LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031523\
Data File : VU053207.D
Acq On : 15 Mar 2023 17:50
Operator : JC/MD
Sample : 01929-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFE5

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\SFAMULM031523WMA.M
Title : VOC Analysis

Signal : TIC: VU053207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	34	42	72	rBV	50834	133395	20.46%	2.562%
2	1.598	74	80	95	rVB	93102	110244	16.91%	2.118%
3	1.913	171	178	195	rVB	75195	101048	15.50%	1.941%
4	2.566	370	381	397	rBV	142744	231511	35.51%	4.447%
5	2.794	446	452	454	rBV2	632	749	0.11%	0.014%
6	2.951	492	501	517	rBV	8273	16127	2.47%	0.310%
7	3.794	760	763	768	rBV2	188	218	0.03%	0.004%
8	3.881	785	790	793	rBV2	206	167	0.03%	0.003%
9	4.321	923	927	930	rBV2	285	224	0.03%	0.004%
10	4.347	930	935	937	rBV2	226	227	0.03%	0.004%
11	4.466	970	972	977	rVB	223	189	0.03%	0.004%
12	4.565	991	1003	1010	rBV2	3760	7582	1.16%	0.146%
13	4.623	1010	1021	1046	rVV	49755	128038	19.64%	2.459%
14	5.057	1141	1156	1176	rBV	120502	261664	40.13%	5.026%
15	5.289	1225	1228	1231	rVB	319	171	0.03%	0.003%
16	5.321	1231	1238	1240	rBV2	189	151	0.02%	0.003%
17	5.340	1240	1244	1247	rBV2	215	187	0.03%	0.004%
18	5.469	1280	1284	1287	rBV2	201	180	0.03%	0.003%
19	5.720	1341	1362	1396	rBV2	238748	652023	100.00%	12.524%
20	5.900	1414	1418	1420	rBV	313	204	0.03%	0.004%
21	6.064	1466	1469	1476	rBV2	185	143	0.02%	0.003%
22	6.244	1511	1525	1548	rBV	180975	343608	52.70%	6.600%
23	6.385	1566	1569	1572	rBV3	326	225	0.03%	0.004%
24	6.405	1572	1575	1578	rVV2	283	257	0.04%	0.005%
25	6.530	1607	1614	1617	rBV2	618	603	0.09%	0.012%
26	6.562	1619	1624	1633	rVV4	1446	2440	0.37%	0.047%
27	6.684	1649	1662	1683	rBV	150261	293329	44.99%	5.634%
28	6.877	1718	1722	1724	rBV	182	147	0.02%	0.003%
29	6.932	1734	1739	1742	rBV2	408	480	0.07%	0.009%
30	7.067	1777	1781	1783	rBV2	204	161	0.02%	0.003%
31	7.183	1812	1817	1823	rVV4	1300	1725	0.26%	0.033%
32	7.221	1827	1829	1833	rVV	224	143	0.02%	0.003%
33	7.308	1852	1856	1859	rVB2	192	151	0.02%	0.003%
34	7.385	1877	1880	1884	rVB2	215	182	0.03%	0.003%
35	7.501	1911	1916	1920	rVB2	172	159	0.02%	0.003%
36	7.562	1922	1935	1954	rVV	88624	156808	24.05%	3.012%

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFE5

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\SFAMULM031523WMA.M
Title : VOC Analysis

