LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 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: VU054805.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	110	rBV	92133	121590	15.48%	1.566%
2	2.554	383	393	405	rVB	143573	228371	29.08%	2.941%
3	2.769	457	460	464	rBV5	1684	1631	0.21%	0.021%
4	2.940	509	513	517	rBV3	531	432	0.06%	0.006%
5	3.033	537	542	547	rBV5	1839	2752	0.35%	0.035%
6	3.190	578	591	613	rVB2	49990	136385	17.37%	1.756%
7	3.470	675	678	680	rBV4	642	489	0.06%	0.006%
8	3.544	697	701	704	rVB4	423	254	0.03%	0.003%
9	3.592	714	716	718	rBV2	653	333	0.04%	0.004%
10	3.673	738	741	743	rBV3	571	372	0.05%	0.005%
11	3.785	771	776	780	rVB5	629	556	0.07%	0.007%
12	3.808	780	783	787	rBV2	632	456	0.06%	0.006%
13	3.933	819	822	825	rBV2	620	416	0.05%	0.005%
14	3.991	837	840	842	rBV	474	377	0.05%	0.005%
15	4.052	854	859	863	rBV3	1051	908	0.12%	0.012%
16	4.113	872	878	882	rVB5	508	638	0.08%	0.008%
17	4.145	882	888	890	rBV3	500	339	0.04%	0.004%
18	4.158	890	892	898	rBV3	354	240	0.03%	0.003%
19	4.213	905	909	910	rBV2	511	404	0.05%	0.005%
20	4.223	910	912	915	rVB3	432	223	0.03%	0.003%
21	4.412	965	971	972	rBV2	510	371	0.05%	0.005%
22	4.464	984	987	990	rBV3	739	594	0.08%	0.008%
23	4.570	1017	1020	1021	rBV	442	293	0.04%	0.004%
24	4.618	1024	1035	1055	rBV	70820	174464	22.22%	2.247%
25	4.923	1128	1130	1132	rBV2	394	233	0.03%	0.003%
26	5.055	1156	1171	1196	rBV	144432	326299	41.55%	4.202%
27	5.325	1250	1255	1258	rBV4	549	589	0.08%	0.008%
28	5.348	1260	1262	1264	rBV3	351	230	0.03%	0.003%
29	5.496	1303	1308	1309	rBV2	510	345	0.04%	0.004%
30	5.567	1327	1330	1333	rVB3	520	380	0.05%	0.005%
31	5.631	1348	1350	1355	rBV2	409	317	0.04%	0.004%
32	5.718	1356	1377	1401	rBV2	275174	762611	97.11%	9.820%
33	5.975	1453	1457	1458	rBV3	1002	553	0.07%	0.007%
34	5.985	1458	1460	1463	rVV	760	485	0.06%	0.006%
35	6.116	1496	1501	1504	rBV3	822	573	0.07%	0.007%
36	6.139	1505	1508	1511	rVB4	833	561	0.07%	0.007%

LSC Area Percent Report

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Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 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	6.245	1528	1541	1558	rBV	278430	522244	66.50%	6.725%
38	6.464	1606	1609	1612	rBV4	563	345	0.04%	0.004%
39	6.550	1624	1636	1644	rBV9	3268	7273	0.93%	0.094%
40	6.685	1666	1678	1699	rBV	183747	352950	44.95%	4.545%
41	7.071	1797	1798	1801	rBV	410	256	0.03%	0.003%
42	7.161	1813	1826	1850	rBV	97284	196146	24.98%	2.526%
43	7.325	1874	1877	1879	rBV2	399	238	0.03%	0.003%
44	7.563	1938	1951	1968	rBV	109947	195277	24.87%	2.515%
45	7.772	2012	2016	2018	rBV2	941	737	0.09%	0.009%
46	7.894	2040	2054	2071	rBV	366422	638337	81.29%	8.220%
47	8.126	2123	2126	2131	rVB2	559	359	0.05%	0.005%
48	8.177	2131	2142	2161	rBV2	77492	133730	17.03%	1.722%
49	8.489	2226	2239	2249	rBV4	5704	11628	1.48%	0.150%
50	8.631	2273	2283	2298	rBV	225697	415100	52.86%	5.345%
51	8.904	2363	2368	2369	rBV2	792	651	0.08%	0.008%
52	9.013	2400	2402	2408	rVB4	1079	1024	0.13%	0.013%
53	9.058	2408	2416	2418	rBV4	1053	965	0.12%	0.012%
54	9.107	2428	2431	2434	rVB3	775	428	0.05%	0.006%
55	9.126	2434	2437	2438	rBV	487	248	0.03%	0.003%
56	9.181	2452	2454	2456	rBV2	499	302	0.04%	0.004%
57	9.415	2514	2527	2548	rBV	398069	674918	85.95%	8.691%
58	9.550	2565	2569	2571	rBV4	623	434	0.06%	0.006%
59	9.566	2571	2574	2575	rBV2	892	590	0.08%	0.008%
60	9.656	2600	2602	2605	rVV3	542	353	0.04%	0.005%
61	9.766	2631	2636	2641	rBV4	594	692	0.09%	0.009%
62	9.795	2643	2645	2651	rVV3	385	445	0.06%	0.006%
63	9.849	2660	2662	2664	rBV2	434	227	0.03%	0.003%
64	9.923	2679	2685	2686	rBV3	582	543	0.07%	0.007%
65	9.978	2699	2702	2709	rVB4	586	703	0.09%	0.009%
66	10.065	2727	2729	2732	rVB2	347	181	0.02%	0.002%
67	10.103	2733	2741	2742	rBV4	1692	1648	0.21%	0.021%
68	10.187	2764	2767	2768	rBV	446	273	0.03%	0.004%
69	10.261	2787	2790	2794	rBV4	612	553	0.07%	0.007%
70	10.280	2794	2796	2797	rBV	612	247	0.03%	0.003%
71	10.316	2798	2807	2816	rVV8	6967	11522	1.47%	0.148%
72	10.396	2830	2832	2834	rBV2	335	224	0.03%	0.003%
73	10.444	2843	2847	2851	rBV4	770	717	0.09%	0.009%
74	10.486	2851	2860	2874	rBV4	23498	39654	5.05%	0.511%
75	10.644	2907	2909	2913	rBV3	409	310	0.04%	0.004%
76	10.663	2913	2915	2916	rBV	583	251	0.03%	0.003%

