LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
Data File : VV021920.D
Acq On : 20 Aug 2021 17:48
Operator : SY/MD
Sample : M3458-18ME
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0B56ME

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\SFAMVLM081621WMA.M
Title : VOC Analysis

Signal : TIC: VV021920.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	113	rVB	126947	190505	14.93%	1.793%
2	2.072	311	321	333	rBV	276189	389752	30.54%	3.668%
3	2.436	422	434	436	rBV6	1602	2457	0.19%	0.023%
4	2.732	523	526	529	rVB4	706	420	0.03%	0.004%
5	2.770	536	538	540	rVB2	515	185	0.01%	0.002%
6	2.963	594	598	601	rBV2	324	249	0.02%	0.002%
7	3.002	608	610	612	rBV3	472	283	0.02%	0.003%
8	3.092	636	638	639	rBV	453	172	0.01%	0.002%
9	3.150	653	656	659	rBV	528	391	0.03%	0.004%
10	3.320	705	709	712	rBV2	436	313	0.02%	0.003%
11	3.355	714	720	722	rBV2	475	426	0.03%	0.004%
12	3.404	733	735	739	rVB2	509	322	0.03%	0.003%
13	3.429	739	743	747	rBV4	261	235	0.02%	0.002%
14	3.455	747	751	753	rVB	371	243	0.02%	0.002%
15	3.629	798	805	808	rBV3	650	532	0.04%	0.005%
16	3.651	810	812	814	rVV	376	198	0.02%	0.002%
17	3.696	820	826	827	rBV2	233	171	0.01%	0.002%
18	3.725	829	835	837	rBV3	472	425	0.03%	0.004%
19	3.838	865	870	873	rBV2	280	279	0.02%	0.003%
20	3.892	878	887	930	rBV	64056	253283	19.85%	2.384%
21	4.342	1012	1027	1058	rBV	186248	485051	38.00%	4.565%
22	4.635	1116	1118	1119	rBV	712	325	0.03%	0.003%
23	4.741	1147	1151	1157	rBV2	661	590	0.05%	0.006%
24	4.793	1163	1167	1169	rBV2	637	374	0.03%	0.004%
25	4.812	1169	1173	1175	rBV2	429	267	0.02%	0.003%
26	4.847	1181	1184	1187	rBV2	428	272	0.02%	0.003%
27	4.886	1193	1196	1197	rBV3	395	237	0.02%	0.002%
28	4.931	1208	1210	1214	rBV3	480	309	0.02%	0.003%
29	5.040	1227	1244	1283	rBV3	513304	1276289	100.00%	12.012%
30	5.339	1322	1337	1356	rBV7	5691	18529	1.45%	0.174%
31	5.545	1399	1401	1403	rVB	620	234	0.02%	0.002%
32	5.613	1409	1422	1449	rBV	460114	960341	75.24%	9.039%
33	5.867	1498	1501	1502	rBV2	396	229	0.02%	0.002%
34	5.905	1502	1513	1532	rVV2	21595	48948	3.84%	0.461%
35	6.069	1552	1564	1597	rVB	264115	577950	45.28%	5.440%
36	6.452	1676	1683	1686	rBV2	525	505	0.04%	0.005%

LSC Area Percent Report

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Operator : SY/MD
Sample : M3458-18ME
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0B56ME

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\SFAMVLM081621WMA.M
Title : VOC Analysis

