LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042934.D
Acq On : 05 Apr 2021 16:34
Operator : SY/MD
Sample : M1903-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

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: VU042934.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	70	80	100	rBV	103911	244947	2.20%	0.712%
2	1.691	100	109	147	rVB	854907	1229403	11.05%	3.571%
3	2.366	295	319	353	rBV3	56596	307562	2.76%	0.893%
4	2.549	353	376	394	rVV	3645141	6500256	58.44%	18.882%
5	2.636	395	403	440	rVV	418096	955271	8.59%	2.775%
6	2.806	442	456	495	rVB2	32933	158339	1.42%	0.460%
7	4.121	833	865	925	rBV4	252314	1468162	13.20%	4.265%
8	4.713	1035	1049	1074	rVB	81527	191201	1.72%	0.555%
9	5.298	1217	1231	1244	rBV2	132043	271995	2.45%	0.790%
10	5.382	1244	1257	1275	rVB	208528	420232	3.78%	1.221%
11	5.710	1344	1359	1396	rBV	146402	320366	2.88%	0.931%
12	6.256	1514	1529	1540	rBV	316199	585150	5.26%	1.700%
13	6.321	1540	1549	1567	rVB2	116733	226046	2.03%	0.657%
14	6.575	1604	1628	1640	rBV3	99239	223745	2.01%	0.650%
15	6.774	1678	1690	1705	rBV	85895	162314	1.46%	0.471%
16	7.906	2028	2042	2055	rBV	467529	818599	7.36%	2.378%
17	8.224	2119	2141	2160	rBV	818982	1409361	12.67%	4.094%
18	8.398	2182	2195	2207	rBV	566792	918215	8.25%	2.667%
19	9.423	2501	2514	2528	rBV	429768	710649	6.39%	2.064%
20	9.690	2582	2597	2618	rBV	2204082	3621649	32.56%	10.520%
21	10.240	2752	2768	2783	rBV2	70973	129969	1.17%	0.378%
22	10.639	2880	2892	2902	rBV	376425	591607	5.32%	1.719%
23	10.713	2902	2915	2934	rVV	7276919	11123843	100.00%	32.313%
24	10.806	2934	2944	2955	rVB	161825	248776	2.24%	0.723%
25	11.121	3031	3042	3055	rVB	135531	206826	1.86%	0.601%
26	11.819	3248	3259	3278	rVB	489837	800325	7.19%	2.325%
27	12.066	3324	3336	3358	rBV	300478	580656	5.22%	1.687%

Sum of corrected areas: 34425464

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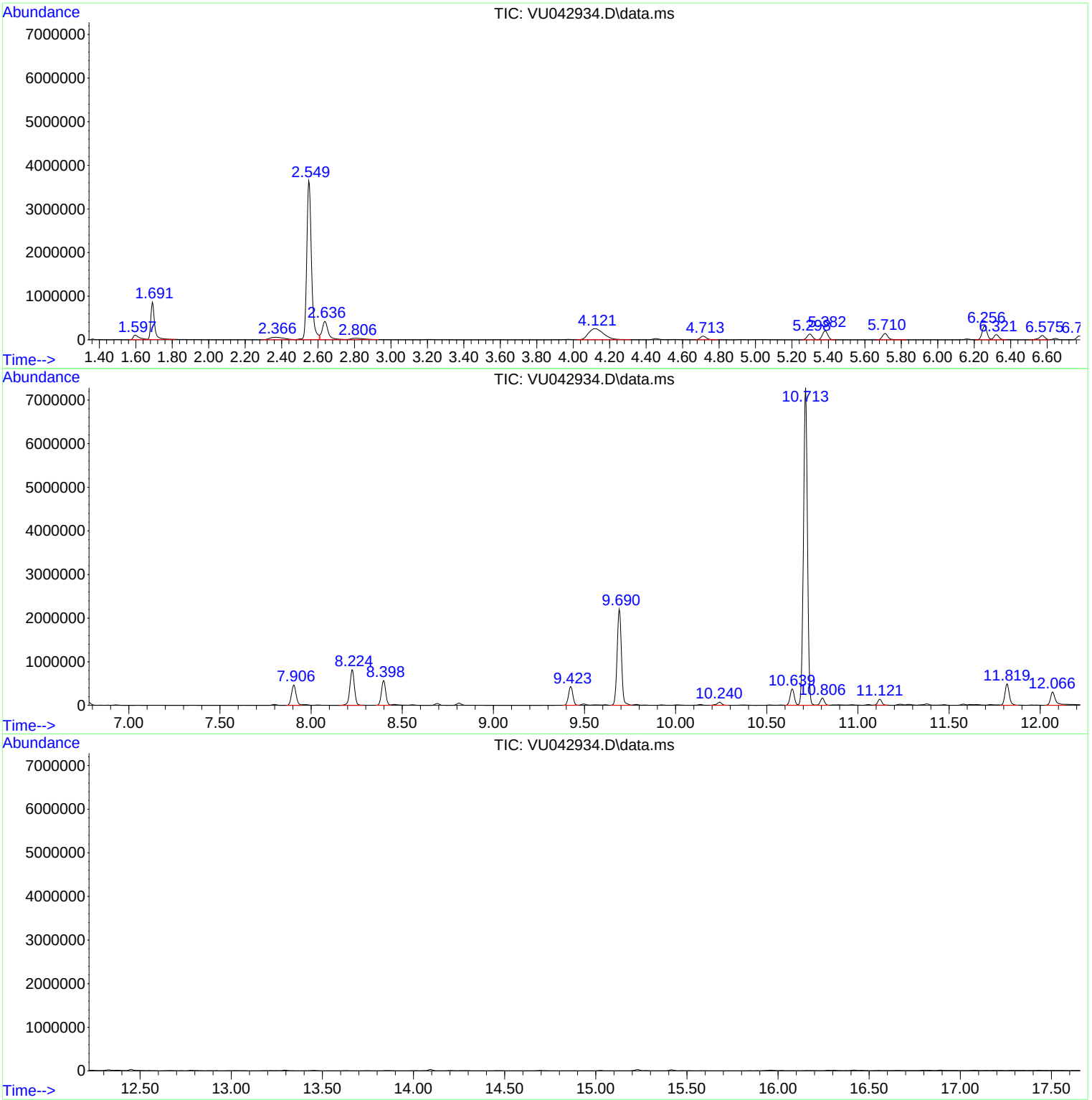
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30809

