

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091322\
 Data File : VN074437.D
 Acq On : 13 Sep 2022 16:51
 Operator : JC\MD
 Sample : N4492-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-09-1.5-11.5-083122

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_N\methods\82N090922W.M
 Title : SW846 8260

Signal : TIC: VN074437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.999	15	19	25	rBV2	106905	145431	11.17%	1.511%
2	2.152	40	45	49	rBV	61220	86368	6.63%	0.897%
3	2.199	49	53	55	rBV	52453	78375	6.02%	0.814%
4	2.234	55	59	63	rVB	106621	141758	10.89%	1.473%
5	2.399	83	87	92	rBV4	47080	78939	6.06%	0.820%
6	2.487	97	102	108	rVV	164192	285683	21.94%	2.968%
7	2.693	129	137	138	rBV3	49273	89826	6.90%	0.933%
8	2.952	175	181	195	rVB	204194	463124	35.57%	4.811%
9	3.857	324	335	347	rBV3	120022	331907	25.49%	3.448%
10	4.140	371	383	394	rBV4	63809	200019	15.36%	2.078%
11	7.251	901	912	921	rBV3	98575	274827	21.11%	2.855%
12	7.951	1022	1031	1036	rBV	201605	468715	36.00%	4.869%
13	8.016	1036	1042	1053	rVB	301712	678169	52.09%	7.045%
14	8.369	1094	1102	1115	rBV	216269	504412	38.74%	5.240%
15	8.904	1182	1193	1203	rBV	485237	958704	73.64%	9.959%
16	9.151	1226	1235	1241	rBV5	16187	32374	2.49%	0.336%
17	10.380	1436	1444	1452	rBV	723789	1301880	100.00%	13.524%
18	10.445	1452	1455	1461	rVB4	15870	27071	2.08%	0.281%
19	11.686	1659	1666	1677	rBV	749463	1288002	98.93%	13.379%
20	12.674	1826	1834	1844	rBV	629521	1020691	78.40%	10.603%
21	13.616	1987	1994	2002	rBV	710218	1170500	89.91%	12.159%

