

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071923\
 Data File : VU054821.D
 Acq On : 19 Jul 2023 15:45
 Operator : MD/SY
 Sample : 03656-16
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 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: VU054821.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	90	95	111	rVB	83585	107252	24.10%	2.524%
2	2.557	384	394	407	rBV	134900	217334	48.84%	5.114%
3	2.997	528	531	532	rBV2	634	360	0.08%	0.008%
4	3.036	538	543	544	rBV4	1451	1104	0.25%	0.026%
5	3.181	575	588	609	rBV3	34294	85437	19.20%	2.010%
6	3.747	761	764	767	rVB2	436	265	0.06%	0.006%
7	3.917	808	817	819	rBV3	412	413	0.09%	0.010%
8	4.123	877	881	883	rVB2	356	246	0.06%	0.006%
9	4.139	883	886	888	rBV	496	271	0.06%	0.006%
10	4.206	904	907	912	rBV2	322	299	0.07%	0.007%
11	4.618	1025	1035	1060	rVV	41107	100328	22.55%	2.361%
12	5.004	1149	1155	1157	rBV2	346	387	0.09%	0.009%
13	5.055	1157	1171	1191	rVV	85987	188401	42.34%	4.433%
14	5.197	1213	1215	1218	rBV	344	279	0.06%	0.007%
15	5.258	1231	1234	1236	rBV2	352	257	0.06%	0.006%
16	5.316	1249	1252	1258	rVB2	676	574	0.13%	0.014%
17	5.412	1279	1282	1286	rVB3	411	289	0.06%	0.007%
18	5.573	1326	1332	1334	rBV	548	463	0.10%	0.011%
19	5.628	1344	1349	1352	rVB	401	302	0.07%	0.007%
