	8.167	2153	2175	2185	rBV	11938108	25811681	22.00%	5.146%
11	8.228	2185	2194	2200	rVV	1209669	2111562	1.80%	0.421%
12	8.273	2200	2208	2234	rVB	2124169	3486561	2.97%	0.695%
13	8.472	2260	2270	2282	rVV	5223246	8577119	7.31%	1.710%
14	8.649	2283	2325	2375	rVB	1379390	7125385	6.07%	1.420%
15	9.128	2428	2474	2505	rBV2	1917008	9181985	7.83%	1.830%
16	9.710	2637	2655	2666	rBV	14462345	25811085	22.00%	5.145%
17	9.771	2666	2674	2677	rVV	827126	1184013	1.01%	0.236%
18	9.800	2678	2683	2692	rVV	1542824	2247299	1.92%	0.448%
19	10.315	2830	2843	2846	rBV	757620	1234352	1.05%	0.246%
20	11.032	3055	3066	3074	rBV	6257676	9217235	7.86%	1.837%
21	11.106	3074	3089	3100	rVB4	2112343	4746600	4.05%	0.946%
22	11.533	3195	3222	3270	rBV2	2391757	8061568	6.87%	1.607%
23	12.225	3425	3437	3442	rBV4	1907492	3339216	2.85%	0.666%
24	12.279	3448	3454	3475	rVB	2562932	3696347	3.15%	0.737%
25	12.578	3533	3547	3565	rBV	1129608	2307836	1.97%	0.460%
26	13.305	3761	3773	3776	rBV2	1625610	2207391	1.88%	0.440%
27	13.353	3784	3788	3809	rVB	2475764	3240055	2.76%	0.646%
28	14.302	4070	4083	4087	rBV2	2129556	3207358	2.73%	0.639%
29	14.328	4088	4091	4107	rVB2	1893366	2292947	1.95%	0.457%
30	15.234	4360	4373	4406	rVB4	1767370	2919752	2.49%	0.582%

Sum of corrected areas: 501630353

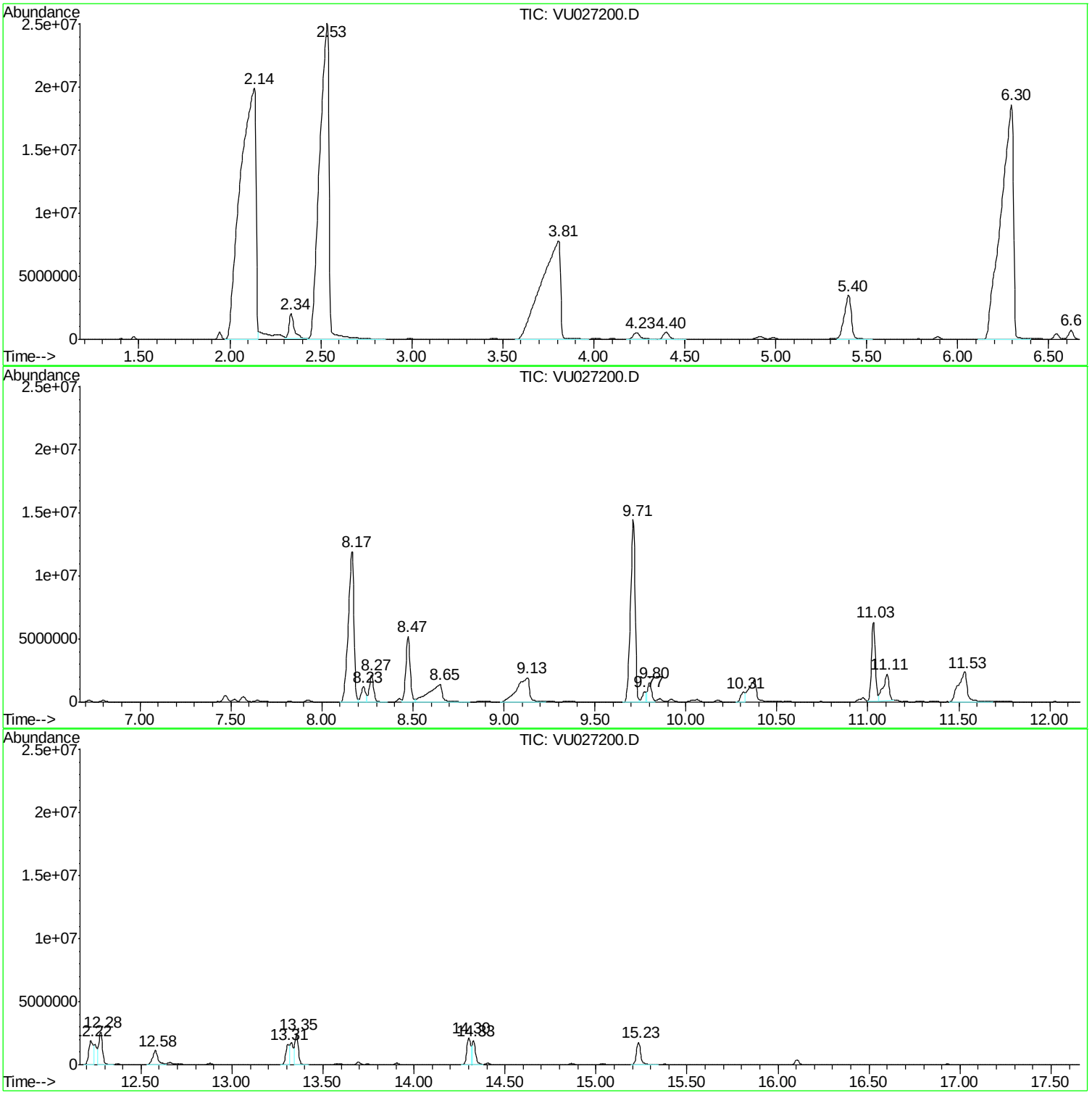
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092618\
Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092618\
Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
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ALS Vial : 41 Sample Multiplier: 1

