LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040521\
Data File : VV020922.D
Acq On : 05 Apr 2021 18:07
Operator : SY/MD
Sample : M1845-09
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : EW1B2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Title : VOC Analysis

Signal : TIC: VV020922.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	77	83	94	rVB2	299199	304337	13.74%	1.723%
2	2.031	302	308	322	rVB	243451	332475	15.01%	1.882%
3	2.108	324	332	353	rVB	525196	762289	34.41%	4.315%
4	3.272	692	694	700	rVB4	786	455	0.02%	0.003%
5	3.304	700	704	709	rVB3	510	428	0.02%	0.002%
6	3.333	709	713	714	rBV2	478	323	0.01%	0.002%
7	3.355	718	720	724	rVV3	351	191	0.01%	0.001%
8	3.400	732	734	735	rBV	319	129	0.01%	0.001%
9	3.458	749	752	753	rBV2	622	351	0.02%	0.002%
10	3.510	763	768	769	rBV3	312	207	0.01%	0.001%
11	3.519	769	771	774	rVV3	323	153	0.01%	0.001%
12	3.548	778	780	782	rVV2	507	327	0.01%	0.002%
13	3.580	786	790	795	rVB2	668	589	0.03%	0.003%
14	3.613	795	800	802	rBV3	651	625	0.03%	0.004%
15	3.629	802	805	808	rBV3	317	252	0.01%	0.001%
16	3.661	810	815	818	rVV2	497	398	0.02%	0.002%
17	3.680	818	821	827	rVB4	537	353	0.02%	0.002%
18	3.722	832	834	836	rBV2	440	285	0.01%	0.002%
19	3.748	840	842	844	rVB2	511	186	0.01%	0.001%
20	3.818	850	864	879	rBV7	13233	33050	1.49%	0.187%
21	3.905	879	891	925	rBV	136102	465566	21.01%	2.636%
22	4.352	1015	1030	1056	rBV	385462	949023	42.84%	5.373%
23	4.596	1104	1106	1109	rVB4	750	319	0.01%	0.002%
24	4.651	1119	1123	1126	rBV5	1174	1015	0.05%	0.006%
25	4.796	1166	1168	1171	rBV2	378	253	0.01%	0.001%
26	4.876	1189	1193	1195	rBV2	586	548	0.02%	0.003%
27	4.892	1195	1198	1200	rVV2	801	455	0.02%	0.003%
28	4.905	1200	1202	1210	rVB4	690	733	0.03%	0.004%
29	4.944	1210	1214	1215	rBV2	487	332	0.01%	0.002%
30	5.047	1229	1246	1276	rBV3	864152	2215459	100.00%	12.542%
31	5.342	1335	1338	1344	rBV6	1138	1214	0.05%	0.007%
32	5.439	1366	1368	1370	rBV2	423	143	0.01%	0.001%
33	5.619	1411	1424	1452	rBV	665303	1336365	60.32%	7.565%
34	5.915	1507	1516	1527	rBV4	17356	31686	1.43%	0.179%
35	6.072	1551	1565	1591	rBV	466641	965097	43.56%	5.464%
36	6.355	1650	1653	1654	rBV2	912	545	0.02%	0.003%

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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_V
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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Title : VOC Analysis

