

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
 Data File : VU025401.D
 Acq On : 13 Jul 2018 20:44
 Operator : MD/SY
 Sample : J3984-08
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB182

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % 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\SOMULM062918WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	0.632	9	13	17	rBV3	684	653	0.02%	0.004%
2	0.728	40	43	47	rBV6	679	618	0.01%	0.004%
3	0.770	51	56	62	rVB5	791	853	0.02%	0.005%
4	0.825	69	73	75	rBV3	955	724	0.02%	0.004%
5	0.944	105	110	114	rVV4	558	592	0.01%	0.003%
6	1.085	145	154	176	rBV	3901938	4325758	100.00%	25.502%
7	1.404	245	253	270	rBV	1911224	2116470	48.93%	12.477%
8	1.561	296	302	308	rBV	147480	143310	3.31%	0.845%
9	1.680	333	339	358	rVB	91105	124910	2.89%	0.736%
10	2.275	515	524	535	rVB	205886	302562	6.99%	1.784%
11	2.381	549	557	577	rVB2	40482	70882	1.64%	0.418%
12	2.481	581	588	600	rBV2	8490	14218	0.33%	0.084%
13	2.612	620	629	643	rBV	45997	76201	1.76%	0.449%
14	2.989	738	746	754	rBV8	4421	8028	0.19%	0.047%
15	3.628	943	945	948	rVB4	1197	581	0.01%	0.003%
16	3.645	948	950	953	rBV2	1138	908	0.02%	0.005%
17	3.712	968	971	974	rBV4	776	575	0.01%	0.003%
18	3.754	981	984	986	rVV3	895	602	0.01%	0.004%
19	3.792	990	996	997	rBV4	874	795	0.02%	0.005%
20	3.815	1001	1003	1010	rVV6	792	645	0.01%	0.004%
21	4.175	1086	1115	1119	rBV	97648	219419	5.07%	1.294%
22	4.230	1122	1132	1160	rVB	436237	1061050	24.53%	6.255%
23	4.651	1248	1263	1285	rVB	181086	420705	9.73%	2.480%
24	4.789	1302	1306	1309	rBV4	1530	1553	0.04%	0.009%
25	4.873	1327	1332	1338	rBV6	1596	2199	0.05%	0.013%
26	4.927	1346	1349	1352	rBV2	784	597	0.01%	0.004%
27	4.973	1359	1363	1365	rBV4	797	704	0.02%	0.004%
28	5.246	1443	1448	1450	rBV5	598	632	0.01%	0.004%
29	5.342	1453	1478	1502	rBV2	345646	1048881	24.25%	6.184%
30	5.590	1552	1555	1558	rVV4	765	640	0.01%	0.004%
31	5.889	1624	1648	1669	rBV	396318	836865	19.35%	4.934%
32	6.333	1771	1786	1803	rBV	231985	473597	10.95%	2.792%
33	6.606	1867	1871	1875	rBV5	1976	2340	0.05%	0.014%
34	6.667	1887	1890	1894	rBV4	1094	655	0.02%	0.004%

