LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042936.D
Acq On : 05 Apr 2021 17:20
Operator : SY/MD
Sample : M1903-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31029

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: VU042936.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	17	rVB	40937	41606	1.87%	0.456%
2	2.353	297	315	351	rVB3	8271	42973	1.94%	0.471%
3	2.639	392	404	415	rBV	16369	31377	1.41%	0.344%
4	2.803	438	455	459	rBV2	12021	26253	1.18%	0.288%
5	4.456	954	969	993	rBV4	45065	113290	5.10%	1.242%
6	5.298	1216	1231	1244	rBV	118167	252209	11.36%	2.765%
7	5.382	1244	1257	1276	rVB	191332	391353	17.63%	4.291%
8	5.710	1344	1359	1394	rBV	135058	311997	14.06%	3.421%
9	6.256	1513	1529	1544	rBV	280615	527409	23.76%	5.783%
10	6.543	1603	1618	1644	rBV	72890	202723	9.13%	2.223%
11	6.883	1707	1724	1738	rBV6	9709	26819	1.21%	0.294%
12	7.906	2028	2042	2054	rBV	435723	743923	33.51%	8.156%
13	7.967	2054	2061	2081	rVB6	20038	43042	1.94%	0.472%
14	8.452	2191	2212	2253	rBV	99687	228909	10.31%	2.510%
15	9.423	2501	2514	2525	rBV	406975	668983	30.14%	7.335%
16	9.491	2525	2535	2578	rVB	315994	576235	25.96%	6.318%
17	10.214	2746	2760	2779	rBV	112443	201261	9.07%	2.207%
18	10.639	2879	2892	2902	rBV	353622	553082	24.92%	6.064%
19	10.690	2902	2908	2922	rVB2	28114	44130	1.99%	0.484%
20	11.237	3066	3078	3084	rBV	56332	88278	3.98%	0.968%
21	11.275	3085	3090	3110	rVV2	44275	80847	3.64%	0.886%
22	11.382	3111	3123	3144	rVB	331754	480981	21.67%	5.274%
23	11.613	3186	3195	3220	rVB	107775	198192	8.93%	2.173%
24	11.729	3221	3231	3238	rBV3	46135	81651	3.68%	0.895%
25	11.819	3248	3259	3278	rVB	446532	718892	32.39%	7.882%
26	12.066	3321	3336	3362	rBV	1309861	2219694	100.00%	24.337%
27	12.179	3364	3371	3394	rVB7	42739	100591	4.53%	1.103%
28	12.555	3482	3488	3501	rVB3	27535	44015	1.98%	0.483%
29	14.198	3988	3999	4016	rBV2	23415	42107	1.90%	0.462%
30	14.291	4016	4028	4041	rVV3	22856	37830	1.70%	0.415%

Sum of corrected areas: 9120652

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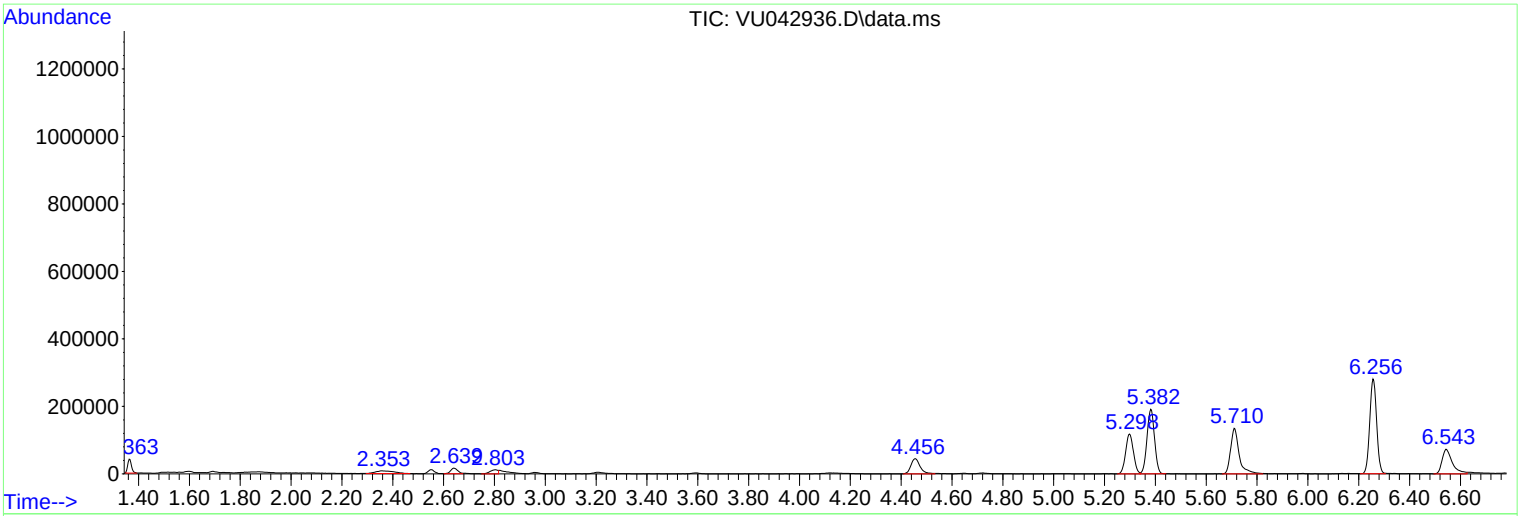
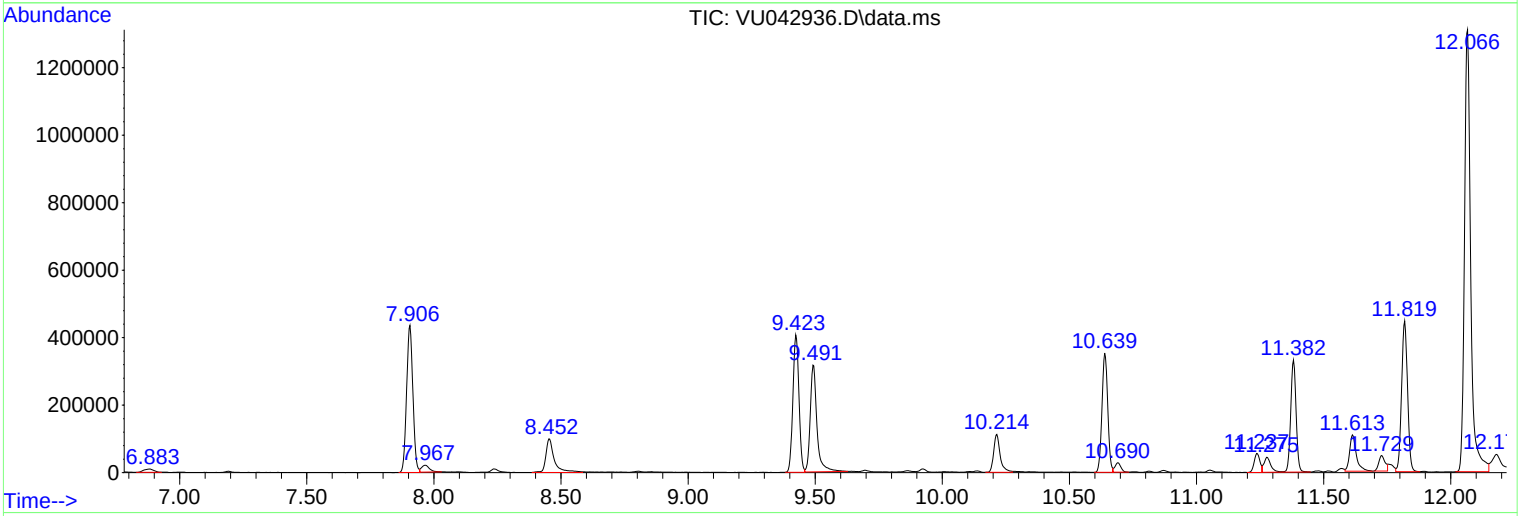
ALS Vial : 16 Sample Multiplier: 1

