LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031769.D
Acq On : 26 Jul 2023 15:13
Operator : SY/MD
Sample : 03754-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BH2Z2

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\SFAMVLM072523WMA.M
Title : VOC Analysis

Signal : TIC: VV031769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	89	rVB	211396	236527	15.22%	1.981%
2	1.532	146	153	173	rVB	196088	244302	15.72%	2.046%
3	2.060	308	317	328	rBV	361954	526625	33.88%	4.411%
4	2.114	329	334	350	rVB	50219	78095	5.02%	0.654%
5	2.452	432	439	442	rBV7	1618	1981	0.13%	0.017%
6	2.571	465	476	490	rVV3	15954	33748	2.17%	0.283%
7	2.664	503	505	511	rVB6	1642	1670	0.11%	0.014%
8	2.706	511	518	521	rBV8	2078	2335	0.15%	0.020%
9	2.748	529	531	536	rVB5	973	950	0.06%	0.008%
10	2.892	572	576	578	rBV2	1139	877	0.06%	0.007%
11	3.124	644	648	652	rBV5	1496	1081	0.07%	0.009%
12	3.320	701	709	711	rBV5	1067	1204	0.08%	0.010%
13	3.333	711	713	717	rVB4	1448	1140	0.07%	0.010%
14	3.355	717	720	724	rBV5	1516	1003	0.06%	0.008%
15	3.458	747	752	755	rVB2	870	740	0.05%	0.006%
16	3.593	791	794	796	rBV2	1184	787	0.05%	0.007%
17	3.793	847	856	884	rBV	130741	382269	24.59%	3.202%
18	4.182	974	977	980	rVV4	1109	802	0.05%	0.007%
19	4.256	985	1000	1027	rVV2	277422	727711	46.81%	6.096%
20	4.616	1109	1112	1118	rVB6	1093	714	0.05%	0.006%
21	4.670	1125	1129	1133	rBV6	1572	1069	0.07%	0.009%
22	4.754	1151	1155	1157	rBV5	1313	1106	0.07%	0.009%
23	4.963	1200	1220	1248	rBV2	577533	1554538	100.00%	13.022%
24	5.207	1294	1296	1299	rVB4	1102	760	0.05%	0.006%
25	5.262	1310	1313	1317	rVB6	1113	819	0.05%	0.007%
26	5.323	1330	1332	1336	rBV4	1566	967	0.06%	0.008%
27	5.371	1344	1347	1350	rBV4	1078	973	0.06%	0.008%
28	5.542	1387	1400	1422	rBV	391878	829349	53.35%	6.947%
29	5.828	1478	1489	1510	rBV2	53488	113713	7.31%	0.953%
30	5.915	1512	1516	1518	rBV5	4254	3513	0.23%	0.029%
31	5.995	1528	1541	1561	rBV	370678	762944	49.08%	6.391%
32	6.252	1618	1621	1626	rBV7	991	889	0.06%	0.007%
33	6.339	1643	1648	1652	rBV6	1631	1369	0.09%	0.011%
34	6.513	1689	1702	1711	rBV6	10560	20881	1.34%	0.175%
35	6.741	1770	1773	1777	rVB5	1181	1071	0.07%	0.009%
36	6.815	1792	1796	1802	rBV4	942	917	0.06%	0.008%

LSC Area Percent Report

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Z2

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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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Title : VOC Analysis