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 Title : VOC Analysis

35	6.738	1909	1912	1914	rBV3	953	726	0.02%	0.004%
36	6.850	1940	1947	1955	rVB9	3270	5646	0.13%	0.033%
37	6.918	1964	1968	1972	rVB4	820	631	0.01%	0.004%
38	7.230	2053	2065	2085	rVV	135212	241457	5.58%	1.423%
39	7.339	2085	2099	2125	rVV	265289	484804	11.21%	2.858%
40	7.506	2149	2151	2154	rBV3	1034	650	0.02%	0.004%
41	7.567	2157	2170	2184	rBV	486351	841699	19.46%	4.962%
42	7.850	2247	2258	2275	rBV	96812	162238	3.75%	0.956%
43	7.937	2282	2285	2287	rBV5	894	628	0.01%	0.004%
44	7.969	2292	2295	2299	rBV4	929	807	0.02%	0.005%
45	8.136	2342	2347	2349	rBV4	861	639	0.01%	0.004%
46	8.181	2352	2361	2370	rVV2	6245	10709	0.25%	0.063%
47	8.310	2389	2401	2419	rBV	327944	570631	13.19%	3.364%
48	8.461	2445	2448	2453	rBV4	1204	1206	0.03%	0.007%
49	8.551	2472	2476	2479	rBV4	561	549	0.01%	0.003%
50	8.686	2516	2518	2523	rVB5	998	602	0.01%	0.004%
51	8.712	2523	2526	2528	rBV2	969	615	0.01%	0.004%
52	8.799	2546	2553	2554	rBV6	851	721	0.02%	0.004%
53	8.950	2589	2600	2616	rVV	54389	92625	2.14%	0.546%
54	9.091	2632	2644	2671	rBV	529604	891220	20.60%	5.254%
55	9.252	2685	2694	2704	rVV3	6117	9696	0.22%	0.057%
56	9.381	2725	2734	2742	rBV2	12516	19445	0.45%	0.115%
57	9.439	2748	2752	2754	rVB5	894	652	0.02%	0.004%
58	9.561	2786	2790	2793	rBV4	1180	1010	0.02%	0.006%
59	9.583	2794	2797	2801	rBV5	882	671	0.02%	0.004%
60	9.738	2841	2845	2850	rBV6	737	845	0.02%	0.005%
61	9.783	2850	2859	2868	rBV2	10845	17233	0.40%	0.102%
62	9.918	2896	2901	2902	rBV2	2427	1929	0.04%	0.011%
63	10.030	2932	2936	2937	rBV3	759	561	0.01%	0.003%
64	10.056	2939	2944	2948	rVB5	1715	2007	0.05%	0.012%
65	10.149	2969	2973	2975	rBV3	795	686	0.02%	0.004%
66	10.168	2975	2979	2981	rVV4	740	591	0.01%	0.003%
67	10.252	2998	3005	3014	rVB4	5507	8285	0.19%	0.049%
68	10.435	3045	3062	3086	rVB	338803	553704	12.80%	3.264%
69	10.612	3107	3117	3125	rBV	8440	14232	0.33%	0.084%
70	10.895	3203	3205	3213	rVB5	510	557	0.01%	0.003%
71	11.139	3278	3281	3284	rBV5	875	540	0.01%	0.003%

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72	11.255	3310	3317	3329	rVB3	8223	12724	0.29%	0.075%
73	11.345	3332	3345	3349	rBV5	3209	5054	0.12%	0.030%
74	11.487	3376	3389	3406	rVB	540277	851490	19.68%	5.020%
75	11.557	3407	3411	3412	rBV3	910	582	0.01%	0.003%
76	11.641	3433	3437	3441	rBV3	670	600	0.01%	0.004%
77	11.744	3465	3469	3471	rBV2	1053	861	0.02%	0.005%
78	11.799	3483	3486	3489	rVV5	1094	629	0.01%	0.004%
79	11.863	3493	3506	3525	rVB	503219	796264	18.41%	4.694%
80	11.985	3542	3544	3546	rBV2	1270	847	0.02%	0.005%
81	12.281	3631	3636	3640	rBV5	631	661	0.02%	0.004%
82	12.422	3676	3680	3683	rBV3	882	703	0.02%	0.004%
83	12.487	3689	3700	3707	rVV2	5126	9339	0.22%	0.055%
84	12.535	3711	3715	3716	rVV2	901	684	0.02%	0.004%
85	12.570	3717	3726	3741	rVV2	30537	47173	1.09%	0.278%
86	12.628	3741	3744	3749	rVB3	728	549	0.01%	0.003%
87	12.776	3785	3790	3794	rVV5	779	856	0.02%	0.005%
88	12.805	3795	3799	3805	rVB5	615	693	0.02%	0.004%
89	12.898	3824	3828	3832	rBV6	603	547	0.01%	0.003%
90	13.008	3858	3862	3864	rBV3	1047	910	0.02%	0.005%
91	13.046	3872	3874	3875	rBV	1314	556	0.01%	0.003%
92	13.117	3891	3896	3901	rVB7	1233	1410	0.03%	0.008%
93	13.207	3916	3924	3929	rBV5	1065	1028	0.02%	0.006%
94	13.332	3953	3963	3971	rBV7	7556	17138	0.40%	0.101%
95	13.831	4116	4118	4122	rVB3	1330	736	0.02%	0.004%
96	14.056	4184	4188	4189	rVV4	1198	764	0.02%	0.005%
97	14.065	4189	4191	4195	rVB4	982	690	0.02%	0.004%
98	14.281	4252	4258	4266	rVB2	4033	5980	0.14%	0.035%
99	14.352	4278	4280	4283	rBV2	946	593	0.01%	0.003%
100	14.901	4448	4451	4454	rBV3	1799	1259	0.03%	0.007%

