LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101022\
Data File : VV028499.D
Acq On : 10 Oct 2022 16:55
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

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\SFAMVLM100722WMA.M
Title : VOC Analysis

Signal : TIC: VV028499.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	75	82	99	rBV	117153	127592	3.21%	0.866%
2	1.564	159	163	179	rVB	105907	120779	3.04%	0.820%
3	2.105	322	331	347	rVB	215244	316724	7.96%	2.149%
4	3.185	654	667	685	rBV	51519	108141	2.72%	0.734%
5	3.423	738	741	743	rBV3	408	278	0.01%	0.002%
6	3.506	765	767	770	rVB2	374	239	0.01%	0.002%
7	3.535	770	776	780	rBV2	444	562	0.01%	0.004%
8	3.564	783	785	789	rVV3	727	399	0.01%	0.003%
9	3.654	811	813	818	rVV4	428	182	0.00%	0.001%
10	3.690	821	824	827	rBV2	328	202	0.01%	0.001%
11	3.818	858	864	865	rBV4	682	499	0.01%	0.003%
12	3.908	880	892	931	rBV2	47838	225844	5.68%	1.533%
13	4.342	1013	1027	1053	rBV	174399	433896	10.91%	2.944%
14	4.757	1153	1156	1159	rVB	449	252	0.01%	0.002%
15	4.773	1159	1161	1165	rBV2	624	510	0.01%	0.003%
16	4.912	1202	1204	1208	rBV2	537	333	0.01%	0.002%
17	4.944	1212	1214	1217	rBV	502	314	0.01%	0.002%
18	5.040	1225	1244	1281	rBV2	438982	1157215	29.09%	7.853%
19	5.355	1340	1342	1345	rBV3	436	193	0.00%	0.001%
20	5.397	1352	1355	1356	rBV2	648	316	0.01%	0.002%
21	5.458	1370	1374	1375	rBV4	605	379	0.01%	0.003%
22	5.516	1388	1392	1394	rBV	442	274	0.01%	0.002%
23	5.535	1394	1398	1400	rBV3	411	308	0.01%	0.002%
24	5.612	1410	1422	1455	rBV	369379	756775	19.03%	5.136%
25	5.854	1495	1497	1499	rBV2	518	223	0.01%	0.002%
26	6.066	1549	1563	1589	rBV2	242936	514863	12.94%	3.494%
27	6.310	1623	1639	1668	rBV	125401	269394	6.77%	1.828%
28	6.558	1714	1716	1718	rVB	490	191	0.00%	0.001%
29	6.574	1718	1721	1722	rBV2	487	253	0.01%	0.002%
30	6.616	1731	1734	1737	rVB3	486	307	0.01%	0.002%
31	6.638	1737	1741	1742	rBV3	746	456	0.01%	0.003%
32	6.667	1748	1750	1754	rVB4	963	588	0.01%	0.004%
33	6.751	1767	1776	1792	rVB3	14907	27946	0.70%	0.190%
34	6.931	1819	1832	1839	rBV	57164	97856	2.46%	0.664%
35	6.982	1840	1848	1872	rVB	148587	275447	6.93%	1.869%
36	7.133	1884	1895	1912	rVB3	86990	169171	4.25%	1.148%

LSC Area Percent Report

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Acq On : 10 Oct 2022 16:55
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

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\SFAMVLM100722WMA.M
Title : VOC Analysis