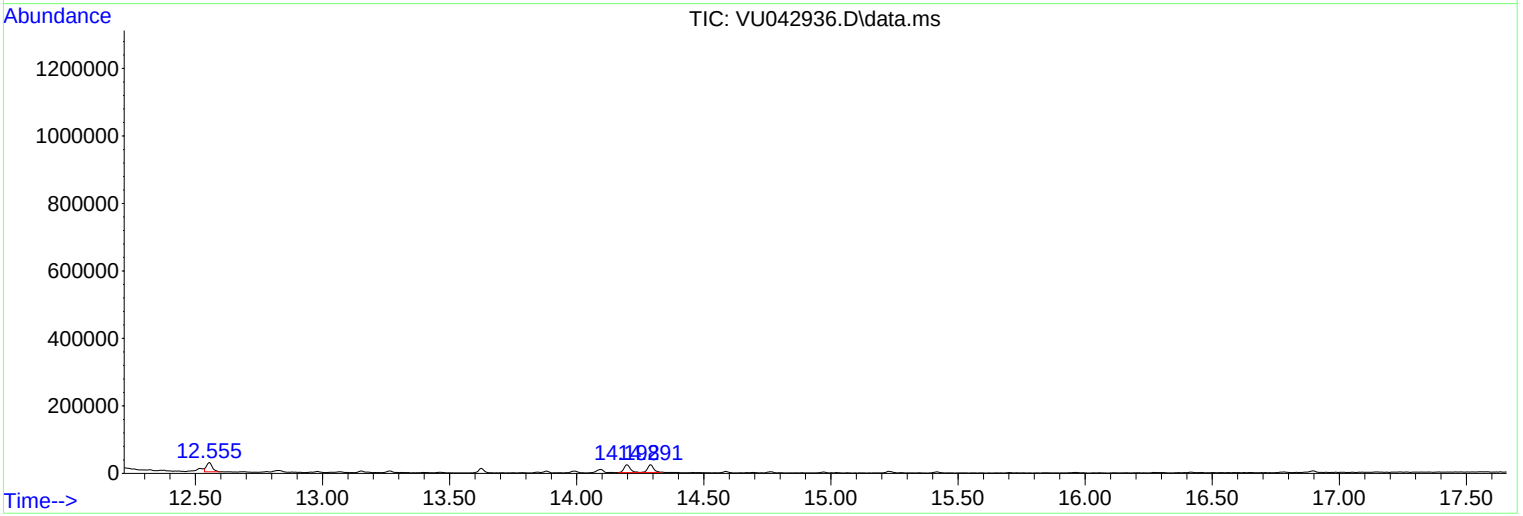
Instrument :
MSVOA_U
ClientSampleId :
31029