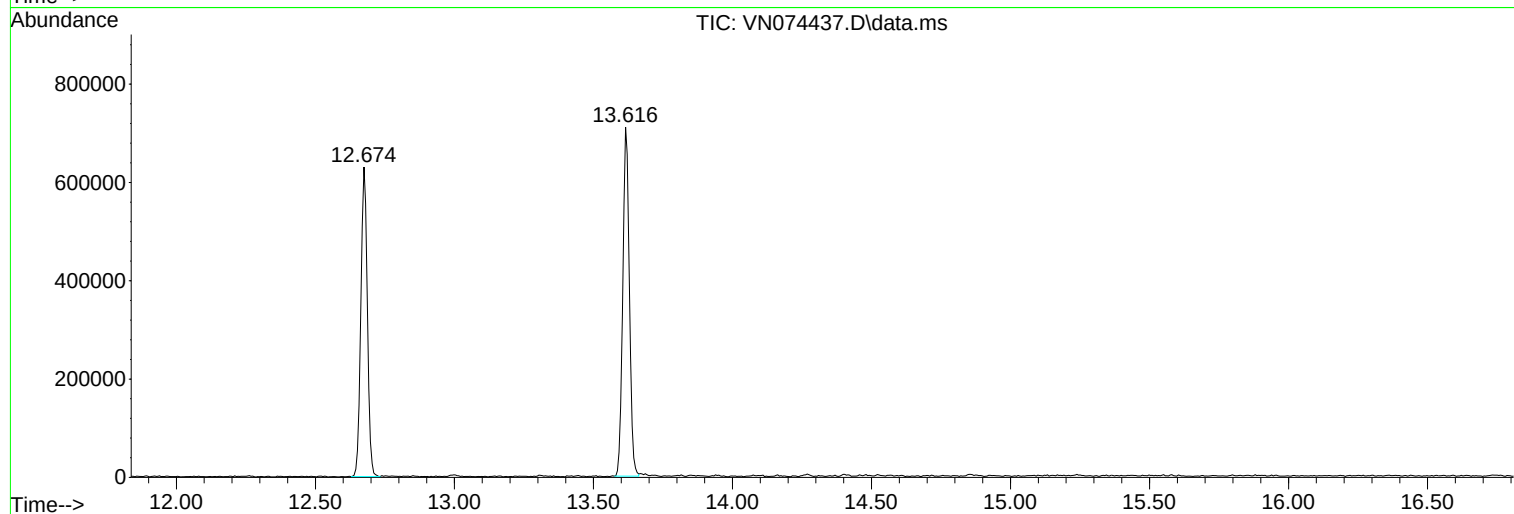
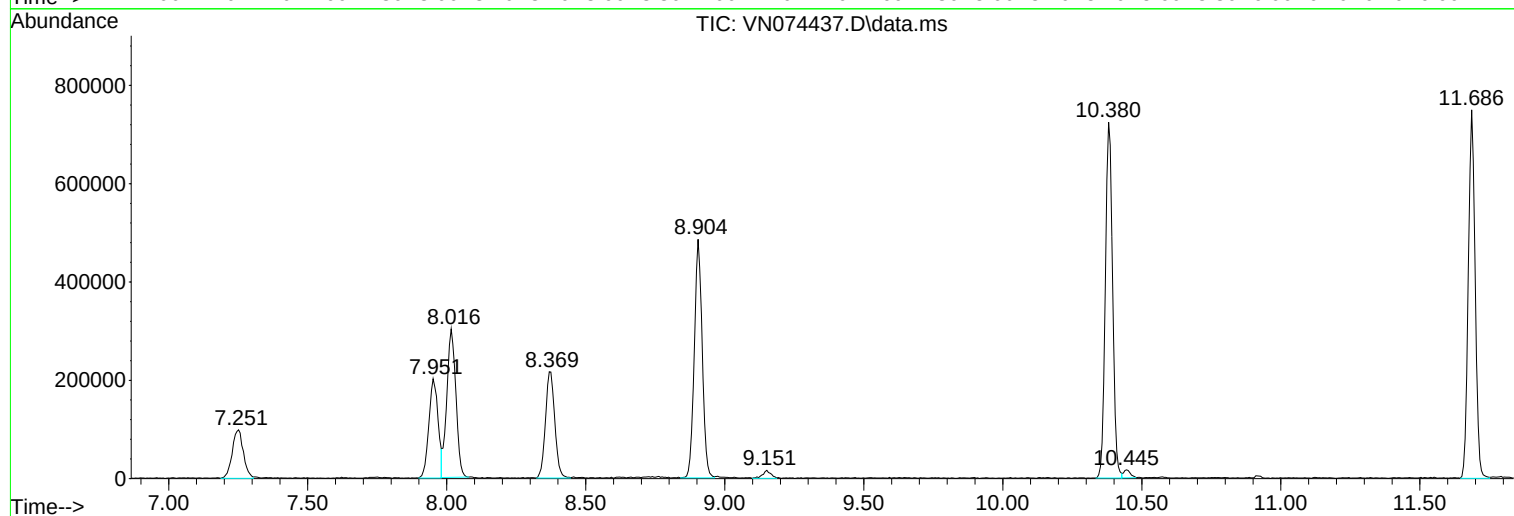
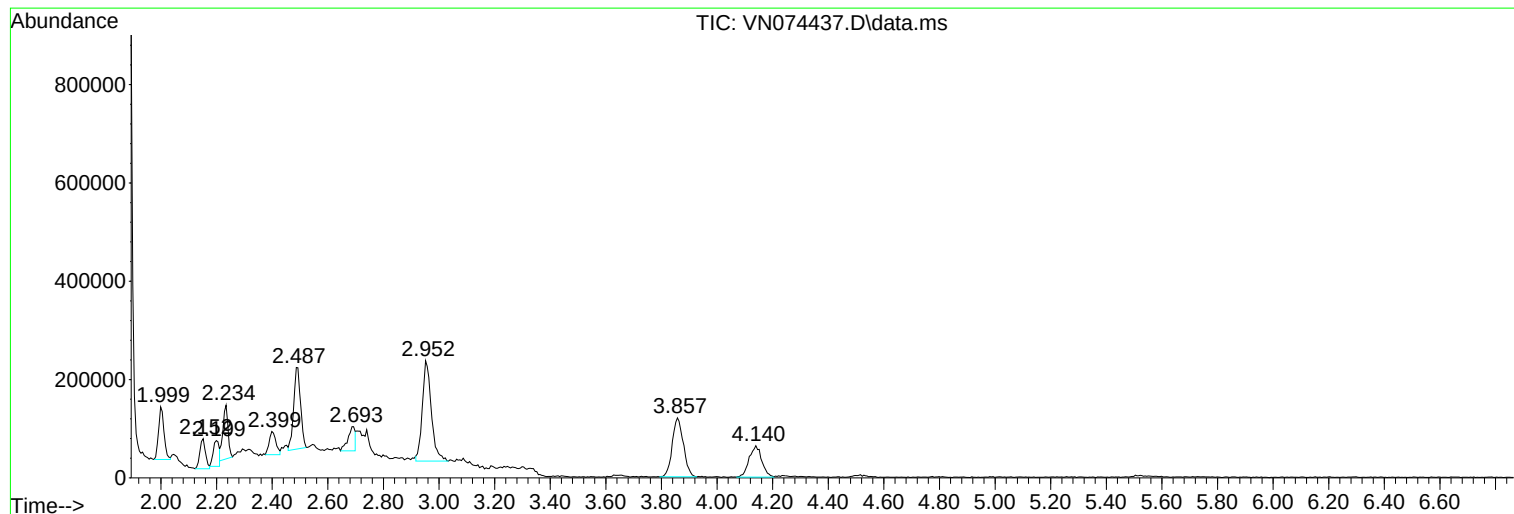
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

