

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
 Data File : VN074806.D
 Acq On : 07 Oct 2022 13:06
 Operator : JC\MD
 Sample : N4977-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 251032-3

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\82N100522W.M

Title : SW846 8260

Signal : TIC: VN074806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	38	44	51	rBV	277347	500399	14.38%	3.667%
2	2.771	119	122	125	rBV2	63997	83990	2.41%	0.615%
3	2.830	128	132	134	rBV3	92605	141507	4.07%	1.037%
4	4.753	450	459	461	rBV6	18696	39176	1.13%	0.287%
5	7.453	908	918	929	rBV	32456	100827	2.90%	0.739%
6	8.177	1032	1041	1046	rBV	442899	1053426	30.27%	7.719%
7	8.235	1046	1051	1060	rVB	372656	817257	23.48%	5.988%
8	8.594	1102	1112	1122	rBV2	549576	1275935	36.66%	9.349%
9	9.106	1190	1199	1212	rBV	569434	1191071	34.22%	8.727%
10	10.571	1439	1448	1464	rBV	1874095	3480546	100.00%	25.503%
11	11.865	1660	1668	1680	rBV	879486	1622925	46.63%	11.891%
12	12.853	1828	1836	1844	rBV	1028208	1748700	50.24%	12.813%
13	13.794	1989	1996	2007	rBV	943159	1592037	45.74%	11.665%

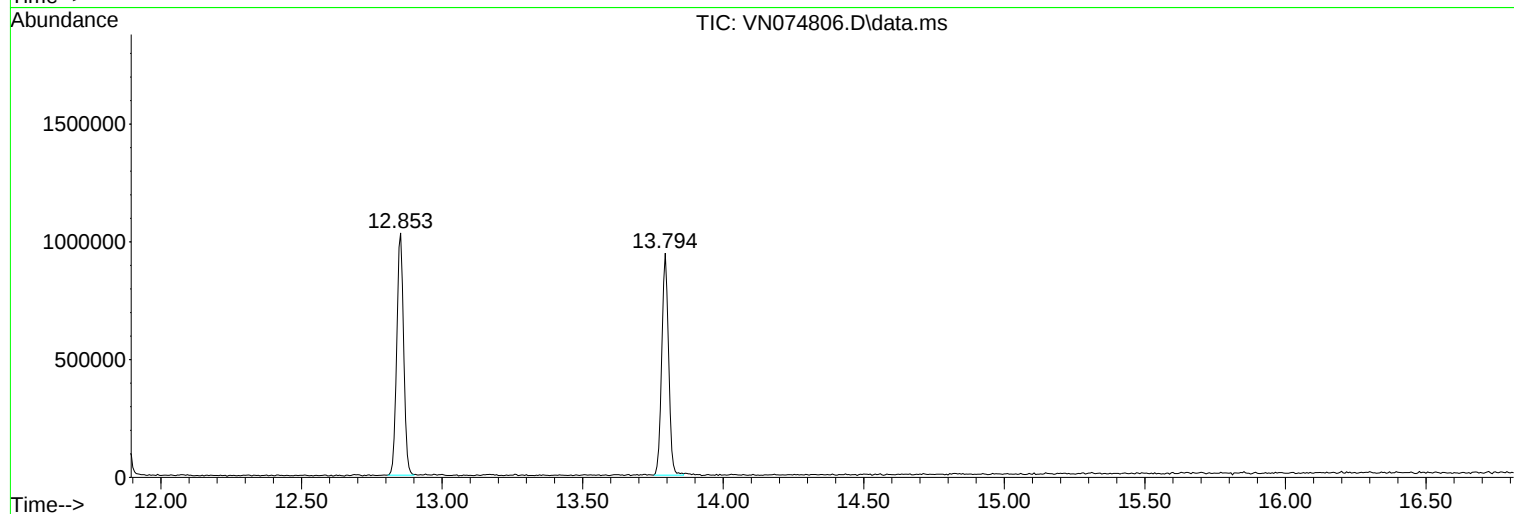
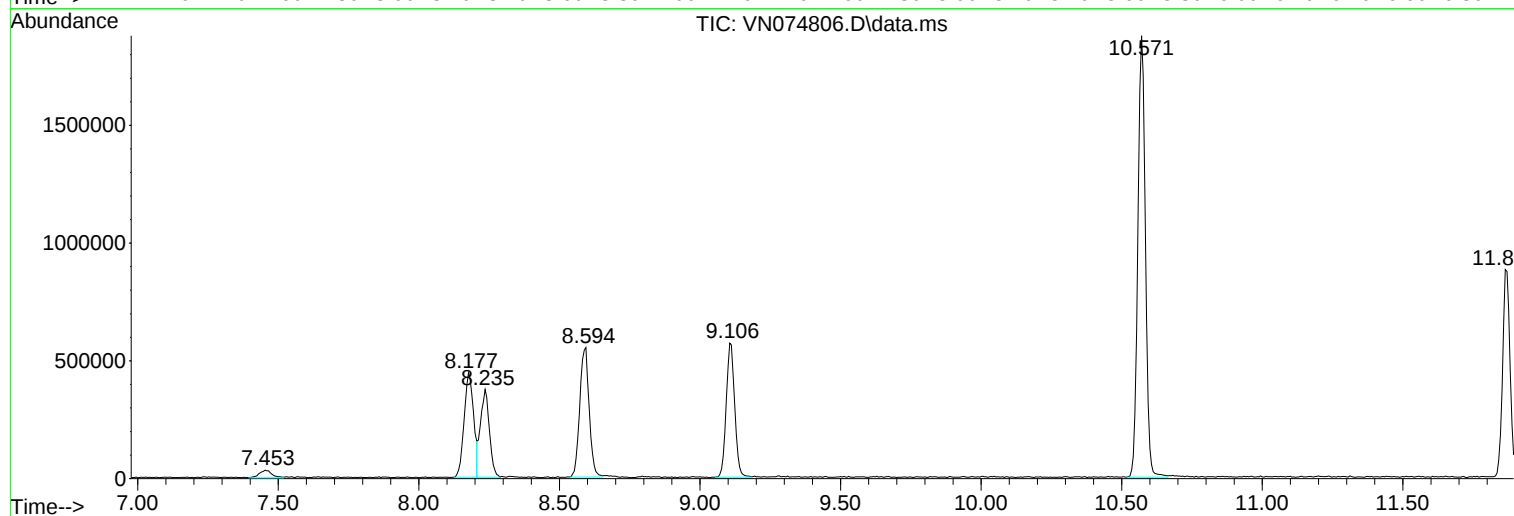
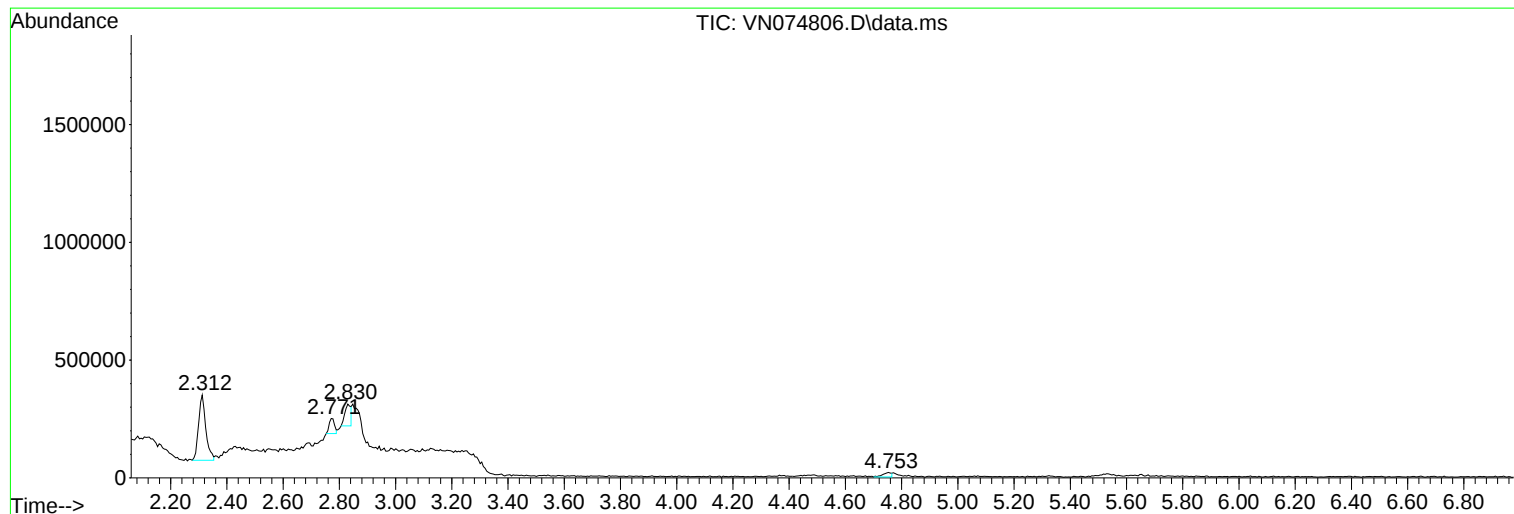
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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



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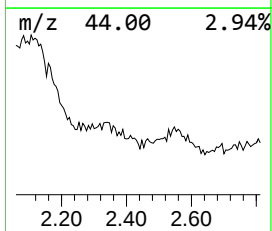
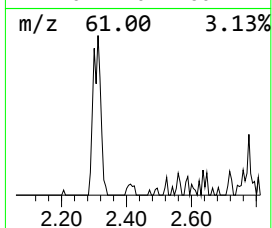
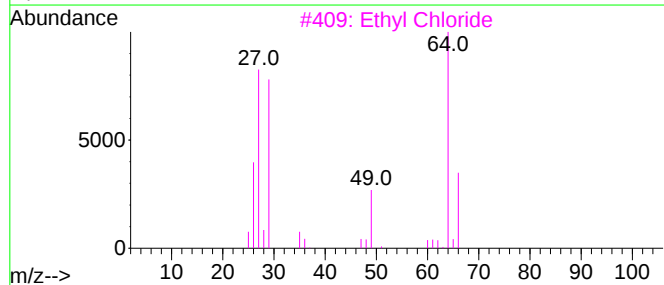
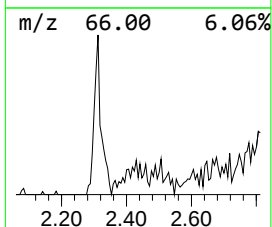
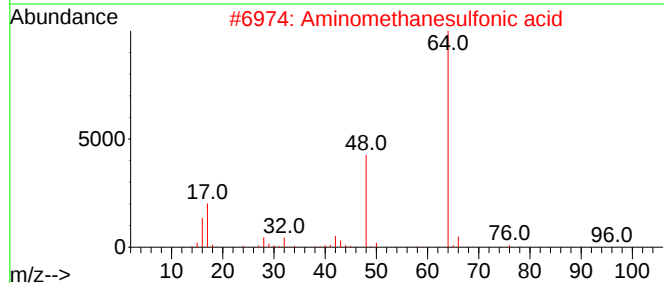
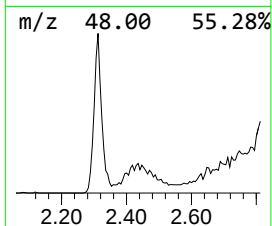
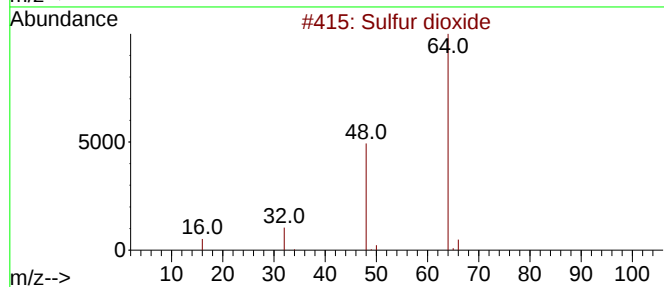
