

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025378.D
 Acq On : 29 Nov 2021 18:31
 Operator : JC/MD
 Sample : M4837-07 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20927

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	64	rBV	8632	9371	1.06%	0.164%
2	2.056	153	159	172	rBV	491614	729888	82.95%	12.751%
3	2.538	229	238	244	rBV	10600	19646	2.23%	0.343%
4	2.946	298	305	313	rVB	5248	11646	1.32%	0.203%
5	3.861	444	455	474	rBV	345433	879939	100.00%	15.372%
6	4.574	562	572	584	rBV	3580	11082	1.26%	0.194%
7	5.391	695	706	720	rBV	73467	211455	24.03%	3.694%
8	5.556	721	733	752	rVB	123564	352079	40.01%	6.151%
9	5.958	789	799	819	rBV	76124	207164	23.54%	3.619%
10	6.763	919	931	948	rBV	193263	457321	51.97%	7.989%
11	7.208	996	1004	1023	rBV	169579	356997	40.57%	6.237%
12	8.653	1234	1241	1249	rBV	400515	622946	70.79%	10.883%
13	9.238	1332	1337	1341	rBV	25810	39305	4.47%	0.687%
14	10.055	1465	1471	1484	rVB	410348	544078	61.83%	9.505%
15	10.579	1552	1557	1565	rBV	78722	112695	12.81%	1.969%
16	11.085	1634	1640	1651	rVB	317312	423228	48.10%	7.394%
17	11.658	1729	1734	1744	rBV	5816	9967	1.13%	0.174%
18	12.024	1789	1794	1803	rVB	420379	524135	59.56%	9.156%
19	12.219	1821	1826	1844	rBV	110197	158471	18.01%	2.768%
20	12.414	1854	1858	1864	rVB	7327	9067	1.03%	0.158%
21	12.591	1881	1887	1899	rBV	18917	33754	3.84%	0.590%

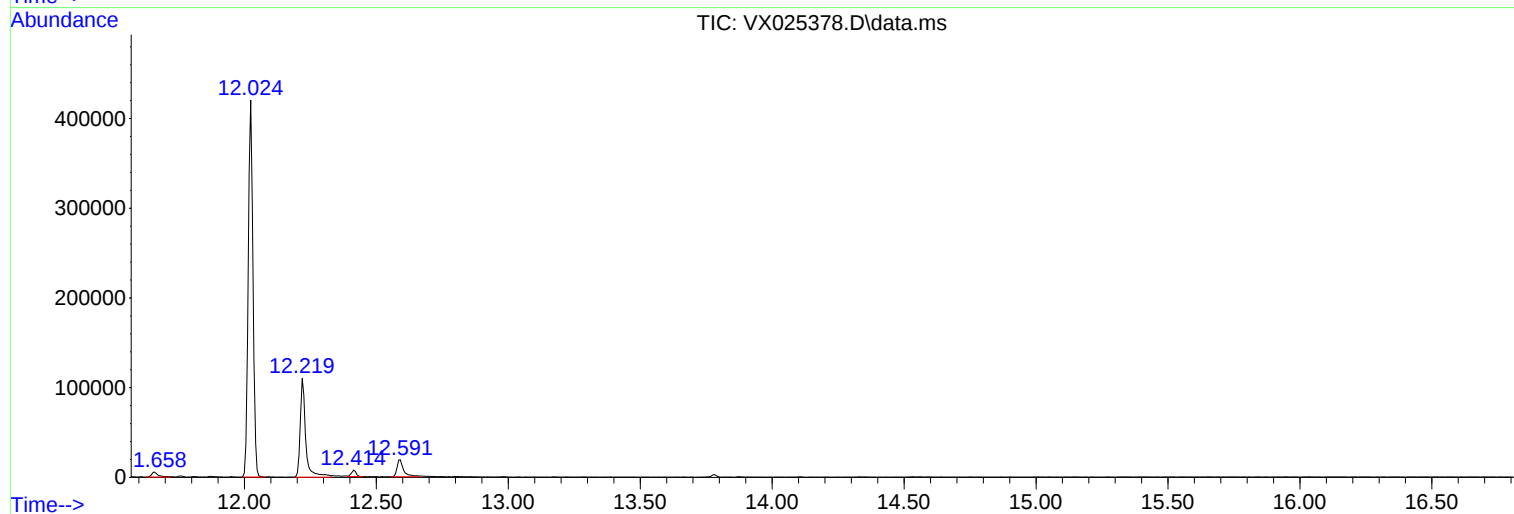
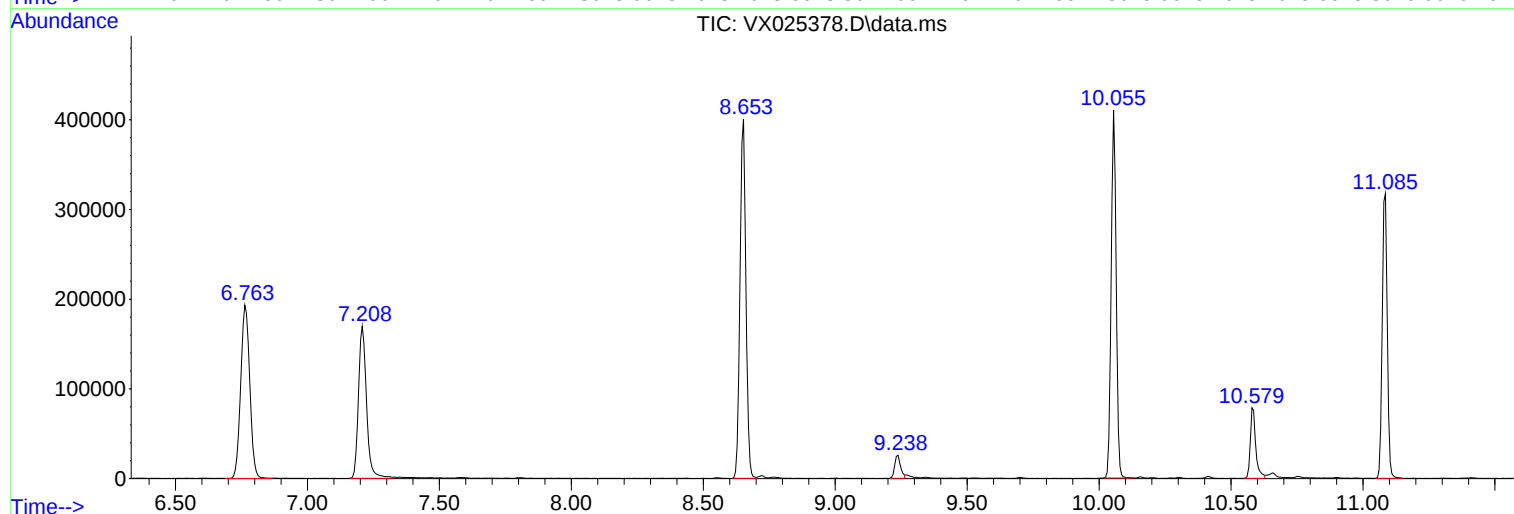
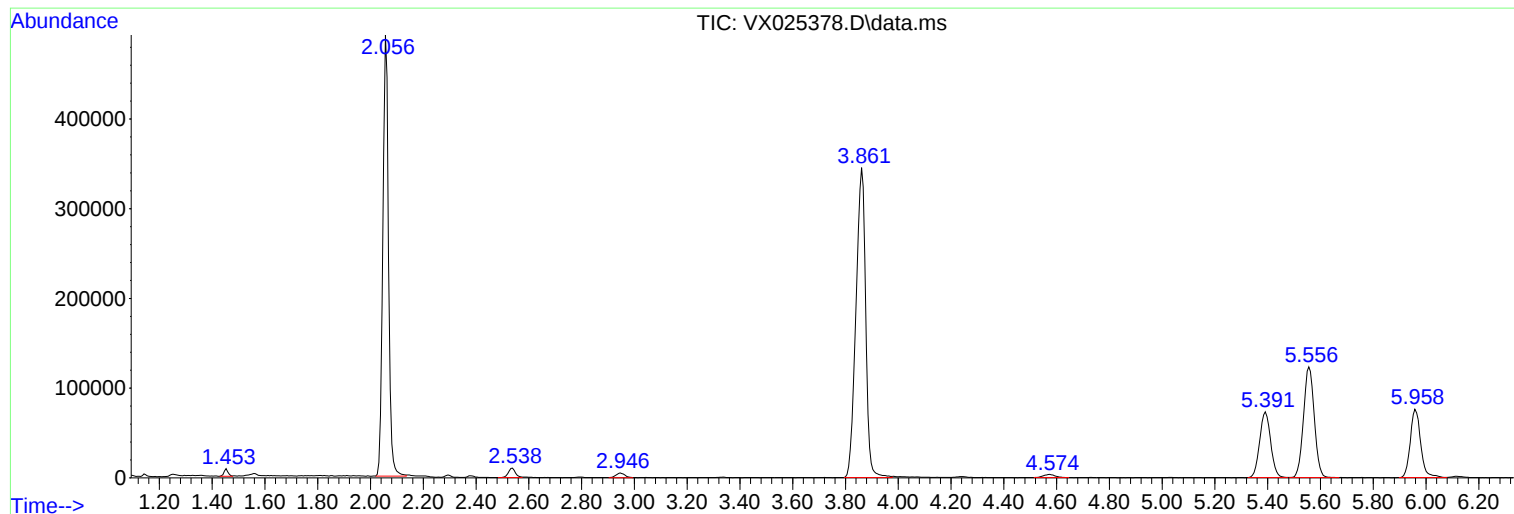
