

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092419\
 Data File : VU034790.D
 Acq On : 24 Sep 2019 22:41
 Operator : JC/SP
 Sample : K4984-06ME 10X
 Misc : 4.99g/5.0ml/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEDLOME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.174	22	26	34	rBV2	7281	8271	0.04%	0.019%
2	1.322	69	72	77	rBV5	4134	3829	0.02%	0.009%
3	1.392	86	94	105	rBV	341648	354905	1.63%	0.814%
4	1.579	129	152	162	rBV4	84011	249585	1.15%	0.572%
5	1.656	168	176	185	rBV	278546	348813	1.61%	0.800%
6	2.254	352	362	386	rVB	526110	828595	3.81%	1.900%
7	2.569	454	460	462	rBV5	1987	2068	0.01%	0.005%
8	2.614	467	474	479	rVV6	1420	2539	0.01%	0.006%
9	2.678	487	494	502	rBV6	4950	7944	0.04%	0.018%
10	2.820	524	538	550	rBV	44543	95776	0.44%	0.220%
11	2.929	567	572	577	rBV5	1187	1195	0.01%	0.003%
12	2.974	583	586	591	rVB5	1494	1276	0.01%	0.003%
13	3.003	591	595	601	rVB8	1487	1436	0.01%	0.003%
14	3.096	621	624	628	rVB3	1678	1209	0.01%	0.003%
15	3.170	639	647	651	rBV5	1513	1868	0.01%	0.004%
16	3.190	651	653	657	rBV3	1232	1130	0.01%	0.003%
17	3.312	688	691	695	rVB3	1933	1079	0.00%	0.002%
18	3.357	702	705	710	rBV5	1298	1076	0.00%	0.002%
19	3.813	841	847	848	rBV5	1265	1214	0.01%	0.003%
20	4.148	939	951	989	rBV2	273721	944909	4.35%	2.167%