37	6.918	1816	1828	1852	rBV	166307	320720	20.63%	2.687%
38	7.249	1920	1931	1963	rBV	532386	969527	62.37%	8.122%
39	7.513	2009	2013	2015	rBV4	2197	1454	0.09%	0.012%
40	7.558	2018	2027	2052	rVV	117870	220060	14.16%	1.843%
41	7.690	2066	2068	2070	rBV3	1421	775	0.05%	0.006%
42	7.966	2151	2154	2156	rBV3	1403	929	0.06%	0.008%
43	8.030	2164	2174	2188	rBV	396546	736892	47.40%	6.173%
44	8.452	2302	2305	2309	rVB6	2157	1653	0.11%	0.014%
45	8.510	2321	2323	2325	rBV2	1320	733	0.05%	0.006%
46	8.625	2357	2359	2362	rBV4	1212	765	0.05%	0.006%
47	8.670	2371	2373	2374	rBV2	1634	720	0.05%	0.006%
48	8.789	2399	2410	2437	rBV	637817	1073260	69.04%	8.991%
49	9.040	2486	2488	2490	rBV3	1822	1109	0.07%	0.009%
50	9.075	2495	2499	2501	rBV4	2174	1865	0.12%	0.016%
51	9.181	2530	2532	2535	rVB4	2600	1168	0.08%	0.010%
52	9.381	2592	2594	2600	rVB6	1336	835	0.05%	0.007%
53	9.429	2606	2609	2614	rVB6	2206	1845	0.12%	0.015%
54	9.455	2614	2617	2620	rBV4	1684	1009	0.06%	0.008%
55	9.500	2629	2631	2639	rVB8	2148	1572	0.10%	0.013%
56	9.567	2650	2652	2656	rBV5	1645	1408	0.09%	0.012%
57	9.667	2681	2683	2686	rBV4	2017	988	0.06%	0.008%
58	9.780	2716	2718	2722	rVB5	1653	1095	0.07%	0.009%
59	9.850	2738	2740	2743	rBV4	1294	853	0.05%	0.007%
60	9.998	2782	2786	2793	rBV8	1507	1707	0.11%	0.014%
61	10.159	2824	2836	2850	rBV	485418	779672	50.15%	6.531%
62	10.329	2882	2889	2900	rVB4	10635	18714	1.20%	0.157%
63	10.455	2924	2928	2930	rBV4	2127	1692	0.11%	0.014%
64	10.493	2938	2940	2946	rBV7	1371	1130	0.07%	0.009%
65	10.574	2963	2965	2969	rBV3	1262	901	0.06%	0.008%
66	10.715	3001	3009	3016	rBV3	3728	5898	0.38%	0.049%
67	10.805	3034	3037	3039	rBV3	1525	869	0.06%	0.007%
68	10.863	3051	3055	3059	rVB6	1842	1364	0.09%	0.011%
69	10.886	3059	3062	3065	rBV4	1298	920	0.06%	0.008%
70	10.989	3091	3094	3095	rBV3	1589	880	0.06%	0.007%
71	11.091	3121	3126	3130	rBV9	1987	2453	0.16%	0.021%
72	11.133	3132	3139	3146	rVV9	7860	12029	0.77%	0.101%
73	11.191	3146	3157	3175	rVV	630797	980071	63.05%	8.210%
74	11.358	3207	3209	3211	rBV3	1146	730	0.05%	0.006%
75	11.410	3223	3225	3228	rVB4	1683	1048	0.07%	0.009%
76	11.426	3228	3230	3232	rBV3	1432	729	0.05%	0.006%

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BH2Z2

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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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Title : VOC Analysis

77	11.497	3242	3252	3262	rBV4	18711	39453	2.54%	0.330%
78	11.567	3263	3274	3290	rVB	645576	1033966	66.51%	8.661%
79	11.947	3383	3392	3404	rVV	33377	54842	3.53%	0.459%
80	12.033	3416	3419	3422	rBV4	2012	1445	0.09%	0.012%
81	12.197	3463	3470	3480	rVB2	8224	12242	0.79%	0.103%
82	12.255	3480	3488	3495	rBV8	14000	21299	1.37%	0.178%
83	12.381	3524	3527	3529	rBV4	1848	1464	0.09%	0.012%
84	12.651	3608	3611	3616	rBV5	1888	1576	0.10%	0.013%
85	12.696	3622	3625	3627	rBV4	1264	718	0.05%	0.006%
86	12.808	3656	3660	3661	rBV5	1000	769	0.05%	0.006%
87	12.969	3707	3710	3712	rBV3	2082	1293	0.08%	0.011%
88	13.005	3717	3721	3724	rBV5	2297	1842	0.12%	0.015%
89	13.027	3725	3728	3732	rVB5	1770	1601	0.10%	0.013%
90	13.384	3835	3839	3844	rVB6	1794	1588	0.10%	0.013%
91	13.406	3844	3846	3849	rBV4	1478	1082	0.07%	0.009%
92	13.776	3959	3961	3965	rVB3	2021	1224	0.08%	0.010%
93	13.795	3965	3967	3971	rBV5	1057	890	0.06%	0.007%
94	13.837	3976	3980	3982	rBV4	3260	2578	0.17%	0.022%
95	13.873	3982	3991	4004	rVB3	30642	51217	3.29%	0.429%
96	13.972	4020	4022	4024	rBV3	1408	722	0.05%	0.006%
97	14.249	4104	4108	4110	rBV4	2107	1506	0.10%	0.013%
98	14.326	4130	4132	4136	rBV5	1976	1695	0.11%	0.014%
99	15.062	4356	4361	4369	rVB10	7574	10285	0.66%	0.086%
100	15.628	4535	4537	4539	rBV3	2311	886	0.06%	0.007%

