LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV020221\
Data File : VV020250.D
Acq On : 02 Feb 2021 20:02
Operator : SY/MD
Sample : M1258-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG531

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\SOMVLM012821WMA.M
Title : VOC Analysis

Signal : TIC: VV020250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.110	3	6	13	rVB	380605	297829	13.95%	1.573%
2	1.254	45	51	58	rBV2	98145	196111	9.19%	1.036%
3	1.306	62	67	78	rVB2	332852	439336	20.58%	2.321%
4	1.569	144	149	161	rVB	224794	262779	12.31%	1.388%
5	2.032	286	293	307	rVV	169878	246827	11.56%	1.304%
6	2.110	308	317	336	rVB	444081	650882	30.49%	3.438%
7	2.299	364	376	382	rBV	33028	53843	2.52%	0.284%
8	3.364	705	707	711	rVB4	897	492	0.02%	0.003%
9	3.438	723	730	733	rBV4	1258	1742	0.08%	0.009%
10	3.508	749	752	761	rVB5	799	1130	0.05%	0.006%
11	3.576	767	773	774	rBV3	640	421	0.02%	0.002%
12	3.685	793	807	824	rBV2	59539	152204	7.13%	0.804%
13	3.891	860	871	903	rBV	144720	440997	20.66%	2.329%
14	4.209	968	970	973	rBV2	700	406	0.02%	0.002%
15	4.225	973	975	980	rVB4	989	791	0.04%	0.004%
16	4.270	985	989	993	rVB5	817	619	0.03%	0.003%
17	4.354	996	1015	1041	rBV	340645	842858	39.48%	4.452%
18	4.640	1101	1104	1106	rBV3	622	471	0.02%	0.002%
19	4.830	1157	1163	1166	rBV5	713	829	0.04%	0.004%
20	4.888	1175	1181	1182	rBV3	424	409	0.02%	0.002%
21	4.901	1182	1185	1187	rVB3	758	441	0.02%	0.002%
22	4.917	1187	1190	1198	rVB4	803	1072	0.05%	0.006%
23	4.971	1204	1207	1211	rBV2	515	444	0.02%	0.002%
24	5.052	1214	1232	1274	rBV2	818243	2134726	100.00%	11.275%
25	5.373	1323	1332	1334	rBV4	6331	7406	0.35%	0.039%
26	5.489	1366	1368	1373	rVB5	1225	829	0.04%	0.004%
27	5.621	1396	1409	1436	rBV	792774	1584062	74.20%	8.367%
28	5.913	1489	1500	1516	rVB7	16685	35410	1.66%	0.187%
29	6.074	1536	1550	1574	rBV	460214	935332	43.82%	4.940%
30	6.219	1589	1595	1596	rBV5	2114	2218	0.10%	0.012%
31	6.257	1600	1607	1623	rVB3	13966	29289	1.37%	0.155%
32	6.418	1653	1657	1662	rVB5	686	601	0.03%	0.003%
33	6.646	1720	1728	1731	rBV4	1312	1427	0.07%	0.008%
34	6.807	1775	1778	1780	rBV	891	622	0.03%	0.003%
35	6.881	1798	1801	1805	rBV3	743	521	0.02%	0.003%
36	6.990	1823	1835	1858	rBV	256201	464654	21.77%	2.454%

LSC Area Percent Report

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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG531

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\SOMVLM012821WMA.M
Title : VOC Analysis

