LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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: VU042937.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	17	rVB	40396	41154	3.02%	0.540%
2	2.639	391	404	429	rVV	58591	115385	8.45%	1.515%
3	4.115	846	863	866	rBV6	6639	15634	1.15%	0.205%
4	4.456	952	969	992	rBV2	37098	94828	6.95%	1.245%
5	5.298	1214	1231	1244	rBV	119544	253322	18.56%	3.325%
6	5.382	1244	1257	1278	rVB	191813	394062	28.87%	5.173%
7	5.710	1343	1359	1393	rBV	136097	313112	22.94%	4.110%
8	6.256	1513	1529	1550	rBV	280170	529527	38.80%	6.951%
9	6.546	1603	1619	1645	rBV2	58951	163135	11.95%	2.141%
10	6.867	1706	1719	1739	rBV7	9121	24817	1.82%	0.326%
11	7.906	2028	2042	2054	rBV	436199	749716	54.93%	9.841%
12	7.964	2054	2060	2077	rVB6	17765	37679	2.76%	0.495%
13	8.237	2133	2145	2161	rBV3	9037	17821	1.31%	0.234%
14	8.456	2202	2213	2237	rBV2	51334	109978	8.06%	1.444%
15	9.423	2501	2514	2525	rBV	409046	668231	48.96%	8.772%
16	9.491	2525	2535	2571	rVB	257265	478213	35.04%	6.277%
17	9.925	2660	2670	2680	rVB	30270	46882	3.44%	0.615%
18	10.214	2749	2760	2781	rBV	99581	181043	13.27%	2.376%
19	10.639	2880	2892	2902	rBV	350810	552308	40.47%	7.250%
20	10.690	2902	2908	2922	rVB	34349	53960	3.95%	0.708%
21	11.240	3065	3079	3085	rBV	53156	86949	6.37%	1.141%
22	11.279	3085	3091	3113	rVV2	41531	79867	5.85%	1.048%
23	11.382	3113	3123	3134	rVB	30332	44963	3.29%	0.590%
24	11.565	3169	3180	3186	rBV3	18898	31161	2.28%	0.409%
25	11.613	3186	3195	3219	rVV2	109058	213437	15.64%	2.802%
26	11.726	3220	3230	3248	rVV	64503	130822	9.59%	1.717%
27	11.819	3248	3259	3274	rVB	447934	707344	51.83%	9.285%
28	12.066	3319	3336	3364	rBV	767733	1364780	100.00%	17.915%
29	12.179	3367	3371	3385	rVB6	20526	37849	2.77%	0.497%
30	12.822	3563	3571	3582	rVB7	7469	14595	1.07%	0.192%
31	14.198	3986	3999	4013	rBV2	19730	34094	2.50%	0.448%
32	14.291	4018	4028	4037	rBV3	20274	31498	2.31%	0.413%

