

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
 Data File : VU025400.D
 Acq On : 13 Jul 2018 20:20
 Operator : MD/SY
 Sample : J3984-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB181

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	0.667	21	24	27	rBV3	594	353	0.01%	0.002%
2	0.741	44	47	51	rVB3	1307	973	0.02%	0.006%
3	0.883	88	91	94	rVV4	567	495	0.01%	0.003%
4	0.950	109	112	116	rBV4	862	608	0.01%	0.004%
5	1.082	136	153	174	rBV	3923045	4431082	100.00%	27.303%
6	1.404	245	253	270	rBV	1665915	1939622	43.77%	11.952%
7	1.561	296	302	319	rVB	116108	124786	2.82%	0.769%
8	1.680	333	339	355	rVB	84384	116018	2.62%	0.715%
9	2.275	514	524	535	rBV	200675	309977	7.00%	1.910%
10	2.378	549	556	580	rVB2	18508	35994	0.81%	0.222%
11	2.484	581	589	603	rBV2	9584	16356	0.37%	0.101%
12	2.609	620	628	643	rVB2	14510	25958	0.59%	0.160%
13	2.812	688	691	694	rBV4	1181	830	0.02%	0.005%
14	2.985	737	745	756	rVB5	6284	11949	0.27%	0.074%
15	3.214	814	816	819	rVB3	1020	529	0.01%	0.003%
16	3.233	819	822	828	rVB6	836	903	0.02%	0.006%
17	3.265	828	832	834	rBV4	1114	866	0.02%	0.005%
18	3.320	846	849	853	rVB4	537	383	0.01%	0.002%
19	3.394	866	872	876	rBV5	851	954	0.02%	0.006%
20	3.452	888	890	894	rVB4	837	494	0.01%	0.003%
21	3.477	894	898	902	rBV6	727	698	0.02%	0.004%
22	3.555	917	922	925	rBV4	570	507	0.01%	0.003%
23	3.600	932	936	938	rVB3	878	460	0.01%	0.003%
24	3.616	938	941	944	rVB3	686	521	0.01%	0.003%
25	3.905	1023	1031	1035	rBV4	682	864	0.02%	0.005%
26	4.037	1069	1072	1077	rBV5	557	563	0.01%	0.003%
27	4.172	1086	1114	1119	rBV	93883	216276	4.88%	1.333%
28	4.227	1122	1131	1162	rVB	409577	981474	22.15%	6.048%
29	4.526	1220	1224	1225	rBV3	773	603	0.01%	0.004%
30	4.648	1246	1262	1280	rBV	176153	408495	9.22%	2.517%
31	4.879	1325	1334	1339	rBV7	1445	2097	0.05%	0.013%
32	4.950	1353	1356	1358	rVB2	640	355	0.01%	0.002%
33	4.972	1358	1363	1365	rBV4	922	941	0.02%	0.006%
34	5.108	1402	1405	1410	rBV6	1003	870	0.02%	0.005%

