

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
 Data File : VX038675.D
 Acq On : 09 Nov 2023 13:09
 Operator : JC/MD
 Sample : 05287-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50131

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\82X110723W.M
 Title : SW846 8260

Signal : TIC: VX038675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	41	46	53	rBV	671420	801685	2.93%	0.718%
2	1.496	63	67	74	rVB	298637	289761	1.06%	0.259%
3	1.752	104	109	120	rVB	279186	365780	1.34%	0.328%
4	1.959	138	143	152	rVB2	142627	291577	1.07%	0.261%
5	2.099	152	166	169	rBV	8123850	21626387	79.10%	19.365%
6	2.160	172	176	180	rVV	179974	317983	1.16%	0.285%
7	2.215	180	185	194	rVB	390607	629683	2.30%	0.564%
8	2.380	206	212	230	rVB	628750	1015539	3.71%	0.909%
9	2.532	230	237	244	rBV	188222	324298	1.19%	0.290%
10	2.752	268	273	282	rVB	203527	377157	1.38%	0.338%
11	3.111	322	332	350	rBV	834945	1941515	7.10%	1.739%
12	4.556	559	569	580	rBV	98644	281729	1.03%	0.252%
13	4.715	581	595	632	rVV	3479395	9907095	36.24%	8.871%
14	5.385	694	705	713	rBV	174927	510393	1.87%	0.457%
15	5.550	724	732	753	rVB	280259	814219	2.98%	0.729%
16	5.958	788	799	803	rBV	164684	416788	1.52%	0.373%
17	6.044	803	813	834	rVV	5451014	14852782	54.33%	13.300%
18	6.763	921	931	953	rVB	427855	1046269	3.83%	0.937%
19	7.202	993	1003	1024	rBV	234092	548531	2.01%	0.491%
20	7.452	1038	1044	1061	rVB	242731	495065	1.81%	0.443%
21	7.897	1105	1117	1137	rBV	132309	278257	1.02%	0.249%
22	8.647	1233	1240	1246	rBV	866554	1437157	5.26%	1.287%
23	8.720	1246	1252	1269	rVB	16336627	27339649	100.00%	24.481%
24	10.055	1459	1471	1483	rBV	984577	1394970	5.10%	1.249%
25	10.195	1488	1494	1505	rVV	1855856	2499340	9.14%	2.238%
26	10.299	1505	1511	1527	rVB	5816067	7892259	28.87%	7.067%
27	10.579	1552	1557	1562	rBV	311832	430798	1.58%	0.386%
28	10.640	1562	1567	1582	rVB	3216360	4130492	15.11%	3.699%
29	11.079	1634	1639	1651	rVB	917112	1178164	4.31%	1.055%
30	11.378	1683	1688	1696	rVV	701575	1169686	4.28%	1.047%
31	11.451	1696	1700	1711	rVB	315724	387470	1.42%	0.347%
32	11.610	1721	1726	1733	rBV	329559	422797	1.55%	0.379%
33	11.750	1745	1749	1756	rVB	1373768	1677167	6.13%	1.502%
34	12.018	1788	1793	1800	rBV	1268162	1587255	5.81%	1.421%
35	12.085	1800	1804	1810	rVB	503915	607178	2.22%	0.544%
36	12.244	1822	1830	1838	rBV2	440689	694356	2.54%	0.622%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

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\82X110723W.M
Title : SW846 8260

37	13.292	1997	2002	2007	rVB2	340112	437725	1.60%	0.392%
38	13.774	2074	2081	2088	rVB	506589	637678	2.33%	0.571%
39	14.225	2149	2155	2163	rBV	160556	283147	1.04%	0.254%
40	14.634	2214	2222	2226	rBV2	205277	337591	1.23%	0.302%

