

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100121\
 Data File : VV022499.D
 Acq On : 02 Oct 2021 06:01
 Operator : SY/MD
 Sample : M4023-09
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AJ8

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\SFAMVLM100121WMA.M
 Title : VOC Analysis

Signal : TIC: VV022499.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	94	rBV2	155368	169151	0.06%	0.036%
2	1.413	113	116	129	rVB4	3642	4258	0.00%	0.001%
3	1.568	156	164	178	rBV	97788	110109	0.04%	0.024%
4	1.777	224	229	236	rVB2	7153	7809	0.00%	0.002%
5	1.841	242	249	263	rVB	40016	51152	0.02%	0.011%
6	2.114	321	334	378	rBV	28071517	42774402	15.69%	9.203%
7	2.507	447	456	470	rVB2	11585	20643	0.01%	0.004%
8	2.606	483	487	489	rBV3	621	442	0.00%	0.000%
9	2.764	525	536	553	rVV	61593	108739	0.04%	0.023%
10	3.037	614	621	624	rVV5	640	775	0.00%	0.000%
11	3.191	652	669	699	rBV	533798	1136851	0.42%	0.245%
12	3.397	729	733	734	rBV3	1032	573	0.00%	0.000%
13	3.532	772	775	779	rBV4	644	468	0.00%	0.000%
14	3.761	841	846	850	rBV4	488	544	0.00%	0.000%
15	3.918	873	895	954	rBV	29621330	74418374	27.30%	16.011%
16	4.359	1017	1032	1064	rVB3	133797	415306	0.15%	0.089%
17	4.626	1089	1115	1170	rBV	21253933	54330595	19.93%	11.689%
18	5.053	1232	1248	1265	rBV2	283714	755080	0.28%	0.162%
19	5.394	1352	1354	1360	rVB3	685	428	0.00%	0.000%
