LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
Acq On : 18 Jul 2023 16:23
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BH2X8

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: VU054810.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	89	95	114	rVB	90200	115176	15.27%	1.500%
2	2.554	383	393	406	rBV	137918	223400	29.61%	2.910%
3	2.625	408	415	429	rVB	21250	36986	4.90%	0.482%
4	3.120	564	569	571	rBV2	470	362	0.05%	0.005%
5	3.184	577	589	614	rVB3	60825	154816	20.52%	2.017%
6	3.451	669	672	674	rVB2	640	358	0.05%	0.005%
7	3.467	674	677	678	rBV	551	339	0.04%	0.004%
8	3.586	711	714	716	rBV	586	390	0.05%	0.005%
9	3.631	725	728	730	rBV3	522	289	0.04%	0.004%
10	3.737	759	761	764	rBV2	487	278	0.04%	0.004%
11	3.808	781	783	786	rBV	486	254	0.03%	0.003%
12	3.898	807	811	814	rBV2	585	479	0.06%	0.006%
13	4.052	856	859	864	rBV4	634	590	0.08%	0.008%
14	4.088	868	870	875	rVB3	761	472	0.06%	0.006%
15	4.113	875	878	881	rBV4	495	330	0.04%	0.004%
16	4.155	888	891	893	rBV	398	240	0.03%	0.003%
17	4.235	914	916	918	rVB3	573	217	0.03%	0.003%
18	4.255	918	922	923	rBV2	407	312	0.04%	0.004%
19	4.300	932	936	939	rBV4	421	369	0.05%	0.005%
20	4.425	969	975	979	rBV4	591	754	0.10%	0.010%
21	4.618	1024	1035	1056	rBV	79957	195855	25.96%	2.551%
22	4.914	1125	1127	1128	rBV	717	335	0.04%	0.004%
23	4.988	1147	1150	1151	rBV3	724	333	0.04%	0.004%
24	5.055	1157	1171	1194	rBV	148013	318448	42.21%	4.148%
25	5.242	1225	1229	1230	rBV2	627	416	0.06%	0.005%
26	5.306	1247	1249	1252	rBV3	469	227	0.03%	0.003%
27	5.560	1325	1328	1331	rVB4	627	376	0.05%	0.005%
28	5.592	1333	1338	1344	rVB5	922	1036	0.14%	0.013%
29	5.624	1344	1348	1349	rBV2	412	314	0.04%	0.004%
30	5.718	1357	1377	1401	rBV2	277001	754419	100.00%	9.827%
31	5.981	1457	1459	1462	rBV3	535	344	0.05%	0.004%
32	6.046	1478	1479	1481	rBV	478	231	0.03%	0.003%
33	6.110	1497	1499	1500	rBV	497	230	0.03%	0.003%
34	6.242	1527	1540	1560	rBV	272618	516012	68.40%	6.722%
35	6.486	1611	1616	1618	rBV	530	505	0.07%	0.007%
36	6.547	1621	1635	1639	rBV7	3027	6771	0.90%	0.088%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
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Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BH2X8

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	6.685	1665	1678	1701	rBV	179292	352435	46.72%	4.591%
38	6.862	1730	1733	1735	rBV2	1089	748	0.10%	0.010%
39	7.036	1785	1787	1789	rBV2	349	236	0.03%	0.003%
40	7.071	1794	1798	1799	rBV2	710	346	0.05%	0.005%
41	7.158	1810	1825	1843	rBV	101559	208894	27.69%	2.721%
42	7.306	1868	1871	1872	rBV3	718	428	0.06%	0.006%
43	7.374	1885	1892	1899	rBV4	1019	1772	0.23%	0.023%
44	7.422	1903	1907	1908	rBV2	350	229	0.03%	0.003%
45	7.448	1910	1915	1918	rVV4	560	504	0.07%	0.007%
46	7.464	1918	1920	1923	rVB3	428	277	0.04%	0.004%
47	7.560	1936	1950	1966	rBV	109714	191734	25.41%	2.498%
48	7.894	2040	2054	2073	rBV	352962	613928	81.38%	7.997%
49	8.177	2129	2142	2157	rBV	73149	128151	16.99%	1.669%
50	8.354	2194	2197	2199	rBV3	483	380	0.05%	0.005%
51	8.435	2218	2222	2224	rBV	539	517	0.07%	0.007%
52	8.631	2272	2283	2297	rBV	239785	438293	58.10%	5.709%
53	8.920	2369	2373	2375	rBV3	423	339	0.04%	0.004%
54	8.965	2384	2387	2390	rBV2	621	402	0.05%	0.005%
55	9.007	2397	2400	2401	rBV2	383	232	0.03%	0.003%
56	9.058	2412	2416	2421	rBV4	806	636	0.08%	0.008%
57	9.094	2424	2427	2430	rBV2	563	471	0.06%	0.006%
58	9.145	2440	2443	2446	rBV2	886	658	0.09%	0.009%
59	9.290	2485	2488	2490	rBV2	448	303	0.04%	0.004%
60	9.415	2514	2527	2551	rBV	397418	658631	87.30%	8.580%
61	9.615	2587	2589	2592	rBV4	896	470	0.06%	0.006%
62	9.653	2598	2601	2604	rBV3	579	440	0.06%	0.006%
63	9.756	2630	2633	2634	rBV	509	307	0.04%	0.004%
64	9.804	2645	2648	2649	rBV2	378	235	0.03%	0.003%
65	9.917	2680	2683	2686	rBV3	393	281	0.04%	0.004%
66	9.933	2686	2688	2693	rVV3	693	555	0.07%	0.007%
67	10.084	2729	2735	2737	rBV4	797	783	0.10%	0.010%
68	10.184	2762	2766	2768	rBV2	802	585	0.08%	0.008%
69	10.235	2779	2782	2784	rBV	769	502	0.07%	0.007%
70	10.316	2798	2807	2815	rBV7	7962	13128	1.74%	0.171%
71	10.406	2831	2835	2839	rBV3	598	560	0.07%	0.007%
72	10.486	2851	2860	2875	rVB4	29318	46641	6.18%	0.608%
73	10.566	2882	2885	2890	rBV2	738	563	0.07%	0.007%
74	10.753	2928	2943	2958	rBV	317362	510889	67.72%	6.655%
75	10.952	3002	3005	3008	rBV2	531	463	0.06%	0.006%
76	11.084	3044	3046	3048	rBV	538	265	0.04%	0.003%

