

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
 Data File : VN073240.D
 Acq On : 29 Jun 2022 14:05
 Operator : JC\MD
 Sample : N3504-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TRE-1616

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_N\methods\82N062822W.M

Title : SW846 8260

Signal : TIC: VN073240.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.381	82	84	206	rBV	43132466	401190388	47.32%	27.277%
2	4.216	277	396	397	rBV	32228093	847829820	100.00%	57.645%
3	4.810	480	497	519	rBV	3512044	10952898	1.29%	0.745%
4	5.504	595	615	649	rBV	8304448	33041823	3.90%	2.247%
5	6.640	789	808	854	rBV2	1685121	10301728	1.22%	0.700%
6	6.992	854	868	898	rVV	5533355	17935510	2.12%	1.219%
7	7.357	911	930	964	rVB	11866981	36817945	4.34%	2.503%
8	8.192	1061	1072	1091	rBV	5539417	15026367	1.77%	1.022%
9	8.798	1164	1175	1188	rBV	5111273	20536743	2.42%	1.396%
10	9.145	1220	1234	1259	rBV	10339472	30663681	3.62%	2.085%
11	12.075	1721	1732	1741	rBV	8655975	14602752	1.72%	0.993%
12	13.710	2002	2010	2017	rVB	7405468	11877404	1.40%	0.808%
13	14.074	2064	2072	2082	rBV	12402900	19999652	2.36%	1.360%

