

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090518\
 Data File : VU026568.D
 Acq On : 06 Sep 2018 01:32
 Operator : MD/SY
 Sample : J4718-13
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEGC9

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\SOMULM082918WMA.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	0.728	41	43	48	rBV	162	183	0.04%	0.004%
2	0.754	48	51	53	rVB	154	104	0.02%	0.002%
3	0.773	53	57	62	rBV	171	241	0.05%	0.005%
4	0.850	78	81	84	rBB	129	110	0.02%	0.002%
5	0.889	85	93	97	rBV	138	265	0.05%	0.006%
6	0.911	97	100	104	rVV	98	103	0.02%	0.002%
7	0.950	110	112	115	rVB	201	133	0.03%	0.003%
8	0.966	115	117	120	rBV	150	130	0.03%	0.003%
9	1.085	136	154	173	rBV	158454	184973	36.93%	4.086%
10	1.182	180	184	189	rBV2	4357	4496	0.90%	0.099%
11	1.394	242	250	259	rBV	70078	81333	16.24%	1.797%
12	1.677	331	338	355	rVB	56127	72915	14.56%	1.611%
13	2.185	487	496	512	rBV	73026	111582	22.28%	2.465%
14	2.268	513	522	534	rVB	110338	164843	32.91%	3.642%
15	2.378	554	556	562	rVB3	700	397	0.08%	0.009%
16	2.587	578	621	624	rBV4	17784	74706	14.92%	1.650%
17	3.397	871	873	878	rVB2	279	199	0.04%	0.004%
18	3.436	878	885	894	rVV2	752	1256	0.25%	0.028%
19	3.484	898	900	903	rVB2	176	98	0.02%	0.002%
20	3.802	992	999	1001	rBV	107	131	0.03%	0.003%
21	3.992	1053	1058	1063	rBV	140	164	0.03%	0.004%
22	4.075	1082	1084	1089	rVB2	214	131	0.03%	0.003%
23	4.124	1089	1099	1100	rBV2	807	933	0.19%	0.021%
24	4.178	1100	1116	1145	rVV	47734	125369	25.03%	2.770%
25	4.407	1185	1187	1190	rBV2	289	196	0.04%	0.004%
26	4.593	1241	1245	1246	rBV	217	132	0.03%	0.003%
27	4.651	1246	1263	1286	rVV	90121	209058	41.74%	4.618%
28	4.738	1288	1290	1293	rVB2	242	116	0.02%	0.003%
29	4.998	1361	1371	1382	rVB5	1551	2627	0.52%	0.058%
30	5.075	1391	1395	1399	rBV	102	106	0.02%	0.002%
31	5.120	1406	1409	1411	rBV2	195	142	0.03%	0.003%
32	5.342	1454	1478	1504	rBV2	167553	500849	100.00%	11.065%
33	5.480	1517	1521	1525	rVB2	209	184	0.04%	0.004%
34	5.519	1530	1533	1537	rVV	92	92	0.02%	0.002%

