

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092421\
 Data File : VU044808.D
 Acq On : 24 Sep 2021 13:37
 Operator : SY/MD
 Sample : M3873-07DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7X7DL

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU044808.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	36	42	64	rBV2	47134	67224	5.34%	0.621%
2	1.604	74	82	97	rBV3	336493	396472	31.48%	3.662%
3	1.909	169	177	192	rVB	137791	188546	14.97%	1.741%
4	1.993	193	203	218	rVB	199865	276876	21.98%	2.557%
5	2.202	261	268	282	rVB	27059	39013	3.10%	0.360%
6	2.469	347	351	362	rVB3	2153	3105	0.25%	0.029%
7	2.568	370	382	400	rBV	249863	419829	33.33%	3.878%
8	2.710	424	426	430	rBV2	251	131	0.01%	0.001%
9	2.729	430	432	437	rBV	197	90	0.01%	0.001%
10	2.755	437	440	444	rVB3	187	112	0.01%	0.001%
11	2.790	445	451	452	rBV2	470	389	0.03%	0.004%
12	2.842	464	467	470	rBV2	174	105	0.01%	0.001%
13	2.922	489	492	493	rBV	175	97	0.01%	0.001%
14	2.964	498	505	508	rBV2	324	402	0.03%	0.004%
15	2.980	508	510	514	rVB	204	127	0.01%	0.001%
16	3.051	518	532	543	rBB3	4124	7764	0.62%	0.072%
17	3.141	548	560	575	rBV	22540	44590	3.54%	0.412%
18	3.292	604	607	611	rVB2	218	184	0.01%	0.002%
