LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082518\
Data File : VU026382.D
Acq On : 25 Aug 2018 19:31
Operator : MD/SY
Sample : J4644-17
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOM7

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_U\METHOD\SOMULM082218WMA.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	0.609	4	6	13	rVB	365	286	0.02%	0.003%
2	0.638	13	15	16	rBV	122	46	0.00%	0.000%
3	0.664	16	23	24	rBV3	463	424	0.04%	0.004%
4	0.699	33	34	40	rVB	330	161	0.01%	0.001%
5	0.728	40	43	45	rBV2	559	368	0.03%	0.003%
6	0.760	50	53	55	rVV	363	243	0.02%	0.002%
7	0.773	55	57	60	rVV	307	181	0.02%	0.002%
8	0.805	62	67	70	rBV2	345	354	0.03%	0.003%
9	0.831	70	75	77	rVV2	294	305	0.03%	0.003%
10	0.857	81	83	85	rBV	150	78	0.01%	0.001%
11	0.892	92	94	97	rVB2	243	130	0.01%	0.001%
12	0.921	97	103	105	rBV2	305	256	0.02%	0.002%
13	1.088	135	155	174	rBV	801908	870348	74.39%	7.676%
14	1.400	244	252	266	rBV2	1102958	1169954	100.00%	10.318%
15	1.680	332	339	350	rVB	109534	137732	11.77%	1.215%
16	2.185	488	496	511	rBV	174215	261412	22.34%	2.305%
17	2.272	515	523	535	rVB	245554	369461	31.58%	3.258%
18	3.500	902	905	907	rBV	281	216	0.02%	0.002%
19	3.612	937	940	943	rBV2	301	180	0.02%	0.002%
20	3.815	1000	1003	1006	rBV2	204	127	0.01%	0.001%
21	3.908	1029	1032	1033	rBV	255	132	0.01%	0.001%
22	4.127	1088	1100	1104	rBV3	7159	14110	1.21%	0.124%
23	4.181	1106	1117	1119	rBV2	92793	151744	12.97%	1.338%
24	4.548	1228	1231	1236	rBV3	365	248	0.02%	0.002%
25	4.571	1236	1238	1239	rBV	222	72	0.01%	0.001%
26	4.651	1245	1263	1289	rBV	201039	471686	40.32%	4.160%
27	4.831	1318	1319	1320	rBV	321	114	0.01%	0.001%
28	4.940	1352	1353	1355	rBV	210	104	0.01%	0.001%
29	4.956	1355	1358	1362	rVB3	347	245	0.02%	0.002%
30	4.982	1363	1366	1367	rBV	431	235	0.02%	0.002%
31	5.024	1377	1379	1380	rBV	402	199	0.02%	0.002%
32	5.210	1434	1437	1441	rBV2	391	289	0.02%	0.003%
33	5.249	1445	1449	1453	rBV2	395	358	0.03%	0.003%
34	5.342	1453	1478	1504	rBV2	384663	1141722	97.59%	10.069%

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ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOM7

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_U\METHOD\SOMULM082218WMA.M
Title : VOC Analysis

