

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072019\
 Data File : VU033351.D
 Acq On : 20 Jul 2019 00:43
 Operator : JC/SP
 Sample : K3890-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A52S1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_U\METHOD\SOMUTR071619WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.392	60	94	108	rBV2	315498	516293	16.73%	4.277%
2	1.688	174	186	211	rVB	741394	1020532	33.07%	8.454%
3	2.264	353	365	375	rBV3	160057	284869	9.23%	2.360%
4	2.312	375	380	388	rVV2	25709	41033	1.33%	0.340%
5	2.363	389	396	408	rVB	39374	61328	1.99%	0.508%
6	2.604	461	471	482	rBV	38347	63879	2.07%	0.529%
7	3.421	706	725	751	rBV	697199	1526599	49.47%	12.647%
8	4.193	944	965	986	rBV2	110630	397555	12.88%	3.293%
9	4.624	1079	1099	1115	rBV	77910	185586	6.01%	1.537%
10	4.887	1163	1181	1198	rBV	486692	1145732	37.13%	9.491%
11	4.964	1198	1205	1221	rVB4	15838	33850	1.10%	0.280%
12	5.315	1292	1314	1340	rBV3	145942	409433	13.27%	3.392%
13	5.865	1472	1485	1504	rBV2	131440	258072	8.36%	2.138%
14	6.164	1566	1578	1599	rVB2	40920	80942	2.62%	0.671%
15	6.312	1609	1624	1641	rBV	102209	201829	6.54%	1.672%
16	7.209	1892	1903	1926	rBV	47022	83903	2.72%	0.695%
17	7.546	1992	2008	2018	rBV	178257	308151	9.99%	2.553%
18	7.617	2018	2030	2061	rVB	1844504	3085699	100.00%	25.563%
19	7.832	2087	2097	2114	rVB2	30822	55163	1.79%	0.457%
20	8.299	2225	2242	2276	rBV	275552	507546	16.45%	4.205%
21	8.971	2436	2451	2468	rBV2	75602	124573	4.04%	1.032%
22	9.074	2471	2483	2505	rBV	207932	348584	11.30%	2.888%
23	9.234	2521	2533	2551	rVB	32914	53429	1.73%	0.443%
24	9.363	2557	2573	2588	rBV2	28292	50058	1.62%	0.415%
25	9.762	2688	2697	2710	rVB	37515	60594	1.96%	0.502%
26	10.299	2855	2864	2876	rVB	41509	66537	2.16%	0.551%
