

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012623\
 Data File : VX033919.D
 Acq On : 26 Jan 2023 19:01
 Operator : JC/MD
 Sample : 01321-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 33902

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\82X011123W.M
 Title : SW846 8260

Signal : TIC: VX033919.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	65	rBV	344202	389344	3.44%	0.905%
2	2.063	151	160	174	rBV	2301605	4645766	41.04%	10.802%
3	2.374	202	211	223	rVB	177204	291252	2.57%	0.677%
4	2.520	227	235	253	rBV	398934	753308	6.65%	1.752%
5	3.111	323	332	345	rVB	59936	142165	1.26%	0.331%
6	5.385	692	705	714	rBV	81598	237869	2.10%	0.553%
7	5.550	723	732	751	rVB	147580	426272	3.77%	0.991%
8	5.952	787	798	804	rBV	81954	220728	1.95%	0.513%
9	6.038	804	812	828	rVB	804883	2115937	18.69%	4.920%
10	6.757	921	930	943	rBV	211273	513920	4.54%	1.195%
11	8.647	1234	1240	1245	rBV	443335	692894	6.12%	1.611%
12	8.720	1245	1252	1271	rVB	7239788	11320688	100.00%	26.322%
13	10.055	1465	1471	1481	rBV	433397	595159	5.26%	1.384%
14	10.195	1488	1494	1505	rBV	1283007	1718182	15.18%	3.995%
15	10.299	1505	1511	1529	rVB	4565478	6213819	54.89%	14.448%
16	10.640	1561	1567	1583	rVB	2805976	3595466	31.76%	8.360%