37	7.310	1939	1950	1973	rBV	527132	923236	23.21%	6.265%
38	7.616	2036	2045	2071	rBV	104700	191904	4.82%	1.302%
39	7.863	2118	2122	2123	rBV4	763	401	0.01%	0.003%
40	7.892	2129	2131	2134	rVB3	445	211	0.01%	0.001%
41	7.934	2134	2144	2145	rBV7	5281	5927	0.15%	0.040%
42	7.998	2162	2164	2167	rVB2	508	312	0.01%	0.002%
43	8.018	2167	2170	2172	rBV3	367	231	0.01%	0.002%
44	8.040	2175	2177	2181	rVB	675	388	0.01%	0.003%
45	8.085	2181	2191	2231	rBV	284163	572768	14.40%	3.887%
46	8.554	2335	2337	2341	rVB2	467	245	0.01%	0.002%
47	8.577	2341	2344	2347	rBV4	772	522	0.01%	0.004%
48	8.616	2353	2356	2358	rBV3	497	393	0.01%	0.003%
49	8.628	2358	2360	2364	rVB4	726	416	0.01%	0.003%
50	8.680	2373	2376	2378	rBV	412	217	0.01%	0.001%
51	8.754	2386	2399	2416	rBV5	4303	8697	0.22%	0.059%
52	8.847	2416	2428	2456	rBV	529807	919743	23.12%	6.242%
53	9.111	2508	2510	2513	rBV2	560	333	0.01%	0.002%
54	9.143	2516	2520	2521	rBV2	532	398	0.01%	0.003%
55	9.198	2534	2537	2539	rBV3	564	323	0.01%	0.002%
56	9.288	2561	2565	2566	rBV2	620	443	0.01%	0.003%
57	9.336	2577	2580	2584	rBV	447	352	0.01%	0.002%
58	9.358	2585	2587	2589	rVB	494	241	0.01%	0.002%
59	9.378	2589	2593	2595	rBV2	523	380	0.01%	0.003%
60	9.413	2598	2604	2607	rBV3	414	473	0.01%	0.003%
61	9.474	2621	2623	2629	rVB2	385	265	0.01%	0.002%
62	9.500	2629	2631	2633	rBV2	437	245	0.01%	0.002%
63	9.538	2638	2643	2644	rBV2	365	290	0.01%	0.002%
64	9.587	2653	2658	2659	rBV2	781	620	0.02%	0.004%
65	9.648	2674	2677	2681	rVB2	514	318	0.01%	0.002%
66	9.728	2689	2702	2729	rBV	680785	1177903	29.61%	7.993%
67	10.207	2838	2851	2877	rVB	335913	542915	13.65%	3.684%
68	10.474	2919	2934	2960	rBV	2405428	3977496	100.00%	26.992%
69	10.866	3050	3056	3059	rBV2	615	554	0.01%	0.004%
70	10.889	3059	3063	3066	rBV2	505	316	0.01%	0.002%
71	10.918	3068	3072	3075	rBV3	593	529	0.01%	0.004%
72	10.937	3075	3078	3081	rBV2	364	246	0.01%	0.002%
73	11.005	3097	3099	3102	rBV3	387	234	0.01%	0.002%
74	11.095	3115	3127	3141	rBV7	8115	16308	0.41%	0.111%
75	11.169	3146	3150	3157	rVB7	3251	3974	0.10%	0.027%
76	11.239	3161	3172	3194	rBV	565899	885488	22.26%	6.009%

LSC Area Percent Report

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Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

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\SFAMVLM100722WMA.M
Title : VOC Analysis

77	11.458	3239	3240	3245	rVB4	493	217	0.01%	0.001%
78	11.516	3256	3258	3259	rBV2	1226	556	0.01%	0.004%
79	11.615	3278	3289	3315	rVB	522200	830277	20.87%	5.634%
80	11.853	3361	3363	3367	rBV3	858	583	0.01%	0.004%
81	11.902	3375	3378	3379	rBV	553	262	0.01%	0.002%
82	12.008	3407	3411	3415	rBV4	386	305	0.01%	0.002%
83	12.030	3415	3418	3421	rBV3	418	244	0.01%	0.002%
84	12.107	3438	3442	3443	rBV3	809	568	0.01%	0.004%
85	12.140	3446	3452	3463	rVB4	5737	9345	0.23%	0.063%
86	12.213	3467	3475	3476	rBV4	1103	1304	0.03%	0.009%
87	12.313	3498	3506	3519	rVB	28122	41801	1.05%	0.284%
88	12.506	3564	3566	3568	rBV2	447	251	0.01%	0.002%
89	12.570	3582	3586	3588	rBV2	758	584	0.01%	0.004%
90	12.657	3612	3613	3616	rBV2	452	244	0.01%	0.002%
91	12.712	3626	3630	3631	rBV2	593	441	0.01%	0.003%
92	12.757	3638	3644	3646	rBV3	806	740	0.02%	0.005%
93	13.011	3717	3723	3725	rBV2	933	788	0.02%	0.005%
94	13.027	3725	3728	3730	rBV	486	260	0.01%	0.002%
95	13.233	3789	3792	3796	rBV4	616	484	0.01%	0.003%
96	13.287	3807	3809	3812	rBV3	409	294	0.01%	0.002%
97	13.422	3849	3851	3853	rBV3	473	218	0.01%	0.001%
98	13.474	3865	3867	3868	rBV3	478	193	0.00%	0.001%
99	13.744	3949	3951	3954	rBV3	546	310	0.01%	0.002%
100	13.975	4020	4023	4027	rBV2	574	469	0.01%	0.003%

