

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061022\
 Data File : VU049032.D
 Acq On : 11 Jun 2022 05:36
 Operator : SY/MD
 Sample : N3249-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXYX2

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\SFAMULM061022WMA.M
 Title : VOC Analysis

Signal : TIC: VU049032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.356	3	5	21	rVB	706227	583672	67.90%	7.276%
2	1.437	23	30	39	rBV	60496	67850	7.89%	0.846%
3	1.588	69	77	86	rBV2	203343	288566	33.57%	3.597%
4	1.633	86	91	96	rVV	72673	75545	8.79%	0.942%
5	1.659	96	99	105	rVB	23701	21962	2.55%	0.274%
6	1.729	112	121	130	rBV4	32546	46361	5.39%	0.578%
7	1.864	157	163	167	rBV3	5880	7882	0.92%	0.098%
8	1.903	167	175	193	rVB	72083	101380	11.79%	1.264%
9	2.089	225	233	243	rBV2	14367	19372	2.25%	0.241%
10	2.150	243	252	262	rVB	20035	28093	3.27%	0.350%
11	2.240	277	280	281	rBV3	843	619	0.07%	0.008%
12	2.314	295	303	312	rVB4	5824	9357	1.09%	0.117%
13	2.404	321	331	345	rVB7	9366	18498	2.15%	0.231%
14	2.565	368	381	393	rVV2	164673	282312	32.84%	3.519%
15	2.630	395	401	415	rVB4	11112	17434	2.03%	0.217%
16	2.800	446	454	462	rBV6	4103	6557	0.76%	0.082%
17	2.858	462	472	482	rVB3	5210	9083	1.06%	0.113%
