

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
 Data File : VX041174.D
 Acq On : 19 Apr 2024 13:41
 Operator : JC/MD
 Sample : P2121-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 4827RE

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\82X041624W.M
 Title : SW846 8260

Signal : TIC: VX041174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	24	rBV	74081	88906	6.54%	1.150%
2	1.368	41	46	54	rVB2	7107	14163	1.04%	0.183%
3	2.398	208	215	227	rBV	33420	66576	4.90%	0.861%
4	3.690	416	427	440	rBV2	32471	91216	6.71%	1.180%
5	3.922	452	465	491	rBV	108337	366522	26.96%	4.743%
6	4.239	506	517	528	rBV2	13309	40941	3.01%	0.530%
7	4.343	528	534	552	rVB5	4054	16665	1.23%	0.216%
8	5.385	694	705	721	rVB	114827	337089	24.79%	4.362%
9	5.550	721	732	751	rBV	198522	573684	42.20%	7.423%
10	5.952	787	798	814	rBV	119140	319848	23.53%	4.139%
11	6.757	921	930	949	rBV	291968	708500	52.11%	9.168%
12	7.257	1007	1012	1026	rBV2	5681	17518	1.29%	0.227%
13	8.647	1233	1240	1249	rBV	605248	944316	69.46%	12.219%
14	8.720	1249	1252	1263	rVB	11006	21163	1.56%	0.274%
15	10.055	1465	1471	1486	rBV	584907	819743	60.29%	10.607%
16	10.756	1581	1586	1598	rBV	34861	61711	4.54%	0.799%
17	11.079	1634	1639	1645	rBV	486688	643958	47.36%	8.333%
18	11.134	1645	1648	1658	rVB2	19096	29254	2.15%	0.379%
19	11.280	1668	1672	1685	rVB	19584	29853	2.20%	0.386%
20	11.390	1685	1690	1699	rBV5	10637	20406	1.50%	0.264%
21	11.573	1716	1720	1723	rBV2	19272	26835	1.97%	0.347%
22	11.604	1723	1725	1732	rVV3	16948	24275	1.79%	0.314%
23	11.683	1733	1738	1747	rVV	1189340	1359567	100.00%	17.593%
24	12.024	1788	1794	1802	rBV	601356	785735	57.79%	10.167%
25	12.219	1821	1826	1836	rBV	117763	210559	15.49%	2.725%
26	12.305	1836	1840	1853	rVB6	12271	36407	2.68%	0.471%
27	13.676	2059	2065	2072	rBV	44625	56668	4.17%	0.733%