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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Data File : VU042934.D
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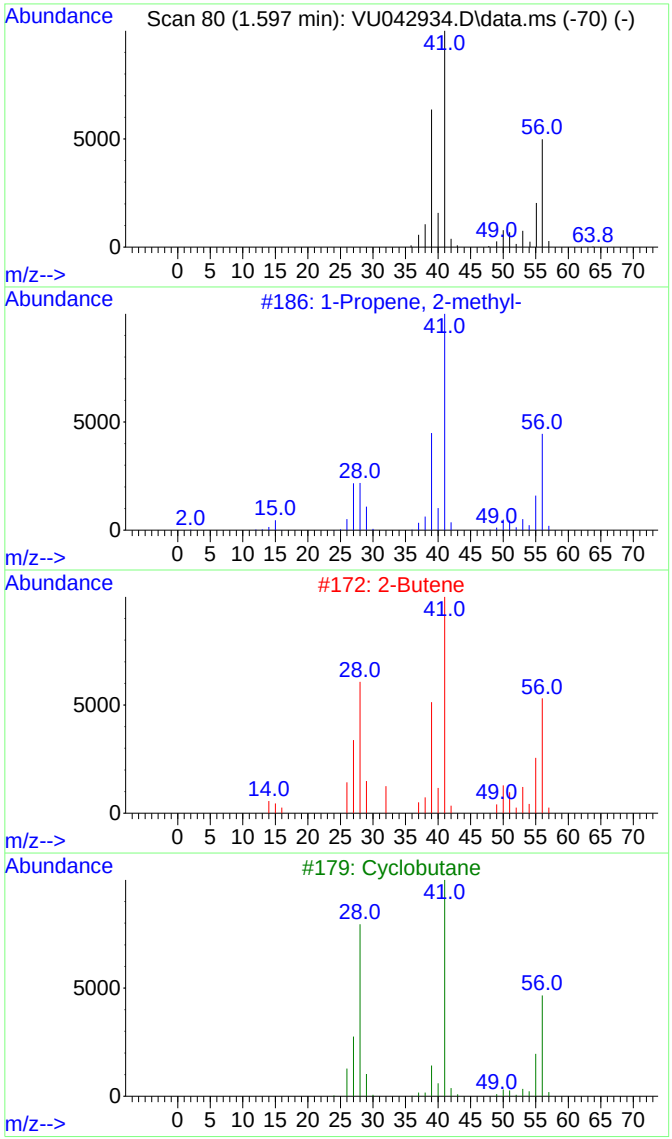
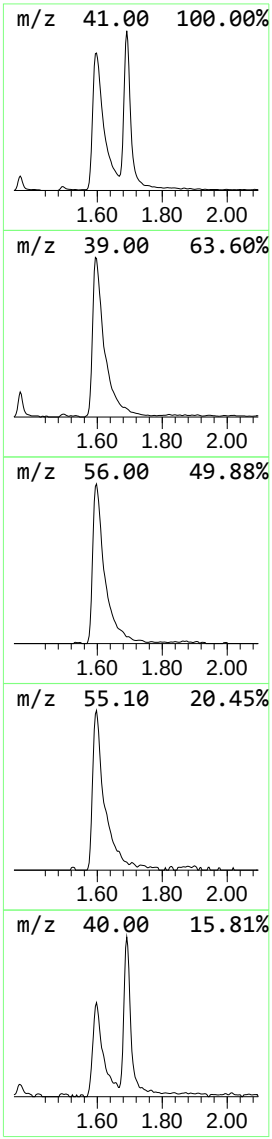
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.597	29.14 ug/l	244947	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	91
2	2-Butene	56	C4H8	000107-01-7	72
3	Cyclobutane	56	C4H8	000287-23-0	49
4	1-Butene	56	C4H8	000106-98-9	49
5	2-Butene, (Z)-	56	C4H8	000590-18-1	47





