LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053262.D
Acq On : 17 Mar 2023 13:16
Operator : JC/MD
Sample : 01929-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFE6

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: VU053262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.462	30	38	52	rBV	71619	111176	18.64%	2.454%
2	1.597	74	80	96	rVB	83199	96317	16.15%	2.126%
3	1.909	170	177	191	rVB	61331	84309	14.14%	1.861%
4	2.565	369	381	392	rBV	122047	196671	32.98%	4.342%
5	2.691	418	420	424	rBV	330	203	0.03%	0.004%
6	2.777	445	447	448	rBV	408	151	0.03%	0.003%
7	3.713	735	738	739	rBV	270	138	0.02%	0.003%
8	3.781	756	759	762	rVB	254	136	0.02%	0.003%
9	3.800	762	765	769	rBV2	208	183	0.03%	0.004%
10	4.015	830	832	834	rBV	127	63	0.01%	0.001%
11	4.028	834	836	839	rVV	226	119	0.02%	0.003%
12	4.260	905	908	909	rBV	119	54	0.01%	0.001%
13	4.388	945	948	949	rBV	126	70	0.01%	0.002%
14	4.459	965	970	972	rBV	271	252	0.04%	0.006%
15	4.610	1006	1017	1043	rBV	50438	123328	20.68%	2.723%
16	5.057	1140	1156	1179	rBV	108004	235533	39.50%	5.200%
17	5.469	1282	1284	1290	rBV	223	110	0.02%	0.002%
18	5.543	1304	1307	1309	rBV	169	110	0.02%	0.002%
19	5.594	1320	1323	1325	rBV	166	143	0.02%	0.003%
20	5.616	1327	1330	1335	rBV	170	216	0.04%	0.005%
21	5.719	1341	1362	1386	rBV2	219262	596347	100.00%	13.165%
22	5.912	1420	1422	1428	rVB	197	100	0.02%	0.002%
23	6.041	1461	1462	1465	rVB	140	57	0.01%	0.001%
24	6.108	1479	1483	1487	rBB	360	306	0.05%	0.007%
25	6.150	1490	1496	1498	rBV	432	511	0.09%	0.011%
26	6.243	1512	1525	1544	rBV	169772	319736	53.62%	7.058%
27	6.424	1579	1581	1584	rBV	150	46	0.01%	0.001%
28	6.446	1584	1588	1590	rBV2	182	116	0.02%	0.003%
29	6.533	1608	1615	1619	rBV5	674	919	0.15%	0.020%
30	6.568	1619	1626	1634	rVB5	1206	1964	0.33%	0.043%
31	6.684	1648	1662	1683	rBV	141052	269014	45.11%	5.939%
32	6.841	1710	1711	1715	rBV	124	48	0.01%	0.001%
33	7.034	1767	1771	1773	rBV2	179	137	0.02%	0.003%
34	7.047	1773	1775	1777	rVV	165	78	0.01%	0.002%
35	7.076	1781	1784	1788	rBV	212	148	0.02%	0.003%
36	7.096	1788	1790	1793	rBV	182	85	0.01%	0.002%

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
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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