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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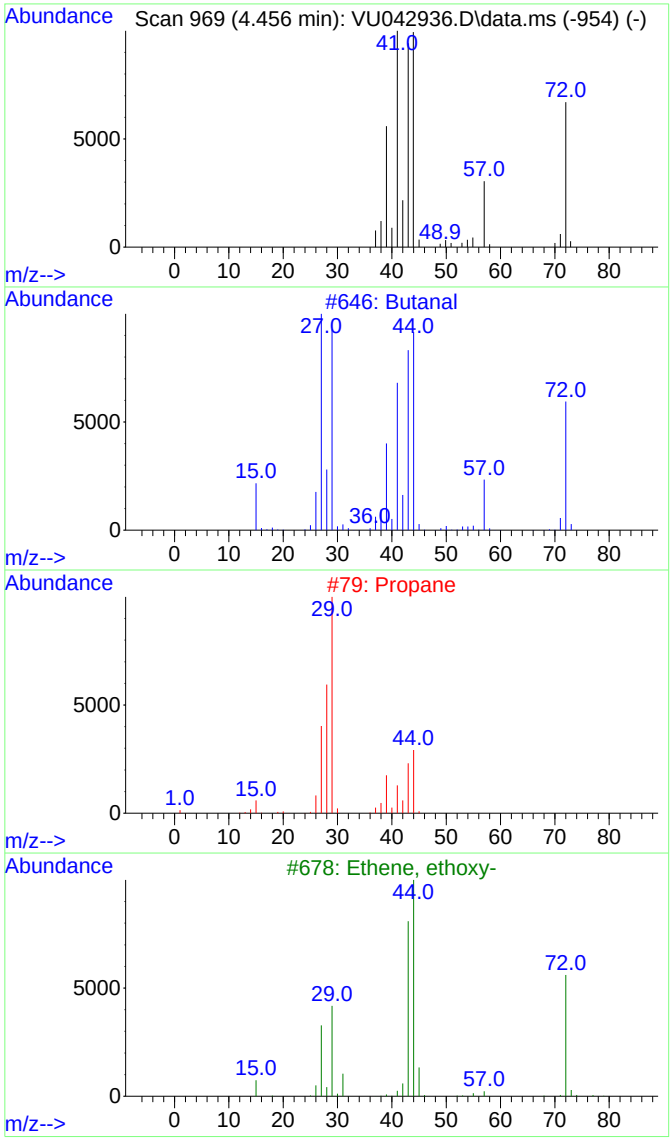
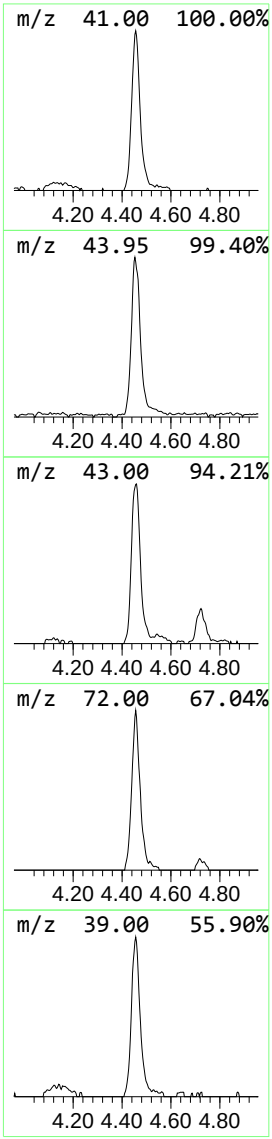
****

Peak Number 1 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.456	14.47 ug/l	113290	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	47
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	35
5	Methacrolein	70	C4H6O	000078-85-3	27





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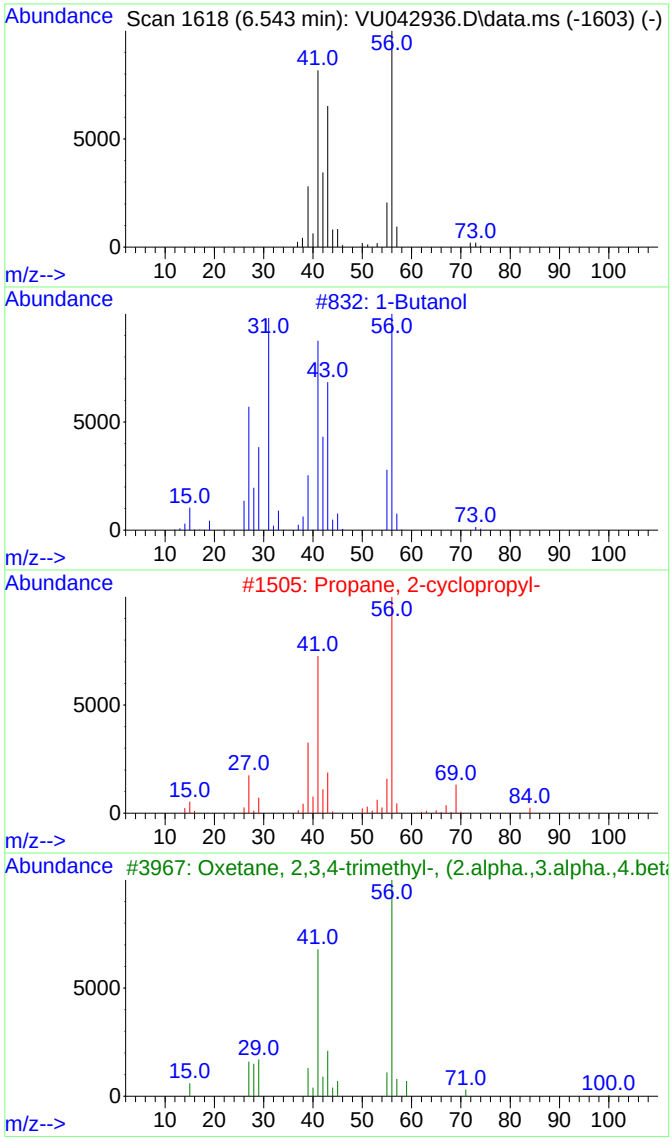
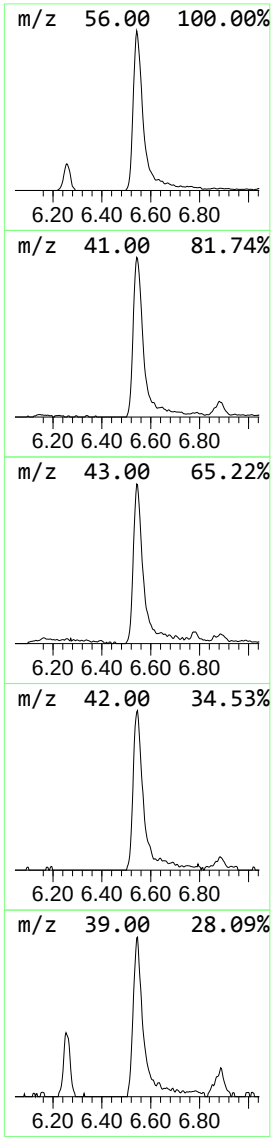
Peak Number 2 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.543	19.22 ug/l	202723	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
4	Isobutylene epoxide	72	C4H8O	000558-30-5	9
5	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9





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Operator : SY/MD
Sample : M1903-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31029