17	10.964	1614	1620	1623	rBV	110941	144108	1.27%	0.335%
18	11.079	1634	1639	1649	rVB	381622	483866	4.27%	1.125%
19	11.305	1669	1676	1683	rBV	141748	176862	1.56%	0.411%
20	11.378	1683	1688	1696	rVV	836424	1395996	12.33%	3.246%
21	11.451	1696	1700	1714	rVB	388236	472957	4.18%	1.100%
22	11.610	1721	1726	1739	rBV	426242	514012	4.54%	1.195%
23	11.750	1744	1749	1756	rBV	1513065	1804600	15.94%	4.196%
24	12.024	1788	1794	1799	rVB	470617	604437	5.34%	1.405%
25	12.085	1799	1804	1816	rVB	570949	691672	6.11%	1.608%
26	12.244	1821	1830	1838	rBV3	394351	665617	5.88%	1.548%
27	12.317	1838	1842	1852	rVB3	127037	183776	1.62%	0.427%
28	12.610	1886	1890	1894	rBV	128789	161627	1.43%	0.376%
29	12.701	1900	1905	1913	rBV2	75108	123318	1.09%	0.287%
30	12.963	1944	1948	1954	rVB	137538	172774	1.53%	0.402%
31	13.170	1977	1982	1986	rVB	102559	128736	1.14%	0.299%
32	13.292	1997	2002	2007	rVB2	243355	318426	2.81%	0.740%
33	13.420	2019	2023	2032	rVB	116797	151627	1.34%	0.353%
34	13.774	2075	2081	2088	rVB	216096	271873	2.40%	0.632%
35	14.231	2149	2156	2160	rBV	151593	252639	2.23%	0.587%
36	14.481	2192	2197	2207	rBV2	118457	173459	1.53%	0.403%

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Instrument :
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ClientSampleId :
33902