37	6.532	1704	1708	1712	rBV2	329	347	0.03%	0.003%
38	6.606	1728	1731	1734	rBV3	383	326	0.03%	0.003%
39	6.741	1770	1773	1775	rBV2	548	371	0.03%	0.003%
40	6.802	1789	1792	1795	rVB4	587	340	0.03%	0.003%
41	6.915	1824	1827	1829	rBV4	666	439	0.03%	0.004%
42	6.989	1838	1850	1880	rBV	136111	277315	21.73%	2.610%
43	7.172	1905	1907	1910	rVB3	474	187	0.01%	0.002%
44	7.259	1930	1934	1935	rBV2	996	699	0.05%	0.007%
45	7.317	1940	1952	1970	rBV	589718	1052289	82.45%	9.904%
46	7.625	2035	2048	2082	rBV	90731	185529	14.54%	1.746%
47	7.857	2117	2120	2121	rBV3	408	253	0.02%	0.002%
48	7.969	2154	2155	2159	rVB	420	195	0.02%	0.002%
49	8.108	2185	2198	2229	rBV3	222021	535968	41.99%	5.044%
50	8.683	2375	2377	2382	rVB3	618	359	0.03%	0.003%
51	8.754	2396	2399	2401	rBV2	471	279	0.02%	0.003%
52	8.854	2419	2430	2458	rVV	667156	1172519	91.87%	11.036%
53	9.085	2500	2502	2504	rBV2	542	295	0.02%	0.003%
54	9.153	2515	2523	2524	rBV6	2211	2545	0.20%	0.024%
55	9.278	2559	2562	2565	rVV2	801	440	0.03%	0.004%
56	9.291	2565	2566	2571	rVV	300	176	0.01%	0.002%
57	9.349	2581	2584	2586	rVV	314	198	0.02%	0.002%
58	9.358	2586	2587	2594	rVB3	344	328	0.03%	0.003%
59	9.426	2603	2608	2610	rBV2	247	204	0.02%	0.002%
60	9.471	2618	2622	2625	rBV2	362	304	0.02%	0.003%
61	9.554	2642	2648	2649	rBV2	1553	1329	0.10%	0.013%
62	9.648	2674	2677	2683	rBV2	323	337	0.03%	0.003%
63	9.680	2683	2687	2690	rBV3	503	436	0.03%	0.004%
64	9.699	2691	2693	2694	rBV	452	177	0.01%	0.002%
65	9.757	2708	2711	2716	rBV3	319	248	0.02%	0.002%
66	9.857	2735	2742	2746	rBV3	897	1032	0.08%	0.010%
67	9.908	2746	2758	2775	rVB3	29670	51384	4.03%	0.484%
68	9.995	2783	2785	2789	rVB2	542	270	0.02%	0.003%
69	10.017	2789	2792	2795	rBV3	416	345	0.03%	0.003%
70	10.130	2816	2827	2838	rBV3	5741	11056	0.87%	0.104%
71	10.223	2844	2856	2879	rVB	366017	603310	47.27%	5.678%
72	10.522	2941	2949	2954	rBV6	2003	3272	0.26%	0.031%
73	10.580	2957	2967	2978	rVV	59452	97756	7.66%	0.920%
74	10.731	3012	3014	3016	rBV	391	244	0.02%	0.002%
75	10.754	3016	3021	3023	rVV4	596	557	0.04%	0.005%
76	10.780	3026	3029	3032	rBV3	401	361	0.03%	0.003%

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Operator : SY/MD
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Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0B56ME

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\SFAMVLM081621WMA.M
Title : VOC Analysis

77	11.008	3096	3100	3102	rBV3	337	266	0.02%	0.003%
78	11.034	3102	3108	3112	rBV6	1435	1735	0.14%	0.016%
79	11.146	3137	3143	3144	rBV3	2735	2323	0.18%	0.022%
80	11.194	3150	3158	3166	rBV2	58260	83970	6.58%	0.790%
81	11.252	3166	3176	3194	rVB	797507	1228301	96.24%	11.561%
82	11.545	3261	3267	3271	rVB7	1320	1624	0.13%	0.015%
83	11.628	3281	3293	3312	rBV	638433	1003378	78.62%	9.444%
84	11.908	3372	3380	3384	rBV7	1733	2574	0.20%	0.024%
85	12.030	3415	3418	3421	rBV3	575	352	0.03%	0.003%
86	12.098	3429	3439	3442	rBV6	3140	4455	0.35%	0.042%
87	12.152	3454	3456	3460	rVB2	514	304	0.02%	0.003%
88	12.204	3469	3472	3475	rBV2	285	231	0.02%	0.002%
89	12.294	3494	3500	3506	rVB4	736	879	0.07%	0.008%
90	12.448	3546	3548	3553	rVB3	569	414	0.03%	0.004%
91	12.474	3553	3556	3558	rBV3	599	394	0.03%	0.004%
92	12.606	3585	3597	3604	rBV6	1548	2273	0.18%	0.021%
93	12.654	3609	3612	3621	rVB3	550	620	0.05%	0.006%
94	13.149	3763	3766	3771	rBV2	430	246	0.02%	0.002%
95	13.432	3852	3854	3855	rBV	515	178	0.01%	0.002%
96	13.516	3875	3880	3893	rVB3	4759	6970	0.55%	0.066%
97	13.683	3930	3932	3937	rVB2	499	380	0.03%	0.004%
98	13.905	3994	4001	4009	rVB2	5365	7097	0.56%	0.067%
99	15.596	4520	4527	4537	rVB6	18551	28803	2.26%	0.271%
100	16.188	4703	4711	4717	rBV6	20815	31827	2.49%	0.300%

