

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042322\
 Data File : VU048253.D
 Acq On : 23 Apr 2022 18:01
 Operator : SY/MD
 Sample : N2488-12
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0HZ5

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU048253.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	34	41	51	rBV	161534	160878	14.54%	1.639%
2	1.600	73	81	99	rVB	128984	165507	14.96%	1.686%
3	1.899	168	174	197	rVB	97981	145614	13.16%	1.483%
4	2.488	354	357	360	rBV3	424	231	0.02%	0.002%
5	2.565	368	381	395	rBV	226277	373729	33.77%	3.807%
6	2.636	395	403	408	rVV	22113	34668	3.13%	0.353%
7	2.684	409	418	438	rVB	228489	401588	36.29%	4.091%
8	2.951	490	501	520	rBV	78348	148698	13.44%	1.515%
9	3.102	547	548	555	rVB2	326	256	0.02%	0.003%
10	3.186	562	574	585	rBV	5681	13183	1.19%	0.134%
11	3.353	623	626	629	rVB2	367	273	0.02%	0.003%
12	3.597	699	702	706	rVV3	285	286	0.03%	0.003%
13	3.616	706	708	714	rVB2	359	299	0.03%	0.003%
14	3.719	736	740	742	rVB2	290	209	0.02%	0.002%
15	4.009	823	830	834	rBV2	303	394	0.04%	0.004%
16	4.063	841	847	852	rVB2	206	251	0.02%	0.003%
17	4.169	875	880	883	rBV2	312	316	0.03%	0.003%
18	4.427	957	960	963	rBV2	285	215	0.02%	0.002%
19	4.452	963	968	971	rBV	278	285	0.03%	0.003%
