LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

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\82X071222W.M
Title : SW846 8260

Signal : TIC: VX030167.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	72	rBV	1678589	1867582	100.00%	22.290%
2	2.069	156	161	166	rBV	18893	28998	1.55%	0.346%
3	2.386	207	213	223	rVB	138879	219329	11.74%	2.618%
4	4.385	534	541	550	rBV	11561	31668	1.70%	0.378%
5	5.391	694	706	720	rBV	104314	304737	16.32%	3.637%
6	5.562	720	734	747	rVB	179975	512071	27.42%	6.112%
7	5.964	789	800	814	rBV	123087	327164	17.52%	3.905%
8	6.129	820	827	841	rBV3	19742	64182	3.44%	0.766%
9	6.769	921	932	943	rBV	304947	732254	39.21%	8.740%
10	6.879	943	950	960	rVB2	20856	52488	2.81%	0.626%
11	8.653	1234	1241	1247	rBV	619141	942293	50.46%	11.247%
12	8.726	1247	1253	1259	rVB	101886	163897	8.78%	1.956%
13	10.055	1463	1471	1485	rBV	610090	817850	43.79%	9.761%
14	11.085	1627	1640	1649	rBV	448328	576573	30.87%	6.882%
15	11.896	1766	1773	1782	rBV	115267	244396	13.09%	2.917%
16	12.024	1789	1794	1804	rVB	595779	730829	39.13%	8.723%
17	12.226	1822	1827	1831	rBV2	39659	72166	3.86%	0.861%
18	12.293	1831	1838	1839	rVV3	141202	290129	15.54%	3.463%
19	12.311	1839	1841	1848	rVV2	163044	296543	15.88%	3.539%
20	12.366	1848	1850	1864	rVB2	40944	103238	5.53%	1.232%

