

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
 Data File : VU042280.D
 Acq On : 05 Feb 2021 14:10
 Operator : SY/MD
 Sample : M1326-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 X2Z54

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\SFAMULM020521WMA.M

Title : VOC Analysis

Signal : TIC: VU042280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.388	9	15	30	rVB	31847	37657	0.25%	0.125%
2	1.485	39	45	50	rBV	42032	40756	0.27%	0.136%
3	1.523	50	57	69	rVB	79728	89951	0.61%	0.299%
4	1.600	74	81	97	rVB	93926	111492	0.75%	0.371%
5	1.880	156	168	176	rBV	885302	1167834	7.86%	3.886%
6	2.137	239	248	262	rVB	98119	143941	0.97%	0.479%
7	2.575	371	384	394	rBV2	241139	480087	3.23%	1.598%
8	2.645	395	406	444	rVB	8338088	14851329	100.00%	49.422%
9	3.369	613	631	658	rBV2	585135	1388141	9.35%	4.619%
10	3.587	694	699	706	rBV4	1105	1683	0.01%	0.006%
11	3.761	750	753	755	rBV2	192	144	0.00%	0.000%
12	3.874	782	788	789	rBV	189	148	0.00%	0.000%
13	4.018	829	833	837	rBV	133	102	0.00%	0.000%
14	4.070	846	849	853	rBV	263	263	0.00%	0.001%
15	4.137	868	870	873	rVV2	163	105	0.00%	0.000%
16	4.211	889	893	898	rBV	101	105	0.00%	0.000%
17	4.304	919	922	926	rVB	212	132	0.00%	0.000%
18	4.642	1010	1027	1066	rBV	77448	234866	1.58%	0.782%
19	4.864	1093	1096	1097	rBV	168	97	0.00%	0.000%
20	4.925	1113	1115	1122	rVB	258	163	0.00%	0.001%
21	5.083	1143	1164	1189	rVV3	201220	632193	4.26%	2.104%
22	5.185	1193	1196	1200	rVV3	260	144	0.00%	0.000%
23	5.324	1218	1239	1256	rBV2	68441	152991	1.03%	0.509%
24	5.533	1289	1304	1321	rBV	97085	209218	1.41%	0.696%
25	5.735	1343	1367	1379	rBV2	302266	817216	5.50%	2.720%
26	5.986	1440	1445	1448	rBV	124	122	0.00%	0.000%
27	6.092	1472	1478	1483	rVB3	601	504	0.00%	0.002%
28	6.121	1483	1487	1488	rBV	258	144	0.00%	0.000%
29	6.195	1505	1510	1513	rVB2	299	207	0.00%	0.001%
30	6.256	1514	1529	1544	rBV	244902	461783	3.11%	1.537%
31	6.404	1569	1575	1588	rVB3	3327	5475	0.04%	0.018%
32	6.459	1589	1592	1596	rBV	288	171	0.00%	0.001%
33	6.549	1610	1620	1629	rVB7	4483	8363	0.06%	0.028%
34	6.591	1630	1633	1634	rBV7	227	111	0.00%	0.000%
35	6.603	1635	1637	1640	rVB	281	146	0.00%	0.000%
36	6.700	1652	1667	1678	rBV	190329	367104	2.47%	1.222%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
 Title : VOC Analysis

37	6.771	1680	1689	1710	rVB	165238	319356	2.15%	1.063%
38	7.025	1749	1768	1793	rVV3	12454	48711	0.33%	0.162%
39	7.224	1813	1830	1852	rVV3	31995	57602	0.39%	0.192%
40	7.382	1870	1879	1891	rVB2	6433	10997	0.07%	0.037%
41	7.500	1907	1916	1919	rBV	93	147	0.00%	0.000%
42	7.574	1926	1939	1945	rBV	116594	201906	1.36%	0.672%
43	7.806	1997	2011	2029	rVV	160621	313015	2.11%	1.042%
44	7.906	2030	2042	2053	rVV	383837	651310	4.39%	2.167%
45	7.976	2054	2064	2083	rVB	441110	747289	5.03%	2.487%
46	8.189	2116	2130	2150	rBV2	123652	210532	1.42%	0.701%
47	8.410	2186	2199	2215	rBV	131241	223770	1.51%	0.745%
48	8.529	2233	2236	2239	rBV2	169	121	0.00%	0.000%
49	8.565	2239	2247	2253	rBV5	1484	2061	0.01%	0.007%
50	8.648	2259	2273	2297	rBV	281805	512130	3.45%	1.704%
51	8.819	2314	2326	2344	rVB	67480	116328	0.78%	0.387%
52	8.931	2349	2361	2381	rBV	100738	171567	1.16%	0.571%
53	9.079	2403	2407	2411	rVV2	186	135	0.00%	0.000%
54	9.217	2446	2450	2453	rBV	205	122	0.00%	0.000%
55	9.304	2474	2477	2483	rVB	169	102	0.00%	0.000%
56	9.426	2501	2515	2535	rVV	342415	563803	3.80%	1.876%
57	9.581	2555	2563	2568	rVB2	899	1056	0.01%	0.004%
58	9.706	2589	2602	2617	rBV	339095	527540	3.55%	1.756%
59	9.825	2634	2639	2645	rBV2	281	288	0.00%	0.001%
60	9.983	2683	2688	2692	rVB2	199	184	0.00%	0.001%
61	10.005	2692	2695	2696	rBV2	183	104	0.00%	0.000%
62	10.121	2720	2731	2752	rBV	174928	277193	1.87%	0.922%
63	10.201	2752	2756	2759	rBV	187	112	0.00%	0.000%
64	10.259	2771	2774	2781	rBV	124	133	0.00%	0.000%
65	10.304	2784	2788	2793	rVB	437	313	0.00%	0.001%
66	10.491	2841	2846	2853	rVB2	751	874	0.01%	0.003%
67	10.555	2862	2866	2870	rBV	231	136	0.00%	0.000%
68	10.767	2919	2932	2957	rBV2	274782	648001	4.36%	2.156%
69	10.899	2969	2973	2974	rBV	236	181	0.00%	0.001%
70	10.934	2981	2984	2987	rBV	212	151	0.00%	0.001%
71	10.986	2990	3000	3014	rVB2	19169	31909	0.21%	0.106%
72	11.095	3027	3034	3041	rBV4	1098	1603	0.01%	0.005%
73	11.185	3059	3062	3067	rVB2	209	155	0.00%	0.001%
74	11.298	3091	3097	3101	rBV3	1685	2332	0.02%	0.008%
75	11.346	3102	3112	3124	rVB	74862	120672	0.81%	0.402%
76	11.475	3139	3152	3173	rVB	515244	794715	5.35%	2.645%