21	4.302	996	999	1003	rVB3	2134	1255	0.01%	0.003%
22	4.344	1010	1012	1014	rBV3	2021	1149	0.01%	0.003%
23	4.389	1025	1026	1035	rVB8	2151	2439	0.01%	0.006%
24	4.620	1081	1098	1119	rBV	417490	986301	4.54%	2.262%
25	4.865	1165	1174	1179	rVV10	3111	4916	0.02%	0.011%
26	4.977	1207	1209	1215	rVB6	2562	2209	0.01%	0.005%
27	5.064	1233	1236	1242	rVB6	1851	1845	0.01%	0.004%
28	5.100	1242	1247	1249	rBV5	1790	1303	0.01%	0.003%
29	5.112	1249	1251	1255	rVB4	1638	1286	0.01%	0.003%
30	5.315	1288	1314	1337	rBV2	883041	2608437	12.01%	5.982%
31	5.466	1356	1361	1362	rBV4	2019	1373	0.01%	0.003%
32	5.707	1430	1436	1441	rBV7	1529	2138	0.01%	0.005%
33	5.772	1451	1456	1460	rVB8	1574	1734	0.01%	0.004%
34	5.862	1471	1484	1505	rBV	741078	1476545	6.80%	3.386%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
 Title : VOC Analysis

35	6.167	1567	1579	1598	rVB4	79262	169537	0.78%	0.389%
36	6.305	1608	1622	1644	rBV	615195	1231079	5.67%	2.823%
37	6.775	1763	1768	1769	rBV4	1384	1237	0.01%	0.003%
38	6.845	1789	1790	1794	rVV3	1820	1307	0.01%	0.003%
39	6.865	1794	1796	1804	rVV7	1953	1958	0.01%	0.004%
40	7.206	1890	1902	1931	rVV	352347	645648	2.97%	1.481%
41	7.321	1931	1938	1949	rVB	4141	7123	0.03%	0.016%
42	7.408	1963	1965	1971	rVB5	1370	1293	0.01%	0.003%
43	7.466	1971	1983	1991	rBV5	6063	10598	0.05%	0.024%