20	5.622	1412	1425	1458	rVV	240408	550417	0.20%	0.118%
21	5.957	1490	1529	1539	rBV4	61640242	272629681	100.00%	58.657%
22	6.661	1741	1748	1760	rVB4	9748	17540	0.01%	0.004%
23	6.992	1841	1851	1872	rBV	98866	179051	0.07%	0.039%
24	7.240	1920	1928	1940	rBV2	9556	18632	0.01%	0.004%
25	7.320	1942	1953	1965	rVV	372831	638654	0.23%	0.137%
26	7.391	1966	1975	2000	rVB	424851	726975	0.27%	0.156%
27	7.625	2039	2048	2071	rBV	68435	118220	0.04%	0.025%
28	7.841	2103	2115	2137	rBV	546415	941235	0.35%	0.203%
29	7.937	2138	2145	2151	rVV2	20947	38719	0.01%	0.008%
30	7.979	2152	2158	2175	rVB	53206	88767	0.03%	0.019%
31	8.092	2183	2193	2221	rBV	156952	324977	0.12%	0.070%
32	8.487	2309	2316	2328	rVB5	7992	13882	0.01%	0.003%
33	8.612	2352	2355	2361	rVB2	673	616	0.00%	0.000%
34	8.767	2394	2403	2409	rBV5	4983	8810	0.00%	0.002%
35	8.854	2419	2430	2451	rBV	423519	686943	0.25%	0.148%
36	8.976	2457	2468	2473	rBV	288617	452070	0.17%	0.097%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
 Title : VOC Analysis

37	9.014	2474	2480	2501	rVV	833891	1260552	0.46%	0.271%
38	9.140	2503	2519	2536	rVV	3532139	5622896	2.06%	1.210%
39	9.227	2539	2546	2566	rVB2	46028	84504	0.03%	0.018%
40	9.545	2632	2645	2674	rBV	2579917	3921002	1.44%	0.844%
41	9.728	2696	2702	2709	rBV4	1324	1491	0.00%	0.000%
42	9.796	2716	2723	2731	rBV9	3496	5036	0.00%	0.001%
