

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010824\
 Data File : VU057424.D
 Acq On : 09 Jan 2024 08:23
 Operator : MD/SY
 Sample : P1058-20
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 YCHH0

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_U\Method\SFAMULM010824WMA.M
 Title : VOC Analysis

Signal : TIC: VU057424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.390	24	31	43	rVB	54672	57369	5.84%	0.735%
2	1.492	55	63	80	rVB	362574	432045	44.01%	5.536%
3	1.599	87	96	107	rBV	104700	127671	13.00%	1.636%
4	1.914	186	194	208	rVB	73889	107054	10.90%	1.372%
5	2.290	309	311	316	rVB2	568	479	0.05%	0.006%
6	2.325	316	322	324	rBV3	716	708	0.07%	0.009%
7	2.560	383	395	410	rBV3	209831	371110	37.80%	4.756%
8	2.647	413	422	443	rVB	30273	78120	7.96%	1.001%
9	3.415	659	661	663	rBV2	571	367	0.04%	0.005%
10	3.631	725	728	734	rBB2	318	261	0.03%	0.003%
11	3.708	748	752	753	rBV	263	194	0.02%	0.002%
12	3.862	790	800	815	rBB2	2580	5166	0.53%	0.066%
13	4.280	927	930	936	rBB	169	216	0.02%	0.003%
14	4.428	972	976	980	rBB2	344	256	0.03%	0.003%
15	4.631	1028	1039	1069	rBV	45343	149683	15.25%	1.918%
16	5.055	1156	1171	1192	rBV2	189064	426778	43.47%	5.469%
17	5.229	1222	1225	1226	rBV2	621	313	0.03%	0.004%
18	5.267	1233	1237	1238	rBV	328	218	0.02%	0.003%
19	5.309	1239	1250	1265	rVB4	11070	23912	2.44%	0.306%
20	5.717	1357	1377	1408	rBV2	355927	981739	100.00%	12.581%
21	5.930	1439	1443	1445	rVB2	396	333	0.03%	0.004%
22	5.949	1445	1449	1450	rBV	279	199	0.02%	0.003%
23	6.242	1527	1540	1564	rBV	315139	616982	62.85%	7.906%
24	6.489	1613	1617	1619	rVB2	390	279	0.03%	0.004%
25	6.531	1624	1630	1634	rBV3	949	1020	0.10%	0.013%
26	6.550	1634	1636	1639	rVB2	439	220	0.02%	0.003%
27	6.605	1647	1653	1656	rBB2	363	395	0.04%	0.005%
28	6.682	1664	1677	1697	rBV	215652	423204	43.11%	5.423%
29	6.994	1771	1774	1777	rBB	358	220	0.02%	0.003%
30	7.190	1832	1835	1838	rBV2	472	326	0.03%	0.004%
31	7.415	1902	1905	1910	rBB	217	208	0.02%	0.003%
32	7.463	1916	1920	1924	rBB	201	200	0.02%	0.003%
33	7.512	1931	1935	1938	rBV2	288	232	0.02%	0.003%
34	7.560	1938	1950	1973	rBV2	116048	212592	21.65%	2.724%
35	7.695	1988	1992	1994	rBV3	532	322	0.03%	0.004%
36	7.708	1994	1996	1998	rVV	398	203	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010824WMA.M
 Title : VOC Analysis