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 Title : VOC Analysis

35	5.545	1538	1541	1545	rVV	258	208	0.04%	0.005%
36	5.615	1558	1563	1567	rBV	330	328	0.07%	0.007%
37	5.731	1597	1599	1602	rVB	184	97	0.02%	0.002%
38	5.770	1609	1611	1614	rVB	278	156	0.03%	0.003%
39	5.789	1615	1617	1619	rBV	130	96	0.02%	0.002%
40	5.889	1633	1648	1677	rBV	195773	378037	75.48%	8.351%
41	5.992	1677	1680	1684	rVV2	377	306	0.06%	0.007%
42	6.011	1684	1686	1690	rVB	165	86	0.02%	0.002%
43	6.194	1734	1743	1745	rBV4	814	1142	0.23%	0.025%
44	6.333	1773	1786	1807	rBV	121381	238526	47.62%	5.269%
45	6.615	1871	1874	1877	rBV	166	166	0.03%	0.004%
46	6.635	1878	1880	1884	rVV	84	87	0.02%	0.002%
47	6.850	1943	1947	1952	rBV3	295	310	0.06%	0.007%
48	6.940	1972	1975	1980	rBV	92	104	0.02%	0.002%
49	7.230	2054	2065	2079	rBV	60756	104188	20.80%	2.302%
50	7.377	2107	2111	2117	rVB2	196	186	0.04%	0.004%
51	7.429	2126	2127	2133	rVB	128	82	0.02%	0.002%
52	7.567	2157	2170	2188	rBV	220510	375901	75.05%	8.304%
53	7.718	2215	2217	2219	rBV	178	94	0.02%	0.002%
54	7.747	2224	2226	2229	rVB2	155	86	0.02%	0.002%
55	7.850	2248	2258	2276	rBV	42487	70681	14.11%	1.561%
56	7.947	2285	2288	2292	rVB	168	123	0.02%	0.003%
57	7.982	2295	2299	2303	rVV2	160	126	0.03%	0.003%
58	8.181	2349	2361	2371	rBV3	7594	15266	3.05%	0.337%
59	8.313	2391	2402	2428	rVB	161147	270288	53.97%	5.971%
60	8.532	2467	2470	2474	rVB	189	136	0.03%	0.003%
61	8.609	2491	2494	2495	rBV	156	94	0.02%	0.002%
62	9.091	2631	2644	2670	rBV	277564	451110	90.07%	9.966%
63	9.258	2692	2696	2699	rBV	181	176	0.04%	0.004%
64	9.406	2730	2742	2754	rBV3	6480	13308	2.66%	0.294%
65	10.017	2929	2932	2935	rBV	102	89	0.02%	0.002%
66	10.255	2996	3006	3020	rBV2	21787	37887	7.56%	0.837%
67	10.432	3049	3061	3077	rBV	172438	272236	54.35%	6.014%
68	10.545	3094	3096	3099	rBV	141	101	0.02%	0.002%
69	10.612	3105	3117	3132	rBV2	4247	7155	1.43%	0.158%
70	10.850	3188	3191	3195	rBV	163	120	0.02%	0.003%
71	10.876	3195	3199	3202	rVB	210	182	0.04%	0.004%

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72	11.014	3239	3242	3245	rBV2	391	311	0.06%	0.007%
73	11.139	3279	3281	3283	rBV	179	128	0.03%	0.003%
74	11.159	3285	3287	3290	rVB2	209	126	0.03%	0.003%
75	11.204	3298	3301	3303	rBV2	155	117	0.02%	0.003%
76	11.268	3319	3321	3325	rVB	206	109	0.02%	0.002%
77	11.294	3326	3329	3337	rVV	147	180	0.04%	0.004%
78	11.329	3337	3340	3345	rVV2	205	176	0.04%	0.004%
79	11.487	3377	3389	3409	rVV	247958	387117	77.29%	8.552%
80	11.676	3445	3448	3450	rBV	183	113	0.02%	0.002%
81	11.757	3468	3473	3478	rBV2	351	395	0.08%	0.009%
82	11.860	3493	3505	3525	rBV	220918	352249	70.33%	7.782%
83	12.483	3690	3699	3707	rVB2	1373	2044	0.41%	0.045%
84	12.535	3713	3715	3717	rBV2	185	94	0.02%	0.002%
85	12.657	3750	3753	3758	rBV2	219	159	0.03%	0.004%
86	12.757	3782	3784	3786	rBV	235	119	0.02%	0.003%
87	12.972	3848	3851	3853	rBV	175	92	0.02%	0.002%
88	13.075	3876	3883	3893	rBV4	1386	1985	0.40%	0.044%
89	13.236	3929	3933	3937	rBV2	287	268	0.05%	0.006%
90	13.307	3952	3955	3958	rBV	236	181	0.04%	0.004%
91	13.358	3969	3971	3974	rBV	214	103	0.02%	0.002%
92	13.442	3992	3997	4001	rBV2	234	288	0.06%	0.006%
93	13.548	4024	4030	4033	rBV2	213	261	0.05%	0.006%
94	13.950	4152	4155	4158	rBV3	304	226	0.05%	0.005%
95	14.030	4179	4180	4183	rVB	271	130	0.03%	0.003%
96	14.191	4227	4230	4235	rBV2	231	208	0.04%	0.005%
97	14.274	4254	4256	4267	rVB2	805	1082	0.22%	0.024%
98	14.506	4325	4328	4334	rBV2	413	393	0.08%	0.009%
99	14.541	4337	4339	4342	rBV	319	170	0.03%	0.004%
100	15.808	4730	4733	4735	rBV2	371	236	0.05%	0.005%

