

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN080320\
 Data File : VN062736.D
 Acq On : 3 Aug 2020 15:25
 Operator : JC/MD
 Sample : L3539-03
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 I-LGC-5

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072120W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.818	3	14	26	rVB	30121	48069	1.55%	0.466%
2	1.921	37	46	60	rVB	64705	89981	2.91%	0.873%
3	2.420	192	201	210	rBV	340418	422038	13.63%	4.093%
4	3.777	603	623	636	rBV	246795	624501	20.17%	6.057%
5	3.854	637	647	667	rVB	87585	226079	7.30%	2.193%
6	4.011	675	696	723	rBV	1173410	3096427	100.00%	30.031%
7	6.792	1543	1561	1583	rBV2	18280	53336	1.72%	0.517%
8	7.548	1780	1796	1808	rBV2	98728	250670	8.10%	2.431%
9	7.625	1808	1820	1843	rVB2	171028	404594	13.07%	3.924%
10	7.992	1917	1934	1956	rBV3	145822	371379	11.99%	3.602%
11	8.551	2093	2108	2126	rBV	270866	558509	18.04%	5.417%
12	9.866	2494	2517	2563	rBV	322601	993627	32.09%	9.637%
13	10.059	2564	2577	2591	rVV	443231	806002	26.03%	7.817%
14	10.230	2619	2630	2645	rVB	29860	52908	1.71%	0.513%
15	11.252	2934	2948	2963	rBV3	21878	41640	1.34%	0.404%
16	11.381	2974	2988	3009	rBV	407089	720533	23.27%	6.988%
17	12.377	3283	3298	3318	rBV	312812	527441	17.03%	5.115%
18	12.963	3467	3480	3492	rBV2	46911	87699	2.83%	0.851%
19	13.320	3578	3591	3607	rBV	346248	581327	18.77%	5.638%
20	15.104	4132	4146	4162	rBV	198536	353975	11.43%	3.433%

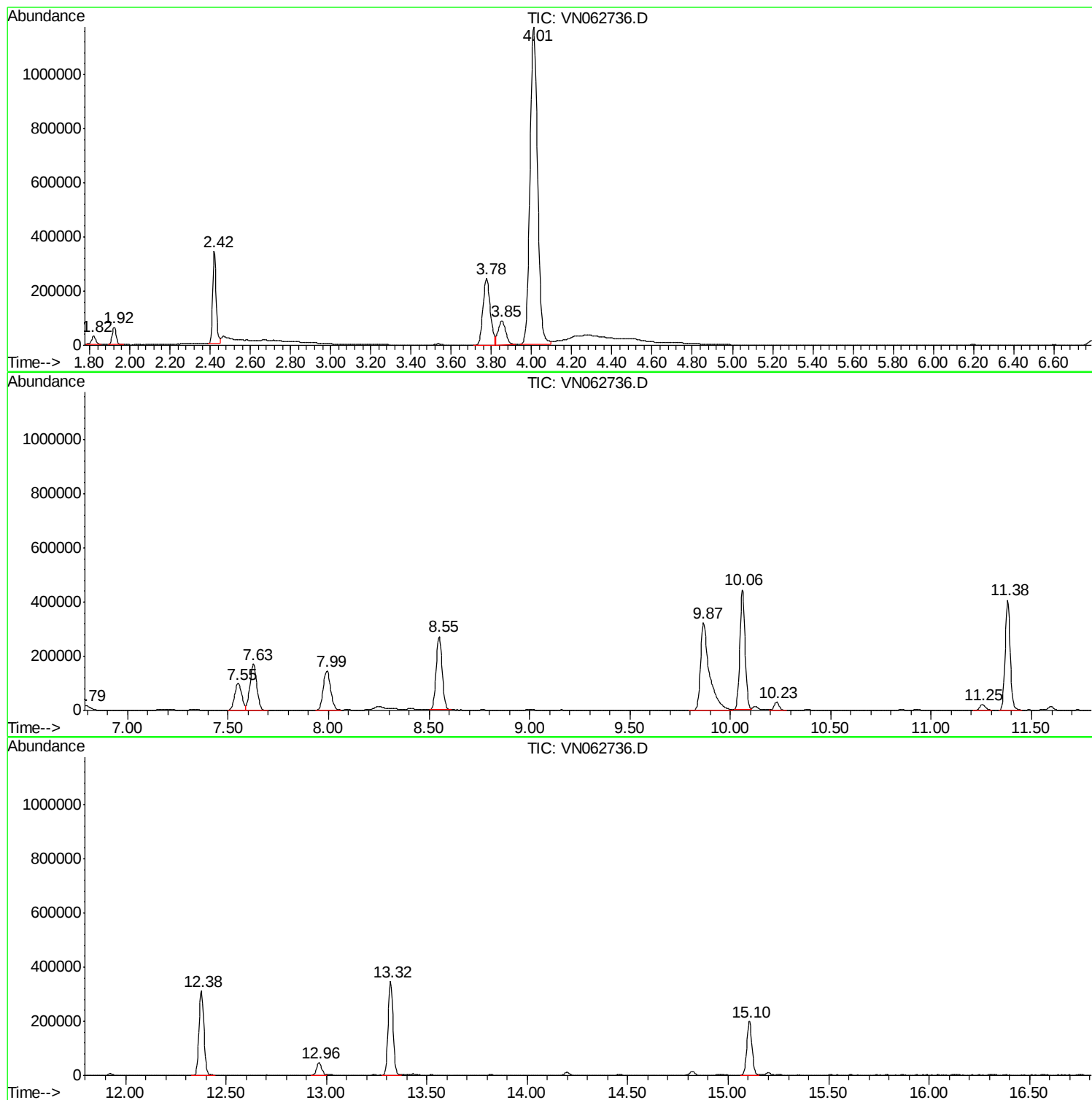
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N072120W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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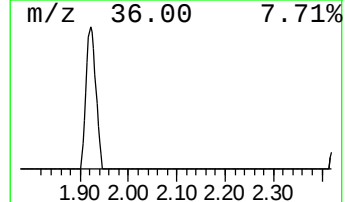
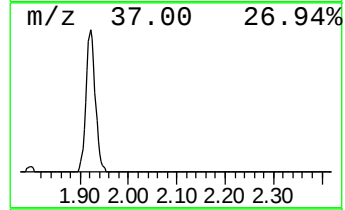
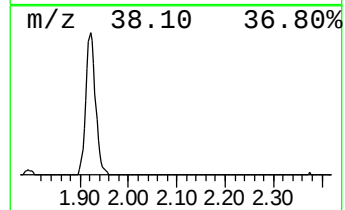