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 Title : VOC Analysis

35	5.204	1431	1435	1439	rBV4	762	862	0.02%	0.005%
36	5.243	1443	1447	1450	rVB2	578	461	0.01%	0.003%
37	5.342	1453	1478	1514	rBV2	325524	1042778	23.53%	6.425%
38	5.554	1541	1544	1548	rBV4	1064	889	0.02%	0.005%
39	5.667	1575	1579	1581	rBV2	960	835	0.02%	0.005%
40	5.699	1586	1589	1596	rVB6	974	812	0.02%	0.005%
41	5.786	1613	1616	1618	rBV4	882	533	0.01%	0.003%
42	5.841	1629	1633	1634	rBV3	762	462	0.01%	0.003%
43	5.886	1634	1647	1675	rBV	349074	731993	16.52%	4.510%
44	6.333	1771	1786	1806	rBV	225610	465471	10.50%	2.868%
45	6.522	1842	1845	1848	rBV4	1107	708	0.02%	0.004%
46	6.606	1867	1871	1872	rBV2	1994	1260	0.03%	0.008%
47	6.751	1913	1916	1918	rBV4	1123	897	0.02%	0.006%
48	6.767	1918	1921	1922	rBV3	1174	690	0.02%	0.004%
49	6.850	1939	1947	1950	rBV9	1066	1439	0.03%	0.009%
50	7.050	2005	2009	2014	rVB6	714	798	0.02%	0.005%
51	7.104	2023	2026	2029	rBV3	919	692	0.02%	0.004%
52	7.230	2049	2065	2082	rBV	126343	228033	5.15%	1.405%
53	7.339	2086	2099	2118	rVV	135689	249214	5.62%	1.536%
54	7.455	2130	2135	2139	rBV5	919	830	0.02%	0.005%
55	7.497	2145	2148	2151	rVB3	768	470	0.01%	0.003%
56	7.567	2156	2170	2184	rBV	468761	836355	18.87%	5.153%
57	7.850	2246	2258	2274	rBV	84219	143801	3.25%	0.886%
58	7.966	2287	2294	2298	rBV8	1318	1961	0.04%	0.012%
59	8.017	2307	2310	2313	rBV4	660	456	0.01%	0.003%
60	8.050	2318	2320	2326	rVB5	841	586	0.01%	0.004%
61	8.111	2337	2339	2345	rBV5	638	528	0.01%	0.003%
62	8.181	2350	2361	2371	rBV2	6045	11150	0.25%	0.069%
63	8.259	2375	2385	2386	rBV6	3730	4849	0.11%	0.030%
64	8.310	2390	2401	2442	rVV	309789	611072	13.79%	3.765%
65	8.950	2592	2600	2611	rVB2	28240	45586	1.03%	0.281%
66	9.091	2633	2644	2680	rVB	491800	871526	19.67%	5.370%
67	9.381	2727	2734	2744	rVB3	11405	17570	0.40%	0.108%