Sum of corrected areas: 11937664

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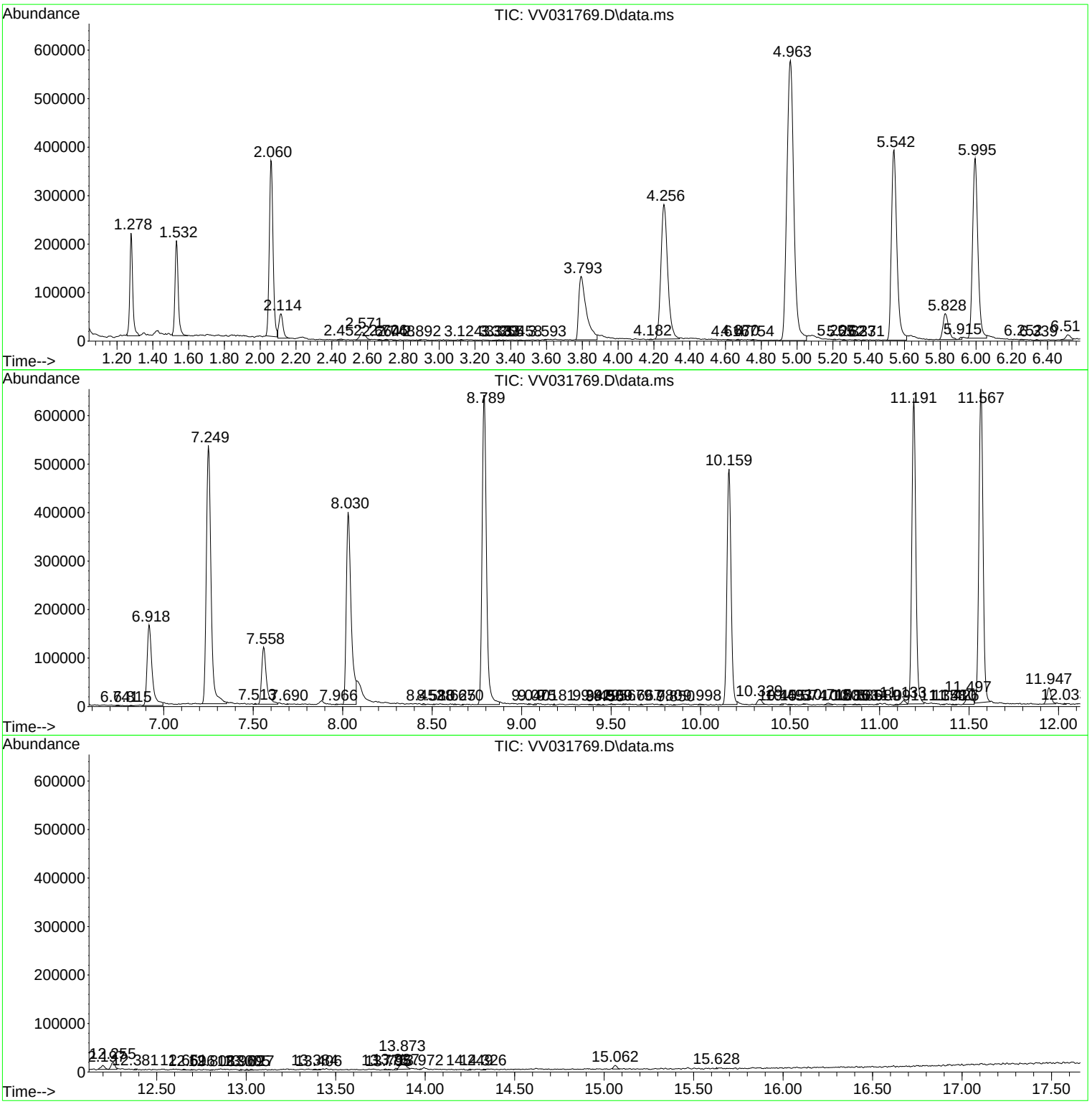
Instrument :
MSVOA_V
ClientSampleId :
BH2Z2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
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Instrument :
MSVOA_V
ClientSampleId :
BH2Z2

