LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054811.D
Acq On : 18 Jul 2023 16:48
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BH2Y4

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\SFAMULM071723WMA.M
Title : VOC Analysis

Signal : TIC: VU054811.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	90	95	111	rVB	91547	114404	15.20%	1.479%
2	2.554	383	393	406	rBV	136325	219013	29.09%	2.831%
3	3.184	573	589	612	rBV4	69750	178389	23.70%	2.306%
4	3.473	677	679	682	rBV2	427	295	0.04%	0.004%
5	3.586	710	714	718	rVB4	1124	962	0.13%	0.012%
6	3.608	718	721	727	rVB3	846	728	0.10%	0.009%
7	3.647	728	733	734	rBV2	594	461	0.06%	0.006%
8	3.689	741	746	748	rBV3	579	495	0.07%	0.006%
9	3.779	770	774	778	rBV4	783	749	0.10%	0.010%
10	3.885	805	807	808	rBV	350	170	0.02%	0.002%
11	4.014	844	847	852	rBV4	628	555	0.07%	0.007%
12	4.068	862	864	867	rBV2	502	350	0.05%	0.005%
13	4.084	867	869	871	rBV2	549	296	0.04%	0.004%
14	4.194	900	903	906	rVB3	571	393	0.05%	0.005%
15	4.248	914	920	921	rBV3	589	504	0.07%	0.007%
16	4.358	952	954	958	rVB	723	387	0.05%	0.005%
17	4.383	958	962	964	rBV2	639	417	0.06%	0.005%
18	4.615	1024	1034	1055	rBV	80991	198373	26.35%	2.565%
19	4.927	1129	1131	1133	rBV2	438	231	0.03%	0.003%
20	4.978	1146	1147	1150	rVB2	370	182	0.02%	0.002%
21	4.997	1151	1153	1155	rBV2	476	180	0.02%	0.002%
22	5.055	1156	1171	1190	rBV	146230	320511	42.58%	4.144%
23	5.303	1245	1248	1249	rBV	460	232	0.03%	0.003%
24	5.325	1253	1255	1256	rBV	412	182	0.02%	0.002%
25	5.361	1264	1266	1269	rBV	276	202	0.03%	0.003%
26	5.409	1279	1281	1284	rVB3	649	325	0.04%	0.004%
27	5.428	1284	1287	1291	rBV3	531	388	0.05%	0.005%
28	5.451	1291	1294	1297	rVB3	634	432	0.06%	0.006%
29	5.467	1297	1299	1304	rVB3	495	355	0.05%	0.005%
30	5.493	1304	1307	1313	rBV3	689	710	0.09%	0.009%
31	5.528	1313	1318	1321	rVB3	745	550	0.07%	0.007%
32	5.563	1324	1329	1335	rBV5	626	829	0.11%	0.011%
33	5.608	1340	1343	1348	rBV3	775	636	0.08%	0.008%
34	5.718	1354	1377	1397	rBV3	272216	749119	99.51%	9.685%
35	5.949	1447	1449	1451	rBV2	498	294	0.04%	0.004%
36	6.120	1499	1502	1505	rBV2	497	324	0.04%	0.004%

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

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\SFAMULM071723WMA.M
Title : VOC Analysis

37	6.245	1528	1541	1562	rBV	284038	543254	72.17%	7.023%
38	6.493	1616	1618	1623	rBV	525	446	0.06%	0.006%
39	6.685	1665	1678	1695	rBV	179571	354400	47.08%	4.582%
40	6.856	1730	1731	1735	rVB	743	358	0.05%	0.005%
41	6.882	1735	1739	1742	rBV	757	545	0.07%	0.007%
42	6.946	1755	1759	1762	rBV2	974	972	0.13%	0.013%
43	7.004	1775	1777	1781	rVB3	531	310	0.04%	0.004%
44	7.026	1781	1784	1788	rBV3	559	452	0.06%	0.006%
45	7.081	1799	1801	1803	rBV3	337	217	0.03%	0.003%
46	7.161	1814	1826	1843	rBV2	100524	200586	26.65%	2.593%
47	7.380	1892	1894	1896	rBV3	469	221	0.03%	0.003%
48	7.396	1896	1899	1901	rBV3	691	350	0.05%	0.005%
49	7.454	1915	1917	1923	rVB4	794	710	0.09%	0.009%
50	7.483	1923	1926	1927	rBV	632	337	0.04%	0.004%
51	7.521	1936	1938	1939	rBV	417	193	0.03%	0.002%
52	7.563	1939	1951	1969	rVV2	103716	186000	24.71%	2.405%
53	7.753	2008	2010	2014	rBV3	701	456	0.06%	0.006%
54	7.894	2041	2054	2070	rBV	348144	611101	81.18%	7.901%
55	8.177	2131	2142	2159	rBV	72682	125370	16.65%	1.621%
56	8.303	2180	2181	2184	rVB	389	193	0.03%	0.002%
57	8.322	2184	2187	2188	rBV2	397	194	0.03%	0.003%
58	8.335	2189	2191	2192	rBV2	598	179	0.02%	0.002%
59	8.357	2197	2198	2203	rVB2	635	417	0.06%	0.005%
60	8.444	2222	2225	2226	rBV2	623	306	0.04%	0.004%
61	8.631	2272	2283	2319	rBV2	238902	471788	62.67%	6.099%
62	8.904	2365	2368	2370	rBV	768	468	0.06%	0.006%
63	8.962	2384	2386	2389	rBV2	386	249	0.03%	0.003%
64	9.029	2404	2407	2411	rBV3	829	715	0.09%	0.009%
65	9.325	2496	2499	2501	rBV2	552	319	0.04%	0.004%
66	9.361	2507	2510	2512	rBV3	539	316	0.04%	0.004%
67	9.415	2515	2527	2553	rVV	418553	683053	90.74%	8.831%
68	9.634	2592	2595	2596	rBV	666	340	0.05%	0.004%
69	9.666	2603	2605	2607	rBV2	750	434	0.06%	0.006%
70	9.869	2667	2668	2672	rBV2	382	270	0.04%	0.003%
71	9.926	2684	2686	2688	rBV2	352	176	0.02%	0.002%
72	10.023	2713	2716	2719	rBV2	656	428	0.06%	0.006%
73	10.058	2724	2727	2728	rBV2	410	249	0.03%	0.003%
74	10.209	2772	2774	2778	rVB3	672	319	0.04%	0.004%
75	10.316	2798	2807	2821	rBV6	9006	14086	1.87%	0.182%
76	10.489	2851	2861	2874	rBV3	33016	50965	6.77%	0.659%

