

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV020222\
 Data File : VV024526.D
 Acq On : 02 Feb 2022 15:47
 Operator : SY/MD
 Sample : N1353-09ME
 Misc : 3.26g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 COVF2ME

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\SFAMVLM020222WMA.M
 Title : VOC Analysis

Signal : TIC: VV024526.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	98	rVB	170333	199538	14.26%	1.674%
2	1.564	156	163	179	rBV	124513	180291	12.88%	1.512%
3	2.092	318	327	340	rBV	249193	353242	25.24%	2.963%
4	2.905	577	580	586	rVB6	1073	907	0.06%	0.008%
5	3.179	659	665	669	rBV8	629	888	0.06%	0.007%
6	3.217	675	677	682	rVB5	822	581	0.04%	0.005%
7	3.693	819	825	829	rVB6	759	819	0.06%	0.007%
8	3.767	845	848	852	rBV5	843	690	0.05%	0.006%
9	3.918	883	895	896	rBV	42588	63260	4.52%	0.531%
10	4.343	1012	1027	1057	rVB	209824	545448	38.98%	4.575%
11	4.632	1114	1117	1120	rBV3	613	511	0.04%	0.004%
12	4.699	1134	1138	1140	rBV4	623	571	0.04%	0.005%
13	5.040	1226	1244	1283	rBV2	560965	1399318	100.00%	11.738%
14	5.291	1319	1322	1328	rBV5	501	564	0.04%	0.005%
15	5.339	1328	1337	1338	rBV5	4307	4583	0.33%	0.038%
16	5.613	1409	1422	1458	rBV	432067	902752	64.51%	7.573%
17	5.799	1477	1480	1483	rBV3	949	624	0.04%	0.005%
18	5.902	1497	1512	1529	rBV3	26980	61408	4.39%	0.515%
19	6.066	1550	1563	1590	rBV	293693	632489	45.20%	5.306%
20	6.207	1598	1607	1620	rBV3	13338	39034	2.79%	0.327%
21	6.918	1820	1828	1835	rBV8	2040	3392	0.24%	0.028%
22	6.985	1838	1849	1874	rVV	178614	351803	25.14%	2.951%
23	7.188	1904	1912	1914	rBV4	1172	1434	0.10%	0.012%
24	7.233	1914	1926	1935	rBV	153425	361775	25.85%	3.035%
25	7.313	1943	1951	1968	rVB	661606	1219036	87.12%	10.226%
26	7.567	2022	2030	2037	rBV5	4835	7014	0.50%	0.059%
27	7.622	2037	2047	2079	rVB	111630	244234	17.45%	2.049%
28	8.127	2183	2204	2231	rBV3	171880	689296	49.26%	5.782%
29	8.349	2265	2273	2285	rBV6	5343	9736	0.70%	0.082%
30	8.471	2308	2311	2314	rVB4	825	526	0.04%	0.004%
31	8.503	2314	2321	2330	rVB9	1610	3015	0.22%	0.025%
32	8.542	2330	2333	2334	rBV3	912	489	0.03%	0.004%
33	8.590	2336	2348	2362	rBV7	6998	16556	1.18%	0.139%
34	8.719	2384	2388	2395	rVB5	962	1265	0.09%	0.011%
35	8.789	2395	2410	2418	rBV4	5588	11121	0.79%	0.093%
36	8.854	2418	2430	2455	rBV	566050	1104970	78.96%	9.269%

