LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

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\SFAMULM051421WMA.M
Title : VOC Analysis

Signal : TIC: VU043730.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	12	rBV3	5775	5315	0.02%	0.009%
2	1.604	74	82	98	rVB2	294013	334267	1.42%	0.581%
3	1.912	170	178	197	rVB2	181461	284515	1.21%	0.494%
4	2.578	370	385	399	rBV3	650403	1289208	5.47%	2.240%
5	2.761	432	442	450	rBV	7561	14275	0.06%	0.025%
6	2.941	495	498	500	rBV	657	493	0.00%	0.001%
7	3.054	525	533	541	rBV7	2195	4212	0.02%	0.007%
8	3.179	557	572	590	rBV	68092	153488	0.65%	0.267%
9	3.285	601	605	610	rVB4	518	468	0.00%	0.001%
10	3.359	617	628	641	rVB3	8682	17173	0.07%	0.030%
11	3.877	766	789	812	rBV	2271680	5400129	22.91%	9.384%
12	4.002	815	828	848	rVB	68053	175992	0.75%	0.306%
13	4.542	985	996	999	rBV4	2324	3723	0.02%	0.006%
14	4.626	1008	1022	1032	rBV	211595	497273	2.11%	0.864%
15	4.813	1072	1080	1093	rVB3	7040	15874	0.07%	0.028%
16	5.073	1143	1161	1180	rBV	332986	732364	3.11%	1.273%
17	5.327	1217	1240	1273	rBV	10471932	23572143	100.00%	40.963%
18	5.732	1346	1366	1415	rVB2	712308	2015113	8.55%	3.502%
19	6.256	1514	1529	1548	rBV	476657	900607	3.82%	1.565%
20	6.555	1605	1622	1625	rBV9	8498	18287	0.08%	0.032%
21	6.700	1649	1667	1684	rBV	437281	841155	3.57%	1.462%
22	6.922	1720	1736	1762	rBV	294021	587440	2.49%	1.021%
23	7.256	1831	1840	1849	rBV5	2984	5172	0.02%	0.009%
24	7.346	1854	1868	1898	rBV	227524	435495	1.85%	0.757%
25	7.523	1909	1923	1931	rBV	316083	569405	2.42%	0.990%
26	7.571	1931	1938	1960	rVB	256645	443904	1.88%	0.771%
27	7.719	1970	1984	2005	rVB	279663	518328	2.20%	0.901%
28	7.906	2026	2042	2056	rBV	900478	1523543	6.46%	2.648%
29	7.976	2056	2064	2075	rVB2	33067	56821	0.24%	0.099%
30	8.185	2116	2129	2145	rBV	160882	271160	1.15%	0.471%
31	8.404	2183	2197	2210	rVB5	8067	19128	0.08%	0.033%
32	8.494	2212	2225	2236	rVB3	3580	6435	0.03%	0.011%
33	8.558	2236	2245	2253	rBV6	4857	7616	0.03%	0.013%
34	8.639	2256	2270	2304	rBV	600403	1075279	4.56%	1.869%
35	8.845	2328	2334	2342	rBV7	2838	4158	0.02%	0.007%
36	8.931	2356	2361	2365	rBV6	566	548	0.00%	0.001%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

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\SFAMULM051421WMA.M
Title : VOC Analysis

37	9.047	2383	2397	2405	rBV9	3617	7339	0.03%	0.013%
38	9.140	2417	2426	2434	rVB6	1240	2155	0.01%	0.004%
39	9.182	2434	2439	2440	rBV3	1312	1086	0.00%	0.002%
40	9.282	2466	2470	2473	rVV4	768	743	0.00%	0.001%
41	9.320	2473	2482	2498	rVV3	12750	23589	0.10%	0.041%
42	9.423	2500	2514	2536	rBV	690212	1278060	5.42%	2.221%
43	9.526	2537	2546	2556	rVV3	28194	49435	0.21%	0.086%
44	9.574	2556	2561	2577	rVB7	2559	5107	0.02%	0.009%
45	9.700	2585	2600	2611	rBV4	6415	12241	0.05%	0.021%
46	9.764	2611	2620	2628	rBV4	3291	5178	0.02%	0.009%
47	9.928	2667	2671	2678	rBV2	391	396	0.00%	0.001%
48	9.996	2685	2692	2699	rBV4	1887	2598	0.01%	0.005%
49	10.047	2699	2708	2717	rVV7	1616	2760	0.01%	0.005%
50	10.111	2719	2728	2742	rVB3	6253	11884	0.05%	0.021%
51	10.263	2761	2775	2795	rBV	2248857	4071860	17.27%	7.076%
52	10.552	2856	2865	2875	rBV2	70013	123240	0.52%	0.214%
53	10.764	2915	2931	2942	rBV	614139	1029125	4.37%	1.788%
54	10.899	2957	2973	2981	rBV8	55554	159079	0.67%	0.276%
55	10.944	2982	2987	2995	rVB	60306	80281	0.34%	0.140%
56	11.037	2995	3016	3034	rBV	3068489	5254160	22.29%	9.131%
57	11.124	3035	3043	3051	rBV2	108218	152829	0.65%	0.266%
58	11.198	3060	3066	3073	rVV	76953	101148	0.43%	0.176%
59	11.243	3074	3080	3089	rVB2	60679	86830	0.37%	0.151%
60	11.298	3089	3097	3103	rBV	18576	27674	0.12%	0.048%
61	11.340	3103	3110	3120	rVB2	43075	61197	0.26%	0.106%
62	11.481	3143	3154	3166	rBV7	15758	37679	0.16%	0.065%
63	11.571	3177	3182	3191	rVB7	6849	9252	0.04%	0.016%
64	11.642	3192	3204	3215	rVV7	16807	36278	0.15%	0.063%
65	11.716	3218	3227	3243	rVB6	27702	46378	0.20%	0.081%
66	11.819	3244	3259	3276	rVV	678382	1105708	4.69%	1.921%
67	11.906	3277	3286	3296	rVB3	23228	35477	0.15%	0.062%
68	12.102	3329	3347	3361	rBV3	140565	233330	0.99%	0.405%
69	12.198	3363	3377	3395	rVV	847594	1425602	6.05%	2.477%
70	12.381	3431	3434	3440	rVB6	1164	1181	0.01%	0.002%
71	12.426	3443	3448	3460	rVB6	3154	4535	0.02%	0.008%
72	12.500	3462	3471	3481	rBV7	4734	9572	0.04%	0.017%
73	12.561	3483	3490	3499	rVB10	6521	10629	0.05%	0.018%
74	12.616	3500	3507	3514	rBV2	9522	12478	0.05%	0.022%
75	12.664	3517	3522	3525	rBV5	3919	4597	0.02%	0.008%
76	12.870	3575	3586	3599	rBV2	28914	45877	0.19%	0.080%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

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\SFAMULM051421WMA.M
Title : VOC Analysis

77	12.951	3600	3611	3628	rVB5	26177	56469	0.24%	0.098%
78	13.118	3659	3663	3670	rBV8	3602	4769	0.02%	0.008%
79	13.156	3670	3675	3684	rVB5	5911	8133	0.03%	0.014%
80	13.262	3700	3708	3723	rVV9	17482	37439	0.16%	0.065%
81	13.333	3725	3730	3740	rVB7	3998	5418	0.02%	0.009%
82	13.401	3747	3751	3757	rBV7	861	1111	0.00%	0.002%
83	13.462	3762	3770	3777	rVB7	3085	5010	0.02%	0.009%
84	13.523	3786	3789	3790	rBV2	831	446	0.00%	0.001%
85	13.629	3817	3822	3829	rVB5	1291	1730	0.01%	0.003%
86	13.732	3847	3854	3862	rVV5	3322	4766	0.02%	0.008%
87	13.790	3868	3872	3880	rVB6	1948	2449	0.01%	0.004%
88	13.825	3880	3883	3885	rBV2	548	422	0.00%	0.001%
89	13.848	3885	3890	3896	rBV6	1553	1613	0.01%	0.003%
90	13.918	3898	3912	3915	rBV4	5020	8361	0.04%	0.015%
91	14.060	3952	3956	3957	rBV2	1172	687	0.00%	0.001%
92	14.092	3963	3966	3973	rVB3	2234	2324	0.01%	0.004%
93	14.176	3984	3992	4000	rBV9	8422	12428	0.05%	0.022%
94	14.291	4022	4028	4038	rVB9	2592	3439	0.01%	0.006%
95	14.336	4038	4042	4046	rBV3	1011	1241	0.01%	0.002%
96	14.526	4097	4101	4107	rVB5	987	957	0.00%	0.002%
97	14.774	4170	4178	4184	rVB6	5327	7075	0.03%	0.012%
98	14.815	4187	4191	4200	rVV6	1016	1351	0.01%	0.002%
99	15.031	4253	4258	4269	rVB7	2469	2961	0.01%	0.005%
100	15.426	4374	4381	4391	rVB8	2508	4678	0.02%	0.008%

