LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

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\82U032421W.M
Title : SW846 8260

Signal : TIC: VU042932.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.366	3	8	21	rVB	52525	54733	7.73%	0.861%
2	1.591	70	78	90	rBV2	16737	25305	3.57%	0.398%
3	1.690	103	109	119	rVB	11422	15094	2.13%	0.238%
4	2.552	367	377	393	rBV	6659	10262	1.45%	0.162%
5	2.642	393	405	418	rBV	12813	25092	3.54%	0.395%
6	2.806	438	456	472	rBV4	5220	17967	2.54%	0.283%
7	3.214	569	583	597	rBV2	5250	15784	2.23%	0.248%
8	3.591	689	700	712	rBV6	3235	7744	1.09%	0.122%
9	3.976	803	820	845	rBV3	23724	71036	10.03%	1.118%
10	4.456	951	969	993	rBV	108966	272503	38.48%	4.289%
11	5.298	1215	1231	1244	rBV	116374	244352	34.50%	3.846%
12	5.382	1244	1257	1278	rVB	181997	372403	52.58%	5.862%
13	5.710	1345	1359	1374	rBV	126908	266629	37.65%	4.197%
14	6.256	1514	1529	1552	rBV	264137	493965	69.74%	7.775%
15	6.549	1607	1620	1648	rBV2	23316	66854	9.44%	1.052%
16	6.886	1713	1725	1737	rBV2	13201	25708	3.63%	0.405%
17	7.906	2025	2042	2055	rBV	415935	708249	100.00%	11.148%
18	7.973	2055	2063	2079	rVB3	18971	35990	5.08%	0.566%
19	8.237	2136	2145	2159	rVB8	3205	7253	1.02%	0.114%
20	8.459	2202	2214	2242	rBV3	31939	75480	10.66%	1.188%
21	8.803	2312	2321	2336	rVB6	7309	13410	1.89%	0.211%
22	9.423	2502	2514	2527	rBV	381784	637507	90.01%	10.034%
23	9.494	2527	2536	2558	rVB	82348	158850	22.43%	2.500%
24	9.700	2592	2600	2608	rVB2	11579	16623	2.35%	0.262%
25	10.111	2713	2728	2733	rBV8	10028	19506	2.75%	0.307%
26	10.217	2748	2761	2785	rBV	35619	74849	10.57%	1.178%
27	10.639	2880	2892	2903	rBV	330461	519480	73.35%	8.177%
28	10.690	2903	2908	2916	rVB3	14375	21373	3.02%	0.336%
29	10.754	2921	2928	2938	rVB	11310	17868	2.52%	0.281%
30	10.877	2955	2966	2984	rBV6	8829	17154	2.42%	0.270%
31	11.050	3012	3020	3029	rVB3	8195	11214	1.58%	0.177%
32	11.240	3069	3079	3086	rBV2	28610	48547	6.85%	0.764%
33	11.278	3086	3091	3111	rVB6	18288	35991	5.08%	0.566%
34	11.381	3112	3123	3143	rVB	153562	226887	32.03%	3.571%
35	11.475	3143	3152	3160	rBV3	7734	11229	1.59%	0.177%
36	11.616	3187	3196	3220	rVB2	50146	100566	14.20%	1.583%

LSC Area Percent Report

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Sample : M1903-03
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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : SW846 8260

37	11.729	3222	3231	3236	rVV2	26160	39950	5.64%	0.629%
38	11.774	3236	3245	3250	rVV	79486	129133	18.23%	2.033%
39	11.819	3250	3259	3279	rVB	419985	682529	96.37%	10.743%
40	12.069	3323	3337	3362	rBV	255213	500516	70.67%	7.878%
41	12.179	3365	3371	3380	rVB7	15060	26407	3.73%	0.416%
42	12.317	3405	3414	3426	rVB2	14921	24805	3.50%	0.390%
43	12.417	3439	3445	3453	rVB4	5765	7559	1.07%	0.119%
44	12.555	3481	3488	3498	rVB5	8927	13303	1.88%	0.209%
45	12.806	3556	3566	3582	rBV5	11298	23369	3.30%	0.368%
46	12.880	3582	3589	3598	rBV3	12366	18024	2.54%	0.284%
47	12.960	3607	3614	3628	rVB8	6666	12168	1.72%	0.192%
48	13.073	3641	3649	3657	rVB	9817	14478	2.04%	0.228%
49	13.629	3815	3822	3830	rVB7	5211	8293	1.17%	0.131%
50	13.883	3889	3901	3912	rBV4	19713	31579	4.46%	0.497%
51	14.095	3959	3967	3975	rVB	14992	22020	3.11%	0.347%
52	14.198	3989	3999	4012	rBV4	13472	21415	3.02%	0.337%
53	14.288	4017	4027	4038	rBV6	9198	15244	2.15%	0.240%
54	14.973	4228	4240	4249	rBV4	5319	8485	1.20%	0.134%
55	15.227	4305	4319	4329	rBV5	5568	10501	1.48%	0.165%