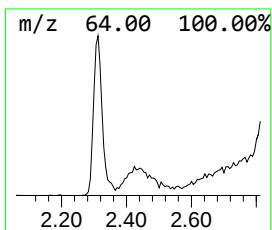
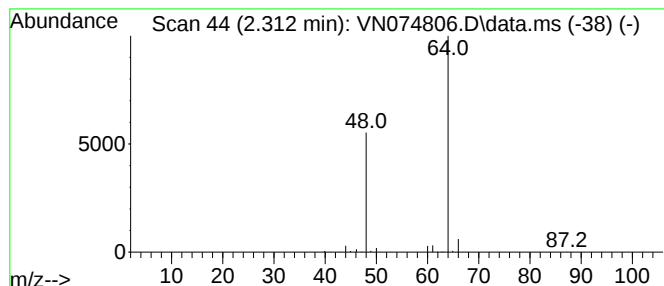
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	30.61 ug/l	500399	Pentafluorobenzene	8.235

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	64
3			Ethyl Chloride	64	C2H5Cl	000075-00-3	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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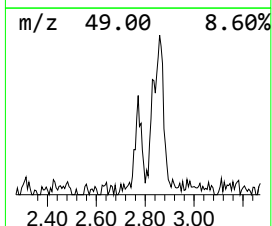
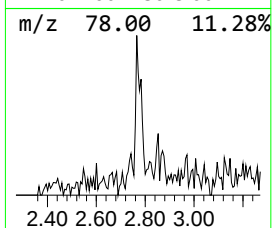
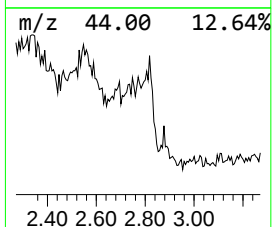
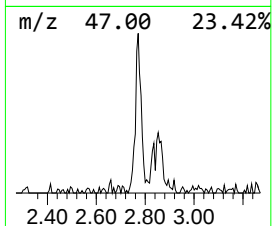
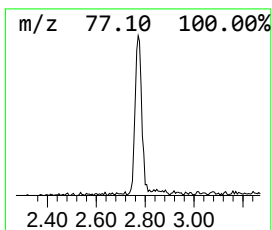
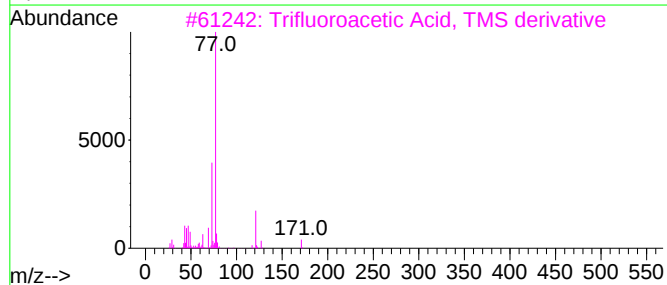
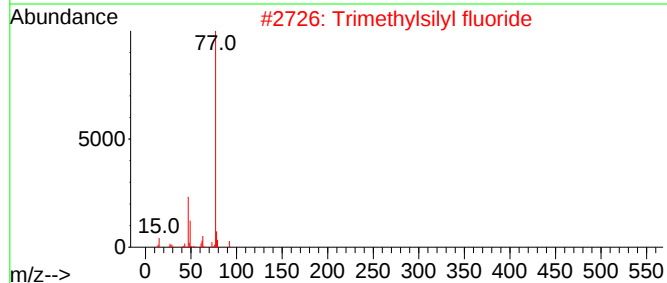
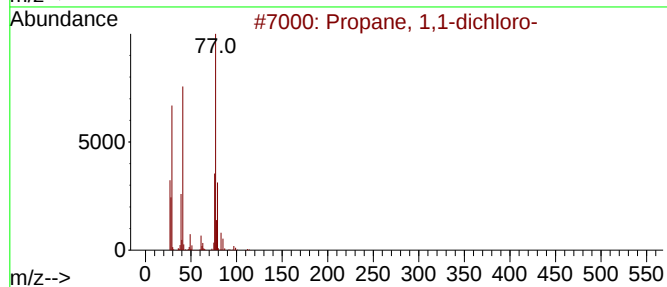
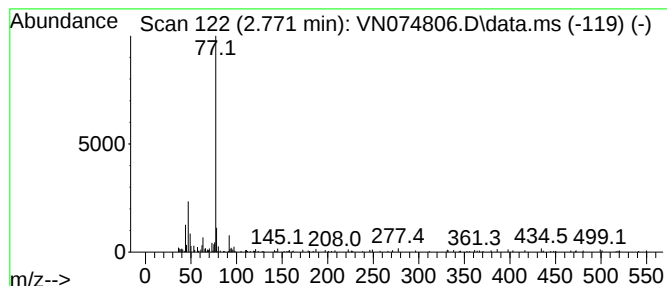