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\82X011123W.M
Title : SW846 8260

37	14.634	2215	2222	2226	rBV2	134690	243652	2.15%	0.567%
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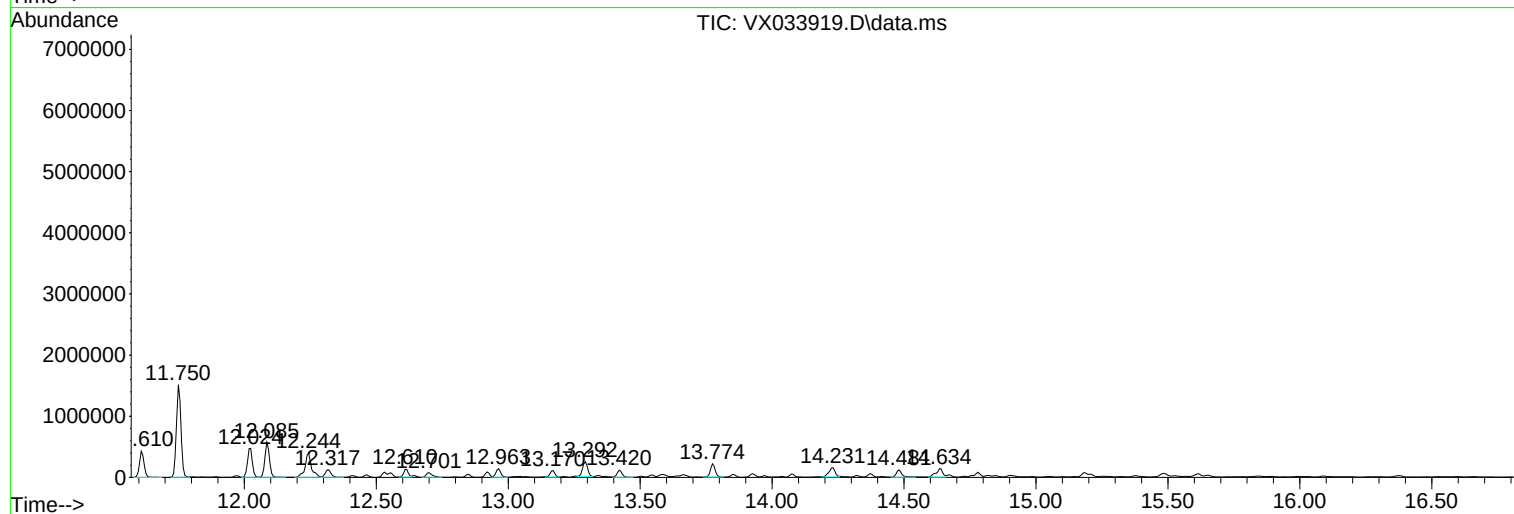
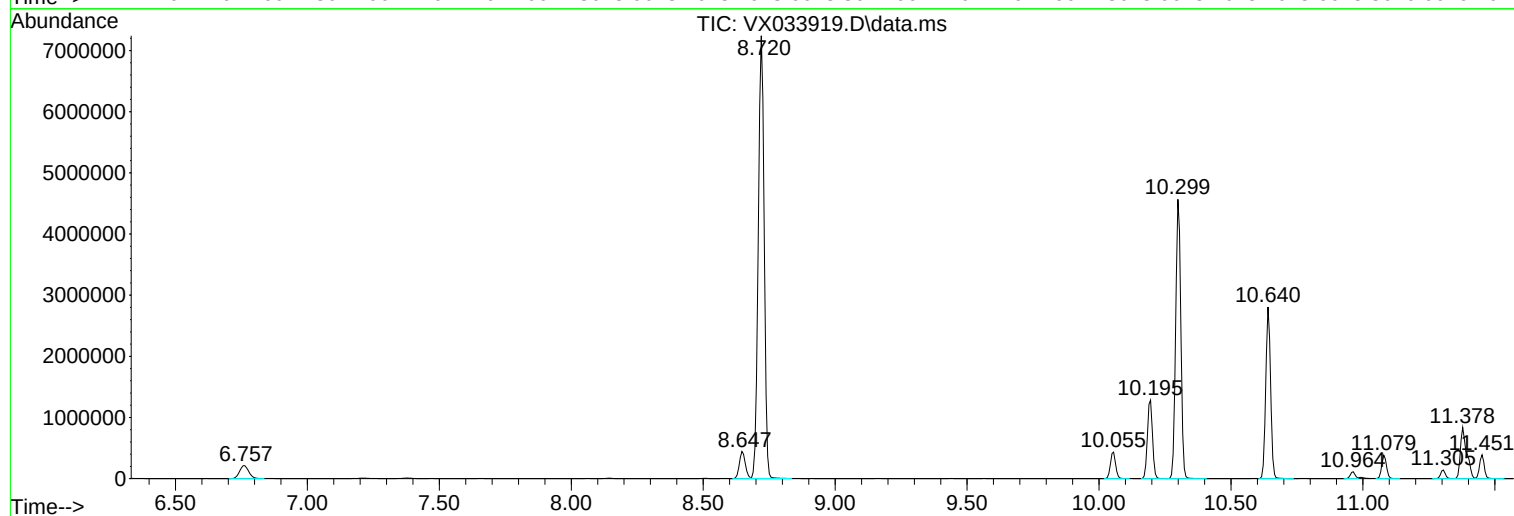
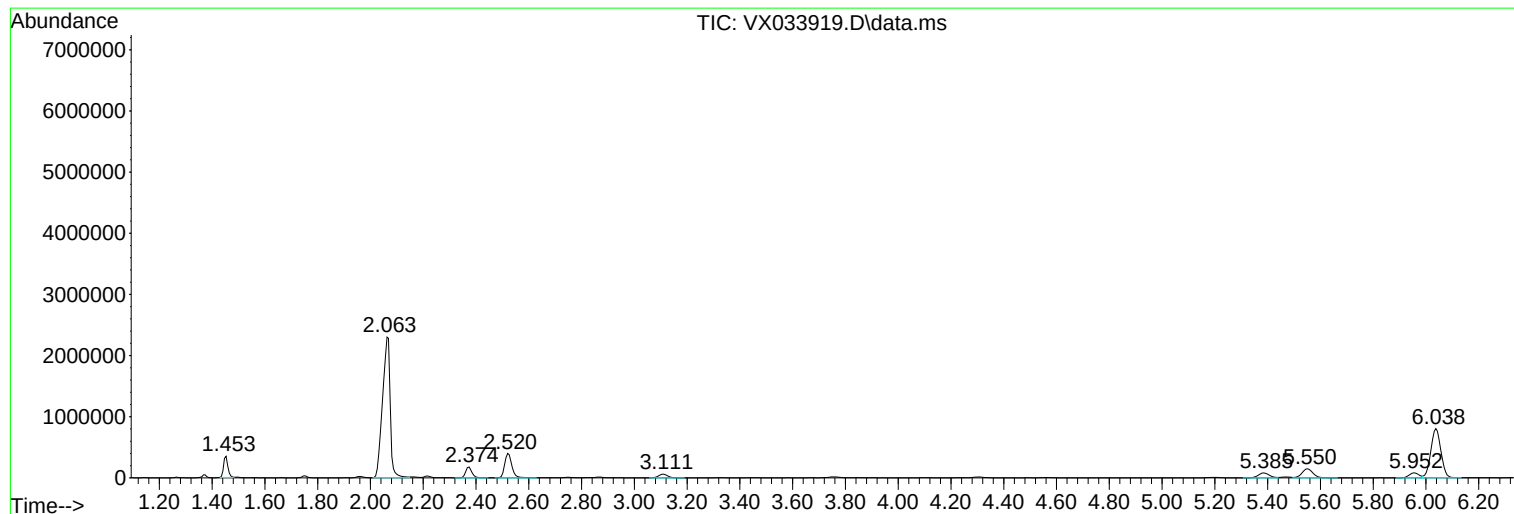
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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



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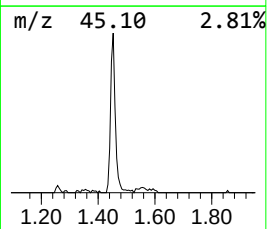
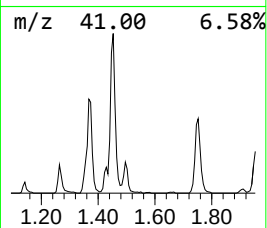
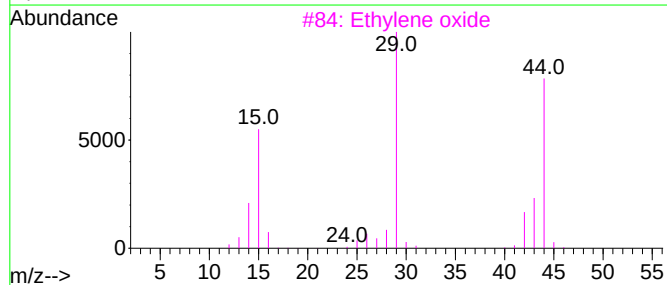
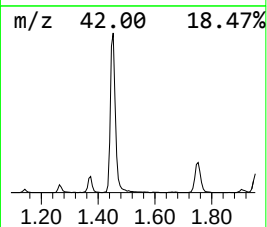
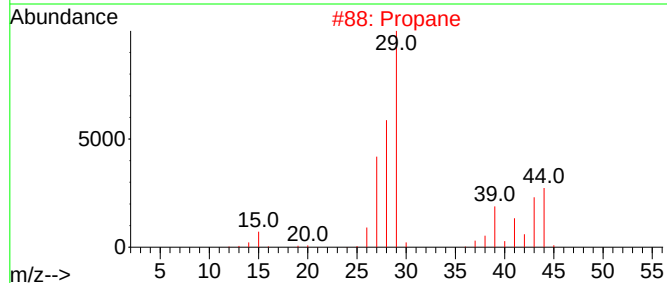
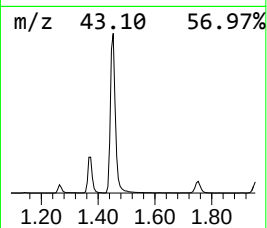
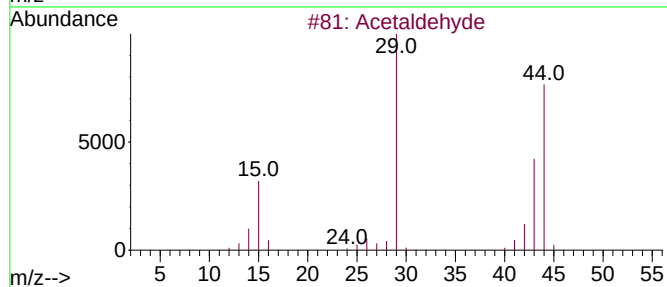
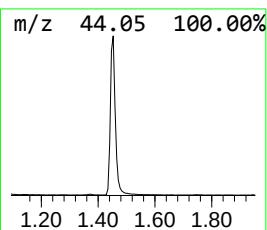
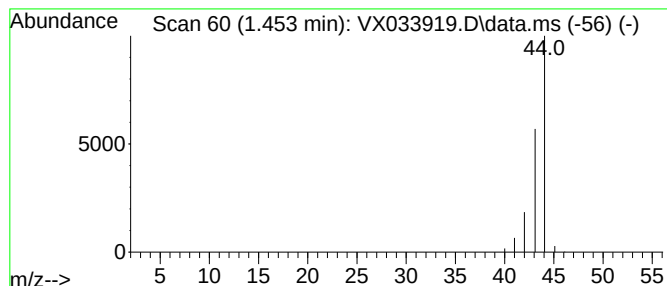
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	45.67 ug/l	389344	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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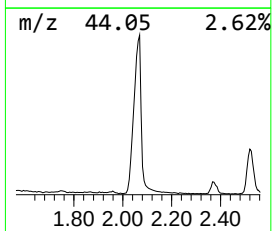
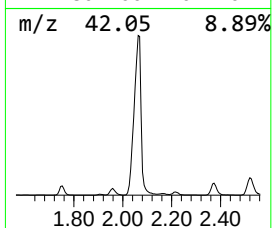
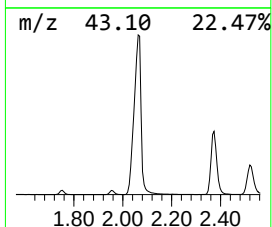
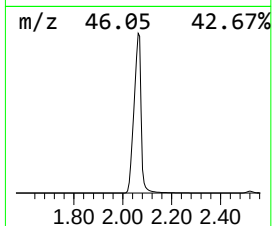
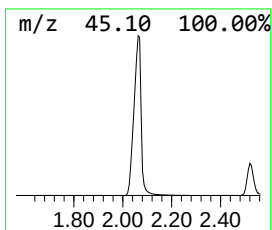