Sum of corrected areas: 6353235

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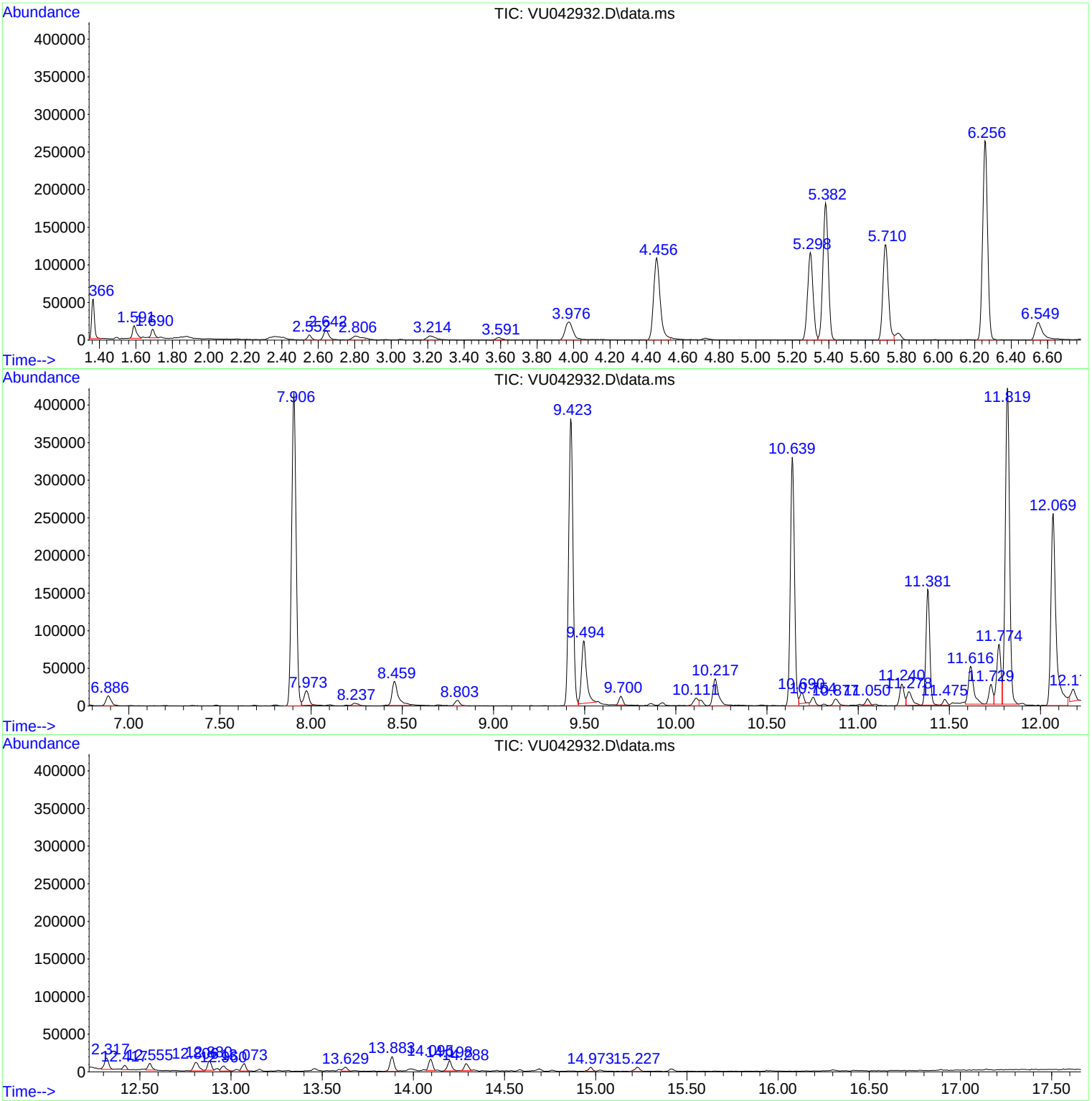
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

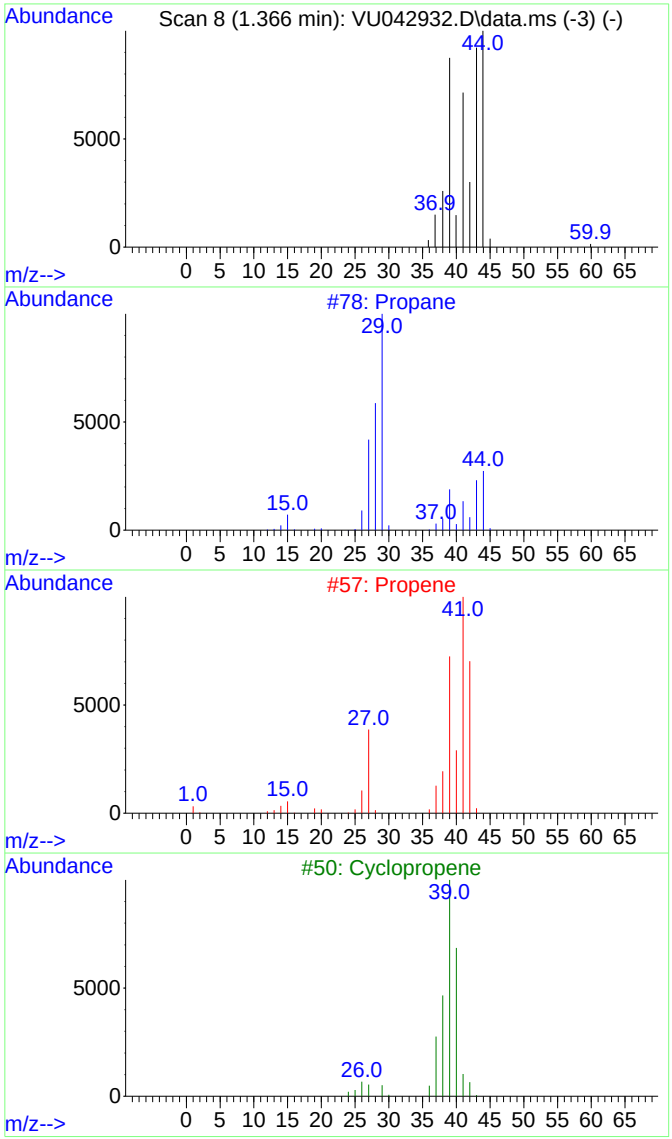
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