LSC Area Percent Report

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Acq On : 18 Jul 2023 14:19
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 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	10.753	2932	2943	2958	rBV	312067	507742	64.66%	6.538%
78	10.872	2977	2980	2981	rBV	633	283	0.04%	0.004%
79	11.158	3060	3069	3079	rBV4	9186	13677	1.74%	0.176%
80	11.251	3096	3098	3101	rVB	641	242	0.03%	0.003%
81	11.293	3106	3111	3121	rVB6	3827	5279	0.67%	0.068%
82	11.412	3144	3148	3152	rBV4	489	427	0.05%	0.005%
83	11.457	3153	3162	3165	rBV3	3313	5355	0.68%	0.069%
84	11.518	3178	3181	3184	rBV2	473	287	0.04%	0.004%
85	11.608	3201	3209	3217	rBV4	17929	28632	3.65%	0.369%
86	11.743	3234	3251	3259	rBV2	37715	68543	8.73%	0.883%
87	11.811	3260	3272	3290	rVB	482188	785287	100.00%	10.113%
88	12.084	3346	3357	3366	rBV7	11672	20826	2.65%	0.268%
89	12.190	3375	3390	3406	rBV	414935	674013	85.83%	8.680%
90	12.457	3464	3473	3480	rBV4	18326	27027	3.44%	0.348%
91	12.524	3486	3494	3514	rVB	165967	257448	32.78%	3.315%
92	12.840	3583	3592	3607	rBV2	44175	69673	8.87%	0.897%
93	13.196	3696	3703	3707	rBV8	2154	3284	0.42%	0.042%
94	13.666	3847	3849	3852	rVB2	951	519	0.07%	0.007%
95	13.846	3897	3905	3916	rVV2	6099	10796	1.37%	0.139%
96	13.897	3919	3921	3924	rVB	695	266	0.03%	0.003%
97	14.032	3955	3963	3974	rBV6	17505	29535	3.76%	0.380%
98	14.476	4081	4101	4117	rBV	158617	269224	34.28%	3.467%
99	15.692	4473	4479	4489	rBV8	4690	7619	0.97%	0.098%
100	15.878	4535	4537	4540	rBV2	1487	733	0.09%	0.009%