20	4.562	998	1002	1004	rBV3	514	456	0.04%	0.005%
21	4.629	1009	1023	1043	rBV	109611	294366	26.60%	2.999%
22	5.063	1141	1158	1186	rVV	191969	424987	38.41%	4.329%
23	5.160	1186	1188	1189	rVV2	598	310	0.03%	0.003%
24	5.202	1190	1201	1225	rVV2	20353	45991	4.16%	0.468%
25	5.292	1227	1229	1241	rVB4	1024	1327	0.12%	0.014%
26	5.382	1255	1257	1260	rBV2	289	236	0.02%	0.002%
27	5.626	1326	1333	1336	rBV2	208	213	0.02%	0.002%
28	5.726	1341	1364	1397	rBV2	414840	1106590	100.00%	11.272%
29	5.970	1431	1440	1443	rBV3	1115	1289	0.12%	0.013%
30	6.250	1512	1527	1550	rVV	371564	707870	63.97%	7.211%
31	6.394	1563	1572	1586	rVB4	8058	16004	1.45%	0.163%
32	6.526	1607	1613	1616	rBV4	846	1087	0.10%	0.011%
33	6.562	1621	1624	1625	rBV2	856	500	0.05%	0.005%
34	6.690	1650	1664	1681	rBV	253415	498618	45.06%	5.079%
35	6.777	1684	1691	1709	rVB2	8173	18762	1.70%	0.191%
36	6.880	1718	1723	1724	rBV2	965	750	0.07%	0.008%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	7.153	1802	1808	1809	rVV2	559	498	0.05%	0.005%
38	7.189	1809	1819	1835	rVB7	4465	9049	0.82%	0.092%
39	7.288	1842	1850	1853	rBV3	379	404	0.04%	0.004%
40	7.359	1867	1872	1875	rBV2	262	249	0.02%	0.003%
41	7.398	1878	1884	1888	rVB2	186	217	0.02%	0.002%