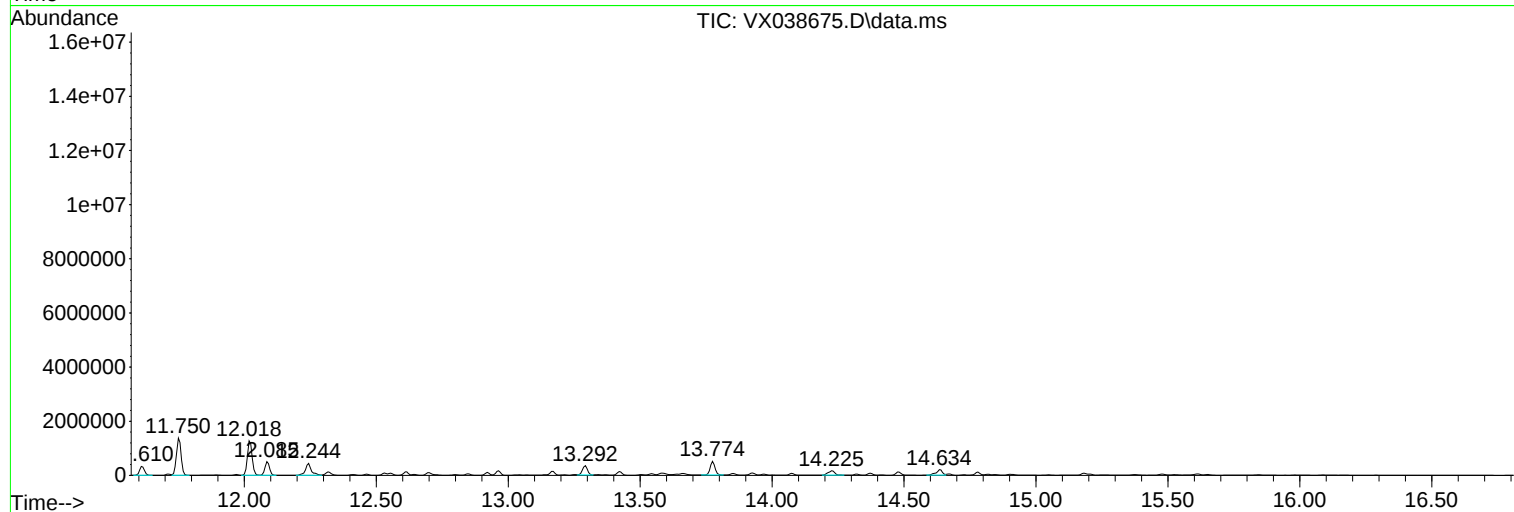
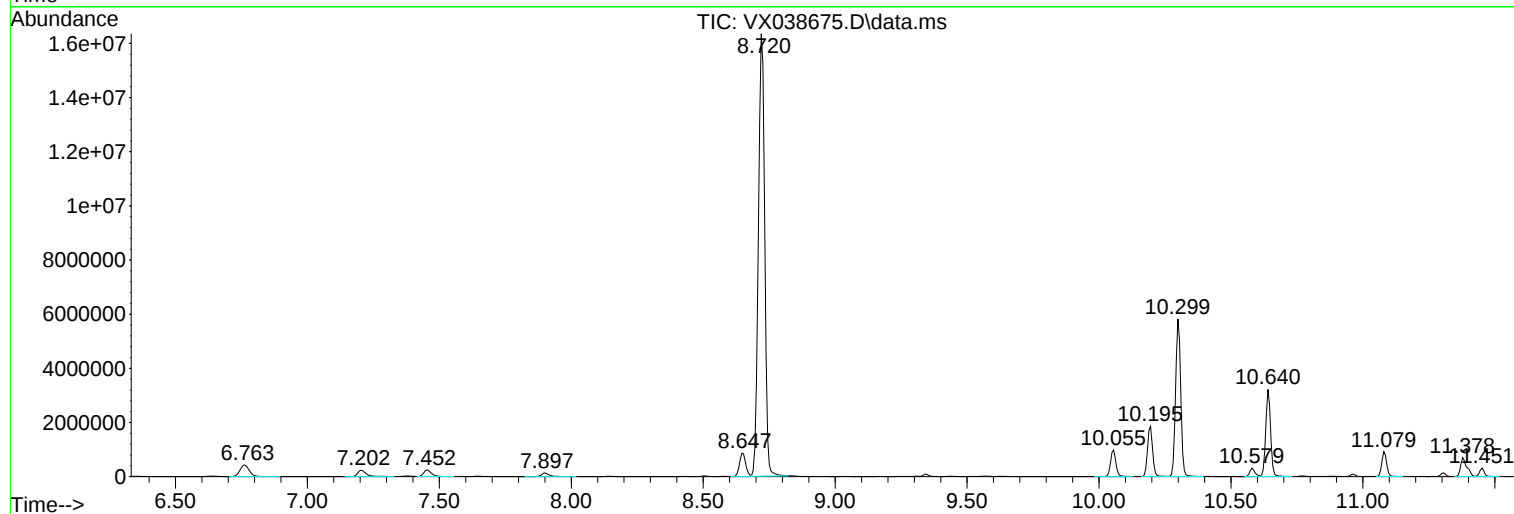
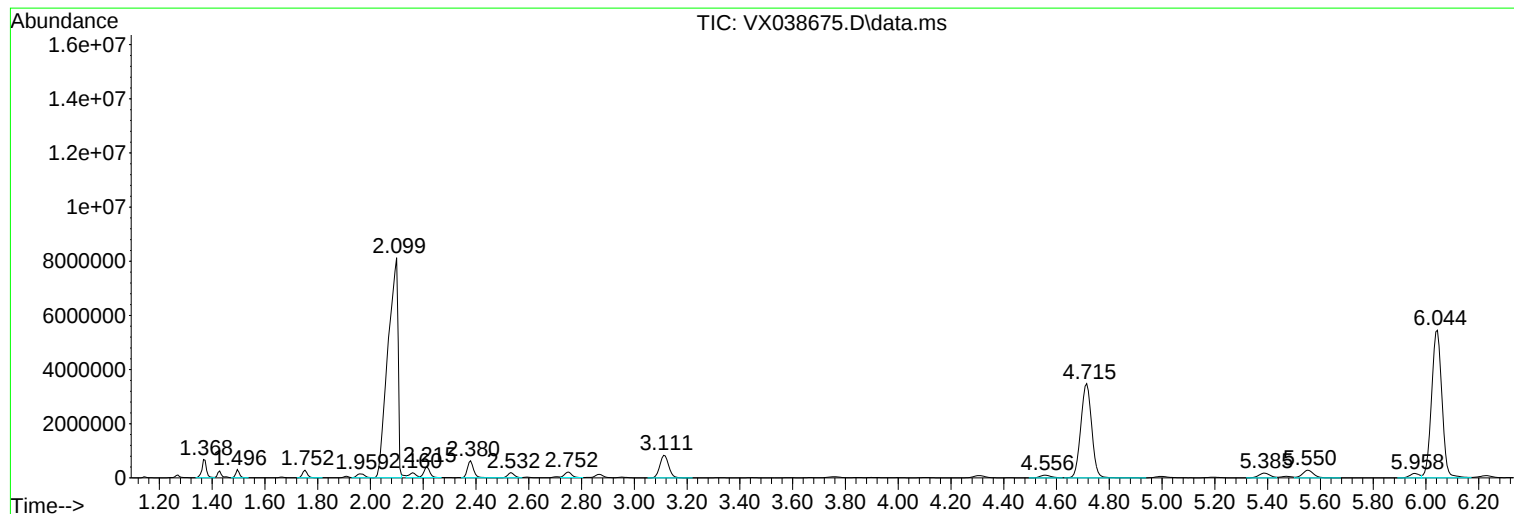
Sum of corrected areas: 111677372

