

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051425\
 Data File : VX046195.D
 Acq On : 14 May 2025 15:32
 Operator : JC/MD
 Sample : Q2033-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TW-WTS-08

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	21	26	35	rBV	12776	21614	4.85%	0.790%
2	1.447	55	59	64	rBV	6858	8188	1.84%	0.299%
3	1.581	70	81	84	rVB5	3858	9406	2.11%	0.344%
4	2.063	153	160	170	rBV	38154	59773	13.40%	2.184%
5	2.288	193	197	203	rBV	3410	5096	1.14%	0.186%
6	2.380	206	212	225	rVB	31488	52730	11.82%	1.926%
7	2.538	229	238	245	rBV2	9920	19939	4.47%	0.728%
8	2.959	297	307	317	rBV2	6175	15442	3.46%	0.564%
9	3.855	446	454	467	rBV2	21847	60397	13.54%	2.206%
10	5.385	693	705	720	rBV	52779	157895	35.40%	5.768%
11	5.544	720	731	747	rBV2	73903	216081	48.44%	7.894%
12	5.952	789	798	808	rBV	62760	166873	37.41%	6.096%
13	6.038	810	812	823	rVB4	3169	6631	1.49%	0.242%
14	6.757	921	930	950	rBV	132094	324226	72.68%	11.845%
15	7.232	1003	1008	1015	rBV5	1844	4962	1.11%	0.181%
16	8.647	1233	1240	1250	rBV	276580	446092	100.00%	16.297%
17	8.720	1250	1252	1262	rVB3	3869	6460	1.45%	0.236%
18	10.049	1465	1470	1482	rBV	284082	404300	90.63%	14.770%
19	10.195	1490	1494	1502	rVB	6881	10279	2.30%	0.376%
20	11.079	1634	1639	1652	rBV	233425	296918	66.56%	10.847%
21	12.018	1788	1793	1802	rBV	280979	341806	76.62%	12.487%
22	12.213	1821	1825	1828	rBV	22641	35618	7.98%	1.301%
23	12.244	1828	1830	1843	rVB	21427	26801	6.01%	0.979%
24	13.774	2075	2081	2092	rBV	29355	39802	8.92%	1.454%

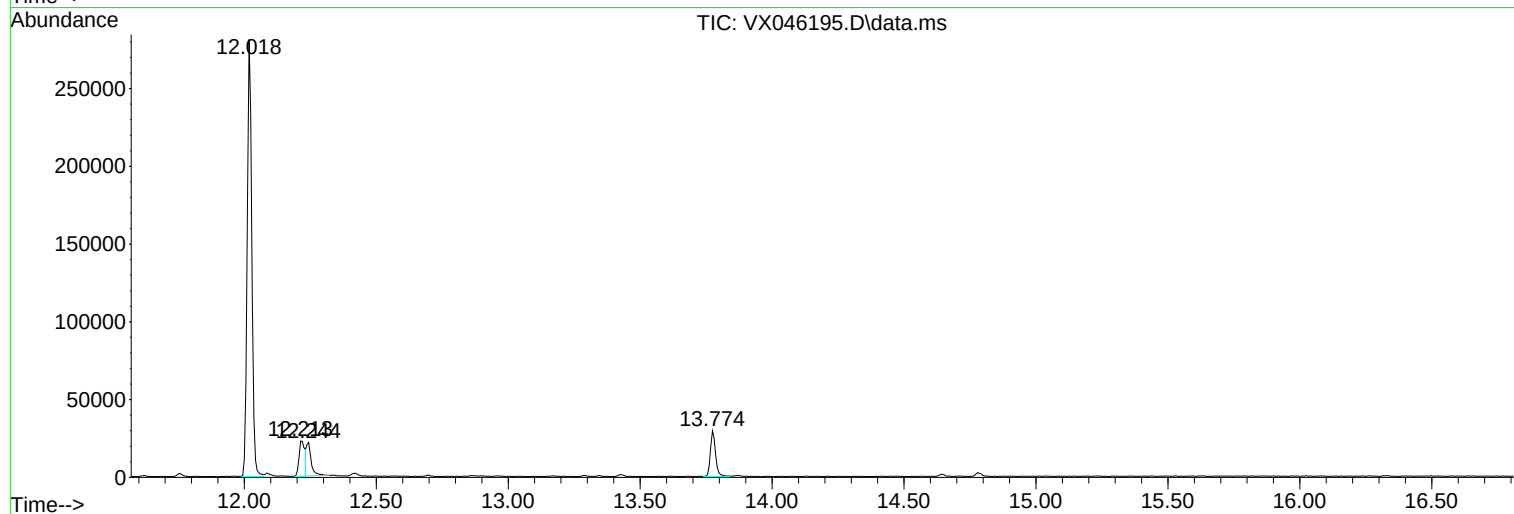
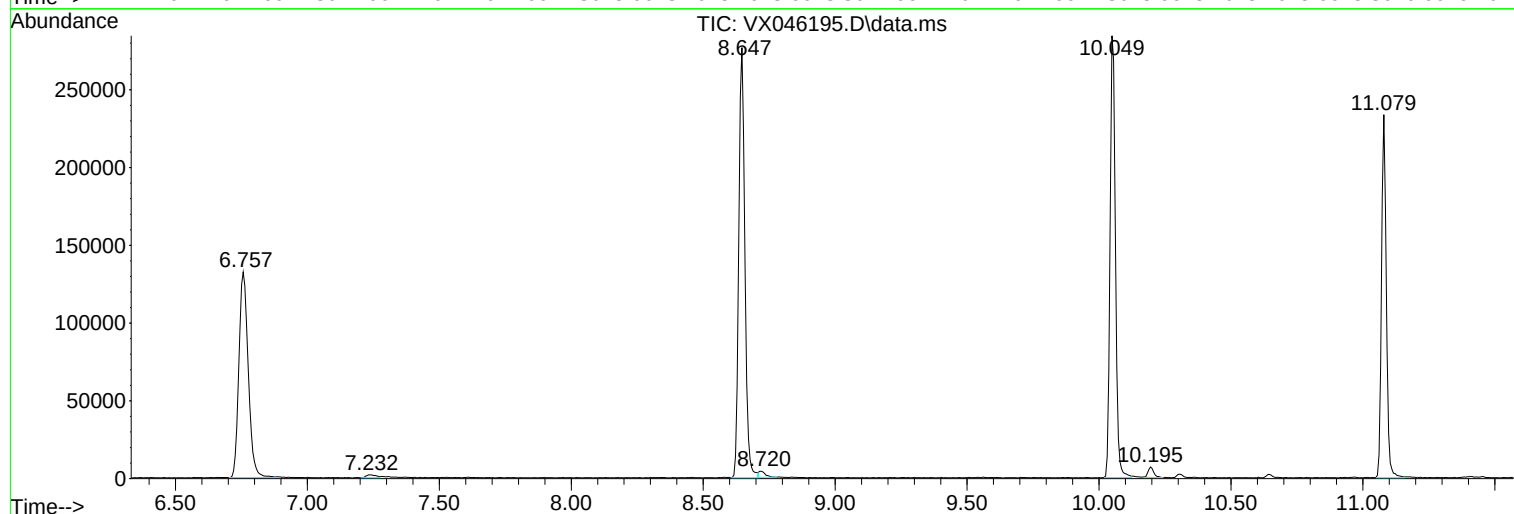