37	6.465	1684	1687	1691	rBV3	1512	1105	0.05%	0.006%
38	6.767	1779	1781	1782	rBV2	473	227	0.01%	0.001%
39	6.838	1798	1803	1807	rVB3	775	780	0.04%	0.004%
40	6.863	1809	1811	1812	rBV	486	146	0.01%	0.001%
41	6.918	1826	1828	1831	rBV	487	207	0.01%	0.001%
42	6.940	1831	1835	1837	rBV2	615	434	0.02%	0.002%
43	6.989	1839	1850	1870	rBV	285814	512096	23.11%	2.899%
44	7.320	1941	1953	1971	rBV	1064329	1831563	82.67%	10.369%
45	7.625	2038	2048	2079	rBV	201285	351804	15.88%	1.992%
46	7.812	2105	2106	2108	rBV	459	237	0.01%	0.001%
47	7.889	2126	2130	2132	rBV3	914	674	0.03%	0.004%
48	8.050	2178	2180	2183	rBV4	583	282	0.01%	0.002%
49	8.095	2183	2194	2228	rBV	527963	1045321	47.18%	5.918%
50	8.445	2301	2303	2306	rBV3	769	450	0.02%	0.003%
51	8.548	2330	2335	2337	rBV3	504	397	0.02%	0.002%
52	8.603	2350	2352	2354	rVB3	813	341	0.02%	0.002%
53	8.657	2367	2369	2374	rVB2	870	601	0.03%	0.003%
54	8.683	2374	2377	2381	rBV3	723	689	0.03%	0.004%
55	8.722	2381	2389	2393	rBV6	5592	7756	0.35%	0.044%
56	8.857	2419	2431	2458	rBV	978742	1607975	72.58%	9.103%
57	9.220	2542	2544	2546	rBV2	457	225	0.01%	0.001%
58	9.291	2564	2566	2568	rVB2	665	291	0.01%	0.002%
59	9.538	2641	2643	2646	rBV	389	268	0.01%	0.002%
60	9.641	2673	2675	2677	rBV	400	178	0.01%	0.001%
61	9.651	2677	2678	2681	rBV2	469	248	0.01%	0.001%
62	9.673	2682	2685	2687	rBV3	815	547	0.02%	0.003%
63	9.780	2716	2718	2721	rBV	361	304	0.01%	0.002%
64	9.818	2728	2730	2732	rBV	374	179	0.01%	0.001%
65	9.834	2732	2735	2737	rVV4	902	516	0.02%	0.003%
66	9.863	2741	2744	2748	rVB3	1216	1092	0.05%	0.006%
67	9.882	2748	2750	2753	rBV2	757	494	0.02%	0.003%
68	9.979	2778	2780	2782	rVB2	370	131	0.01%	0.001%
69	10.021	2782	2793	2806	rBV	130477	218808	9.88%	1.239%
70	10.220	2843	2855	2872	rBV	728685	1134428	51.21%	6.422%
71	10.439	2920	2923	2924	rBV	467	313	0.01%	0.002%
72	10.513	2943	2946	2947	rBV2	668	373	0.02%	0.002%
73	10.590	2963	2970	2976	rBV7	2115	3628	0.16%	0.021%
74	10.641	2984	2986	2991	rBV4	890	661	0.03%	0.004%
75	10.725	3007	3012	3015	rBV3	662	625	0.03%	0.004%
76	10.747	3016	3019	3024	rVV4	1179	918	0.04%	0.005%

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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : EW1B2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Title : VOC Analysis

77	10.812	3037	3039	3042	rVB3	905	371	0.02%	0.002%
78	10.898	3063	3066	3067	rBV2	1121	599	0.03%	0.003%
79	10.924	3067	3074	3083	rVB6	6240	10179	0.46%	0.058%
80	11.101	3126	3129	3133	rBV4	934	870	0.04%	0.005%
81	11.152	3138	3145	3153	rVV8	3573	5328	0.24%	0.030%
82	11.255	3165	3177	3194	rBV	1062738	1610424	72.69%	9.117%
83	11.474	3242	3245	3254	rVB7	1318	1611	0.07%	0.009%
84	11.545	3260	3267	3280	rVB8	5821	11072	0.50%	0.063%
85	11.632	3282	3294	3315	rVB	1149700	1785147	80.58%	10.106%
86	11.924	3384	3385	3387	rBV2	642	290	0.01%	0.002%
87	11.982	3401	3403	3406	rBV	599	385	0.02%	0.002%
88	12.050	3422	3424	3426	rBV	992	563	0.03%	0.003%
89	12.599	3592	3595	3598	rBV3	1174	855	0.04%	0.005%
90	12.654	3610	3612	3616	rVB2	849	444	0.02%	0.003%
91	12.738	3636	3638	3641	rBV	553	232	0.01%	0.001%
92	12.789	3652	3654	3657	rBV2	657	402	0.02%	0.002%
93	12.837	3659	3669	3682	rVV2	64699	98559	4.45%	0.558%
94	13.033	3728	3730	3732	rBV2	516	270	0.01%	0.002%
95	13.191	3776	3779	3781	rBV2	797	436	0.02%	0.002%
96	13.255	3797	3799	3802	rBV3	1048	646	0.03%	0.004%
97	13.342	3824	3826	3829	rBV3	447	286	0.01%	0.002%
98	13.741	3949	3950	3953	rVB2	1130	336	0.02%	0.002%
99	14.255	4108	4110	4111	rBV	884	423	0.02%	0.002%
100	14.992	4336	4339	4342	rBV4	1410	1053	0.05%	0.006%