35	5.458	1512	1514	1519	rBV3	391	372	0.03%	0.003%
36	5.545	1538	1541	1542	rBV	426	218	0.02%	0.002%
37	5.799	1618	1620	1622	rBV	504	209	0.02%	0.002%
38	5.889	1634	1648	1675	rBV	369707	722607	61.76%	6.373%
39	6.085	1704	1709	1711	rBV2	645	484	0.04%	0.004%
40	6.152	1728	1730	1734	rBV2	389	223	0.02%	0.002%
41	6.191	1734	1742	1753	rVB7	3618	6895	0.59%	0.061%
42	6.255	1759	1762	1765	rBV2	283	198	0.02%	0.002%
43	6.332	1771	1786	1806	rBV	263553	518514	44.32%	4.573%
44	6.506	1837	1840	1843	rBV3	271	174	0.01%	0.002%
45	6.599	1867	1869	1871	rBV	180	119	0.01%	0.001%
46	6.644	1878	1883	1887	rBV3	445	412	0.04%	0.004%
47	6.725	1900	1908	1912	rVB2	355	394	0.03%	0.003%
48	6.750	1912	1916	1920	rBV2	374	273	0.02%	0.002%
49	6.824	1937	1939	1940	rBV2	303	142	0.01%	0.001%
50	6.950	1975	1978	1982	rVB	315	282	0.02%	0.002%
51	6.972	1982	1985	1990	rVB2	299	253	0.02%	0.002%
52	7.001	1990	1994	2001	rBV3	476	727	0.06%	0.006%
53	7.059	2006	2012	2015	rBV3	378	482	0.04%	0.004%
54	7.127	2030	2033	2035	rBV	274	191	0.02%	0.002%
55	7.230	2053	2065	2086	rBV	142723	248799	21.27%	2.194%
56	7.361	2104	2106	2107	rBV	262	100	0.01%	0.001%
57	7.451	2132	2134	2135	rBV	188	97	0.01%	0.001%
58	7.567	2154	2170	2191	rBV	531087	908758	77.67%	8.014%
59	7.779	2232	2236	2241	rBV2	503	435	0.04%	0.004%
60	7.808	2243	2245	2246	rBV	164	50	0.00%	0.000%
61	7.850	2246	2258	2274	rBV	106372	178439	15.25%	1.574%
62	8.188	2352	2363	2373	rBV2	35201	87752	7.50%	0.774%
63	8.313	2394	2402	2421	rVB	341867	566025	48.38%	4.992%
64	8.648	2504	2506	2508	rBV	395	156	0.01%	0.001%
65	8.757	2537	2540	2542	rBV2	310	219	0.02%	0.002%
66	8.905	2585	2586	2587	rBV2	237	80	0.01%	0.001%
67	8.921	2588	2591	2594	rVV3	445	408	0.03%	0.004%
68	8.953	2594	2601	2613	rVB6	2508	4874	0.42%	0.043%
69	9.091	2631	2644	2670	rBV	547932	895061	76.50%	7.894%
70	9.252	2691	2694	2697	rBV2	428	319	0.03%	0.003%
71	9.339	2718	2721	2723	rBV	217	141	0.01%	0.001%

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ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOM7

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_U\METHOD\SOMULM082218WMA.M
Title : VOC Analysis

72	9.377	2730	2733	2741	rVB3	994	1059	0.09%	0.009%
73	9.419	2743	2746	2750	rBV2	436	301	0.03%	0.003%
74	9.474	2760	2763	2768	rBV2	409	332	0.03%	0.003%
75	9.496	2768	2770	2773	rVB	355	192	0.02%	0.002%
76	9.519	2775	2777	2780	rBV2	262	170	0.01%	0.001%
77	9.692	2827	2831	2835	rVB2	394	281	0.02%	0.002%
78	9.718	2835	2839	2842	rBV2	639	531	0.05%	0.005%
79	9.863	2878	2884	2885	rBV	350	365	0.03%	0.003%
80	9.898	2892	2895	2898	rBV2	374	321	0.03%	0.003%
81	9.940	2904	2908	2909	rBV3	390	297	0.03%	0.003%
82	9.975	2916	2919	2920	rBV	138	79	0.01%	0.001%
83	10.011	2927	2930	2932	rBV	230	118	0.01%	0.001%
84	10.062	2944	2946	2951	rVB2	465	333	0.03%	0.003%
85	10.165	2975	2978	2982	rBV2	593	540	0.05%	0.005%
86	10.255	2994	3006	3028	rBV2	88275	154481	13.20%	1.362%
87	10.390	3046	3048	3049	rBV	285	130	0.01%	0.001%
88	10.432	3049	3061	3083	rVB	369884	596485	50.98%	5.260%
89	10.622	3112	3120	3133	rVB2	16562	31211	2.67%	0.275%
90	10.754	3158	3161	3163	rBV	415	279	0.02%	0.002%
91	10.879	3195	3200	3207	rVB3	1508	1783	0.15%	0.016%
92	10.908	3207	3209	3213	rBV2	348	297	0.03%	0.003%
93	11.078	3260	3262	3265	rBV2	463	278	0.02%	0.002%
94	11.123	3274	3276	3279	rBV	345	223	0.02%	0.002%
95	11.210	3301	3303	3304	rBV	227	103	0.01%	0.001%
96	11.487	3377	3389	3406	rBV	560164	868320	74.22%	7.658%
97	11.747	3462	3470	3483	rBV3	12285	19680	1.68%	0.174%
98	11.863	3492	3506	3522	rBV	571928	911640	77.92%	8.040%
99	12.307	3641	3644	3646	rBV	479	290	0.02%	0.003%
100	13.072	3875	3882	3891	rVB5	6947	10499	0.90%	0.093%