37	7.733	2002	2004	2007	rVB2	497	286	0.03%	0.004%
38	7.759	2008	2012	2015	rBV	292	235	0.02%	0.003%
39	7.891	2040	2053	2074	rBV	425103	756459	77.05%	9.694%
40	8.110	2118	2121	2124	rVB2	529	427	0.04%	0.005%
41	8.174	2130	2141	2166	rBV2	81777	151282	15.41%	1.939%
42	8.267	2168	2170	2173	rVB2	377	204	0.02%	0.003%
43	8.306	2179	2182	2186	rBV	205	203	0.02%	0.003%
44	8.357	2195	2198	2203	rBB	309	258	0.03%	0.003%
45	8.396	2206	2210	2213	rBB2	268	226	0.02%	0.003%
46	8.486	2234	2238	2242	rBB	247	214	0.02%	0.003%
47	8.563	2257	2262	2264	rBV	309	269	0.03%	0.003%
48	8.643	2273	2287	2318	rBV3	175980	390263	39.75%	5.001%
49	8.920	2369	2373	2377	rVB2	446	311	0.03%	0.004%
50	8.942	2378	2380	2383	rBV	318	219	0.02%	0.003%
51	9.151	2442	2445	2449	rBV	283	242	0.02%	0.003%
52	9.357	2504	2509	2511	rBV	198	219	0.02%	0.003%
53	9.412	2514	2526	2559	rBV	422902	746062	75.99%	9.560%
54	9.589	2577	2581	2583	rBV2	544	499	0.05%	0.006%
55	9.634	2591	2595	2598	rBV	229	206	0.02%	0.003%
56	9.669	2602	2606	2610	rBV	254	311	0.03%	0.004%
57	9.759	2631	2634	2635	rBV2	531	234	0.02%	0.003%
58	9.994	2703	2707	2710	rBV2	318	290	0.03%	0.004%
59	10.029	2715	2718	2720	rBV	347	221	0.02%	0.003%
60	10.097	2736	2739	2742	rBV2	425	295	0.03%	0.004%
61	10.396	2830	2832	2837	rVV	367	246	0.03%	0.003%
62	10.454	2847	2850	2856	rBB	213	256	0.03%	0.003%
63	10.482	2856	2859	2862	rBV	272	238	0.02%	0.003%
64	10.528	2866	2873	2879	rBV3	937	1495	0.15%	0.019%
65	10.595	2890	2894	2897	rBV	267	230	0.02%	0.003%
66	10.704	2925	2928	2931	rVB	334	236	0.02%	0.003%
67	10.753	2931	2943	2963	rBV	291213	474254	48.31%	6.077%
68	10.865	2974	2978	2980	rBV2	651	476	0.05%	0.006%
69	10.894	2983	2987	2991	rVB2	531	456	0.05%	0.006%
70	10.933	2991	2999	3006	rBV5	1355	1776	0.18%	0.023%
71	11.241	3091	3095	3098	rBV	314	268	0.03%	0.003%
72	11.730	3243	3247	3248	rBV	378	251	0.03%	0.003%
73	11.807	3259	3271	3293	rBV	375961	608951	62.03%	7.803%
74	12.032	3337	3341	3344	rBV	410	336	0.03%	0.004%
75	12.058	3344	3349	3351	rBV	378	380	0.04%	0.005%
76	12.187	3377	3389	3408	rBV	386715	636787	64.86%	8.160%

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Integration Parameters: LSCINT.P

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Peak Location: TOP

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77	12.299	3422	3424	3431	rVB3	645	632	0.06%	0.008%
78	12.331	3431	3434	3437	rBV2	388	243	0.02%	0.003%
79	12.556	3501	3504	3508	rVB2	342	219	0.02%	0.003%
80	12.682	3541	3543	3551	rVB	239	224	0.02%	0.003%
81	12.756	3564	3566	3567	rBV	613	284	0.03%	0.004%
82	12.929	3617	3620	3624	rVB	383	261	0.03%	0.003%
83	13.196	3698	3703	3712	rBV	215	315	0.03%	0.004%
84	13.515	3800	3802	3805	rVB	455	185	0.02%	0.002%
85	13.531	3805	3807	3809	rBV	381	193	0.02%	0.002%
86	13.640	3838	3841	3845	rVB	571	390	0.04%	0.005%
87	13.679	3849	3853	3857	rBV2	420	370	0.04%	0.005%
88	13.711	3859	3863	3867	rBV2	273	219	0.02%	0.003%
89	13.804	3889	3892	3895	rBV	234	210	0.02%	0.003%
90	13.865	3908	3911	3916	rVB2	432	247	0.03%	0.003%
91	14.032	3960	3963	3966	rBV2	395	268	0.03%	0.003%
92	14.051	3966	3969	3970	rBV2	324	191	0.02%	0.002%
93	14.418	4078	4083	4085	rBV	603	385	0.04%	0.005%
94	14.598	4133	4139	4141	rBV3	350	330	0.03%	0.004%
95	14.720	4174	4177	4179	rBV2	423	245	0.02%	0.003%
96	14.814	4202	4206	4207	rBV2	323	217	0.02%	0.003%
97	14.900	4231	4233	4235	rBV2	384	186	0.02%	0.002%
98	14.942	4243	4246	4252	rVB2	436	392	0.04%	0.005%
99	14.968	4252	4254	4257	rBV	474	330	0.03%	0.004%
100	15.244	4337	4340	4341	rBV2	609	390	0.04%	0.005%