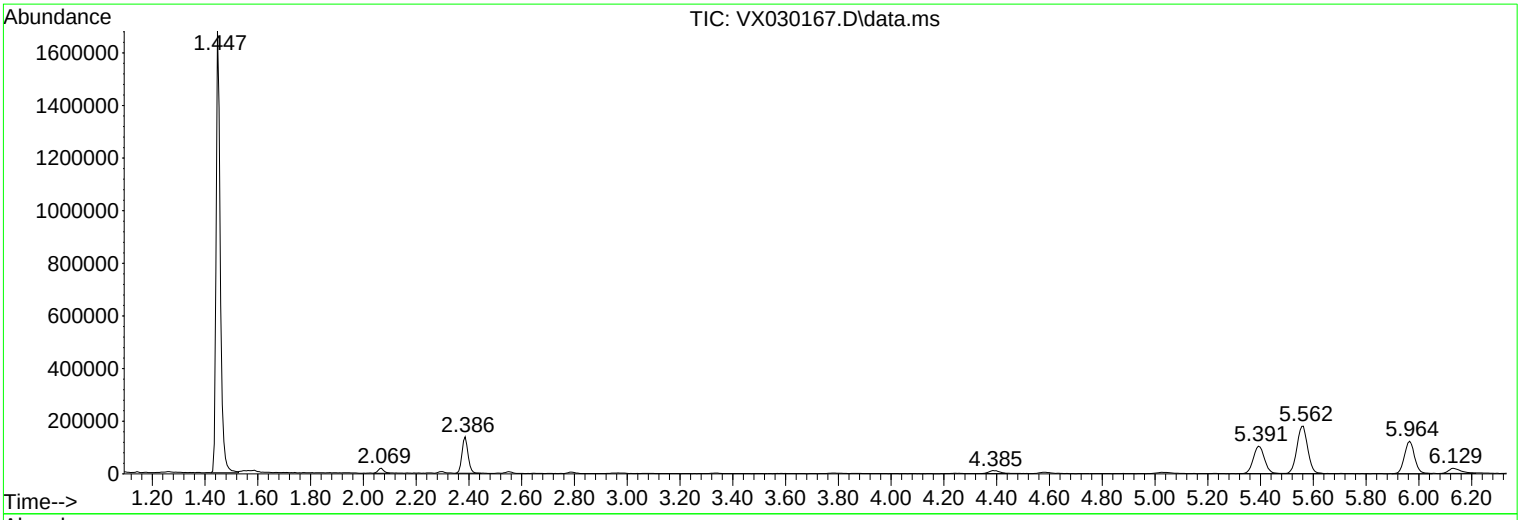
Sum of corrected areas: 8378387

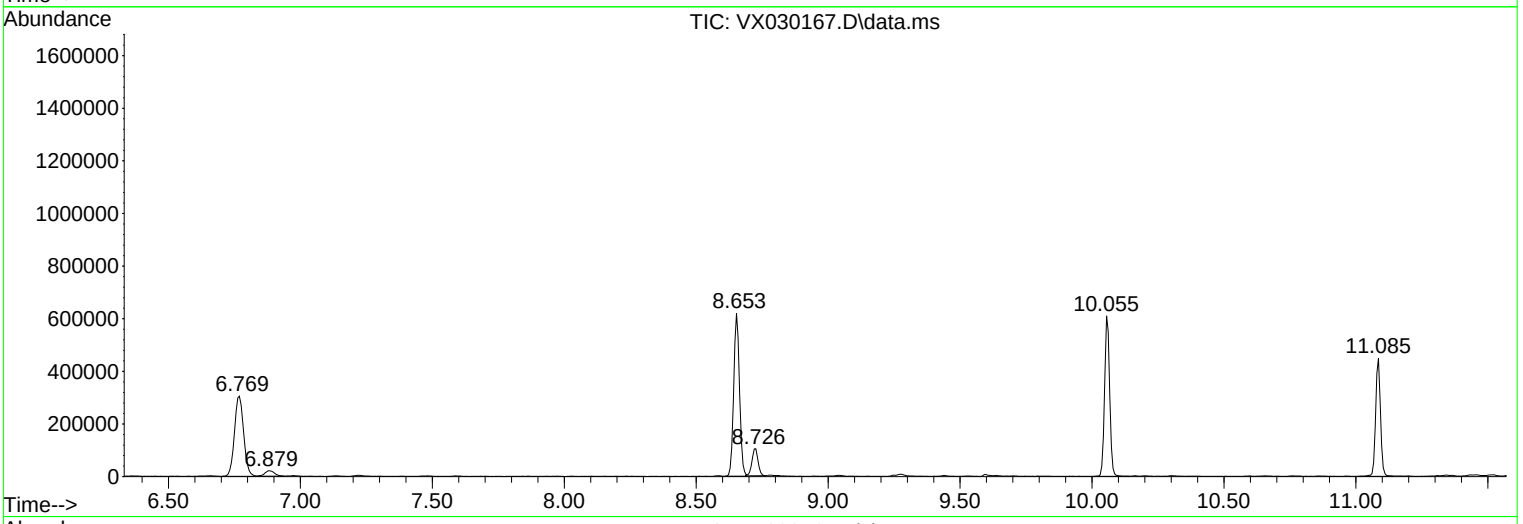
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