42	7.504	1914	1917	1921	rBV2	290	268	0.02%	0.003%
43	7.568	1921	1937	1958	rBV	112567	202459	18.30%	2.062%
44	7.677	1960	1971	1986	rVB2	12990	24738	2.24%	0.252%
45	7.758	1993	1996	2001	rBV3	335	267	0.02%	0.003%
46	7.803	2002	2010	2017	rVV6	1754	2859	0.26%	0.029%
47	7.899	2026	2040	2056	rBV	473146	829801	74.99%	8.453%
48	8.182	2114	2128	2144	rBV2	85087	146842	13.27%	1.496%
49	8.256	2147	2151	2155	rVV4	436	376	0.03%	0.004%
50	8.388	2188	2192	2194	rBV2	316	267	0.02%	0.003%
51	8.475	2217	2219	2226	rVB3	736	599	0.05%	0.006%
52	8.504	2226	2228	2231	rVB	412	258	0.02%	0.003%
53	8.555	2241	2244	2247	rBV3	377	257	0.02%	0.003%
54	8.639	2254	2270	2297	rBV2	356838	674054	60.91%	6.866%
55	8.957	2366	2369	2375	rVB3	521	528	0.05%	0.005%
56	9.031	2387	2392	2396	rBV2	263	220	0.02%	0.002%
57	9.240	2450	2457	2461	rBV2	242	345	0.03%	0.004%
58	9.417	2499	2512	2556	rBV	532764	918578	83.01%	9.357%
59	9.568	2556	2559	2562	rBV	258	225	0.02%	0.002%
60	9.693	2594	2598	2601	rVV2	427	386	0.03%	0.004%
61	9.745	2608	2614	2617	rBV2	277	282	0.03%	0.003%
62	9.783	2617	2626	2631	rBV3	1753	2368	0.21%	0.024%
63	9.832	2638	2641	2645	rVB	290	235	0.02%	0.002%
64	9.999	2685	2693	2705	rVB4	2275	3483	0.31%	0.035%
65	10.108	2725	2727	2731	rVV2	335	237	0.02%	0.002%