Sum of corrected areas: 11339020

LSC Report - Integrated Chromatogram

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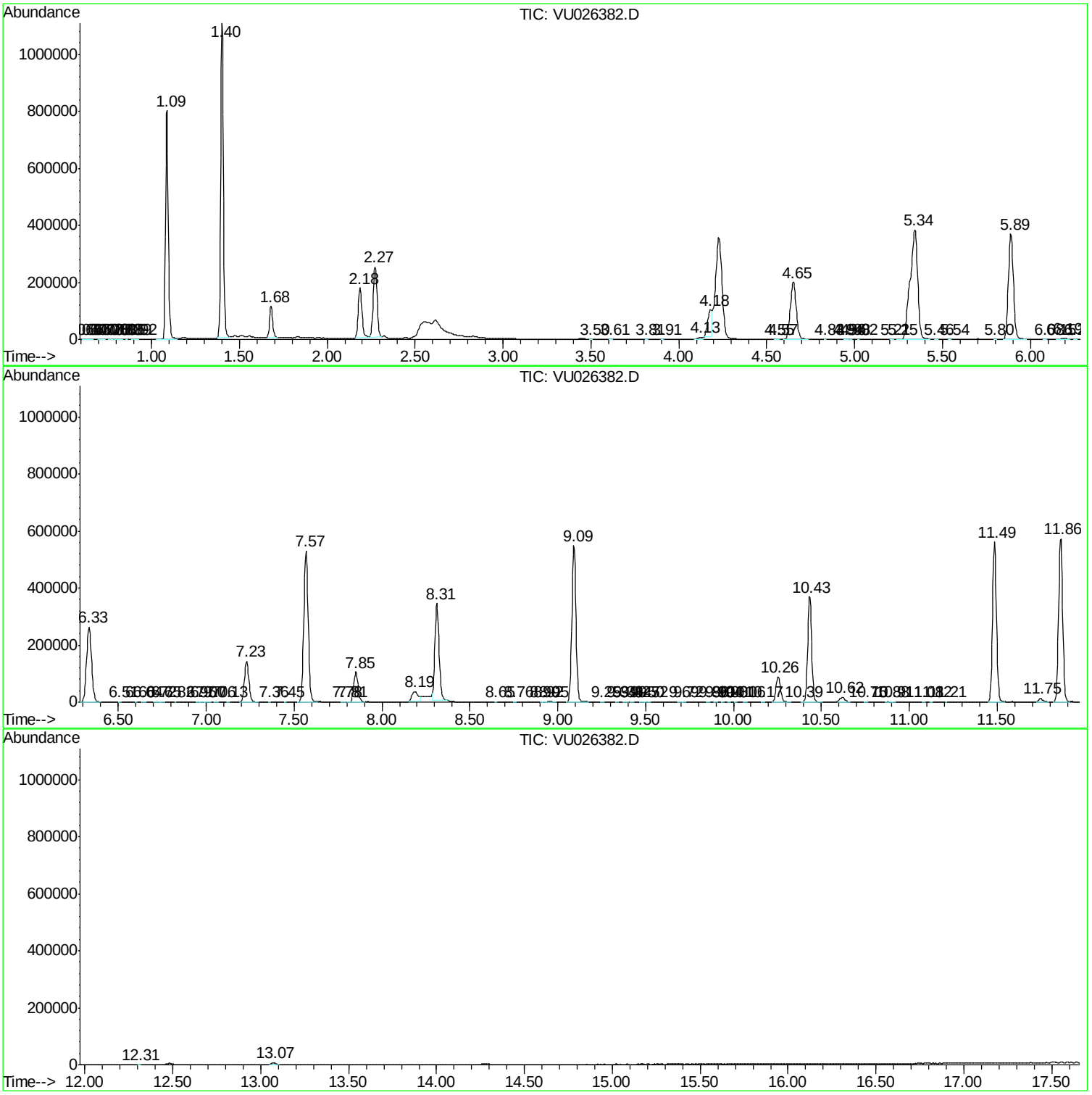
Instrument : MSVOA_U
ClientSampleId : ETOM7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082218WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082518\
Data File : VU026382.D
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Quant Title : VOC Analysis