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	7.141	1801	1804	1806	rBV	183	138	0.02%	0.003%
38	7.153	1806	1808	1809	rBV	248	120	0.02%	0.003%
39	7.292	1848	1851	1856	rBV	248	204	0.03%	0.005%
40	7.353	1869	1870	1872	rBV	123	47	0.01%	0.001%
41	7.391	1880	1882	1885	rBV	180	146	0.02%	0.003%
42	7.562	1922	1935	1952	rBV	79451	137597	23.07%	3.038%
43	7.687	1969	1974	1980	rVB3	946	1228	0.21%	0.027%
44	7.723	1983	1985	1988	rVB	211	113	0.02%	0.002%
45	7.739	1988	1990	1992	rBV	156	67	0.01%	0.001%
46	7.774	1999	2001	2002	rBV	139	76	0.01%	0.002%
47	7.893	2025	2038	2057	rBV	275595	469712	78.76%	10.369%
48	8.173	2114	2125	2143	rBV2	53324	91605	15.36%	2.022%
49	8.359	2181	2183	2185	rBV	143	78	0.01%	0.002%
50	8.401	2194	2196	2200	rBV	146	91	0.02%	0.002%
51	8.626	2256	2266	2298	rVV2	157363	289117	48.48%	6.383%
52	8.790	2313	2317	2319	rVV2	898	498	0.08%	0.011%
53	8.803	2319	2321	2325	rVB2	198	140	0.02%	0.003%
54	8.841	2331	2333	2337	rBB	195	90	0.02%	0.002%
55	8.899	2350	2351	2353	rBV	111	43	0.01%	0.001%
56	9.092	2408	2411	2413	rBV	163	141	0.02%	0.003%
57	9.105	2413	2415	2419	rVV2	218	181	0.03%	0.004%
58	9.128	2419	2422	2425	rVV	191	129	0.02%	0.003%
59	9.234	2452	2455	2459	rBV	191	199	0.03%	0.004%
60	9.272	2460	2467	2471	rVV2	553	711	0.12%	0.016%
61	9.411	2498	2510	2536	rBV	233834	386367	64.79%	8.529%
62	9.558	2553	2556	2559	rBV2	334	174	0.03%	0.004%
63	9.587	2563	2565	2566	rBV	127	51	0.01%	0.001%
64	9.613	2571	2573	2577	rVB	193	107	0.02%	0.002%
65	9.636	2577	2580	2582	rBV2	169	99	0.02%	0.002%
66	9.819	2633	2637	2638	rBV	235	165	0.03%	0.004%
67	9.890	2656	2659	2665	rVB	210	136	0.02%	0.003%
68	9.915	2665	2667	2671	rBB2	222	140	0.02%	0.003%
69	10.240	2764	2768	2771	rBV	225	122	0.02%	0.003%
70	10.266	2772	2776	2779	rBV2	201	207	0.03%	0.005%
71	10.391	2812	2815	2817	rBV2	149	105	0.02%	0.002%
72	10.568	2861	2870	2882	rBV2	18540	28799	4.83%	0.636%
73	10.616	2882	2885	2886	rBV	174	99	0.02%	0.002%
74	10.751	2914	2927	2944	rBV	188244	299075	50.15%	6.602%
75	10.964	2990	2993	2995	rVB	134	56	0.01%	0.001%
76	11.060	3021	3023	3027	rBV	237	135	0.02%	0.003%

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFE6

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	11.198	3064	3066	3069	rBV2	171	95	0.02%	0.002%
78	11.218	3070	3072	3074	rBV	170	81	0.01%	0.002%
79	11.372	3118	3120	3124	rVB	220	95	0.02%	0.002%
80	11.468	3147	3150	3152	rBV	185	105	0.02%	0.002%
81	11.591	3185	3188	3189	rBV	163	76	0.01%	0.002%
82	11.703	3221	3223	3224	rBV	159	53	0.01%	0.001%
83	11.806	3244	3255	3273	rBV	231450	370348	62.10%	8.176%
84	12.189	3361	3374	3394	rBV	250685	395785	66.37%	8.737%
85	12.439	3449	3452	3455	rVB	347	196	0.03%	0.004%
86	12.475	3461	3463	3465	rBV2	174	96	0.02%	0.002%
87	12.803	3558	3565	3568	rVB2	239	260	0.04%	0.006%
88	13.401	3743	3751	3762	rBV3	8570	12869	2.16%	0.284%
89	13.574	3802	3805	3807	rBV	120	51	0.01%	0.001%
90	13.668	3829	3834	3835	rBV	229	175	0.03%	0.004%
91	14.098	3962	3968	3971	rBV2	636	657	0.11%	0.015%
92	14.626	4130	4132	4137	rBV	225	220	0.04%	0.005%
93	14.825	4192	4194	4196	rBV2	283	137	0.02%	0.003%
94	14.864	4203	4206	4210	rBV2	212	208	0.03%	0.005%
95	14.902	4214	4218	4221	rBV2	322	238	0.04%	0.005%
96	14.992	4243	4246	4248	rBV2	298	207	0.03%	0.005%
97	15.066	4267	4269	4271	rBV	227	136	0.02%	0.003%
98	15.147	4292	4294	4296	rVB	257	99	0.02%	0.002%
99	15.497	4400	4403	4404	rBV	372	245	0.04%	0.005%
100	15.520	4408	4410	4413	rBV3	233	169	0.03%	0.004%