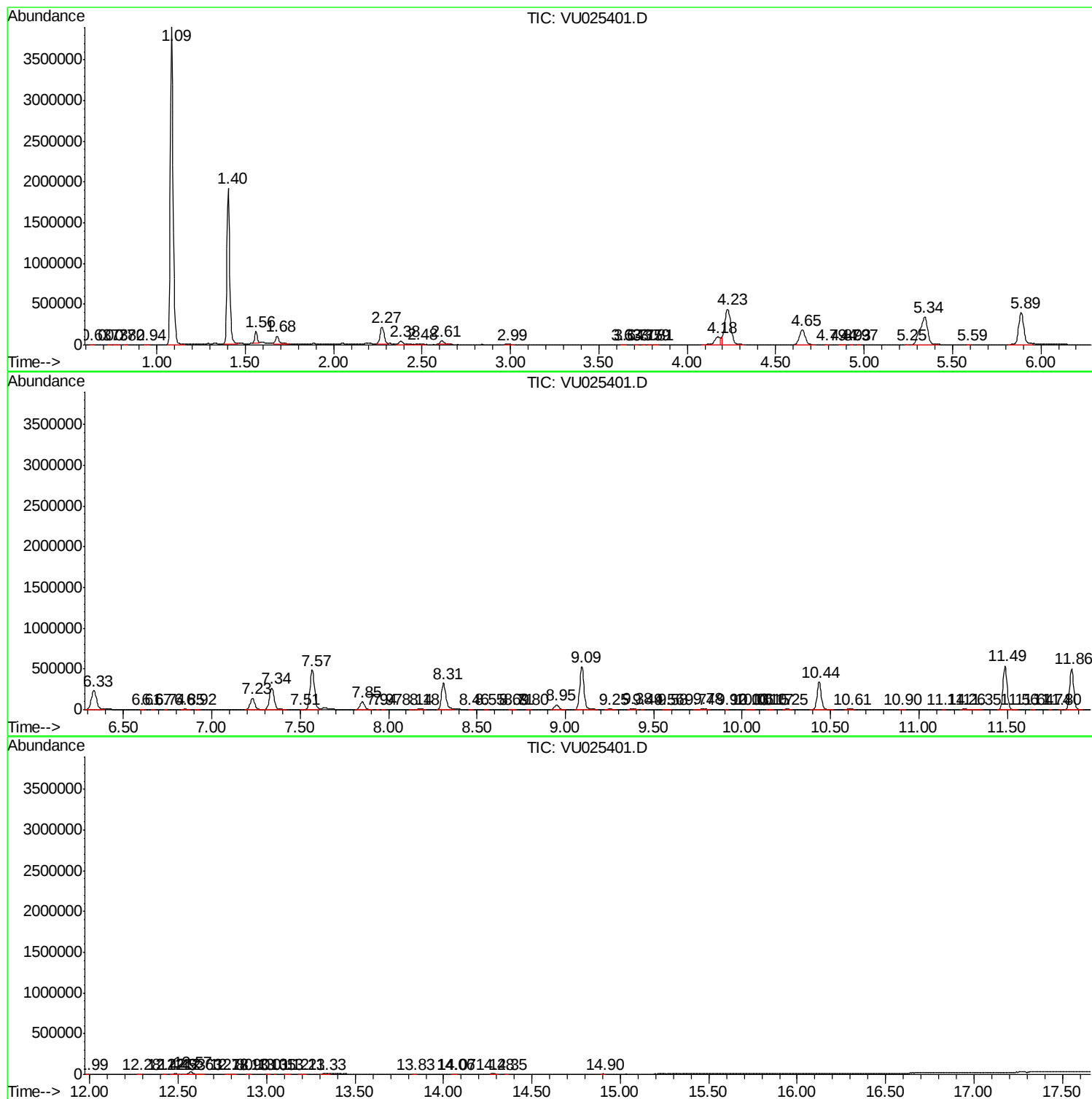
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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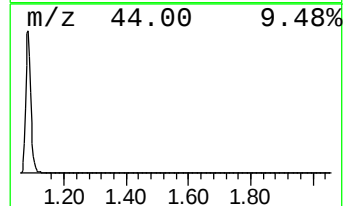
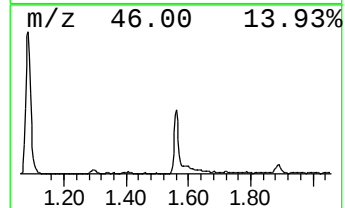
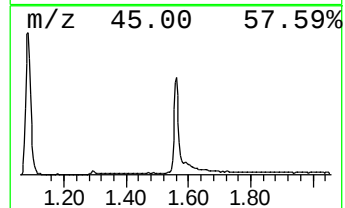
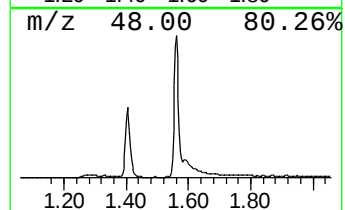
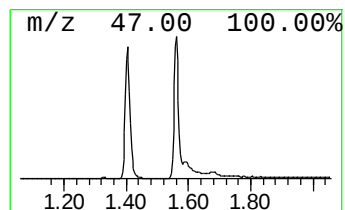
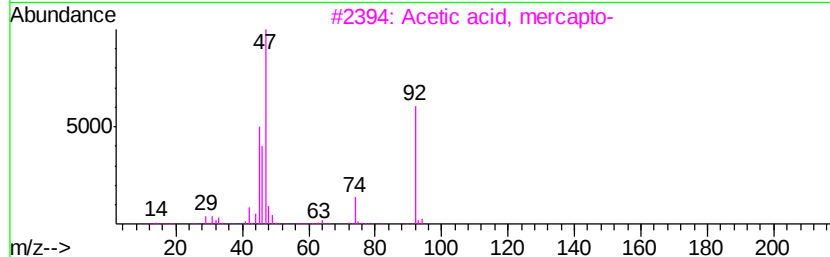
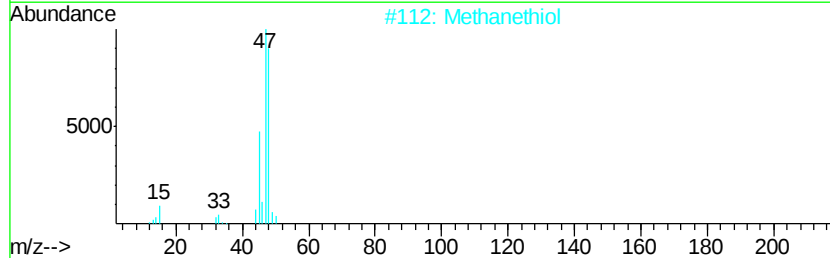