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Data File : VU042934.D
Acq On : 05 Apr 2021 16:34
Operator : SY/MD
Sample : M1903-05
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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

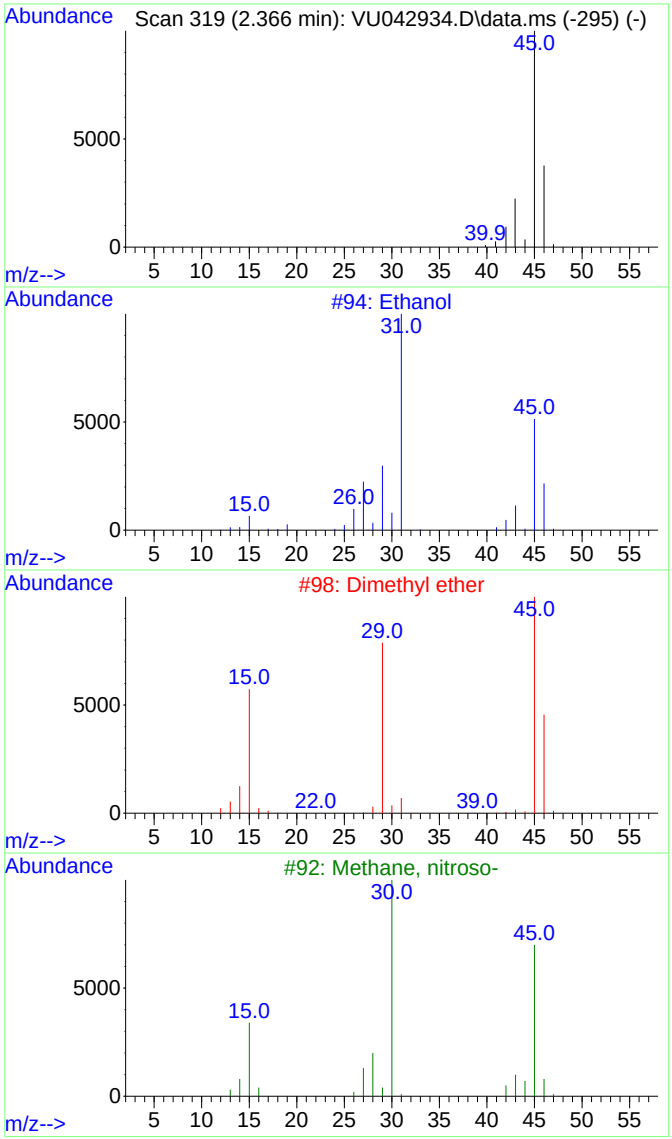
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

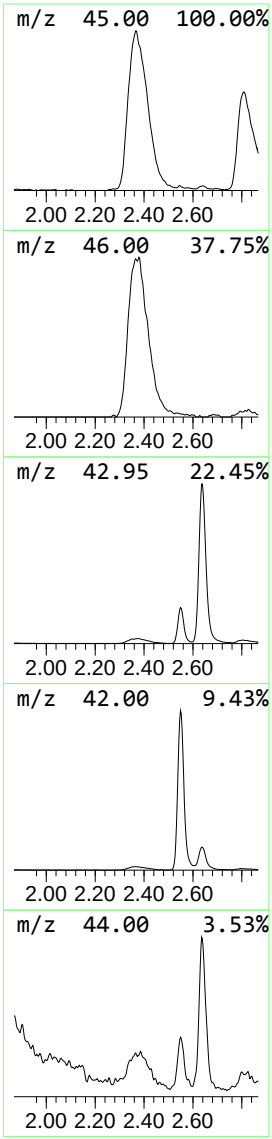
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.366	36.59 ug/l	307562	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	L-Lactic acid	90	C3H6O3	000079-33-4	2





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Data File : VU042934.D
Acq On : 05 Apr 2021 16:34
Operator : SY/MD
Sample : M1903-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

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

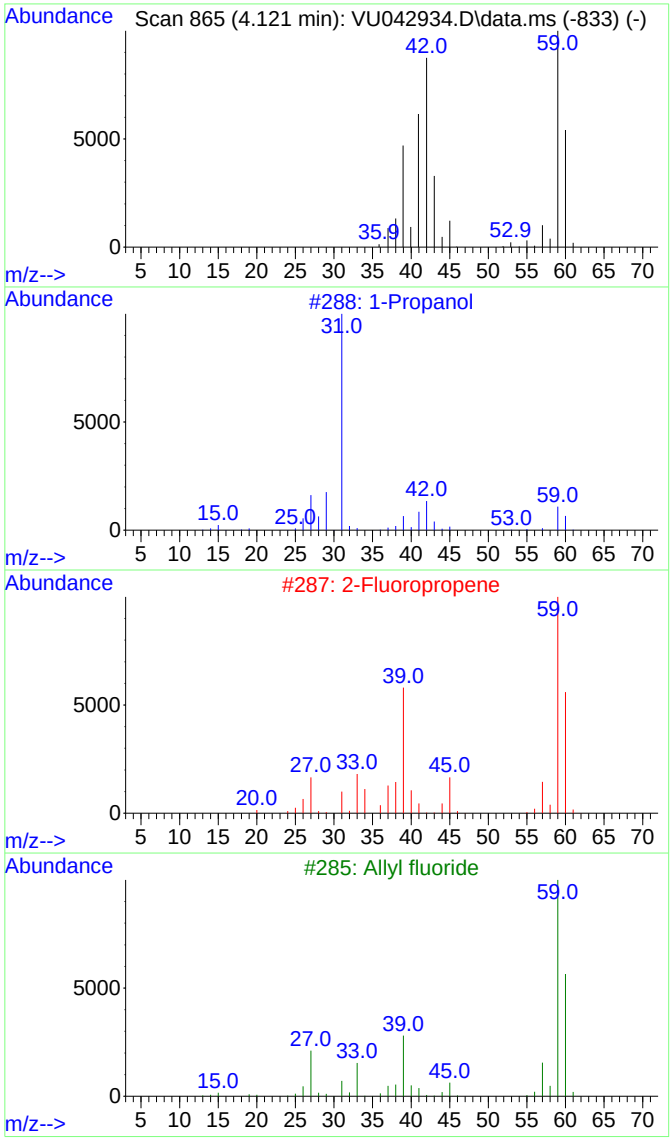
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