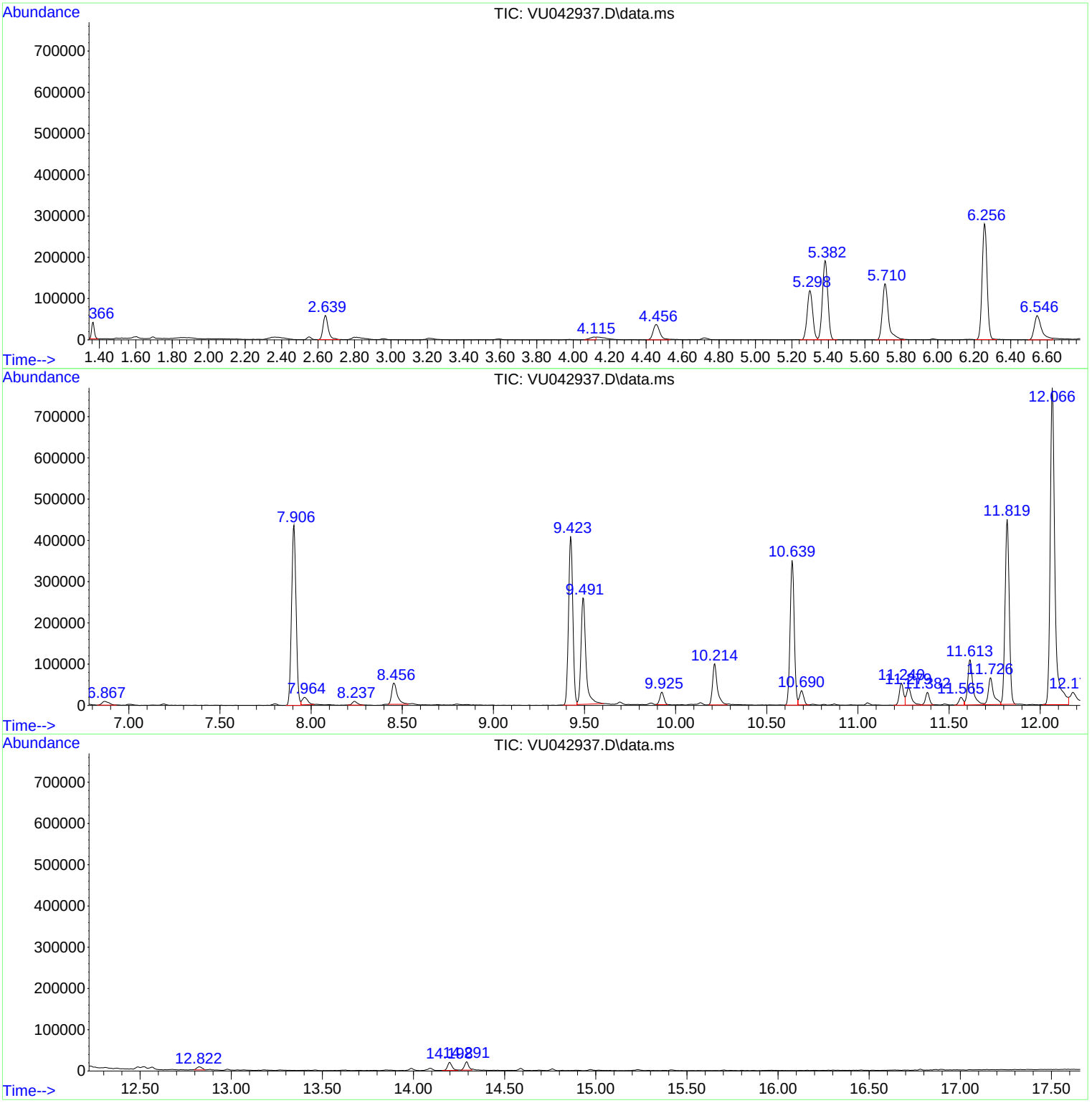
Sum of corrected areas: 7618166

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31030

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 : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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

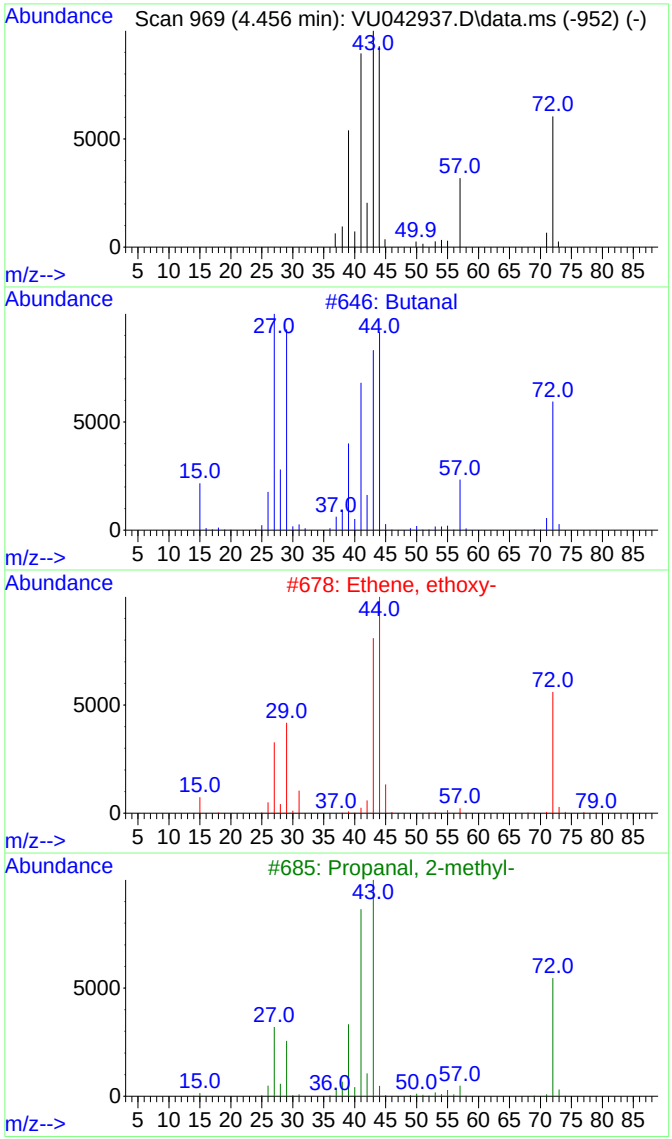
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

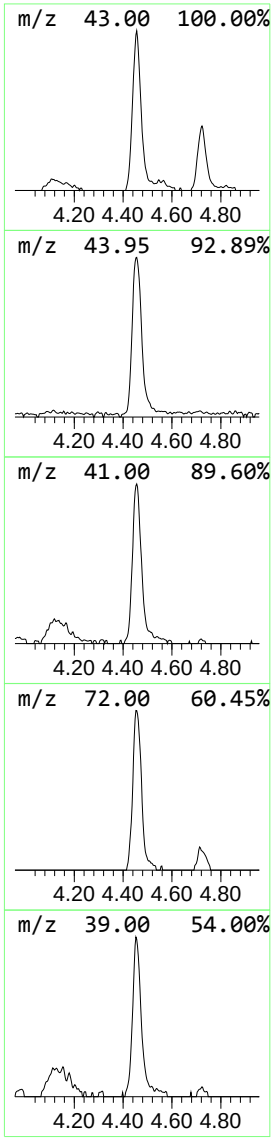
****

Peak Number 1 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.456	12.03 ug/l	94828	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25
5	Methacrolein	70	C4H6O	000078-85-3	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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

