

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072823\
 Data File : VV031777.D
 Acq On : 28 Jul 2023 10:29
 Operator : SY/MD
 Sample : 03754-16
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 4 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: VV031777.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	66	74	89	rVB	196628	222456	13.85%	1.789%
2	1.529	145	152	167	rVB	186609	223427	13.91%	1.797%
3	2.056	306	316	328	rBV	367769	549053	34.18%	4.415%
4	2.111	328	333	350	rVB	39211	66686	4.15%	0.536%
5	2.336	399	403	405	rBV5	1457	1042	0.06%	0.008%
6	2.407	421	425	427	rVB5	1137	862	0.05%	0.007%
7	2.497	451	453	457	rBV4	1147	930	0.06%	0.007%
8	2.564	461	474	488	rBV4	17460	41047	2.55%	0.330%
9	2.687	508	512	514	rBV6	1851	1309	0.08%	0.011%
10	2.979	600	603	607	rVB5	1574	1464	0.09%	0.012%
11	3.011	607	613	616	rBV7	1599	2007	0.12%	0.016%
12	3.092	635	638	641	rBV3	1341	1080	0.07%	0.009%
13	3.117	644	646	651	rVV6	1693	1544	0.10%	0.012%
14	3.162	654	660	662	rVV6	1178	1093	0.07%	0.009%
15	3.217	673	677	679	rBV4	1094	961	0.06%	0.008%
16	3.407	734	736	743	rVB6	1193	1301	0.08%	0.010%
17	3.439	743	746	751	rBV5	2207	1856	0.12%	0.015%
18	3.484	751	760	762	rBV7	1244	1459	0.09%	0.012%
19	3.558	781	783	789	rVB5	1272	990	0.06%	0.008%
20	3.593	789	794	795	rBV3	2920	2232	0.14%	0.018%
