LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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	32	40	46	rBV2	10677	12216	1.02%	0.198%
2	1.398	60	70	78	rBV2	17544	28680	2.39%	0.464%
3	1.472	85	93	103	rBV	68406	75603	6.30%	1.224%
4	2.013	253	261	274	rVB2	12542	18136	1.51%	0.294%
5	2.244	323	333	345	rVB	23359	37017	3.08%	0.599%
6	2.321	345	357	371	rBV	168172	266536	22.20%	4.317%
7	2.443	383	395	411	rBV	46896	82620	6.88%	1.338%
8	2.614	436	448	467	rBV	52995	91436	7.62%	1.481%
9	2.826	499	514	532	rVB	19518	42122	3.51%	0.682%
10	3.604	744	756	777	rBV2	52271	127901	10.65%	2.071%
11	3.984	858	874	902	rBV2	114498	287609	23.95%	4.658%
12	4.266	951	962	983	rVB	13957	33685	2.81%	0.546%
13	4.881	1138	1153	1170	rBV2	72912	160963	13.41%	2.607%
14	4.980	1170	1184	1203	rVV2	113607	248732	20.72%	4.028%
15	5.308	1271	1286	1298	rBV2	88645	192008	15.99%	3.110%
16	5.389	1299	1311	1328	rVB	96738	212925	17.73%	3.448%
17	5.884	1451	1465	1485	rBV	190971	369976	30.82%	5.992%
18	6.167	1542	1553	1581	rBV	43453	95928	7.99%	1.554%
19	6.530	1649	1666	1675	rBV4	6834	14841	1.24%	0.240%
20	6.704	1703	1720	1757	rBV	681050	1200623	100.00%	19.444%
21	7.562	1975	1987	2000	rBV	298554	517820	43.13%	8.386%
22	7.636	2000	2010	2029	rVB	90942	160419	13.36%	2.598%
23	8.131	2156	2164	2182	rBV2	7363	15327	1.28%	0.248%
24	8.459	2255	2266	2277	rBV6	14051	30582	2.55%	0.495%
25	8.524	2277	2286	2301	rVB	45623	73655	6.13%	1.193%
26	9.086	2449	2461	2479	rBV	254111	424684	35.37%	6.878%
27	9.173	2479	2488	2503	rVB2	15577	27009	2.25%	0.437%
28	9.372	2540	2550	2561	rBV2	29833	48015	4.00%	0.778%
29	9.781	2669	2677	2685	rBV3	12343	20717	1.73%	0.336%
30	9.896	2702	2713	2737	rBV2	21057	42059	3.50%	0.681%
31	10.305	2827	2840	2854	rBV	195687	309476	25.78%	5.012%
32	10.919	3015	3031	3037	rBV2	9145	13978	1.16%	0.226%
33	11.064	3063	3076	3088	rBV	42744	63681	5.30%	1.031%
34	11.147	3094	3102	3110	rBV3	8211	12130	1.01%	0.196%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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	11.292	3130	3147	3158	rVV4	20470	40280	3.35%	0.652%
36	11.440	3184	3193	3196	rBV3	10142	13911	1.16%	0.225%
37	11.482	3196	3206	3220	rVB	236167	365845	30.47%	5.925%
38	11.710	3266	3277	3280	rBV2	57513	75308	6.27%	1.220%
39	11.739	3280	3286	3309	rVB	154807	259668	21.63%	4.205%
40	11.980	3351	3361	3372	rVB3	16302	25360	2.11%	0.411%
41	13.520	3825	3840	3860	rBV3	20182	35303	2.94%	0.572%