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 Title : VOC Analysis

77	11.549	3173	3175	3178	rVB	188	127	0.00%	0.000%
78	11.610	3191	3194	3196	rBV2	473	289	0.00%	0.001%
79	11.754	3234	3239	3245	rVB2	796	868	0.01%	0.003%
80	11.822	3245	3260	3282	rBV2	395929	966819	6.51%	3.217%
81	12.031	3308	3325	3339	rBV	25188	41944	0.28%	0.140%
82	12.150	3357	3362	3363	rBV	215	156	0.00%	0.001%
83	12.201	3365	3378	3401	rVB	393313	626684	4.22%	2.085%
84	12.285	3403	3404	3407	rBV	196	114	0.00%	0.000%
85	12.340	3419	3421	3423	rBV2	376	189	0.00%	0.001%
86	12.526	3475	3479	3487	rBV	278	297	0.00%	0.001%
87	12.561	3487	3490	3492	rBV	186	111	0.00%	0.000%
88	12.690	3525	3530	3535	rVB3	1279	1225	0.01%	0.004%
89	12.954	3603	3612	3618	rBV2	7523	11794	0.08%	0.039%
90	13.008	3619	3629	3642	rVV	87217	137042	0.92%	0.456%
91	13.066	3645	3647	3650	rVB2	215	122	0.00%	0.000%
92	13.124	3662	3665	3669	rBV	233	154	0.00%	0.001%
93	13.339	3723	3732	3740	rBV3	9502	14046	0.09%	0.047%
94	13.555	3794	3799	3809	rBV3	958	1185	0.01%	0.004%
95	13.802	3873	3876	3880	rBV	260	166	0.00%	0.001%
96	13.851	3884	3891	3898	rVV4	1176	1477	0.01%	0.005%
97	14.095	3959	3967	3979	rVB2	1573	2438	0.02%	0.008%
98	14.208	4000	4002	4004	rBV	235	119	0.00%	0.000%
99	14.240	4008	4012	4017	rBV	241	285	0.00%	0.001%
100	14.339	4031	4043	4061	rVB	306688	478982	3.23%	1.594%