Sum of corrected areas: 4529803

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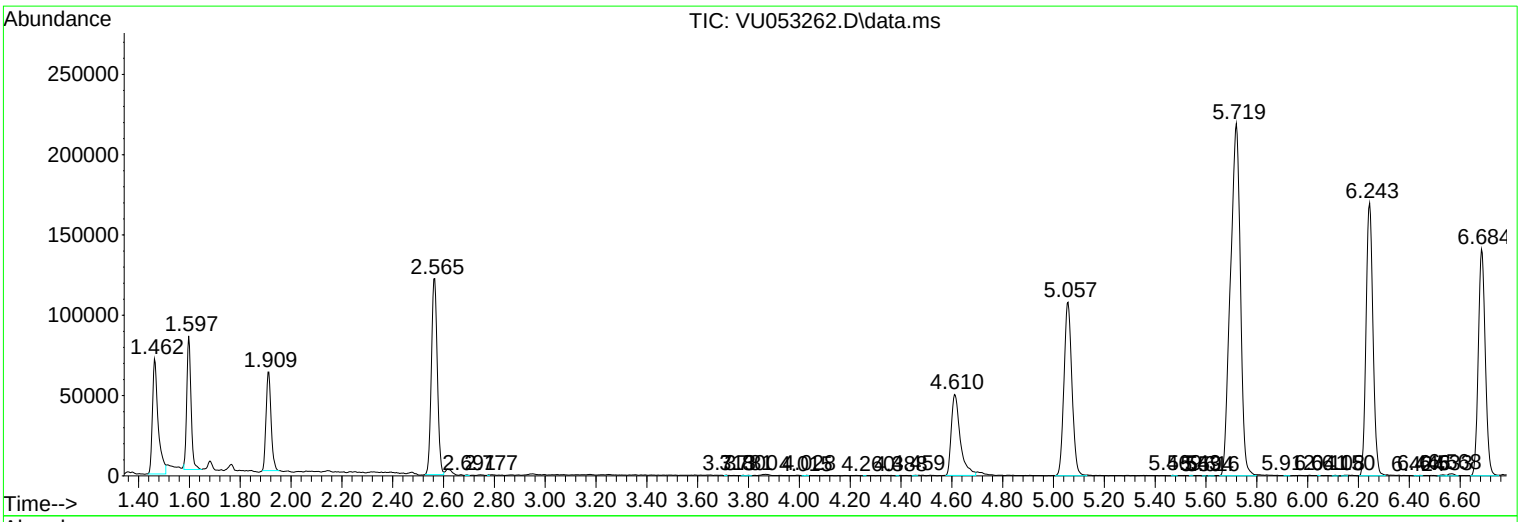
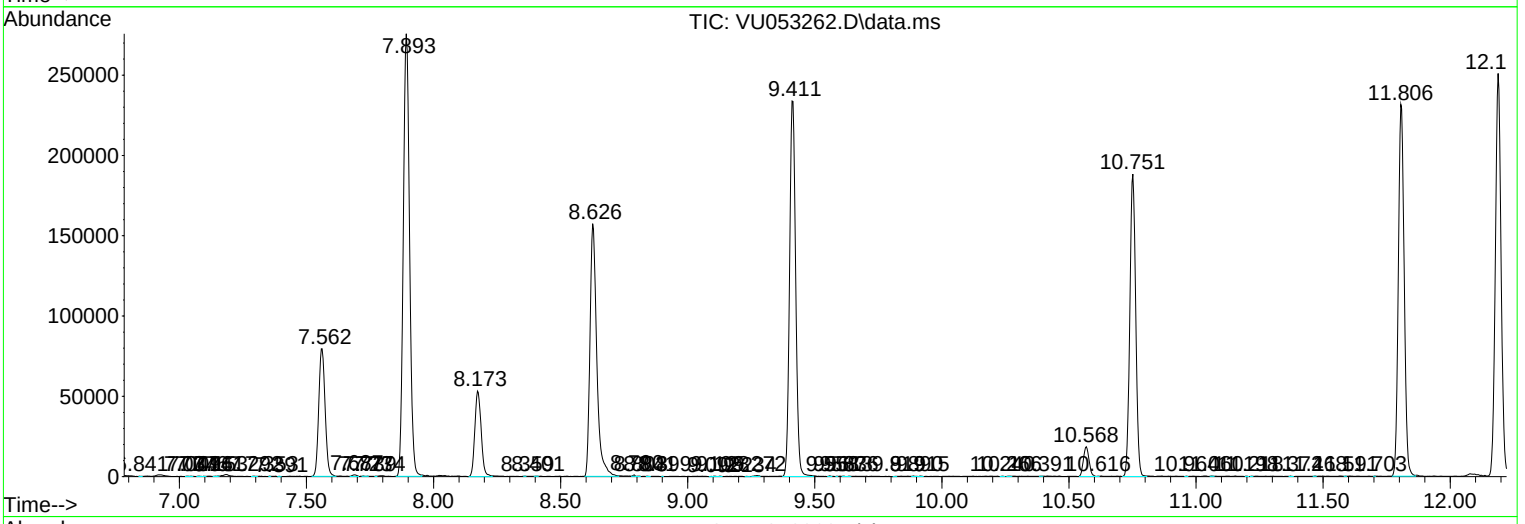
ALS Vial : 10 Sample Multiplier: 1