37	7.318	1924	1937	1959	rBV	1007642	1748691	81.92%	9.236%
38	7.534	1996	2004	2015	rVB2	8354	14482	0.68%	0.076%
39	7.624	2020	2032	2050	rBV	181999	310919	14.56%	1.642%
40	7.830	2092	2096	2099	rBV3	887	753	0.04%	0.004%
41	7.888	2109	2114	2117	rBV5	427	409	0.02%	0.002%
42	7.926	2121	2126	2128	rBV2	803	629	0.03%	0.003%
43	7.945	2128	2132	2134	rBV3	905	690	0.03%	0.004%
44	7.981	2134	2143	2155	rVV4	23965	40669	1.91%	0.215%
45	8.042	2160	2162	2167	rVB5	903	579	0.03%	0.003%
46	8.090	2167	2177	2212	rBV	515265	977421	45.79%	5.163%
47	8.437	2281	2285	2288	rVB6	641	498	0.02%	0.003%
48	8.486	2297	2300	2304	rVV3	632	557	0.03%	0.003%
49	8.717	2365	2372	2382	rBV5	5799	10147	0.48%	0.054%
50	8.801	2395	2398	2403	rBV4	722	662	0.03%	0.003%
51	8.855	2403	2415	2444	rBV	1212456	1950050	91.35%	10.300%
52	9.116	2489	2496	2498	rBV5	2224	2520	0.12%	0.013%
53	9.235	2528	2533	2536	rBV3	577	593	0.03%	0.003%
54	9.305	2550	2555	2556	rBV3	1702	1107	0.05%	0.006%
55	9.322	2557	2560	2564	rVB4	1650	1320	0.06%	0.007%
56	9.408	2582	2587	2593	rVB4	639	630	0.03%	0.003%
57	9.453	2598	2601	2603	rBV2	780	566	0.03%	0.003%
58	9.659	2661	2665	2667	rBV	589	451	0.02%	0.002%
59	9.701	2674	2678	2681	rBV4	555	423	0.02%	0.002%
60	9.740	2687	2690	2692	rVV2	701	427	0.02%	0.002%
61	9.778	2697	2702	2708	rVB3	1029	1188	0.06%	0.006%
62	10.032	2771	2781	2788	rBV5	2166	3717	0.17%	0.020%
63	10.167	2818	2823	2824	rVV2	777	688	0.03%	0.004%
64	10.219	2828	2839	2862	rVB	717988	1125405	52.72%	5.944%
65	10.318	2867	2870	2873	rVB3	698	439	0.02%	0.002%
66	10.550	2937	2942	2946	rVB5	675	672	0.03%	0.004%
67	10.794	3009	3018	3019	rBV5	2134	2082	0.10%	0.011%
68	10.846	3031	3034	3037	rBV2	567	457	0.02%	0.002%
69	10.916	3053	3056	3065	rBV6	539	704	0.03%	0.004%
70	10.971	3070	3073	3075	rBV2	643	440	0.02%	0.002%
71	11.177	3131	3137	3145	rBV7	1135	1606	0.08%	0.008%
72	11.254	3148	3161	3195	rBV	1351256	2053925	96.21%	10.849%
73	11.482	3230	3232	3241	rVB6	983	1167	0.05%	0.006%
74	11.543	3247	3251	3261	rVB6	1199	1666	0.08%	0.009%
75	11.630	3265	3278	3301	rBV	1207520	1862661	87.26%	9.838%
76	11.849	3343	3346	3350	rBV3	895	697	0.03%	0.004%

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Instrument : MSVOA_V
ClientSampleId : BG531

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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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM012821WMA.M
Title : VOC Analysis

77	11.891	3350	3359	3365	rVV8	1847	2890	0.14%	0.015%
78	11.977	3381	3386	3388	rBV2	653	637	0.03%	0.003%
79	12.029	3398	3402	3405	rBV2	863	667	0.03%	0.004%
80	12.164	3438	3444	3447	rBV4	787	718	0.03%	0.004%
81	12.196	3451	3454	3461	rVB3	548	495	0.02%	0.003%
82	12.370	3502	3508	3517	rVB7	1423	2555	0.12%	0.013%
83	12.408	3517	3520	3524	rBV3	619	530	0.02%	0.003%
84	12.450	3529	3533	3540	rVB4	1448	1316	0.06%	0.007%
85	12.485	3540	3544	3547	rBV2	828	624	0.03%	0.003%
86	12.665	3595	3600	3602	rBV4	801	804	0.04%	0.004%
87	12.772	3630	3633	3636	rBV2	517	425	0.02%	0.002%
88	12.836	3649	3653	3660	rVB6	1577	1674	0.08%	0.009%
89	12.910	3673	3676	3679	rVB2	550	433	0.02%	0.002%
90	12.942	3682	3686	3688	rBV3	752	447	0.02%	0.002%
91	13.238	3775	3778	3780	rBV3	835	614	0.03%	0.003%
92	13.344	3808	3811	3814	rBV4	675	440	0.02%	0.002%
93	13.424	3833	3836	3840	rBV4	568	505	0.02%	0.003%
94	13.849	3965	3968	3971	rBV2	901	615	0.03%	0.003%
95	14.128	4053	4055	4059	rBV2	499	442	0.02%	0.002%
96	14.263	4095	4097	4102	rVB2	839	697	0.03%	0.004%
97	14.386	4132	4135	4137	rBV2	768	422	0.02%	0.002%
98	14.498	4168	4170	4175	rBV	560	439	0.02%	0.002%
99	14.575	4189	4194	4195	rBV2	946	684	0.03%	0.004%
100	15.222	4392	4395	4399	rBV4	973	682	0.03%	0.004%