27	10.418	2889	2901	2912	rBV	100591	164809	5.34%	1.365%
28	10.646	2961	2972	2985	rBV2	41700	67955	2.20%	0.563%
29	11.466	3216	3227	3248	rBV2	237278	395747	12.83%	3.278%
30	11.752	3304	3316	3332	rBV2	72198	124603	4.04%	1.032%
31	11.845	3334	3345	3364	rVV	203766	346297	11.22%	2.869%

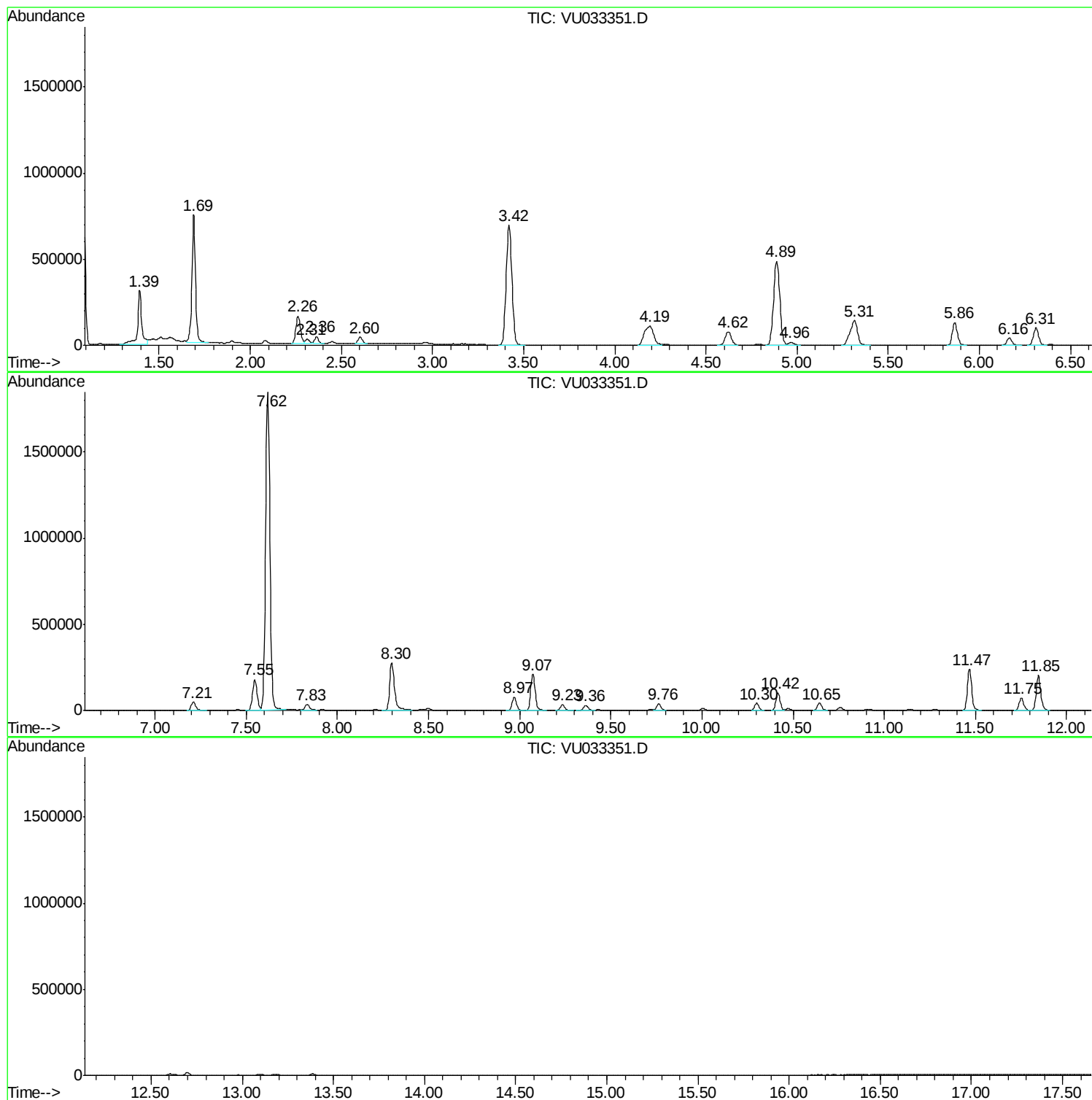
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ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A52S1

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR071619WMA.M
Quant Title : TRACE VOA SOM01.0

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



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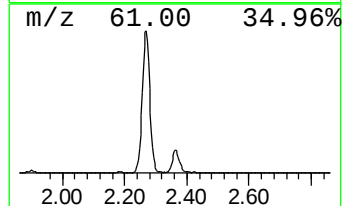
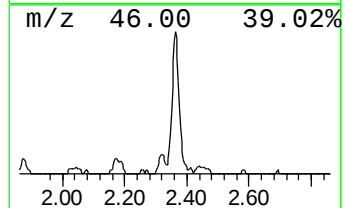
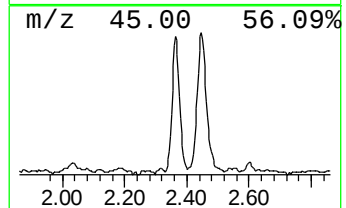
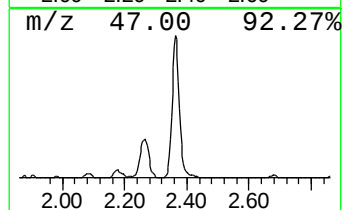
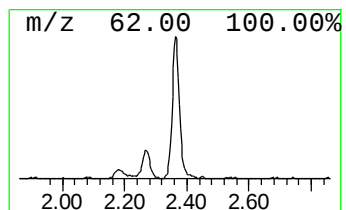
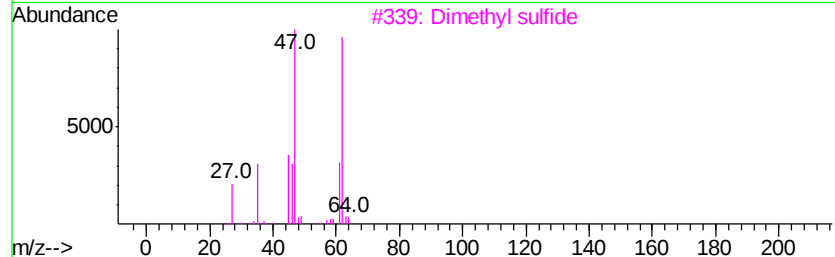