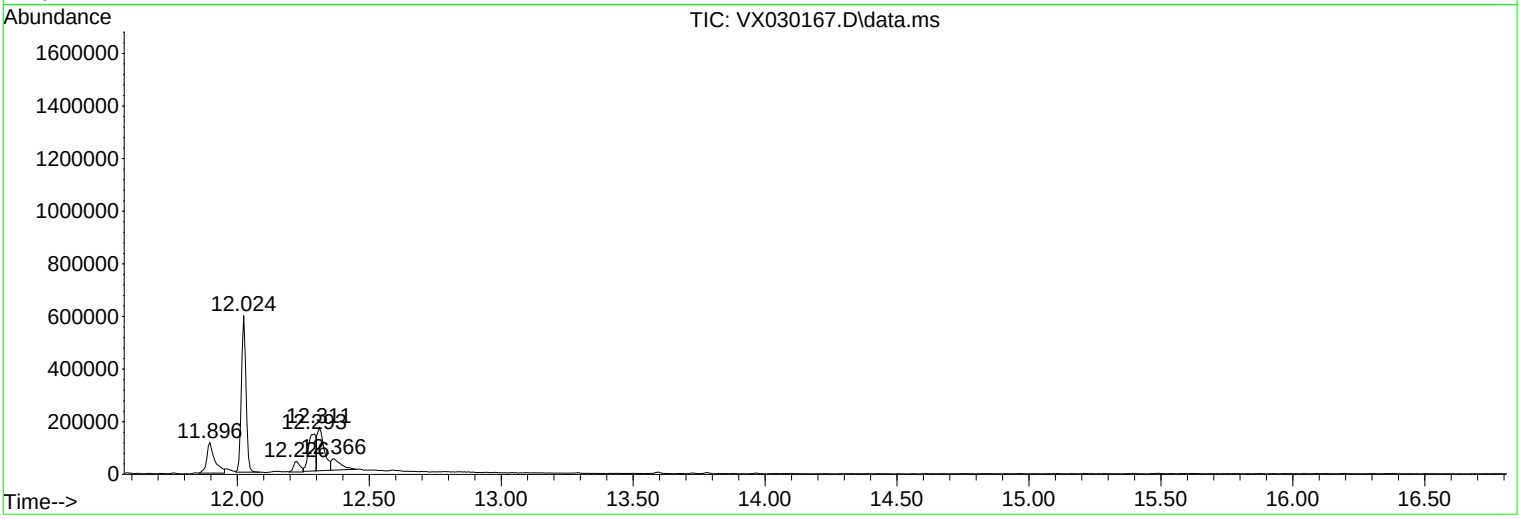
Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

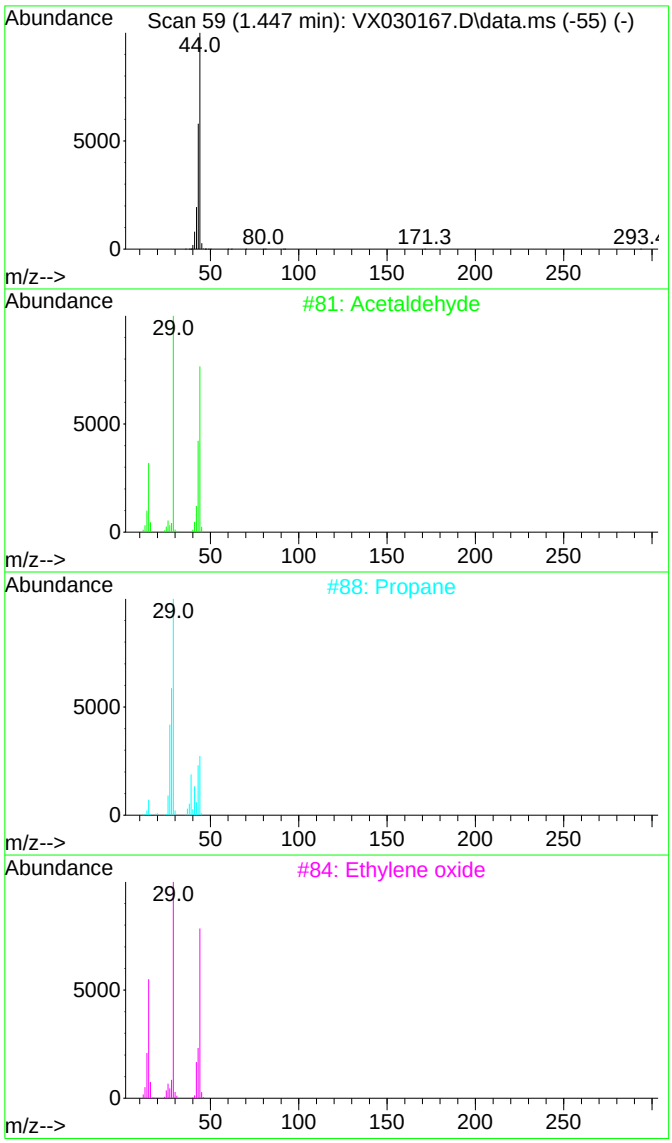
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