19	3.359	617	628	644	rVB	10648	20736	1.65%	0.192%
20	3.420	644	647	649	rBV	147	101	0.01%	0.001%
21	3.443	651	654	658	rVB2	179	133	0.01%	0.001%
22	3.530	677	681	683	rBV	215	129	0.01%	0.001%
23	3.697	729	733	737	rVB2	213	226	0.02%	0.002%
24	3.719	737	740	742	rBV	179	113	0.01%	0.001%
25	3.732	742	744	746	rBV	135	97	0.01%	0.001%
26	3.816	766	770	773	rBV	187	184	0.01%	0.002%
27	3.848	777	780	782	rBV	176	96	0.01%	0.001%
28	3.986	819	823	827	rVB	318	258	0.02%	0.002%
29	4.067	845	848	852	rVV2	180	124	0.01%	0.001%
30	4.102	856	859	862	rBV2	161	117	0.01%	0.001%
31	4.134	867	869	873	rVB2	174	132	0.01%	0.001%
32	4.163	873	878	883	rBV2	209	222	0.02%	0.002%
33	4.227	890	898	905	rBV2	226	473	0.04%	0.004%
34	4.263	905	909	913	rBV2	138	143	0.01%	0.001%
35	4.311	919	924	927	rBV2	100	111	0.01%	0.001%
36	4.536	981	994	1008	rVB2	10112	23487	1.86%	0.217%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	4.671	1008	1036	1066	rBV2	363433	1143606	90.80%	10.563%
38	4.870	1096	1098	1101	rBV2	301	160	0.01%	0.001%
39	4.903	1105	1108	1110	rBV2	223	139	0.01%	0.001%
40	4.944	1117	1121	1124	rBV	118	94	0.01%	0.001%
41	4.967	1124	1128	1133	rVV3	225	228	0.02%	0.002%
42	5.070	1141	1160	1183	rBV	223931	486526	38.63%	4.494%