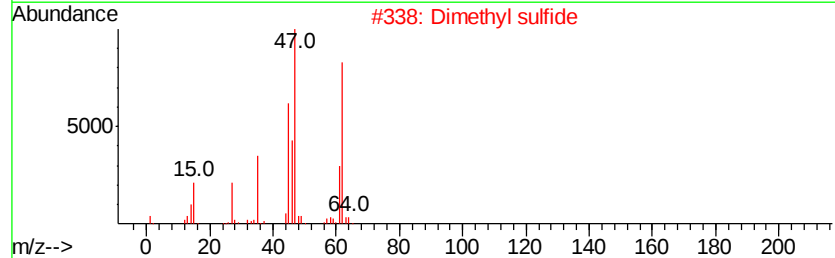
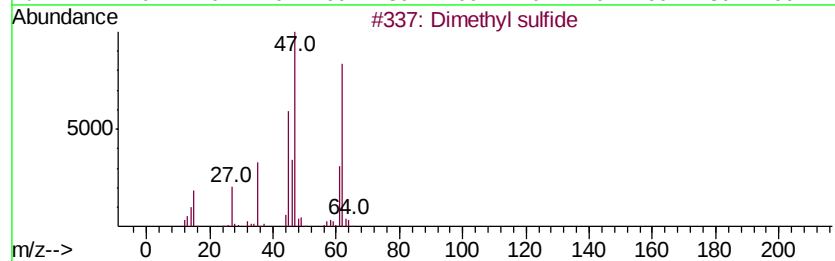
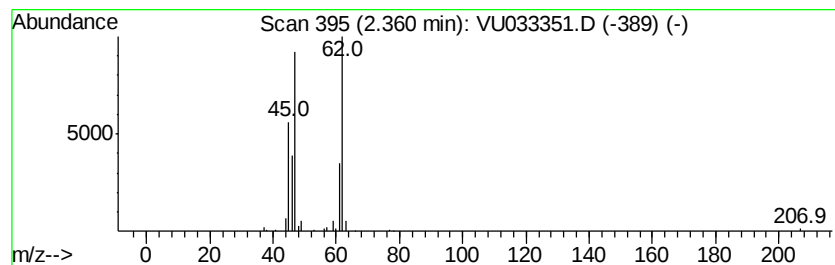
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Dimethyl sulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.36	1.19 ug/L	61328	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethyl sulfide	62	C2H6S	000075-18-3	91
2		Dimethyl sulfide	62	C2H6S	000075-18-3	91
3		Dimethyl sulfide	62	C2H6S	000075-18-3	91
4		Dimethyl sulfide	62	C2H6S	000075-18-3	91
5		Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83



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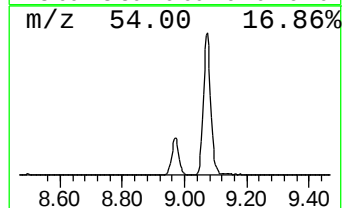
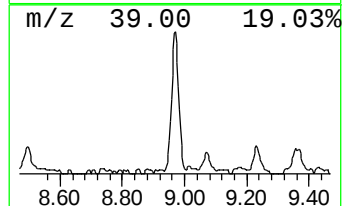
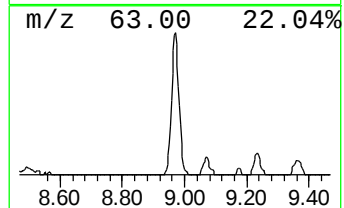
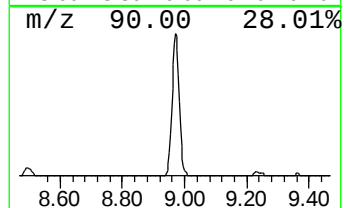
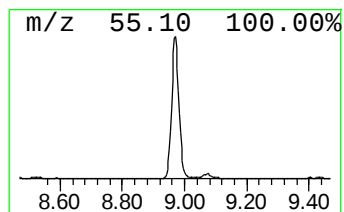
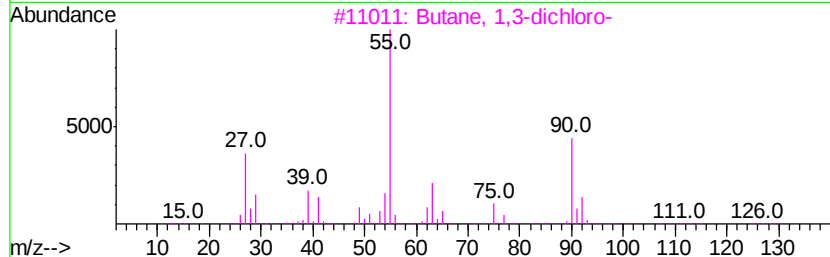