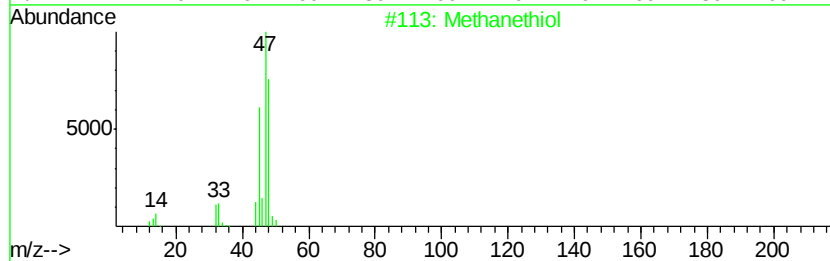
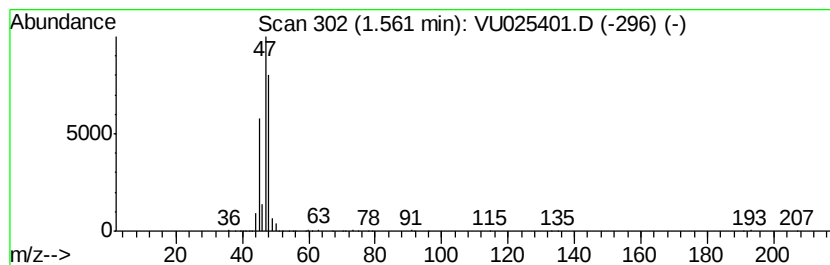
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Methanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.56	8.56 ug/L	143310	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	91
2		Methanethiol	48	CH4S	000074-93-1	90
3		Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
4		Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
5		Methional	104	C4H8OS	003268-49-3	9