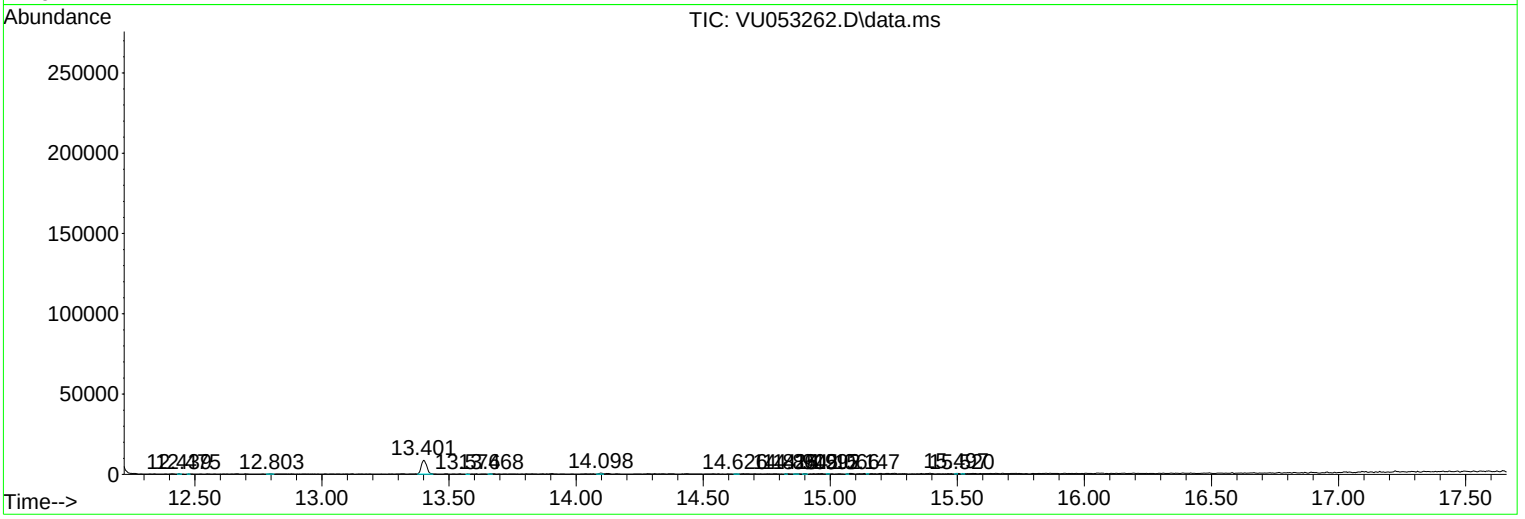
Instrument :
MSVOA_U
ClientSampleId :
EYFE6

