

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
 Data File : VX021211.D
 Acq On : 15 Mar 2021 19:41
 Operator : JC/MD
 Sample : M1647-20
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP4-41735-30780

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\82X031521W.M

Title : SW846 8260

Signal : TIC: VX021211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.340	205	213	222	rBV	6811914	11084630	100.00%	68.780%
2	2.422	222	227	246	rVB	569861	895308	8.08%	5.555%
3	3.940	469	485	500	rBV	575840	1546358	13.95%	9.595%
4	5.470	734	745	761	rVB	54080	155296	1.40%	0.964%
5	5.629	761	772	784	rBV	84196	231120	2.09%	1.434%
6	6.029	830	840	848	rBV	61443	163109	1.47%	1.012%
7	6.829	965	976	996	rBV	139721	333479	3.01%	2.069%
8	8.694	1286	1293	1300	rBV	284145	449856	4.06%	2.791%
9	10.094	1522	1531	1543	rBV	306127	428599	3.87%	2.659%
10	11.118	1700	1705	1711	rBV	248008	322344	2.91%	2.000%
11	12.059	1860	1865	1872	rVB	311690	377667	3.41%	2.343%
12	12.253	1892	1898	1911	rBV	68699	128198	1.16%	0.795%

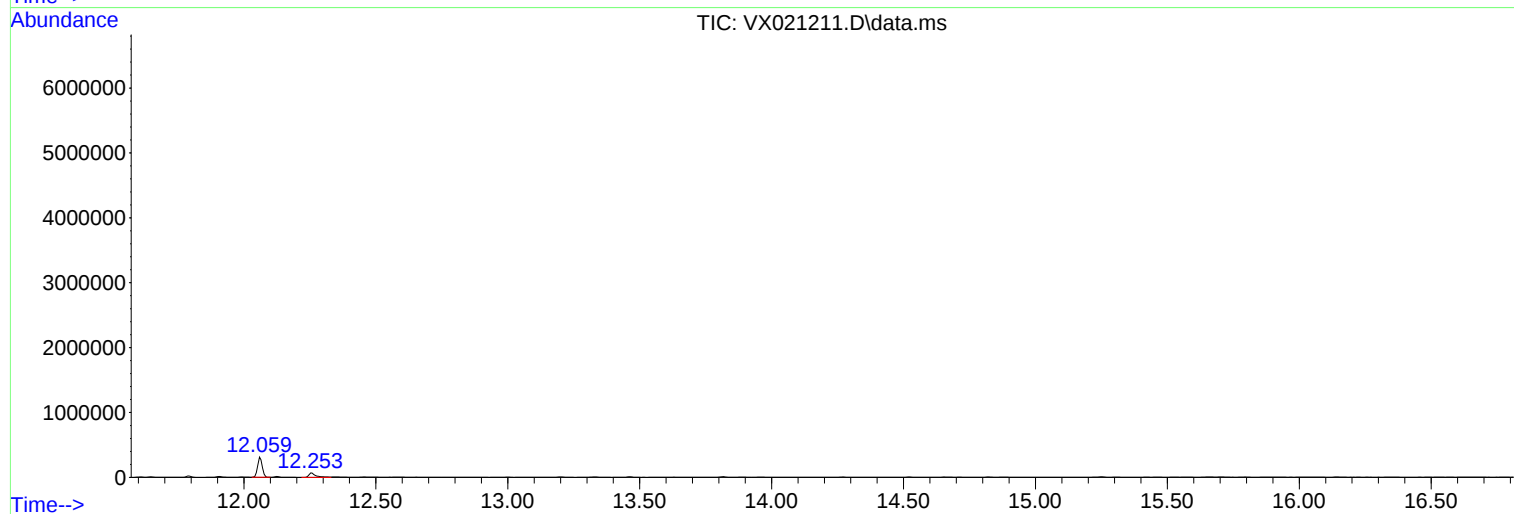
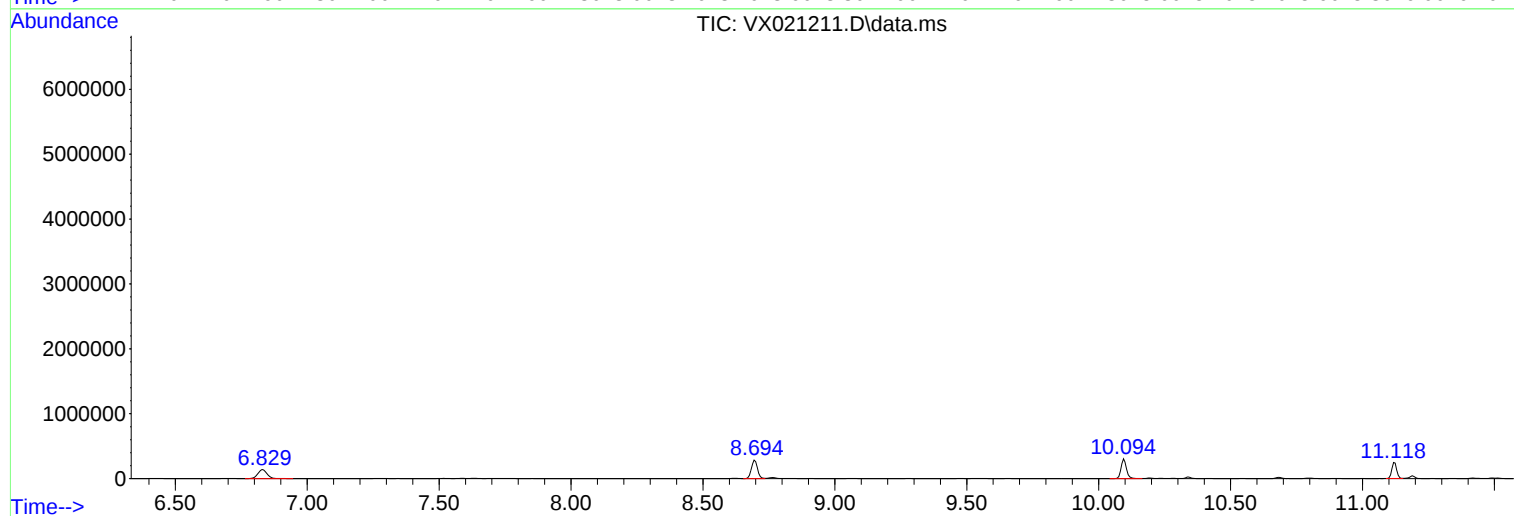
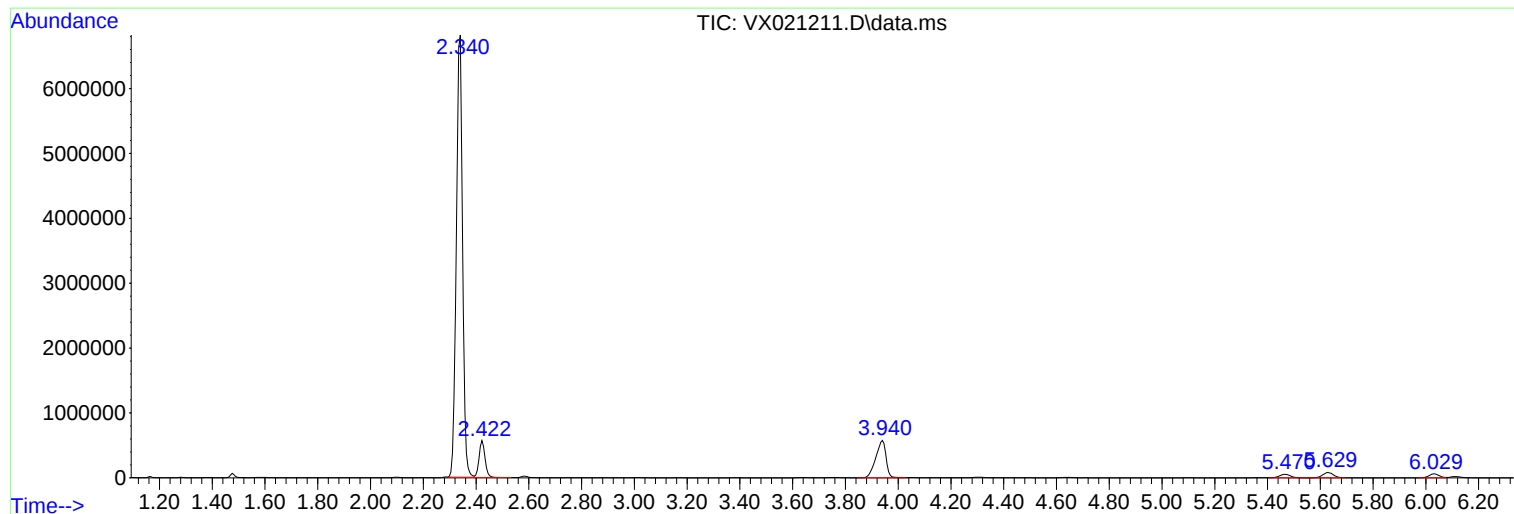
Sum of corrected areas: 16115964