37	7.649	1959	1962	1963	rBV	264	179	0.03%	0.003%
38	7.684	1969	1973	1978	rBV4	645	665	0.10%	0.013%
39	7.893	2024	2038	2054	rBV	306272	527732	80.94%	10.137%
40	8.176	2114	2126	2147	rBV	61532	104518	16.03%	2.008%
41	8.318	2168	2170	2172	rBV	288	142	0.02%	0.003%
42	8.414	2195	2200	2203	rVV2	246	255	0.04%	0.005%
43	8.440	2205	2208	2211	rVB2	309	175	0.03%	0.003%
44	8.466	2211	2216	2220	rBV2	185	208	0.03%	0.004%
45	8.546	2236	2241	2245	rBV2	202	190	0.03%	0.004%
46	8.630	2254	2267	2294	rBV2	170683	324434	49.76%	6.232%
47	8.790	2314	2317	2322	rVB3	727	523	0.08%	0.010%
48	8.861	2334	2339	2342	rBV2	189	246	0.04%	0.005%
49	8.903	2349	2352	2355	rBV2	203	143	0.02%	0.003%
50	9.115	2413	2418	2424	rVV2	189	195	0.03%	0.004%
51	9.199	2438	2444	2447	rBV	187	214	0.03%	0.004%
52	9.266	2461	2465	2467	rBV2	469	349	0.05%	0.007%
53	9.411	2498	2510	2535	rVV	261141	438670	67.28%	8.426%
54	9.559	2550	2556	2557	rBV2	348	305	0.05%	0.006%
55	9.630	2575	2578	2581	rBV	255	192	0.03%	0.004%
56	9.755	2613	2617	2622	rVB2	318	319	0.05%	0.006%
57	10.019	2695	2699	2702	rBV2	257	188	0.03%	0.004%
58	10.060	2707	2712	2715	rBV2	249	239	0.04%	0.005%
59	10.099	2721	2724	2729	rVB3	326	264	0.04%	0.005%
60	10.244	2761	2769	2772	rBV2	475	443	0.07%	0.009%
61	10.298	2780	2786	2787	rBV	165	147	0.02%	0.003%
62	10.411	2819	2821	2827	rVB	242	148	0.02%	0.003%
63	10.456	2832	2835	2840	rBV2	238	263	0.04%	0.005%
64	10.565	2859	2869	2888	rVB	24431	39187	6.01%	0.753%
65	10.752	2914	2927	2946	rVB	212109	339213	52.02%	6.516%
66	10.884	2966	2968	2972	rVB	252	194	0.03%	0.004%
67	10.909	2972	2976	2979	rBV	152	160	0.02%	0.003%
68	10.957	2988	2991	2994	rVV2	197	157	0.02%	0.003%
69	11.015	3005	3009	3014	rBV	296	226	0.03%	0.004%
70	11.060	3019	3023	3029	rBV2	222	213	0.03%	0.004%
71	11.112	3034	3039	3041	rBV2	232	227	0.03%	0.004%
72	11.195	3061	3065	3068	rBV2	216	175	0.03%	0.003%
73	11.215	3068	3071	3073	rVB	257	149	0.02%	0.003%
74	11.253	3080	3083	3087	rBV2	230	179	0.03%	0.003%
75	11.314	3098	3102	3106	rBV2	289	240	0.04%	0.005%
76	11.462	3144	3148	3150	rBV	384	302	0.05%	0.006%

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFE5

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\SFAMULM031523WMA.M
Title : VOC Analysis

77	11.504	3158	3161	3167	rBV2	229	290	0.04%	0.006%
78	11.575	3177	3183	3188	rVB3	454	525	0.08%	0.010%
79	11.633	3197	3201	3205	rBV2	143	145	0.02%	0.003%
80	11.806	3243	3255	3281	rBV	294438	469704	72.04%	9.022%
81	11.938	3294	3296	3300	rVB	390	235	0.04%	0.005%
82	11.983	3305	3310	3314	rBV	178	192	0.03%	0.004%
83	12.006	3314	3317	3320	rVB	206	141	0.02%	0.003%
84	12.067	3326	3336	3338	rBV2	3675	4310	0.66%	0.083%
85	12.189	3362	3374	3393	rBV	289686	470685	72.19%	9.041%
86	12.440	3449	3452	3455	rVB	244	171	0.03%	0.003%
87	12.552	3482	3487	3490	rVB2	282	285	0.04%	0.005%
88	12.768	3550	3554	3559	rBV2	426	519	0.08%	0.010%
89	13.044	3635	3640	3645	rVB2	244	209	0.03%	0.004%
90	13.250	3701	3704	3708	rBV	259	154	0.02%	0.003%
91	13.398	3741	3750	3763	rBV3	18679	29895	4.58%	0.574%
92	13.536	3789	3793	3795	rBV2	214	187	0.03%	0.004%
93	13.961	3922	3925	3926	rBV	287	165	0.03%	0.003%
94	14.009	3935	3940	3943	rBV	212	181	0.03%	0.003%
95	14.092	3963	3966	3968	rBV	480	302	0.05%	0.006%
96	14.234	4007	4010	4014	rBV	237	197	0.03%	0.004%
97	14.272	4017	4022	4024	rBV2	235	204	0.03%	0.004%
98	14.324	4036	4038	4040	rBV2	259	141	0.02%	0.003%
99	14.356	4046	4048	4050	rBV	310	162	0.02%	0.003%
100	14.690	4149	4152	4155	rBV	314	157	0.02%	0.003%