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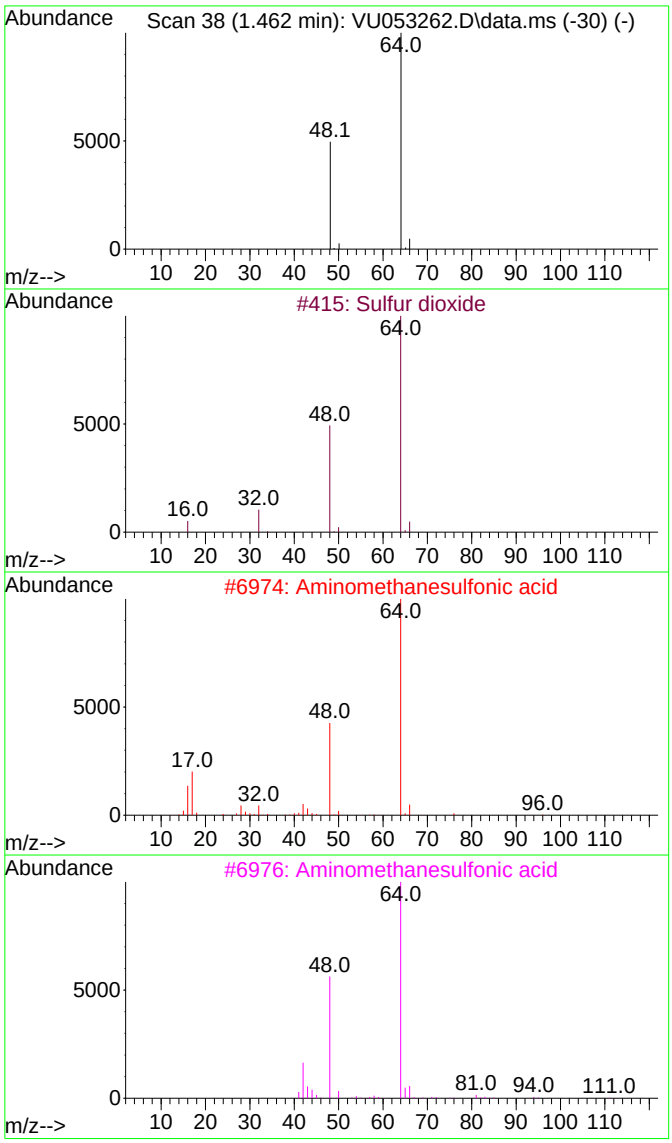
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

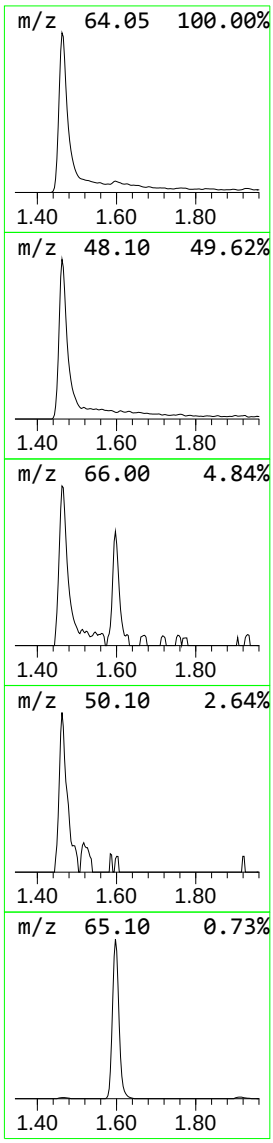
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.462	17.39 ug/L	111176	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	74
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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MSVOA_U
ClientSampleId :
EYFE6