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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BH2Y4

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_U\Method\SFAMULM071723WMA.M
Title : VOC Analysis

77	10.586	2889	2891	2894	rBV3	762	499	0.07%	0.006%
78	10.685	2918	2922	2923	rBV2	540	461	0.06%	0.006%
79	10.753	2931	2943	2959	rBV	311608	501761	66.65%	6.487%
80	11.087	3045	3047	3048	rBV	1015	419	0.06%	0.005%
81	11.158	3061	3069	3078	rBV3	9751	14515	1.93%	0.188%
82	11.528	3181	3184	3185	rBV2	506	317	0.04%	0.004%
83	11.608	3200	3209	3227	rVB6	23046	43588	5.79%	0.564%
84	11.676	3227	3230	3231	rBV	767	379	0.05%	0.005%
85	11.714	3235	3242	3243	rBV3	8472	8334	1.11%	0.108%
86	11.807	3260	3271	3289	rVB	447381	752778	100.00%	9.732%
87	12.190	3379	3390	3409	rVB	383309	622215	82.66%	8.044%
88	12.348	3437	3439	3443	rVB3	741	471	0.06%	0.006%
89	12.373	3443	3447	3449	rBV4	1451	1132	0.15%	0.015%
90	12.454	3465	3472	3483	rBV6	18933	29525	3.92%	0.382%
91	12.524	3485	3494	3516	rVB	184600	291618	38.74%	3.770%
92	12.840	3583	3592	3604	rBV3	47606	74177	9.85%	0.959%
93	13.360	3752	3754	3757	rBV2	699	437	0.06%	0.006%
94	13.512	3799	3801	3803	rBV2	721	368	0.05%	0.005%
95	13.839	3898	3903	3914	rVB10	2978	5352	0.71%	0.069%
96	14.032	3954	3963	3977	rBV4	24175	41309	5.49%	0.534%
97	14.164	4000	4004	4005	rBV	1837	1310	0.17%	0.017%
98	14.444	4083	4091	4092	rBV3	13441	14113	1.87%	0.182%
99	14.476	4094	4101	4121	rVB	184290	284900	37.85%	3.683%
100	14.769	4190	4192	4196	rBV4	777	602	0.08%	0.008%