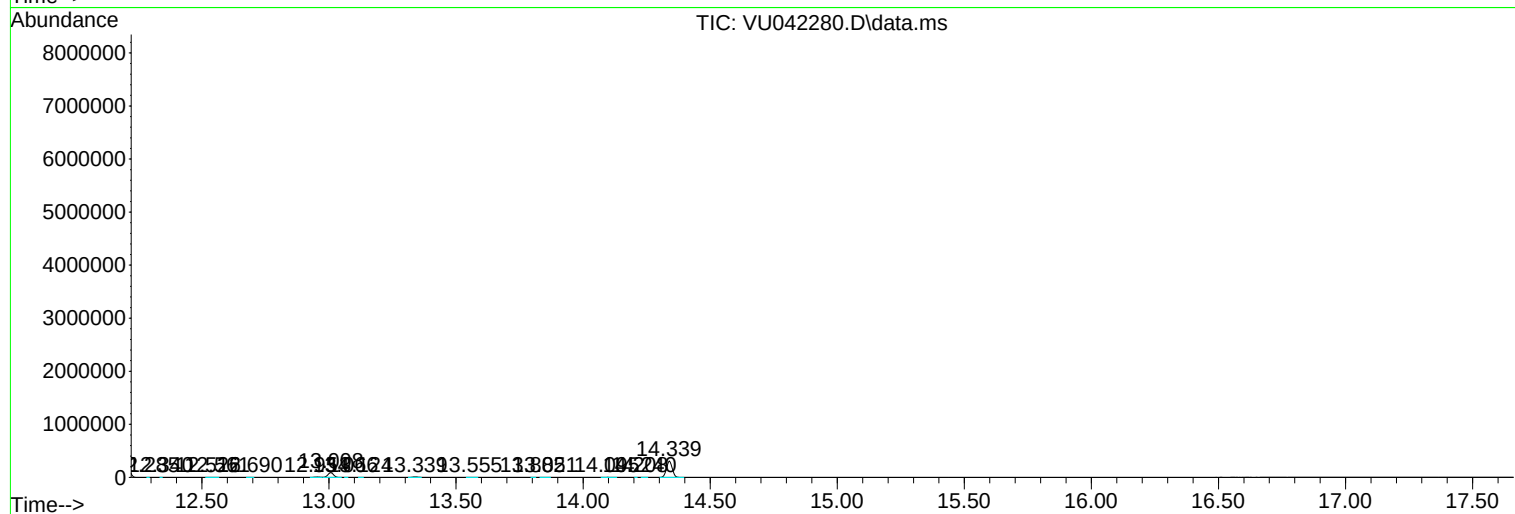
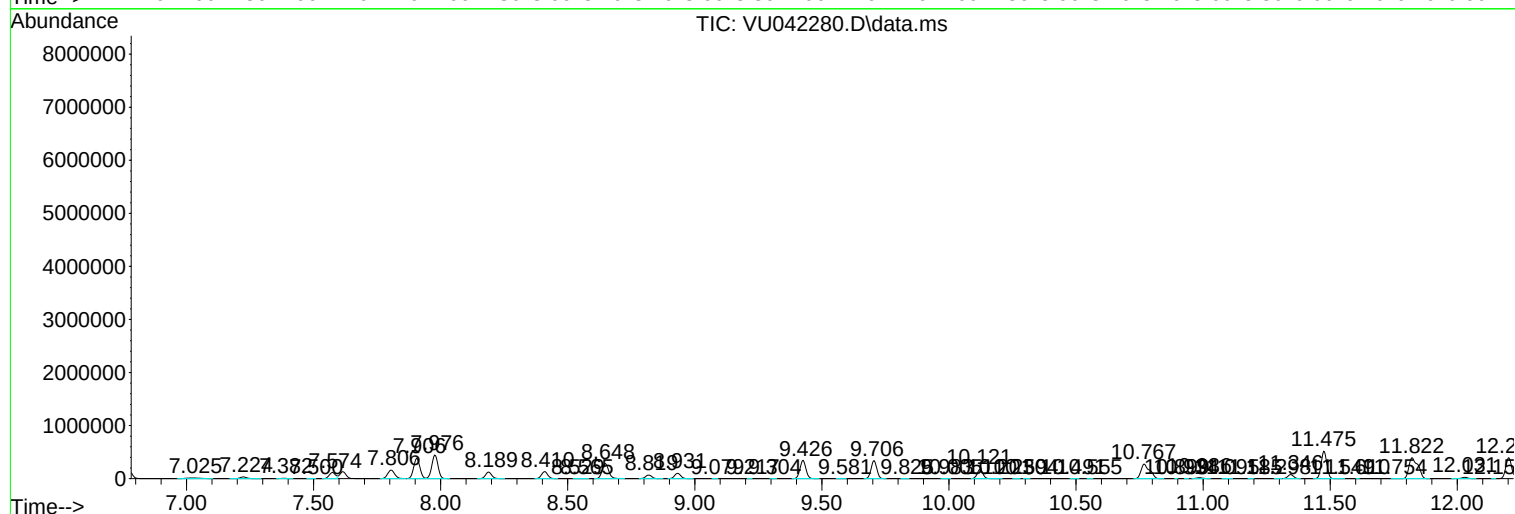
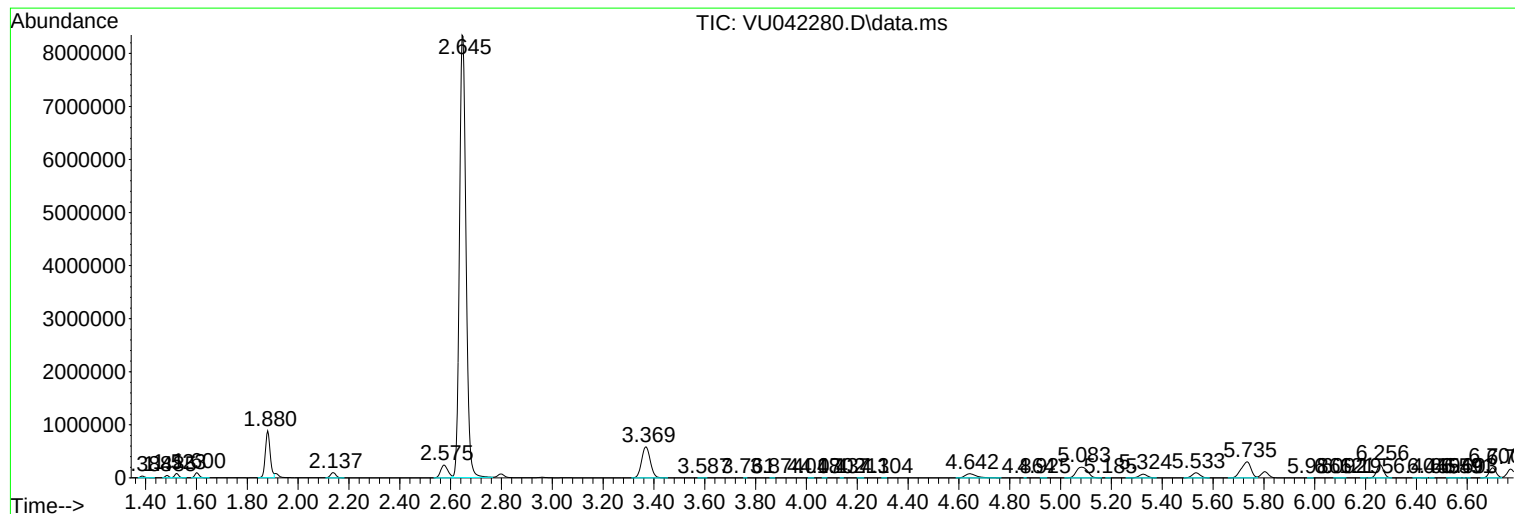
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