LSC Area Percent Report

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Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BH2X8

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

77	11.158	3061	3069	3079	rBV4	9937	15330	2.03%	0.200%
78	11.293	3103	3111	3121	rBV7	4377	7872	1.04%	0.103%
79	11.534	3183	3186	3187	rBV2	960	556	0.07%	0.007%
80	11.608	3195	3209	3227	rVB6	23034	44278	5.87%	0.577%
81	11.679	3229	3231	3234	rBV3	389	266	0.04%	0.003%
82	11.714	3234	3242	3243	rBV5	9693	10127	1.34%	0.132%
83	11.807	3259	3271	3288	rVB	445748	725871	96.22%	9.456%
84	12.010	3331	3334	3338	rVB5	1287	835	0.11%	0.011%
85	12.081	3345	3356	3369	rBV7	13765	26668	3.53%	0.347%
86	12.190	3378	3390	3408	rBV	393268	625873	82.96%	8.153%
87	12.351	3437	3440	3443	rBV2	689	511	0.07%	0.007%
88	12.454	3462	3472	3479	rBV4	19358	30019	3.98%	0.391%
89	12.524	3485	3494	3511	rVB	183417	279411	37.04%	3.640%
90	12.840	3580	3592	3604	rBV2	49145	79676	10.56%	1.038%
91	13.036	3649	3653	3654	rBV3	1339	865	0.11%	0.011%
92	13.380	3758	3760	3761	rBV2	661	255	0.03%	0.003%
93	13.544	3807	3811	3814	rBV5	1784	1676	0.22%	0.022%
94	13.843	3895	3904	3918	rVB5	3635	8357	1.11%	0.109%
95	13.897	3918	3921	3924	rBV3	675	365	0.05%	0.005%
96	13.914	3924	3926	3928	rBV2	502	287	0.04%	0.004%
97	14.032	3954	3963	3975	rBV4	21361	36126	4.79%	0.471%
98	14.444	4081	4091	4092	rBV3	12586	13556	1.80%	0.177%
99	14.476	4094	4101	4115	rVB	166929	257465	34.13%	3.354%
100	14.868	4220	4223	4226	rBV3	1015	898	0.12%	0.012%