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.771 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.771	5.14 ug/l	83990	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dichloro-	112	C3H6Cl2	000078-99-9	40
2			Trimethylsilyl fluoride	92	C3H9FSi	000420-56-4	39
3			Trifluoroacetic Acid, TMS deriva...	186	C5H9F3O2Si	000400-53-3	38
4			tert-Butyldimethylfluorosilane	134	C6H15FSi	1000366-62-3	38
5			Perfluoropropionic acid, TMS der...	236	C6H9F5O2Si	024930-02-7	36



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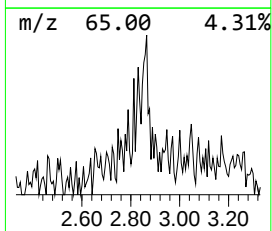
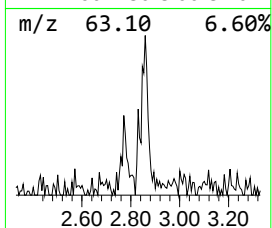
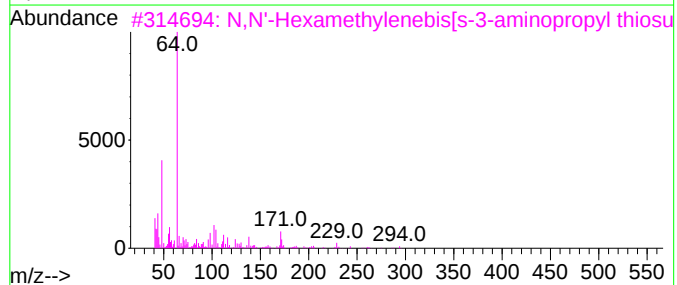
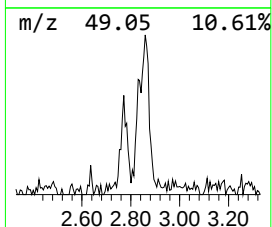
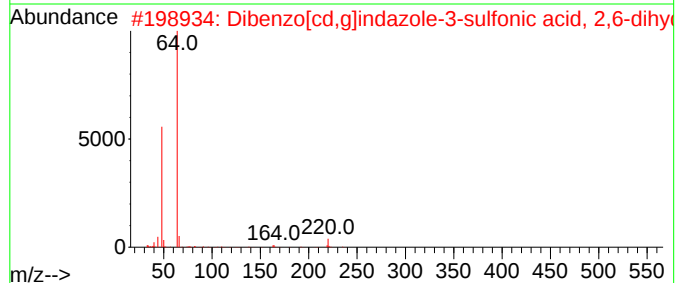
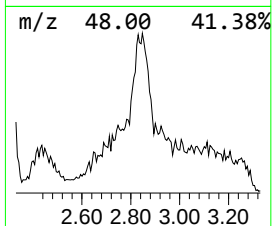
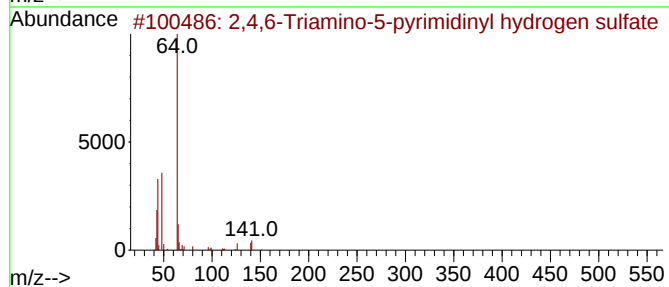
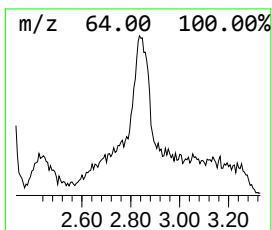
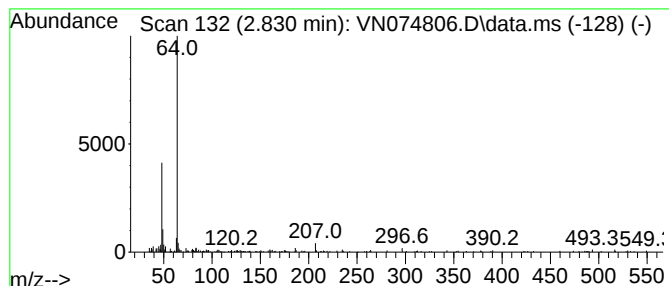