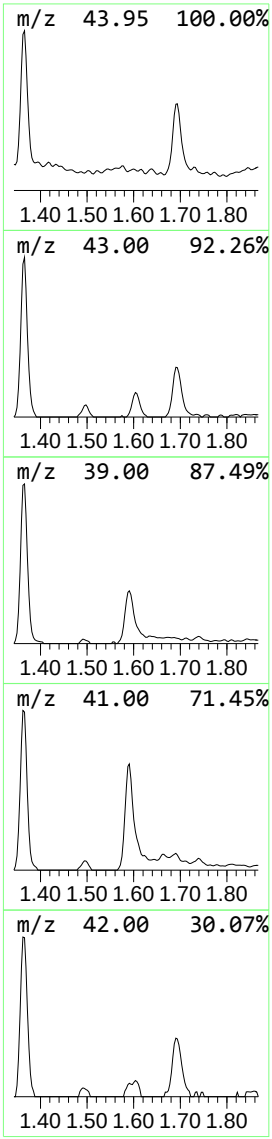
****

Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.366	7.35 ug/l	54733	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Propene	42	C3H6	000115-07-1	9
3	Cyclopropene	40	C3H4	002781-85-3	4
4	2-Isopropoxyethylamine	103	C5H13NO	081731-43-3	2
5	Alanine	89	C3H7NO2	000056-41-7	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

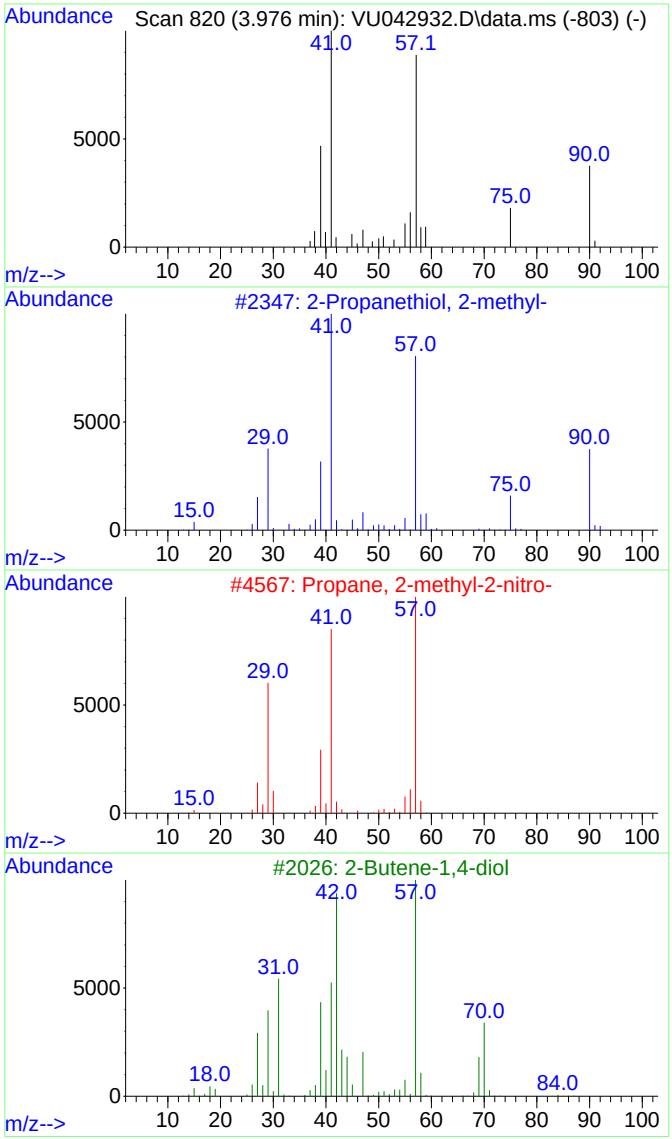
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

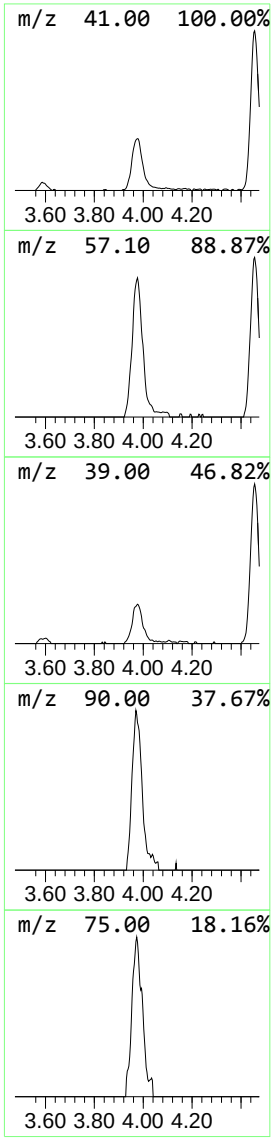
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.976	9.54 ug/l	71036	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	53
2	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
3	2-Butene-1,4-diol	88	C4H8O2	000110-64-5	23
4	2-Butanethiol	90	C4H10S	000513-53-1	9
5	Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	9





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Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