18	2.951	495	501	503	rBV3	968	985	0.11%	0.012%
19	3.015	512	521	529	rBV5	3576	6425	0.75%	0.080%
20	3.089	541	544	549	rBV2	264	333	0.04%	0.004%
21	3.179	564	572	584	rVB4	2909	5761	0.67%	0.072%
22	3.324	608	617	619	rBV3	719	772	0.09%	0.010%
23	3.347	619	624	625	rBV2	1086	707	0.08%	0.009%
24	3.388	635	637	643	rVB2	353	295	0.03%	0.004%
25	3.443	643	654	665	rBV4	2689	5525	0.64%	0.069%
26	3.584	690	698	709	rBV8	2818	6021	0.70%	0.075%
27	3.646	714	717	719	rVB2	462	290	0.03%	0.004%
28	3.691	727	731	735	rVB	269	260	0.03%	0.003%
29	3.713	735	738	743	rBV2	251	261	0.03%	0.003%
30	3.748	746	749	752	rBV	358	252	0.03%	0.003%
31	3.867	769	786	806	rBV2	69223	163571	19.03%	2.039%
32	4.157	872	876	878	rBV2	589	485	0.06%	0.006%
33	4.253	900	906	909	rBV3	568	653	0.08%	0.008%
34	4.620	1007	1020	1030	rBV	105332	249782	29.06%	3.114%
35	4.768	1063	1066	1071	rVV4	510	468	0.05%	0.006%
36	4.887	1101	1103	1112	rVB3	578	688	0.08%	0.009%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
 Title : VOC Analysis

37	5.064	1141	1158	1181	rBV	166809	366361	42.62%	4.567%
38	5.314	1221	1236	1252	rBV	59356	132168	15.38%	1.648%
39	5.514	1296	1298	1303	rBV4	275	291	0.03%	0.004%
