

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070221\
 Data File : VV021596.D
 Acq On : 02 Jul 2021 14:28
 Operator : SY/MD
 Sample : M2914-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBK50

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\SFAMVLM062921WMA.M

Title : VOC Analysis

Signal : TIC: VV021596.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	76	82	95	rVB	172594	174528	11.28%	1.367%
2	1.561	155	162	176	rVB	147434	170215	11.00%	1.333%
3	2.105	321	331	346	rBV	318665	461984	29.86%	3.619%
4	2.291	382	389	397	rBV	5290	7739	0.50%	0.061%
5	2.391	415	420	424	rBV3	370	430	0.03%	0.003%
6	2.426	429	431	434	rBV2	442	265	0.02%	0.002%
7	2.503	448	455	461	rBV5	1408	1998	0.13%	0.016%
8	2.571	474	476	481	rVB3	501	332	0.02%	0.003%
9	2.600	482	485	488	rBV4	587	395	0.03%	0.003%
10	2.642	494	498	502	rBV4	754	520	0.03%	0.004%
11	3.095	633	639	641	rBV5	388	316	0.02%	0.002%
12	3.127	647	649	656	rVB5	355	341	0.02%	0.003%
13	3.327	707	711	712	rBV5	494	291	0.02%	0.002%
14	3.616	798	801	807	rBV4	540	583	0.04%	0.005%
15	3.870	870	880	923	rBV	120415	328798	21.25%	2.576%
16	4.150	965	967	970	rVB3	597	303	0.02%	0.002%
17	4.262	1000	1002	1005	rVB3	603	322	0.02%	0.003%
18	4.346	1011	1028	1053	rBV	243855	605505	39.14%	4.743%
19	4.580	1098	1101	1104	rBV3	504	428	0.03%	0.003%
20	4.635	1115	1118	1122	rBV4	294	271	0.02%	0.002%
21	4.674	1127	1130	1133	rVV2	493	304	0.02%	0.002%
22	5.043	1226	1245	1276	rBV2	601721	1547154	100.00%	12.119%
23	5.317	1327	1330	1336	rVV4	805	588	0.04%	0.005%
24	5.368	1342	1346	1349	rVB2	433	385	0.02%	0.003%
25	5.420	1357	1362	1365	rBV4	543	497	0.03%	0.004%
26	5.439	1367	1368	1373	rVB3	795	512	0.03%	0.004%
27	5.526	1390	1395	1397	rBV3	563	565	0.04%	0.004%
28	5.613	1408	1422	1451	rBV	521321	1041297	67.30%	8.157%
29	5.905	1502	1513	1530	rBV4	14922	32127	2.08%	0.252%
30	5.982	1535	1537	1543	rBV5	676	673	0.04%	0.005%
31	6.069	1550	1564	1585	rBV	338422	688875	44.53%	5.396%
32	6.195	1601	1603	1605	rBV3	1021	542	0.04%	0.004%
33	6.291	1631	1633	1636	rVB3	602	291	0.02%	0.002%
34	6.314	1636	1640	1642	rBV5	357	294	0.02%	0.002%
35	6.458	1679	1685	1690	rBV3	448	609	0.04%	0.005%
36	6.542	1706	1711	1714	rBV3	441	300	0.02%	0.002%