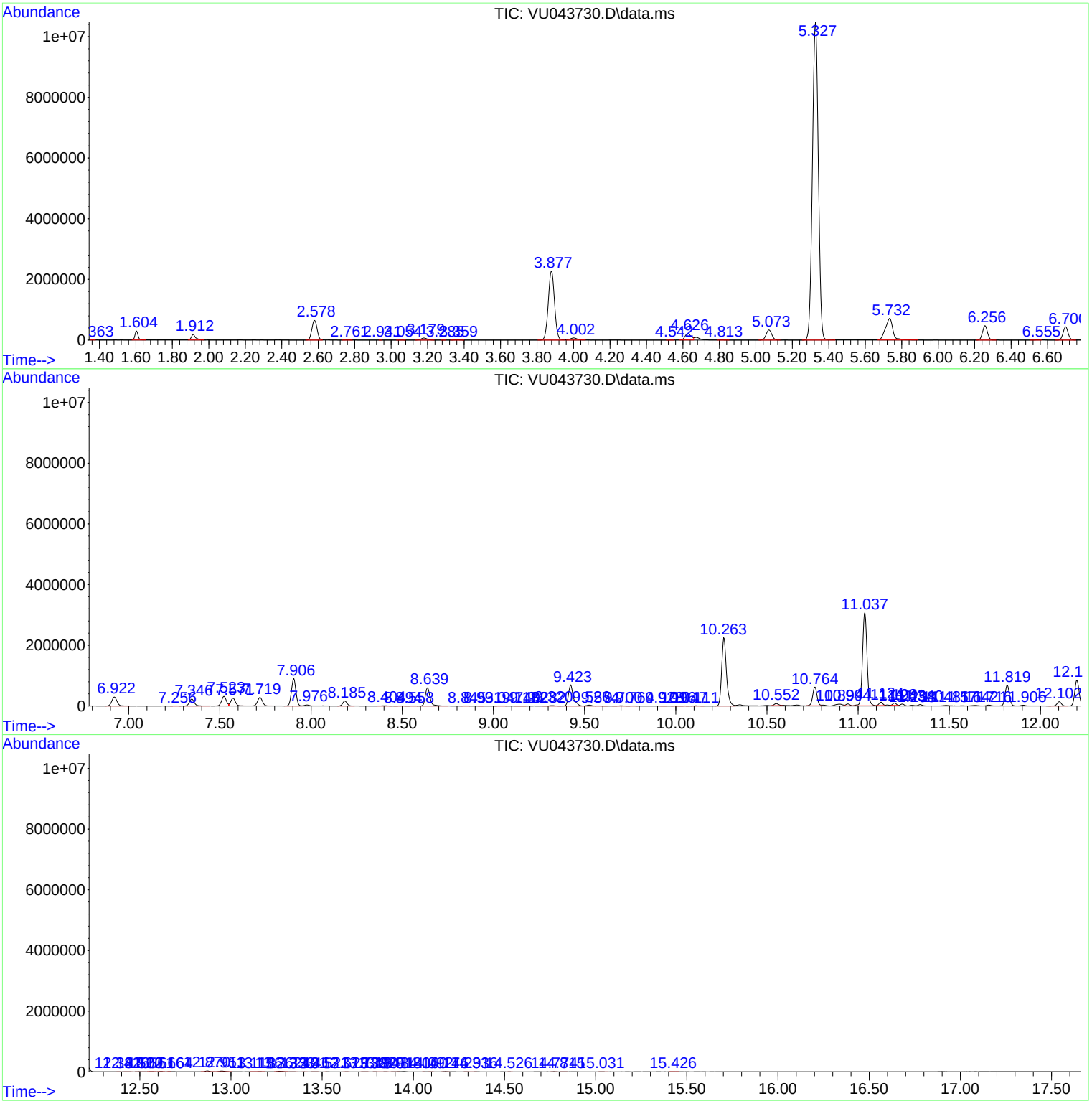
Sum of corrected areas: 57544350

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

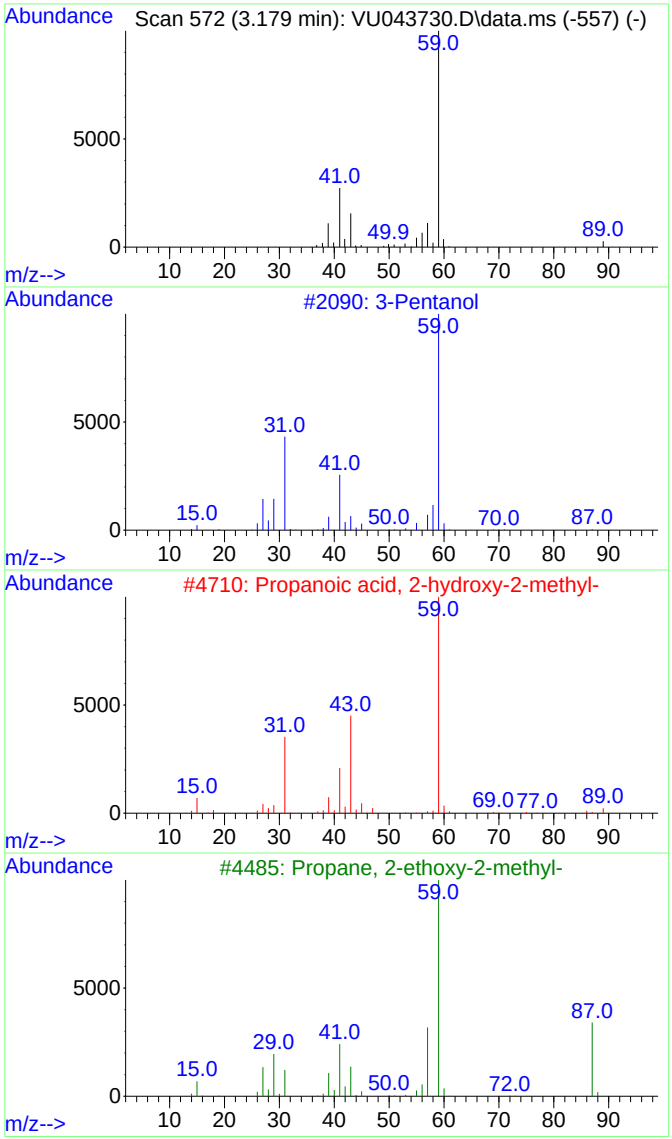
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

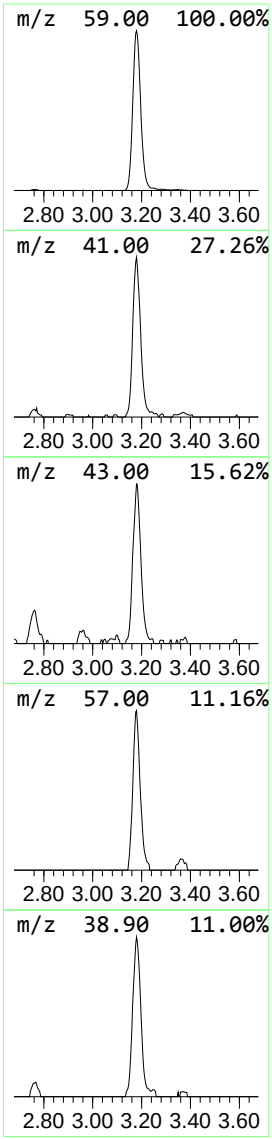
****

Peak Number 1 unknown-01 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.179	8.52 ug/L	153488	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol	88	C5H12O	000584-02-1	40
2	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	39
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	39
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
5	5-Hexyn-3-ol	98	C6H10O	019780-84-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

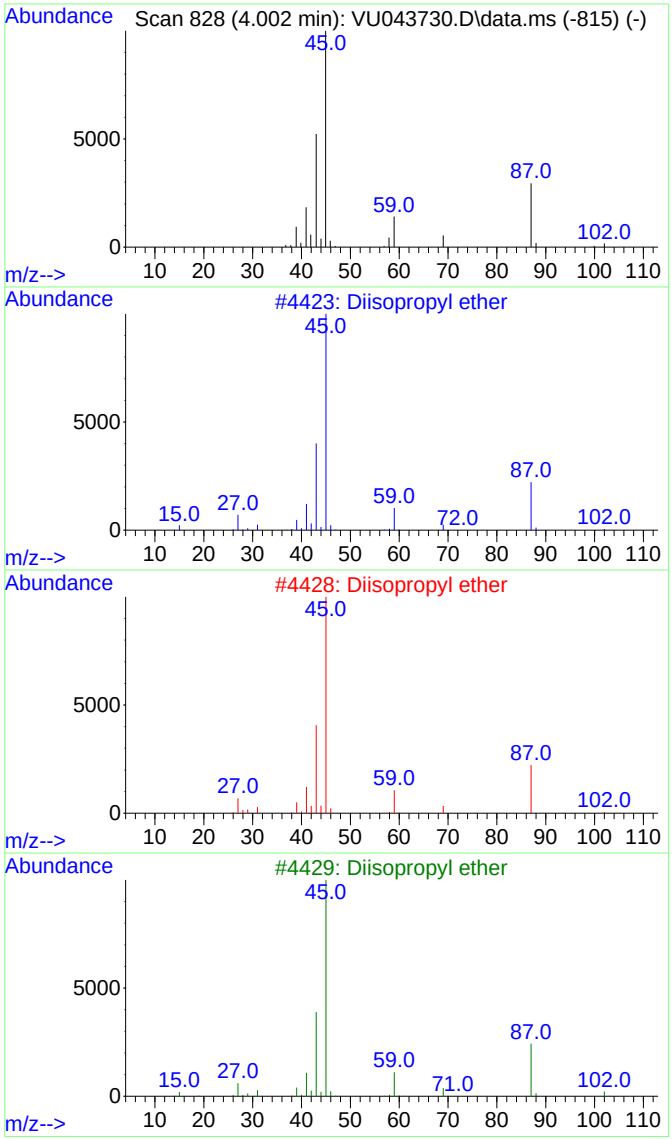
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