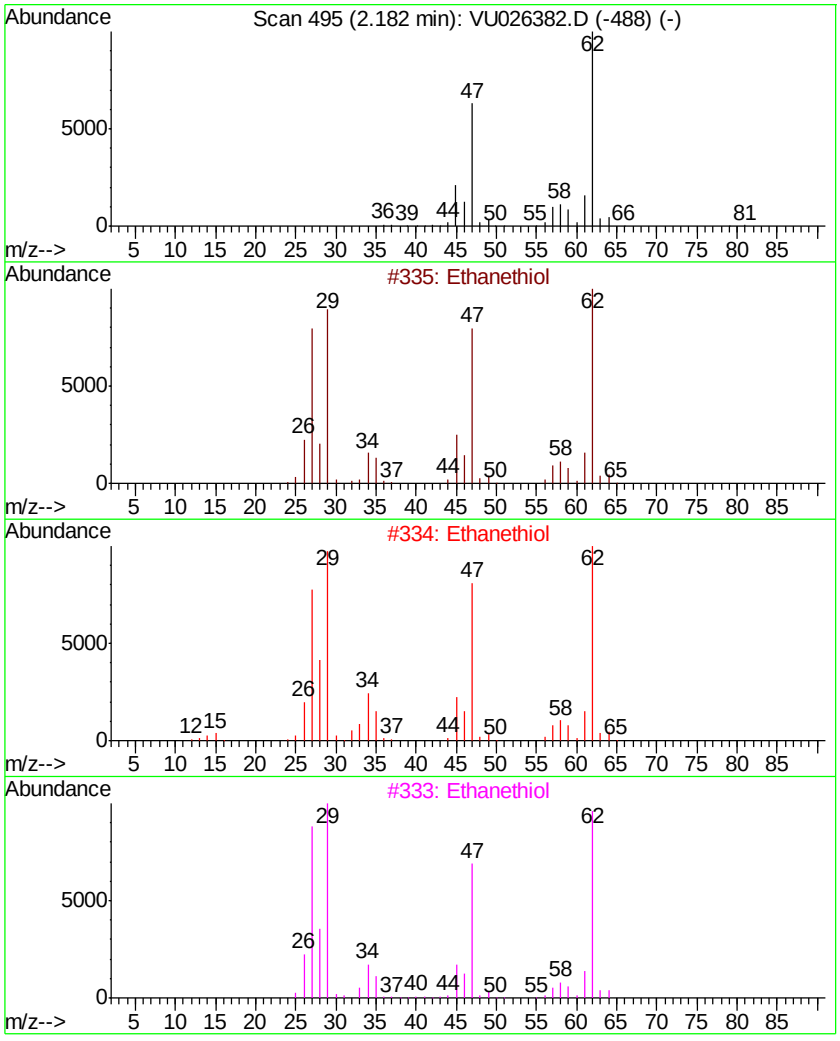
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

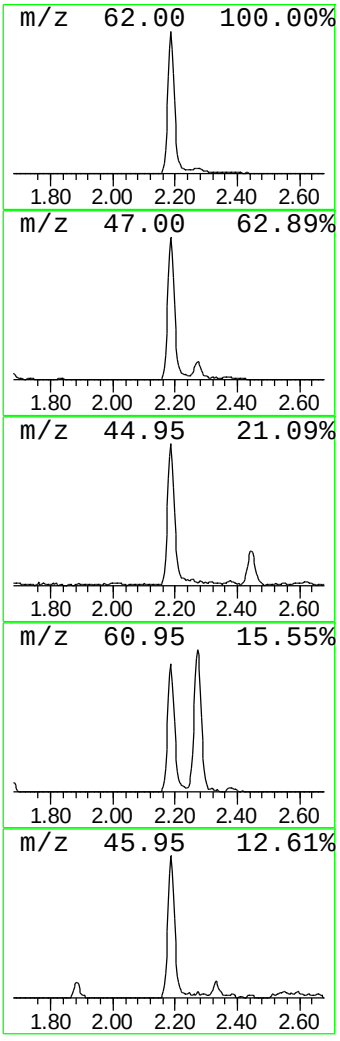
****

Peak Number 2 Ethanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	18.09 ug/L	261412	1,4-Difluorobenzene	5.89

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	91
5	Ethanethiol	62	C2H6S	000075-08-1	91





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Instrument : MSVOA_U
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082218WMA.M
Quant Title : VOC Analysis