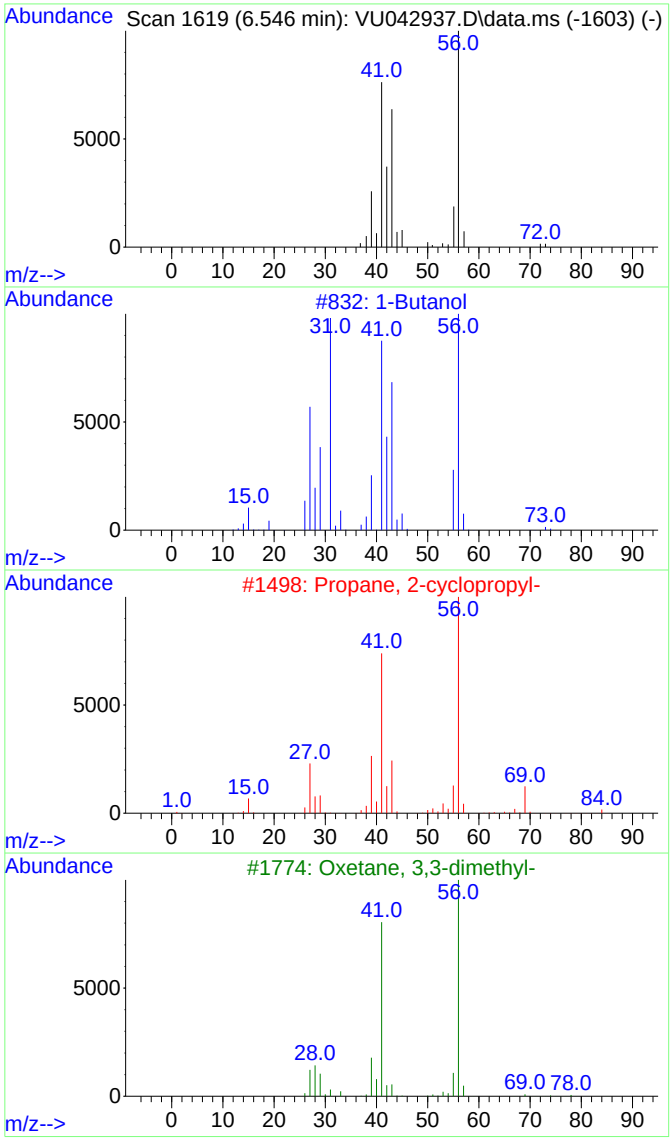
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

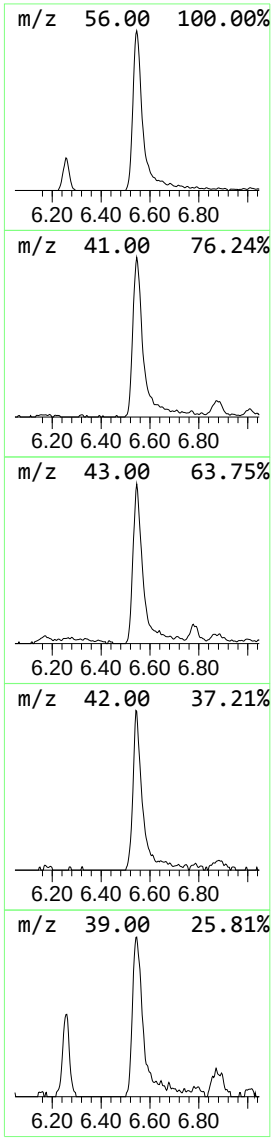
****

Peak Number 2 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.546	15.40 ug/l	163135	1,4-Difluorobenzene	6.256

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	38
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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

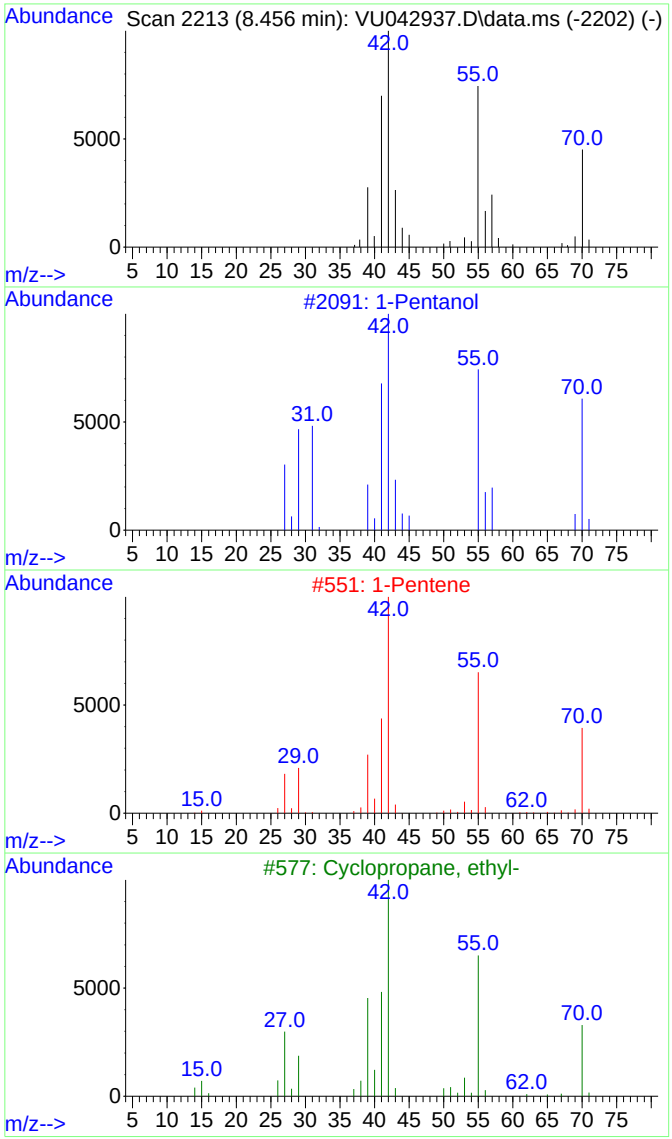
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