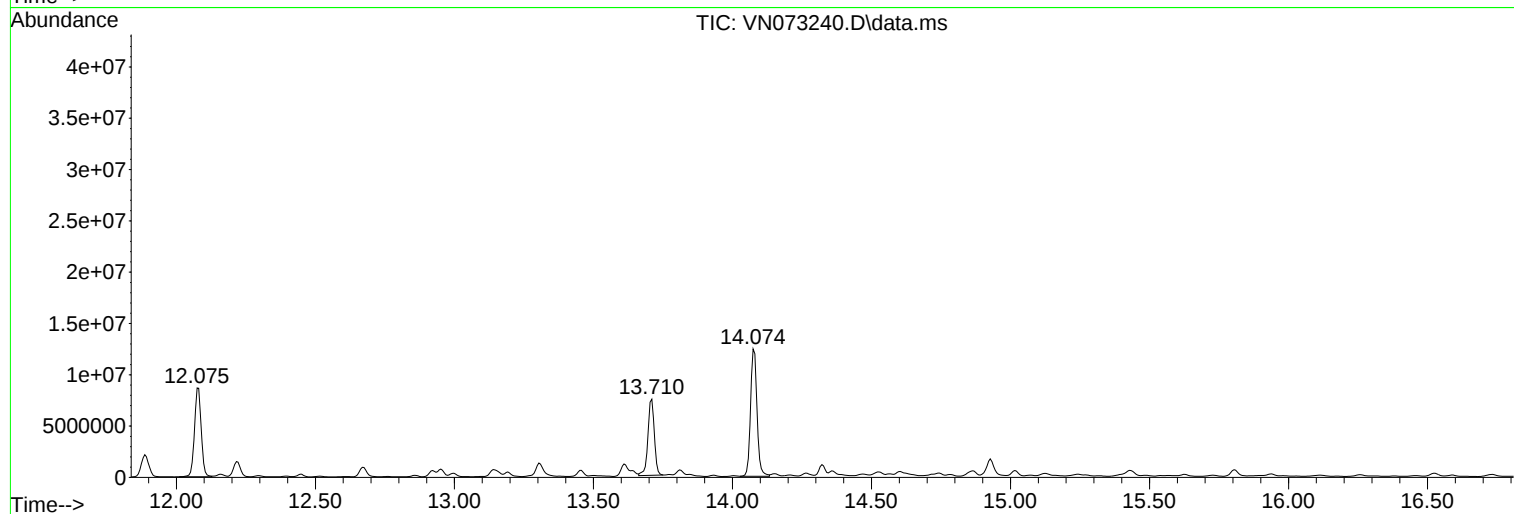
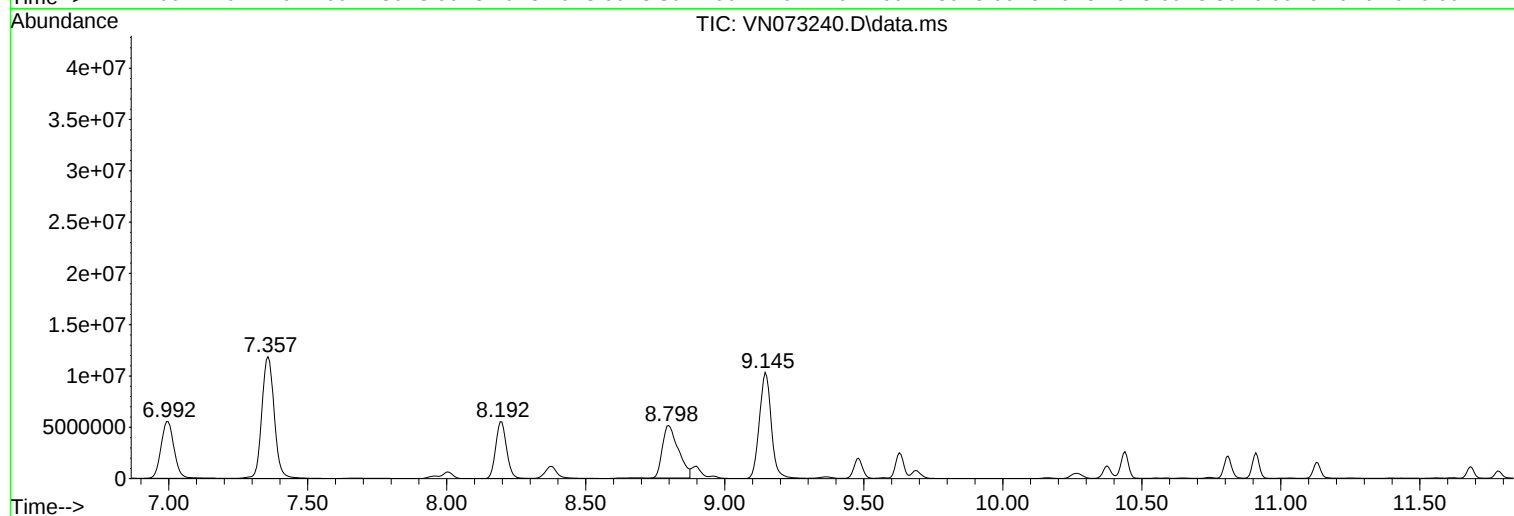
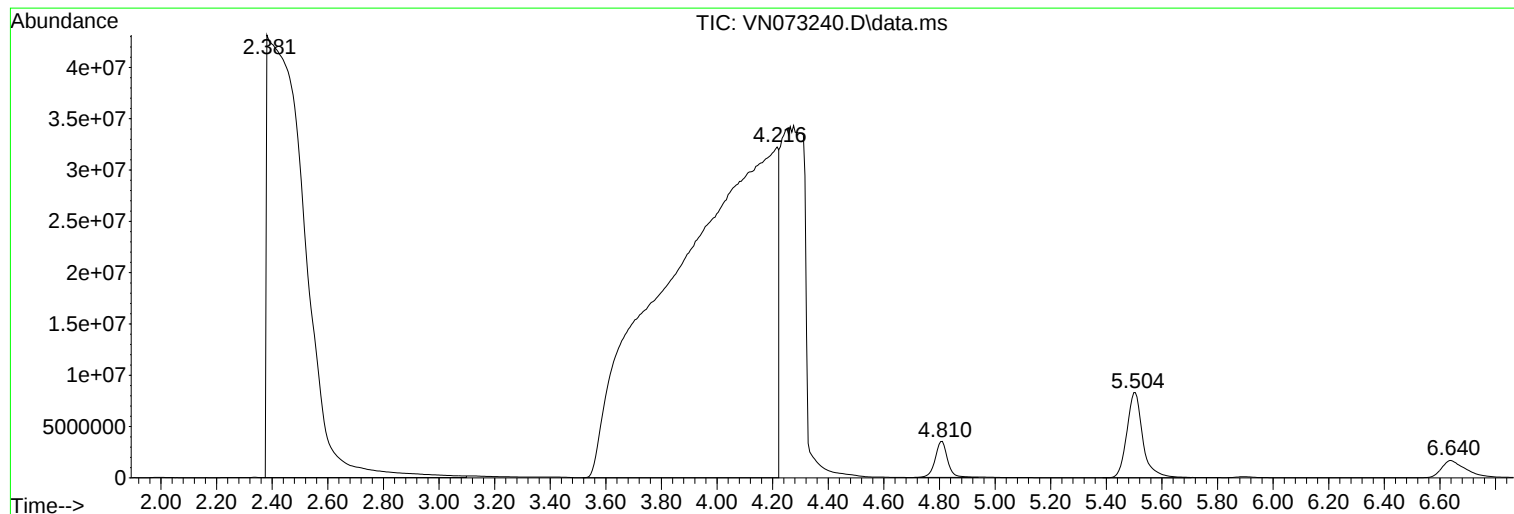
Sum of corrected areas: 1470776711