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



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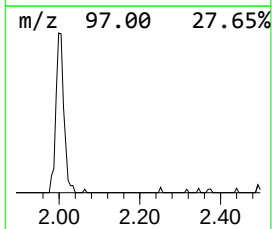
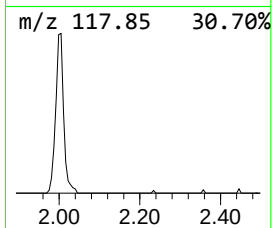
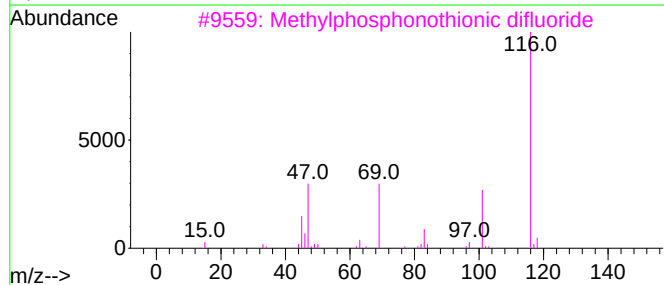
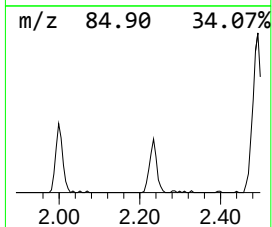
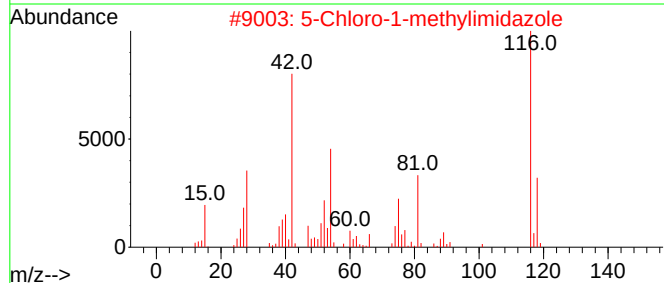
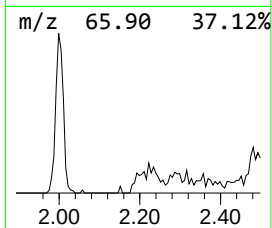
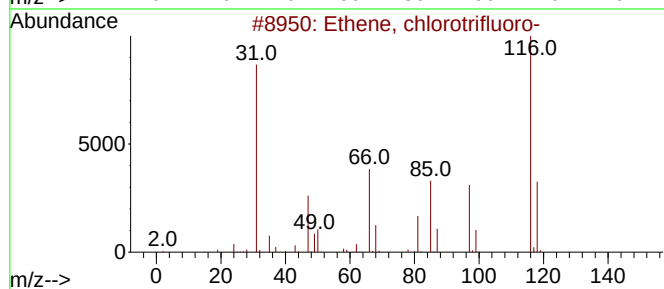
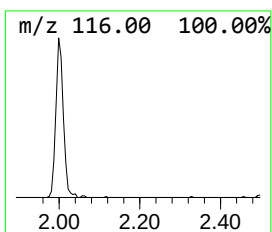
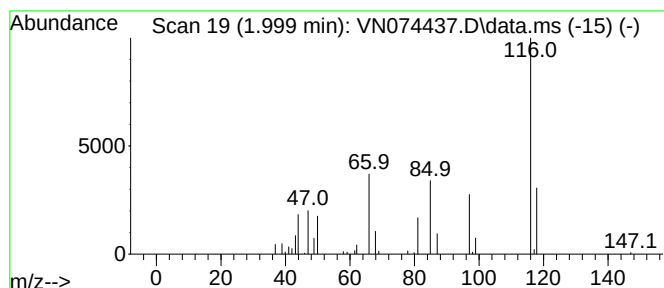
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethene, chlorotrifluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.999	10.72 ug/l	145431	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethene, chlorotrifluoro-	116	C2ClF3	000079-38-9	96
2			5-Chloro-1-methylimidazole	116	C4H5ClN2	000872-49-1	9
3			Methylphosphonothionic difluoride	116	CH3F2PS	000753-72-0	9
4			D-Alanine, N-ethoxycarbonyl-, un...	315	C17H33NO4	1000347-75-4	9
5			D-Alanine, N-ethoxycarbonyl-, oc...	273	C14H27NO4	1000347-75-1	9