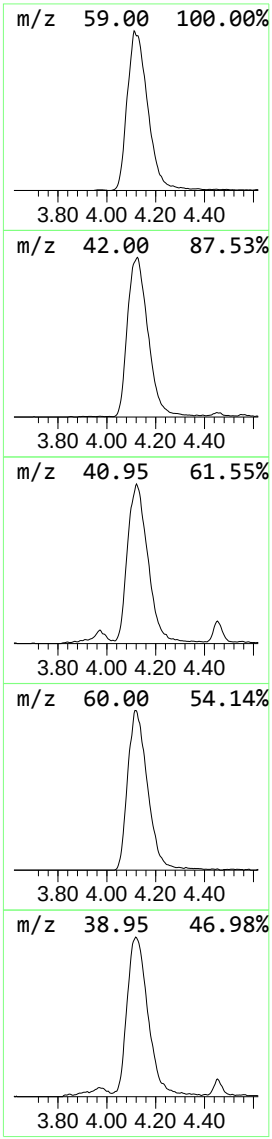
****

Peak Number 4 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.121	174.69 ug/l	1468160	Pentafluorobenzene	5.382

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	62
3	Allyl fluoride	60	C3H5F	000818-92-8	32
4	Cyclopropane	42	C3H6	000075-19-4	25
5	Propene	42	C3H6	000115-07-1	17





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Data File : VU042934.D
Acq On : 05 Apr 2021 16:34
Operator : SY/MD
Sample : M1903-05
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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

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

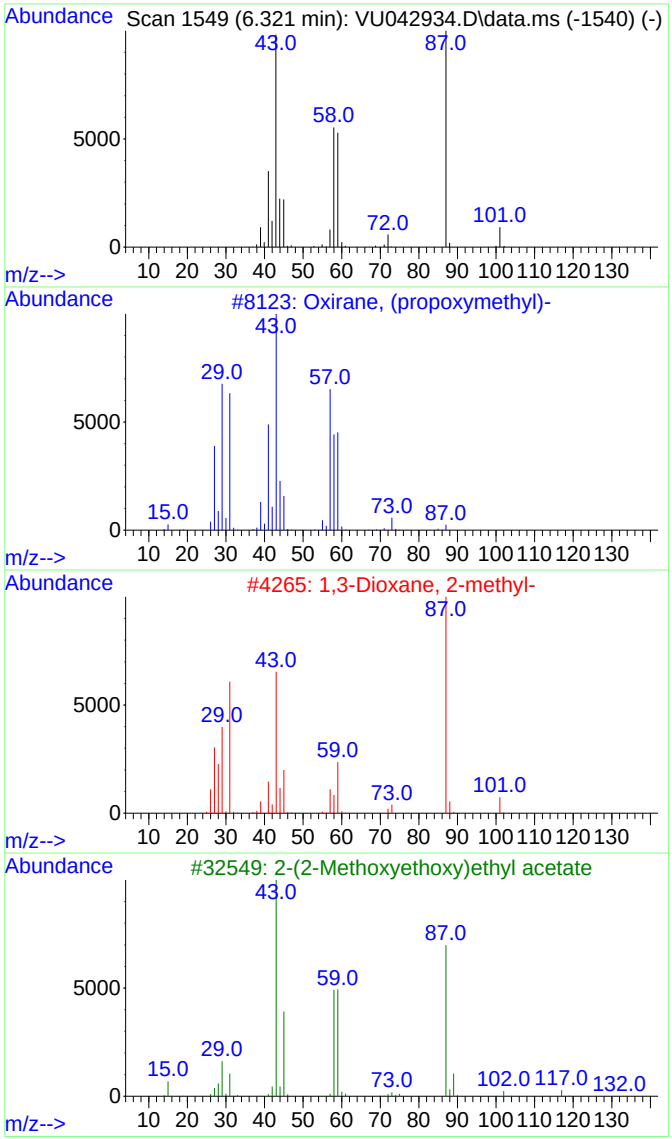
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

