LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

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\82U120618W.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	1.302	33	40	46	rBV2	6920	7451	1.27%	0.145%
2	1.399	60	70	79	rVB3	12325	18191	3.10%	0.354%
3	1.473	84	93	104	rBV	39501	45154	7.70%	0.879%
4	1.572	114	124	135	rVB6	5837	10567	1.80%	0.206%
5	2.013	252	261	273	rVB	15760	23064	3.93%	0.449%
6	2.244	322	333	345	rBB	11027	17475	2.98%	0.340%
7	2.322	345	357	370	rBV	46769	74058	12.63%	1.441%
8	2.444	383	395	410	rBV	38868	68289	11.64%	1.329%
9	2.614	436	448	467	rBV	73120	124824	21.28%	2.429%
10	2.826	498	514	533	rBV3	18000	39605	6.75%	0.771%
11	3.186	614	626	638	rBV2	3000	6700	1.14%	0.130%
12	3.604	745	756	782	rBV2	28033	70399	12.00%	1.370%
13	3.984	859	874	901	rBV	95381	239491	40.83%	4.661%
14	4.196	925	940	952	rBV2	4554	12961	2.21%	0.252%
15	4.267	952	962	987	rVV2	11832	30094	5.13%	0.586%
16	4.389	990	1000	1016	rVB3	3295	7401	1.26%	0.144%
17	4.881	1138	1153	1170	rBV	70726	157036	26.77%	3.056%
18	4.981	1171	1184	1205	rVB2	107334	236390	40.30%	4.601%
19	5.309	1271	1286	1298	rBV	84494	179465	30.60%	3.493%
20	5.389	1299	1311	1331	rVB	86230	185003	31.54%	3.601%
21	5.884	1449	1465	1487	rBV	180081	348751	59.46%	6.788%
22	6.170	1544	1554	1579	rBV2	29822	65491	11.17%	1.275%
23	6.530	1653	1666	1675	rBV4	5026	11001	1.88%	0.214%
24	6.704	1706	1720	1750	rBV	328117	586562	100.00%	11.416%
25	7.463	1944	1956	1967	rBV2	9610	16981	2.90%	0.330%
26	7.562	1974	1987	2000	rBV	282668	490885	83.69%	9.554%
27	7.636	2000	2010	2029	rVB	86728	154956	26.42%	3.016%
28	8.132	2152	2164	2177	rBV3	5735	11815	2.01%	0.230%
29	8.463	2256	2267	2276	rBV6	10141	25603	4.36%	0.498%
30	8.521	2276	2285	2305	rVB	90890	146168	24.92%	2.845%
31	9.087	2447	2461	2481	rBV	243665	402682	68.65%	7.837%
32	9.173	2481	2488	2503	rVV3	11067	20538	3.50%	0.400%
33	9.247	2503	2511	2522	rVB2	6844	9670	1.65%	0.188%
34	9.373	2539	2550	2565	rBV	35275	57615	9.82%	1.121%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

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\82U120618W.M
Title : SW846 8260

35	9.604	2610	2622	2634	rBV3	3917	6549	1.12%	0.127%
36	9.781	2659	2677	2696	rBV7	18012	36680	6.25%	0.714%
37	9.897	2703	2713	2733	rBV3	17108	41845	7.13%	0.814%
38	10.305	2829	2840	2854	rBV	186294	290251	49.48%	5.649%
39	10.369	2854	2860	2869	rVB4	5037	7538	1.29%	0.147%
40	10.588	2913	2928	2936	rBV2	3515	6661	1.14%	0.130%
41	10.678	2945	2956	2963	rBV	16155	26227	4.47%	0.510%
42	10.771	2975	2985	3001	rVB3	9595	14329	2.44%	0.279%
43	10.916	3016	3030	3037	rBV4	7269	11732	2.00%	0.228%
44	10.967	3037	3046	3062	rVV4	12441	25551	4.36%	0.497%
45	11.064	3066	3076	3091	rBV	34231	50594	8.63%	0.985%
46	11.148	3091	3102	3115	rVB2	33292	51168	8.72%	0.996%
47	11.215	3115	3123	3130	rBV2	7686	12169	2.07%	0.237%
48	11.263	3131	3138	3141	rVV3	7463	10860	1.85%	0.211%
49	11.292	3141	3147	3162	rVB	18108	30460	5.19%	0.593%
50	11.440	3180	3193	3196	rBV6	7653	11414	1.95%	0.222%
51	11.482	3196	3206	3225	rVV	217727	344345	58.71%	6.702%
52	11.569	3226	3233	3246	rVB	8615	12309	2.10%	0.240%
53	11.742	3274	3287	3313	rBV	123544	215206	36.69%	4.188%
54	11.858	3316	3323	3337	rVB9	4499	9970	1.70%	0.194%
55	11.980	3351	3361	3369	rBV	13066	19860	3.39%	0.387%