43	9.934	2750	2766	2781	rBV2	32195	54011	0.02%	0.012%
44	10.008	2781	2789	2792	rBV3	2146	2935	0.00%	0.001%
45	10.101	2815	2818	2822	rVB5	1265	824	0.00%	0.000%
46	10.217	2842	2854	2867	rBV	236463	372974	0.14%	0.080%
47	10.323	2884	2887	2890	rBV4	1122	739	0.00%	0.000%
48	10.358	2890	2898	2906	rBV3	11863	19029	0.01%	0.004%
49	10.452	2918	2927	2932	rBV2	10779	15258	0.01%	0.003%
50	10.545	2948	2956	2963	rBV3	7021	9205	0.00%	0.002%
51	10.741	3009	3017	3024	rVV2	5052	7568	0.00%	0.002%
52	10.847	3042	3050	3056	rBV6	2724	3806	0.00%	0.001%
53	10.918	3063	3072	3075	rBV	13173	17294	0.01%	0.004%
54	10.956	3076	3084	3094	rVB	76098	123595	0.05%	0.027%
55	11.030	3102	3107	3115	rBV5	900	1082	0.00%	0.000%
56	11.088	3118	3125	3137	rVB9	4786	7393	0.00%	0.002%
57	11.149	3137	3144	3146	rBV4	1129	1107	0.00%	0.000%
58	11.172	3146	3151	3154	rBV5	2391	2640	0.00%	0.001%
59	11.249	3163	3175	3194	rBV	492502	745829	0.27%	0.160%
60	11.349	3194	3206	3217	rVV5	7093	14669	0.01%	0.003%
61	11.432	3226	3232	3239	rVB4	1343	1926	0.00%	0.000%
62	11.535	3256	3264	3275	rBV5	14421	22496	0.01%	0.005%
63	11.625	3280	3292	3307	rVV	378687	585631	0.21%	0.126%
64	11.690	3310	3312	3322	rVV8	3517	3642	0.00%	0.001%
65	11.767	3333	3336	3338	rVV3	860	596	0.00%	0.000%
66	11.783	3338	3341	3345	rVV5	952	863	0.00%	0.000%