40	5.597	1317	1324	1327	rBV	390	388	0.05%	0.005%
41	5.620	1327	1331	1336	rBV2	254	260	0.03%	0.003%
42	5.726	1342	1364	1377	rBV2	306959	859607	100.00%	10.716%
43	5.887	1405	1414	1427	rVV5	1324	2780	0.32%	0.035%
44	5.964	1434	1438	1440	rVV2	473	361	0.04%	0.005%
45	5.977	1440	1442	1449	rVB2	805	722	0.08%	0.009%
46	6.012	1449	1453	1455	rBV2	319	249	0.03%	0.003%
47	6.031	1457	1459	1464	rVV2	364	265	0.03%	0.003%
48	6.134	1488	1491	1496	rVB2	265	271	0.03%	0.003%
49	6.192	1502	1509	1512	rBV2	351	424	0.05%	0.005%
50	6.247	1512	1526	1544	rBV	262493	498381	57.98%	6.213%
51	6.430	1580	1583	1587	rVB2	328	251	0.03%	0.003%
52	6.543	1605	1618	1632	rBV5	17066	32631	3.80%	0.407%
53	6.690	1649	1664	1682	rBV2	203906	401996	46.77%	5.011%
54	6.793	1693	1696	1699	rBV4	710	452	0.05%	0.006%
55	6.867	1710	1719	1721	rBV2	276	341	0.04%	0.004%
56	6.887	1721	1725	1728	rVV2	406	304	0.04%	0.004%
57	6.928	1734	1738	1741	rBV2	313	268	0.03%	0.003%
58	6.961	1741	1748	1750	rBV3	2117	2040	0.24%	0.025%
59	7.314	1852	1858	1859	rBV	288	304	0.04%	0.004%
60	7.366	1869	1874	1879	rBV2	419	465	0.05%	0.006%
61	7.565	1923	1936	1955	rBV	86246	151213	17.59%	1.885%
62	7.681	1967	1972	1976	rBV4	701	861	0.10%	0.011%
