

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025377.D
 Acq On : 29 Nov 2021 18:08
 Operator : JC/MD
 Sample : M4837-14 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20934

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: VX025377.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.057	152	159	174	rBV	529391	797466	74.94%	13.026%
2	2.532	230	237	244	rBV	12847	23154	2.18%	0.378%
3	3.867	443	456	477	rBV	408376	1064203	100.00%	17.383%
4	5.391	694	706	720	rBV2	72732	210175	19.75%	3.433%
5	5.556	722	733	747	rVB	125274	352166	33.09%	5.752%
6	5.958	786	799	808	rBV	77613	202989	19.07%	3.316%
7	6.763	921	931	950	rBV	192314	456338	42.88%	7.454%
8	7.208	995	1004	1020	rBV	213830	441318	41.47%	7.209%
9	8.653	1233	1241	1248	rBV	391732	623250	58.56%	10.180%
10	8.720	1248	1252	1257	rVB	8574	12269	1.15%	0.200%
11	9.232	1331	1336	1348	rBV	32255	55078	5.18%	0.900%
12	10.055	1465	1471	1480	rVB	406740	541658	50.90%	8.848%
13	10.579	1551	1557	1565	rBV	104517	145698	13.69%	2.380%
14	10.659	1565	1570	1580	rVB2	10467	19840	1.86%	0.324%
15	11.079	1634	1639	1654	rVB	318900	422238	39.68%	6.897%
16	11.658	1729	1734	1740	rBV	7474	11396	1.07%	0.186%
17	12.024	1788	1794	1802	rBV	414481	522629	49.11%	8.537%
18	12.219	1821	1826	1838	rBV	110735	152285	14.31%	2.487%
19	12.414	1855	1858	1863	rVB	13517	16089	1.51%	0.263%
20	12.585	1880	1886	1905	rBV	28690	51828	4.87%	0.847%

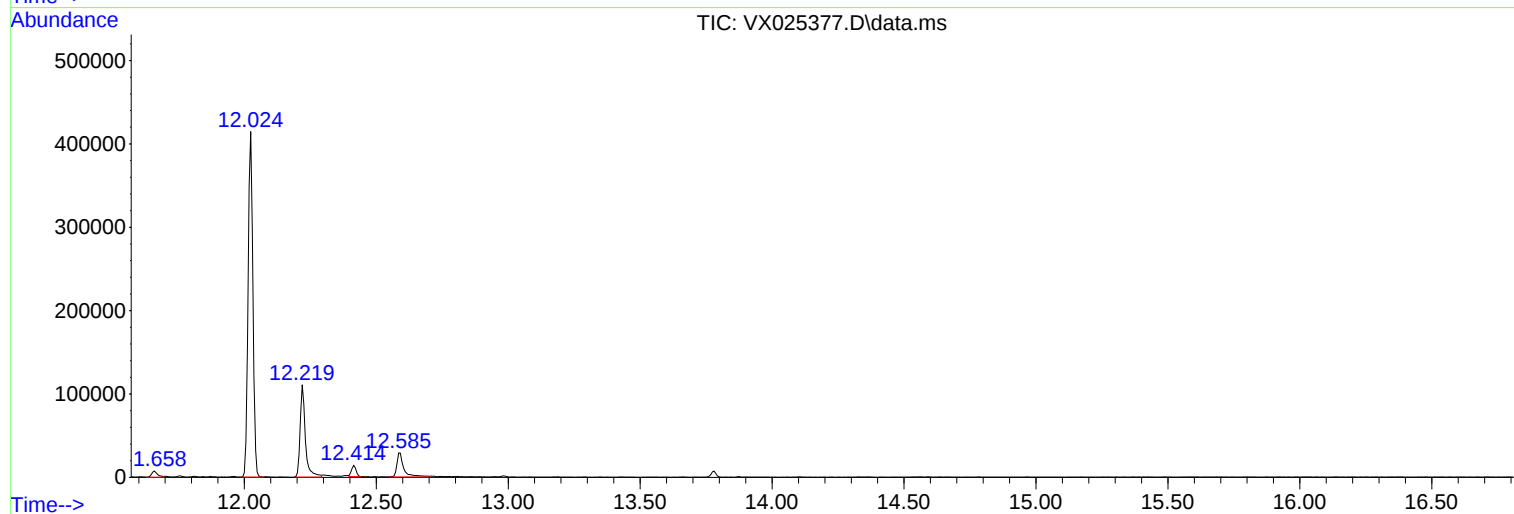
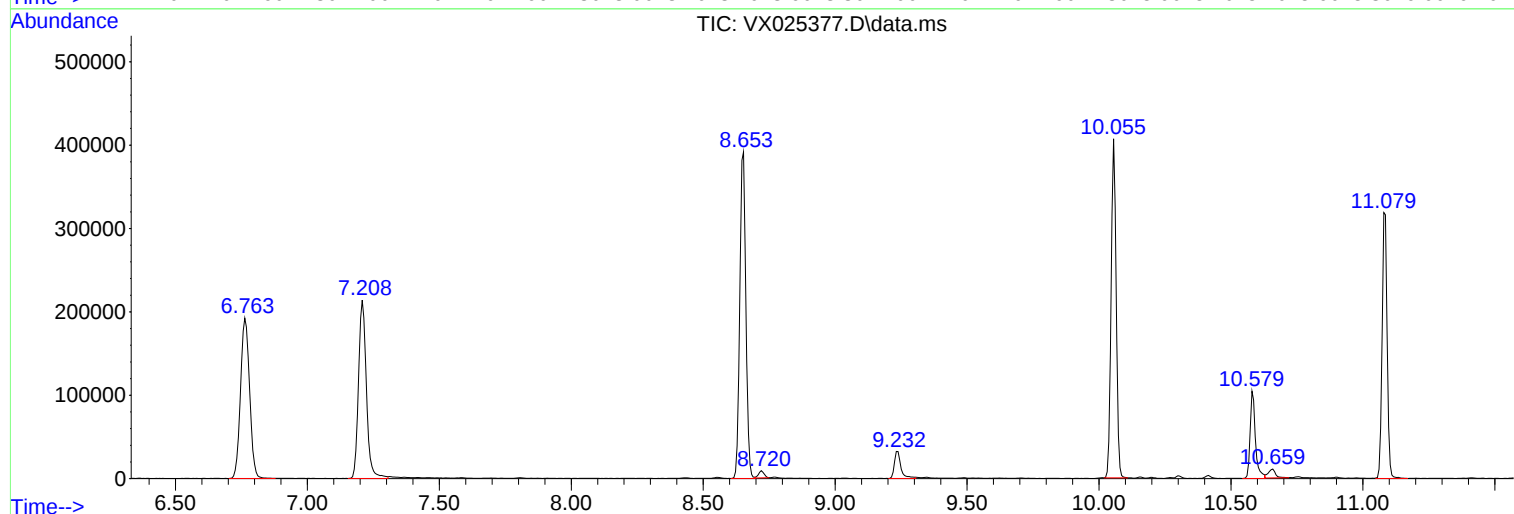