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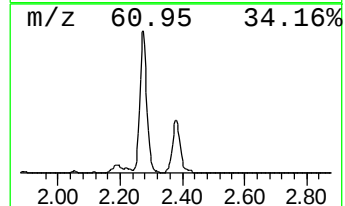
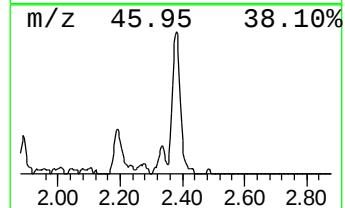
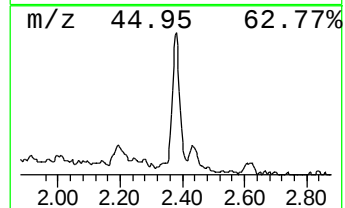
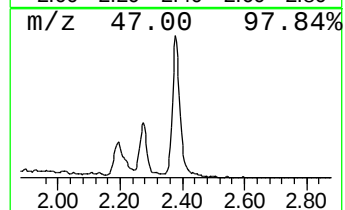
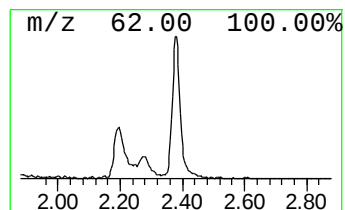
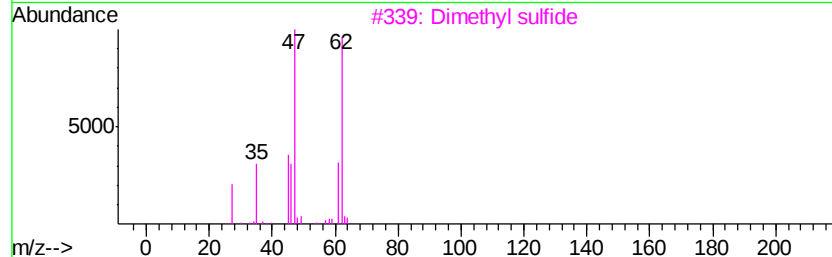
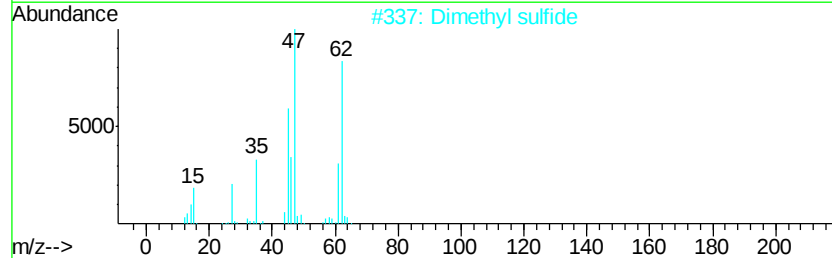
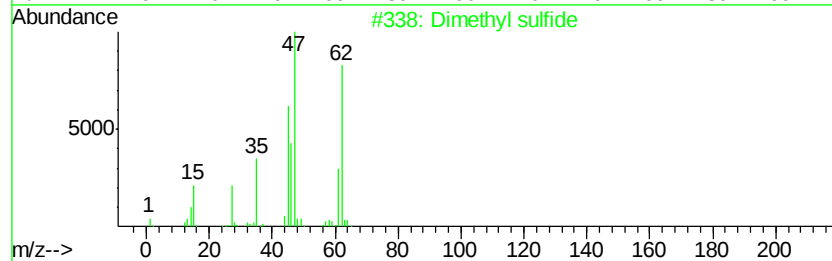
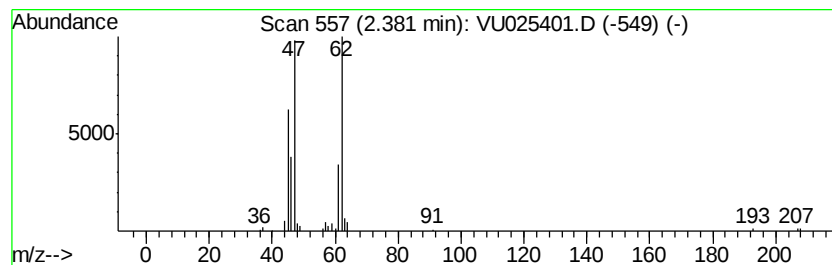
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Quant Title : VOC Analysis