20	5.721	1358	1378	1397	rBV2	160308	435230	97.81%	10.241%
21	5.939	1442	1446	1450	rVB3	368	285	0.06%	0.007%
22	5.968	1453	1455	1461	rVB	414	299	0.07%	0.007%
23	6.004	1461	1466	1468	rBV3	428	422	0.09%	0.010%
24	6.245	1526	1541	1563	rBV	170723	324674	72.97%	7.640%
25	6.685	1665	1678	1695	rBV2	106647	207805	46.70%	4.890%
26	6.853	1726	1730	1732	rBV	620	429	0.10%	0.010%
27	6.894	1738	1743	1745	rVV	382	305	0.07%	0.007%
28	6.930	1751	1754	1757	rVV2	389	268	0.06%	0.006%
29	7.161	1813	1826	1843	rBV3	26613	57245	12.86%	1.347%
30	7.255	1853	1855	1859	rBV2	365	245	0.06%	0.006%
31	7.406	1899	1902	1908	rBV2	331	337	0.08%	0.008%
32	7.441	1908	1913	1917	rBV2	403	409	0.09%	0.010%
33	7.467	1917	1921	1925	rBV	311	262	0.06%	0.006%
34	7.563	1939	1951	1971	rBV	60466	108041	24.28%	2.542%
35	7.650	1975	1978	1983	rVB3	674	519	0.12%	0.012%
36	7.692	1986	1991	1992	rBV4	757	635	0.14%	0.015%

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

37	7.894	2041	2054	2072	rBV	204817	354859	79.75%	8.350%
38	8.042	2098	2100	2103	rBV2	550	336	0.08%	0.008%
39	8.116	2118	2123	2127	rVB3	640	467	0.10%	0.011%
40	8.177	2131	2142	2161	rVV2	41580	73574	16.53%	1.731%
41	8.248	2162	2164	2169	rVB3	553	286	0.06%	0.007%
42	8.271	2169	2171	2174	rVB	738	341	0.08%	0.008%
43	8.354	2194	2197	2201	rVB	488	329	0.07%	0.008%