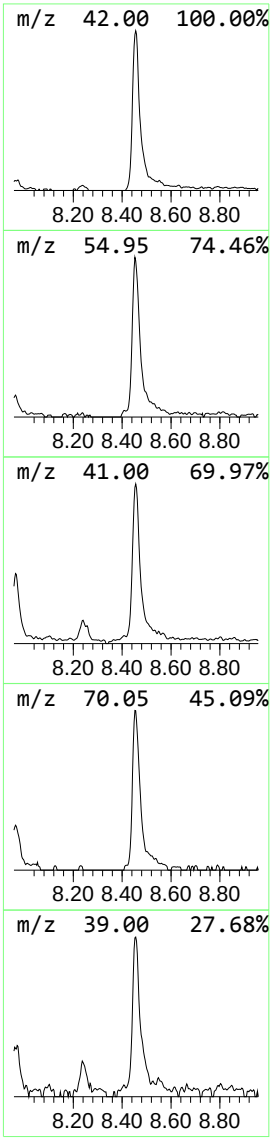
****

Peak Number 3 1-Pentanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.456	8.23 ug/l	109978	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	86
2	1-Pentene	70	C5H10	000109-67-1	80
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
4	Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	40
5	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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

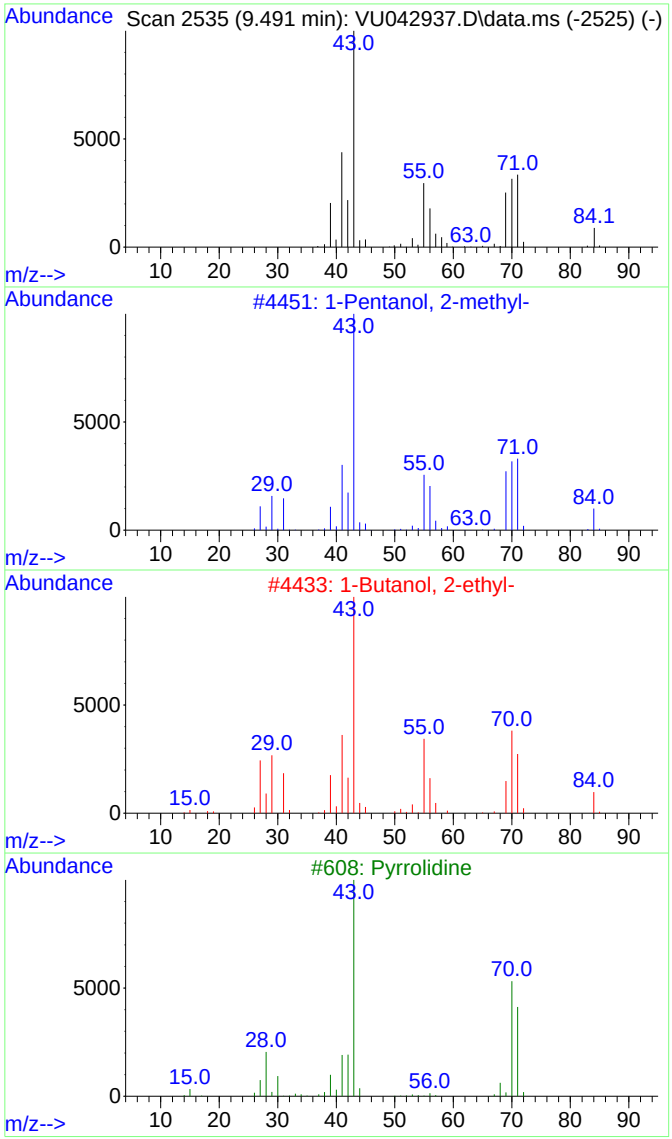
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

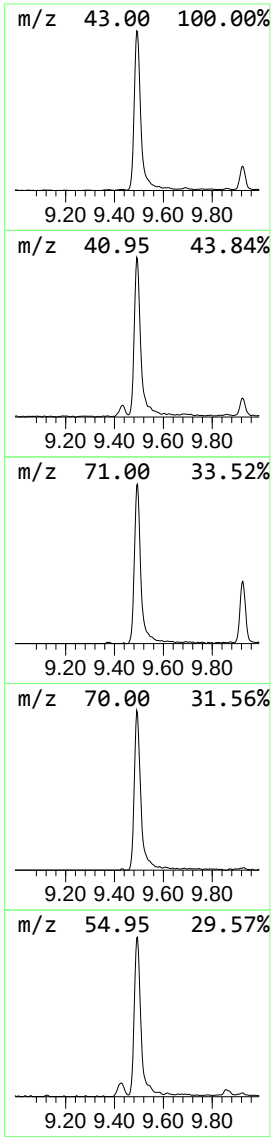
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.491	35.78 ug/l	478213	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	45
4	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	45
5	Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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