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

Peak Number 3 Dimethyl sulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	4.23 ug/L	70882	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2		Dimethyl sulfide	62	C2H6S	000075-18-3	94
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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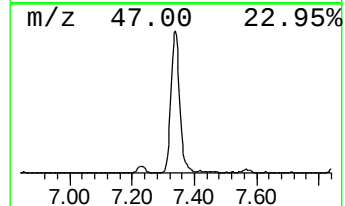
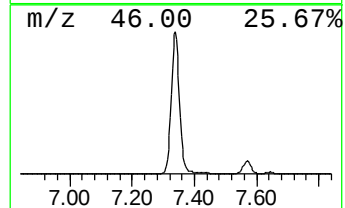
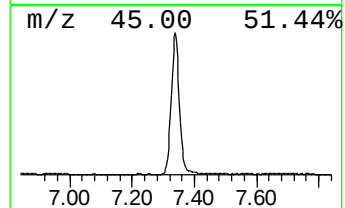
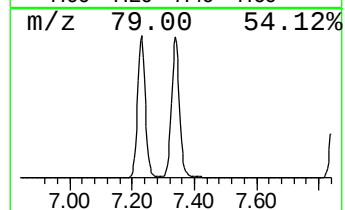
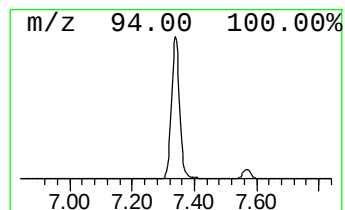
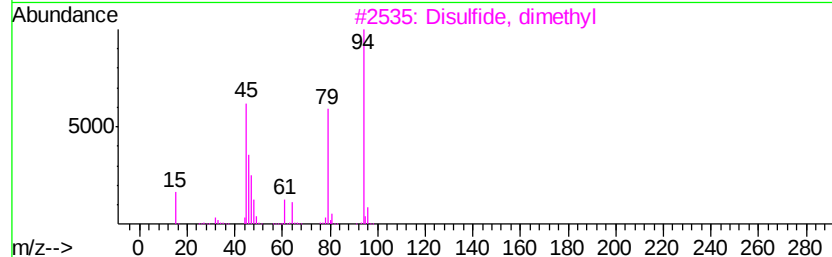
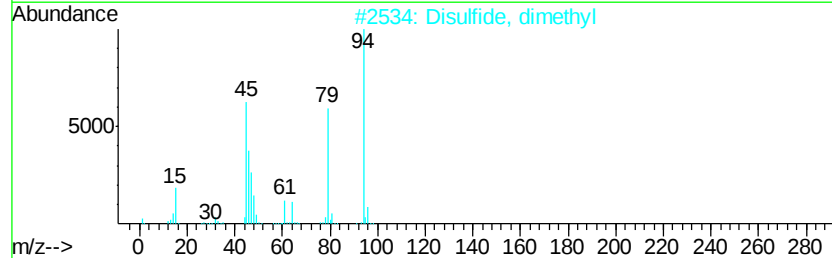
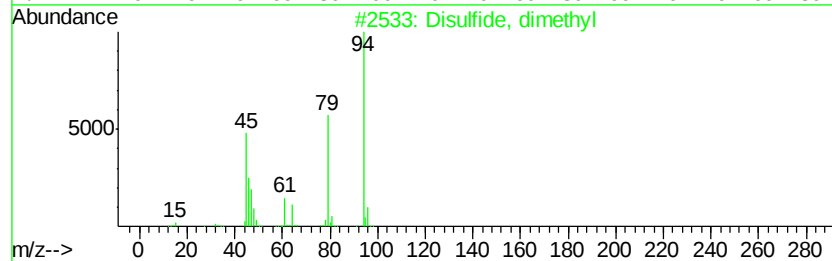
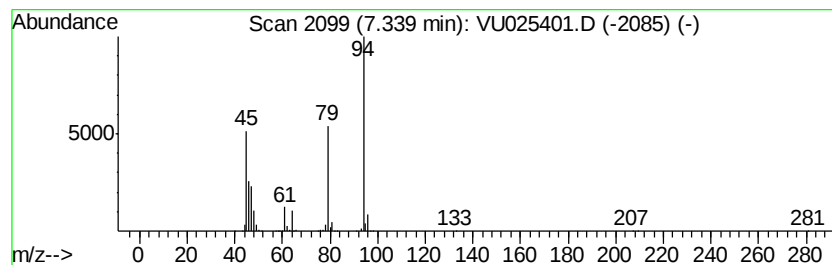
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

Peak Number 5 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	28.97 ug/L	484804	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2		Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
3		Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
4		Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
5		Disulfide, dimethyl	94	C2H6S2	000624-92-0	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
Data File : VU025401.D
Acq On : 13 Jul 2018 20:44
Operator : MD/SY
Sample : J3984-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB182