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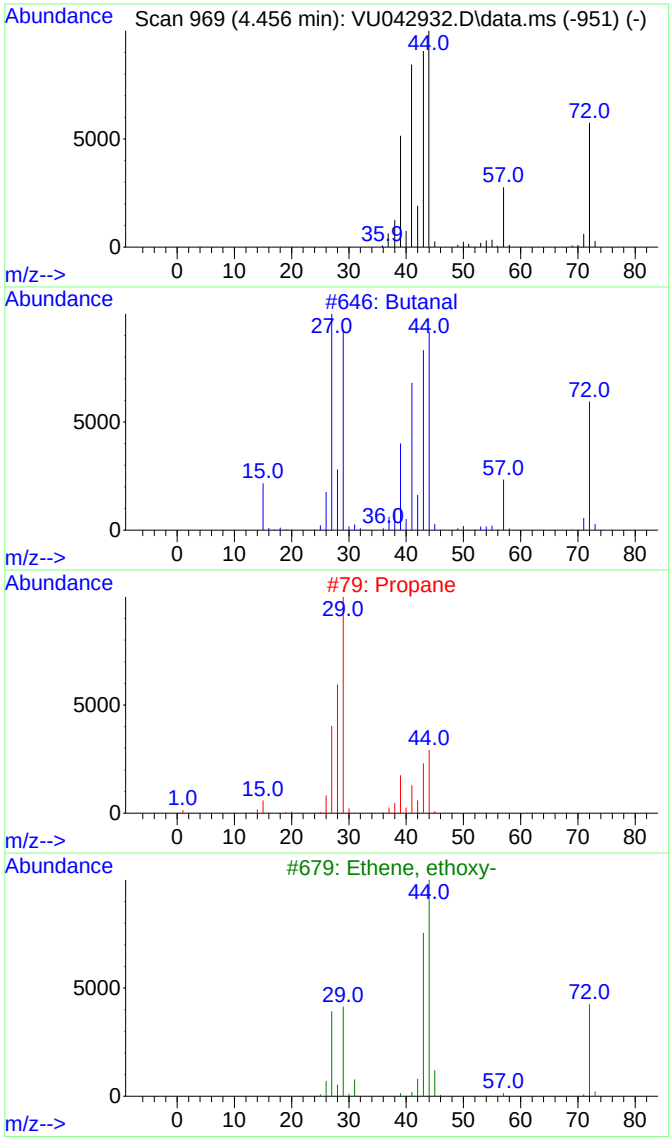
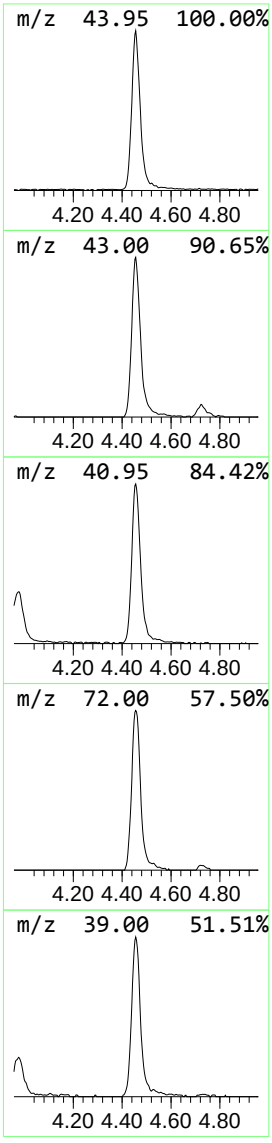
Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.456	36.59 ug/l	272503	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propane	44	C3H8	000074-98-6	59
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	Methacrolein	70	C4H6O	000078-85-3	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

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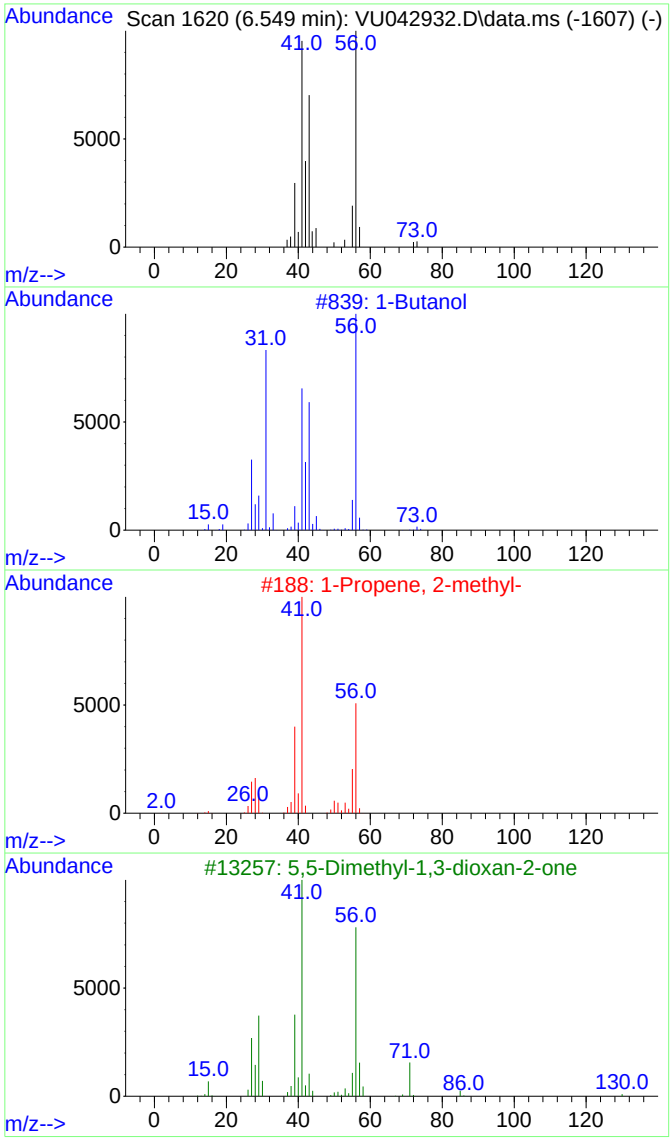
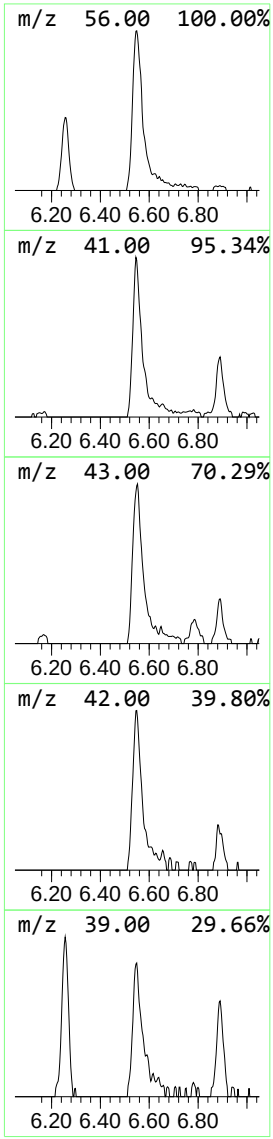
Peak Number 4 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.549	6.77 ug/l	66854	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	78
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	40
3	5,5-Dimethyl-1,3-dioxan-2-one	130	C6H10O3	003592-12-9	9
4	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
5	Cyclopropanecarboxaldehyde	70	C4H6O	001489-69-6	9





