LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 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: VU042904.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	71	79	101	rBV	17317	27307	4.24%	0.499%
2	1.691	101	109	134	rBV	74775	103342	16.04%	1.889%
3	2.356	298	316	338	rVB3	8268	31252	4.85%	0.571%
4	2.549	363	376	395	rBV	297951	532866	82.70%	9.740%
5	2.639	395	404	427	rVB	31618	66698	10.35%	1.219%
6	4.105	840	860	894	rBV7	23575	109931	17.06%	2.009%
7	4.723	1041	1052	1069	rVB	5116	12479	1.94%	0.228%
8	5.298	1216	1231	1244	rBV2	103894	221298	34.35%	4.045%
9	5.382	1244	1257	1280	rVB	164952	337280	52.35%	6.165%
10	5.713	1344	1360	1380	rBV	116590	237709	36.89%	4.345%
11	6.256	1513	1529	1542	rBV	242258	454105	70.48%	8.301%
12	6.327	1542	1551	1564	rVB2	10427	20646	3.20%	0.377%
13	6.575	1611	1628	1642	rBV3	12432	26502	4.11%	0.484%
14	6.784	1680	1693	1710	rBV	6549	13032	2.02%	0.238%
15	7.906	2028	2042	2059	rBV	379075	644324	100.00%	11.778%
16	8.227	2122	2142	2158	rBV	52380	91558	14.21%	1.674%
17	8.401	2185	2196	2208	rBV2	31111	51282	7.96%	0.937%
18	8.694	2278	2287	2299	rBV3	3942	6466	1.00%	0.118%
19	9.423	2501	2514	2531	rBV	348572	570467	88.54%	10.428%
20	9.497	2531	2537	2549	rVB7	3957	7149	1.11%	0.131%
21	9.690	2584	2597	2619	rBV	170303	280877	43.59%	5.134%
22	10.243	2754	2769	2781	rBV5	5172	10242	1.59%	0.187%
23	10.639	2880	2892	2904	rBV	289414	463400	71.92%	8.471%
24	10.713	2904	2915	2935	rVV	330391	527148	81.81%	9.636%
25	10.806	2935	2944	2956	rVB3	7133	11014	1.71%	0.201%
26	11.121	3032	3042	3057	rVB2	8657	14142	2.19%	0.259%
27	11.819	3247	3259	3276	rVB	363582	582254	90.37%	10.643%
28	12.073	3327	3338	3351	rBV3	8215	15866	2.46%	0.290%