44	8.631	2272	2283	2315	rBV2	124021	240919	54.14%	5.669%
45	8.795	2331	2334	2339	rVB3	914	710	0.16%	0.017%
46	8.843	2345	2349	2352	rVB3	496	297	0.07%	0.007%
47	8.875	2356	2359	2361	rBV	383	292	0.07%	0.007%
48	8.975	2387	2390	2394	rVB2	473	327	0.07%	0.008%
49	9.113	2429	2433	2439	rBV	546	535	0.12%	0.013%
50	9.219	2460	2466	2468	rBV2	371	259	0.06%	0.006%
51	9.415	2514	2527	2549	rBV	245813	407528	91.59%	9.590%
52	9.528	2559	2562	2566	rVB2	427	393	0.09%	0.009%
53	9.611	2586	2588	2594	rVB2	483	345	0.08%	0.008%
54	9.672	2603	2607	2608	rBV	304	250	0.06%	0.006%
55	9.692	2610	2613	2614	rBV2	559	308	0.07%	0.007%
56	9.881	2668	2672	2674	rBV2	355	318	0.07%	0.007%
57	10.058	2722	2727	2729	rBV2	321	332	0.07%	0.008%
58	10.142	2748	2753	2758	rBV5	745	763	0.17%	0.018%
59	10.258	2786	2789	2793	rBV3	293	295	0.07%	0.007%
60	10.312	2802	2806	2807	rBV3	1245	771	0.17%	0.018%
61	10.425	2839	2841	2844	rVB2	485	254	0.06%	0.006%
62	10.486	2853	2860	2870	rVV6	7847	11564	2.60%	0.272%
63	10.647	2907	2910	2914	rBV2	373	315	0.07%	0.007%
64	10.753	2927	2943	2957	rBV	176950	284303	63.89%	6.690%
65	11.004	3016	3021	3023	rBV2	495	499	0.11%	0.012%
66	11.026	3026	3028	3033	rVV3	854	651	0.15%	0.015%
67	11.081	3040	3045	3047	rBV3	312	283	0.06%	0.007%
68	11.296	3105	3112	3114	rBV4	1272	1441	0.32%	0.034%