Sum of corrected areas: 5205984

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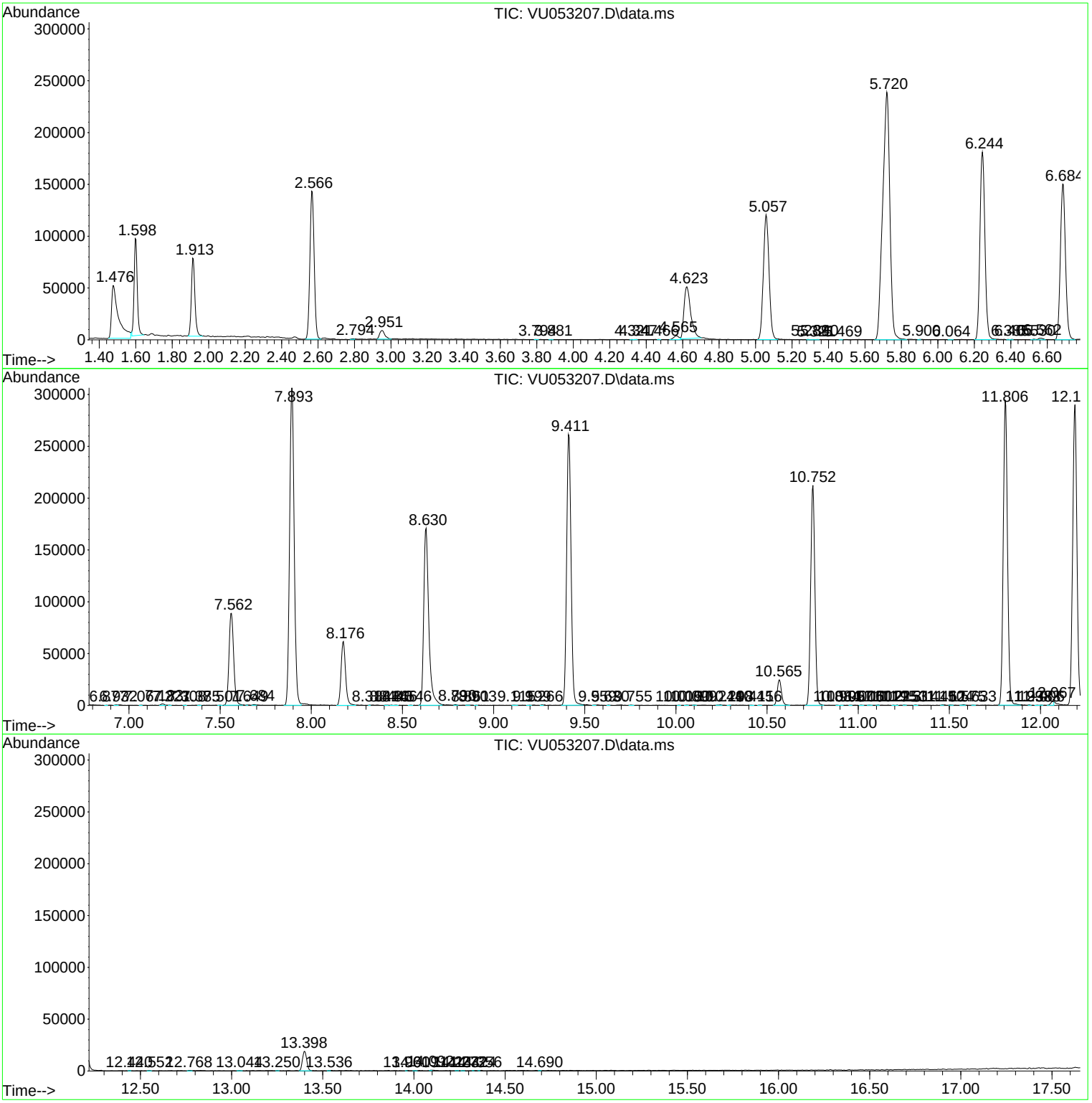
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFE5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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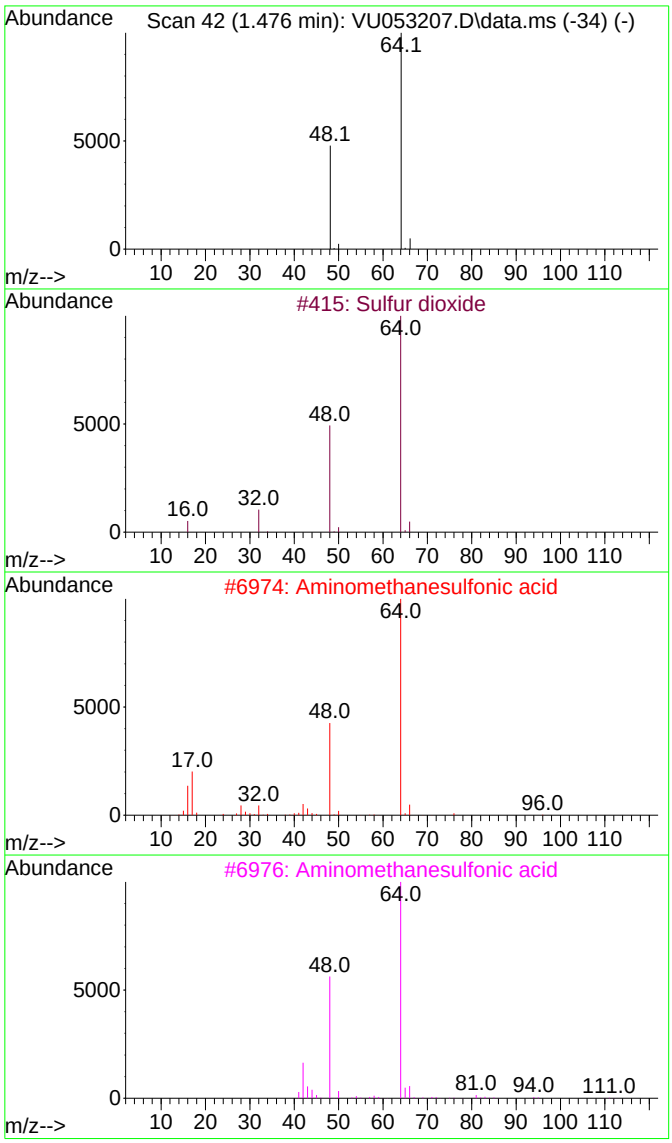
Quant Title : VOC Analysis