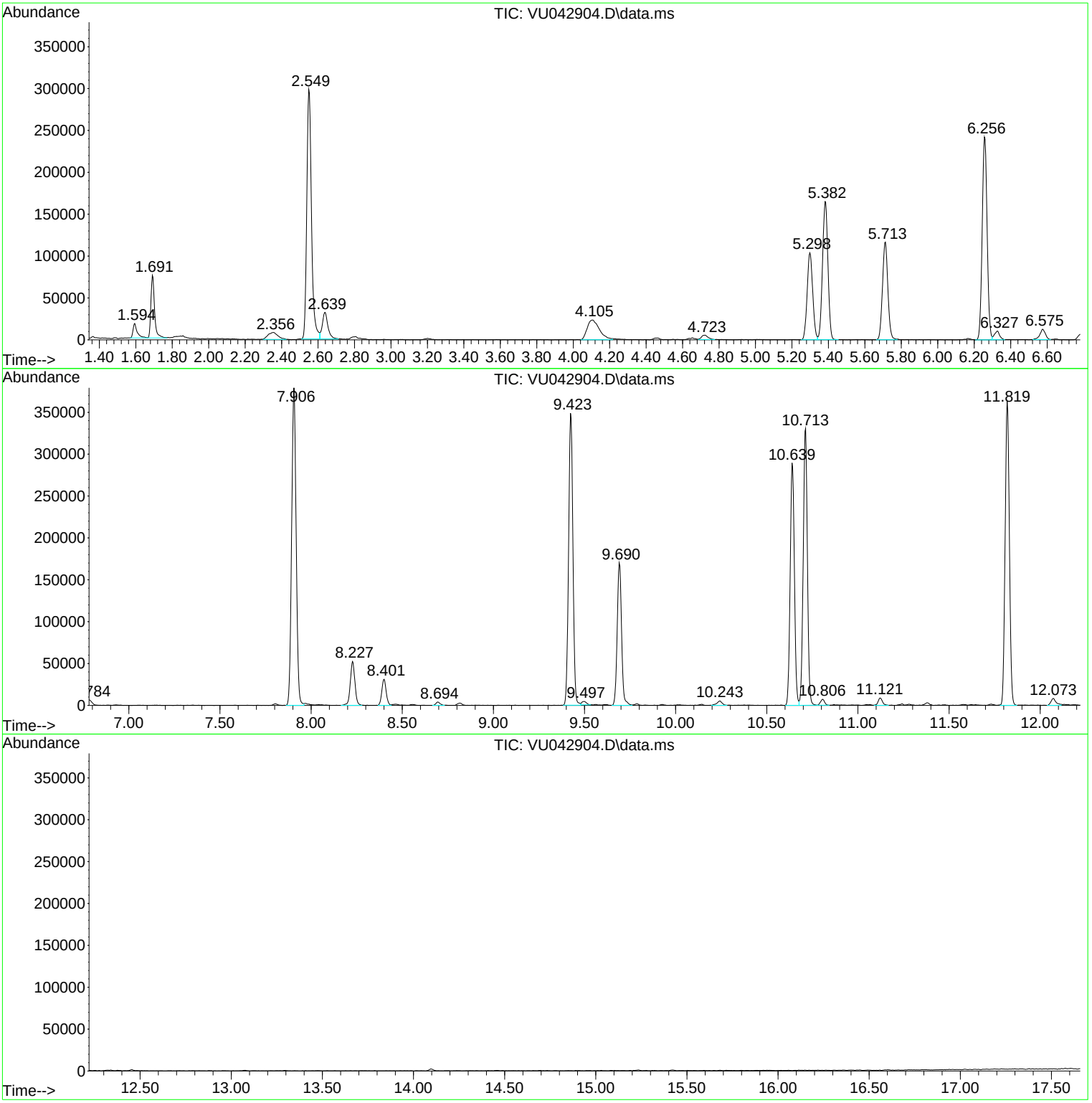
Sum of corrected areas: 5470636

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

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

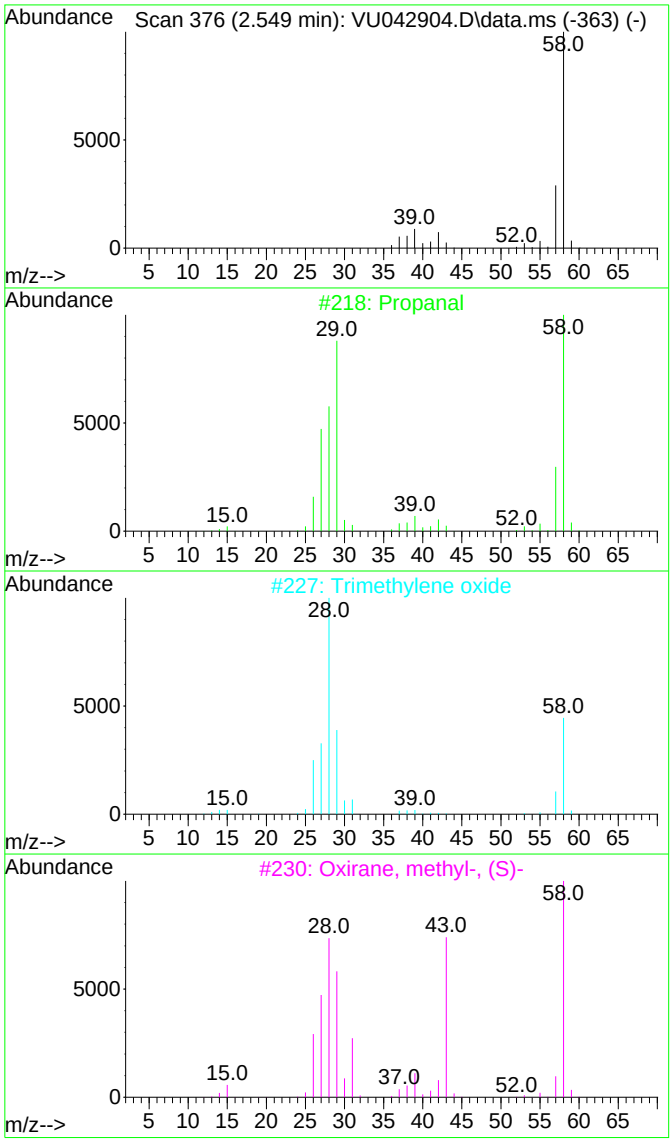
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

