

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
 Data File : VU043045.D
 Acq On : 13 Apr 2021 12:46
 Operator : SY/MD
 Sample : M1952-03 100X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 30820

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\82U041221W.M
 Title : SW846 8260

Signal : TIC: VU043045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.691	101	109	135	rVB	138120	190797	17.99%	2.969%
2	2.549	366	376	392	rBV	30944	56112	5.29%	0.873%
3	2.642	392	405	429	rVB	32062	75647	7.13%	1.177%
4	2.813	437	458	506	rBV	34289	213705	20.16%	3.325%
5	4.125	837	866	922	rBV4	156369	1060283	100.00%	16.497%
6	4.456	958	969	990	rVB5	6967	17331	1.63%	0.270%
7	4.726	1043	1053	1068	rVB3	4706	11120	1.05%	0.173%
8	5.298	1216	1231	1245	rBV	128366	274615	25.90%	4.273%
9	5.382	1245	1257	1279	rVB	202945	414153	39.06%	6.444%
10	5.710	1343	1359	1372	rBV	146992	300660	28.36%	4.678%
11	5.784	1373	1382	1397	rVB	24669	50463	4.76%	0.785%
12	6.256	1514	1529	1549	rBV	301962	568455	53.61%	8.845%
13	6.558	1607	1623	1642	rBV2	6829	20850	1.97%	0.324%
14	7.906	2027	2042	2054	rBV	476948	811296	76.52%	12.623%
15	7.976	2054	2064	2076	rVB	66372	114623	10.81%	1.783%
16	8.462	2205	2215	2235	rBV5	10111	24391	2.30%	0.379%
17	8.735	2292	2300	2312	rVB2	14052	23009	2.17%	0.358%
18	9.423	2501	2514	2528	rBV	430979	705392	66.53%	10.975%
19	9.497	2529	2537	2554	rVV2	16861	37274	3.52%	0.580%
20	9.574	2554	2561	2573	rVB3	6405	10802	1.02%	0.168%
21	9.700	2583	2600	2611	rVB2	31987	55663	5.25%	0.866%
22	10.108	2716	2727	2740	rVB3	20675	37010	3.49%	0.576%
23	10.639	2880	2892	2909	rBV	362005	566413	53.42%	8.813%
24	11.475	3143	3152	3164	rVB3	11111	16335	1.54%	0.254%
25	11.819	3240	3259	3277	rBV	444833	701653	66.18%	10.917%
26	12.320	3405	3415	3426	rVB	8974	14140	1.33%	0.220%
27	14.095	3955	3967	3979	rBV	33882	54960	5.18%	0.855%