Sum of corrected areas: 14735894

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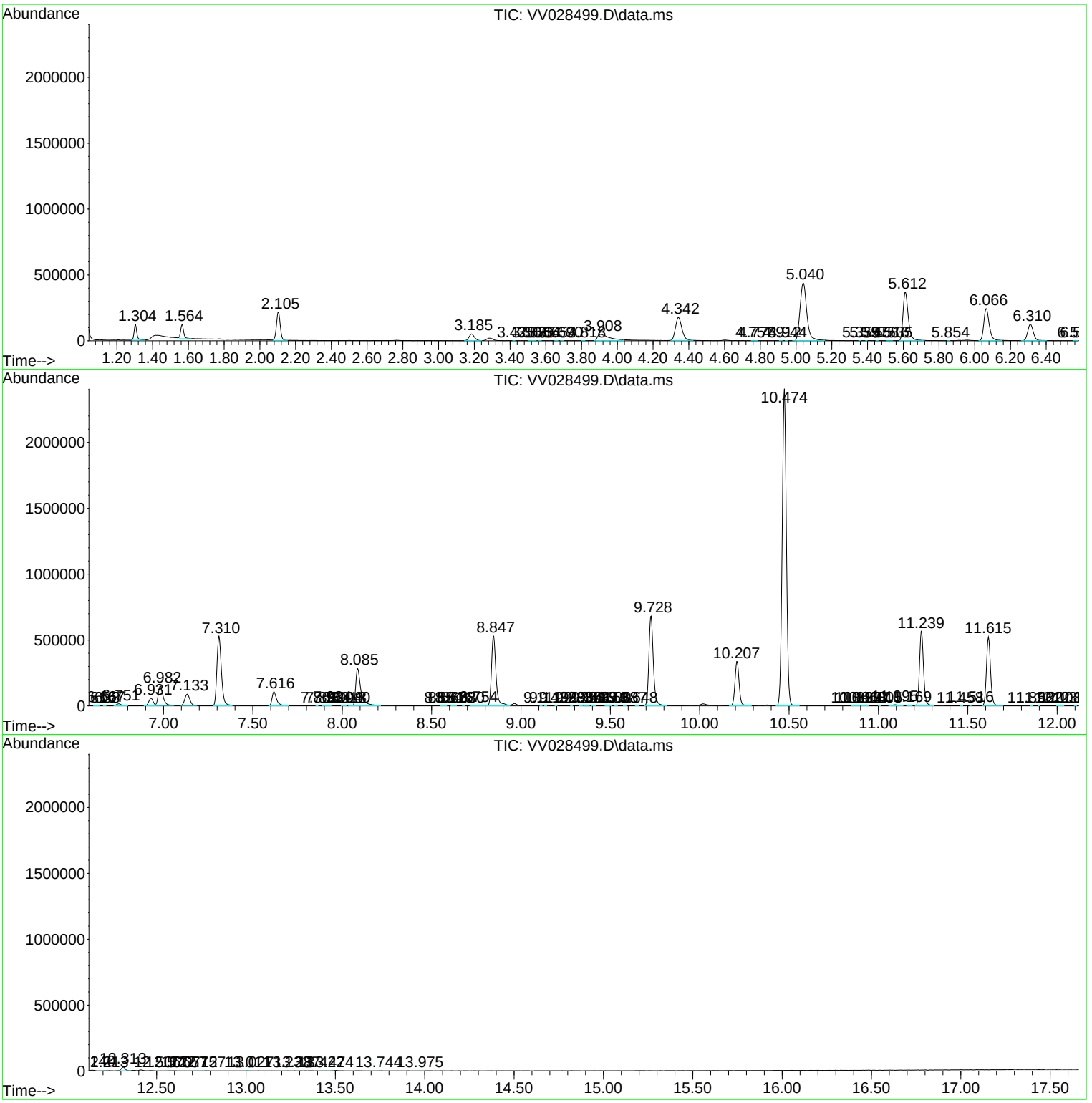
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101022\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