Sum of corrected areas: 10624904

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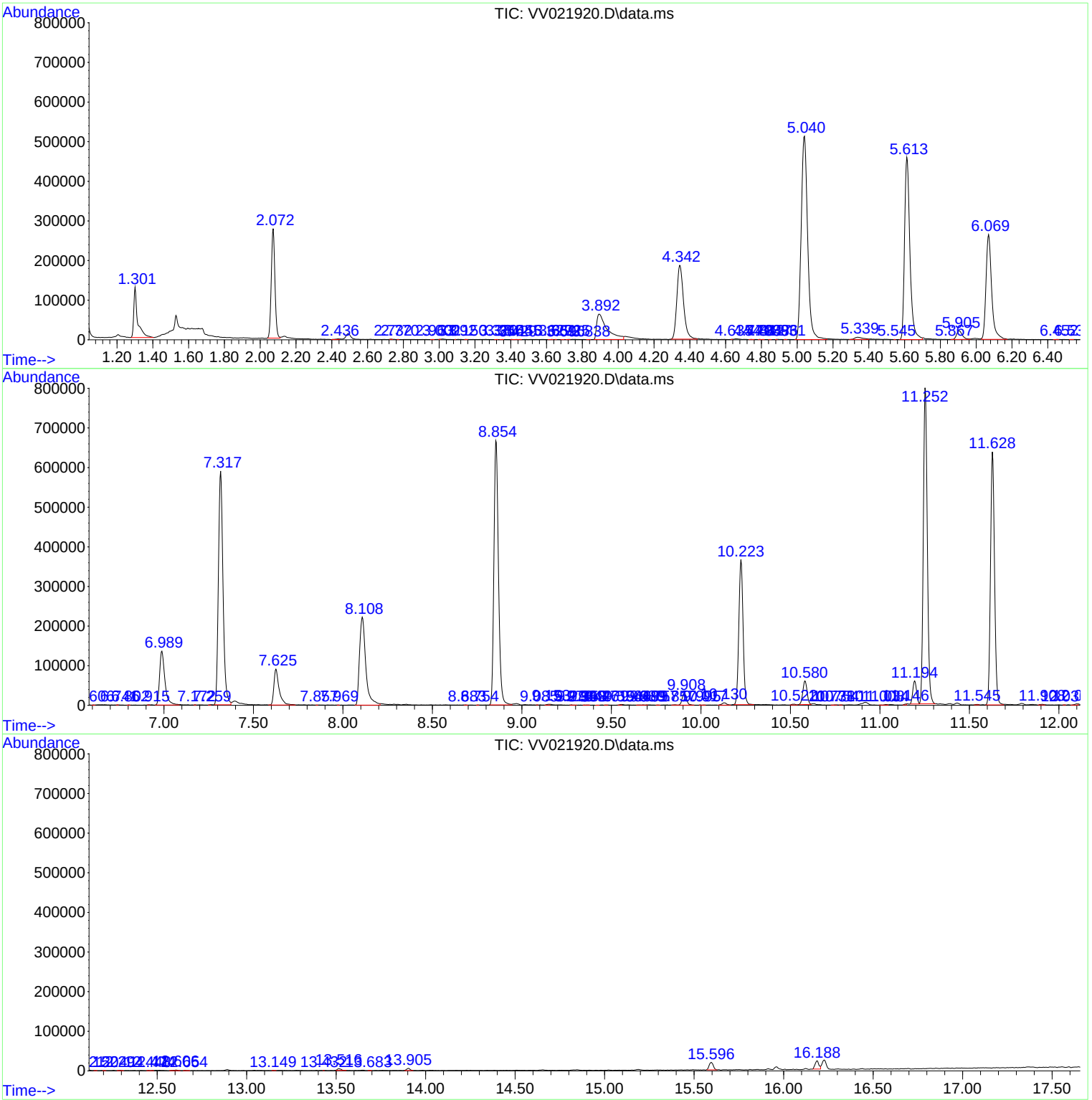
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0B56ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
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Instrument :
MSVOA_V
ClientSampleId :
C0B56ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

