

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071923\
 Data File : VU054819.D
 Acq On : 19 Jul 2023 14:39
 Operator : MD/SY
 Sample : 03656-16
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH2X9

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\SFAMULM071723WMA.M
 Title : VOC Analysis

Signal : TIC: VU054819.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	90	96	112	rVB	77978	101507	13.48%	1.483%
2	2.554	383	393	406	rBV	126896	205477	27.30%	3.001%
3	3.190	578	591	613	rVB3	28516	82215	10.92%	1.201%
4	3.422	660	663	665	rBV3	665	461	0.06%	0.007%
5	3.454	670	673	677	rVB3	851	491	0.07%	0.007%
6	3.480	677	681	683	rBV3	686	588	0.08%	0.009%
7	3.557	704	705	706	rBV3	368	75	0.01%	0.001%
8	3.840	788	793	798	rBV3	515	533	0.07%	0.008%
9	4.155	889	891	892	rBV	327	124	0.02%	0.002%
10	4.380	960	961	963	rVB	313	105	0.01%	0.002%
11	4.422	972	974	976	rBV2	661	360	0.05%	0.005%
12	4.489	993	995	997	rBV2	626	289	0.04%	0.004%
13	4.618	1024	1035	1058	rBV	78862	188863	25.09%	2.759%
14	5.055	1157	1171	1192	rBV	142376	309245	41.08%	4.517%