67	11.866	3363	3367	3370	rBV3	734	571	0.00%	0.000%
68	11.902	3373	3378	3381	rVV3	478	492	0.00%	0.000%
69	11.937	3381	3389	3400	rVV7	2338	4063	0.00%	0.001%
70	12.014	3406	3413	3422	rVV7	2552	3500	0.00%	0.001%
71	12.108	3436	3442	3446	rBV4	752	908	0.00%	0.000%
72	12.188	3461	3467	3475	rBV5	2505	3498	0.00%	0.001%
73	12.252	3479	3487	3493	rBV7	5472	8338	0.00%	0.002%
74	12.384	3520	3528	3539	rVB3	4281	6858	0.00%	0.001%
75	12.603	3589	3596	3606	rVV8	6970	11128	0.00%	0.002%
76	12.648	3606	3610	3616	rVB5	851	805	0.00%	0.000%

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 Title : VOC Analysis

77	12.879	3677	3682	3689	rVB5	1165	1505	0.00%	0.000%
78	12.944	3694	3702	3715	rVB4	25259	36554	0.01%	0.008%
79	13.079	3742	3744	3751	rVB4	510	517	0.00%	0.000%
80	13.136	3751	3762	3774	rBV3	26890	40582	0.01%	0.009%
81	13.448	3853	3859	3867	rBV7	1852	2027	0.00%	0.000%
82	13.506	3871	3877	3878	rBV3	949	850	0.00%	0.000%
83	13.567	3889	3896	3904	rBV6	3190	4597	0.00%	0.001%
84	13.667	3924	3927	3933	rVB3	706	454	0.00%	0.000%
85	14.136	4069	4073	4076	rBV2	797	641	0.00%	0.000%
86	14.474	4176	4178	4184	rVB4	515	480	0.00%	0.000%
87	14.638	4224	4229	4232	rBV2	515	685	0.00%	0.000%
88	14.738	4256	4260	4264	rVB2	462	451	0.00%	0.000%
89	14.860	4295	4298	4302	rVV5	573	431	0.00%	0.000%
90	14.982	4330	4336	4343	rBV4	591	838	0.00%	0.000%