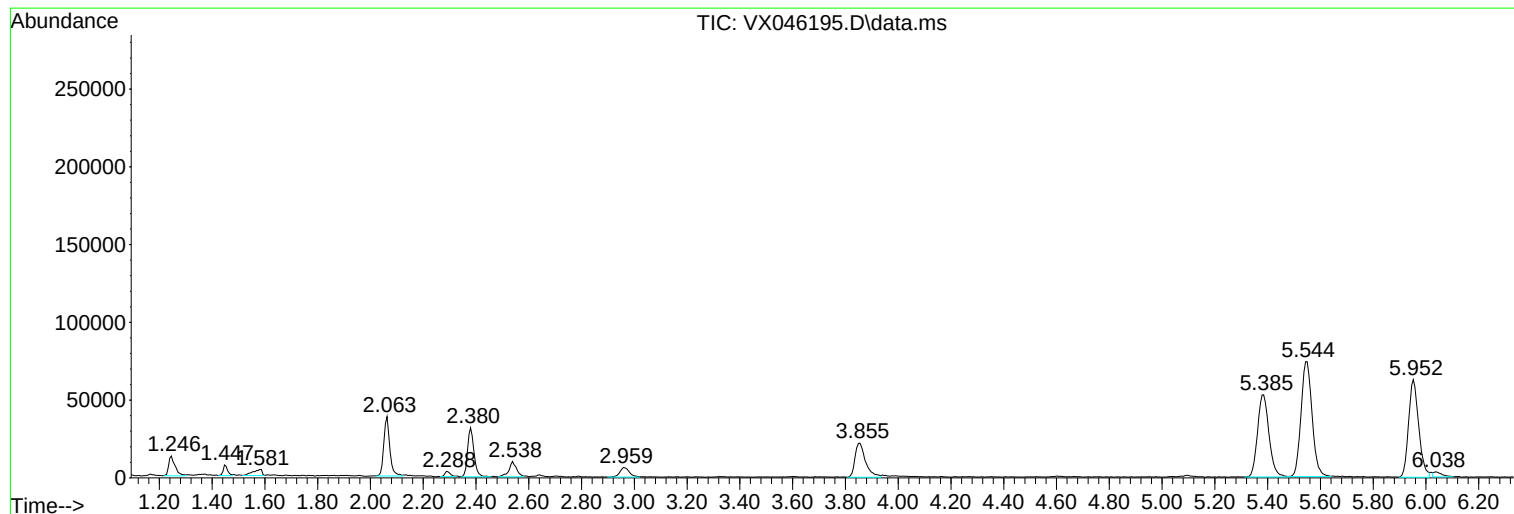
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



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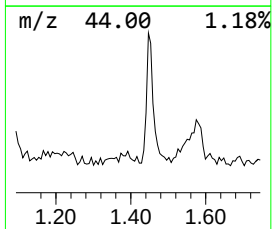
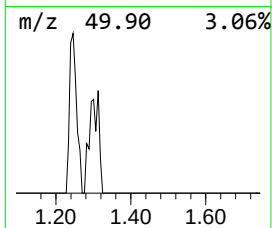
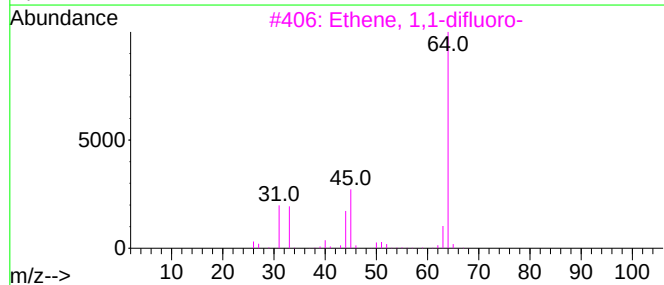
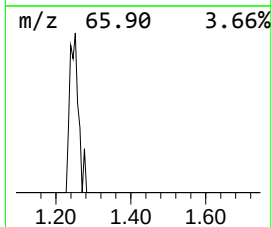
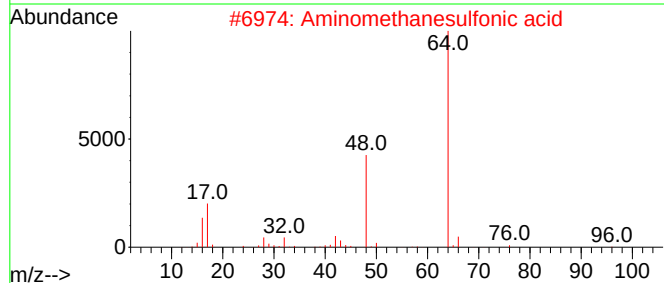
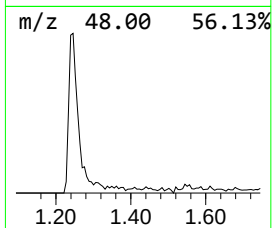
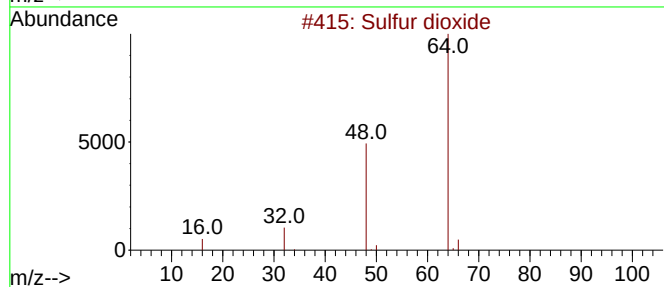
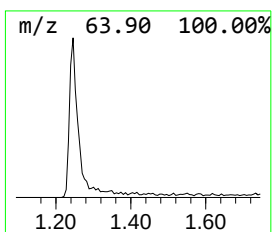
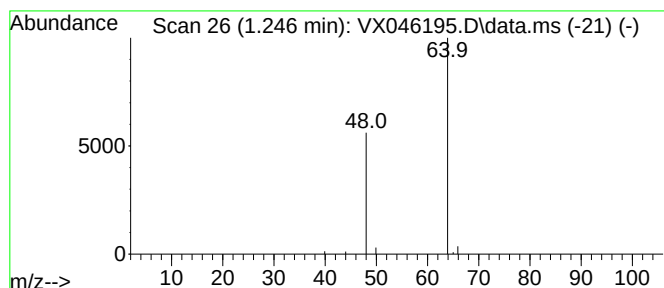
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	5.00 ug/l	21614	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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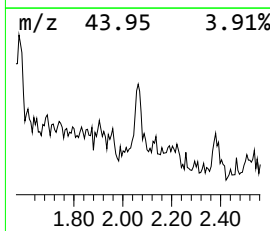
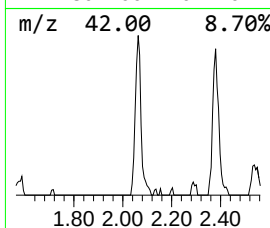