68	9.783	2853	2859	2867	rVB3	9384	13303	0.30%	0.082%
69	9.918	2897	2901	2904	rBV4	2085	2169	0.05%	0.013%
70	10.300	3016	3020	3021	rBV3	811	629	0.01%	0.004%
71	10.435	3050	3062	3081	rVB	331639	542414	12.24%	3.342%

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Title : VOC Analysis

72	10.612	3109	3117	3125	rVB2	8387	13889	0.31%	0.086%
73	10.705	3142	3146	3150	rBV4	808	687	0.02%	0.004%
74	11.011	3238	3241	3243	rBV2	667	383	0.01%	0.002%
75	11.114	3270	3273	3276	rBV4	603	445	0.01%	0.003%
76	11.133	3276	3279	3280	rBV3	810	443	0.01%	0.003%
77	11.255	3310	3317	3328	rVB2	8222	12857	0.29%	0.079%
78	11.345	3335	3345	3352	rBV8	2999	5765	0.13%	0.036%
79	11.487	3377	3389	3408	rBV	531351	820863	18.53%	5.058%
80	11.712	3457	3459	3465	rBV3	826	656	0.01%	0.004%
81	11.863	3494	3506	3522	rBV	501644	808714	18.25%	4.983%
82	11.969	3536	3539	3542	rBV3	1161	1025	0.02%	0.006%
83	12.072	3565	3571	3579	rBV6	2711	4057	0.09%	0.025%
84	12.152	3591	3596	3599	rBV4	781	759	0.02%	0.005%
85	12.181	3602	3605	3607	rVB3	723	396	0.01%	0.002%
86	12.200	3607	3611	3614	rBV3	850	575	0.01%	0.004%
87	12.397	3668	3672	3674	rVB3	567	404	0.01%	0.002%
88	12.570	3715	3726	3741	rBV3	36296	57043	1.29%	0.351%
89	12.988	3853	3856	3858	rBV3	1252	960	0.02%	0.006%
90	13.049	3868	3875	3880	rBV7	2907	4017	0.09%	0.025%
91	13.162	3904	3910	3914	rVB5	864	1148	0.03%	0.007%
92	13.184	3914	3917	3920	rBV3	980	756	0.02%	0.005%
93	13.226	3927	3930	3933	rBV3	752	569	0.01%	0.004%
94	13.258	3937	3940	3944	rVB5	1064	778	0.02%	0.005%
95	13.336	3951	3964	3967	rBV10	6317	10634	0.24%	0.066%
96	13.869	4127	4130	4132	rBV3	1151	738	0.02%	0.005%
97	14.236	4240	4244	4250	rVB6	1311	1573	0.04%	0.010%
98	14.281	4250	4258	4266	rBV	5312	9570	0.22%	0.059%
99	14.438	4304	4307	4309	rBV2	1045	791	0.02%	0.005%
100	14.477	4317	4319	4326	rVB7	1011	665	0.02%	0.004%