Sum of corrected areas: 5138054

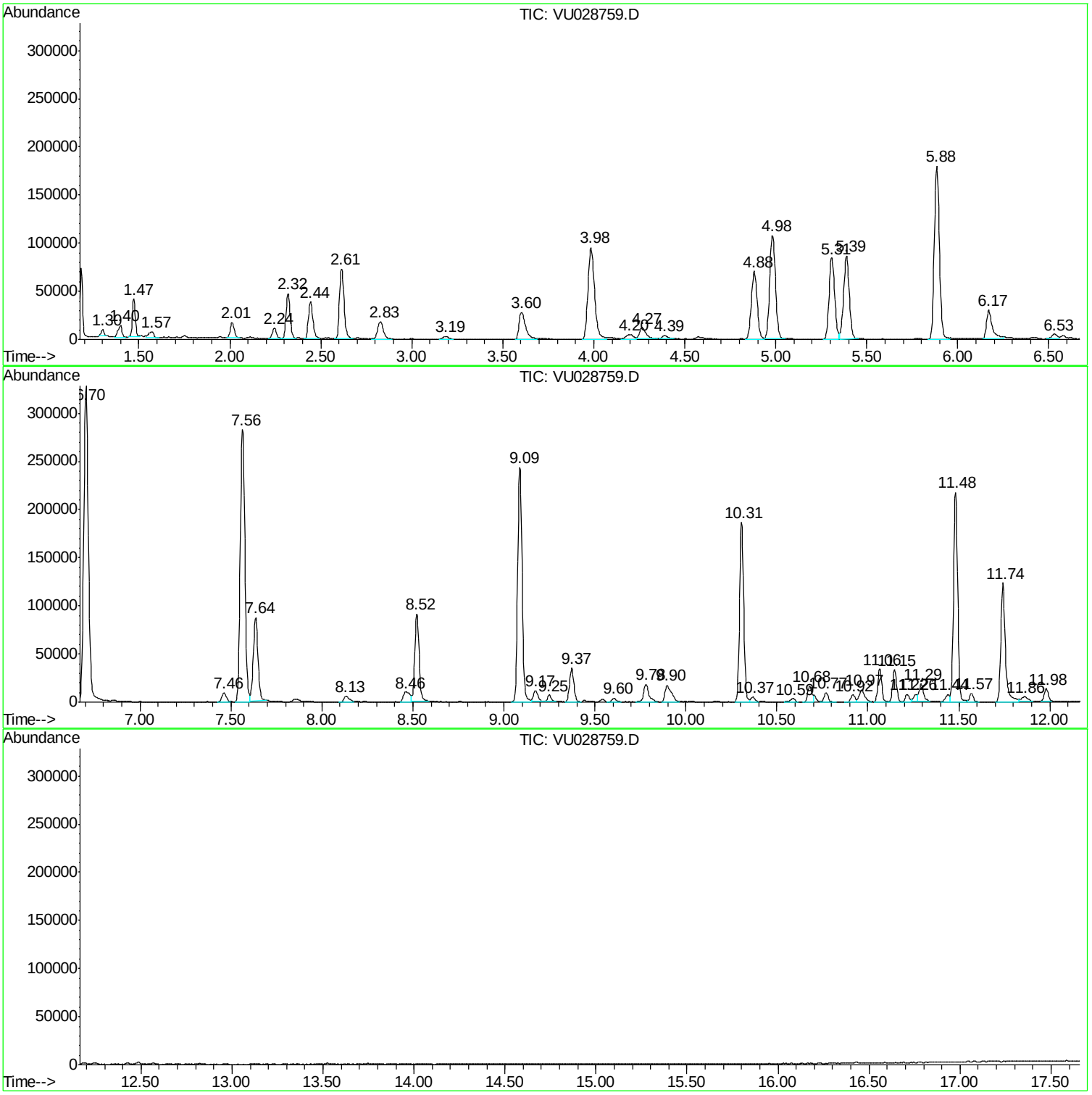
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.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\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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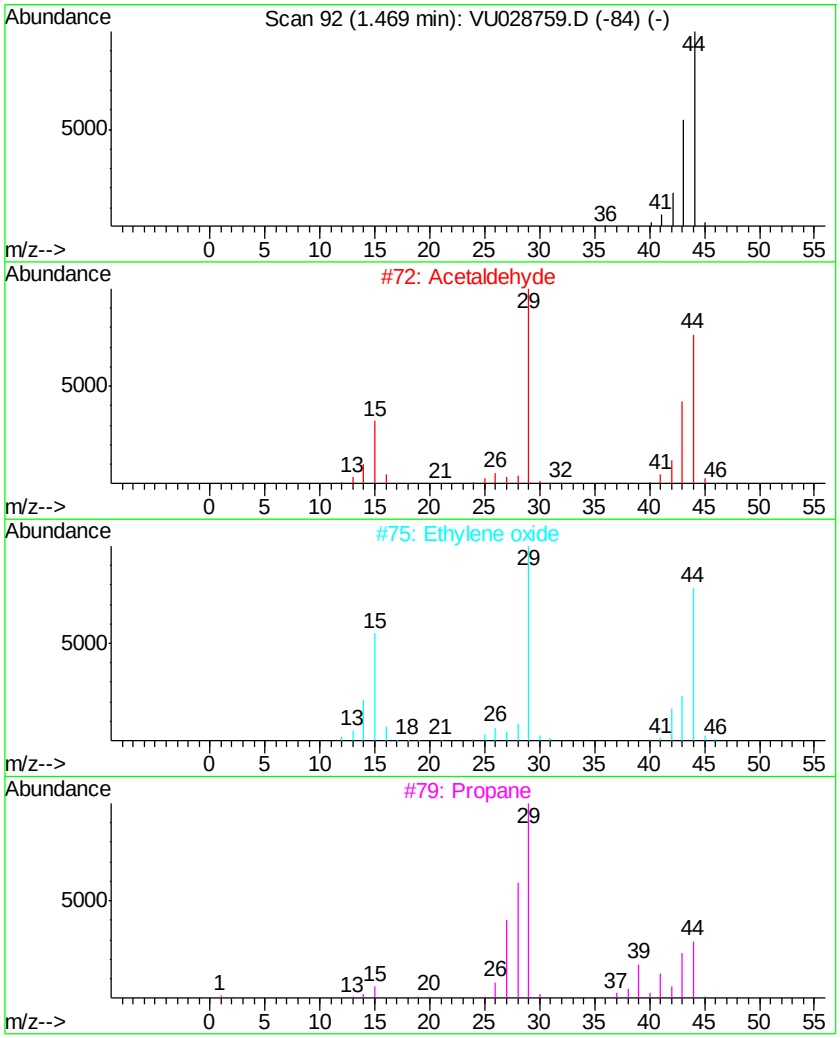
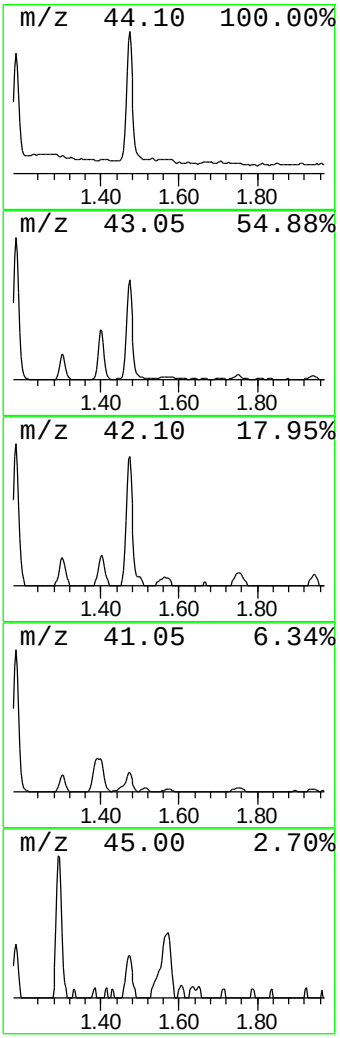
Peak Number 1 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	9.55 ug/l	45154	Pentafluorobenzene	4.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Alanine	89	C3H7NO2	000056-41-7	4
5	1,2-Propanediamine	74	C3H10N2	000078-90-0	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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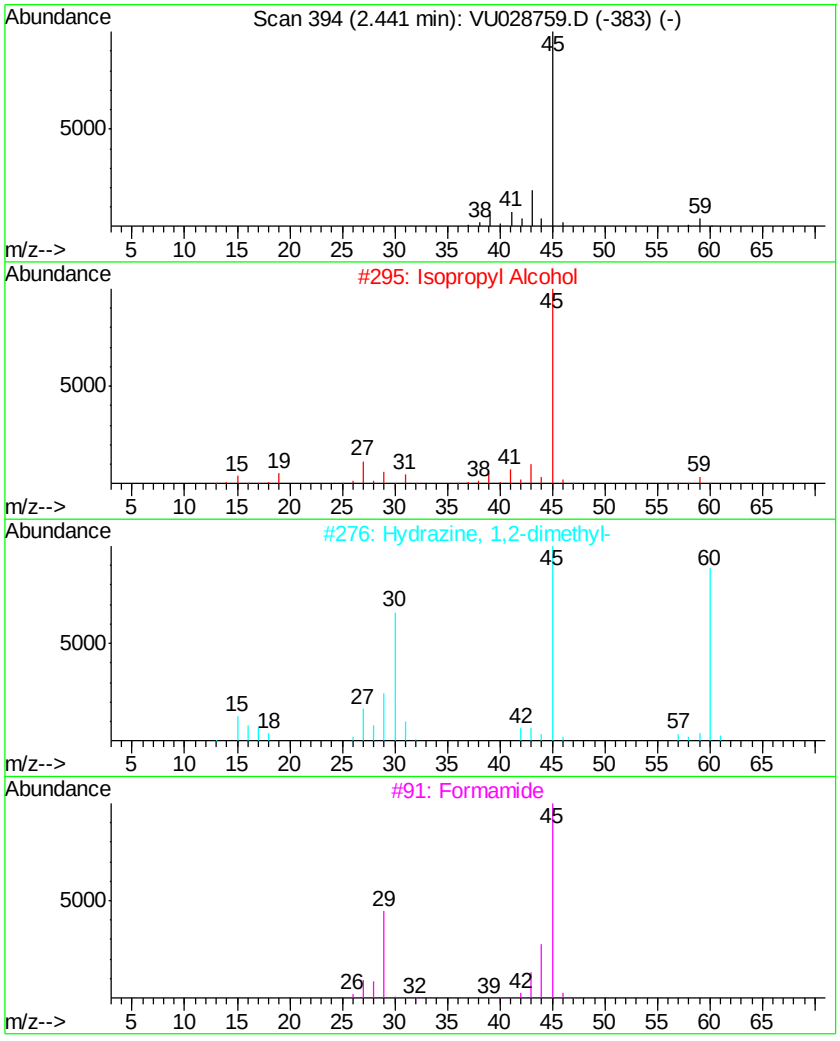