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

TIC Library : C:\DATABASE\NIST11.L
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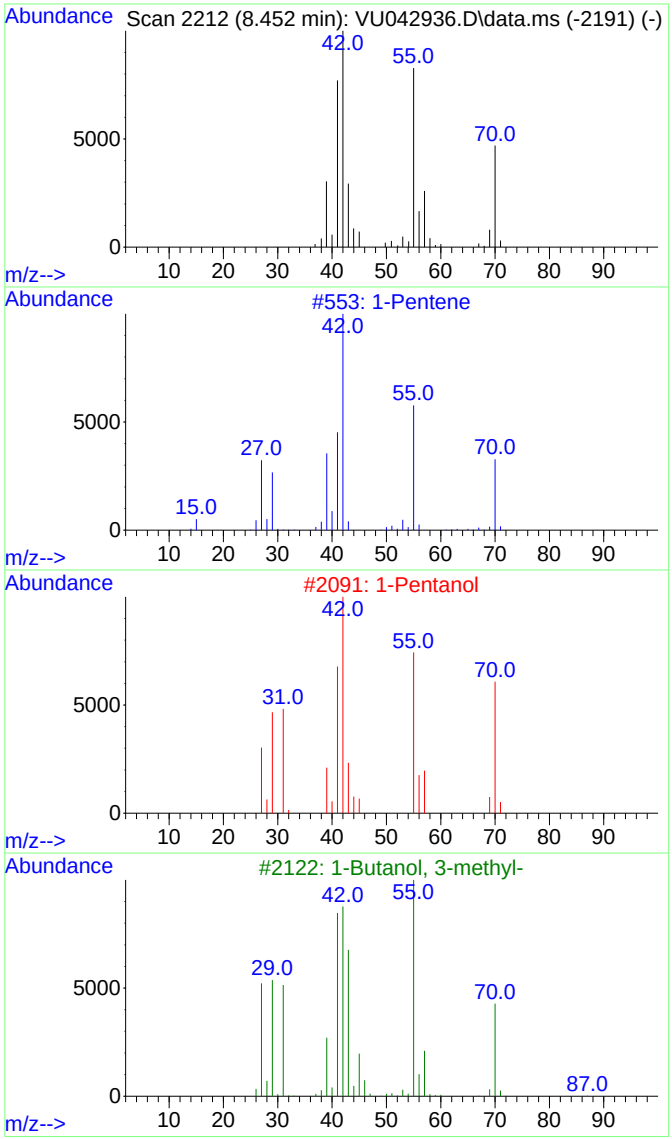
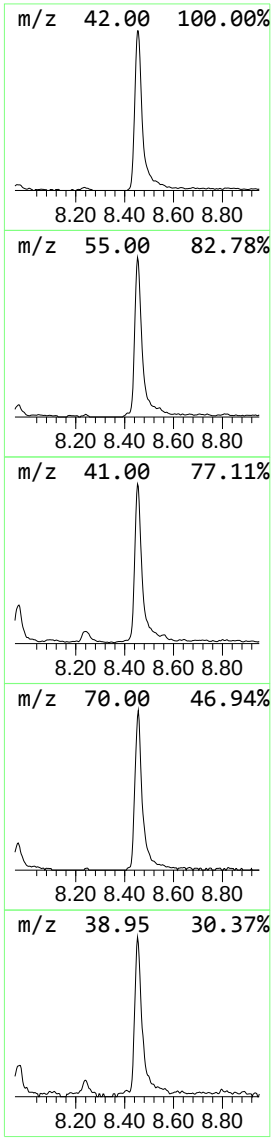
Peak Number 3 1-Pentene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.452	17.11 ug/l	228909	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	72
2	1-Pentanol	88	C5H12O	000071-41-0	72
3	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	50
4	2-Pentene	70	C5H10	000109-68-2	38
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	38





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Sample : M1903-07
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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31029

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

TIC Library : C:\DATABASE\NIST11.L
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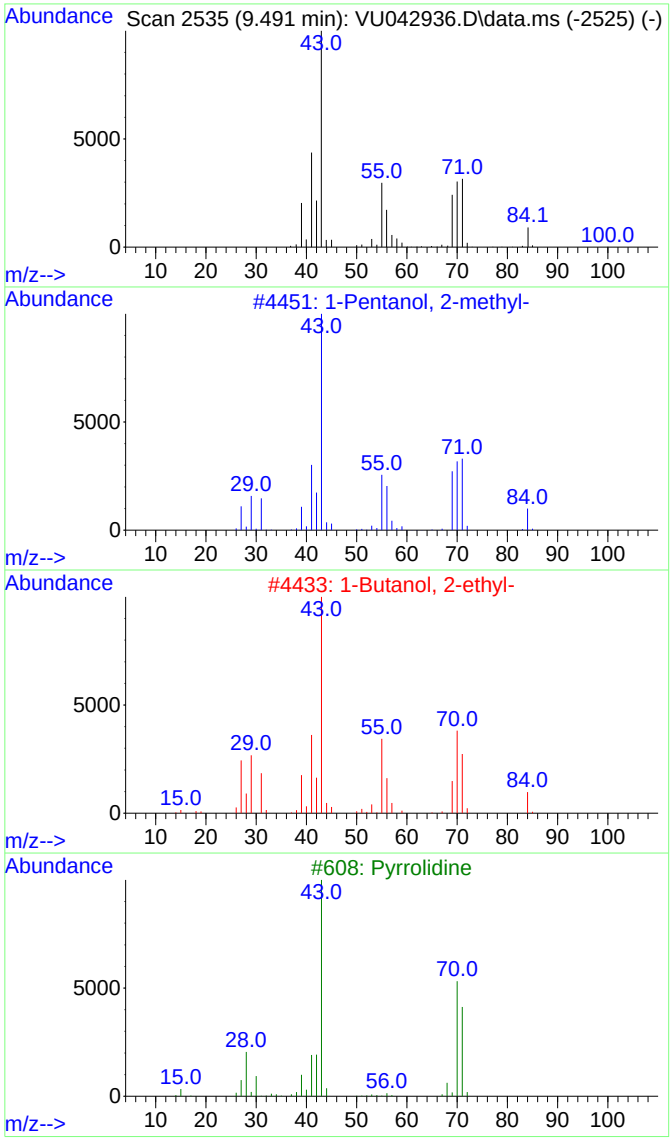
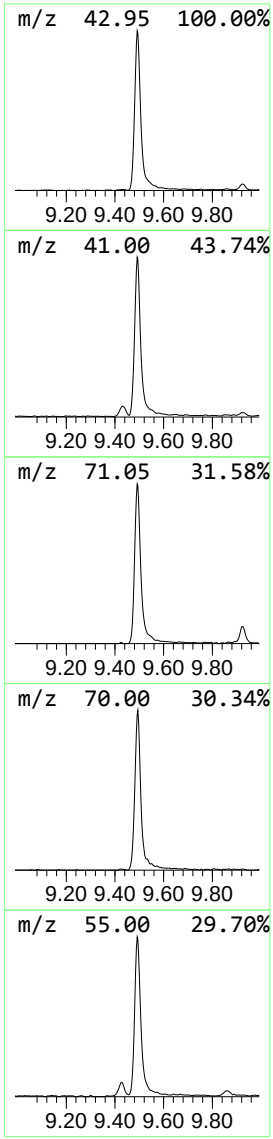
****
Peak Number 4 1-Pentanol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.491	43.07 ug/l	576235	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
3	Pyrrolidine	71	C4H9N	000123-75-1	42
4	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	42
5	Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	40