Sum of corrected areas: 17664249

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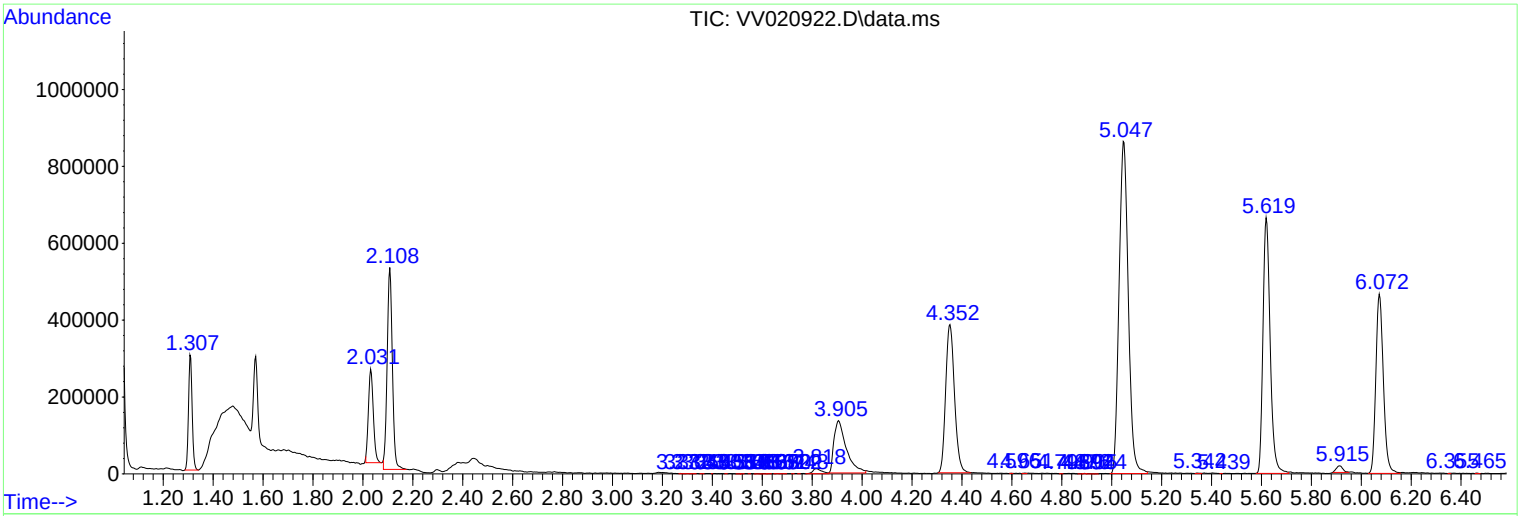
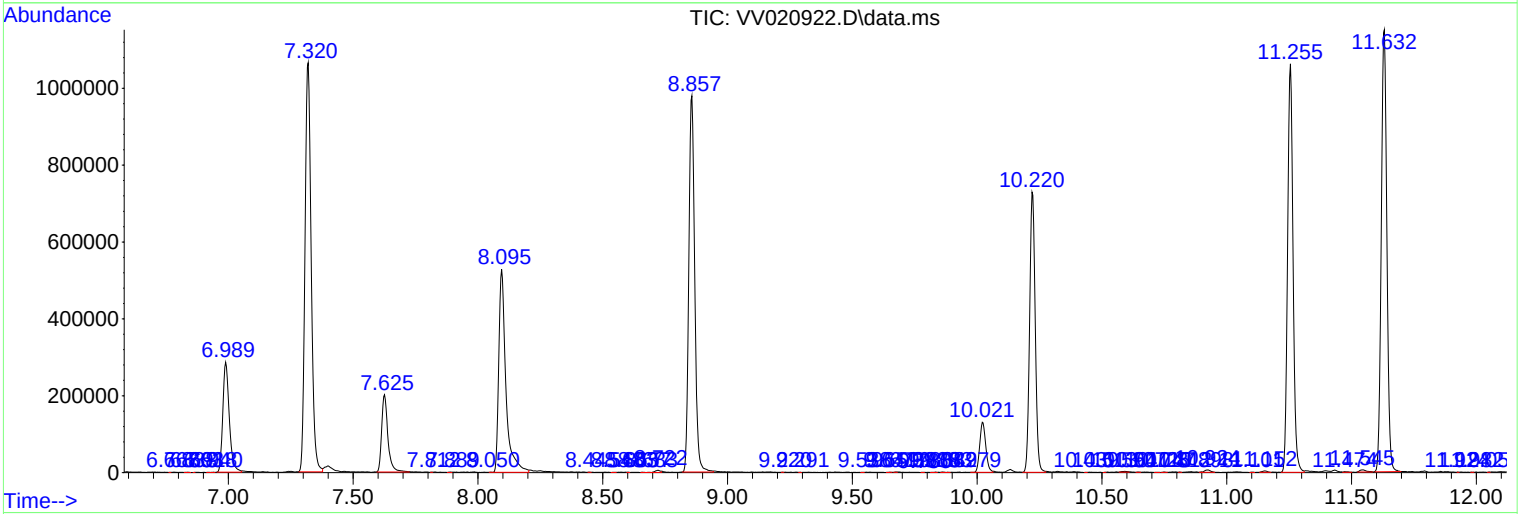