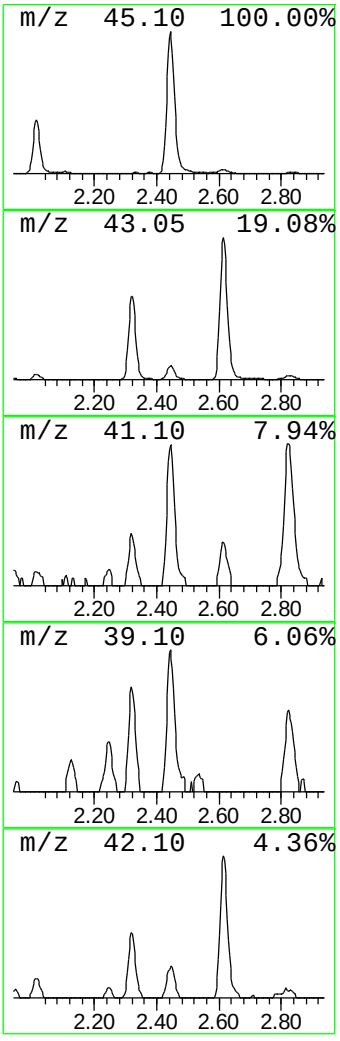
Peak Number 2 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	14.44 ug/l	68289	Pentafluorobenzene	4.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	Formamide	45	CH3NO	000075-12-7	7
4	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5	2-Butanol	74	C4H10O	000078-92-2	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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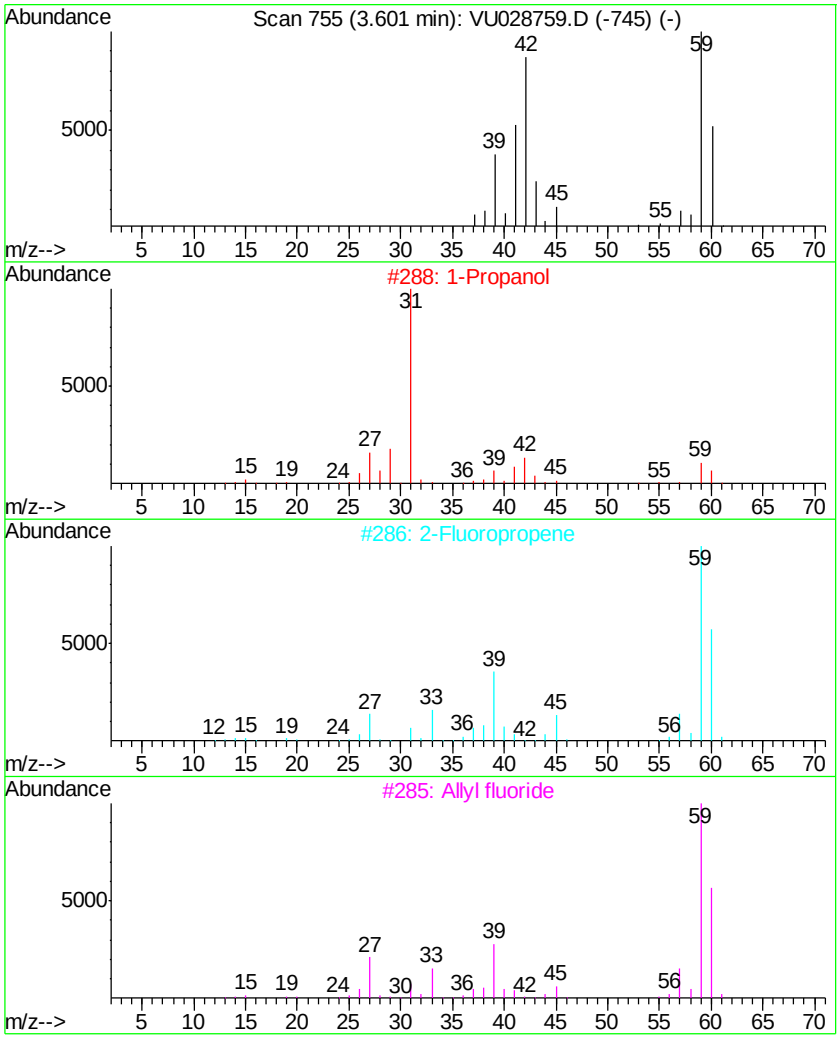
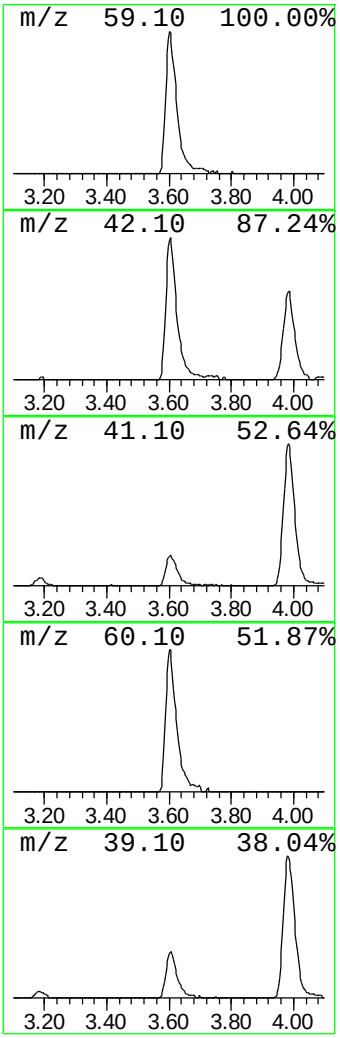
Peak Number 3 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	14.89 ug/l	70399	Pentafluorobenzene	4.98