28	14.140	2137	2141	2146	rBV2	12531	15941	1.17%	0.206%

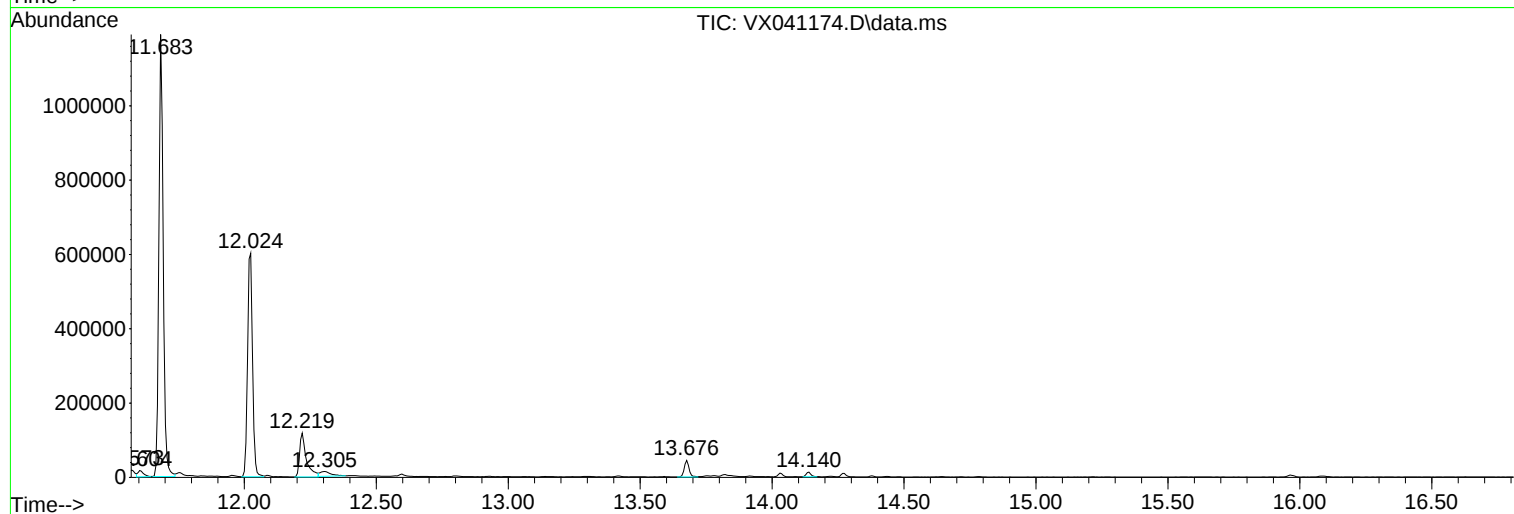
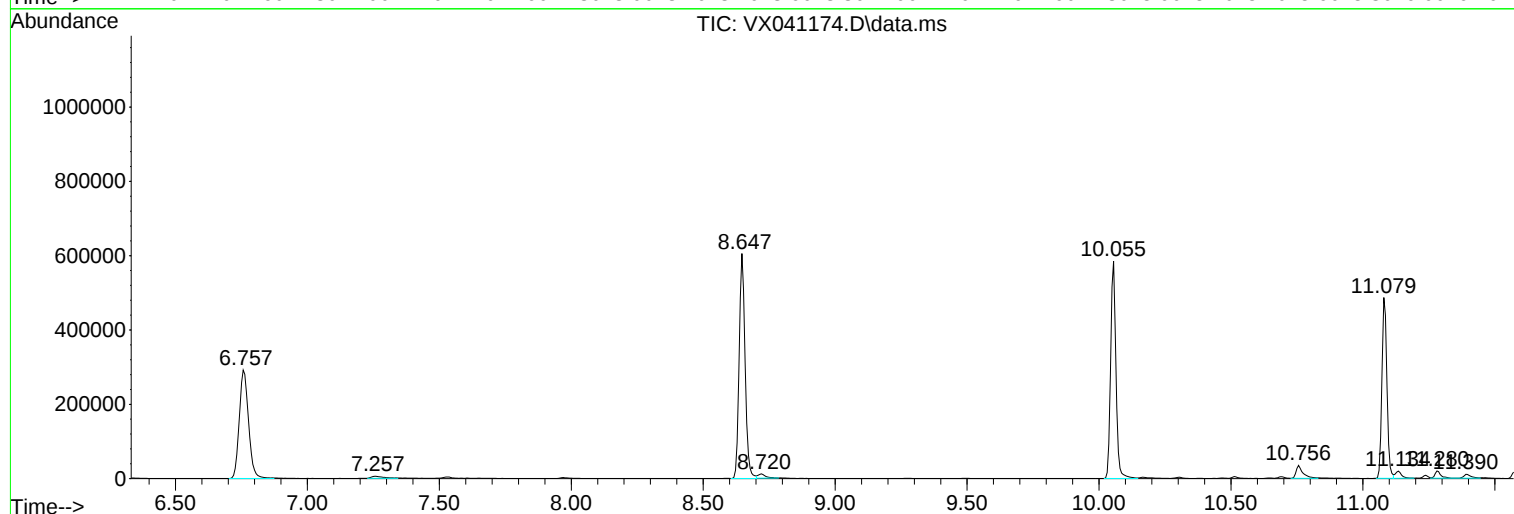
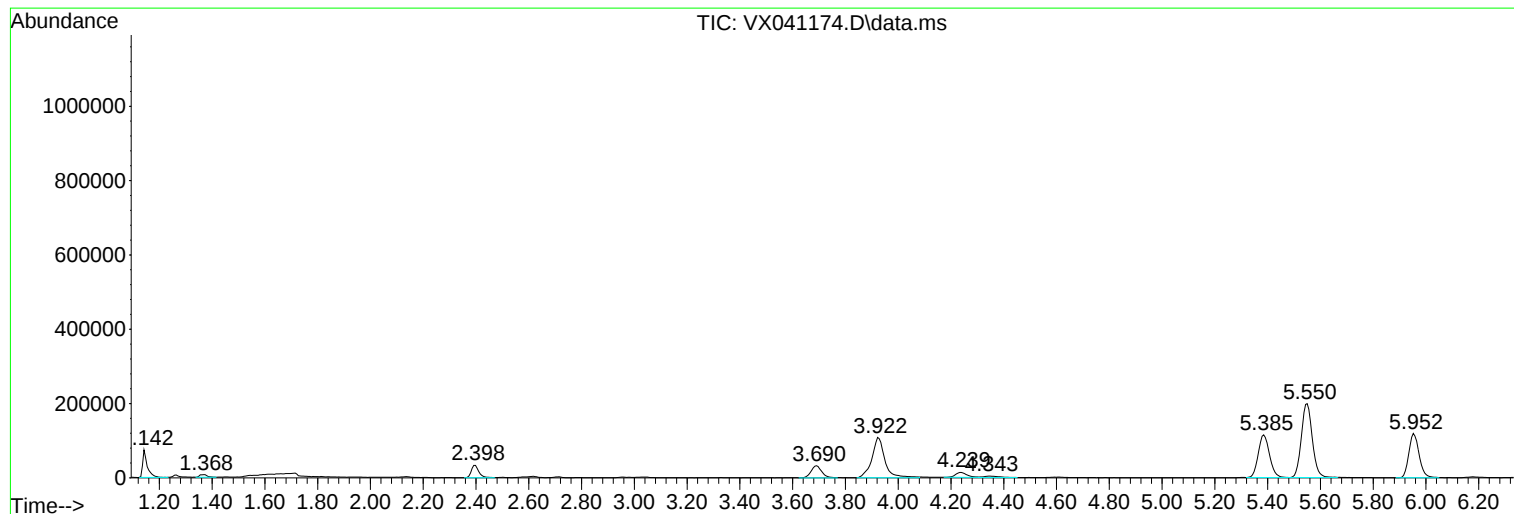
Sum of corrected areas: 7728019

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
Data File : VX041174.D
Acq On : 19 Apr 2024 13:41
Operator : JC/MD
Sample : P2121-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4827RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041624W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
Data File : VX041174.D
Acq On : 19 Apr 2024 13:41
Operator : JC/MD
Sample : P2121-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4827RE

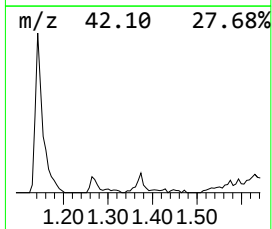
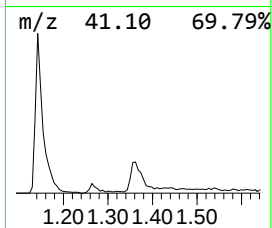
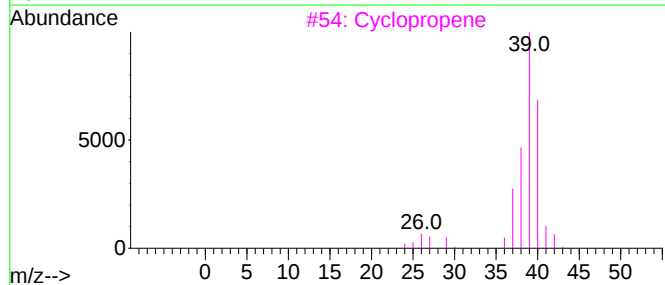
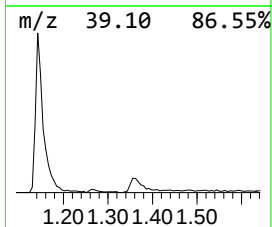
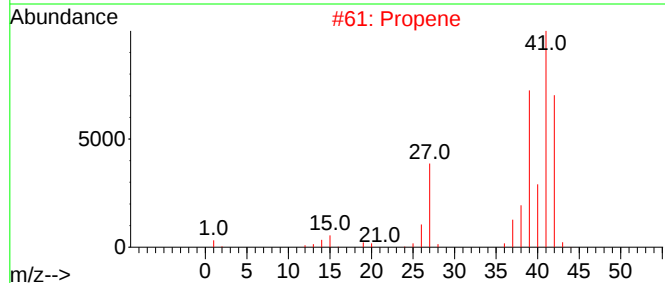
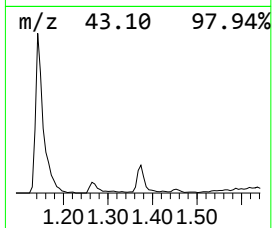