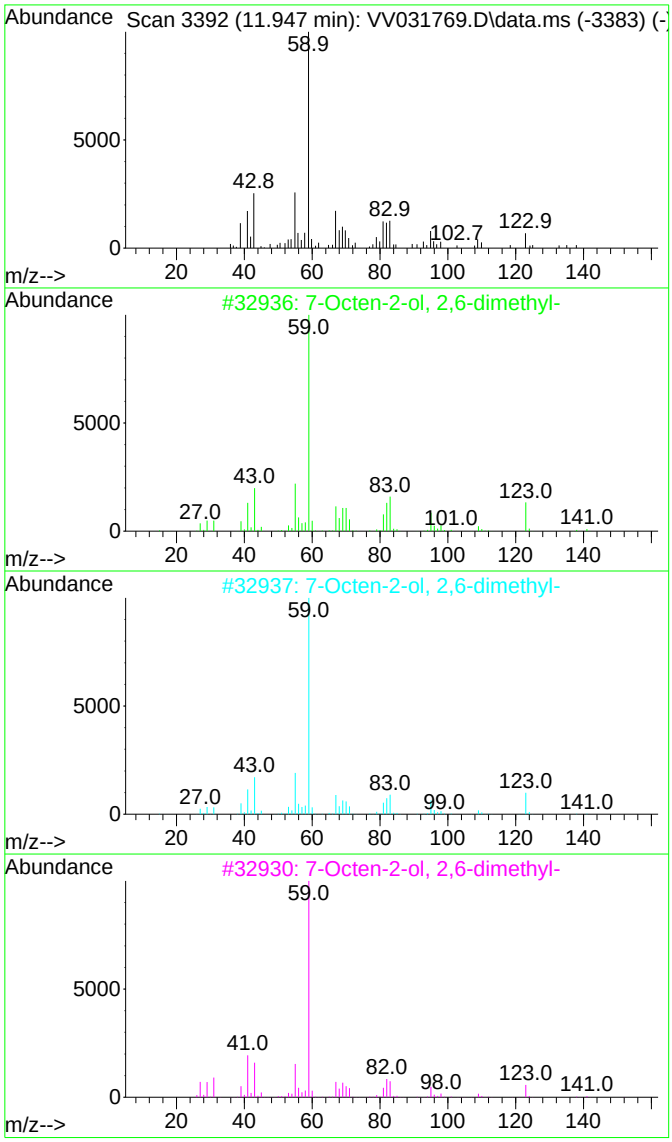
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