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Operator : SY/MD
Sample : M1903-03
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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

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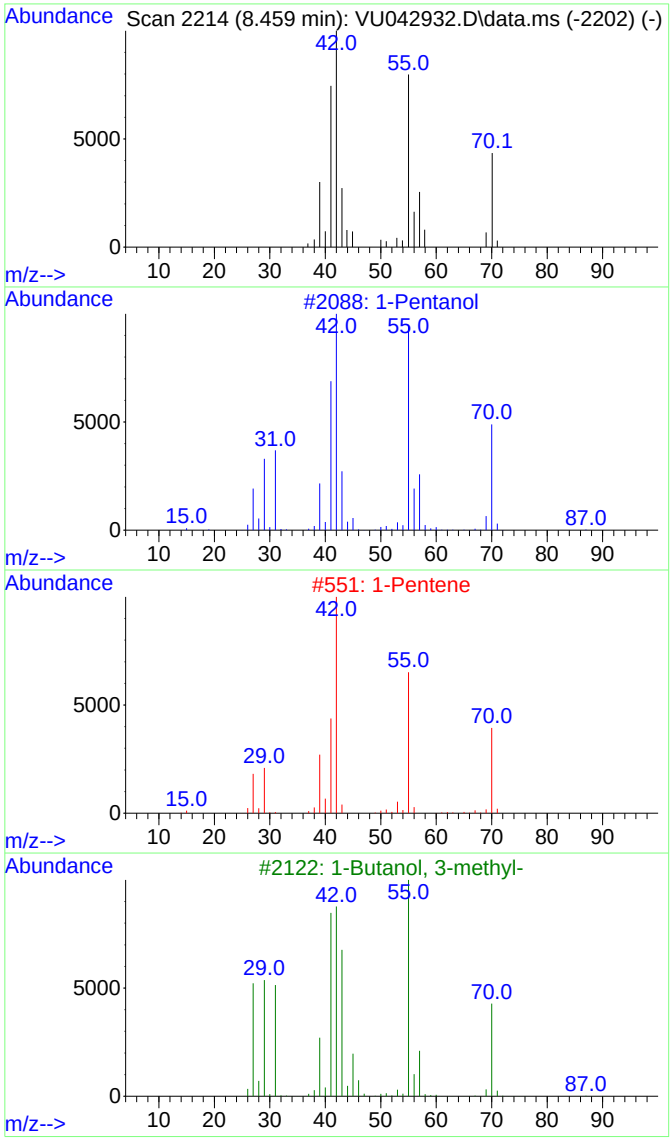
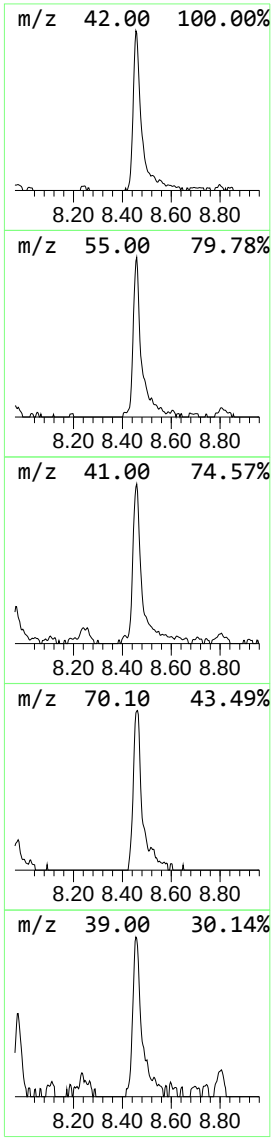
Peak Number 5 1-Pentanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.459	5.92 ug/l	75480	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	83
2	1-Pentene	70	C5H10	000109-67-1	72
3	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	64
4	Cyclopentane	70	C5H10	000287-92-3	45
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

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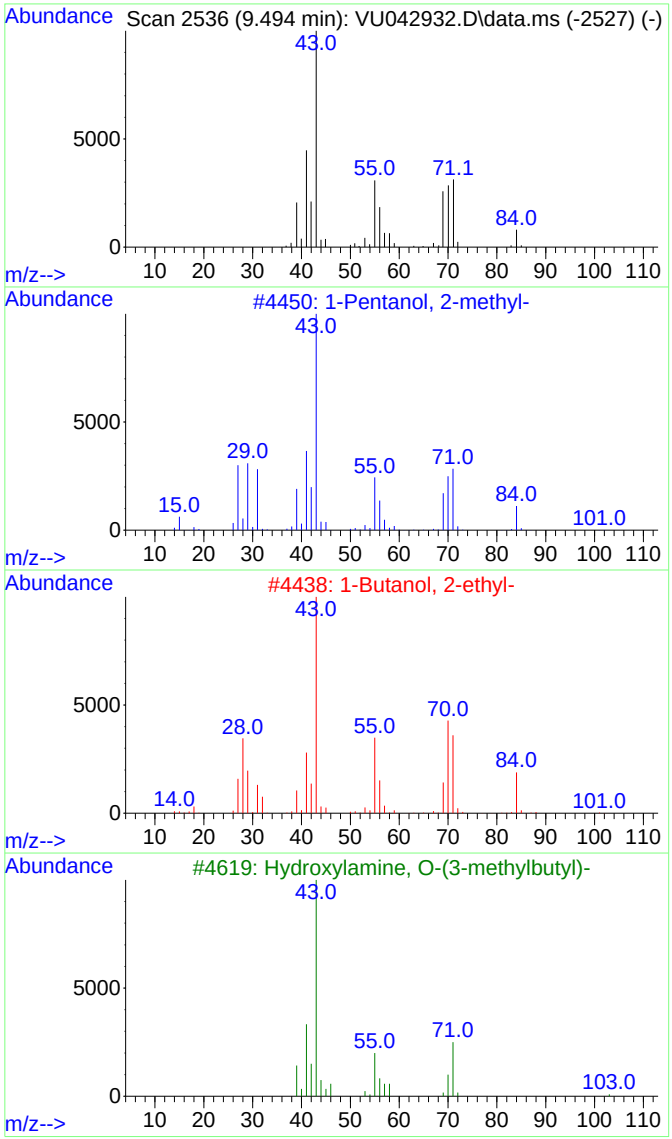
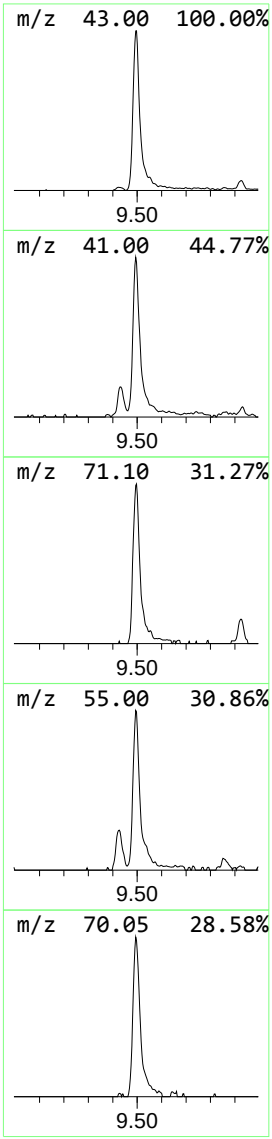
Peak Number 6 1-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.494	12.46 ug/l	158850	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	86
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	72
3	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	40
4	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	36
5	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	36