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 Title : VOC Analysis

37	6.622	1727	1736	1752	rBV7	3952	10507	0.68%	0.082%
38	6.683	1753	1755	1759	rVV4	1299	1079	0.07%	0.008%
39	6.725	1763	1768	1773	rVV6	657	673	0.04%	0.005%
40	6.986	1837	1849	1868	rBV	201861	365004	23.59%	2.859%
41	7.156	1895	1902	1903	rBV6	1922	1940	0.13%	0.015%
42	7.314	1939	1951	1970	rBV	742770	1288105	83.26%	10.090%
43	7.622	2035	2047	2065	rBV	135673	237494	15.35%	1.860%
44	7.777	2093	2095	2103	rVB4	534	539	0.03%	0.004%
45	8.085	2180	2191	2227	rBV	413902	745822	48.21%	5.842%
46	8.455	2303	2306	2311	rVB3	440	352	0.02%	0.003%
47	8.635	2359	2362	2364	rBV4	522	339	0.02%	0.003%
48	8.854	2417	2430	2456	rBV	754190	1228493	79.40%	9.623%
49	9.059	2490	2494	2502	rVB4	797	871	0.06%	0.007%
50	9.149	2511	2522	2534	rVV8	2806	5591	0.36%	0.044%
51	9.394	2592	2598	2601	rBV5	735	834	0.05%	0.007%
52	9.593	2657	2660	2667	rVB4	332	275	0.02%	0.002%
53	9.641	2670	2675	2680	rBV5	703	655	0.04%	0.005%
54	9.677	2685	2686	2690	rVB2	437	264	0.02%	0.002%
55	9.702	2690	2694	2695	rBV2	534	296	0.02%	0.002%
56	9.738	2701	2705	2706	rBV2	434	303	0.02%	0.002%
57	9.905	2753	2757	2759	rBV2	363	275	0.02%	0.002%
58	10.008	2785	2789	2791	rVV4	432	335	0.02%	0.003%
59	10.063	2802	2806	2810	rVB3	619	517	0.03%	0.004%
60	10.127	2818	2826	2834	rBV7	1641	2624	0.17%	0.021%
61	10.217	2842	2854	2880	rVB	477450	741829	47.95%	5.811%
62	10.313	2880	2884	2886	rBV5	475	404	0.03%	0.003%
63	10.358	2894	2898	2901	rBV3	1013	869	0.06%	0.007%
64	10.452	2920	2927	2931	rBV6	3112	4105	0.27%	0.032%
65	10.670	2988	2995	2996	rBV3	766	749	0.05%	0.006%
66	10.696	2997	3003	3013	rVB3	3380	5207	0.34%	0.041%
67	10.764	3022	3024	3028	rVB2	766	407	0.03%	0.003%
68	10.818	3034	3041	3045	rBV4	958	1303	0.08%	0.010%
69	10.921	3065	3073	3081	rVB	6736	9234	0.60%	0.072%
70	10.989	3090	3094	3095	rBV2	532	293	0.02%	0.002%
71	11.024	3097	3105	3116	rVV7	3385	6299	0.41%	0.049%
72	11.088	3116	3125	3135	rVB6	7165	11896	0.77%	0.093%
73	11.143	3138	3142	3148	rBV6	827	1098	0.07%	0.009%
74	11.249	3164	3175	3188	rBV	813396	1250180	80.81%	9.793%
75	11.445	3230	3236	3246	rVB2	7641	10665	0.69%	0.084%
76	11.535	3259	3264	3275	rVB7	3451	4776	0.31%	0.037%

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 Title : VOC Analysis

77	11.625	3280	3292	3307	rBV	748665	1174957	75.94%	9.204%
78	11.744	3328	3329	3334	rBV4	775	614	0.04%	0.005%
79	11.921	3373	3384	3392	rBV	41588	68652	4.44%	0.538%
80	11.966	3393	3398	3412	rVB3	14227	23680	1.53%	0.185%
81	12.088	3434	3436	3438	rBV2	655	453	0.03%	0.004%
82	12.181	3459	3465	3468	rBV5	1044	1375	0.09%	0.011%
83	12.464	3546	3553	3563	rVB3	10012	14792	0.96%	0.116%
84	12.551	3572	3580	3584	rBV4	7065	9965	0.64%	0.078%
85	12.783	3645	3652	3658	rBV9	7497	11569	0.75%	0.091%
86	12.847	3663	3672	3681	rVV3	31071	47738	3.09%	0.374%
87	13.017	3722	3725	3727	rBV2	823	533	0.03%	0.004%
88	13.043	3731	3733	3735	rBV3	1022	603	0.04%	0.005%
89	13.185	3770	3777	3787	rVB5	6846	11527	0.75%	0.090%
90	13.416	3829	3849	3859	rBV4	31135	68595	4.43%	0.537%
91	13.513	3871	3879	3895	rVB2	16675	31429	2.03%	0.246%
92	13.593	3895	3904	3925	rBV2	27303	62616	4.05%	0.490%
93	13.808	3964	3971	3989	rVV6	16384	34034	2.20%	0.267%
94	13.882	3989	3994	4003	rVB9	4079	5497	0.36%	0.043%
95	14.024	4032	4038	4048	rVB3	18178	25147	1.63%	0.197%
96	14.197	4084	4092	4109	rVB2	26300	39990	2.58%	0.313%
97	14.336	4128	4135	4141	rBV6	3188	4876	0.32%	0.038%
98	14.609	4214	4220	4224	rBV4	9111	11416	0.74%	0.089%
99	16.435	4781	4788	4802	rVB	38362	60404	3.90%	0.473%
100	17.098	4988	4994	5005	rVB3	27484	42446	2.74%	0.332%