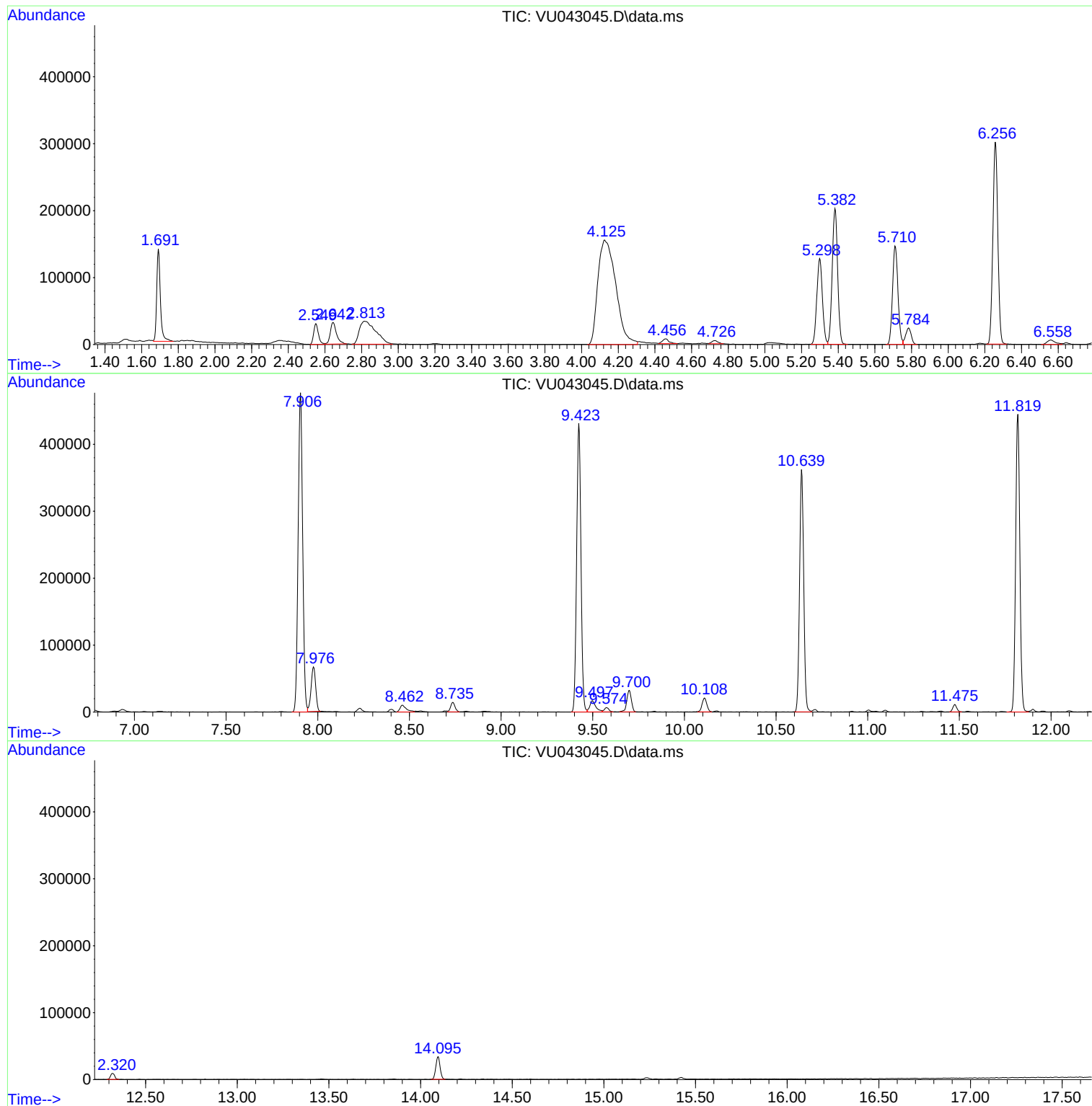
Sum of corrected areas: 6427152

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043045.D
Acq On : 13 Apr 2021 12:46
Operator : SY/MD
Sample : M1952-03 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30820

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043045.D
Acq On : 13 Apr 2021 12:46
Operator : SY/MD
Sample : M1952-03 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30820