69	11.434	3151	3155	3156	rBV2	427	270	0.06%	0.006%
70	11.547	3187	3190	3192	rBV2	467	286	0.06%	0.007%
71	11.608	3198	3209	3217	rBV5	4976	7867	1.77%	0.185%
72	11.743	3237	3251	3259	rVV7	11451	19919	4.48%	0.469%
73	11.811	3259	3272	3290	rVV	278860	444971	100.00%	10.471%
74	11.984	3321	3326	3328	rBV2	397	345	0.08%	0.008%
75	12.065	3343	3351	3352	rBV3	3457	3403	0.76%	0.080%
76	12.132	3369	3372	3375	rBV2	695	438	0.10%	0.010%

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77	12.190	3379	3390	3406	rVB	228898	366590	82.39%	8.626%
78	12.454	3465	3472	3479	rBV8	4155	6502	1.46%	0.153%
79	12.528	3485	3495	3511	rBV2	46986	73828	16.59%	1.737%
80	12.714	3549	3553	3560	rVV3	734	937	0.21%	0.022%
81	12.769	3567	3570	3574	rBV3	656	611	0.14%	0.014%
82	12.839	3583	3592	3605	rBV6	10914	17828	4.01%	0.420%
83	13.007	3641	3644	3646	rBV	533	348	0.08%	0.008%
84	13.106	3673	3675	3678	rBV	433	340	0.08%	0.008%
85	13.164	3689	3693	3695	rBV2	301	261	0.06%	0.006%
86	13.373	3756	3758	3760	rBV	616	278	0.06%	0.007%
87	13.868	3910	3912	3915	rVB3	500	265	0.06%	0.006%
88	14.032	3958	3963	3976	rVB8	4504	6923	1.56%	0.163%
89	14.145	3992	3998	4003	rBV3	721	672	0.15%	0.016%
90	14.177	4004	4008	4012	rBV3	424	404	0.09%	0.010%
91	14.254	4028	4032	4035	rBV2	299	289	0.06%	0.007%