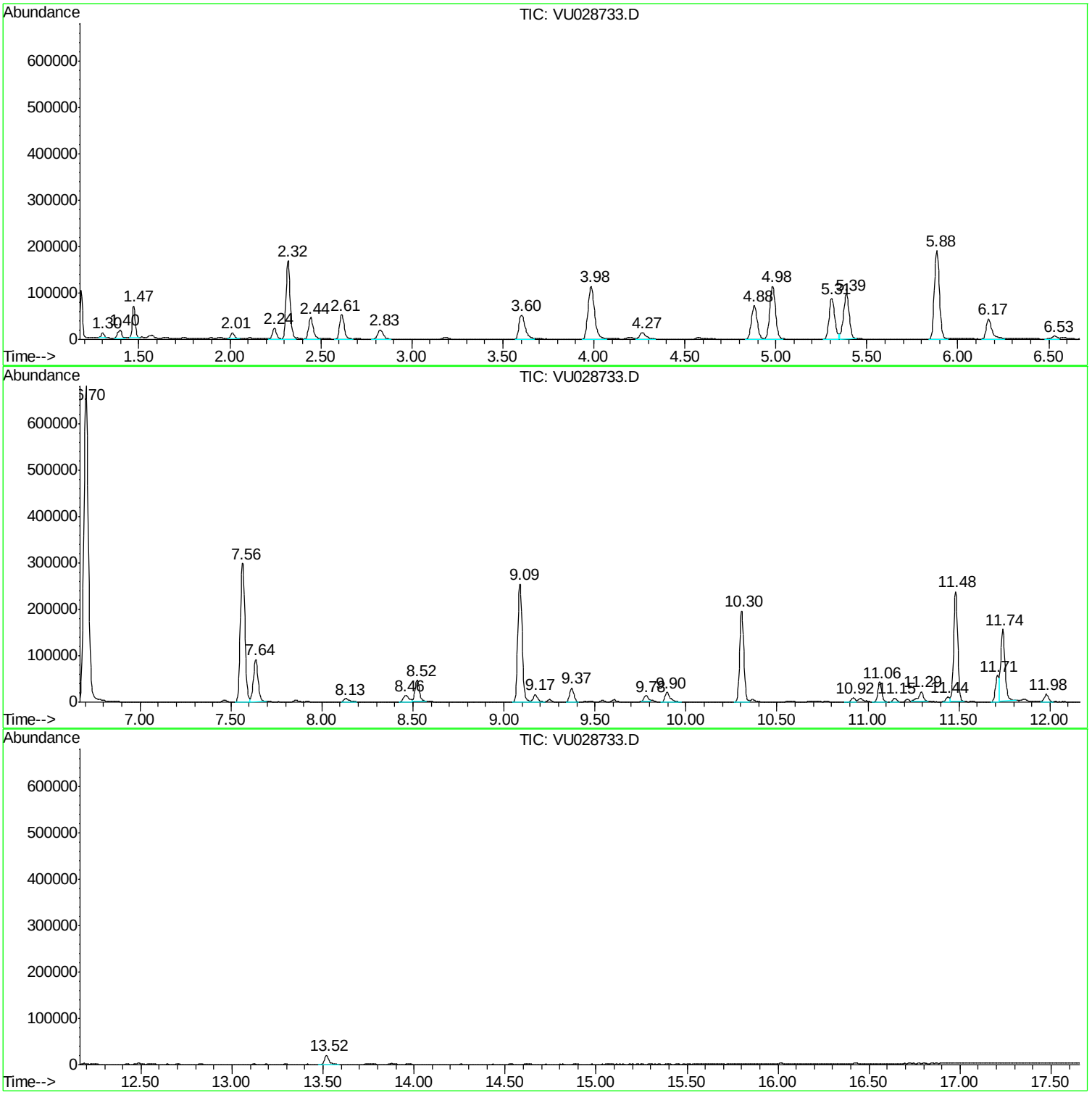
Sum of corrected areas: 6174784

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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 : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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

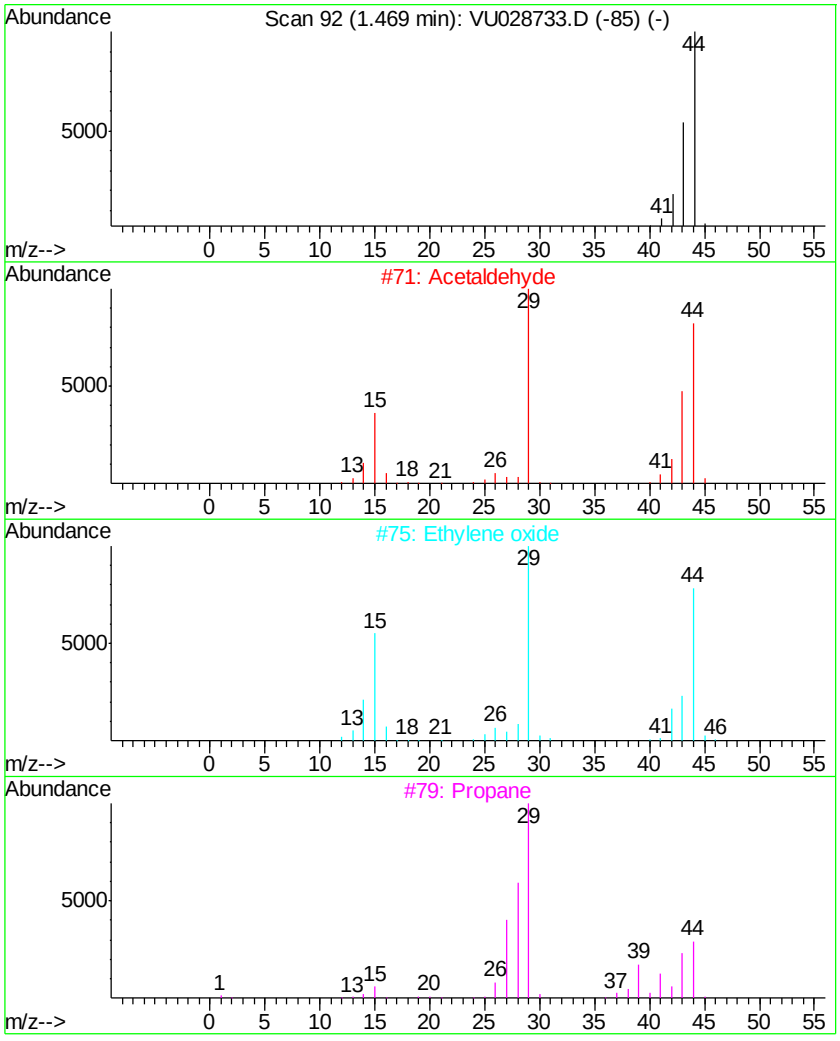
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

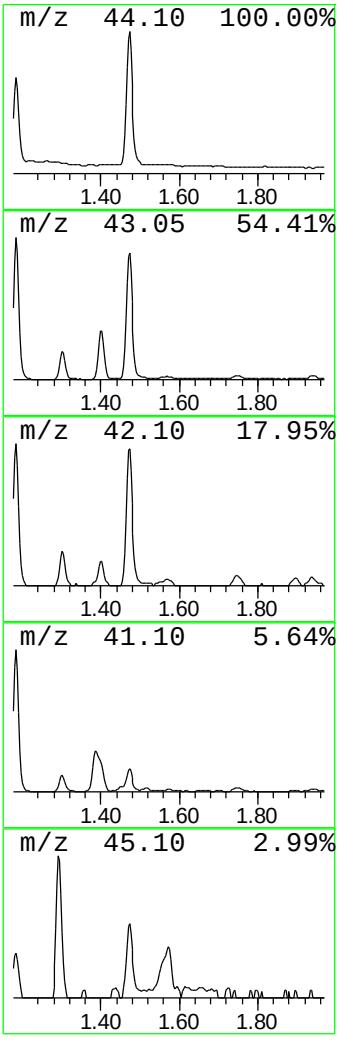
****

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	15.20 ug/l	75603	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	(R)-(-)-2-Amino-1-propanol	75	C3H9NO	035320-23-1	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 : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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