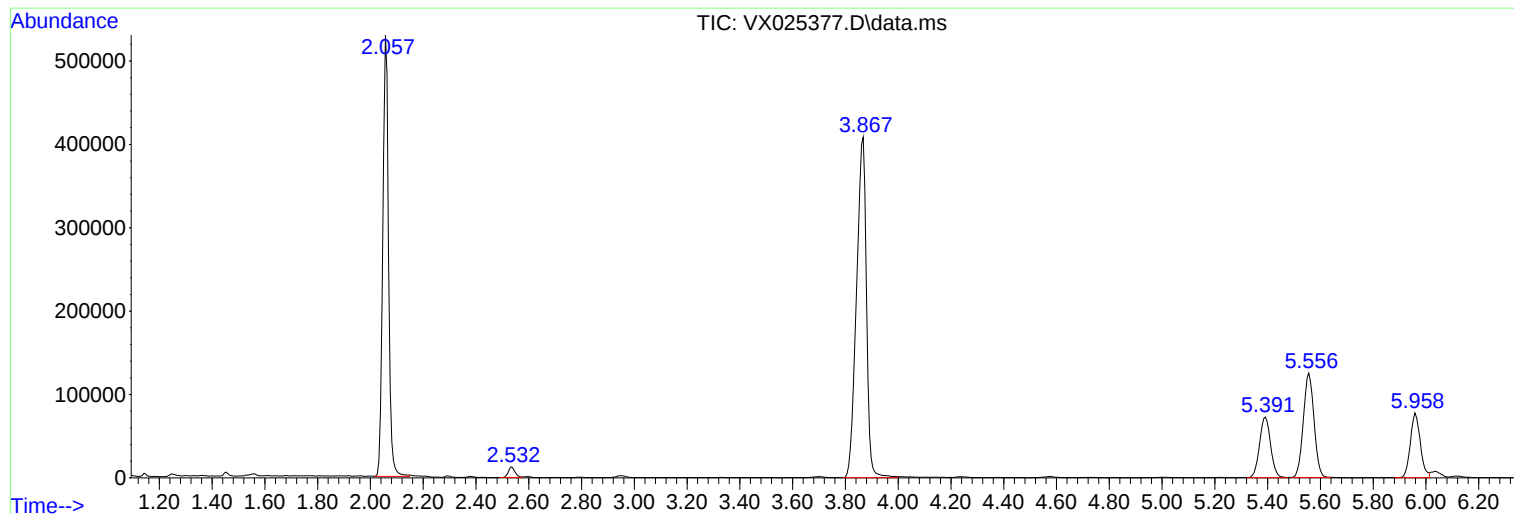
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Quant Title : SW846 8260

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



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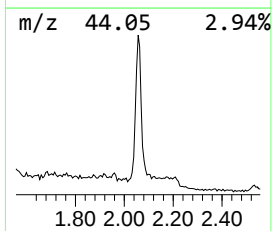
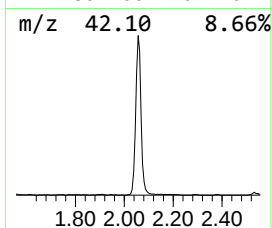
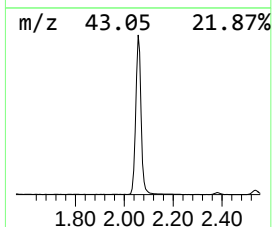
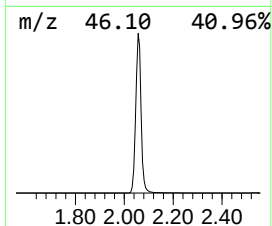
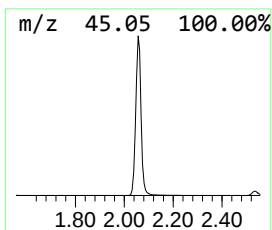
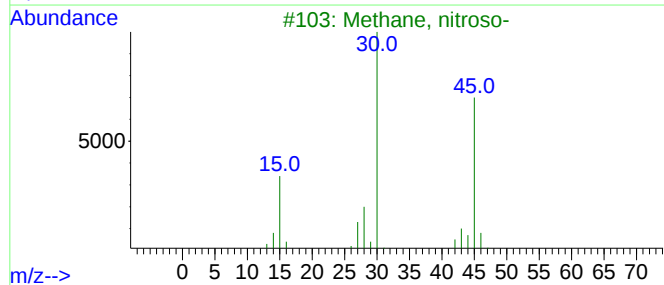
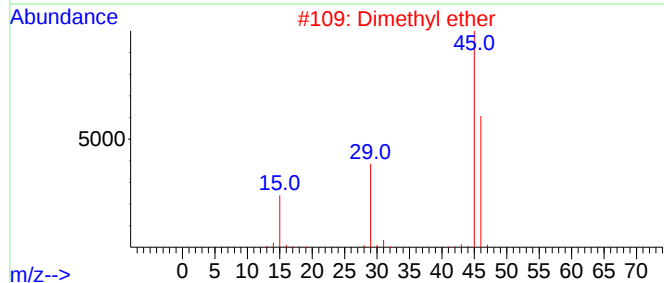
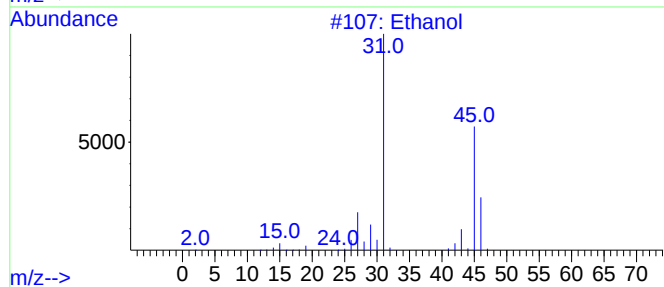
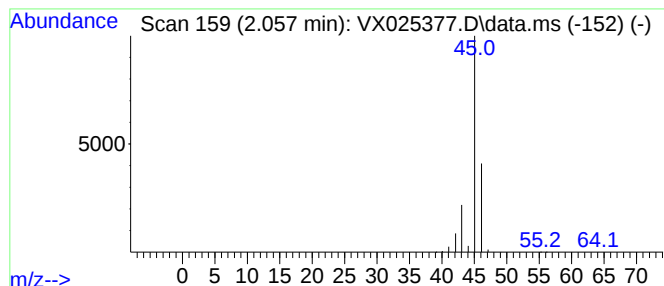
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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.