Sum of corrected areas: 7734945

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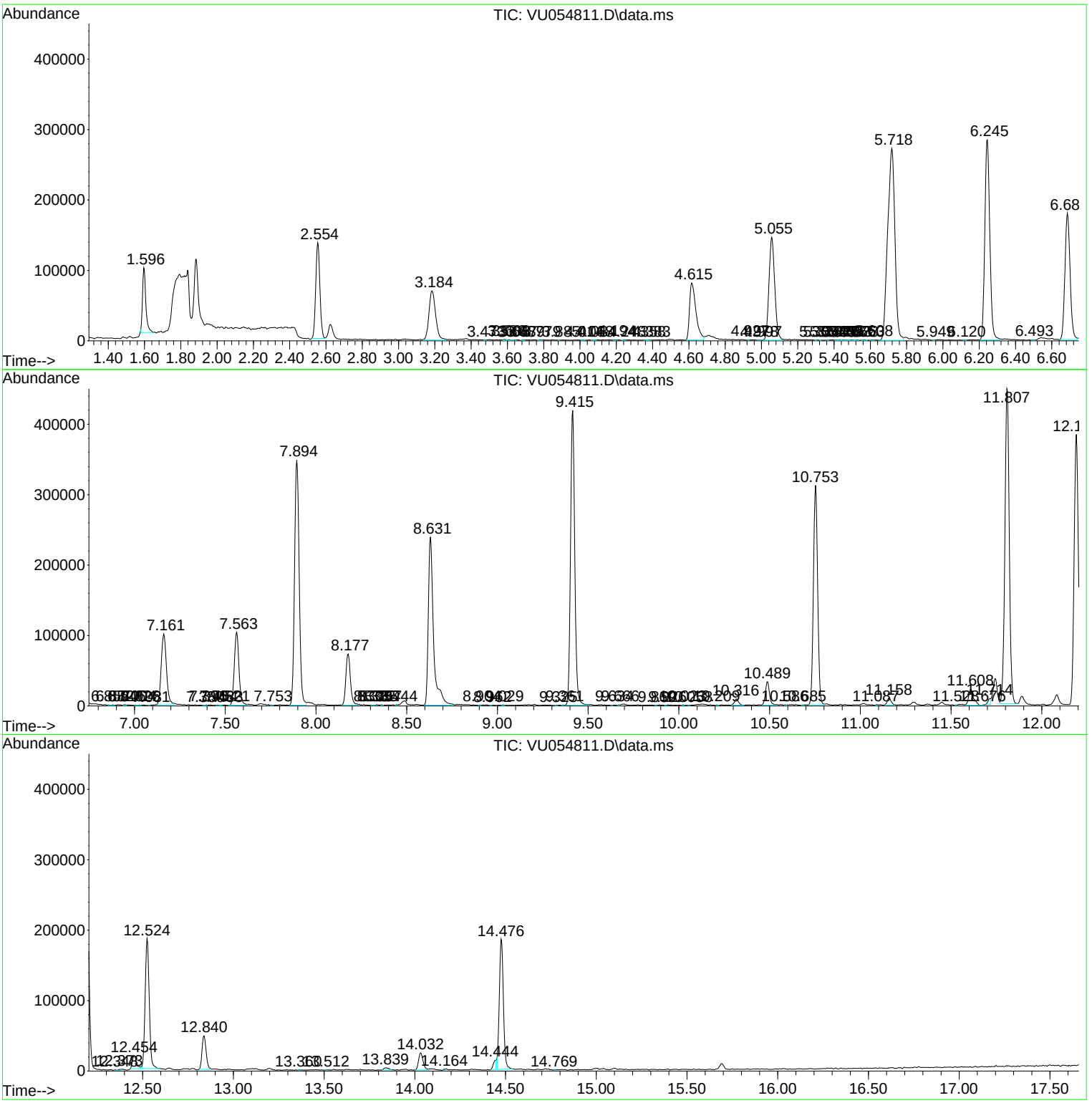
Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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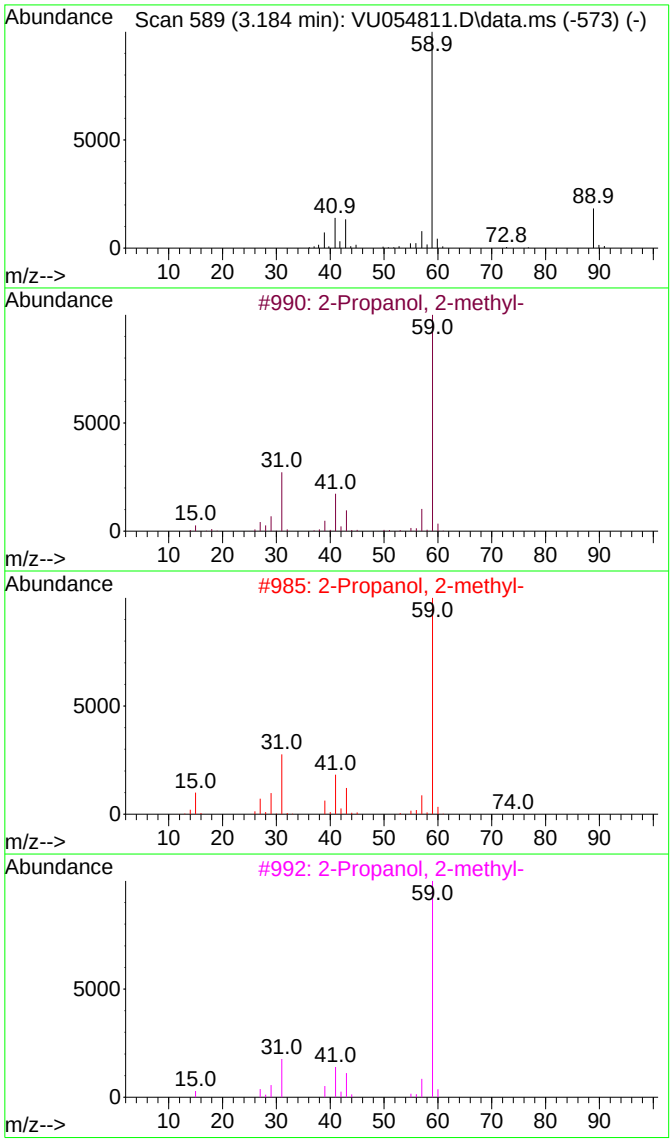
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

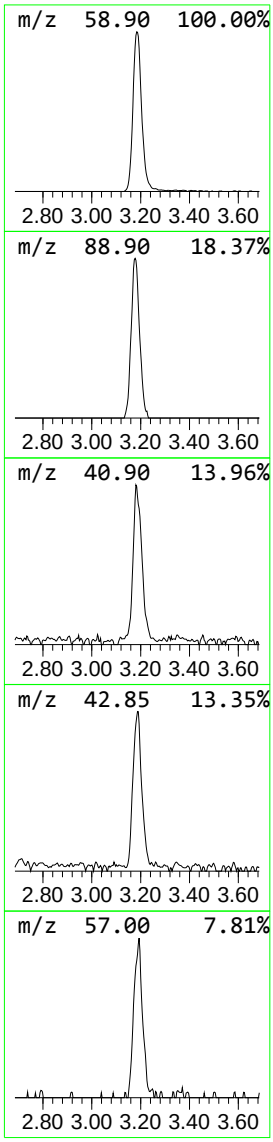
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.184	16.42 ug/L	178389	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
4	3-Pentanol	88	C5H12O	000584-02-1	39
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054811.D
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