92	14.341	4054	4059	4063	rBV3	630	592	0.13%	0.014%
93	14.479	4095	4102	4116	rVB2	44028	66046	14.84%	1.554%
94	14.859	4216	4220	4223	rBV2	670	586	0.13%	0.014%
95	14.936	4241	4244	4248	rBV	520	446	0.10%	0.010%
96	14.991	4257	4261	4263	rBV2	571	403	0.09%	0.009%
97	15.000	4263	4264	4267	rVV2	529	293	0.07%	0.007%
98	15.135	4304	4306	4309	rBV2	543	367	0.08%	0.009%
99	15.685	4475	4477	4480	rBV2	1052	616	0.14%	0.014%
100	16.450	4711	4715	4717	rBV3	1101	950	0.21%	0.022%

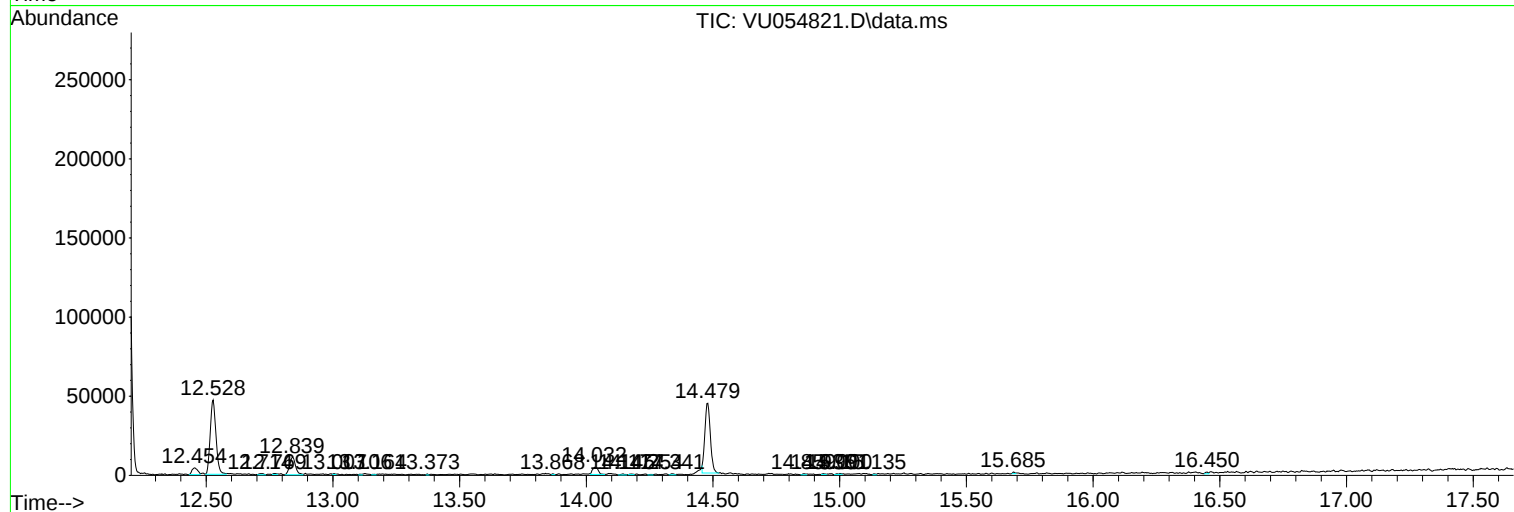
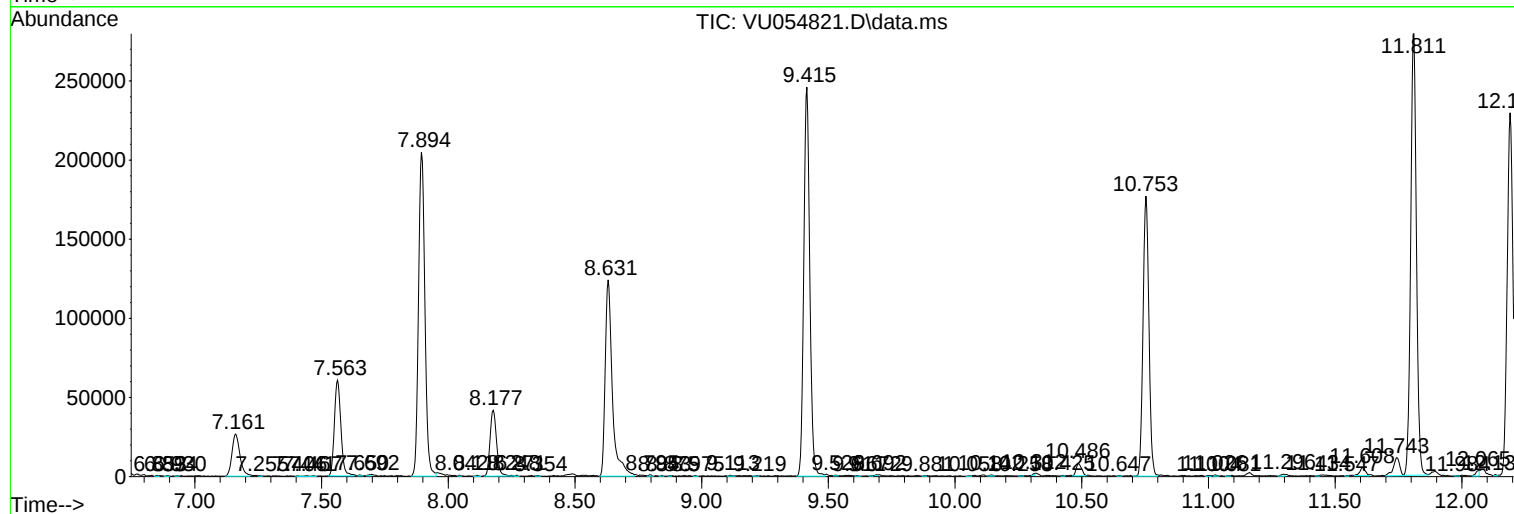
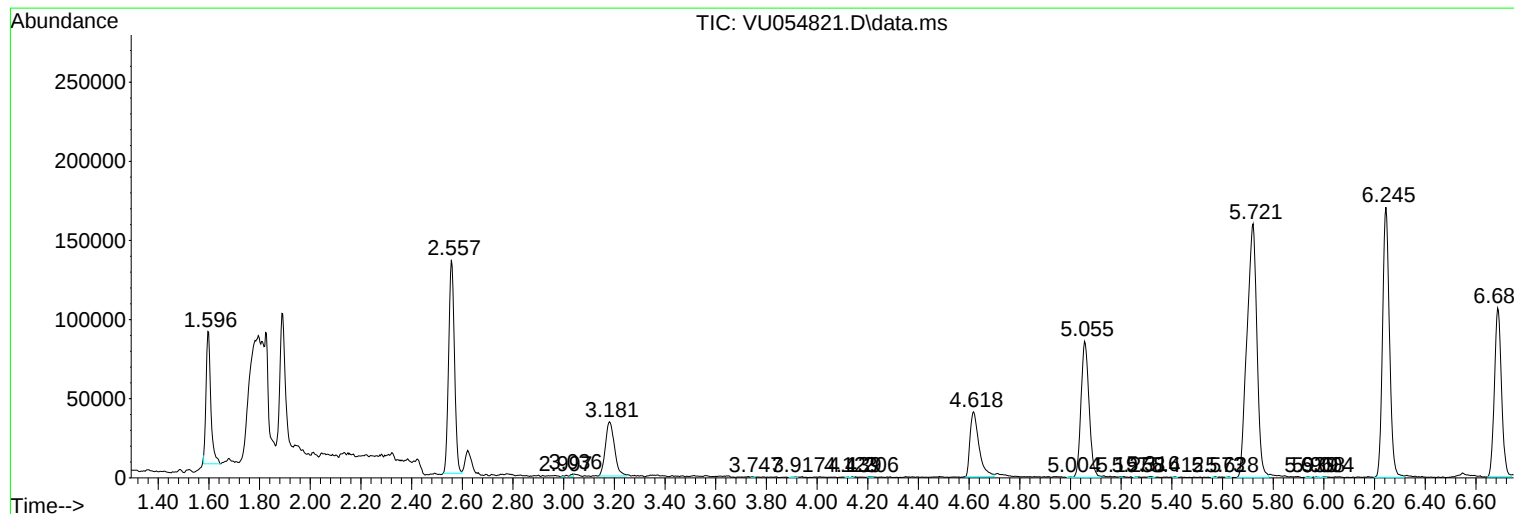
Sum of corrected areas: 4249689

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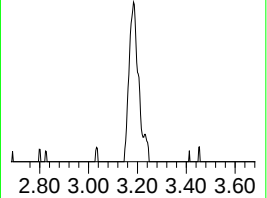
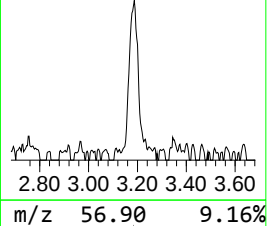
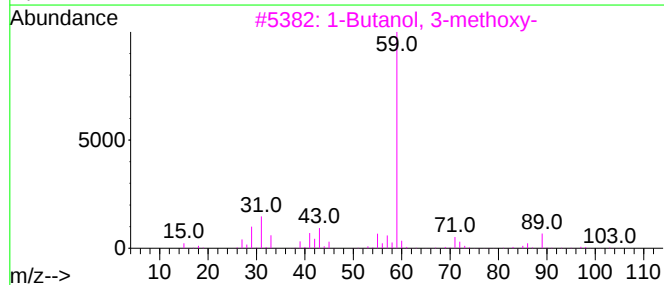
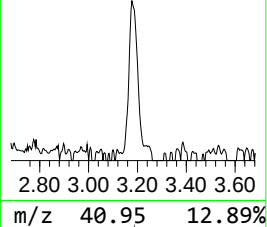
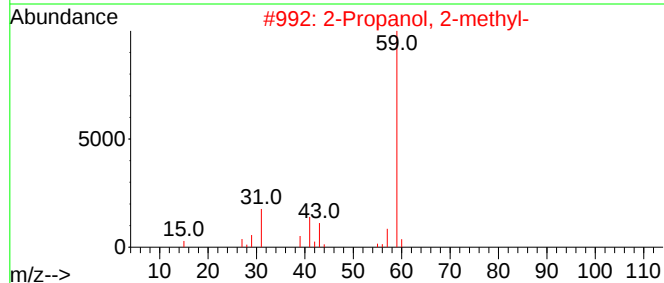
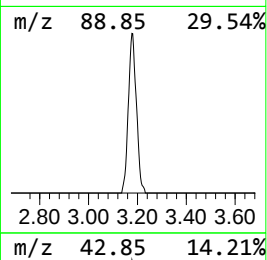
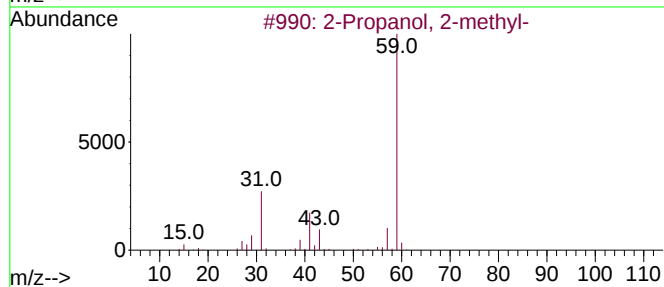
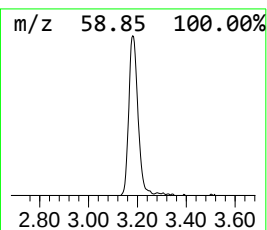
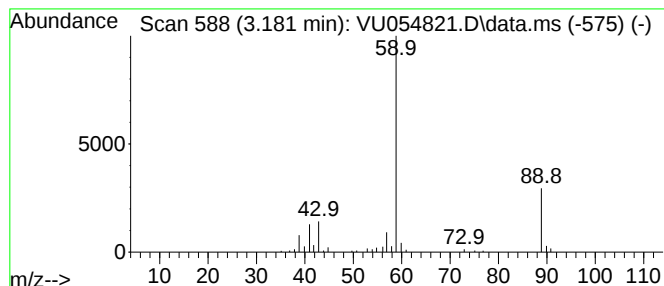
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.181	13.16 ug/L	85437	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	53
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	42
3	1-Butanol, 3-methoxy-			104	C5H12O2	002517-43-3	39