Sum of corrected areas: 18932492

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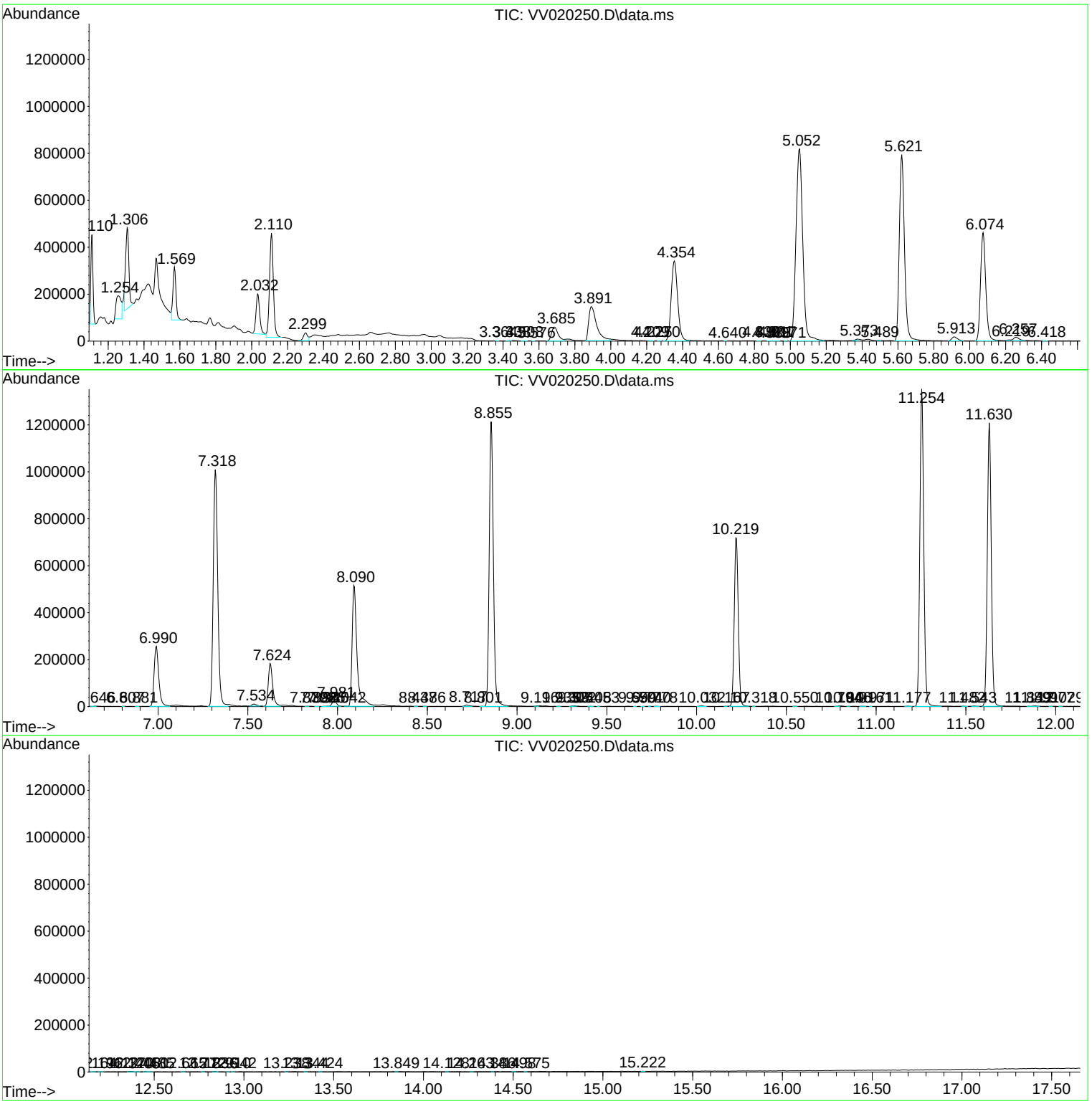
Instrument :
MSVOA_V
ClientSampleId :
BG531

