

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX041720\
 Data File : VX015750.D
 Acq On : 17 Apr 2020 19:48
 Operator : JC/SP
 Sample : L2305-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 I-L-C-1

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_X\METHOD\82X032720W.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	1.064	25	29	37	rBV	4469533	5100262	3.81%	0.996%
2	1.131	37	40	45	rBV	2061202	3072511	2.30%	0.600%
3	1.174	45	47	56	rVB	2959597	3232273	2.42%	0.631%
4	1.564	108	111	161	rVB	52742333	133767888	100.00%	26.125%
5	2.253	218	224	245	rBV	3057411	6392511	4.78%	1.248%
6	2.417	245	251	256	rBV	2980900	4669058	3.49%	0.912%
7	2.551	266	273	274	rBV4	66659200	102085300	76.32%	19.937%
8	5.472	741	752	762	rBV2	583664	1688369	1.26%	0.330%
9	5.630	768	778	796	rVB	1022267	2857141	2.14%	0.558%
10	6.032	832	844	850	rBV	630049	1641424	1.23%	0.321%
11	6.118	850	858	873	rVB	4799306	12462547	9.32%	2.434%
12	6.386	895	902	909	rBV2	698629	2027519	1.52%	0.396%
13	6.837	967	976	988	rBV	1575994	3723583	2.78%	0.727%