15	5.364	1262	1267	1270	rBV3	876	979	0.13%	0.014%
16	5.605	1340	1342	1344	rBV	392	120	0.02%	0.002%
17	5.621	1344	1347	1349	rBV2	393	282	0.04%	0.004%
18	5.717	1357	1377	1404	rBV2	273181	748434	99.43%	10.933%
19	5.971	1453	1456	1460	rBV3	896	697	0.09%	0.010%
20	6.039	1472	1477	1482	rBV4	1011	1462	0.19%	0.021%
21	6.090	1491	1493	1496	rBV	425	259	0.03%	0.004%
22	6.110	1496	1499	1504	rVB3	709	520	0.07%	0.008%
23	6.171	1515	1518	1521	rVB3	554	417	0.06%	0.006%
24	6.193	1521	1525	1526	rBV	499	262	0.03%	0.004%
25	6.245	1528	1541	1563	rVV	272339	528461	70.20%	7.719%
26	6.685	1666	1678	1695	rBV	176791	343376	45.62%	5.016%
27	7.078	1798	1800	1803	rBV2	182	91	0.01%	0.001%
28	7.090	1803	1804	1805	rBV2	361	120	0.02%	0.002%
29	7.161	1815	1826	1851	rVB	47718	99633	13.24%	1.455%
30	7.299	1865	1869	1872	rBV4	771	600	0.08%	0.009%
31	7.447	1914	1915	1917	rVB	332	106	0.01%	0.002%
32	7.476	1918	1924	1925	rBV4	1146	891	0.12%	0.013%
33	7.563	1939	1951	1973	rBV	101644	188574	25.05%	2.755%
34	7.685	1985	1989	1990	rBV4	1285	975	0.13%	0.014%