Sum of corrected areas: 7676617

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
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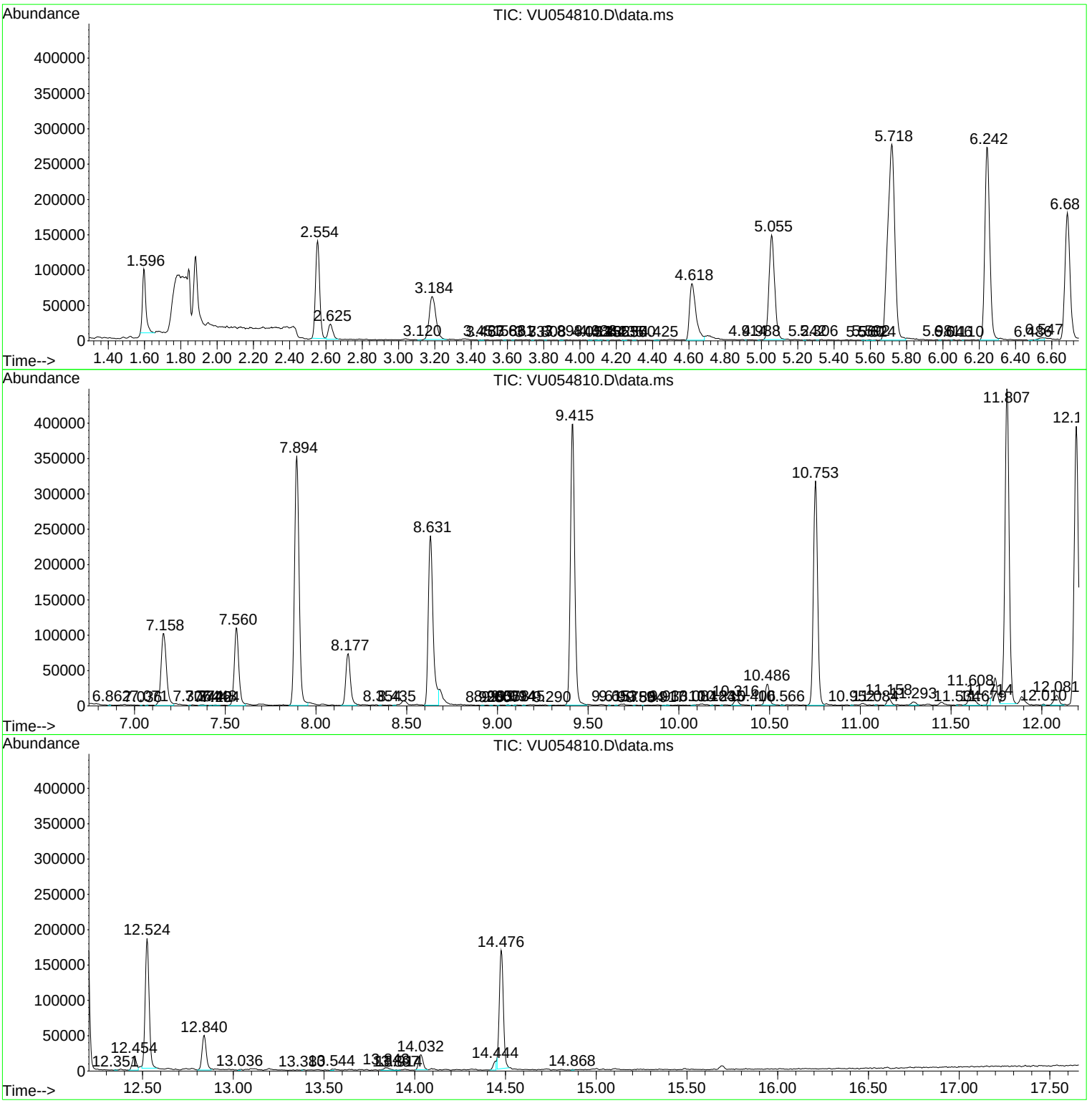
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

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\
Data File : VU054810.D
Acq On : 18 Jul 2023 16:23
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

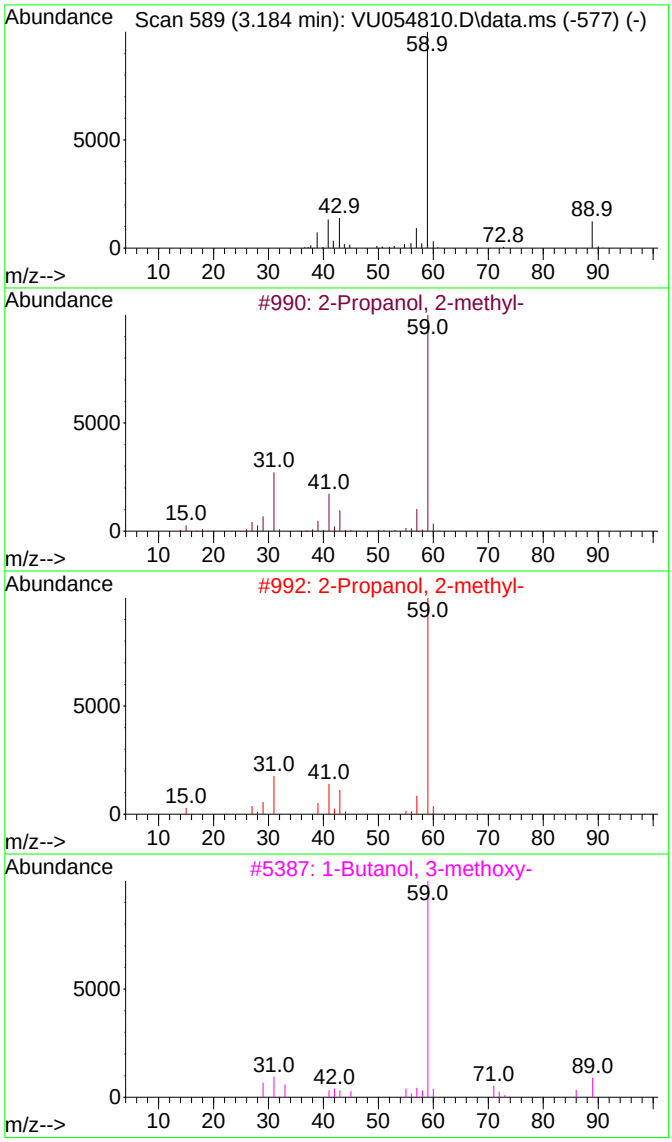
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