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	46
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	9
5	Acetaldoxime	59	C2H5NO	000107-29-9	7





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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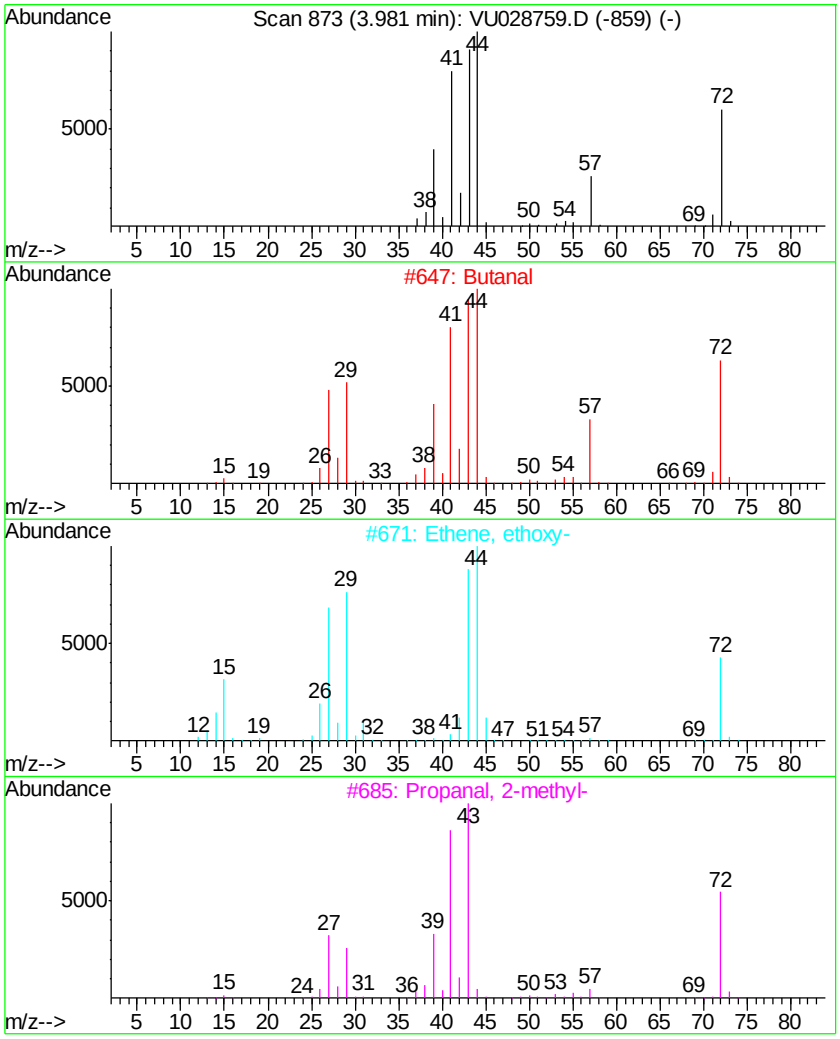
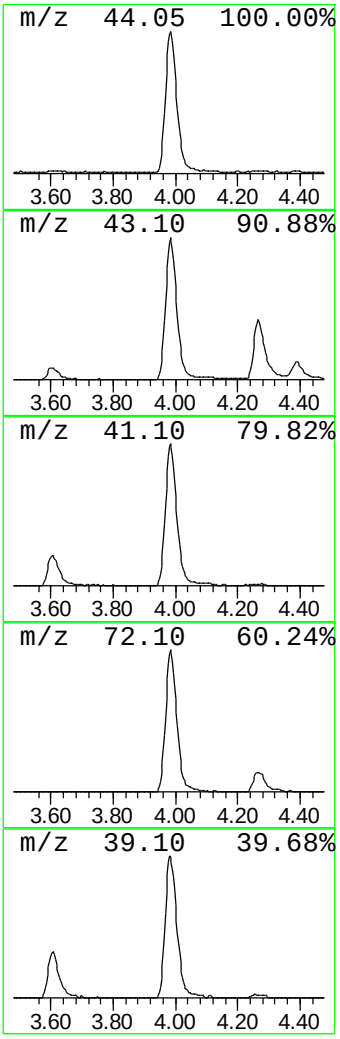
Peak Number 4 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	50.66 ug/l	239491	Pentafluorobenzene	4.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	17