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Integrator: RTE

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 Title : VOC Analysis

37	9.018	2467	2481	2501	rVB	32543	67141	4.80%	0.563%
38	9.140	2501	2519	2533	rBV	150878	285365	20.39%	2.394%
39	9.317	2569	2574	2575	rBV2	1076	858	0.06%	0.007%
40	9.471	2608	2622	2633	rBV9	6787	15618	1.12%	0.131%
41	9.548	2636	2646	2663	rVB2	56749	100742	7.20%	0.845%
42	9.677	2678	2686	2687	rBV5	2317	2535	0.18%	0.021%
43	9.718	2689	2699	2717	rVV2	70443	140670	10.05%	1.180%
44	10.014	2786	2791	2798	rBV7	1948	2456	0.18%	0.021%
45	10.088	2804	2814	2817	rBV9	2702	4173	0.30%	0.035%
46	10.124	2818	2825	2837	rVB4	8195	15148	1.08%	0.127%
47	10.223	2842	2856	2875	rBV	326205	594233	42.47%	4.985%
48	10.368	2894	2901	2904	rBV8	1717	2571	0.18%	0.022%
49	10.455	2918	2928	2935	rBV3	10953	19807	1.42%	0.166%
50	10.577	2961	2966	2981	rVB2	19540	28765	2.06%	0.241%
51	10.741	3007	3017	3035	rVB10	6544	17248	1.23%	0.145%
52	10.834	3035	3046	3051	rBV7	2286	3925	0.28%	0.033%
53	10.879	3053	3060	3065	rBV3	6778	9619	0.69%	0.081%
54	10.918	3065	3072	3084	rVB3	23169	37358	2.67%	0.313%
55	11.027	3096	3106	3107	rBV6	3365	3437	0.25%	0.029%
56	11.252	3165	3176	3195	rBV	669276	1039696	74.30%	8.721%
57	11.339	3196	3203	3211	rBV2	9882	14850	1.06%	0.125%
58	11.625	3281	3292	3311	rVB	621138	997953	71.32%	8.371%
59	11.789	3334	3343	3351	rBV2	21838	32125	2.30%	0.269%
60	11.918	3377	3383	3386	rBV4	3093	3834	0.27%	0.032%
61	11.985	3401	3404	3408	rBV6	1918	2031	0.15%	0.017%
62	12.249	3485	3486	3487	rBB	441	913	0.07%	0.008%
63	12.316	3505	3507	3515	rVB7	1167	1138	0.08%	0.010%
64	12.371	3515	3524	3529	rBV8	3719	5960	0.43%	0.050%
65	12.413	3529	3537	3546	rVB6	4596	7509	0.54%	0.063%
66	12.464	3546	3553	3561	rBV5	9119	14028	1.00%	0.118%
67	12.632	3603	3605	3609	rBV4	861	479	0.03%	0.004%
68	12.712	3625	3630	3631	rBV3	641	497	0.04%	0.004%
69	12.844	3668	3671	3673	rBV3	704	503	0.04%	0.004%
70	12.889	3678	3685	3695	rVB7	7324	10545	0.75%	0.088%
71	13.162	3766	3770	3773	rVV5	1015	913	0.07%	0.008%
72	13.197	3777	3781	3785	rVB6	766	759	0.05%	0.006%
73	13.268	3801	3803	3812	rVB5	1310	1227	0.09%	0.010%
74	13.342	3823	3826	3830	rBV2	749	724	0.05%	0.006%
75	13.480	3865	3869	3871	rBV3	582	475	0.03%	0.004%
76	13.509	3871	3878	3879	rBV5	2006	1771	0.13%	0.015%

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 ClientSampleId :
 C0VF2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
 Title : VOC Analysis

77	13.664	3923	3926	3929	rBV4	722	497	0.04%	0.004%
78	13.696	3933	3936	3940	rBV3	1099	810	0.06%	0.007%
79	13.802	3963	3969	3970	rBV3	560	641	0.05%	0.005%
80	13.924	4003	4007	4010	rVB4	819	664	0.05%	0.006%
81	13.943	4010	4013	4018	rBV4	788	721	0.05%	0.006%
82	13.969	4018	4021	4024	rBV2	710	509	0.04%	0.004%
83	14.040	4036	4043	4050	rVB8	1049	1636	0.12%	0.014%
84	14.123	4066	4069	4073	rVB3	652	543	0.04%	0.005%
85	14.146	4073	4076	4078	rBV	654	485	0.03%	0.004%
86	14.259	4105	4111	4114	rBV3	476	511	0.04%	0.004%
87	14.329	4130	4133	4137	rVV4	862	604	0.04%	0.005%
88	14.419	4158	4161	4164	rVB4	815	531	0.04%	0.004%
89	14.471	4173	4177	4183	rVB5	713	868	0.06%	0.007%
90	14.541	4197	4199	4205	rVB6	627	567	0.04%	0.005%
91	14.586	4210	4213	4217	rBV3	724	722	0.05%	0.006%
92	14.776	4269	4272	4274	rVV3	754	499	0.04%	0.004%
93	14.853	4291	4296	4300	rBV5	956	1142	0.08%	0.010%
94	15.107	4372	4375	4380	rVB	2997	2126	0.15%	0.018%
95	15.139	4380	4385	4388	rBV8	913	910	0.07%	0.008%
96	15.175	4394	4396	4399	rBV3	987	678	0.05%	0.006%
97	15.352	4448	4451	4454	rBV4	591	496	0.04%	0.004%
98	15.570	4515	4519	4522	rBV3	648	553	0.04%	0.005%
99	15.866	4608	4611	4616	rBV3	869	910	0.07%	0.008%
100	16.101	4682	4684	4688	rBV4	1065	810	0.06%	0.007%