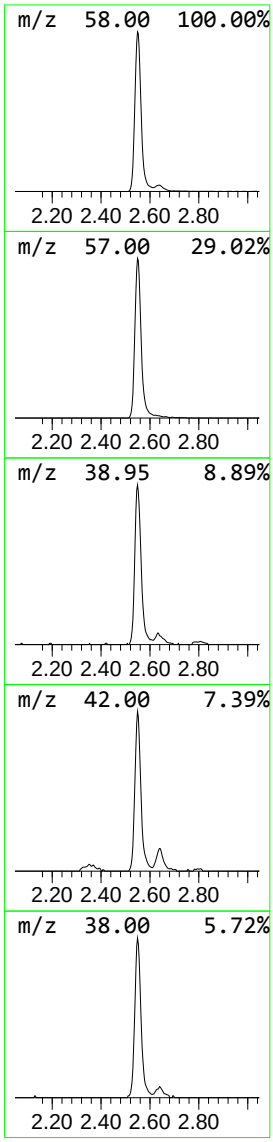
****

Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.549	78.99 ug/l	532866	Pentafluorobenzene	5.385

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
4	Propylene oxide	58	C3H6O	000075-56-9	7
5	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

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

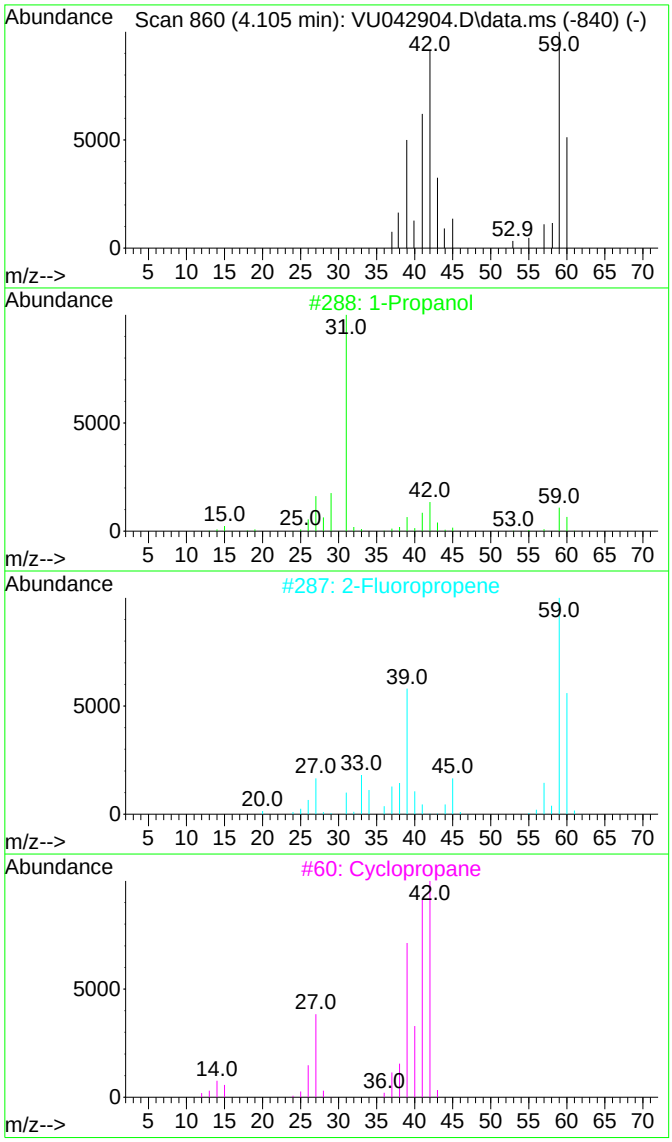
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

