LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031523\
Data File : VU053208.D
Acq On : 15 Mar 2023 18:13
Operator : JC/MD
Sample : 01929-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFE7

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: VU053208.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	35	43	71	rBV	43740	116045	19.10%	2.409%
2	1.600	75	81	96	rVB	87114	101766	16.75%	2.112%
3	1.912	171	178	192	rVB	69216	94508	15.56%	1.962%
4	2.565	370	381	396	rBV	132927	215123	35.41%	4.465%
5	3.816	767	770	771	rBV	190	94	0.02%	0.002%
6	3.841	776	778	779	rBV	197	81	0.01%	0.002%
7	4.038	838	839	840	rBV	268	72	0.01%	0.001%
8	4.079	850	852	853	rBV2	131	73	0.01%	0.002%
9	4.337	930	932	934	rBV	144	54	0.01%	0.001%
10	4.475	972	975	977	rBV	135	64	0.01%	0.001%
11	4.620	1009	1020	1053	rBV	45790	122467	20.16%	2.542%
12	4.964	1125	1127	1129	rBV	162	102	0.02%	0.002%
13	5.057	1141	1156	1175	rBV	111357	243044	40.01%	5.045%
14	5.173	1189	1192	1196	rBV2	242	152	0.03%	0.003%
15	5.198	1196	1200	1202	rBV2	181	135	0.02%	0.003%
16	5.327	1237	1240	1244	rBV2	198	199	0.03%	0.004%
17	5.369	1251	1253	1255	rVB	184	52	0.01%	0.001%
18	5.407	1261	1265	1267	rBV2	126	117	0.02%	0.002%
19	5.465	1280	1283	1287	rBV2	210	178	0.03%	0.004%
20	5.620	1329	1331	1333	rVB	179	74	0.01%	0.002%
21	5.719	1341	1362	1383	rBV2	225273	607507	100.00%	12.610%
22	5.880	1407	1412	1415	rBV2	353	376	0.06%	0.008%
23	5.931	1425	1428	1431	rVB	263	169	0.03%	0.004%
24	5.948	1431	1433	1434	rBV	150	67	0.01%	0.001%
25	6.243	1512	1525	1543	rBV	175758	335292	55.19%	6.960%
26	6.372	1558	1565	1568	rBV2	281	343	0.06%	0.007%
27	6.423	1578	1581	1584	rBV2	315	275	0.05%	0.006%
28	6.443	1584	1587	1589	rVV	149	115	0.02%	0.002%
29	6.497	1602	1604	1607	rBV2	257	153	0.03%	0.003%
30	6.526	1611	1613	1619	rVB2	395	257	0.04%	0.005%
31	6.568	1619	1626	1634	rVV4	1483	2602	0.43%	0.054%
32	6.600	1634	1636	1639	rVB	246	137	0.02%	0.003%
33	6.684	1648	1662	1680	rBV	140161	274327	45.16%	5.694%
34	6.783	1689	1693	1697	rBV	514	437	0.07%	0.009%
35	6.812	1697	1702	1708	rVB3	536	507	0.08%	0.011%
36	6.996	1756	1759	1761	rBV	156	94	0.02%	0.002%

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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_U\Method\SFAMULM031523WMA.M
Title : VOC Analysis