2.057	113.22 ug/l	797466	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
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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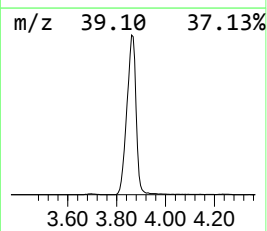
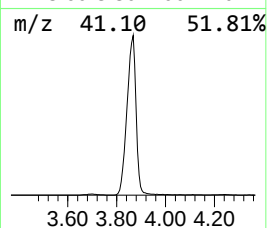
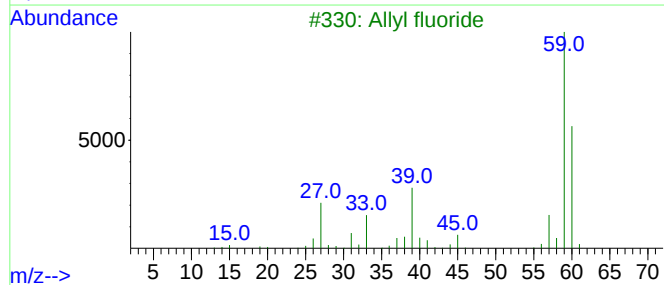
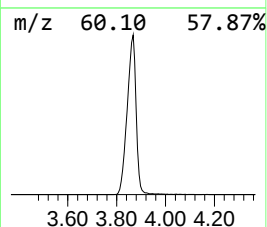
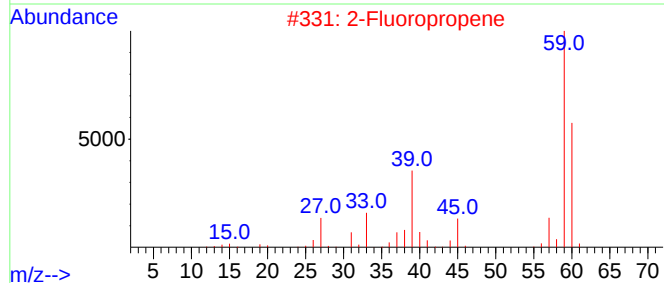
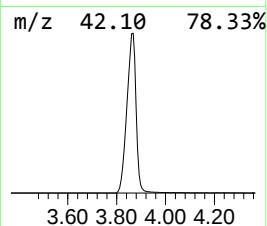
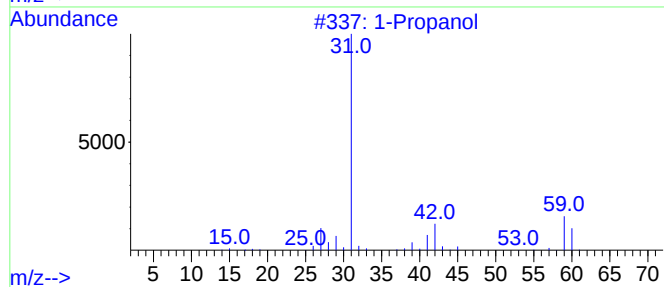
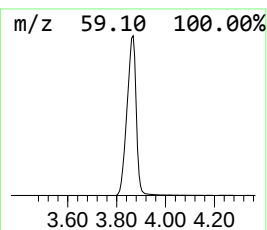
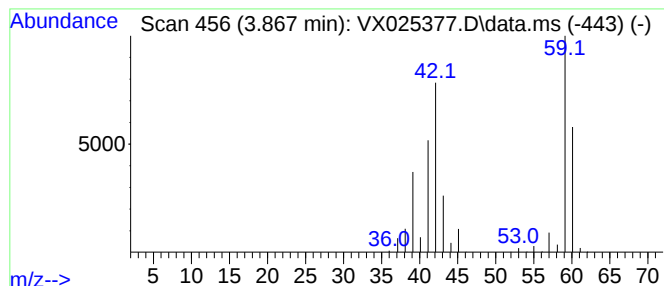
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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.