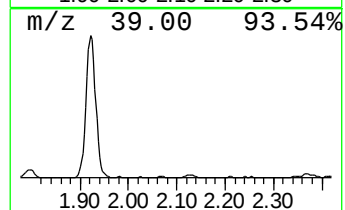
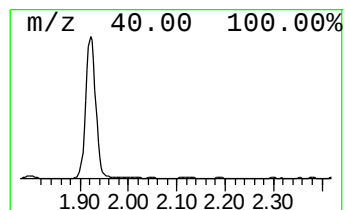
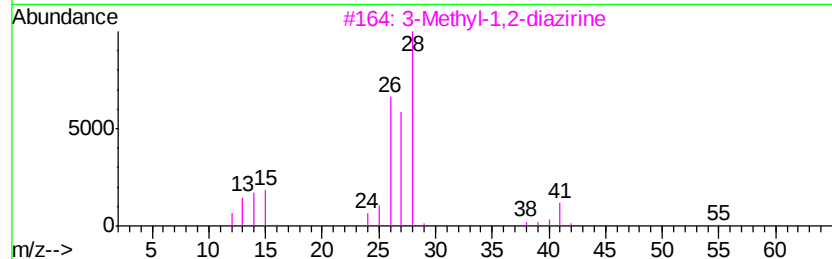
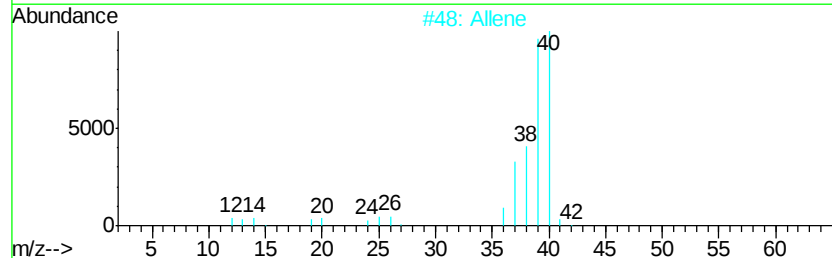
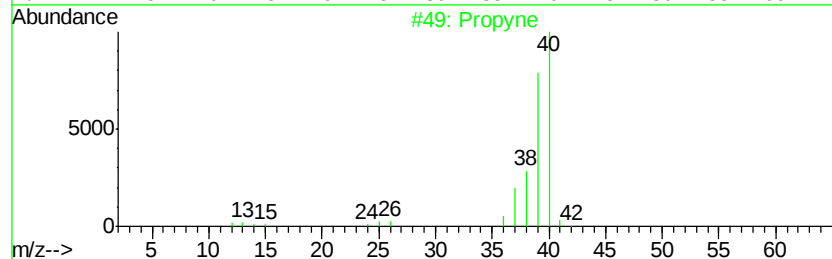
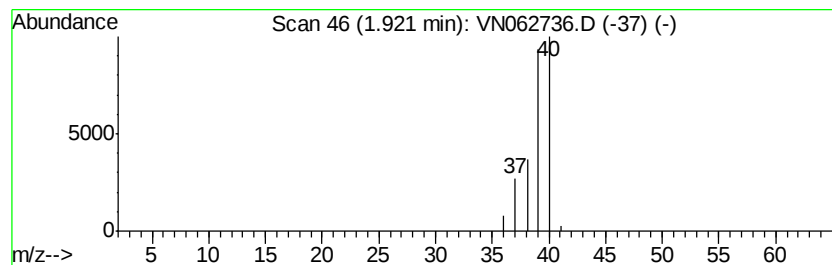
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N072120W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propyne Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.92	11.12 ug/l	89981	Pentafluorobenzene	7.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyne		40	C3H4	000074-99-7	90
2	Allene		40	C3H4	000463-49-0	90
3	3-Methyl-1,2-diazirine		56	C2H4N2	1000305-83-7	1
4	1-Butanamine, 2-methyl-		87	C5H13N	000096-15-1	1
5	Ethane, nitro-		75	C2H5NO2	000079-24-3	1



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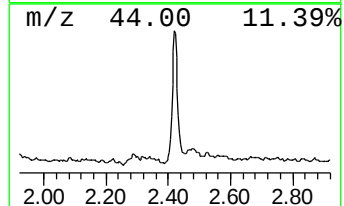
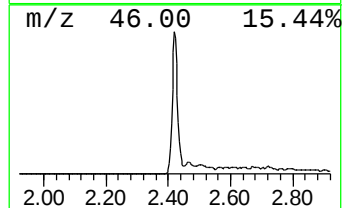
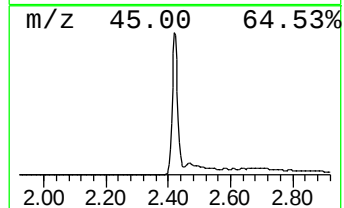