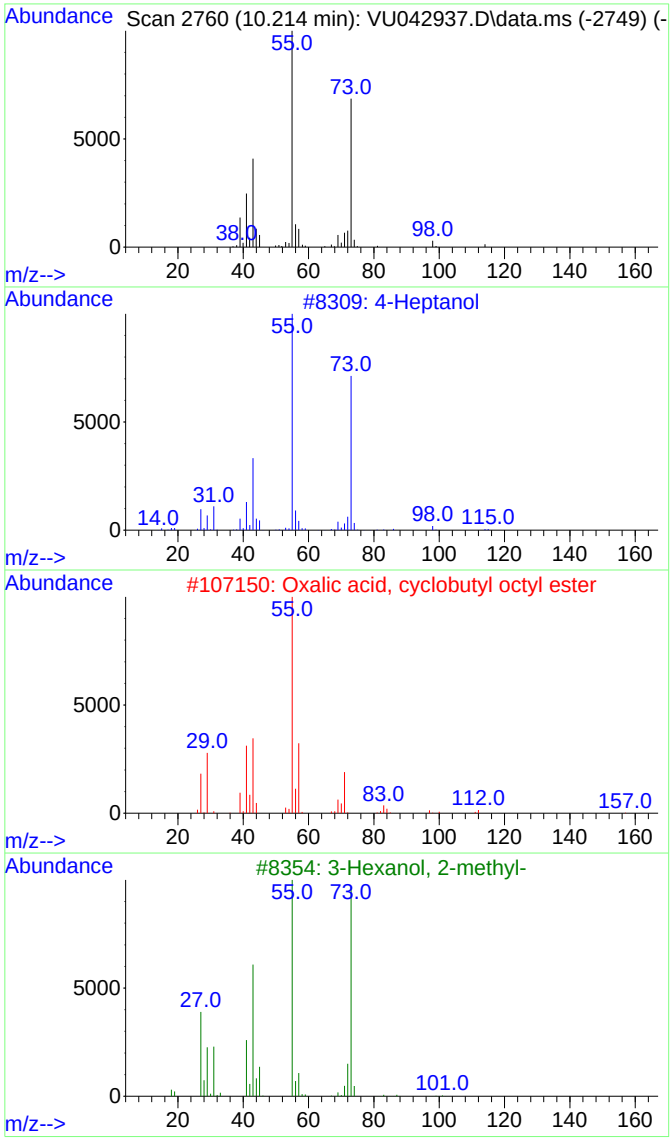
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

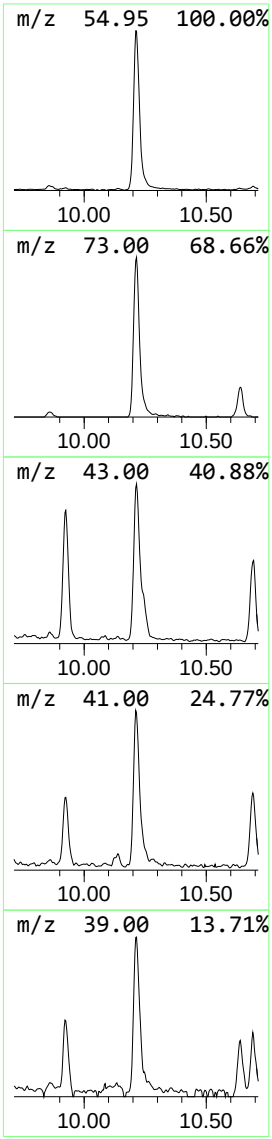
****

Peak Number 5 4-Heptanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.214	13.55 ug/l	181043	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	78
2	Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	43
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	42
4	Oxalic acid, cyclobutyl heptyl e...	242	C13H22O4	1000309-69-8	37
5	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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

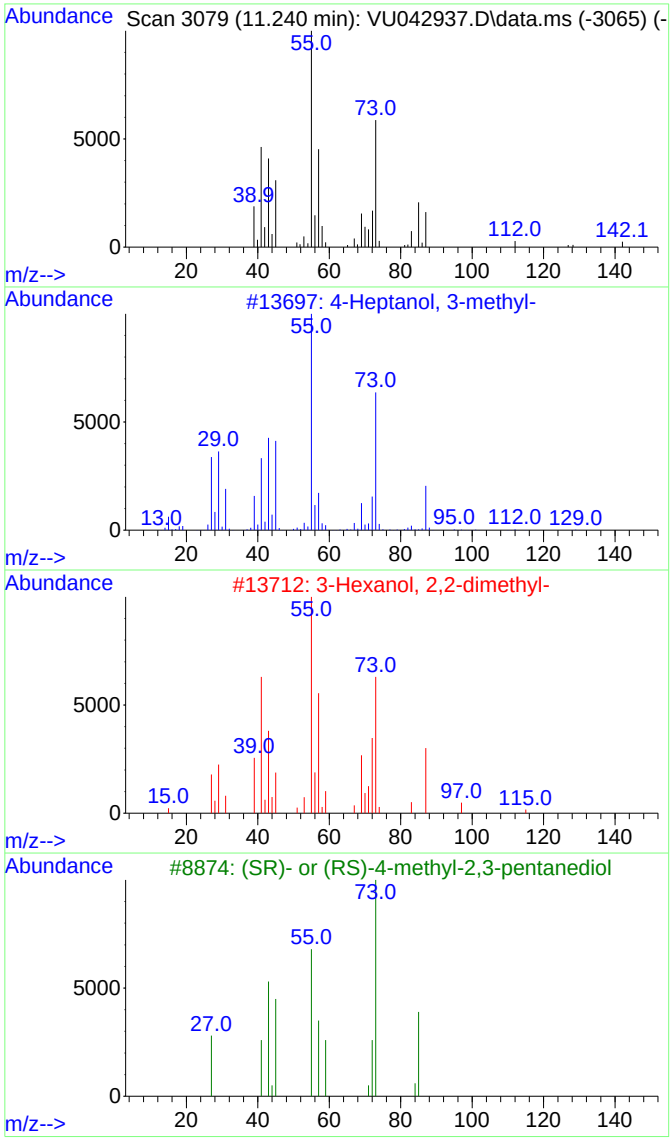
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