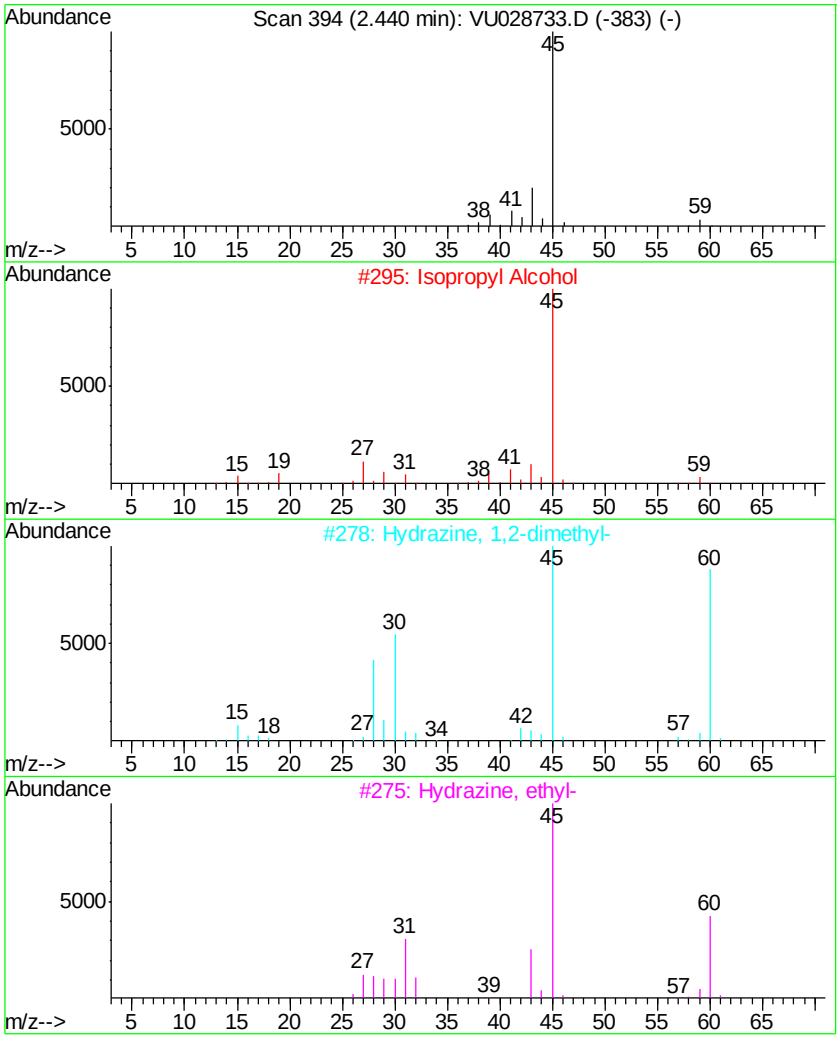
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