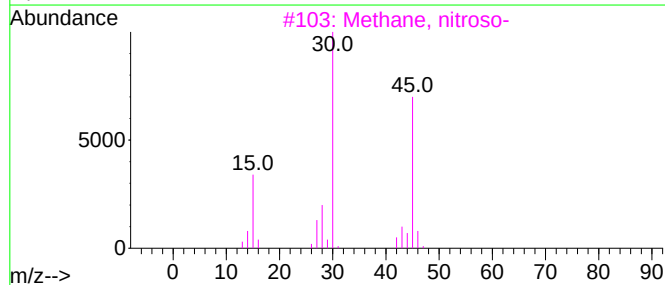
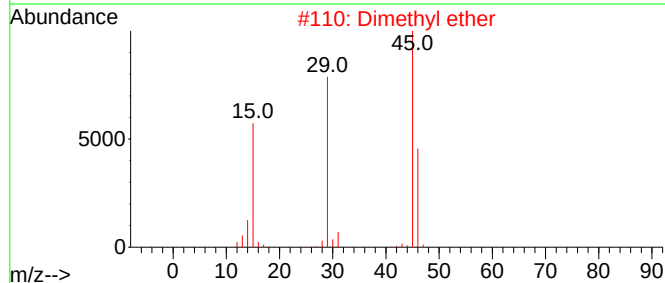
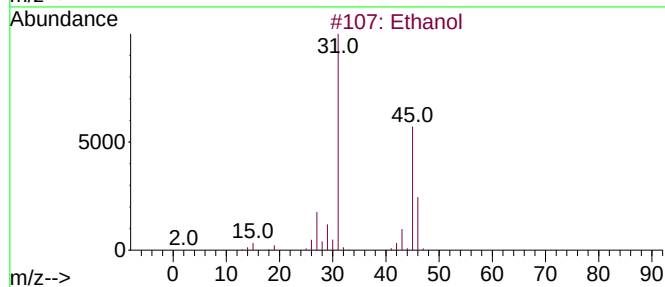
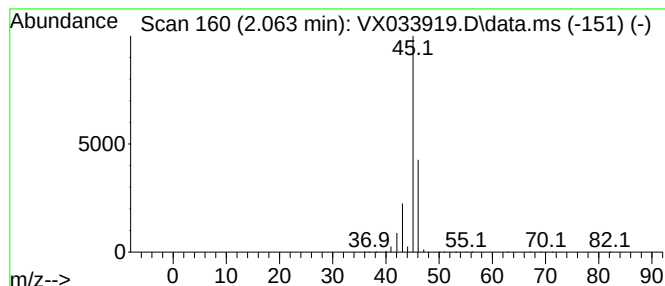
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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	544.93 ug/l	4645770	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	78
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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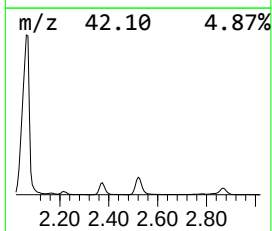
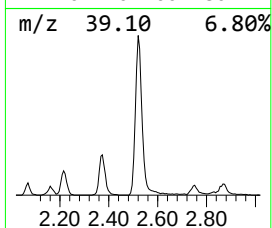
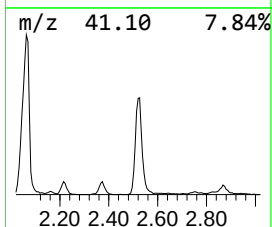
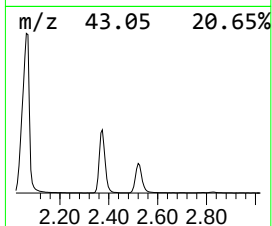
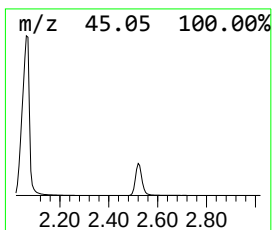
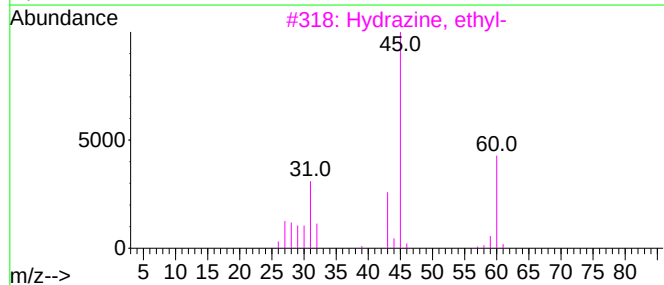
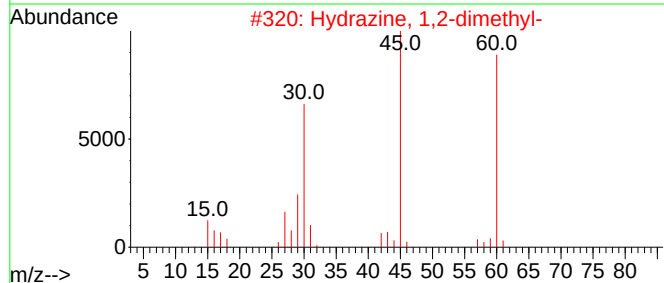
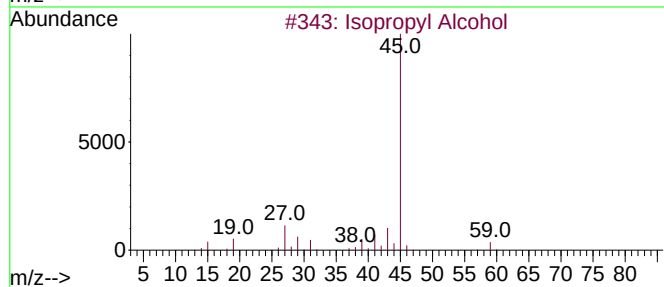
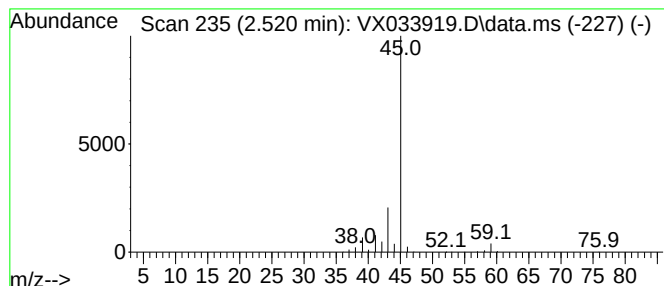
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.520	88.36 ug/l	753308	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4			Formamide	45	CH3NO	000075-12-7	5
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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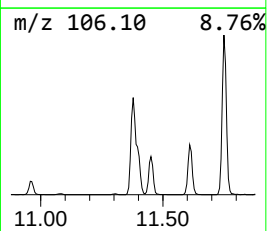
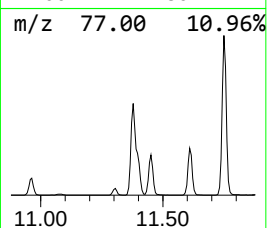
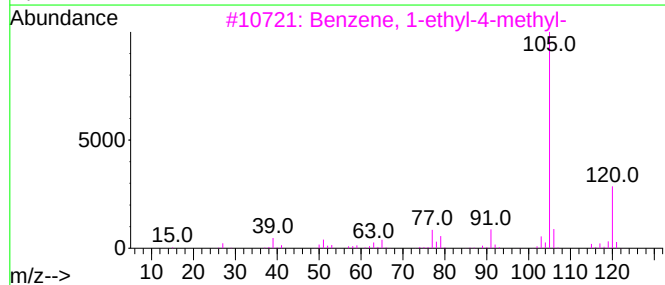
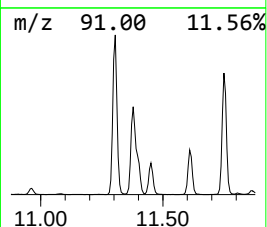