21	3.728	834	836	841	rVB5	1222	934	0.06%	0.008%
22	3.789	841	855	884	rBV2	150619	448891	27.94%	3.610%
23	4.252	979	999	1029	rBV	291241	762342	47.45%	6.131%
24	4.500	1074	1076	1080	rBV5	2035	1598	0.10%	0.013%
25	4.564	1092	1096	1101	rBV8	1384	1581	0.10%	0.013%
26	4.609	1108	1110	1116	rVB7	1839	1610	0.10%	0.013%
27	4.677	1127	1131	1135	rVB5	1498	1310	0.08%	0.011%
28	4.841	1180	1182	1187	rVB6	1829	1462	0.09%	0.012%
29	4.867	1187	1190	1193	rBV4	1215	860	0.05%	0.007%
30	4.886	1193	1196	1200	rBV4	878	924	0.06%	0.007%
31	4.957	1200	1218	1247	rBV2	594322	1606564	100.00%	12.920%
32	5.207	1293	1296	1302	rVB8	1822	1482	0.09%	0.012%
33	5.484	1378	1382	1385	rBV5	1148	1056	0.07%	0.008%
34	5.539	1385	1399	1420	rBV	398222	843110	52.48%	6.780%
35	5.825	1476	1488	1506	rBV2	55676	118901	7.40%	0.956%
36	5.921	1512	1518	1523	rBV7	3319	5204	0.32%	0.042%

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

37	5.992	1527	1540	1560	rVV	387601	796223	49.56%	6.403%
38	6.323	1639	1643	1645	rVB4	1625	990	0.06%	0.008%
39	6.407	1667	1669	1672	rBV4	1349	1006	0.06%	0.008%
40	6.510	1692	1701	1713	rBV3	8930	20258	1.26%	0.163%
41	6.648	1741	1744	1748	rVB5	1338	1016	0.06%	0.008%
42	6.754	1774	1777	1781	rVB3	1504	919	0.06%	0.007%
43	6.918	1812	1828	1848	rBV	165099	320094	19.92%	2.574%