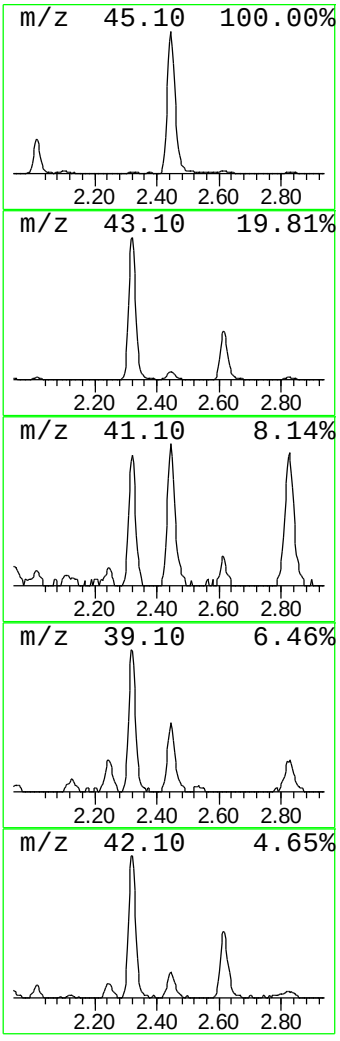
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	16.61 ug/l	82620	Pentafluorobenzene	4.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4	Ethylamine	45	C2H7N	000075-04-7	5
5	Formamide	45	CH3NO	000075-12-7	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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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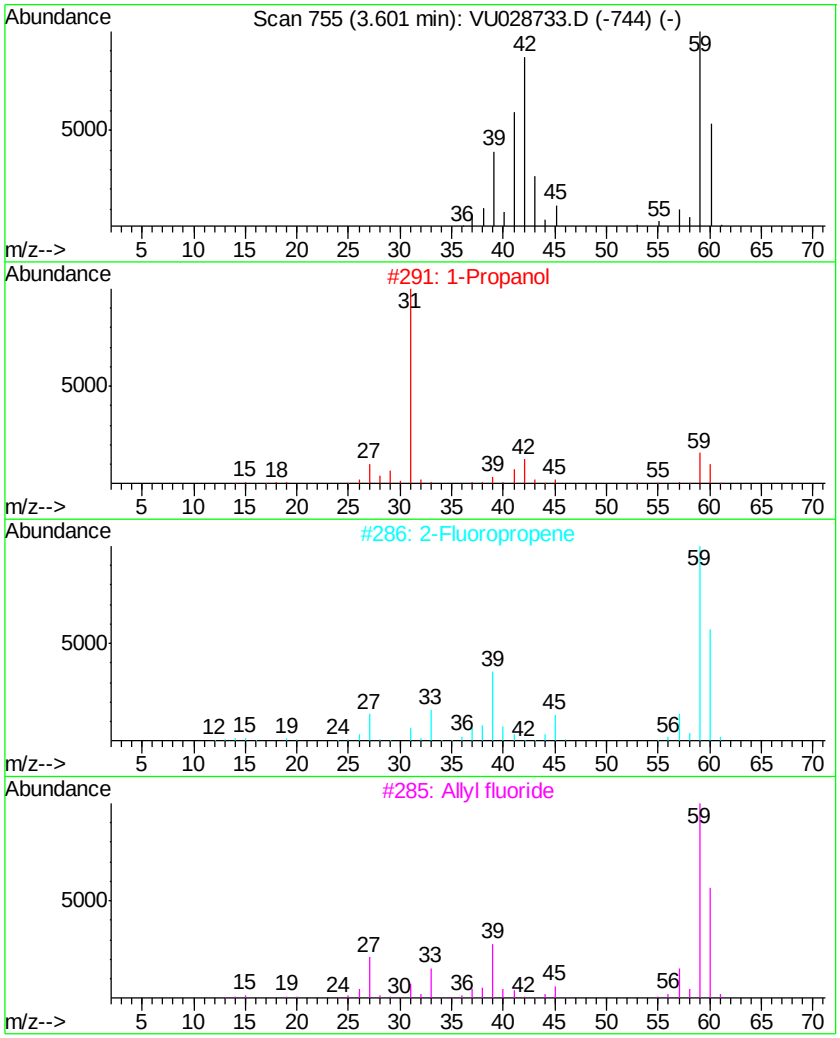
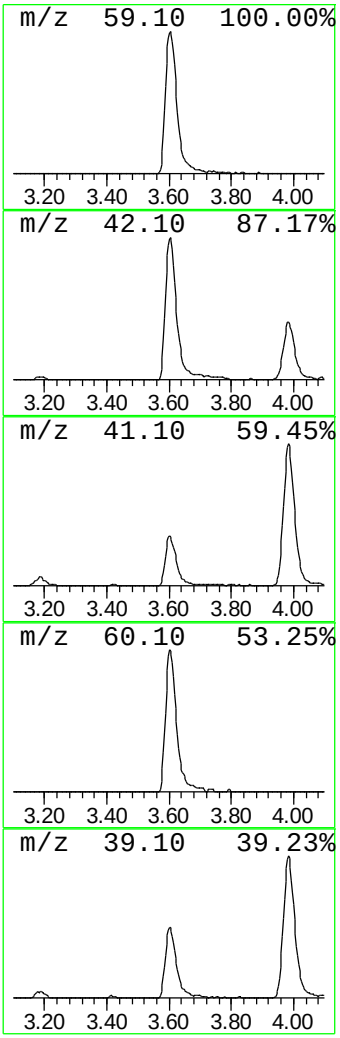
Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	25.71 ug/l	127901	Pentafluorobenzene	4.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	59
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	9
5	Cyclopropane	42	C3H6	000075-19-4	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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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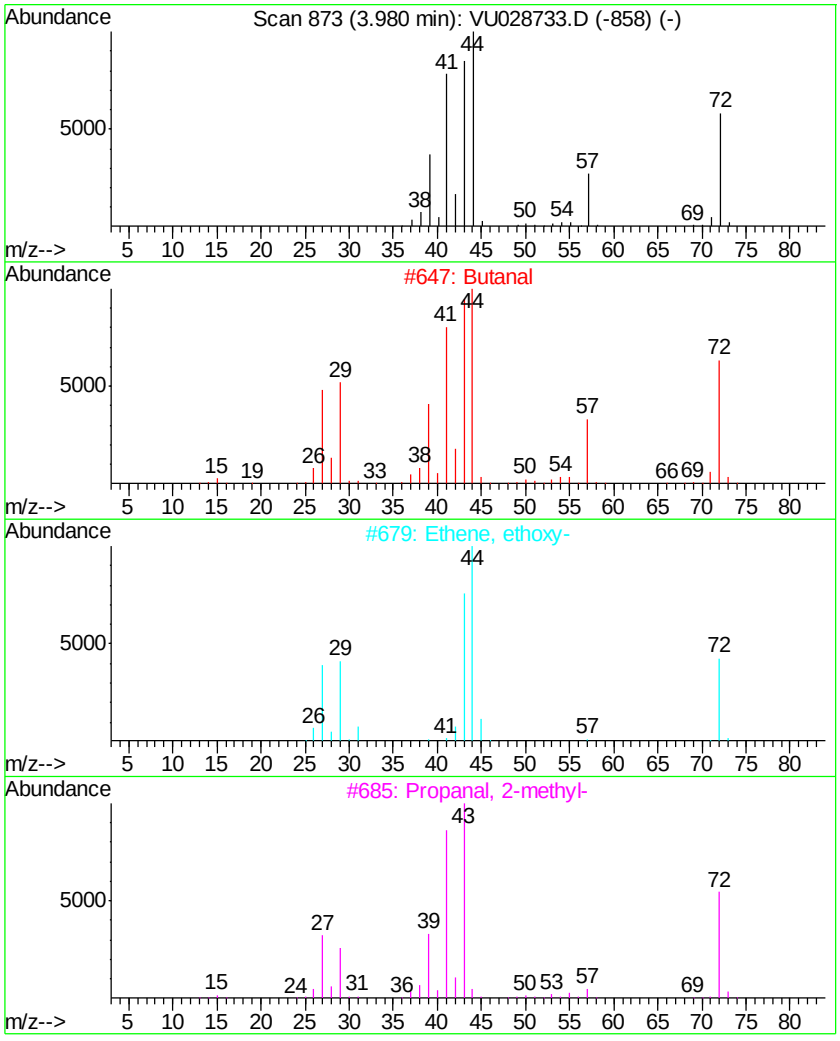
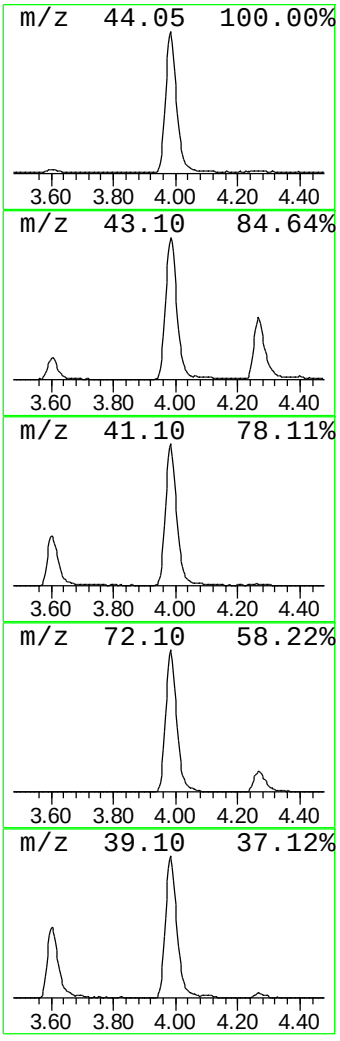
Peak Number 4 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	57.82 ug/l	287609	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	64
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	27
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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