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM012821WMA.M
Quant Title : VOC Analysis

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



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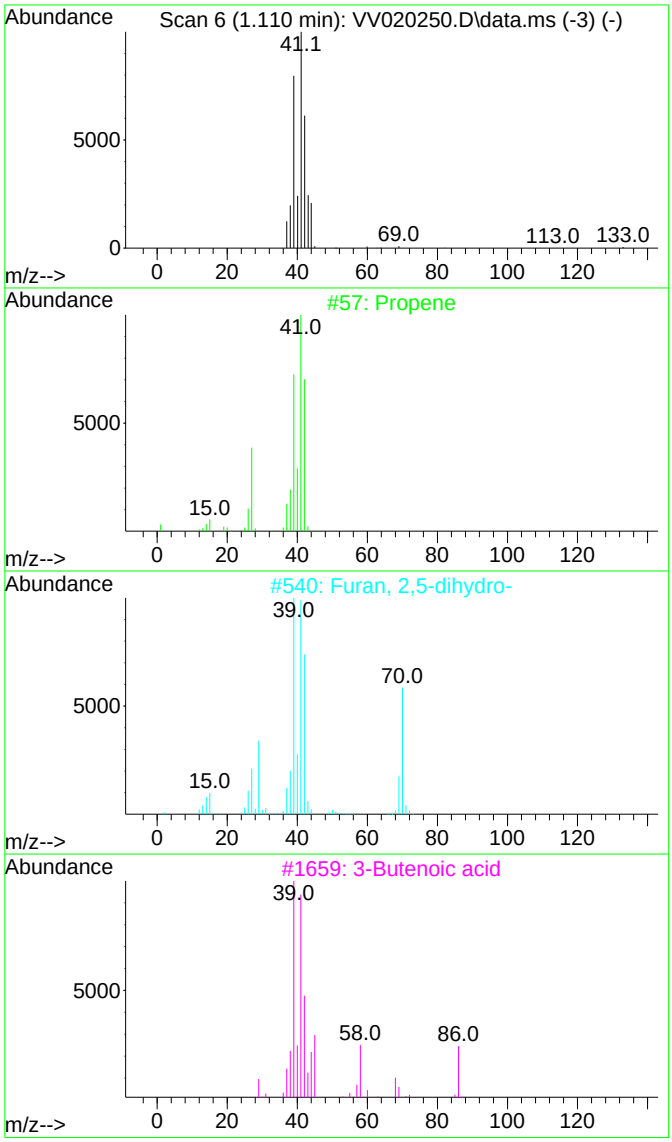
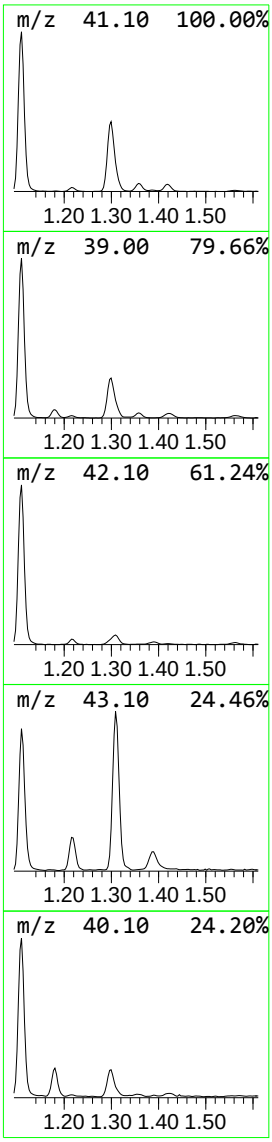
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.110	9.40 ug/L	297829	1,4-Difluorobenzene	5.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	78
3	3-Butenoic acid	86	C4H6O2	000625-38-7	78
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	78
5	Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	74