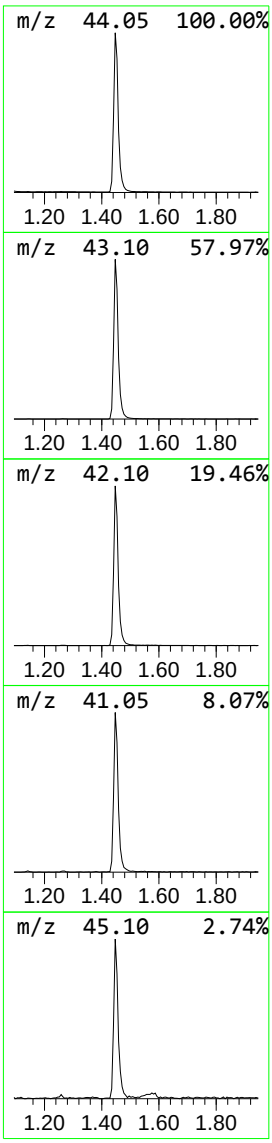
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	182.36 ug/l	1867580	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

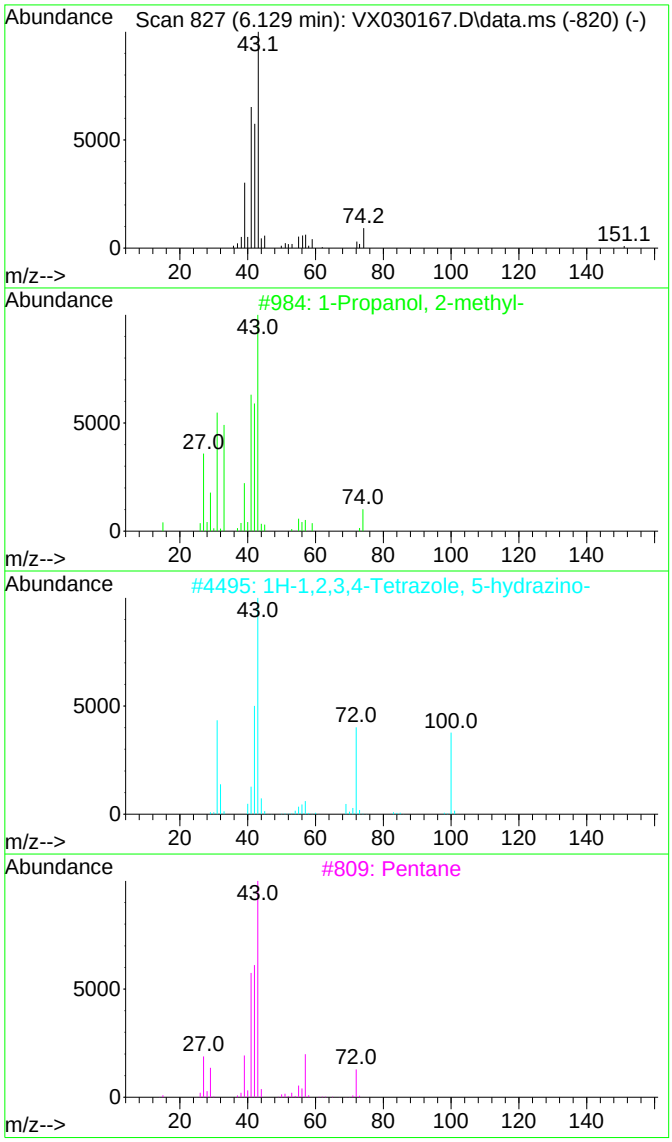
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

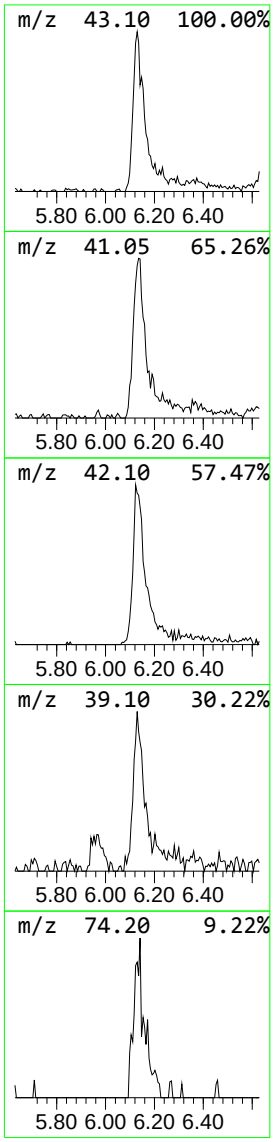
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.129	6.27 ug/l	64182	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	87
2	1H-1,2,3,4-Tetrazole, 5-hydrazino-	100	CH4N6	1000337-72-7	38
3	Pentane	72	C5H12	000109-66-0	36
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	32
5	3-Buten-1-ol	72	C4H8O	000627-27-0	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