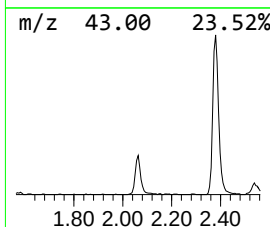
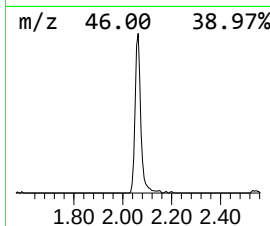
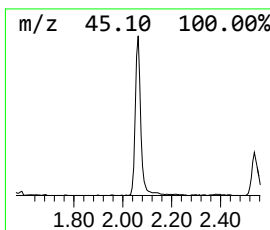
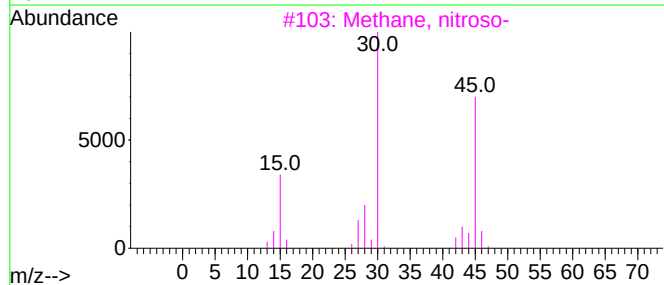
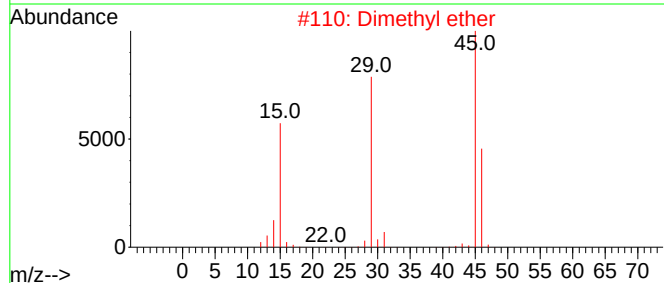
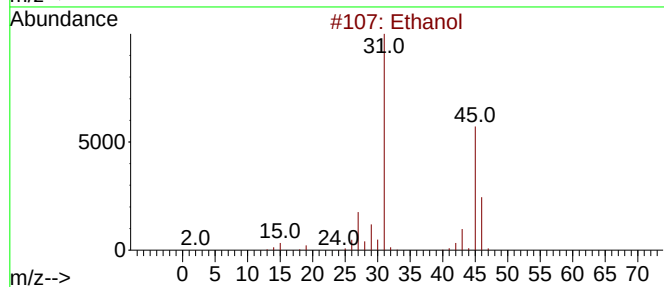
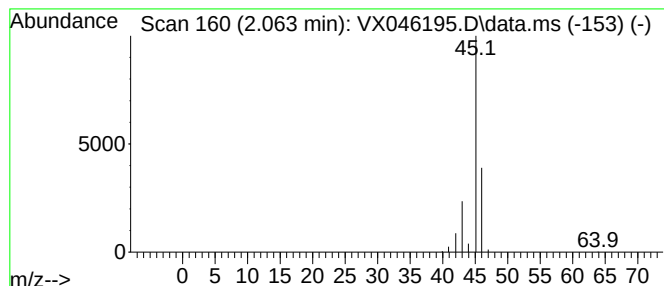
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	13.83 ug/l	59773	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	74
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Oxalic acid			90	C2H2O4	000144-62-7	4



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TW-WTS-08

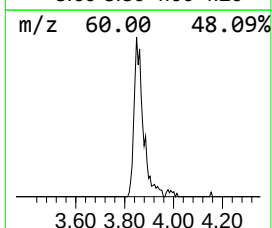
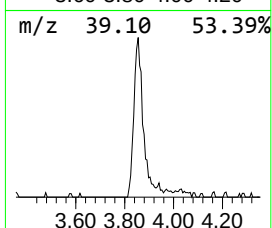
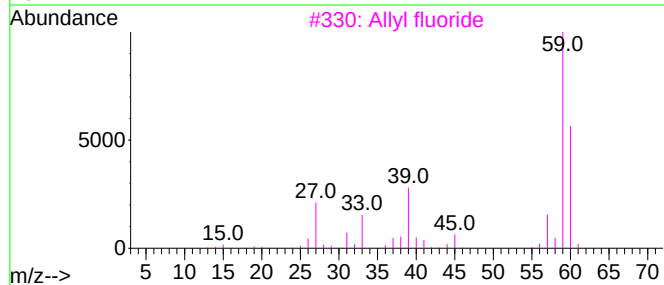
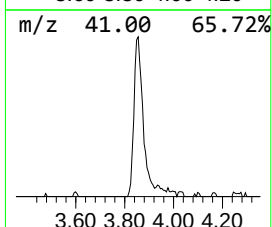
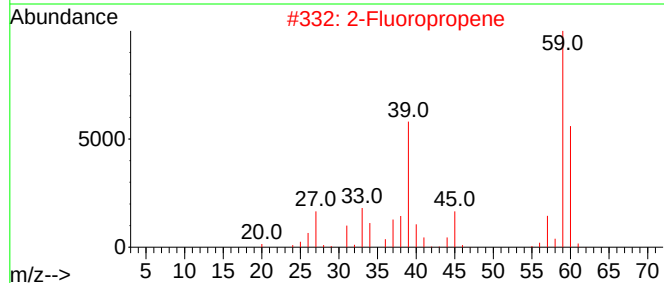