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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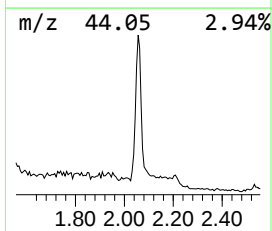
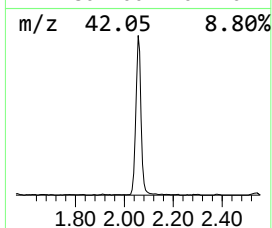
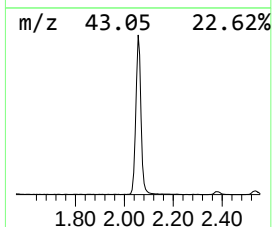
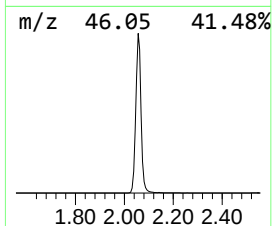
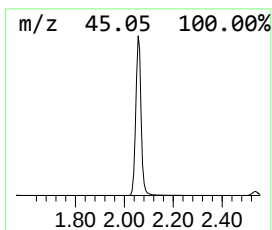
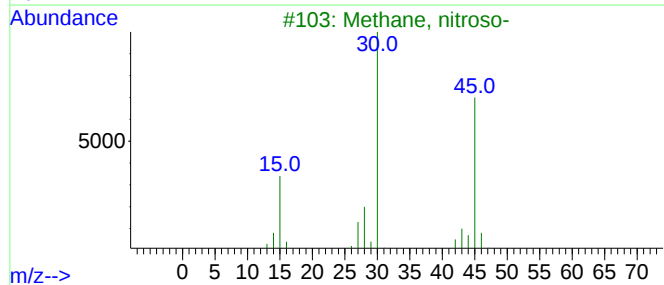
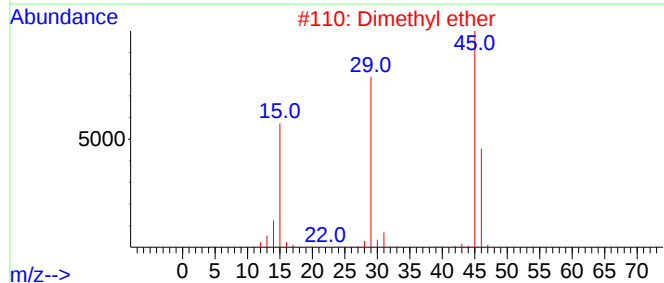
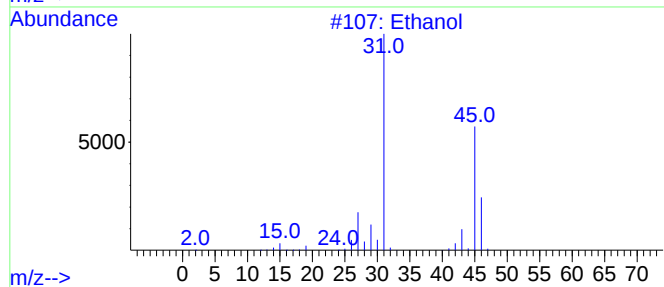
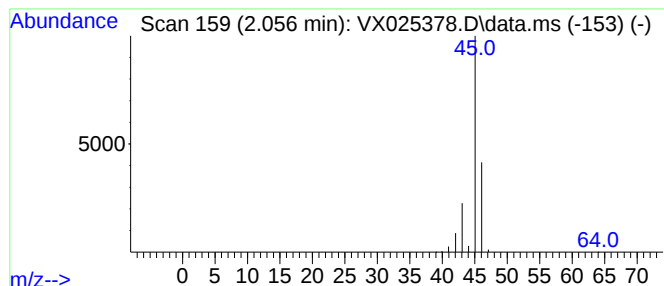
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	103.65 ug/l	729888	Pentafluorobenzene	5.556

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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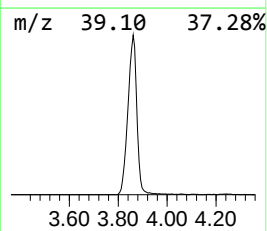
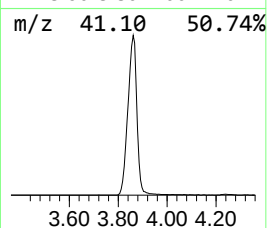