44	7.002	1851	1854	1858	rVB	14525	9634	0.60%	0.077%
45	7.246	1919	1930	1952	rBV	558579	1005559	62.59%	8.087%
46	7.387	1970	1974	1976	rBV3	2035	1633	0.10%	0.013%
47	7.555	2016	2026	2057	rVV	125383	237491	14.78%	1.910%
48	7.879	2118	2127	2134	rBV9	3485	6355	0.40%	0.051%
49	7.947	2144	2148	2153	rVB7	2258	2153	0.13%	0.017%
50	8.030	2162	2174	2189	rBV	395444	760765	47.35%	6.118%
51	8.622	2354	2358	2360	rBV4	1246	951	0.06%	0.008%
52	8.683	2374	2377	2383	rBV8	2005	1656	0.10%	0.013%
53	8.789	2399	2410	2439	rBV	664092	1122871	69.89%	9.030%
54	9.088	2498	2503	2508	rVB8	2229	2843	0.18%	0.023%
55	9.162	2524	2526	2532	rVB5	1118	867	0.05%	0.007%
56	9.397	2596	2599	2603	rVB5	1652	1079	0.07%	0.009%
57	9.680	2684	2687	2692	rVB5	1857	1375	0.09%	0.011%
58	9.722	2696	2700	2702	rBV4	2132	1639	0.10%	0.013%
59	9.866	2741	2745	2747	rBV5	1794	1525	0.09%	0.012%
60	9.889	2748	2752	2754	rVV5	2066	1524	0.09%	0.012%
61	9.953	2770	2772	2776	rBV5	1935	1901	0.12%	0.015%
62	10.085	2810	2813	2820	rBV8	1646	2093	0.13%	0.017%
63	10.159	2820	2836	2860	rBV	505535	818281	50.93%	6.581%
64	10.333	2884	2890	2892	rBV6	3251	3392	0.21%	0.027%
65	10.439	2920	2923	2925	rBV4	1260	967	0.06%	0.008%
66	10.471	2930	2933	2937	rVV4	1866	1531	0.10%	0.012%
67	10.587	2967	2969	2972	rVB3	2201	950	0.06%	0.008%
68	10.715	3004	3009	3012	rBV5	1556	1551	0.10%	0.012%
