

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020224\
 Data File : VX040080.D
 Acq On : 02 Feb 2024 12:35
 Operator : JC/MD
 Sample : P1342-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MR-317AP-GW-20240131-0

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\82X013024W.M
 Title : SW846 8260

Signal : TIC: VX040080.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	56	59	70	rVB	542791	623953	23.69%	9.539%
2	2.063	152	160	175	rBV	1612111	2634062	100.00%	40.269%
3	3.849	445	453	468	rBV3	16422	44607	1.69%	0.682%
4	5.099	648	658	670	rVB2	14064	45241	1.72%	0.692%
5	5.385	695	705	718	rBV	60010	176134	6.69%	2.693%
6	5.550	722	732	750	rVV2	100534	282568	10.73%	4.320%
7	5.958	788	799	811	rBV2	67809	182961	6.95%	2.797%
8	6.763	920	931	947	rBV	158313	385718	14.64%	5.897%
9	7.214	1000	1005	1014	rBV3	11535	29339	1.11%	0.449%
10	8.647	1234	1240	1247	rBV	343573	528346	20.06%	8.077%
11	8.720	1247	1252	1258	rVB	46635	75538	2.87%	1.155%
12	10.055	1465	1471	1481	rBV	345045	480810	18.25%	7.351%
13	11.079	1634	1639	1649	rBV	288426	365755	13.89%	5.592%
14	11.756	1745	1750	1760	rBV	23651	34245	1.30%	0.524%
15	12.018	1788	1793	1801	rBV	377896	490030	18.60%	7.492%
16	12.219	1819	1826	1838	rBV	74097	132508	5.03%	2.026%
17	12.951	1942	1946	1954	rVB3	16976	29304	1.11%	0.448%

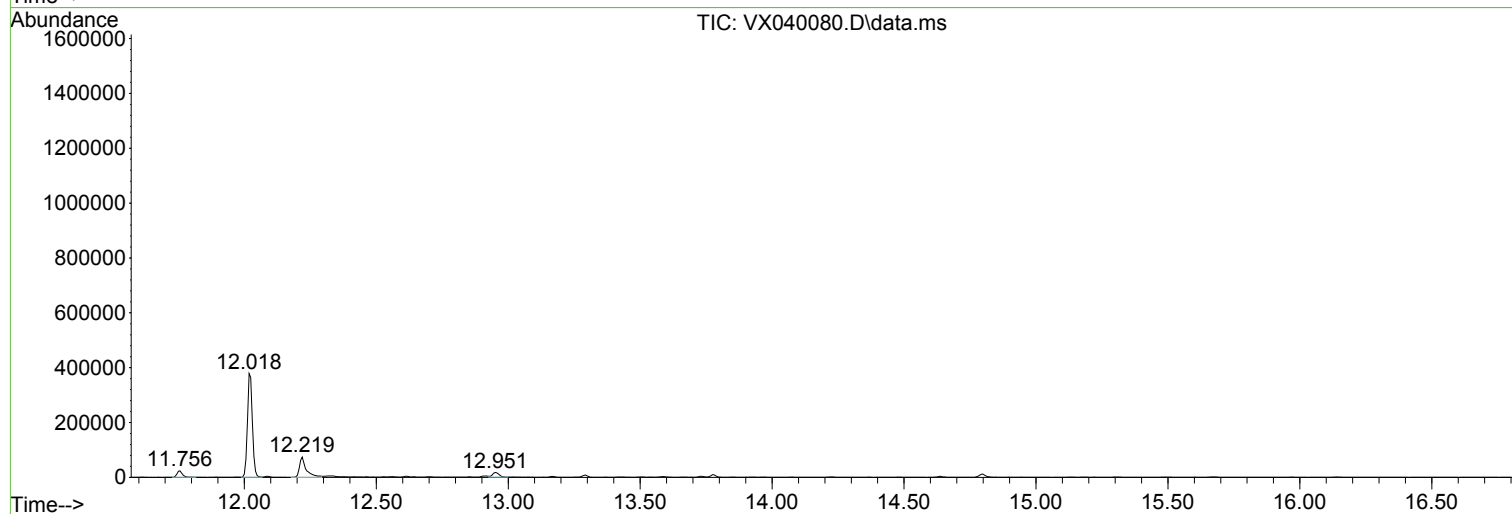
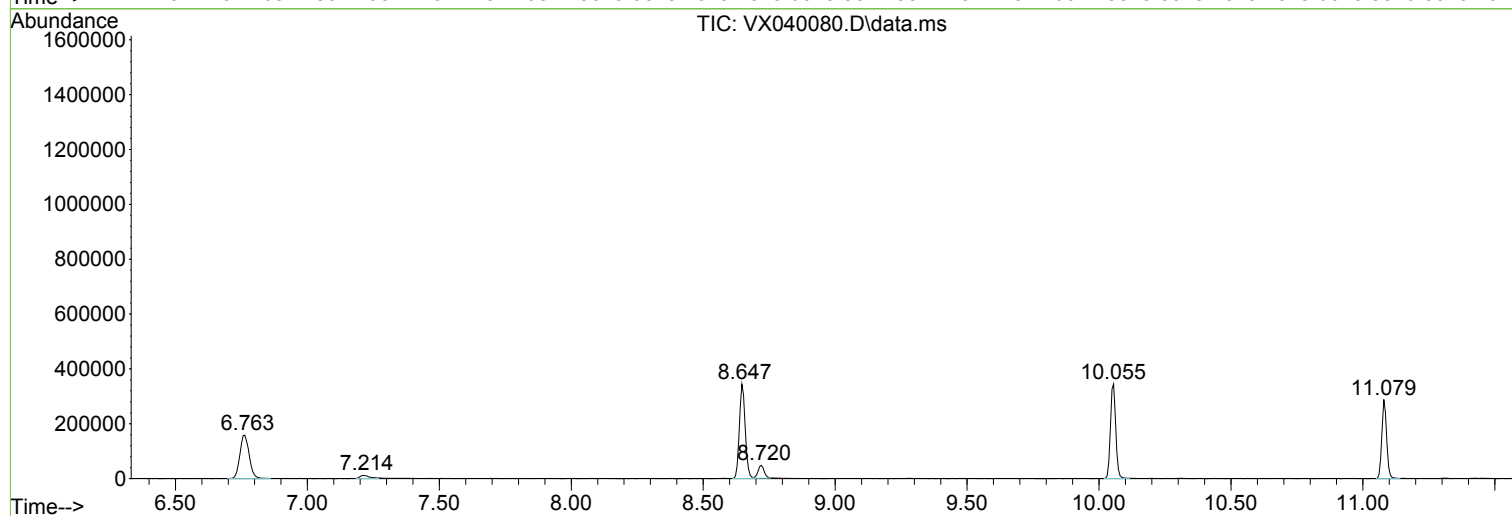
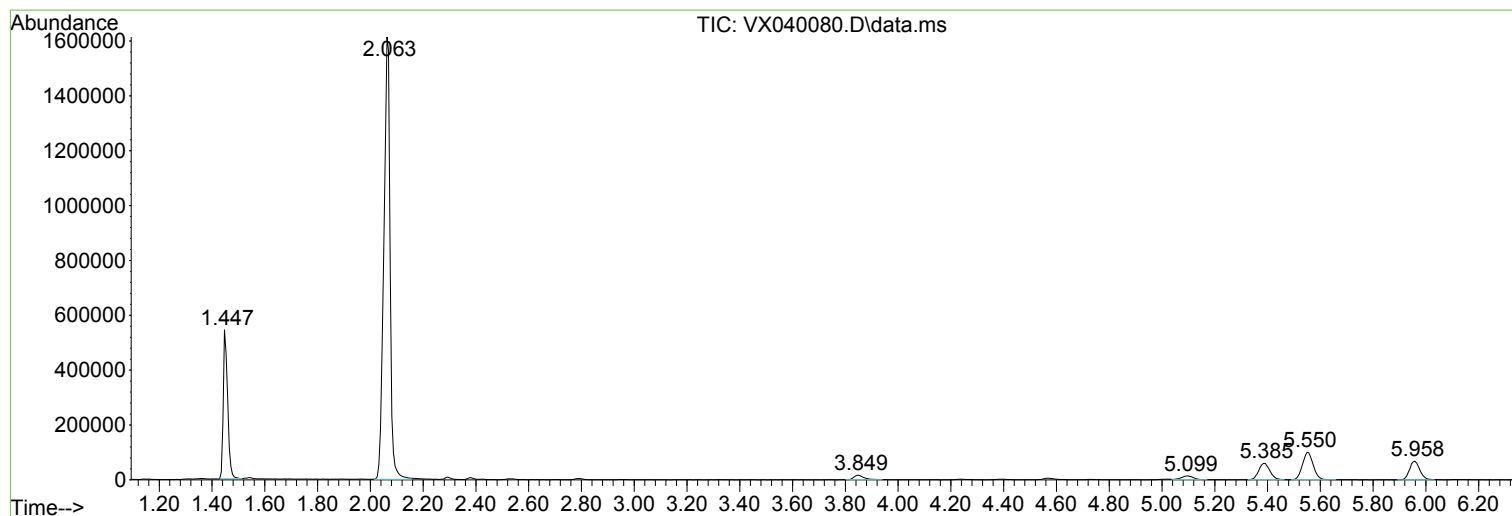
Sum of corrected areas: 6541119

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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