63	7.899	2024	2040	2056	rBV	357490	616895	71.76%	7.690%
64	7.967	2058	2061	2073	rVB3	5039	7236	0.84%	0.090%
65	8.179	2115	2127	2145	rVV2	62177	104432	12.15%	1.302%
66	8.340	2174	2177	2183	rVB	407	319	0.04%	0.004%
67	8.407	2195	2198	2202	rVB2	380	262	0.03%	0.003%
68	8.472	2213	2218	2227	rVB4	1126	1446	0.17%	0.018%
69	8.552	2233	2243	2253	rBV3	19528	33213	3.86%	0.414%
70	8.633	2256	2268	2300	rBV2	272830	544596	63.35%	6.789%
71	8.787	2314	2316	2322	rVB4	1090	873	0.10%	0.011%
72	9.256	2458	2462	2471	rBV	329	408	0.05%	0.005%
73	9.417	2499	2512	2531	rBV	367877	615187	71.57%	7.669%
74	9.645	2579	2583	2587	rBV2	343	302	0.04%	0.004%
75	9.694	2595	2598	2605	rVB4	731	617	0.07%	0.008%
76	10.095	2720	2723	2727	rVV3	422	403	0.05%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
 Title : VOC Analysis

77	10.189	2750	2752	2760	rVB2	233	267	0.03%	0.003%
78	10.237	2763	2767	2773	rVB2	310	441	0.05%	0.005%
79	10.459	2833	2836	2842	rVB2	372	415	0.05%	0.005%
80	10.488	2842	2845	2847	rBV	455	270	0.03%	0.003%
81	10.558	2864	2867	2871	rVV2	249	268	0.03%	0.003%
82	10.755	2915	2928	2951	rVV	311493	510144	59.35%	6.359%
83	10.893	2962	2971	2979	rVB3	2327	2781	0.32%	0.035%
84	11.314	3100	3102	3110	rVB2	401	485	0.06%	0.006%