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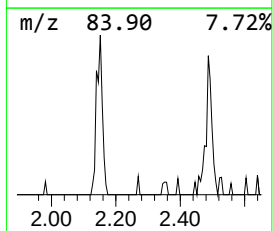
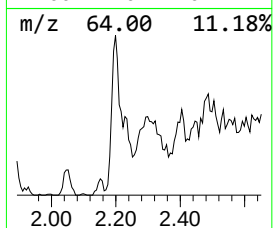
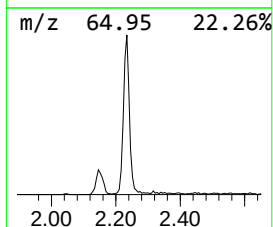
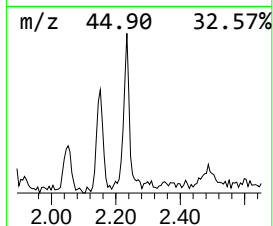
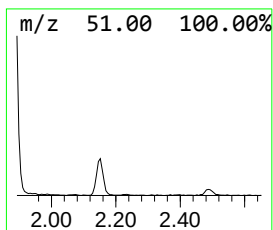
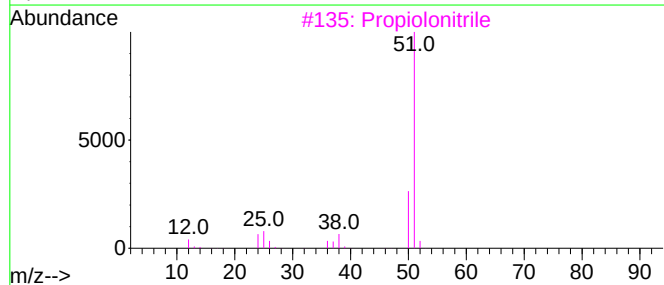
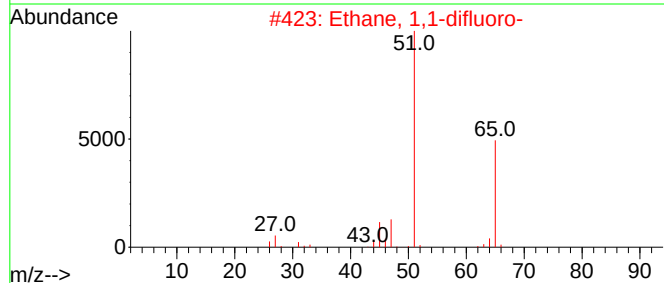
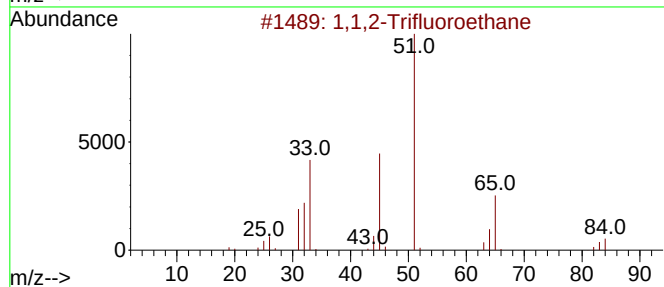
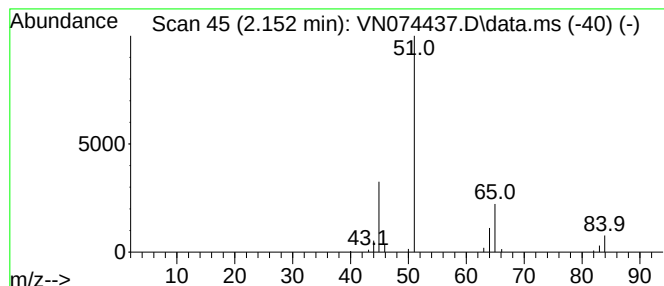
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

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

Peak Number 2 1,1,2-Trifluoroethane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	6.37 ug/l	86368	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,2-Trifluoroethane			84	C2H3F3	000430-66-0	74
2	Ethane, 1,1-difluoro-			66	C2H4F2	000075-37-6	43
3	Propiolonitrile			51	C3HN	001070-71-9	3
4	Difluoromethyl trifluoromethanes...			200	C2HF5O3S	001885-46-7	1
5	Difluorochloromethane			86	CHClF2	000075-45-6	1