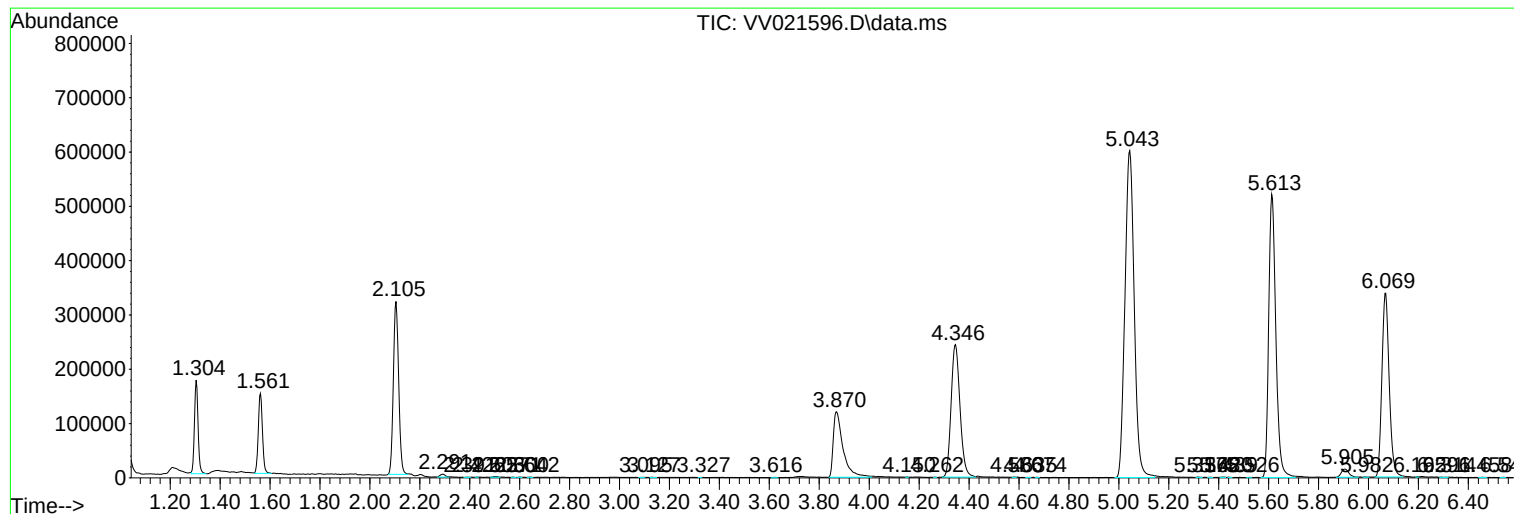
Sum of corrected areas: 12765986

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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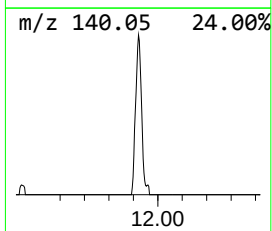
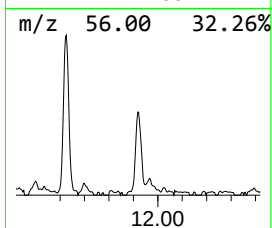
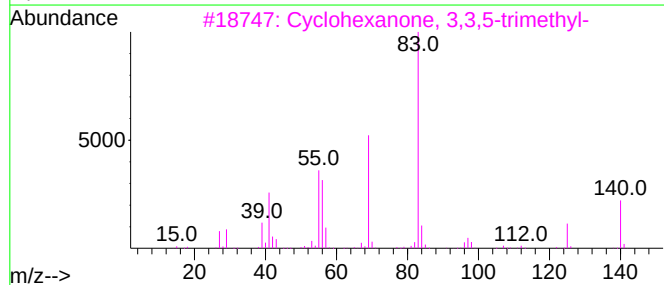
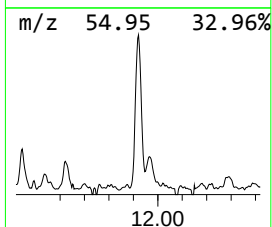
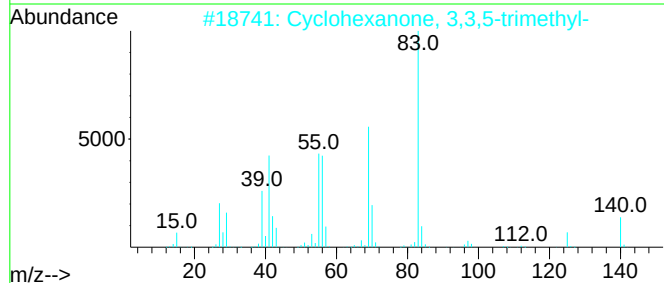
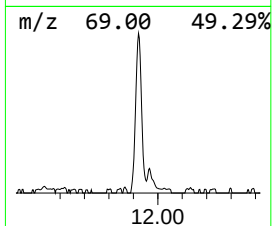
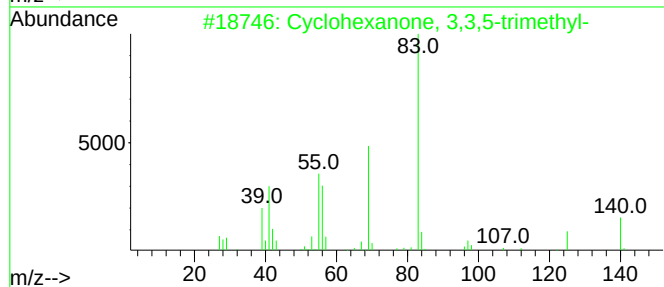
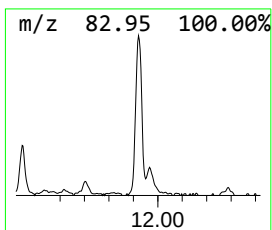
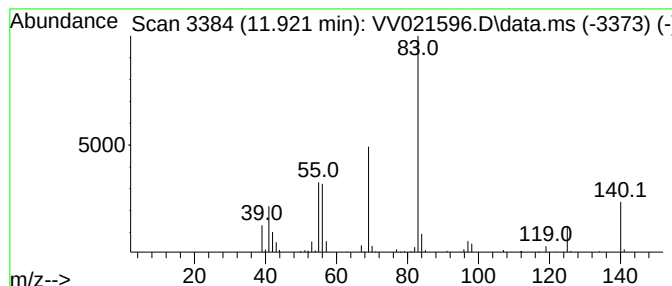
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Cyclohexanone, 3,3,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	2.75 ug/L	68652	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	96
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	90
4			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N02	042282-85-9	47
5			1,3-Cyclohexanedione, 5,5-dimethyl-	140	C8H12O2	000126-81-8	47