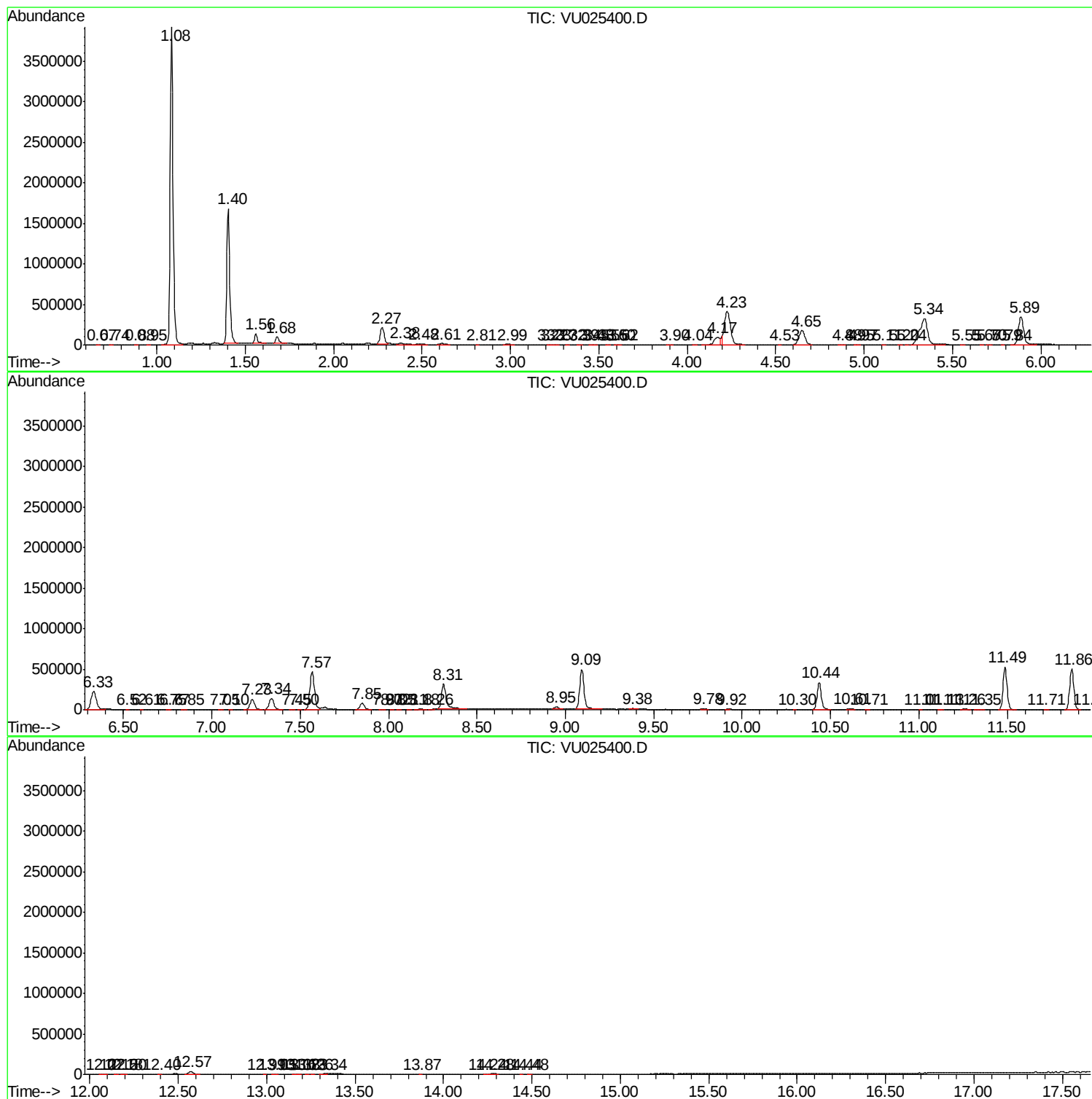
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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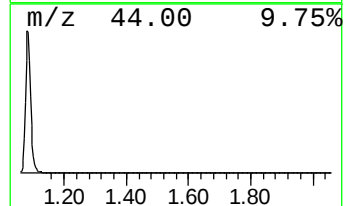
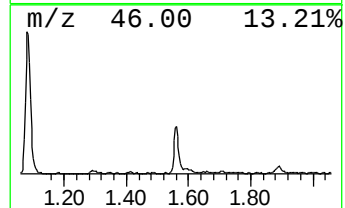
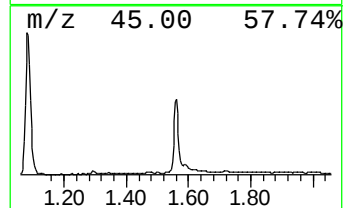
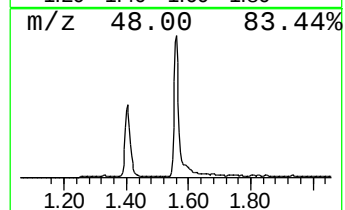
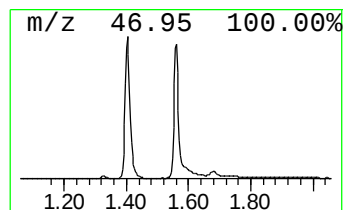
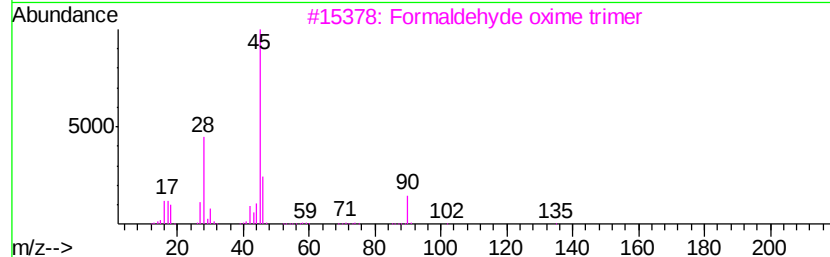
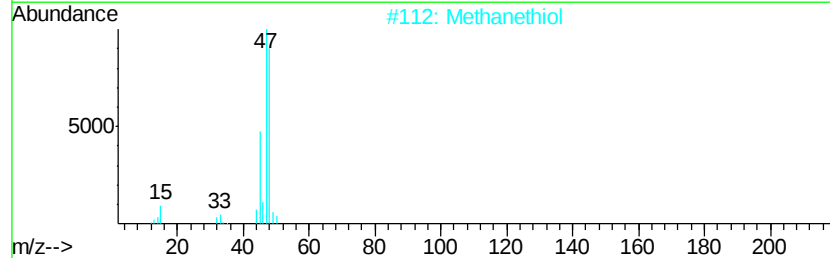
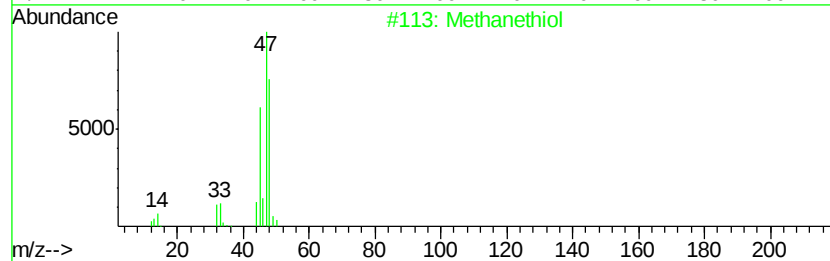
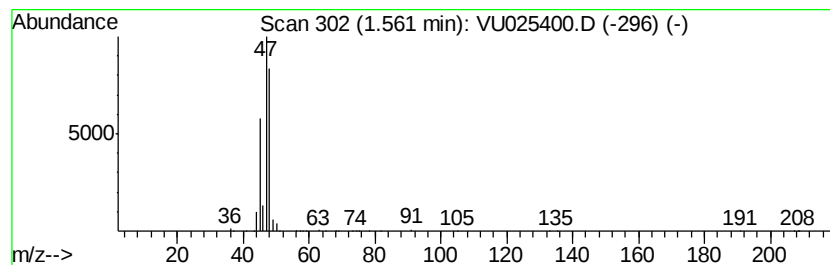
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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	8.52 ug/L	124786	1,4-Difluorobenzene	5.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methanethiol	48	CH4S	000074-93-1	91
2		Methanethiol	48	CH4S	000074-93-1	90
3		Formaldehyde oxime trimer	135	C3H9N3O3	1000234-87-0	9
4		Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
5		Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9