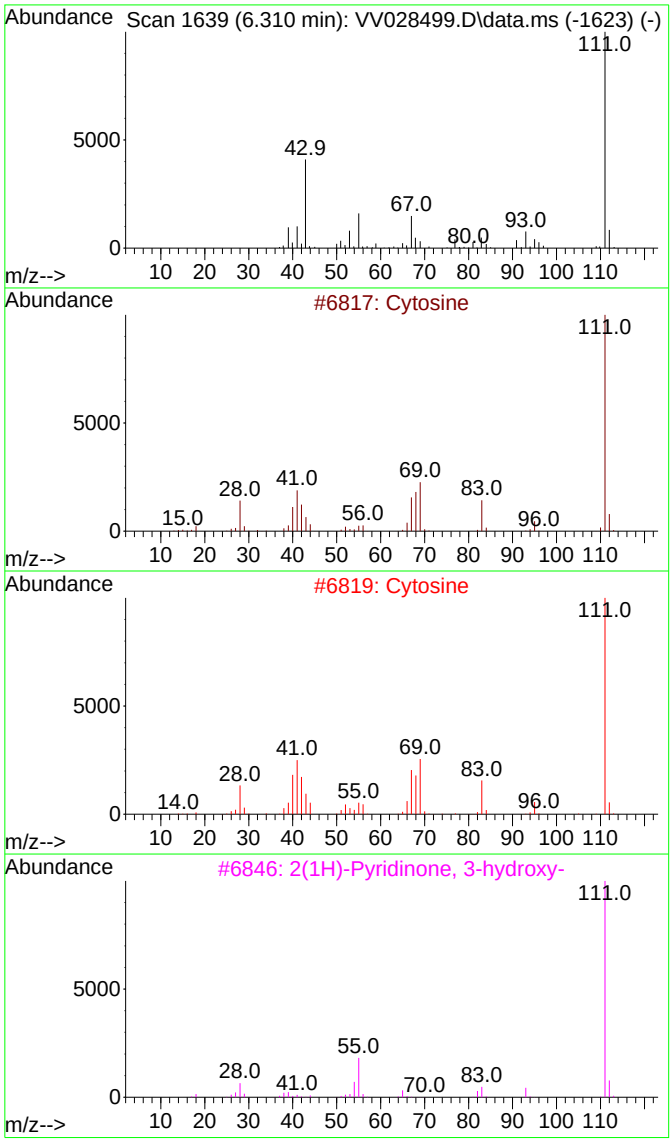
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

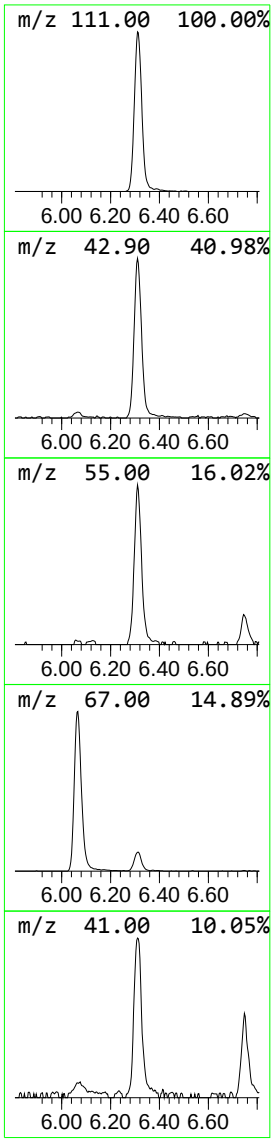
****

Peak Number 1 Cytosine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.310	17.80 ug/L	269394	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cytosine	111	C4H5N3O	000071-30-7	64
2	Cytosine	111	C4H5N3O	000071-30-7	64
3	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	59
4	2-Heptenoic acid, 4-nitrophenyl ...	249	C13H15NO4	1000406-90-6	53
5	Cytosine	111	C4H5N3O	000071-30-7	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101022\
Data File : VV028499.D
Acq On : 10 Oct 2022 16:55
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