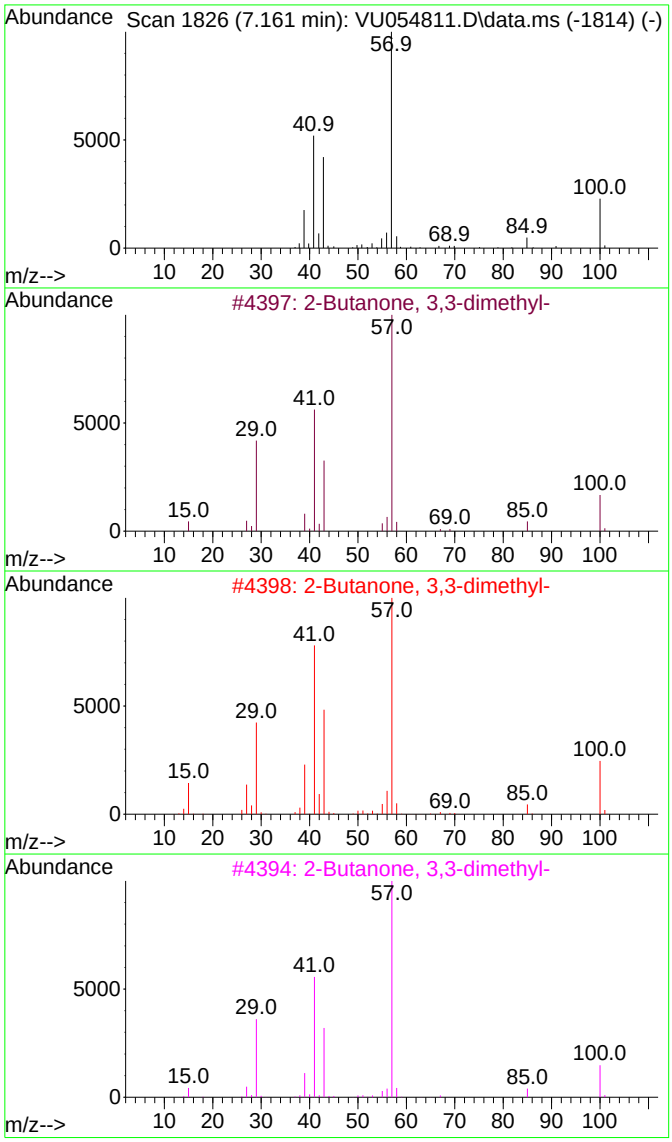
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

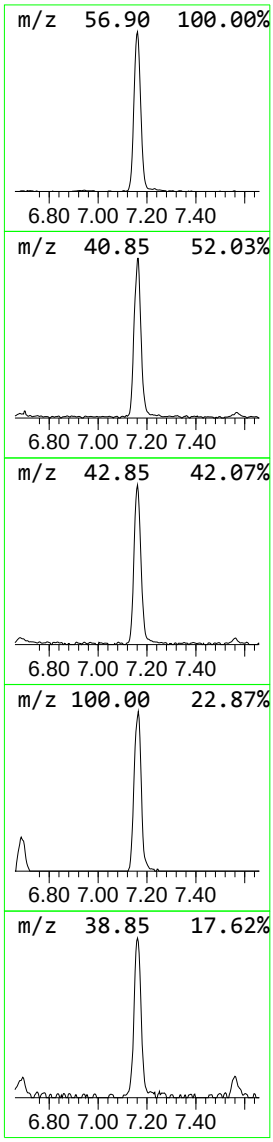
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.161	18.46 ug/L	200586	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	90
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	83
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
5	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64





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MSVOA_U
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BH2Y4

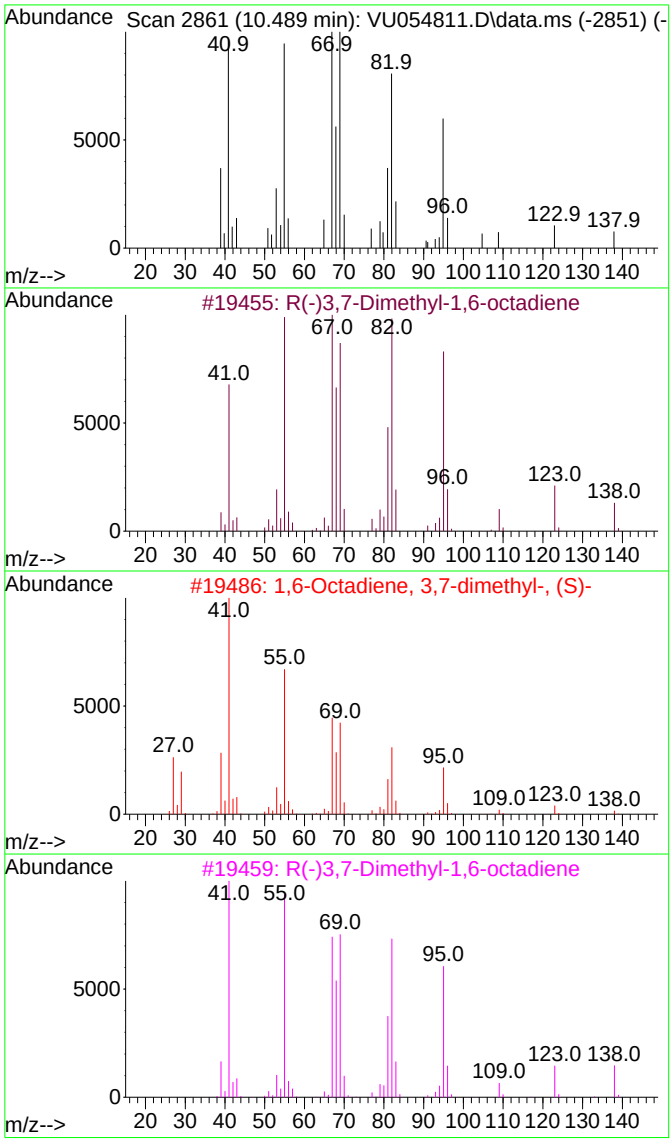
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