91	15.017	4343	4347	4351	rVV3	451	450	0.00%	0.000%
92	15.101	4371	4373	4375	rBV	1248	722	0.00%	0.000%
93	15.522	4500	4504	4506	rBV5	628	459	0.00%	0.000%
94	15.545	4508	4511	4516	rBV3	706	572	0.00%	0.000%
95	15.638	4535	4540	4542	rBV3	441	441	0.00%	0.000%
96	15.702	4557	4560	4561	rBV	855	450	0.00%	0.000%
97	15.738	4568	4571	4576	rBV4	526	501	0.00%	0.000%
98	16.062	4668	4672	4674	rBV4	560	510	0.00%	0.000%
99	16.429	4782	4786	4789	rBV5	838	666	0.00%	0.000%
100	16.448	4789	4792	4795	rVB3	948	708	0.00%	0.000%

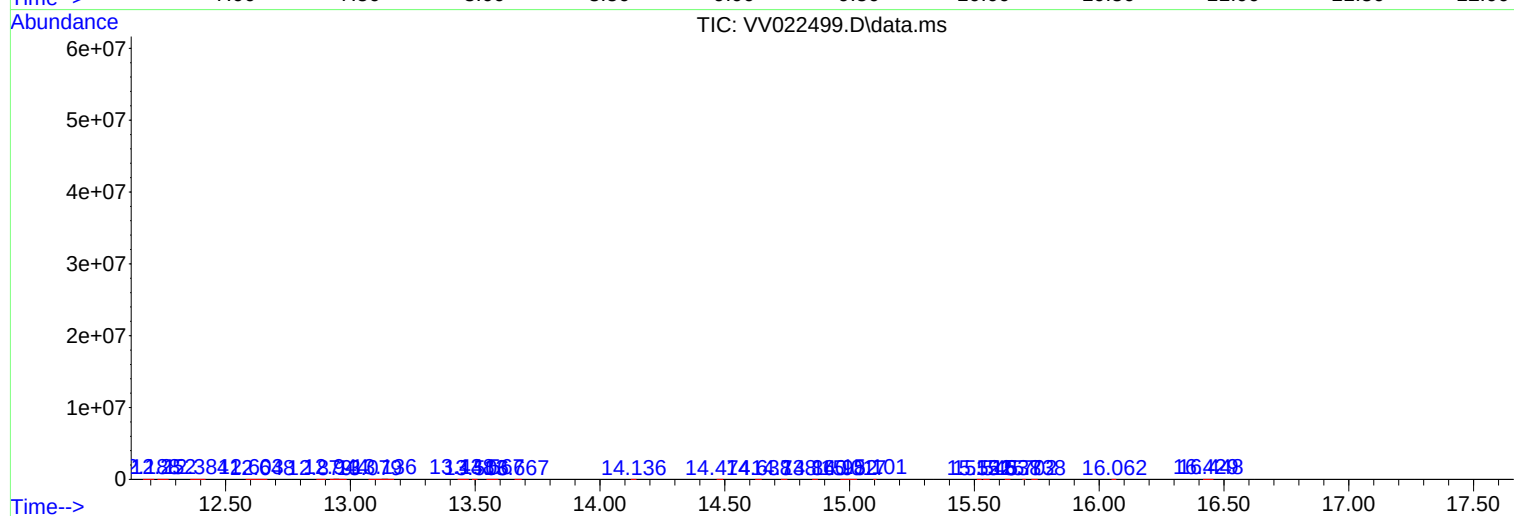
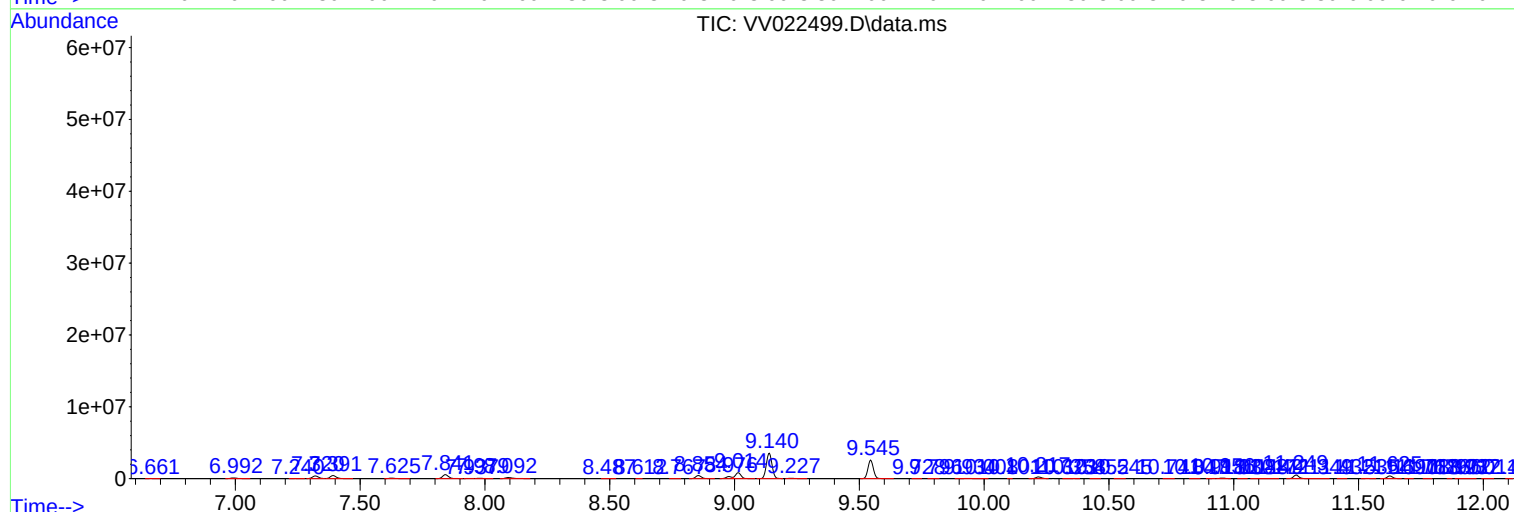
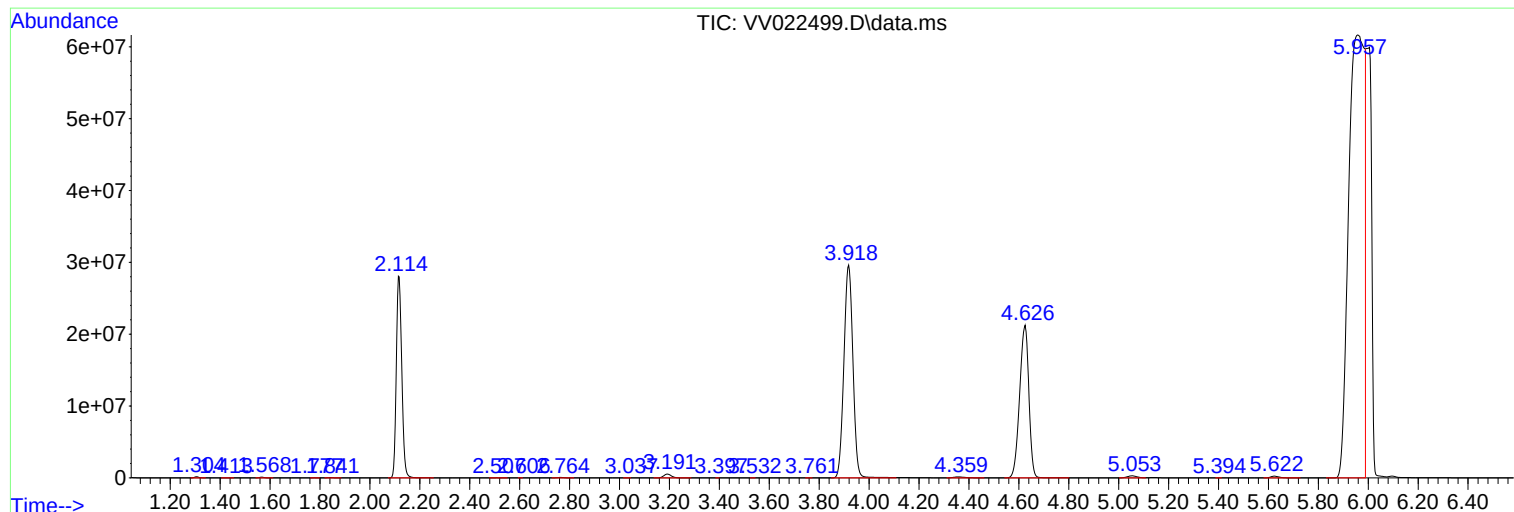
Sum of corrected areas: 464787733

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Instrument :
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ClientSampleId :
C0AJ8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.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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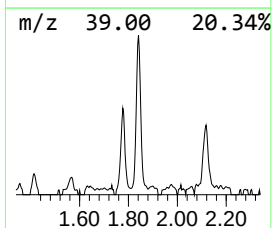
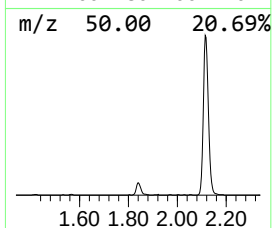
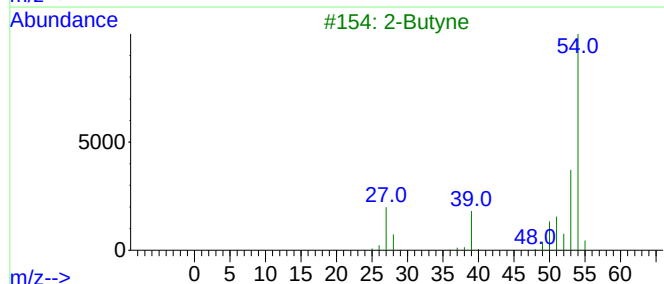
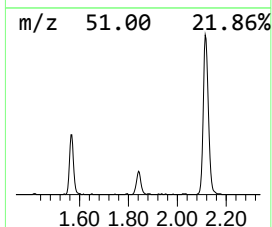
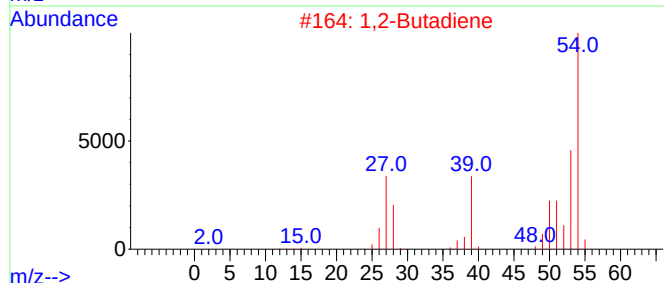
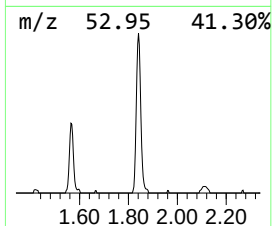
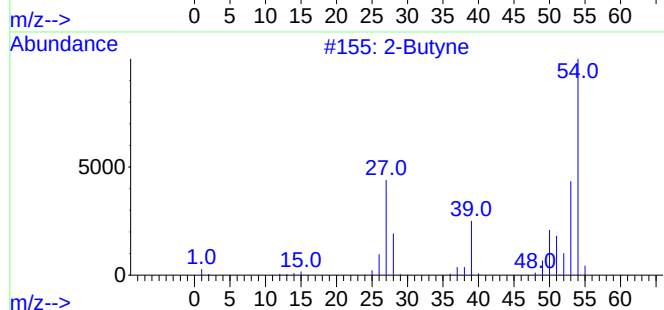
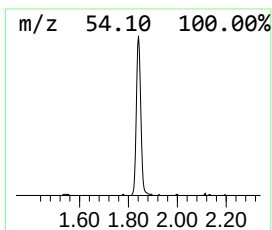
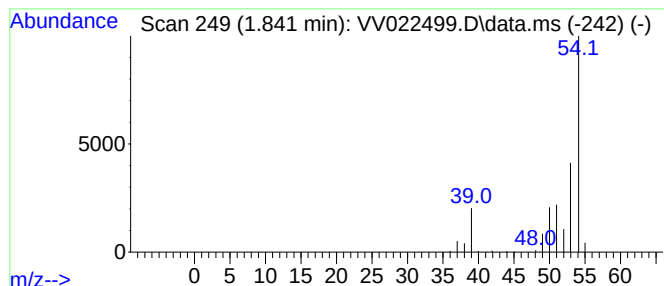