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

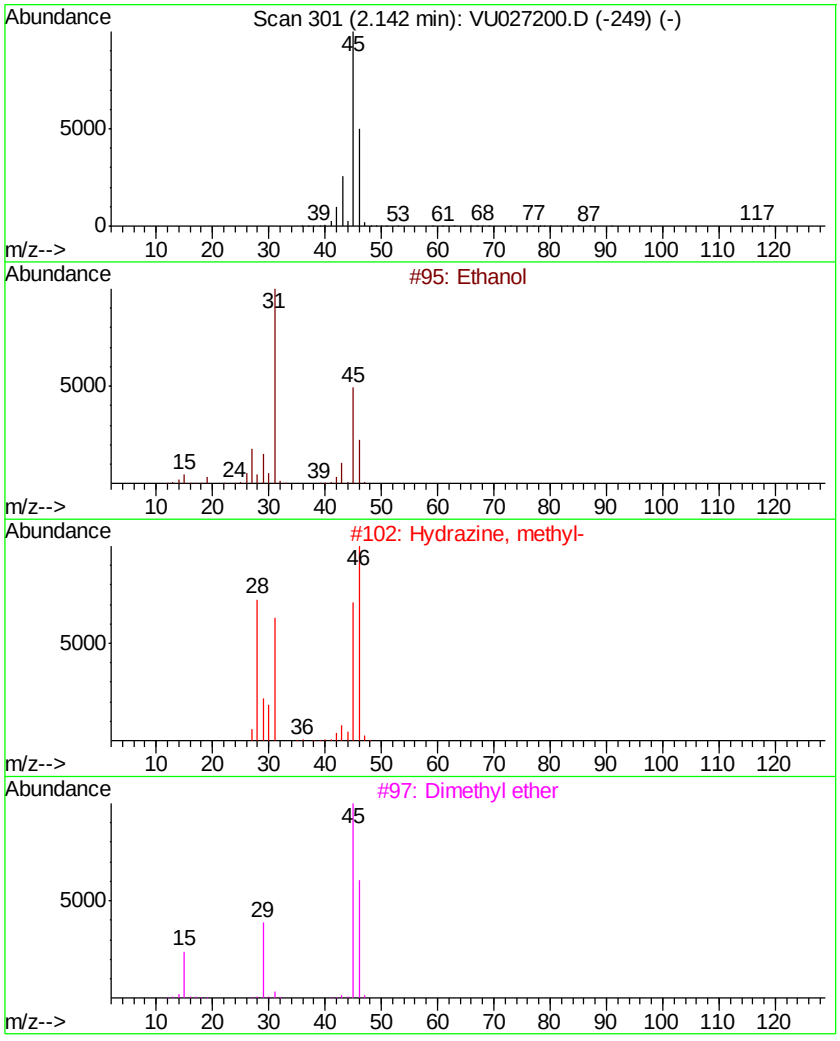
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

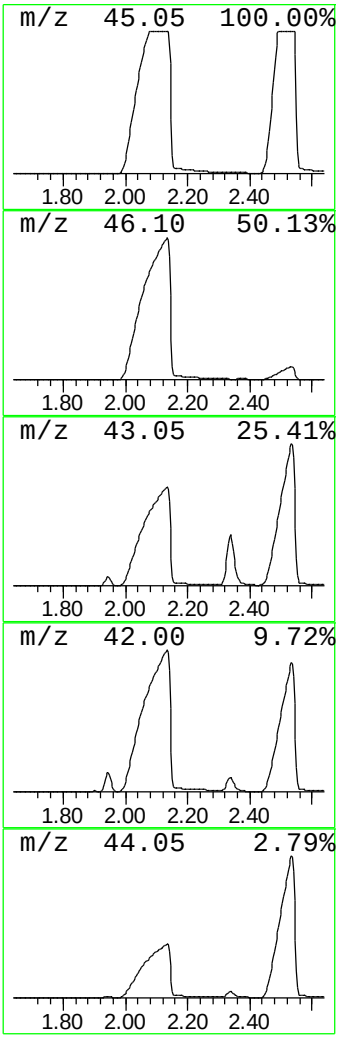
****

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	625.17 ug/l	117330000	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	78
2	Hydrazine, methyl-	46	CH6N2	000060-34-4	9
3	Dimethyl ether	46	C2H6O	000115-10-6	9
4	Methane, nitroso-	45	CH3NO	000865-40-7	4
5	Ethene, fluoro-	46	C2H3F	000075-02-5	4





Library Search Compound Report

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Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