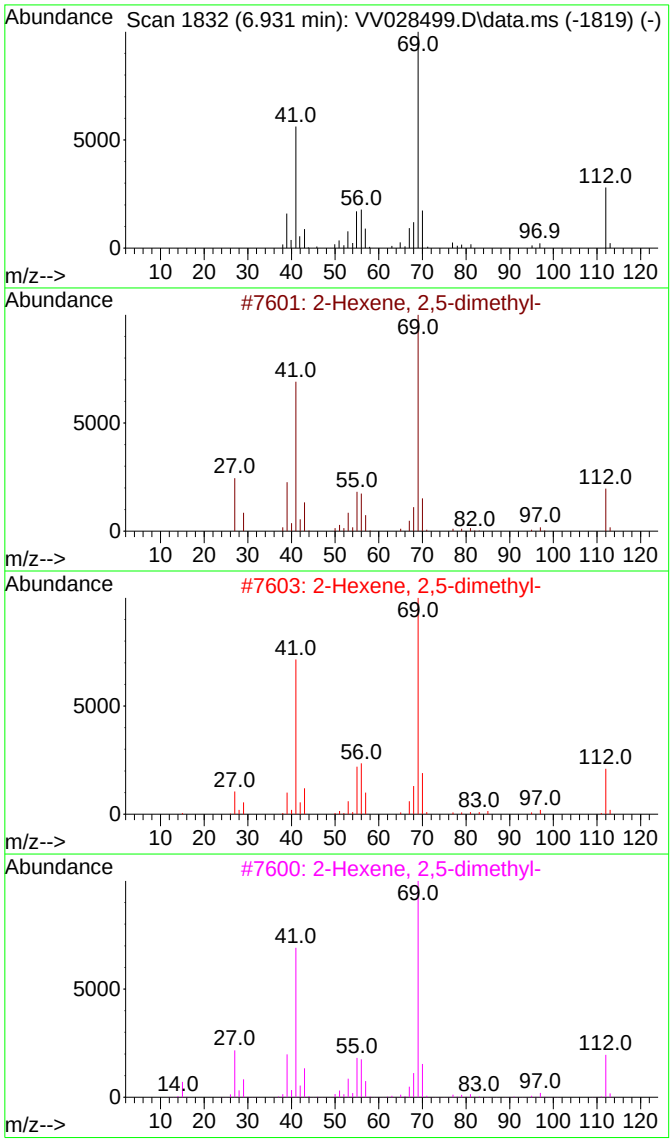
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

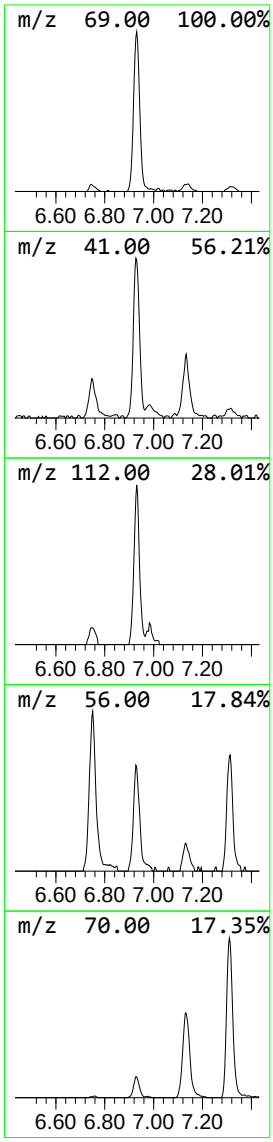
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.931	6.47 ug/L	97856	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	91
2	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	91
3	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	91
4	2-Methyl-2-heptene	112	C8H16	000627-97-4	86
5	3-Hexene, 2,5-dimethyl-, (E)-	112	C8H16	000692-70-6	83