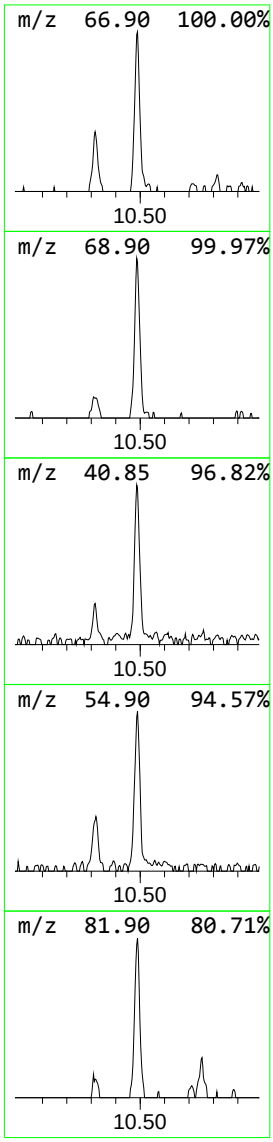
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 R(-)3,7-Dimethyl-1,6-octadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.489	3.73 ug/L	50965	Chlorobenzene-d5	9.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	97
2	1,6-Octadiene, 3,7-dimethyl-, (S)-	138	C10H18	010281-55-7	94
3	R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	86
4	Cyclohexaneethanol, .beta.-methyl-	142	C9H18O	005442-00-2	50
5	1,6-Octadiene, 2,6-dimethyl-, (Z)-	138	C10H18	006874-34-6	47





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Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

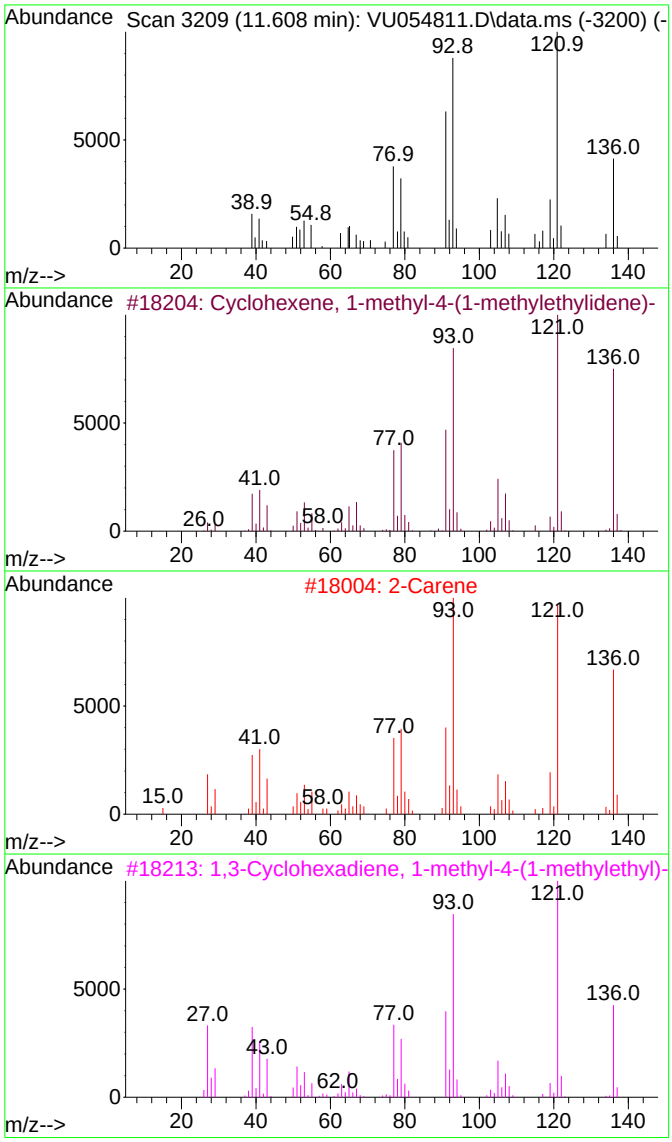
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

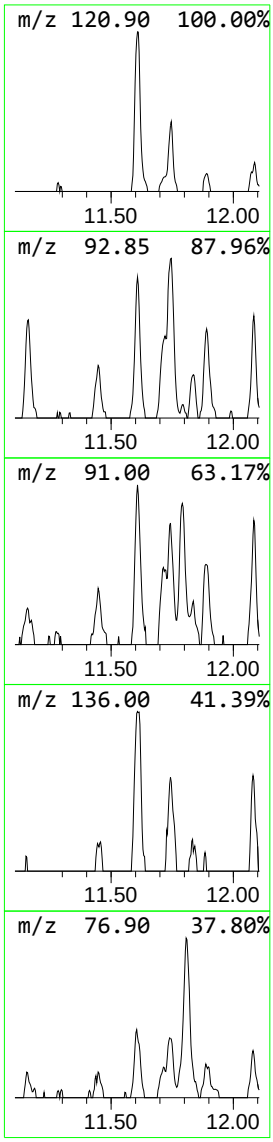
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.608	2.90 ug/L	43588	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	97
2	2-Carene	136	C10H16	000554-61-0	96
3	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	96
4	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	95
5	Bicyclo[4.1.0]hept-2-ene, 3,7,7-...	136	C10H16	004497-92-1	95