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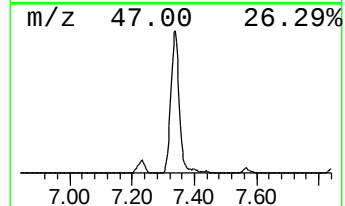
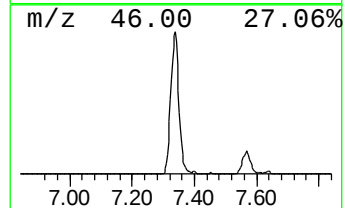
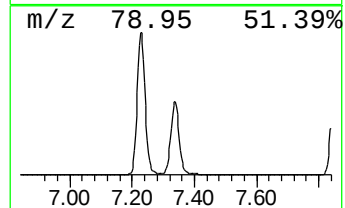
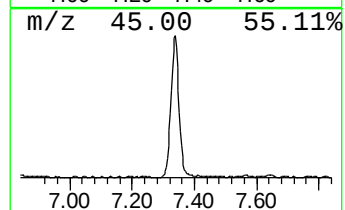
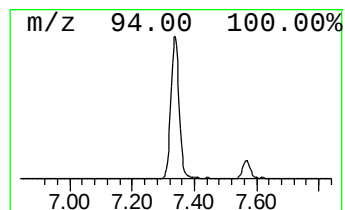
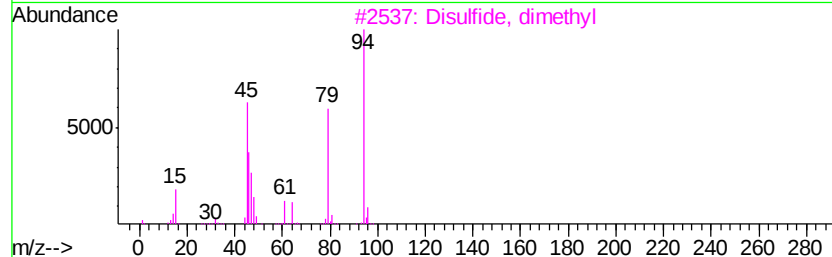
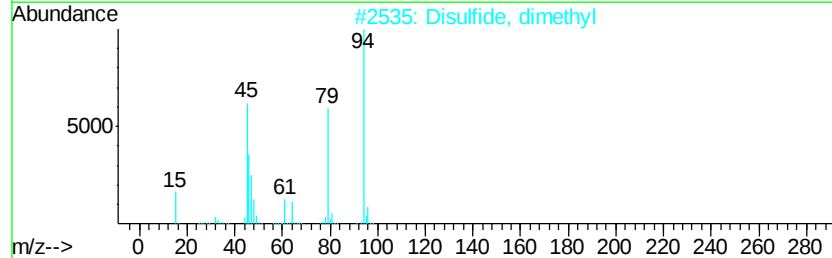
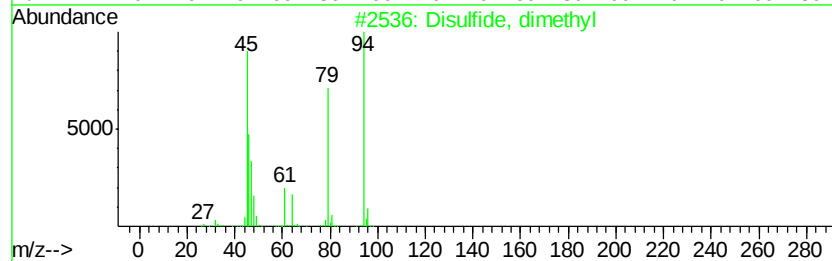
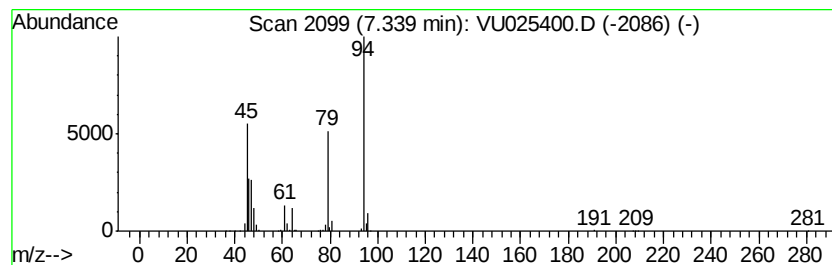
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	17.02 ug/L	249214	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	97
5		Disulfide, dimethyl	94	C2H6S2	000624-92-0	96