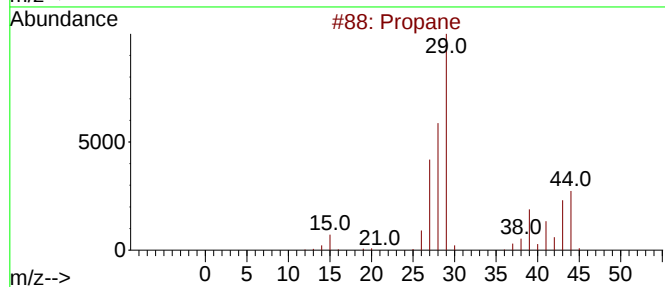
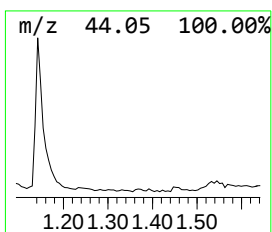
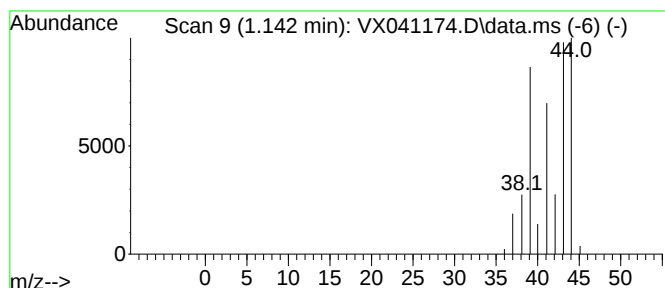
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041624W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	7.75 ug/l	88906	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	83
2	Propene			42	C3H6	000115-07-1	9
3	Cyclopropene			40	C3H4	002781-85-3	2
4	Alanine			89	C3H7NO2	000056-41-7	2
5	Butanenitrile			69	C4H7N	000109-74-0	2



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
Data File : VX041174.D
Acq On : 19 Apr 2024 13:41
Operator : JC/MD
Sample : P2121-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4827RE

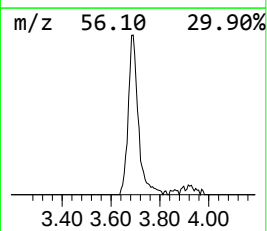
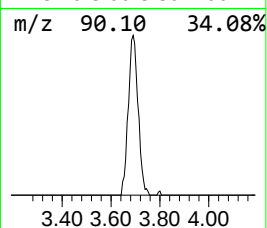
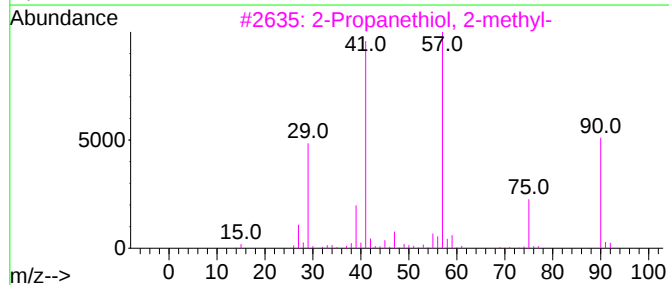
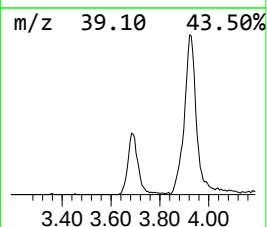
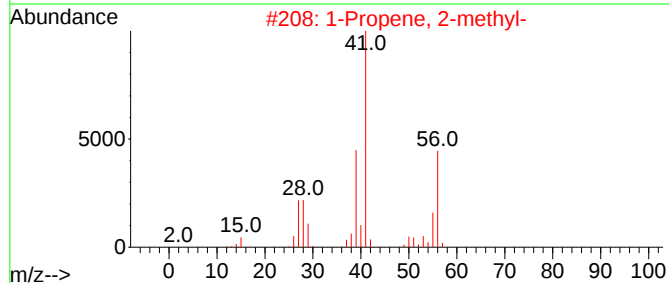
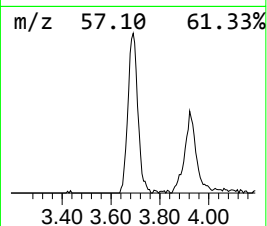