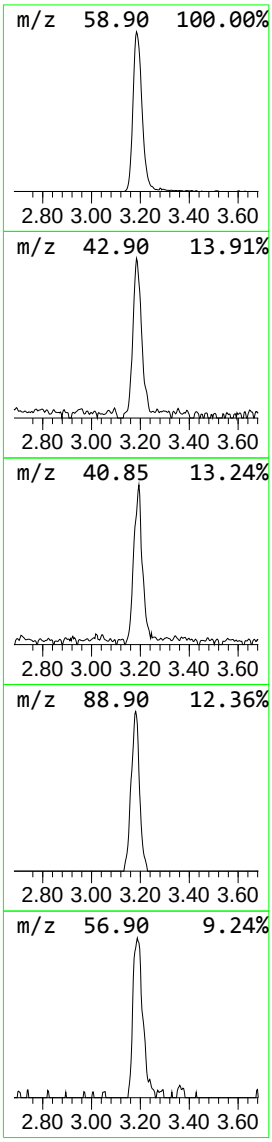
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.184	15.00 ug/L	154816	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	40
4	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	39
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
Acq On : 18 Jul 2023 16:23
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

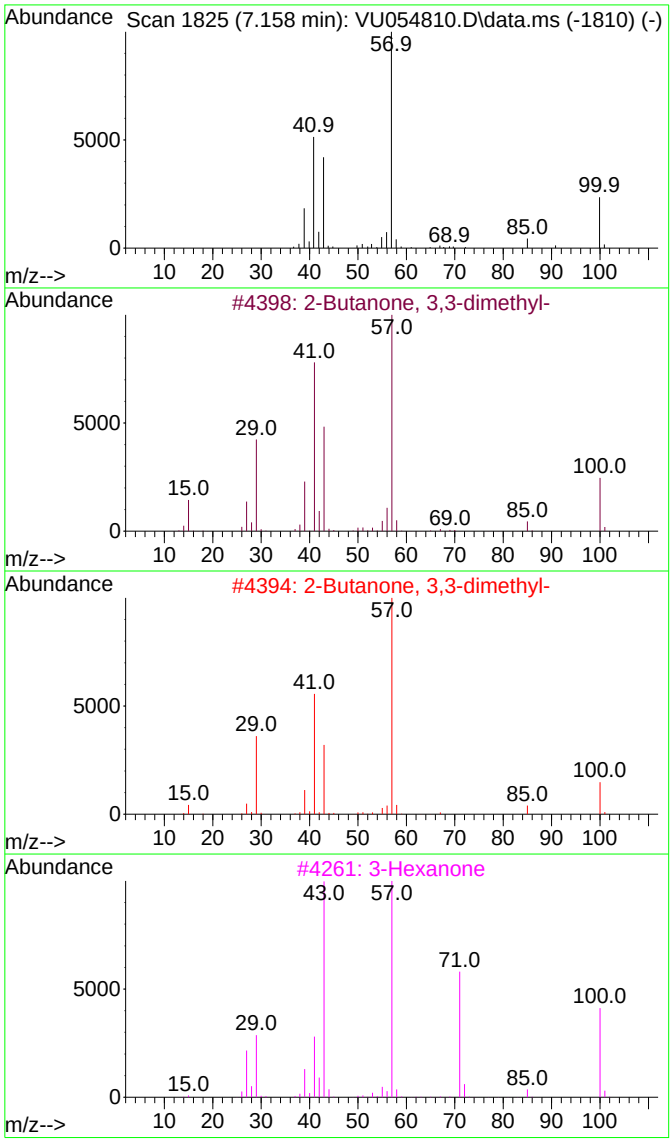
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

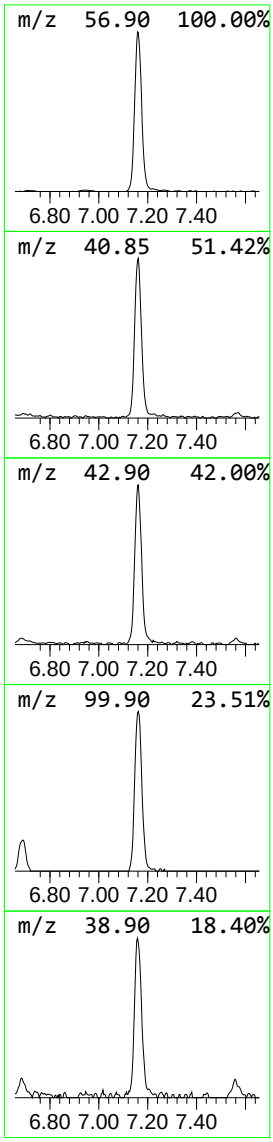
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.158	20.24 ug/L	208894	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	83
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72
3	3-Hexanone	100	C6H12O	000589-38-8	64
4	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	56
5	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