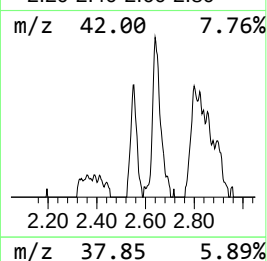
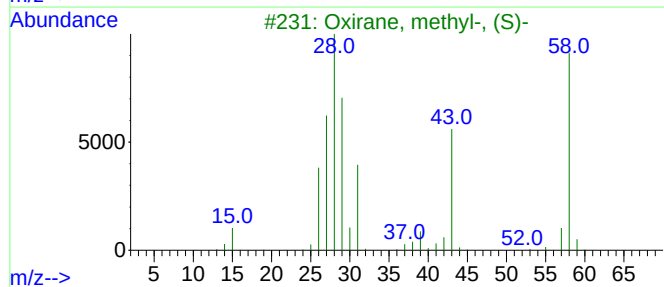
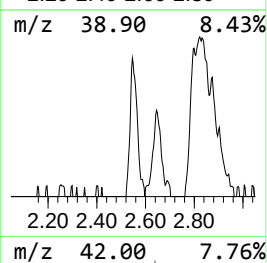
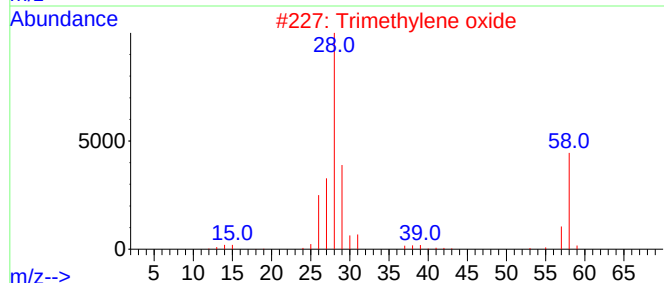
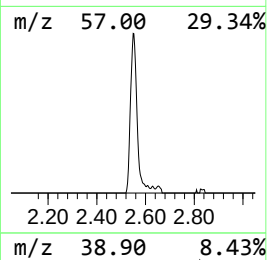
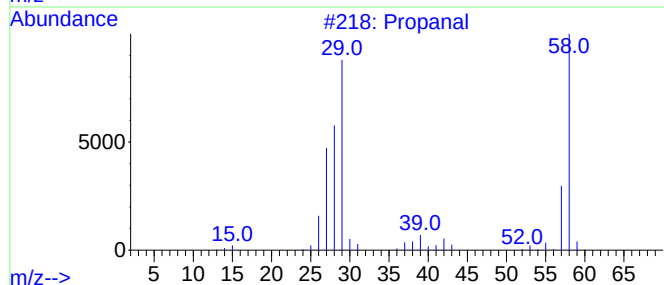
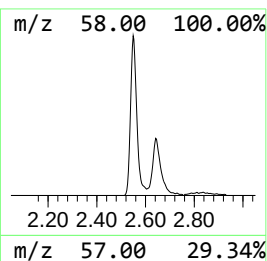
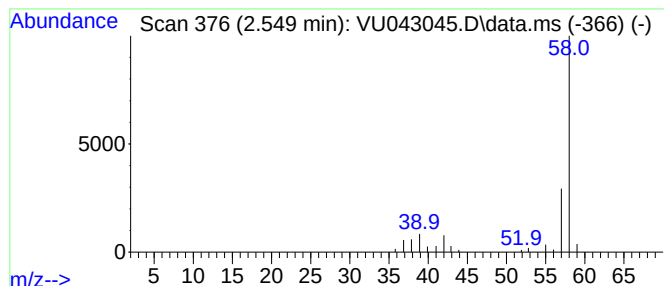
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.549	6.77 ug/l	56112	Pentafluorobenzene	5.382

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	72
2			Trimethylene oxide	58	C3H6O	000503-30-0	56
3			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	9
4			Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	9
5			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043045.D
Acq On : 13 Apr 2021 12:46
Operator : SY/MD
Sample : M1952-03 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30820