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MW-09-1.5-11.5-083122

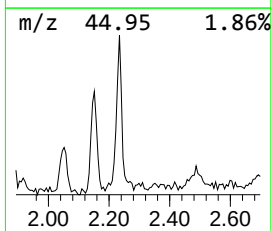
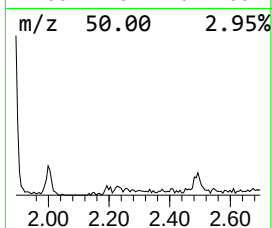
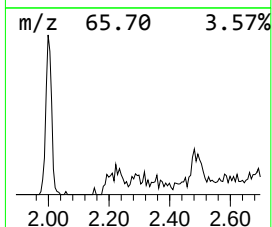
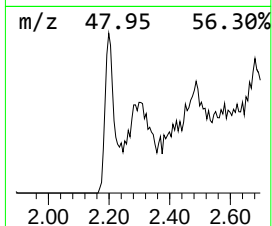
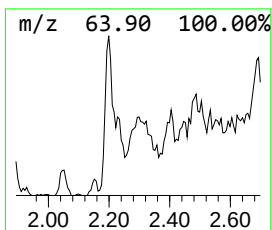
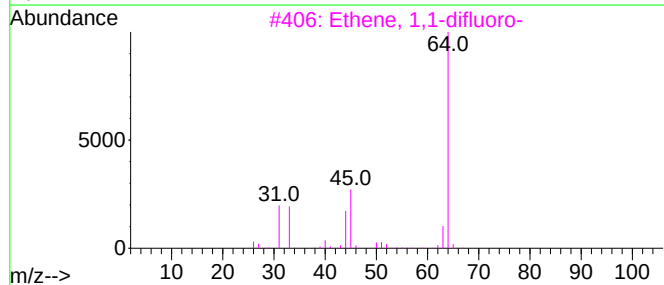
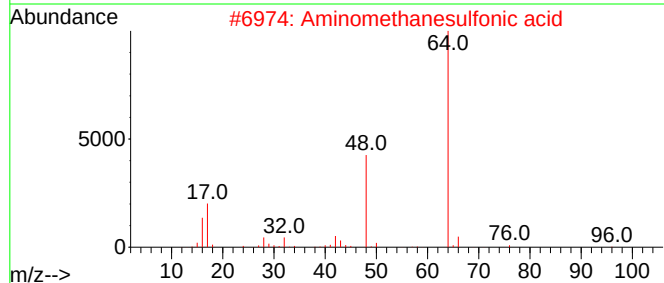
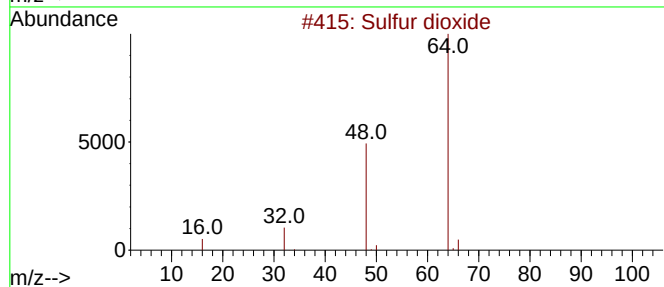
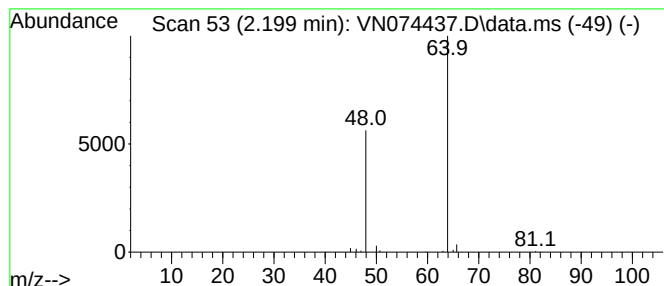
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Quant Title : SW846 8260

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

Peak Number 3 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	5.78 ug/l	78375	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	4
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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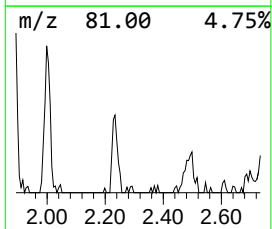
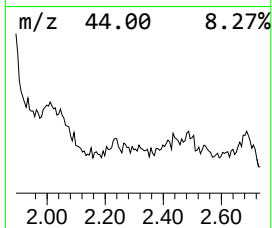
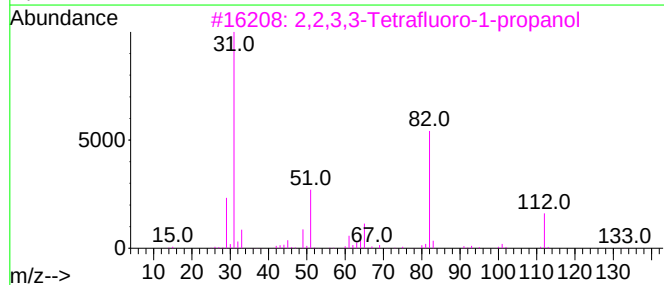
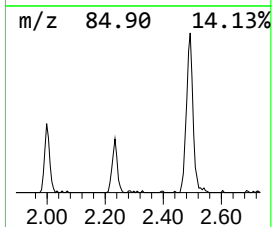
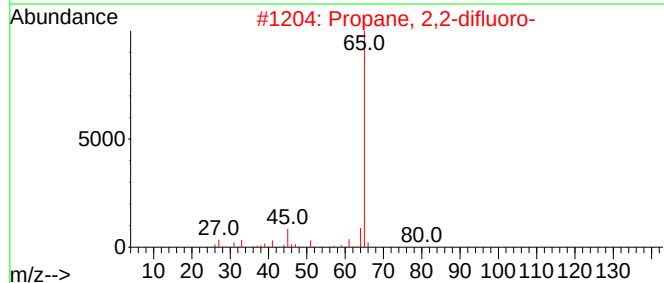
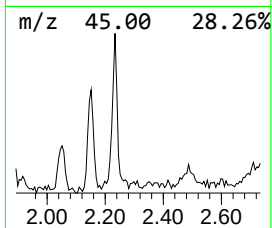
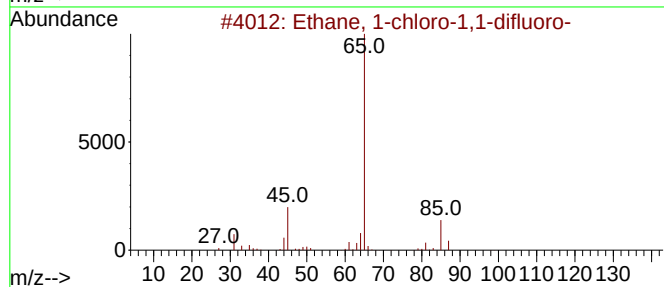
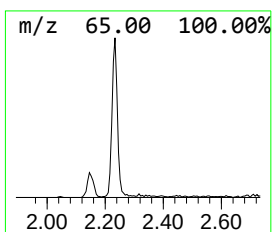
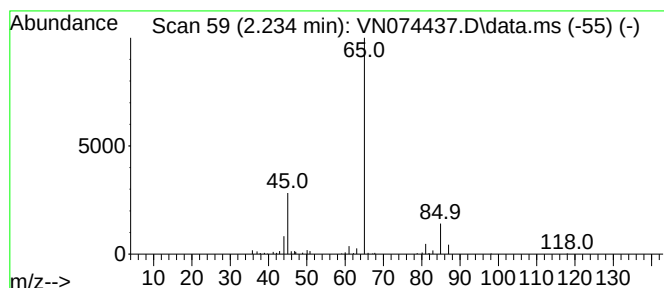
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Quant Title : SW846 8260