85	11.478	3151	3153	3155	rBV	444	270	0.03%	0.003%
86	11.812	3245	3257	3275	rBV	326560	521516	60.67%	6.501%
87	12.018	3317	3321	3324	rBV2	367	329	0.04%	0.004%
88	12.192	3362	3375	3393	rBV2	347114	569977	66.31%	7.105%
89	12.497	3467	3470	3473	rBV	405	327	0.04%	0.004%
90	12.645	3512	3516	3519	rBV	321	274	0.03%	0.003%
91	13.128	3662	3666	3673	rBV3	446	574	0.07%	0.007%
92	13.211	3689	3692	3697	rVB	457	305	0.04%	0.004%
93	13.356	3734	3737	3741	rBV	353	269	0.03%	0.003%
94	13.507	3780	3784	3788	rBV2	394	349	0.04%	0.004%
95	13.970	3925	3928	3931	rBV2	351	285	0.03%	0.004%
96	14.613	4121	4128	4131	rBV3	452	672	0.08%	0.008%
97	15.906	4526	4530	4535	rBV4	959	1085	0.13%	0.014%
98	15.976	4547	4552	4554	rBV3	1217	1028	0.12%	0.013%
99	16.131	4597	4600	4603	rBV4	737	572	0.07%	0.007%
100	16.362	4669	4672	4677	rVB6	989	995	0.12%	0.012%

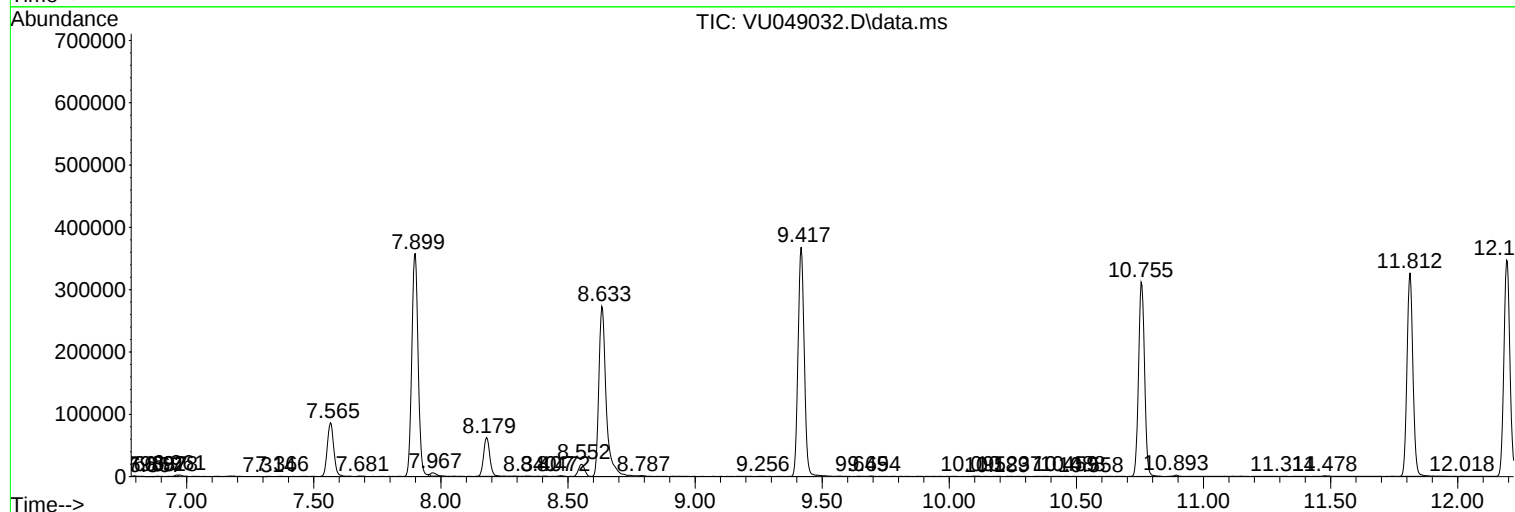
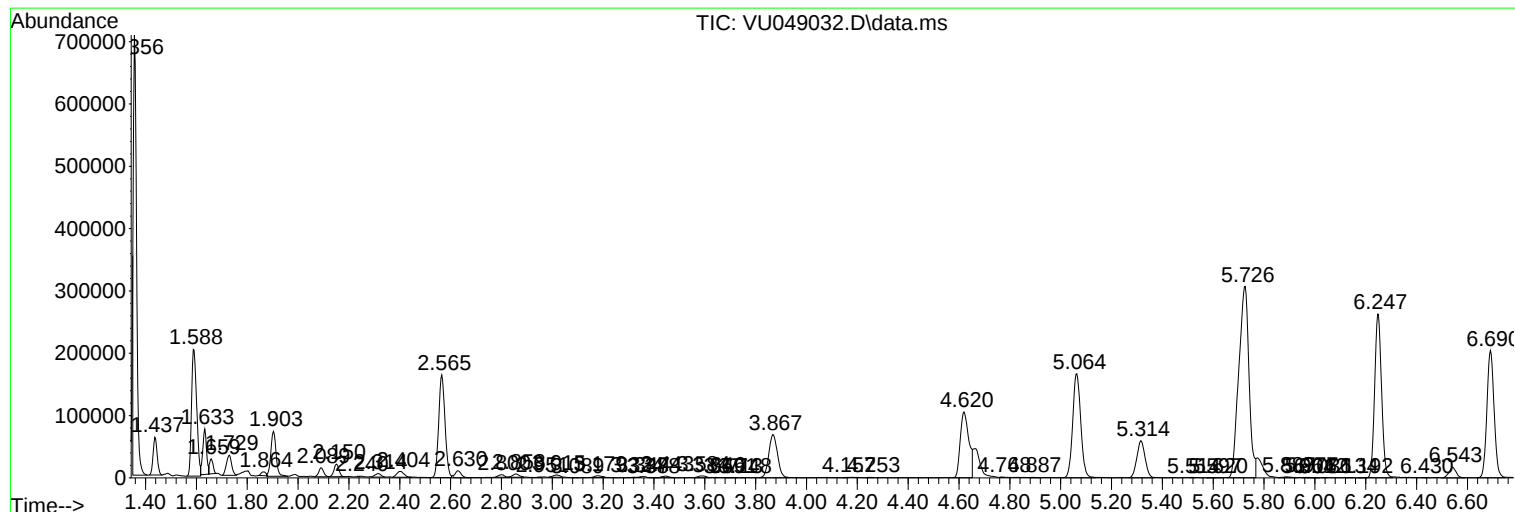
Sum of corrected areas: 8021818

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061022\
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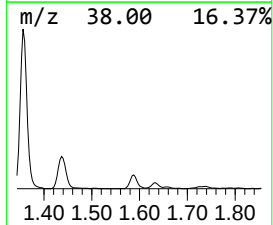
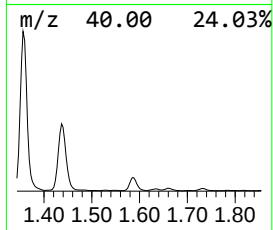
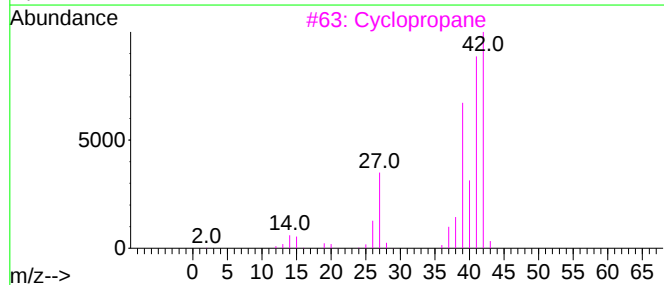