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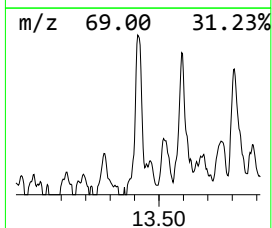
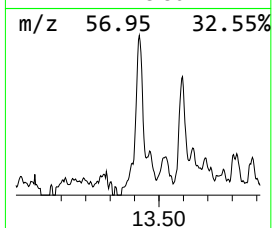
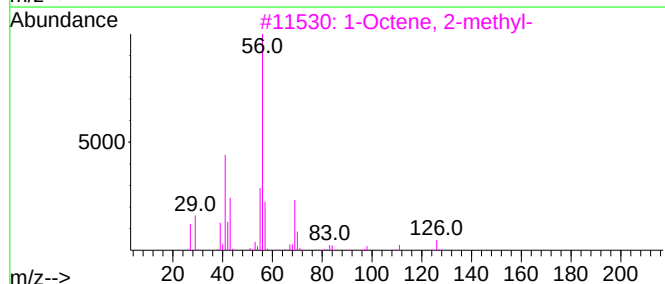
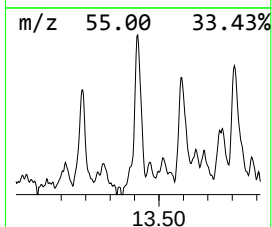
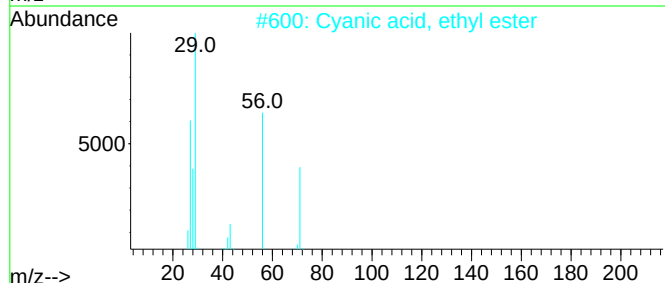
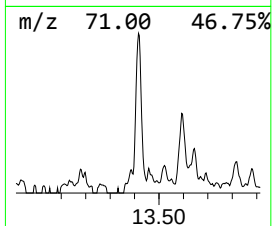
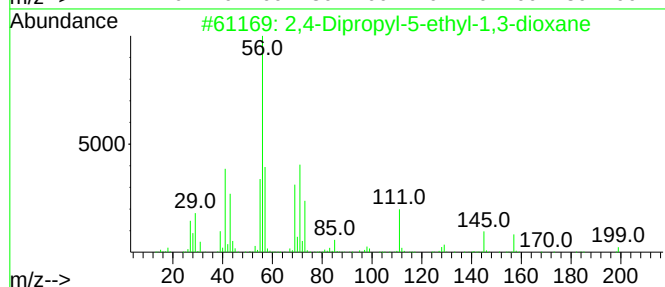
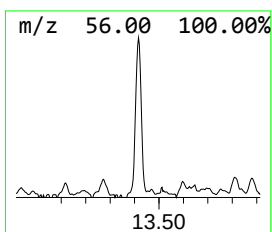
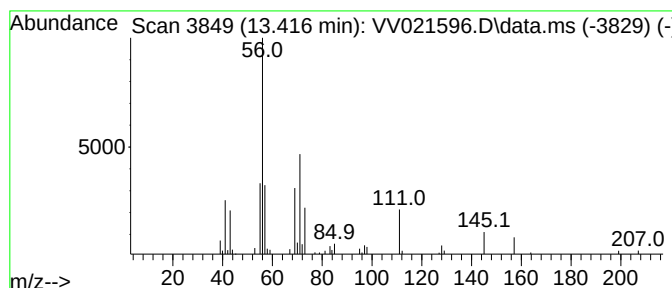
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Quant Title : VOC Analysis

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

Peak Number 3 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.416	2.74 ug/L	68595	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	83
2			Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	47
3			1-Octene, 2-methyl-	126	C9H18	004588-18-5	35
4			1-Decene, 2-methyl-	154	C11H22	013151-27-4	35
5			Cyclopentanone, 2,2,5,5-tetramet...	140	C9H16O	004541-35-9	27