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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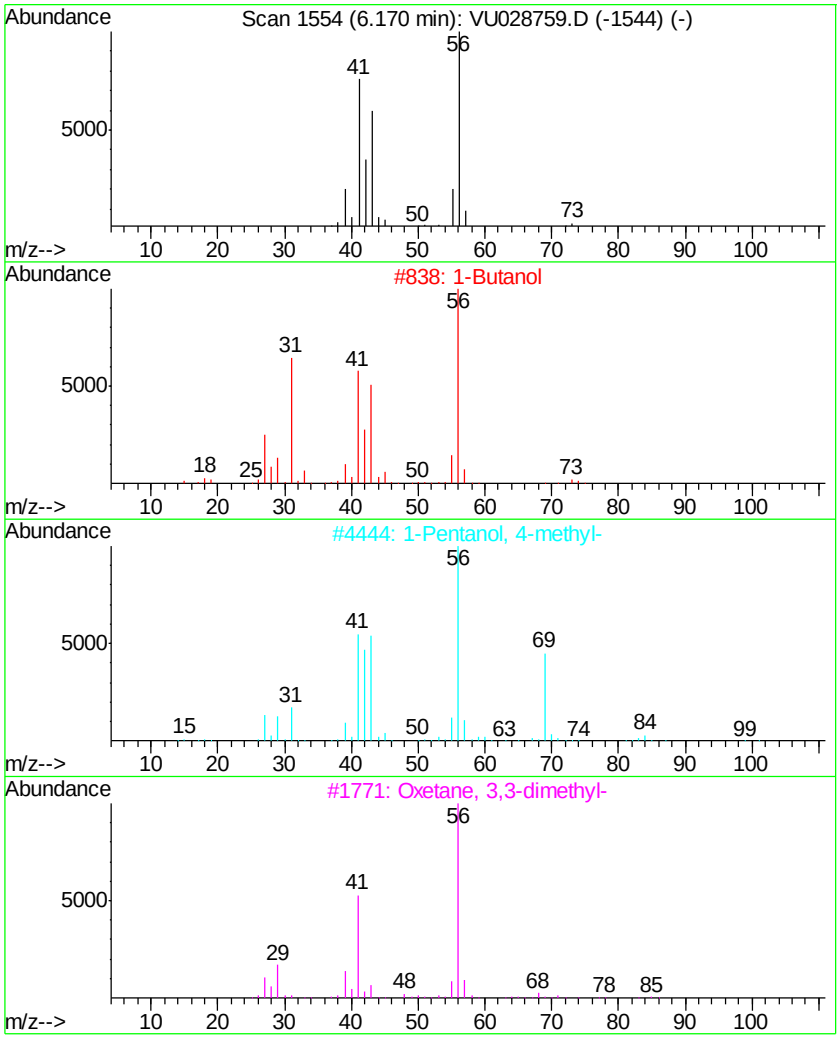
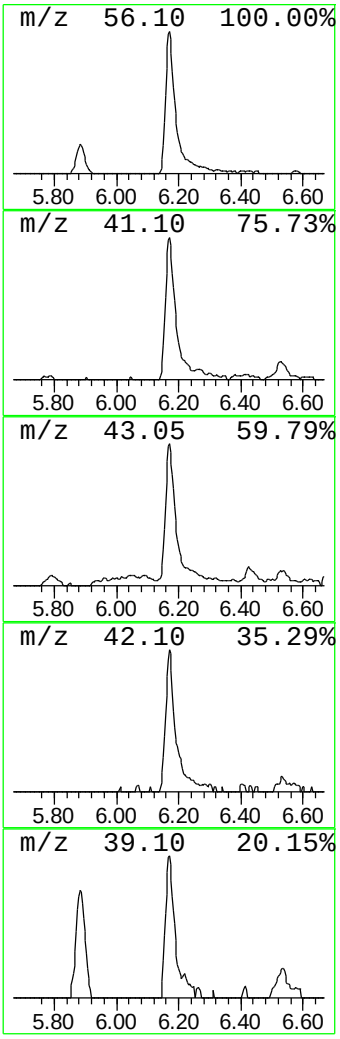
Peak Number 5 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.17	9.39 ug/l	65491	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	40
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
4	Isobutylene epoxide	72	C4H8O	000558-30-5	9
5	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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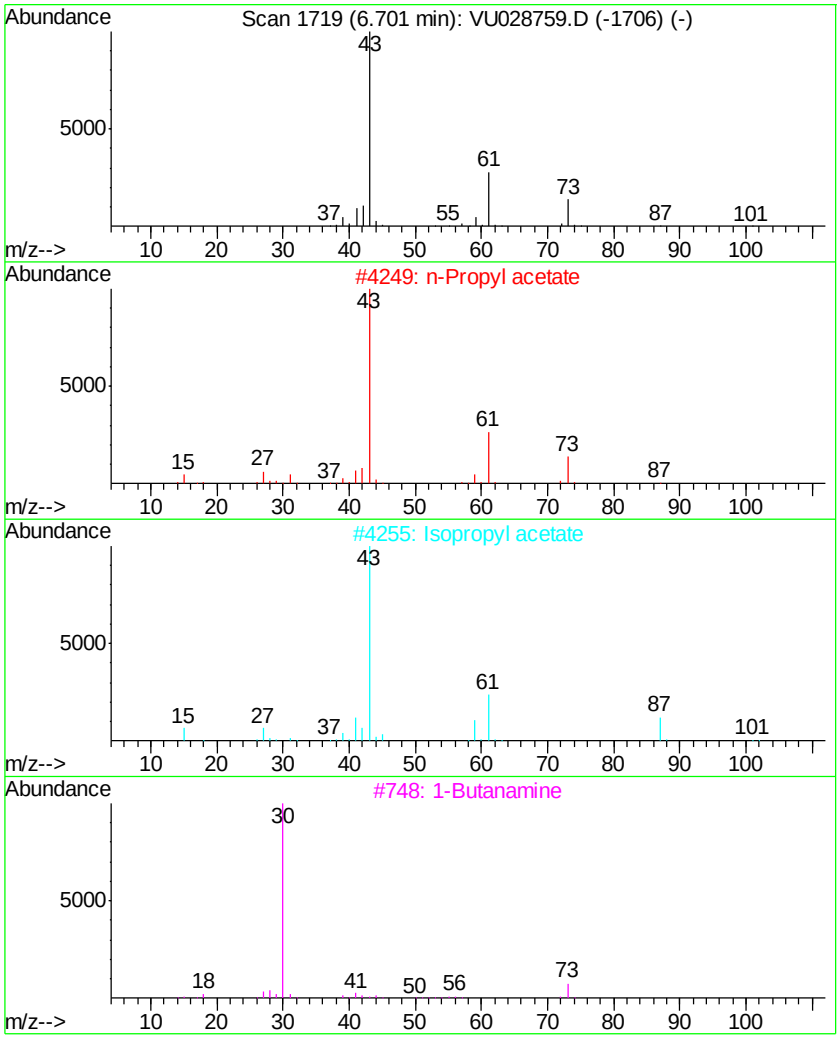
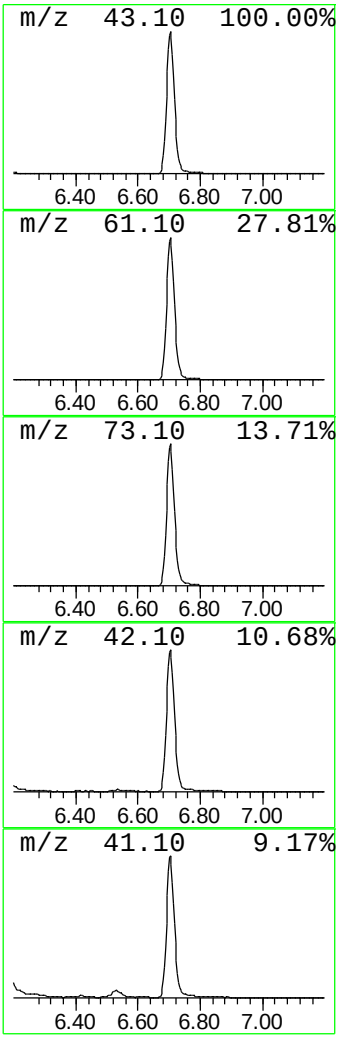
Peak Number 6 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	84.09 ug/l	586562	1,4-Difluorobenzene	5.88