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Instrument : MSVOA_U
ClientSampleId : 31029

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
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TIC Library : C:\DATABASE\NIST11.L
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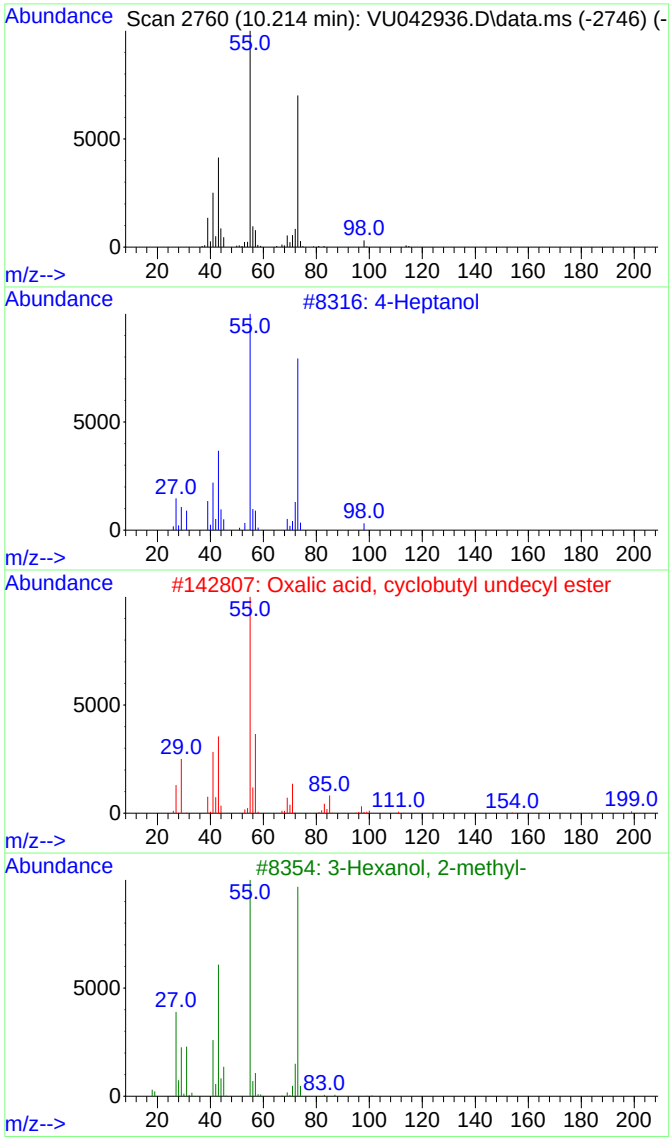
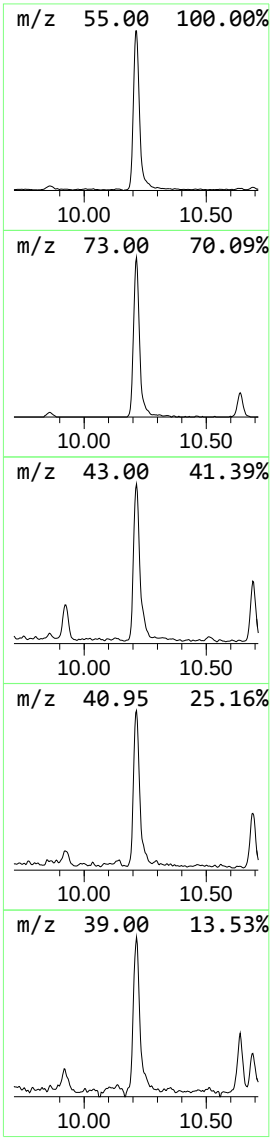
****

Peak Number 5 4-Heptanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.214	15.04 ug/l	201261	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	86
2	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	43
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37
4	Oxalic acid, cyclobutyl heptyl e...	242	C13H22O4	1000309-69-8	37
5	Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	37