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021211.D
Acq On : 15 Mar 2021 19:41
Operator : JC/MD
Sample : M1647-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP4-41735-30780

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021211.D
Acq On : 15 Mar 2021 19:41
Operator : JC/MD
Sample : M1647-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP4-41735-30780

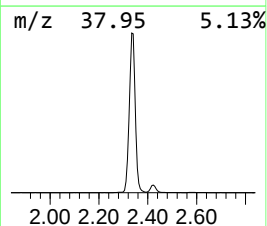
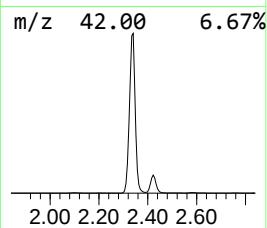
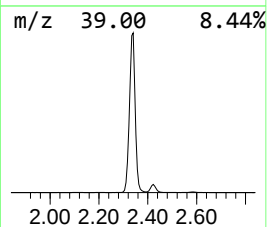
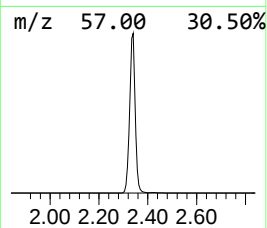
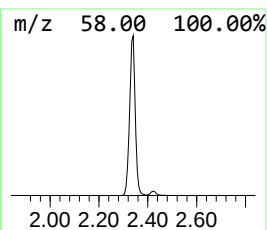
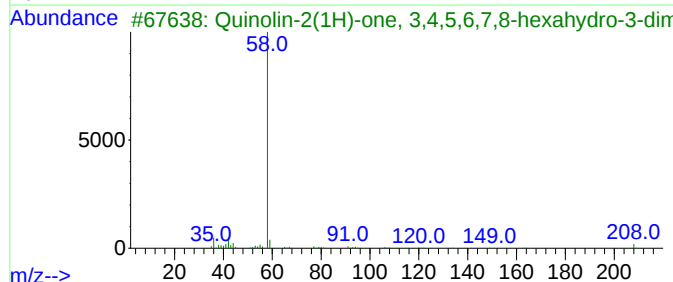
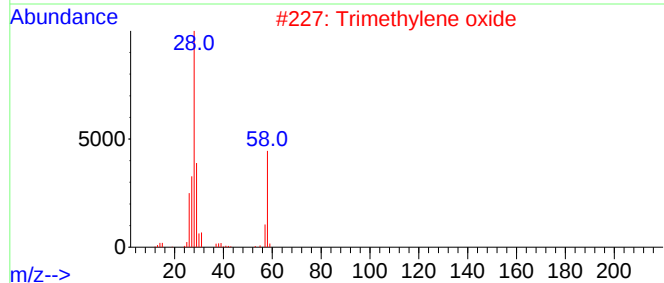
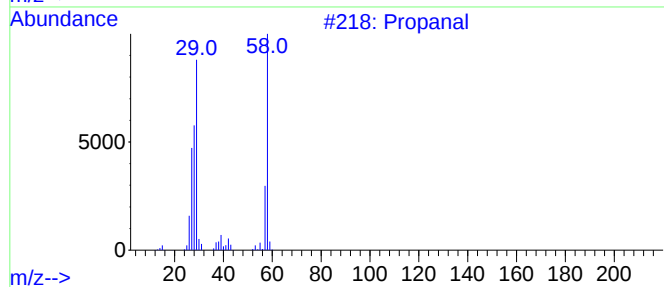
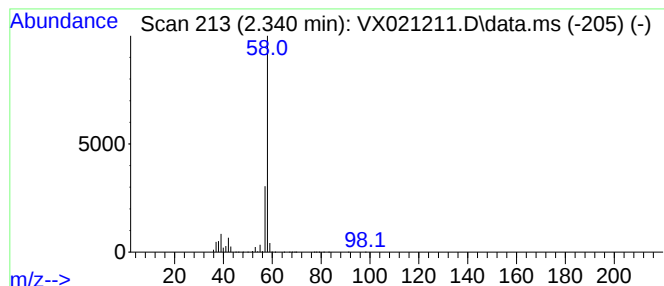
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	2398.02 ug/l	11084600	Pentafluorobenzene	5.629