44	7.543	1993	2007	2028	rBV	1214509	2155081	9.92%	4.942%
45	7.752	2071	2072	2076	rVB4	1869	1208	0.01%	0.003%
46	7.826	2076	2095	2113	rBV	246730	449844	2.07%	1.032%
47	7.990	2143	2146	2150	rVB6	2098	1636	0.01%	0.004%
48	8.206	2196	2213	2229	rBV	13055208	21723518	100.00%	49.818%
49	8.289	2230	2239	2273	rVB	937441	1733054	7.98%	3.974%
50	8.456	2289	2291	2298	rVB7	3729	3060	0.01%	0.007%
51	8.588	2325	2332	2336	rVV8	5298	7512	0.03%	0.017%
52	8.720	2370	2373	2376	rBV4	2547	2259	0.01%	0.005%
53	8.739	2376	2379	2385	rVB7	2707	2063	0.01%	0.005%
54	8.797	2390	2397	2402	rVV5	4629	7461	0.03%	0.017%
55	8.823	2402	2405	2409	rVV6	3447	3517	0.02%	0.008%
56	8.842	2409	2411	2416	rVV4	2889	2655	0.01%	0.006%
57	8.887	2417	2425	2436	rVB3	15906	27820	0.13%	0.064%
58	8.964	2442	2449	2452	rBV7	1503	1787	0.01%	0.004%
59	9.013	2454	2464	2469	rBV3	13247	23336	0.11%	0.054%
60	9.067	2469	2481	2512	rVB	1085128	1793619	8.26%	4.113%
61	9.231	2525	2532	2535	rBV8	2393	2446	0.01%	0.006%
62	9.328	2552	2562	2565	rBV10	4045	6241	0.03%	0.014%
63	9.382	2572	2579	2584	rVV7	5632	7300	0.03%	0.017%
64	9.424	2584	2592	2603	rVB3	30229	46951	0.22%	0.108%
65	9.623	2649	2654	2656	rVV6	1480	1401	0.01%	0.003%
66	9.691	2667	2675	2687	rVB6	8269	17432	0.08%	0.040%
67	9.759	2693	2696	2698	rBV3	1627	1275	0.01%	0.003%