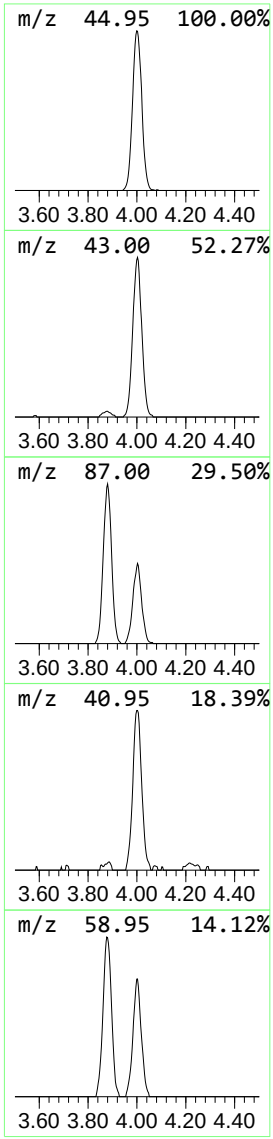
****

Peak Number 2 Diisopropyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.002	9.77 ug/L	175992	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl ether	102	C6H14O	000108-20-3	78
2	Diisopropyl ether	102	C6H14O	000108-20-3	78
3	Diisopropyl ether	102	C6H14O	000108-20-3	72
4	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64
5	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

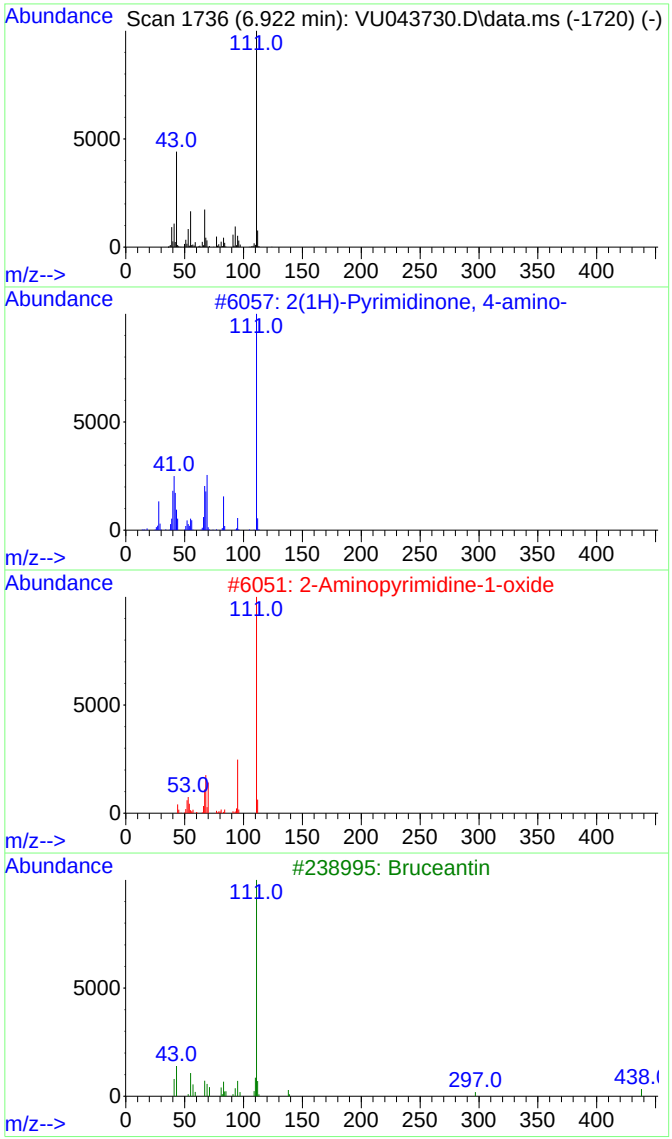
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

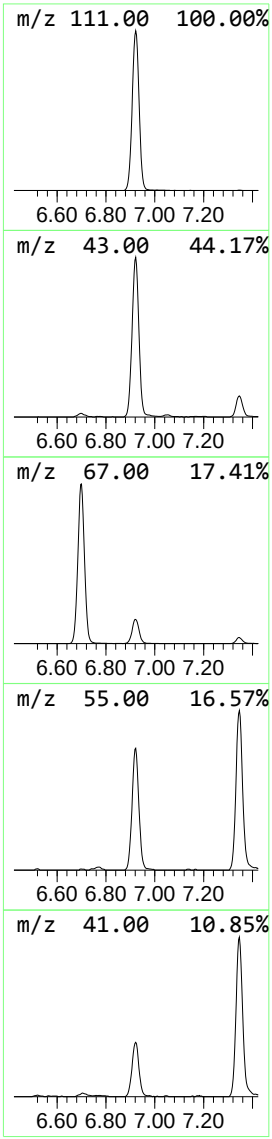
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.922	32.61 ug/L	587440	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	59
3	Bruceantin	548	C28H36O11	041451-75-6	50
4	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	45
5	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

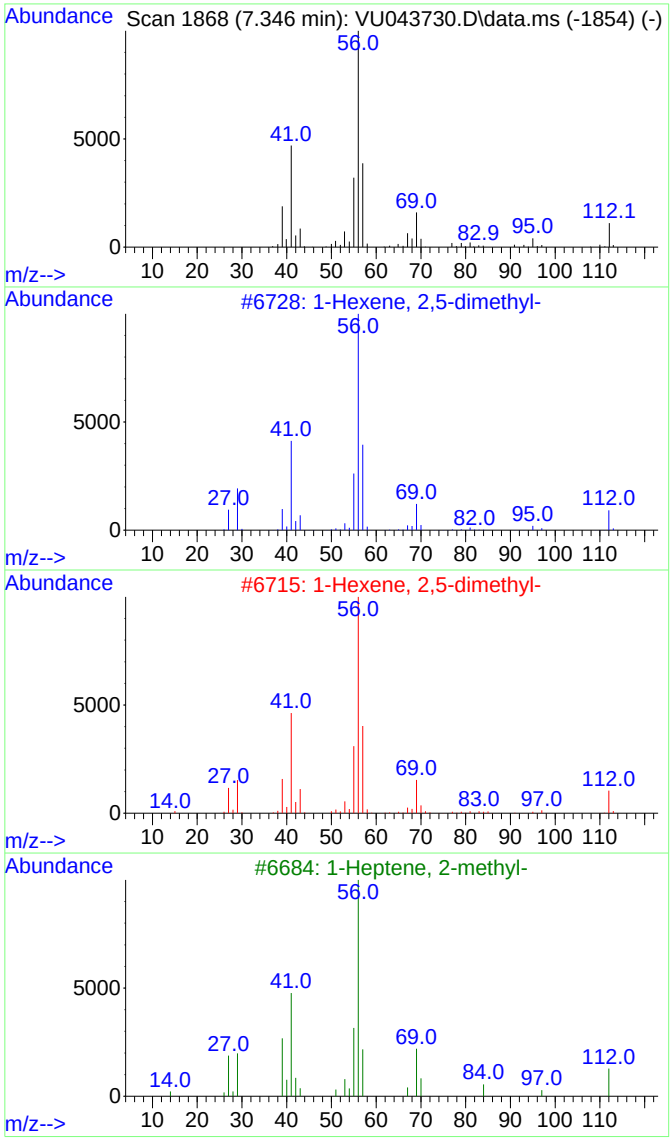
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

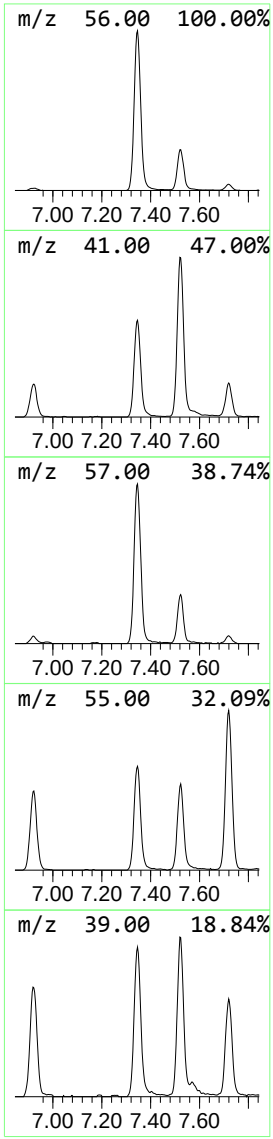
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.346	24.18 ug/L	435495	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	91
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	90
3	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	72
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	64
5	2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

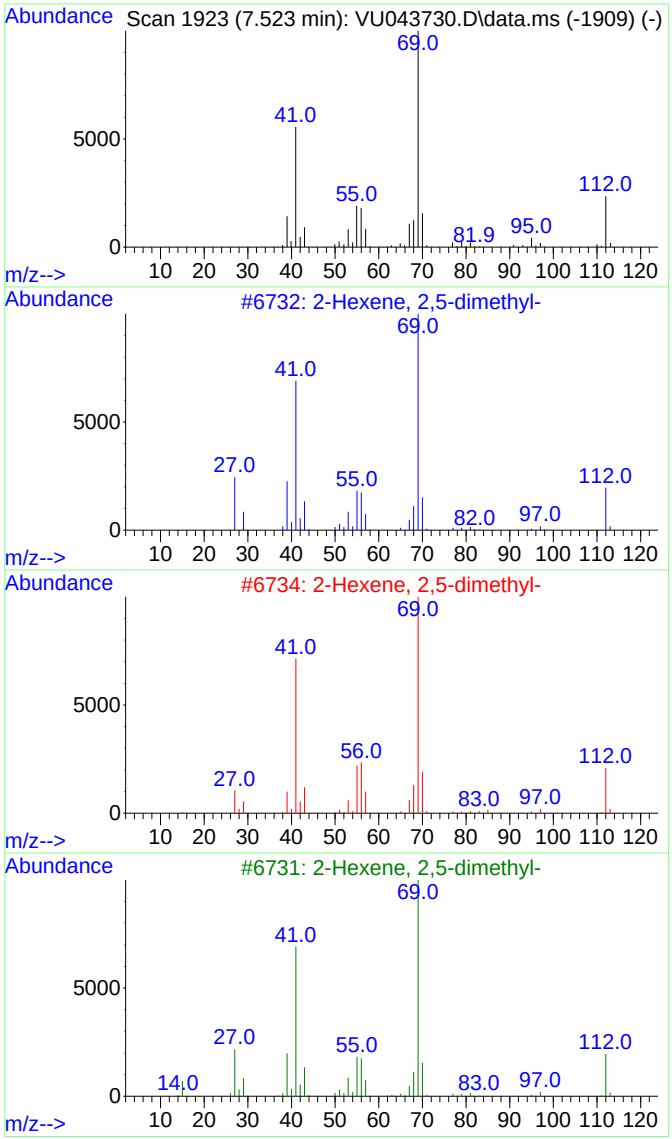
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