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



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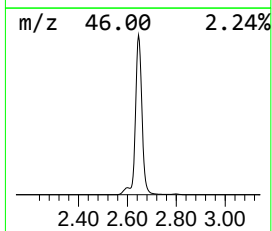
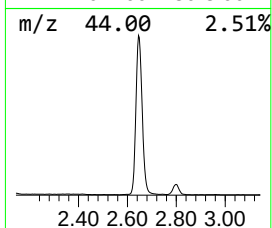
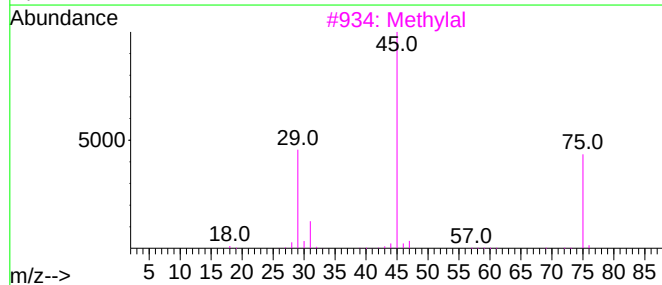
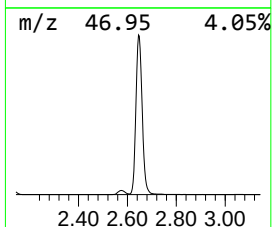
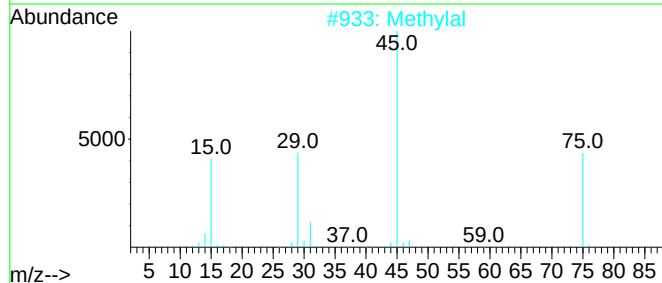
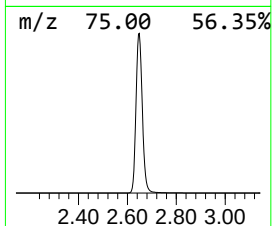
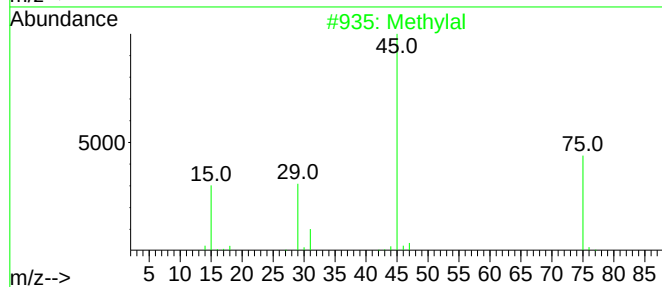
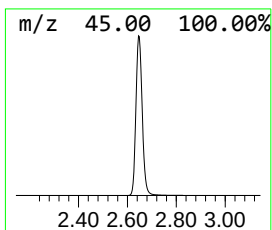
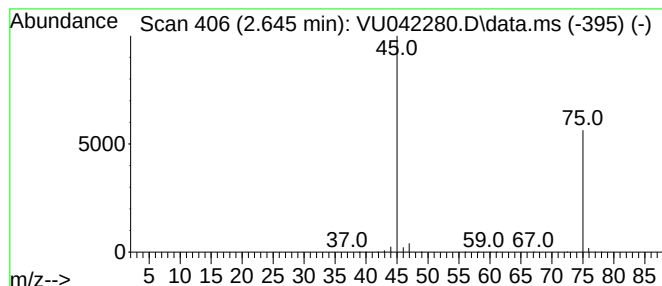
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methylal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.645	1608.04 ug/L	14851300	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylal			76	C3H8O2	000109-87-5	78
2	Methylal			76	C3H8O2	000109-87-5	78
3	Methylal			76	C3H8O2	000109-87-5	59
4	Methanamine, N,N-dimethyl-, N-oxide			75	C3H9NO	001184-78-7	7
5	Ethanethioamide			75	C2H5NS	000062-55-5	5