68	9.791	2704	2706	2708	rBV4	2109	1245	0.01%	0.003%
69	9.926	2735	2748	2758	rVB7	13288	25496	0.12%	0.058%
70	9.977	2760	2764	2767	rBV4	1949	1669	0.01%	0.004%
71	10.022	2767	2778	2785	rBV4	14504	28254	0.13%	0.065%

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Integration Parameters: LSCINT.P

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72	10.132	2804	2812	2817	rBV9	5617	9674	0.04%	0.022%
73	10.202	2825	2834	2837	rBV7	6644	9677	0.04%	0.022%
74	10.234	2838	2844	2850	rVB8	6326	8330	0.04%	0.019%
75	10.299	2853	2864	2869	rBV9	10483	18685	0.09%	0.043%
76	10.408	2887	2898	2914	rBV	846814	1398686	6.44%	3.208%
77	10.508	2927	2929	2933	rVB5	2592	1851	0.01%	0.004%
78	10.575	2947	2950	2951	rBV3	1887	1199	0.01%	0.003%
79	10.607	2953	2960	2961	rBV6	4689	5043	0.02%	0.012%
80	10.672	2975	2980	2981	rBV5	5045	4444	0.02%	0.010%
81	10.730	2990	2998	3008	rBV8	13738	24944	0.11%	0.057%
82	10.794	3009	3018	3028	rVV2	41209	62589	0.29%	0.144%
83	10.884	3041	3046	3050	rBV7	2556	3011	0.01%	0.007%
84	10.942	3059	3064	3068	rBV7	4636	5815	0.03%	0.013%
85	11.051	3091	3098	3103	rBV7	7374	10236	0.05%	0.023%
86	11.096	3103	3112	3117	rBV6	14272	25118	0.12%	0.058%
87	11.254	3153	3161	3165	rBV9	9005	12858	0.06%	0.029%
88	11.312	3170	3179	3188	rVB9	8332	19491	0.09%	0.045%
89	11.376	3189	3199	3206	rBV7	17686	32043	0.15%	0.073%