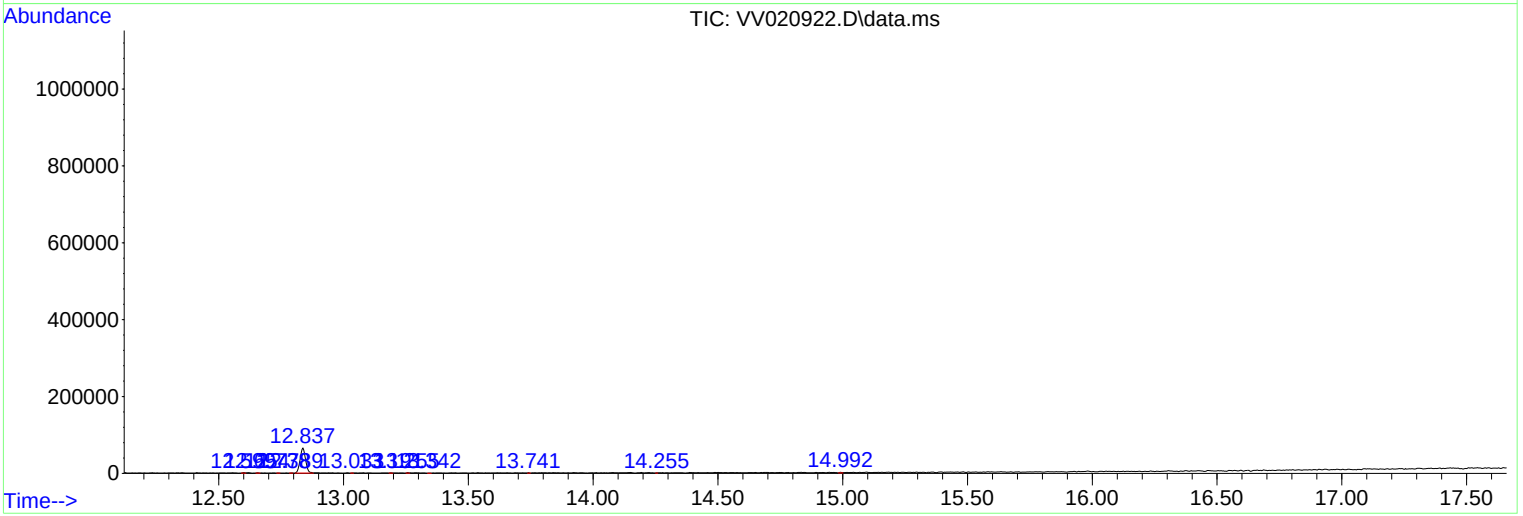
Instrument :
MSVOA_V
ClientSampleId :
EW1B2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