35	7.795	2016	2023	2025	rBV5	979	1011	0.13%	0.015%
36	7.894	2041	2054	2071	rBV	349528	597191	79.34%	8.723%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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\SFAMULM071723WMA.M
 Title : VOC Analysis

37	8.129	2125	2127	2130	rBV2	371	195	0.03%	0.003%
38	8.174	2131	2141	2157	rVV	71804	123070	16.35%	1.798%
39	8.576	2264	2266	2269	rBV2	437	252	0.03%	0.004%
40	8.630	2271	2283	2315	rBV2	162340	319190	42.40%	4.662%
41	8.833	2342	2346	2347	rBV2	1061	674	0.09%	0.010%
42	8.901	2364	2367	2371	rBV5	616	478	0.06%	0.007%
43	9.020	2403	2404	2405	rBV5	492	146	0.02%	0.002%
44	9.264	2479	2480	2483	rBV3	402	135	0.02%	0.002%
45	9.283	2485	2486	2487	rBV3	436	135	0.02%	0.002%
46	9.412	2514	2526	2548	rBV	401544	672468	89.34%	9.823%
47	9.675	2601	2608	2609	rBV4	971	888	0.12%	0.013%
48	9.692	2609	2613	2614	rBV	1473	1046	0.14%	0.015%
49	9.962	2695	2697	2699	rBV2	468	280	0.04%	0.004%
50	10.077	2730	2733	2735	rBV3	710	557	0.07%	0.008%
51	10.235	2779	2782	2787	rBV3	591	757	0.10%	0.011%
52	10.315	2802	2807	2814	rVB6	3878	4637	0.62%	0.068%