90	11.459	3214	3225	3248	rBV	967863	1612267	7.42%	3.697%
91	11.685	3289	3295	3306	rVB	11183	21697	0.10%	0.050%
92	11.836	3330	3342	3363	rBV	1103336	1835103	8.45%	4.208%
93	12.003	3389	3394	3400	rBV4	22492	28929	0.13%	0.066%
94	12.209	3453	3458	3466	rVB9	10827	15135	0.07%	0.035%
95	12.485	3535	3544	3554	rVB9	31564	62467	0.29%	0.143%
96	12.591	3571	3577	3580	rBV4	17129	22103	0.10%	0.051%
97	12.701	3604	3611	3624	rVB10	33305	62765	0.29%	0.144%
98	13.109	3732	3738	3752	rVB10	20914	39597	0.18%	0.091%
99	13.768	3937	3943	3954	rBV7	29582	47607	0.22%	0.109%
100	15.829	4579	4584	4594	rVB5	74180	103563	0.48%	0.237%

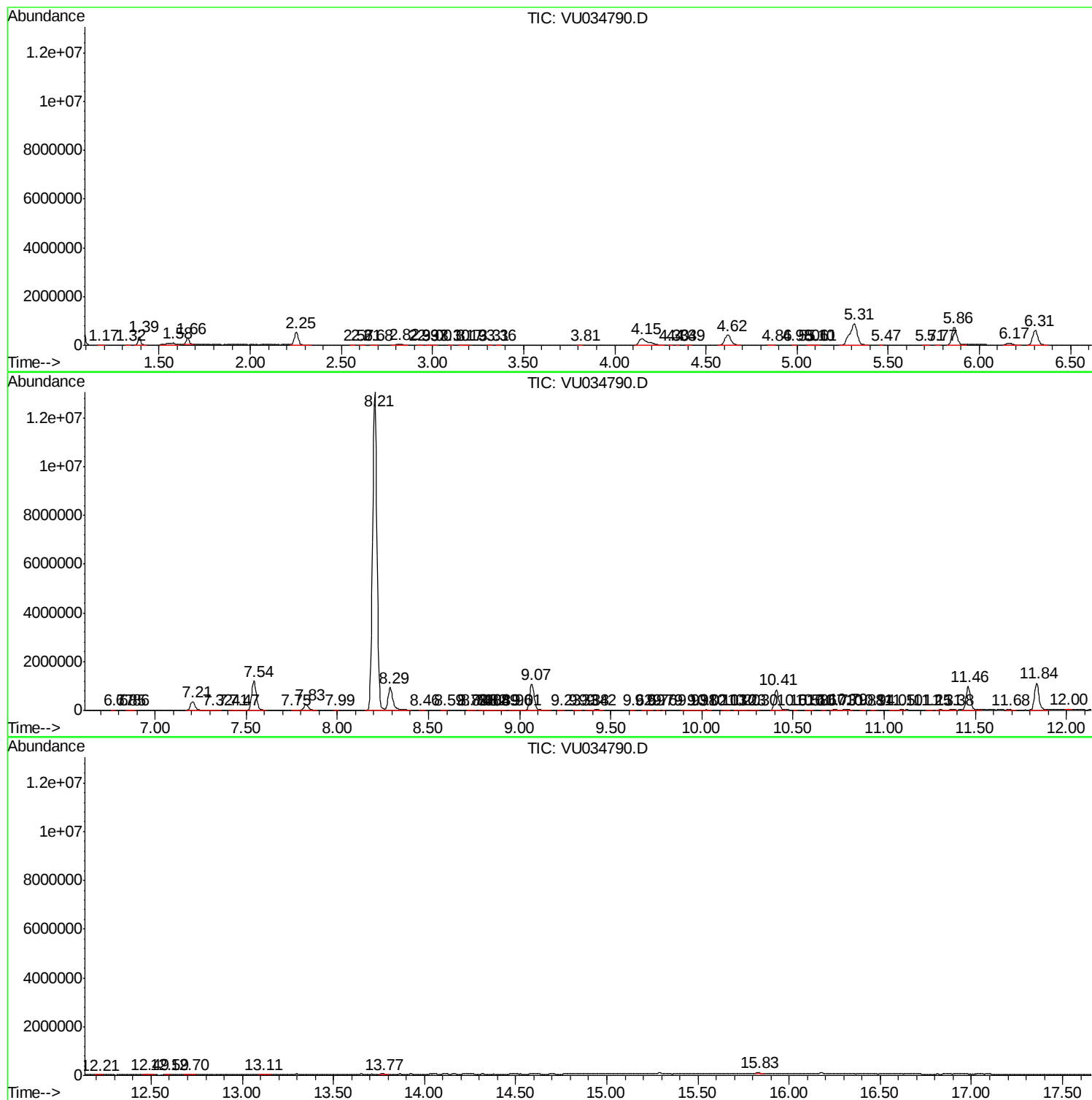
Sum of corrected areas: 43605494

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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEDLOME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 28 Sample Multiplier: 1

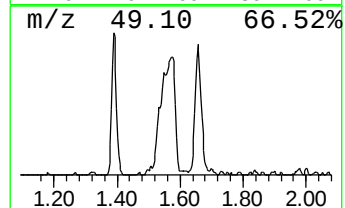
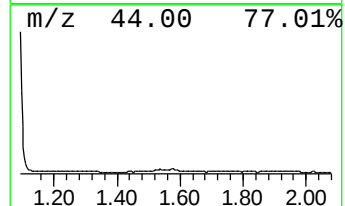
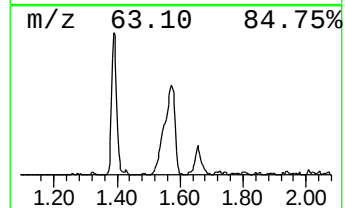
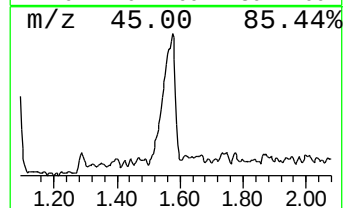
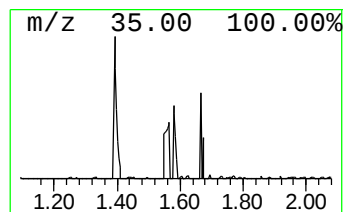
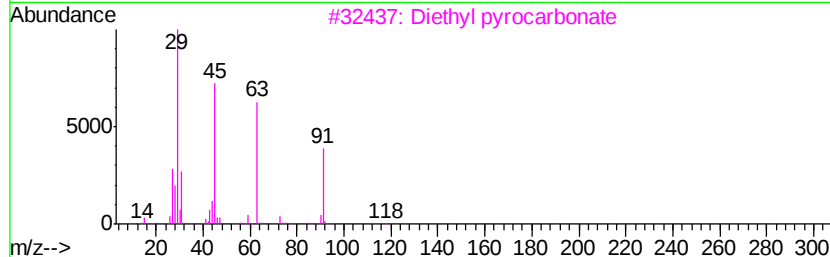
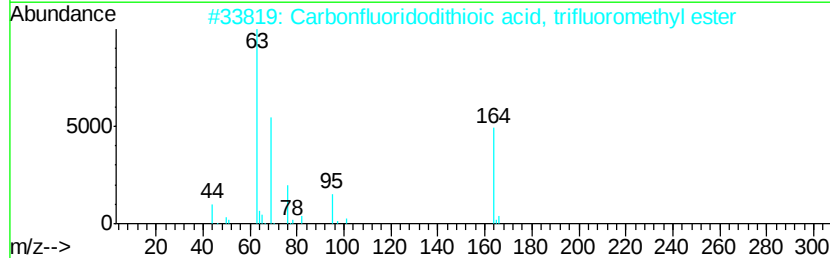
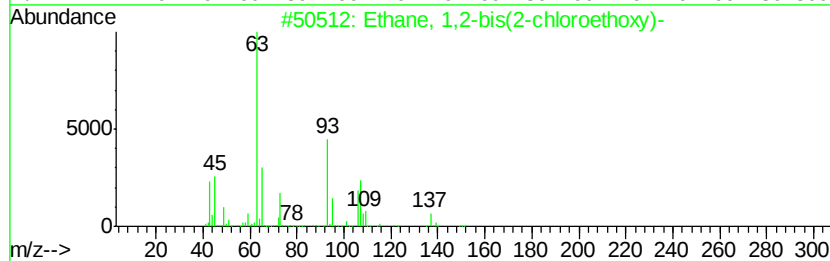
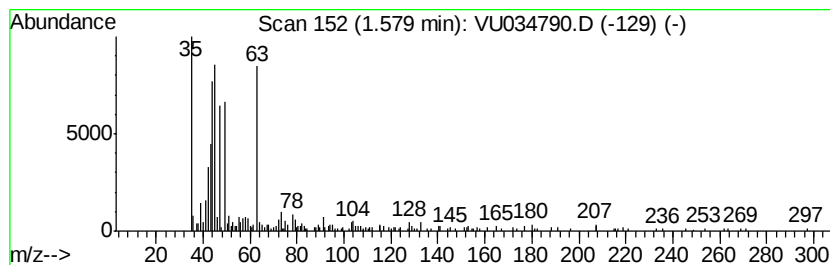
Instrument :
MSVOA_U
ClientSampleId :