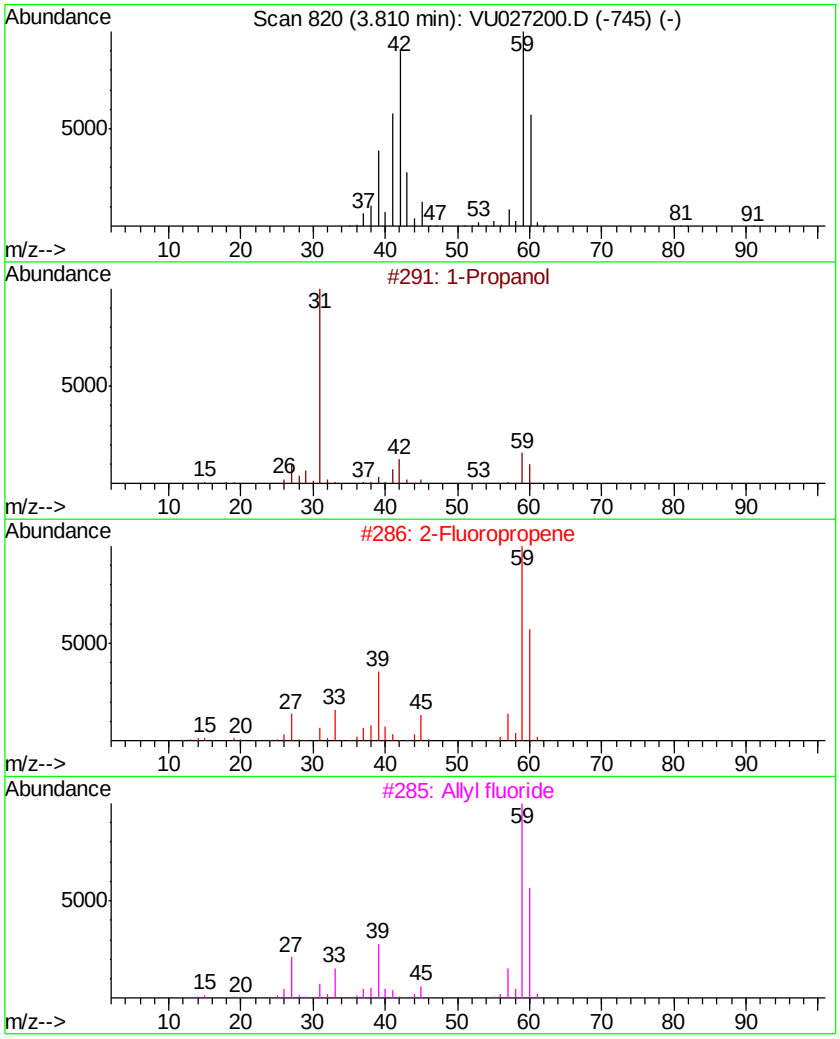
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

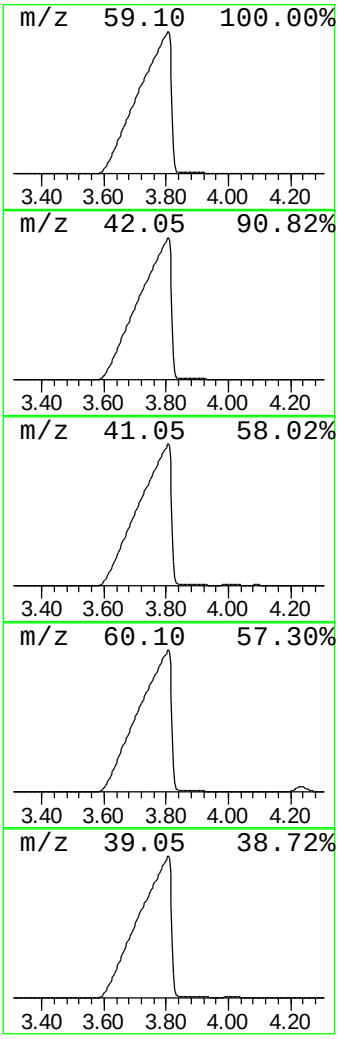
****

Peak Number 3 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.81	305.01 ug/l	57244100	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	2-Fluoropropene	60	C3H5F	001184-60-7	47
3	Allyl fluoride	60	C3H5F	000818-92-8	32
4	Cyclopropane	42	C3H6	000075-19-4	9
5	Propene	42	C3H6	000115-07-1	9





Library Search Compound Report

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Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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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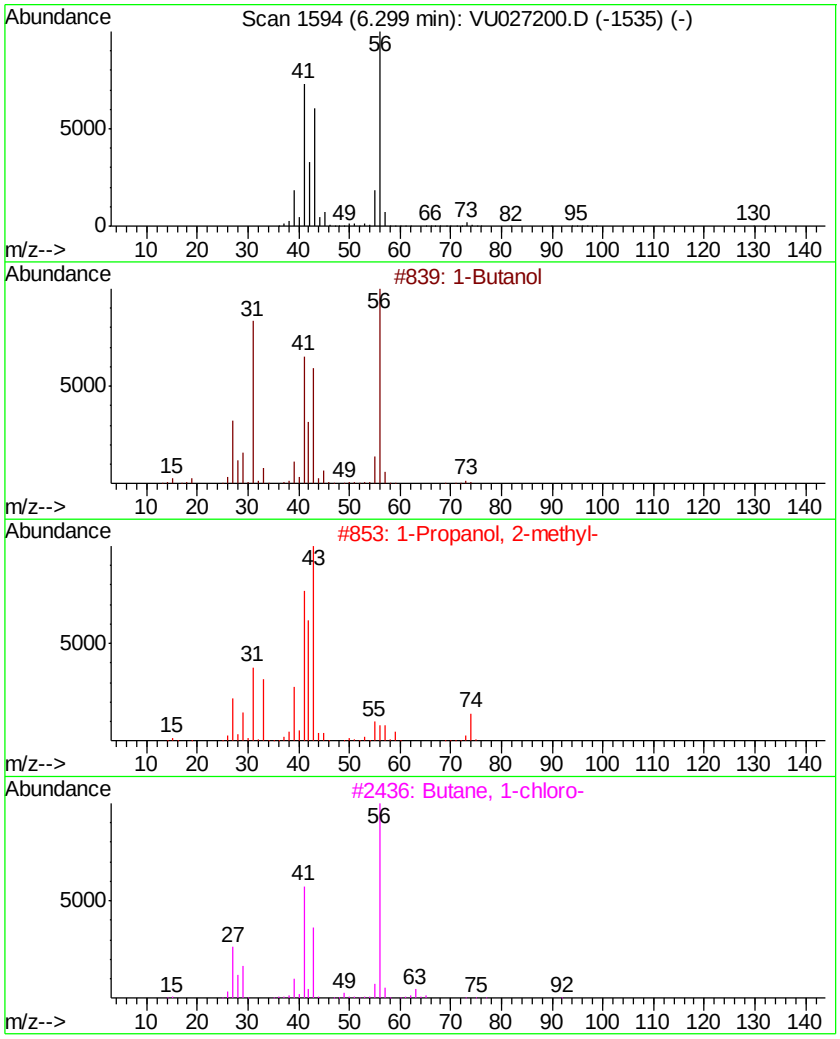
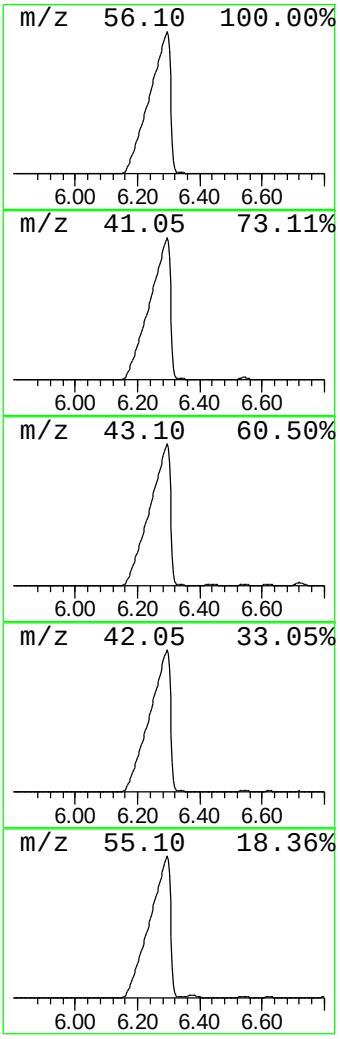
Peak Number 4 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.30	50.00 ug/l	88762700	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	12
3	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092618\
Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