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	56
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5			Propylene oxide	58	C3H6O	000075-56-9	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021211.D
Acq On : 15 Mar 2021 19:41
Operator : JC/MD
Sample : M1647-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP4-41735-30780

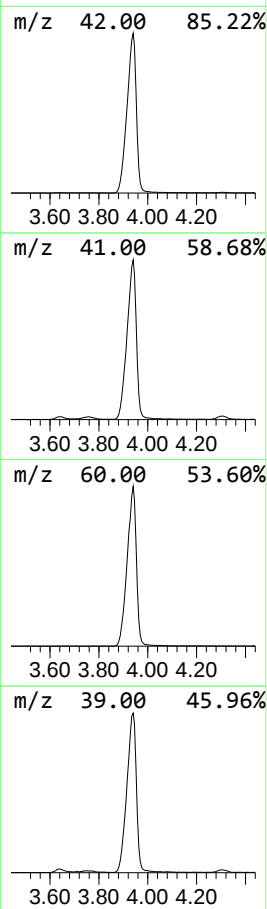
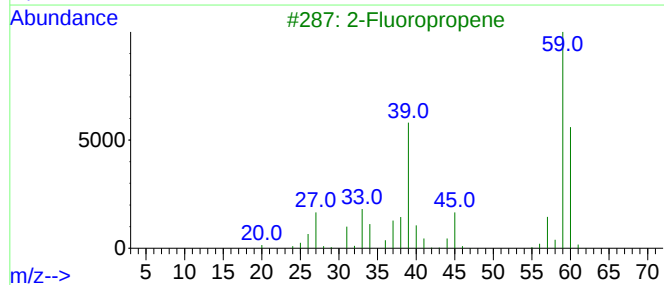
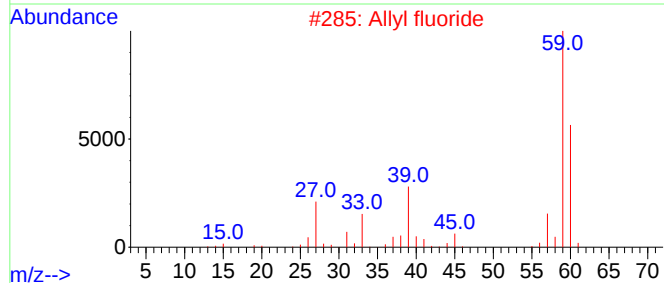
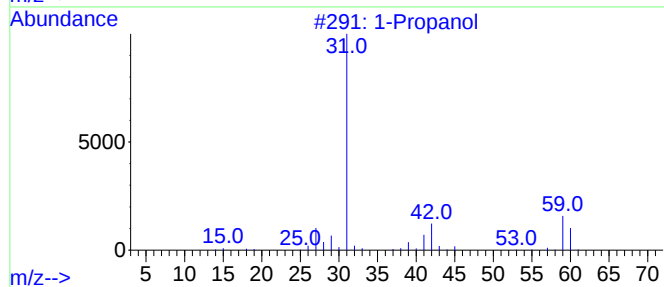
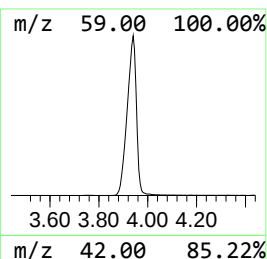
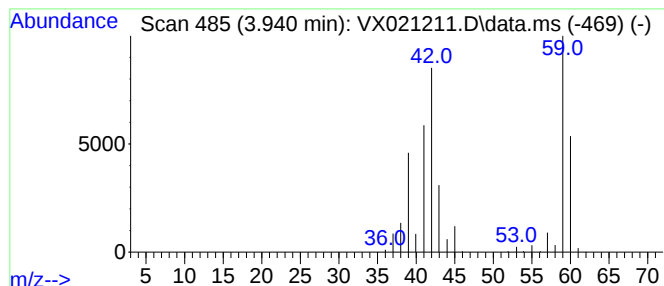
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.940	334.54 ug/l	1546360	Pentafluorobenzene	5.629

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	64
2		Allyl fluoride	60	C3H5F	000818-92-8	38
3		2-Fluoropropene	60	C3H5F	001184-60-7	38
4		Propene	42	C3H6	000115-07-1	25
5		Cyclopropane	42	C3H6	000075-19-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021211.D
Acq On : 15 Mar 2021 19:41
Operator : JC/MD
Sample : M1647-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP4-41735-30780