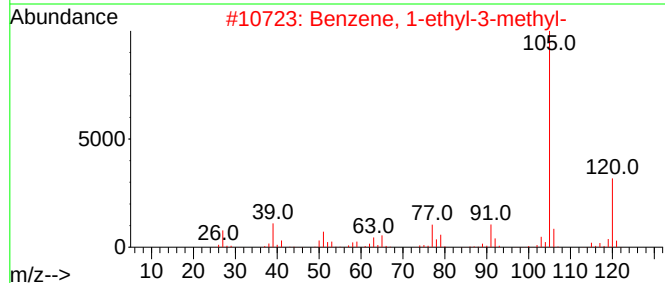
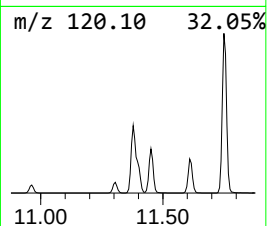
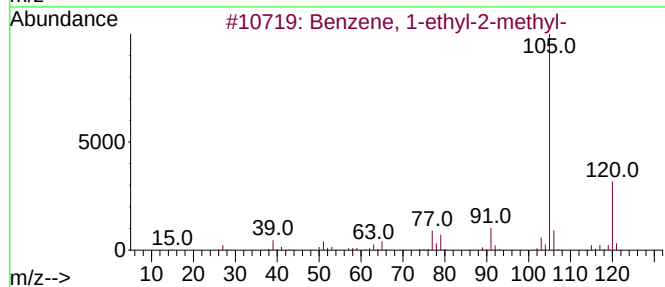
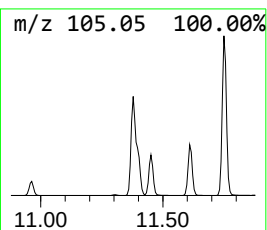
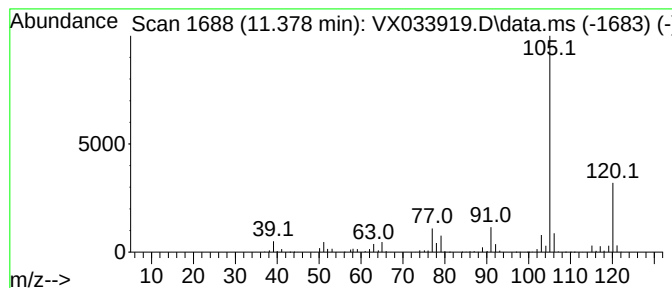
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	115.48 ug/l	1396000	1,4-Dichlorobenzene-d4	12.024

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-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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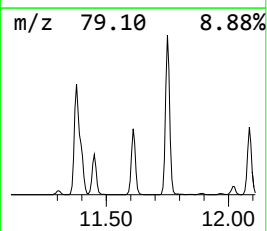
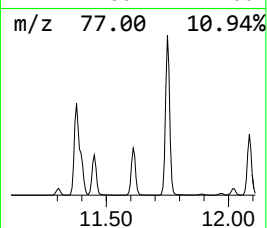
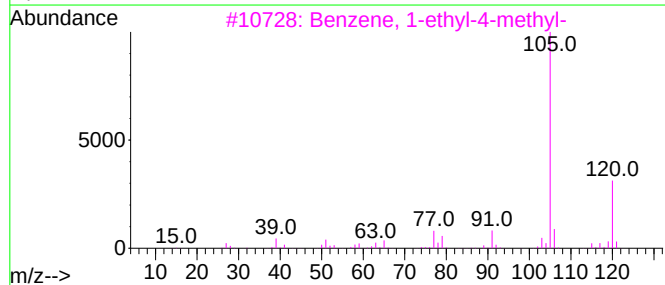
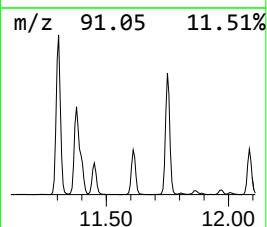
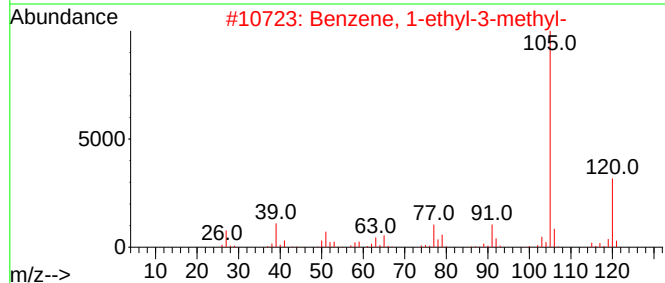
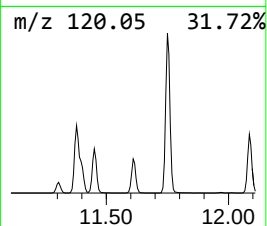
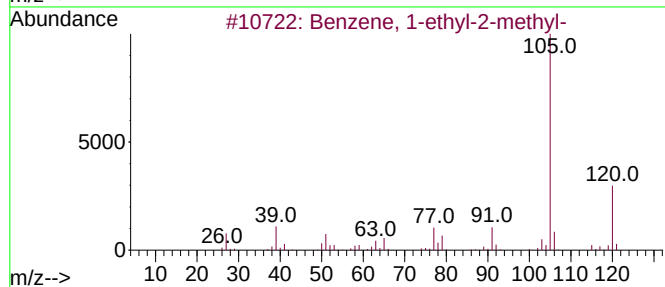
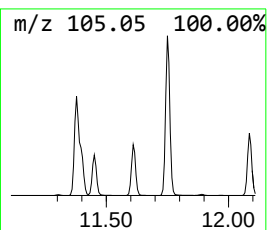
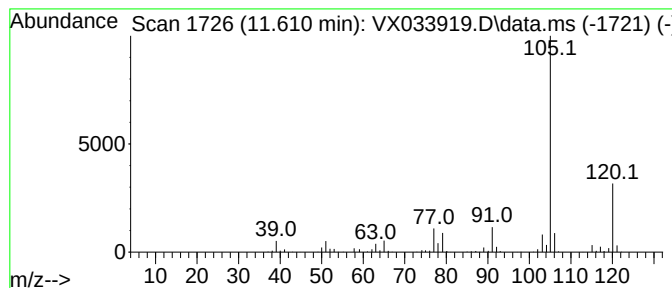
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	42.52 ug/l	514012	1,4-Dichlorobenzene-d4	12.024

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	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012623\
Data File : VX033919.D
Acq On : 26 Jan 2023 19:01
Operator : JC/MD
Sample : 01321-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33902

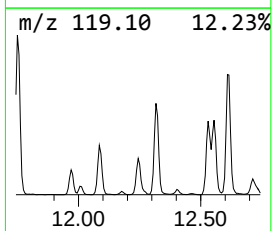