69	10.844	3046	3049	3051	rBV4	1782	1120	0.07%	0.009%
70	10.998	3095	3097	3099	rBV2	1486	867	0.05%	0.007%
71	11.133	3130	3139	3146	rVV10	12979	20395	1.27%	0.164%
72	11.191	3146	3157	3177	rVB	670447	1039791	64.72%	8.362%
73	11.413	3223	3226	3229	rBV5	1239	930	0.06%	0.007%
74	11.500	3243	3253	3262	rBV3	13324	28410	1.77%	0.228%
75	11.564	3263	3273	3294	rVB	692010	1099330	68.43%	8.841%
76	11.947	3382	3392	3411	rVV2	35006	59010	3.67%	0.475%

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 Title : VOC Analysis

77	12.069	3426	3430	3435	rVB7	1854	1588	0.10%	0.013%
78	12.156	3454	3457	3461	rVB5	2006	1176	0.07%	0.009%
79	12.178	3461	3464	3465	rBV3	1991	1129	0.07%	0.009%
80	12.255	3478	3488	3498	rBV5	17858	29816	1.86%	0.240%
81	12.310	3503	3505	3509	rVB5	2013	1107	0.07%	0.009%
82	12.484	3557	3559	3564	rBV6	1411	1161	0.07%	0.009%
83	12.583	3586	3590	3592	rBV5	2381	1898	0.12%	0.015%
84	13.008	3720	3722	3725	rBV3	1833	866	0.05%	0.007%
85	13.069	3736	3741	3746	rBV7	1730	1867	0.12%	0.015%
86	13.210	3777	3785	3793	rVB10	3892	5646	0.35%	0.045%
87	13.551	3887	3891	3893	rBV3	1655	1171	0.07%	0.009%
88	13.689	3927	3934	3941	rBV9	4443	5868	0.37%	0.047%
89	13.744	3947	3951	3954	rBV4	1484	1239	0.08%	0.010%
90	13.873	3977	3991	4006	rBV3	34318	61719	3.84%	0.496%
91	14.140	4072	4074	4078	rVB2	2387	1595	0.10%	0.013%