14	8.465	1233	1243	1252	rBV	14268253	24678411	18.45%	4.820%
15	8.697	1275	1281	1287	rBV	3317628	5174355	3.87%	1.011%
16	8.770	1287	1293	1303	rVV	4394791	6963815	5.21%	1.360%
17	8.892	1307	1313	1322	rVB	7262759	10962206	8.19%	2.141%
18	9.062	1334	1341	1347	rBV	1029882	1572619	1.18%	0.307%
19	9.629	1432	1434	1445	rVB2	812572	1347861	1.01%	0.263%
20	9.977	1482	1491	1499	rBV	1378183	2013062	1.50%	0.393%
21	10.099	1506	1511	1515	rBV	3486682	4717120	3.53%	0.921%
22	10.239	1529	1534	1538	rBV	2051432	2752985	2.06%	0.538%
23	10.343	1542	1551	1562	rVB2	9153561	16077790	12.02%	3.140%
24	10.684	1603	1607	1615	rVB	3601630	4901378	3.66%	0.957%
25	11.123	1674	1679	1685	rBV	3260857	4045512	3.02%	0.790%
26	11.702	1768	1774	1784	rVB	8224343	10956166	8.19%	2.140%
27	11.794	1784	1789	1794	rVB	2374690	2862395	2.14%	0.559%
28	12.001	1816	1823	1827	rBV	1191383	1557739	1.16%	0.304%
29	12.062	1827	1833	1839	rVB2	4439259	5815948	4.35%	1.136%
30	12.129	1839	1844	1850	rBV	1649222	2211833	1.65%	0.432%
31	13.208	2016	2021	2027	rBV2	1368061	1929916	1.44%	0.377%