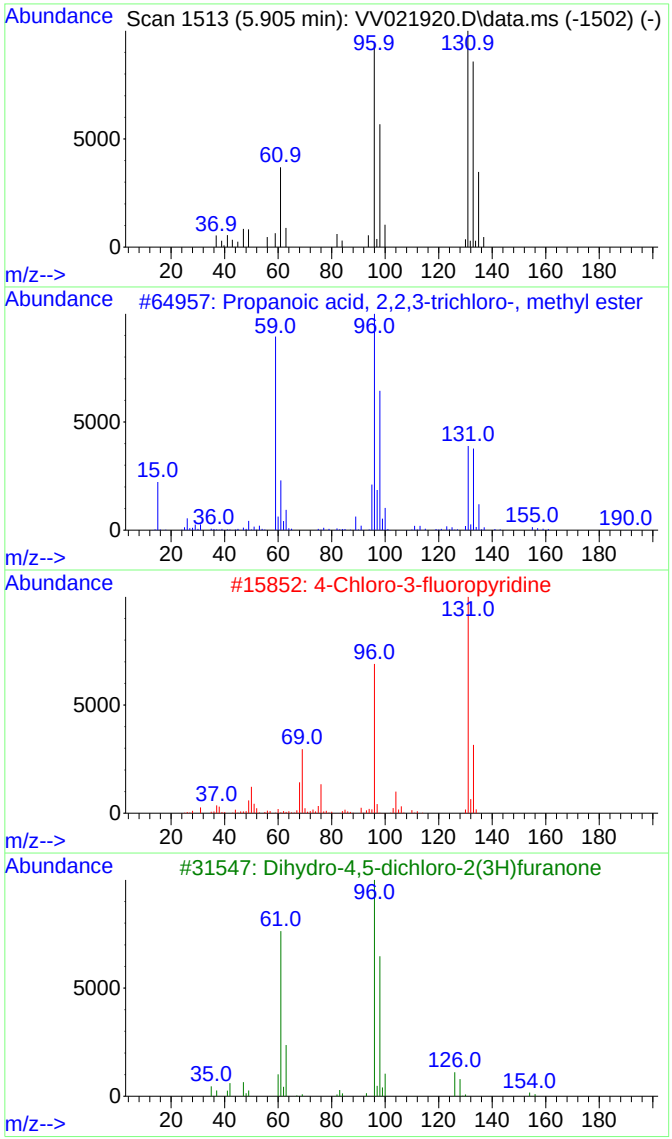
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

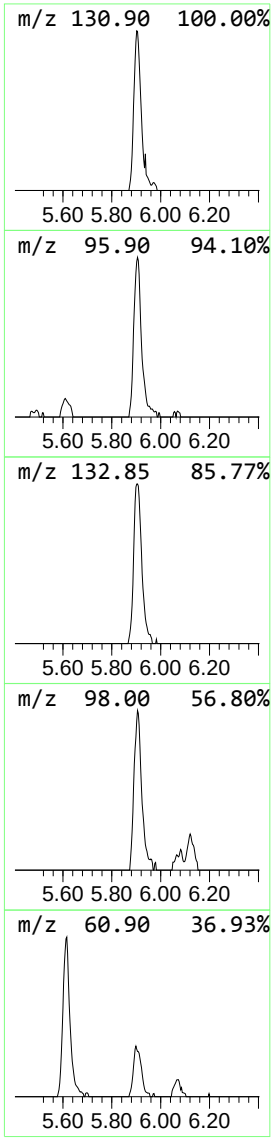
****

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	2.55 ug/L	48948	1,4-Difluorobenzene	5.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	38
2	4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
3	Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	27
4	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	27
5	2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
Data File : VV021920.D
Acq On : 20 Aug 2021 17:48
Operator : SY/MD
Sample : M3458-18ME
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0B56ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