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Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

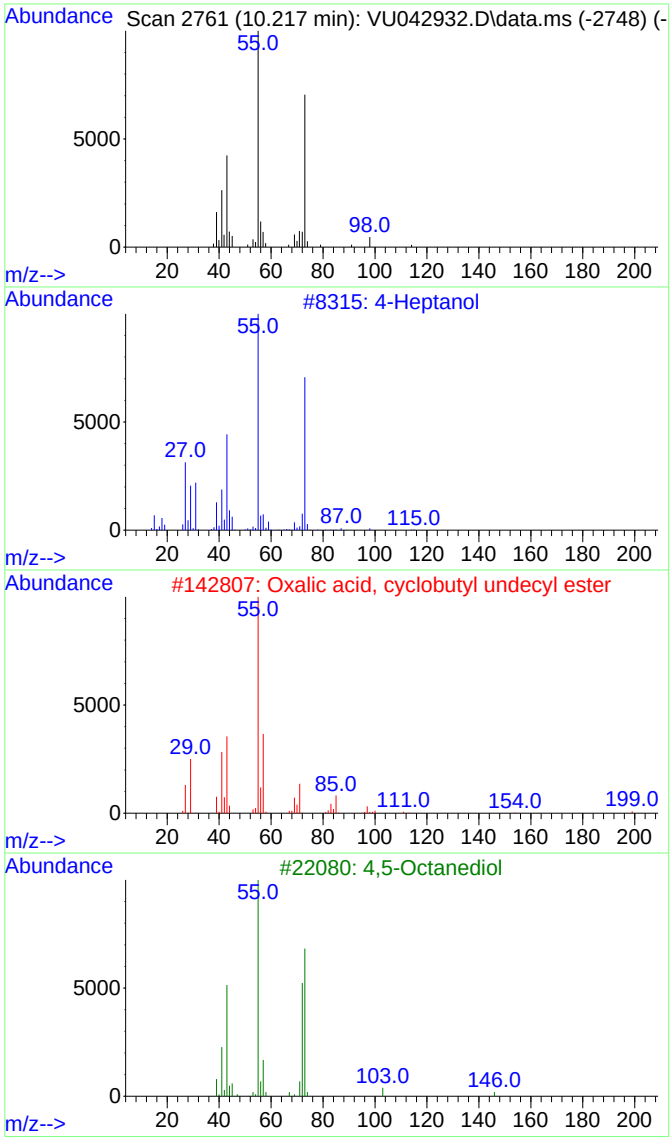
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

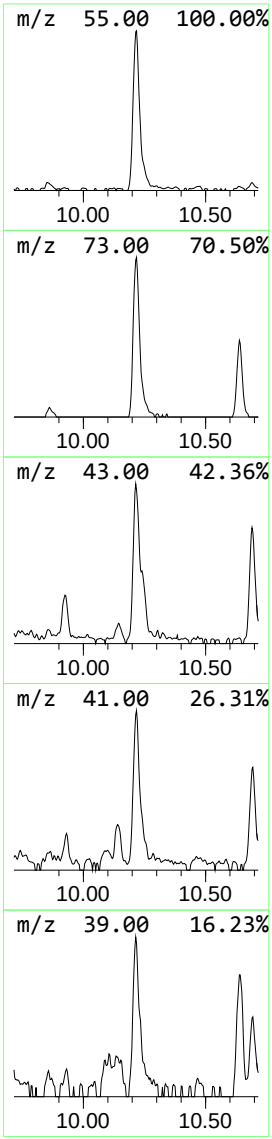
****

Peak Number 7 4-Heptanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.217	5.87 ug/l	74849	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	50
2	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	47
3	4,5-Octanediol	146	C8H18O2	022607-10-9	38
4	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	28
5	DL-4,5-Octanediol	146	C8H18O2	022520-40-7	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