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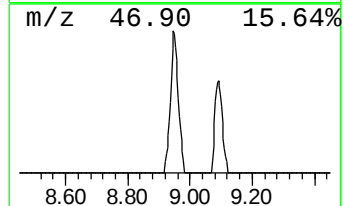
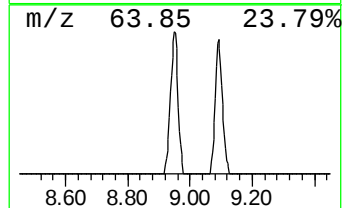
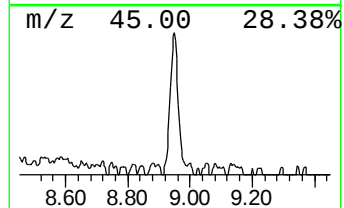
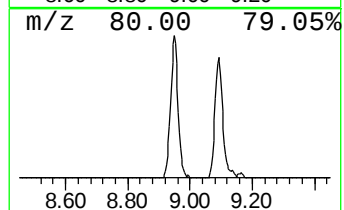
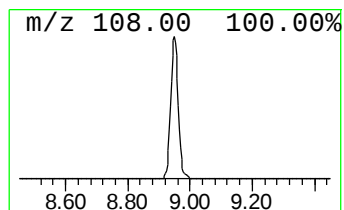
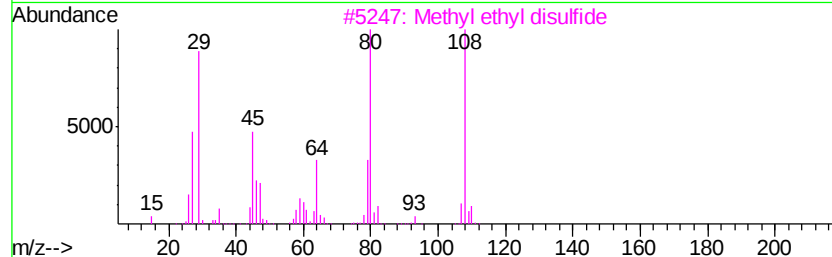
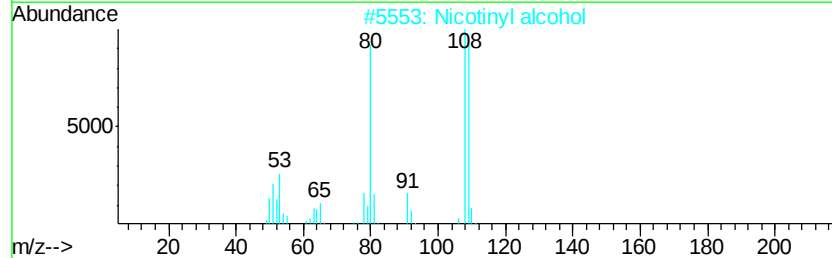
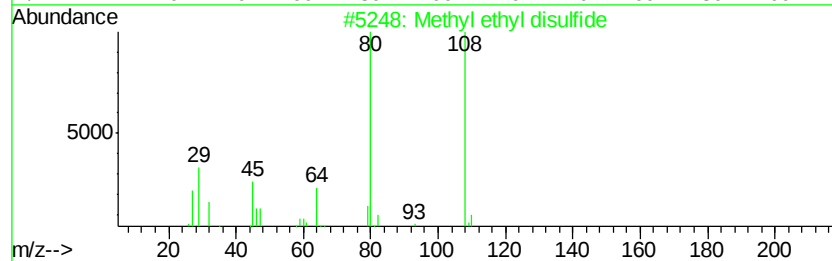
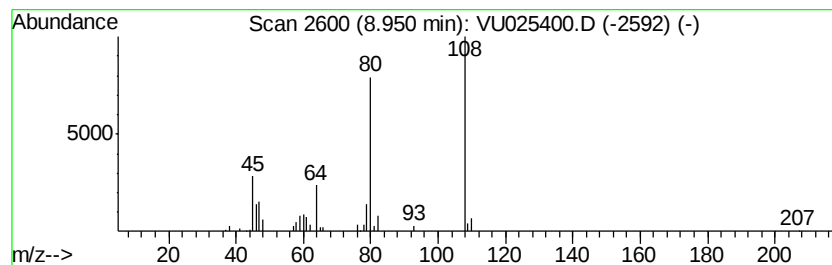
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Quant Title : VOC Analysis