66	10.243	2760	2769	2782	rBV3	3362	5473	0.49%	0.056%
67	10.484	2841	2844	2849	rVB3	376	365	0.03%	0.004%
68	10.520	2849	2855	2856	rBV	242	243	0.02%	0.002%
69	10.571	2863	2871	2878	rVV5	2200	3446	0.31%	0.035%
70	10.668	2896	2901	2909	rBV5	1361	2028	0.18%	0.021%
71	10.758	2917	2929	2951	rVB	407882	648390	58.59%	6.605%
72	10.889	2965	2970	2971	rBV3	933	729	0.07%	0.007%
73	10.992	2999	3002	3004	rBV2	369	293	0.03%	0.003%
74	11.118	3033	3041	3047	rBV4	1254	1718	0.16%	0.018%
75	11.227	3071	3075	3077	rBV2	282	274	0.02%	0.003%
76	11.285	3091	3093	3098	rVB2	430	367	0.03%	0.004%

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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

77	11.471	3139	3151	3168	rBV2	20989	33889	3.06%	0.345%
78	11.581	3174	3185	3187	rBV2	2764	3274	0.30%	0.033%
79	11.696	3214	3221	3227	rVB5	1144	1625	0.15%	0.017%
80	11.748	3230	3237	3245	rVB4	2539	3706	0.33%	0.038%
81	11.812	3245	3257	3278	rBV	518484	846734	76.52%	8.625%
82	11.889	3278	3281	3284	rBV2	374	270	0.02%	0.003%
83	11.973	3303	3307	3310	rVB4	1224	835	0.08%	0.009%
84	12.012	3316	3319	3324	rBV4	562	545	0.05%	0.006%
85	12.069	3327	3337	3347	rVV4	3027	5350	0.48%	0.054%
86	12.108	3347	3349	3353	rVV	579	417	0.04%	0.004%