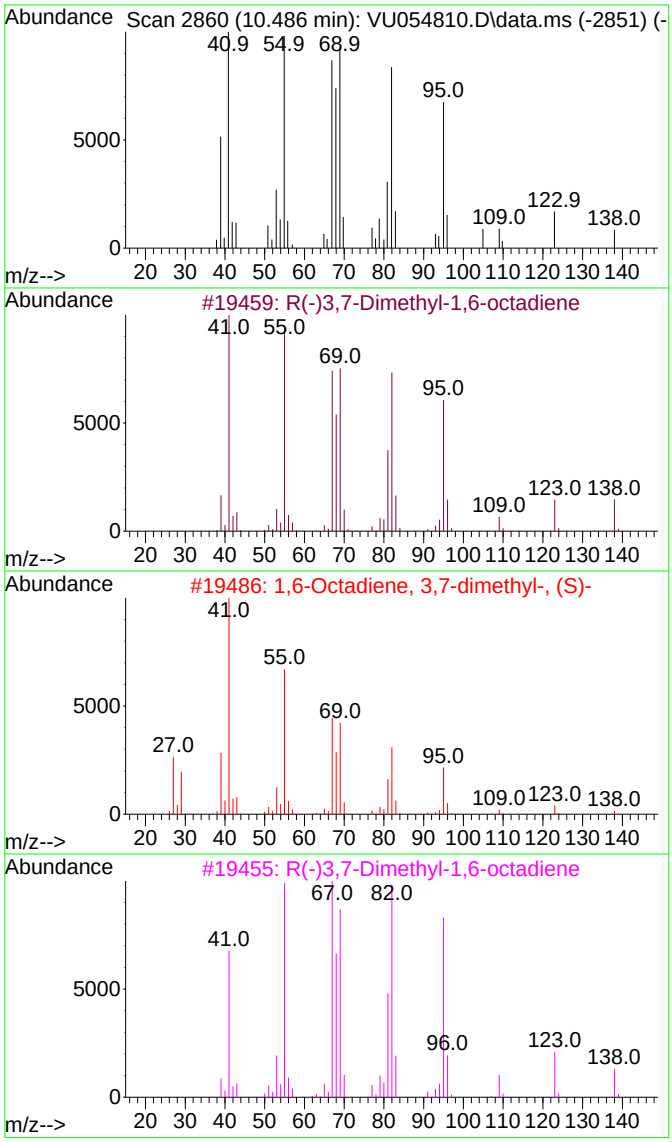
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

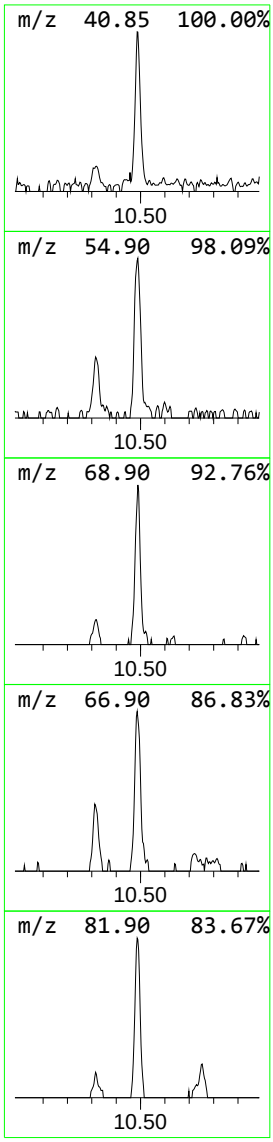
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.486	3.54 ug/L	46641	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	94
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	93
4	.alpha.-CITRONELLENE	138	C10H18	006874-35-7	50
5	Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	001195-31-9	49