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

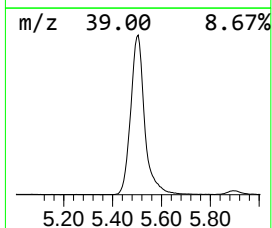
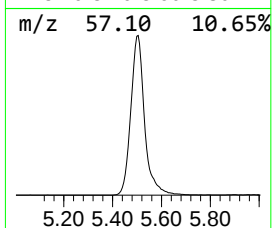
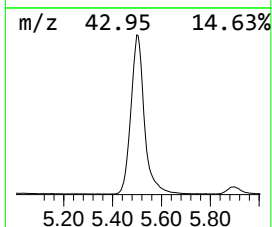
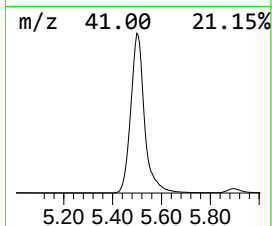
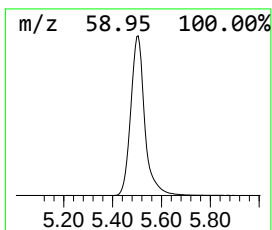
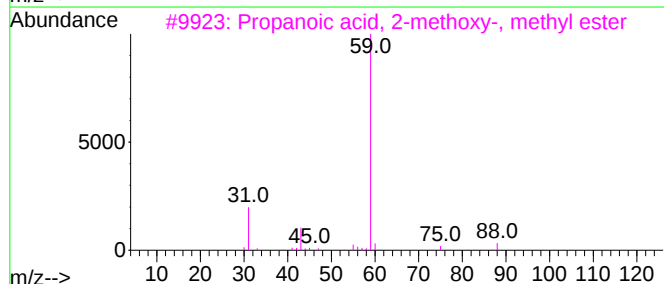
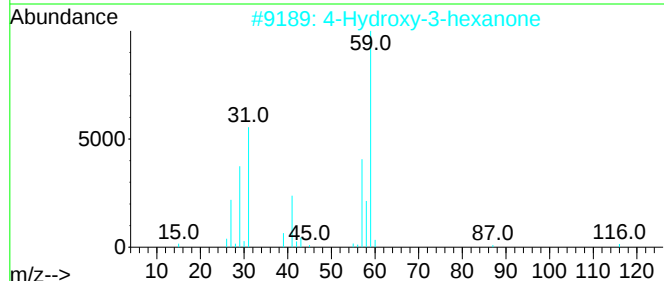
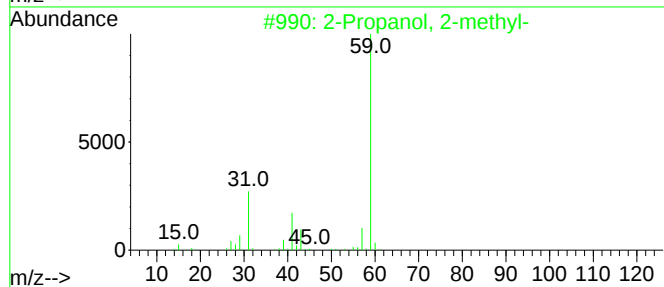
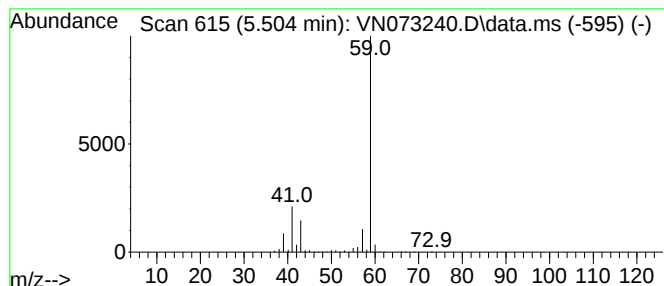
Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.504	109.95 ug/l	33041800	Pentafluorobenzene	8.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	83
2	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
3	Propanoic acid, 2-methoxy-, meth...	118	C5H10O3	017639-76-8	9
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

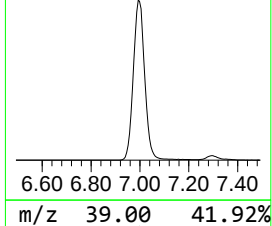
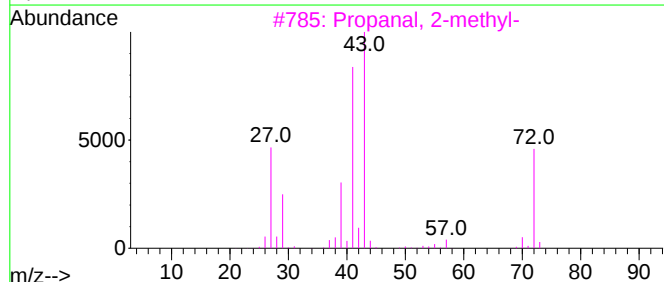
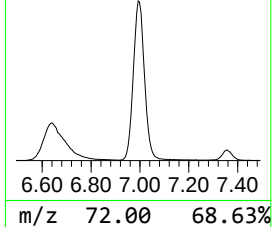
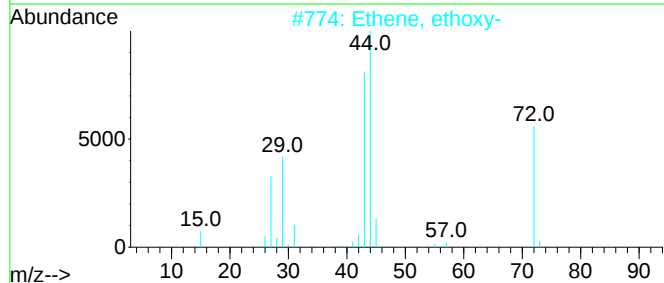
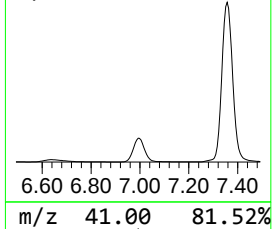
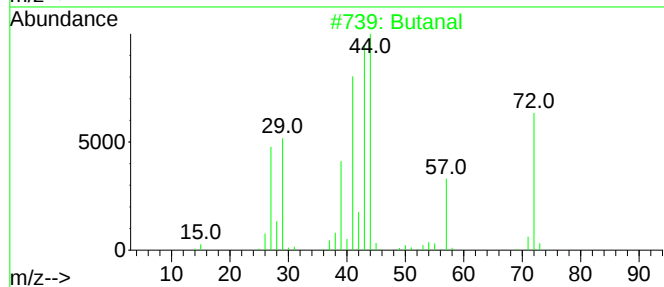
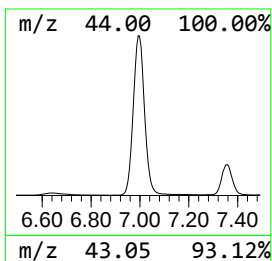
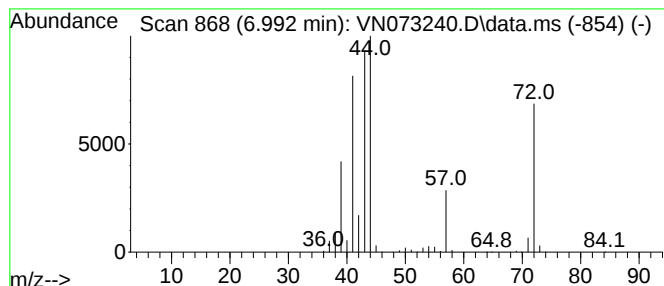
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.992	59.68 ug/l	17935500	Pentafluorobenzene	8.004