87	12.195	3360	3376	3397	rVV	460928	770050	69.59%	7.844%
88	12.333	3413	3419	3423	rBV3	501	519	0.05%	0.005%
89	12.384	3433	3435	3439	rBV3	343	302	0.03%	0.003%
90	12.478	3459	3464	3467	rBV4	691	562	0.05%	0.006%
91	12.622	3506	3509	3511	rBV2	401	253	0.02%	0.003%
92	12.777	3547	3557	3568	rBV6	6297	10656	0.96%	0.109%
93	12.883	3585	3590	3592	rBV2	478	412	0.04%	0.004%
94	12.966	3612	3616	3621	rBV4	470	404	0.04%	0.004%
95	13.735	3850	3855	3861	rVB5	603	650	0.06%	0.007%
96	13.841	3879	3888	3899	rBV2	22507	34338	3.10%	0.350%
97	14.330	4032	4040	4050	rVB3	9052	12910	1.17%	0.132%
98	14.860	4196	4205	4217	rBV	23340	38067	3.44%	0.388%
99	15.384	4366	4368	4370	rBV2	900	408	0.04%	0.004%
100	15.838	4505	4509	4513	rBV3	808	982	0.09%	0.010%

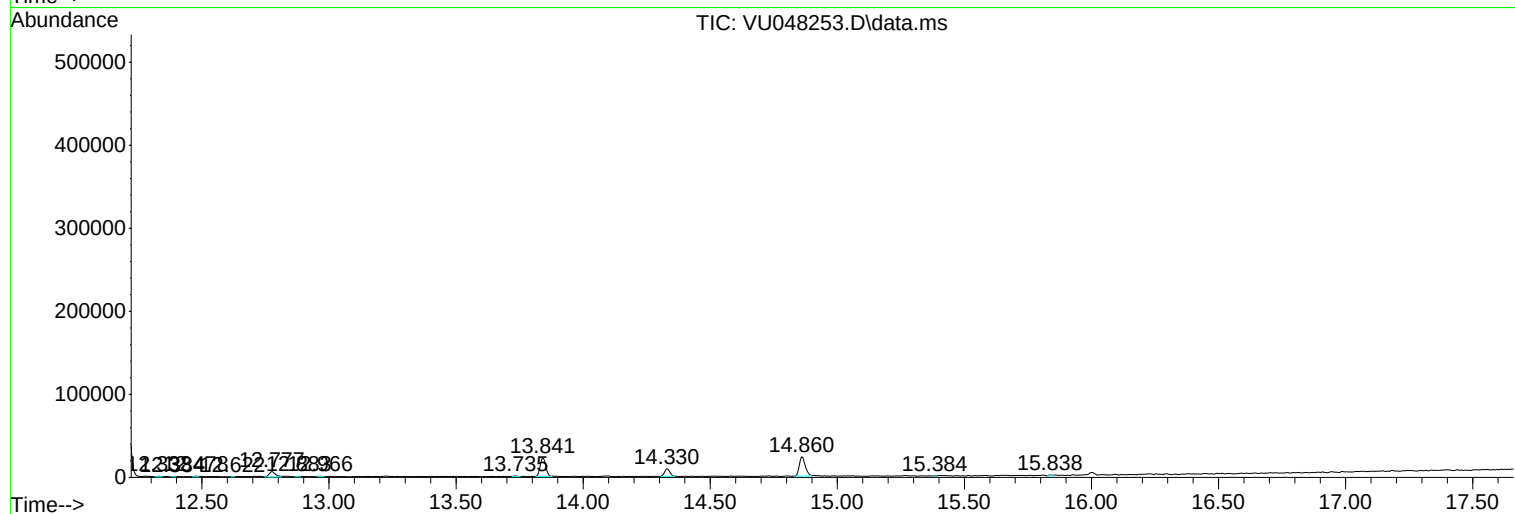
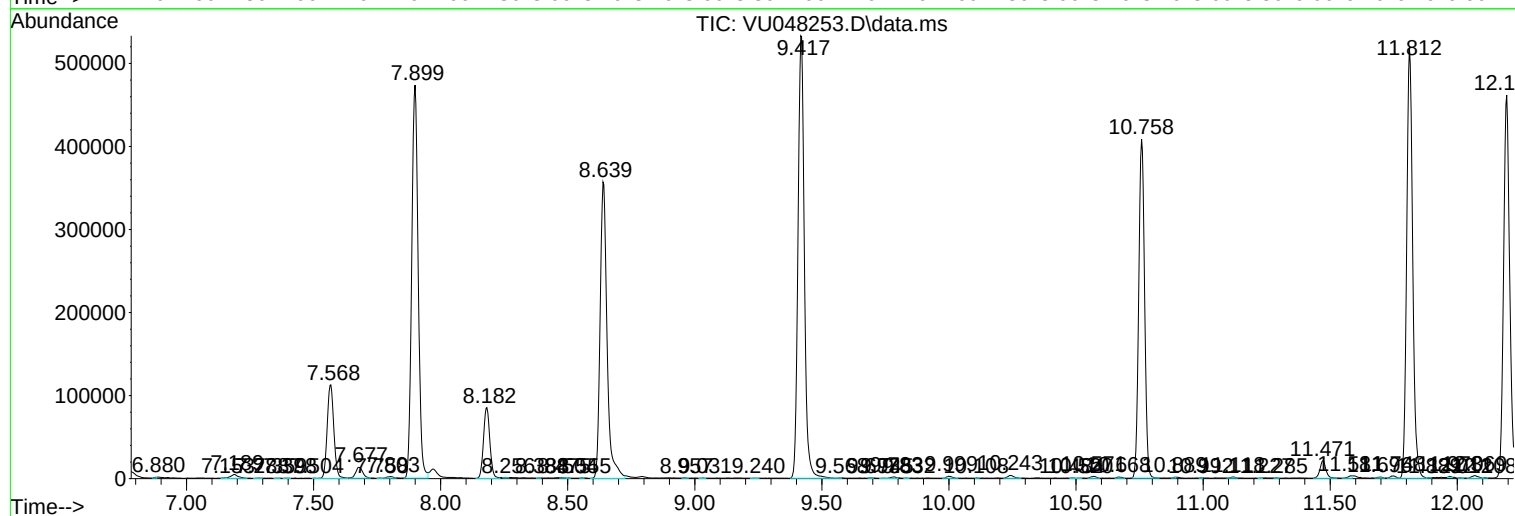
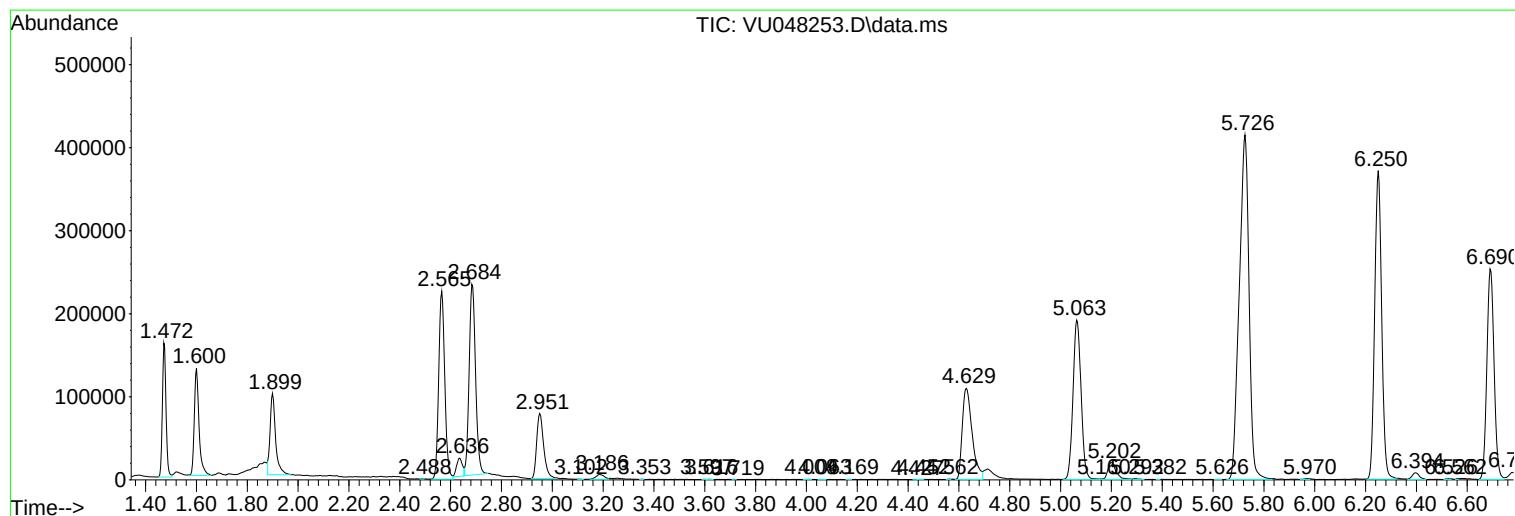
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ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0HZ5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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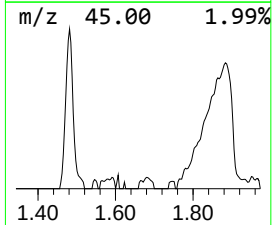
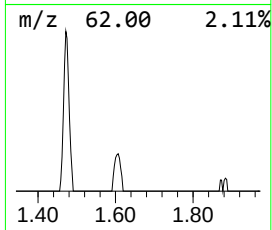
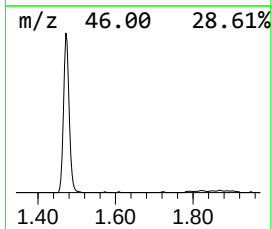
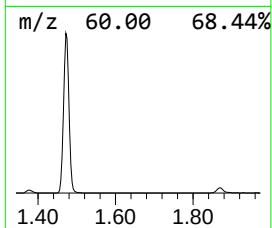