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ClientSampleId : BG531

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM012821WMA.M
Quant Title : VOC Analysis

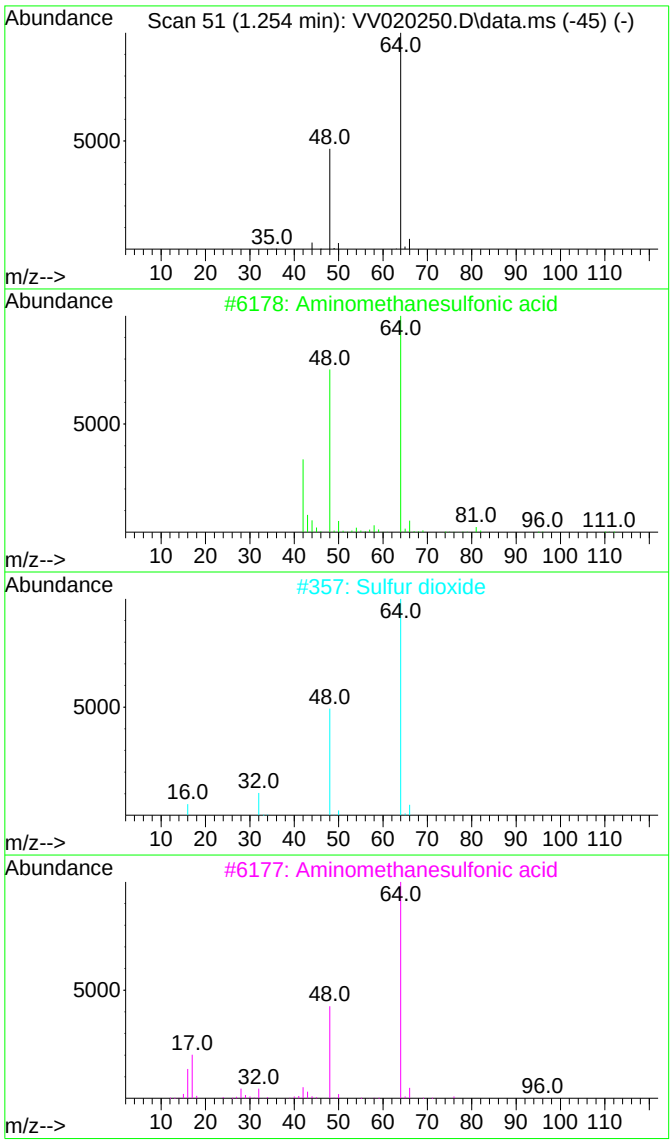
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

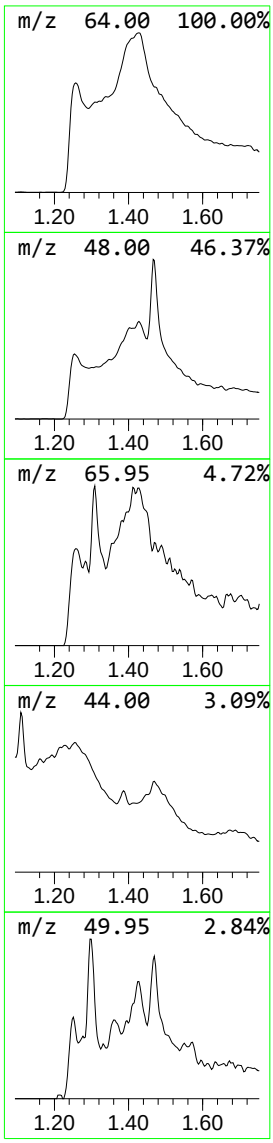
****

Peak Number 2 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.254	6.19 ug/L	196111	1,4-Difluorobenzene	5.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2	Sulfur dioxide	64	O2S	007446-09-5	83
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM012821WMA.M
Quant Title : VOC Analysis