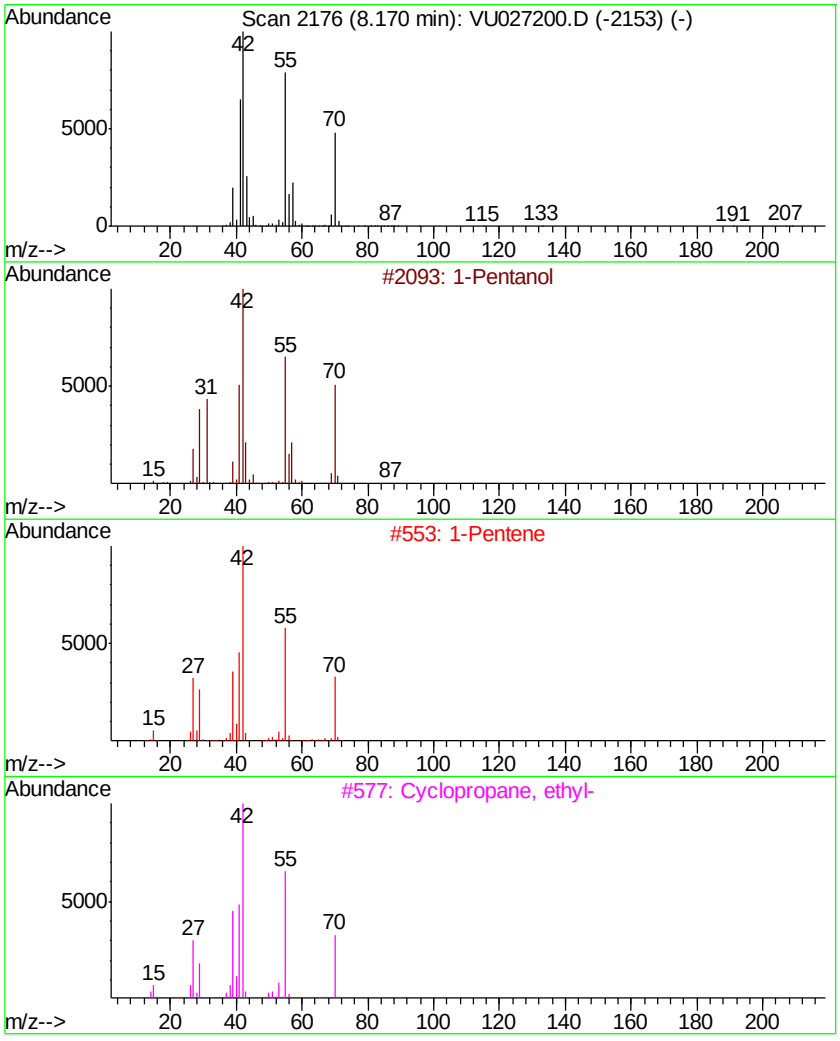
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

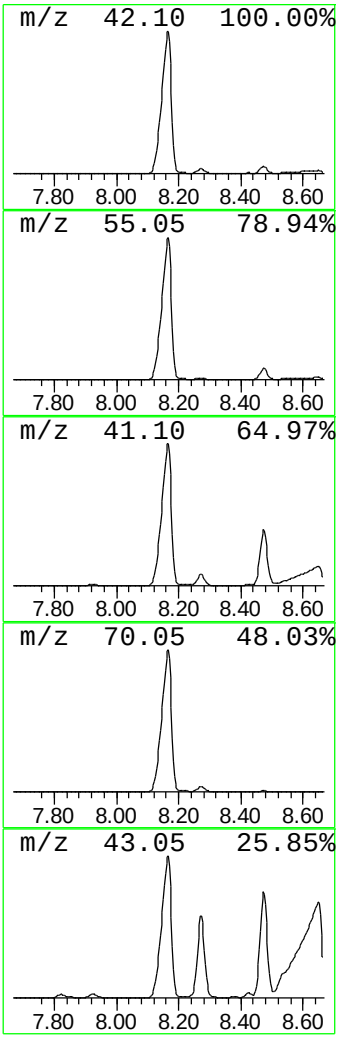
****

Peak Number 5 1-Pentanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	140.56 ug/l	25811700	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	1-Pentene	70	C5H10	000109-67-1	72
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
4	Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	43
5	Formic acid, pentyl ester	116	C6H12O2	000638-49-3	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092618\
Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