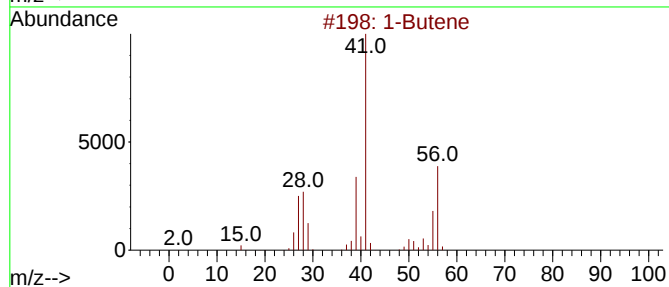
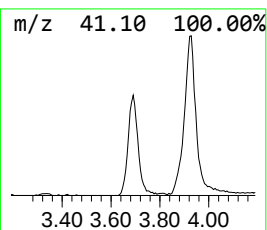
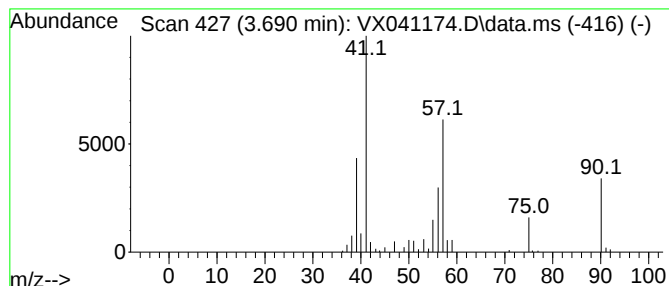
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041624W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.690	7.95 ug/l	91216	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene			56	C4H8	000106-98-9	52
2	1-Propene, 2-methyl-			56	C4H8	000115-11-7	49
3	2-Propanethiol, 2-methyl-			90	C4H10S	000075-66-1	43
4	Propanethial, S-oxide			90	C3H6OS	032157-29-2	40
5	Nitroxide, bis(1,1-dimethylethyl)			144	C8H18NO	002406-25-9	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
Data File : VX041174.D
Acq On : 19 Apr 2024 13:41
Operator : JC/MD
Sample : P2121-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4827RE

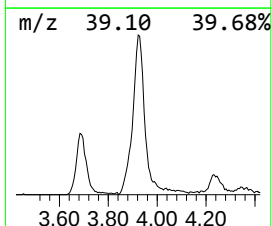
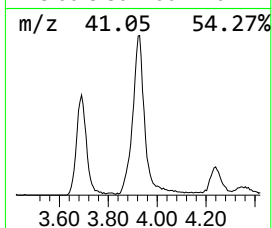
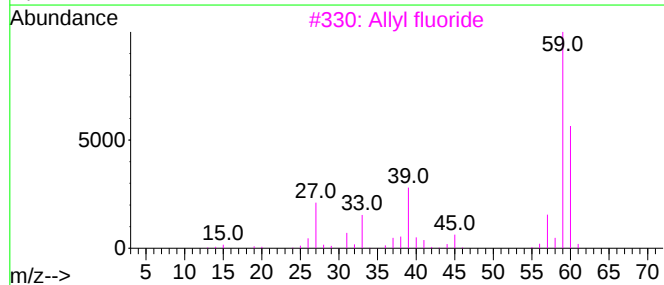
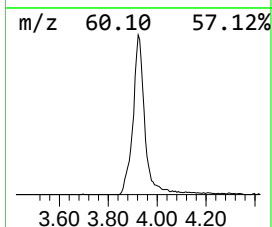