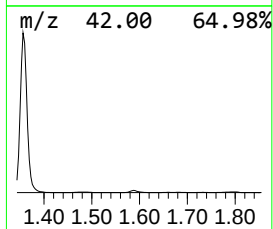
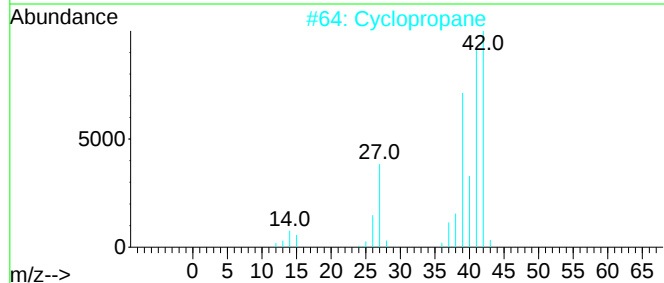
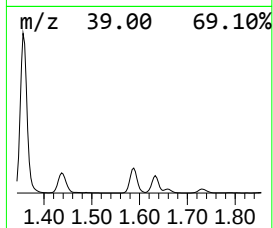
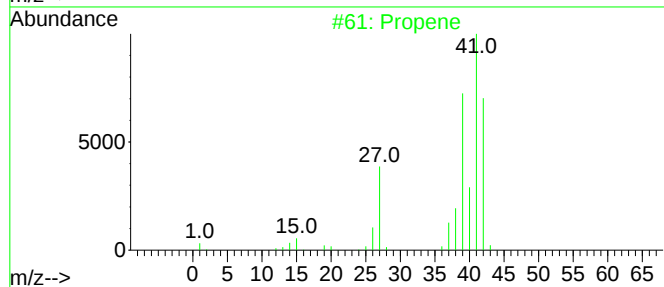
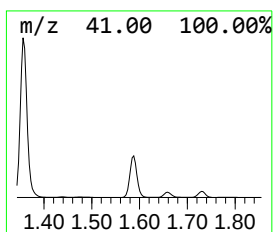
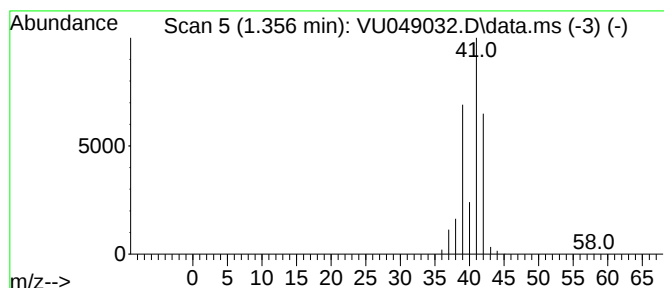
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.356	58.56 ug/L	583672	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	86
3			Cyclopropane	42	C3H6	000075-19-4	78
4			Propene	42	C3H6	000115-07-1	50
5			Cyclopropane	42	C3H6	000075-19-4	37



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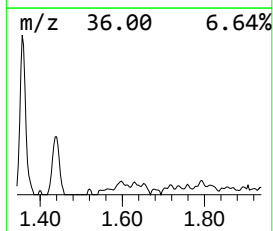
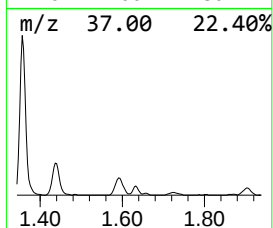
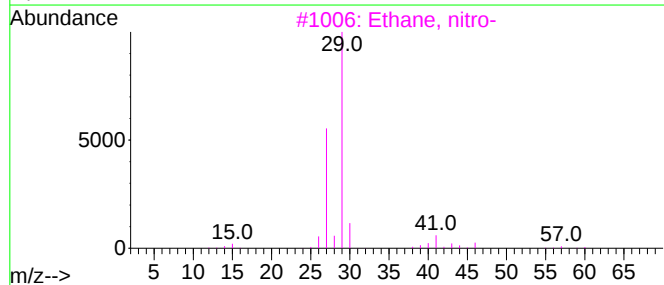
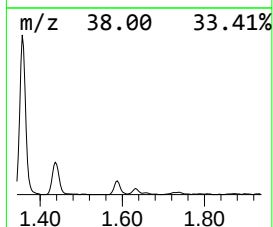
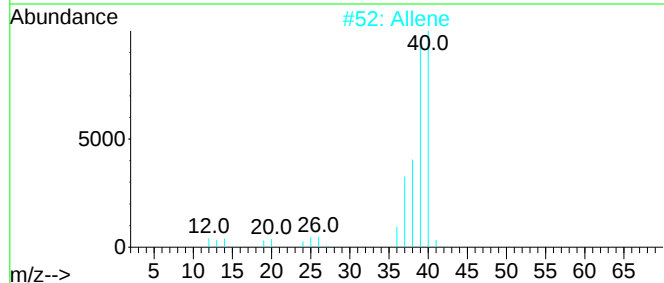
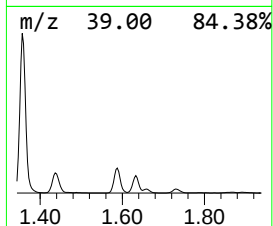
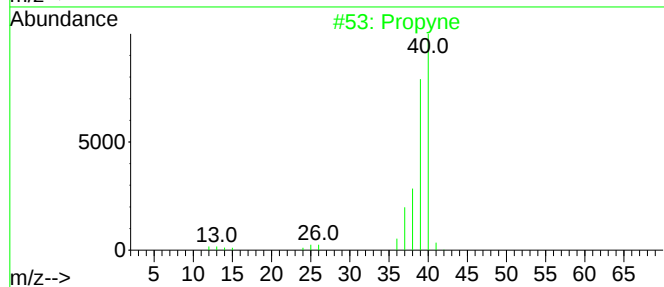
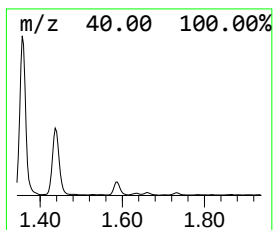
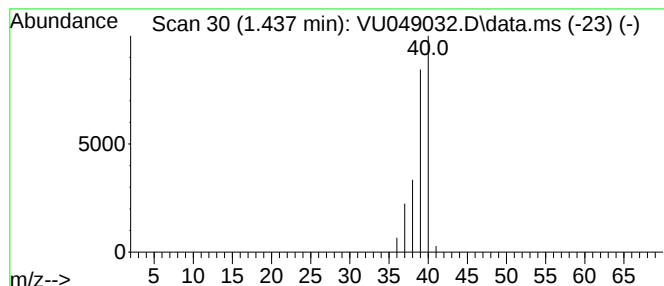
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Propyne Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.437	6.81 ug/L	67850	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propyne	40	C3H4	000074-99-7	90
2			Allene	40	C3H4	000463-49-0	90