43	5.205	1199	1202	1204	rBV2	141	99	0.01%	0.001%
44	5.263	1217	1220	1223	rBV2	315	238	0.02%	0.002%
45	5.285	1223	1227	1229	rVV	308	245	0.02%	0.002%
46	5.301	1229	1232	1235	rVB3	341	277	0.02%	0.003%
47	5.391	1247	1260	1274	rBV3	11565	24546	1.95%	0.227%
48	5.565	1311	1314	1317	rBV2	228	153	0.01%	0.001%
49	5.597	1317	1324	1331	rBV2	576	857	0.07%	0.008%
50	5.729	1343	1365	1399	rBV2	462733	1259438	100.00%	11.633%
51	6.118	1482	1486	1492	rVB2	386	413	0.03%	0.004%
52	6.153	1495	1497	1499	rVB2	158	82	0.01%	0.001%
53	6.253	1512	1528	1557	rBV	350514	660909	52.48%	6.104%
54	6.539	1607	1617	1628	rVB7	3800	7688	0.61%	0.071%
55	6.600	1632	1636	1640	rBV2	161	130	0.01%	0.001%
56	6.697	1651	1666	1685	rBV	292957	574137	45.59%	5.303%
57	6.803	1695	1699	1700	rBV3	358	264	0.02%	0.002%
58	6.944	1739	1743	1746	rBV2	153	125	0.01%	0.001%
59	6.986	1753	1756	1758	rBV	162	105	0.01%	0.001%
60	7.050	1770	1776	1777	rBV2	497	431	0.03%	0.004%
61	7.186	1811	1818	1829	rVB5	1451	2399	0.19%	0.022%
62	7.449	1897	1900	1906	rVB2	151	125	0.01%	0.001%
63	7.568	1924	1937	1962	rBV	154275	268905	21.35%	2.484%
64	7.697	1967	1977	1980	rBV4	815	1325	0.11%	0.012%
65	7.787	2002	2005	2007	rBV2	131	82	0.01%	0.001%