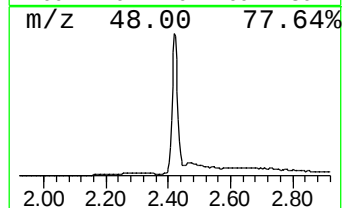
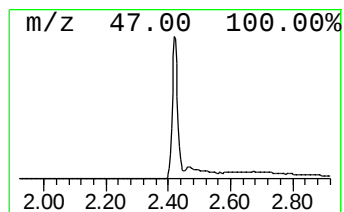
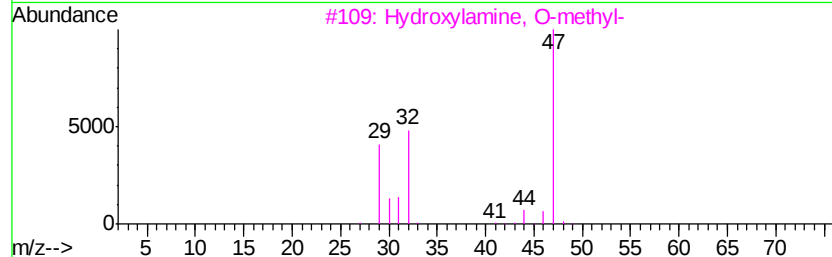
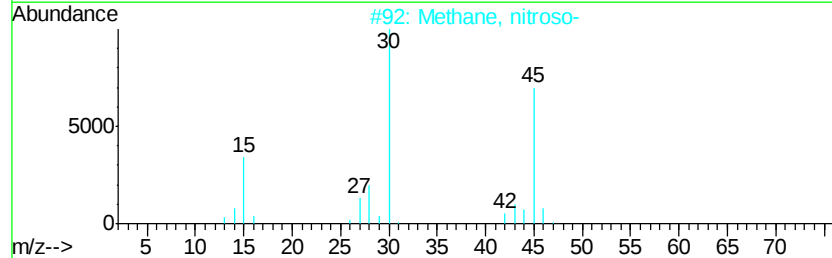
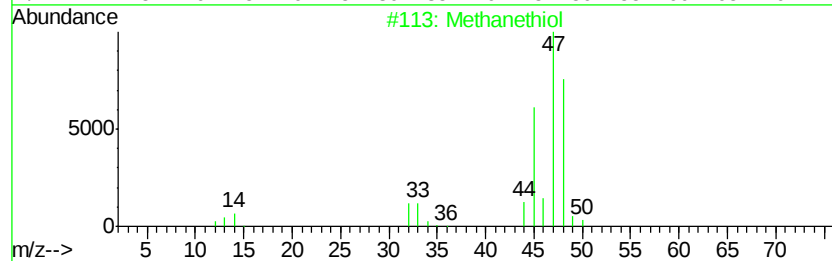
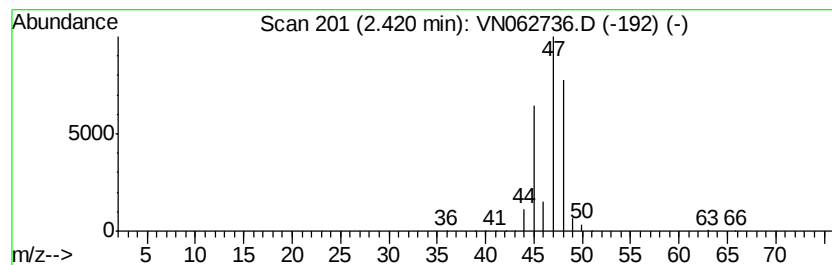
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.42	52.16 ug/l	422038	Pentafluorobenzene	7.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methanethiol	48	CH4S	000074-93-1	91
2		Methane, nitroso-	45	CH3NO	000865-40-7	5
3		Hvdroxylamine, O-methyl-	47	CH5NO	000067-62-9	4
4		Ethane, fluoro-	48	C2H5F	000353-36-6	4
5		Formamide	45	CH3NO	000075-12-7	4



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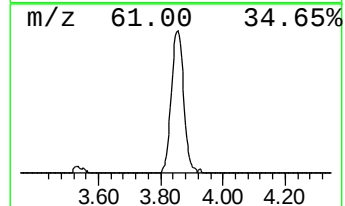
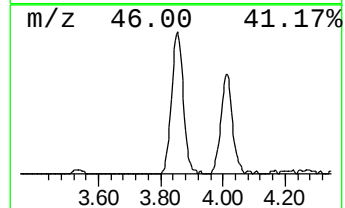
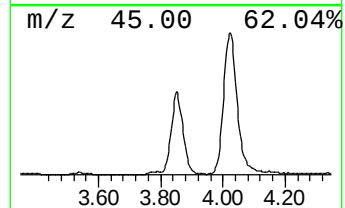
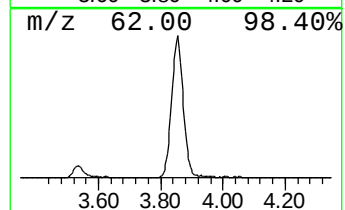
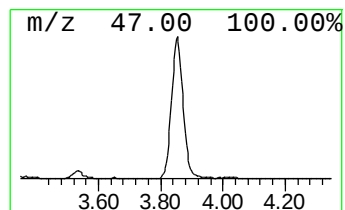