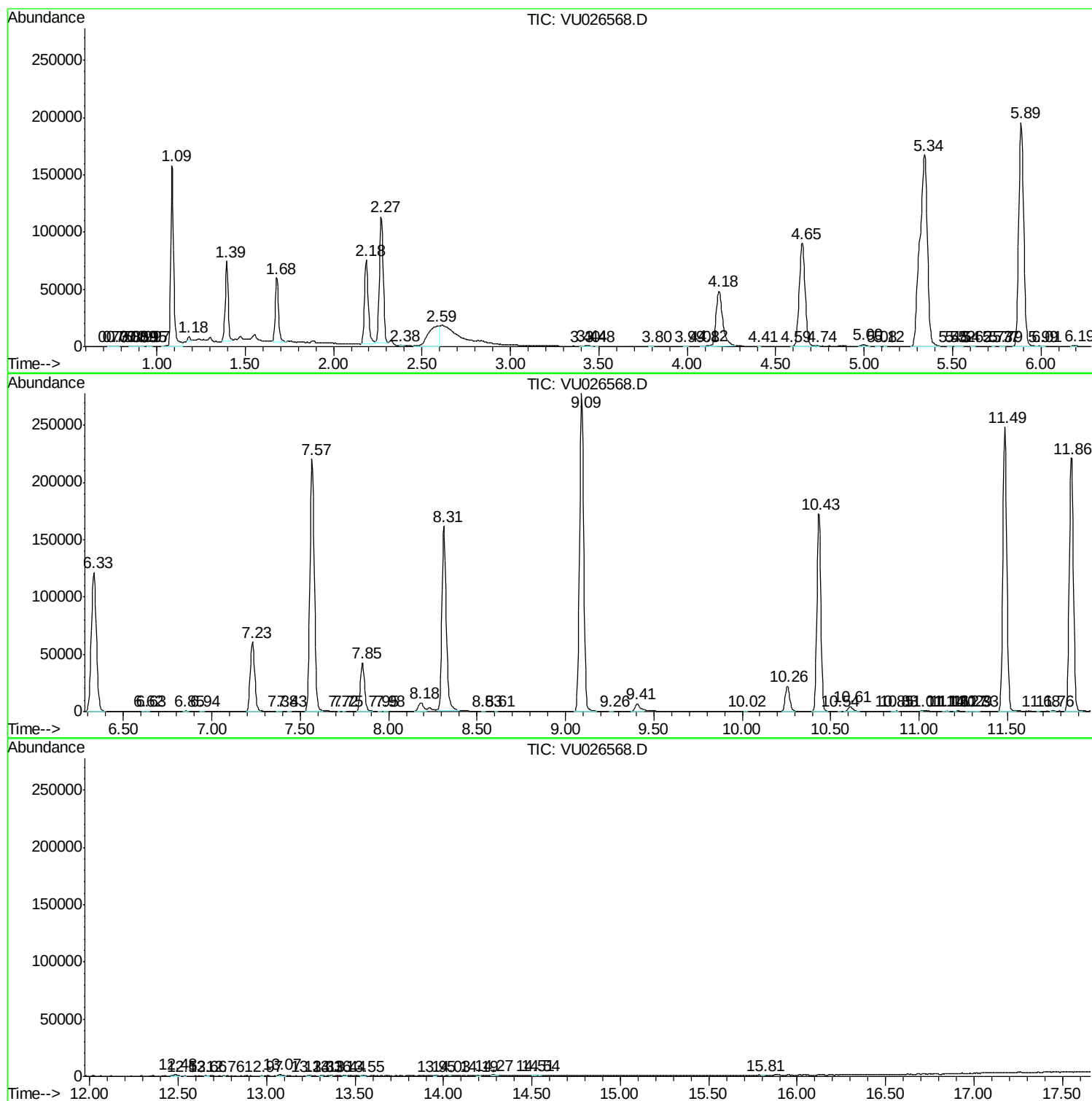
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Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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