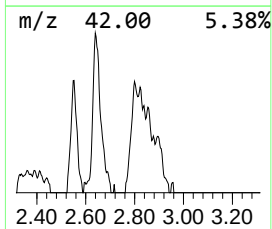
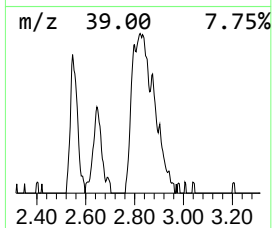
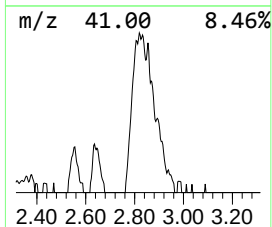
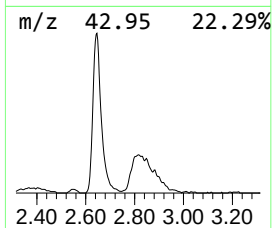
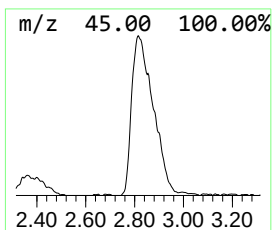
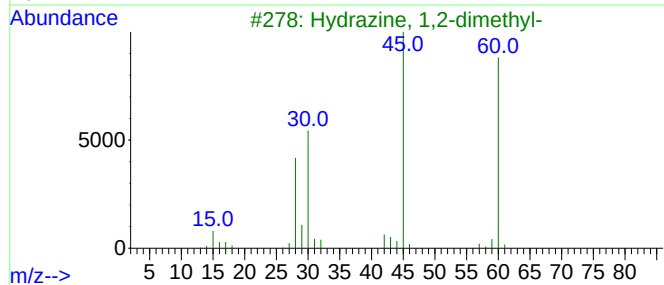
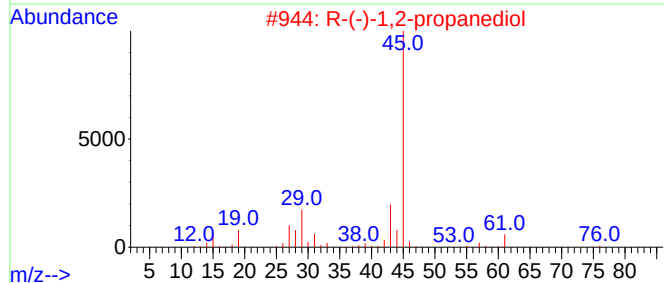
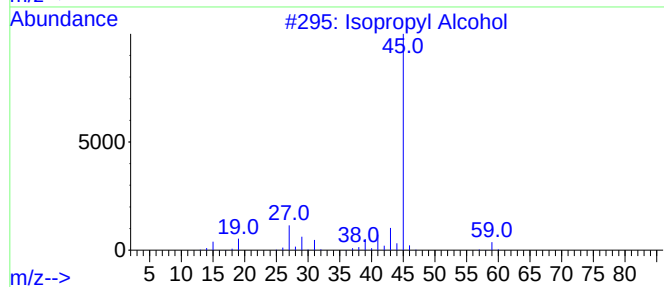
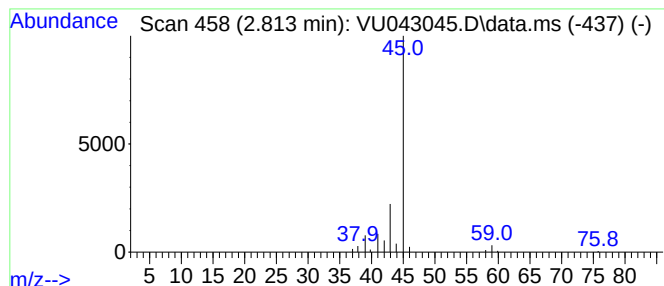
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.813	25.80 ug/l	213705	Pentafluorobenzene	5.382

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4		(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
5		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043045.D
Acq On : 13 Apr 2021 12:46
Operator : SY/MD
Sample : M1952-03 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30820