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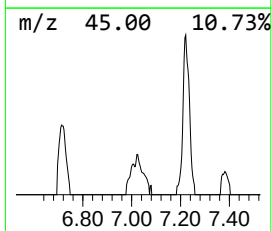
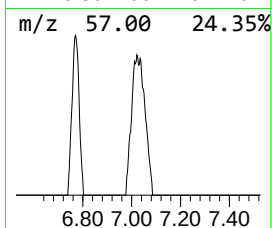
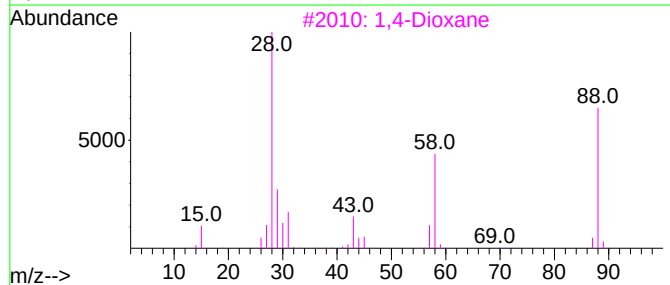
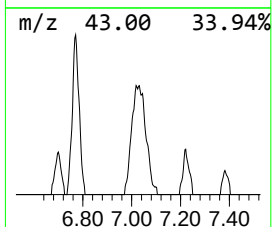
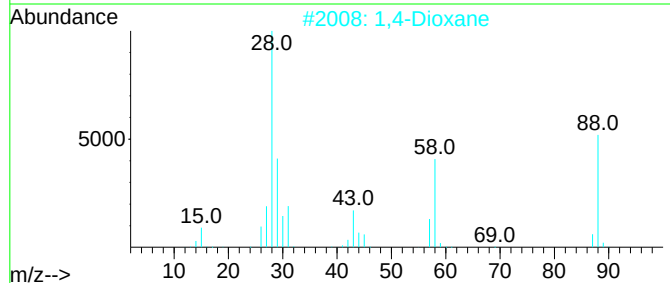
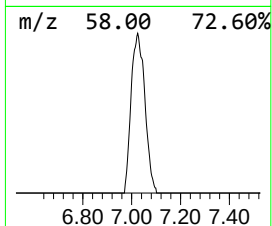
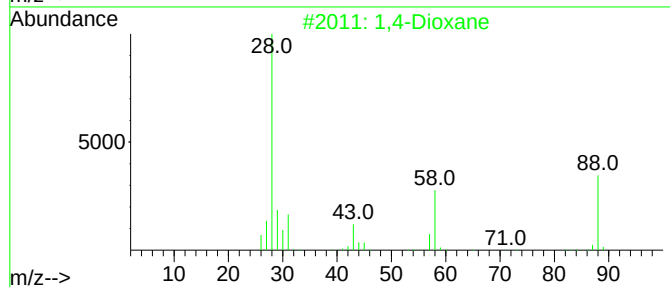
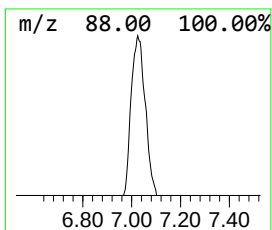
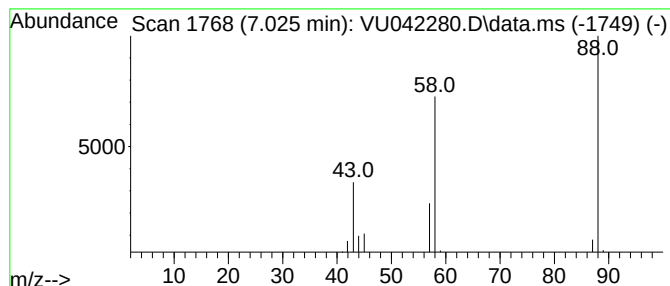
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1,4-Dioxane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.025	5.27 ug/L	48711	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane			88	C4H8O2	000123-91-1	91
2	1,4-Dioxane			88	C4H8O2	000123-91-1	91
3	1,4-Dioxane			88	C4H8O2	000123-91-1	90
4	1,4-Dioxane			88	C4H8O2	000123-91-1	90
5	Urea, N,N'-dimethyl-			88	C3H8N2O	000096-31-1	40