3.867	151.09 ug/l	1064200	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	43
4	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	17
5	Cyclopropane			42	C3H6	000075-19-4	12



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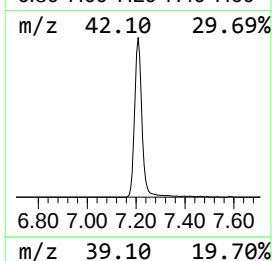
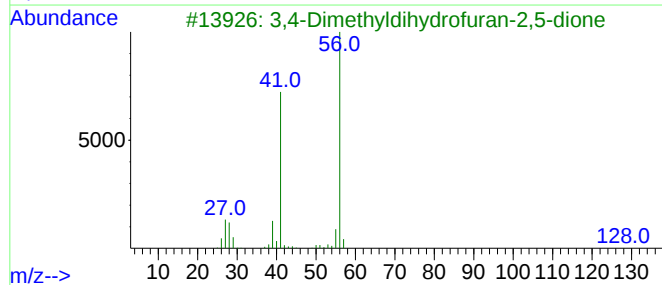
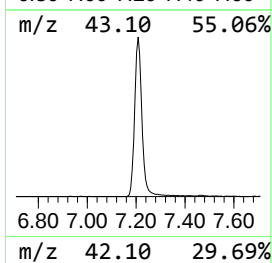
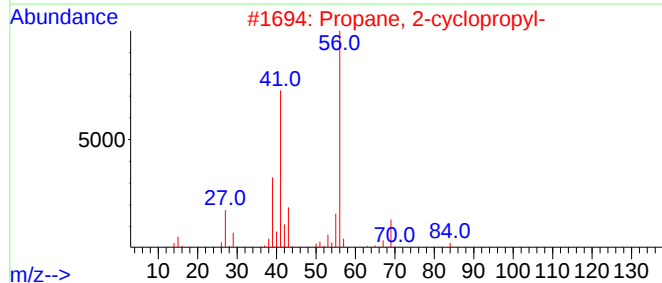
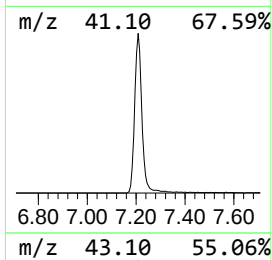
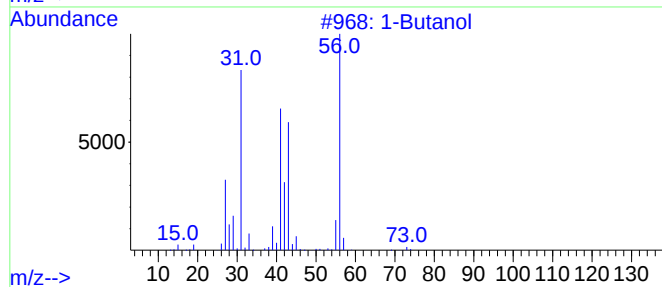
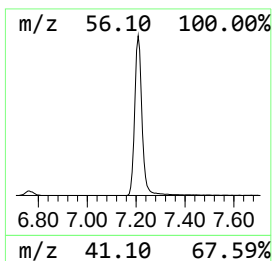
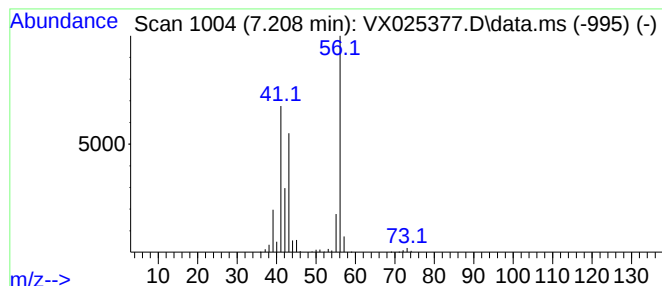
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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	48.35 ug/l	441318	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	91
2	Propane, 2-cyclopropyl-			84	C6H12	003638-35-5	33
3	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	9
4	Oxetane, 3,3-dimethyl-			86	C5H10O	006921-35-3	9