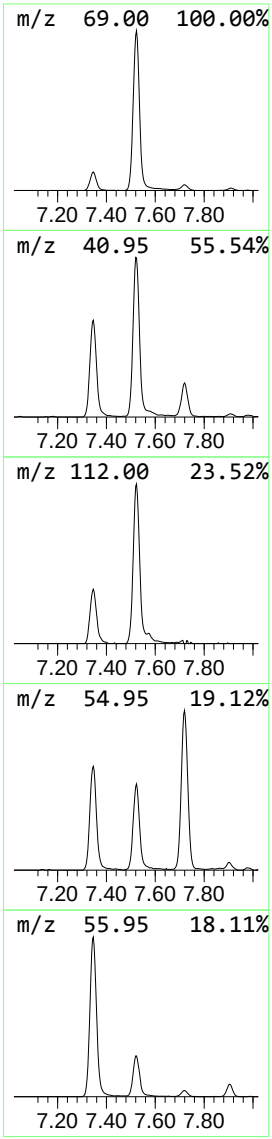
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	31.61 ug/L	569405	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90
2	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90
3	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90
4	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90
5	3-Hexene, 2,5-dimethyl-, (E)-	112	C8H16	000692-70-6	78





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Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

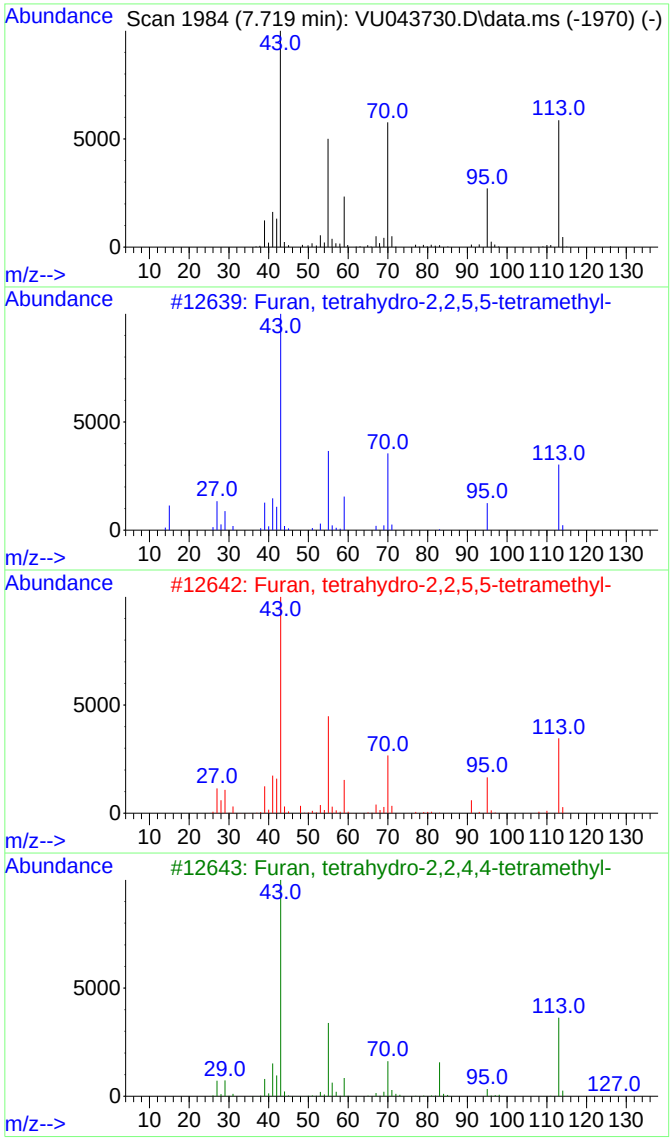
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

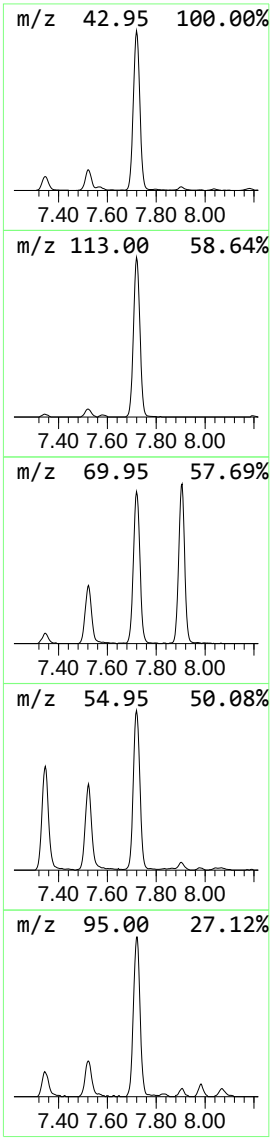
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.719	28.78 ug/L	518328	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	72
3	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
4	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
5	1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	47





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Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

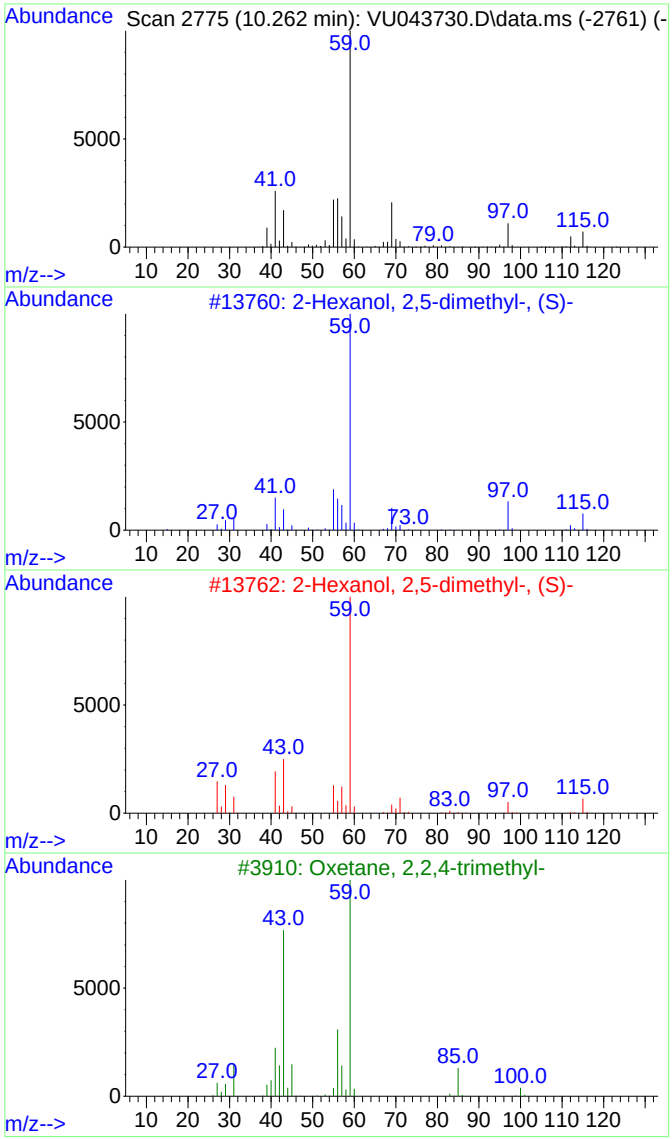
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

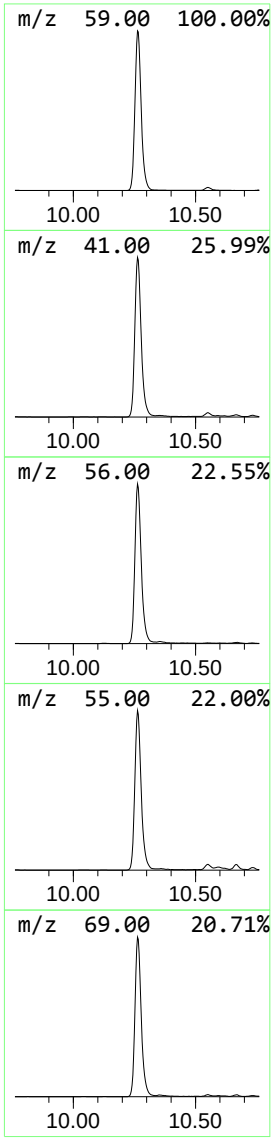
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.262	159.30 ug/L	4071860	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
2	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	64
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	50
4	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	47
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	42





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Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