3			Ethane, nitro-	75	C2H5NO2	000079-24-3	1
4			3-Methyl-1,2-diazirine	56	C2H4N2	1000305-83-7	1
5			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	1



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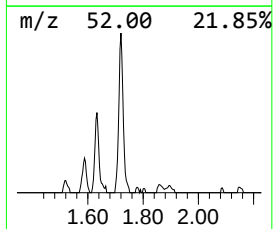
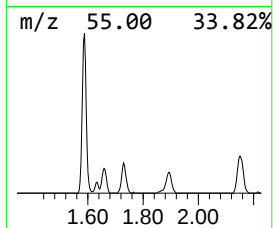
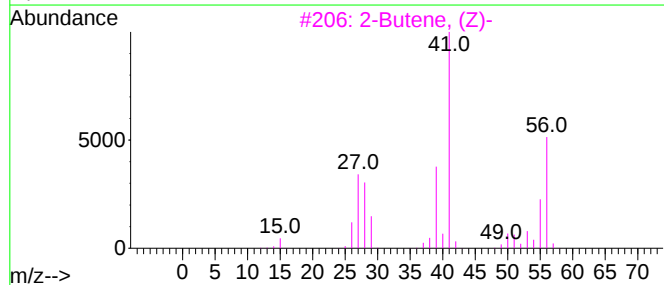
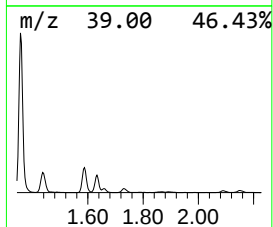
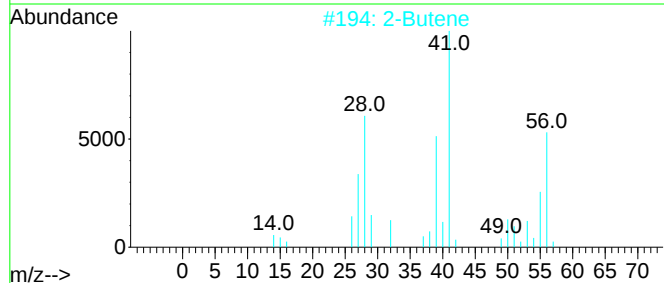
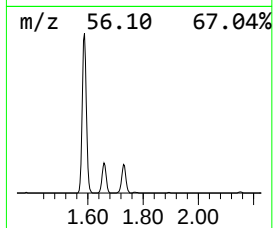
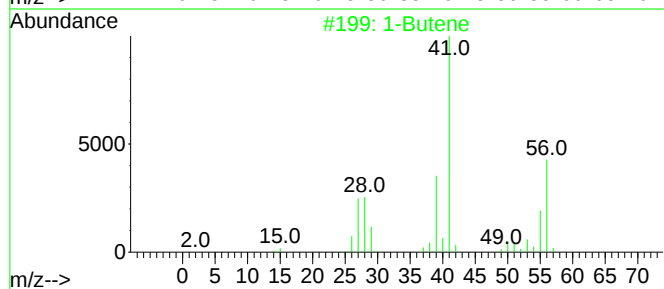
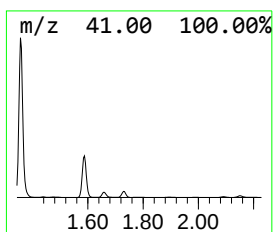
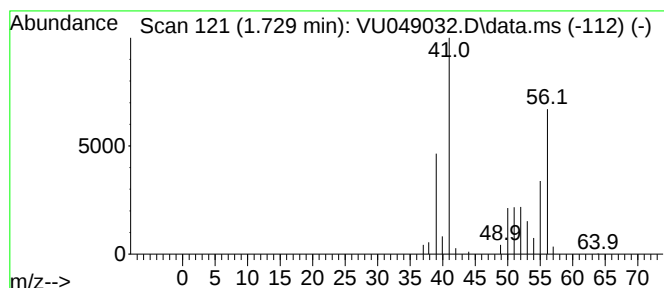
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.729	4.65 ug/L	46361	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene			56	C4H8	000106-98-9	43
2	2-Butene			56	C4H8	000107-01-7	38
3	2-Butene, (Z)-			56	C4H8	000590-18-1	38
4	2-Butene, (E)-			56	C4H8	000624-64-6	38
5	1-Propene, 2-methyl-			56	C4H8	000115-11-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061022\
Data File : VU049032.D
Acq On : 11 Jun 2022 05:36
Operator : SY/MD
Sample : N3249-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXYX2

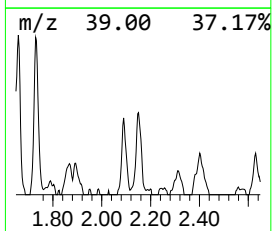
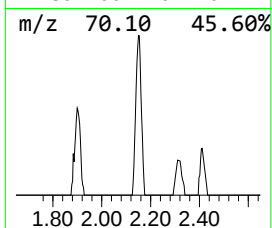