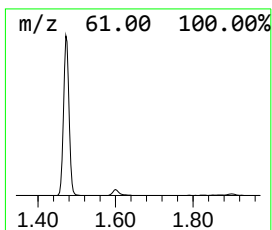
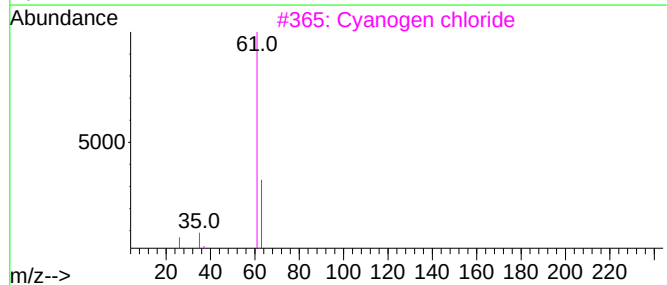
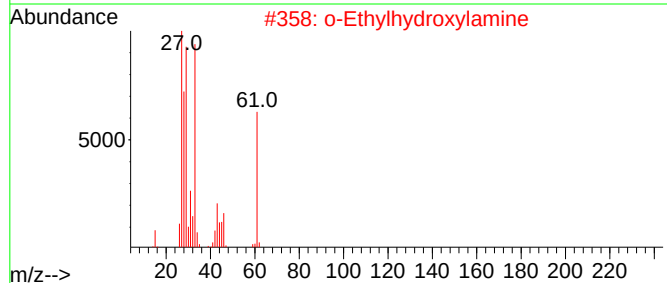
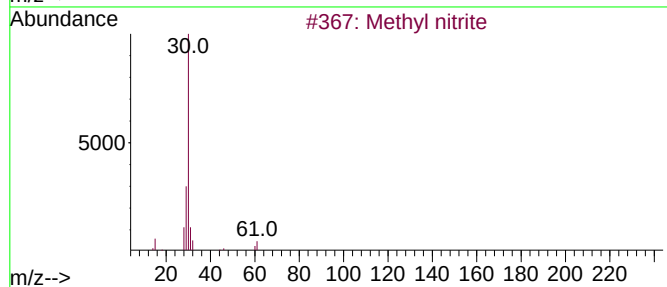
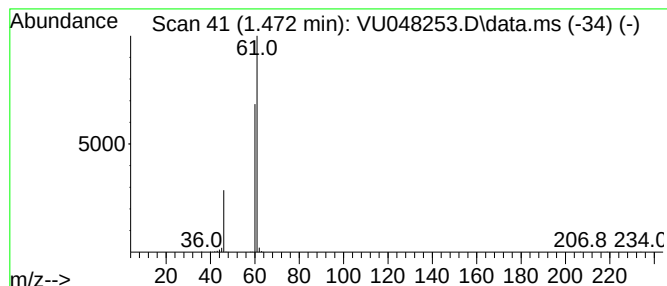
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
1.472	11.36 ug/L	160878	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
3			Cyanogen chloride	61	CClN	000506-77-4	4
4			Cyanogen chloride	61	CClN	000506-77-4	4
5			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4



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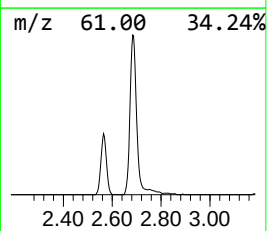
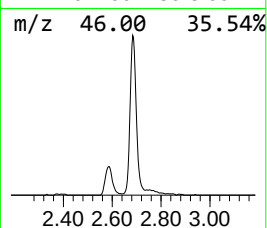
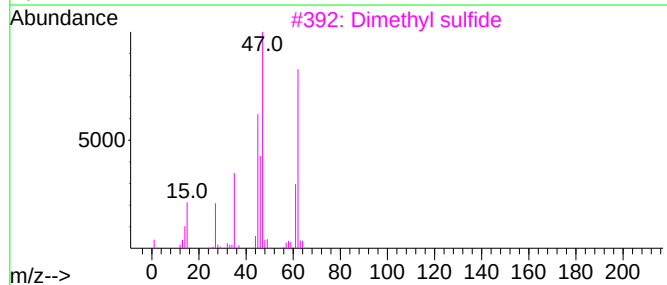
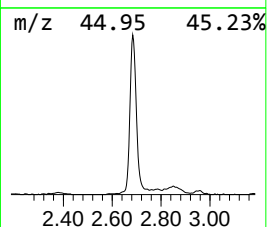
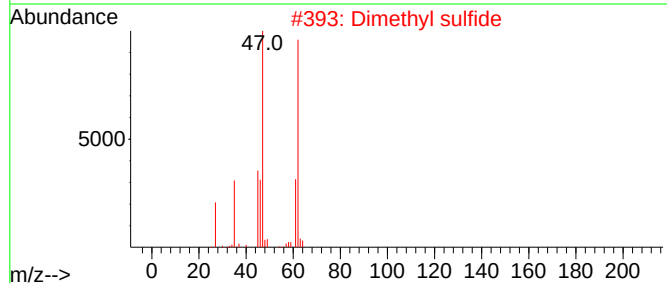
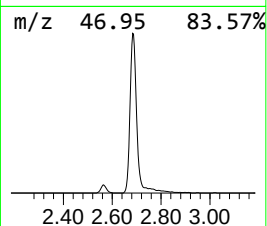
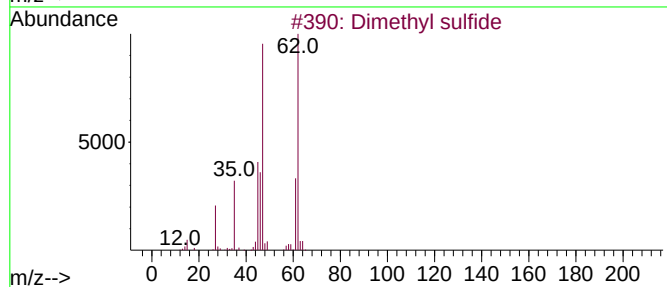
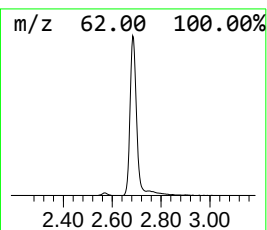
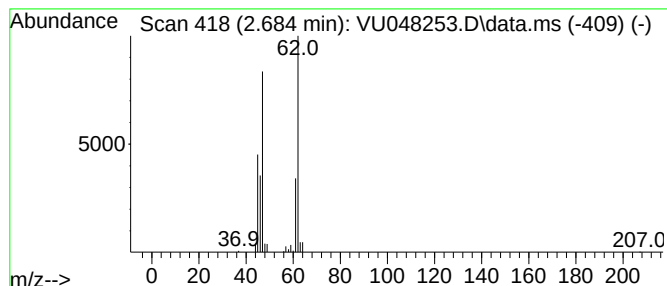
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.684	28.37 ug/L	401588	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Dimethyl sulfide	62	C2H6S	000075-18-3	91
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	91
5			Dimethyl sulfide	62	C2H6S	000075-18-3	90



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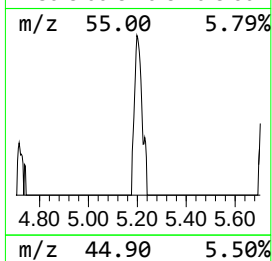