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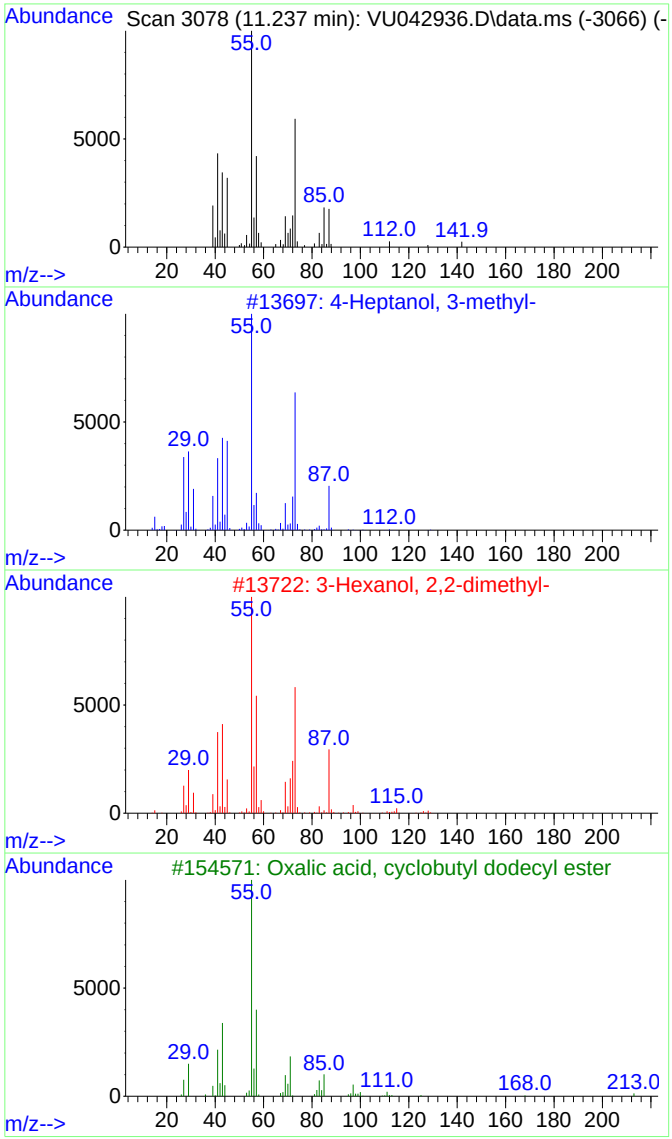
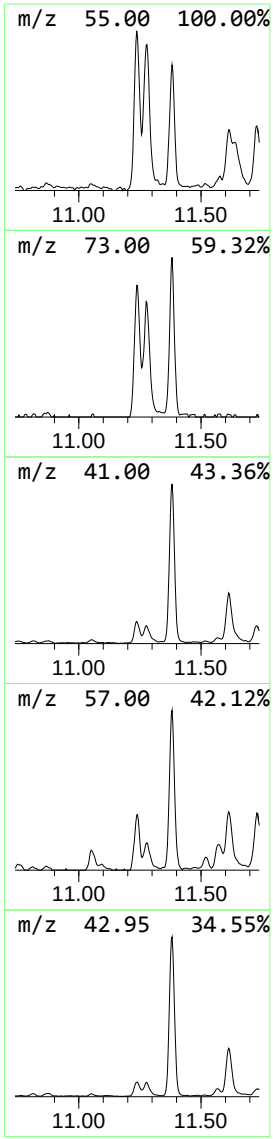
****
Peak Number 6 4-Heptanol, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.237	6.14 ug/l	88278	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	80
2	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	39
3	Oxalic acid, cyclobutyl dodecyl ...	312	C18H32O4	1000309-70-3	38
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37
5	Pentane, 1-(2-butenyloxy)-, (E)-	142	C9H18O	054004-26-1	35





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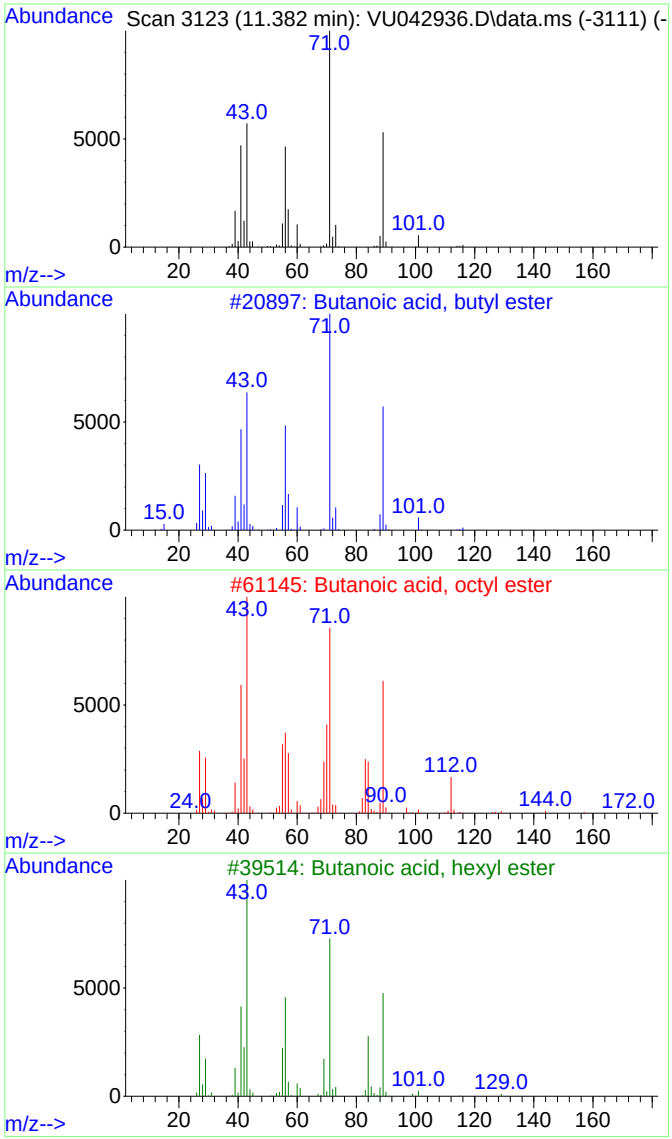
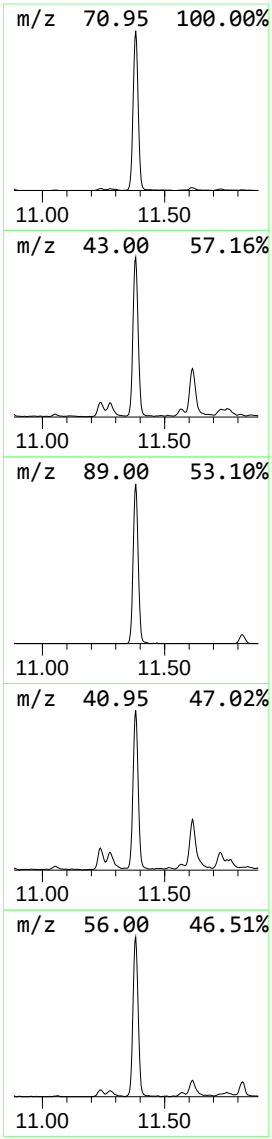
****
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.382	33.45 ug/l	480981	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, octyl ester	200	C12H24O2	000110-39-4	72
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	56