66	7.806	2008	2011	2015	rVB2	263	188	0.01%	0.002%
67	7.903	2026	2041	2056	rBV	530502	909959	72.25%	8.405%
68	7.973	2057	2063	2073	rVB	8269	13195	1.05%	0.122%
69	8.182	2116	2128	2143	rBV	106939	180594	14.34%	1.668%
70	8.298	2159	2164	2167	rBV3	301	284	0.02%	0.003%
71	8.478	2211	2220	2224	rBV2	266	399	0.03%	0.004%
72	8.568	2244	2248	2250	rBV	209	205	0.02%	0.002%
73	8.639	2257	2270	2311	rBV	473585	834370	66.25%	7.707%
74	9.275	2465	2468	2470	rBV	132	86	0.01%	0.001%
75	9.420	2499	2513	2532	rBV	497905	811030	64.40%	7.491%
76	9.571	2556	2560	2567	rBV2	344	423	0.03%	0.004%

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Integration Parameters: LSCINT.P

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Peak Location: TOP

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Peak separation: 5

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Title : VOC Analysis

77	9.697	2594	2599	2608	rVB4	582	859	0.07%	0.008%
78	9.735	2608	2611	2614	rVB	132	84	0.01%	0.001%
79	9.854	2642	2648	2657	rBV2	229	433	0.03%	0.004%
80	10.102	2722	2725	2731	rBV2	422	360	0.03%	0.003%
81	10.214	2755	2760	2764	rBV	216	288	0.02%	0.003%
82	10.401	2815	2818	2820	rBV	183	129	0.01%	0.001%