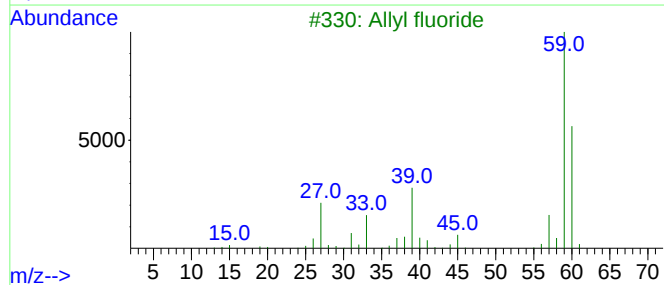
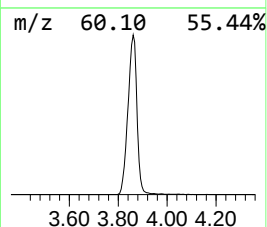
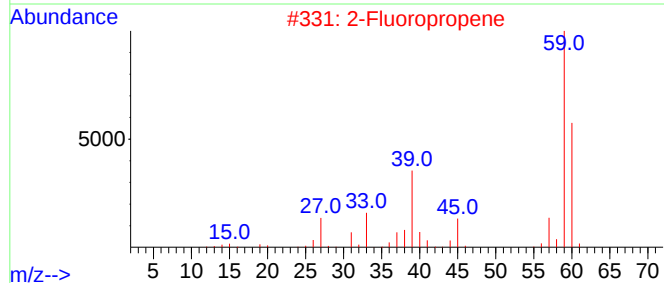
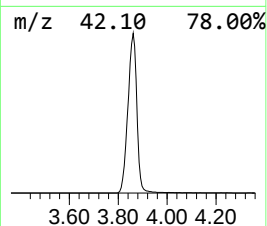
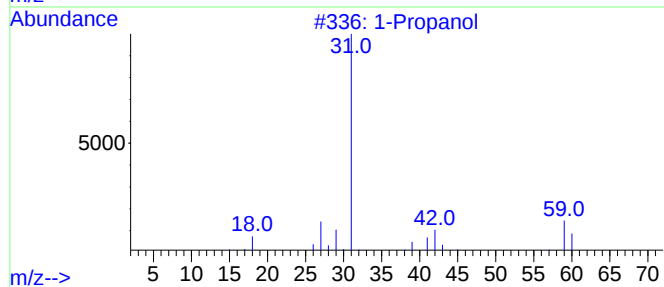
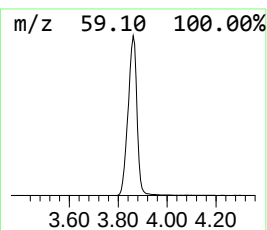
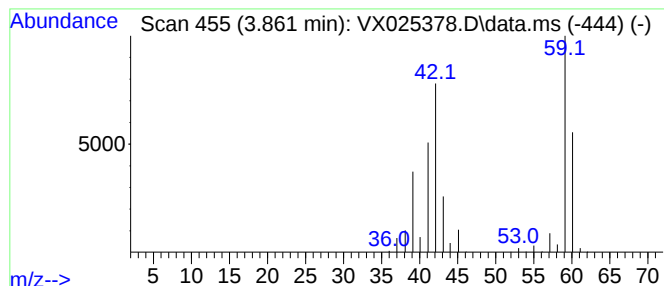
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.861	124.96 ug/l	879939	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	78
2	2-Fluoropropene			60	C3H5F	001184-60-7	49
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	23
5	Cyclopropane			42	C3H6	000075-19-4	16



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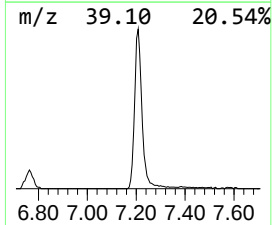
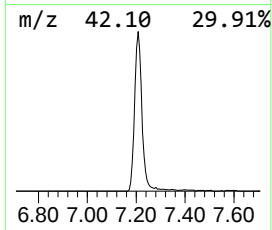
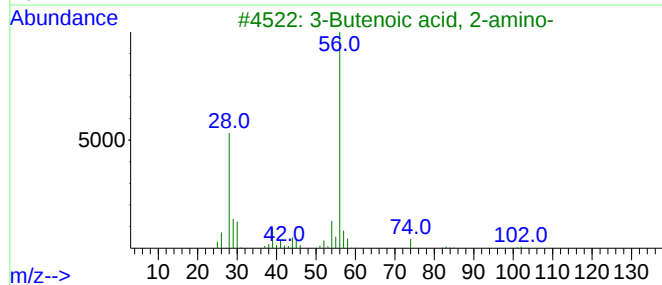