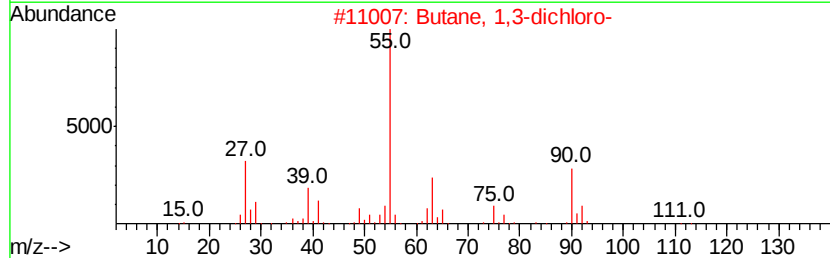
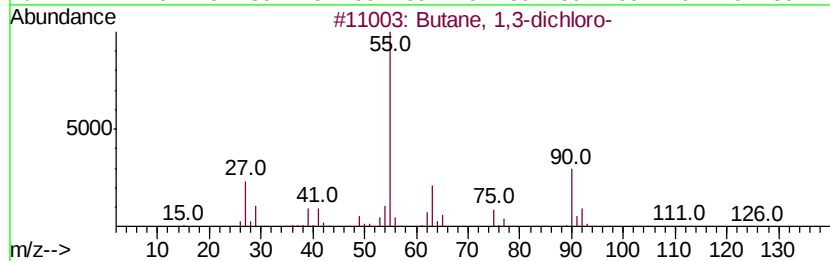
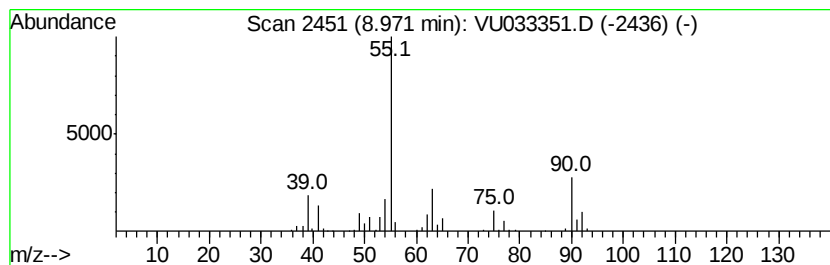
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Butane, 1,3-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	1.79 ug/L	124573	Chlorobenzene-d5	9.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 1,3-dichloro-	126	C4H8Cl2	001190-22-3	90
2		Butane, 1,3-dichloro-	126	C4H8Cl2	001190-22-3	90
3		Butane, 1,3-dichloro-	126	C4H8Cl2	001190-22-3	83
4		2-Butene, 1-chloro-	90	C4H7Cl	000591-97-9	74
5		1-Propene, 1-chloro-2-methyl-	90	C4H7Cl	000513-37-1	68



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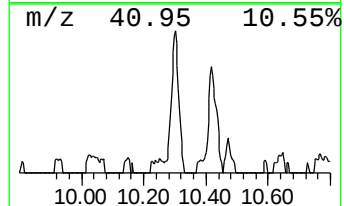
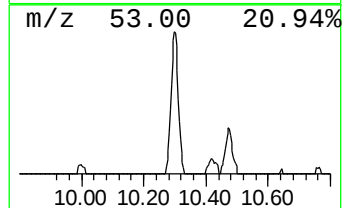
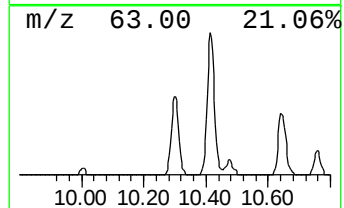
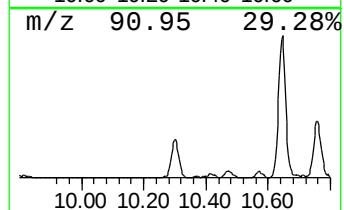
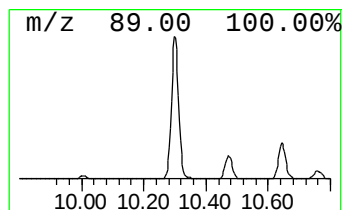
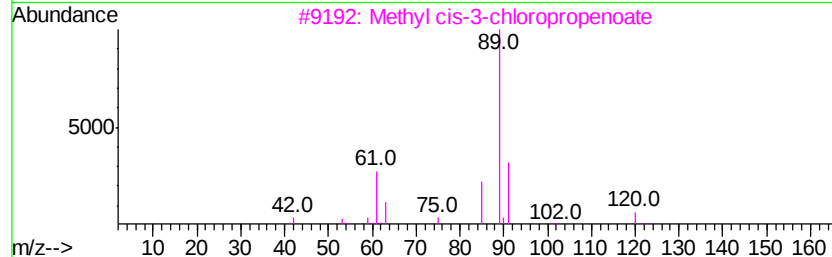