Sum of corrected areas: 7765504

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Data File : VU054805.D
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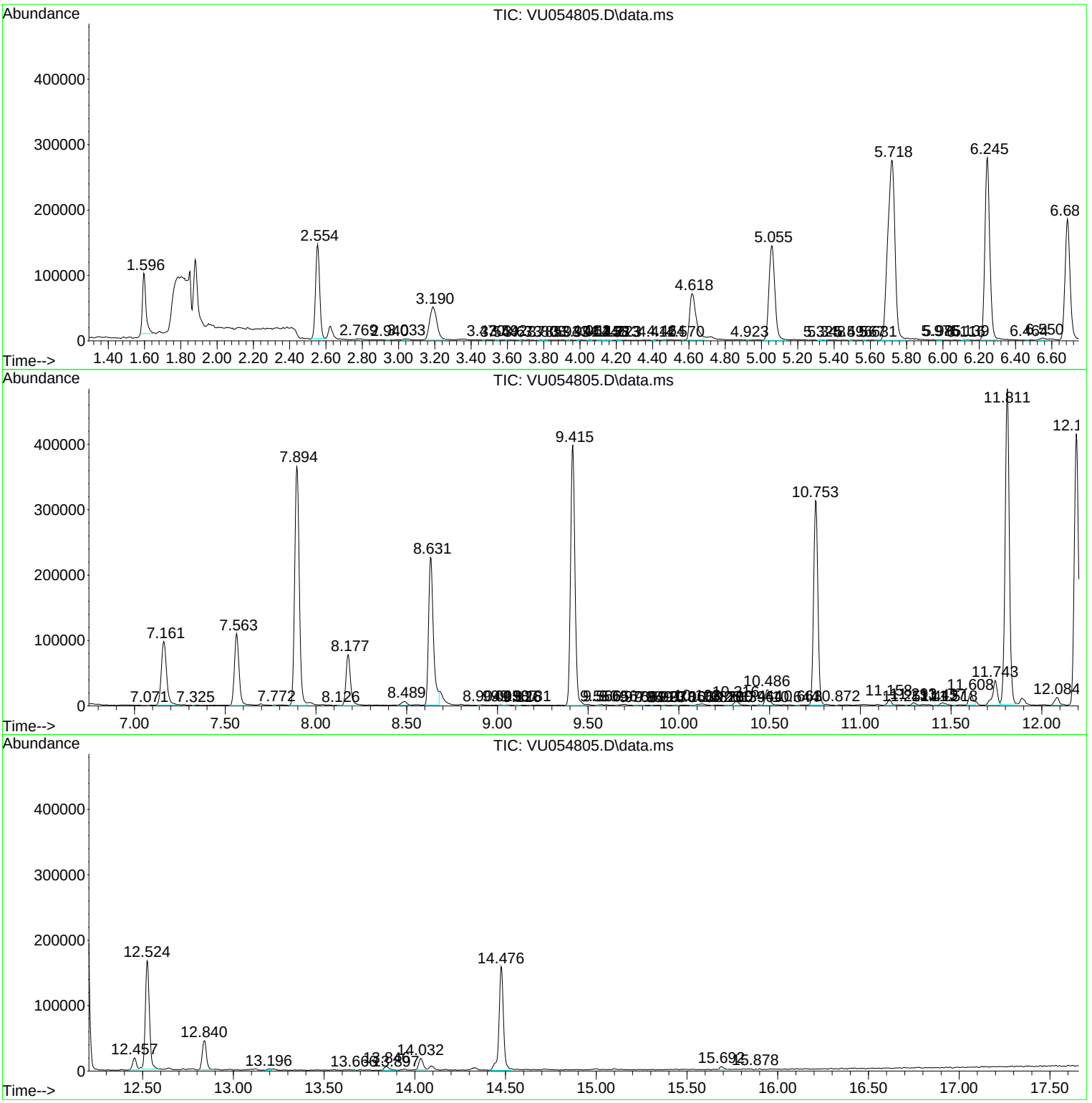
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

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 : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

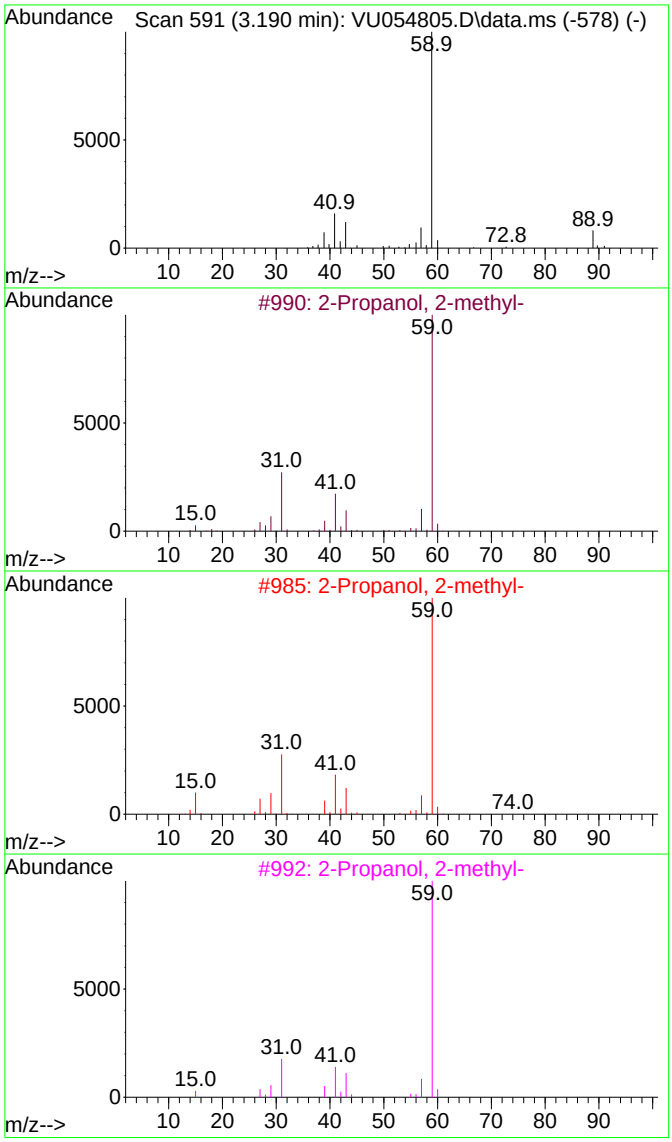
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