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

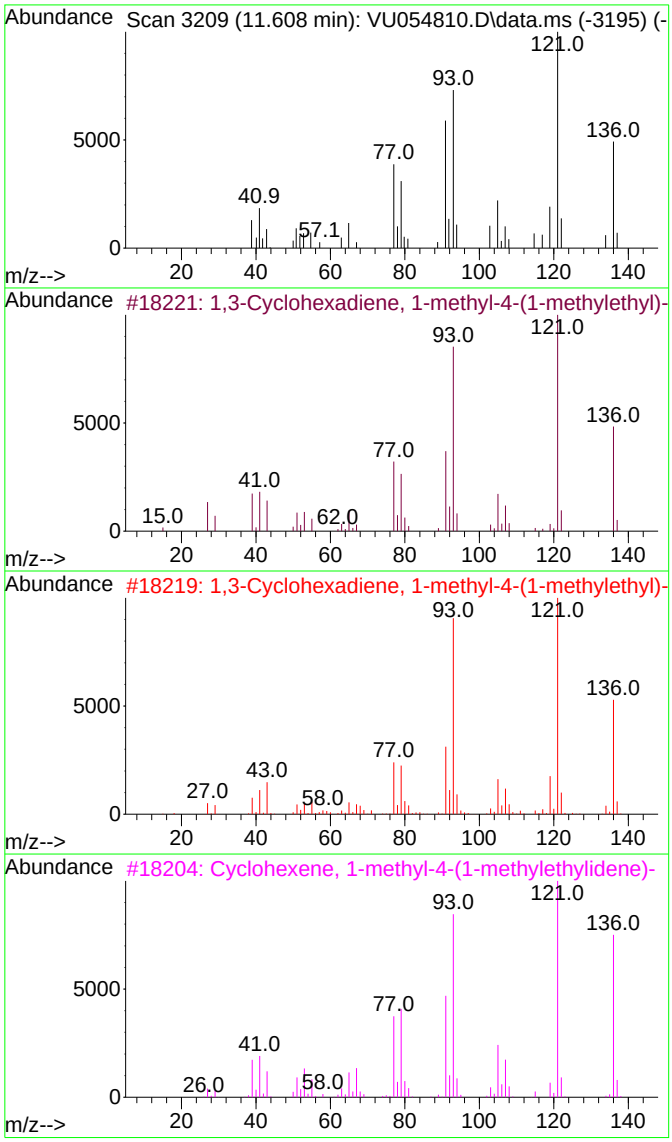
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

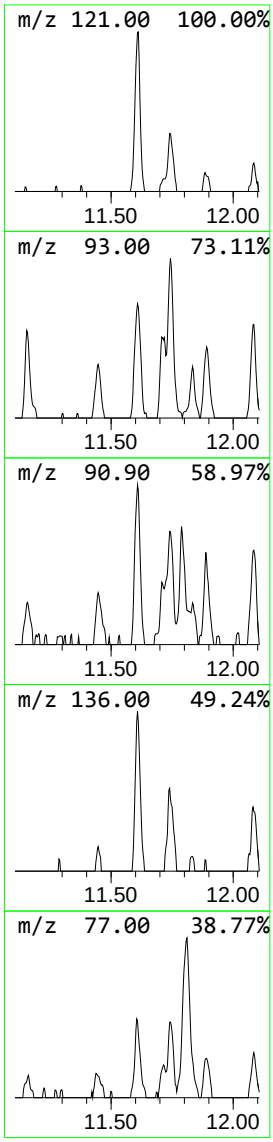
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Cyclohexadiene, 1-methy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.608	3.05 ug/L	44278	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	97
2	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	95
3	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	87
4	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	87
5	Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
Acq On : 18 Jul 2023 16:23
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

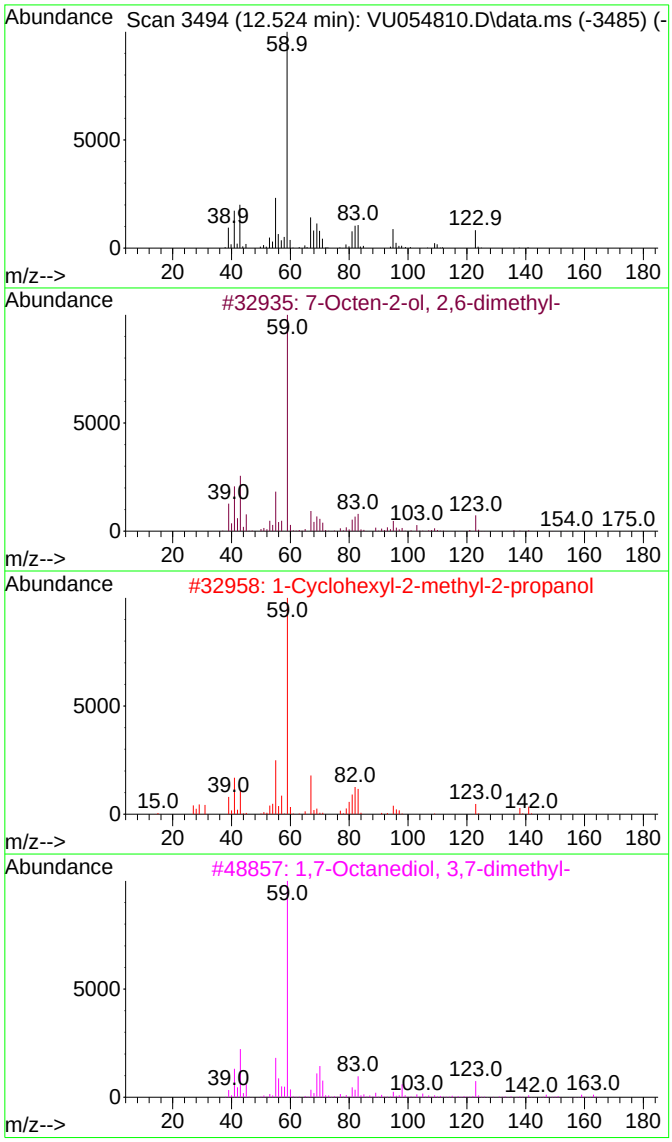
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