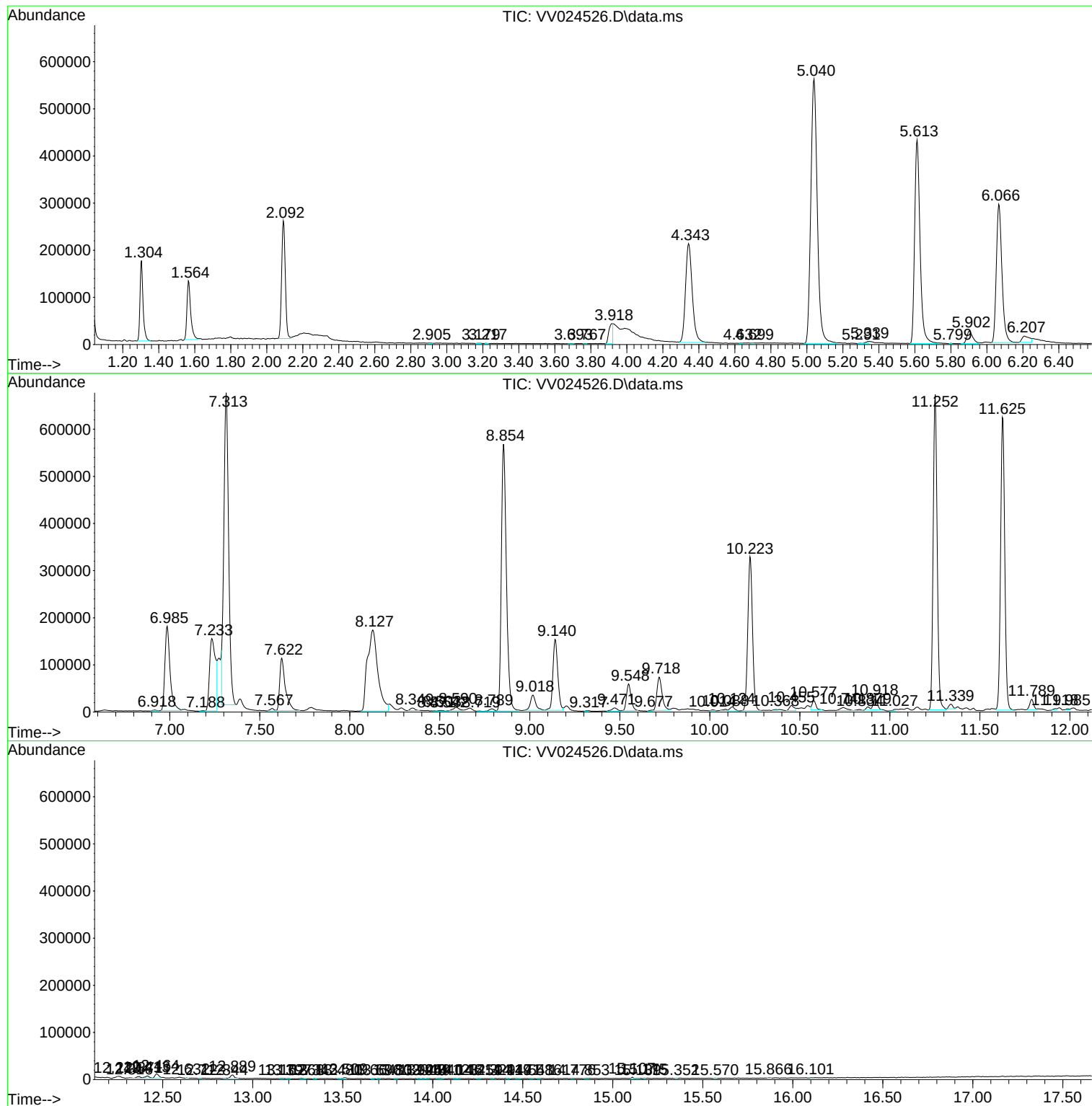
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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C0VF2ME