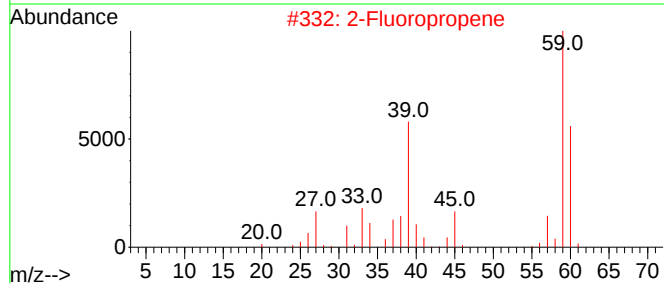
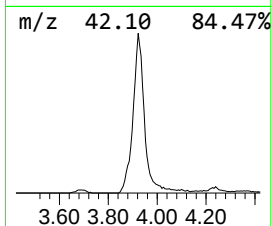
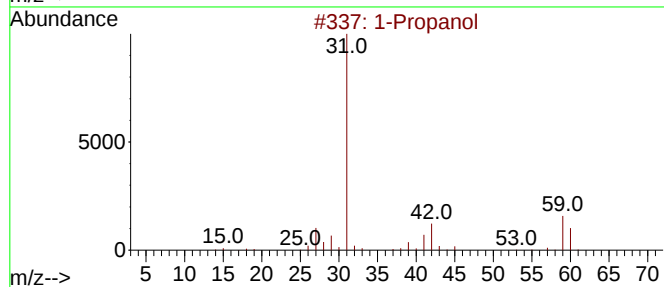
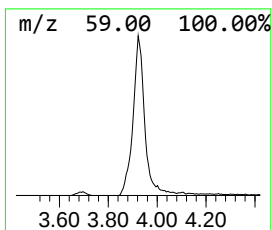
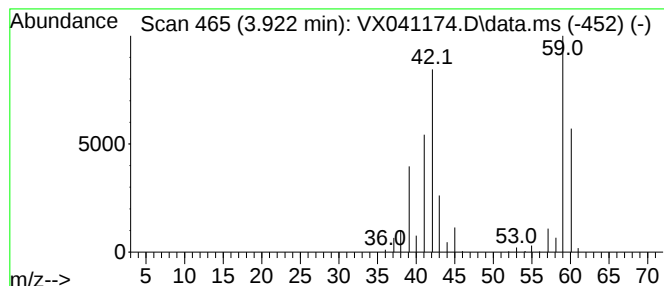
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041624W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.922	31.94 ug/l	366522	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	59
2	2-Fluoropropene			60	C3H5F	001184-60-7	58
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	25
5	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
Data File : VX041174.D
Acq On : 19 Apr 2024 13:41
Operator : JC/MD
Sample : P2121-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4827RE

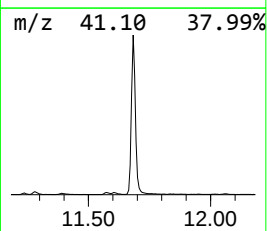
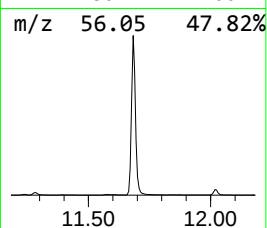
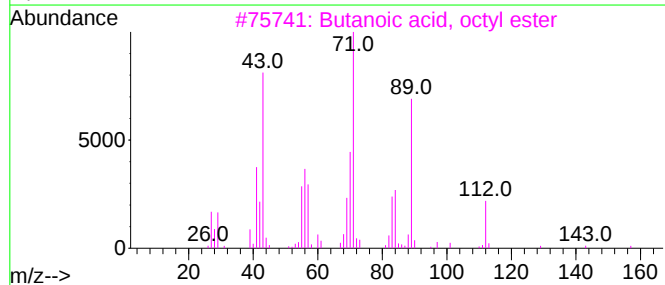
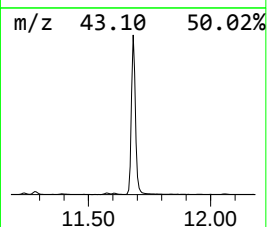
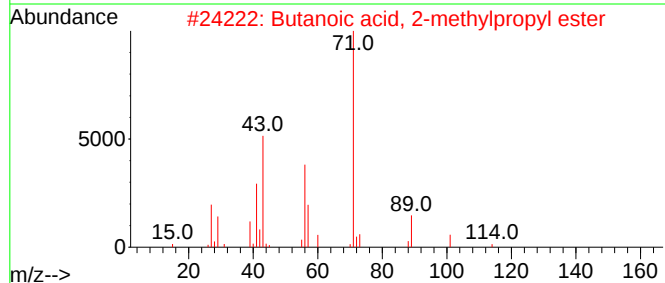