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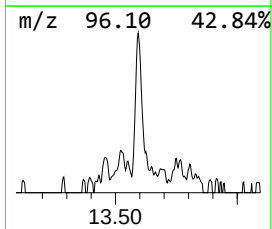
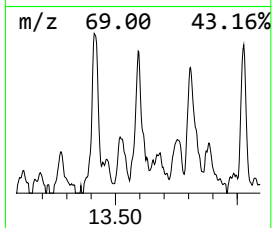
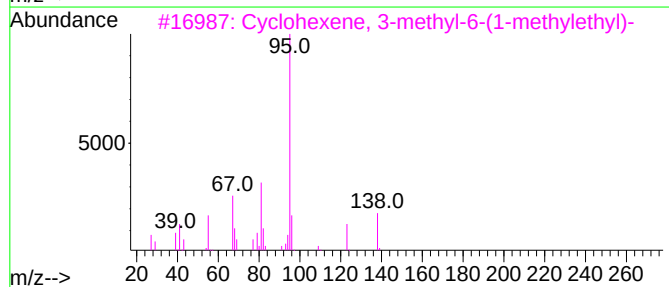
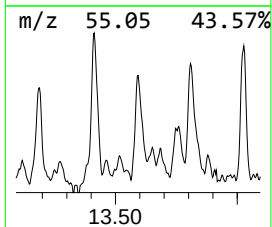
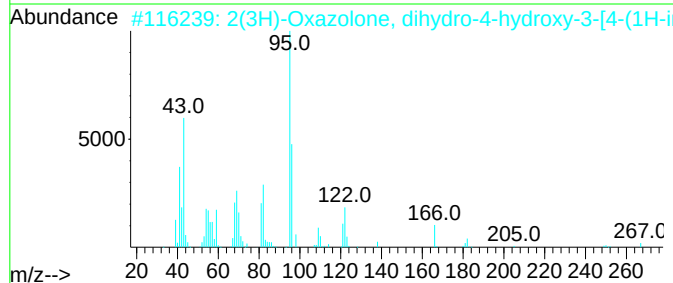
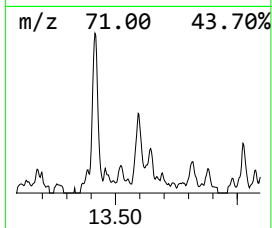
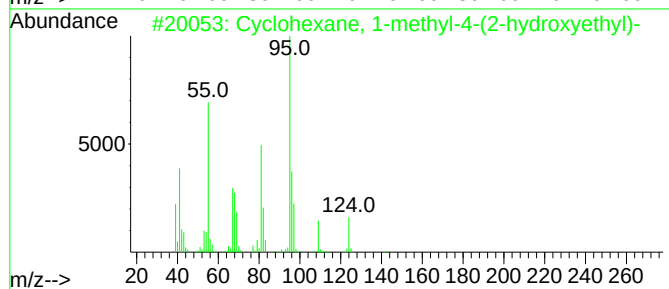
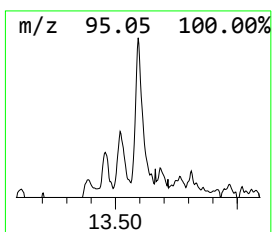
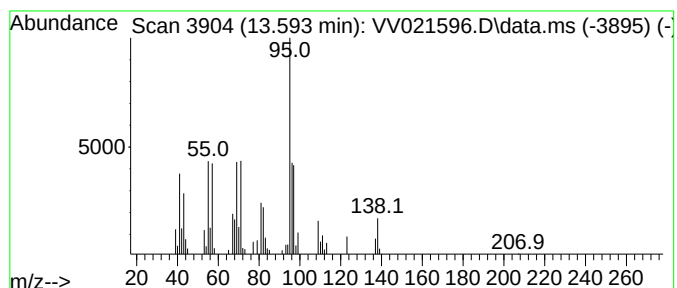
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.593	2.50 ug/L	62616	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-4-(2-hydro...	142	C9H18O	004916-87-4	47
2			2(3H)-Oxazolone, dihydro-4-hydro...	267	C13H21N3O3	1000319-29-4	43
3			Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	38
4			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	35
5			4-Methyl-1-prop-1-ynyl-cyclohexanol	152	C10H16O	1000362-94-7	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070221\
Data File : VV021596.D
Acq On : 02 Jul 2021 14:28
Operator : SY/MD
Sample : M2914-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBK50

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone, ...	11.921	2.8	ug/L	68652	3	11.249	1250180	50.0
2,4-Dipropyl-5-...	13.416	2.7	ug/L	68595	3	11.249	1250180	50.0
unknown-01	13.593	2.5	ug/L	62616	3	11.249	1250180	50.0