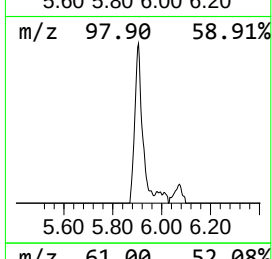
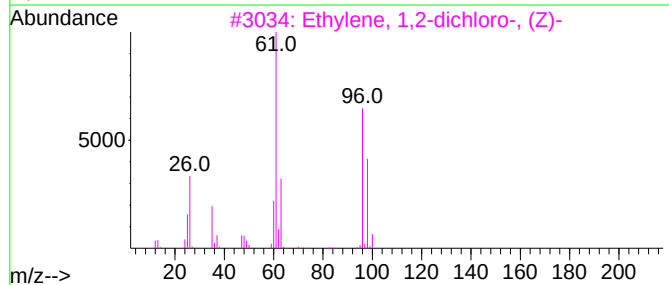
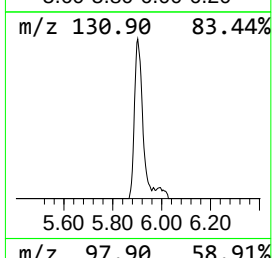
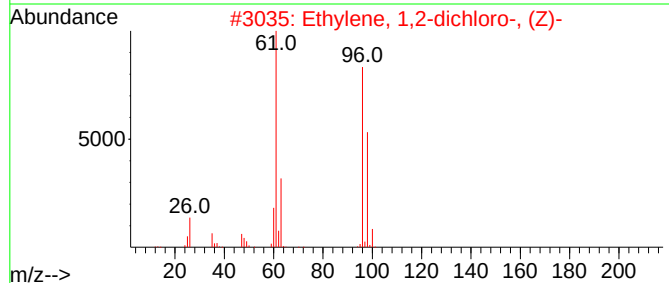
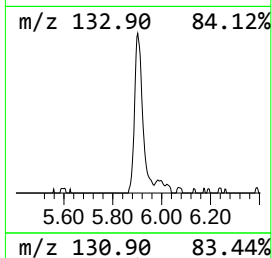
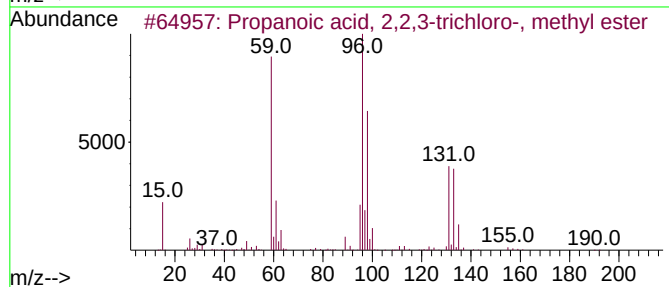
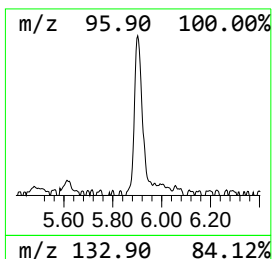
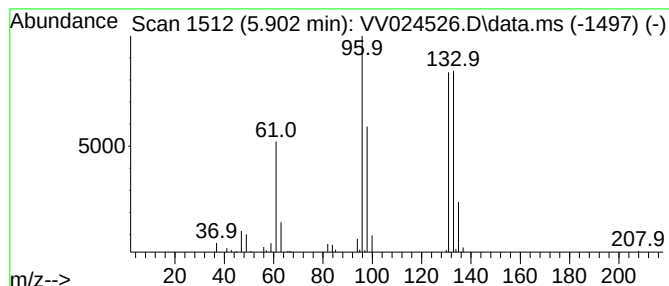
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.40 ug/L	61408	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
4			Ethene, 1,1-dichloro-	96	C2H2Cl2	000075-35-4	38
5			Ethene, 1,1-dichloro-	96	C2H2Cl2	000075-35-4	38



