LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

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_X\METHOD\82X121319W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	43	rBV	909571	1138929	15.52%	3.235%
2	1.168	43	46	52	rVB2	390633	343930	4.69%	0.977%
3	1.399	78	84	88	rBV	59347	74059	1.01%	0.210%
4	1.485	94	98	104	rBV	153130	168891	2.30%	0.480%
5	2.344	233	239	246	rBV	59481	88152	1.20%	0.250%
6	2.430	246	253	265	rBV	4574799	7336727	100.00%	20.842%
7	2.588	272	279	286	rVB	41560	83837	1.14%	0.238%
8	3.027	343	351	360	rBV2	40348	91066	1.24%	0.259%
9	3.777	464	474	485	rVB2	44933	128274	1.75%	0.364%
10	4.325	553	564	578	rBV	154198	421557	5.75%	1.198%
11	5.490	744	755	768	rBV	295445	845316	11.52%	2.401%
12	5.655	771	782	796	rVB	541628	1530370	20.86%	4.347%
13	6.051	837	847	855	rBV	337153	864764	11.79%	2.457%
14	6.136	855	861	870	rVB	117247	302147	4.12%	0.858%
15	6.849	967	978	990	rBV	827251	1944835	26.51%	5.525%
16	7.288	1044	1050	1060	rBV2	44915	106180	1.45%	0.302%
17	8.709	1276	1283	1289	rBV	1714886	2654404	36.18%	7.540%
18	8.776	1289	1294	1307	rVB	3965196	6151798	83.85%	17.476%
19	9.056	1328	1340	1342	rBV4	44806	124708	1.70%	0.354%
20	10.105	1506	1512	1521	rVB	1634446	2292884	31.25%	6.513%
21	10.245	1531	1535	1544	rVB	205928	270561	3.69%	0.769%
22	10.355	1546	1553	1559	rVB	758576	1040330	14.18%	2.955%
23	10.696	1603	1609	1621	rBV2	271767	411331	5.61%	1.168%
24	11.129	1674	1680	1686	rBV	1395123	1839864	25.08%	5.227%
25	11.623	1756	1761	1764	rBV	136803	186122	2.54%	0.529%
26	11.733	1773	1779	1785	rBV	261112	298956	4.07%	0.849%
27	11.916	1804	1809	1817	rVV	181228	252796	3.45%	0.718%
28	12.038	1821	1829	1831	rVV2	182386	257501	3.51%	0.731%
29	12.074	1831	1835	1842	rVB	1835544	2244800	30.60%	6.377%
30	12.202	1852	1856	1862	rVV	71098	110634	1.51%	0.314%
31	12.263	1862	1866	1878	rVV	688946	913071	12.45%	2.594%
32	12.464	1894	1899	1904	rVB	59002	75137	1.02%	0.213%
33	13.830	2119	2123	2129	rVV	140043	189321	2.58%	0.538%
34	13.897	2129	2134	2141	rVV2	64585	110074	1.50%	0.313%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

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_X\METHOD\82X121319W.M
Title : SW846 8260

35	13.964	2141	2145	2152	rVB	55588	77109	1.05%	0.219%
36	14.501	2226	2233	2238	rBV	169050	231886	3.16%	0.659%