83	10.446	2829	2832	2834	rBV	130	99	0.01%	0.001%
84	10.677	2895	2904	2913	rBV2	1725	2707	0.21%	0.025%
85	10.761	2917	2930	2950	rBV	404582	651984	51.77%	6.022%
86	10.864	2958	2962	2963	rBV	520	315	0.03%	0.003%
87	11.118	3037	3041	3042	rBV2	174	121	0.01%	0.001%
88	11.427	3134	3137	3140	rBV	173	162	0.01%	0.001%
89	11.465	3141	3149	3158	rVB4	1666	2714	0.22%	0.025%
90	11.581	3182	3185	3188	rBV2	260	192	0.02%	0.002%
91	11.690	3216	3219	3222	rBV3	541	459	0.04%	0.004%
92	11.745	3234	3236	3239	rBV	315	201	0.02%	0.002%
93	11.816	3246	3258	3278	rBV	450479	703717	55.88%	6.500%
94	11.954	3295	3301	3302	rBV2	552	583	0.05%	0.005%
95	12.044	3327	3329	3331	rBV	168	84	0.01%	0.001%
96	12.092	3342	3344	3347	rVB	206	89	0.01%	0.001%
97	12.195	3360	3376	3398	rBV	484993	783808	62.23%	7.240%
98	12.333	3417	3419	3425	rVB3	481	249	0.02%	0.002%
99	12.362	3426	3428	3431	rBV2	211	92	0.01%	0.001%
100	14.098	3962	3968	3972	rBV2	479	678	0.05%	0.006%

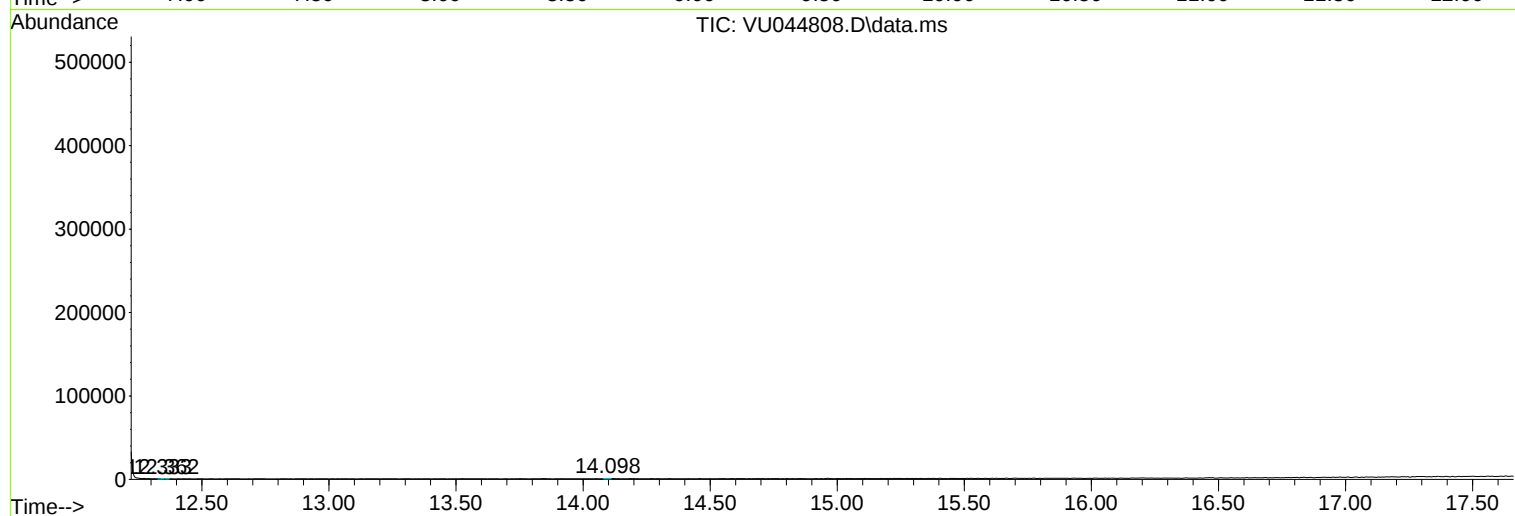
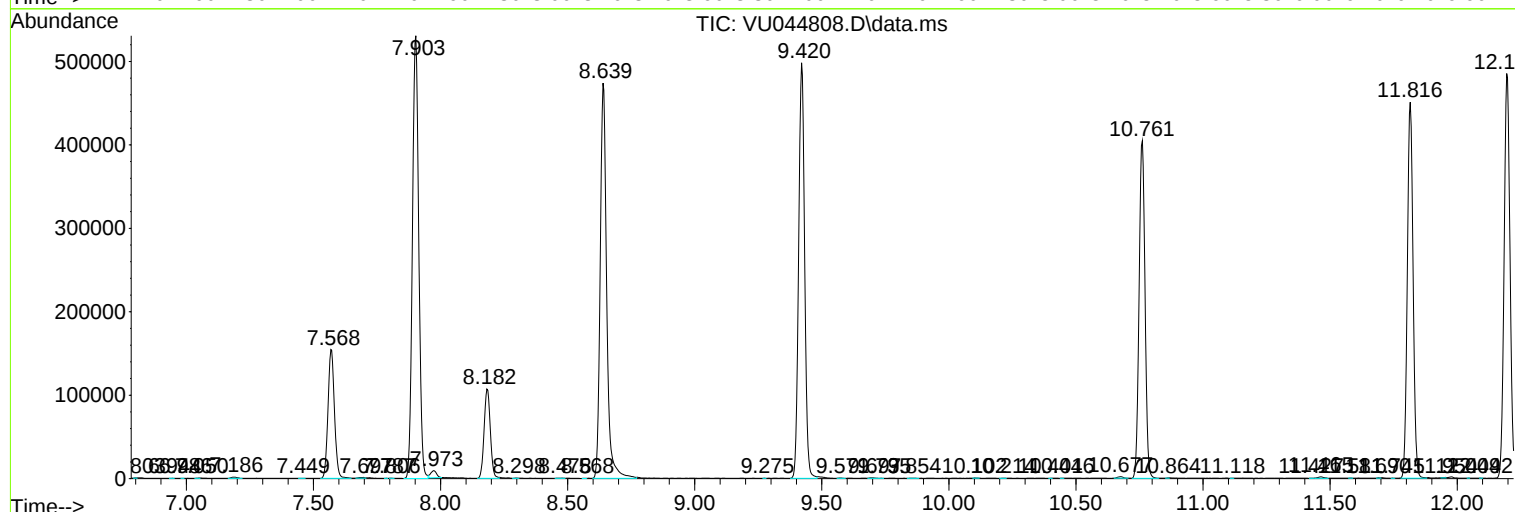
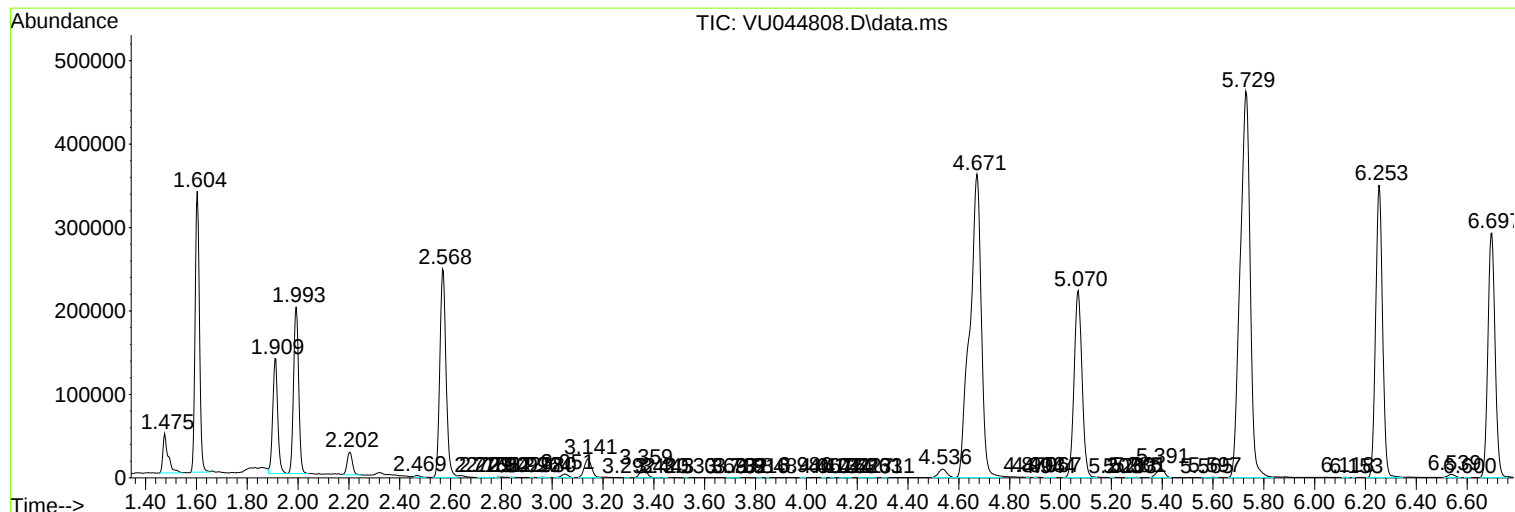
Sum of corrected areas: 10826804

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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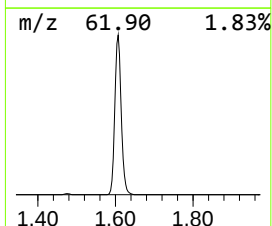