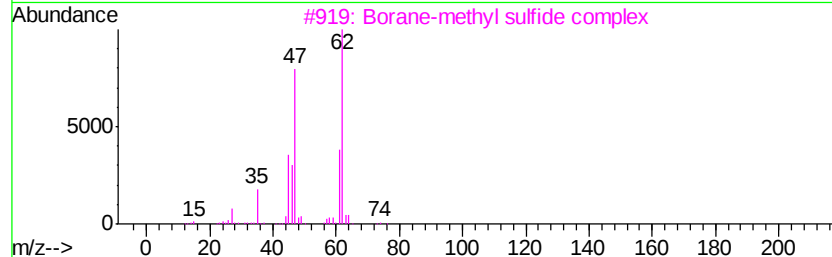
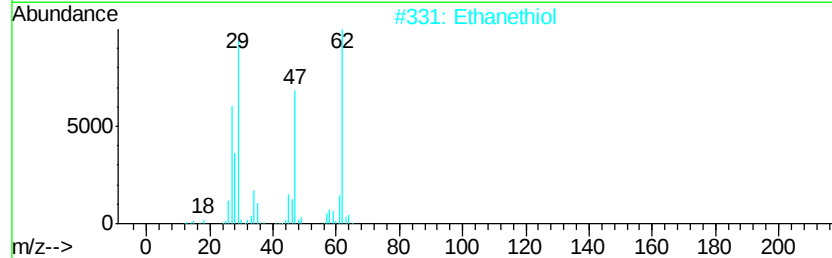
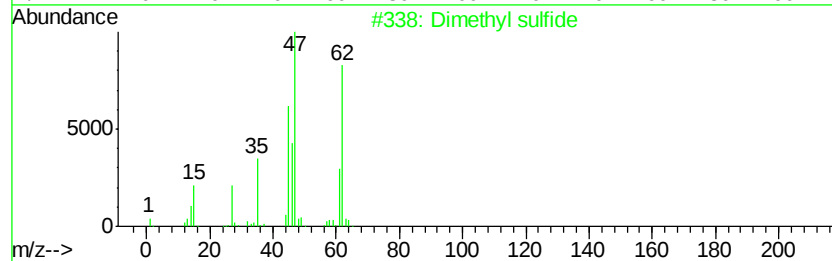
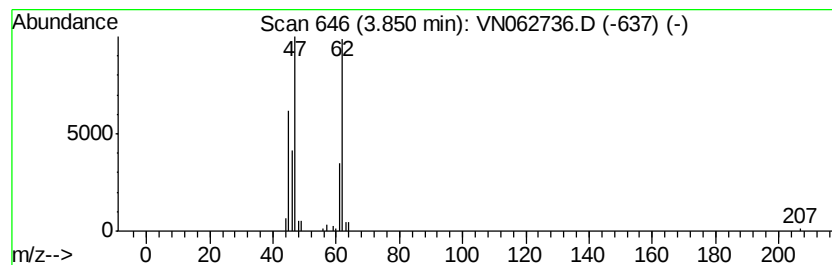
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.85	27.94 ug/l	226079	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethyl sulfide	62	C2H6S	000075-18-3	91
2		Ethanethiol	62	C2H6S	000075-08-1	72
3		Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	64
4		Acetic acid, mercapto-, methyl e...	106	C3H6O2S	002365-48-2	22
5		Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	14



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ClientSampleId :
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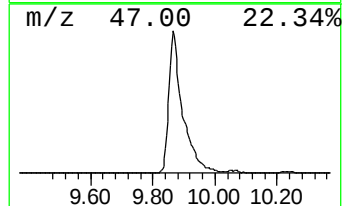
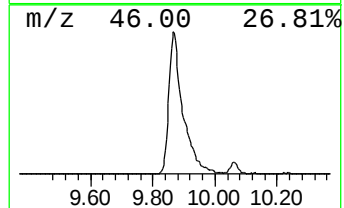
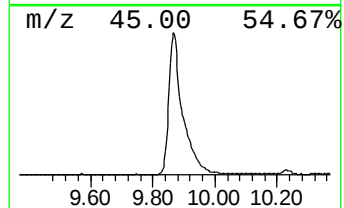
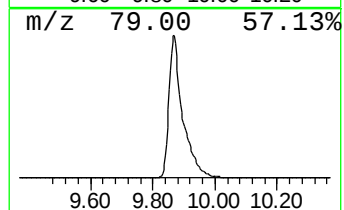
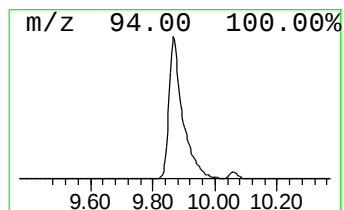