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







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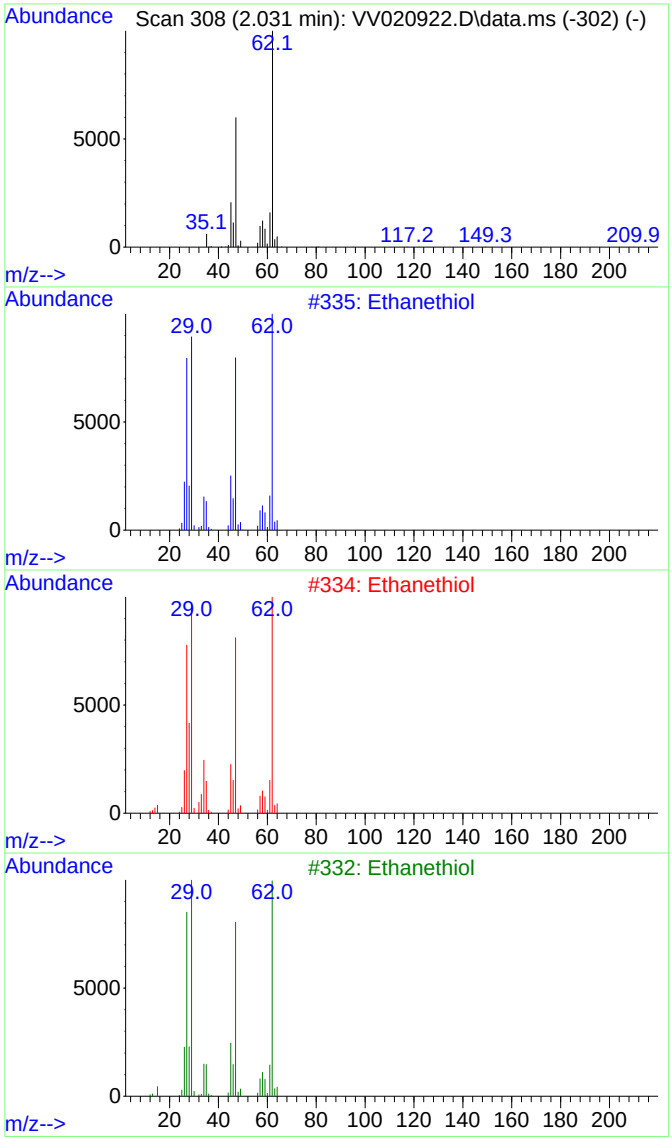
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

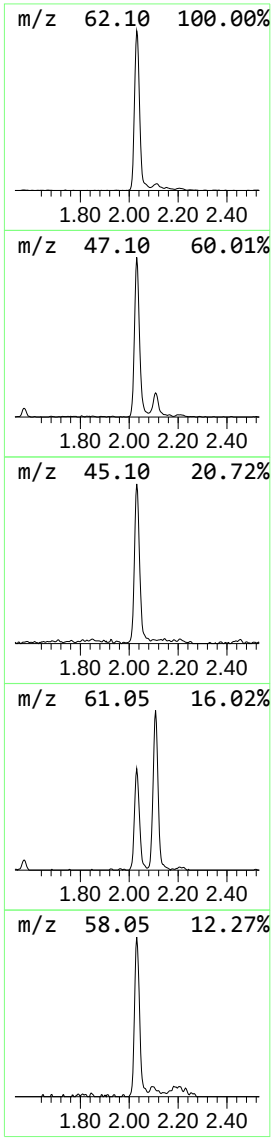
****

Peak Number 1 Ethanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.031	12.44 ug/L	332475	1,4-Difluorobenzene	5.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	87
5	Ethanethiol	62	C2H6S	000075-08-1	87