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	50
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

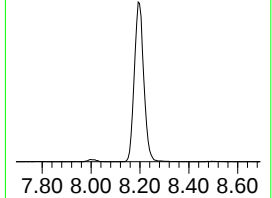
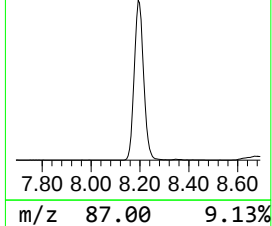
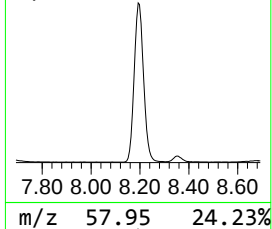
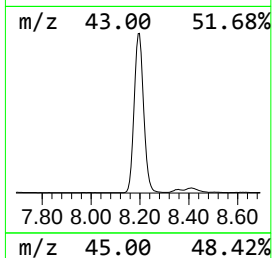
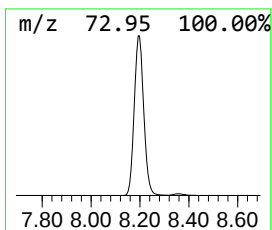
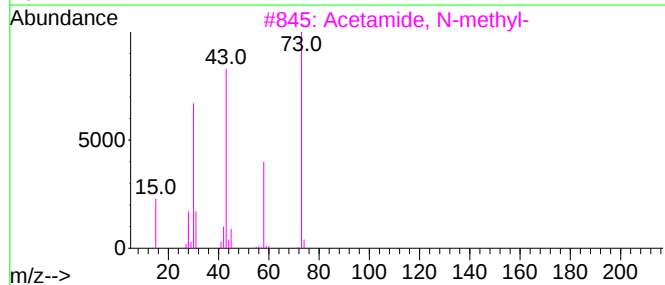
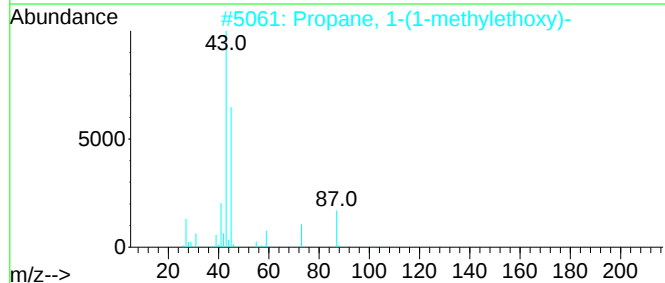
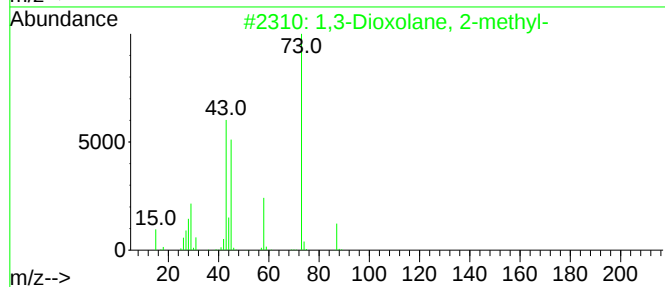
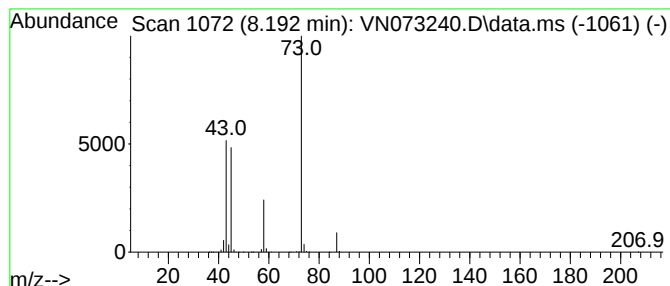
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxolane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.192	50.00 ug/l	15026400	Pentafluorobenzene	8.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	33
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4			3-Methylbutan-2-yl propyl carbonate	174	C9H18O3	1000372-83-4	28
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