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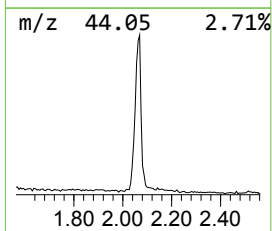
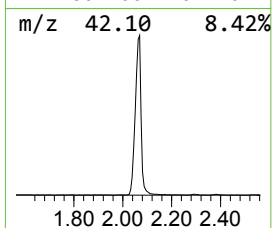
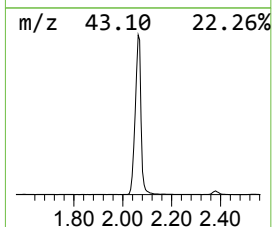
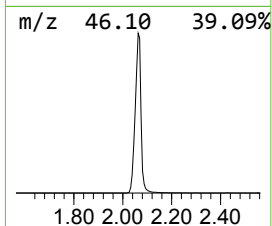
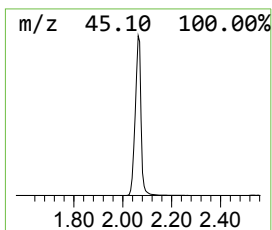
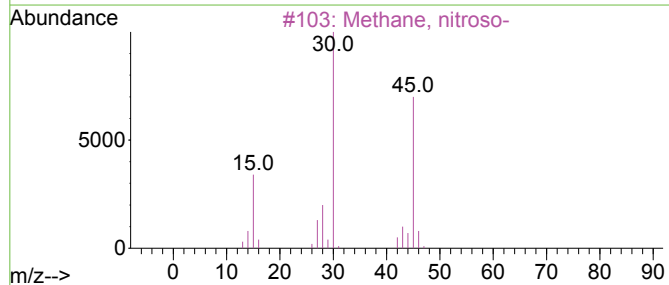
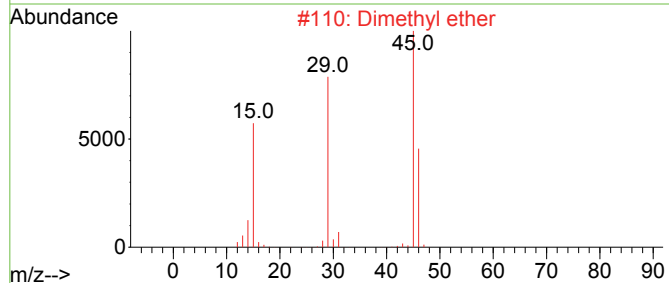
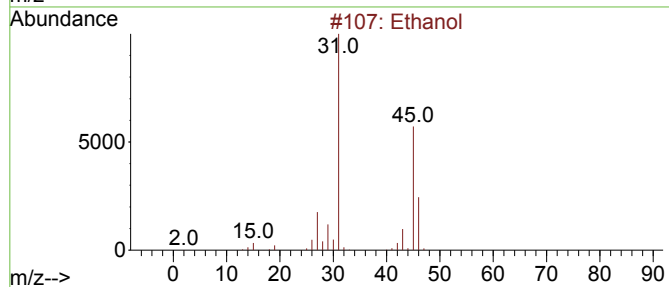
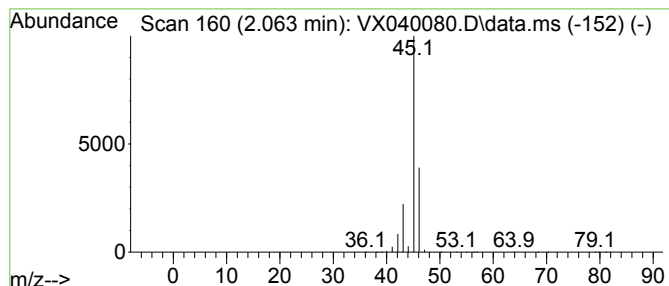
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	466.09 ug/l	2634060	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
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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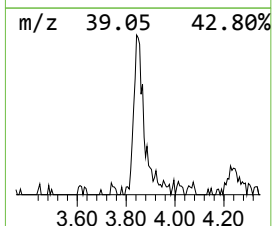