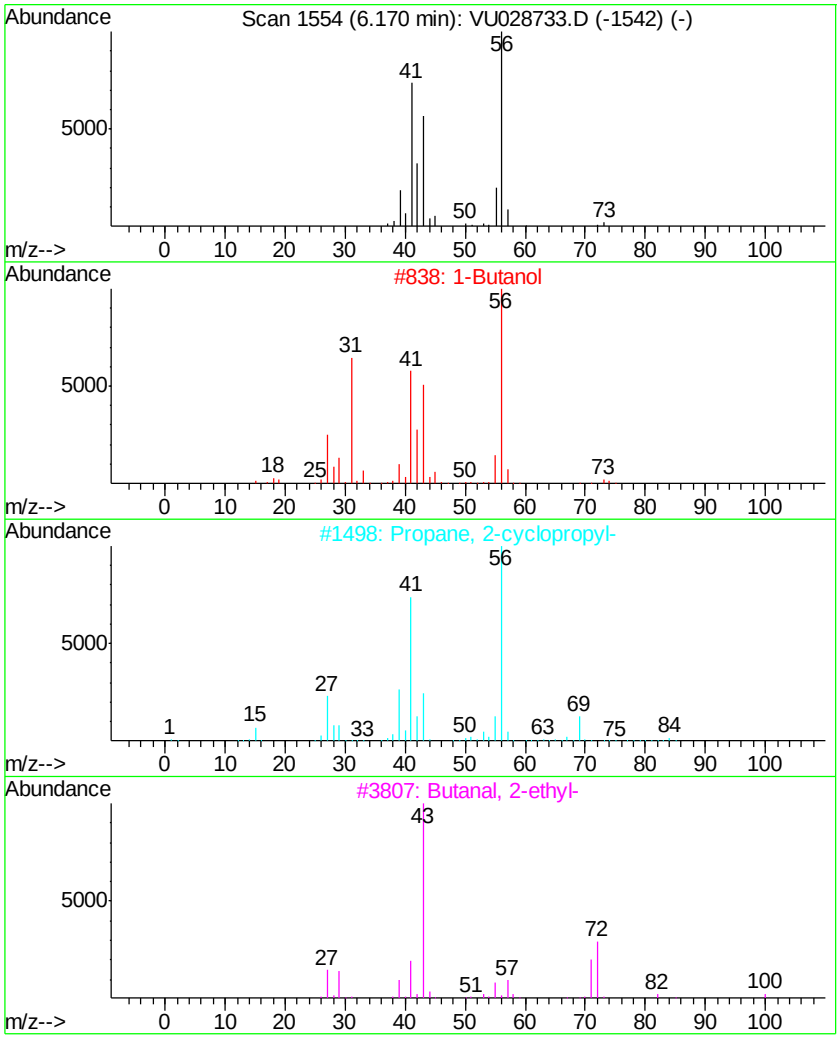
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

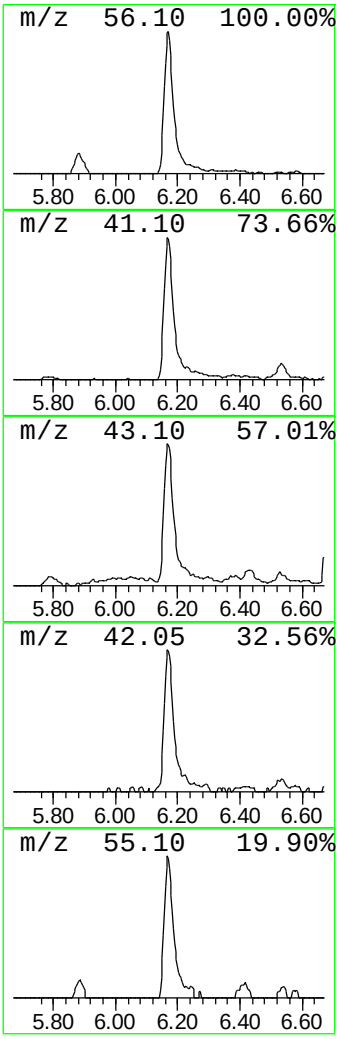
****

Peak Number 5 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.17	12.96 ug/l	95928	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
3	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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

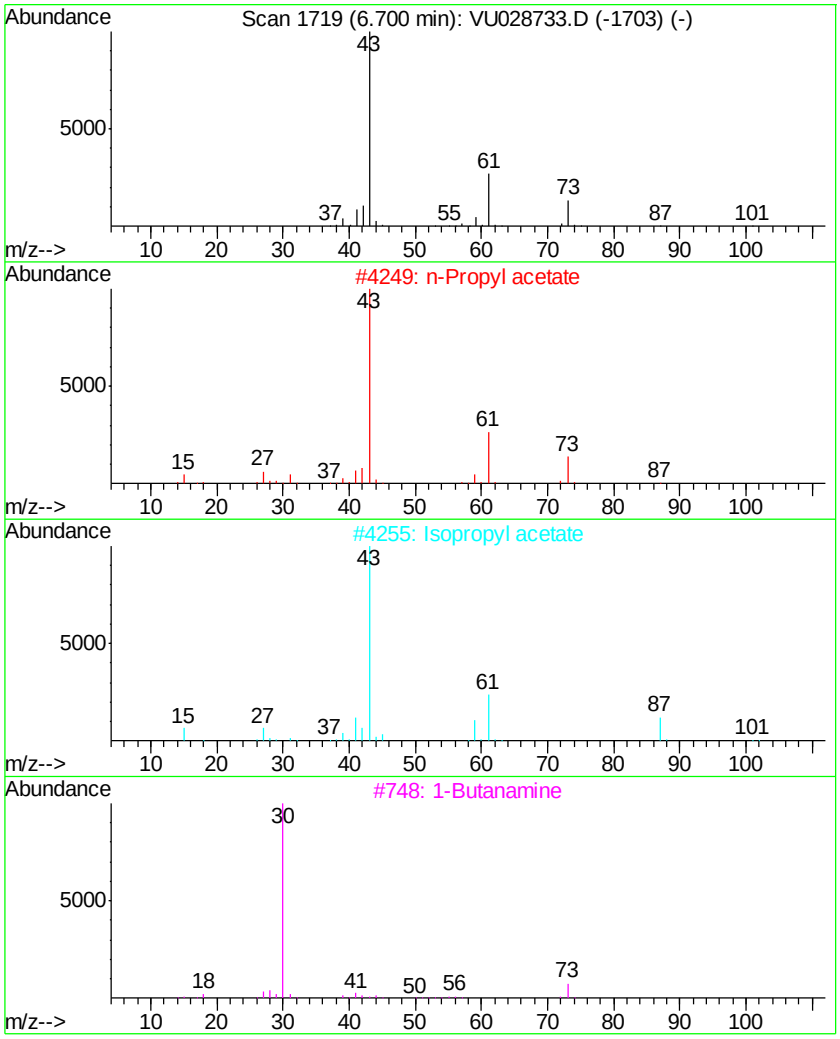
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