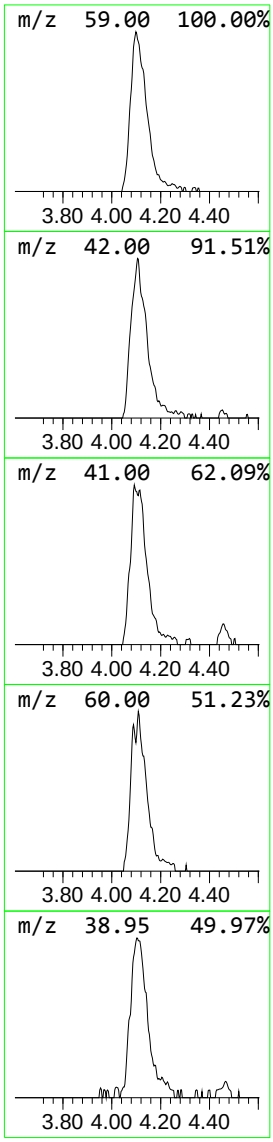
****

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.105	16.30 ug/l	109931	Pentafluorobenzene	5.385

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	50
3	Cyclopropane	42	C3H6	000075-19-4	17
4	Allyl fluoride	60	C3H5F	000818-92-8	9
5	Acetaldoxime	59	C2H5NO	000107-29-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30809

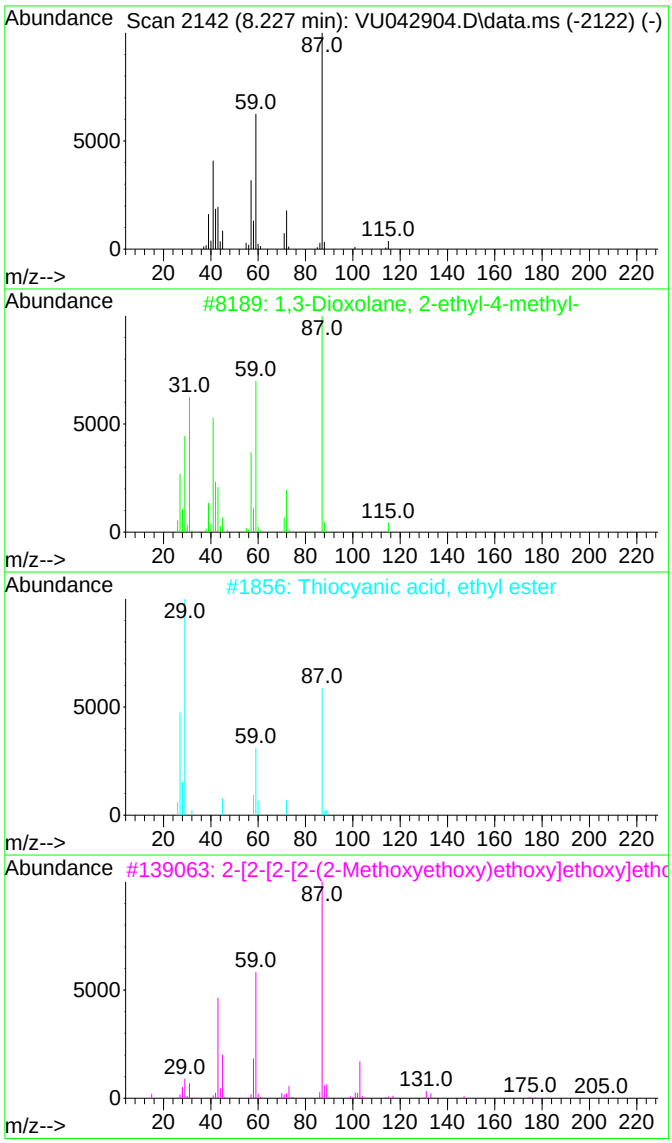
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

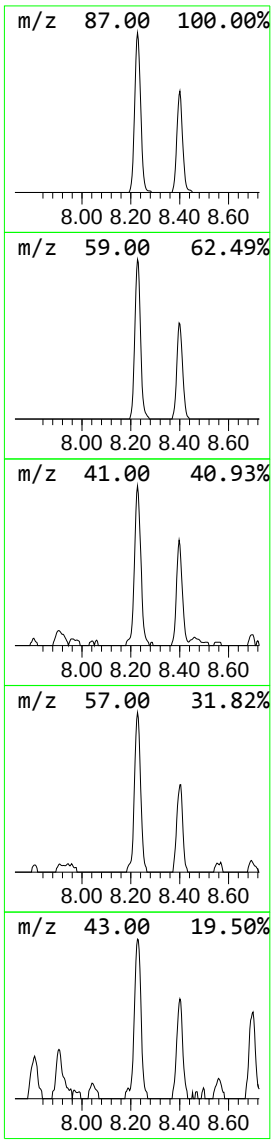
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.227	8.02 ug/l	91558	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	90
2	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	72
3	2-[2-[2-[2-(2-Methoxyethoxy)etho...	294	C13H26O7	1000351-91-3	50
4	Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	45
5	2-[2-[2-(2-Methoxyethoxy)ethoxy]...	250	C11H22O6	1000351-91-4	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30809