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

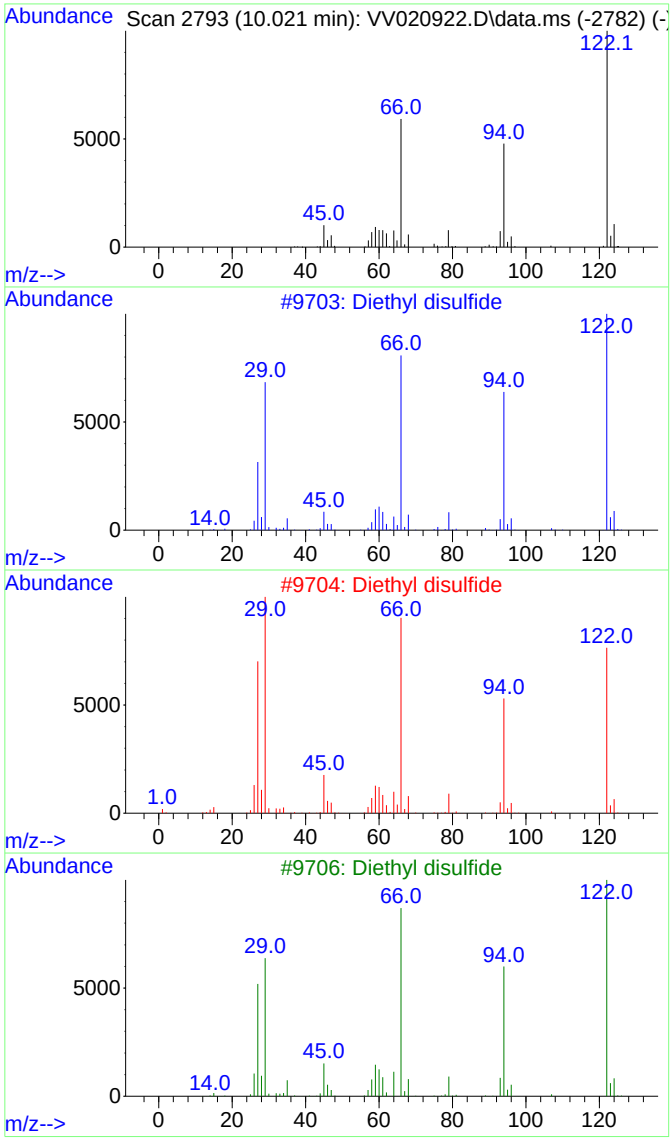
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

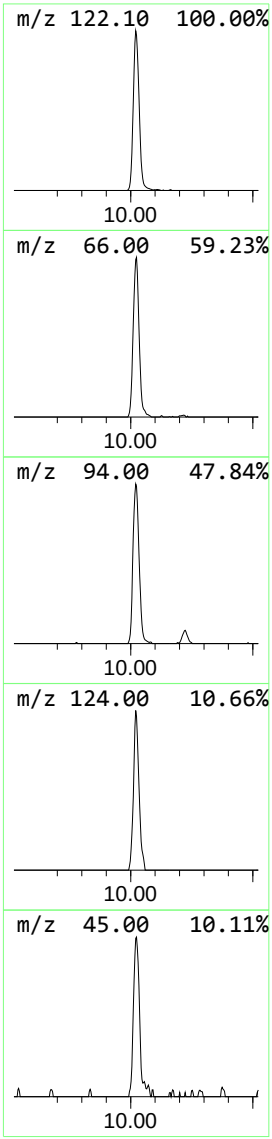
****

Peak Number 3 Diethyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.021	6.80 ug/L	218808	Chlorobenzene-d5	8.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl disulfide	122	C4H10S2	000110-81-6	94
2	Diethyl disulfide	122	C4H10S2	000110-81-6	91
3	Diethyl disulfide	122	C4H10S2	000110-81-6	91
4	Diethyl sulfone	122	C4H10O2S	000597-35-3	42
5	Diethyl sulfone	122	C4H10O2S	000597-35-3	33





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ClientSampleId : EW1B2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