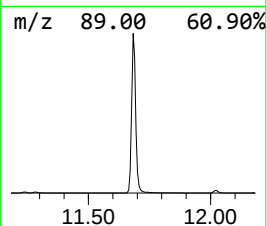
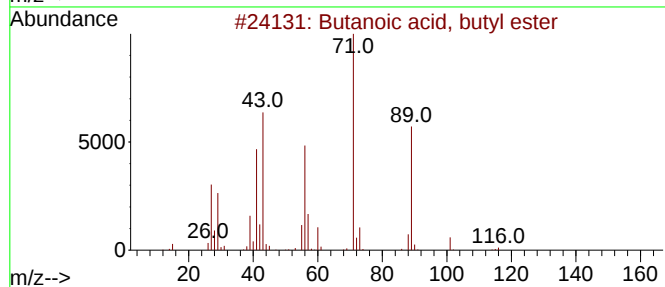
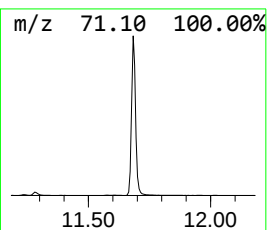
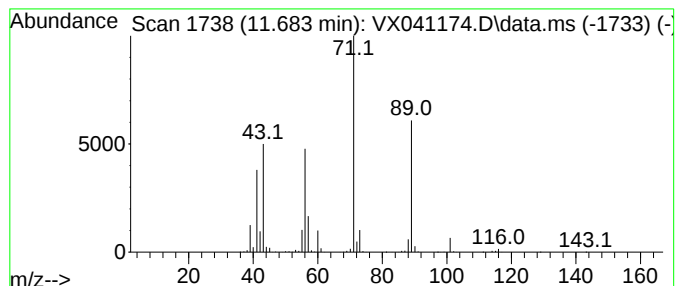
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041624W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	86.52 ug/l	1359570	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	91
2			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
4			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
Data File : VX041174.D
Acq On : 19 Apr 2024 13:41
Operator : JC/MD
Sample : P2121-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4827RE

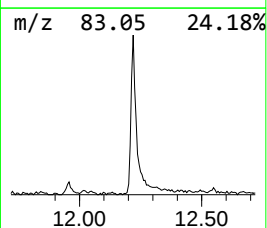
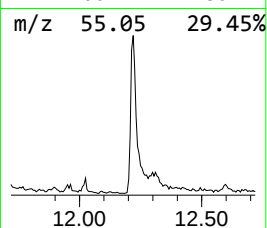
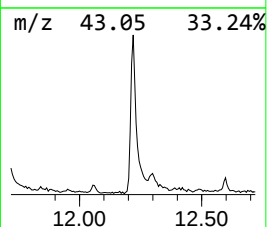
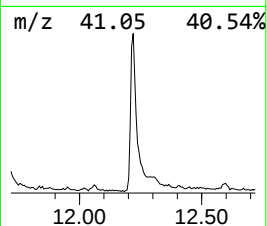
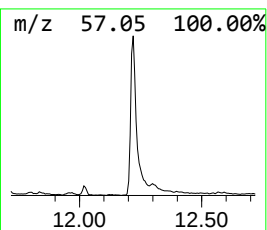
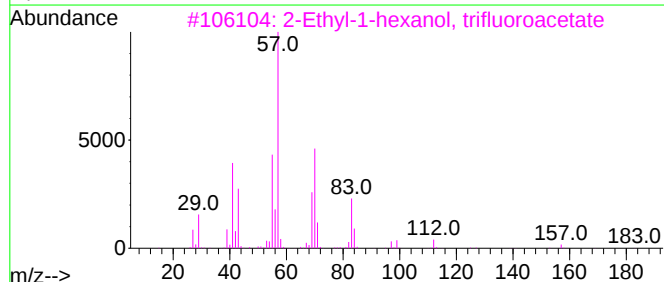
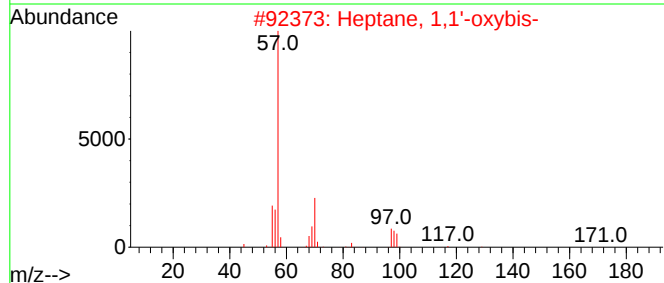