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

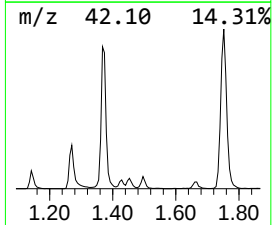
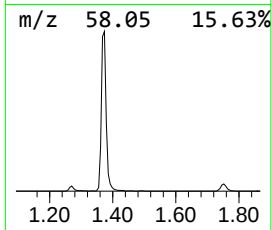
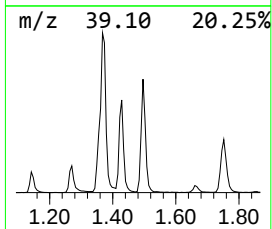
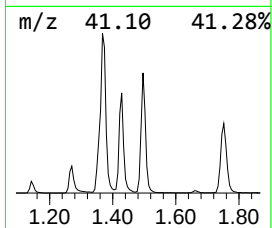
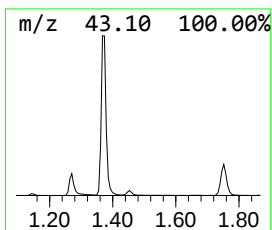
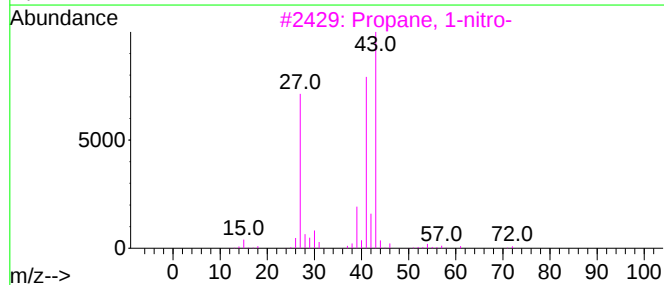
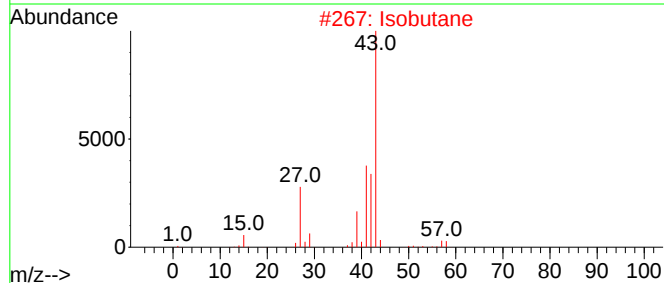
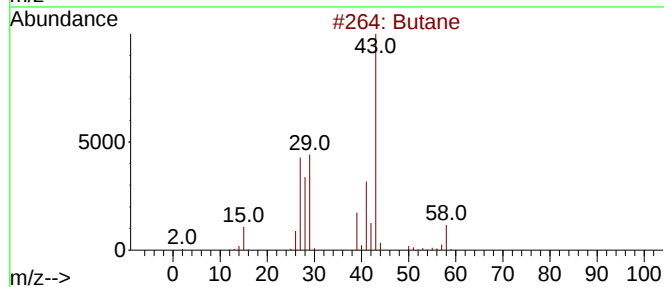
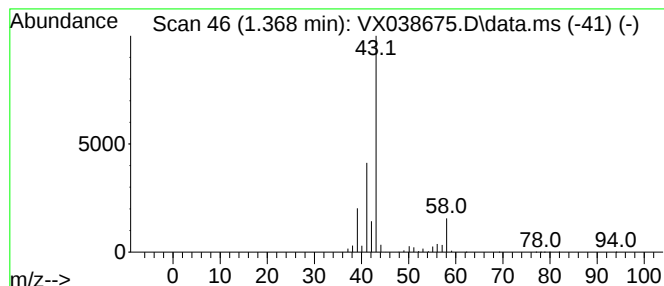
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	49.23 ug/l	801685	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	72
2	Isobutane			58	C4H10	000075-28-5	9
3	Propane, 1-nitro-			89	C3H7NO2	000108-03-2	9
4	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
5	Acetone			58	C3H6O	000067-64-1	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

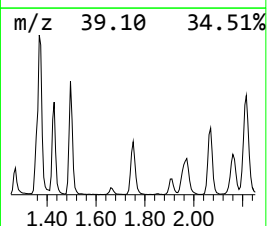
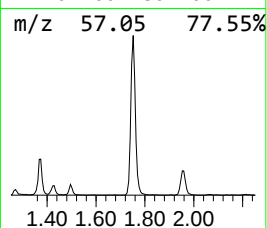
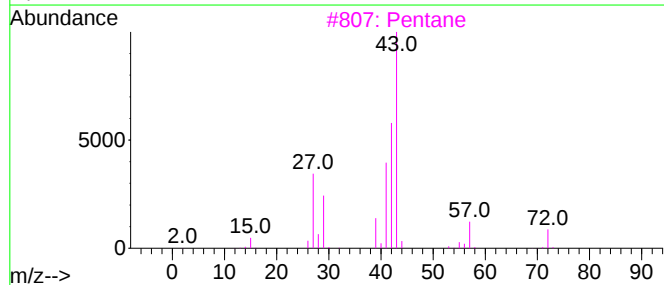
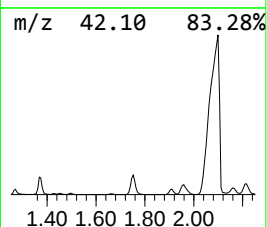
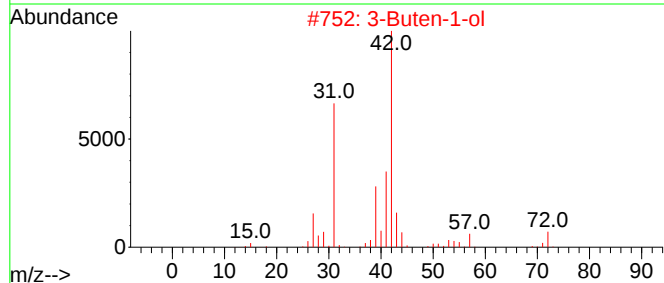
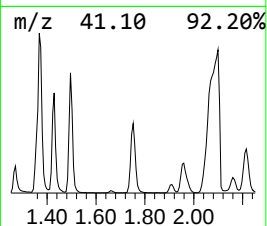
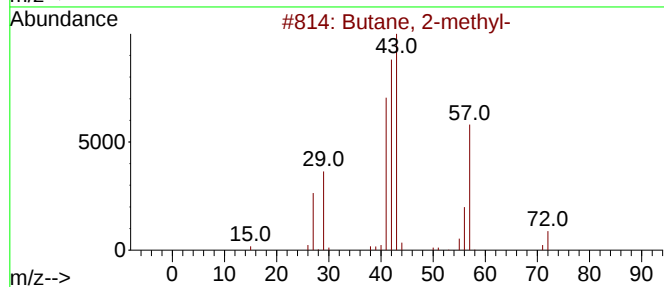
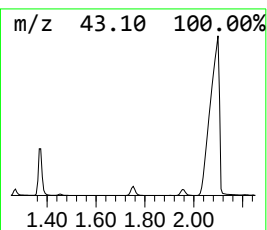
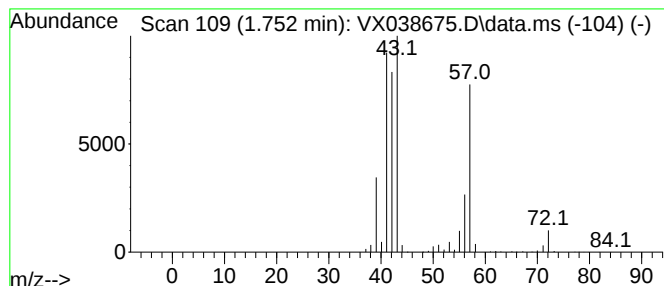
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	22.46 ug/l	365780	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	42
4			Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
5			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