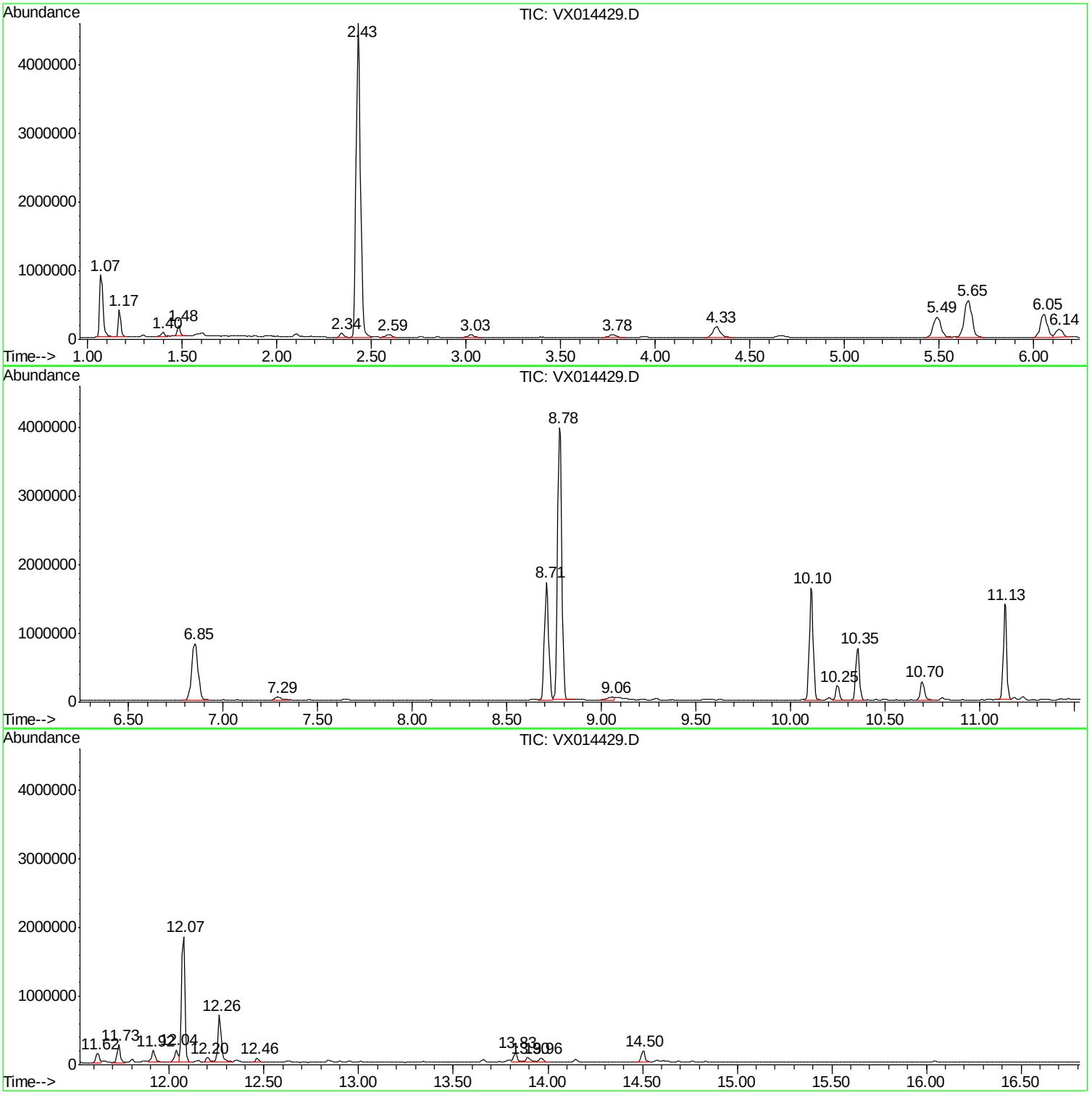
Sum of corrected areas: 35202321

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

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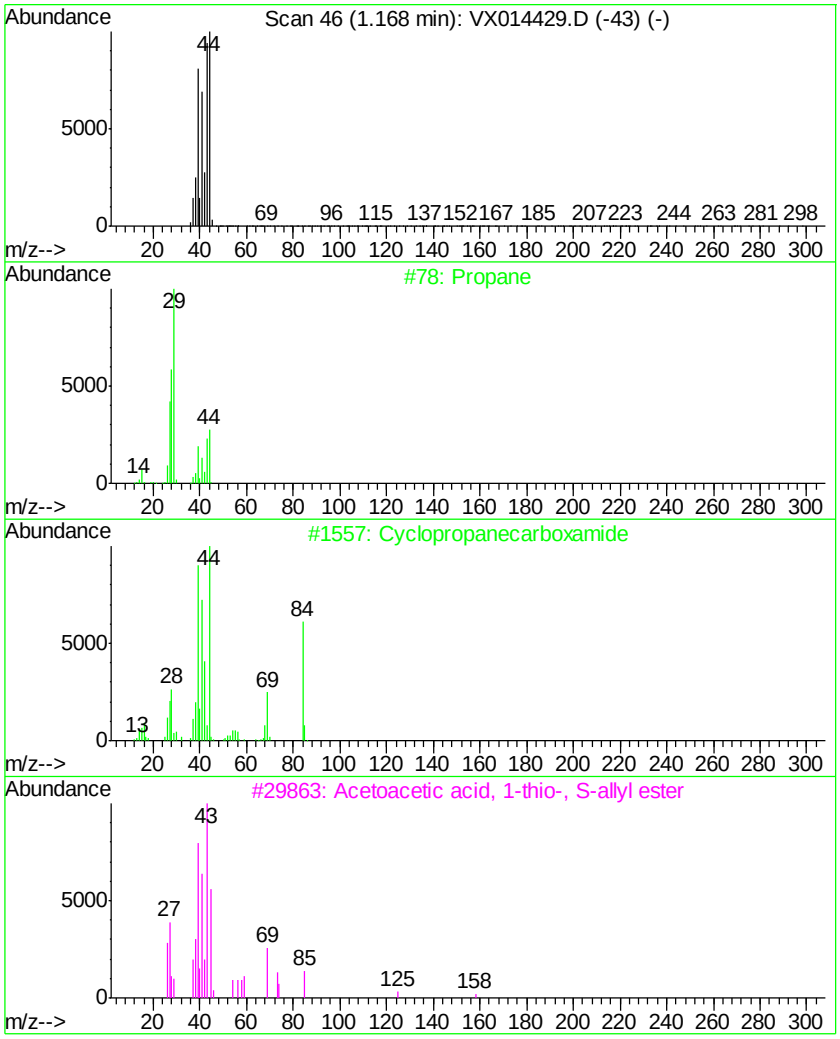
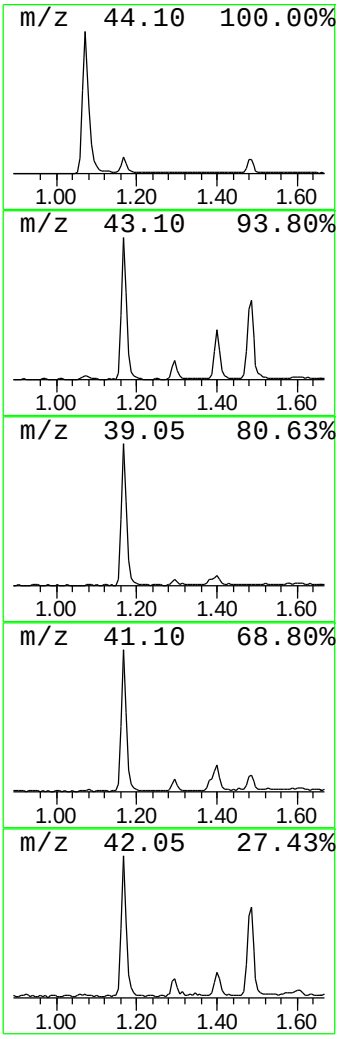
Peak Number 2 Propane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.17	11.24 ug/l	343930	Pentafluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	43
3	Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	39
4	3-Butenoic acid	86	C4H6O2	000625-38-7	36
5	2-Nonynoic acid	154	C9H14O2	001846-70-4	33