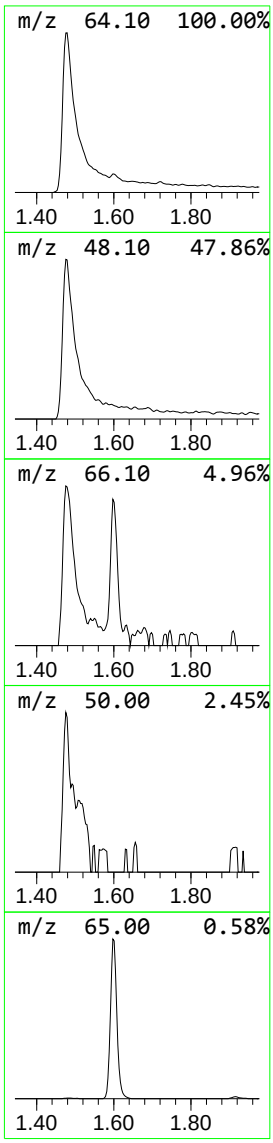
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.476	19.41 ug/L	133395	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Sulfur dioxide	64	O2S	007446-09-5	4





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Instrument :
MSVOA_U
ClientSampleId :
EYFE5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

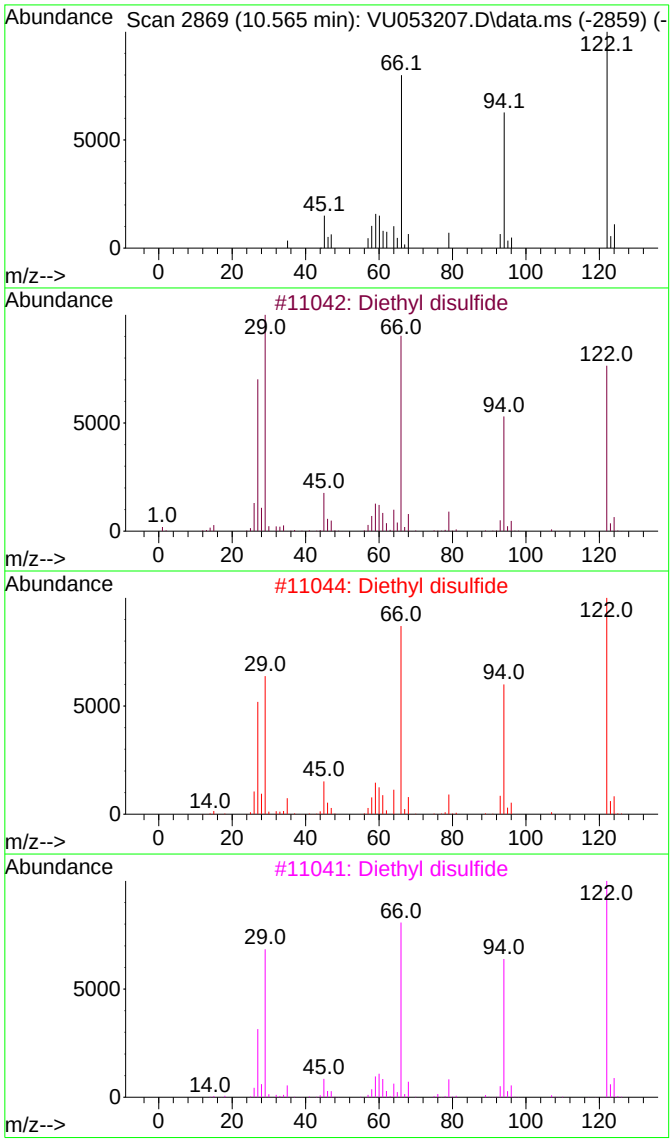
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

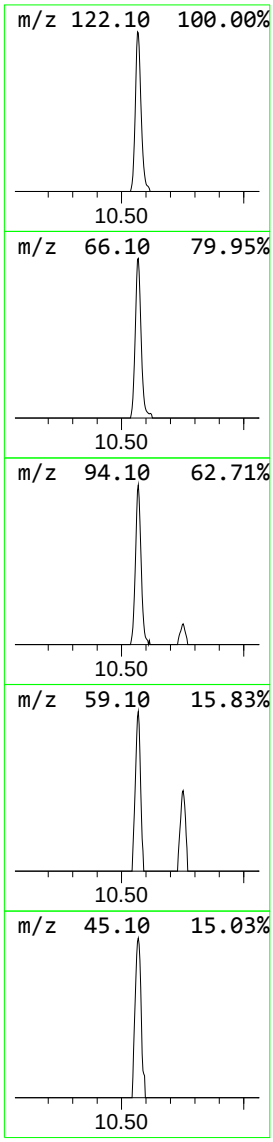
****

Peak Number 3 Diethyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.565	4.47 ug/L	39187	Chlorobenzene-d5	9.411

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	83
4	Benzene, ethoxy-	122	C8H10O	000103-73-1	50
5	6-exo-Methyl-5-exo-norbornenol	124	C8H12O	060362-83-6	50





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MSVOA_U
ClientSampleId :
EYFE5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