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

Peak Number 5 Methyl ethyl disulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	2.62 ug/L	45586	Chlorobenzene-d5	9.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ethyl disulfide	108	C3H8S2	020333-39-5	72
2			Nicotinyl alcohol	109	C6H7NO	000100-55-0	64
3			Methyl ethyl disulfide	108	C3H8S2	020333-39-5	64
4			Disulfide, methyl propyl	122	C4H10S2	002179-60-4	59
5			Methyl n-butyl disulfide	136	C5H12S2	060779-24-0	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
Data File : VU025400.D
Acq On : 13 Jul 2018 20:20
Operator : MD/SY
Sample : J3984-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB181

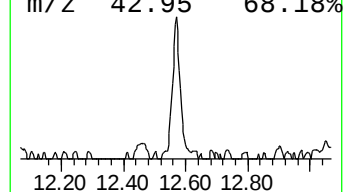
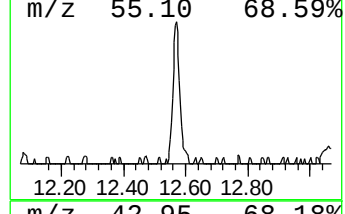
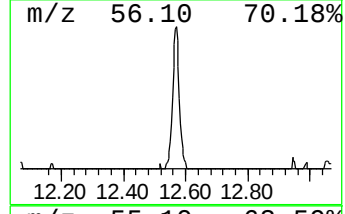
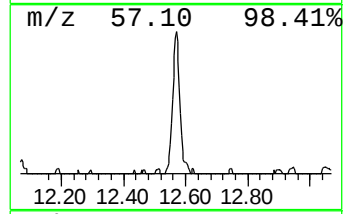
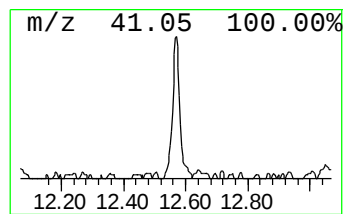
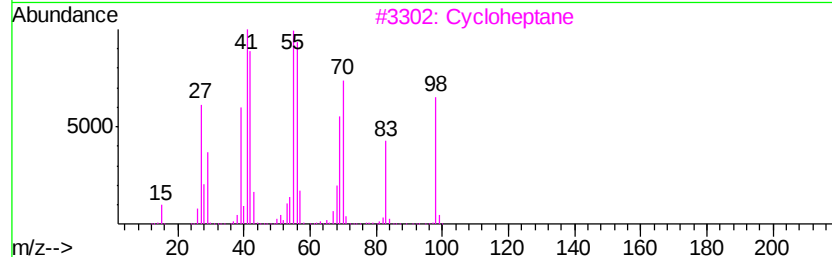
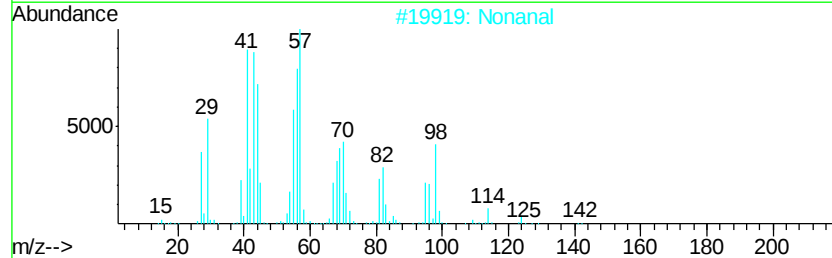
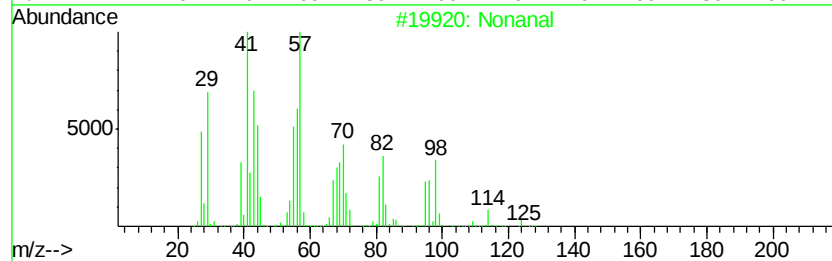
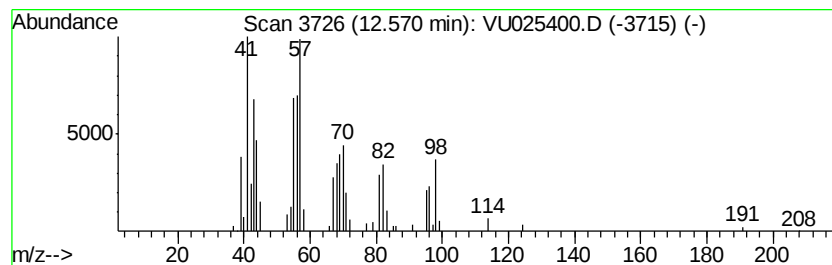
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Quant Title : VOC Analysis

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

Peak Number 6 Nonanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.47 ug/L	57043	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	90
2	Nonanal		142	C9H18O	000124-19-6	78
3	Cycloheptane		98	C7H14	000291-64-5	41
4	Cyclohexanol, 2-methyl-, cis-		114	C7H14O	007443-70-1	38
5	Cyclohexanol, 2-methyl-		114	C7H14O	000583-59-5	35



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Instrument :
MSVOA_U
ClientSampleId :
DB181

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	8.5	ug/L	124786	1	5.89	731993	50.0
Disulfide, dimethyl	7.34	17.0	ug/L	249214	1	5.89	731993	50.0
Methyl ethyl disu...	8.95	2.6	ug/L	45586	2	9.09	871526	50.0
Nonanal	12.57	3.5	ug/L	57043	3	11.49	820863	50.0