92	14.355	4138	4141	4145	rBV5	2045	1892	0.12%	0.015%
93	14.410	4155	4158	4161	rBV4	1521	1092	0.07%	0.009%
94	14.590	4209	4214	4216	rBV4	1991	1892	0.12%	0.015%
95	14.715	4250	4253	4256	rBV5	1514	1035	0.06%	0.008%
96	14.786	4272	4275	4277	rBV4	2487	1436	0.09%	0.012%
97	14.969	4328	4332	4338	rVB7	1636	1864	0.12%	0.015%
98	15.027	4347	4350	4353	rBV3	1407	969	0.06%	0.008%
99	15.062	4356	4361	4366	rBV8	2423	2816	0.18%	0.023%
100	15.927	4625	4630	4632	rBV4	2442	2436	0.15%	0.020%

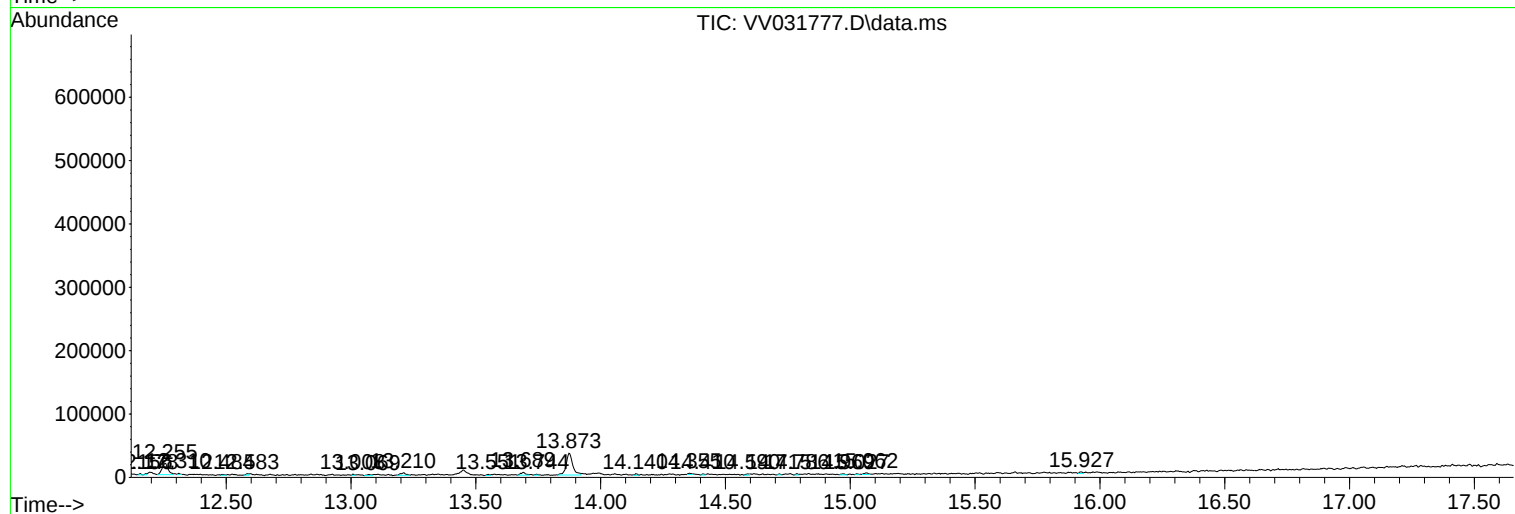
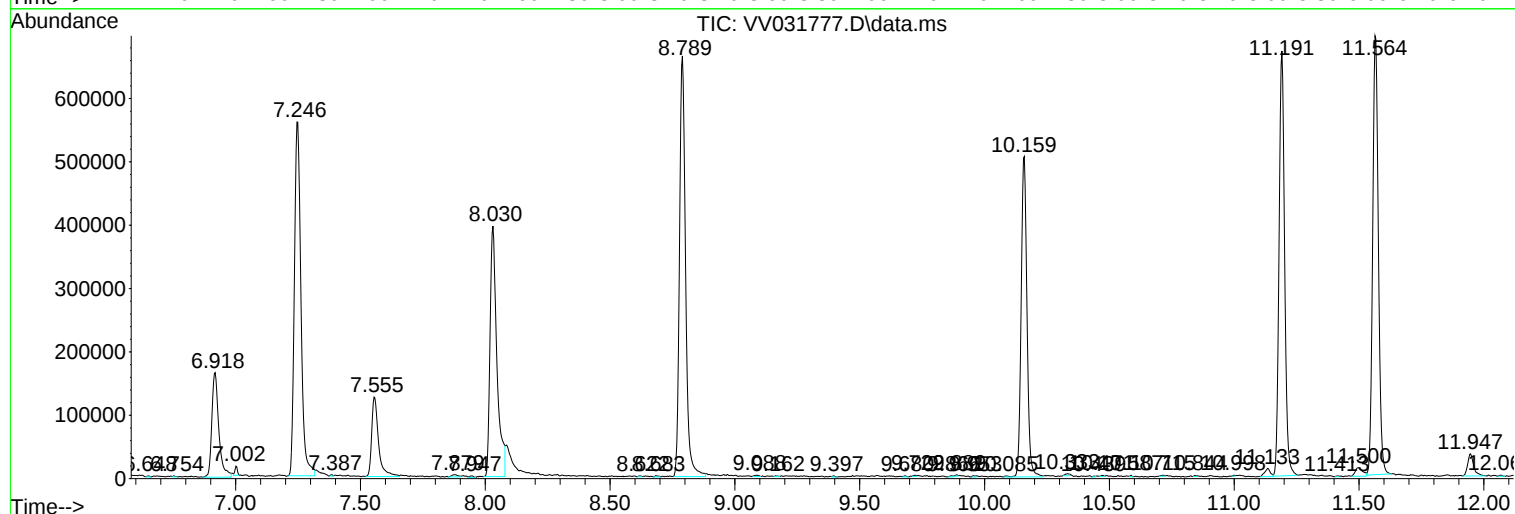
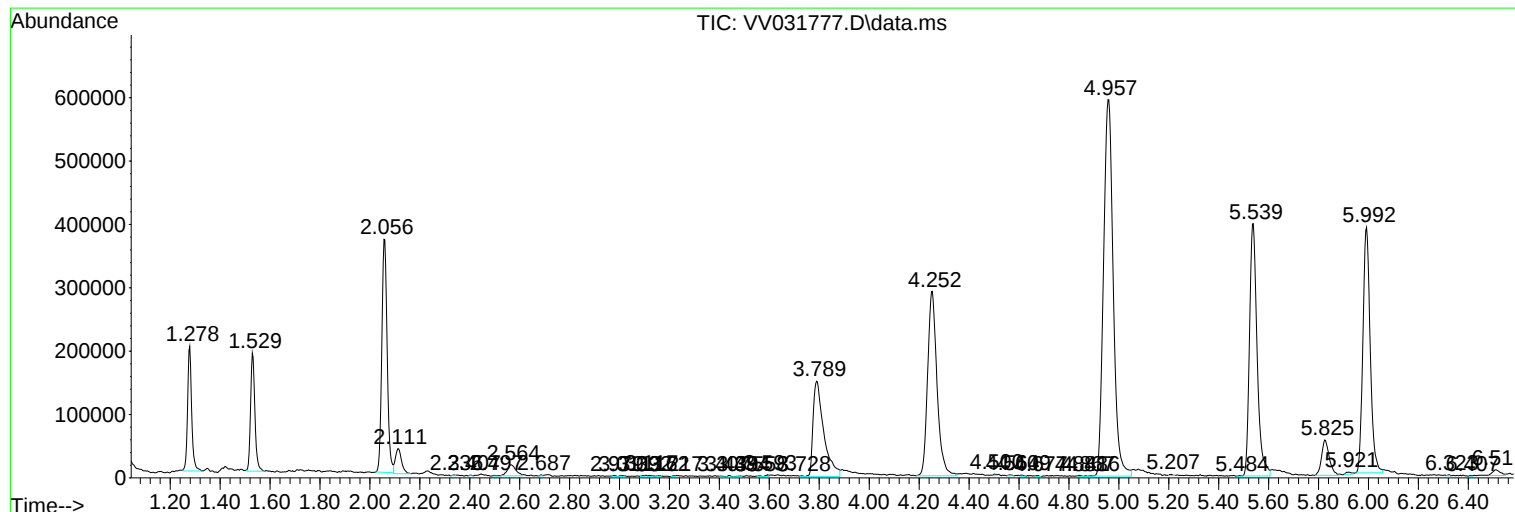
Sum of corrected areas: 12434851

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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



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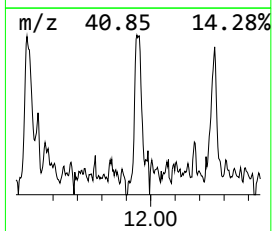
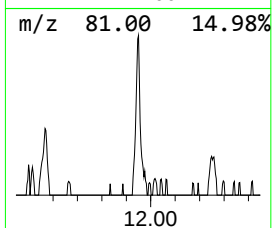
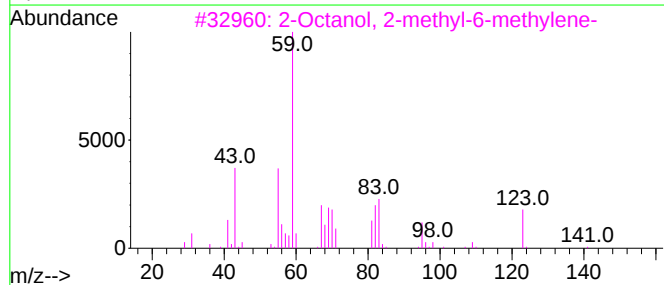
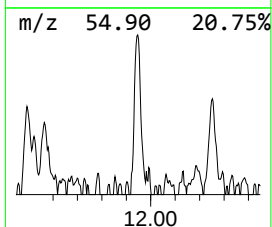
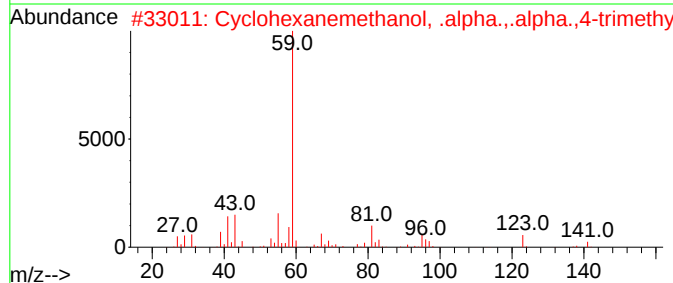
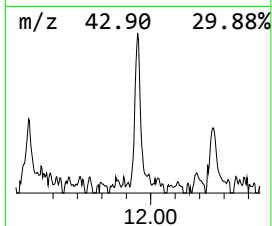
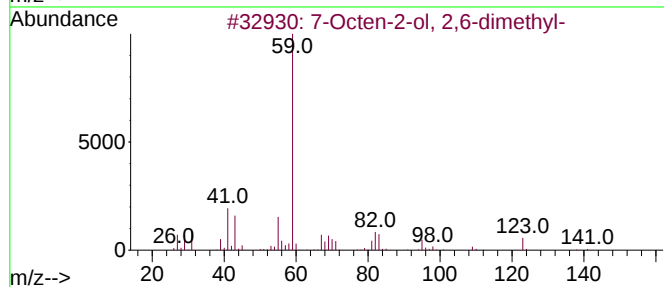
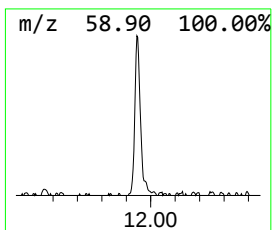
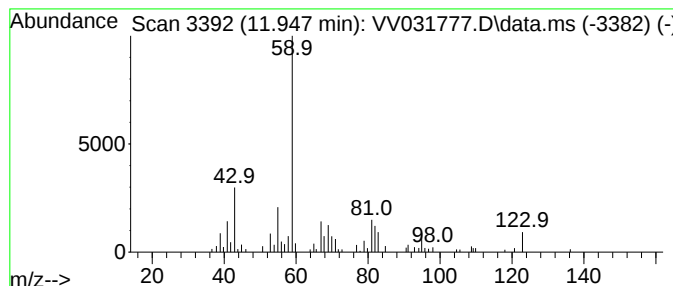
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.947	2.84 ug/L	59010	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	72