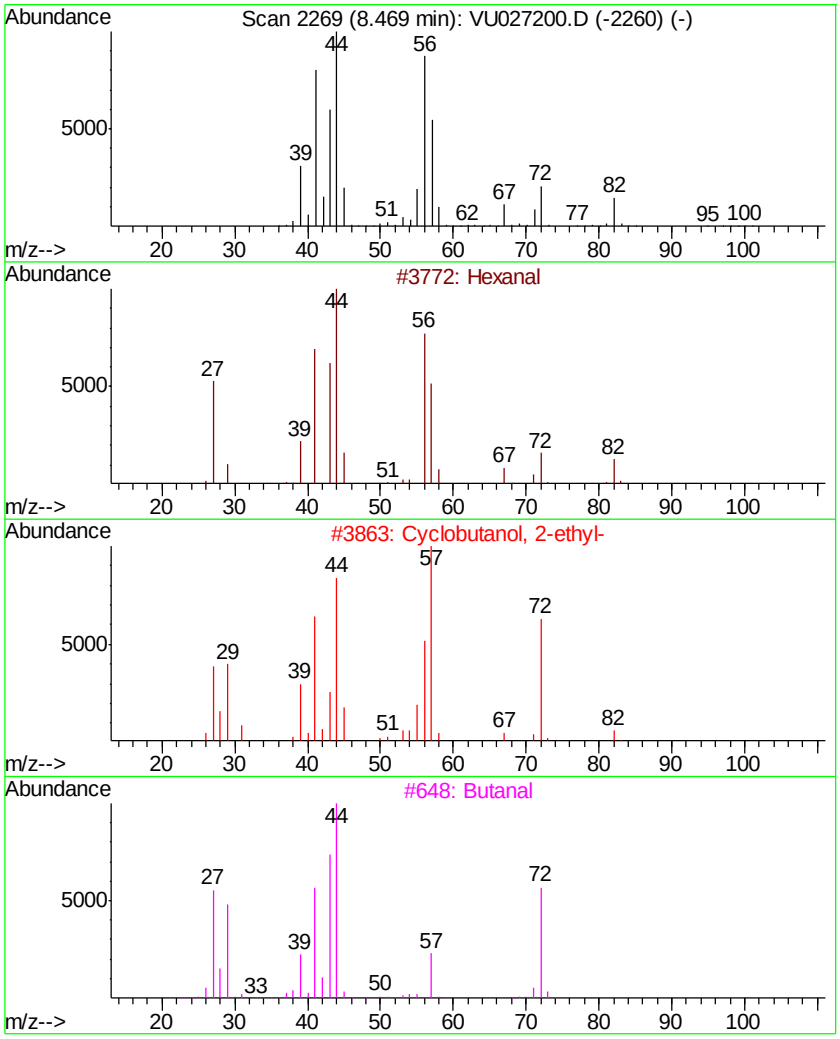
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

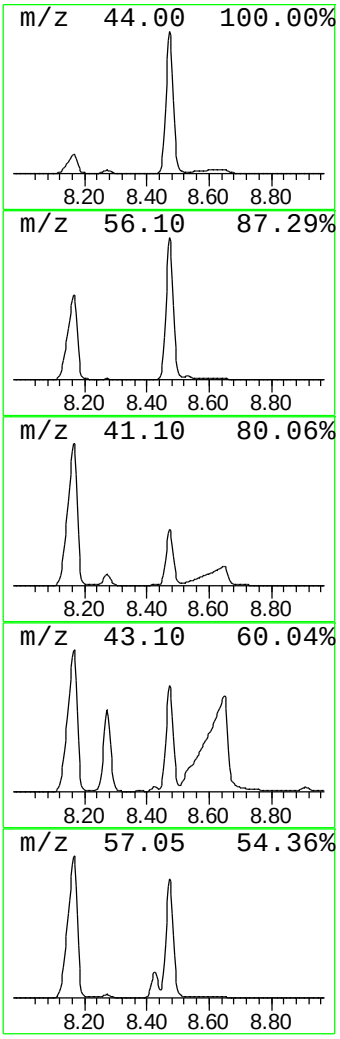
****

Peak Number 6 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	46.71 ug/l	8577120	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	36
3	Butanal	72	C4H8O	000123-72-8	35
4	Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	32
5	Butanal, 3-methyl-	86	C5H10O	000590-86-3	32





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092618\
Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