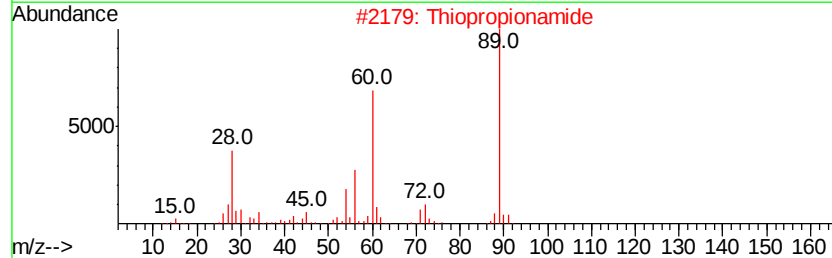
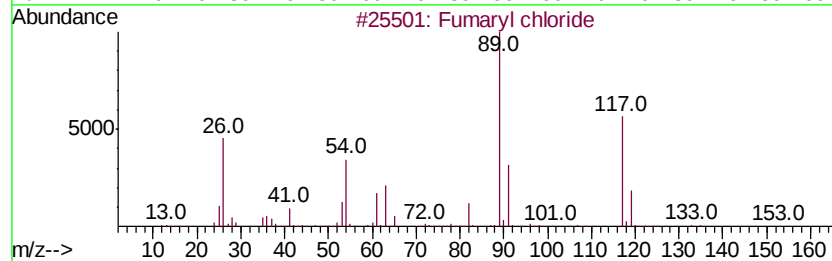
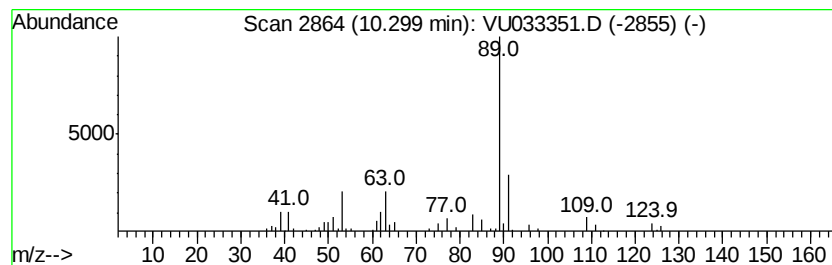
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	0.84 ug/L	66537	1,4-Dichlorobenzene-d4	11.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Fumaryl chloride	152	C4H2Cl2O2	000627-63-4	39
2		Thiopropionamide	89	C3H7NS	000631-58-3	38
3		Methyl cis-3-chloropropenoate	120	C4H5ClO2	1000144-78-7	38
4		Methyl trans-3-chloropropenoate	120	C4H5ClO2	1000144-78-8	38
5		Fumaryl chloride	152	C4H2Cl2O2	000627-63-4	9



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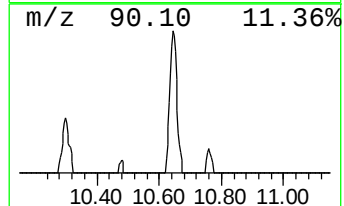
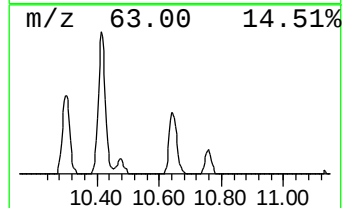
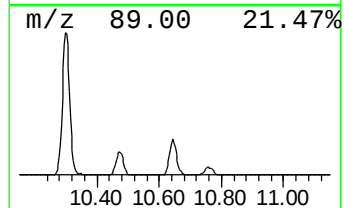
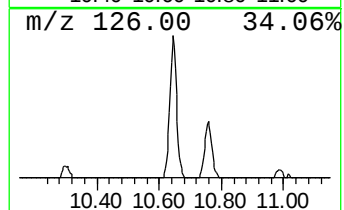
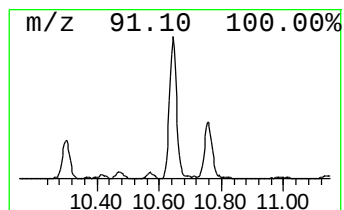
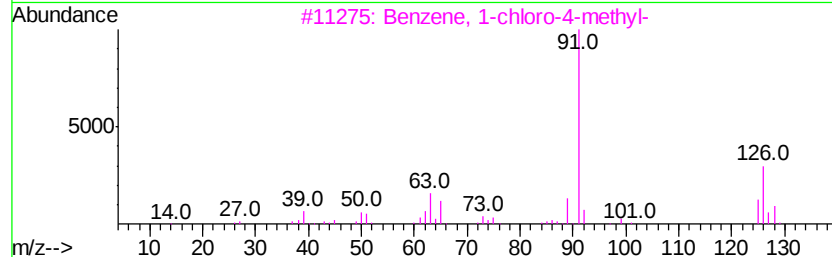
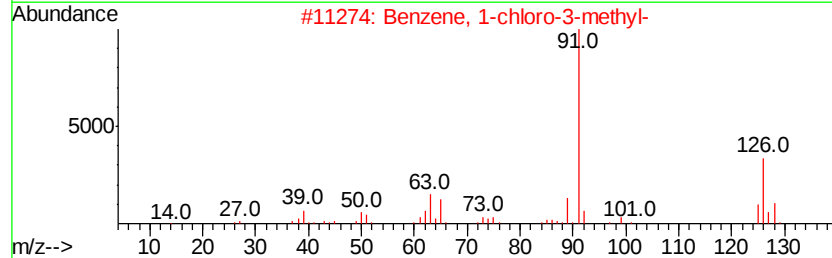