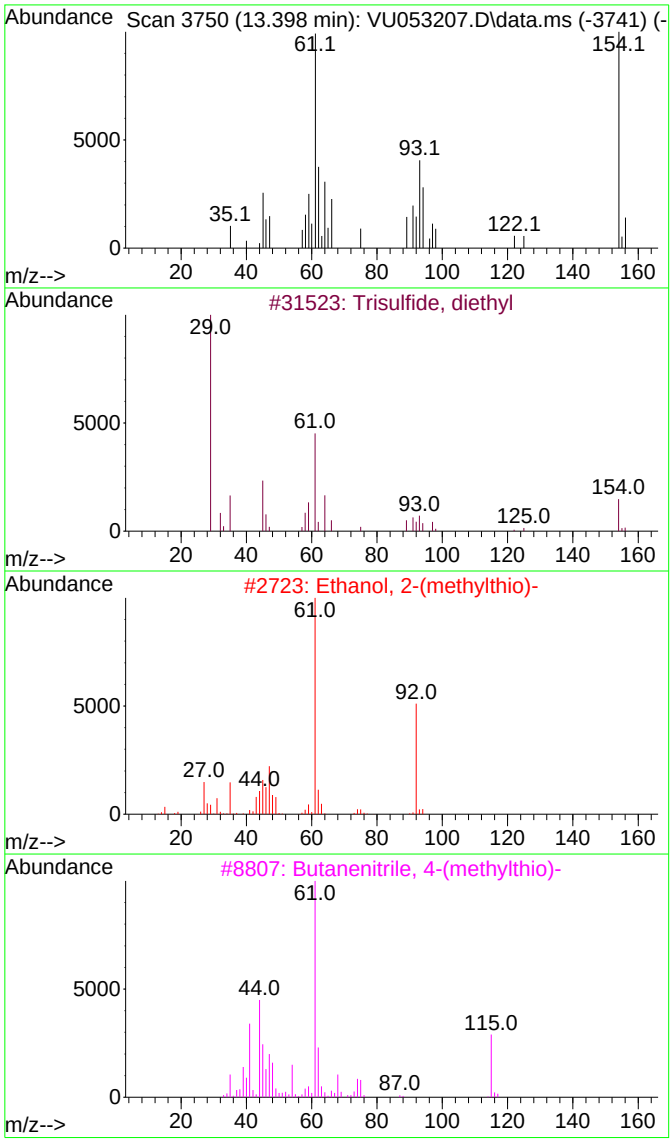
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

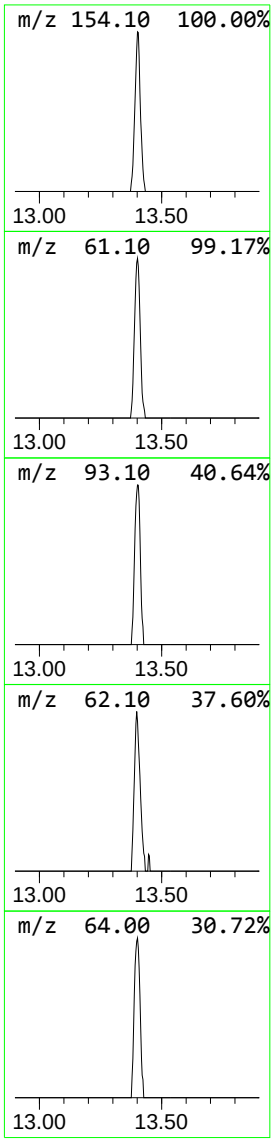
****

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.398	3.18 ug/L	29895	1,4-Dichlorobenzene-d4	11.806

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, diethyl	154	C4H10S3	003600-24-6	22
2	Ethanol, 2-(methylthio)-	92	C3H8OS	005271-38-5	14
3	Butanenitrile, 4-(methylthio)-	115	C5H9NS	059121-24-3	14
4	1-Nitro-2-propanol	105	C3H7NO3	003156-73-8	12
5	1,2-Propanediol, 3-(methylthio)-	122	C4H10O2S	022551-26-4	12





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.476	19.4	ug/L	133395	1	6.244	343608	50.0
Diethyl disulfide	10.565	4.5	ug/L	39187	2	9.411	438670	50.0
unknown-01	13.398	3.2	ug/L	29895	3	11.806	469704	50.0