37	7.009	1761	1763	1767	rVB	327	149	0.02%	0.003%
38	7.185	1812	1818	1819	rBV2	835	803	0.13%	0.017%
39	7.385	1877	1880	1882	rBV2	286	208	0.03%	0.004%
40	7.443	1896	1898	1902	rBB	167	72	0.01%	0.001%
41	7.562	1923	1935	1953	rBV	81016	144084	23.72%	2.991%
42	7.893	2025	2038	2059	rBV	281131	487336	80.22%	10.116%
43	8.044	2082	2085	2088	rVB	438	168	0.03%	0.003%
44	8.060	2088	2090	2092	rBV	230	98	0.02%	0.002%
45	8.076	2092	2095	2097	rBV2	273	186	0.03%	0.004%
46	8.176	2113	2126	2141	rBV2	55741	95619	15.74%	1.985%
47	8.404	2195	2197	2198	rBV2	147	67	0.01%	0.001%
48	8.468	2214	2217	2221	rBV2	294	220	0.04%	0.005%
49	8.539	2236	2239	2241	rBV2	196	118	0.02%	0.002%
50	8.558	2241	2245	2247	rBV2	263	213	0.04%	0.004%
51	8.629	2256	2267	2294	rBV2	155618	296132	48.75%	6.147%
52	8.819	2322	2326	2328	rBV2	263	224	0.04%	0.005%
53	8.906	2350	2353	2356	rBV2	224	179	0.03%	0.004%
54	8.963	2369	2371	2372	rBV	170	73	0.01%	0.002%
55	9.018	2387	2388	2391	rBV	157	86	0.01%	0.002%
56	9.124	2417	2421	2424	rVB2	214	166	0.03%	0.003%
57	9.179	2436	2438	2440	rBV	163	99	0.02%	0.002%
58	9.346	2488	2490	2492	rVB	147	78	0.01%	0.002%
59	9.414	2498	2511	2535	rBV	249999	417130	68.66%	8.659%
60	9.562	2555	2557	2559	rVB	311	107	0.02%	0.002%
61	9.680	2592	2594	2597	rBV	163	59	0.01%	0.001%
62	9.693	2597	2598	2601	rVB	150	81	0.01%	0.002%
63	9.735	2609	2611	2613	rBV	160	95	0.02%	0.002%
64	9.870	2650	2653	2656	rVB2	244	172	0.03%	0.004%
65	10.108	2724	2727	2728	rBV	312	160	0.03%	0.003%
66	10.195	2752	2754	2757	rVB	201	95	0.02%	0.002%
67	10.314	2788	2791	2794	rBV2	181	117	0.02%	0.002%
68	10.407	2817	2820	2823	rVB	181	92	0.02%	0.002%
69	10.446	2830	2832	2837	rVB2	195	121	0.02%	0.003%
70	10.475	2838	2841	2844	rBV3	298	224	0.04%	0.005%
71	10.568	2860	2870	2882	rBV2	19783	31233	5.14%	0.648%
72	10.751	2913	2927	2944	rBV	198018	315138	51.87%	6.541%
73	11.340	3107	3110	3111	rBV	175	104	0.02%	0.002%
74	11.401	3127	3129	3133	rBB	123	37	0.01%	0.001%
75	11.504	3159	3161	3164	rBV	171	86	0.01%	0.002%
76	11.536	3168	3171	3174	rBV	210	109	0.02%	0.002%

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MSVOA_U
ClientSampleId :
EYFE7

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\SFAMULM031523WMA.M
Title : VOC Analysis

77	11.555	3174	3177	3180	rBV2	262	180	0.03%	0.004%
78	11.729	3228	3231	3236	rVB	291	204	0.03%	0.004%
79	11.751	3236	3238	3240	rBV	160	77	0.01%	0.002%
80	11.806	3243	3255	3280	rBV	282585	448316	73.80%	9.306%
81	12.188	3361	3374	3392	rBV	268433	435943	71.76%	9.049%
82	13.401	3743	3751	3763	rVB2	15781	22788	3.75%	0.473%
83	13.516	3784	3787	3791	rBV2	229	203	0.03%	0.004%
84	13.577	3803	3806	3809	rBV	332	211	0.03%	0.004%
85	14.098	3964	3968	3969	rBV2	611	382	0.06%	0.008%
86	14.790	4179	4183	4191	rBV2	442	575	0.09%	0.012%
87	14.819	4191	4192	4194	rBV2	238	99	0.02%	0.002%