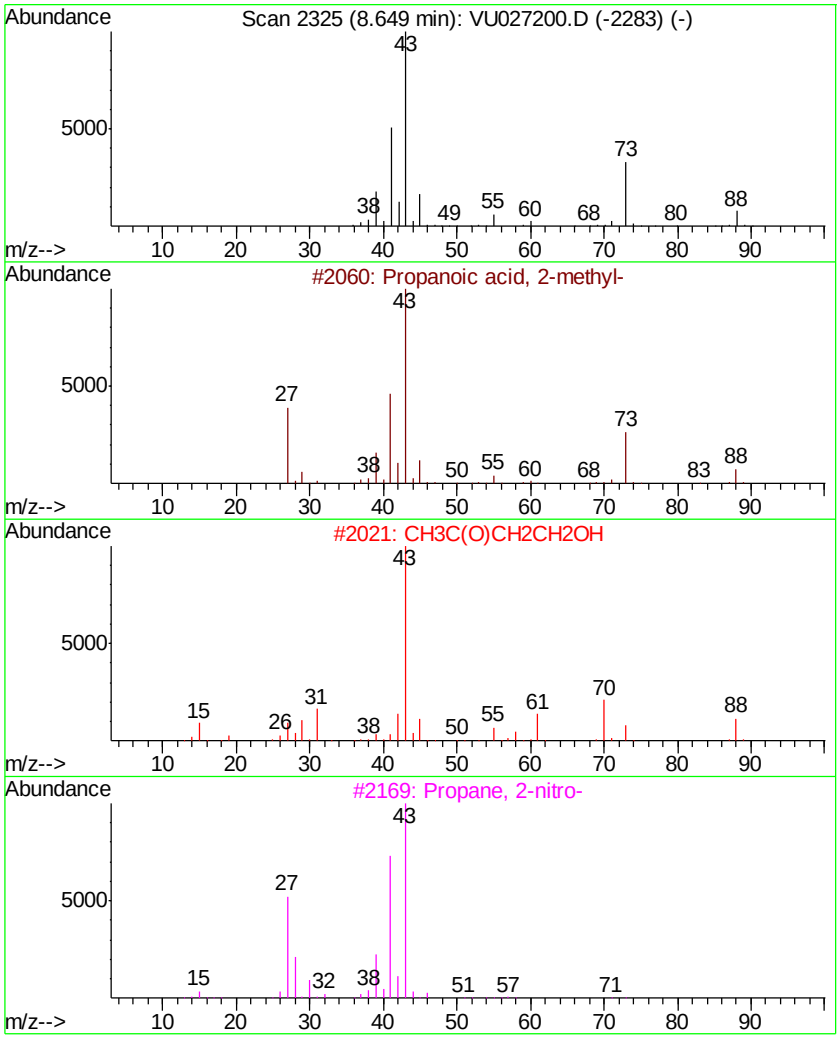
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

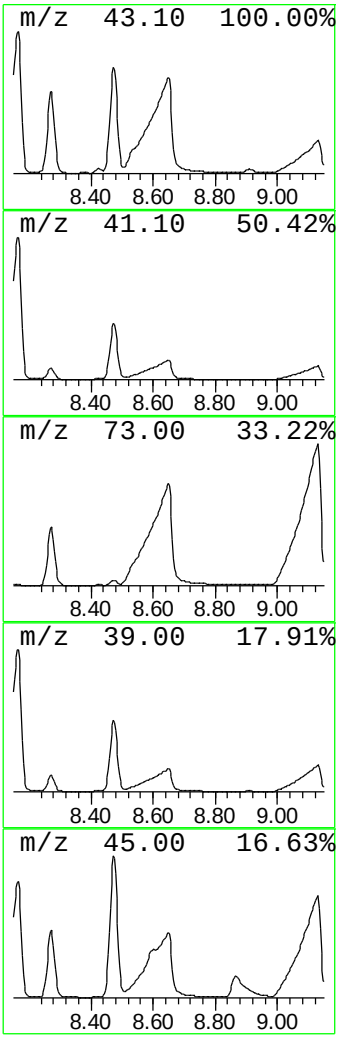
****

Peak Number 7 Propanoic acid, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	38.80 ug/l	7125390	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	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9
3	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
4	Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	9
5	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9





Library Search Compound Report

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Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

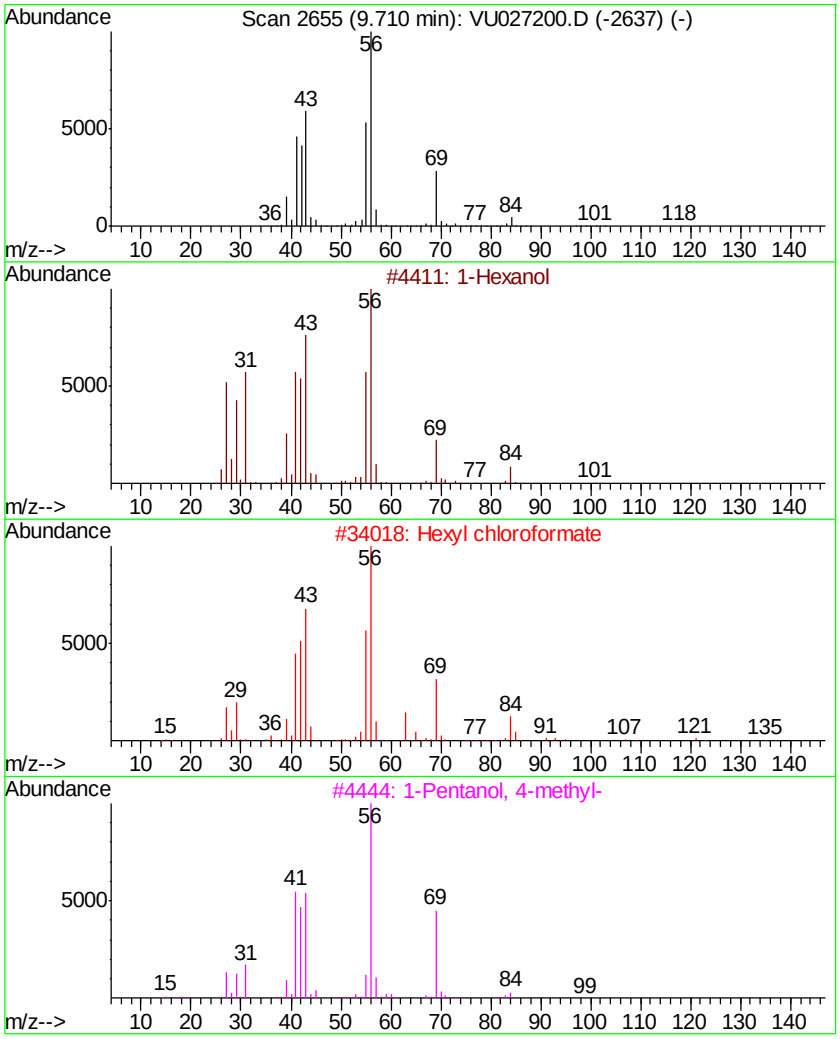
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