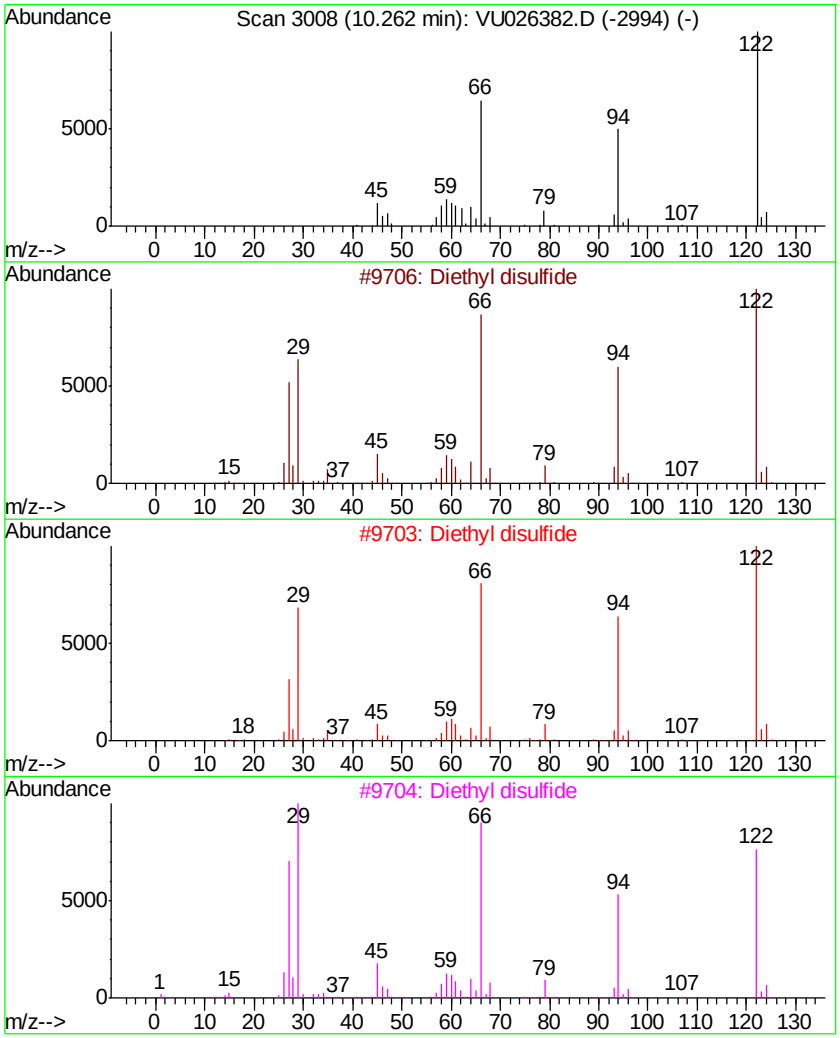
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

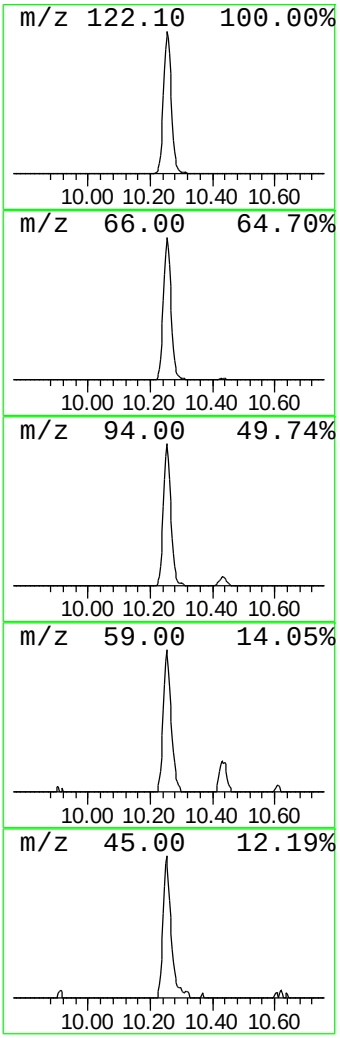
****

Peak Number 5 Diethyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	8.63 ug/L	154481	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl disulfide	122	C4H10S2	000110-81-6	95
2	Diethyl disulfide	122	C4H10S2	000110-81-6	91
3	Diethyl disulfide	122	C4H10S2	000110-81-6	45
4	5-exo-Methyl-5-norbornenol	124	C8H12O	003212-13-3	38
5	6-exo-Methyl-5-exo-norbornenol	124	C8H12O	060362-83-6	38





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	2.18	18.1	ug/L	261412	1	5.89	722607	50.0
Diethyl disulfide	10.26	8.6	ug/L	154481	2	9.09	895061	50.0