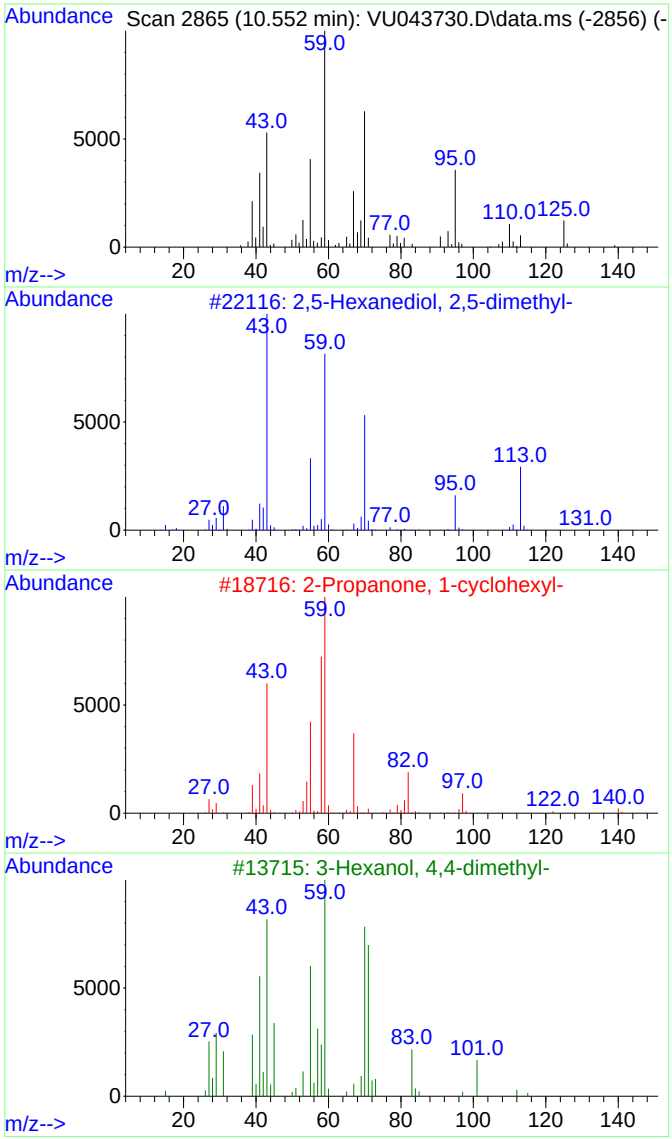
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

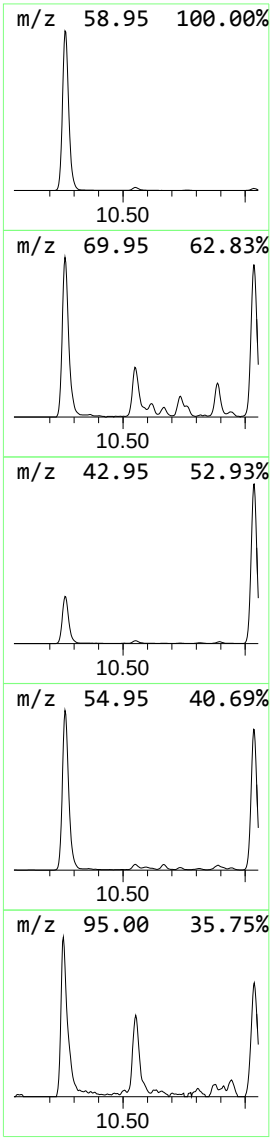
****

Peak Number 9 unknown-02 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.552	4.82 ug/L	123240	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	40
2	2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	32
3	3-Hexanol, 4,4-dimethyl-	130	C8H18O	019550-09-5	28
4	6-Methylheptane-1,6-diol	146	C8H18O2	005392-57-4	25
5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	17





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Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

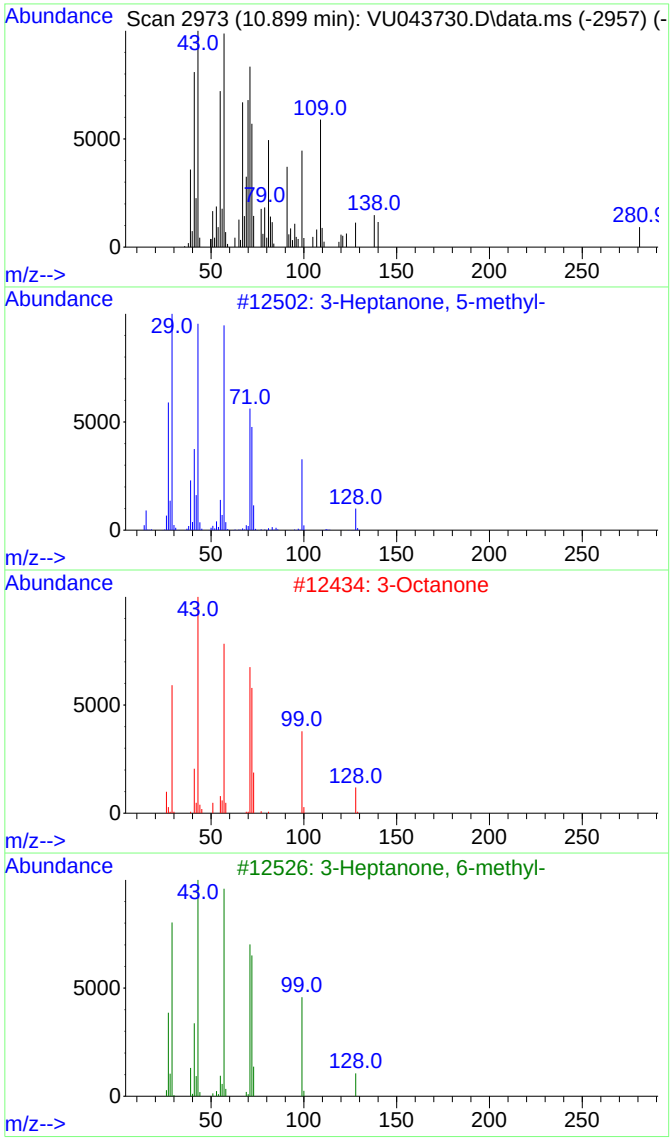
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

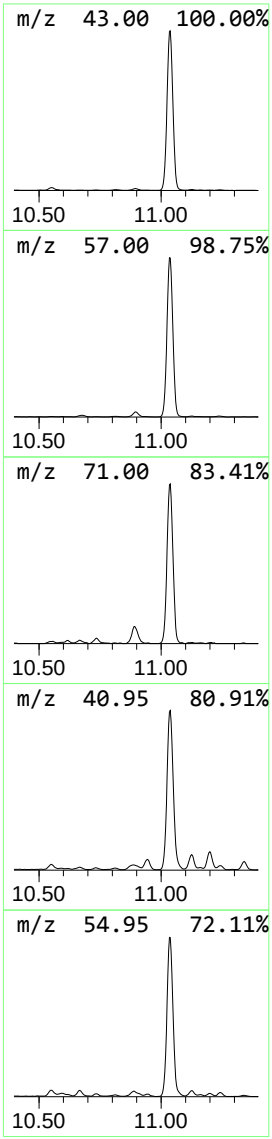
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 3-Heptanone, 5-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.899	7.19 ug/L	159079	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	50
2	3-Octanone	128	C8H16O	000106-68-3	50
3	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	45
4	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	38
5	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	38





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Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

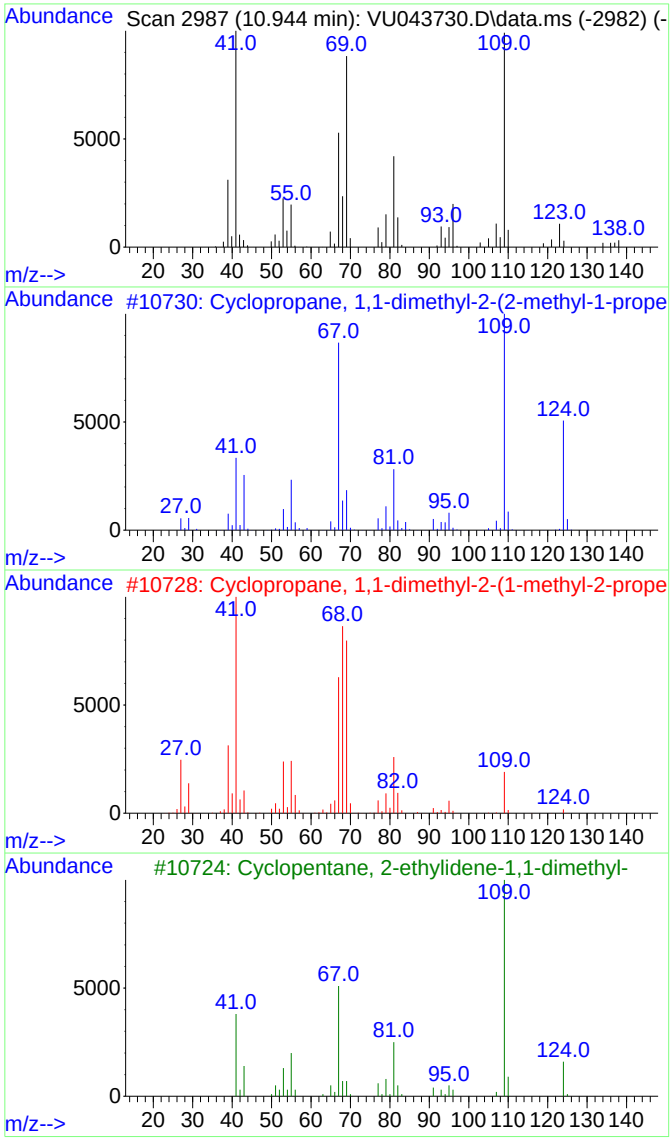
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

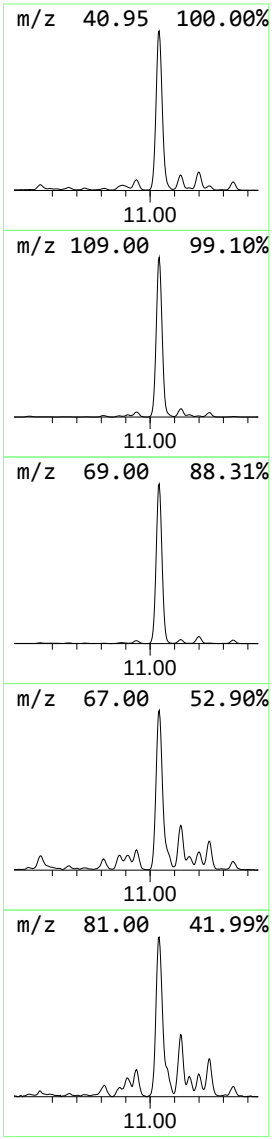
****

Peak Number 11 unknown-03 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.944	3.63 ug/L	80281	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	033422-32-1	43
2	Cyclopropane, 1,1-dimethyl-2-(1-...	124	C9H16	074779-84-3	43
3	Cyclopentane, 2-ethylidene-1,1-d...	124	C9H16	056324-66-4	38
4	1,4-Hexadiene, 3-ethyl-4,5-dimet...	138	C10H18	1000154-09-2	38
5	2,4-Heptadiene, 2,6-dimethyl-	124	C9H16	004634-87-1	38