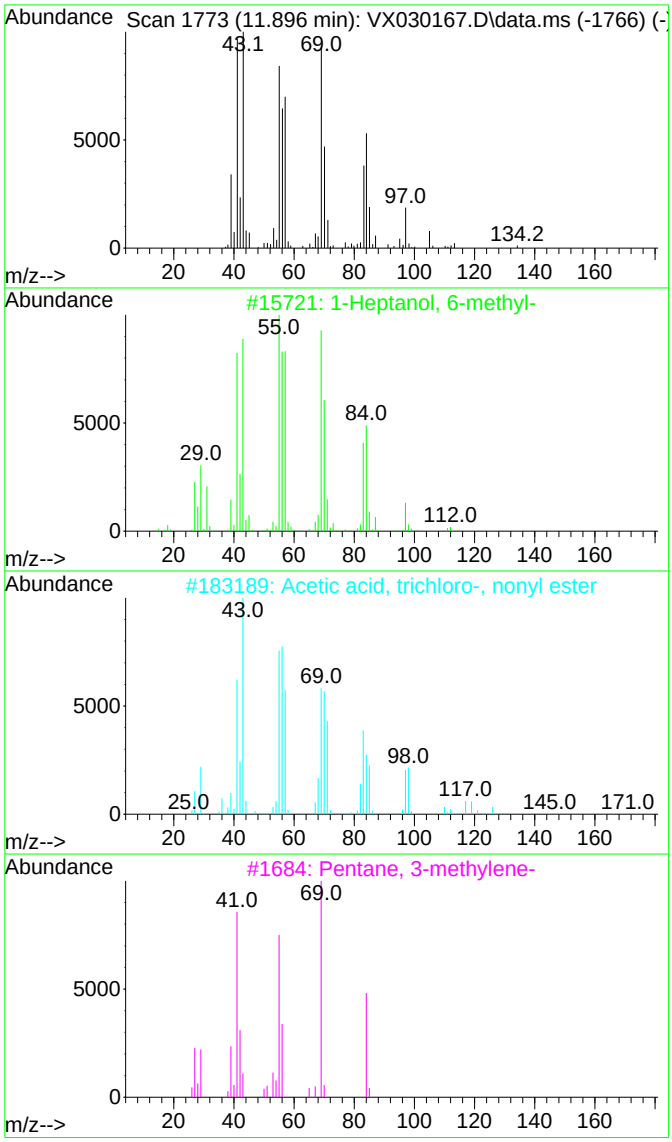
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

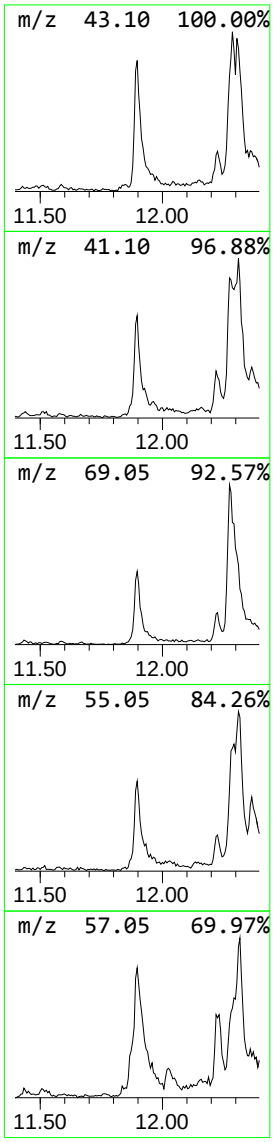
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Heptanol, 6-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.896	16.72 ug/l	244396	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	90
2	Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	50
3	Pentane, 3-methylene-	84	C6H12	000760-21-4	49
4	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	47
5	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