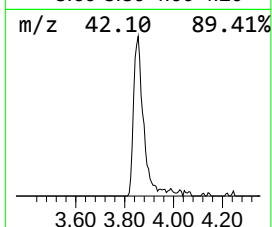
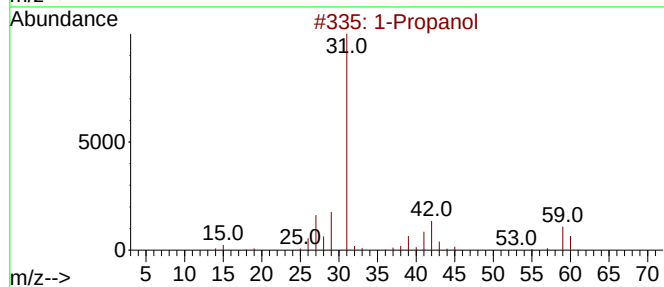
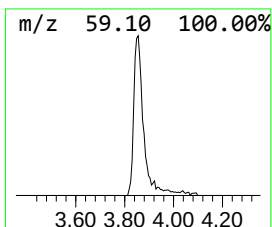
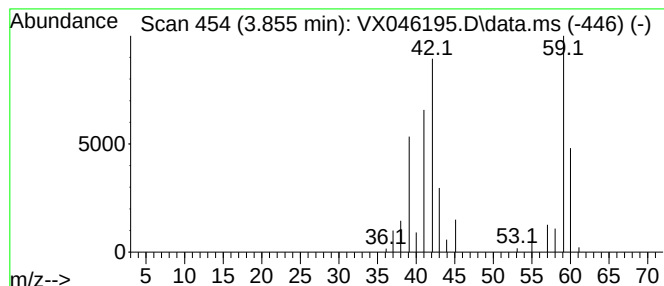
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.855	13.98 ug/l	60397	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	52
2		2-Fluoropropene	60	C3H5F	001184-60-7	49
3		Allyl fluoride	60	C3H5F	000818-92-8	35
4		Propene	42	C3H6	000115-07-1	32
5		Cyclopropane	42	C3H6	000075-19-4	32



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ClientSampleId :
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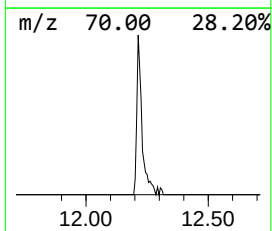
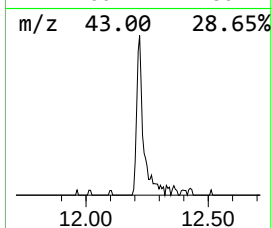
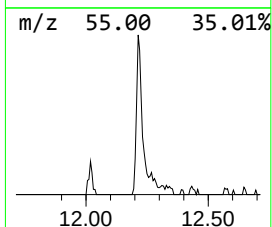
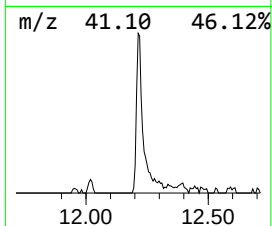
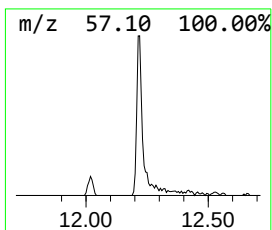