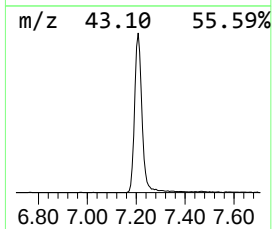
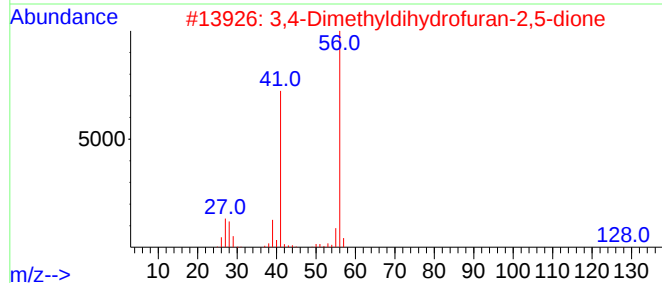
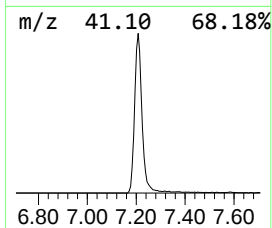
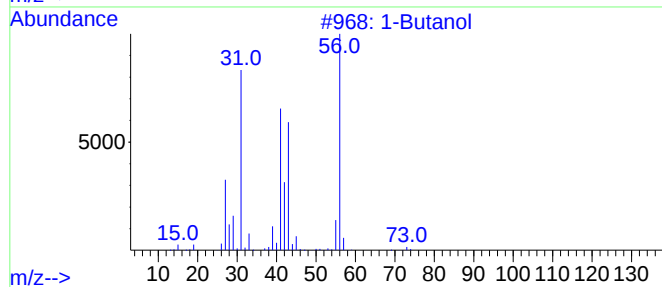
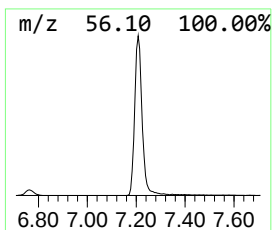
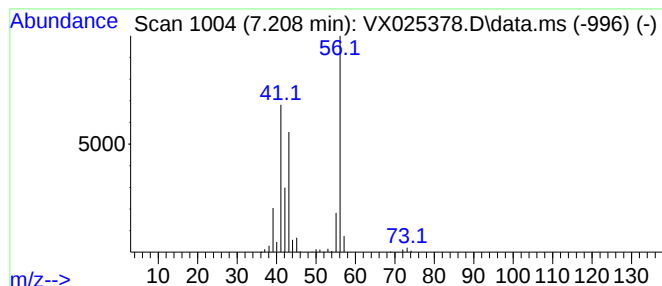
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	39.03 ug/l	356997	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
3			3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
4			Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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20927

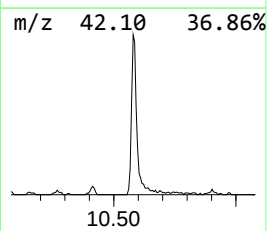
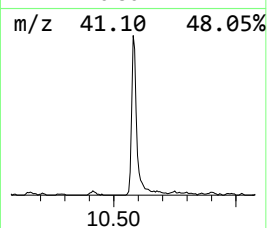
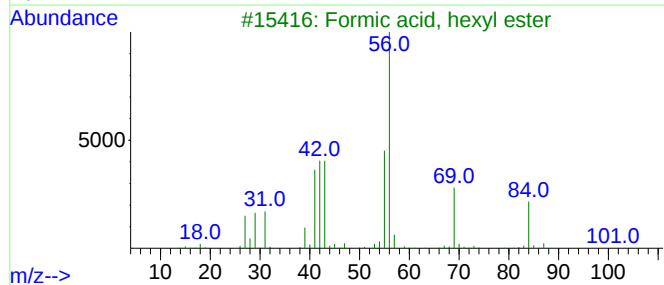
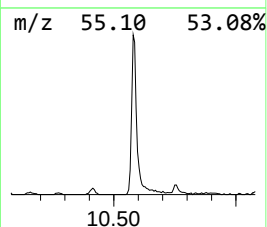
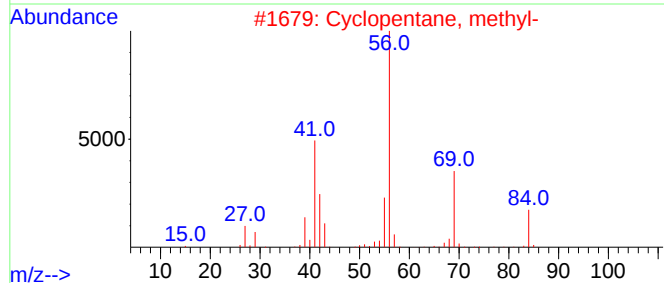