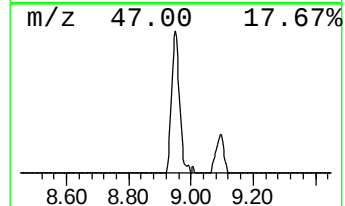
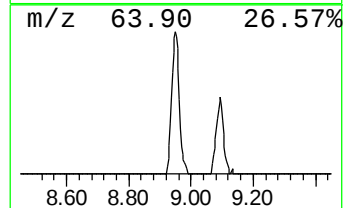
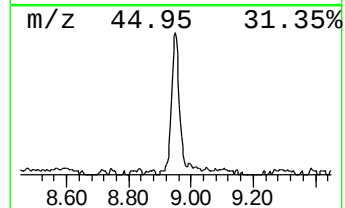
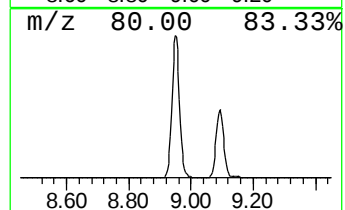
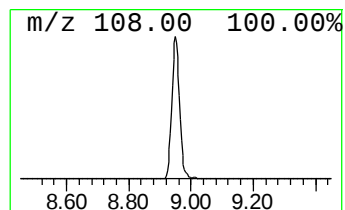
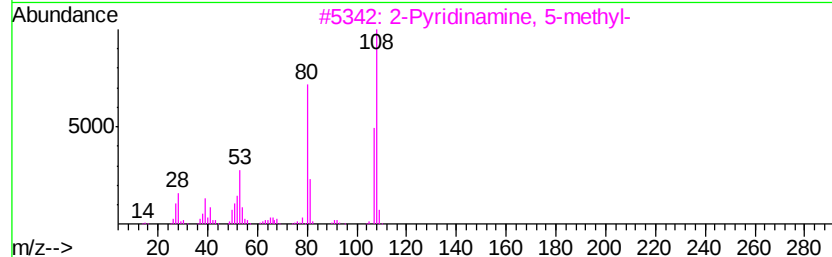
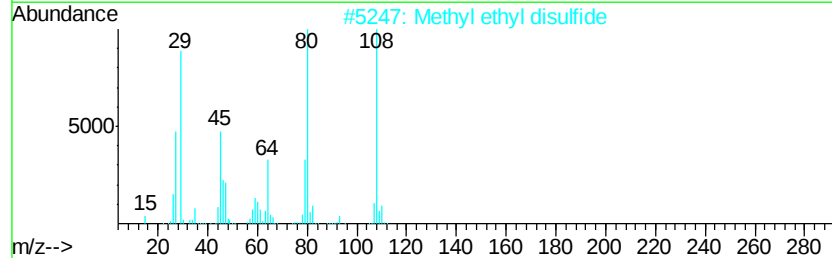
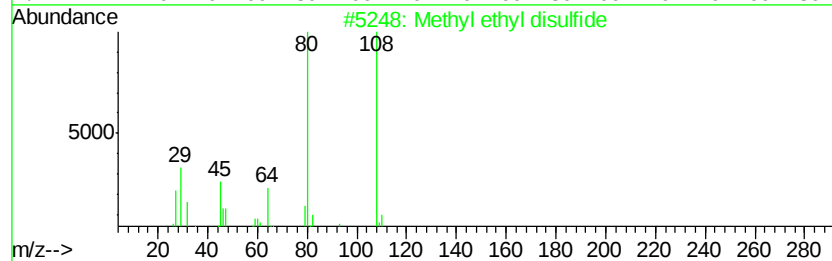
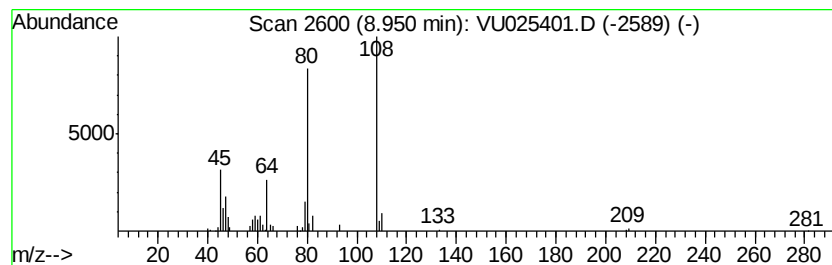
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Quant Title : VOC Analysis

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

Peak Number 6 Methyl ethyl disulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	5.20 ug/L	92625	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	90	
2	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	64	
3	2-Pyridinamine, 5-methyl-	108	C6H8N2	001603-41-4	64	
4	Nicotinyl alcohol	109	C6H7NO	000100-55-0	64	
5	Dimethyl phosphite	110	C2H7O3P	000868-85-9	53	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
Data File : VU025401.D
Acq On : 13 Jul 2018 20:44
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Sample : J3984-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB182