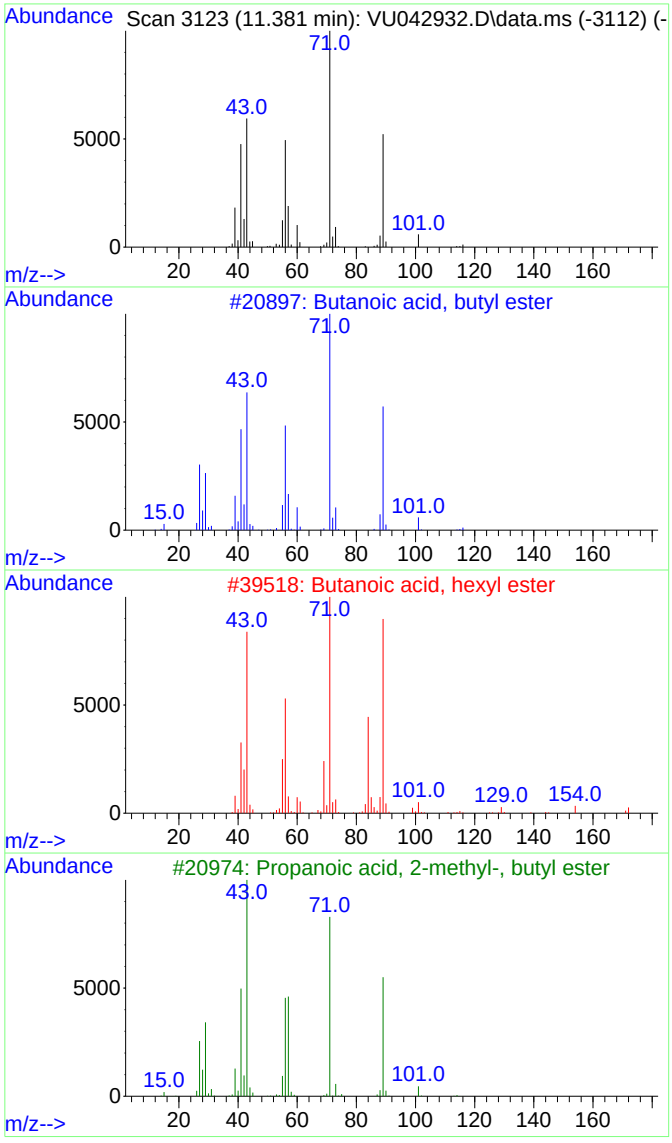
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

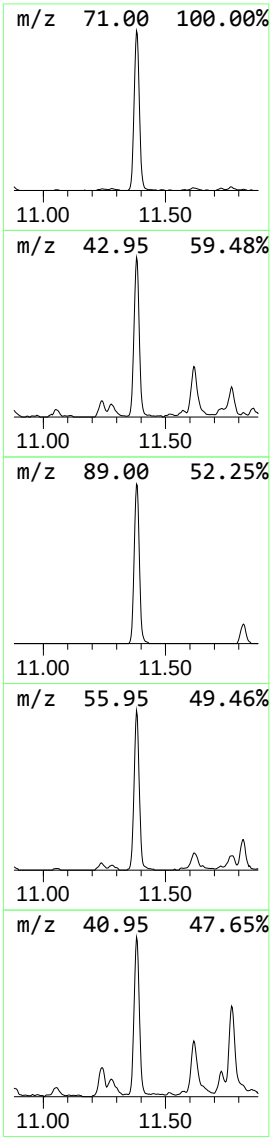
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.381	16.62 ug/l	226887	1,4-Dichlorobenzene-d4	11.819

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	74
3	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	53





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Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

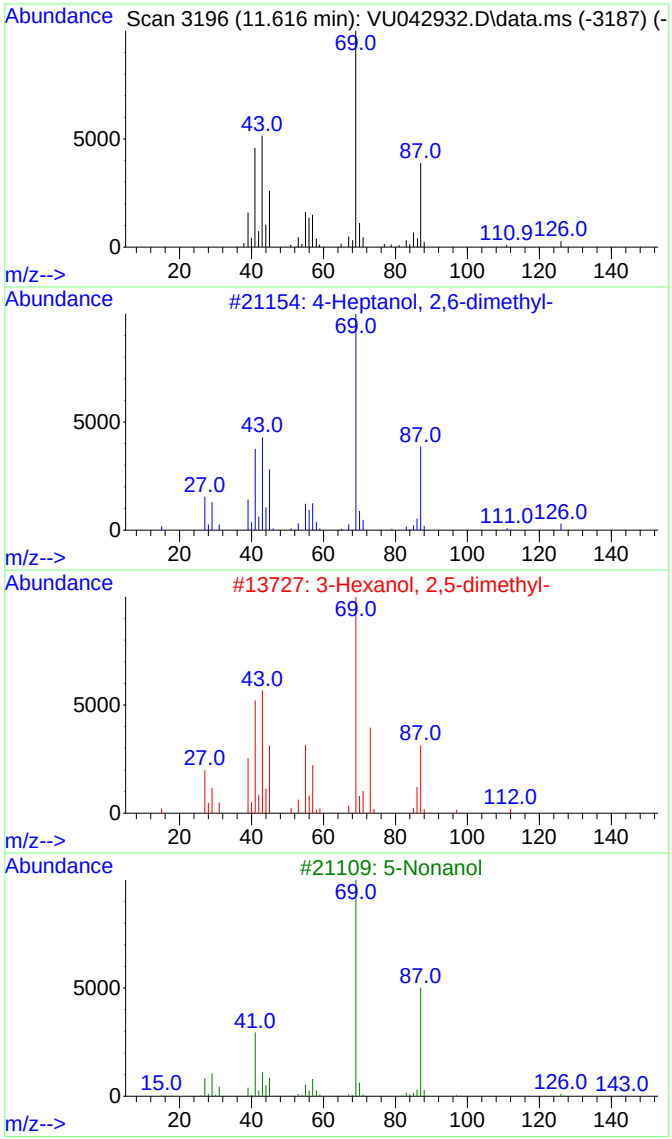
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