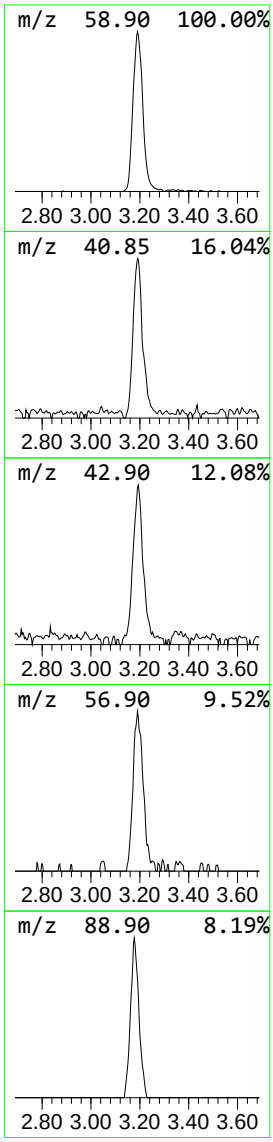
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.190	13.06 ug/L	136385	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	72
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
5	Ethanol, 2-ethoxy-	90	C4H10O2	000110-80-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

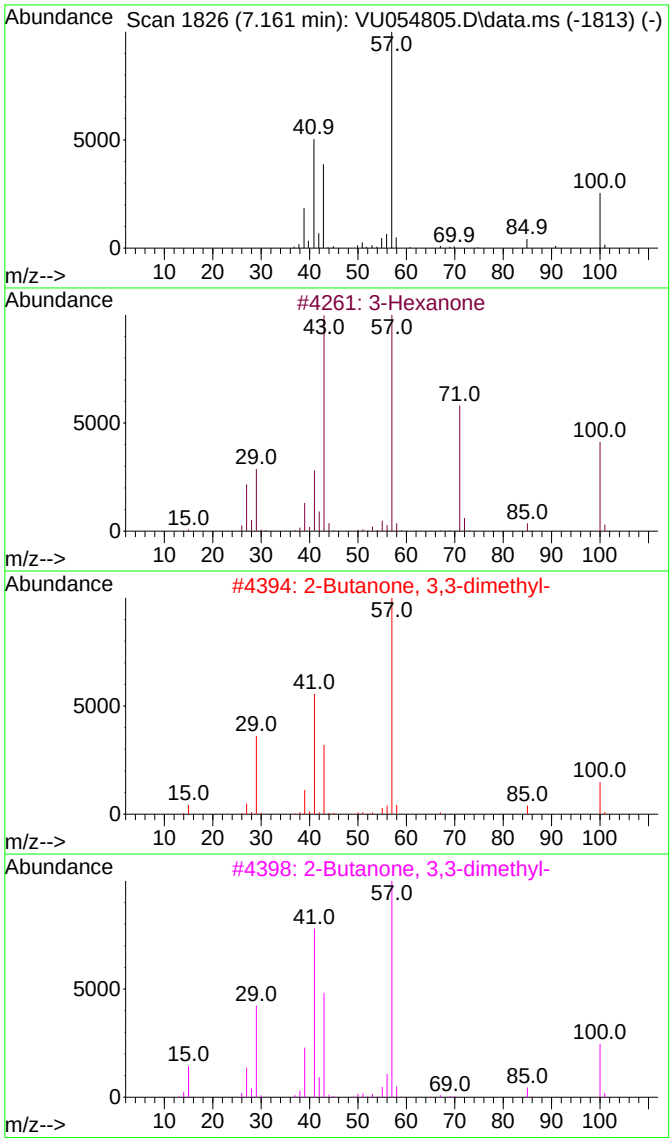
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

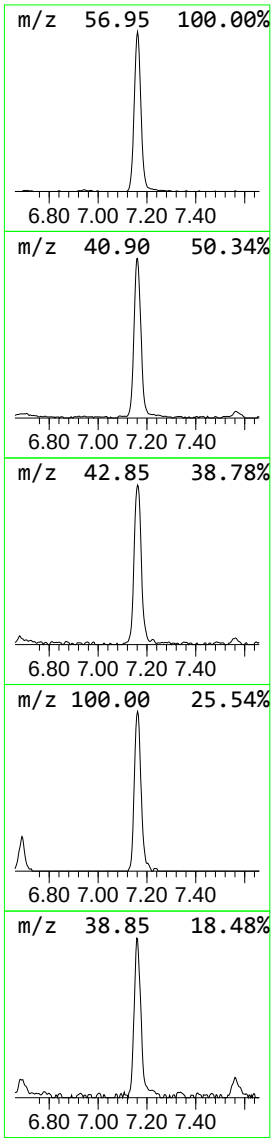
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Hexanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.161	18.78 ug/L	196146	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone	100	C6H12O	000589-38-8	64
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	59
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 : VU054805.D
Acq On : 18 Jul 2023 14:19
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