53	10.376	2825	2826	2827	rBV	340	93	0.01%	0.001%
54	10.386	2827	2829	2831	rBV	423	229	0.03%	0.003%
55	10.486	2852	2860	2876	rVB4	14870	23901	3.18%	0.349%
56	10.556	2880	2882	2883	rBV	533	223	0.03%	0.003%
57	10.753	2931	2943	2959	rBV	329305	533076	70.82%	7.787%
58	10.901	2986	2989	2990	rBV2	510	297	0.04%	0.004%
59	11.071	3039	3042	3046	rBV3	649	555	0.07%	0.008%
60	11.296	3106	3112	3118	rBV6	2490	3761	0.50%	0.055%
61	11.444	3151	3158	3167	rBV7	2067	4772	0.63%	0.070%
62	11.608	3203	3209	3223	rVB6	11736	19596	2.60%	0.286%
63	11.666	3223	3227	3228	rBV	430	288	0.04%	0.004%
64	11.714	3235	3242	3243	rBV4	4533	3760	0.50%	0.055%
65	11.807	3260	3271	3288	rVB	476359	752745	100.00%	10.996%
66	12.077	3345	3355	3372	rBV9	9695	20285	2.69%	0.296%
67	12.190	3378	3390	3407	rBV	398674	643672	85.51%	9.402%
68	12.450	3464	3471	3484	rBV8	9277	15893	2.11%	0.232%
69	12.527	3486	3495	3511	rVB	82534	132273	17.57%	1.932%
70	12.839	3585	3592	3605	rVB5	20074	31968	4.25%	0.467%
71	13.351	3749	3751	3752	rBV	538	190	0.03%	0.003%