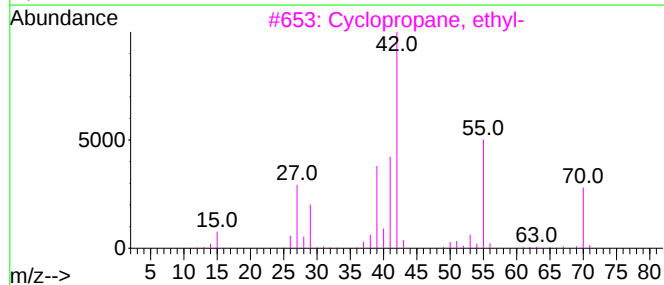
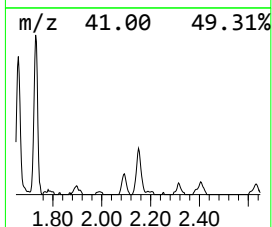
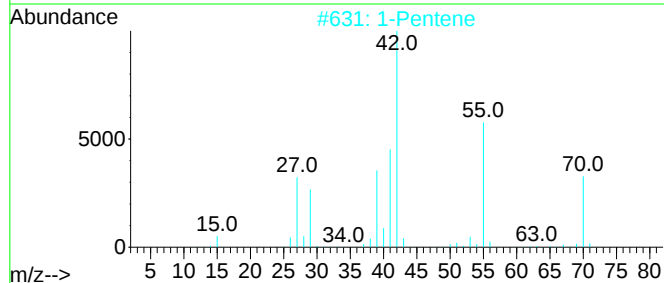
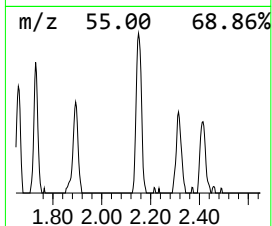
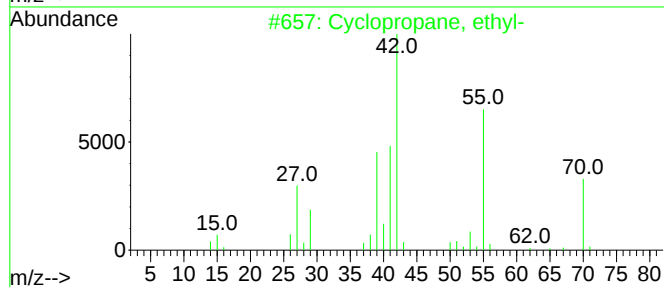
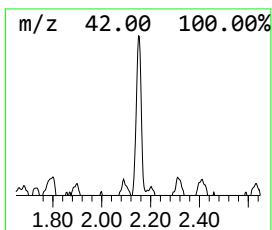
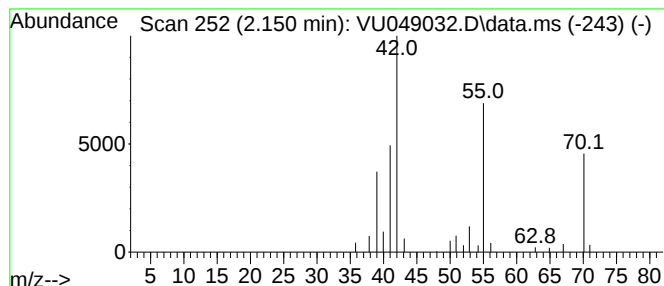
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic2.150 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.150	2.82 ug/L	28093	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	86
2			1-Pentene	70	C5H10	000109-67-1	86
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	86
4			1-Pentene	70	C5H10	000109-67-1	86
5			Cyclopentane	70	C5H10	000287-92-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061022\
Data File : VU049032.D
Acq On : 11 Jun 2022 05:36
Operator : SY/MD
Sample : N3249-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXYX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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
(DEL) Alkane: S...	1.356	58.6	ug/L	583672	1	6.247	498381	50.0
Propyne	1.437	6.8	ug/L	67850	1	6.247	498381	50.0
(DEL) Alkane: S...	1.729	4.7	ug/L	46361	1	6.247	498381	50.0
(DEL) Alkane: C...	2.150	2.8	ug/L	28093	1	6.247	498381	50.0