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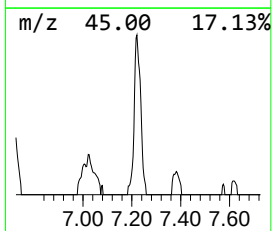
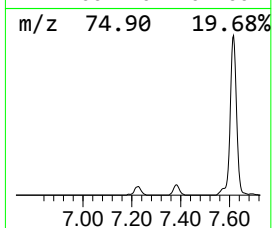
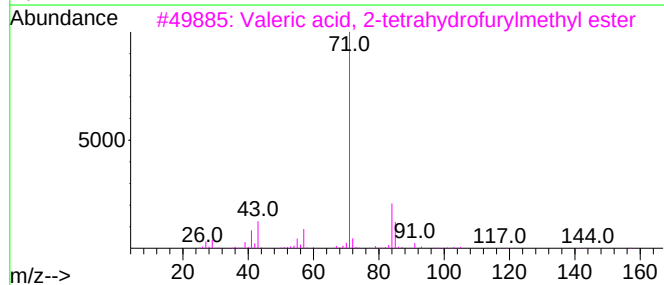
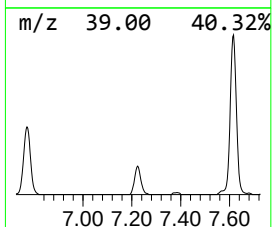
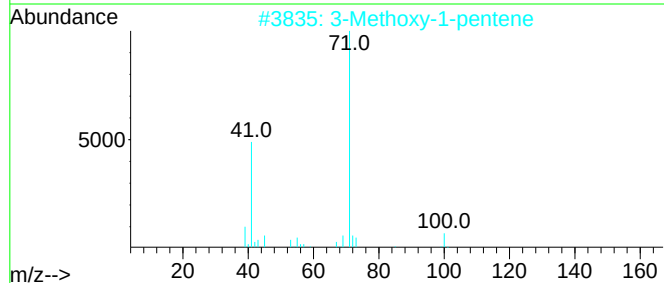
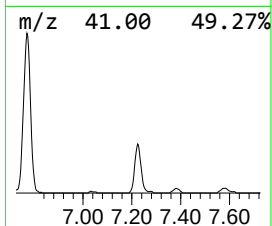
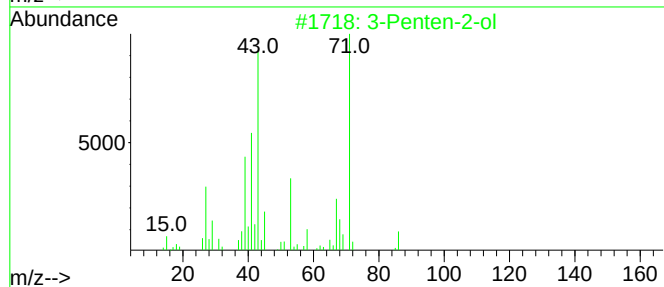
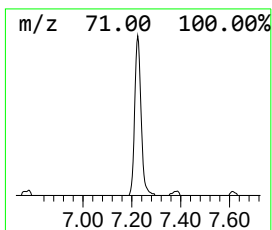
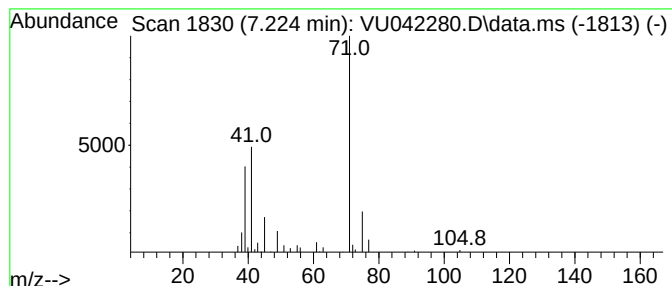
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	6.24 ug/L	57602	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-ol	86	C5H10O	001569-50-2	39
2			3-Methoxy-1-pentene	100	C6H12O	014092-18-3	23
3			Valeric acid, 2-tetrahydrofurylm...	186	C10H18O3	005451-86-5	9
4			Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	9
5			Butanoic acid, 2-pentenyl ester,...	156	C9H16O2	042125-13-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042280.D
Acq On : 05 Feb 2021 14:10
Operator : SY/MD
Sample : M1326-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z54

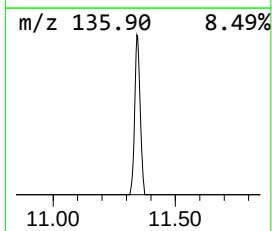
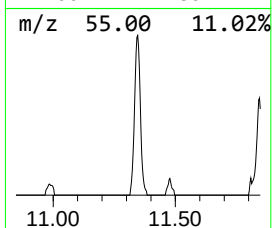
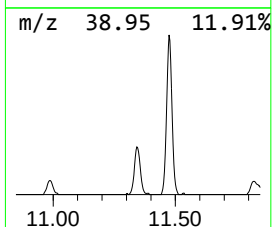
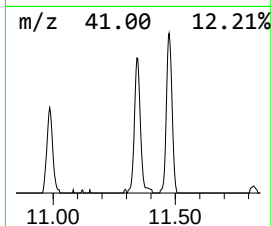
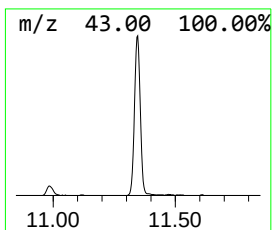
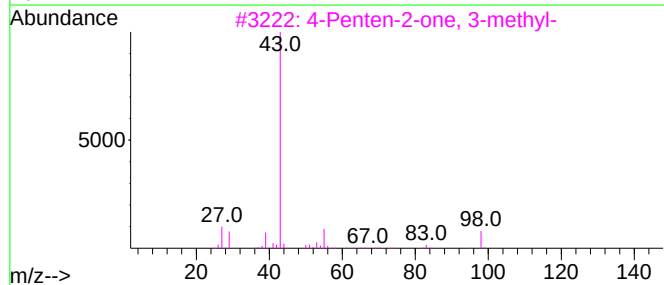
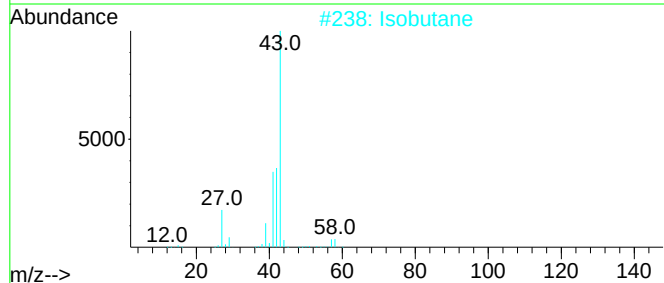
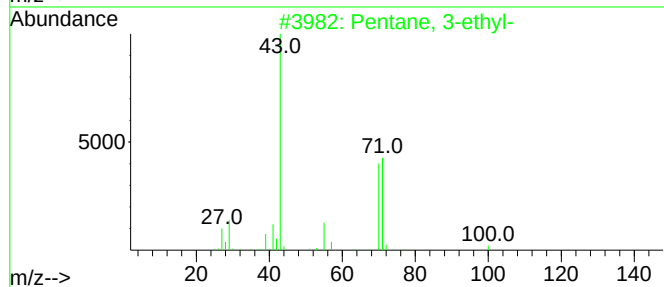
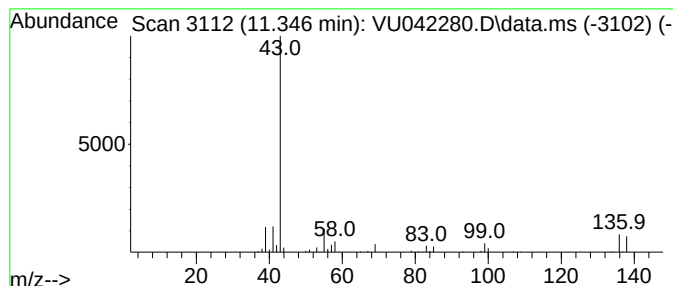
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.346	6.24 ug/L	120672	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-ethyl-	100	C7H16	000617-78-7	35
2			Isobutane	58	C4H10	000075-28-5	32
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	12
4			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5			Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042280.D
Acq On : 05 Feb 2021 14:10
Operator : SY/MD
Sample : M1326-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z54