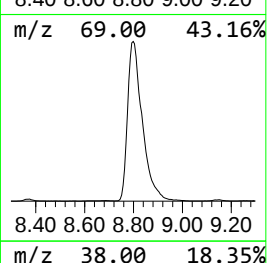
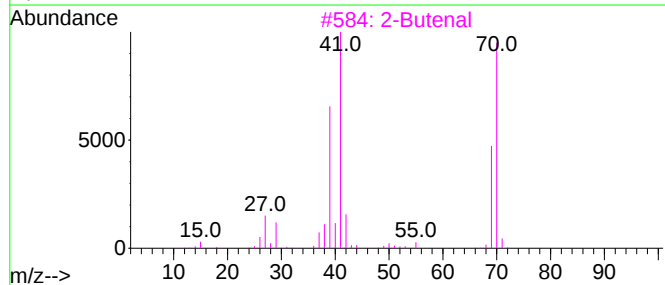
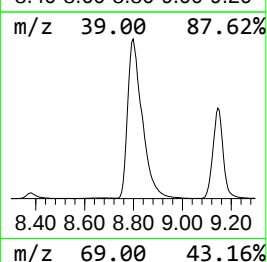
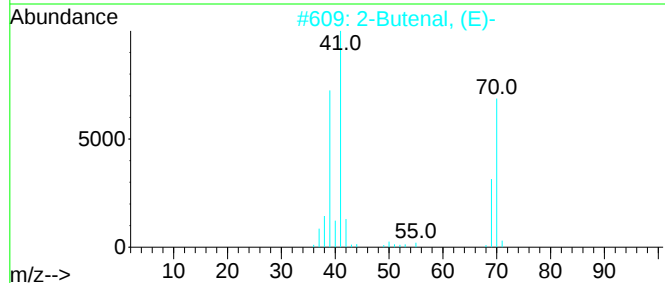
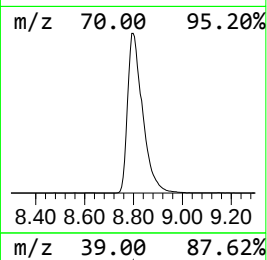
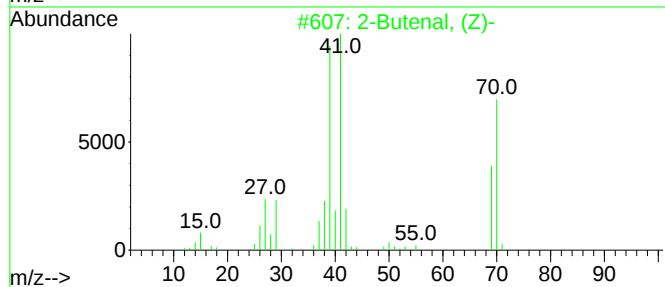
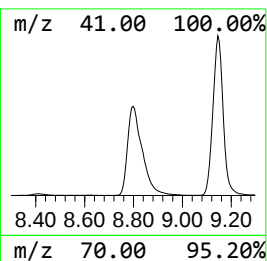
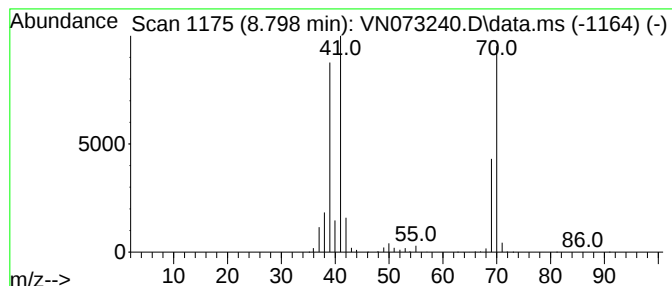
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Butenal, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.798	50.00 ug/l	20536700	1,4-Difluorobenzene	8.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butenal, (Z)-	70	C4H6O	015798-64-8	91
2		2-Butenal, (E)-	70	C4H6O	000123-73-9	91
3		2-Butenal	70	C4H6O	004170-30-3	91
4		Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	90
5		Methacrolein	70	C4H6O	000078-85-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