72	13.457	3779	3784	3785	rBV	1061	678	0.09%	0.010%
73	13.498	3795	3797	3798	rBV	409	126	0.02%	0.002%
74	13.521	3802	3804	3807	rBV	710	467	0.06%	0.007%
75	14.479	4093	4102	4123	rVB2	77286	127354	16.92%	1.860%

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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\SFAMULM071723WMA.M
Title : VOC Analysis

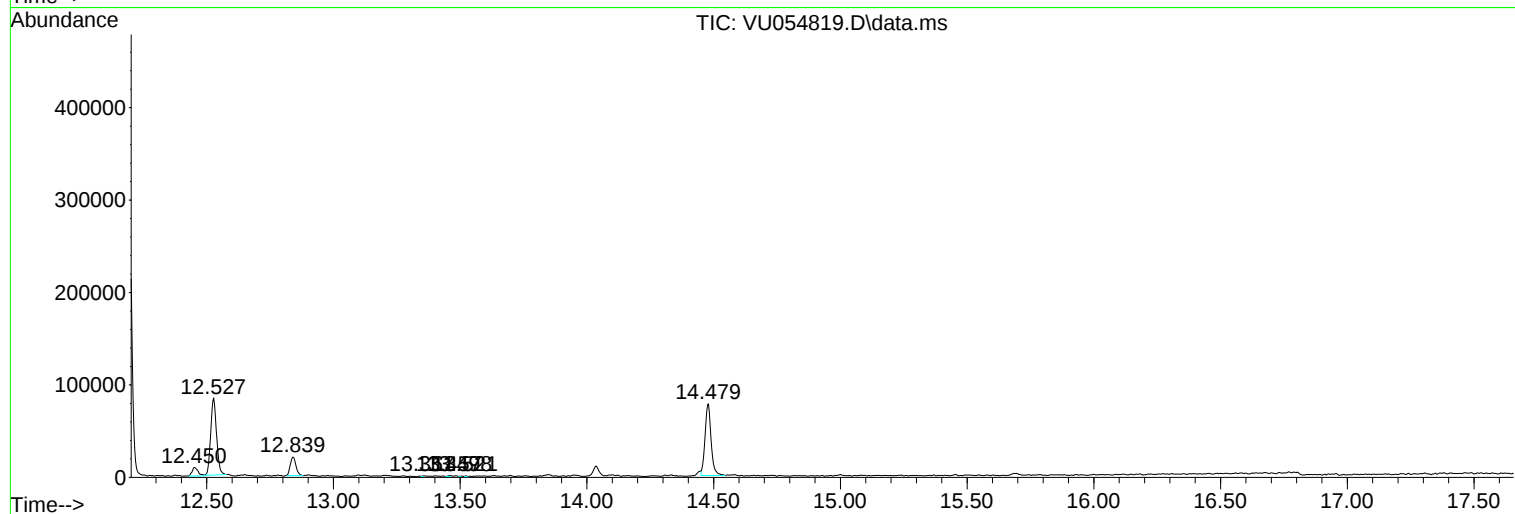
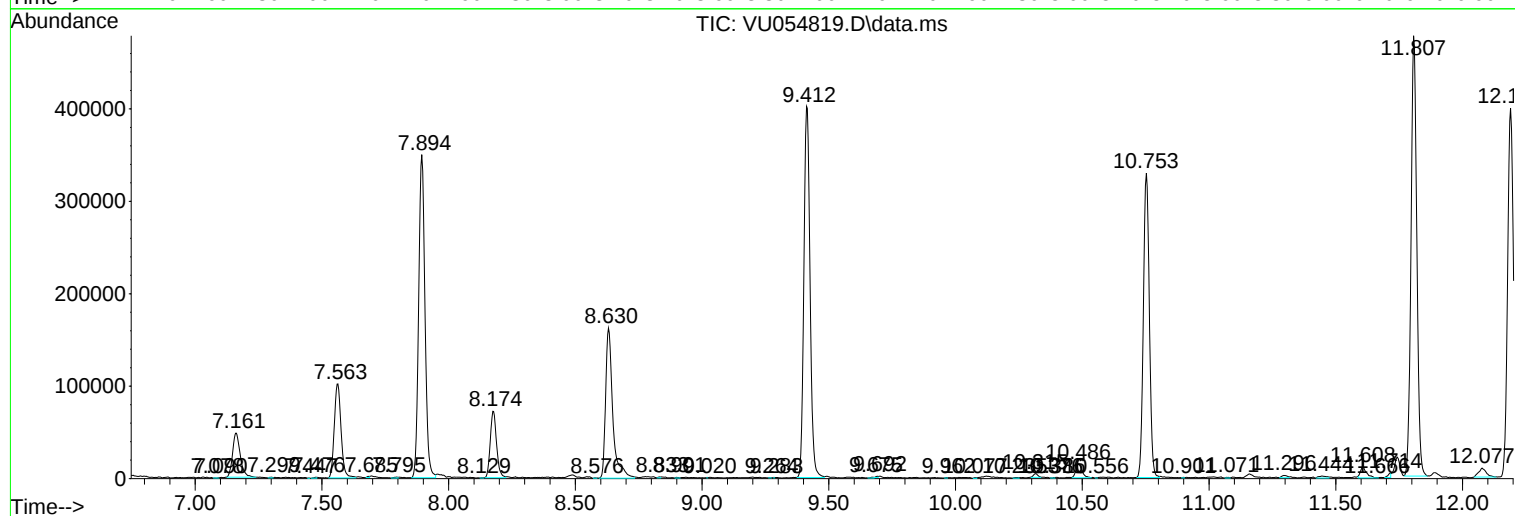
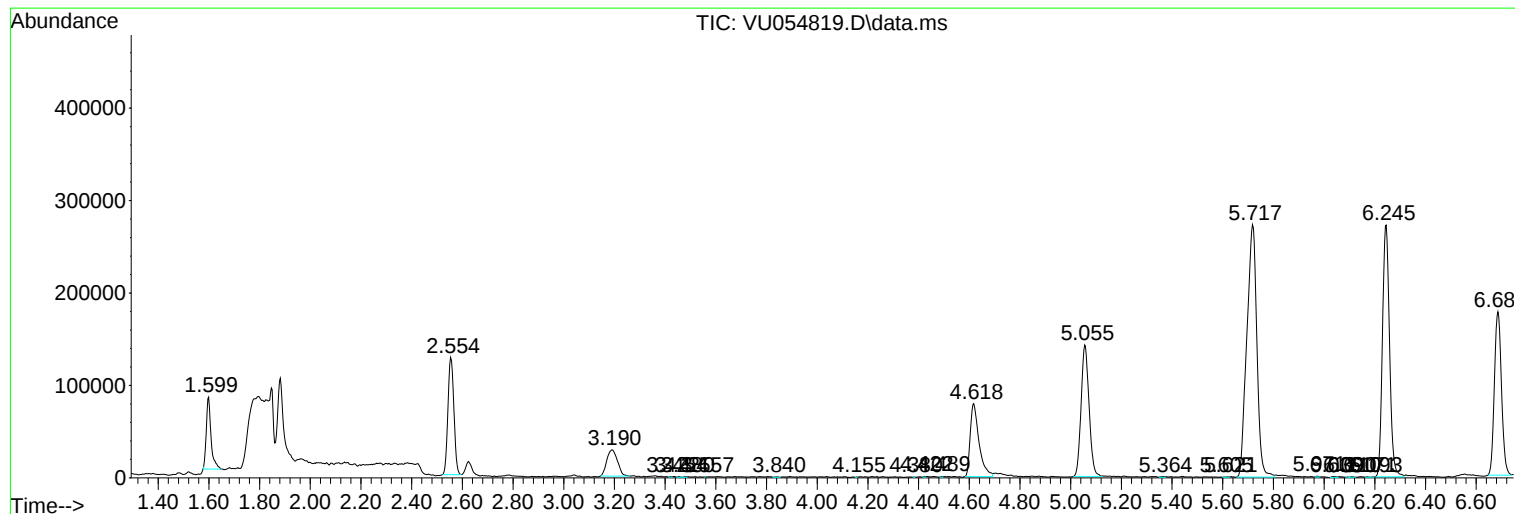
Sum of corrected areas: 6845904

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X9

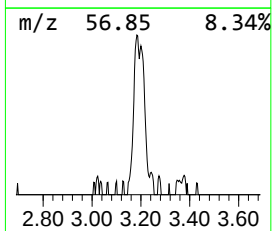
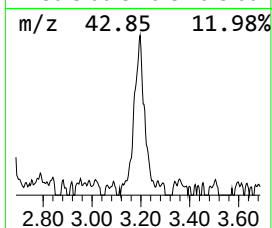
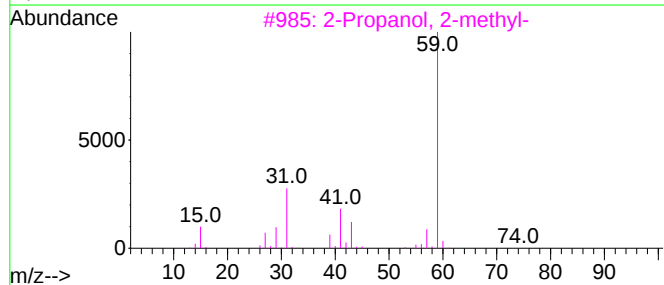
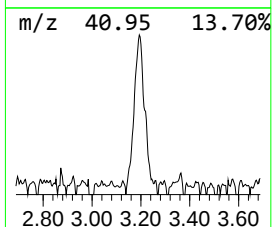
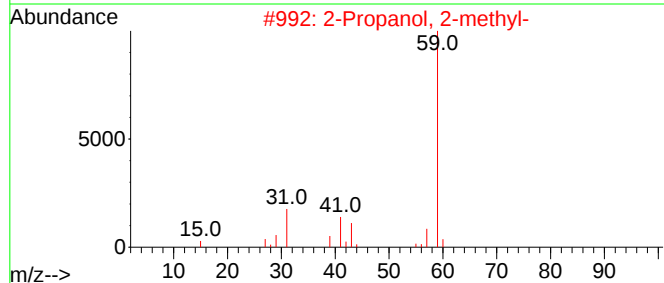
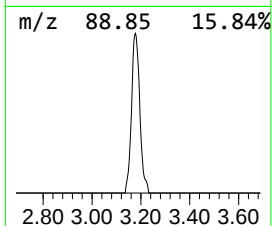
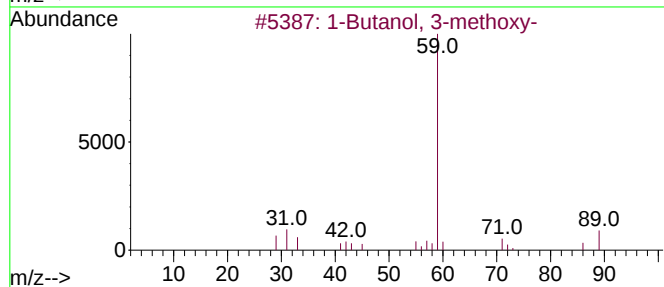
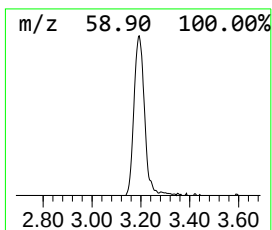
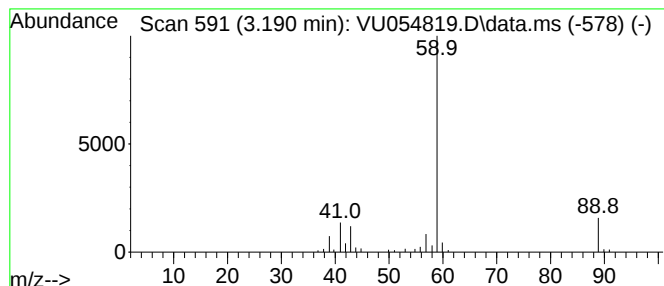
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 1-Butanol, 3-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.190	7.78 ug/L	82215	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 3-methoxy-			104	C5H12O2	002517-43-3	78