32	13.702	2094	2102	2107	rBV	1011109	1517864	1.13%	0.296%
33	13.824	2116	2122	2127	rBV2	70981838	102906136	76.93%	20.098%
34	13.909	2132	2136	2143	rVB	6354778	8016242	5.99%	1.566%

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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

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Title : SW846 8260

35	14.677	2258	2262	2270	rVB	2894713	3705225	2.77%	0.724%
36	14.824	2281	2286	2293	rVB	2027771	2627224	1.96%	0.513%

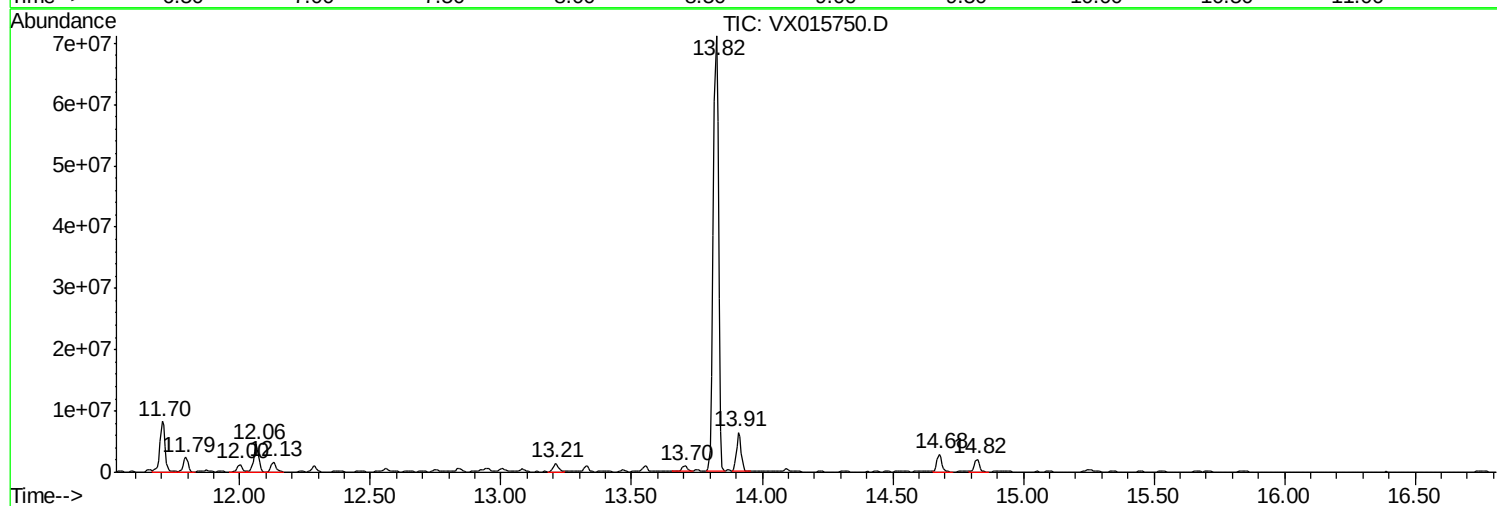
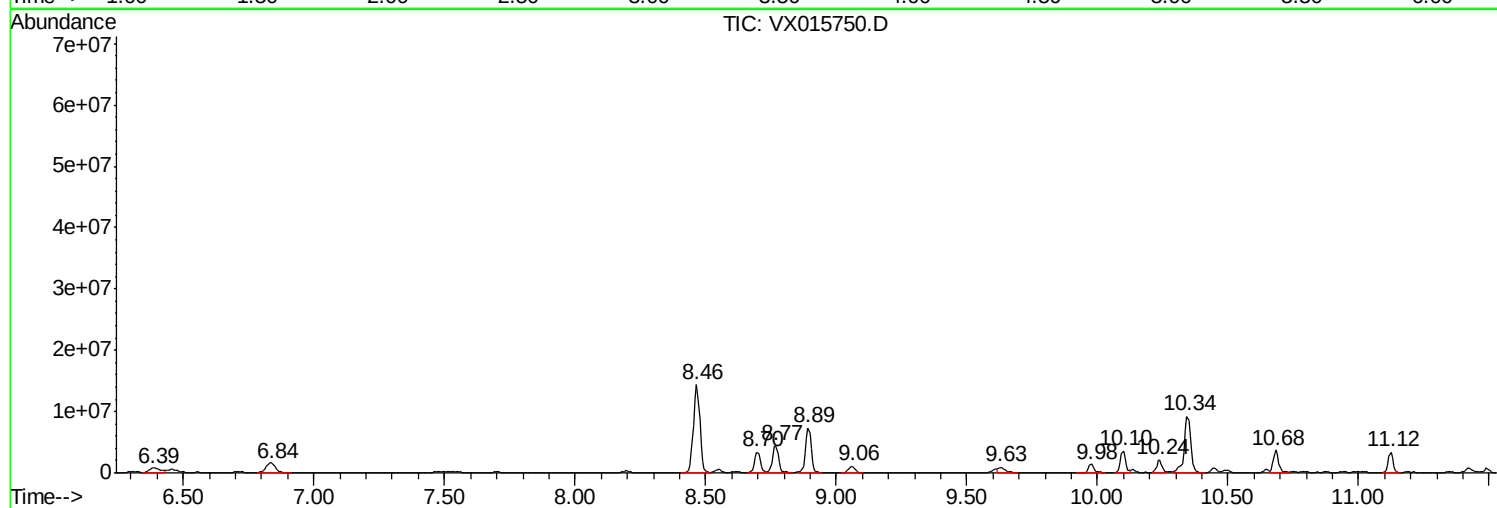
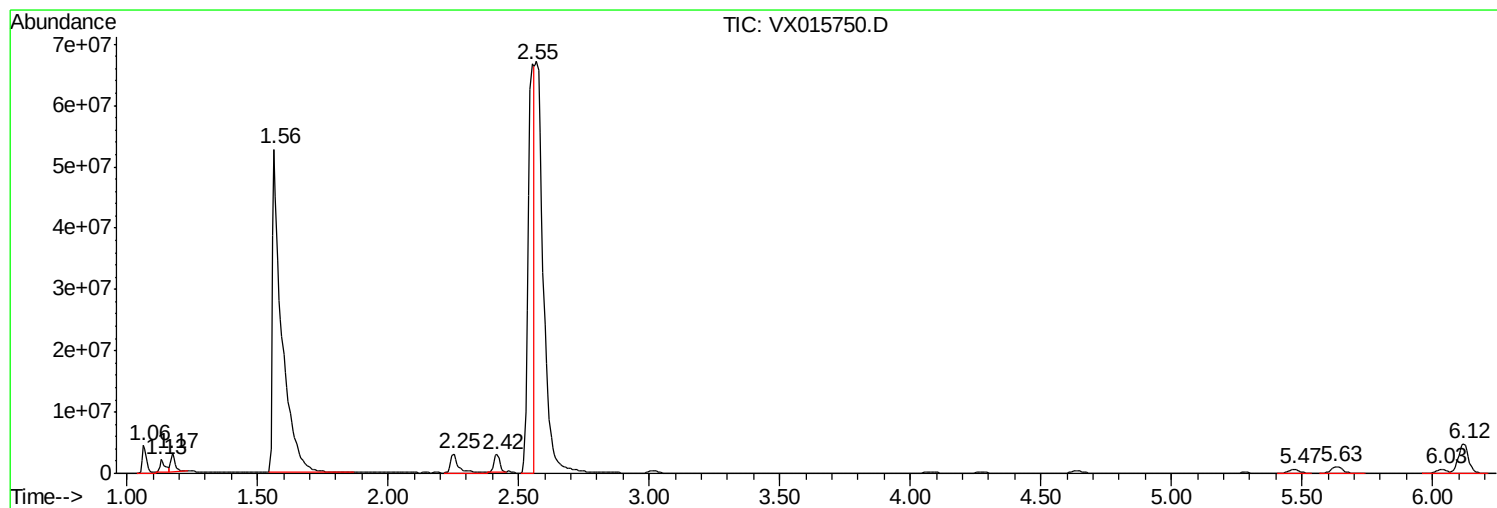
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Quant Title : SW846 8260

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



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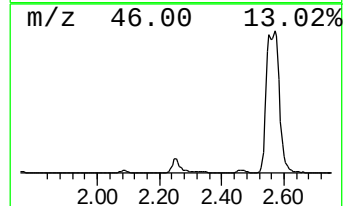
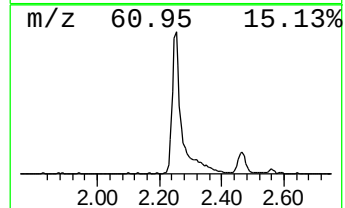
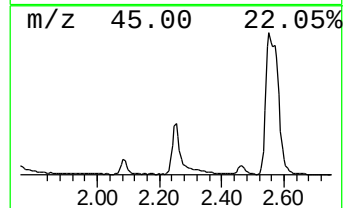
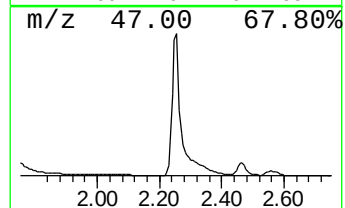
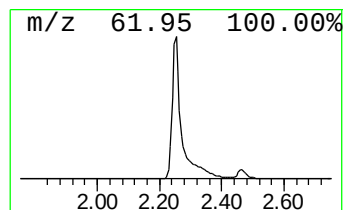