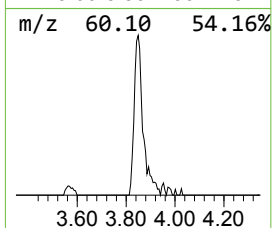
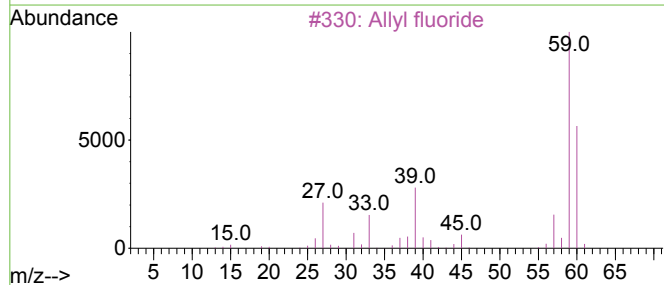
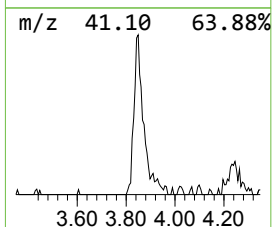
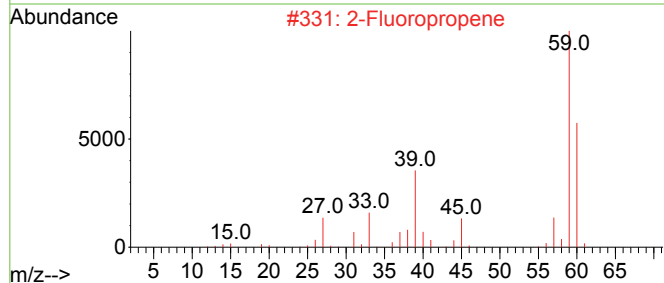
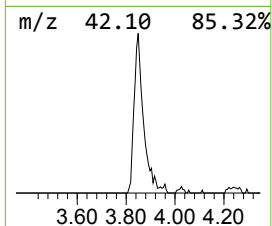
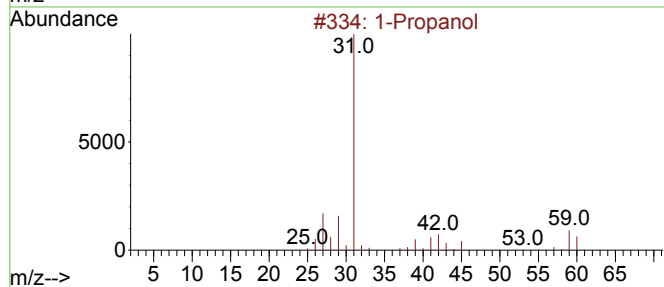
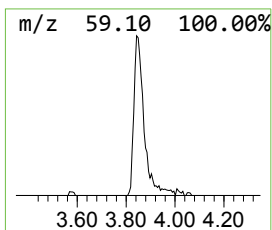
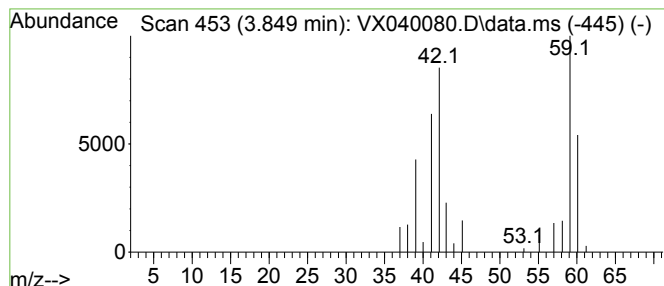
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Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.849	7.89 ug/l	44607	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	50
2	2-Fluoropropene			60	C3H5F	001184-60-7	49
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	32
5	Propene			42	C3H6	000115-07-1	9



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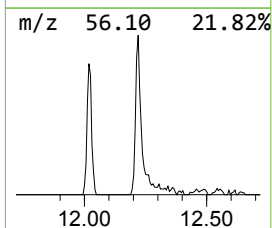
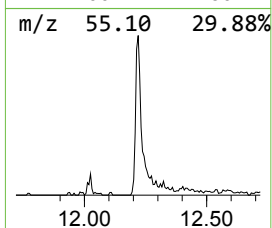