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

Peak Number 4 Ethane, 1-chloro-1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	10.45 ug/l	141758	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	74
2			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	9
3			2,2,3,3-Tetrafluoro-1-propanol	132	C3H4F4O	000076-37-9	1
4			Propane, 1-chloro-2,2-difluoro-	114	C3H5ClF2	000420-99-5	1
5			Propane, 1,1,2,2-tetrafluoro-	116	C3H4F4	040723-63-5	1



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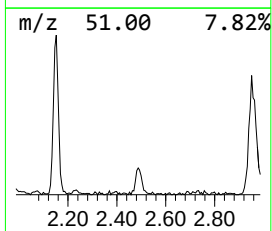
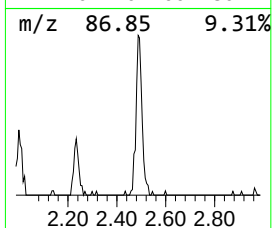
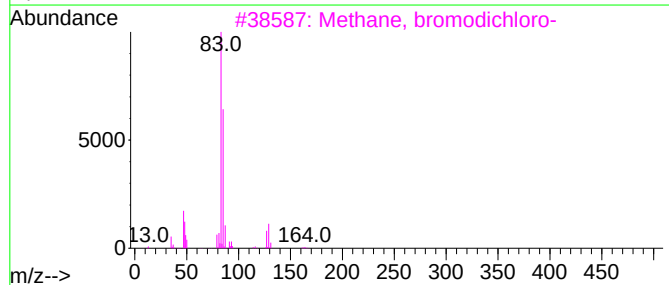
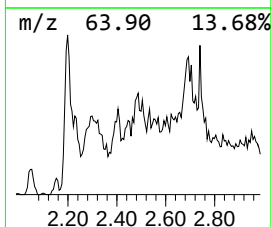
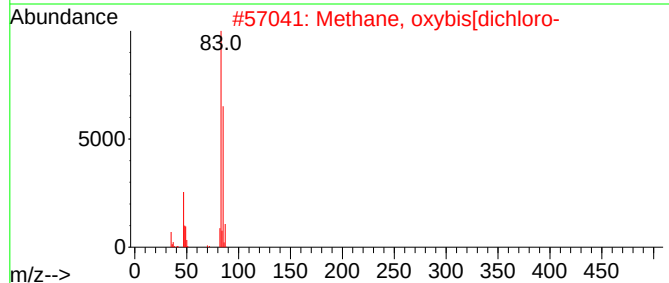
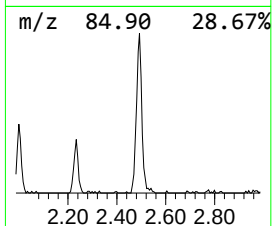
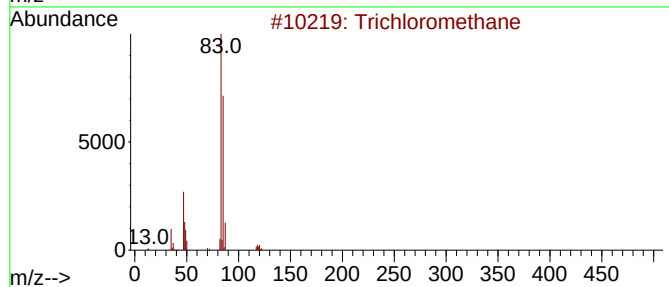
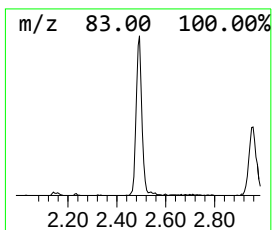
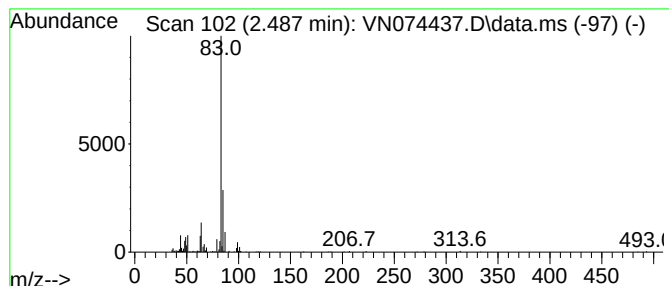
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown2.487 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.487	21.06 ug/l	285683	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloromethane	118	CHCl3	000067-66-3	37
2			Methane, oxybis[dichloro-	182	C2H2Cl4O	020524-86-1	25
3			Methane, bromodichloro-	162	CHBrCl2	000075-27-4	9
4			Methane, dichloronitro-	129	CHCl2NO2	007119-89-3	9
5			3-Methyl-2-butenic acid, tridec...	278	C18H30O2	1000299-31-7	9