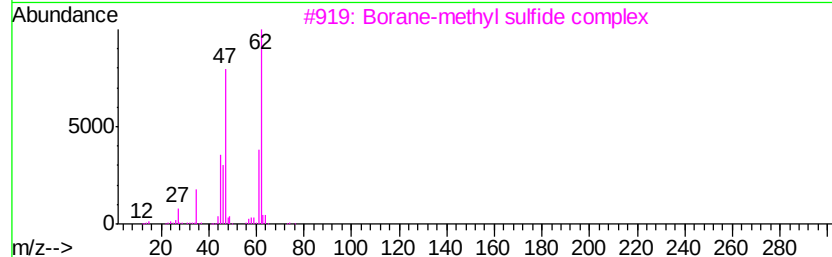
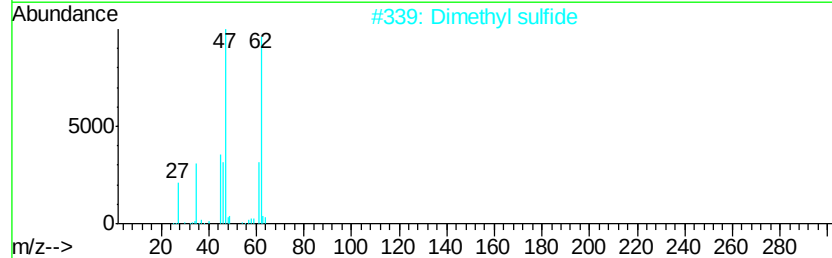
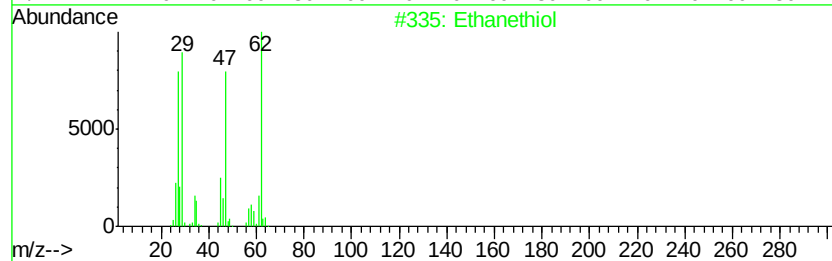
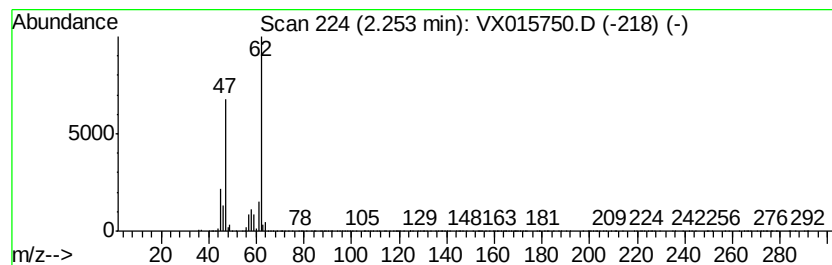
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 5 Ethanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	111.87 ug/l	6392510	Pentafluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol		62	C2H6S	000075-08-1	91
2	Dimethyl sulfide		62	C2H6S	000075-18-3	78
3	Borane-methyl sulfide complex		76	C2H9BS	013292-87-0	25
4	Ethene, chloro-		62	C2H3Cl	000075-01-4	9
5	Phosphine, ethyl-		62	C2H7P	000593-68-0	9



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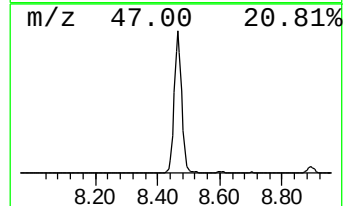
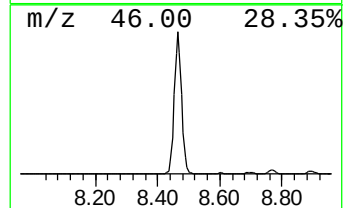
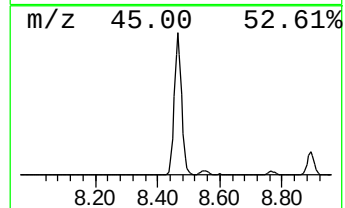
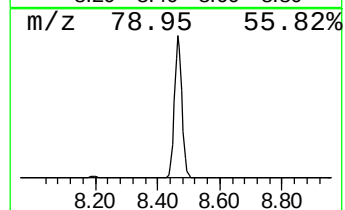
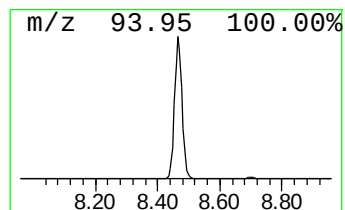
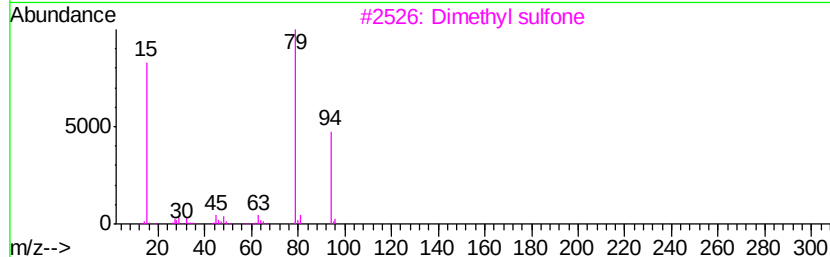
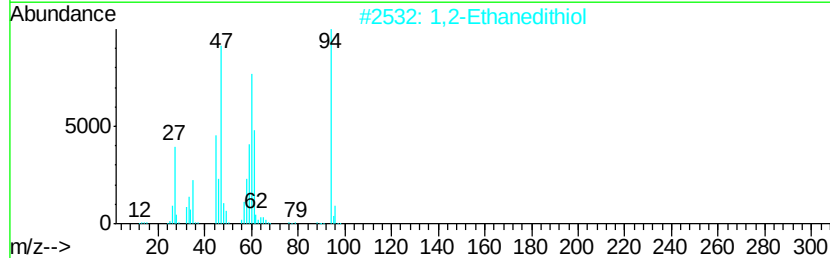
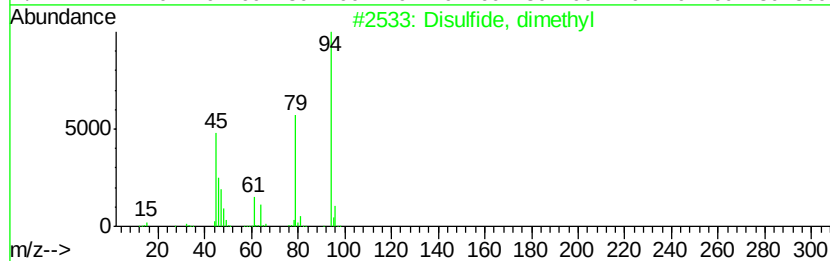
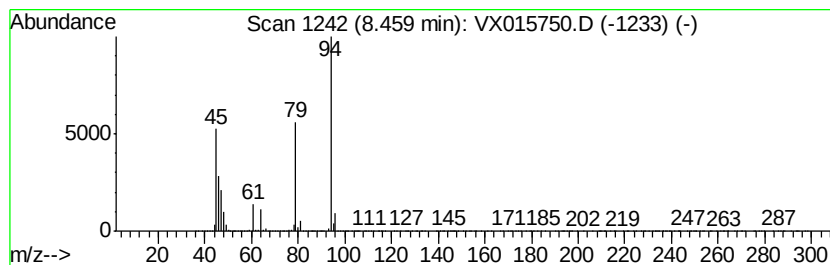