5	.alpha.-Amino-.gamma.-butyrolactone			101	C4H7NO2	001192-20-7	9



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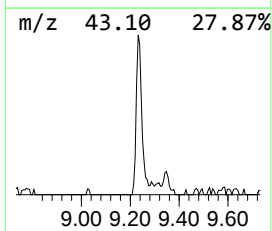
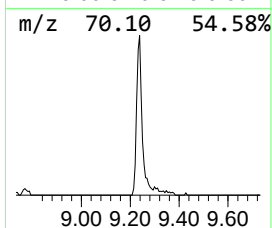
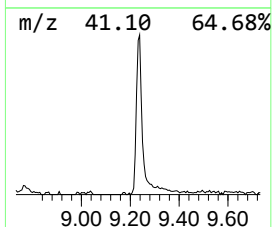
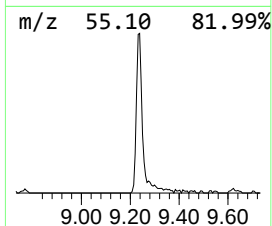
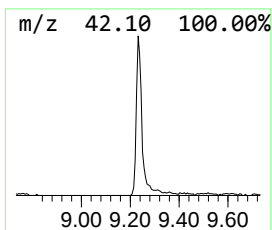
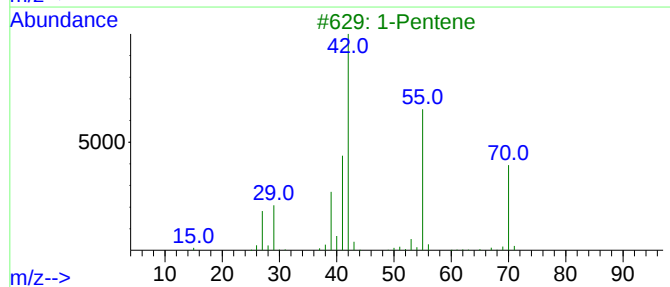
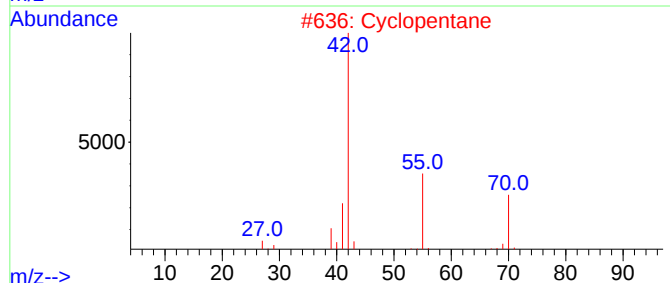
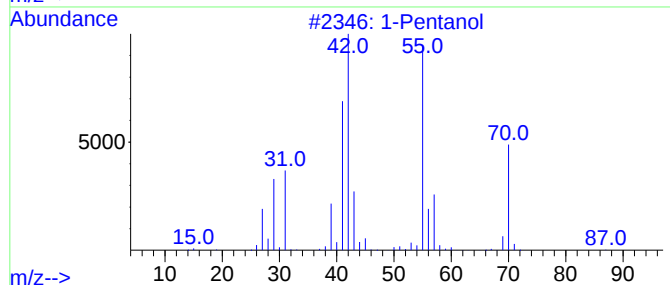
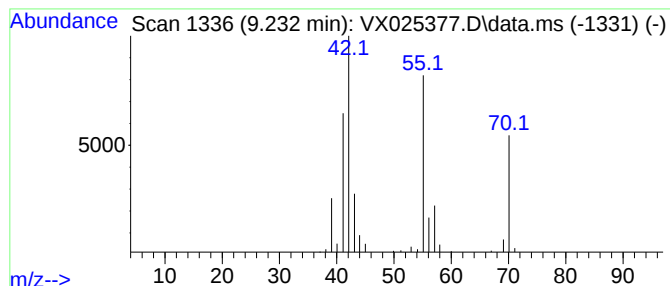
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Pentanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	5.08 ug/l	55078	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol	88	C5H12O	000071-41-0	90
2			Cyclopentane	70	C5H10	000287-92-3	72
3			1-Pentene	70	C5H10	000109-67-1	72
4			Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	40
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	38



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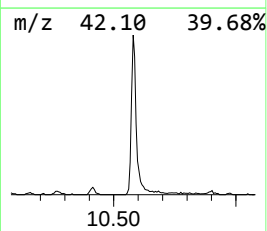