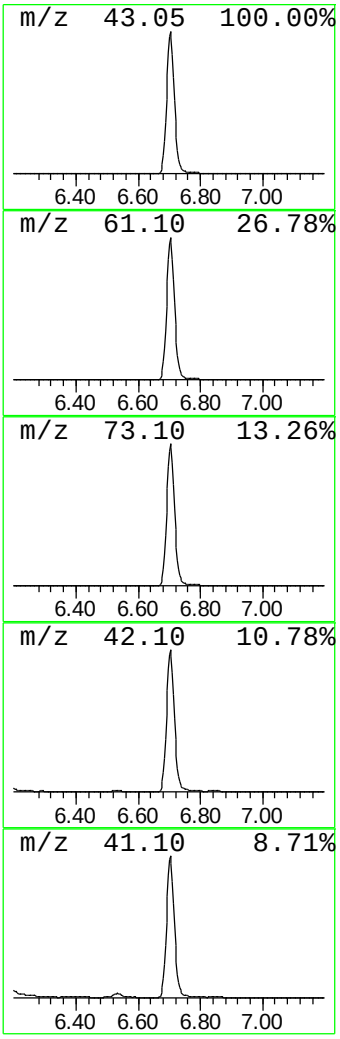
****

Peak Number 6 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	162.26 ug/l	1200620	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	36
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Acetic acid, 2-fluoroethyl ester	106	C4H7FO2	1000367-87-9	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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

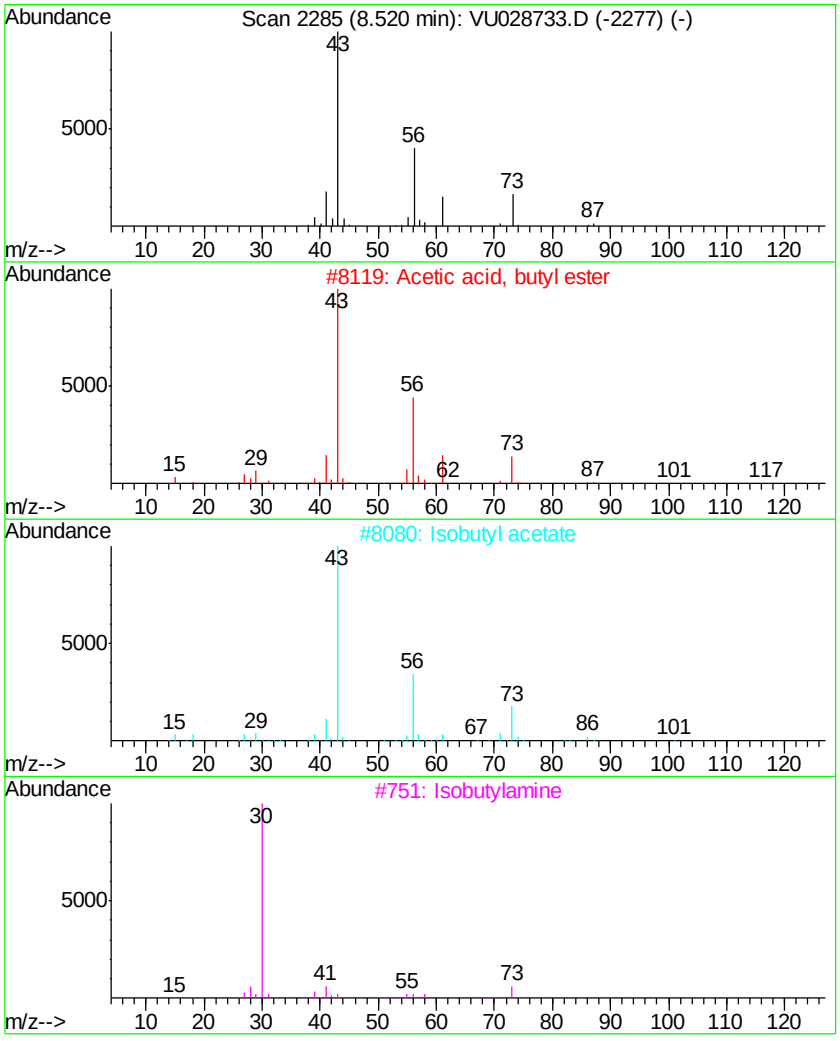
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

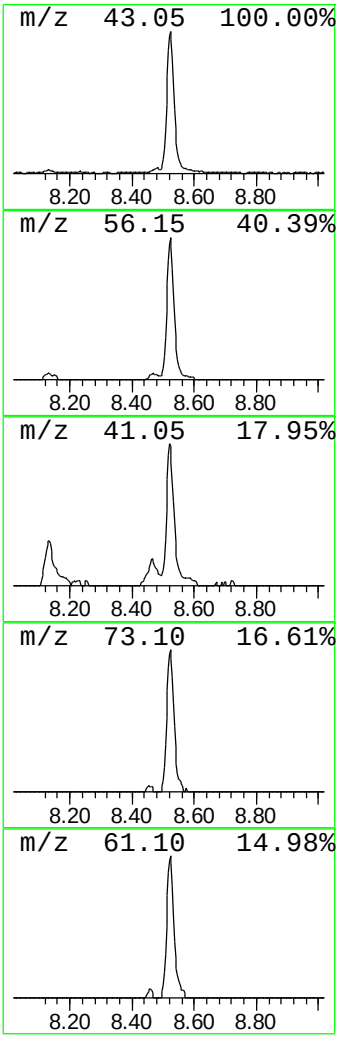
****

Peak Number 7 Acetic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	8.67 ug/l	73655	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	sec-Butyl acetate	116	C6H12O2	000105-46-4	9
5	2,2-Dimethyl-1,3-propanediamine	102	C5H14N2	007328-91-8	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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