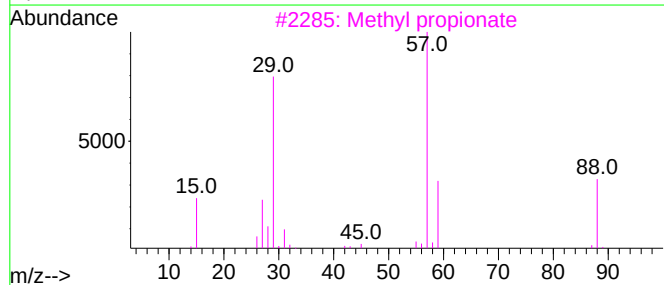
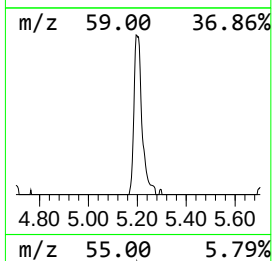
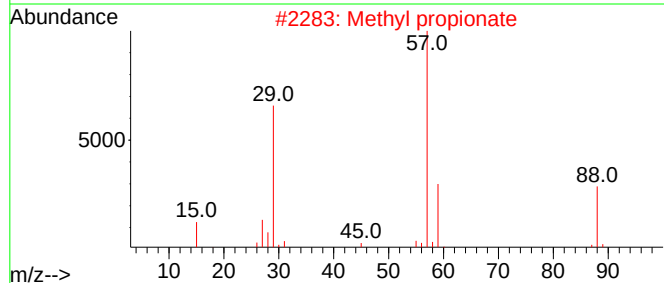
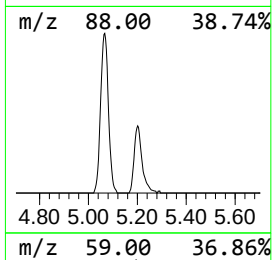
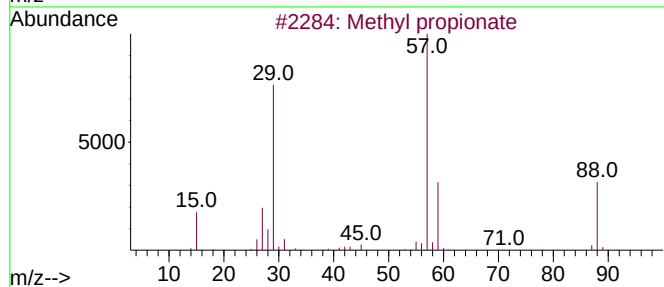
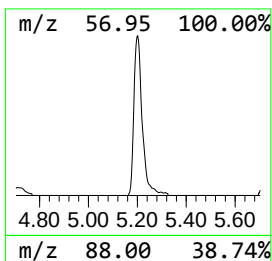
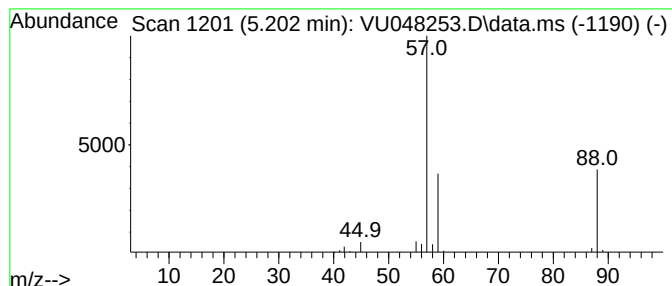
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Methyl propionate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.202	3.25 ug/L	45991	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl propionate			88	C4H8O2	000554-12-1	90
2	Methyl propionate			88	C4H8O2	000554-12-1	90
3	Methyl propionate			88	C4H8O2	000554-12-1	90
4	Methyl propionate			88	C4H8O2	000554-12-1	83
5	Methyl propionate			88	C4H8O2	000554-12-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042322\
Data File : VU048253.D
Acq On : 23 Apr 2022 18:01
Operator : SY/MD
Sample : N2488-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0HZ5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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
unknown-01	1.472	11.4	ug/L	160878	1	6.250	707870	50.0
Dimethyl sulfide	2.684	28.4	ug/L	401588	1	6.250	707870	50.0
Methyl propionate	5.202	3.3	ug/L	45991	1	6.250	707870	50.0