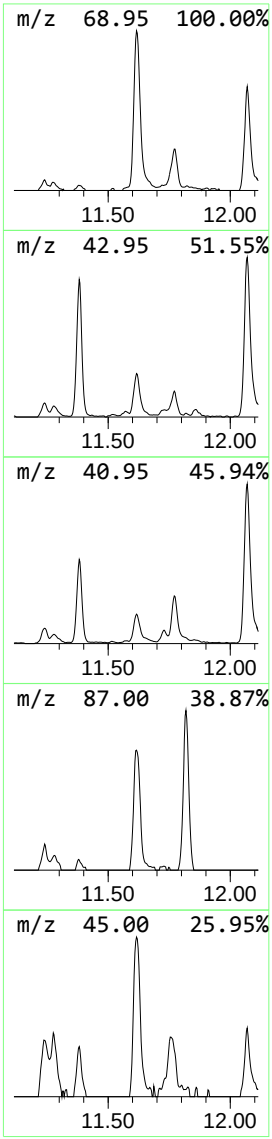
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4-Heptanol, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	7.37 ug/l	100566	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2	3-Hexanol, 2,5-dimethyl-	130	C8H18O	019550-07-3	72
3	5-Nonanol	144	C9H20O	000623-93-8	72
4	1,2-Hexanediol	118	C6H14O2	006920-22-5	72
5	1-Octyn-4-ol	126	C8H14O	052517-92-7	64





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Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

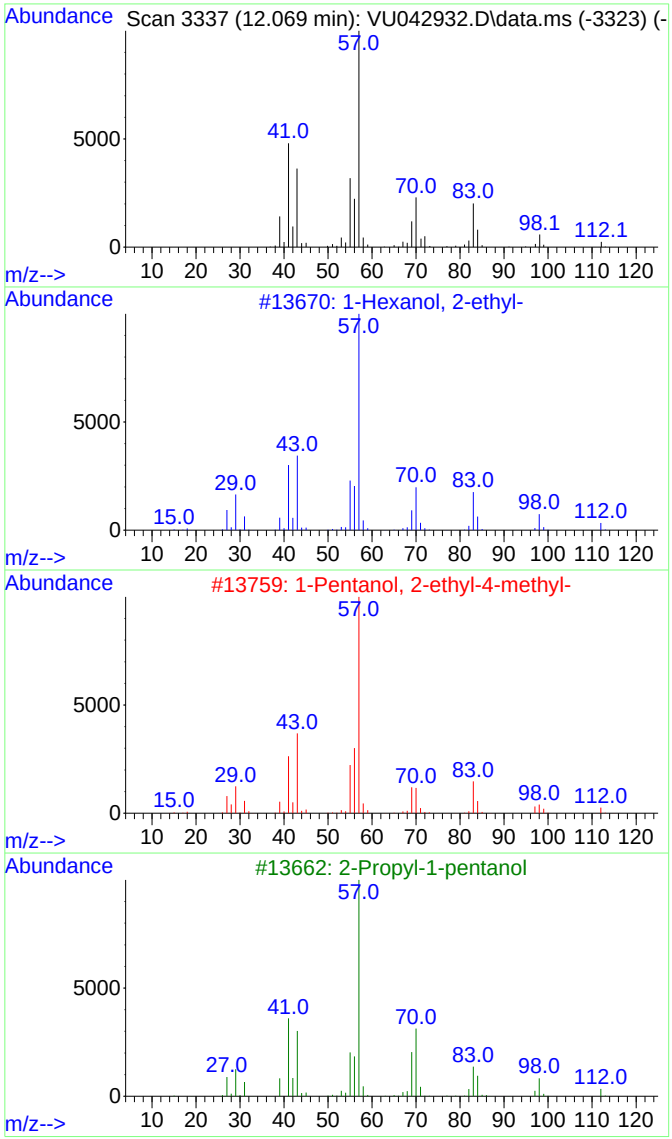
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

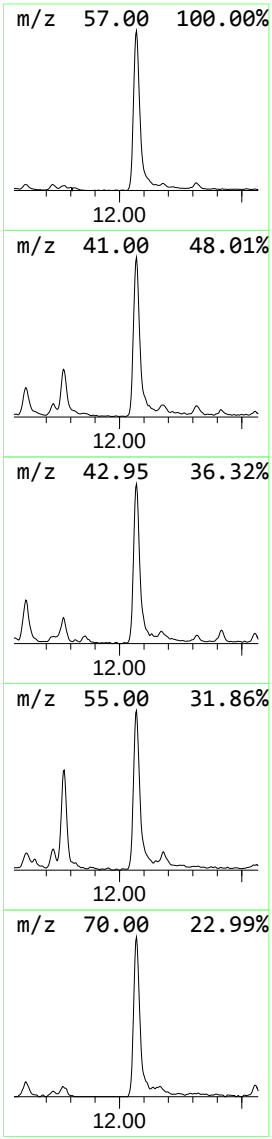
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	36.67 ug/l	500516	1,4-Dichlorobenzene-d4	11.819

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	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	45
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042932.D
Acq On : 05 Apr 2021 15:48
Operator : SY/MD
Sample : M1903-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30792

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.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
Propane	1.366	7.3	ug/l	54733	1	5.382	372403	50.0
2-Propanethiol,...	3.976	9.5	ug/l	71036	1	5.382	372403	50.0
Butanal	4.456	36.6	ug/l	272503	1	5.382	372403	50.0
1-Butanol	6.549	6.8	ug/l	66854	2	6.259	493965	50.0
1-Pentanol	8.459	5.9	ug/l	75480	3	9.423	637507	50.0
1-Pentanol, 2-m...	9.494	12.5	ug/l	158850	3	9.423	637507	50.0
4-Heptanol	10.217	5.9	ug/l	74849	3	9.423	637507	50.0
Butanoic acid, ...	11.381	16.6	ug/l	226887	4	11.819	682529	50.0
4-Heptanol, 2,6...	11.616	7.4	ug/l	100566	4	11.819	682529	50.0
1-Hexanol, 2-et...	12.069	36.7	ug/l	500516	4	11.819	682529	50.0