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Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

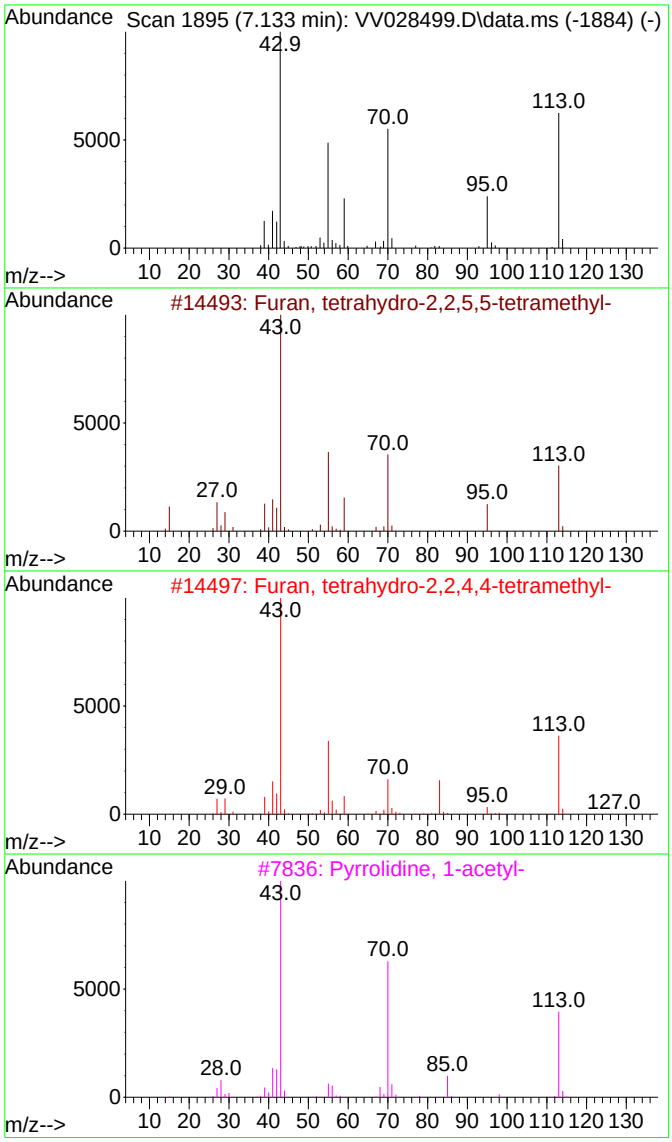
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

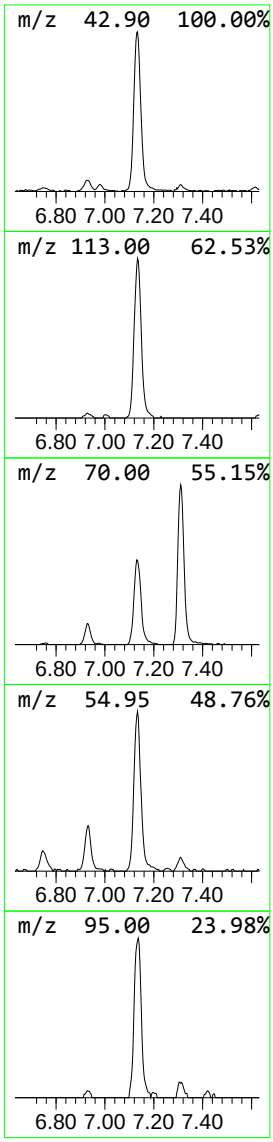
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.133	11.18 ug/L	169171	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	53
2	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3	Pyrrolidine, 1-acetyl-	113	C6H11NO	004030-18-6	53
4	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	52
5	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50