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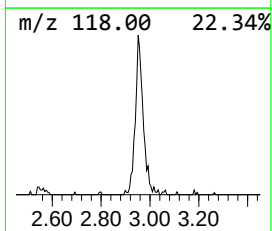
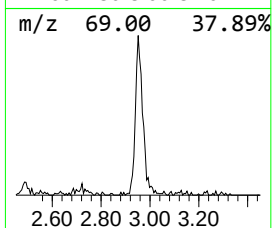
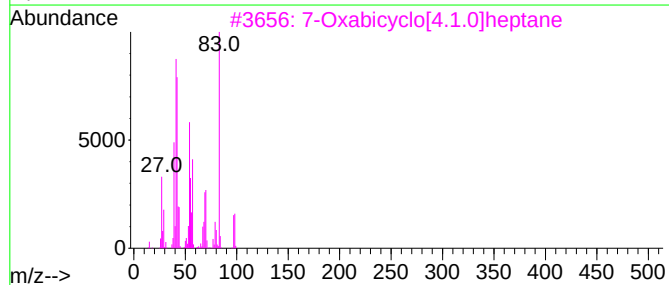
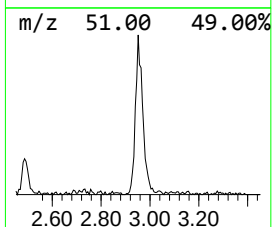
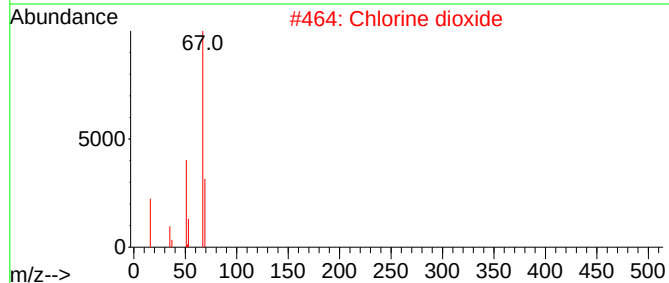
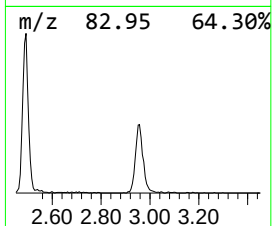
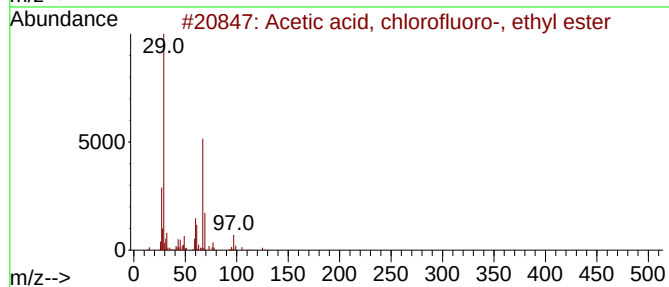
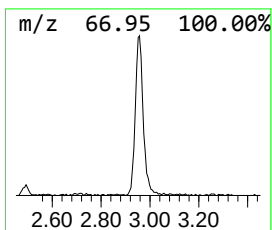
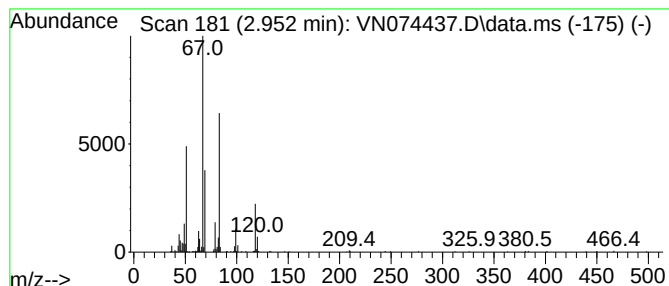
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Quant Title : SW846 8260

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

Peak Number 7 unknown2.952 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.952	34.15 ug/l	463124	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, chlorofluoro-, ethy...	140	C4H6ClF02	000401-56-9	17
2			Chlorine dioxide	67	ClO2	010049-04-4	9
3			7-Oxabicyclo[4.1.0]heptane	98	C6H10O	000286-20-4	9
4			2-Cyclopentene-1-methanol	98	C6H10O	013668-59-2	9
5			Sulfuryl chloride fluoride	118	ClF02S	013637-84-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091322\
Data File : VN074437.D
Acq On : 13 Sep 2022 16:51
Operator : JC\MD
Sample : N4492-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-09-1.5-11.5-083122