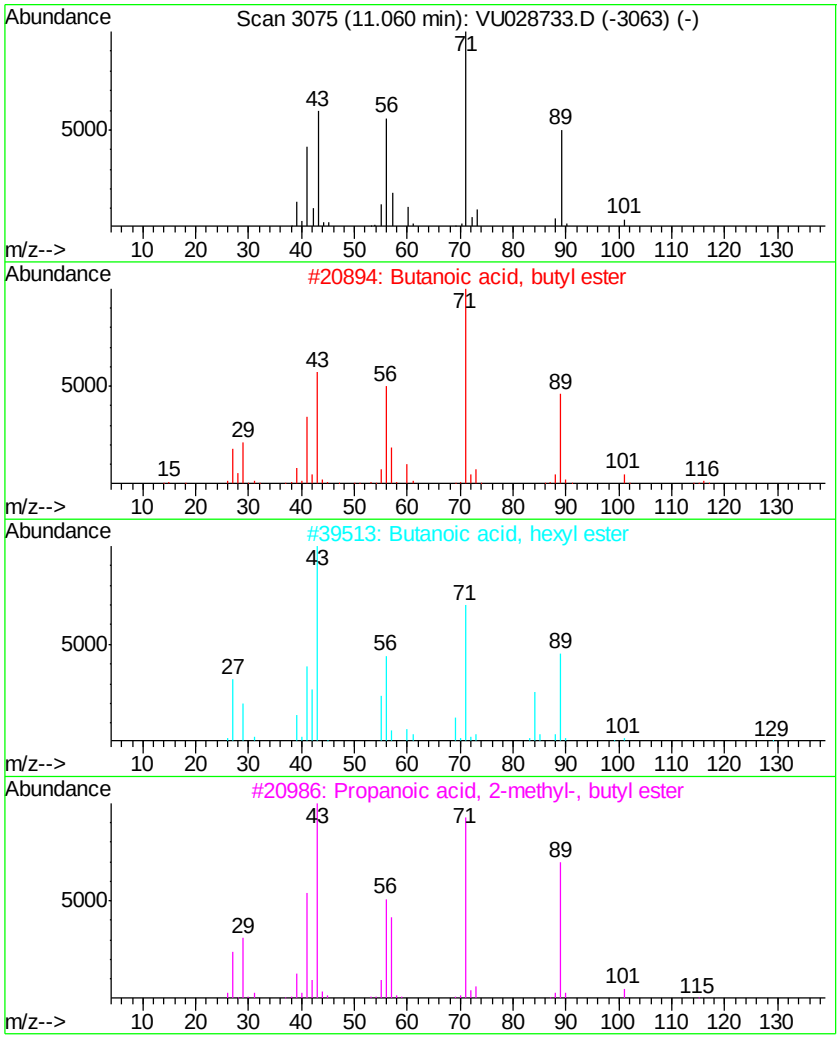
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

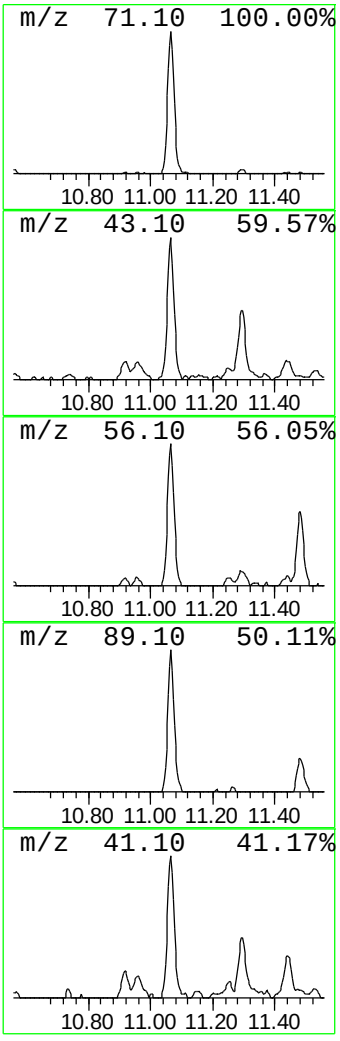
****

Peak Number 8 Butanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	8.70 ug/l	63681	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-, butyl...	144	C8H16O2	000097-87-0	64
4	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59
5	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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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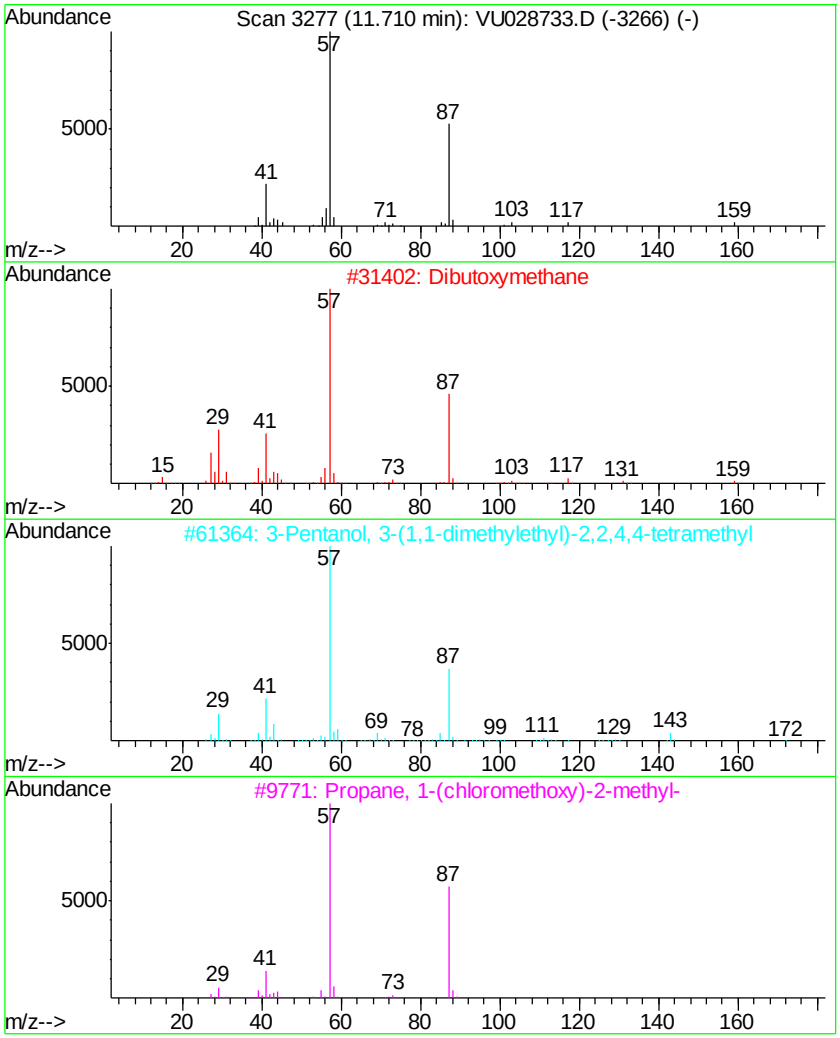
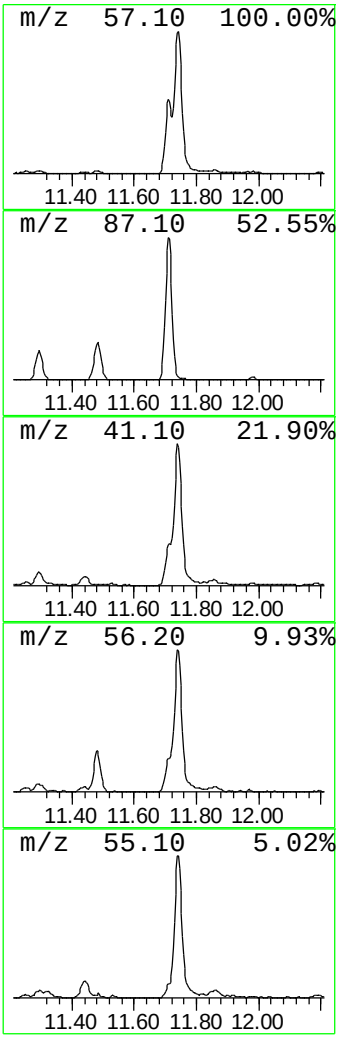
Peak Number 9 Dibutoxymethane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	10.29 ug/l	75308	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibutoxymethane	160	C9H20O2	002568-90-3	72
2	3-Pentanol, 3-(1,1-dimethylethyl...	200	C13H28O	041902-42-5	59
3	Propane, 1-(chloromethoxy)-2-met...	122	C5H11ClO	034180-11-5	53
4	Morpholine	87	C4H9NO	000110-91-8	42
5	Propane, 1,1'-[methylenebis(oxy)...	160	C9H20O2	002568-91-4	39