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

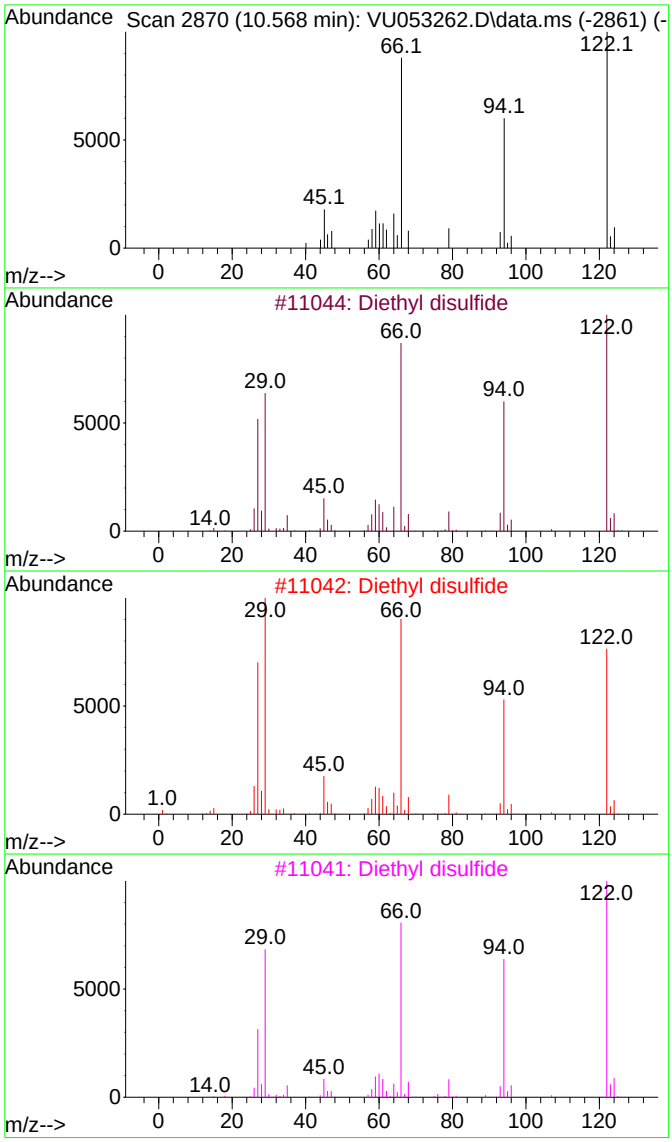
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

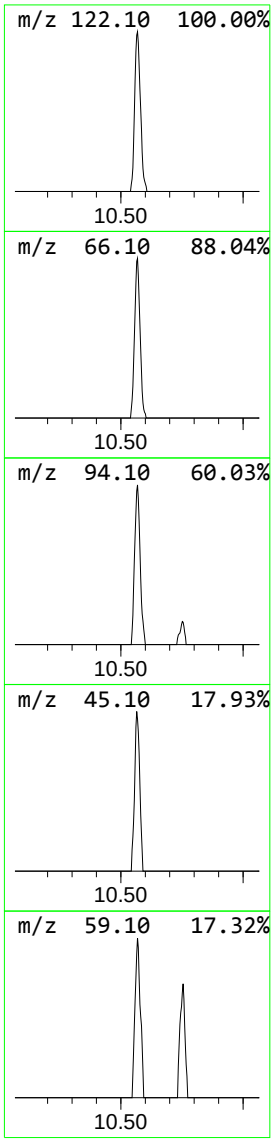
****

Peak Number 3 Diethyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.568	3.73 ug/L	28799	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	94
3	Diethyl disulfide	122	C4H10S2	000110-81-6	91
4	2-Propenal, 3-(2-furanyl)-	122	C7H6O2	000623-30-3	50
5	6-exo-Methyl-5-endo-norbornenol	124	C8H12O	041414-52-2	50





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	1.462	17.4	ug/L	111176	1	6.243	319736	50.0
Diethyl disulfide	10.568	3.7	ug/L	28799	2	9.414	386367	50.0