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Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

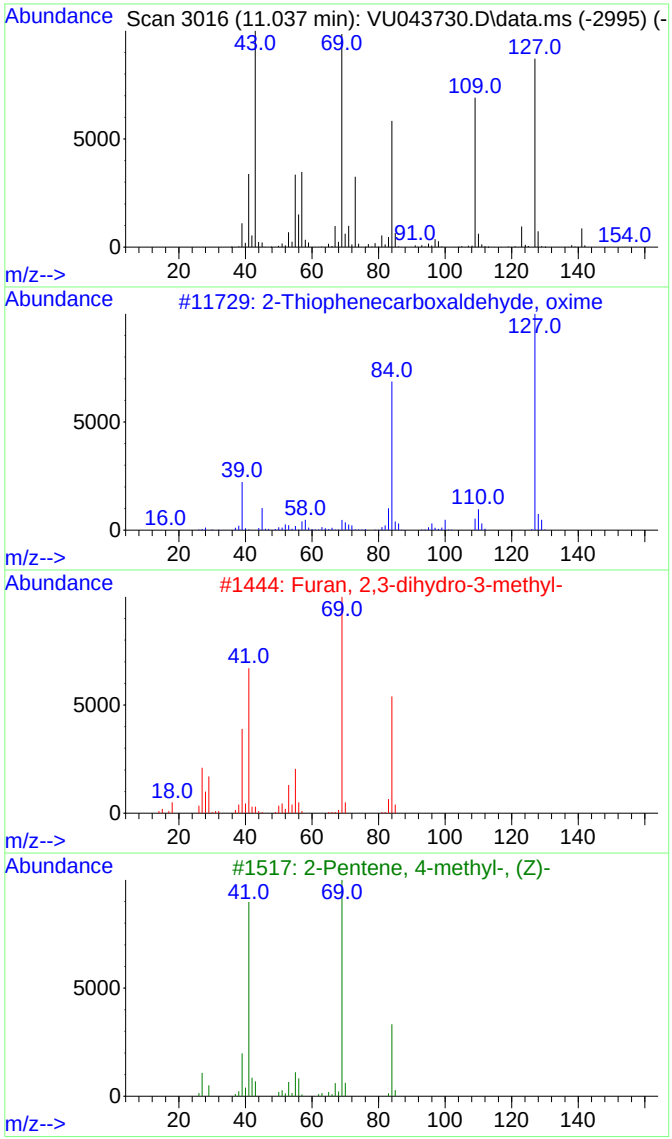
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

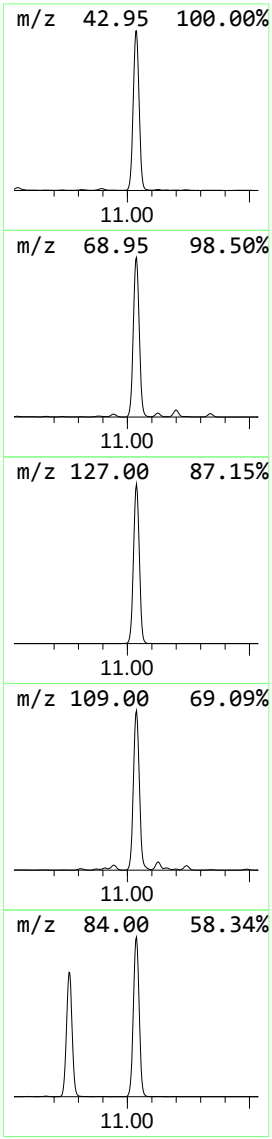
****

Peak Number 12 unknown-04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.037	237.59 ug/L	5254160	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
2	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	30
3	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27
4	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
5	Pentane, 3-methylene-	84	C6H12	000760-21-4	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

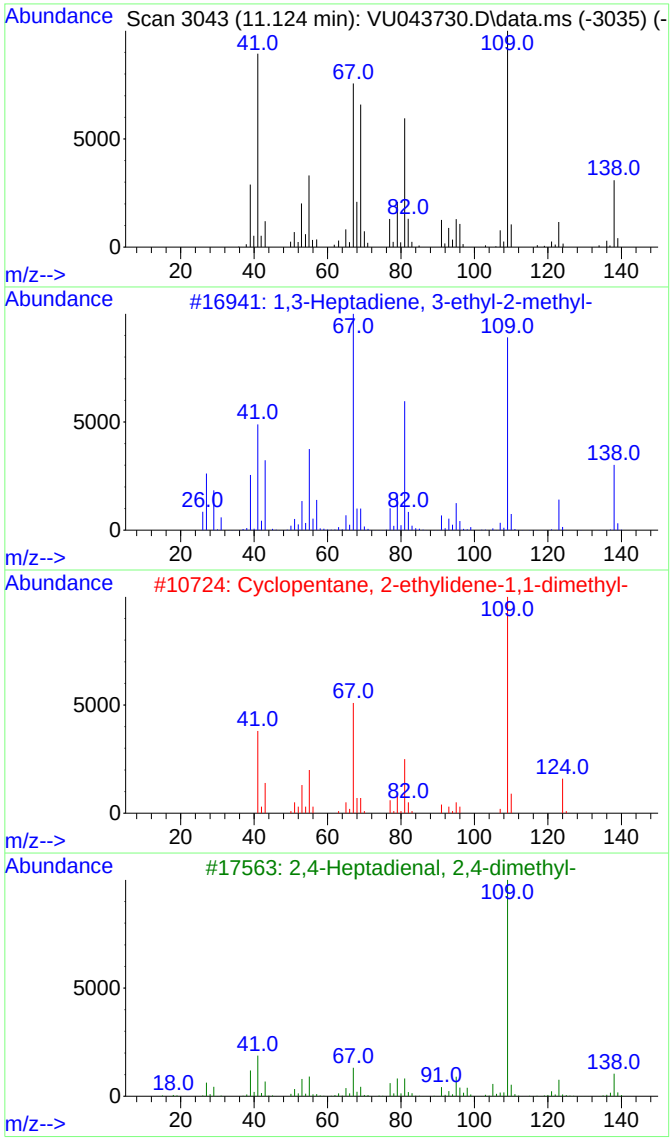
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

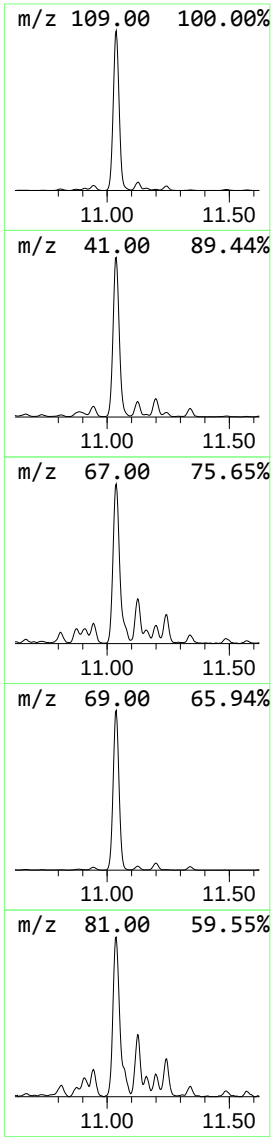
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 1,3-Heptadiene, 3-ethyl-2-m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.124	6.91 ug/L	152829	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Heptadiene, 3-ethyl-2-methyl-	138	C10H18	061142-35-6	83
2	Cyclopentane, 2-ethylidene-1,1-d...	124	C9H16	056324-66-4	64
3	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	64
4	9-Oxabicyclo[3.3.1]non-6-en-3-one	138	C8H10O2	1000190-65-0	50
5	4-Octyne	110	C8H14	001942-45-6	46





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Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

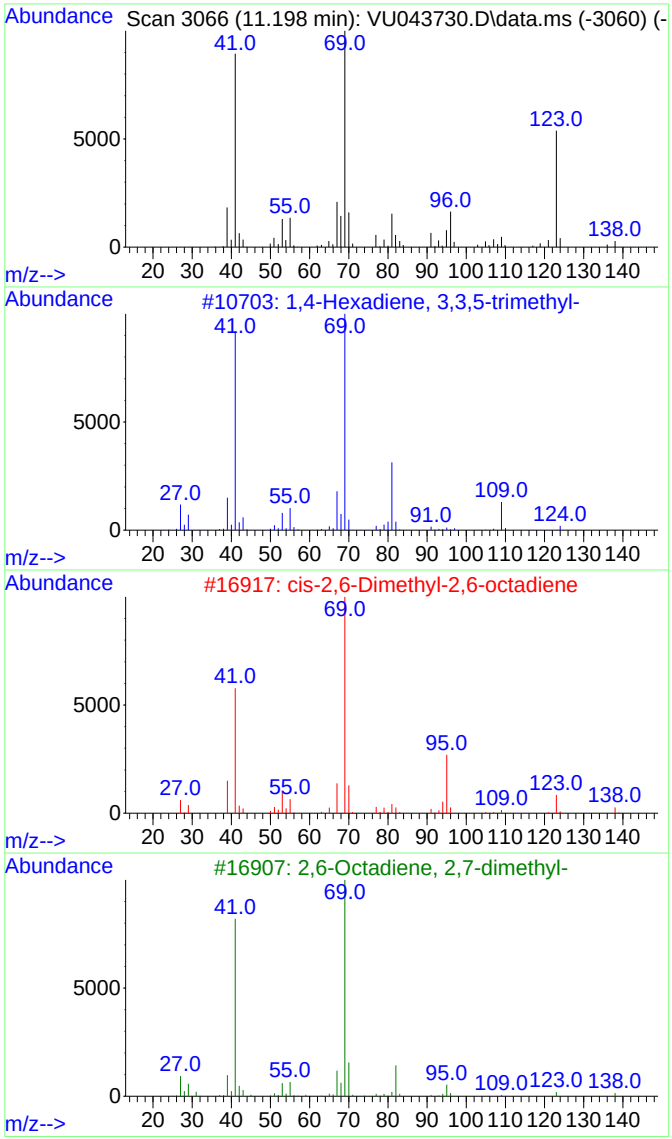
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