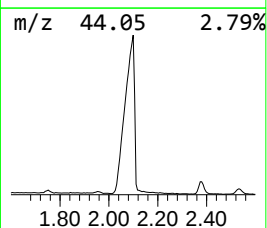
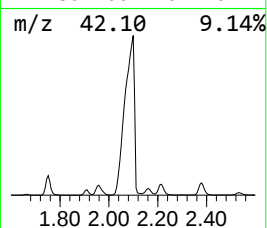
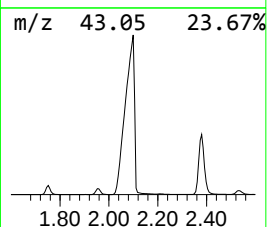
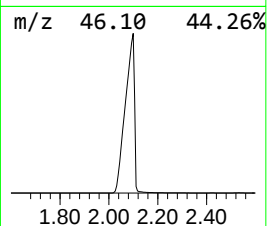
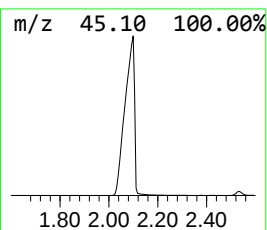
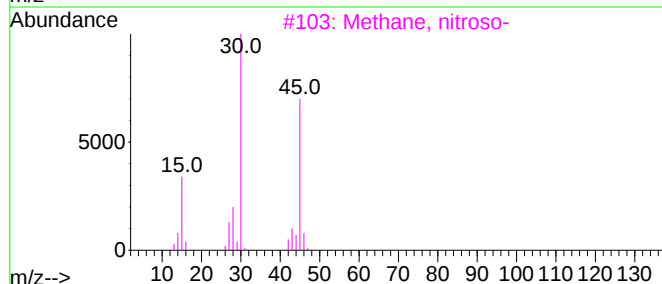
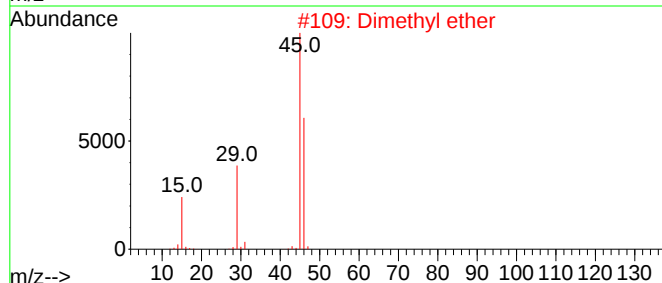
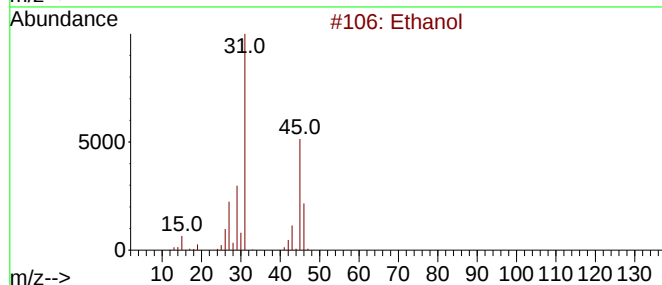
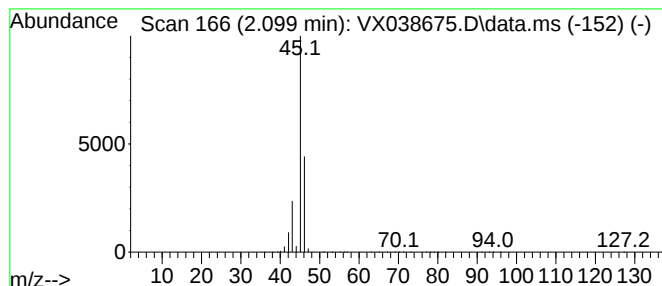
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	1328.04 ug/l	21626400	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	86
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			L-Lactic acid	90	C3H6O3	000079-33-4	2



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

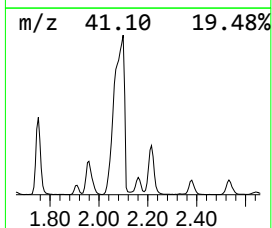
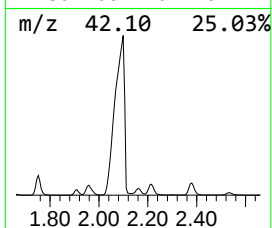
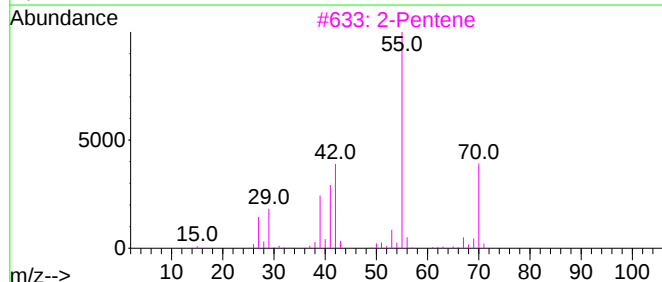
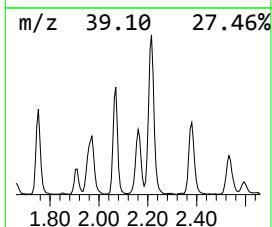
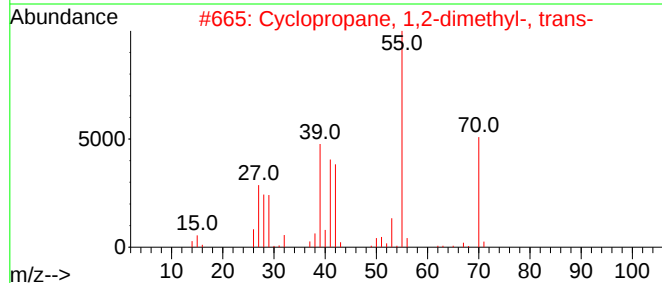
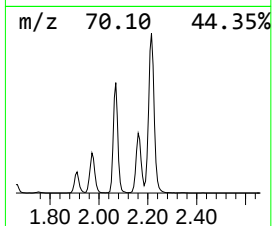
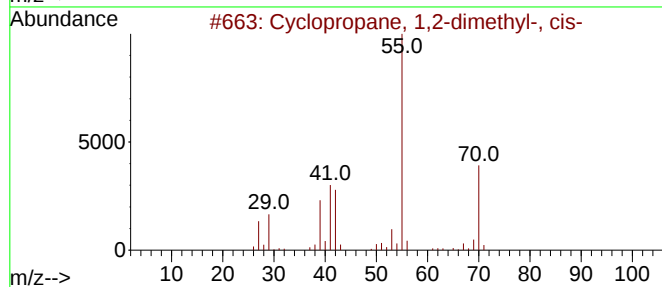
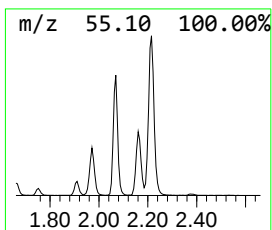
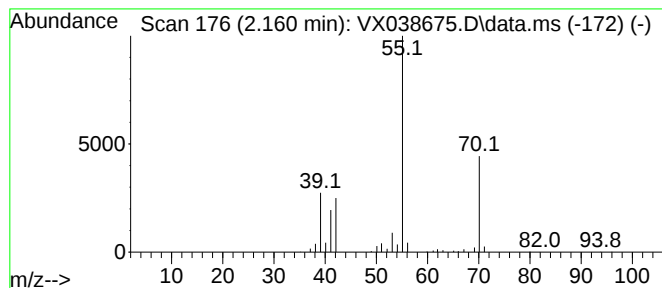
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.160	19.53 ug/l	317983	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86
3			2-Pentene	70	C5H10	000109-68-2	86
4			2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
5			2-Pentene, (E)-	70	C5H10	000646-04-8	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