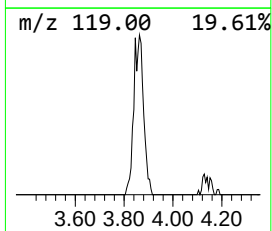
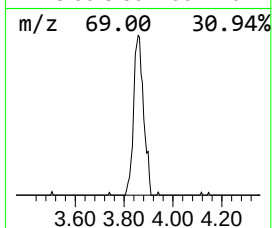
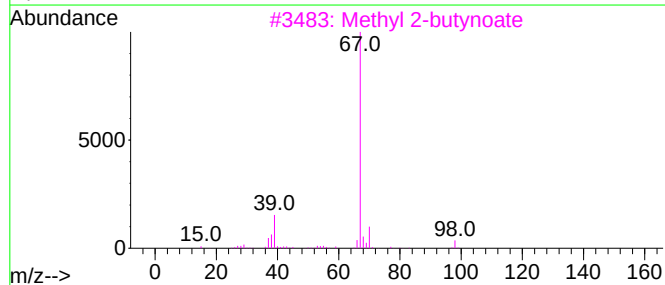
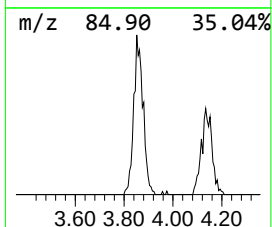
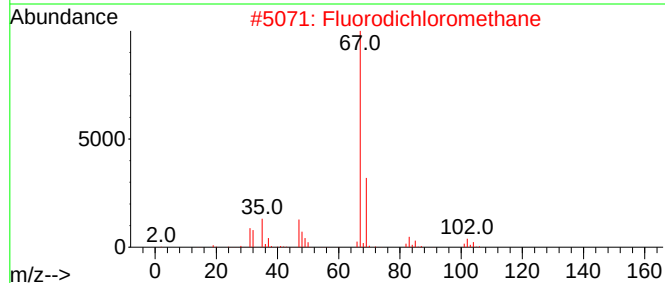
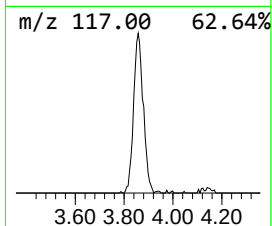
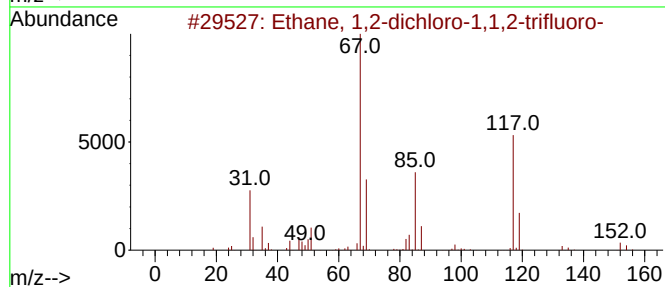
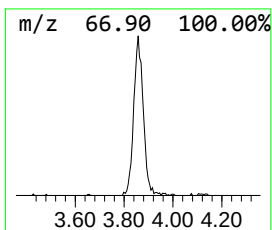
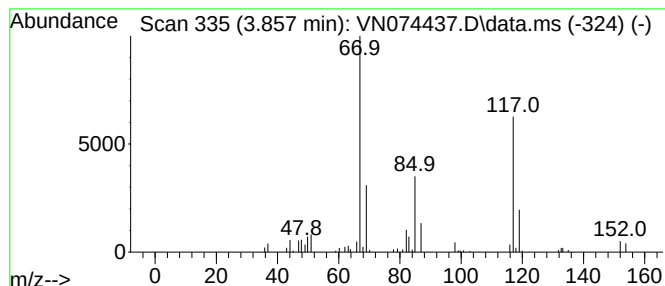
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

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

Peak Number 8 Ethane, 1,2-dichloro-1,1,2-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.857	24.47 ug/l	331907	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HCl2F3	000354-23-4	91
2			Fluorodichloromethane	102	CHCl2F	000075-43-4	38
3			Methyl 2-butynoate	98	C5H6O2	023326-27-4	16
4			Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	062338-02-7	16
5			1,3-Isobenzofurandione, hexahydr...	154	C8H10O3	014166-21-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091322\
Data File : VN074437.D
Acq On : 13 Sep 2022 16:51
Operator : JC\MD
Sample : N4492-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-09-1.5-11.5-083122

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.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
Ethene, chlorot...	1.999	10.7	ug/l	145431	1	8.016	678169	50.0
1,1,2-Trifluoro...	2.152	6.4	ug/l	86368	1	8.016	678169	50.0
Sulfur dioxide	2.199	5.8	ug/l	78375	1	8.016	678169	50.0
Ethane, 1-chlor...	2.234	10.4	ug/l	141758	1	8.016	678169	50.0
unknown2.487	2.487	21.1	ug/l	285683	1	8.016	678169	50.0
Aminomethanesul...	2.693	6.6	ug/l	89826	1	8.016	678169	50.0
unknown2.952	2.952	34.1	ug/l	463124	1	8.016	678169	50.0
Ethane, 1,2-dic...	3.857	24.5	ug/l	331907	1	8.016	678169	50.0