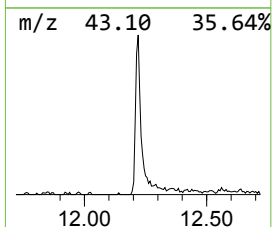
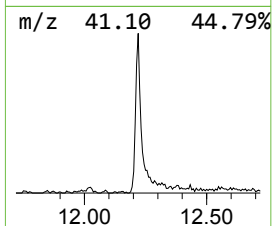
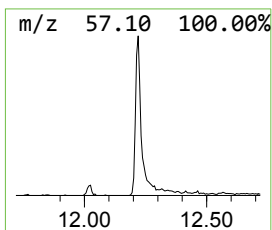
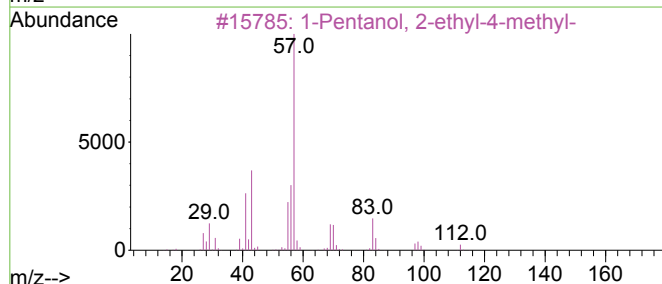
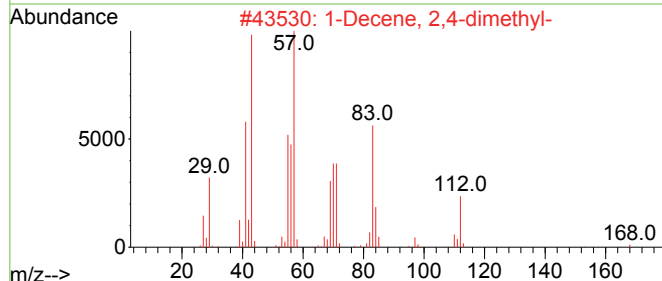
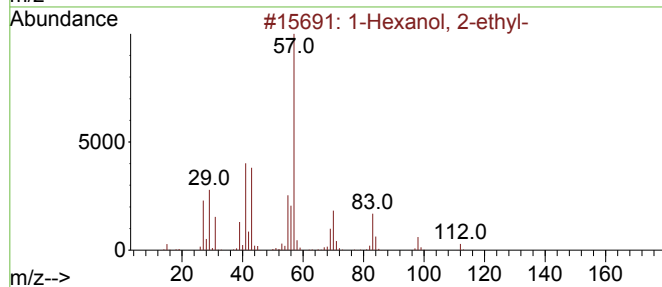
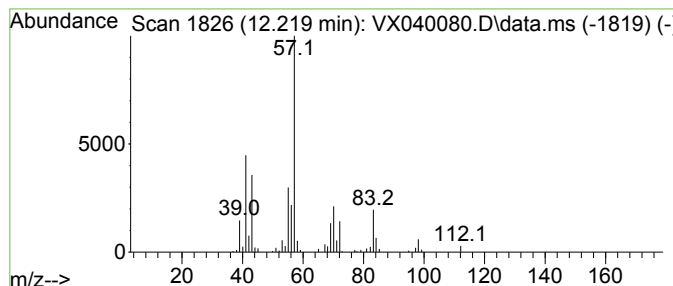
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	13.52 ug/l	132508	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	86
2			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



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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	2.063	466.1	ug/l	2634060	1	5.550	282568	50.0
1-Propanol	3.849	7.9	ug/l	44607	1	5.550	282568	50.0
1-Hexanol, 2-et...	12.219	13.5	ug/l	132508	4	12.024	490030	50.0