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

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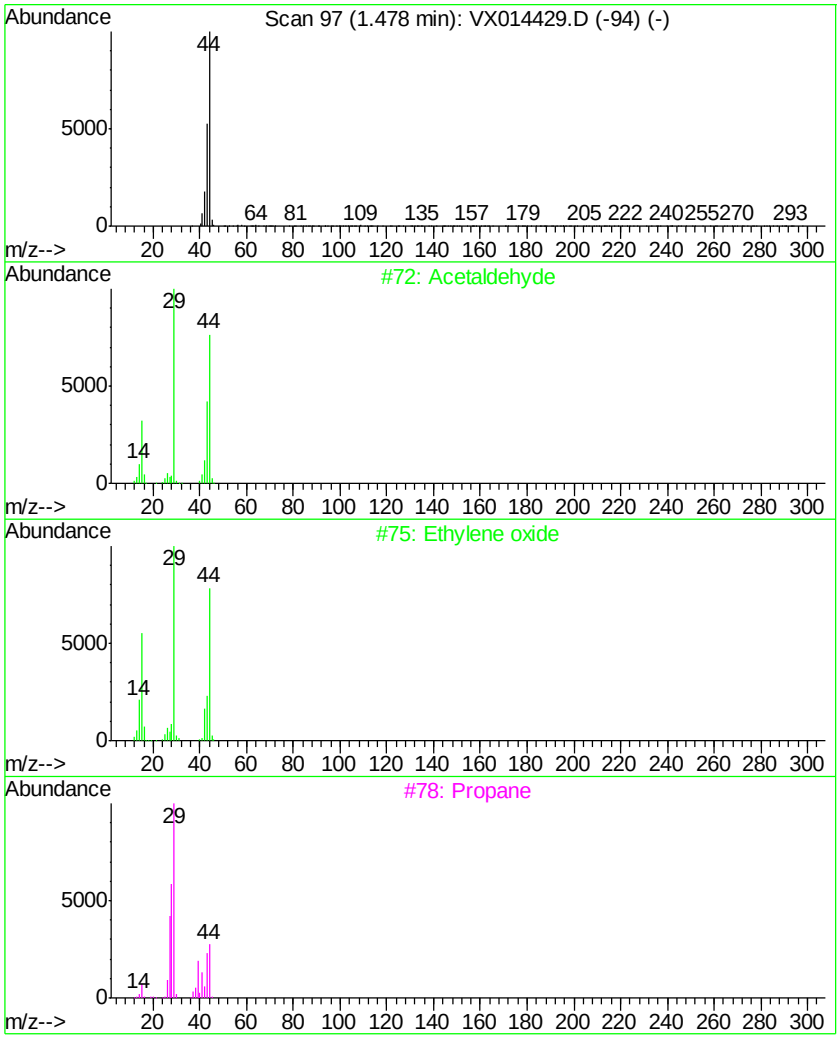
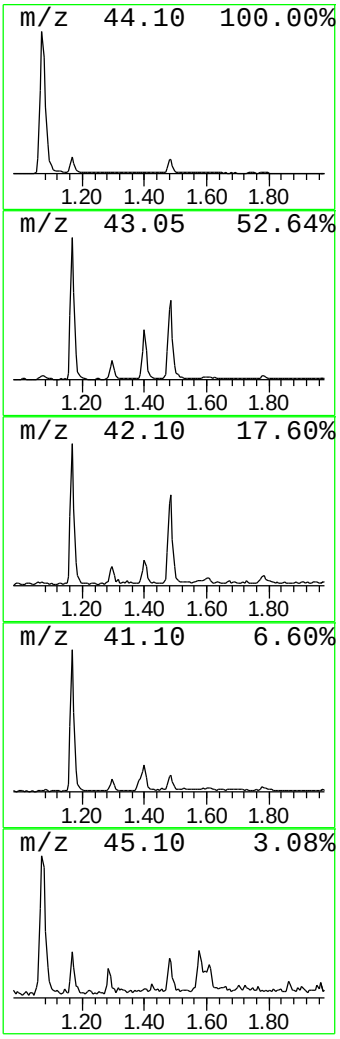
Peak Number 3 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	5.52 ug/l	168891	Pentafluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Ethylene oxide	44	C2H4O	000075-21-8	9
3	Propane	44	C3H8	000074-98-6	5
4	Cystine	240	C6H12N2O4S2	000056-89-3	5
5	Carbon dioxide	44	CO2	000124-38-9	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