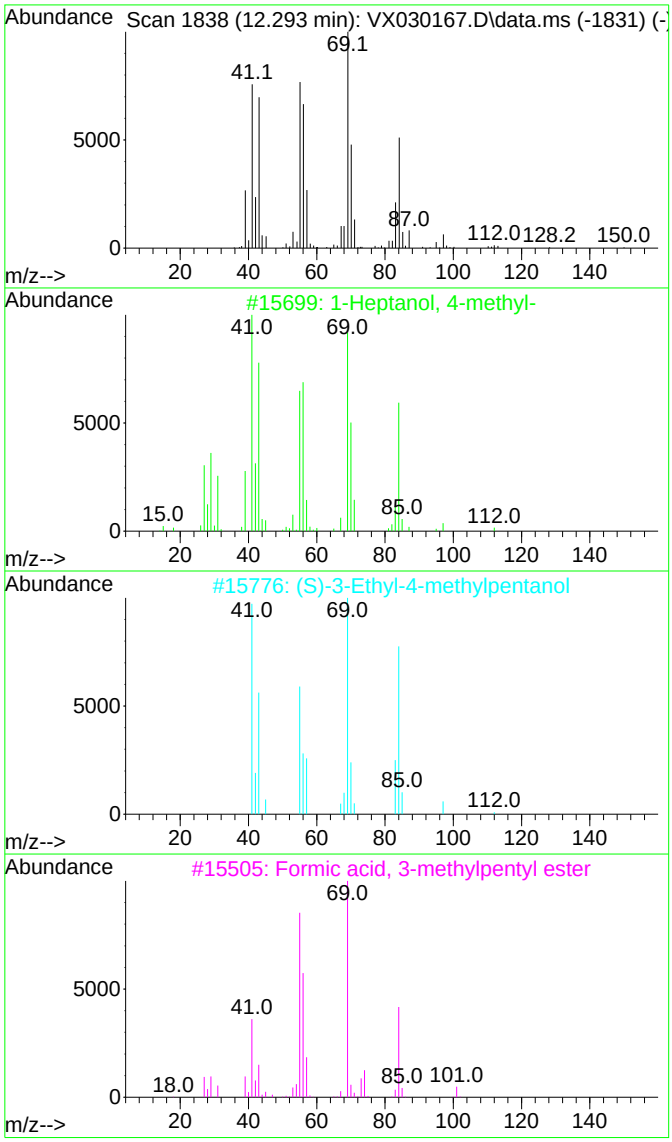
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

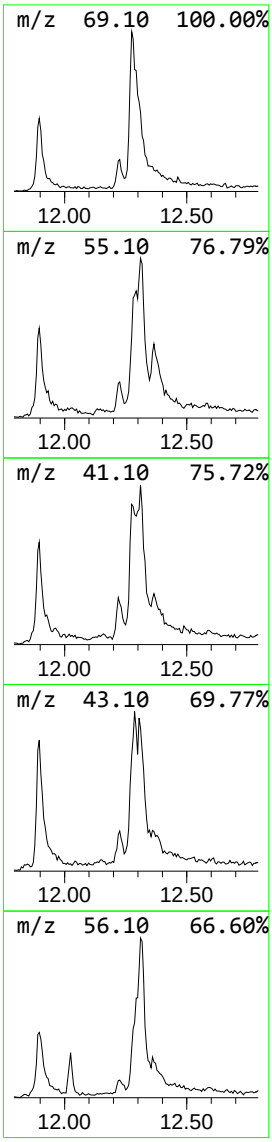
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heptanol, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.293	19.85 ug/l	290129	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	72
2	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	64
3	Formic acid, 3-methylpentyl ester	130	C7H14O2	1000368-21-3	53
4	3-Nonene, 2-methyl-	140	C10H20	053966-53-3	53
5	4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