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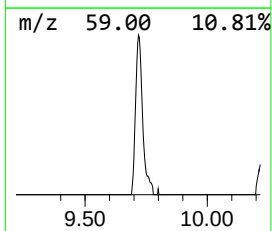
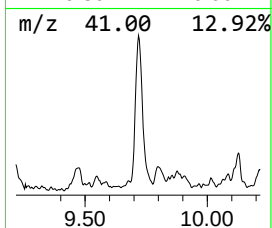
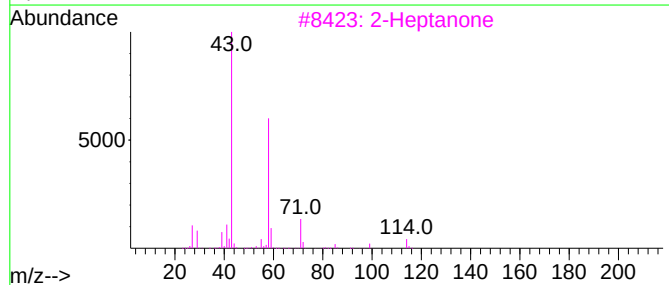
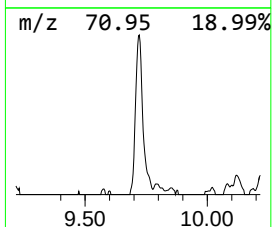
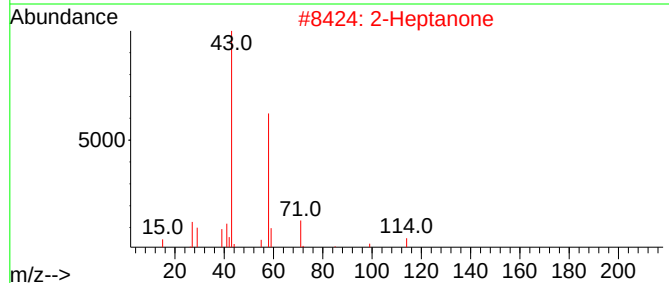
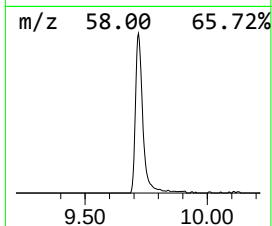
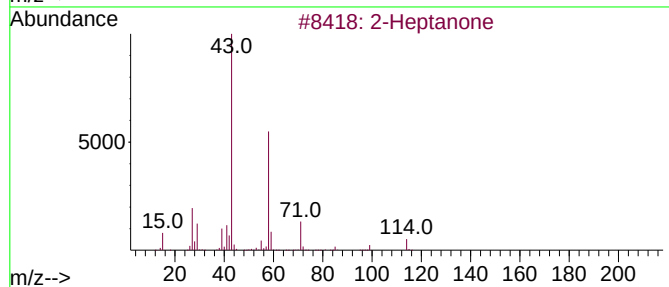
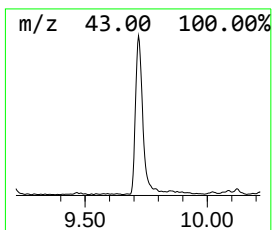
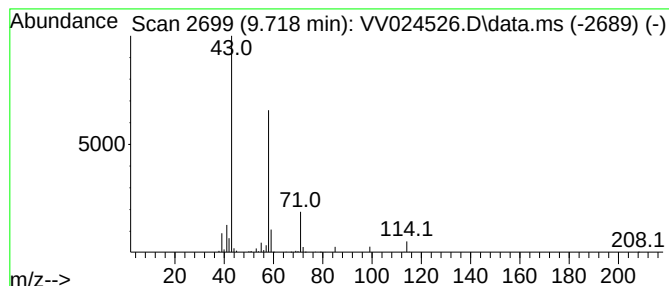
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Quant Title : VOC Analysis

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

Peak Number 3 2-Heptanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.718	6.37 ug/L	140670	Chlorobenzene-d5	8.854

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	91
2	2-Heptanone			114	C7H14O	000110-43-0	91
3	2-Heptanone			114	C7H14O	000110-43-0	91
4	2-Heptanone			114	C7H14O	000110-43-0	87
5	2-Hexanone, 5-methyl-			114	C7H14O	000110-12-3	86



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.902	3.4	ug/L	61408	1	5.613	902752	50.0
2-Heptanone	9.718	6.4	ug/L	140670	2	8.854	1104970	50.0