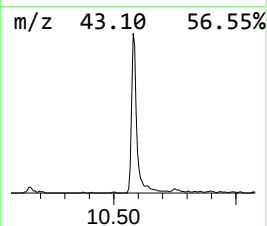
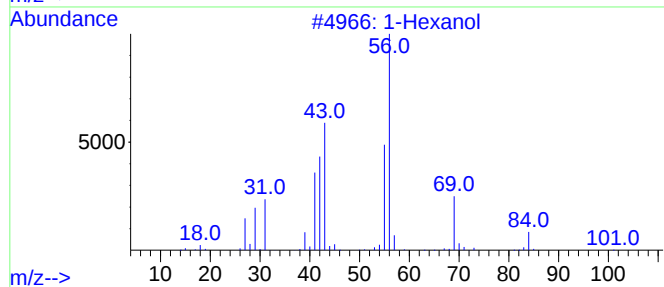
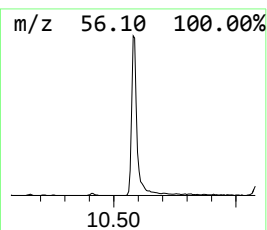
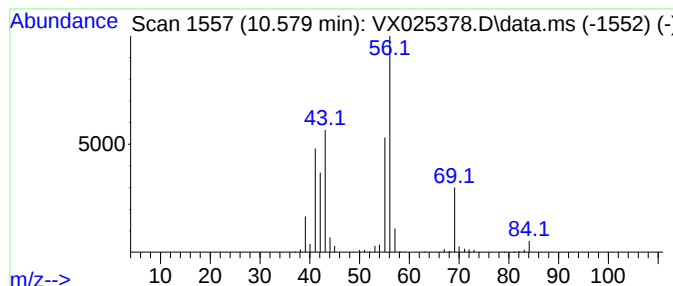
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Quant Title : SW846 8260

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

Peak Number 4 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.579	10.36 ug/l	112695	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	90
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	78
3			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
4			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	74
5			Cyclopropane, propyl-	84	C6H12	002415-72-7	72



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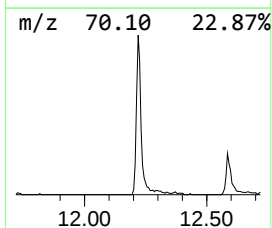