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ClientSampleId :
BFYZ9

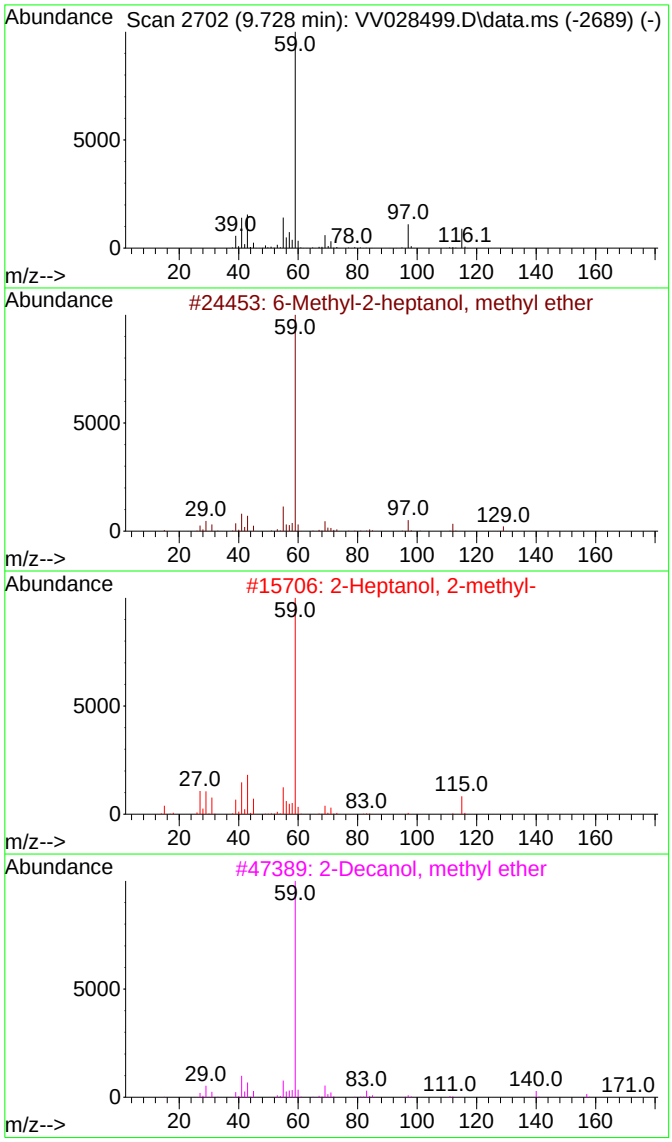
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

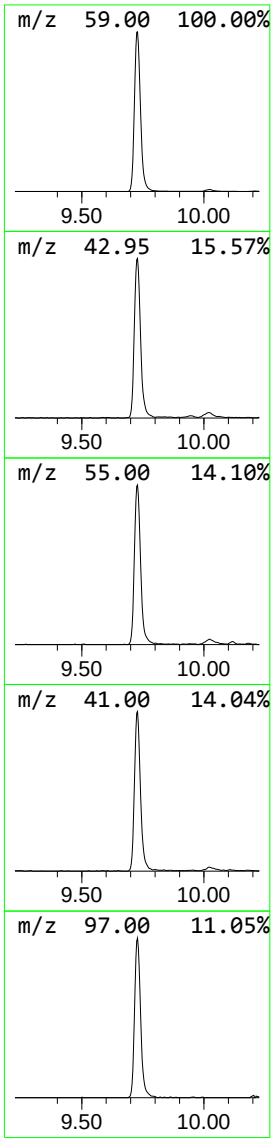
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 6-Methyl-2-heptanol, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	64.03 ug/L	1177900	Chlorobenzene-d5	8.847

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	78
2	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	72
3	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	64
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50





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Data File : VV028499.D
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Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