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	331.38 ug/l	24678400	1,4-Difluorobenzene	6.84

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		Methanesulfonylacetic acid	138	C3H6O4S	002516-97-4	9
5		Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	7



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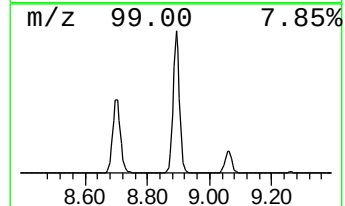
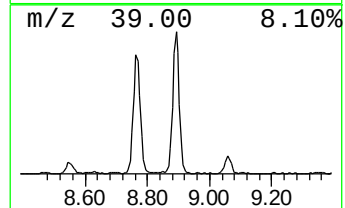
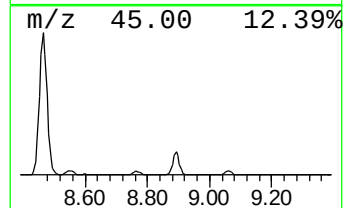
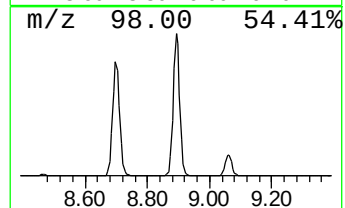
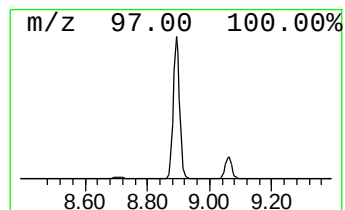
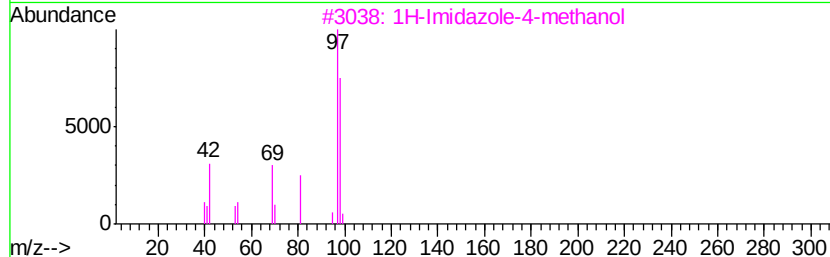
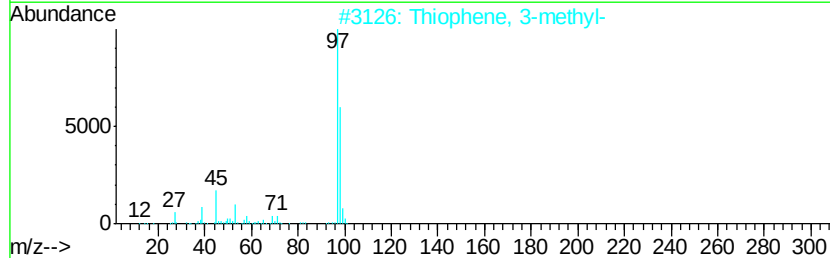
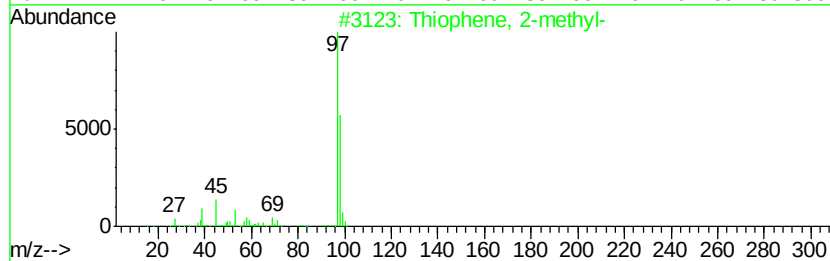
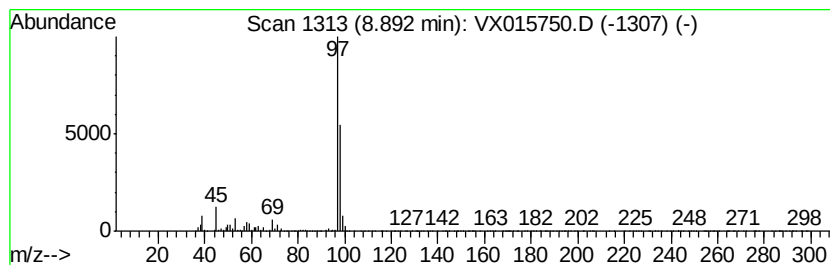
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Thiophene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	116.20 ug/l	10962200	Chlorobenzene-d5	10.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Thiophene, 2-methyl-	98	C5H6S	000554-14-3	95
2		Thiophene, 3-methyl-	98	C5H6S	000616-44-4	91
3		1H-Imidazole-4-methanol	98	C4H6N2O	000822-55-9	39