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	64
3	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	50
4	3-Pentanol			88	C5H12O	000584-02-1	39
5	2,3-Butanediol, 2,3-dimethyl-			118	C6H14O2	000076-09-5	39



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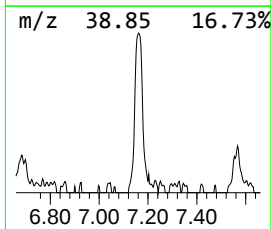
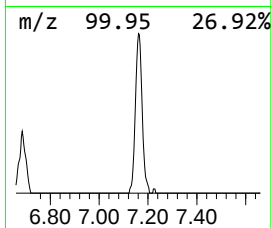
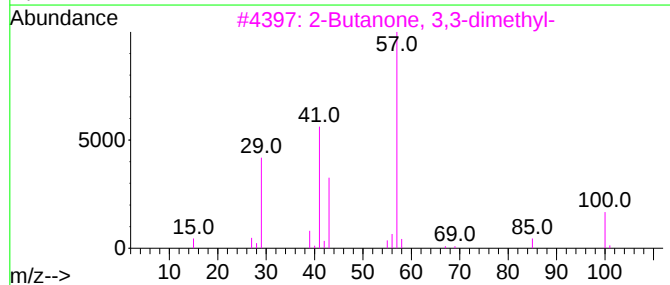
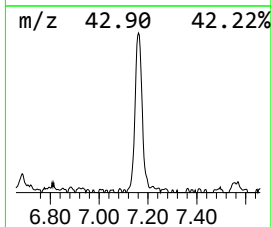
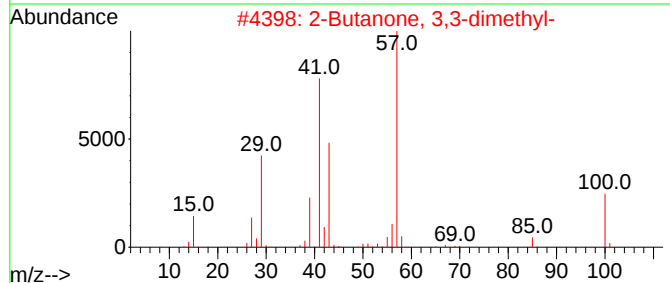
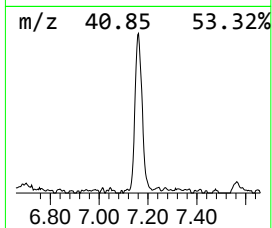
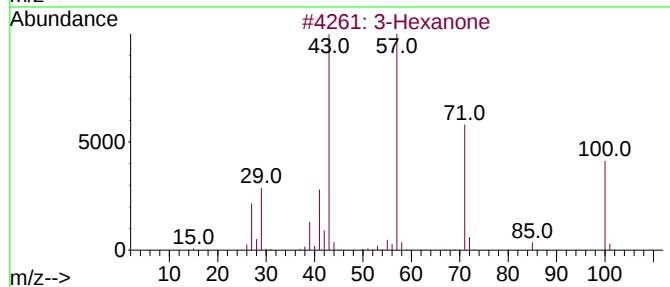
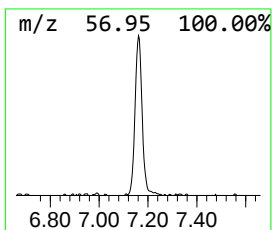
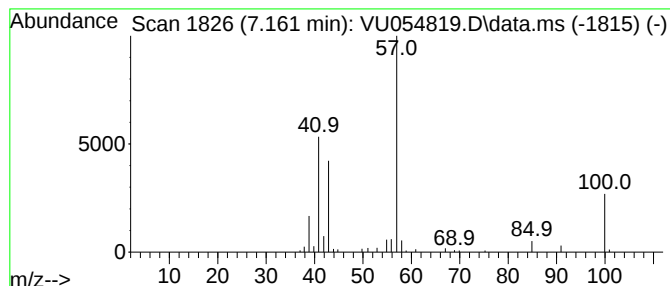
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 3-Hexanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.161	9.43 ug/L	99633	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanone	100	C6H12O	000589-38-8	59
2			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	50