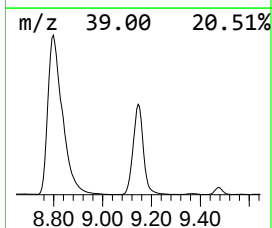
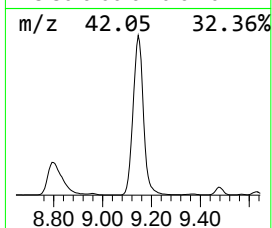
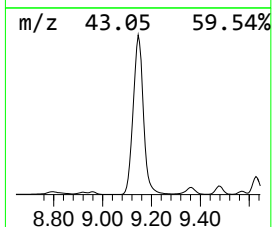
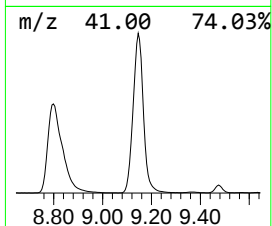
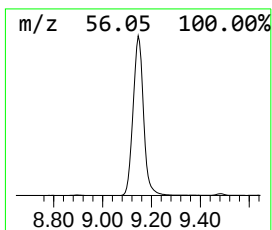
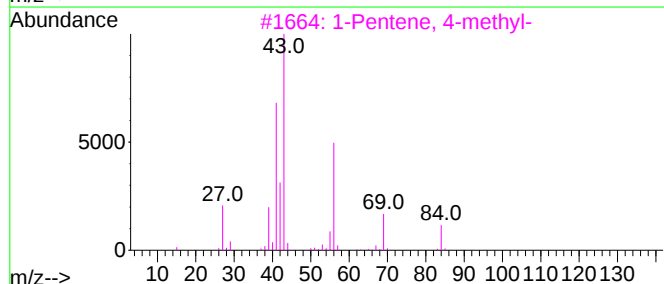
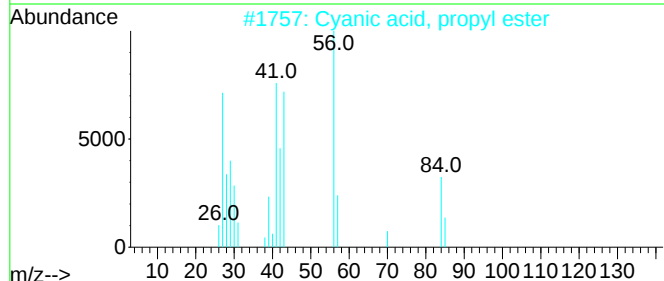
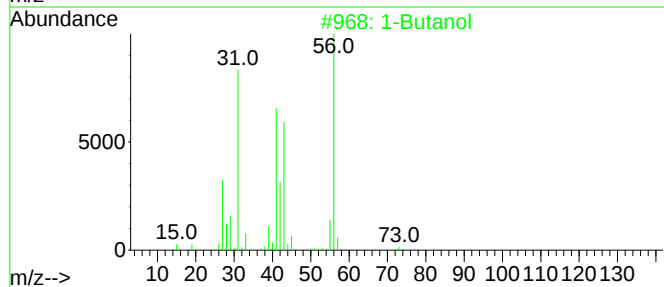
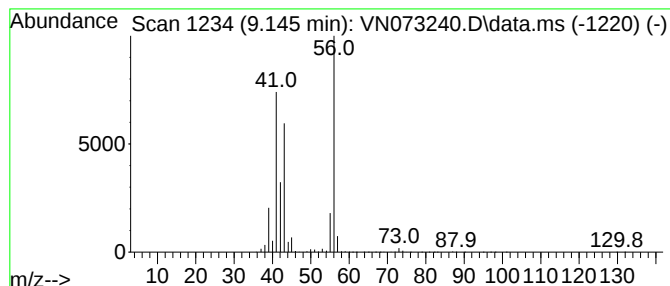
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.145	74.66 ug/l	30663700	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	56
3			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	40
4			1-Hexanol	102	C6H14O	000111-27-3	39
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

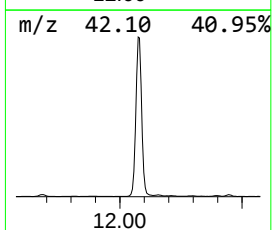
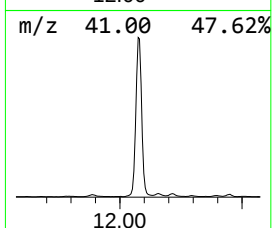
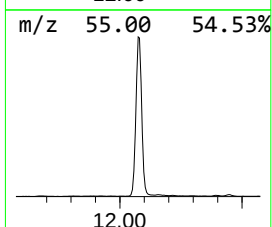
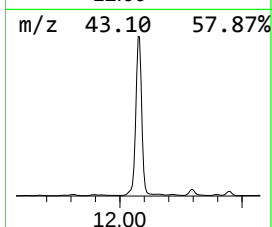
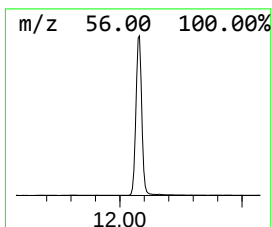
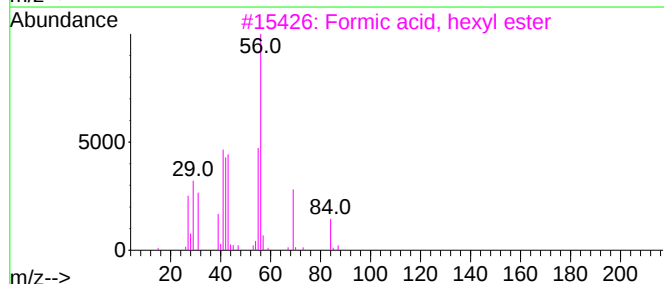
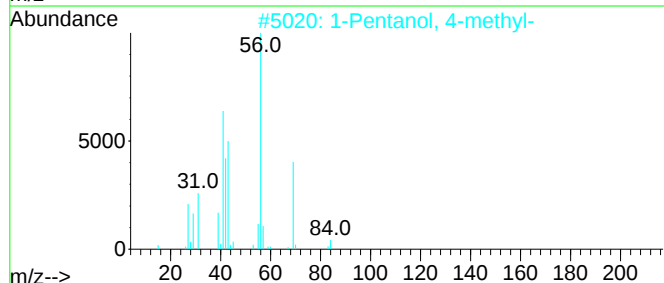
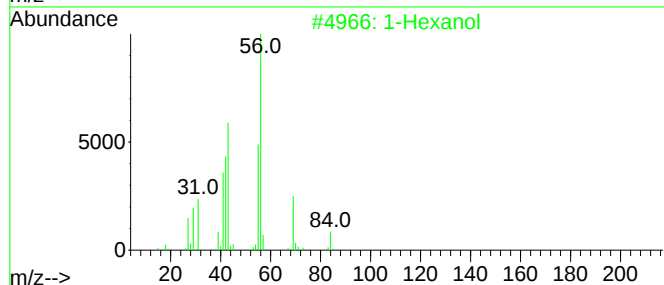
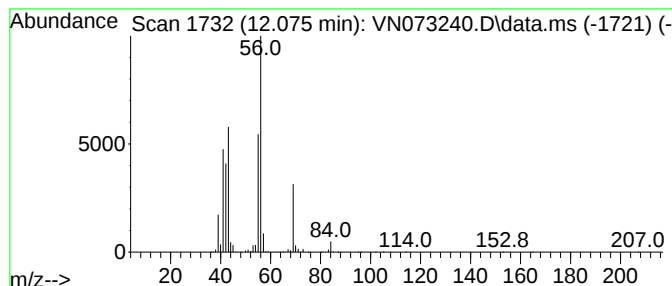
Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.075	50.00 ug/l	14602800	Chlorobenzene-d5	11.680	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	86
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
3	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
4	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	72
5	2-Ethylthiolane, S,S-dioxide	148	C6H12O2S	010178-59-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