Sum of corrected areas: 4817574

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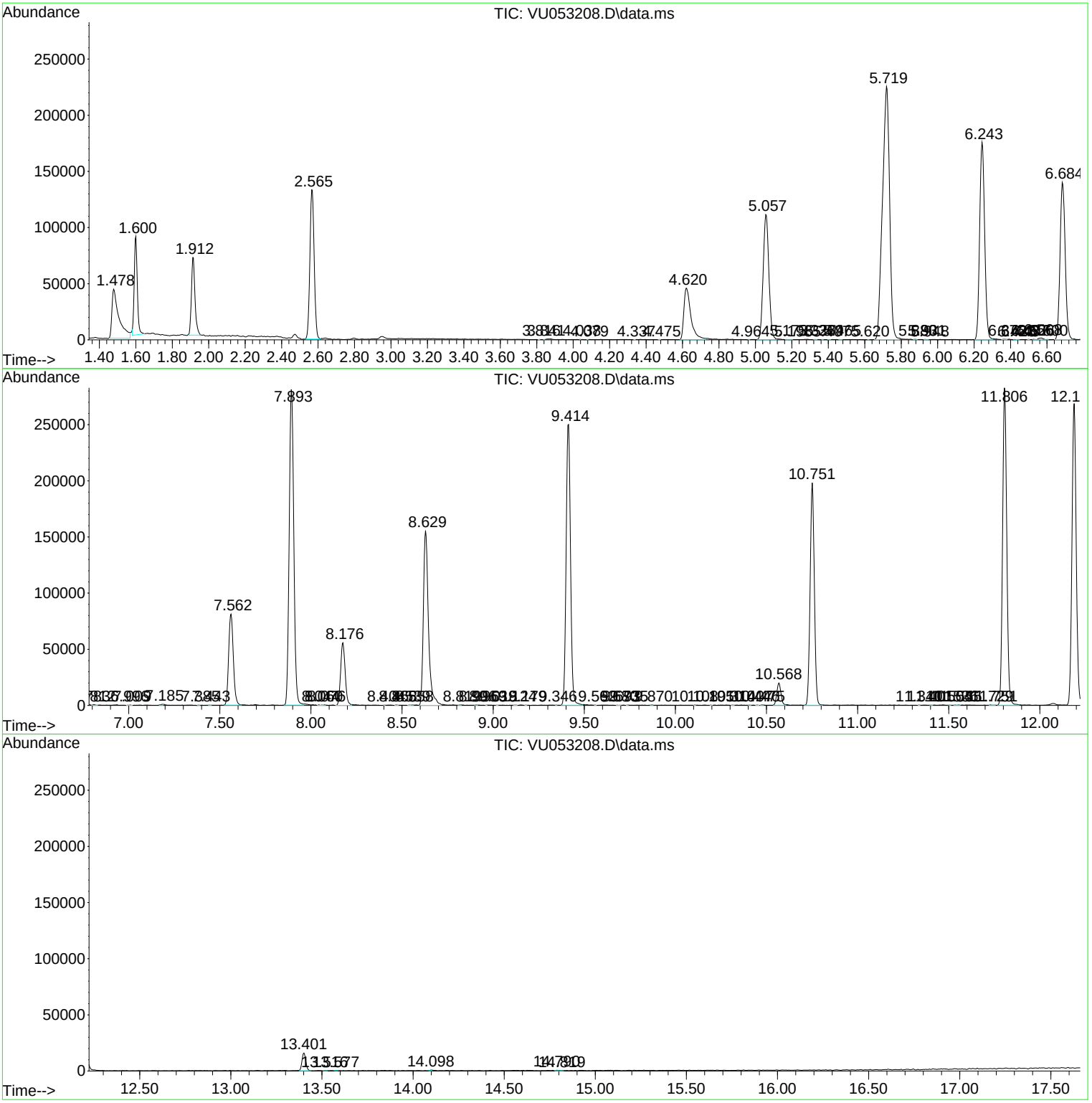
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