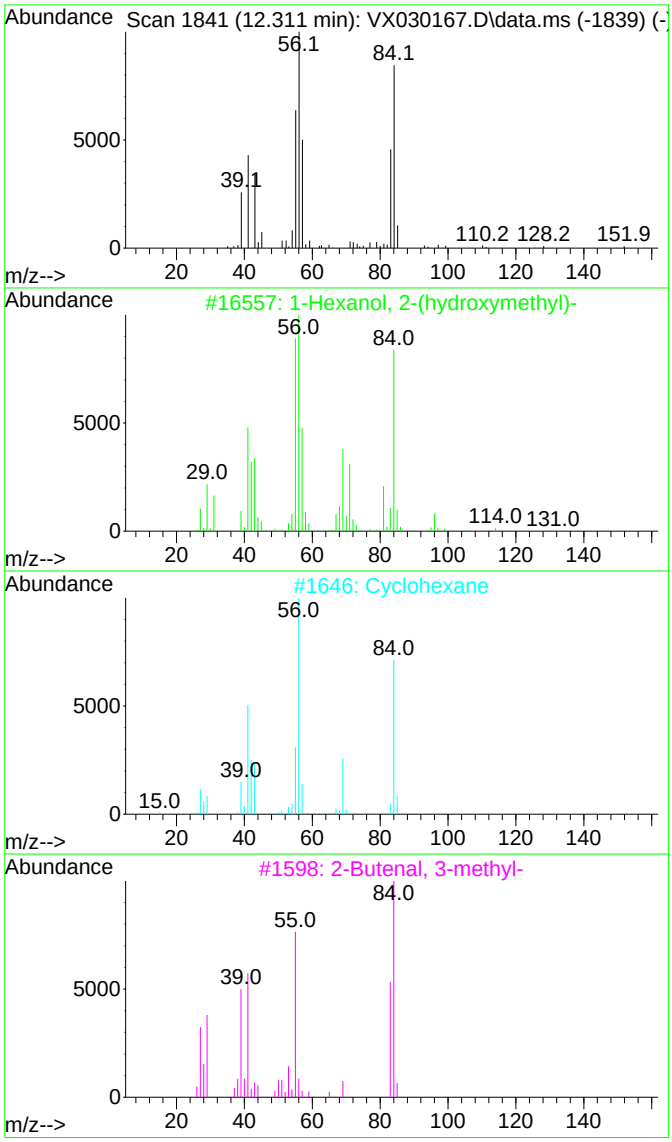
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

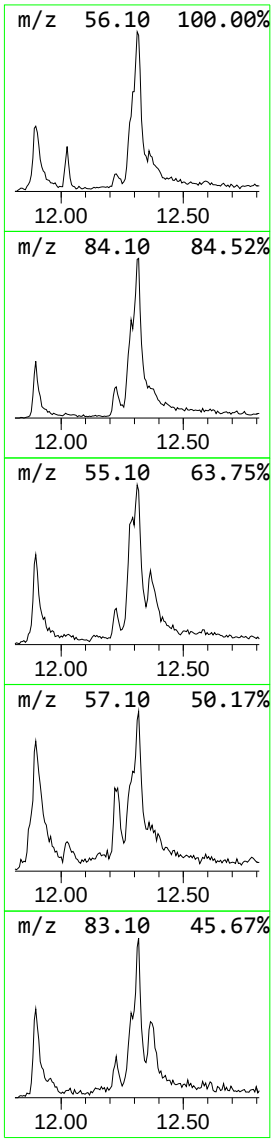
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-(hydroxymethyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.311	20.29 ug/l	296543	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-(hydroxymethyl)-	132	C7H16O2	1000326-00-5	64
2	Cyclohexane	84	C6H12	000110-82-7	64
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	49
4	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	49
5	1-Silacyclo-3-pentene	84	C4H8Si	007049-25-4	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