2			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	50
3			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	50
4			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	50
5			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	50



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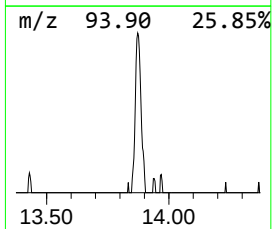
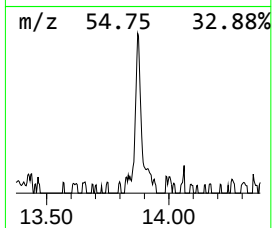
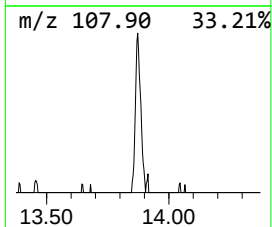
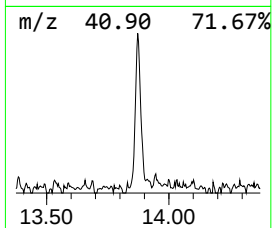
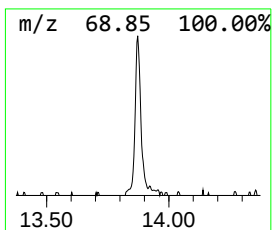
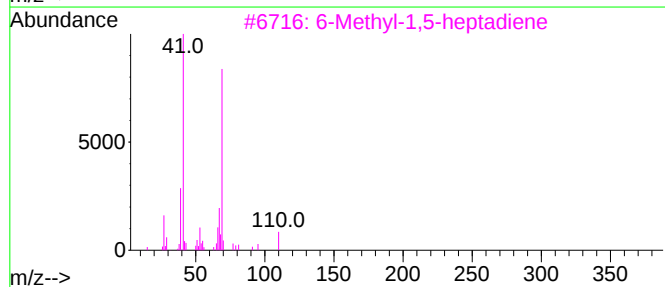
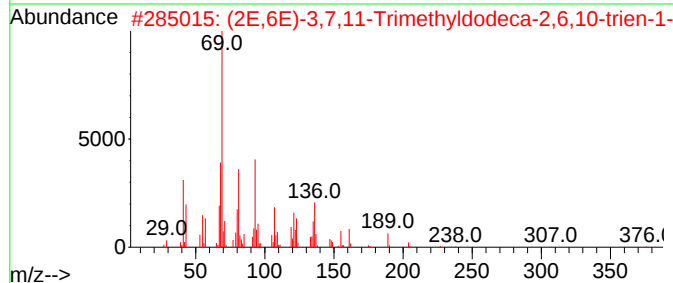
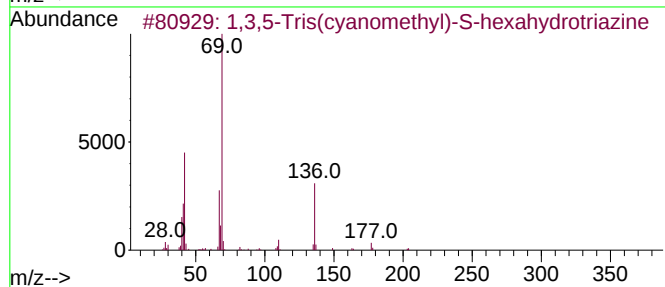
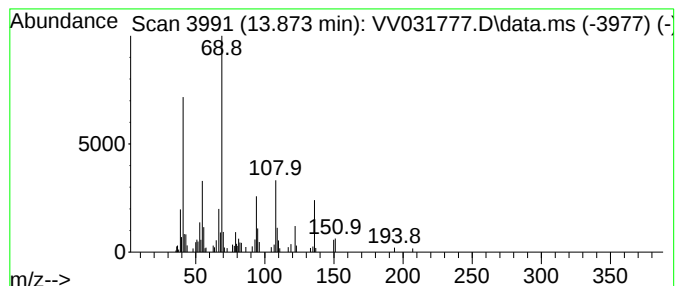
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Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	2.97 ug/L	61719	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	47
2			(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	45
3			6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	38
4			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	38
5			Cyclopropanecarboxaldehyde, 2-me...	166	C11H18O	097231-35-1	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
7-Octen-2-ol, 2...	11.947	2.8	ug/L	59010	3	11.191	1039790	50.0
unknown-01	13.873	3.0	ug/L	61719	3	11.191	1039790	50.0