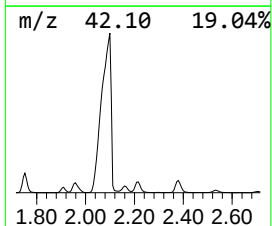
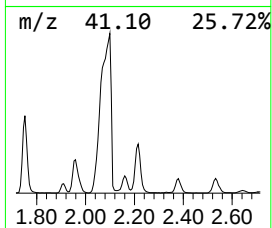
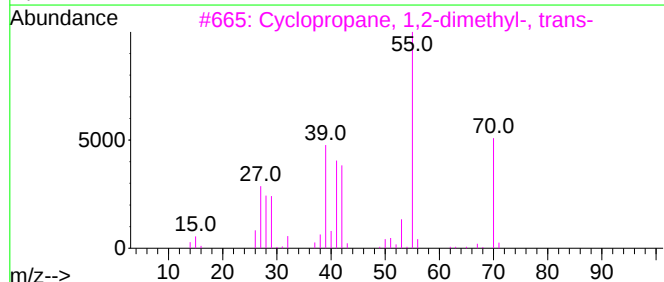
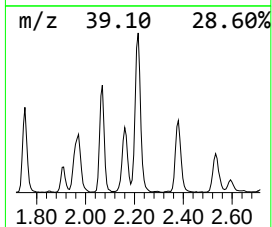
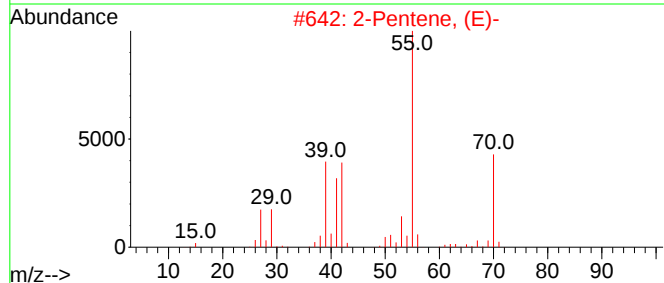
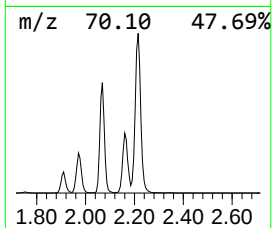
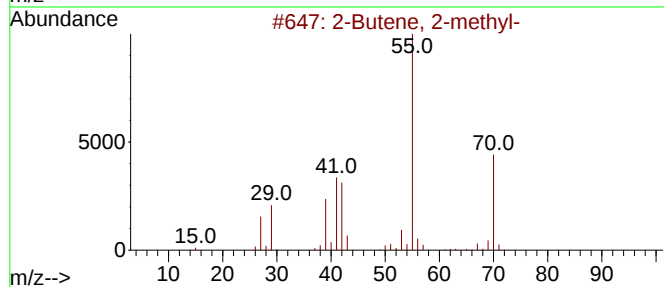
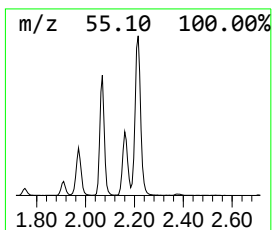
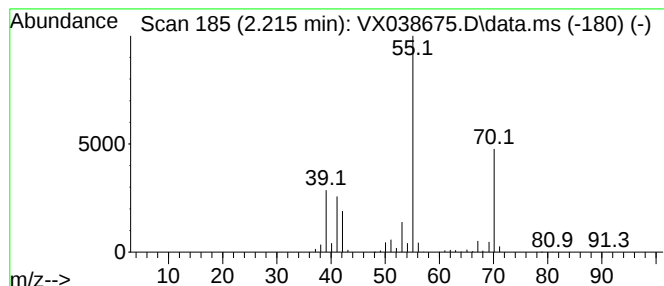
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 5 2-Butene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	38.67 ug/l	629683	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2			2-Pentene, (E)-	70	C5H10	000646-04-8	87
3			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
4			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	81
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