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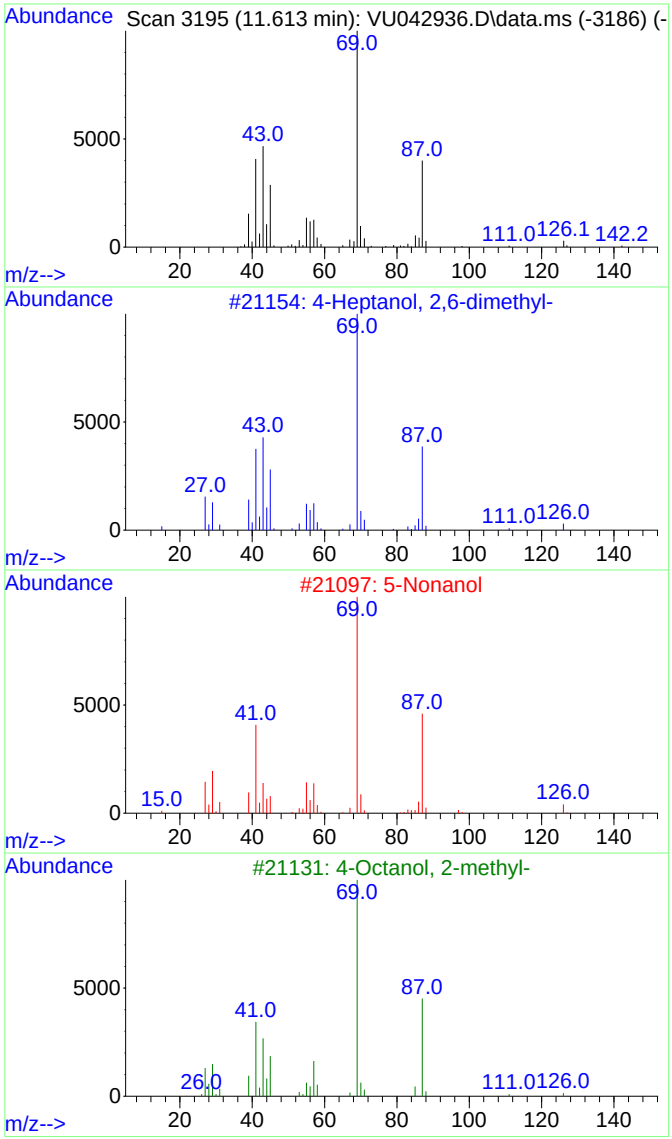
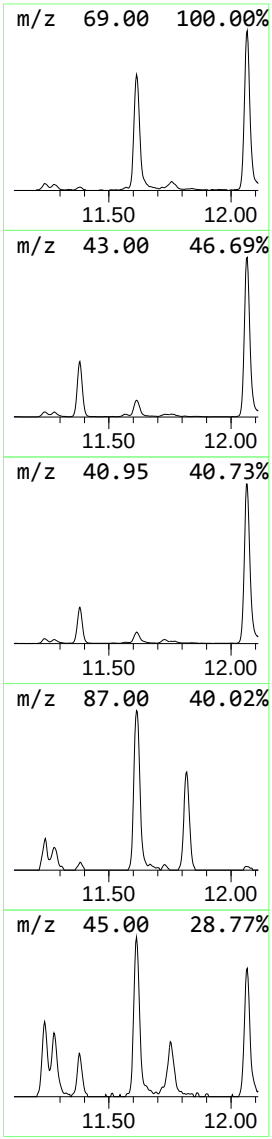
****
Peak Number 8 4-Heptanol, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.613	13.78 ug/l	198192	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	90
2	5-Nonanol	144	C9H20O	000623-93-8	78
3	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	78
4	5-Decanol	158	C10H22O	005205-34-5	72
5	3-Hexanol, 2,5-dimethyl-	130	C8H18O	019550-07-3	72





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Sample : M1903-07
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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
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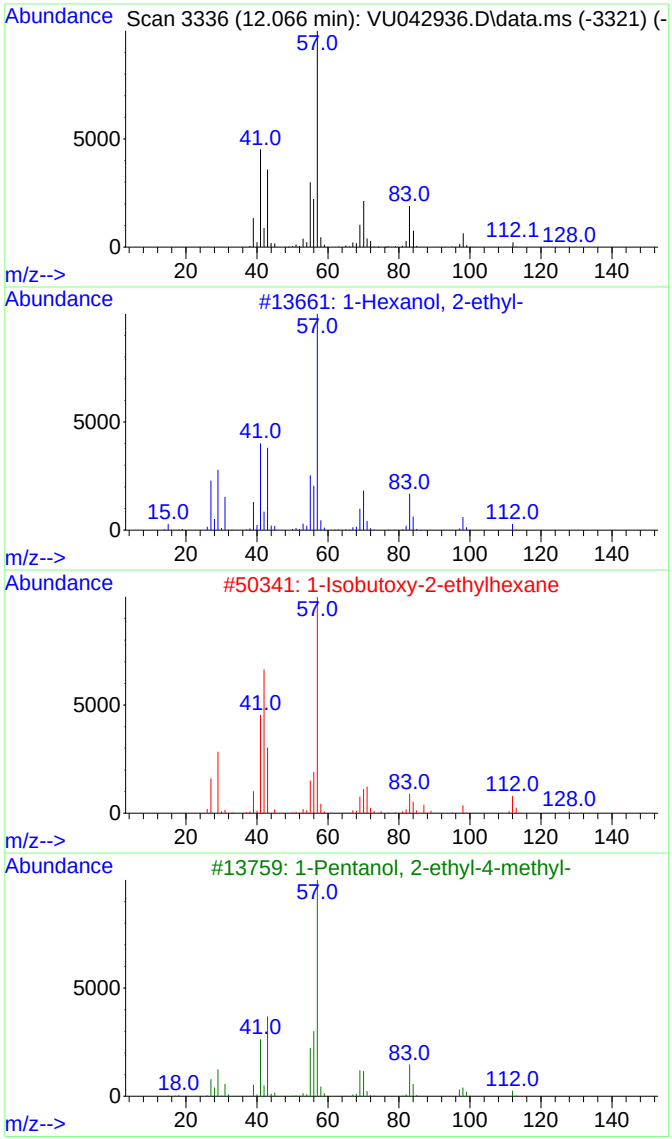
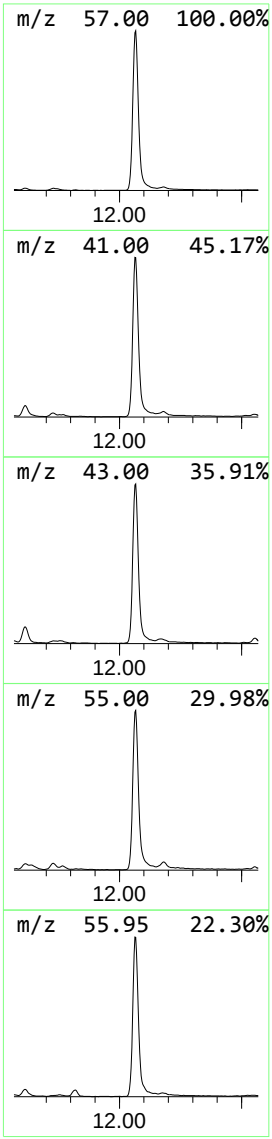
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.067	154.38 ug/l	2219690	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	83
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5	Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042936.D
Acq On : 05 Apr 2021 17:20
Operator : SY/MD
Sample : M1903-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31029