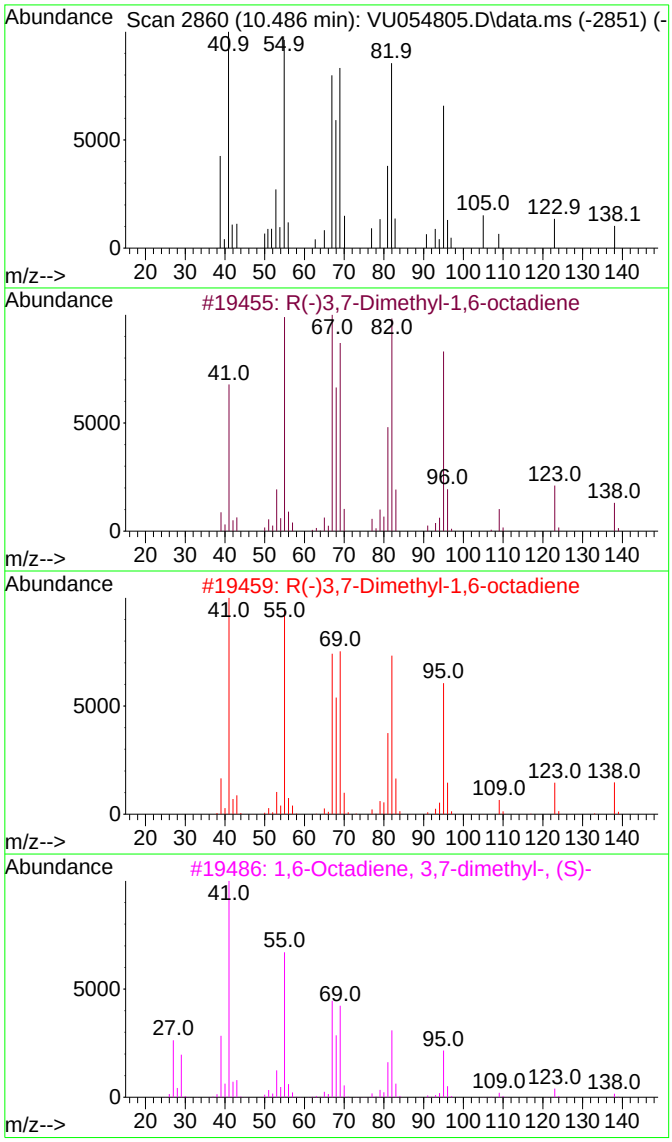
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

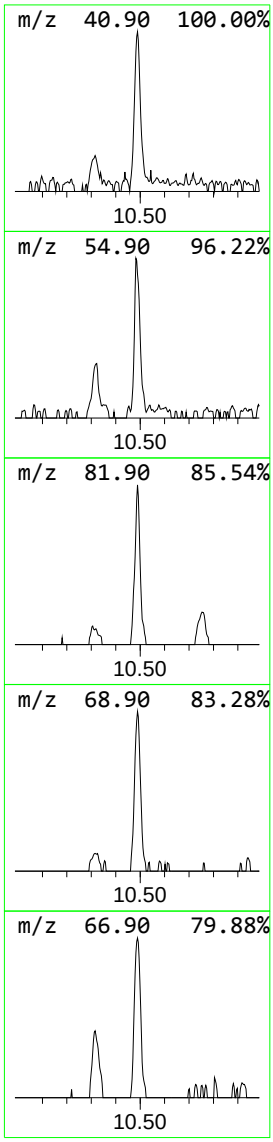
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 R(-)3,7-Dimethyl-1,6-octadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.486	2.94 ug/L	39654	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	96
2	R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	96
3	1,6-Octadiene, 3,7-dimethyl-, (S)-	138	C10H18	010281-55-7	94
4	Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	38
5	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