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Butyne Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.841	4.65 ug/L	51152	1,4-Difluorobenzene	5.625

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butyne			54	C4H6	000503-17-3	87
2	1,2-Butadiene			54	C4H6	000590-19-2	86
3	2-Butyne			54	C4H6	000503-17-3	86
4	1-Butyne			54	C4H6	000107-00-6	78
5	2-Butyne			54	C4H6	000503-17-3	78



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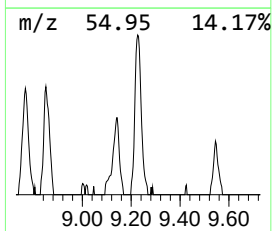
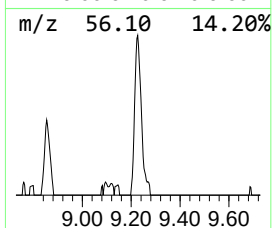
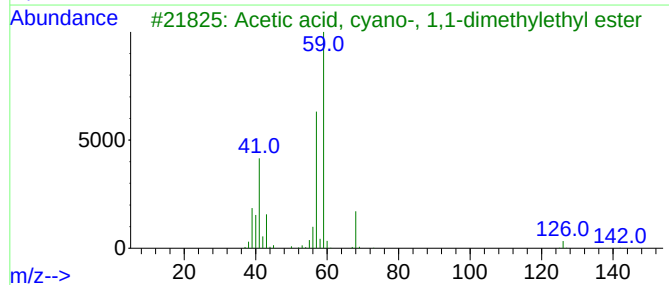
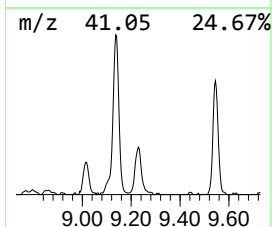
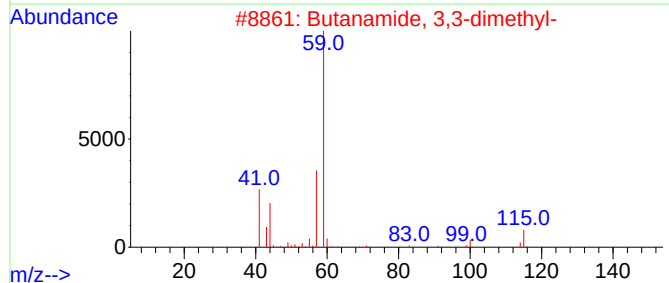
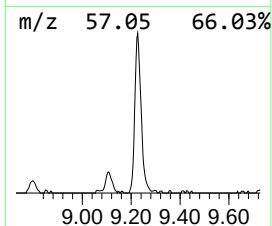
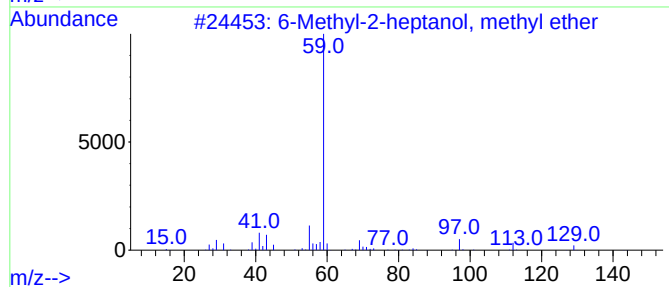
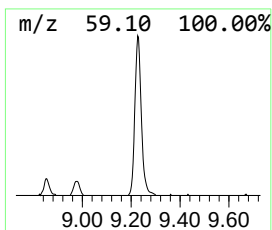
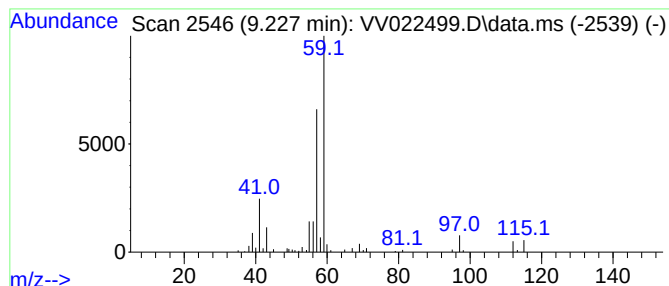
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 6-Methyl-2-heptanol, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.227	6.15 ug/L	84504	Chlorobenzene-d5	8.854

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	59
2			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	59
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	50
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	45
5			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	40