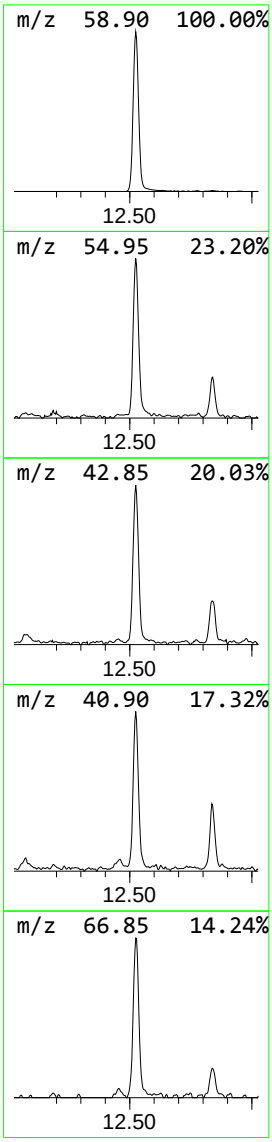
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.525	19.25 ug/L	279411	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
2	1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	72
3	1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	64
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	64
5	3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-96-4	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
Acq On : 18 Jul 2023 16:23
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

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

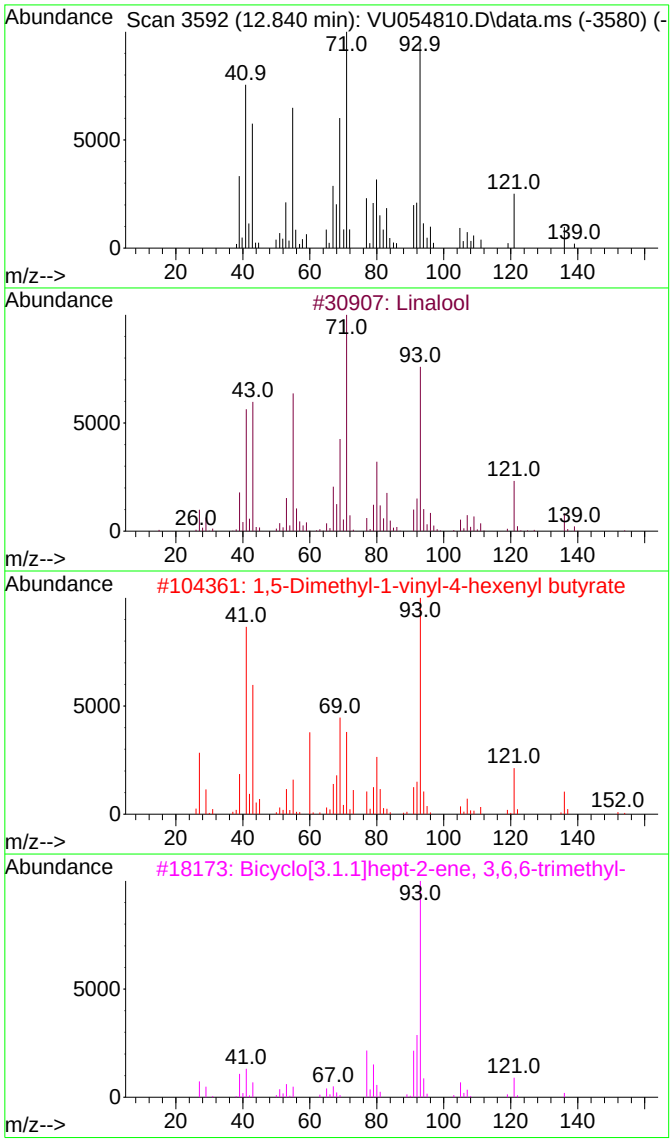
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

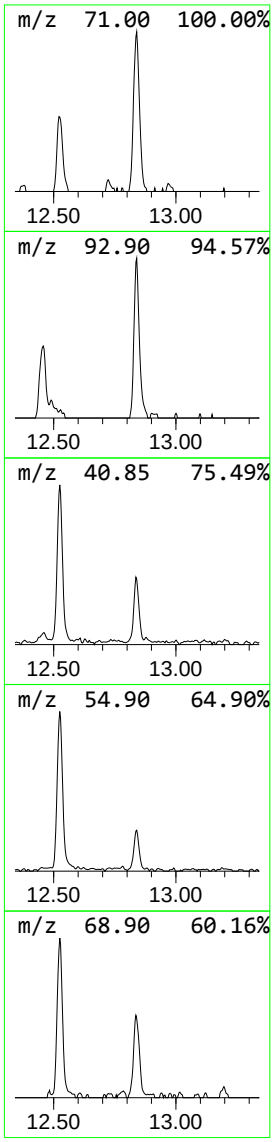
****

Peak Number 7 Linalool Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.840	5.49 ug/L	79676	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Linalool	154	C10H18O	000078-70-6	64
2	1,5-Dimethyl-1-vinyl-4-hexenyl b...	224	C14H24O2	000078-36-4	52
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	50
4	(+)-3-Carene	136	C10H16	000498-15-7	49
5	3-Carene	136	C10H16	013466-78-9	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
Acq On : 18 Jul 2023 16:23
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