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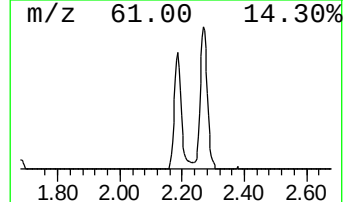
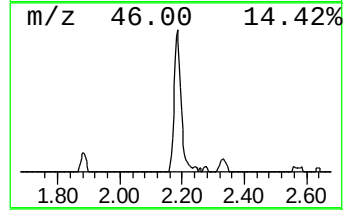
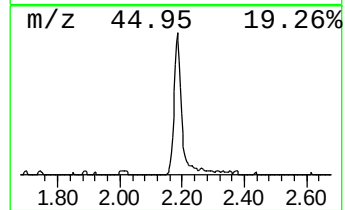
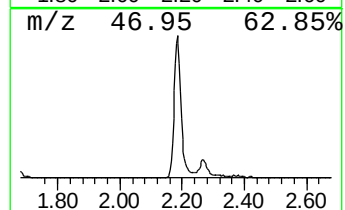
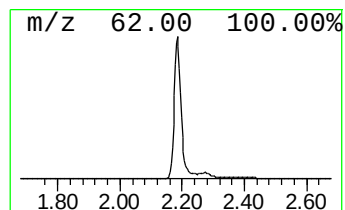
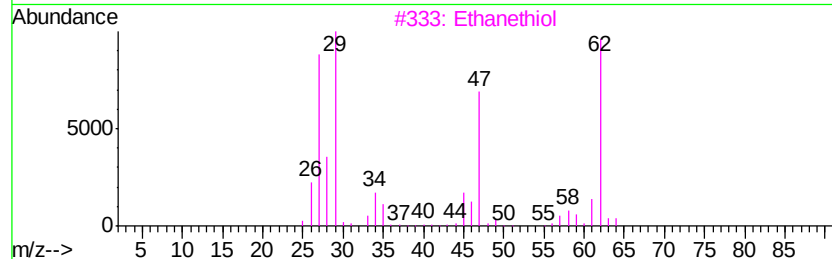
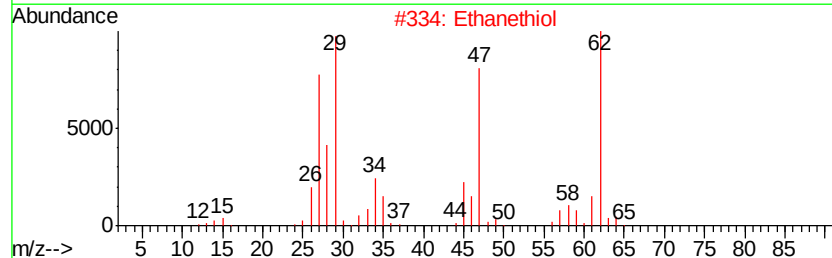
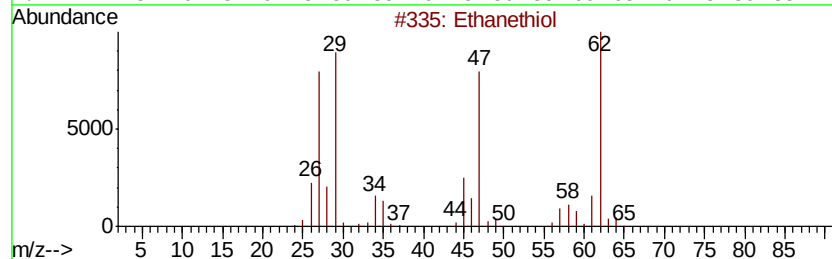
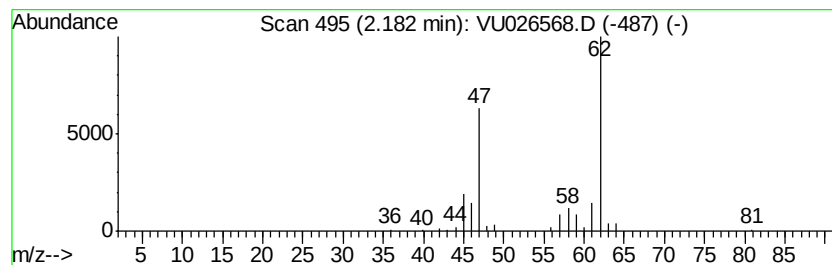
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	14.76 ug/L	111582	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanethiol	62	C2H6S	000075-08-1	91
2		Ethanethiol	62	C2H6S	000075-08-1	91
3		Ethanethiol	62	C2H6S	000075-08-1	91
4		Ethanethiol	62	C2H6S	000075-08-1	91
5		Ethanethiol	62	C2H6S	000075-08-1	91