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Peak Number 3 2,4,6-Triamino-5-pyrimidiny... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.830	8.66 ug/l	141507	Pentafluorobenzene	8.235	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	64
2	Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	43
3	N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	43
4	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	43
5	Sulfur dioxide	64	O2S	007446-09-5	9



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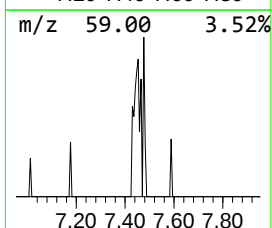
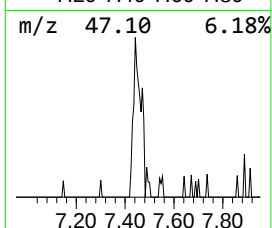
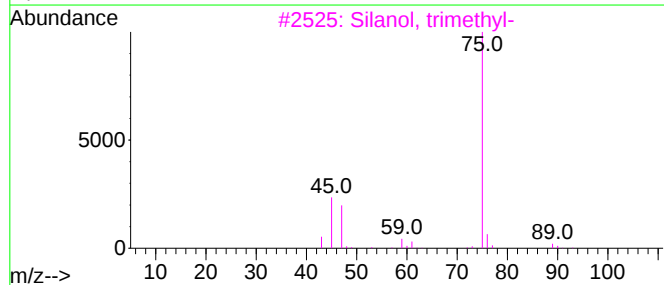
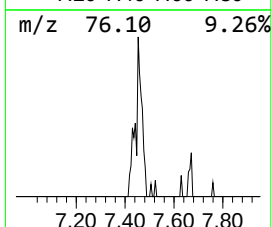
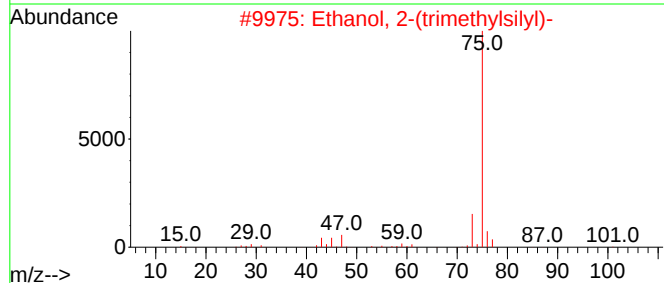
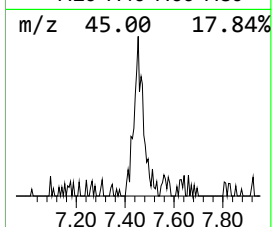
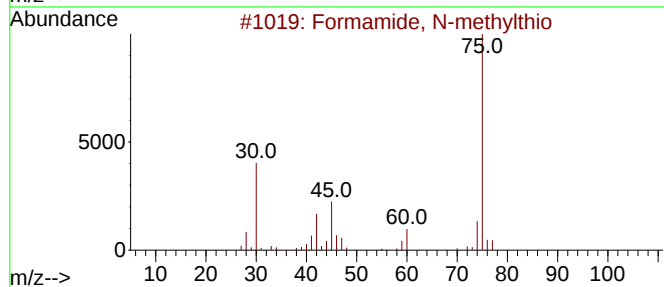