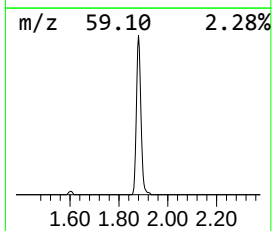
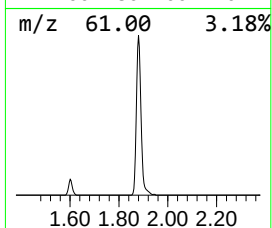
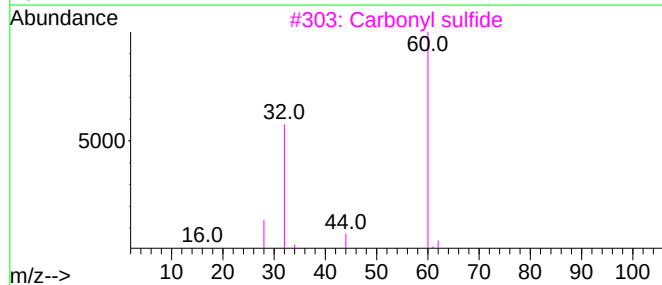
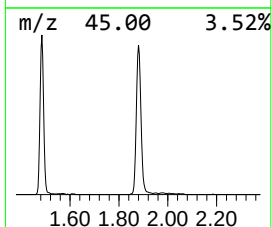
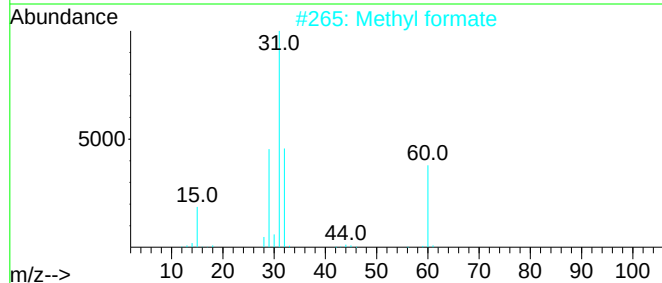
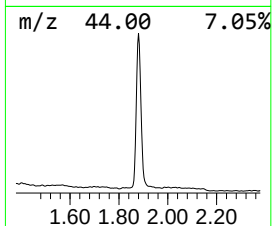
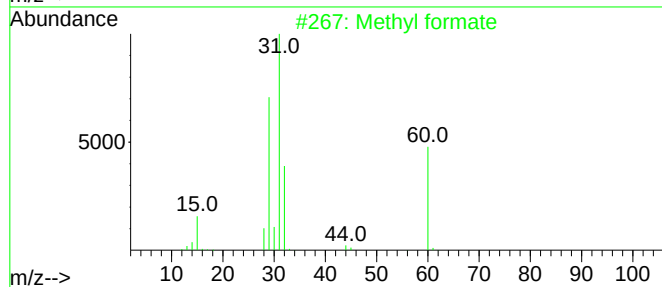
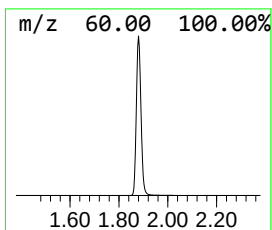
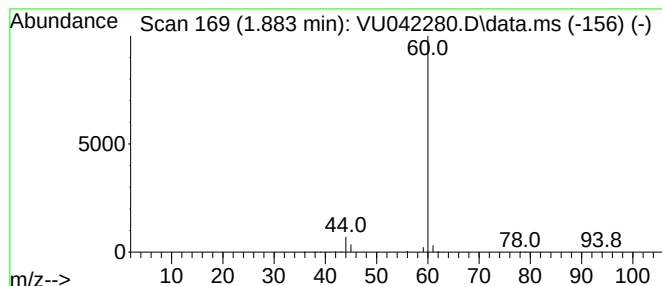
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.880	126.45 ug/L	1167830	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl formate	60	C2H4O2	000107-31-3	7
2			Methyl formate	60	C2H4O2	000107-31-3	7
3			Carbonyl sulfide	60	COS	000463-58-1	5
4			Urea	60	CH4N2O	000057-13-6	5
5			Methyl formate	60	C2H4O2	000107-31-3	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042280.D
Acq On : 05 Feb 2021 14:10
Operator : SY/MD
Sample : M1326-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z54