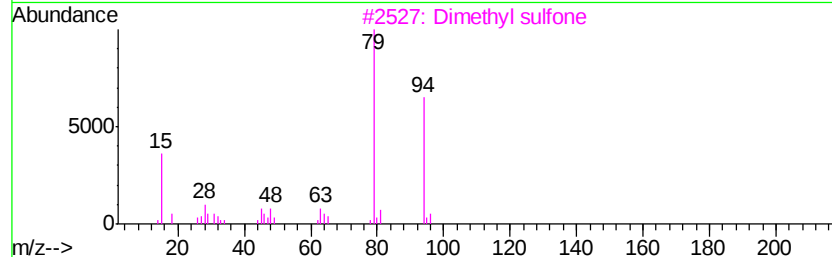
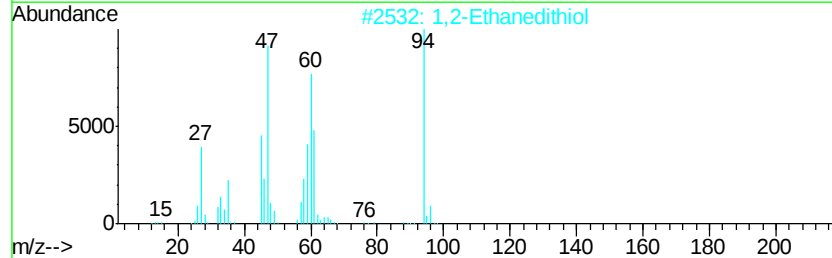
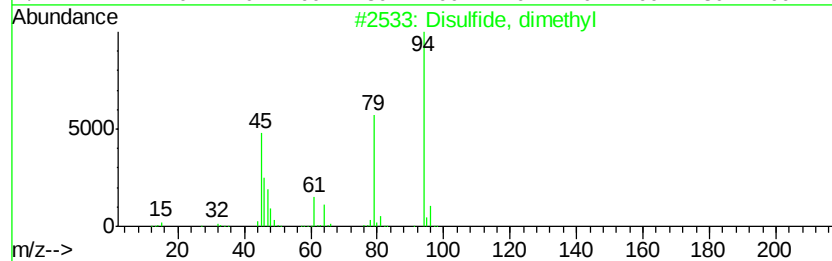
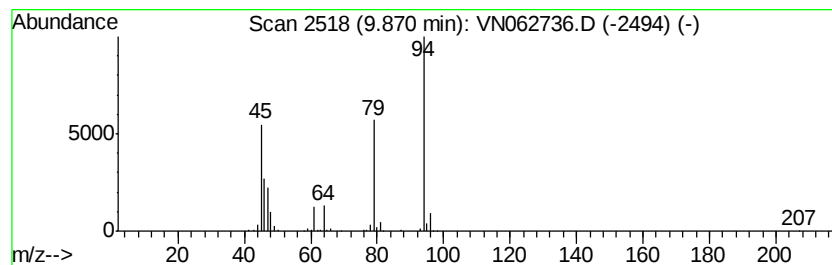
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	88.95 ug/l	993627	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2		1,2-Ethanedithiol	94	C2H6S2	000540-63-6	52
3		Dimethyl sulfone	94	C2H6O2S	000067-71-0	46
4		Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	7
5		Dimethyl ether	46	C2H6O	000115-10-6	5



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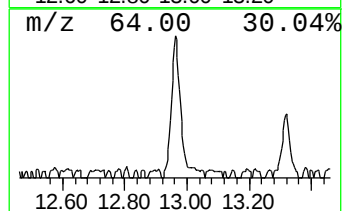
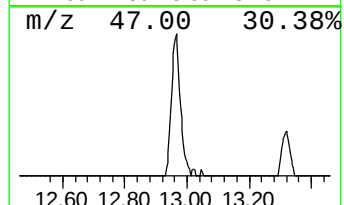
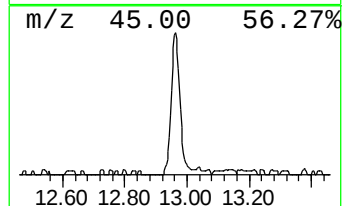
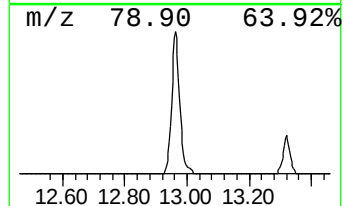
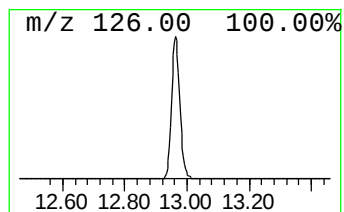
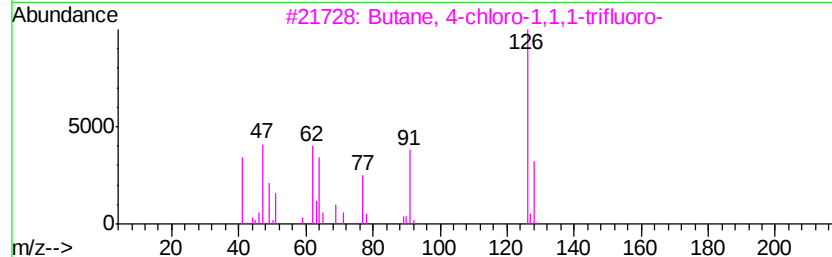
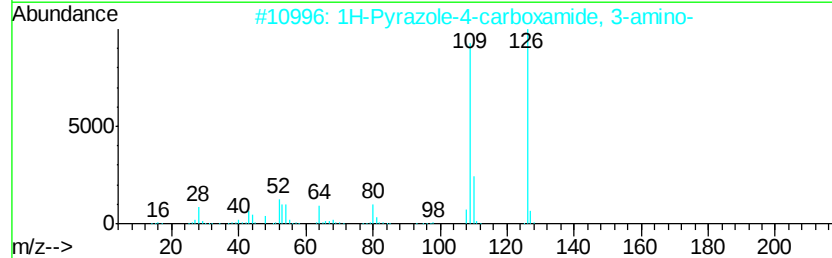
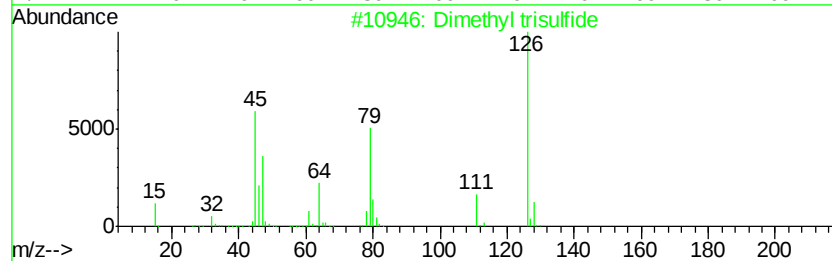