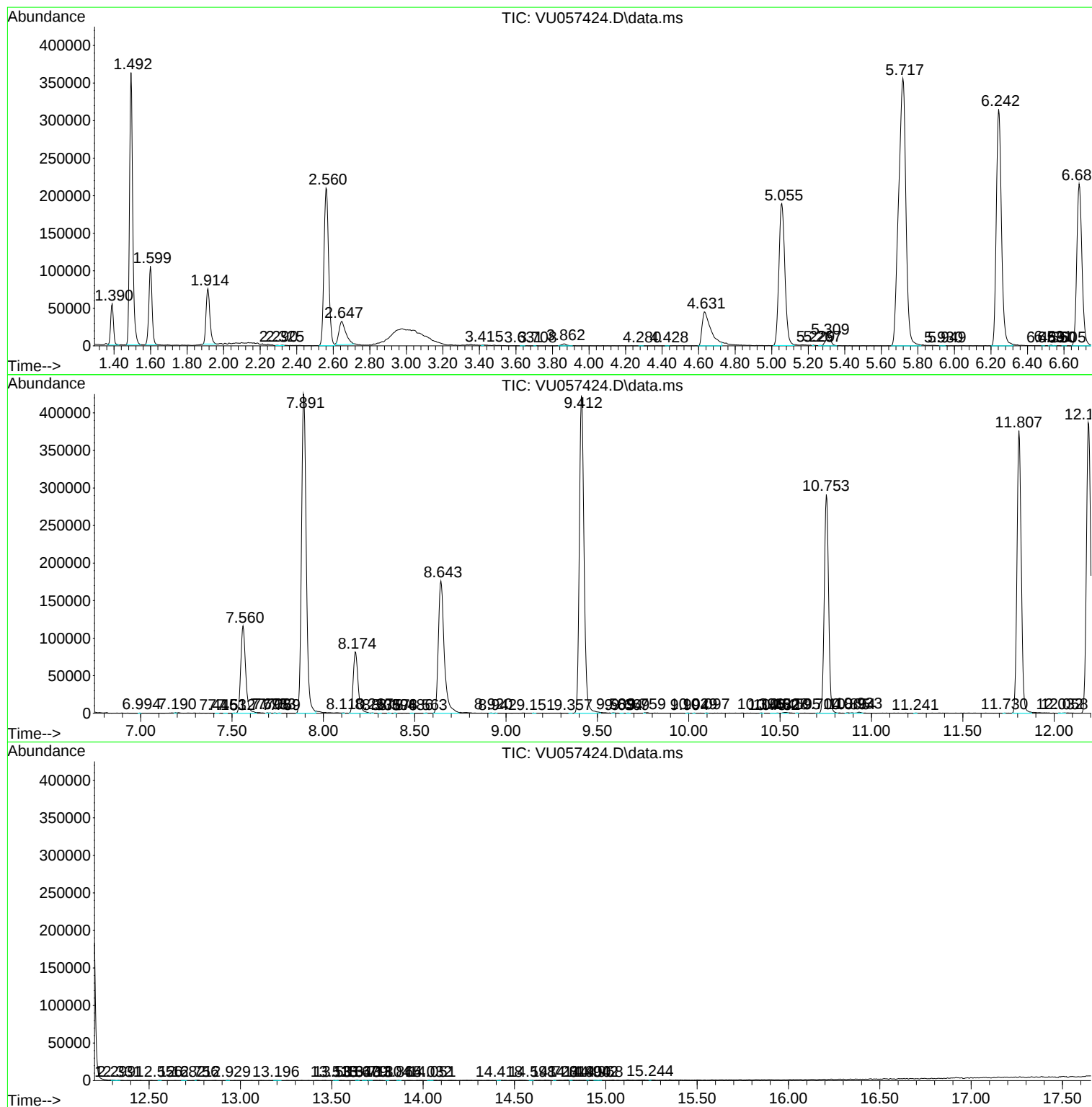
Sum of corrected areas: 7803591

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010824WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YCHH0