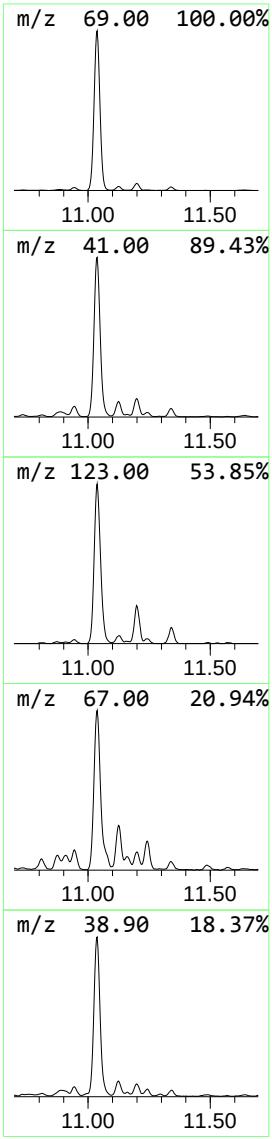
****

Peak Number 14 unknown-05 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.198	4.57 ug/L	101148	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Hexadiene, 3,3,5-trimethyl-	124	C9H16	074753-00-7	47
2	cis-2,6-Dimethyl-2,6-octadiene	138	C10H18	002492-22-0	47
3	2,6-Octadiene, 2,7-dimethyl-	138	C10H18	016736-42-8	46
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	43
5	6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

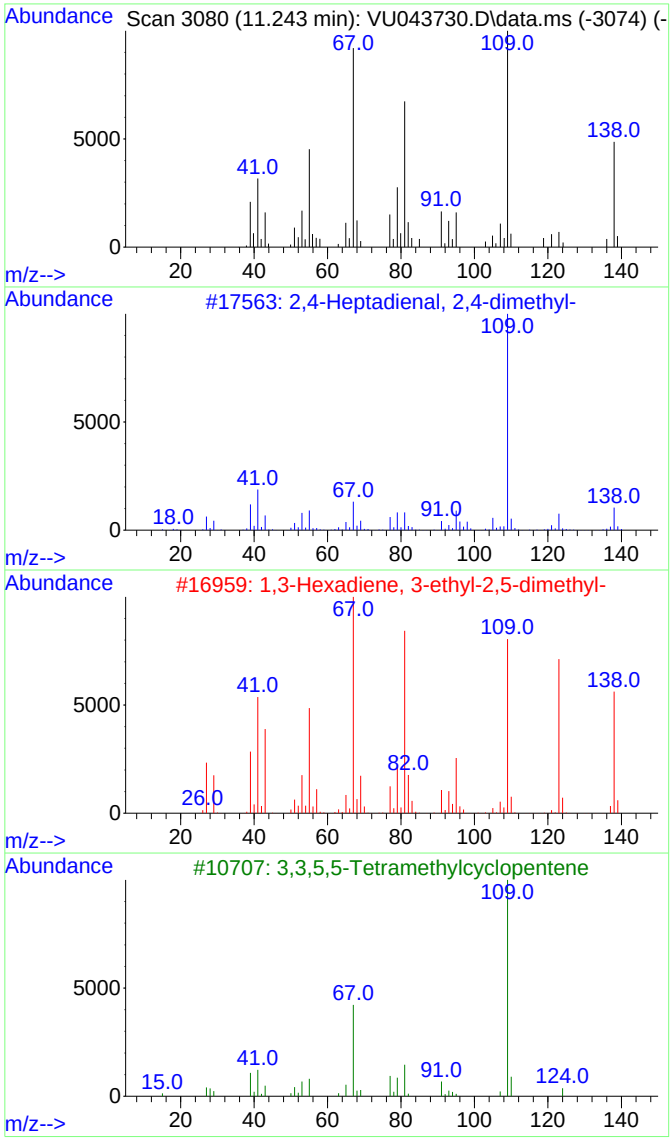
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

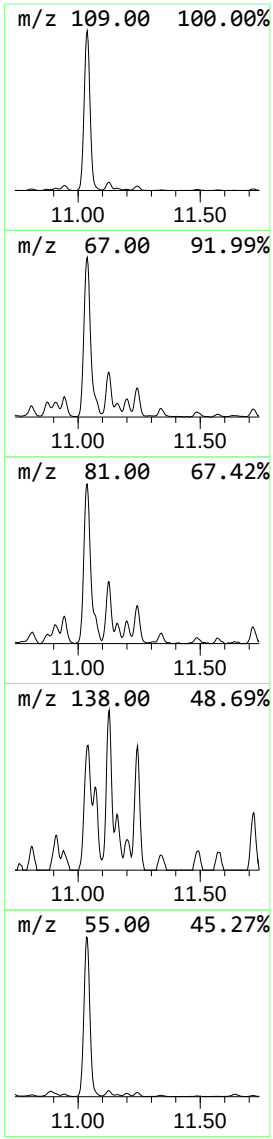
****

Peak Number 15 2,4-Heptadienal, 2,4-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.243	3.93 ug/L	86830	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	72
2	1,3-Hexadiene, 3-ethyl-2,5-dimet...	138	C10H18	062338-07-2	62
3	3,3,5,5-Tetramethylcyclopentene	124	C9H16	038667-10-6	50
4	Bicyclo[2.2.1]heptan-2-one, 3-et...	138	C9H14O	054345-87-8	47
5	1,3-Heptadiene, 3-ethyl-2-methyl-	138	C10H18	061142-35-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

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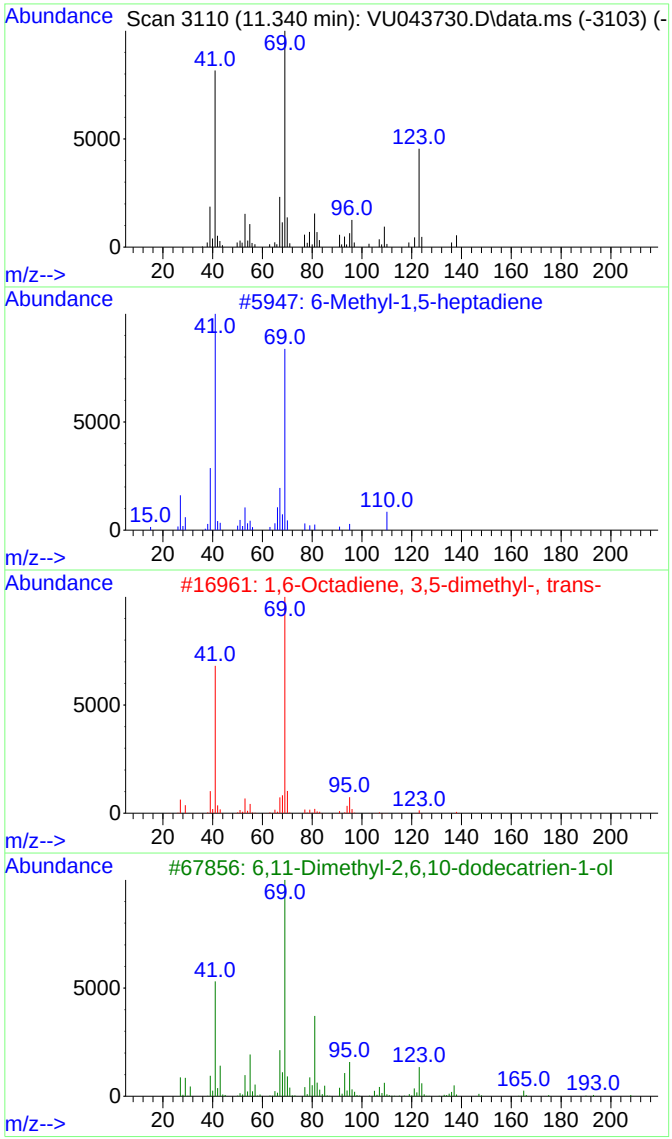
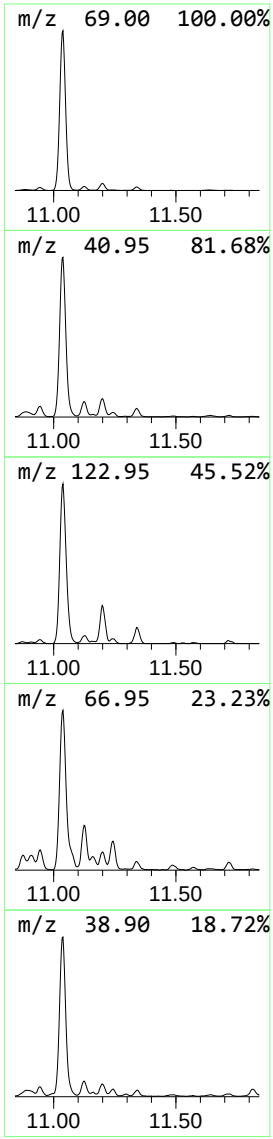
Peak Number 16 unknown-06 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.340	2.77 ug/L	61197	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	43
2	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	43
3	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	42
4	4-Hexen-1-ol, 2-ethenyl-2,5-dime...	154	C10H18O	050598-21-5	40
5	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