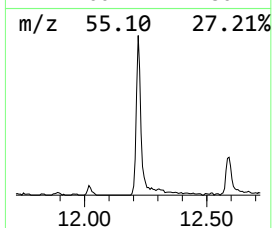
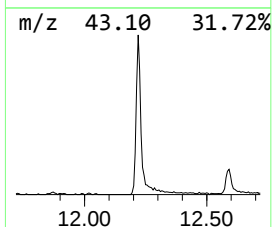
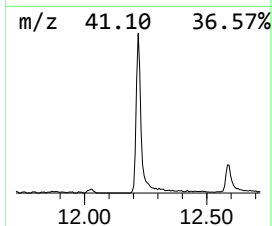
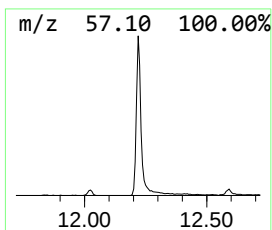
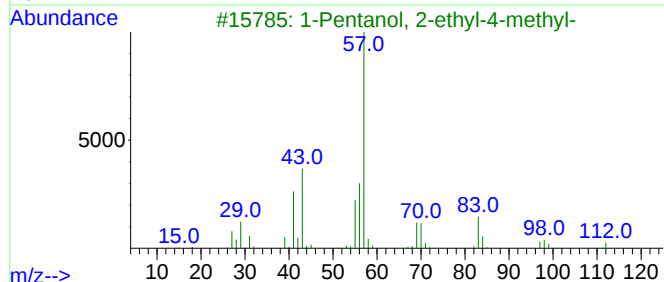
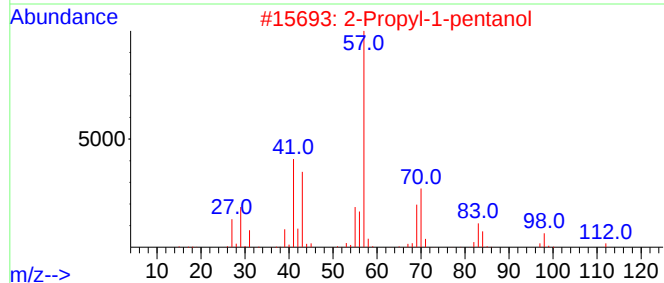
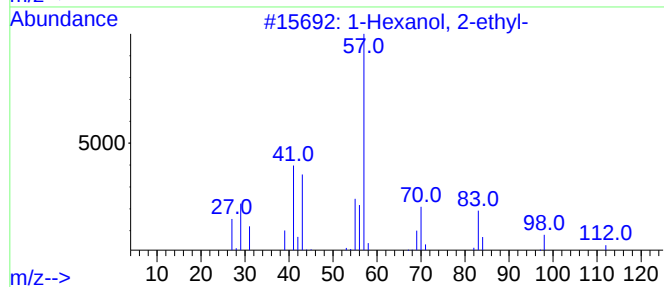
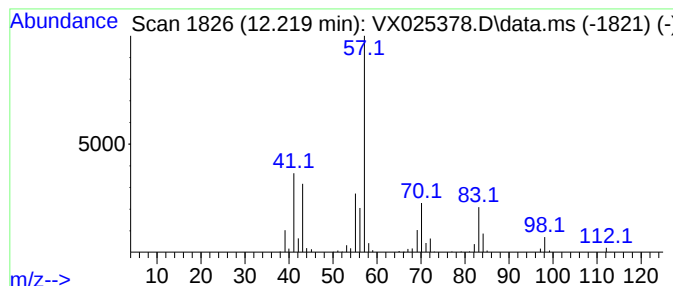
Instrument :
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.219	15.12 ug/l	158471	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.056	103.7	ug/l	729888	1	5.556	352079	50.0
1-Propanol	3.861	125.0	ug/l	879939	1	5.556	352079	50.0
1-Butanol	7.208	39.0	ug/l	356997	2	6.763	457321	50.0
1-Hexanol	10.579	10.4	ug/l	112695	3	10.055	544078	50.0
1-Hexanol, 2-et...	12.219	15.1	ug/l	158471	4	12.024	524135	50.0