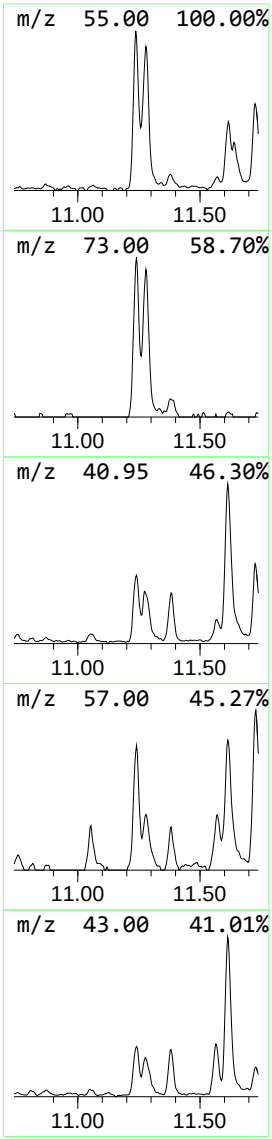
****

Peak Number 6 4-Heptanol, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.240	6.15 ug/l	86949	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	53
2	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	42
3	(SR)- or (RS)-4-methyl-2,3-penta...	118	C6H14O2	006702-10-9	37
4	2-Propenoic acid, methyl ester	86	C4H6O2	000096-33-3	27
5	Oxalic acid, cyclobutyl dodecyl ...	312	C18H32O4	1000309-70-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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

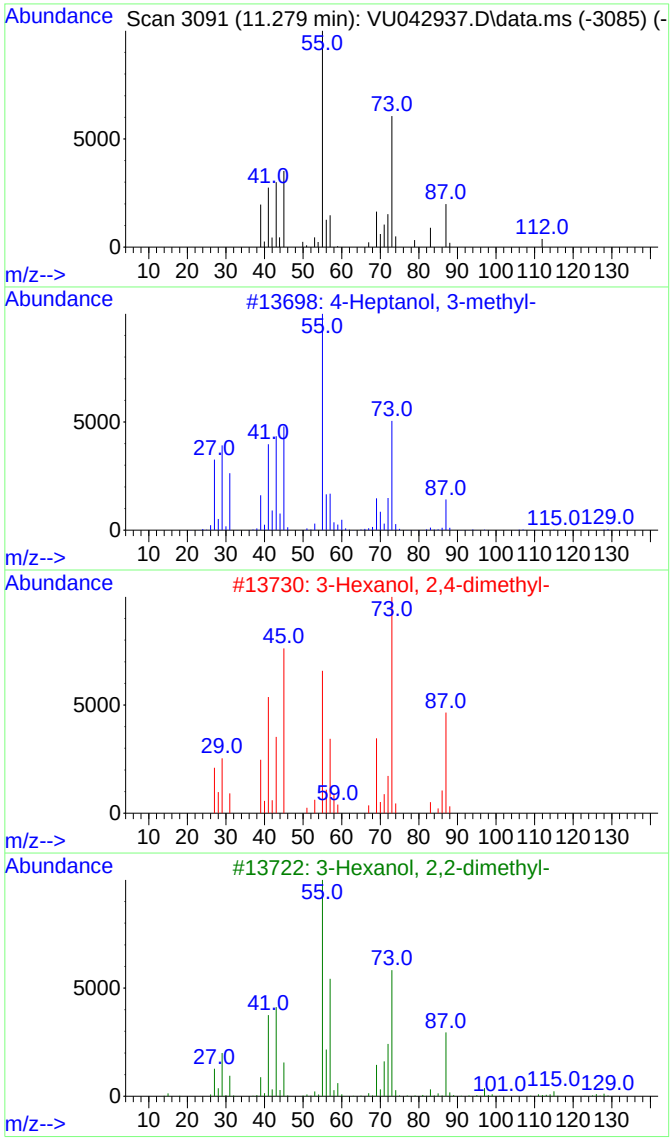
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

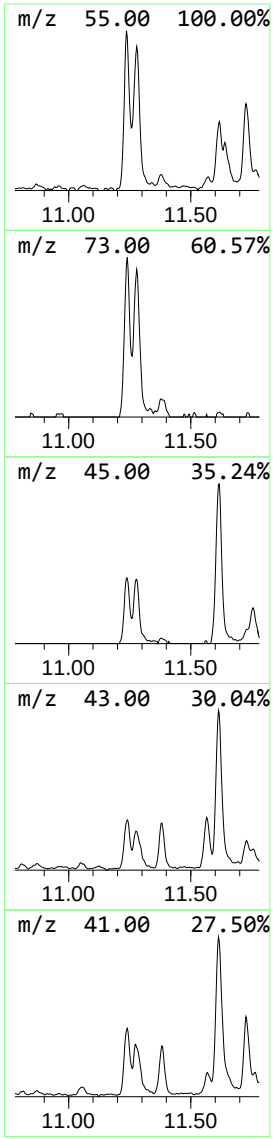
****

Peak Number 7 unknown11.279 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.279	5.65 ug/l	79867	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	50
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	42
3	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	39
4	4-Heptanol	116	C7H16O	000589-55-9	38
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