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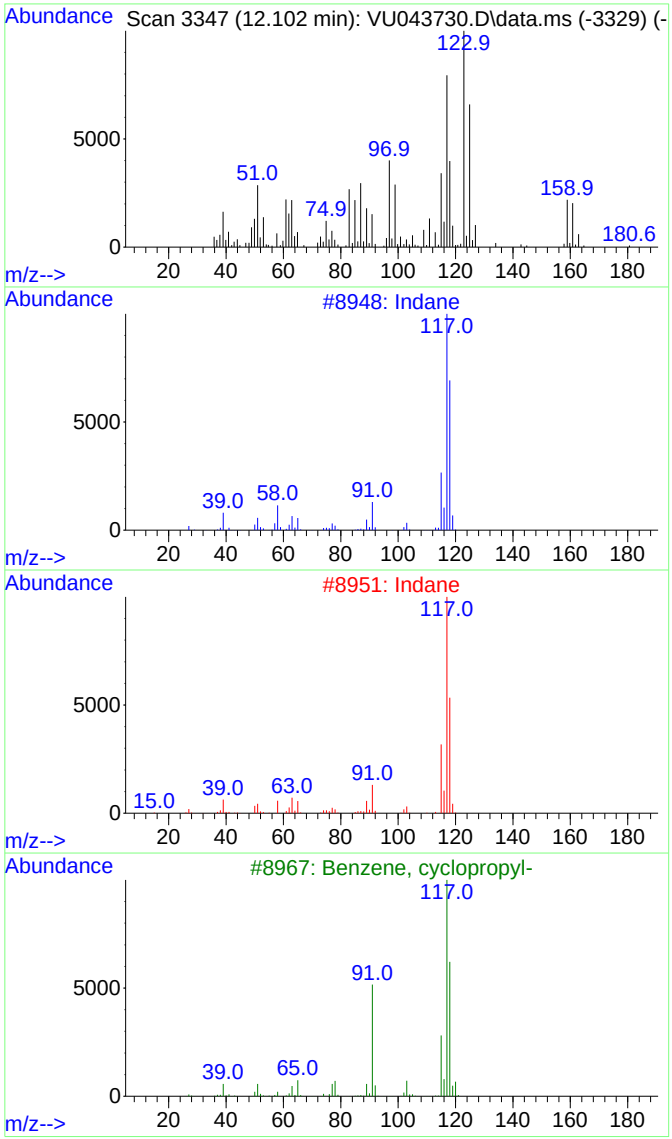
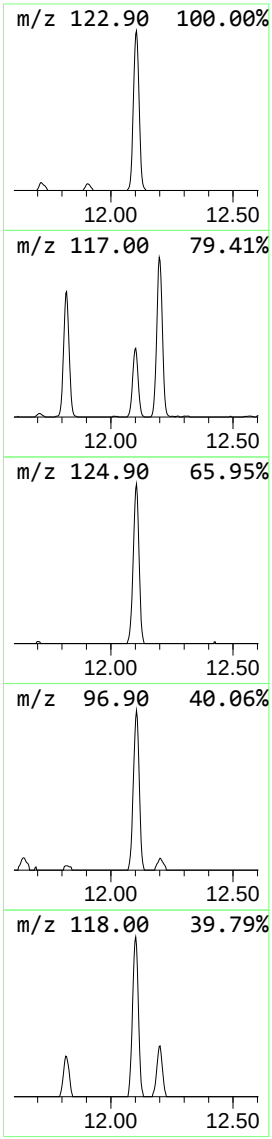
Peak Number 17 unknown-07 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.102	10.55 ug/L	233330	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	20
2	Indane	118	C9H10	000496-11-7	18
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	14
4	Indolizine	117	C8H7N	000274-40-8	14
5	Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	14





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

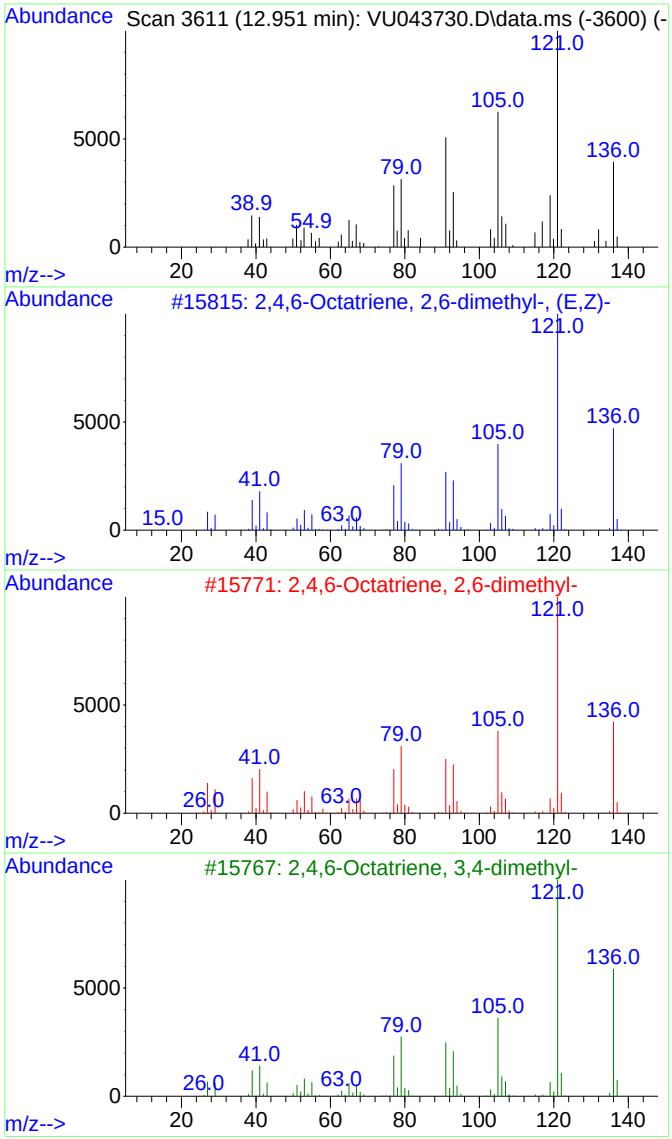
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

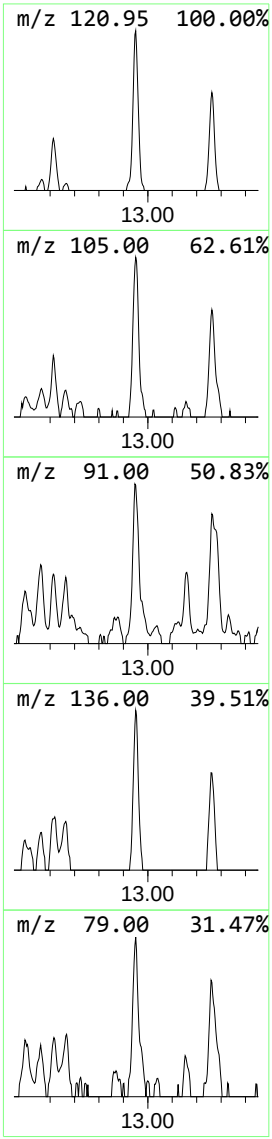
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 2,4,6-Octatriene, 2,6-dimet... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.951	2.55 ug/L	56469	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Octatriene, 2,6-dimethyl-,...	136	C10H16	007216-56-0	93
2	2,4,6-Octatriene, 2,6-dimethyl-	136	C10H16	000673-84-7	90
3	2,4,6-Octatriene, 3,4-dimethyl-	136	C10H16	057396-75-5	87
4	1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	87
5	2,4,6-Octatriene, 2,6-dimethyl-,...	136	C10H16	007216-56-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043730.D
Acq On : 14 May 2021 03:52
Operator : SY/MD
Sample : M2350-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.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
unknown-01	3.179	8.5	ug/L	153488	1	6.256	900607	50.0
Diisopropyl ether	4.002	9.8	ug/L	175992	1	6.256	900607	50.0
2(1H)-Pyrimidin...	6.922	32.6	ug/L	587440	1	6.256	900607	50.0
(DEL) Alkane: S...	7.346	24.2	ug/L	435495	1	6.256	900607	50.0
(DEL) Alkane: S...	7.523	31.6	ug/L	569405	1	6.256	900607	50.0
Furan, tetrahyd...	7.719	28.8	ug/L	518328	1	6.256	900607	50.0
2-Hexanol, 2,5-...	10.262	159.3	ug/L	4071860	2	9.423	1278060	50.0
unknown-02	10.552	4.8	ug/L	123240	2	9.423	1278060	50.0
3-Heptanone, 5-...	10.899	7.2	ug/L	159079	3	11.819	1105710	50.0
unknown-03	10.944	3.6	ug/L	80281	3	11.819	1105710	50.0
unknown-04	11.037	237.6	ug/L	5254160	3	11.819	1105710	50.0
1,3-Heptadiene,...	11.124	6.9	ug/L	152829	3	11.819	1105710	50.0
unknown-05	11.198	4.6	ug/L	101148	3	11.819	1105710	50.0
2,4-Heptadienal...	11.243	3.9	ug/L	86830	3	11.819	1105710	50.0
unknown-06	11.340	2.8	ug/L	61197	3	11.819	1105710	50.0
unknown-07	12.102	10.6	ug/L	233330	3	11.819	1105710	50.0
2,4,6-Octatrien...	12.951	2.5	ug/L	56469	3	11.819	1105710	50.0