BEDLOME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.58	8.45 ug/L	249585	1,4-Difluorobenzene	5.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	23
2	Carbonfluoridodithioic acid, tri...	164	C2F4S2	000371-73-3	17
3	Diethyl pyrocarbonate	162	C6H10O5	001609-47-8	16
4	Ethane, 1-bromo-2-chloro-	142	C2H4BrCl	000107-04-0	10
5	2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	9



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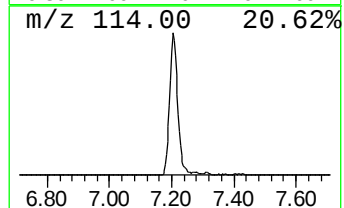
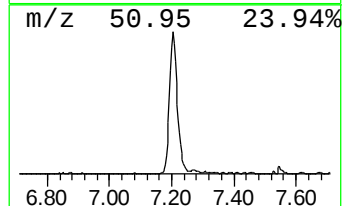
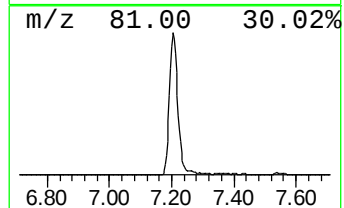
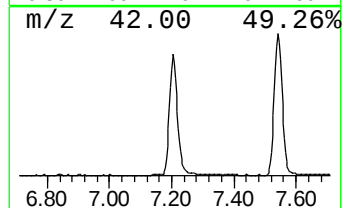
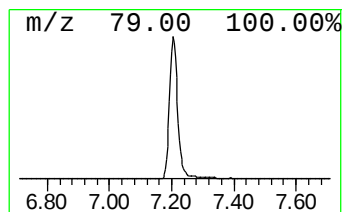
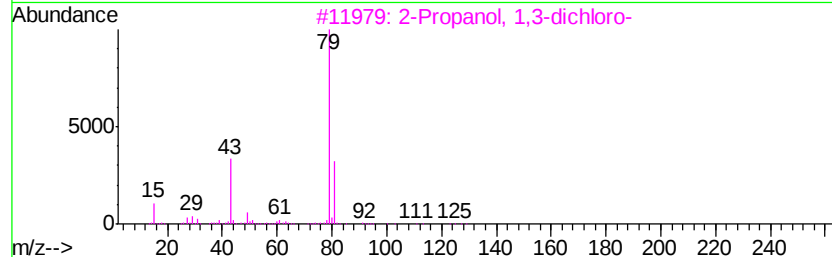
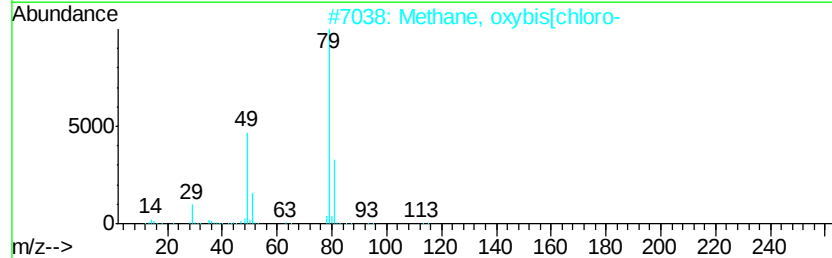
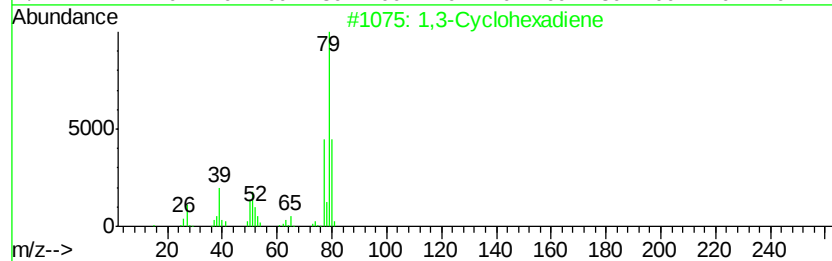
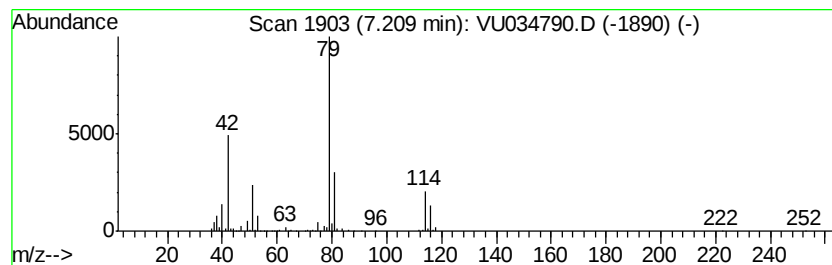
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	21.86 ug/L	645648	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
2		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	23
3		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	17
4		1,3-Cyclohexadiene	80	C6H8	000592-57-4	9
5		1,3-Cyclohexadiene	80	C6H8	000592-57-4	9



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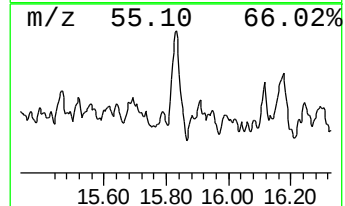
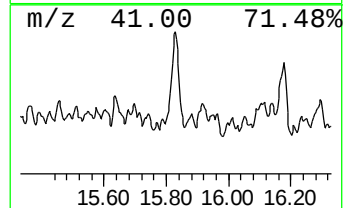