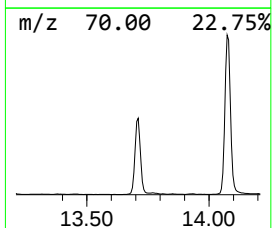
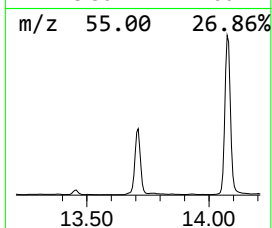
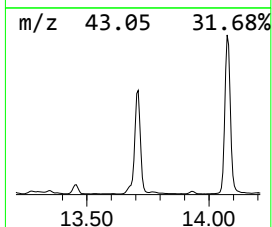
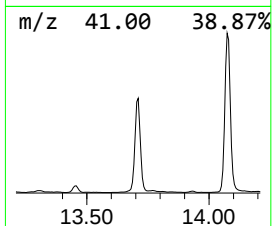
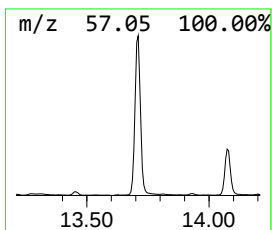
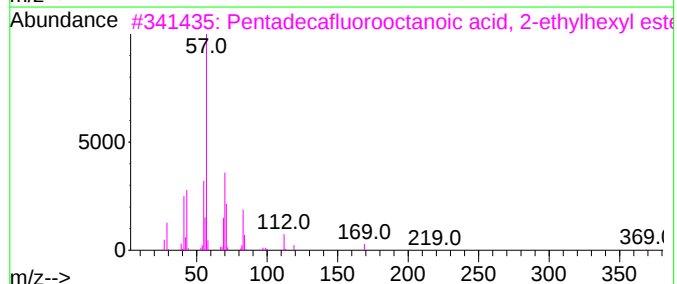
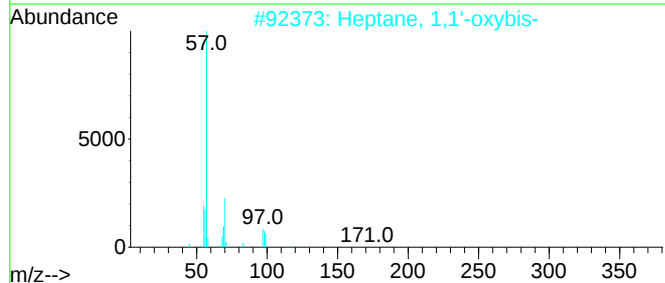
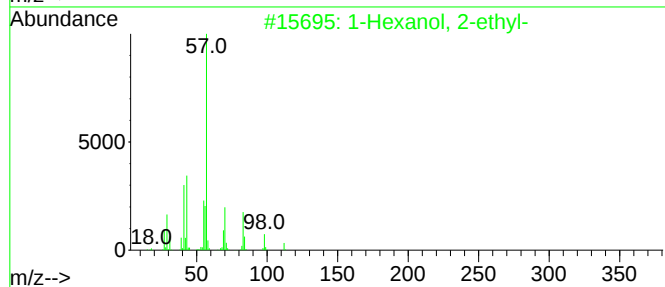
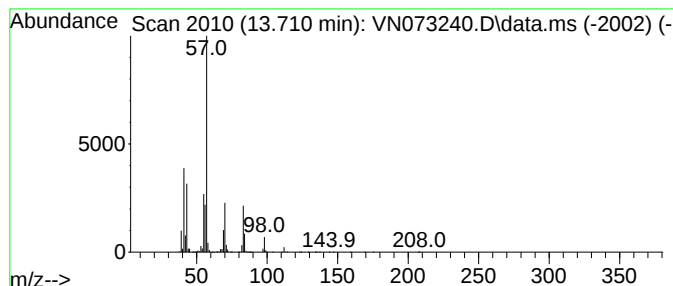
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	50.00 ug/l	11877400	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