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

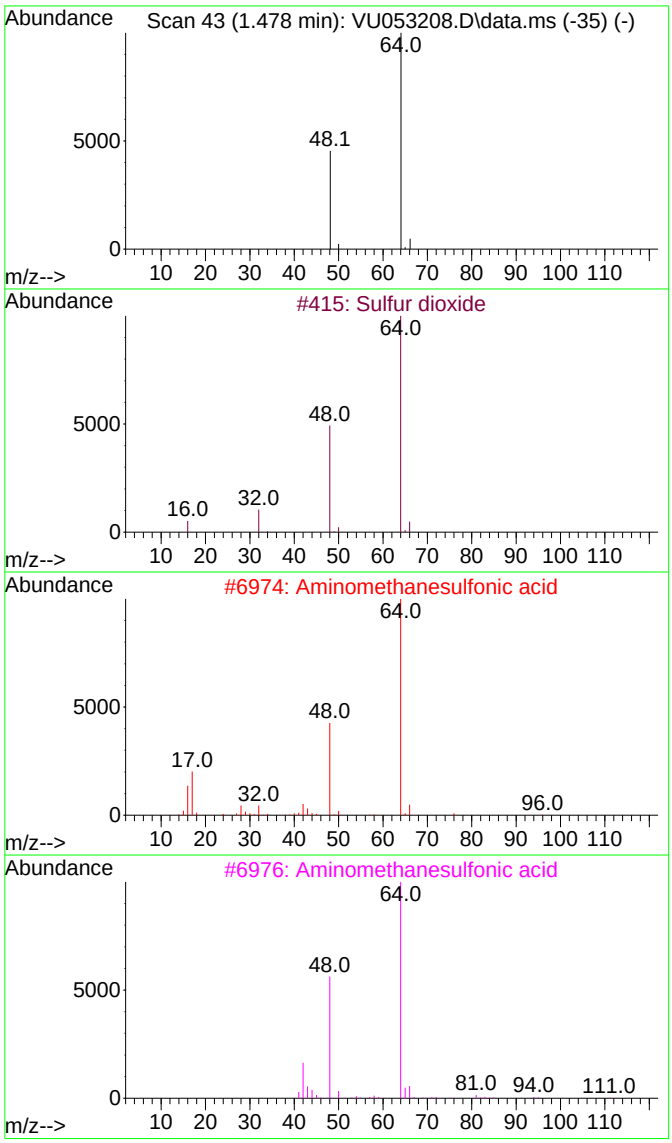
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

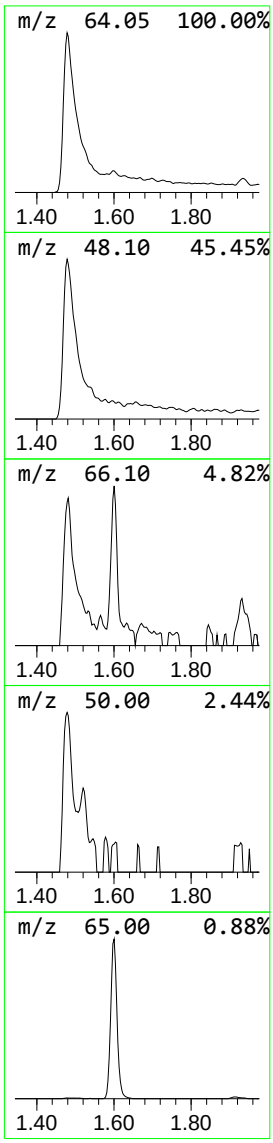
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	17.31 ug/L	116045	1,4-Difluorobenzene	6.243

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	5





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Instrument :
MSVOA_U
ClientSampleId :
EYFE7