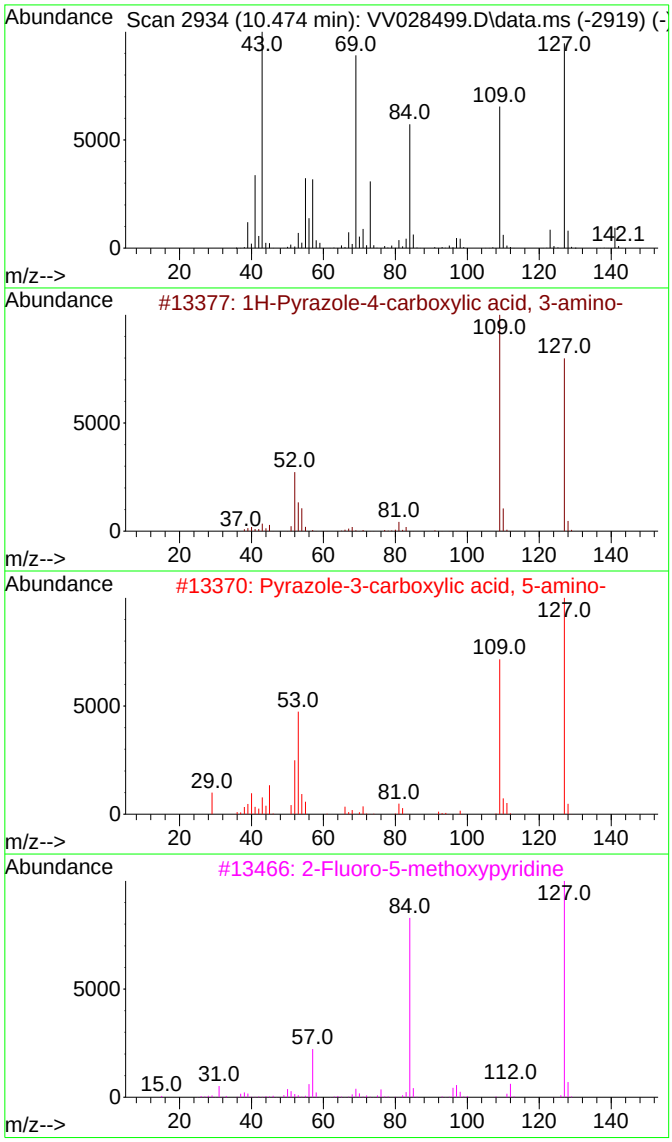
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

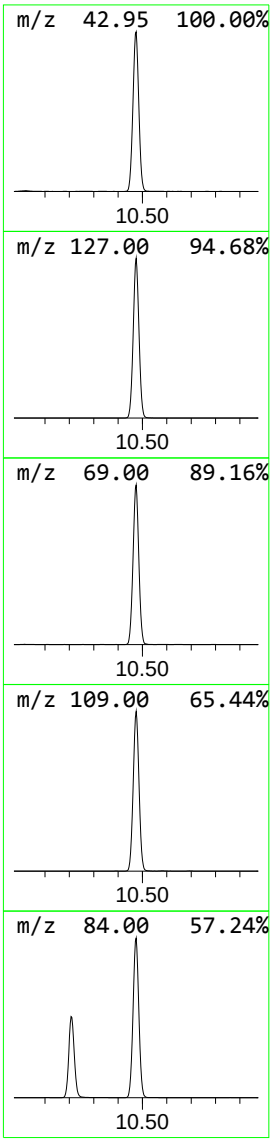
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.474	224.59 ug/L	3977500	1,4-Dichlorobenzene-d4	11.243

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	38
2	Pyrazole-3-carboxylic acid, 5-am...	127	C4H5N3O2	124004-31-5	35
3	2-Fluoro-5-methoxypyridine	127	C6H6FNO	136888-79-4	35
4	2-Fluoro-5-methoxypyridine	127	C6H6FNO	136888-79-4	35
5	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101022\
Data File : VV028499.D
Acq On : 10 Oct 2022 16:55
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.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
Cytosine	6.310	17.8	ug/L	269394	1	5.612	756775	50.0
(DEL) Alkane: S...	6.931	6.5	ug/L	97856	1	5.612	756775	50.0
Furan, tetrahyd...	7.133	11.2	ug/L	169171	1	5.612	756775	50.0
6-Methyl-2-hept...	9.728	64.0	ug/L	1177900	2	8.847	919743	50.0
unknown-01	10.474	224.6	ug/L	3977500	3	11.243	885488	50.0