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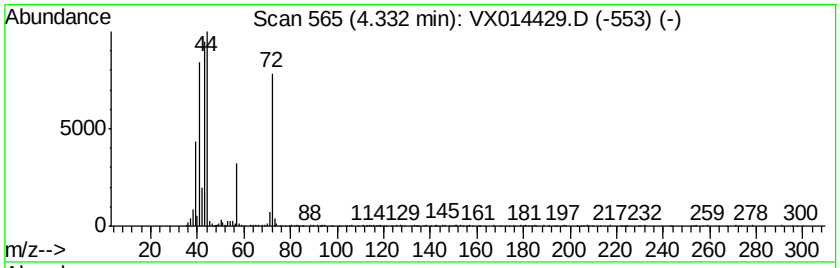
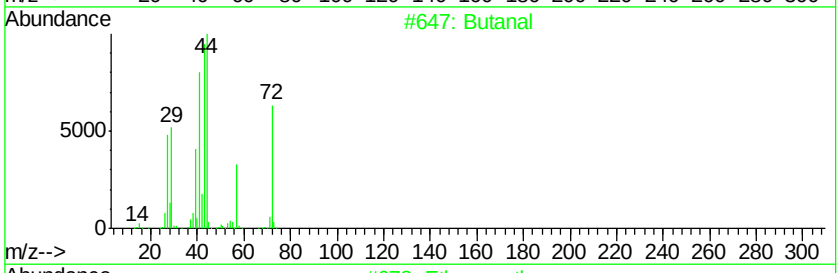
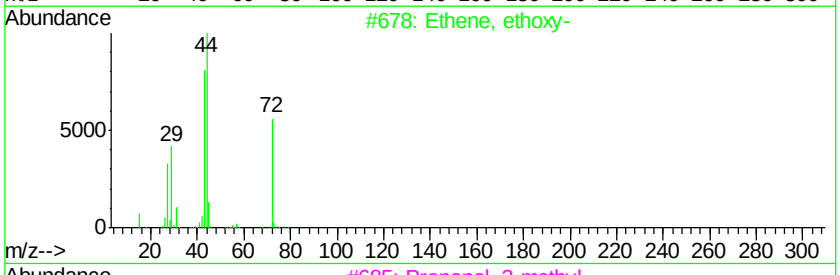
Peak Number 4 Butanal Concentration Rank 3

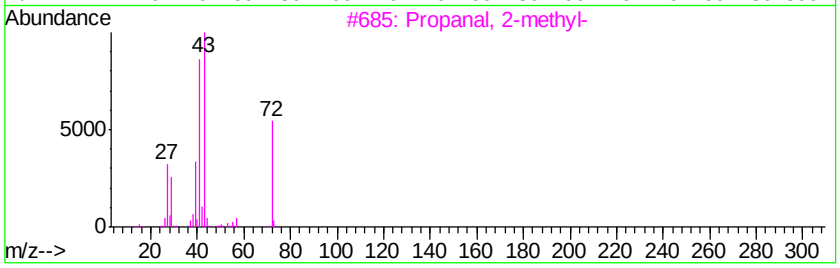
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	13.77 ug/l	421557	Pentafluorobenzene	5.65

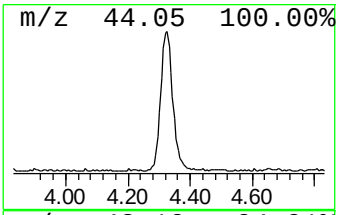
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	Adenine-9-propanoic acid, .alpha...	322	C13H18N6O4	055387-36-5	37
5	Isobutylene epoxide	72	C4H8O	000558-30-5	22