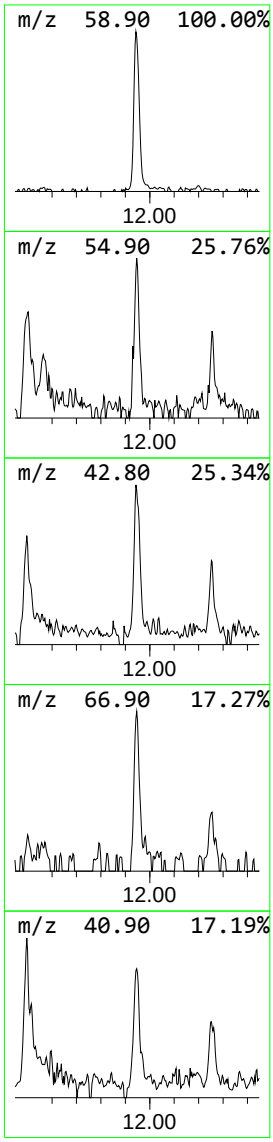
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.947	2.80 ug/L	54842	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
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	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
5	1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031769.D
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MSVOA_V
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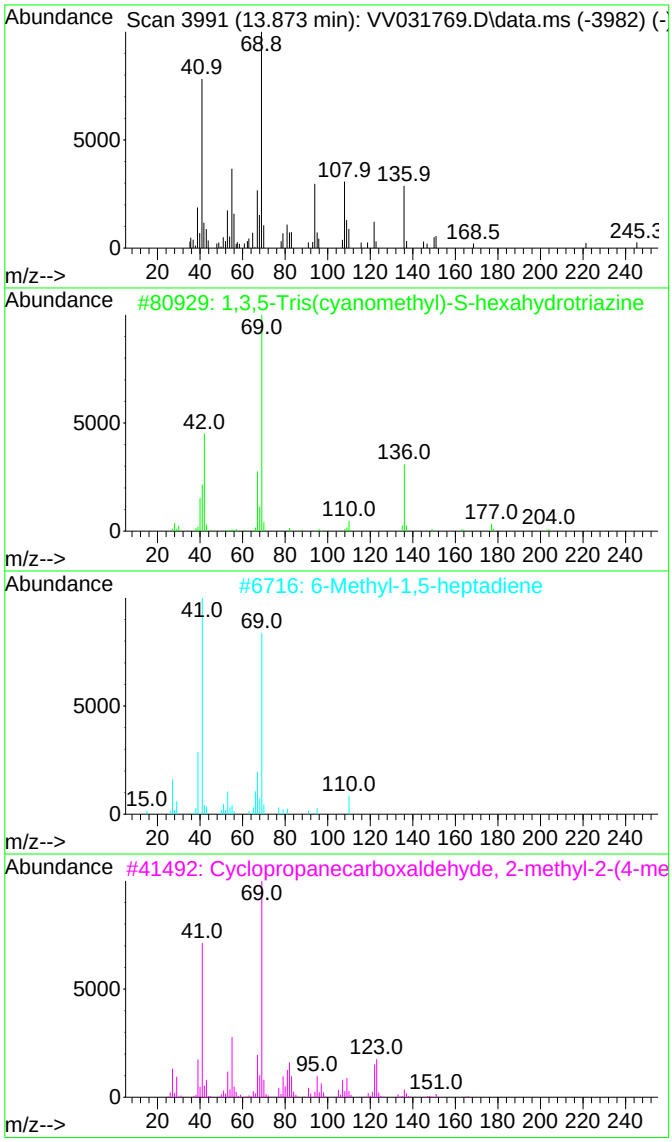
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

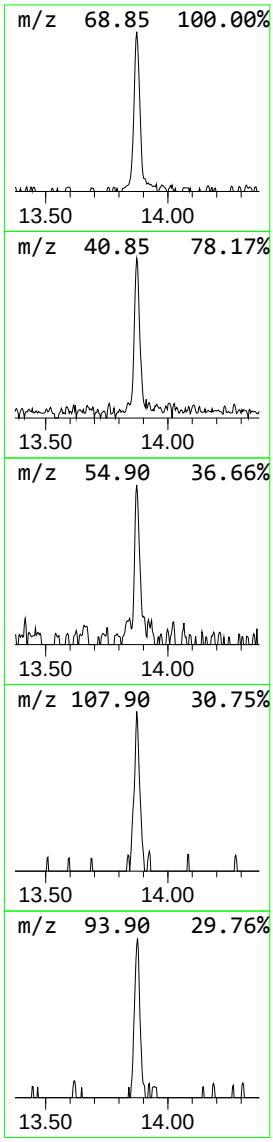
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	2.61 ug/L	51217	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Tris(cyanomethyl)-S-hexahy...	204	C9H12N6	004560-87-6	40
2	6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	38
3	Cyclopropanecarboxaldehyde, 2-me...	166	C11H18O	097231-35-1	38
4	Pentane, 2,4-dibromo-	228	C5H10Br2	019398-53-9	38
5	4-Hexenenitrile, 2,5-dimethyl-2-...	191	C13H21N	069340-56-3	38





Tentatively Identified Compound (LSC) summary

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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
7-Octen-2-ol, 2...	11.947	2.8	ug/L	54842	3	11.191	980071	50.0
unknown-01	13.873	2.6	ug/L	51217	3	11.191	980071	50.0