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

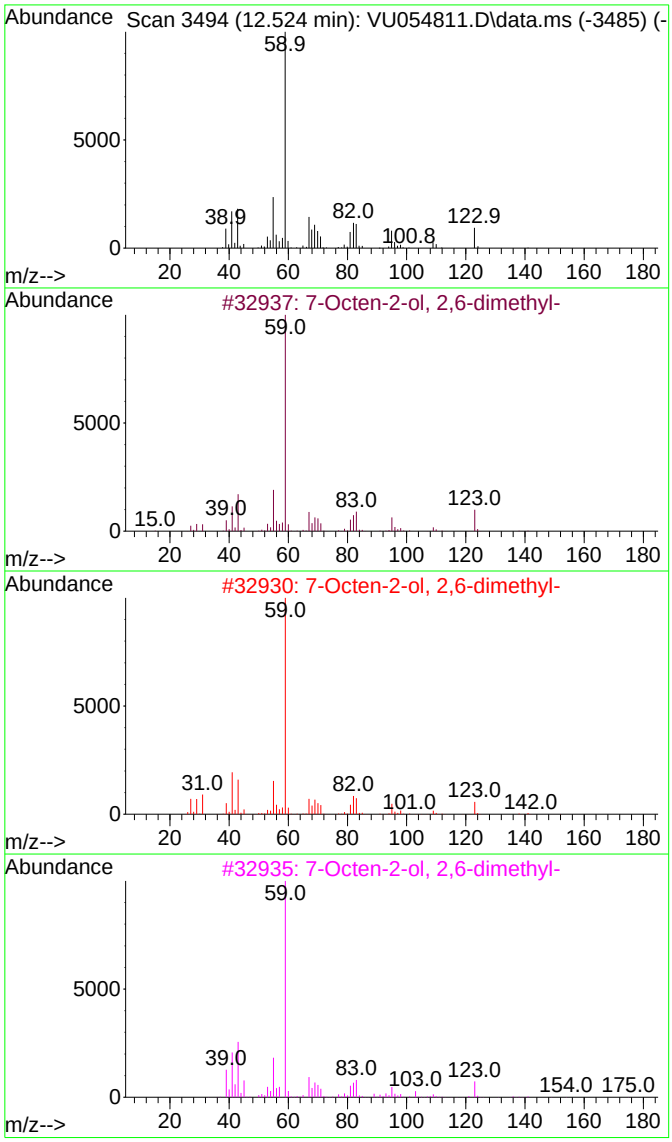
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

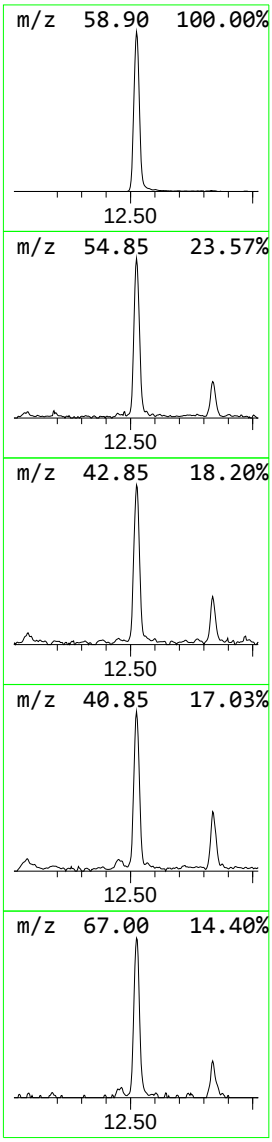
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.524	19.37 ug/L	291618	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	90
2	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
3	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
4	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	78
5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	50





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Data File : VU054811.D
Acq On : 18 Jul 2023 16:48
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

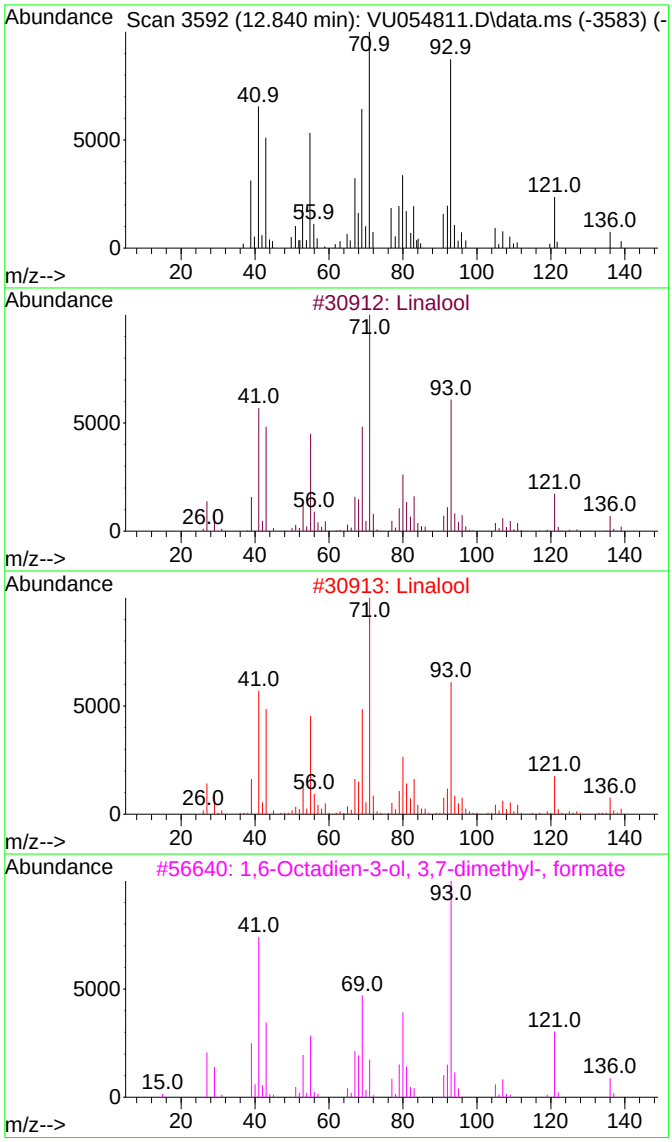
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