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

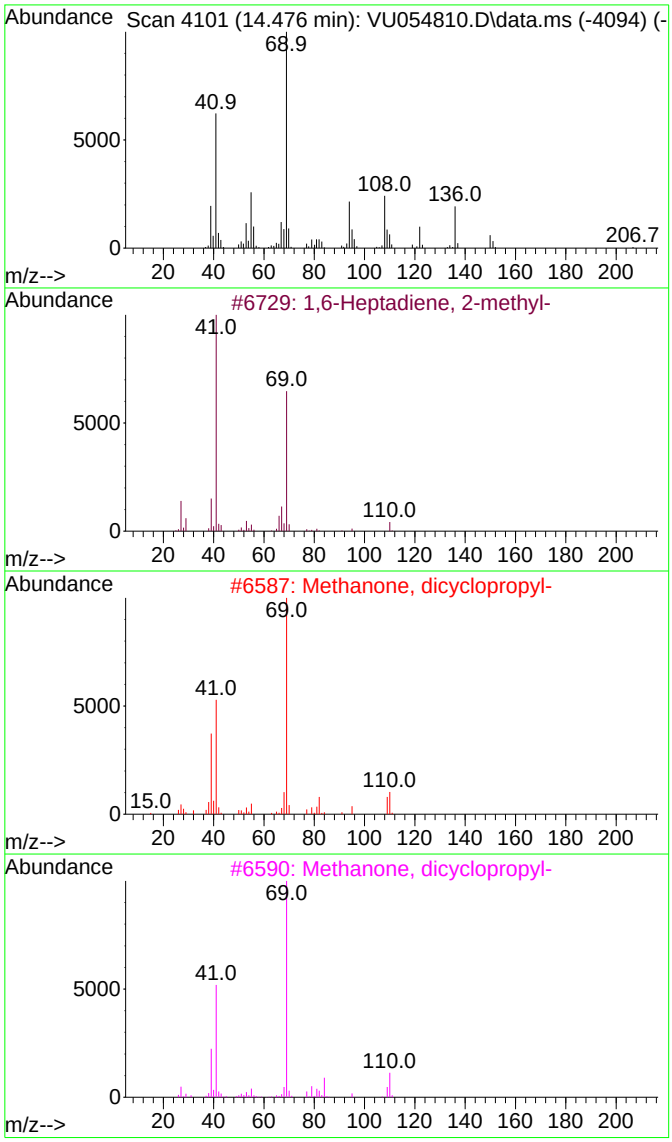
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

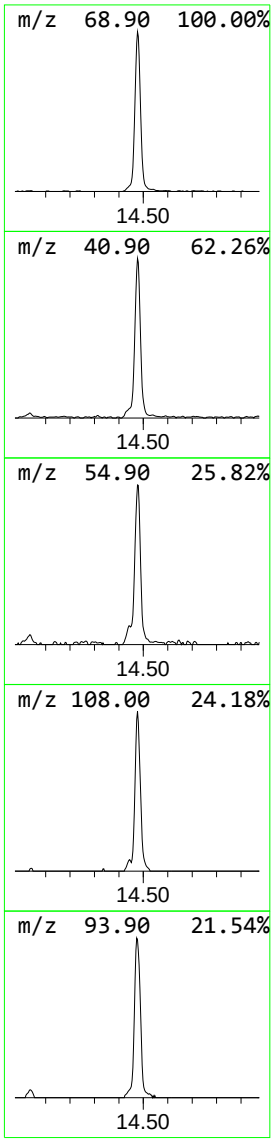
****

Peak Number 8 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.476	17.73 ug/L	257465	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Heptadiene, 2-methyl-	110	C8H14	013643-06-6	38
2	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38
3	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38
4	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054810.D
Acq On : 18 Jul 2023 16:23
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

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	15.0	ug/L	154816	1	6.245	516012	50.0
2-Butanone, 3,3...	7.158	20.2	ug/L	208894	1	6.245	516012	50.0
R(-)3,7-Dimethy...	10.486	3.5	ug/L	46641	2	9.415	658631	50.0
1,3-Cyclohexadi...	11.608	3.0	ug/L	44278	3	11.807	725871	50.0
7-Octen-2-ol, 2...	12.525	19.3	ug/L	279411	3	11.807	725871	50.0
Linalool	12.840	5.5	ug/L	79676	3	11.807	725871	50.0
unknown-01	14.476	17.7	ug/L	257465	3	11.807	725871	50.0