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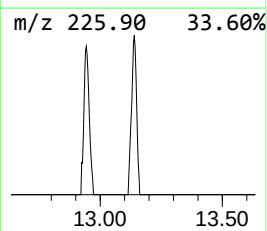
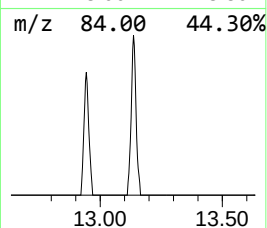
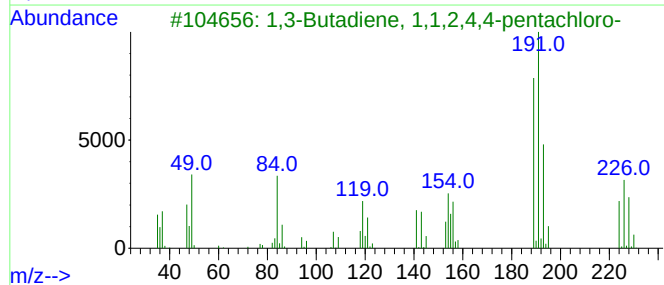
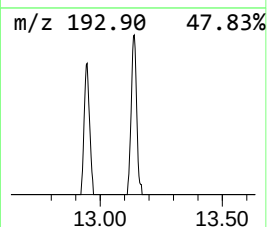
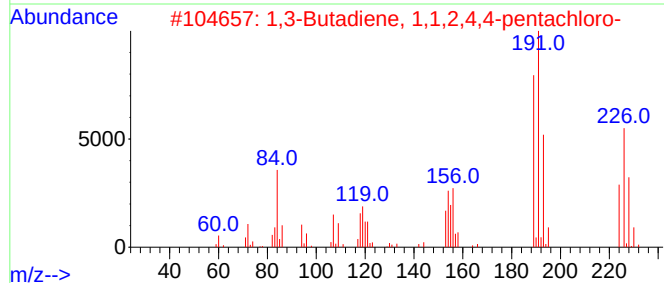
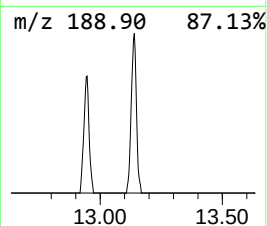
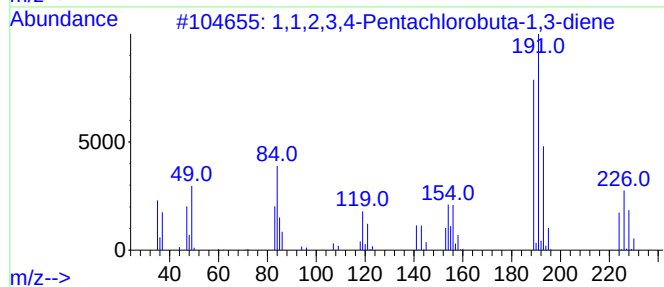
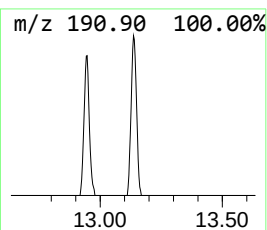
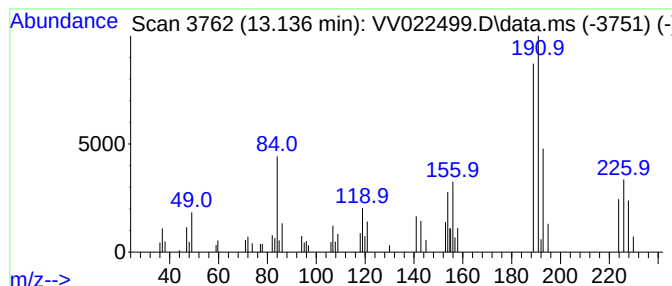
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1,1,2,3,4-Pentachlorobuta-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.136	2.72 ug/L	40582	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HCl5	1010487-10-4	98		
2	1,3-Butadiene, 1,1,2,4,4-pentachloro-	224	C4HCl5	021400-41-9	91		
3	1,3-Butadiene, 1,1,2,4,4-pentachloro-	224	C4HCl5	021400-41-9	91		
4	Thiophene-3-carbonyl chloride, 4-	224	C5H2BrClO5	072899-51-5	50		
5	2-Thiophenecarbonyl chloride, 5-	224	C5H2BrClO5	031555-60-9	50		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100121\
Data File : VV022499.D
Acq On : 02 Oct 2021 06:01
Operator : SY/MD
Sample : M4023-09
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AJ8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butyne	1.841	4.7	ug/L	51152	1	5.625	550417	50.0
6-Methyl-2-hept...	9.227	6.2	ug/L	84504	2	8.854	686943	50.0
1,1,2,3,4-Penta...	13.136	2.7	ug/L	40582	3	11.249	745829	50.0