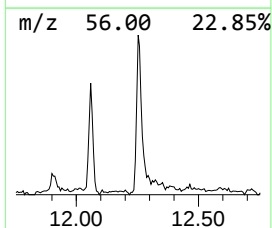
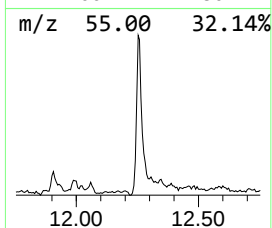
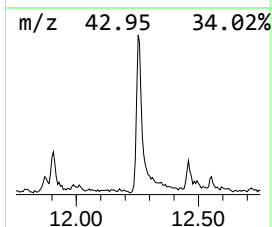
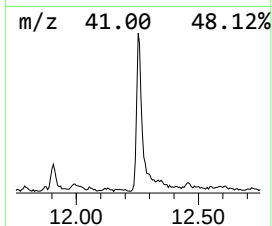
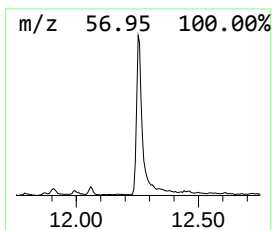
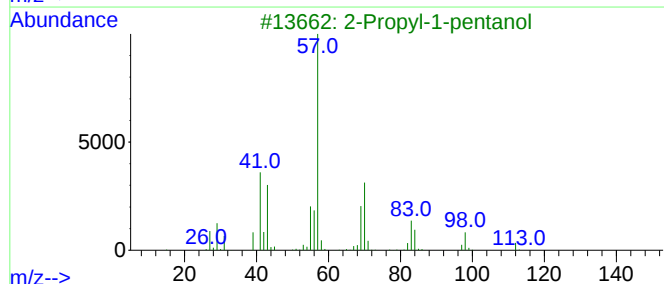
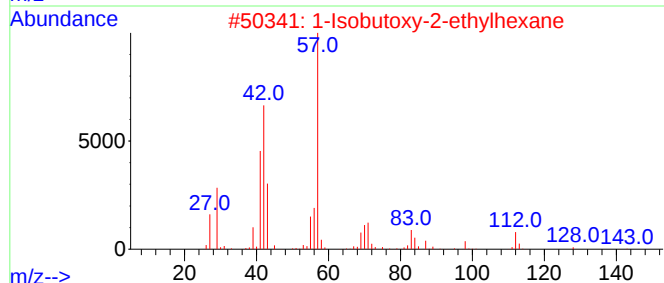
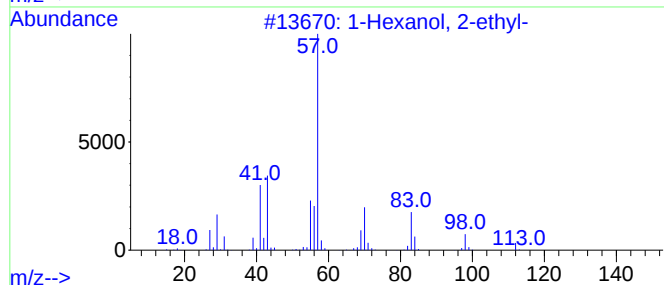
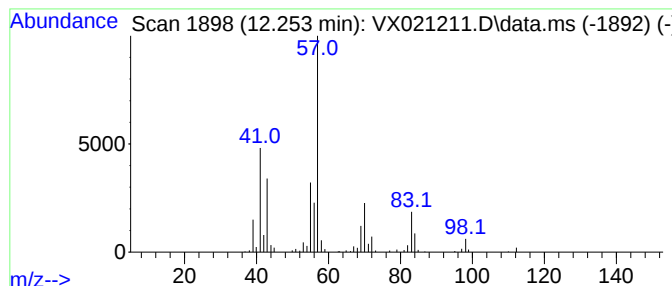
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	16.97 ug/l	128198	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	59
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021211.D
Acq On : 15 Mar 2021 19:41
Operator : JC/MD
Sample : M1647-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP4-41735-30780

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	2.340	2398.0	ug/l	11084600	1	5.629	231120	50.0
1-Propanol	3.940	334.5	ug/l	1546360	1	5.629	231120	50.0
1-Hexanol, 2-et...	12.253	17.0	ug/l	128198	4	12.059	377667	50.0