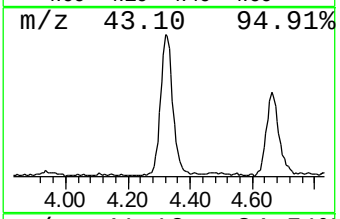


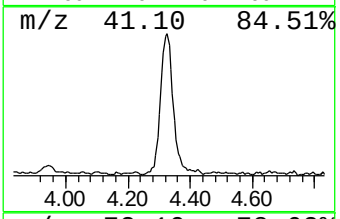


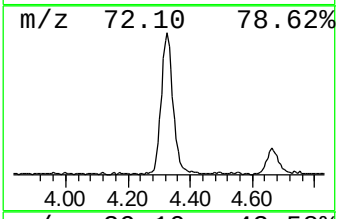


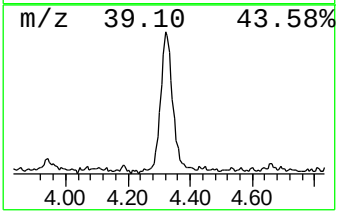












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

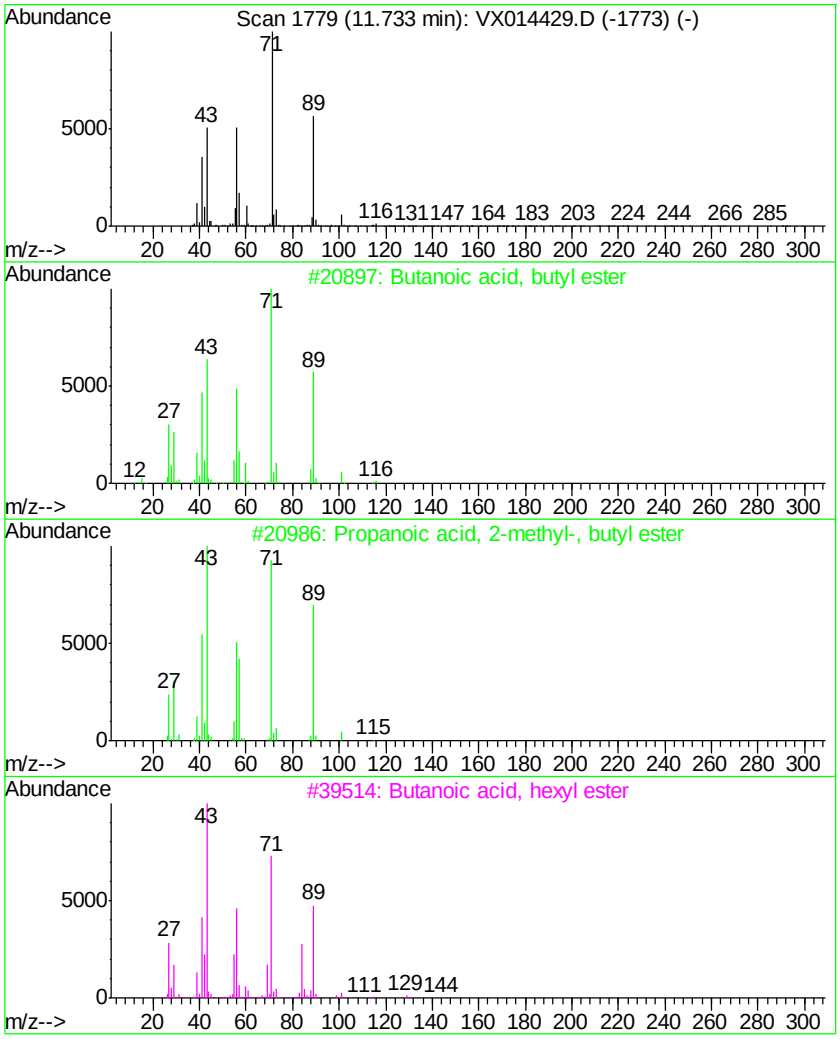
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

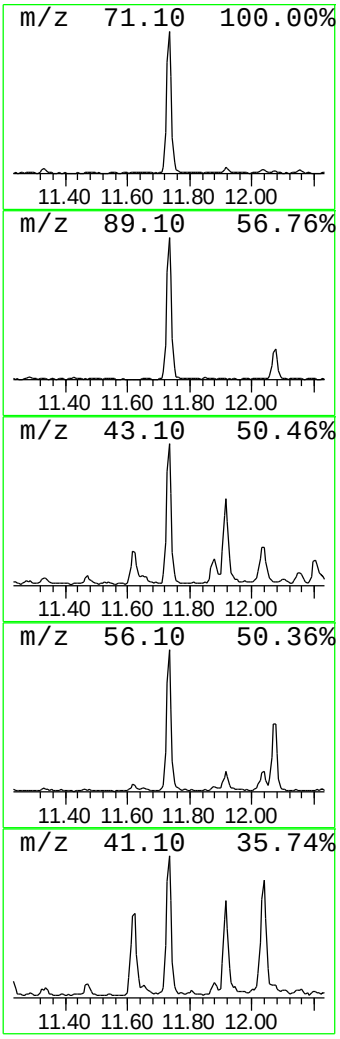
****

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	6.66 ug/l	298956	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	78
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