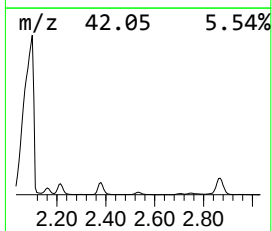
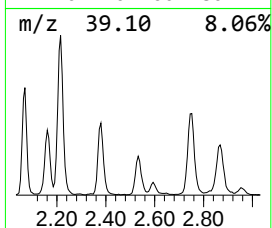
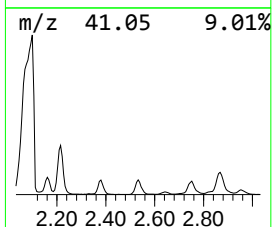
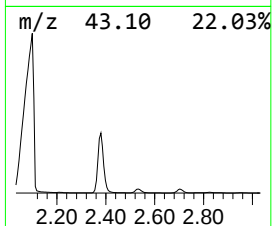
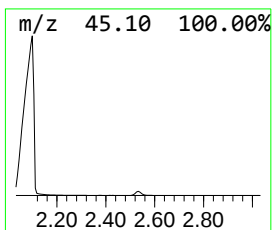
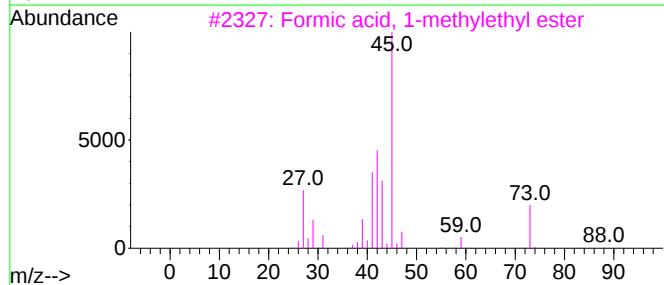
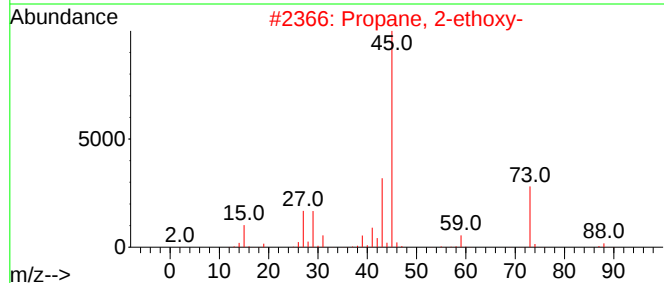
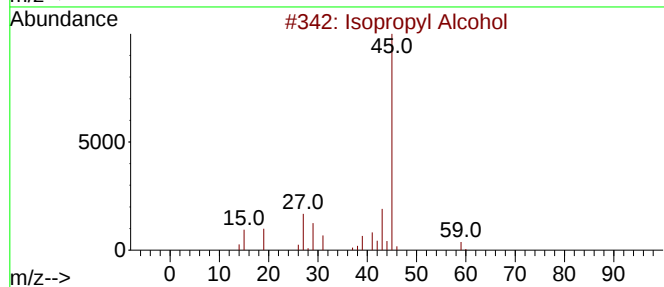
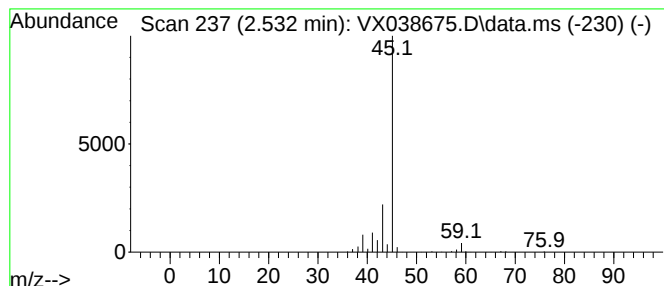
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 6 Isopropyl Alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	19.91 ug/l	324298	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
3			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

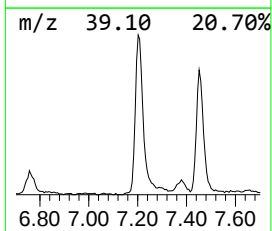
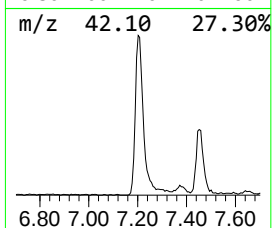
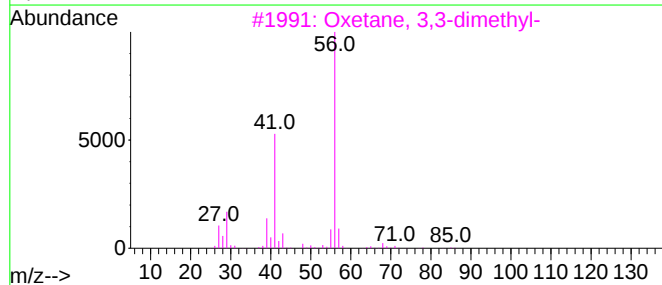
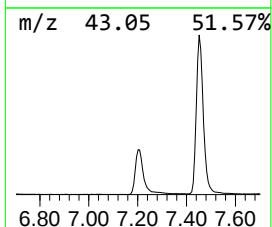
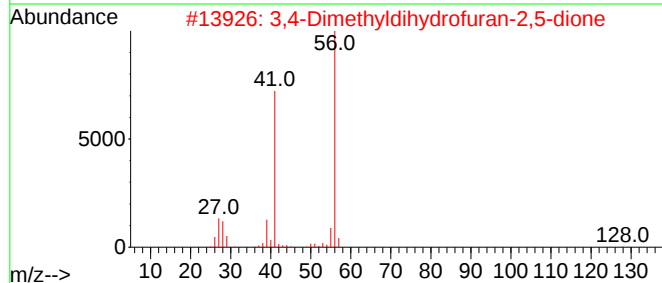
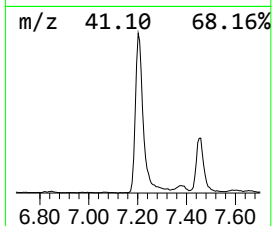
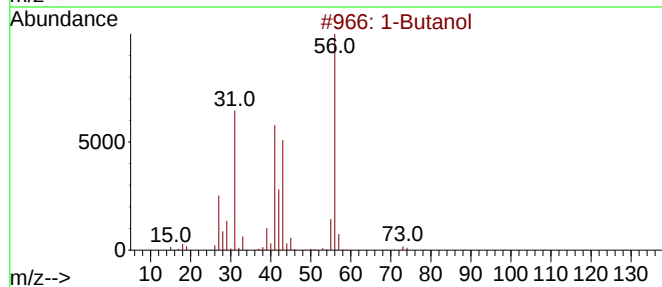
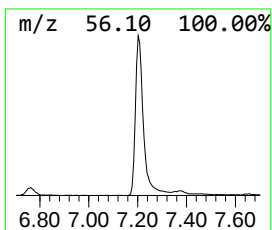
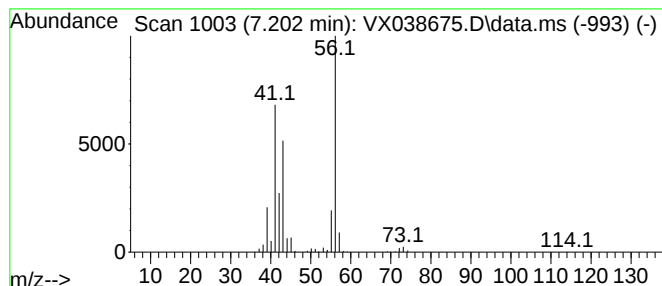
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.202	26.21 ug/l	548531	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	86
2	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	40
3	Oxetane, 3,3-dimethyl-			86	C5H10O	006921-35-3	38
4	Butane, 1-chloro-			92	C4H9Cl	000109-69-3	9
5	Formic acid, butyl ester			102	C5H10O2	000592-84-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