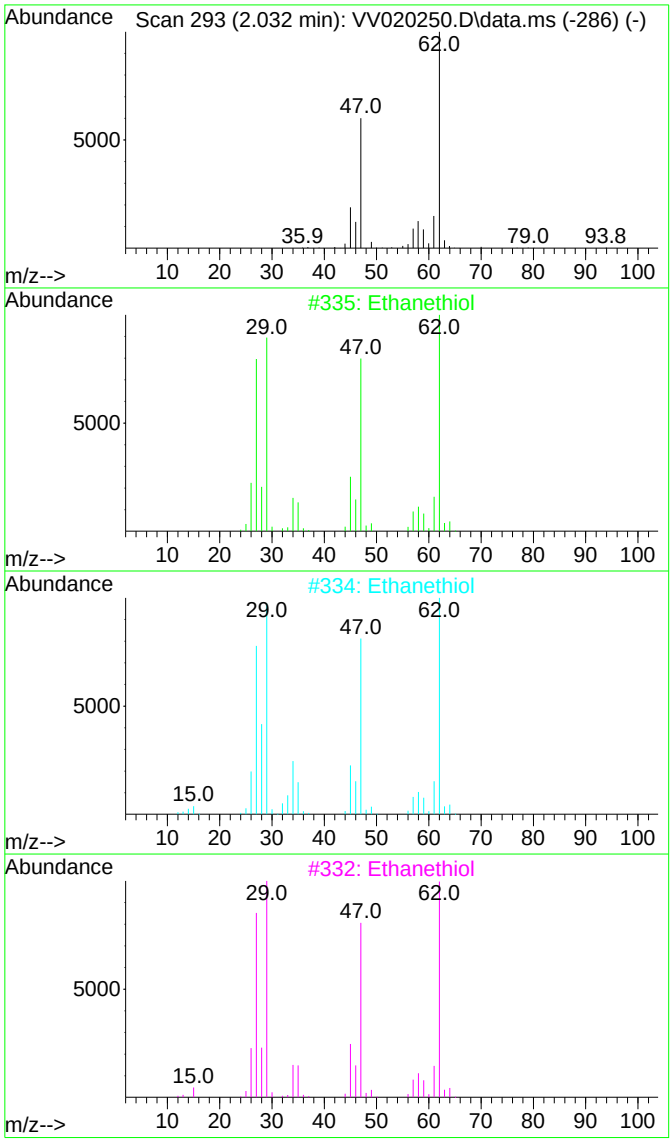
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

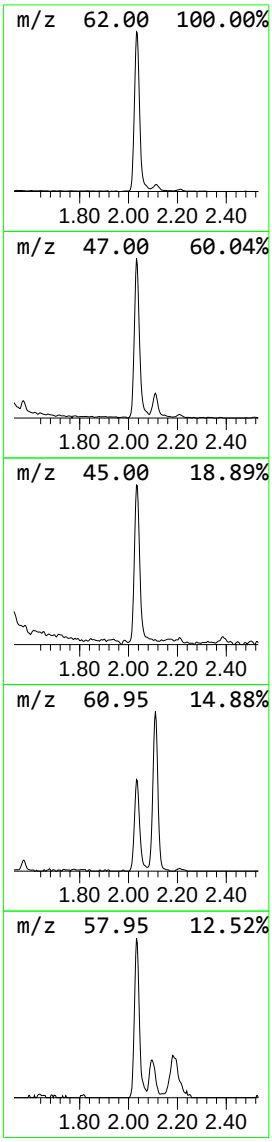
****

Peak Number 3 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.032	7.79 ug/L	246827	1,4-Difluorobenzene	5.621

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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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM012821WMA.M
Quant Title : VOC Analysis