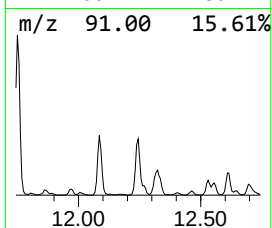
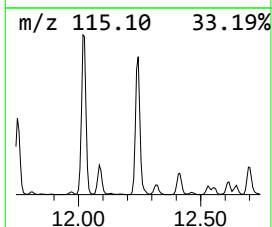
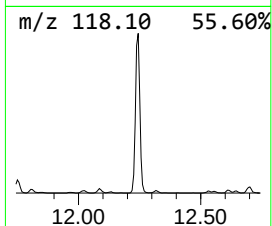
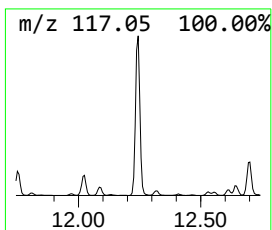
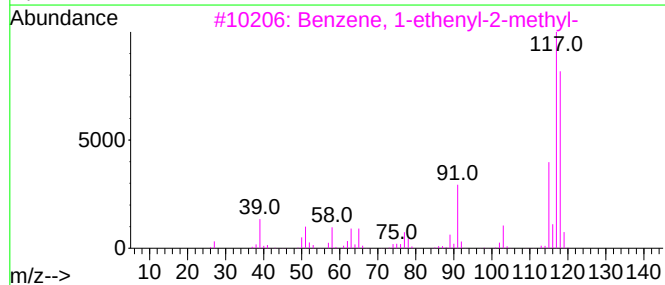
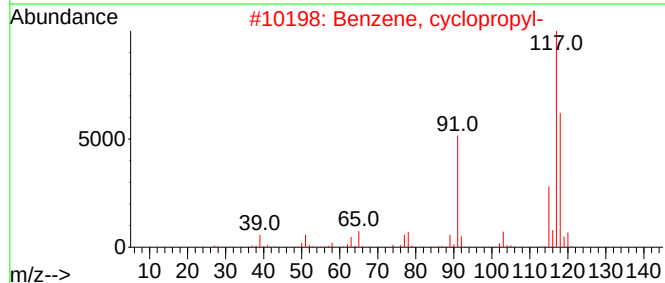
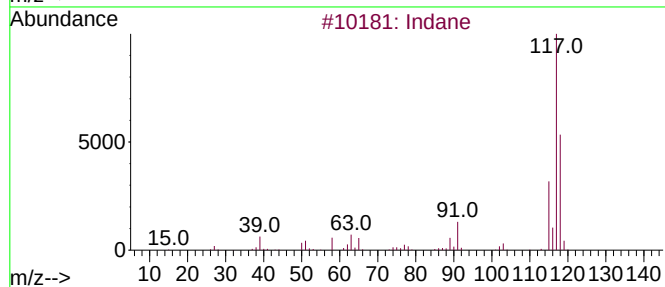
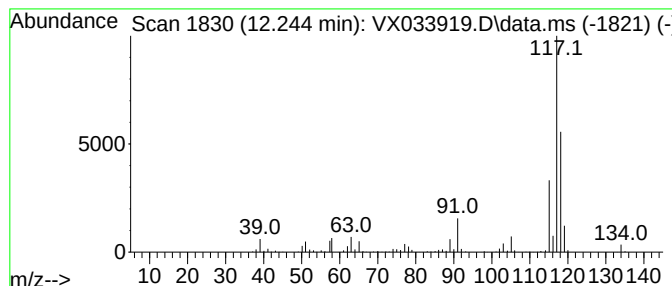
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	55.06 ug/l	665617	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	81
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
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\VX012623\
Data File : VX033919.D
Acq On : 26 Jan 2023 19:01
Operator : JC/MD
Sample : 01321-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33902

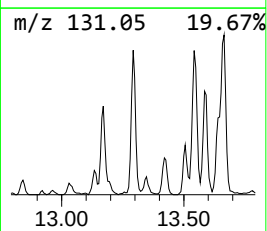
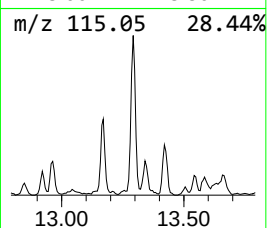
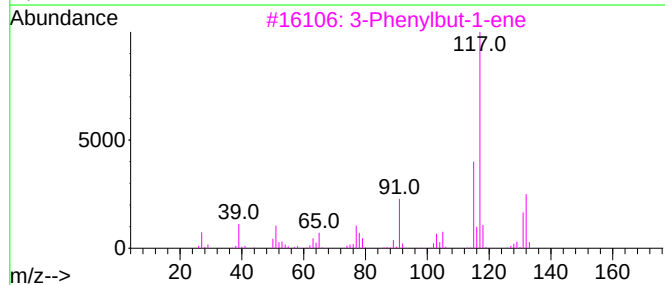
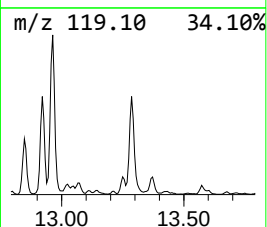
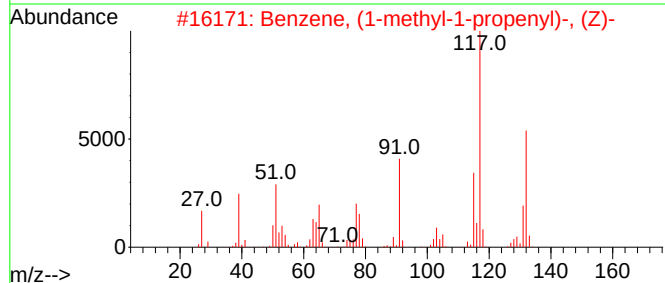
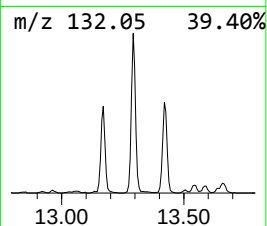
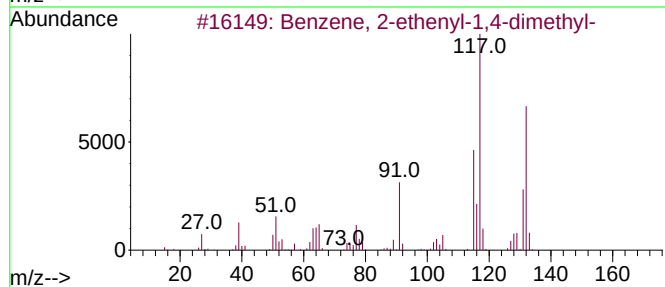
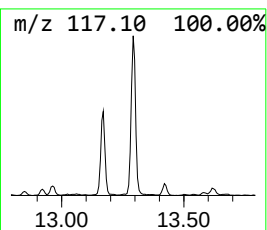
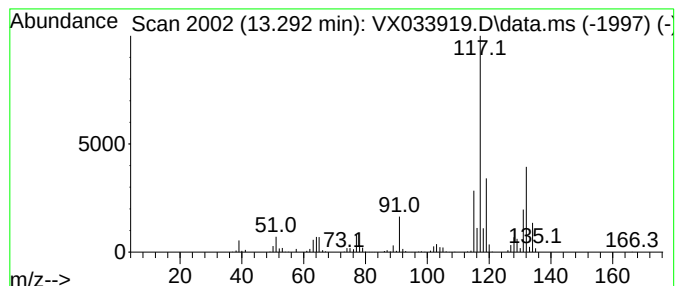
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	26.34 ug/l	318426	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	83
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	80