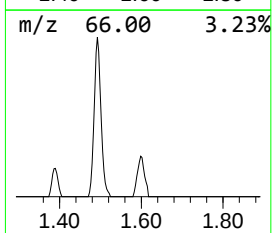
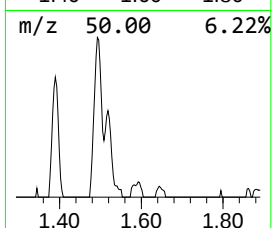
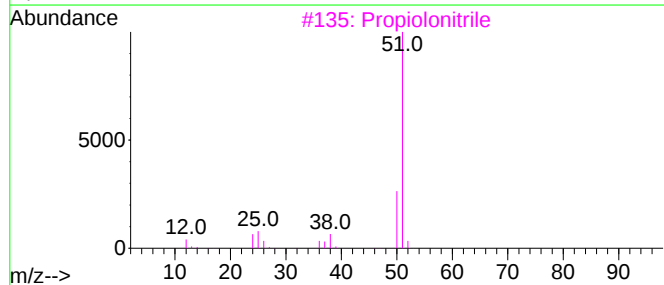
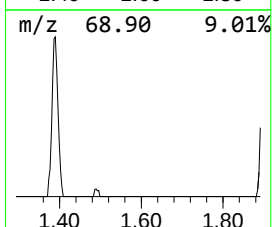
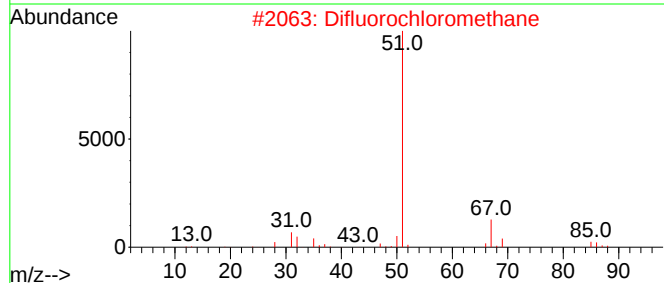
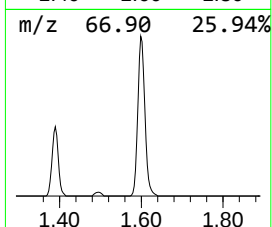
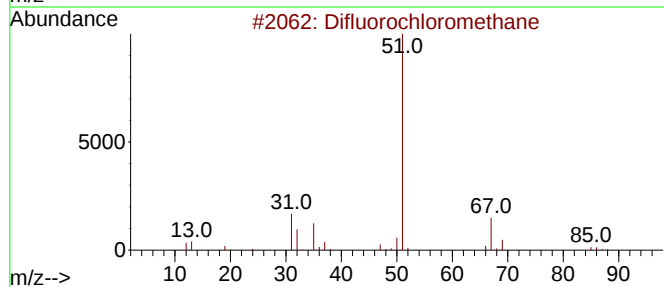
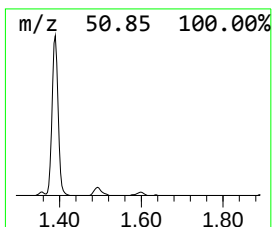
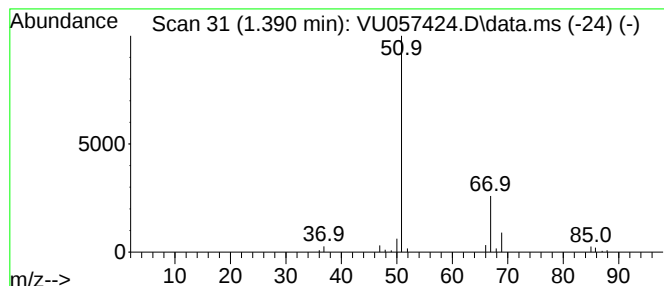
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010824WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.390	4.65 ug/L	57369	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Difluorochloromethane	86	CHClF2	000075-45-6	90
2			Difluorochloromethane	86	CHClF2	000075-45-6	90
3			Propiolonitrile	51	C3HN	001070-71-9	4
4			2-p-Nitrobenzoyl-1,3,5-tribenzyl...	569	C33H31NO8	1000129-85-6	4
5			1-Buten-3-yne, 1-chloro-, (Z)-	86	C4H3Cl	020374-90-7	2