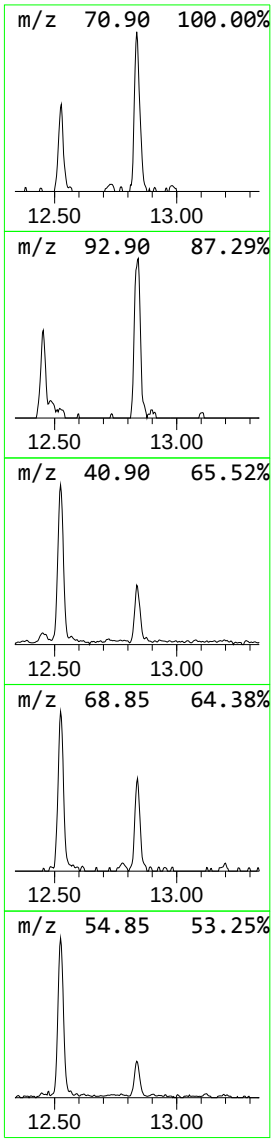
****

Peak Number 7 Linalool Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.839	4.93 ug/L	74177	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Linalool	154	C10H18O	000078-70-6	64
2	Linalool	154	C10H18O	000078-70-6	64
3	1,6-Octadien-3-ol, 3,7-dimethyl-...	182	C11H18O2	000115-99-1	49
4	1,5-Dimethyl-1-vinyl-4-hexenyl b...	224	C14H24O2	000078-36-4	49
5	.beta.-Ocimene	136	C10H16	013877-91-3	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054811.D
Acq On : 18 Jul 2023 16:48
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

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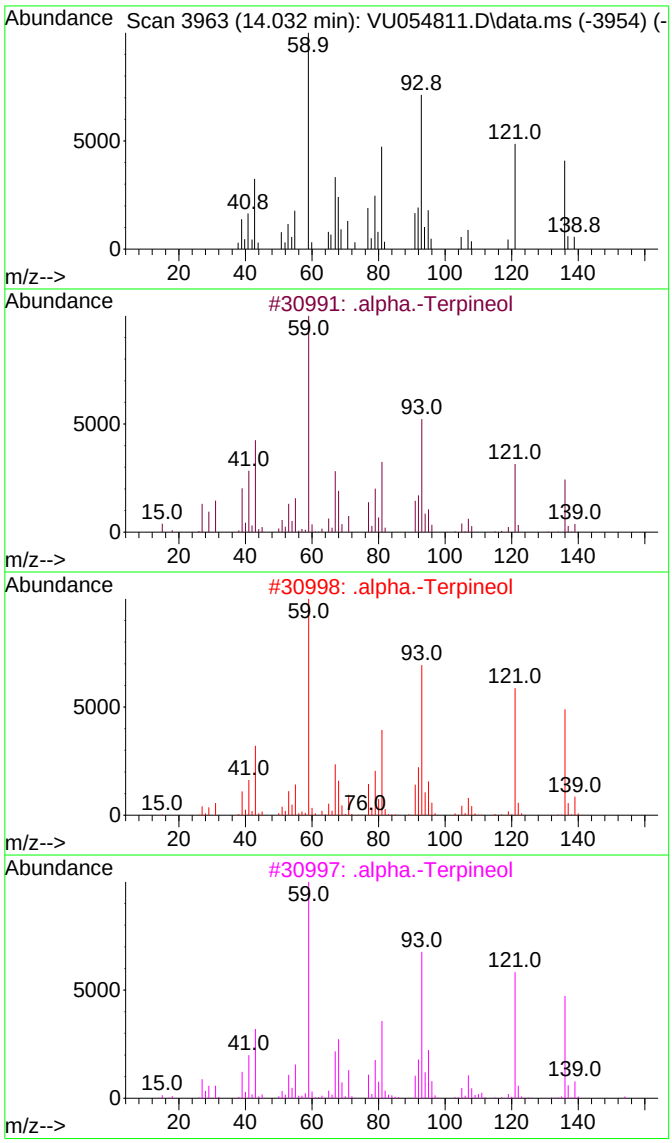
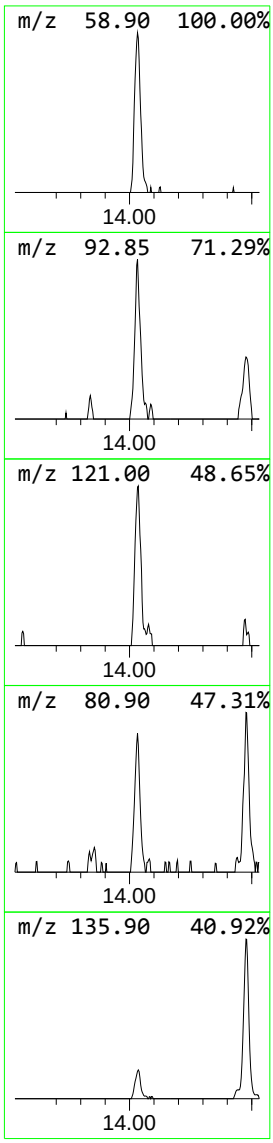
Peak Number 8 .alpha.-Terpineol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.032	2.74 ug/L	41309	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Terpineol	154	C10H18O	000098-55-5	86
2	.alpha.-Terpineol	154	C10H18O	000098-55-5	80
3	.alpha.-Terpineol	154	C10H18O	000098-55-5	80
4	(+)-4-Carene	136	C10H16	029050-33-7	64
5	3-Cyclohexene-1-methanol, .alpha...	154	C10H18O	007785-53-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054811.D
Acq On : 18 Jul 2023 16:48
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