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	80
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012623\
Data File : VX033919.D
Acq On : 26 Jan 2023 19:01
Operator : JC/MD
Sample : 01321-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33902

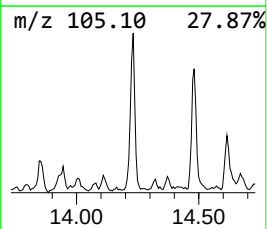
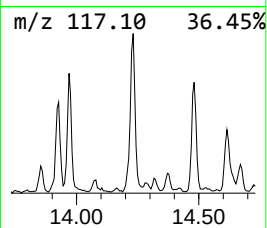
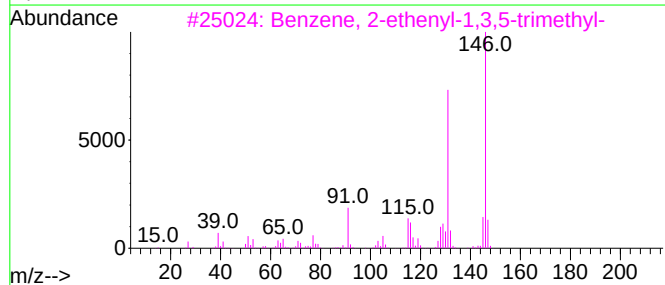
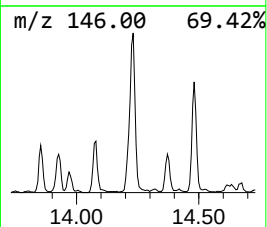
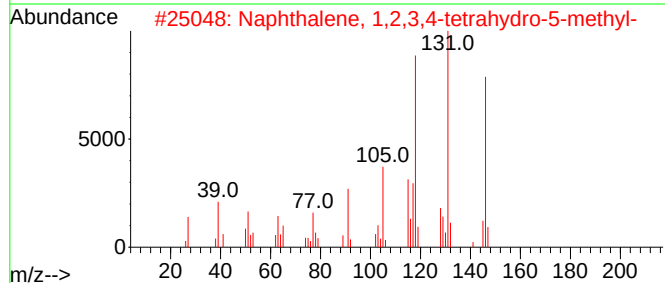
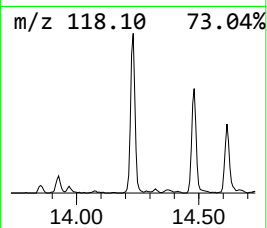
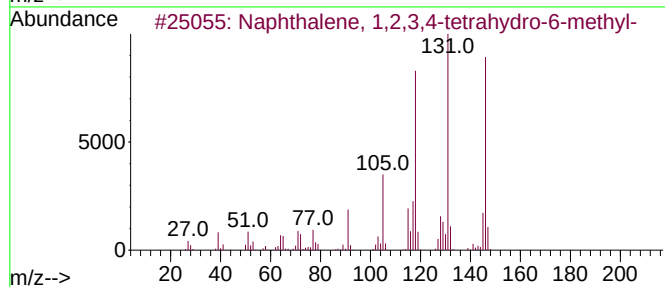
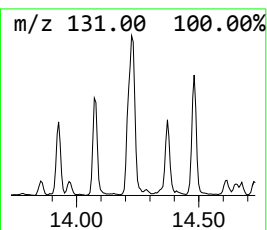
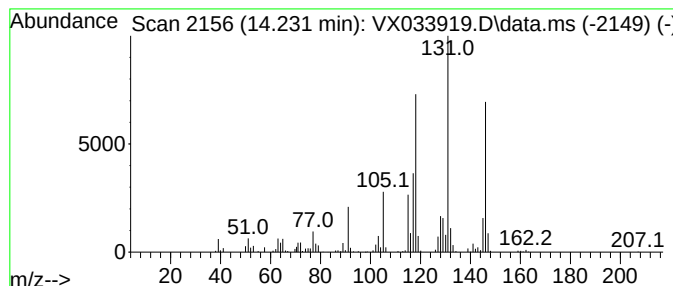
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	20.90 ug/l	252639	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	97
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	96
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	86
4			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	76
5			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX012623\
Data File : VX033919.D
Acq On : 26 Jan 2023 19:01
Operator : JC/MD
Sample : 01321-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33902

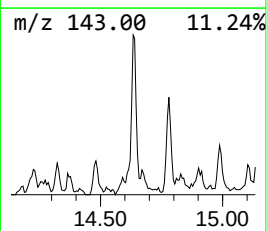
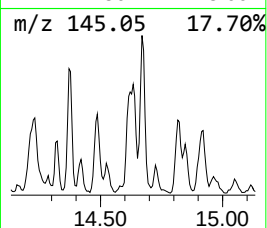
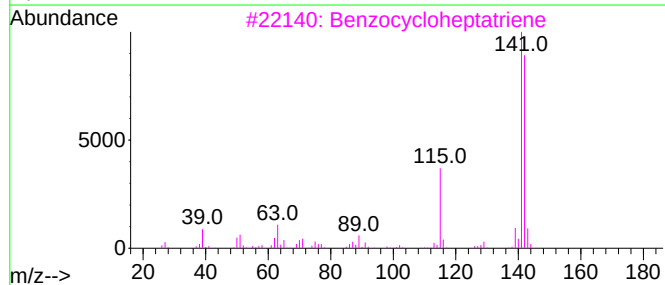