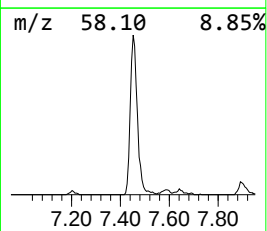
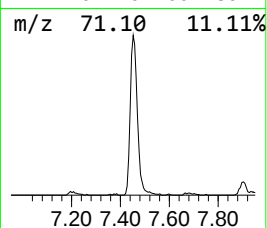
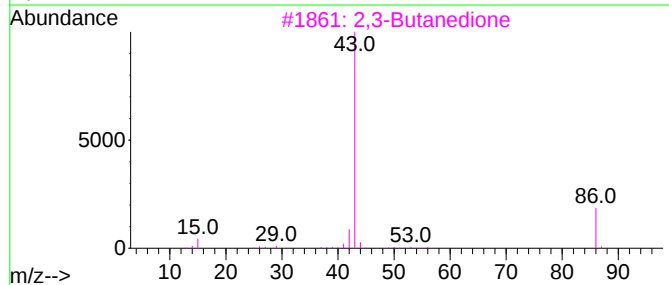
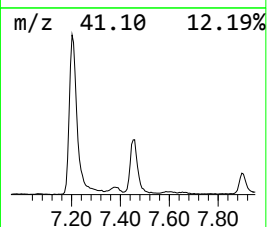
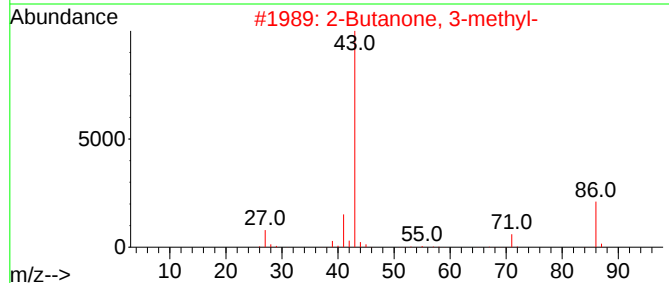
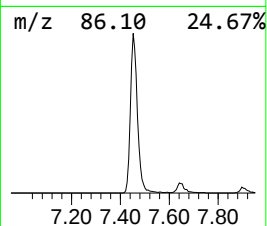
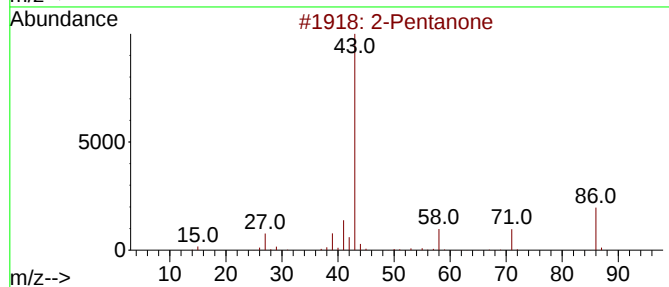
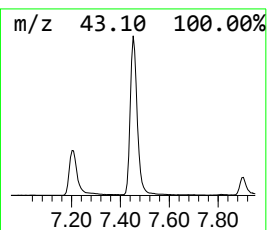
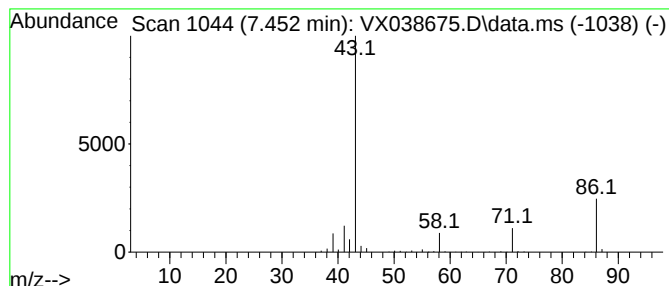
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 8 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.452	23.66 ug/l	495065	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	87
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3			2,3-Butanedione	86	C4H6O2	000431-03-8	37
4			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9
5			2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

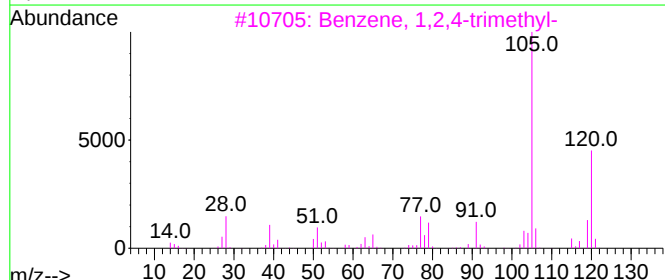
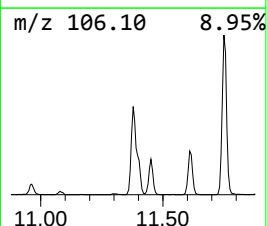
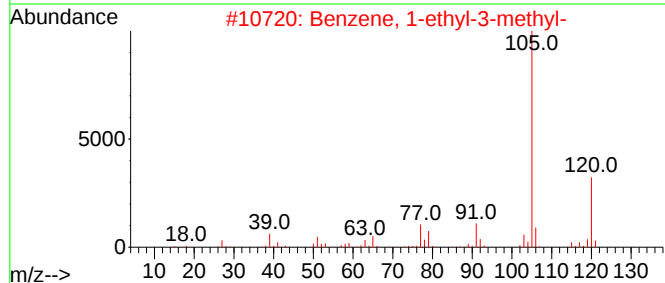
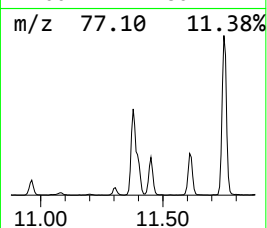
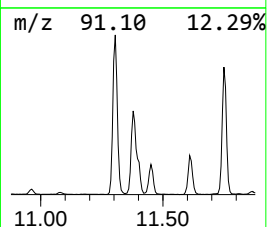
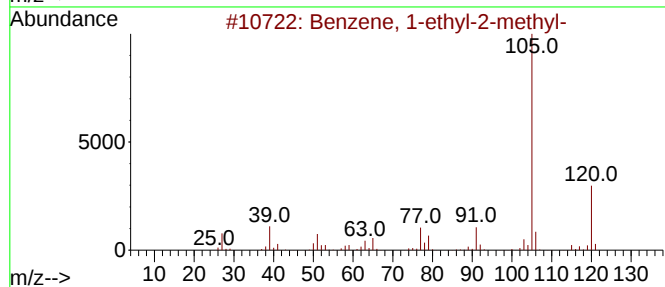
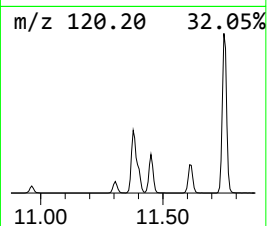
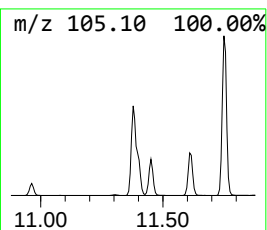
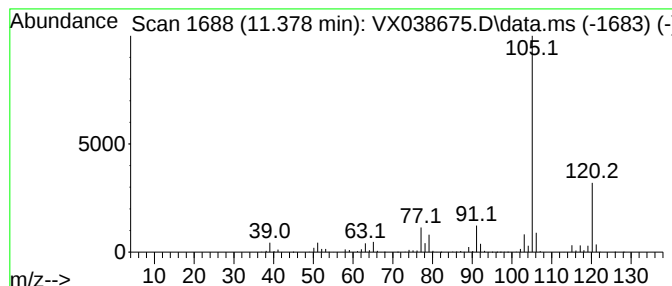
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	36.85 ug/l	1169690	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