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

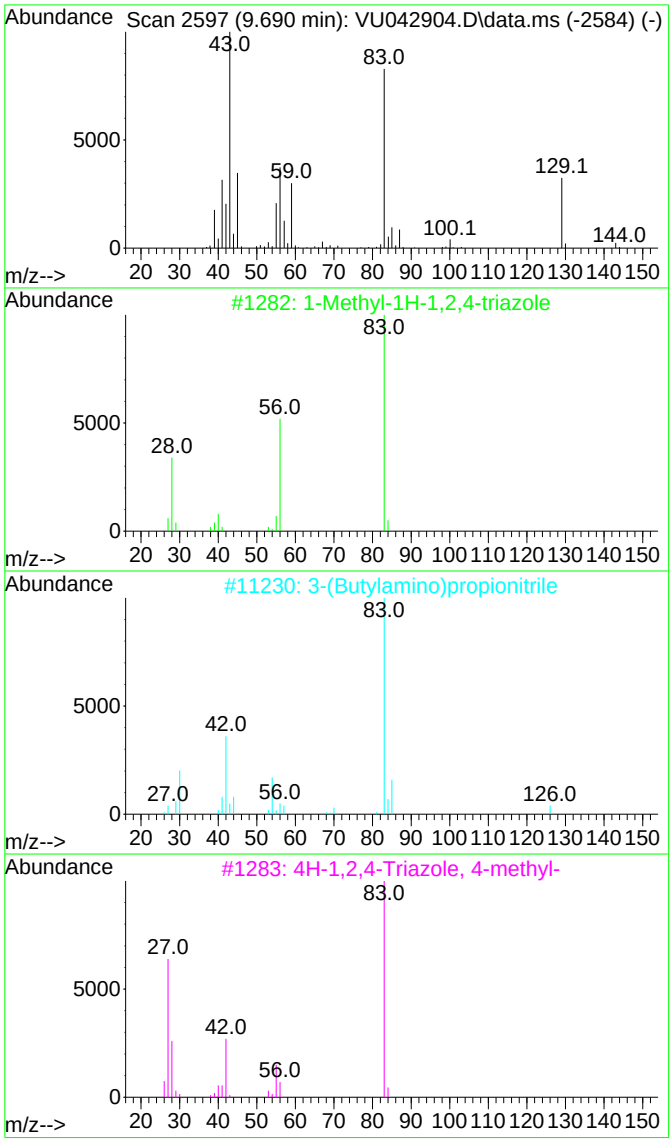
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

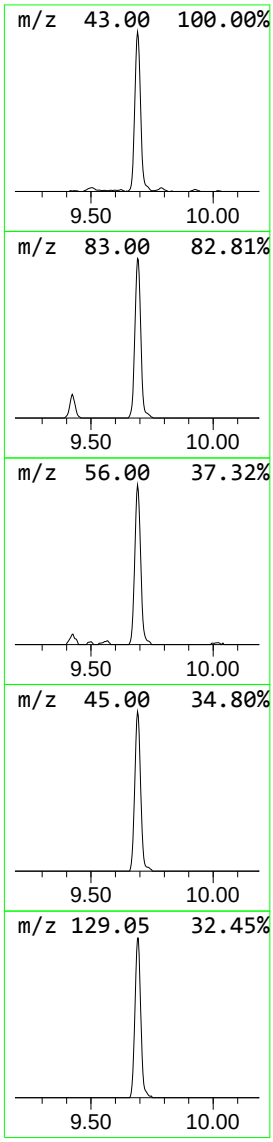
****

Peak Number 5 unknown9.690 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.690	24.62 ug/l	280877	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	38
2	3-(Butylamino)propionitrile	126	C7H14N2	000693-51-6	37
3	4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	32
4	1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	28
5	Oxalic acid, cyclohexyl isobutyl...	228	C12H20O4	1000309-30-4	17