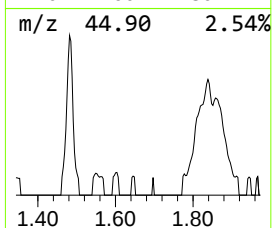
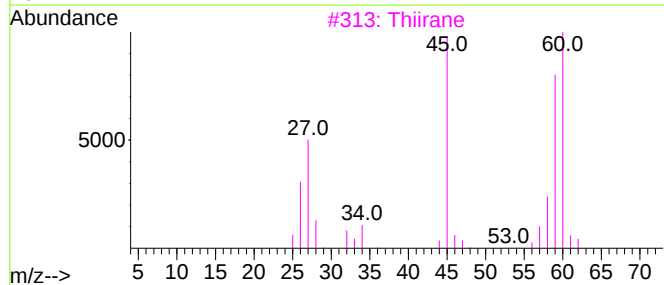
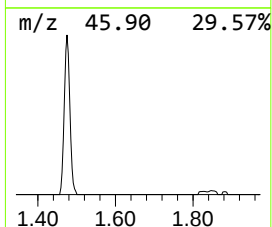
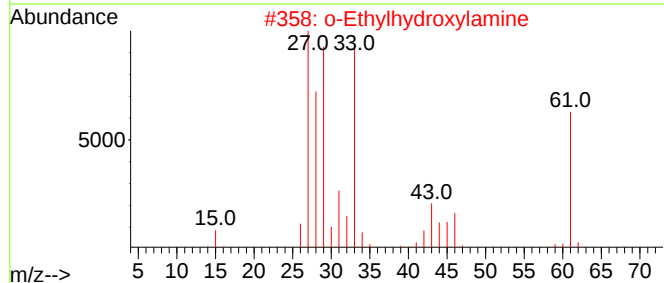
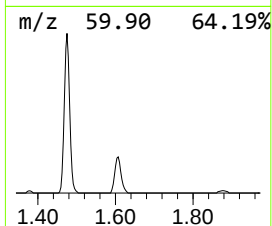
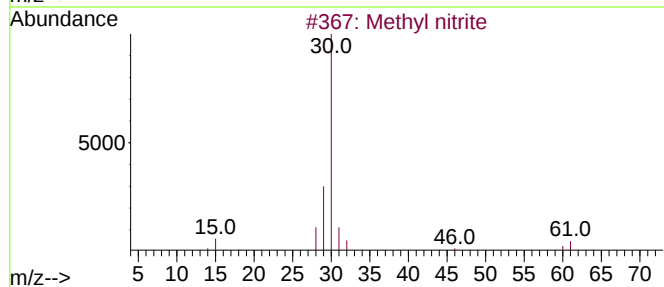
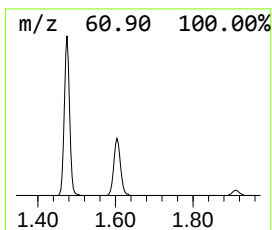
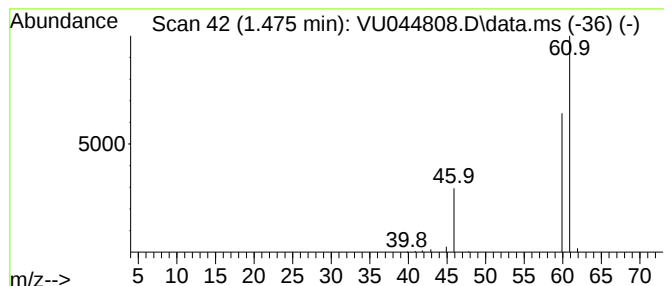
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.475	5.09 ug/L	67224	1,4-Difluorobenzene	6.253

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			Thiirane	60	C2H4S	000420-12-2	4
4			Ethyne, chloro-	60	C2HCl	000593-63-5	4
5			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4



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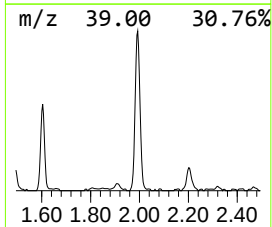
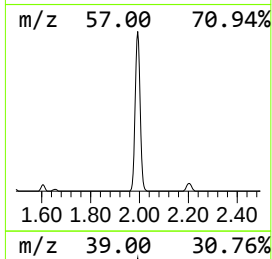
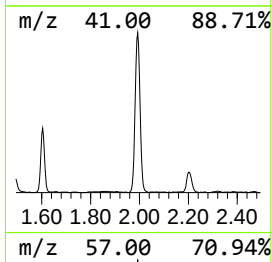
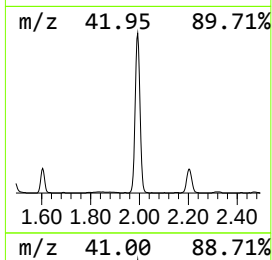
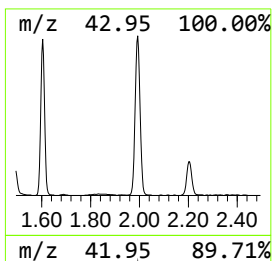
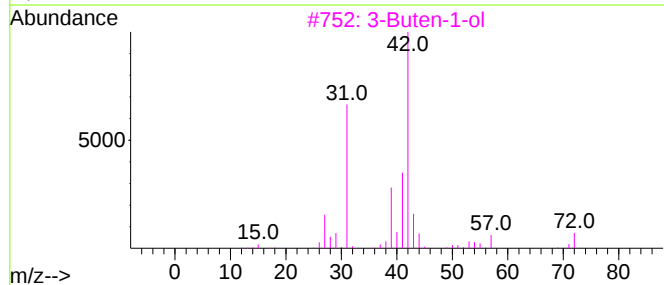
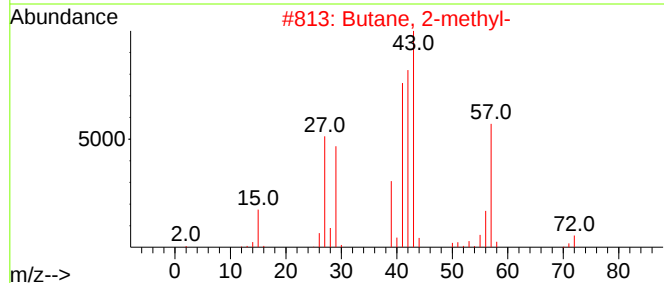
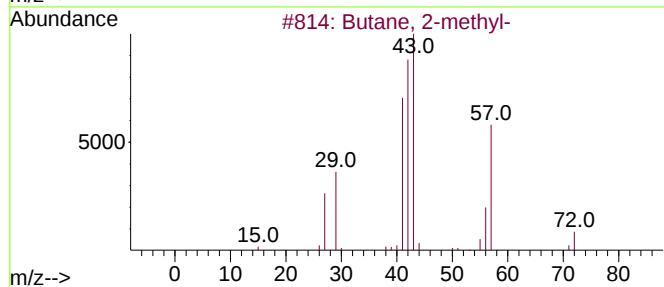
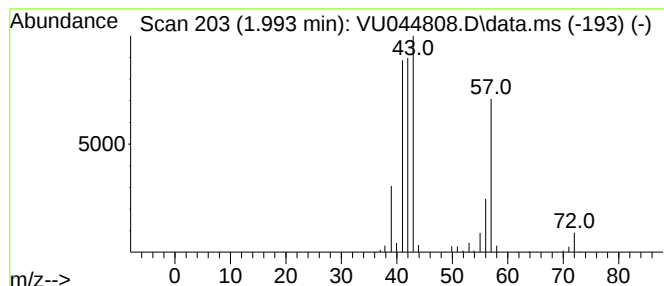
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.993	20.95 ug/L	276876	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	87