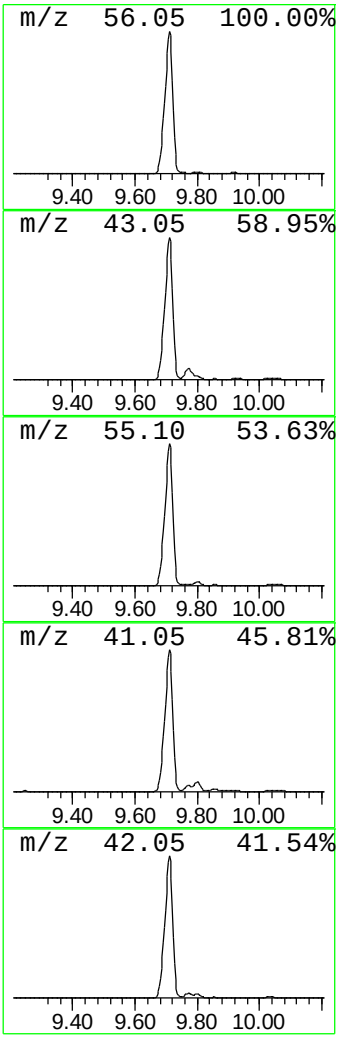
****

Peak Number 8 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.71	140.55 ug/l	25811100	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	83
3	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	56
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	42





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ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

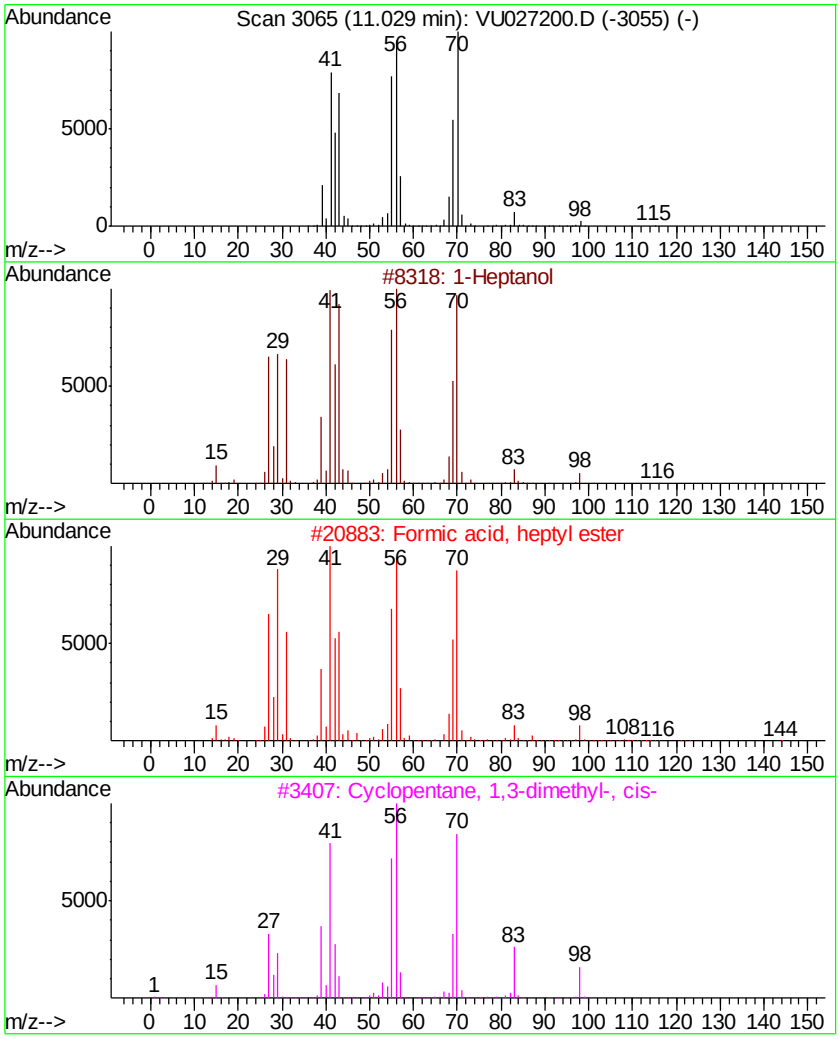
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

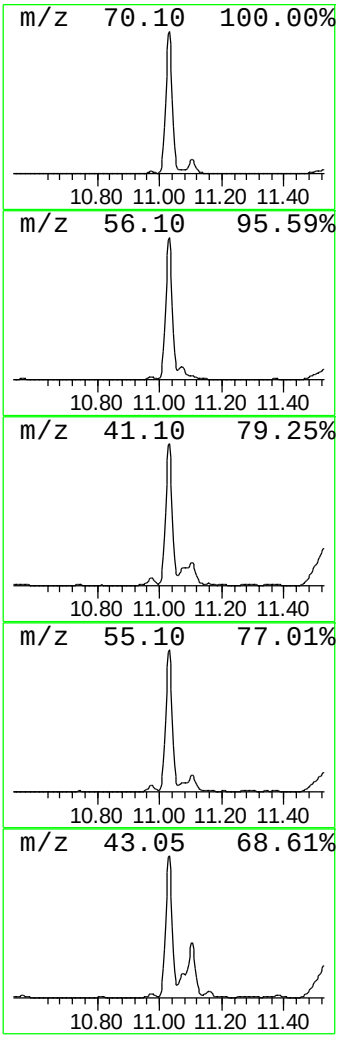
****

Peak Number 9 1-Heptanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.03	57.17 ug/l	9217240	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol	116	C7H16O	000111-70-6	90
2	Formic acid, heptyl ester	144	C8H16O2	000112-23-2	74
3	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	72
4	Cyclobutanone, 2,2-dimethyl-	98	C6H10O	001192-14-9	72
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	64