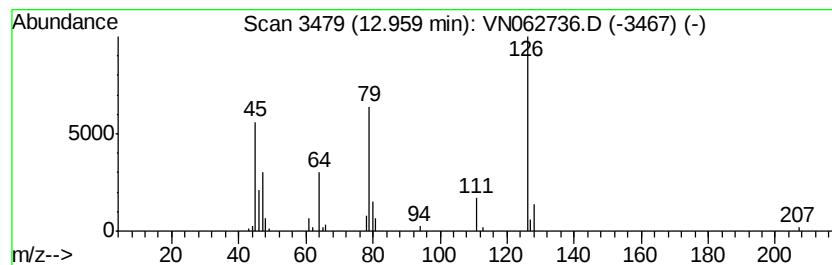
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Dimethyl trisulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.96	7.54 ug/l	87699	1,4-Dichlorobenzene-d4	13.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl trisulfide	126	C2H6S3	003658-80-8	91
2	1H-Pyrazole-4-carboxamide, 3-amino-	126	C4H6N4O	005334-31-6	27
3	Butane, 4-chloro-1,1,1-trifluoro-	146	C4H6ClF3	000406-85-9	23
4	1,3,5-Benzenetriol	126	C6H6O3	000108-73-6	16
5	S-(2,2,2-Trifluoroethyl) methane...	194	C3H5F3O2S2	069466-44-0	12



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propyne	1.92	11.1	ug/l	89981	1	7.63	404594	50.0
Methanethiol	2.42	52.2	ug/l	422038	1	7.63	404594	50.0
Dimethyl sulfide	3.85	27.9	ug/l	226079	1	7.63	404594	50.0
Disulfide, dimethyl	9.87	89.0	ug/l	993627	2	8.55	558509	50.0
Dimethyl trisulfide	12.96	7.5	ug/l	87699	4	13.32	581327	50.0