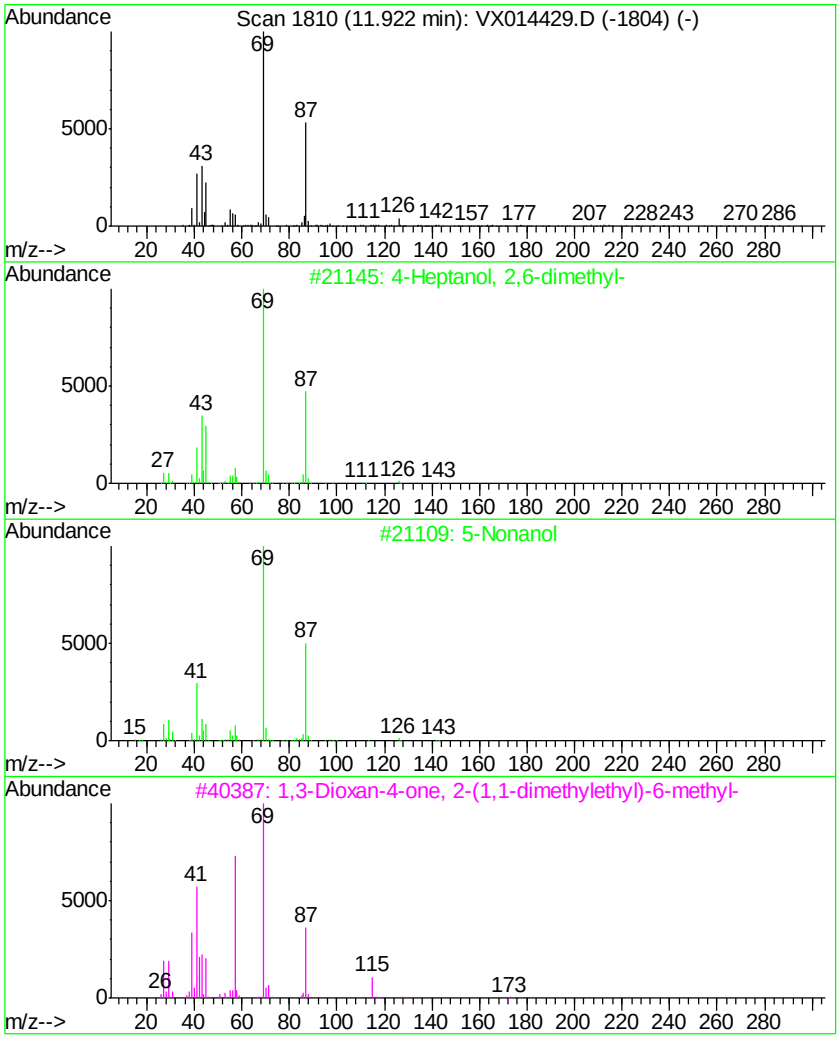
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

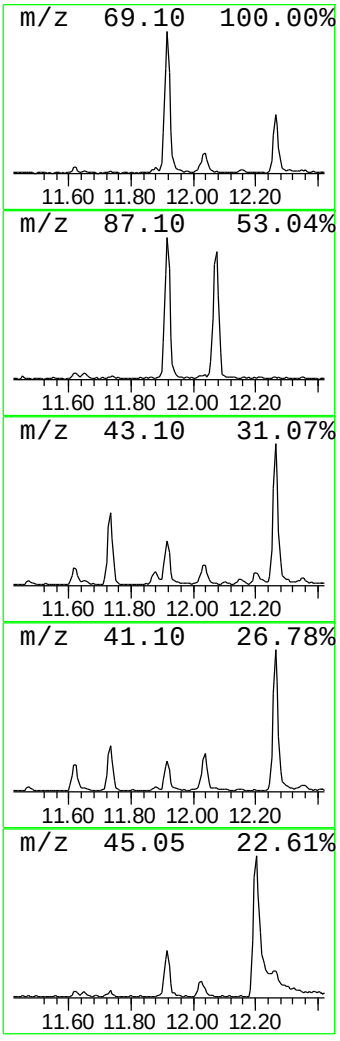
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.63 ug/l	252796	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	78
2	5-Nonanol	144	C9H20O	000623-93-8	64
3	1,3-Dioxan-4-one, 2-(1,1-dimethy...	172	C9H16O3	113505-75-2	64
4	1,2-Hexanediol	118	C6H14O2	006920-22-5	64
5	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	64