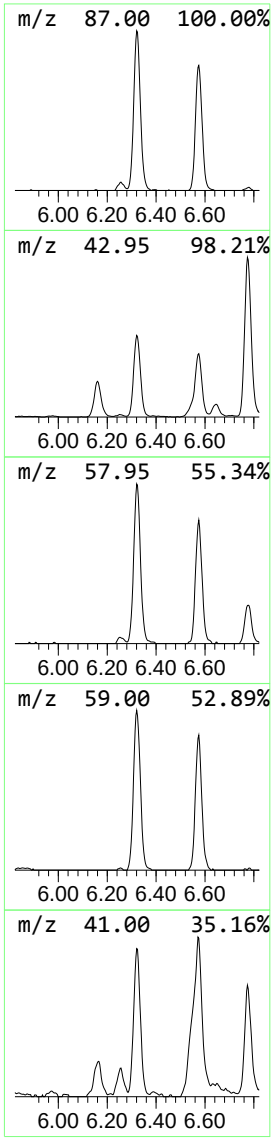
****

Peak Number 5 unknown6.321 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.321	19.32 ug/l	226046	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	47
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	42
3	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	38
4	Monomethyl malonate	118	C4H6O4	016695-14-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	23





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

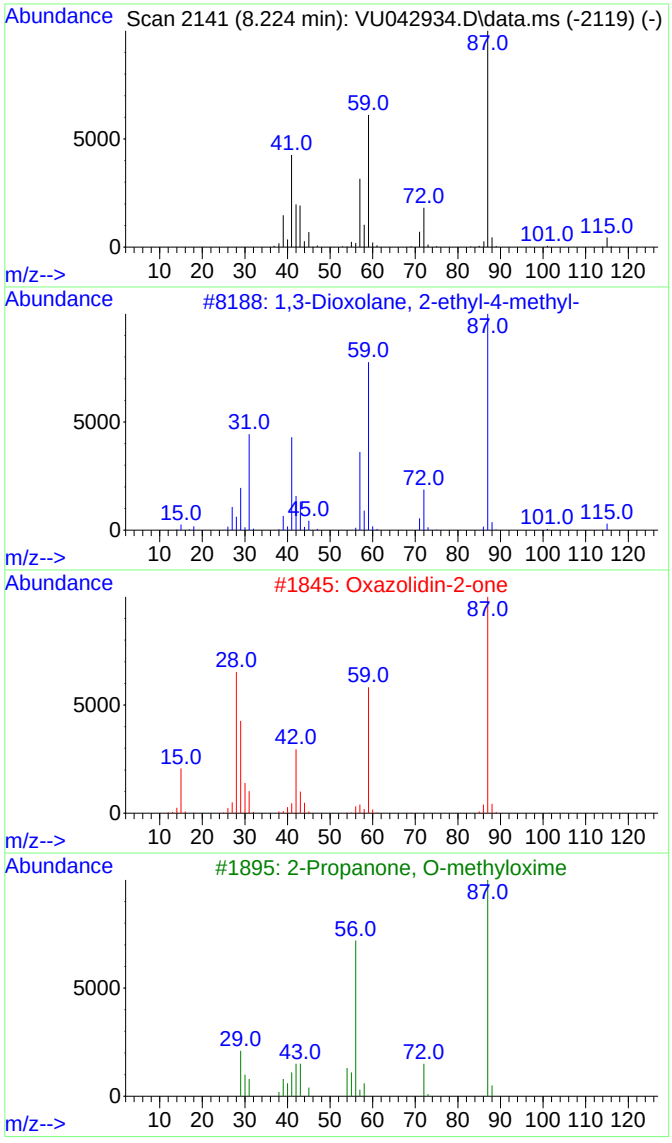
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

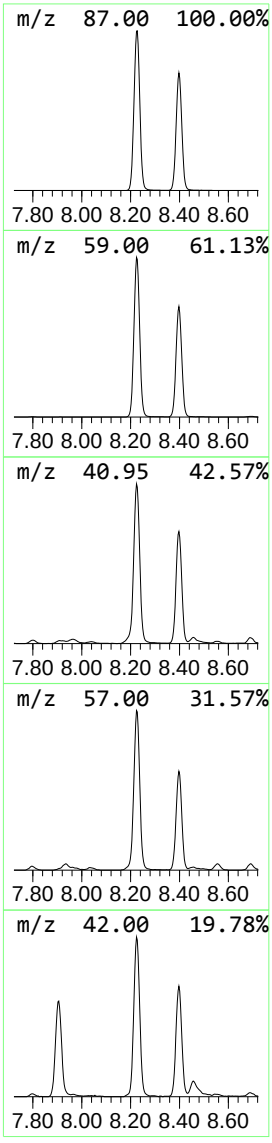
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.224	99.16 ug/l	1409360	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	86
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	58
4	Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	42
5	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	36





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Instrument : MSVOA_U
ClientSampleId : 30809