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

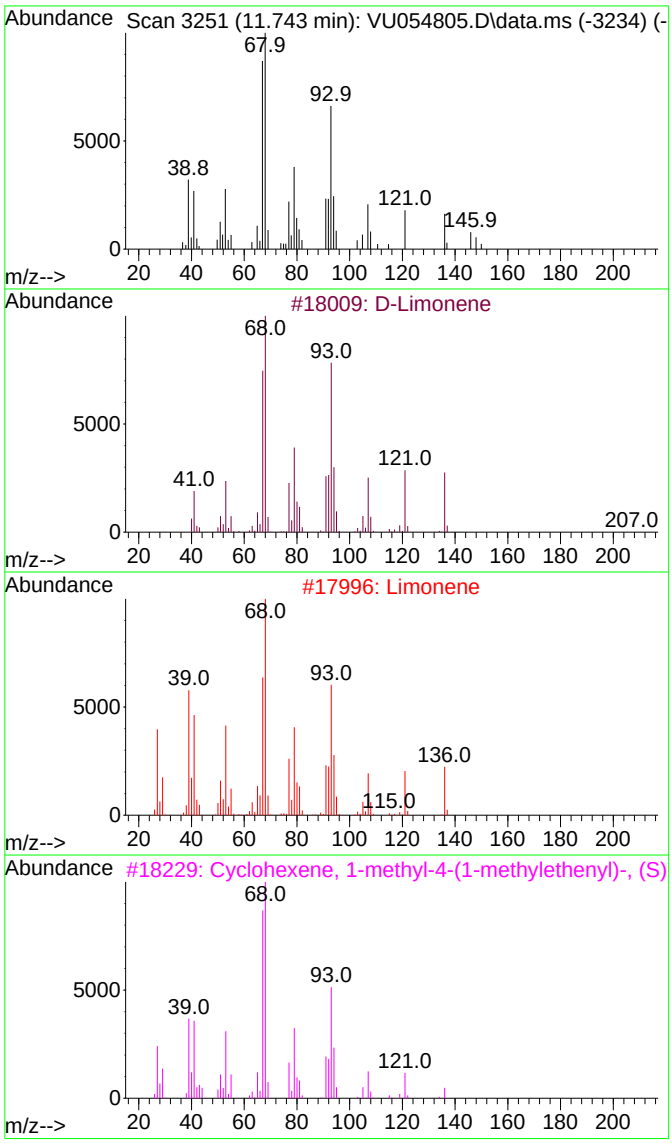
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

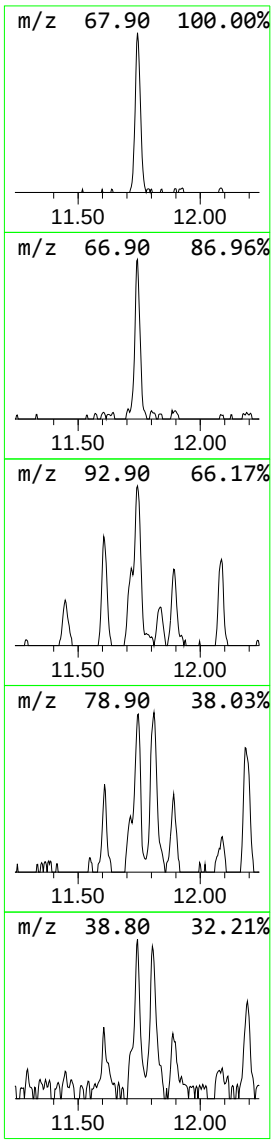
****

Peak Number 5 D-Limonene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.743	4.36 ug/L	68543	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	98
2	Limonene	136	C10H16	000138-86-3	91
3	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	90
4	Limonene	136	C10H16	000138-86-3	89
5	D-Limonene	136	C10H16	005989-27-5	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

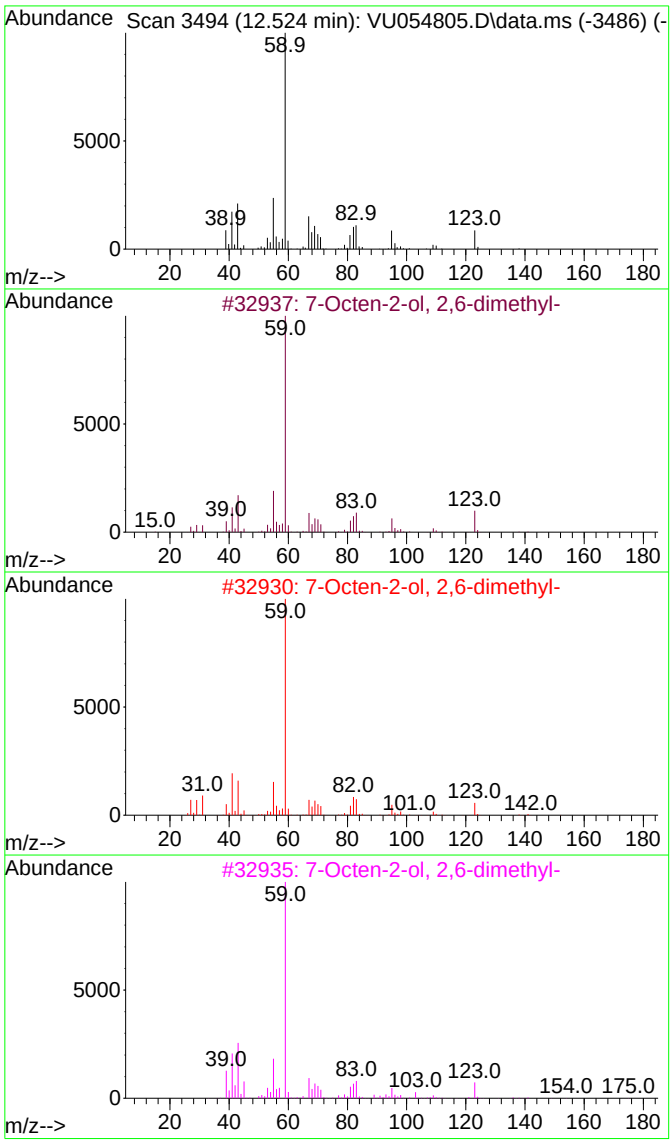
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