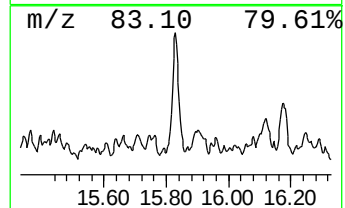
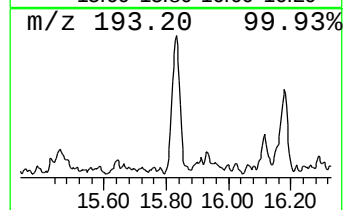
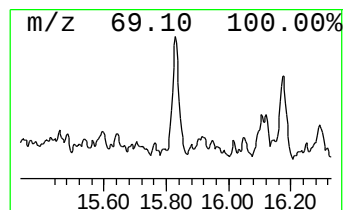
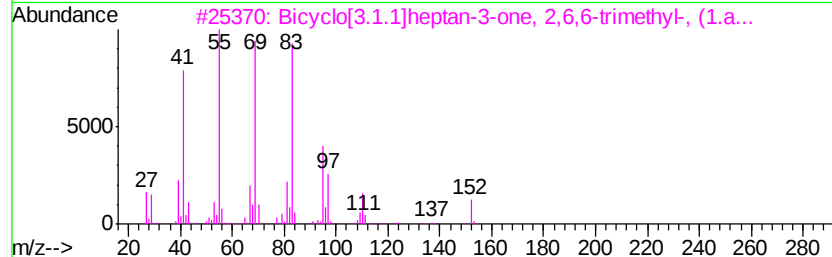
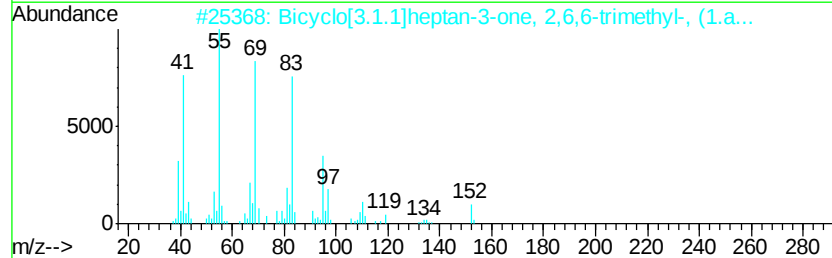
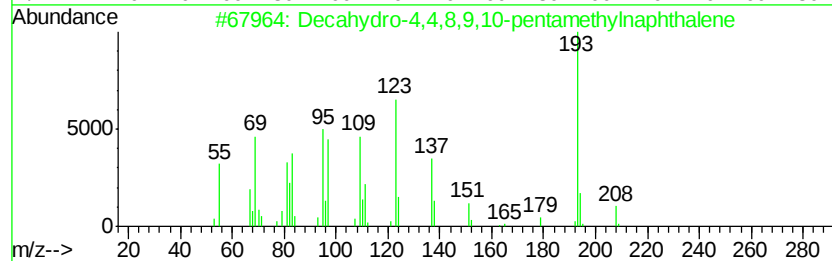
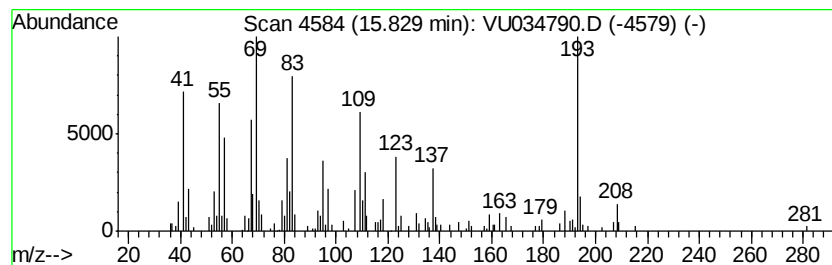
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	3.21 ug/L	103563	1,4-Dichlorobenzene-d4	11.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Decahydro-4,4,8,9,10-pentamethyl...	208 C15H28	080655-44-3 43
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152 C10H16O	015358-88-0 38
3		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152 C10H16O	000547-60-4 30
4		1-(p-Fluorophenyl)-4-piperidone	193 C11H12FNO	1000238-56-7 14
5		Cyclopentane, (2-methylbutyl)-	140 C10H20	053366-38-4 14



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092419\
Data File : VU034790.D
Acq On : 24 Sep 2019 22:41
Operator : JC/SP
Sample : K4984-06ME 10X
Misc : 4.99g/5.0ml/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEDLOME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.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
unknown-01	1.58	8.4	ug/L	249585	1	5.86	1476550	50.0
unknown-02	7.21	21.9	ug/L	645648	1	5.86	1476550	50.0
unknown-03	15.83	3.2	ug/L	103563	3	11.46	1612270	50.0