3			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	50
4			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	45
5			Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	43



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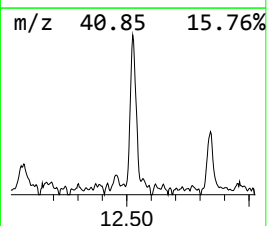
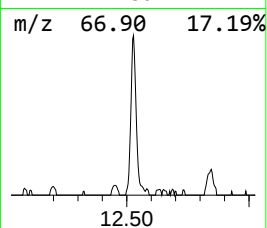
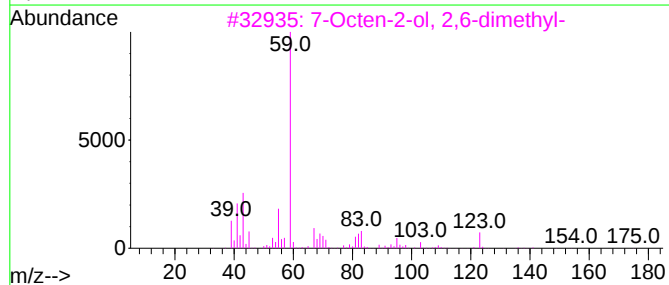
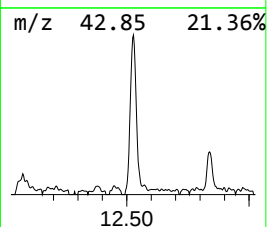
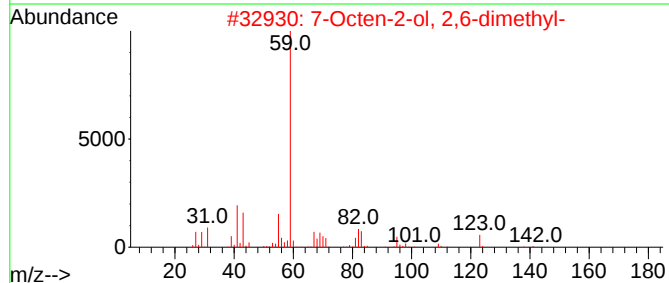
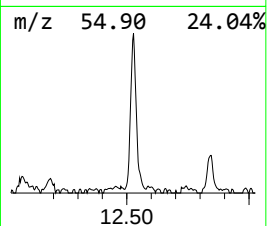
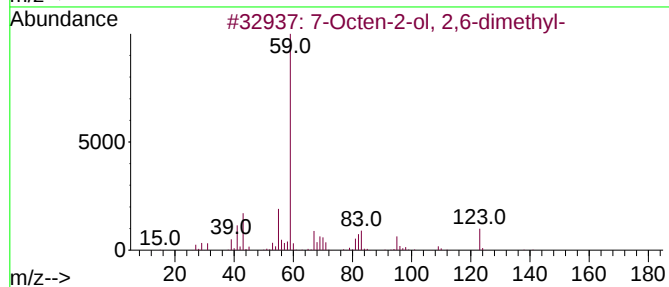
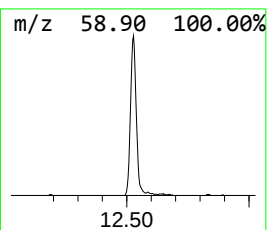
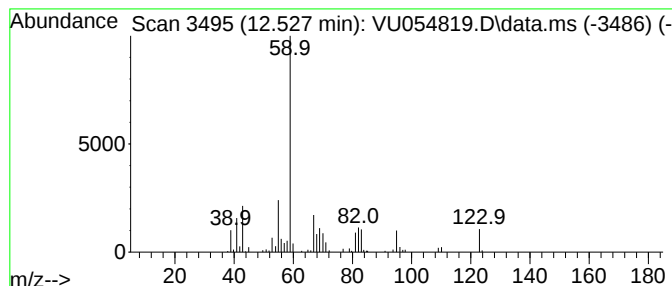
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	8.79 ug/L	132273	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	59
4			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	56
5			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	56



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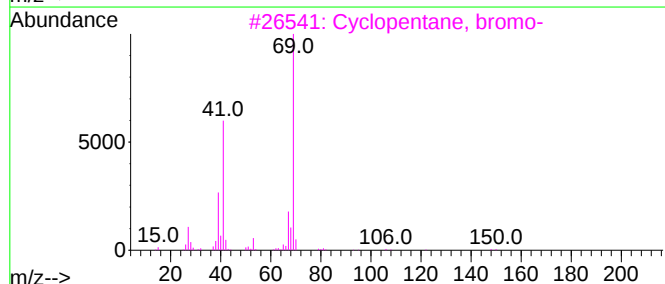
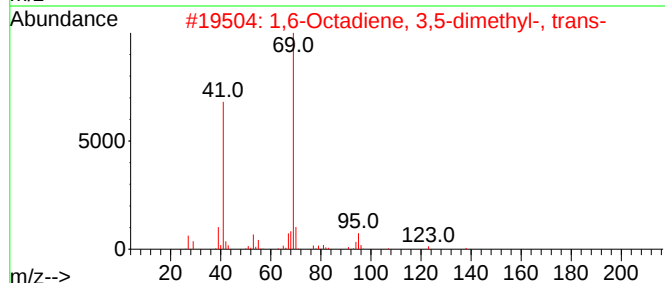
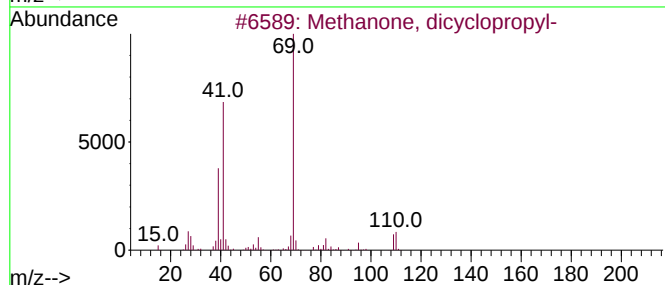
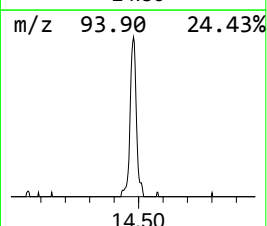