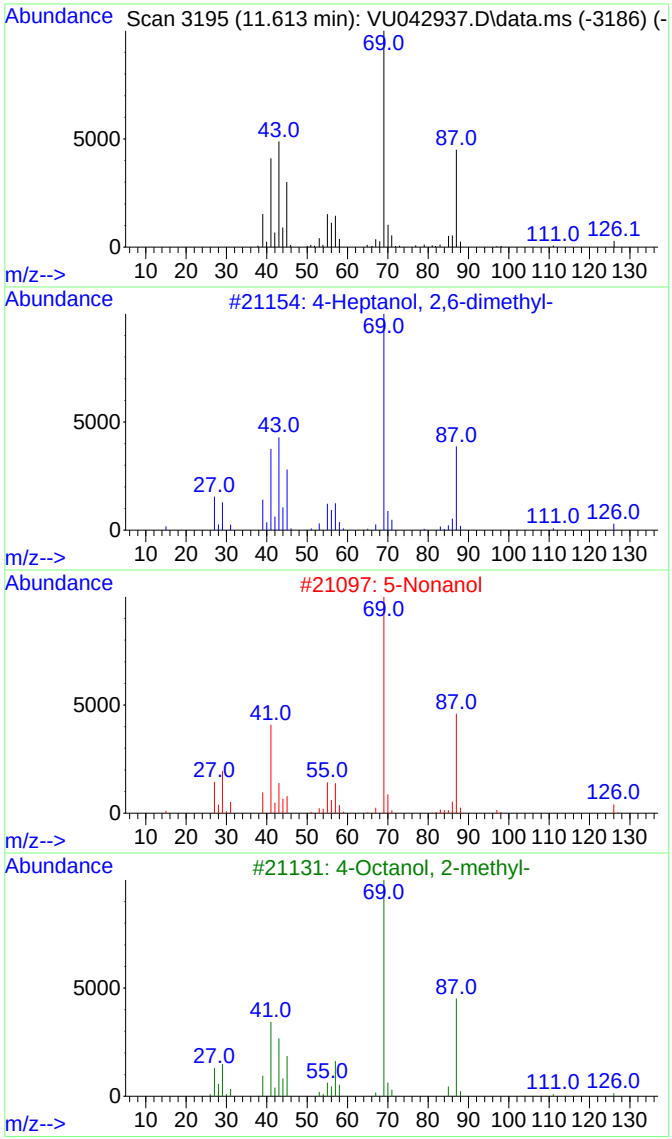
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

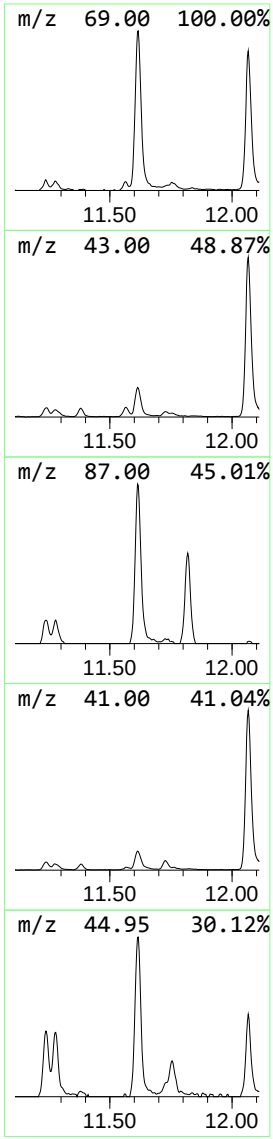
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.613	15.09 ug/l	213437	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	72
4	3-Heptanol, 2,2-dimethyl-	144	C9H20O	019549-70-3	64
5	4,5-Octanediol, 2,7-dimethyl-	174	C10H22O2	1000153-20-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

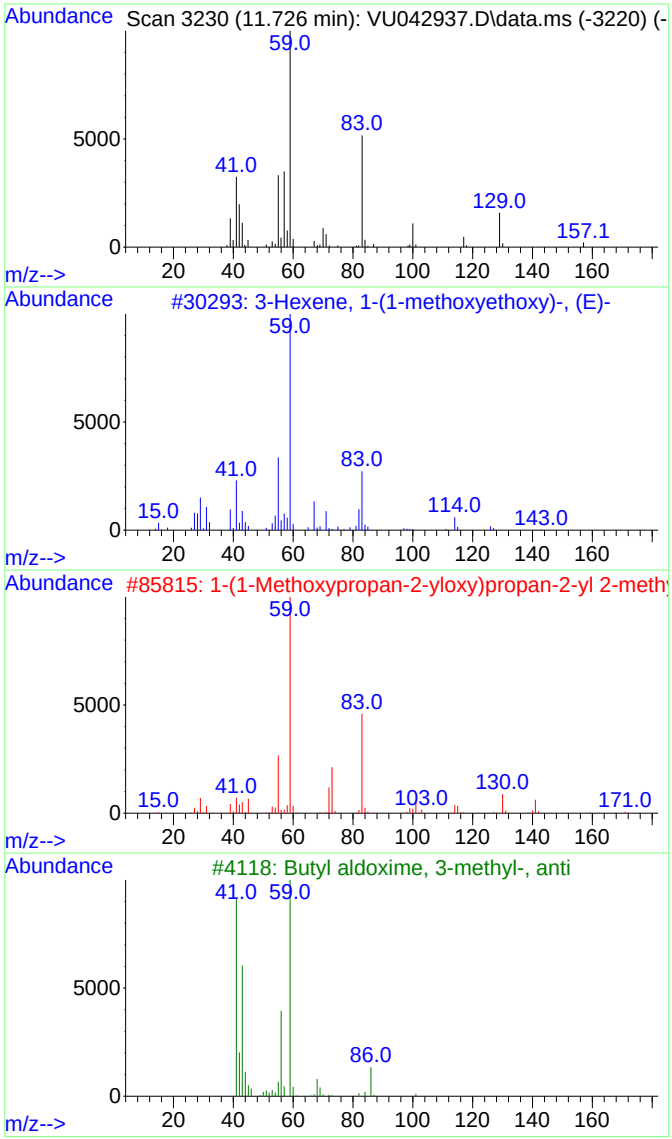
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