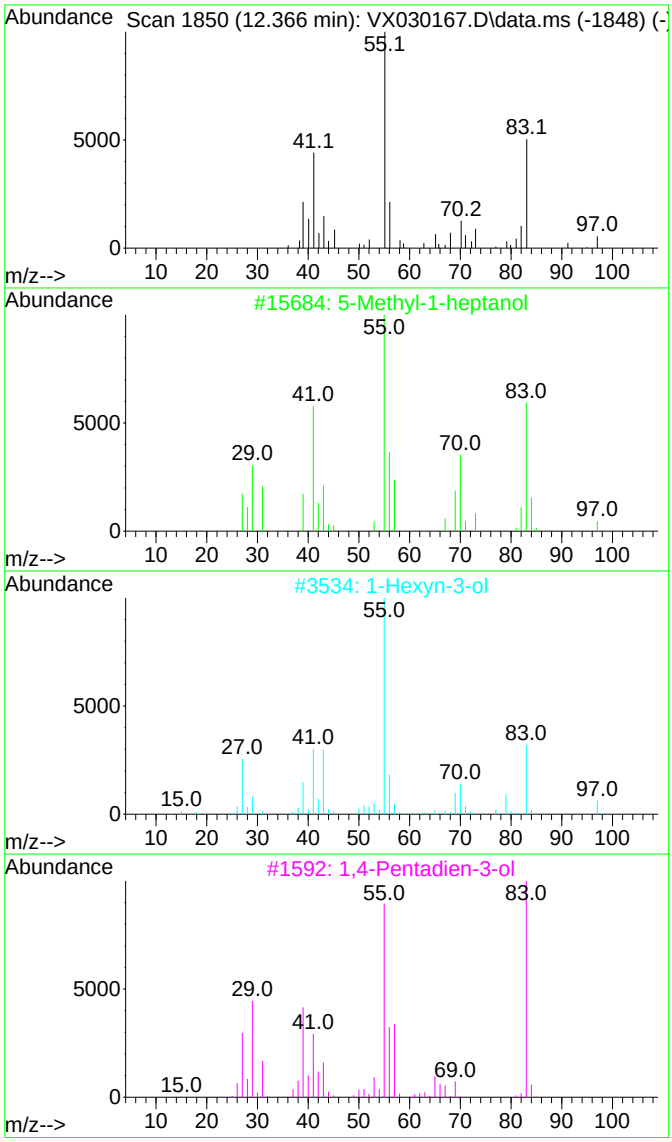
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

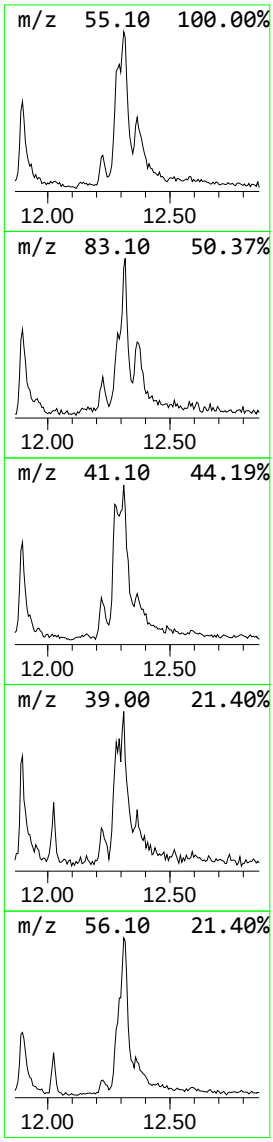
****

Peak Number 6 unknown12.366 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.366	7.06 ug/l	103238	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-1-heptanol	130	C8H18O	007212-53-5	33
2	1-Hexyn-3-ol	98	C6H10O	000105-31-7	33
3	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	25
4	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	25
5	Cyclohexane, nitro-	129	C6H11NO2	001122-60-7	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030167.D
Acq On : 21 Jul 2022 17:15
Operator : JC/MD
Sample : N3781-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0020

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.447	182.4	ug/l	1867580	1	5.562	512071	50.0
1-Propanol, 2-m...	6.129	6.3	ug/l	64182	1	5.562	512071	50.0
1-Heptanol, 6-m...	11.896	16.7	ug/l	244396	4	12.024	730829	50.0
1-Heptanol, 4-m...	12.293	19.9	ug/l	290129	4	12.024	730829	50.0
1-Hexanol, 2-(h...	12.311	20.3	ug/l	296543	4	12.024	730829	50.0
unknown12.366	12.366	7.1	ug/l	103238	4	12.024	730829	50.0