4		4-Methyl-2-pyrazolin-5-one	98	C4H6N2O	013315-23-6	25
5		Propennitrile, 3-ethoxy-2-(2-thi...	257	C10H11N03S2	1000267-97-5	16



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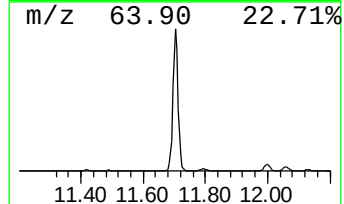
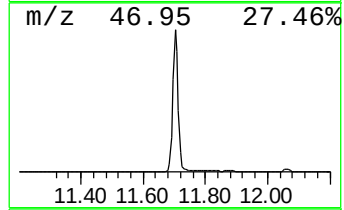
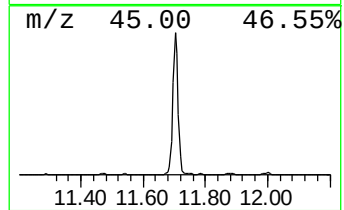
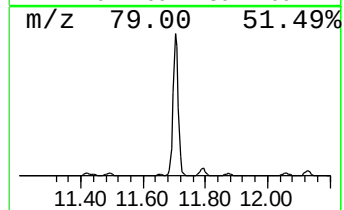
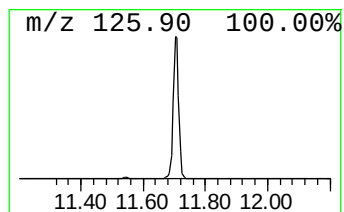
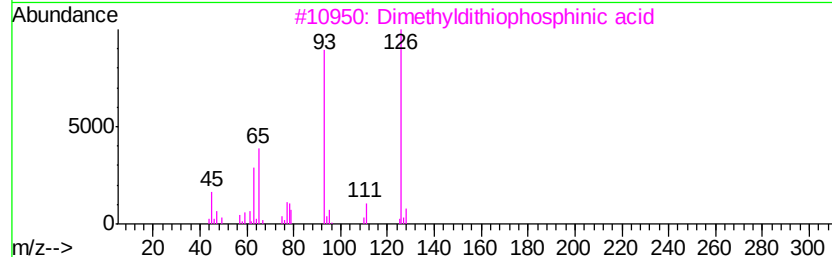
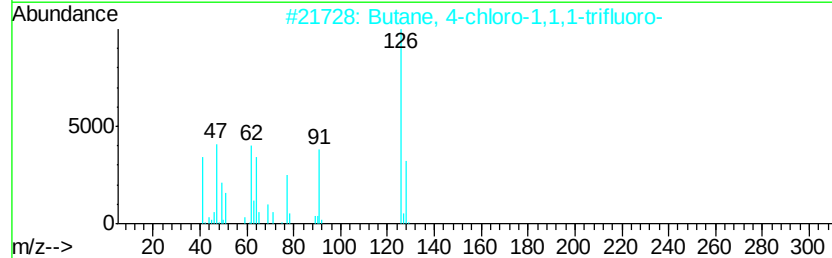
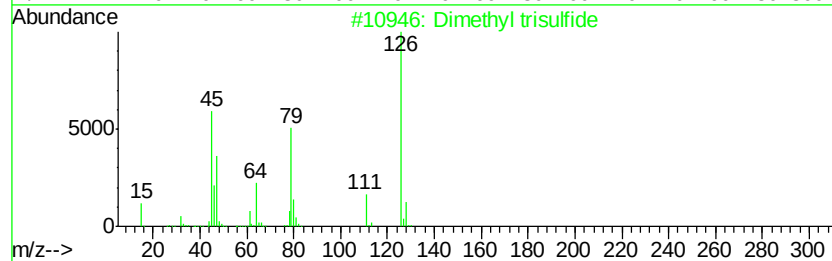
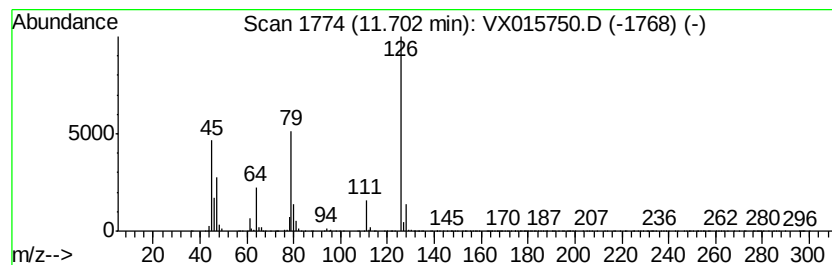
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Dimethyl trisulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	94.19 ug/l	10956200	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dimethyl trisulfide	126 C2H6S3	003658-80-8 97
2		Butane, 4-chloro-1,1,1-trifluoro-	146 C4H6ClF3	000406-85-9 23
3		Dimethyldithiophosphinic acid	126 C2H7PS2	016367-68-3 16
4		1,3,5-Benzenetriol	126 C6H6O3	000108-73-6 16
5		2,4,6-Trihydroxybenzoic acid	170 C7H6O5	000083-30-7 16