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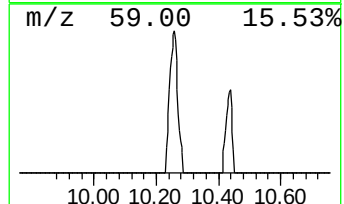
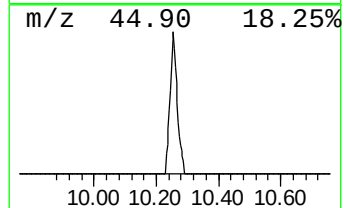
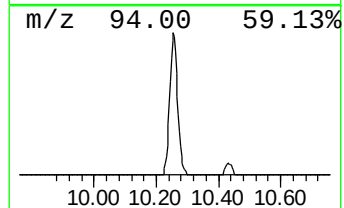
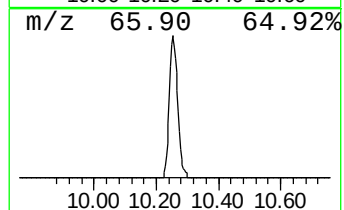
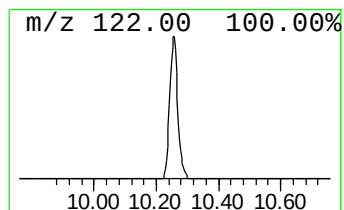
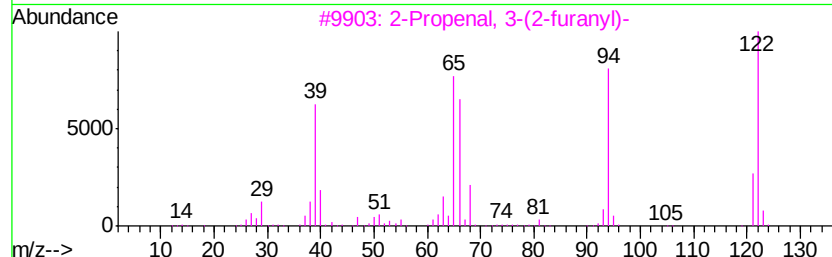
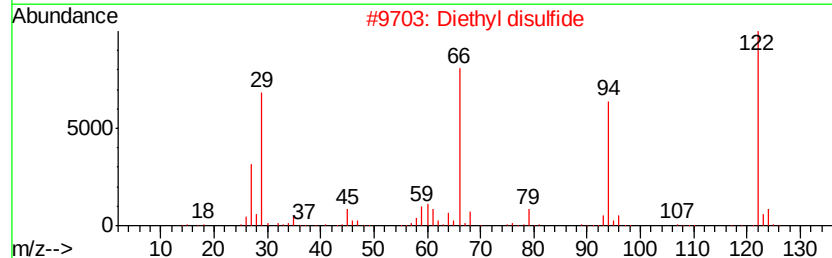
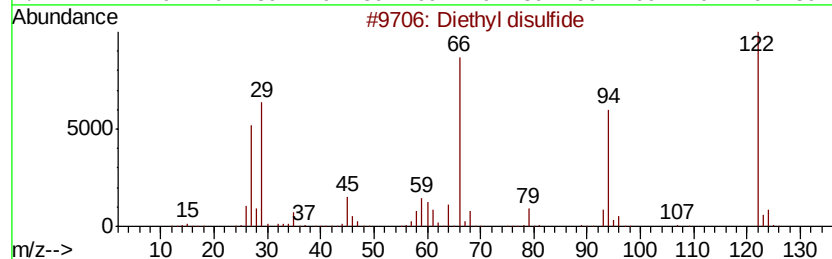
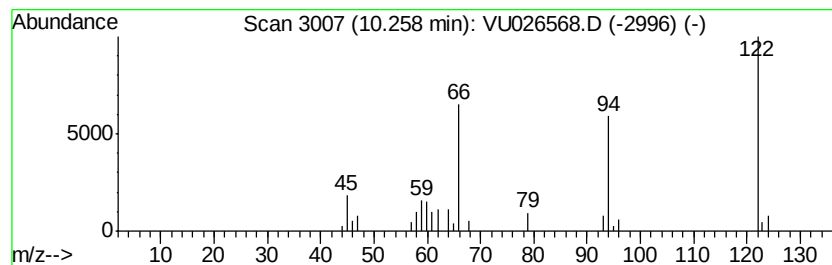
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Quant Title : VOC Analysis

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

Peak Number 5 Diethyl disulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	4.20 ug/L	37887	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyl disulfide	122	C4H10S2	000110-81-6	87
2		Diethyl disulfide	122	C4H10S2	000110-81-6	83
3		2-Propenal, 3-(2-furanvl)-	122	C7H6O2	000623-30-3	38
4		Diethyl disulfide	122	C4H10S2	000110-81-6	38
5		Benzene, ethoxy-	122	C8H10O	000103-73-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanethiol	2.18	14.8	ug/L	111582	1	5.89	378037	50.0
Diethyl disulfide	10.26	4.2	ug/L	37887	2	9.09	451110	50.0