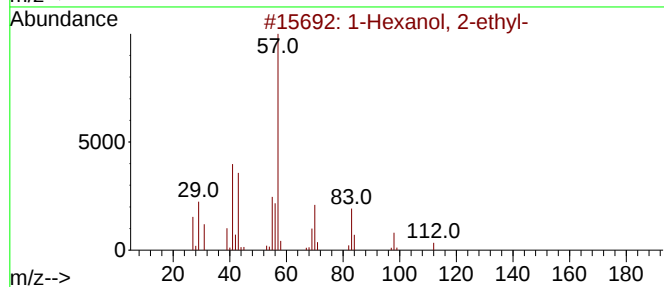
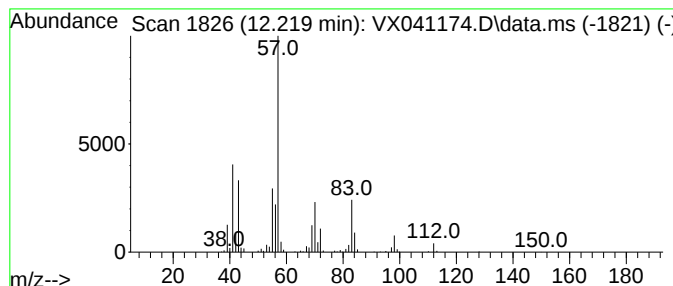
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041624W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	13.40 ug/l	210559	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			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
3			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041924\
Data File : VX041174.D
Acq On : 19 Apr 2024 13:41
Operator : JC/MD
Sample : P2121-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4827RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041624W.M
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
Propane	1.142	7.8	ug/l	88906	1	5.550	573684	50.0
1-Butene	3.690	8.0	ug/l	91216	1	5.550	573684	50.0
1-Propanol	3.922	31.9	ug/l	366522	1	5.550	573684	50.0
Butanoic acid, ...	11.683	86.5	ug/l	1359570	4	12.024	785735	50.0
1-Hexanol, 2-et...	12.219	13.4	ug/l	210559	4	12.024	785735	50.0