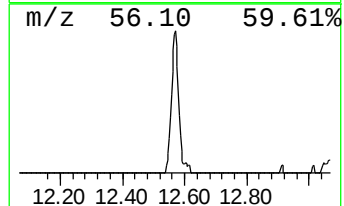
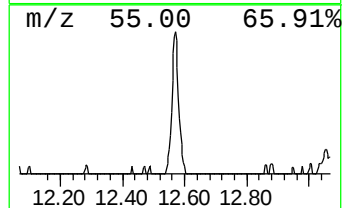
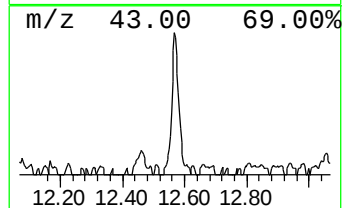
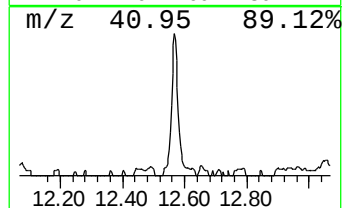
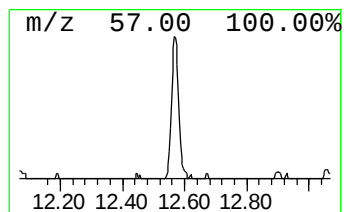
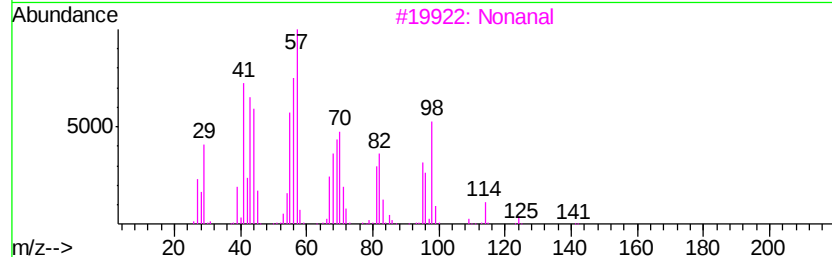
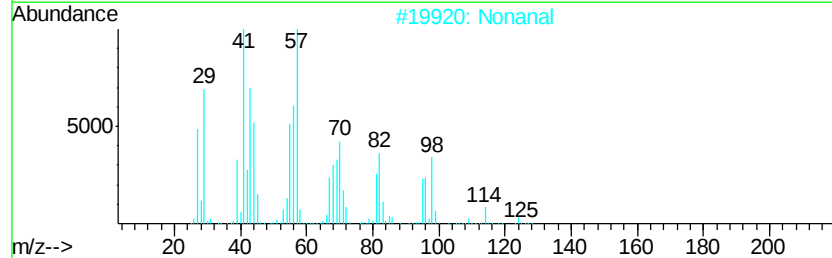
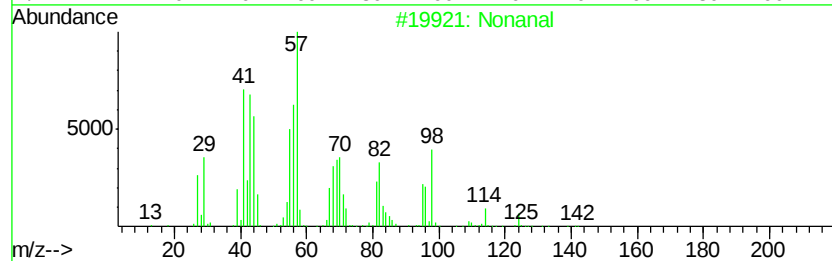
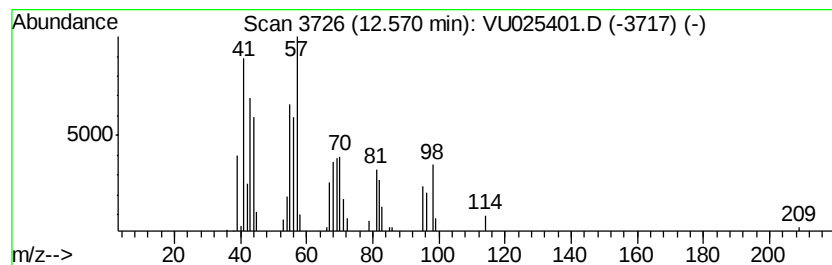
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Nonanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	2.77 ug/L	47173	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	91
2	Nonanal		142	C9H18O	000124-19-6	91
3	Nonanal		142	C9H18O	000124-19-6	90
4	1-Methyl-2-pyrrolidone-4-carboxa...		142	C6H10N2O2	089677-16-7	35
5	Cyclohexanol, 4-methyl-, cis-		114	C7H14O	007731-28-4	30



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB182

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.56	8.6	ug/L	143310	1	5.89	836865	50.0
Dimethyl sulfide	2.38	4.2	ug/L	70882	1	5.89	836865	50.0
Disulfide, dimethyl	7.34	29.0	ug/L	484804	1	5.89	836865	50.0
Methyl ethyl disu...	8.95	5.2	ug/L	92625	2	9.09	891220	50.0
Nonanal	12.57	2.8	ug/L	47173	3	11.49	851490	50.0