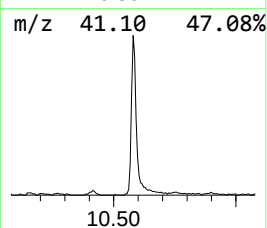
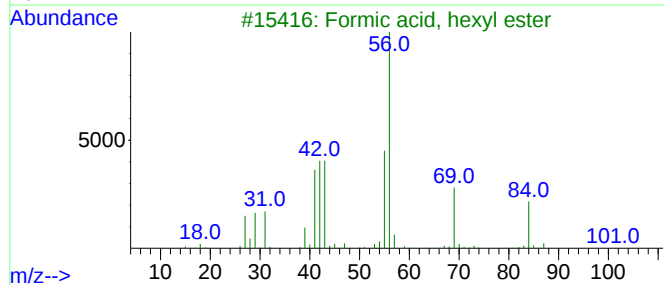
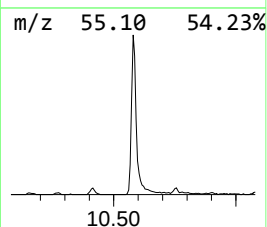
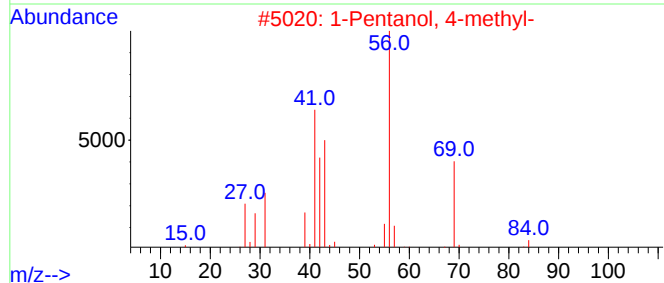
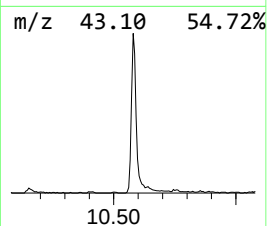
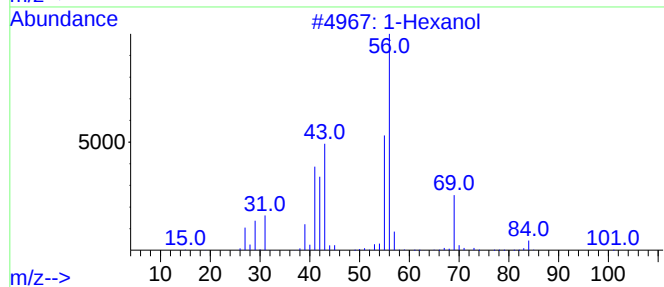
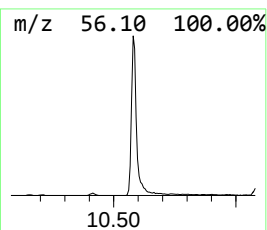
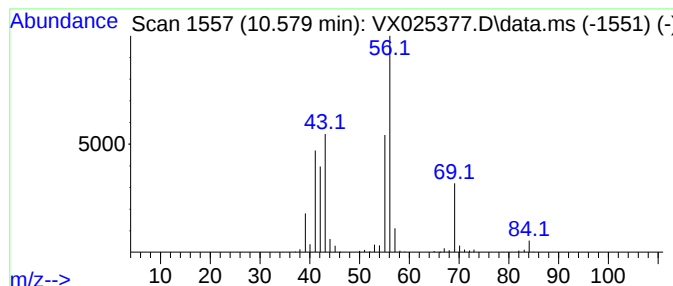
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.579	13.45 ug/l	145698	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	83
2			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
3			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
4			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
5			Cyclopropane, propyl-	84	C6H12	002415-72-7	59



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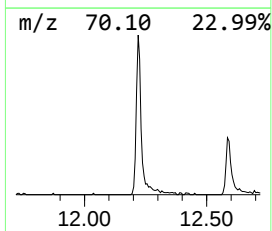
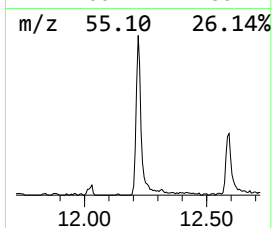
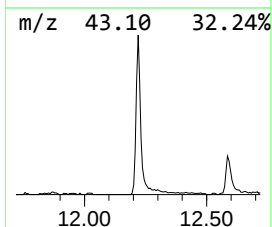
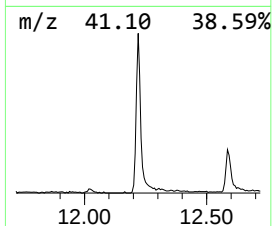