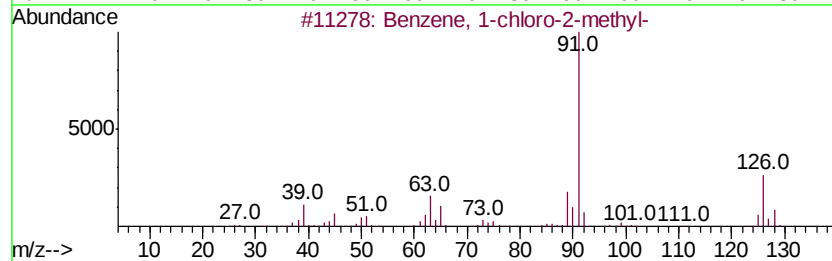
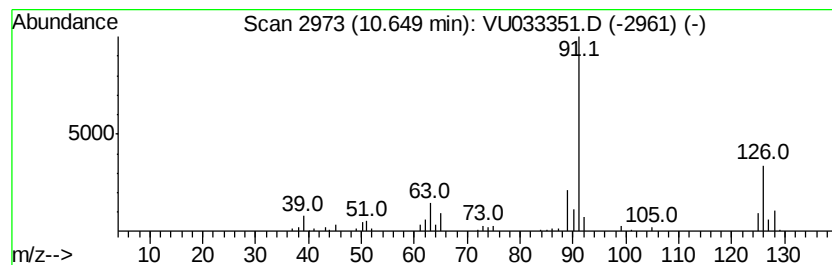
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzene, 1-chloro-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	0.86 ug/L	67955	1,4-Dichlorobenzene-d4	11.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	96
2		Benzene, 1-chloro-3-methyl-	126	C7H7Cl	000108-41-8	95
3		Benzene, 1-chloro-4-methyl-	126	C7H7Cl	000106-43-4	95
4		Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94
5		Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94



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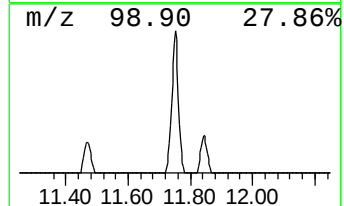
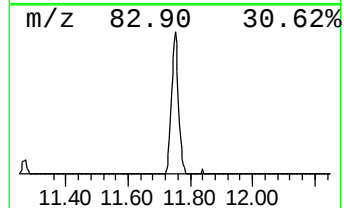
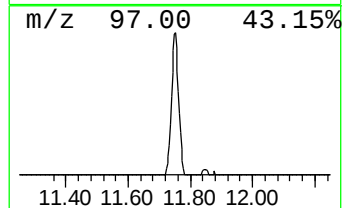
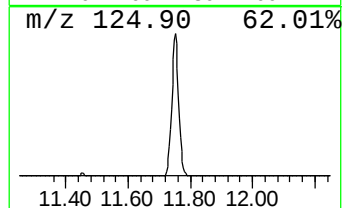
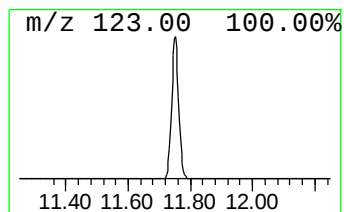
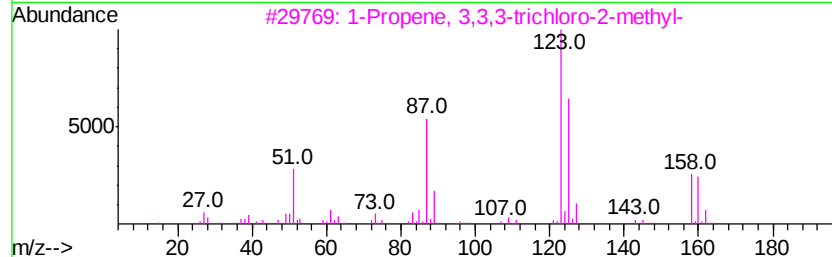
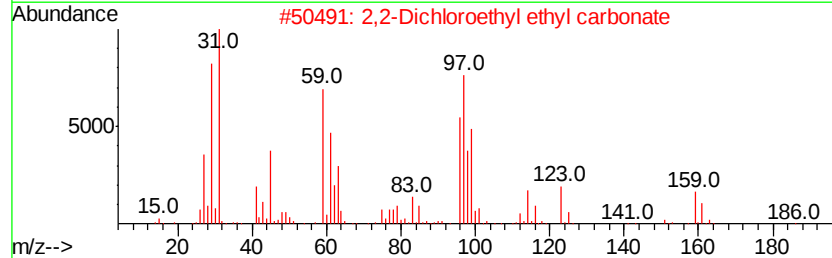