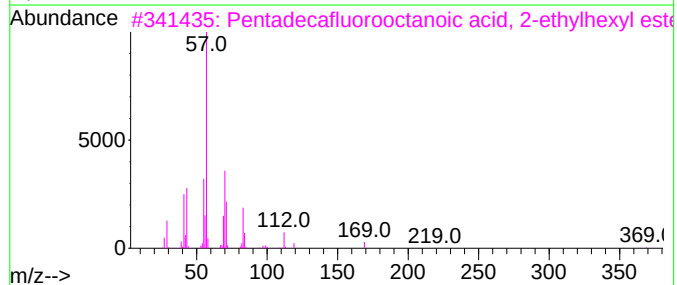
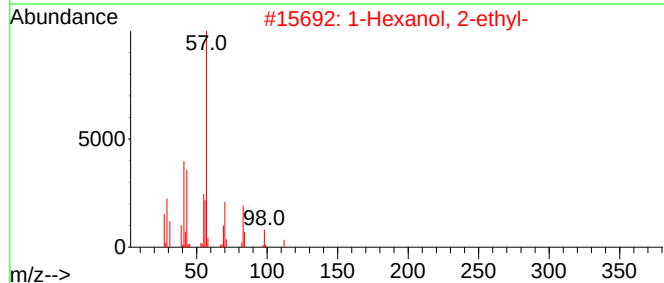
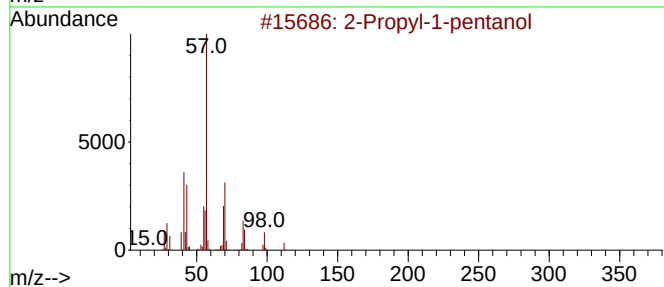
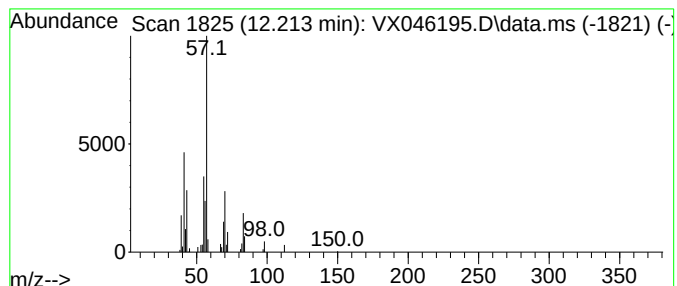
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Quant Title : SW846 8260

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

Peak Number 4 2-Propyl-1-pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	5.21 ug/l	35618	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	59
4			2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	50
5			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	5.0	ug/l	21614	1	5.550	216081	50.0
Ethanol	2.063	13.8	ug/l	59773	1	5.550	216081	50.0
1-Propanol	3.855	14.0	ug/l	60397	1	5.550	216081	50.0
2-Propyl-1-pent...	12.213	5.2	ug/l	35618	4	12.018	341806	50.0