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

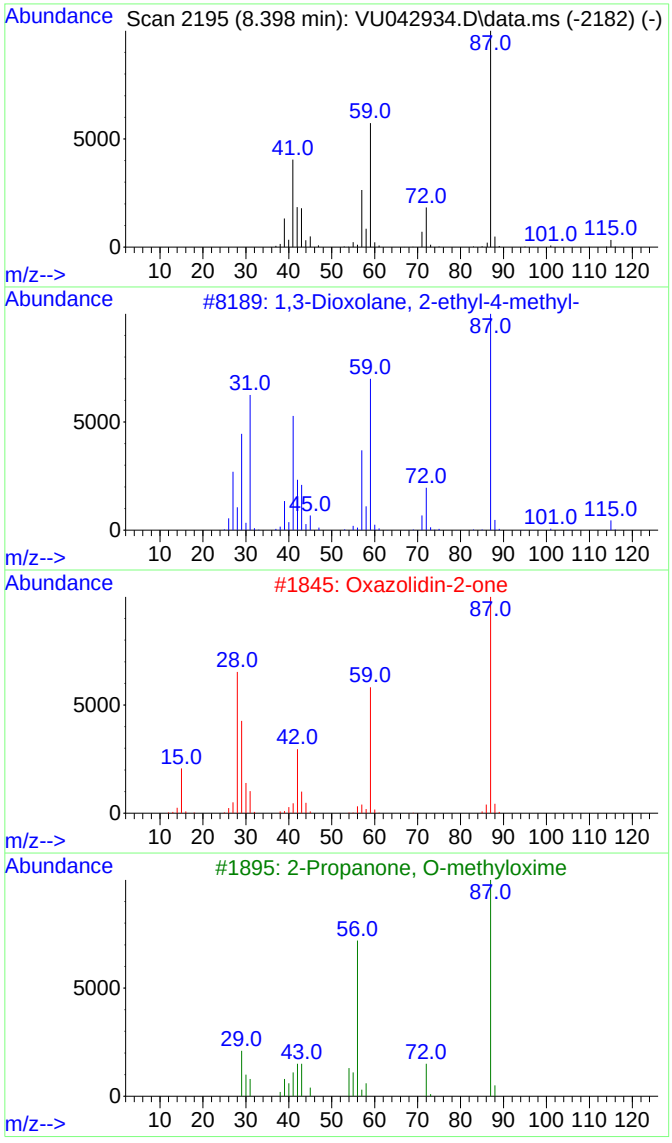
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

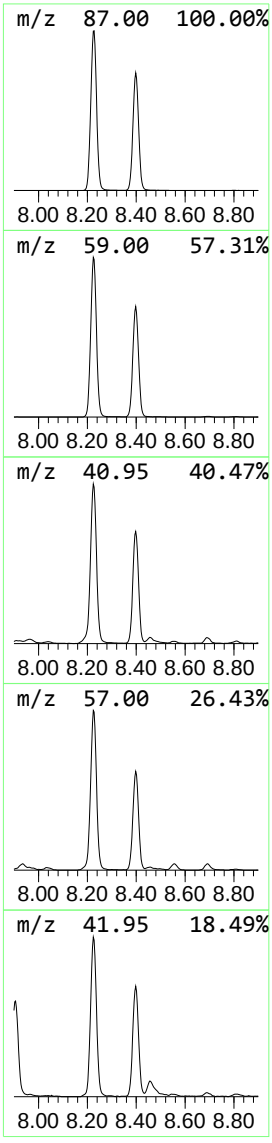
****

Peak Number 7 Oxazolidin-2-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.398	64.60 ug/l	918215	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	95
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	56
3	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
4	Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	50
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50





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ClientSampleId : 30809

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

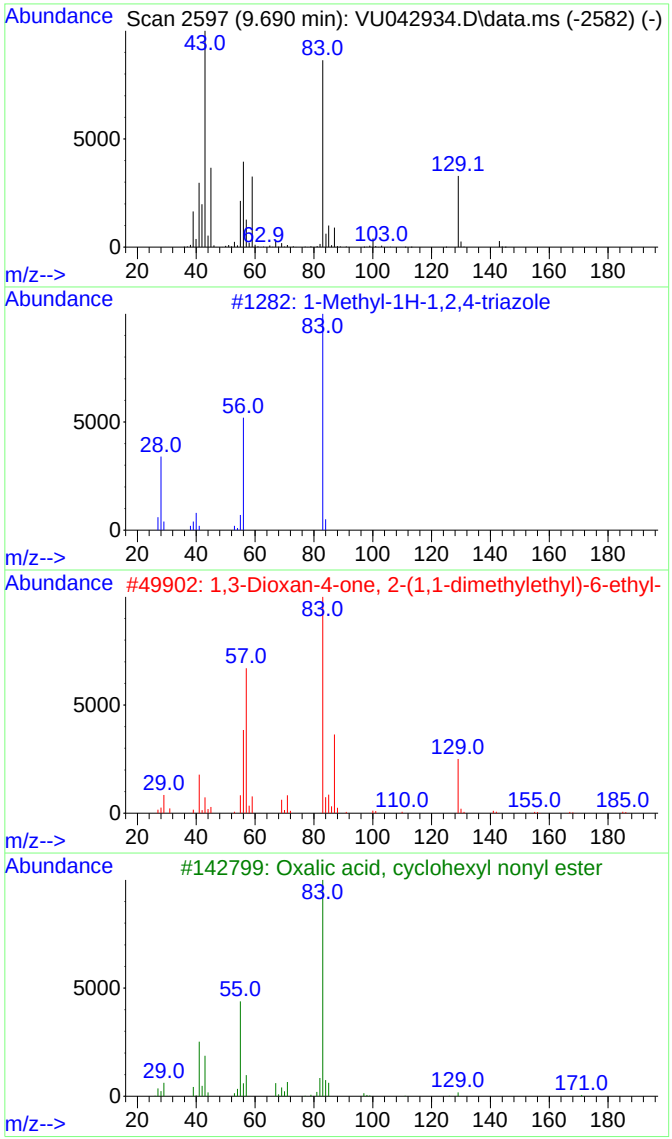
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