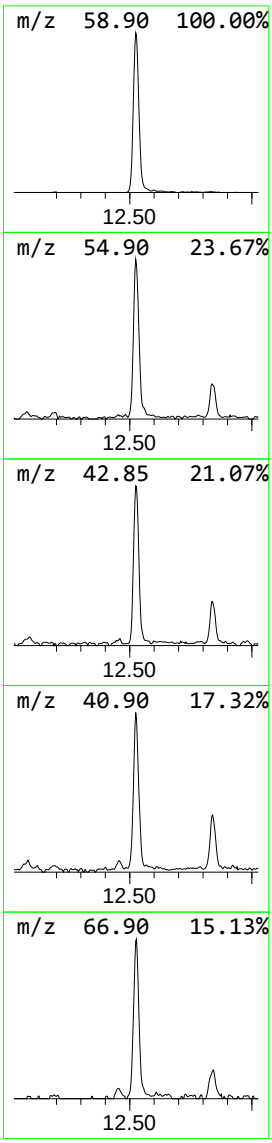
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.525	16.39 ug/L	257448	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	72
3	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
4	3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-96-4	50
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	50





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Data File : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

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

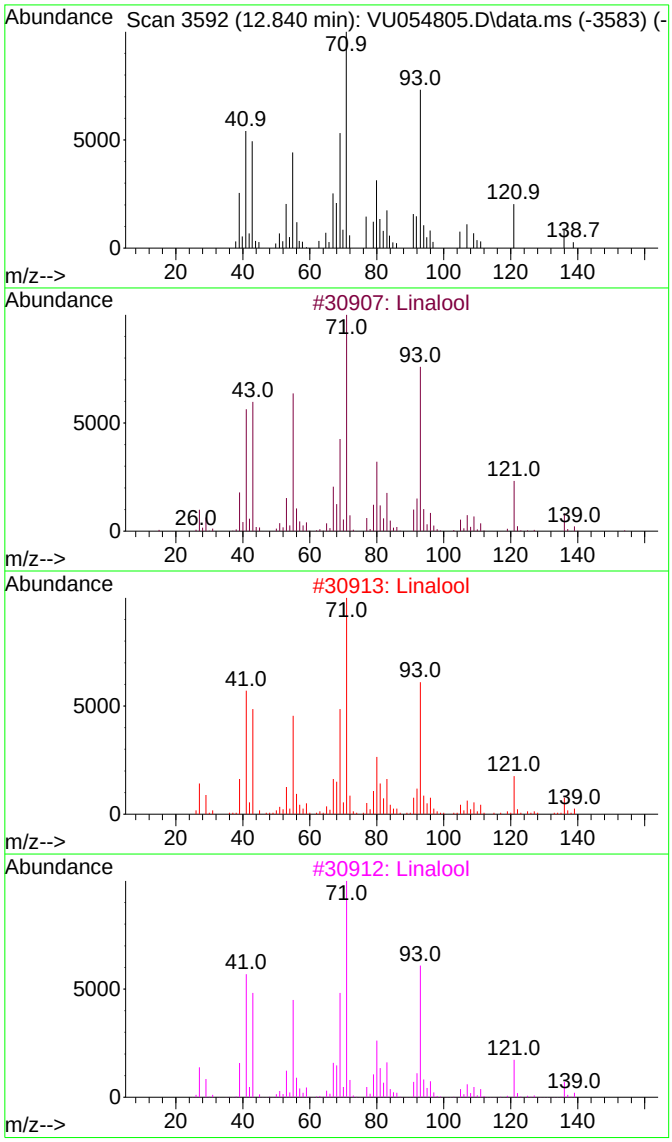
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

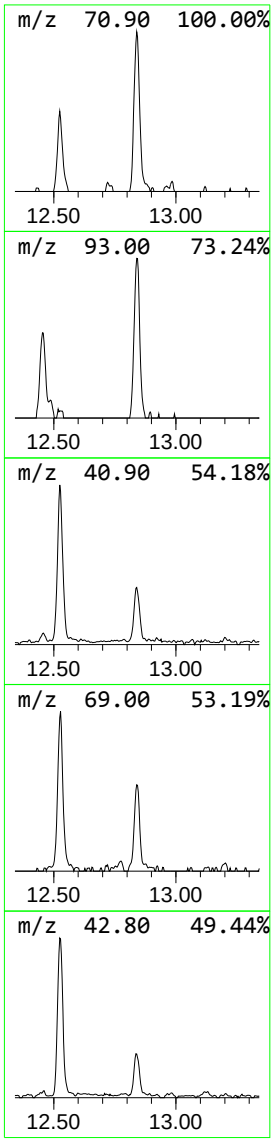
****

Peak Number 7 Linalool Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.840	4.44 ug/L	69673	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Linalool	154	C10H18O	000078-70-6	83
2	Linalool	154	C10H18O	000078-70-6	68
3	Linalool	154	C10H18O	000078-70-6	68
4	Linalool	154	C10H18O	000078-70-6	64
5	Hexanoic acid, 1-ethenyl-1,5-dim...	252	C16H28O2	007779-23-9	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X8