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	9
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

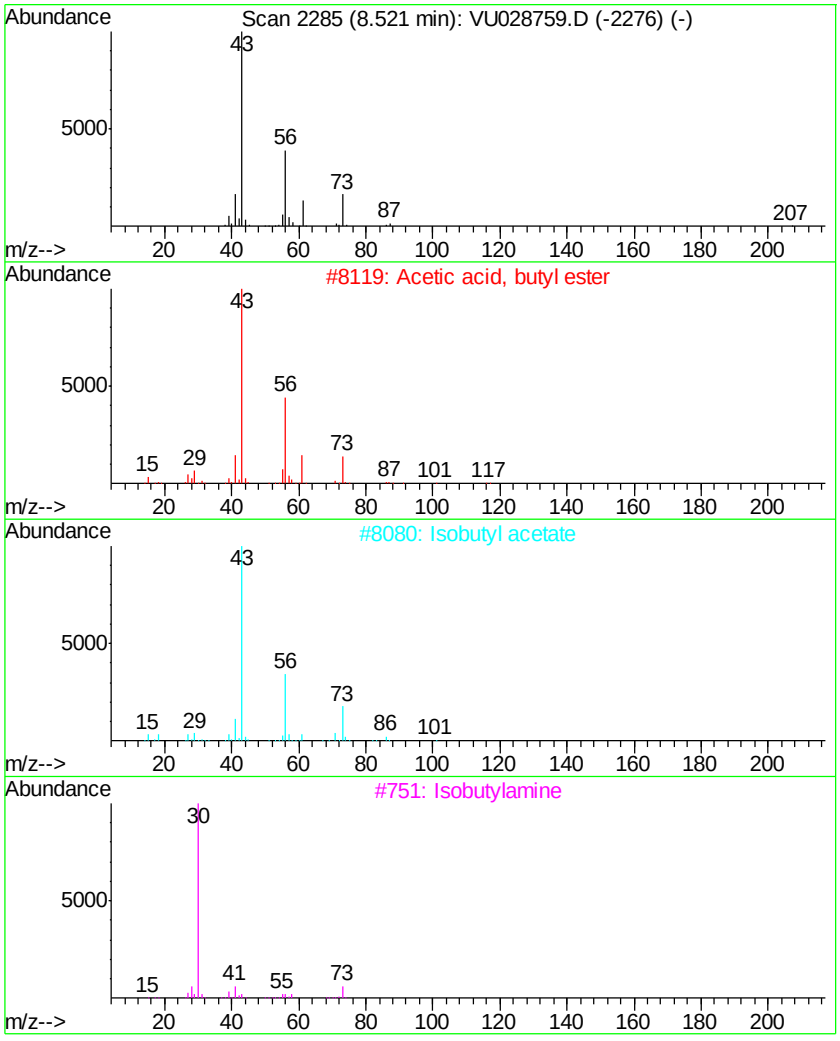
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

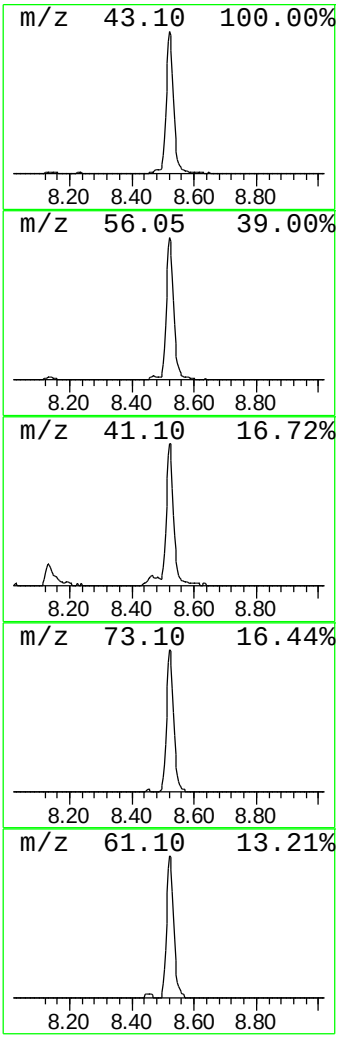
****

Peak Number 7 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	18.15 ug/l	146168	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutyl acetate	116	C6H12O2	000110-19-0	56
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Octanoic acid, hexyl ester	228	C14H28O2	001117-55-1	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