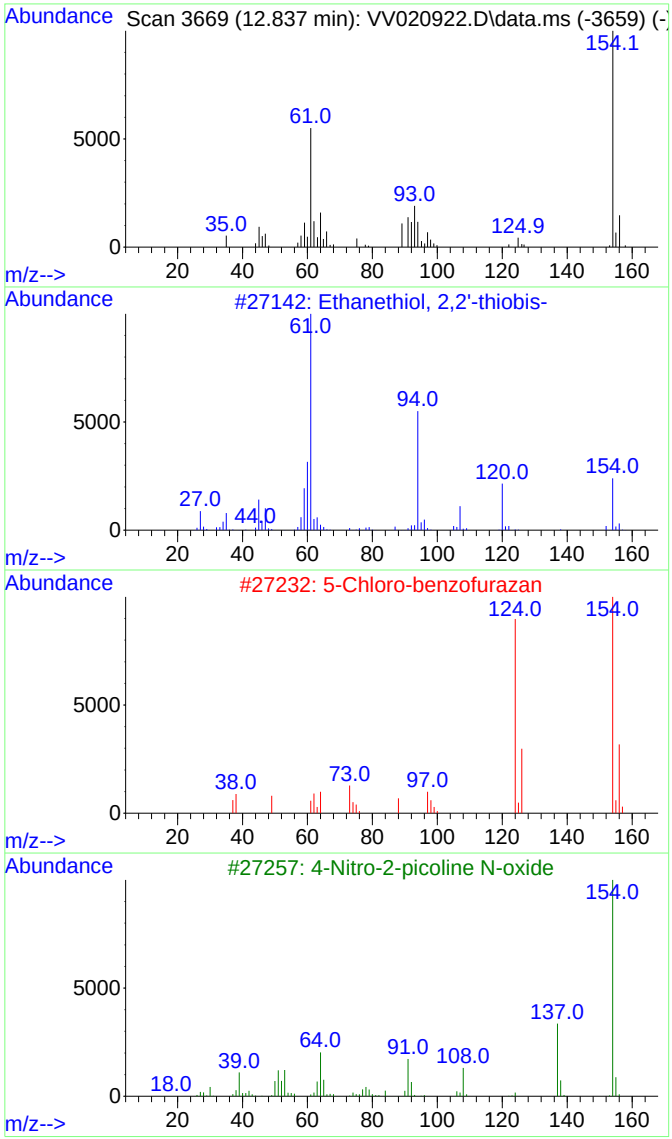
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

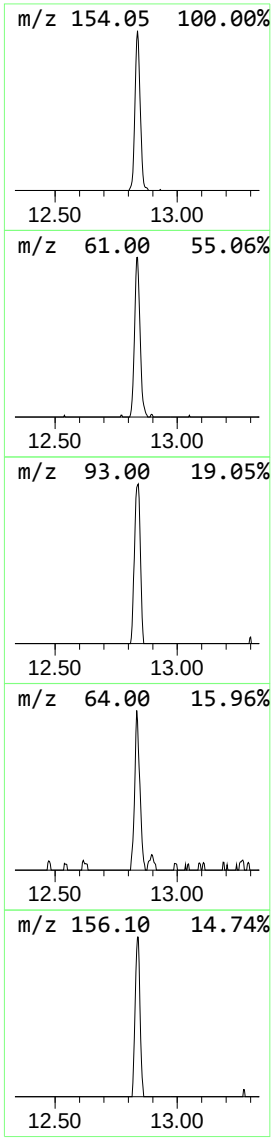
****

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.837	3.06 ug/L	98559	1,4-Dichlorobenzene-d4	11.255

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol, 2,2'-thiobis-	154	C4H10S3	003570-55-6	47
2	5-Chloro-benzofurazan	154	C6H3ClN2O	019155-86-3	43
3	4-Nitro-2-picoline N-oxide	154	C6H6N2O3	005470-66-6	16
4	2-(Dimethyl phosphino)-ethyl pho...	122	C4H12P2	054772-64-4	14
5	Benzoic acid, 4-mercapto-	154	C7H6O2S	001074-36-8	12





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanethiol	2.031	12.4	ug/L	332475	1	5.619	1336370	50.0
Diethyl disulfide	10.021	6.8	ug/L	218808	2	8.857	1607980	50.0
unknown-01	12.837	3.1	ug/L	98559	3	11.255	1610420	50.0