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 30809

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

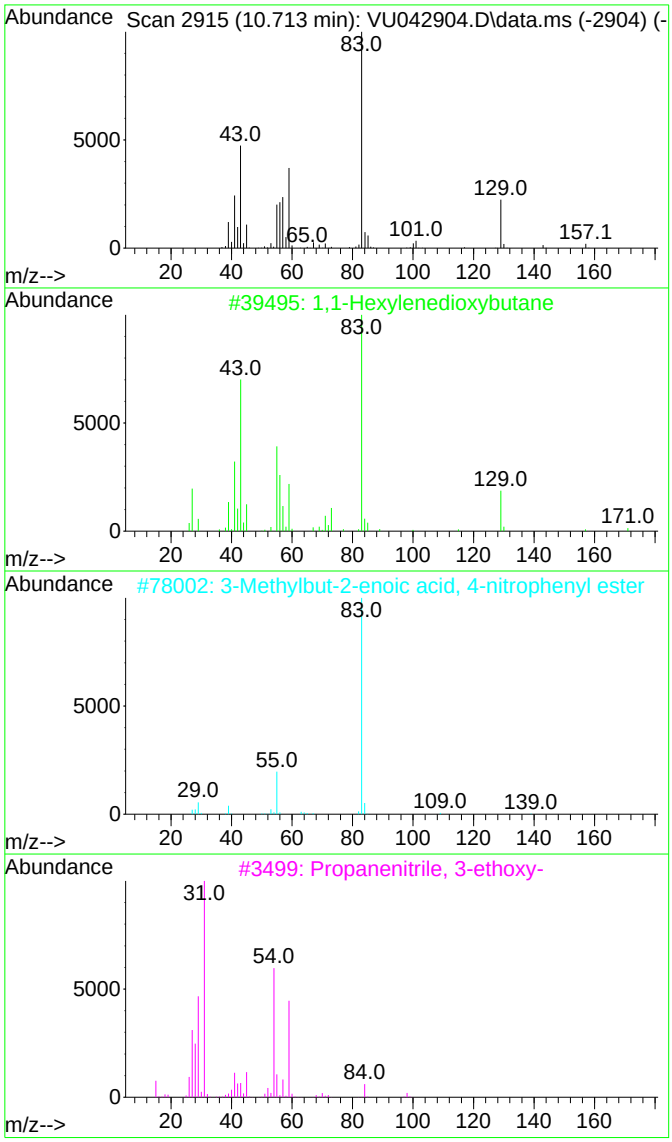
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

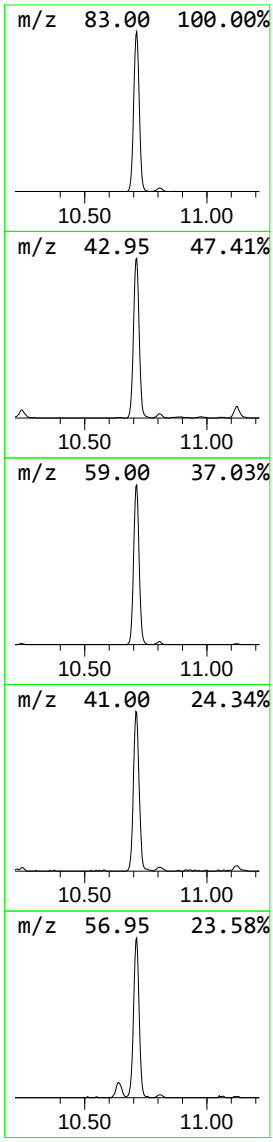
****

Peak Number 6 1,1-Hexylenedioxybutane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.713	45.27 ug/l	527148	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	64
2	3-Methylbut-2-enoic acid, 4-nitr...	221	C11H11NO4	1000307-59-8	25
3	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	10
4	.alpha.-Amino-2,5-dihydro-5-meth...	157	C7H11NO3	018455-25-9	9
5	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040221\
Data File : VU042904.D
Acq On : 02 Apr 2021 18:32
Operator : SY/MD
Sample : M1903-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanal	2.549	79.0	ug/l	532866	1	5.385	337280	50.0
1-Propanol	4.105	16.3	ug/l	109931	1	5.385	337280	50.0
1,3-Dioxolane, ...	8.227	8.0	ug/l	91558	3	9.423	570467	50.0
unknown9.690	9.690	24.6	ug/l	280877	3	9.423	570467	50.0
1,1-Hexylenedio...	10.713	45.3	ug/l	527148	4	11.819	582254	50.0