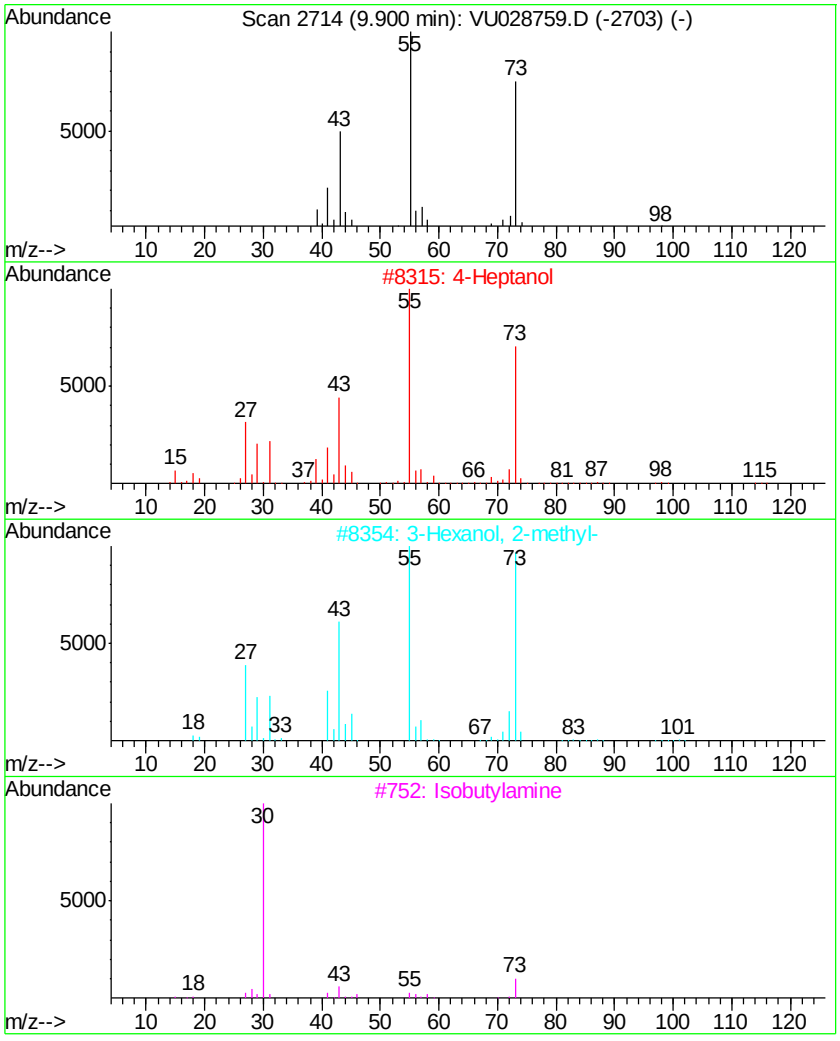
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

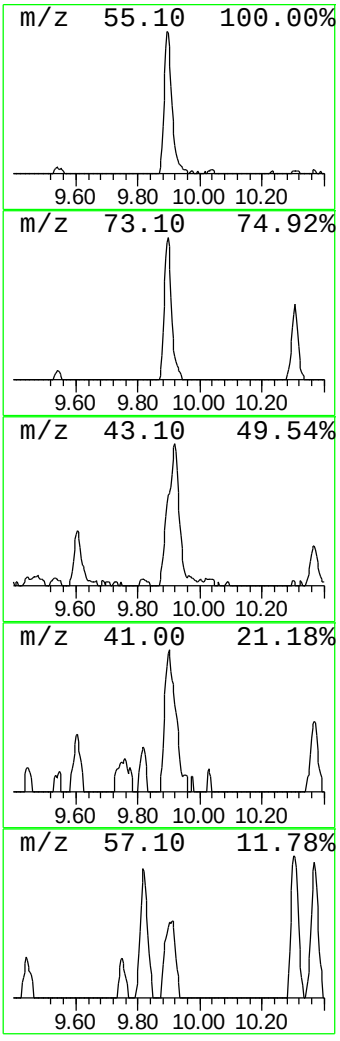
****

Peak Number 8 4-Heptanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	5.20 ug/l	41845	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	83
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	56
3	Isobutylamine	73	C4H11N	000078-81-9	42
4	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	17
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12





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Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

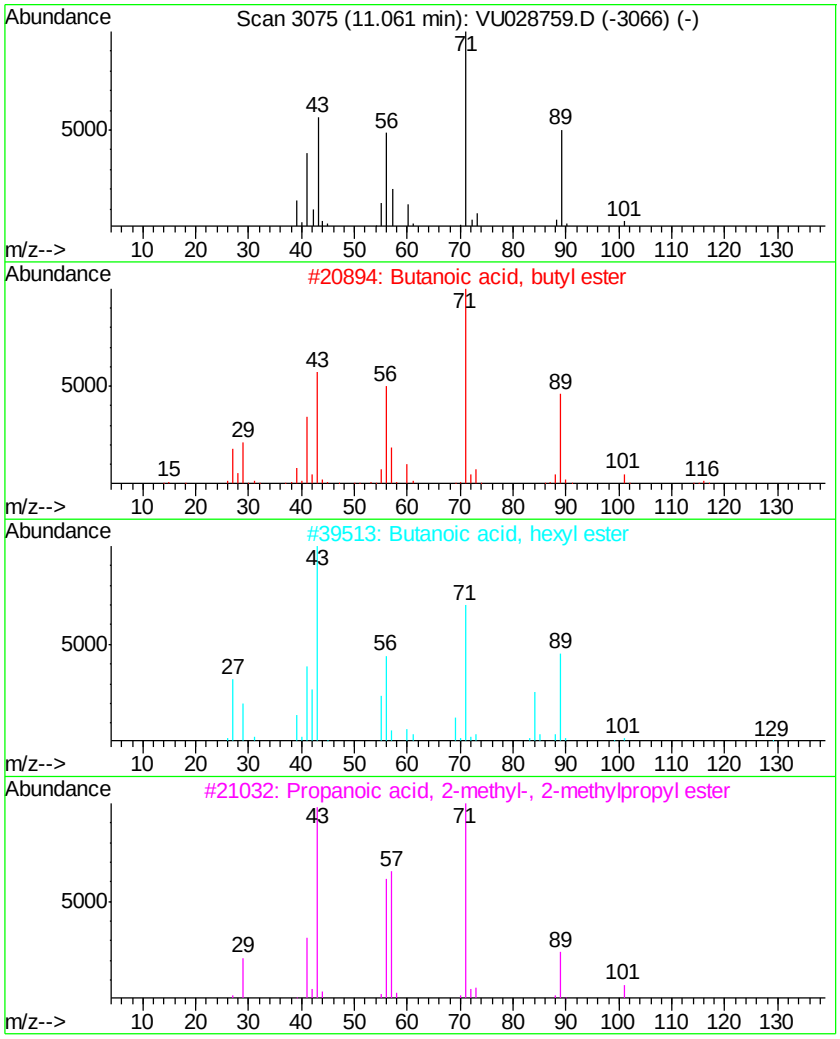
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