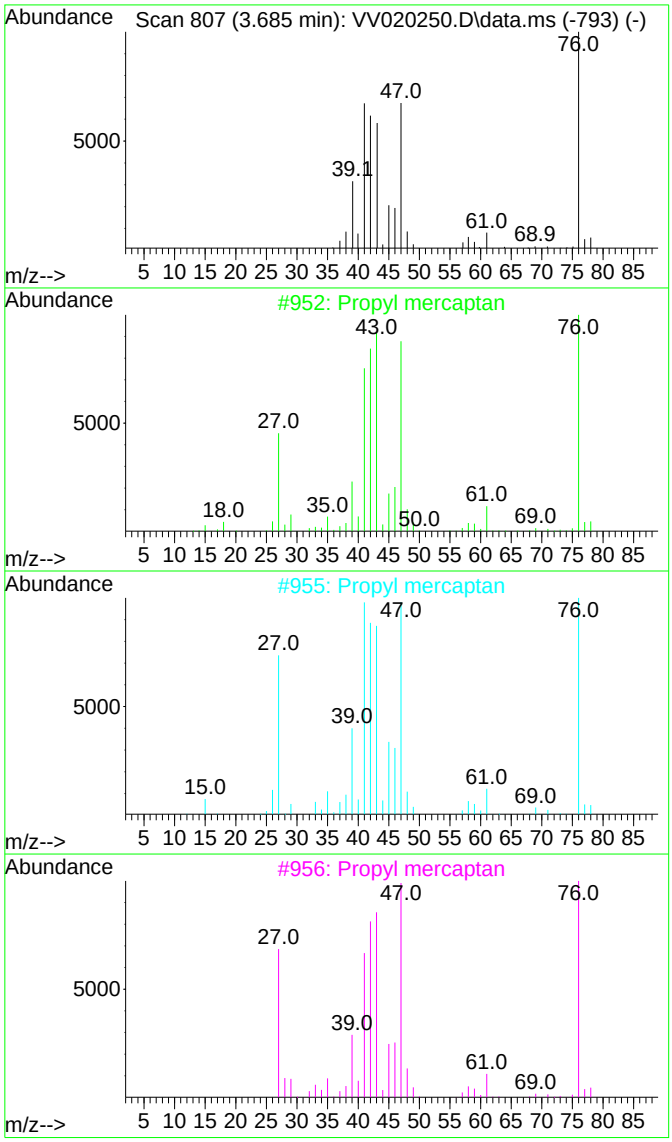
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

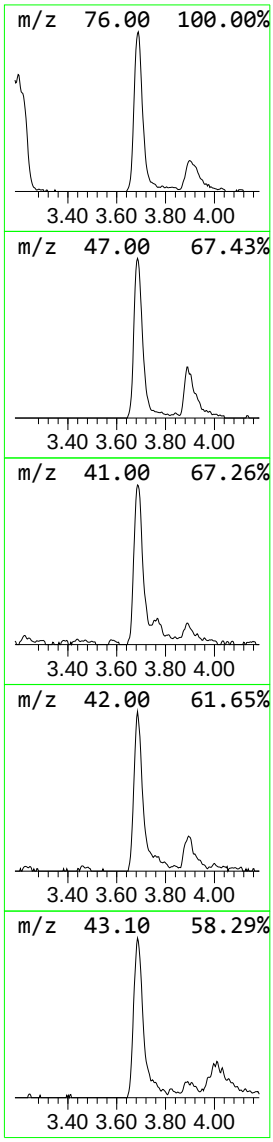
****

Peak Number 4 Propyl mercaptan Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.685	4.80 ug/L	152204	1,4-Difluorobenzene	5.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	91
2	Propyl mercaptan	76	C3H8S	000107-03-9	91
3	Propyl mercaptan	76	C3H8S	000107-03-9	87
4	Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	83
5	Thiourea	76	CH4N2S	000062-56-6	45





Tentatively Identified Compound (LSC) summary

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ClientSampleId : BG531

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM012821WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.110	9.4	ug/L	297829	1	5.621	1584060	50.0
Sulfur dioxide	1.254	6.2	ug/L	196111	1	5.621	1584060	50.0
Ethanethiol	2.032	7.8	ug/L	246827	1	5.621	1584060	50.0
Propyl mercaptan	3.685	4.8	ug/L	152204	1	5.621	1584060	50.0