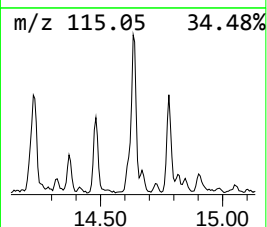
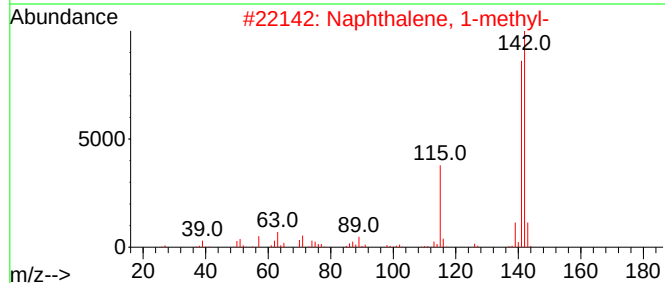
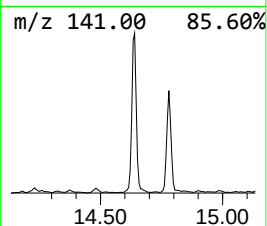
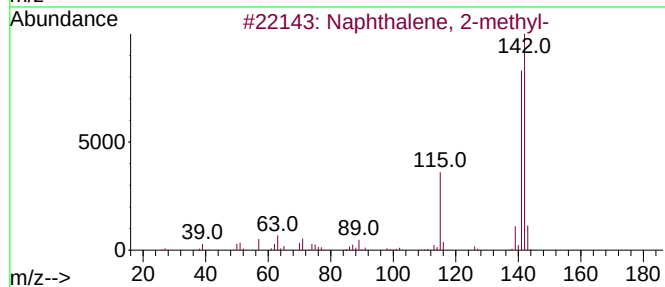
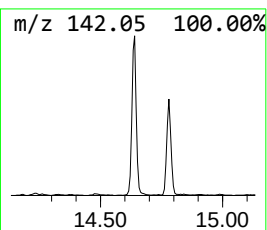
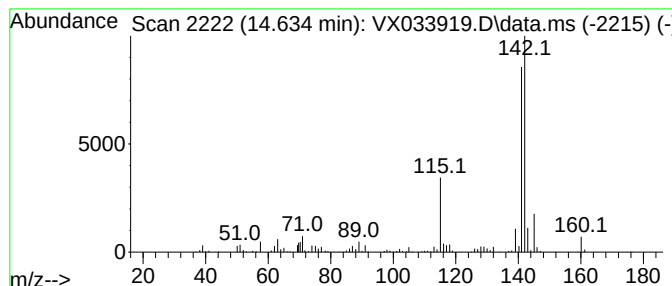
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	20.16 ug/l	243652	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	83
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012623\
Data File : VX033919.D
Acq On : 26 Jan 2023 19:01
Operator : JC/MD
Sample : 01321-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33902

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.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
Acetaldehyde	1.453	45.7	ug/l	389344	1	5.550	426272	50.0
Ethanol	2.063	544.9	ug/l	4645770	1	5.550	426272	50.0
Isopropyl Alcohol	2.520	88.4	ug/l	753308	1	5.550	426272	50.0
Benzene, 1-ethy...	11.378	115.5	ug/l	1396000	4	12.024	604437	50.0
Benzene, 1-ethy...	11.610	42.5	ug/l	514012	4	12.024	604437	50.0
Indane	12.244	55.1	ug/l	665617	4	12.024	604437	50.0
Benzene, 2-ethe...	13.292	26.3	ug/l	318426	4	12.024	604437	50.0
Naphthalene, 1,...	14.231	20.9	ug/l	252639	4	12.024	604437	50.0
Naphthalene, 2-...	14.634	20.2	ug/l	243652	4	12.024	604437	50.0