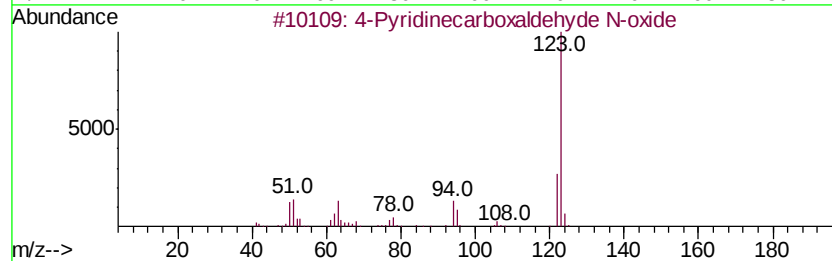
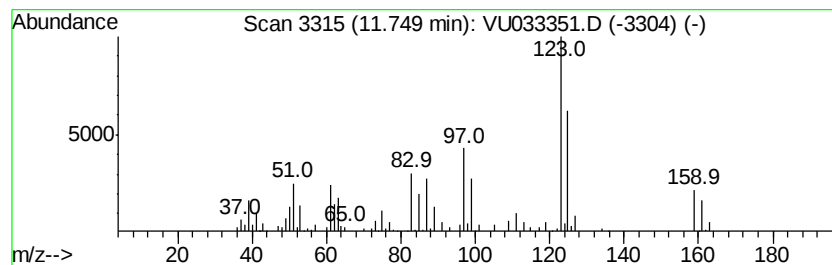
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.75	1.57 ug/L	124603	1,4-Dichlorobenzene-d4	11.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridinecarboxaldehyde N-oxide	123	C6H5NO2	007216-42-4	27
2	2,2-Dichloroethyl ethyl carbonate	186	C5H8Cl2O3	1000373-78-3	25
3	1-Propene, 3,3,3-trichloro-2-met...	158	C4H5Cl3	004749-27-3	16
4	Methyl 3,3-dichloropropenoate	154	C4H4Cl2O2	002257-46-7	16
5	Benzoyl chloride, 2-fluoro-	158	C7H4ClFO	000393-52-2	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl sulfide	2.36	1.2	ug/L	61328	1	5.86	258072	5.0
Butane, 1,3-dichl...	8.97	1.8	ug/L	124573	2	9.07	348584	5.0
unknown-01	10.30	0.8	ug/L	66537	3	11.47	395747	5.0
Benzene, 1-chloro...	10.65	0.9	ug/L	67955	3	11.47	395747	5.0
unknown-02	11.75	1.6	ug/L	124603	3	11.47	395747	5.0