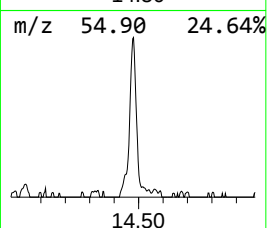
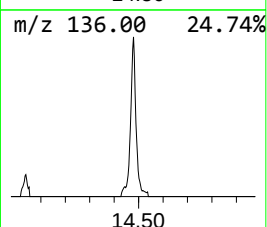
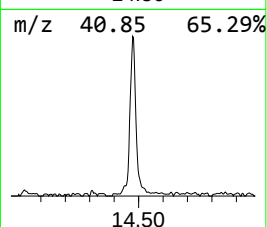
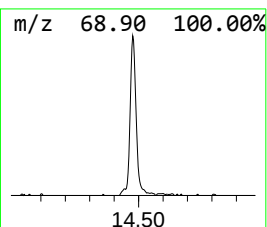
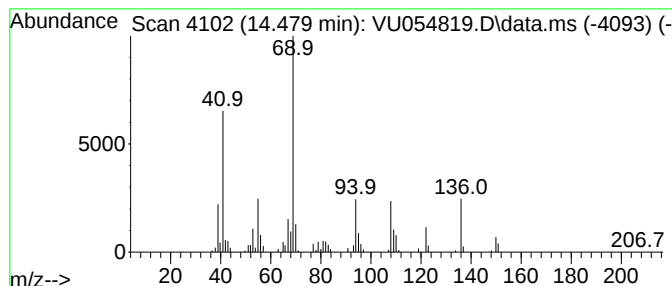
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.479	8.46 ug/L	127354	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	43
2			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	38
3			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	38
4			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38
5			Geranyl formate	182	C11H18O2	000105-86-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071923\
Data File : VU054819.D
Acq On : 19 Jul 2023 14:39
Operator : MD/SY
Sample : 03656-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.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
1-Butanol, 3-me...	3.190	7.8	ug/L	82215	1	6.245	528461	50.0
3-Hexanone	7.161	9.4	ug/L	99633	1	6.245	528461	50.0
7-Octen-2-ol, 2...	12.527	8.8	ug/L	132273	3	11.807	752745	50.0
unknown-01	14.479	8.5	ug/L	127354	3	11.807	752745	50.0