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Data File : VU027200.D
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Operator : MD/SY
Sample : J5048-03
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ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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

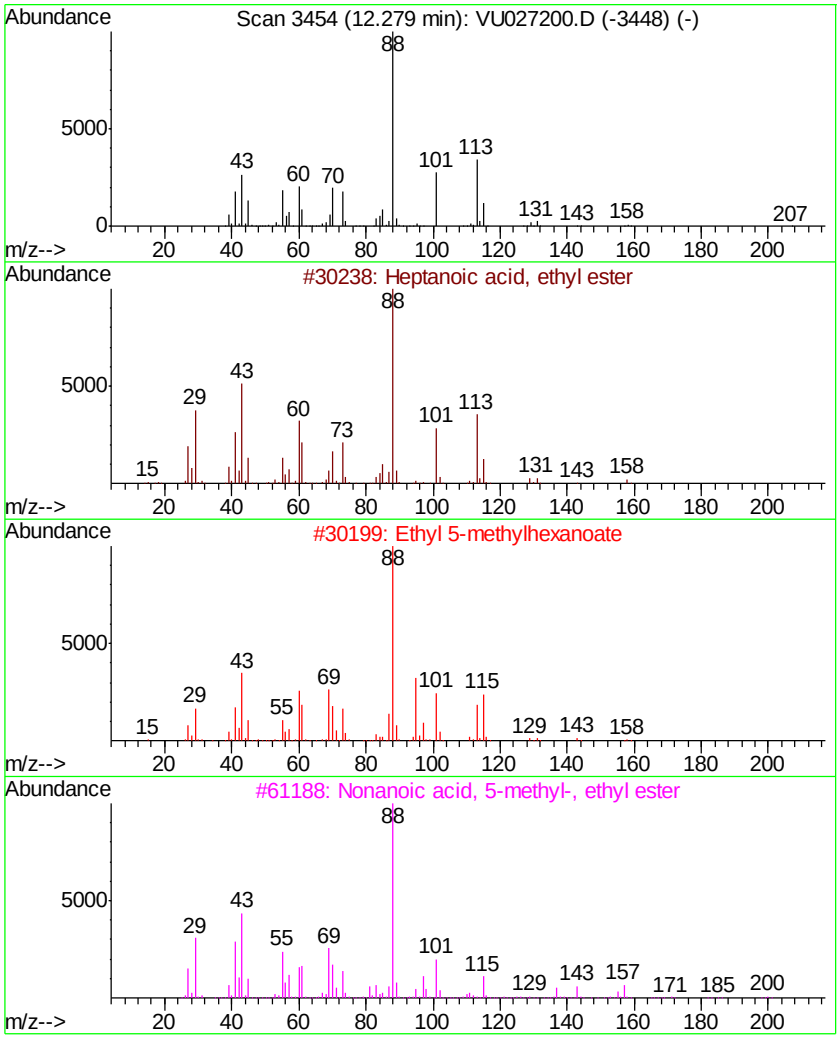
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

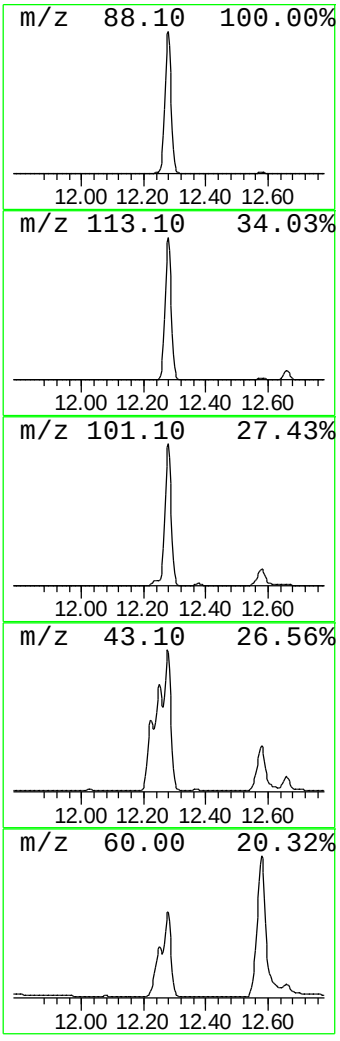
****

Peak Number 10 Heptanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	22.93 ug/l	3696350	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	90
2	Ethyl 5-methylhexanoate	158	C9H18O2	010236-10-9	56
3	Nonanoic acid, 5-methyl-, ethyl ...	200	C12H24O2	116530-40-6	50
4	Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	45
5	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092618\
Data File : VU027200.D
Acq On : 27 Sep 2018 00:47
Operator : MD/SY
Sample : J5048-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MW-57-SEP18

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	2.14	625.2	ug/l	117330000	1	4.99	9383860	50.0
1-Propanol	3.81	305.0	ug/l	57244100	1	4.99	9383860	50.0
1-Butanol	6.30	50.0	ug/l	88762700	2	5.89	88762700	50.0
1-Pentanol	8.17	140.6	ug/l	25811700	3	9.09	9181990	50.0
Hexanal	8.47	46.7	ug/l	8577120	3	9.09	9181990	50.0
Propanoic acid, 2...	8.65	38.8	ug/l	7125390	3	9.09	9181990	50.0
1-Hexanol	9.71	140.6	ug/l	25811100	3	9.09	9181990	50.0
1-Heptanol	11.03	57.2	ug/l	9217240	4	11.49	8061570	50.0
Heptanoic acid, e...	12.28	22.9	ug/l	3696350	4	11.49	8061570	50.0