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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

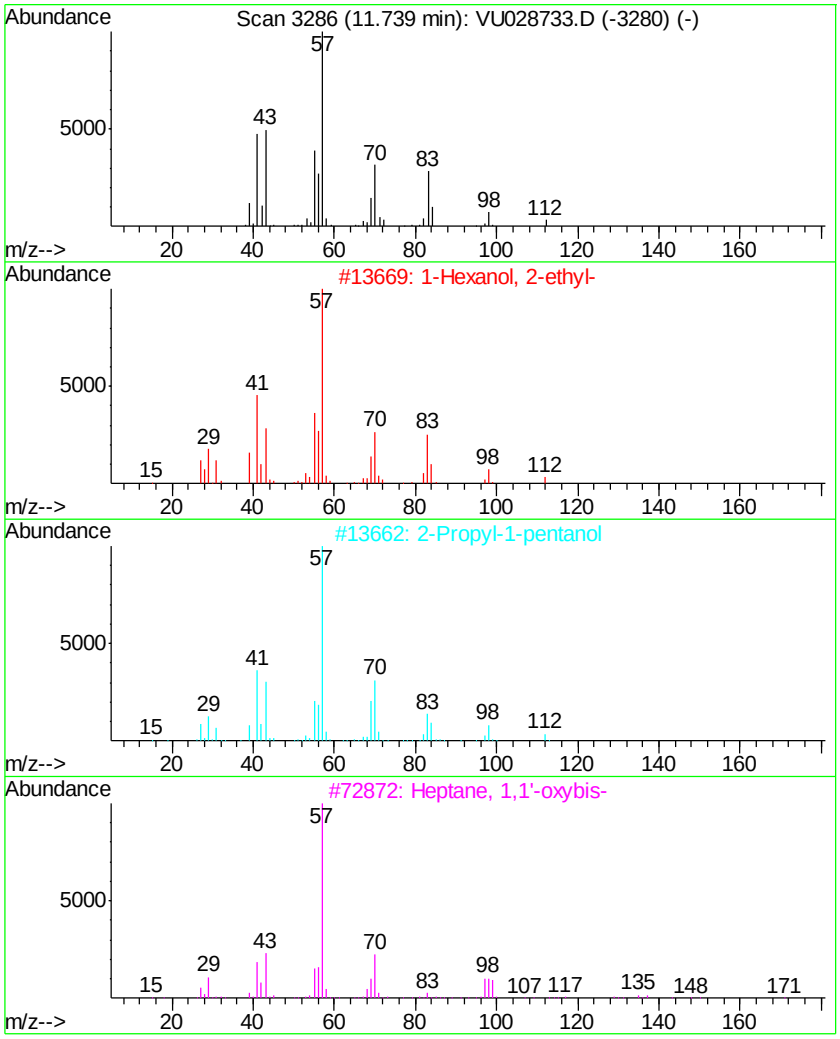
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

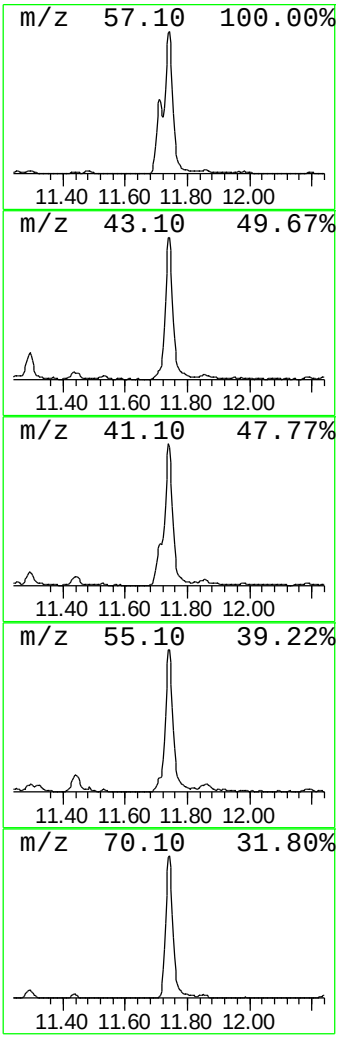
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	35.49 ug/l	259668	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	86
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	45
5	1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028733.D
Acq On : 17 Dec 2018 20:20
Operator : MD/SY
Sample : J6390-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30104

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	15.2	ug/l	75603	1	4.98	248732	50.0
Isopropyl Alcohol	2.44	16.6	ug/l	82620	1	4.98	248732	50.0
1-Propanol	3.60	25.7	ug/l	127901	1	4.98	248732	50.0
Butanal	3.98	57.8	ug/l	287609	1	4.98	248732	50.0
1-Butanol	6.17	13.0	ug/l	95928	2	5.88	369976	50.0
n-Propyl acetate	6.70	162.3	ug/l	1200620	2	5.88	369976	50.0
Acetic acid, buty...	8.52	8.7	ug/l	73655	3	9.09	424684	50.0
Butanoic acid, bu...	11.06	8.7	ug/l	63681	4	11.48	365845	50.0
Dibutoxymethane	11.71	10.3	ug/l	75308	4	11.48	365845	50.0
1-Hexanol, 2-ethyl-	11.74	35.5	ug/l	259668	4	11.48	365845	50.0