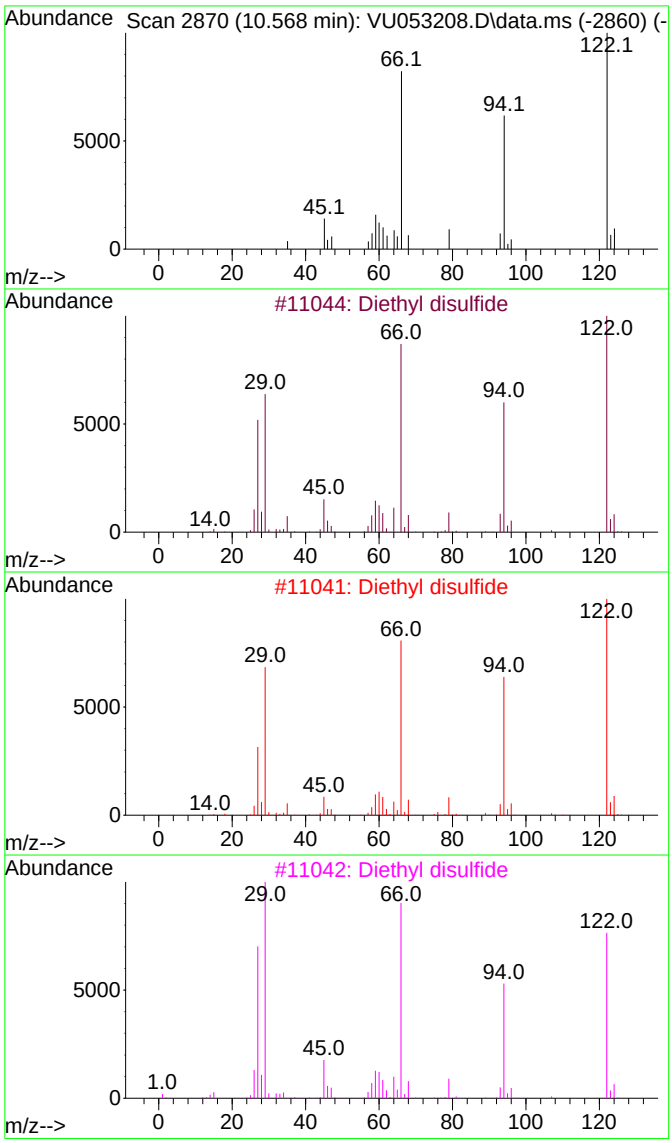
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

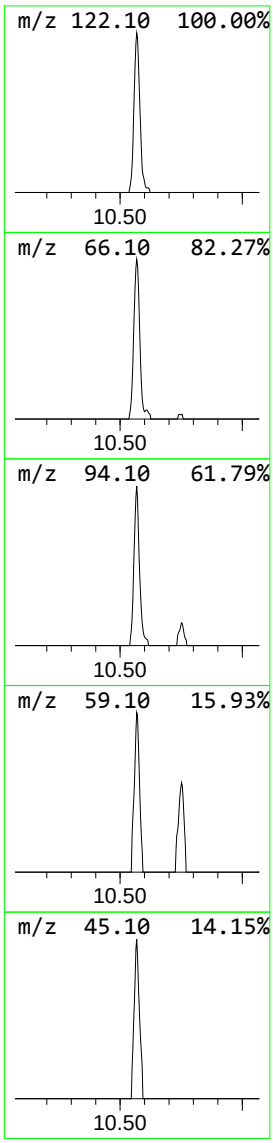
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Diethyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.568	3.74 ug/L	31233	Chlorobenzene-d5	9.414

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	Propanedinitrile, (ethoxymethyle...	122	C6H6N2O	000123-06-8	64
5	Diethyl sulfone	122	C4H10O2S	000597-35-3	53