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

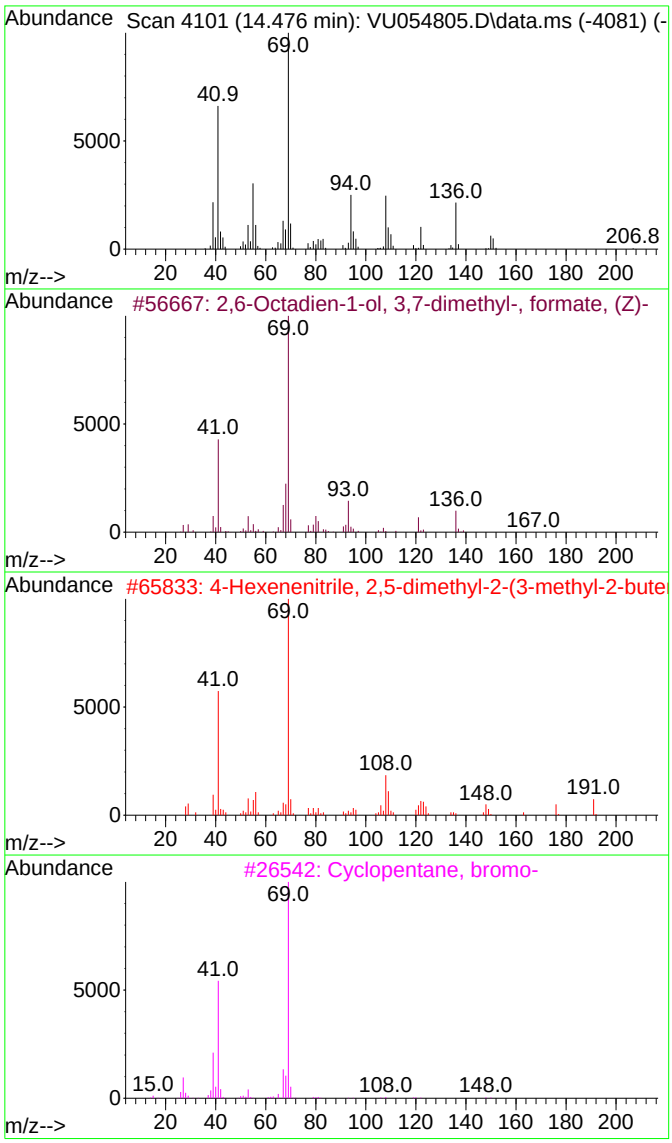
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

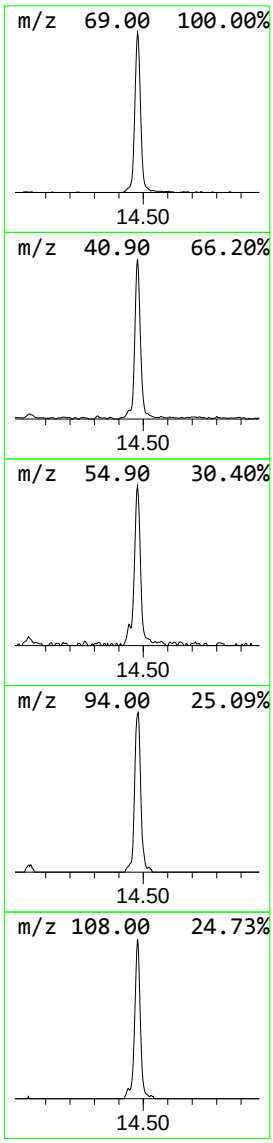
****

Peak Number 8 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.476	17.14 ug/L	269224	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Octadien-1-ol, 3,7-dimethyl-...	182	C11H18O2	002142-94-1	43
2	4-Hexenenitrile, 2,5-dimethyl-2-...	191	C13H21N	069340-56-3	40
3	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	38
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	38
5	Pentane, 1,5-dibromo-	228	C5H10Br2	000111-24-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054805.D
Acq On : 18 Jul 2023 14:19
Operator : MD/SY
Sample : 03656-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 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...	3.190	13.1	ug/L	136385	1	6.245	522244	50.0
3-Hexanone	7.161	18.8	ug/L	196146	1	6.245	522244	50.0
R(-)3,7-Dimethy...	10.486	2.9	ug/L	39654	2	9.415	674918	50.0
D-Limonene	11.743	4.4	ug/L	68543	3	11.811	785287	50.0
7-Octen-2-ol, 2...	12.525	16.4	ug/L	257448	3	11.811	785287	50.0
Linalool	12.840	4.4	ug/L	69673	3	11.811	785287	50.0
unknown-01	14.476	17.1	ug/L	269224	3	11.811	785287	50.0