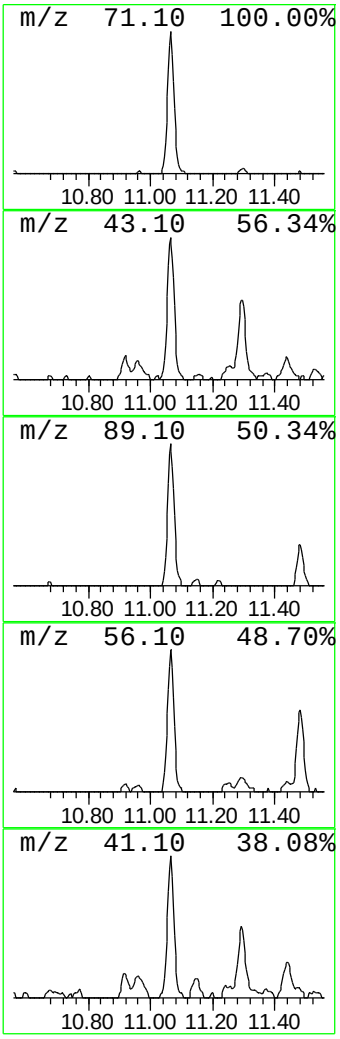
****

Peak Number 9 Butanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	7.35 ug/l	50594	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	56
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

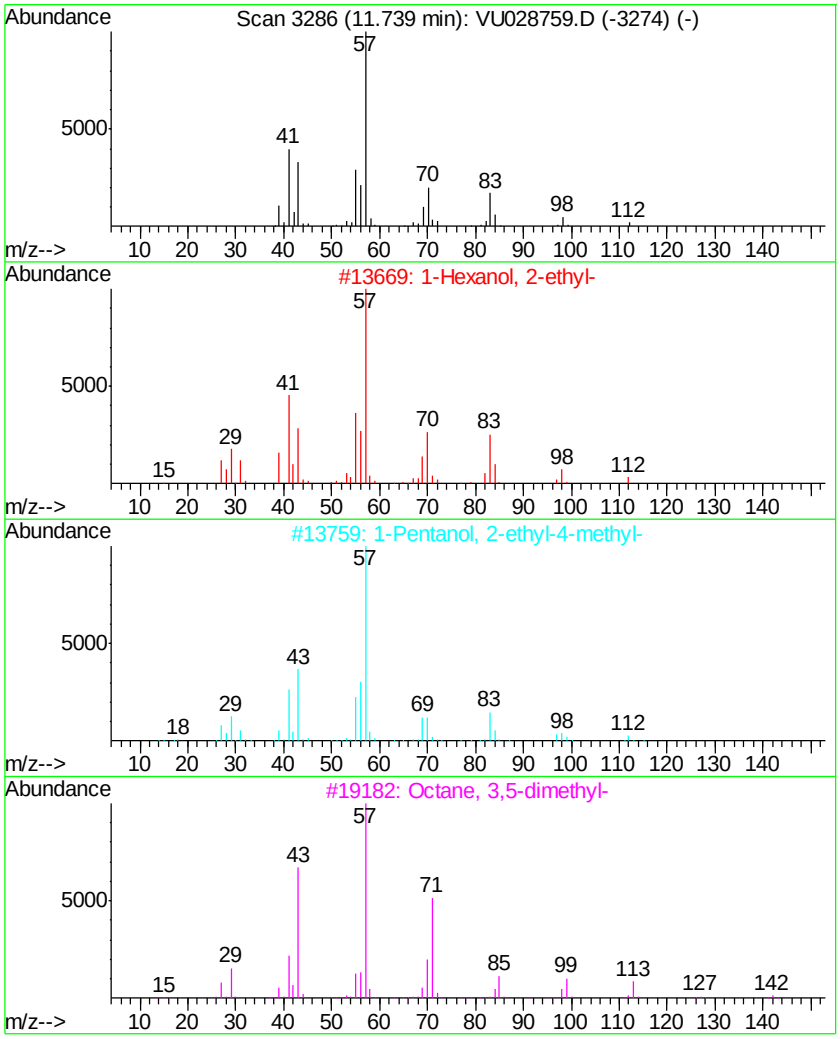
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

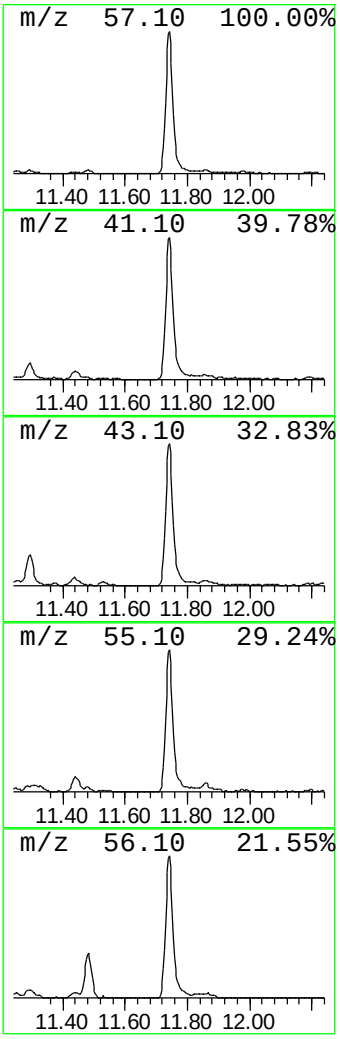
****

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	31.25 ug/l	215206	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	59
4	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028759.D
Acq On : 18 Dec 2018 07:36
Operator : MD/SY
Sample : J6390-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30099

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.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
Acetaldehyde	1.47	9.6	ug/l	45154	1	4.98	236390	50.0
Isopropyl Alcohol	2.44	14.4	ug/l	68289	1	4.98	236390	50.0
1-Propanol	3.60	14.9	ug/l	70399	1	4.98	236390	50.0
Butanal	3.98	50.7	ug/l	239491	1	4.98	236390	50.0
1-Butanol	6.17	9.4	ug/l	65491	2	5.88	348751	50.0
n-Propyl acetate	6.70	84.1	ug/l	586562	2	5.88	348751	50.0
Acetic acid, buty...	8.52	18.1	ug/l	146168	3	9.09	402682	50.0
4-Heptanol	9.90	5.2	ug/l	41845	3	9.09	402682	50.0
Butanoic acid, bu...	11.06	7.3	ug/l	50594	4	11.48	344345	50.0
1-Hexanol, 2-ethyl-	11.74	31.3	ug/l	215206	4	11.48	344345	50.0