Library Search Compound Report

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Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

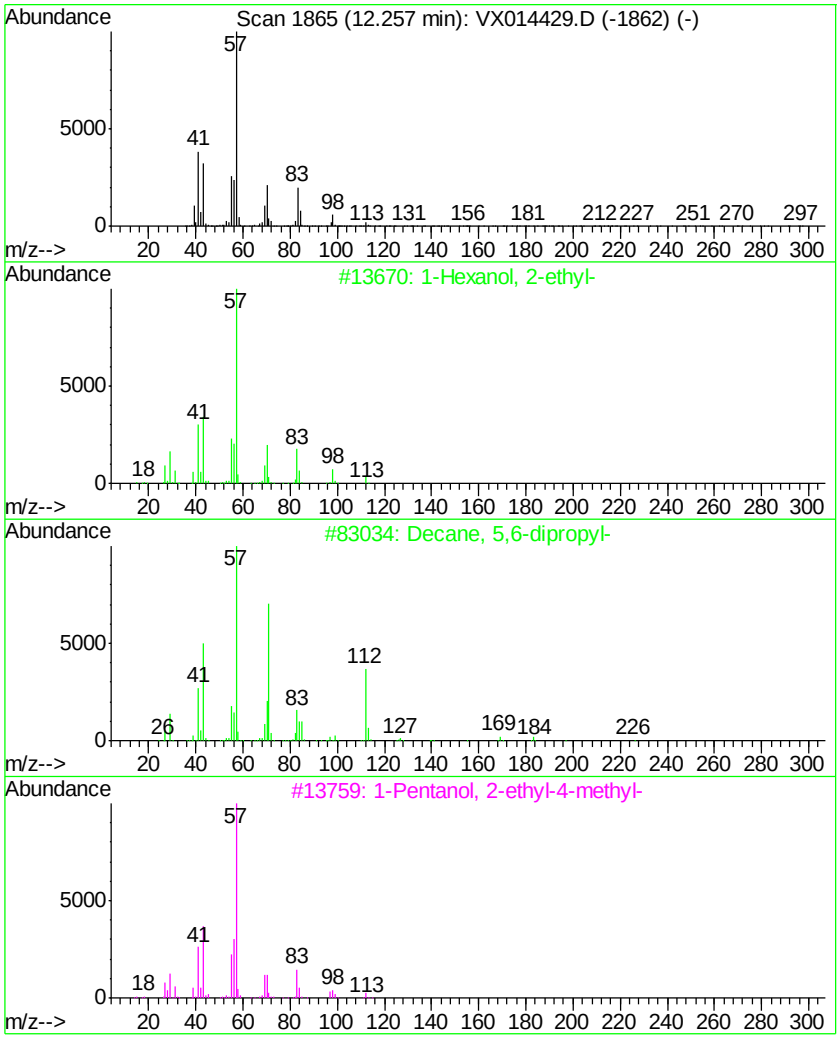
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

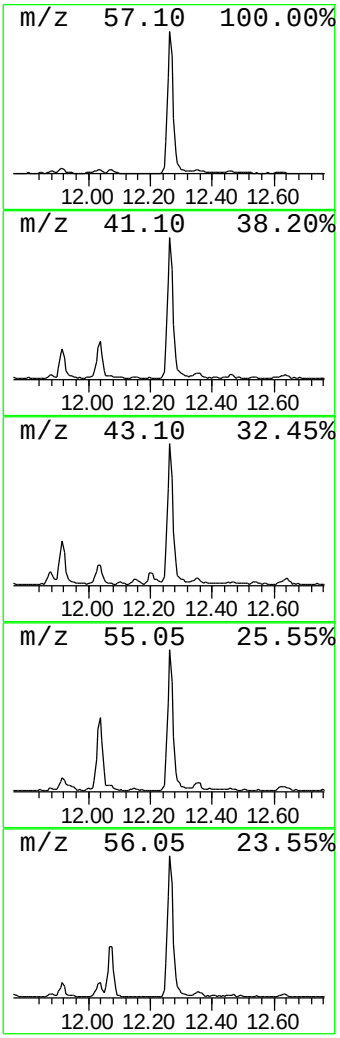
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	20.34 ug/l	913071	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	64
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