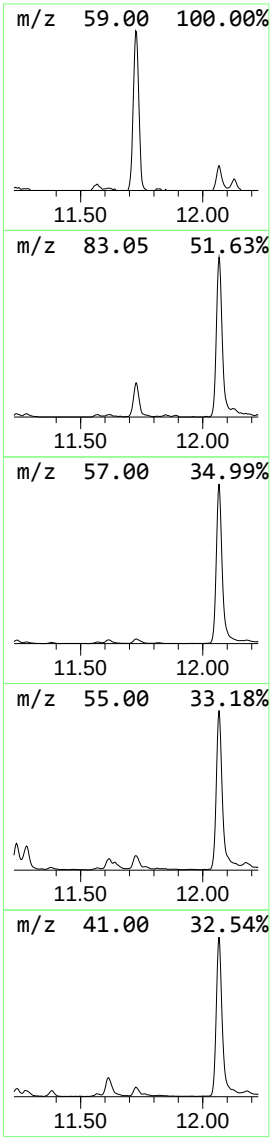
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 3-Hexene, 1-(1-methoxyethox... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.726	9.25 ug/l	130822	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-97-5	53
2	1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	45
3	Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	38
4	3-Decanol	158	C10H22O	001565-81-7	37
5	3-Octanol	130	C8H18O	000589-98-0	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

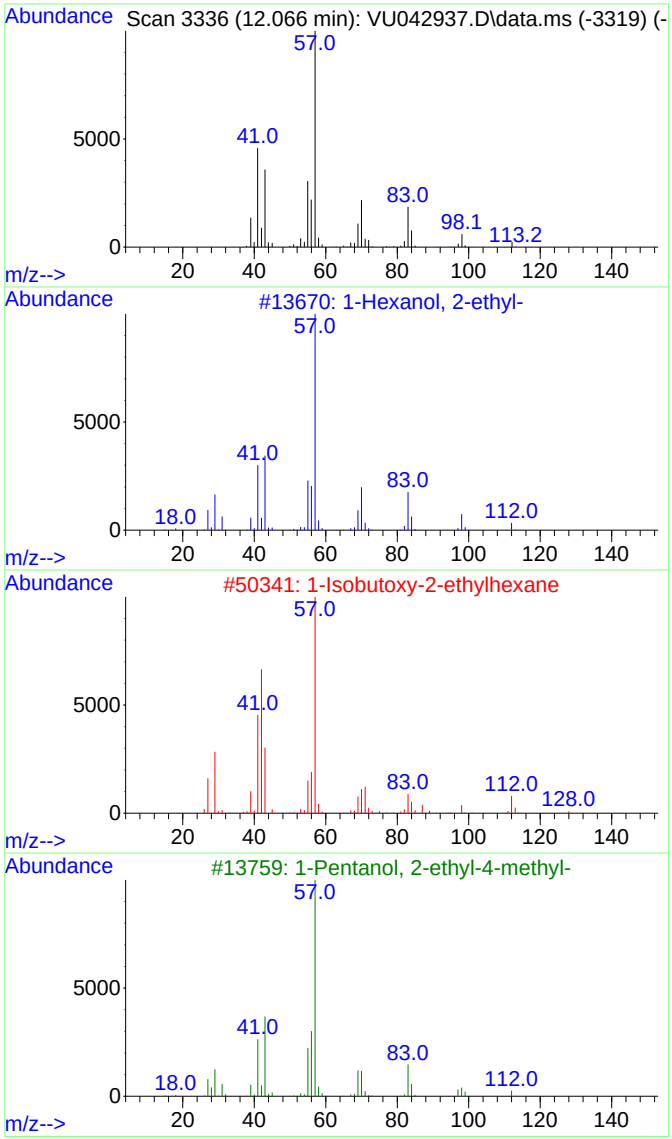
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

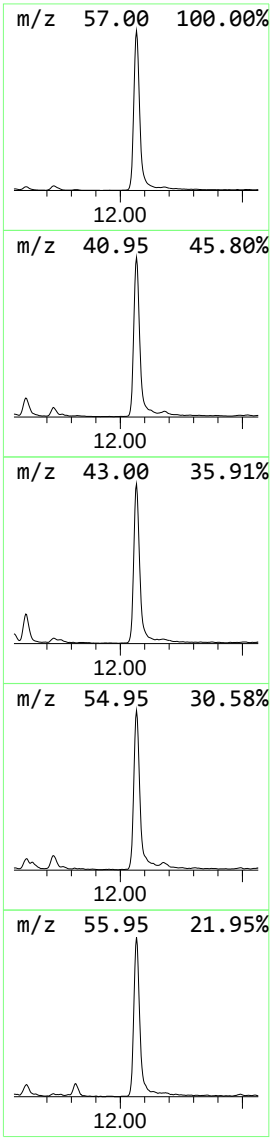
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.066	96.47 ug/l	1364780	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	74
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	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042937.D
Acq On : 05 Apr 2021 17:43
Operator : SY/MD
Sample : M1903-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 31030

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	12.0	ug/l	94828	1	5.382	394062	50.0
1-Butanol	6.546	15.4	ug/l	163135	2	6.256	529527	50.0
1-Pentanol	8.456	8.2	ug/l	109978	3	9.423	668231	50.0
1-Pentanol, 2-m...	9.491	35.8	ug/l	478213	3	9.423	668231	50.0
4-Heptanol	10.214	13.6	ug/l	181043	3	9.423	668231	50.0
4-Heptanol, 3-m...	11.240	6.2	ug/l	86949	4	11.819	707344	50.0
unknown11.279	11.279	5.7	ug/l	79867	4	11.819	707344	50.0
4-Heptanol, 2,6...	11.613	15.1	ug/l	213437	4	11.819	707344	50.0
3-Hexene, 1-(1-...	11.726	9.3	ug/l	130822	4	11.819	707344	50.0
1-Hexanol, 2-et...	12.066	96.5	ug/l	1364780	4	11.819	707344	50.0