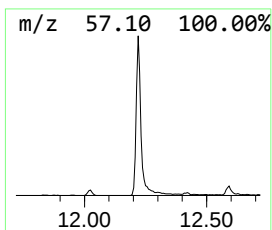
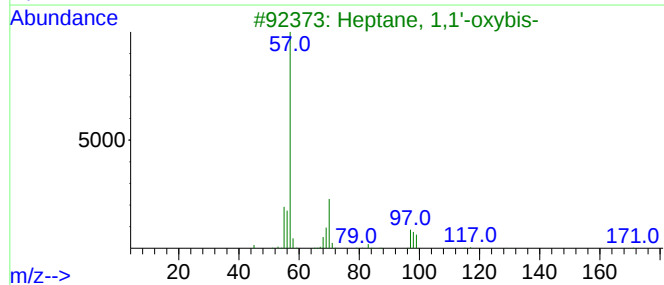
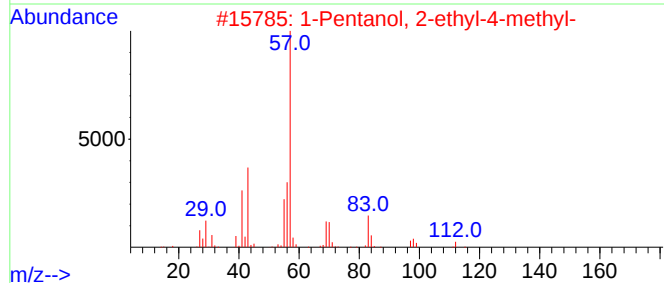
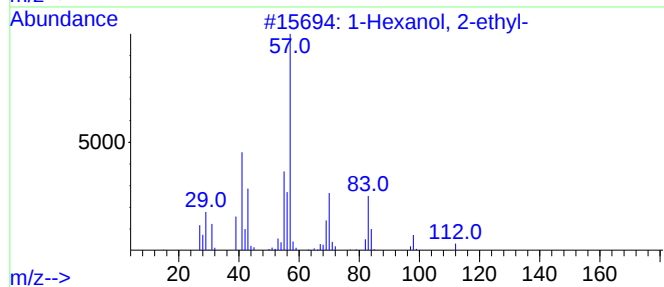
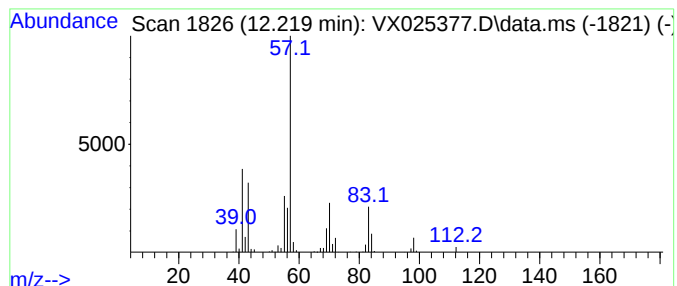
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	14.57 ug/l	152285	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	90
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025377.D
Acq On : 29 Nov 2021 18:08
Operator : JC/MD
Sample : M4837-14 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20934

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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
Ethanol	2.057	113.2	ug/l	797466	1	5.556	352166	50.0
1-Propanol	3.867	151.1	ug/l	1064200	1	5.556	352166	50.0
1-Butanol	7.208	48.4	ug/l	441318	2	6.763	456338	50.0
1-Pentanol	9.232	5.1	ug/l	55078	3	10.055	541658	50.0
1-Hexanol	10.579	13.4	ug/l	145698	3	10.055	541658	50.0
1-Hexanol, 2-et...	12.219	14.6	ug/l	152285	4	12.024	522629	50.0