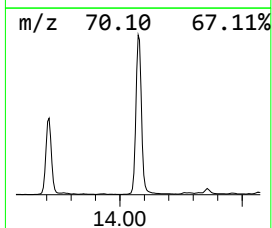
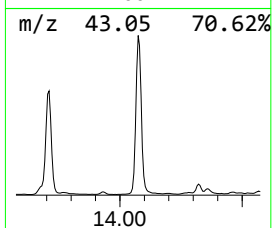
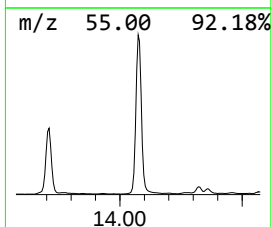
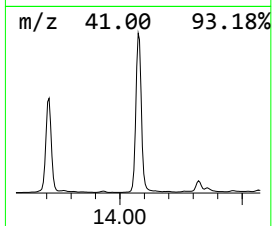
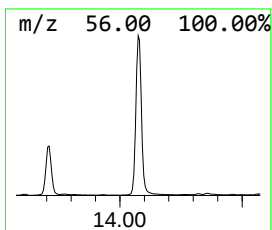
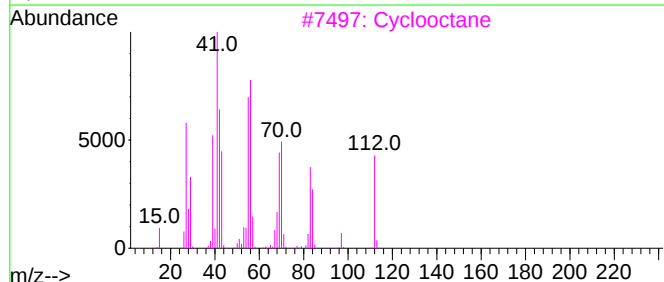
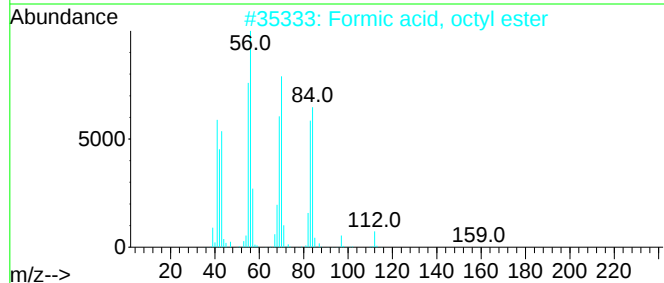
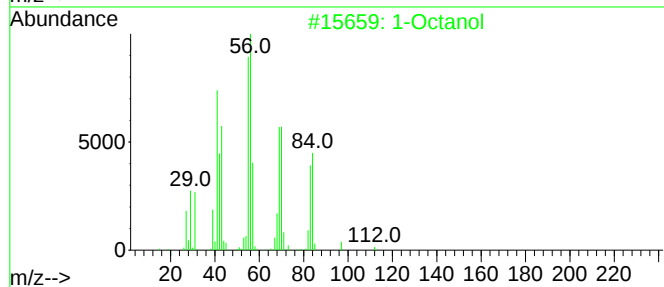
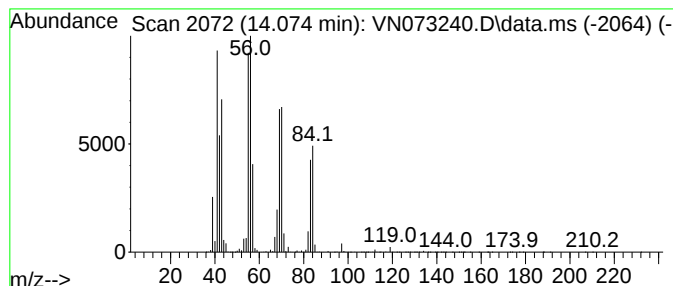
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	84.19 ug/l	19999700	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol			130	C8H18O	000111-87-5	91
2	Formic acid, octyl ester			158	C9H18O2	000112-32-3	90
3	Cyclooctane			112	C8H16	000292-64-8	80
4	Cyclopropane, pentyl-			112	C8H16	002511-91-3	78
5	1-Nonanol			144	C9H20O	000143-08-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073240.D
Acq On : 29 Jun 2022 14:05
Operator : JC\MD
Sample : N3504-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1616

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-m...	5.504	110.0	ug/l	33041800	1	8.004	15026400	50.0
Butanal	6.992	59.7	ug/l	17935500	1	8.004	15026400	50.0
1,3-Dioxolane, ...	8.192	50.0	ug/l	15026400	1	8.004	15026400	50.0
2-Butenal, (Z)-	8.798	50.0	ug/l	20536700	2	8.898	20536700	50.0
1-Butanol	9.145	74.7	ug/l	30663700	2	8.898	20536700	50.0
1-Hexanol	12.075	50.0	ug/l	14602800	3	11.680	14602800	50.0
1-Hexanol, 2-et...	13.710	50.0	ug/l	11877400	4	13.610	11877400	50.0
1-Octanol	14.074	84.2	ug/l	19999700	4	13.610	11877400	50.0