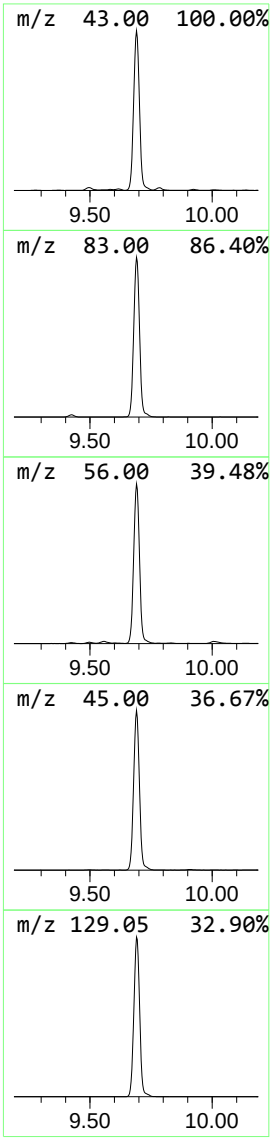
****

Peak Number 8 unknown9.690 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.690	254.81 ug/l	3621650	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	37
2	1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	36
3	Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	25
4	Trichloroacetic acid, hexyl ester	246	C8H13Cl3O2	037587-86-3	14
5	Oxalic acid, cyclohexyl butyl ester	228	C12H20O4	1000309-30-5	12





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Instrument : MSVOA_U
ClientSampleId : 30809

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Quant Title : SW846 8260

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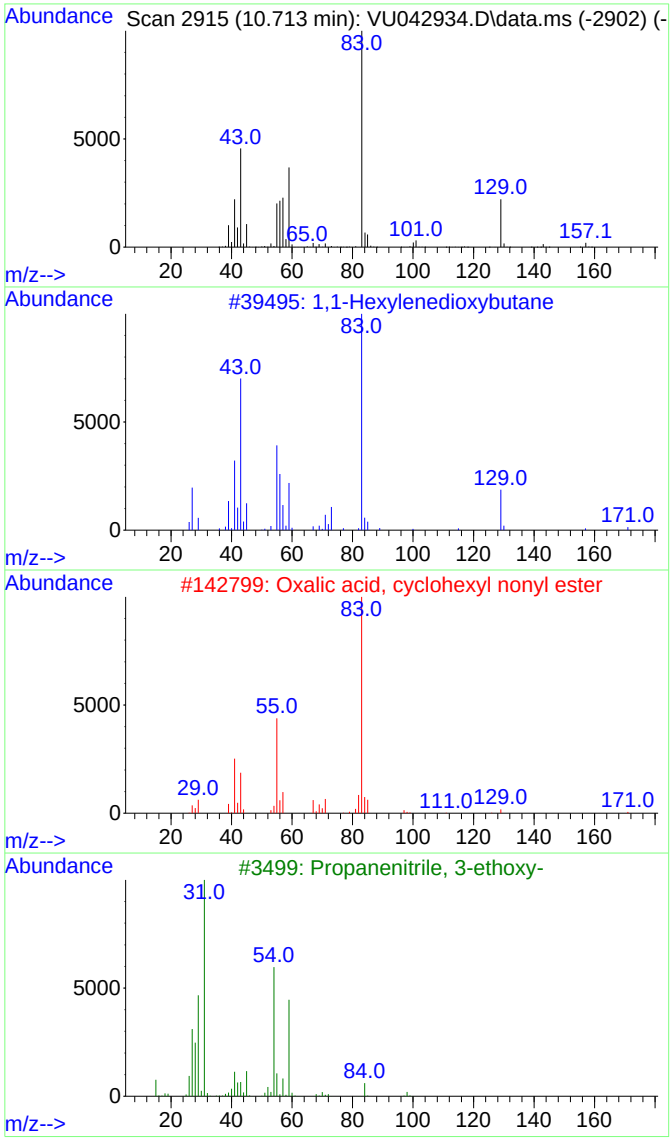
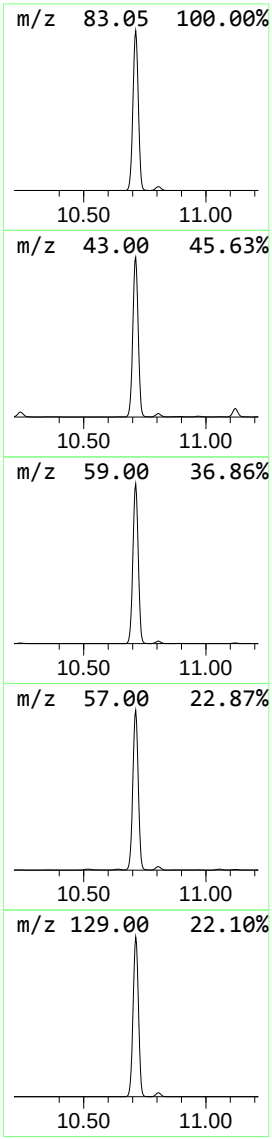
****