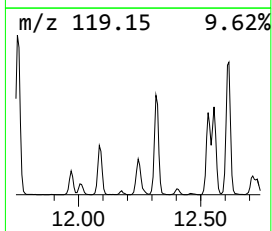
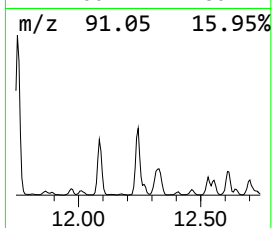
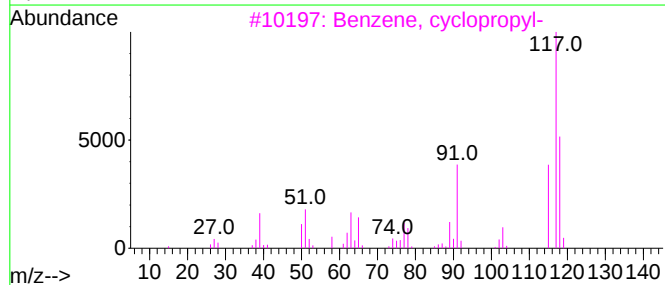
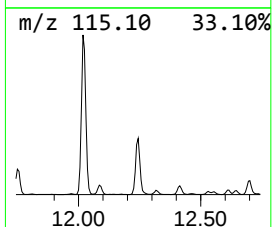
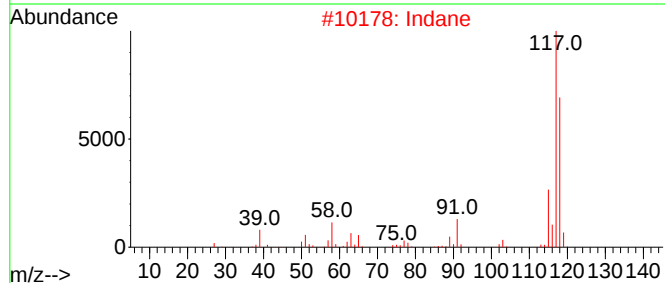
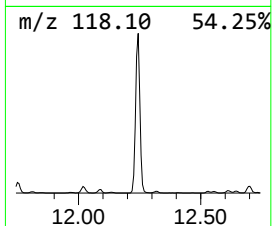
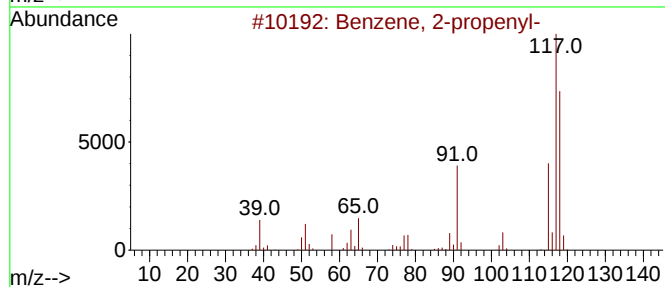
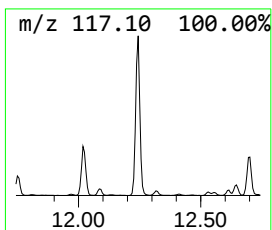
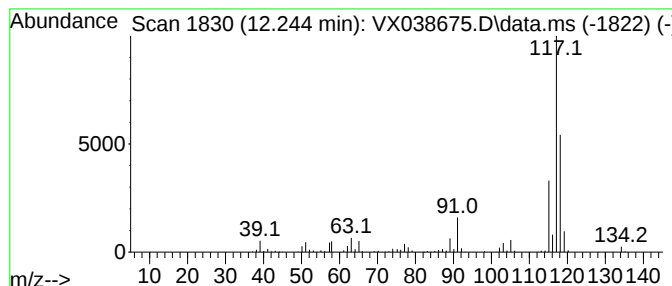
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-propenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	21.87 ug/l	694356	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
2			Indane	118	C9H10	000496-11-7	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
Data File : VX038675.D
Acq On : 09 Nov 2023 13:09
Operator : JC/MD
Sample : 05287-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.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
Butane	1.368	49.2	ug/l	801685	1	5.556	814219	50.0
Butane, 2-methyl-	1.752	22.5	ug/l	365780	1	5.556	814219	50.0
Ethanol	2.099	1328.0	ug/l	21626400	1	5.556	814219	50.0
Cyclopropane, 1...	2.160	19.5	ug/l	317983	1	5.556	814219	50.0
2-Butene, 2-met...	2.215	38.7	ug/l	629683	1	5.556	814219	50.0
Isopropyl Alcohol	2.532	19.9	ug/l	324298	1	5.556	814219	50.0
1-Butanol	7.202	26.2	ug/l	548531	2	6.763	1046270	50.0
2-Pentanone	7.452	23.7	ug/l	495065	2	6.763	1046270	50.0
Benzene, 1-ethy...	11.378	36.9	ug/l	1169690	4	12.018	1587260	50.0
Benzene, 2-prop...	12.244	21.9	ug/l	694356	4	12.018	1587260	50.0