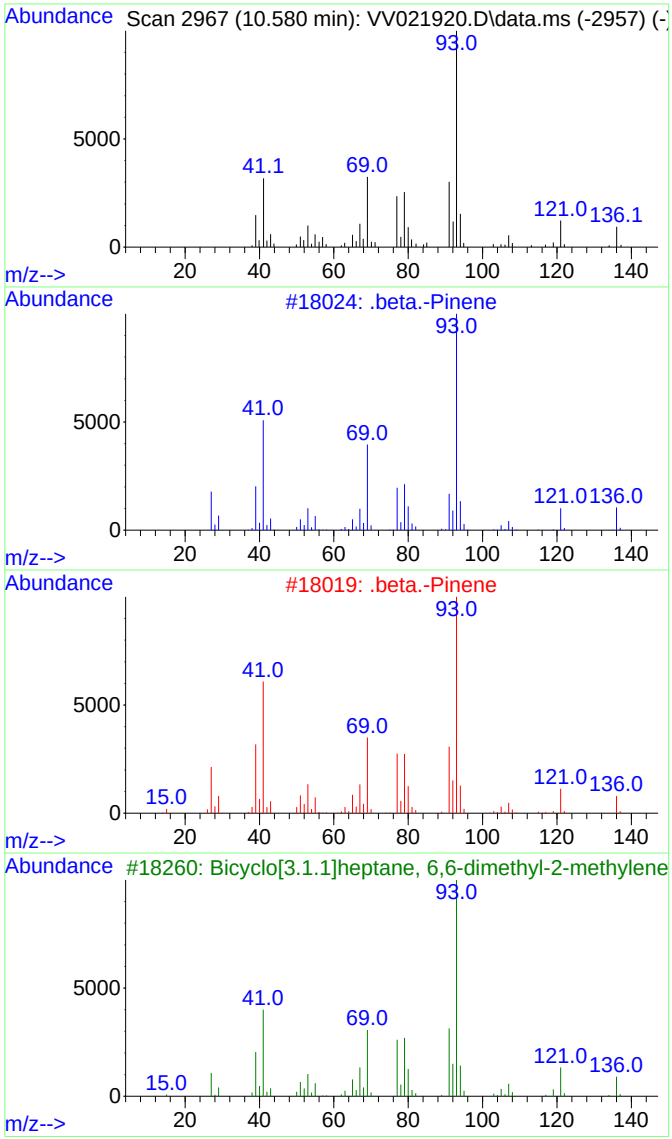
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

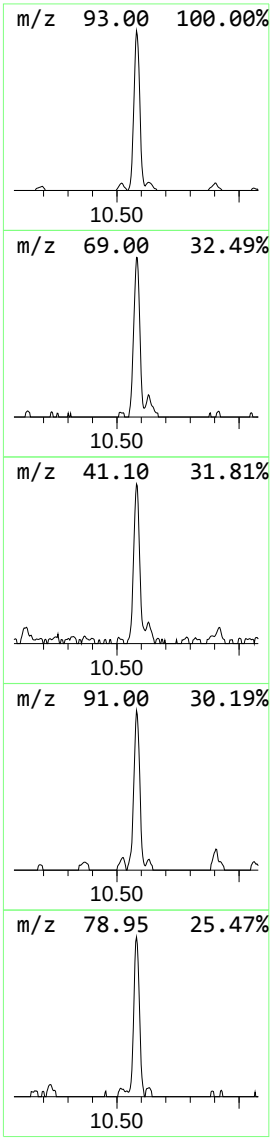
****

Peak Number 3 .beta.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	3.98 ug/L	97756	1,4-Dichlorobenzene-d4	11.252

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	97
2	.beta.-Pinene	136	C10H16	000127-91-3	97
3	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	95
4	.beta.-Pinene	136	C10H16	000127-91-3	94
5	.alpha.-Pinene	136	C10H16	000080-56-8	93





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0B56ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