Peak Number 9 1,1-Hexylenedioxybutane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.713	694.96 ug/l	11123800	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	78
2	Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	28
3	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	10
4	Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1000309-30-7	10
5	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	9





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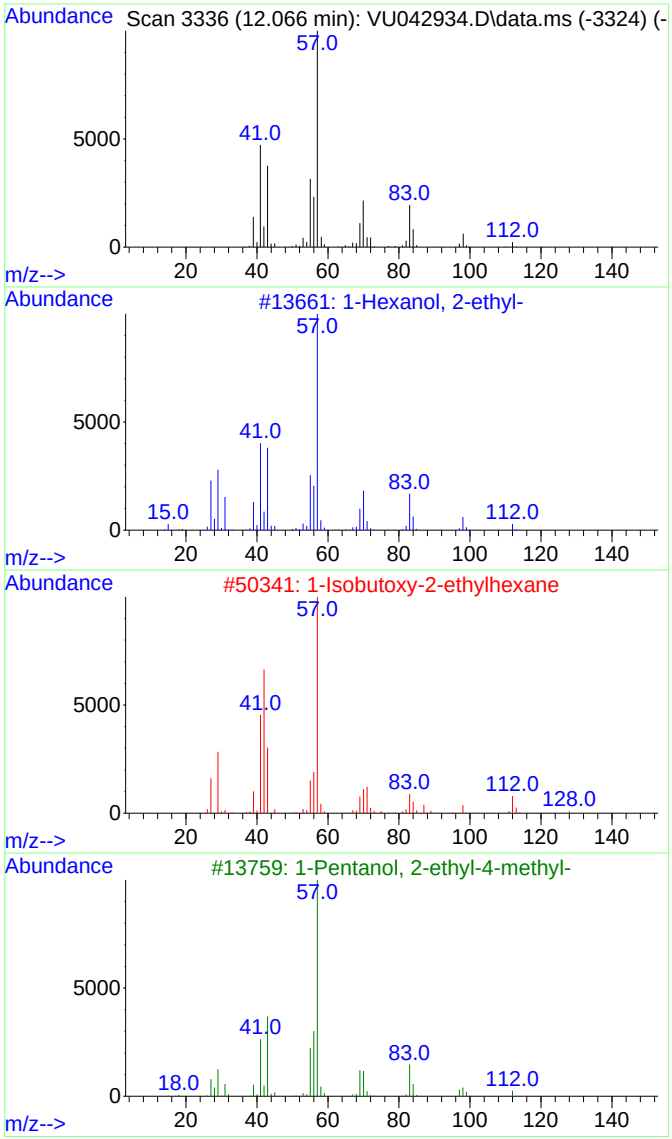
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

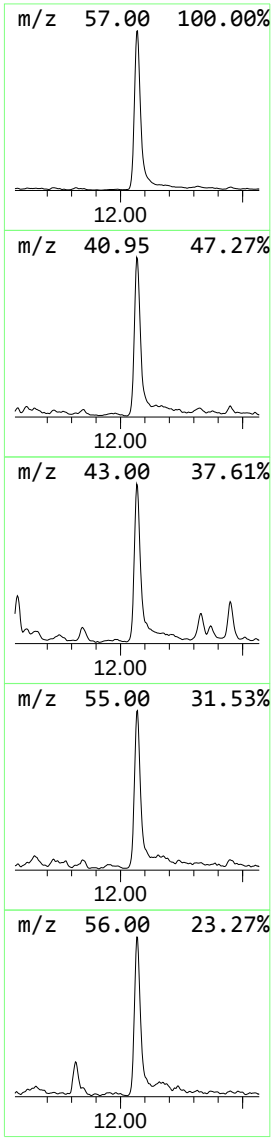
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.067	36.28 ug/l	580656	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	72
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	50





Tentatively Identified Compound (LSC) summary

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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
1-Propene, 2-me...	1.597	29.1	ug/l	244947	1	5.382	420232	50.0
Ethanol	2.366	36.6	ug/l	307562	1	5.382	420232	50.0
1-Propanol	4.121	174.7	ug/l	1468160	1	5.382	420232	50.0
unknown6.321	6.321	19.3	ug/l	226046	2	6.256	585150	50.0
1,3-Dioxolane, ...	8.224	99.2	ug/l	1409360	3	9.423	710649	50.0
Oxazolidin-2-one	8.398	64.6	ug/l	918215	3	9.423	710649	50.0
unknown9.690	9.690	254.8	ug/l	3621650	3	9.423	710649	50.0
1,1-Hexylenedio...	10.713	695.0	ug/l	11123800	4	11.819	800325	50.0
1-Hexanol, 2-et...	12.067	36.3	ug/l	580656	4	11.819	800325	50.0