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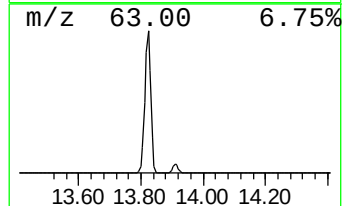
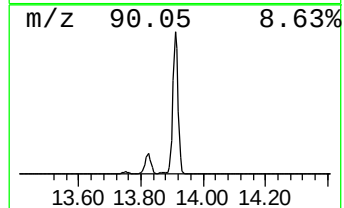
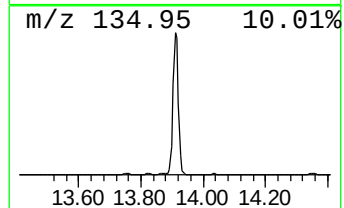
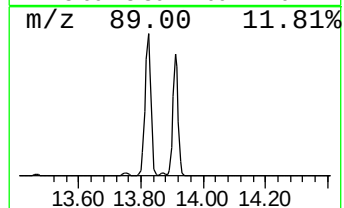
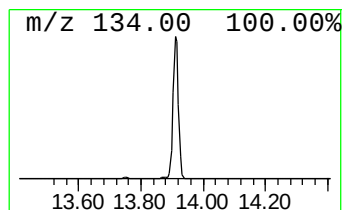
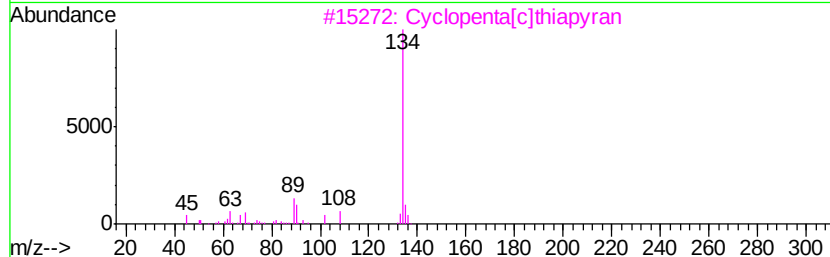
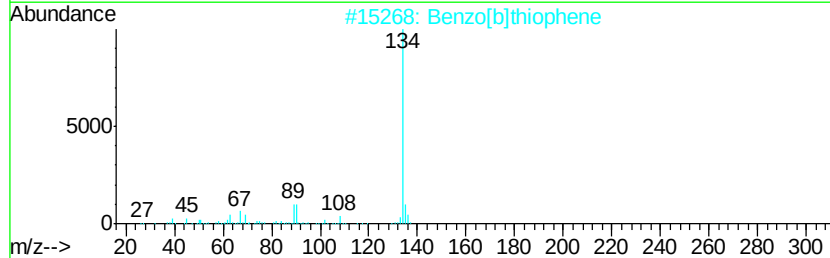
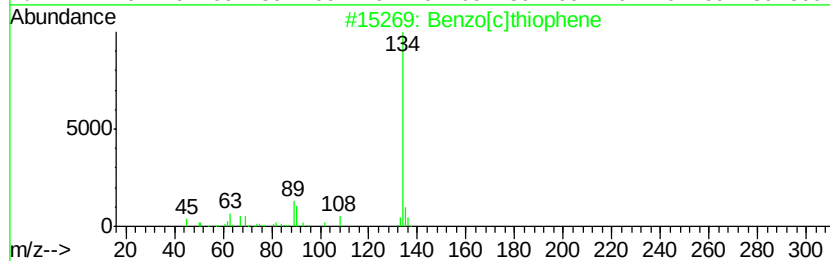
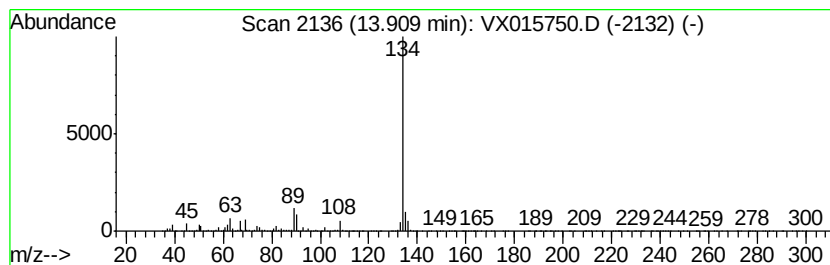
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzo[c]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	68.92 ug/l	8016240	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2		Benzo[b]thiophene	134	C8H6S	000095-15-8	95
3		Cyclopenta[c]thiopyran	134	C8H6S	000270-63-3	94
4		2H-Benzimidazol-2-one, 1,3-dihydro-	134	C7H6N2O	000615-16-7	45
5		Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015750.D
Acq On : 17 Apr 2020 19:48
Operator : JC/SP
Sample : L2305-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
I-L-C-1

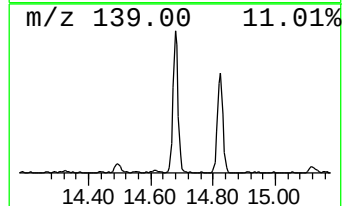
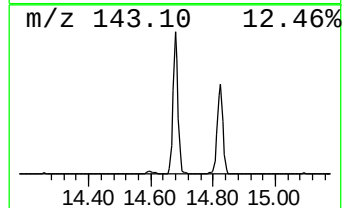
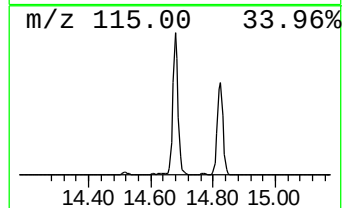