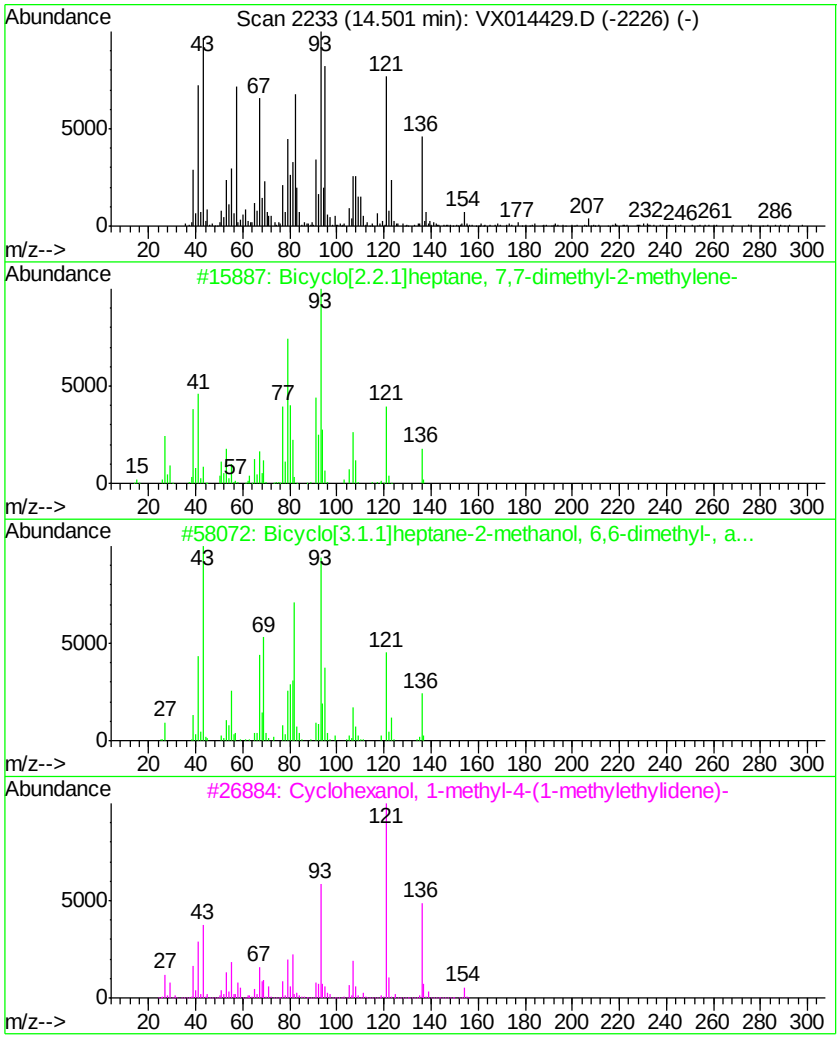
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

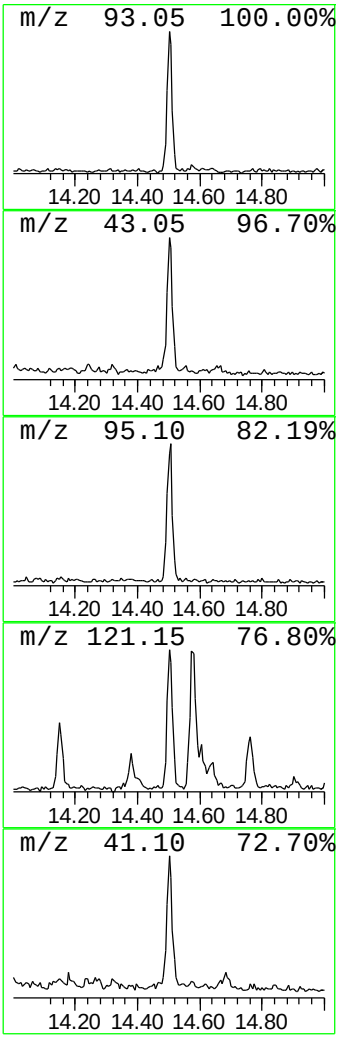
****

Peak Number 8 Bicyclo[2.2.1]heptane, 7,7-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	5.16 ug/l	231886	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	91
2	Bicyclo[3.1.1]heptane-2-methanol...	196	C12H20O2	029021-36-1	72
3	Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	000586-81-2	53
4	(-)-trans-Myrtanyl acatate	196	C12H20O2	1000157-78-3	52
5	2-Methyl-trans-3a,4,7,7a-tetrahy...	136	C10H16	1000145-84-2	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014429.D
Acq On : 06 Jan 2020 15:55
Operator : JC/SP
Sample : K6484-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 40335-40338

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.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	1.17	11.2	ug/l	343930	1	5.65	1530370	50.0
Acetaldehyde	1.48	5.5	ug/l	168891	1	5.65	1530370	50.0
Butanal	4.33	13.8	ug/l	421557	1	5.65	1530370	50.0
Butanoic acid, bu...	11.73	6.7	ug/l	298956	4	12.07	2244800	50.0
4-Heptanol, 2,6-d...	11.92	5.6	ug/l	252796	4	12.07	2244800	50.0
1-Hexanol, 2-ethyl-	12.26	20.3	ug/l	913071	4	12.07	2244800	50.0
Bicyclo[2.2.1]hep...	14.50	5.2	ug/l	231886	4	12.07	2244800	50.0