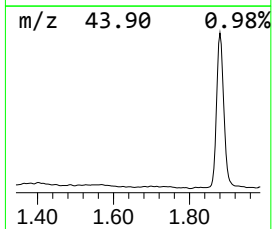
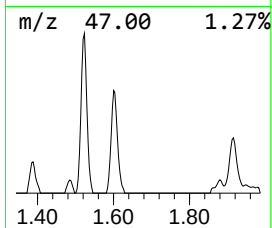
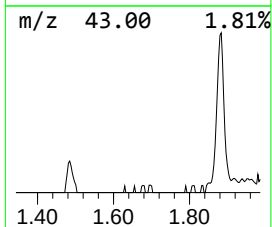
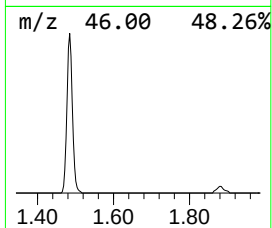
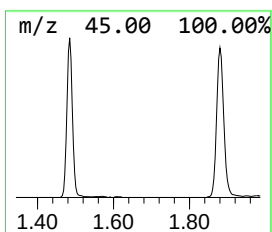
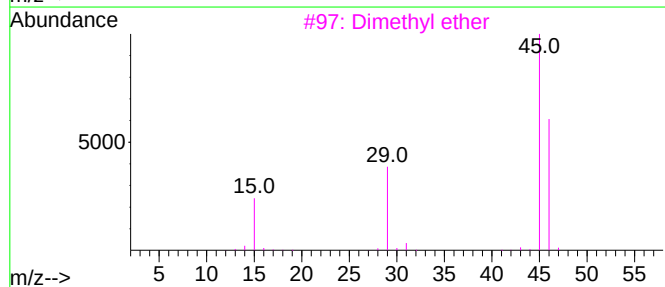
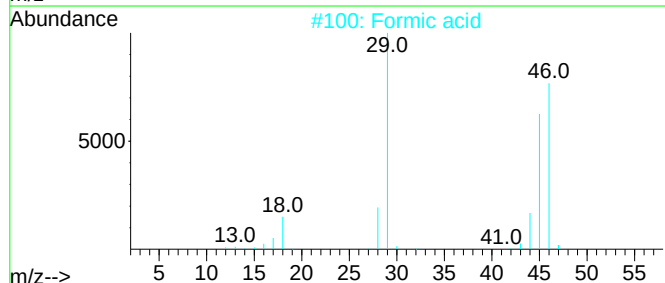
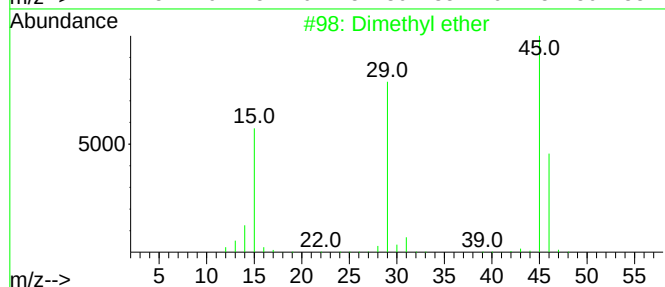
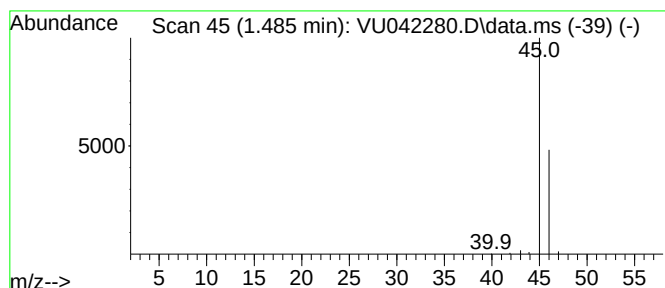
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Dimethyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.485	4.41 ug/L	40756	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	64
2			Formic acid	46	CH2O2	000064-18-6	37
3			Dimethyl ether	46	C2H6O	000115-10-6	9
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042280.D
Acq On : 05 Feb 2021 14:10
Operator : SY/MD
Sample : M1326-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z54

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.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
Methylal	2.645	1608.0	ug/L	14851300	1	6.256	461783	50.0
1,4-Dioxane	7.025	5.3	ug/L	48711	1	6.256	461783	50.0
unknown-02	7.224	6.2	ug/L	57602	1	6.256	461783	50.0
(DEL) Alkane: S...	11.346	6.2	ug/L	120672	3	11.822	966819	50.0
unknown-01	1.880	126.5	ug/L	1167830	1	6.256	461783	50.0
Dimethyl ether	1.485	4.4	ug/L	40756	1	6.256	461783	50.0