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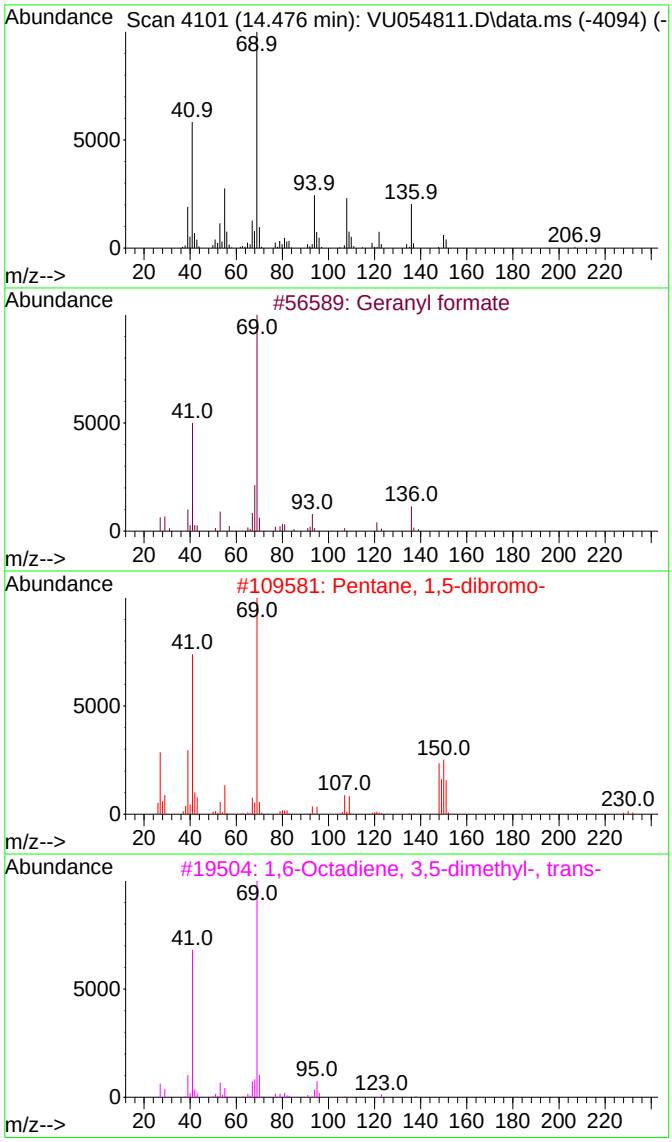
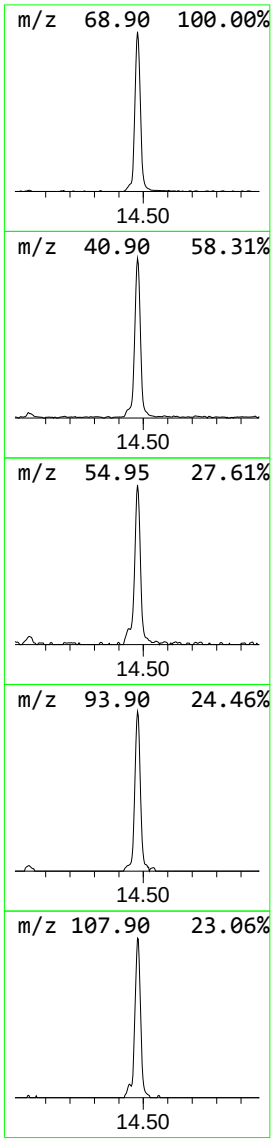
Peak Number 9 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.476	18.92 ug/L	284900	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Geranyl formate	182	C11H18O2	000105-86-2	47
2	Pentane, 1,5-dibromo-	228	C5H10Br2	000111-24-0	43
3	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	38
4	6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	38
5	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054811.D
Acq On : 18 Jul 2023 16:48
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.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
2-Propanol, 2-m...	3.184	16.4	ug/L	178389	1	6.245	543254	50.0
2-Butanone, 3,3...	7.161	18.5	ug/L	200586	1	6.245	543254	50.0
R(-)3,7-Dimethy...	10.489	3.7	ug/L	50965	2	9.415	683053	50.0
Cyclohexene, 1-...	11.608	2.9	ug/L	43588	3	11.811	752778	50.0
7-Octen-2-ol, 2...	12.524	19.4	ug/L	291618	3	11.811	752778	50.0
Linalool	12.839	4.9	ug/L	74177	3	11.811	752778	50.0
.alpha.-Terpineol	14.032	2.7	ug/L	41309	3	11.811	752778	50.0
unknown-01	14.476	18.9	ug/L	284900	3	11.811	752778	50.0