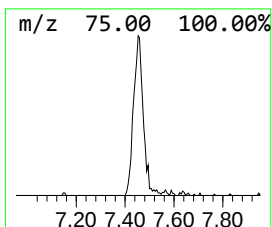
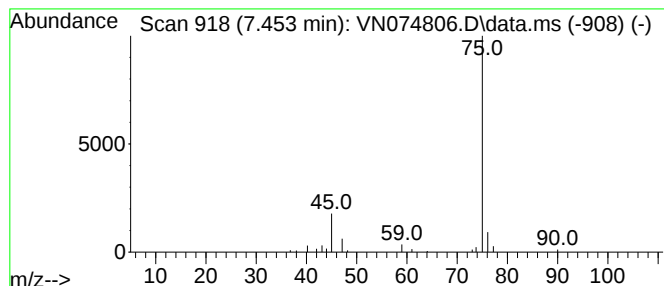
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Peak Number 4 Formamide, N-methylthio Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.453	6.17 ug/l	100827	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-methylthio	75	C2H5NS	018952-41-5	64
2			Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	56
3			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	43
4			tert-Butyldimethylsilanol	132	C6H16OSi	018173-64-3	9
5			Silanol, dimethyl(1,1,2-trimethy...	160	C8H20OSi	055644-10-5	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	30.6	ug/l	500399	1	8.235	817257	50.0
unknown2.771	2.771	5.1	ug/l	83990	1	8.235	817257	50.0
2,4,6-Triamino-...	2.830	8.7	ug/l	141507	1	8.235	817257	50.0
Formamide, N-me...	7.453	6.2	ug/l	100827	1	8.235	817257	50.0