2		Butane, 2-methyl-	72	C5H12	000078-78-4	86
3		3-Buten-1-ol	72	C4H8O	000627-27-0	47
4		Pentane	72	C5H12	000109-66-0	45
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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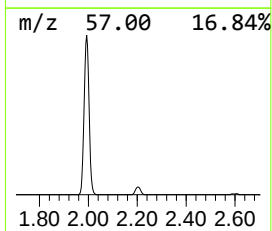
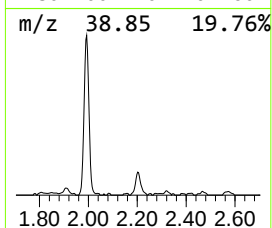
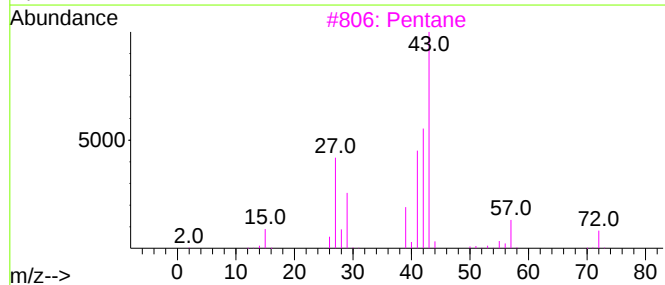
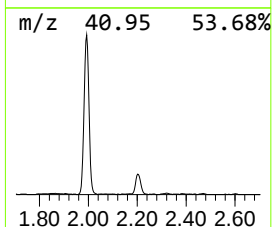
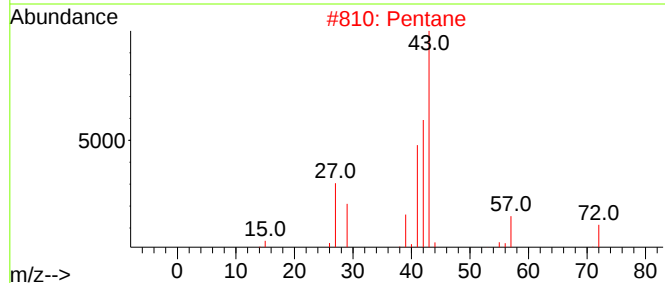
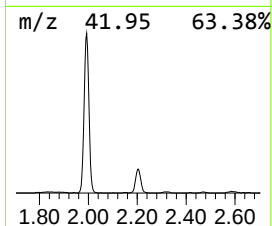
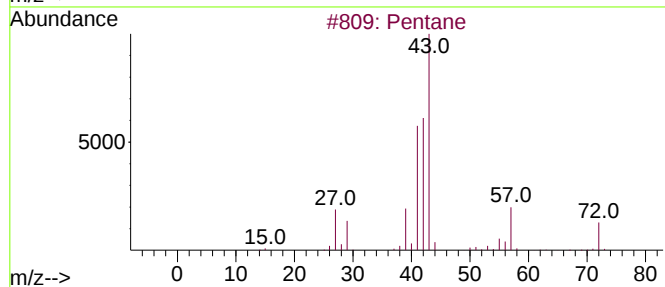
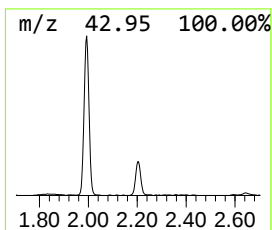
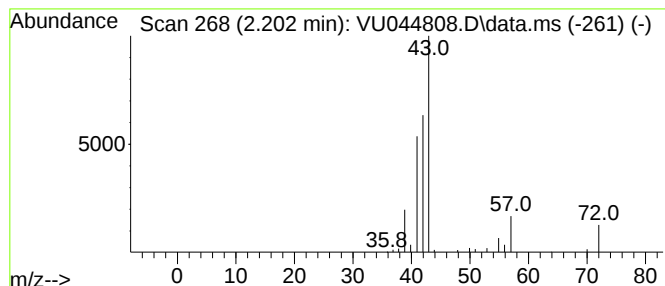
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.202	2.95 ug/L	39013	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Pentane	72	C5H12	000109-66-0	86
3	Pentane	72	C5H12	000109-66-0	86
4	Pentane	72	C5H12	000109-66-0	86
5	Pentane	72	C5H12	000109-66-0	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092421\
Data File : VU044808.D
Acq On : 24 Sep 2021 13:37
Operator : SY/MD
Sample : M3873-07DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7X7DL

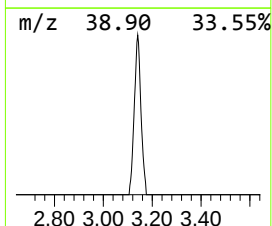