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

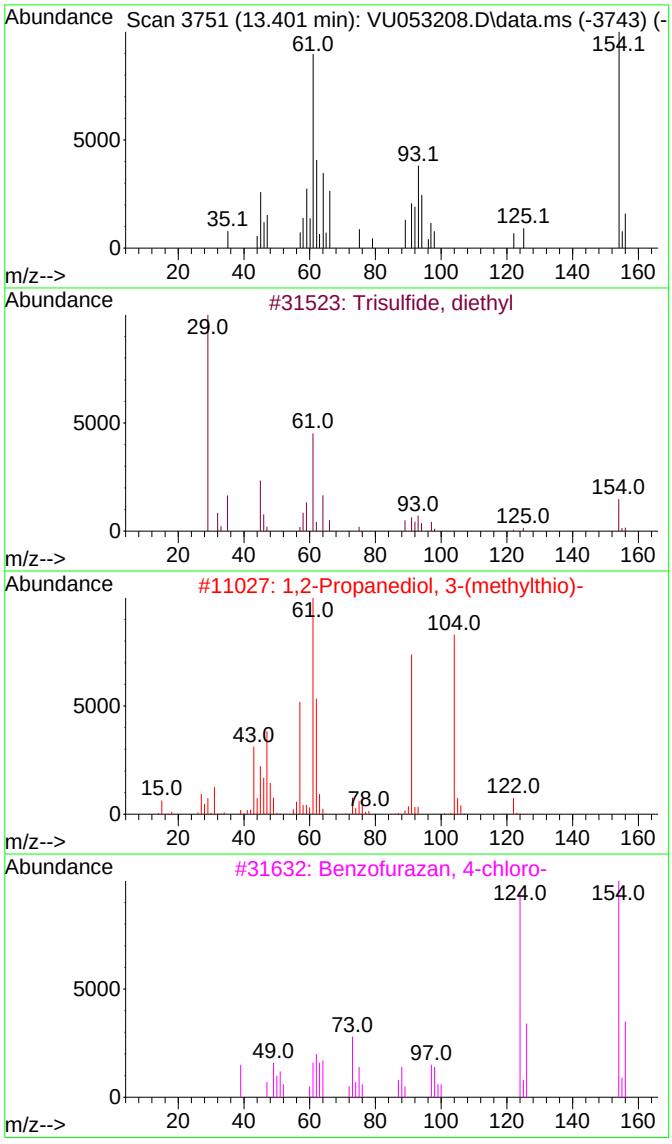
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

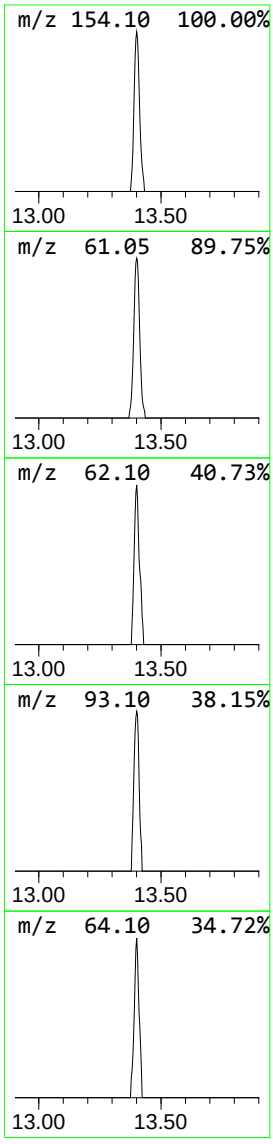
****

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.401	2.54 ug/L	22788	1,4-Dichlorobenzene-d4	11.806

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, diethyl	154	C4H10S3	003600-24-6	38
2	1,2-Propanediol, 3-(methylthio)-	122	C4H10O2S	022551-26-4	25
3	Benzofurazan, 4-chloro-	154	C6H3ClN2O	007116-16-7	23
4	1,2-Propanediol, 3-(methylthio)-	122	C4H10O2S	022551-26-4	10
5	Phenol, 3,5-dimethoxy-	154	C8H10O3	000500-99-2	10





Tentatively Identified Compound (LSC) summary

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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	1.478	17.3	ug/L	116045	1	6.243	335292	50.0
Diethyl disulfide	10.568	3.7	ug/L	31233	2	9.414	417130	50.0
unknown-01	13.401	2.5	ug/L	22788	3	11.806	448316	50.0