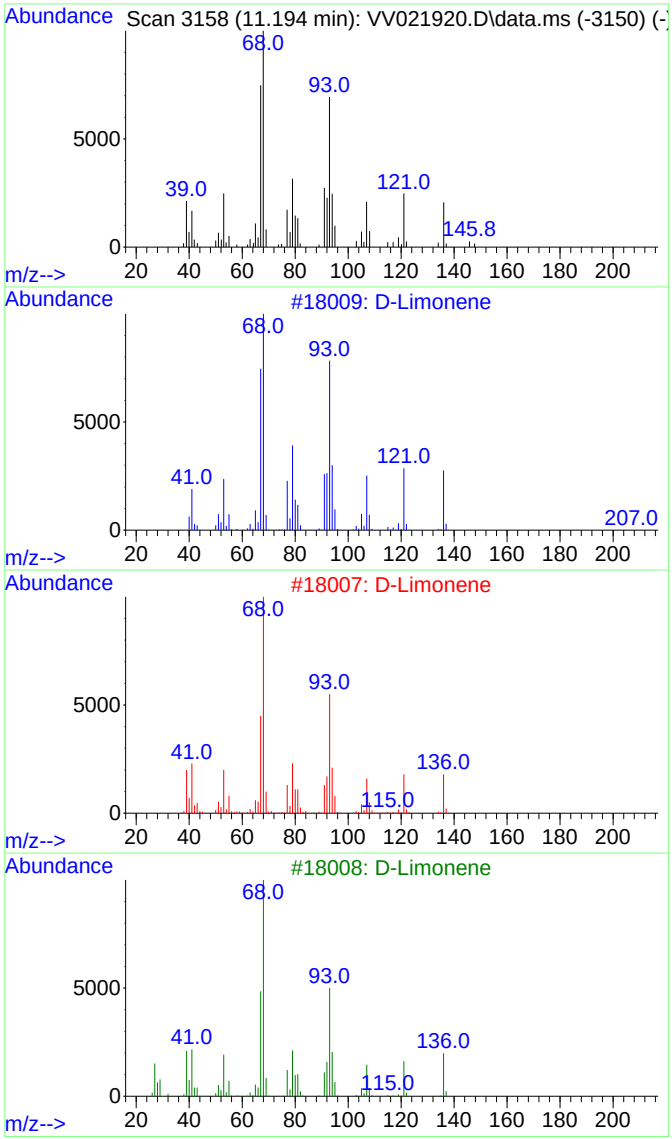
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

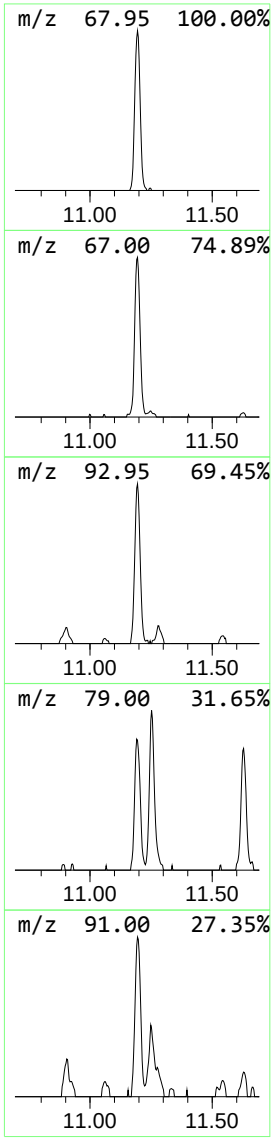
****

Peak Number 4 D-Limonene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.194	3.42 ug/L	83970	1,4-Dichlorobenzene-d4	11.252

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	98
2	D-Limonene	136	C10H16	005989-27-5	96
3	D-Limonene	136	C10H16	005989-27-5	96
4	D-Limonene	136	C10H16	005989-27-5	94
5	Limonene	136	C10H16	000138-86-3	89





Tentatively Identified Compound (LSC) summary

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ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0B56ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.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
unknown-01	5.905	2.5	ug/L	48948	1	5.613	960341	50.0
.beta.-Pinene	10.580	4.0	ug/L	97756	3	11.252	1228300	50.0
D-Limonene	11.194	3.4	ug/L	83970	3	11.252	1228300	50.0