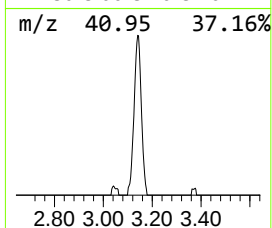
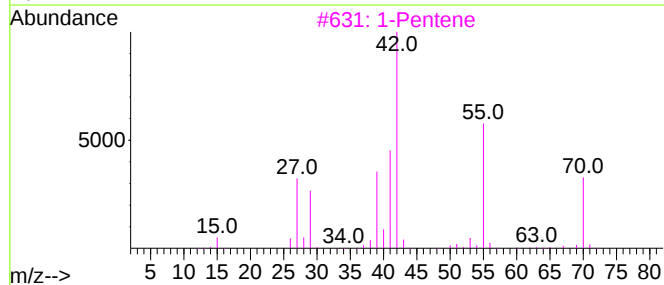
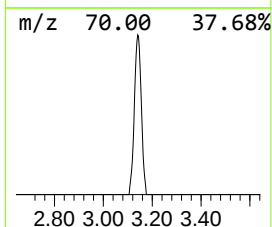
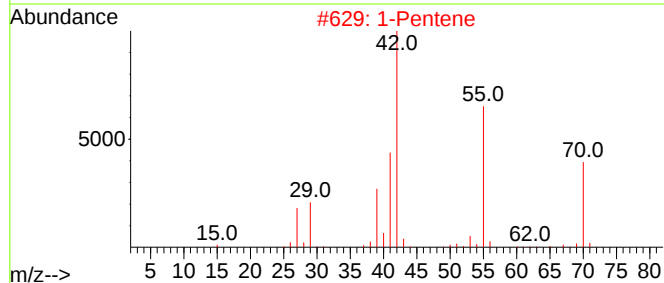
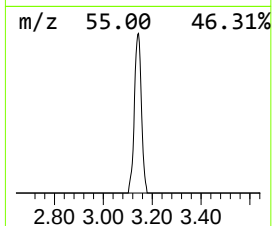
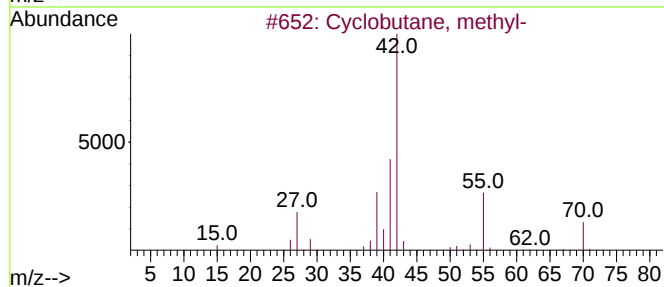
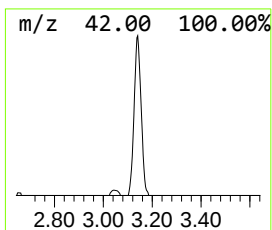
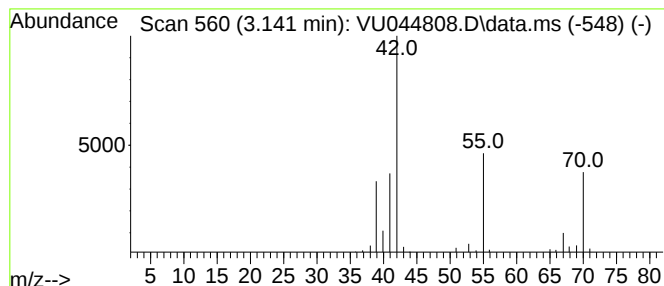
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic3.141 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.141	3.37 ug/L	44590	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2			1-Pentene	70	C5H10	000109-67-1	80
3			1-Pentene	70	C5H10	000109-67-1	80
4			Cyclopentane	70	C5H10	000287-92-3	80
5			Cyclopentane	70	C5H10	000287-92-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092421\
Data File : VU044808.D
Acq On : 24 Sep 2021 13:37
Operator : SY/MD
Sample : M3873-07DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7X7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.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	1.475	5.1	ug/L	67224	1	6.253	660909	50.0
(DEL) Alkane: S...	1.993	20.9	ug/L	276876	1	6.253	660909	50.0
(DEL) Alkane: S...	2.202	3.0	ug/L	39013	1	6.253	660909	50.0
(DEL) Alkane: C...	3.141	3.4	ug/L	44590	1	6.253	660909	50.0