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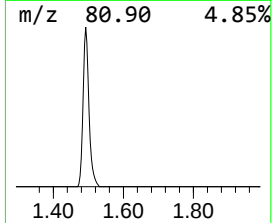
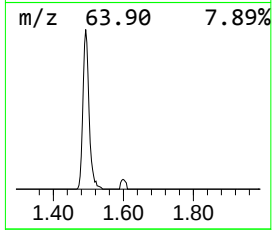
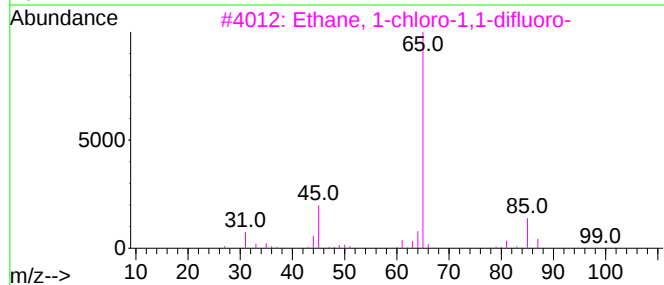
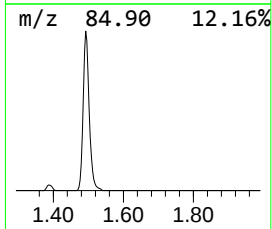
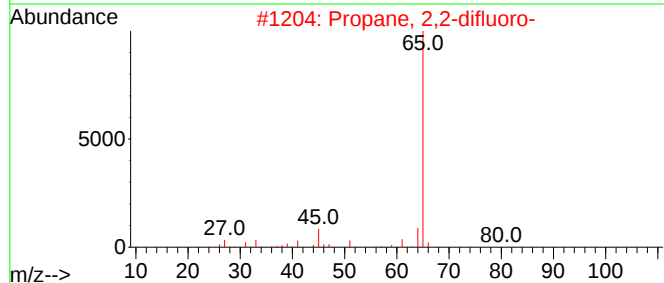
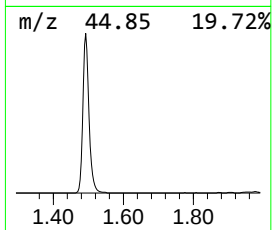
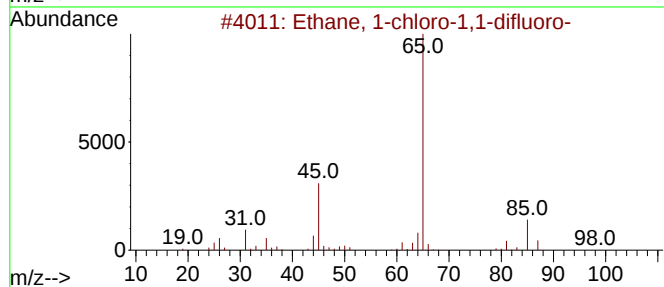
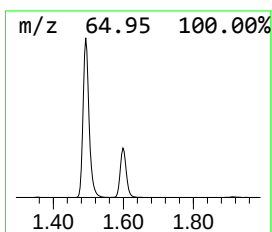
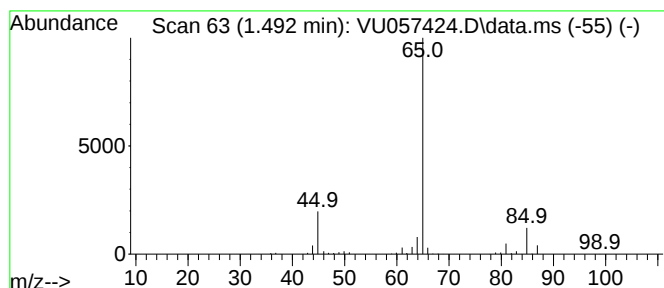
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010824WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.492	35.01 ug/L	432045	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	43		
2	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	43		
3	Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	38		
4	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2		
5	2,2-Difluoropropionic acid	110	C3H4F2O2	000373-96-6	2		



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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
unknown-01	1.390	4.7	ug/L	57369	1	6.242	616982	50.0
unknown-02	1.492	35.0	ug/L	432045	1	6.242	616982	50.0