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

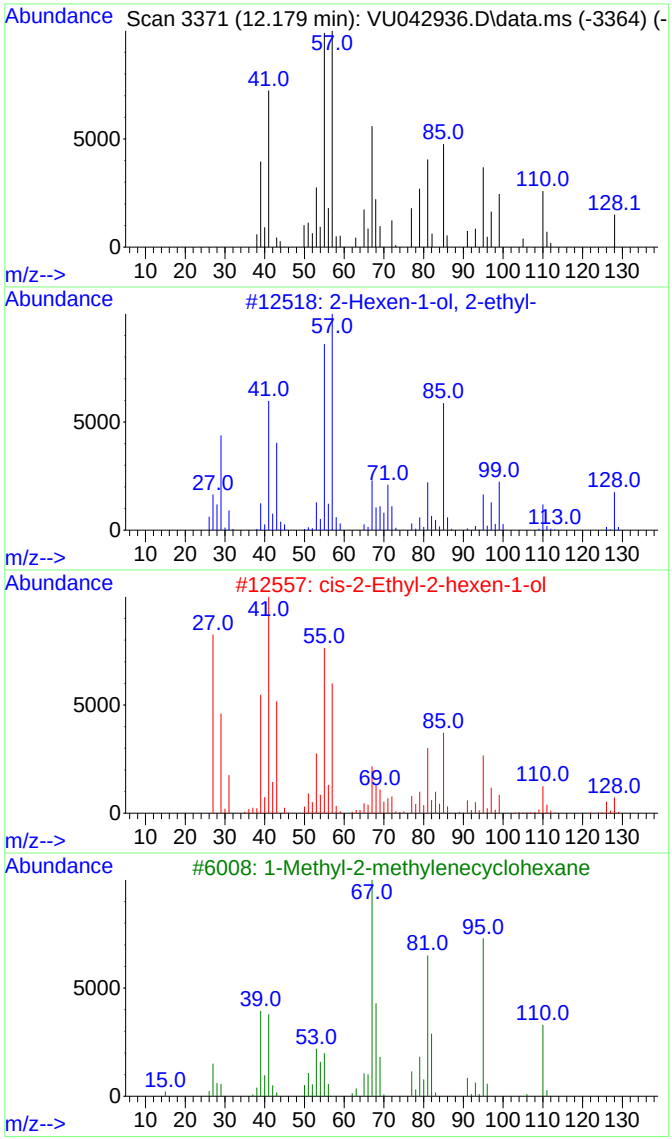
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

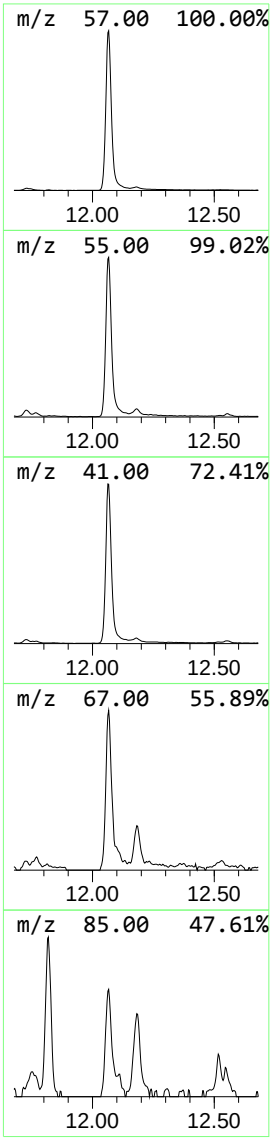
****

Peak Number 10 2-Hexen-1-ol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.179	7.00 ug/l	100591	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexen-1-ol, 2-ethyl-	128	C8H16O	050639-00-4	53
2	cis-2-Ethyl-2-hexen-1-ol	128	C8H16O	1000139-52-4	46
3	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	45
4	1-Methylcycloheptene	110	C8H14	055308-20-8	43
5	Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042936.D
Acq On : 05 Apr 2021 17:20
Operator : SY/MD
Sample : M1903-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31029

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
Butanal	4.456	14.5	ug/l	113290	1	5.382	391353	50.0
1-Butanol	6.543	19.2	ug/l	202723	2	6.256	527409	50.0
1-Pentene	8.452	17.1	ug/l	228909	3	9.423	668983	50.0
1-Pentanol, 2-m...	9.491	43.1	ug/l	576235	3	9.423	668983	50.0
4-Heptanol	10.214	15.0	ug/l	201261	3	9.423	668983	50.0
4-Heptanol, 3-m...	11.237	6.1	ug/l	88278	4	11.819	718892	50.0
Butanoic acid, ...	11.382	33.5	ug/l	480981	4	11.819	718892	50.0
4-Heptanol, 2,6...	11.613	13.8	ug/l	198192	4	11.819	718892	50.0
1-Hexanol, 2-et...	12.067	154.4	ug/l	2219690	4	11.819	718892	50.0
2-Hexen-1-ol, 2...	12.179	7.0	ug/l	100591	4	11.819	718892	50.0