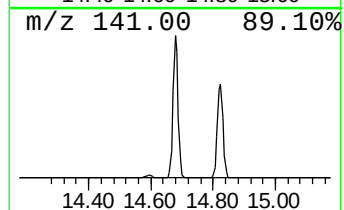
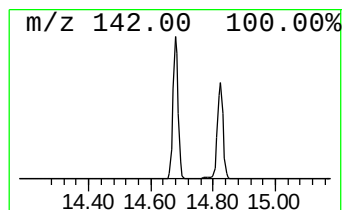
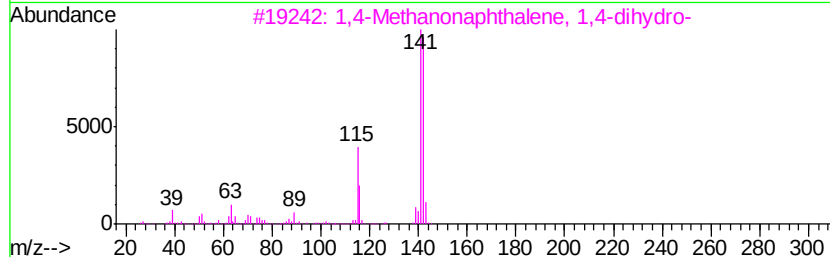
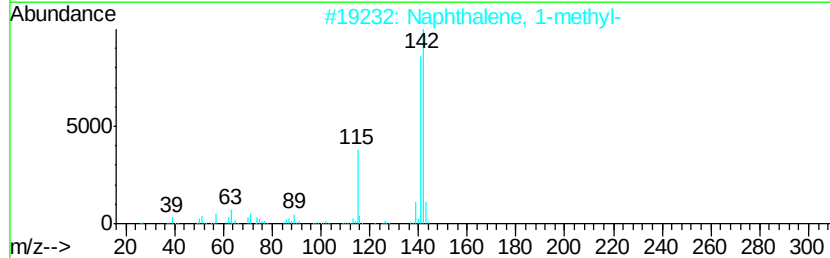
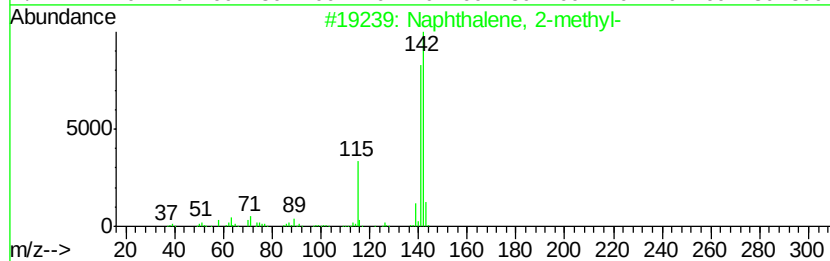
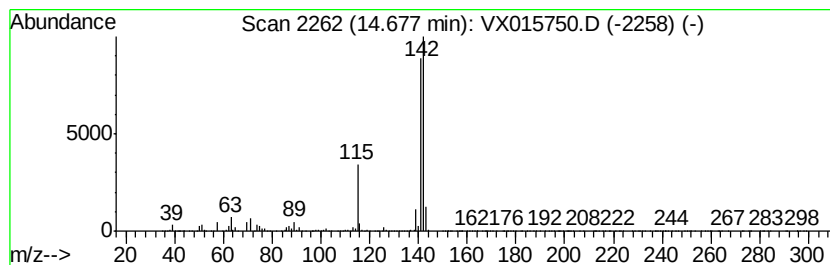
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	31.85 ug/l	3705230	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihydro-	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041720\
Data File : VX015750.D
Acq On : 17 Apr 2020 19:48
Operator : JC/SP
Sample : L2305-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
I-L-C-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanethiol	2.25	111.9	ug/l	6392510	1	5.64	2857140	50.0
Disulfide, dimethyl	8.46	331.4	ug/l	24678400	2	6.84	3723580	50.0
Thiophene, 2-methyl-	8.89	116.2	ug/l	10962200	3	10.10	4717120	50.0
Dimethyl trisulfide	11.70	94.2	ug/l	10956200	4	12.06	5815950	50.0
Benzo[c]thiophene	13.91	68.9	ug/l	8016240	4	12.06	5815950	50.0
Naphthalene, 1-me...	14.68	31.9	ug/l	3705230	4	12.06	5815950	50.0