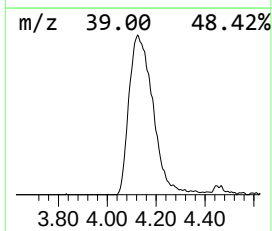
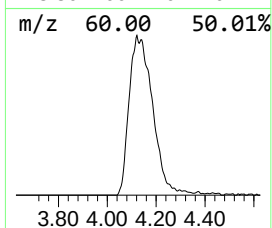
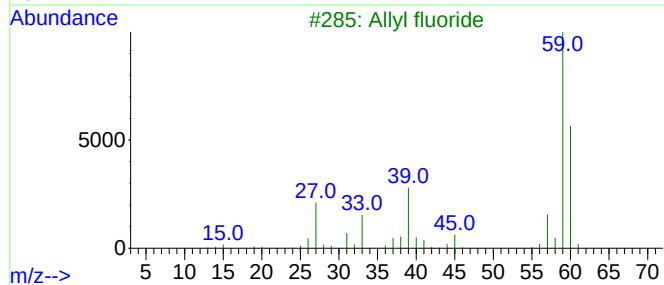
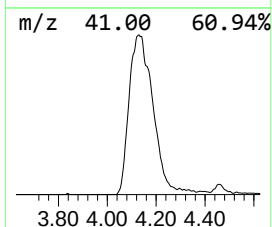
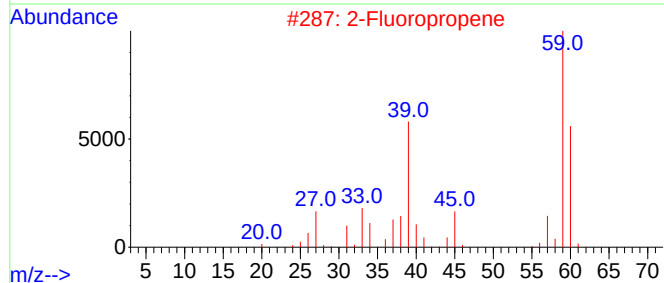
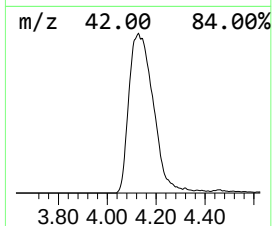
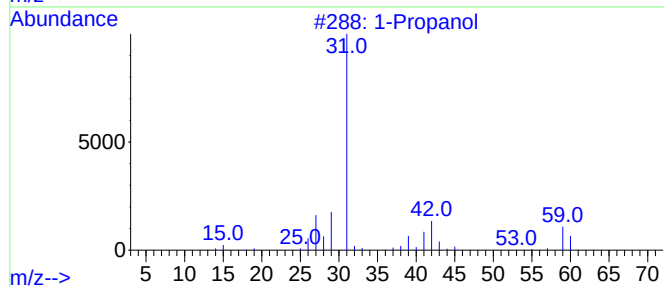
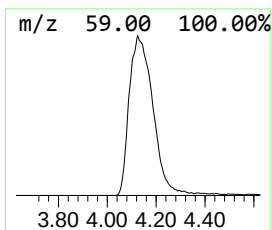
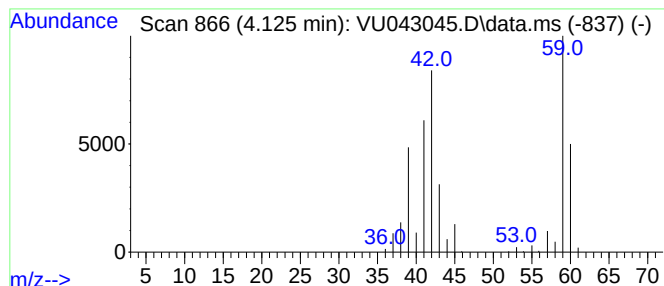
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.125	128.01 ug/l	1060280	Pentafluorobenzene	5.382

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	62
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	25
5	Propene			42	C3H6	000115-07-1	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043045.D
Acq On : 13 Apr 2021 12:46
Operator : SY/MD
Sample : M1952-03 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
30820

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.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	2.549	6.8	ug/l	56112	1	5.382	414153	50.0
Isopropyl Alcohol	2.813	25.8	ug/l	213705	1	5.382	414153	50.0
1-Propanol	4.125	128.0	ug/l	1060280	1	5.382	414153	50.0