4	2,3-Butanediol, 2,3-dimethyl-			118	C6H14O2	000076-09-5	38
5	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	36



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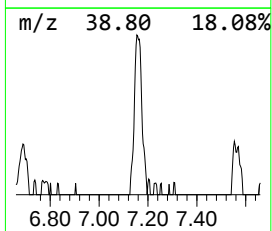
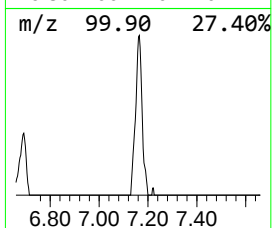
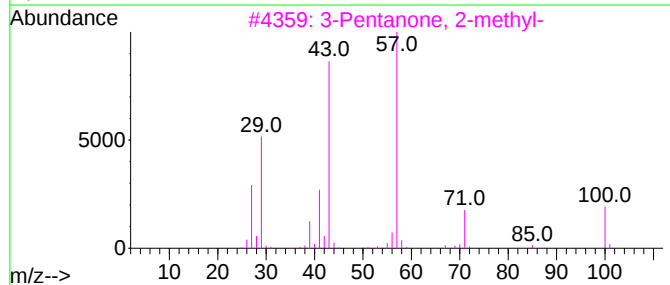
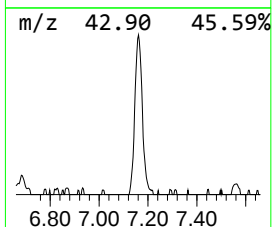
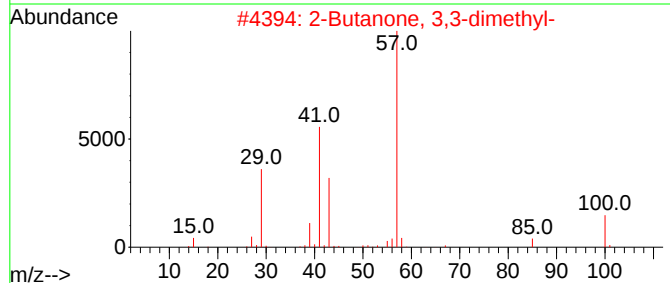
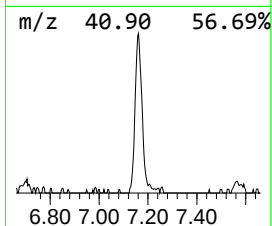
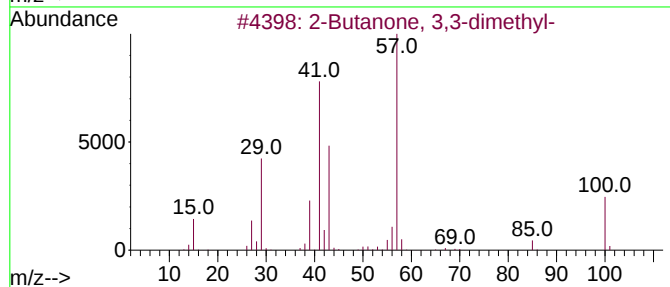
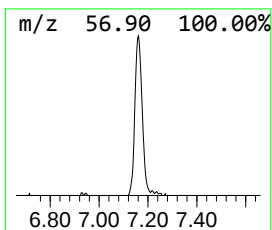
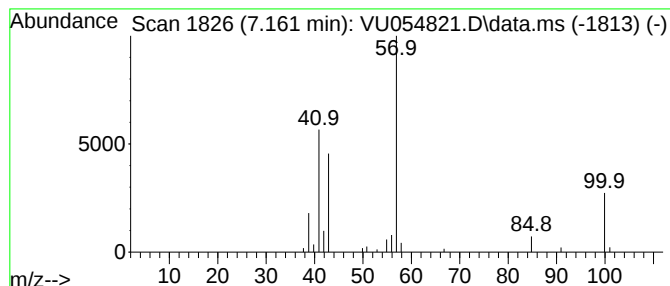
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Quant Title : VOC Analysis

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

Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.161	8.82 ug/L	57245	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	78	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	64	
3	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	58	
4	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	58	
5	Diazene, bis(1,1-dimethylethyl)-		142	C8H18N2	000927-83-3	50	



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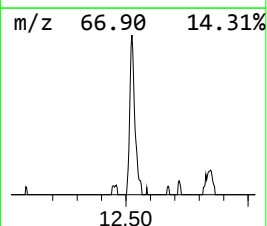
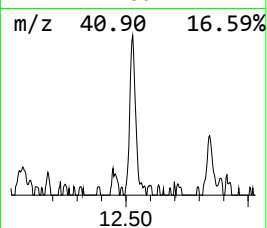
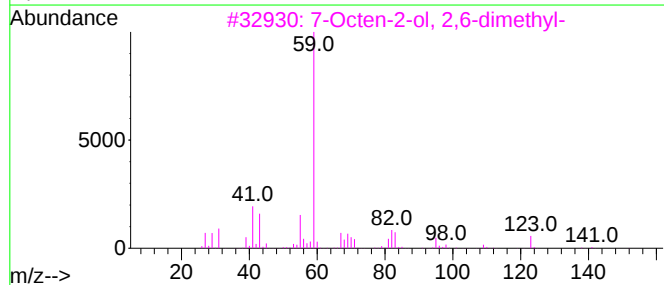
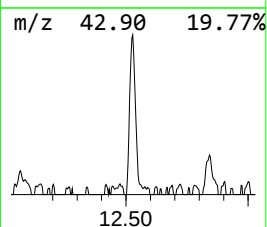
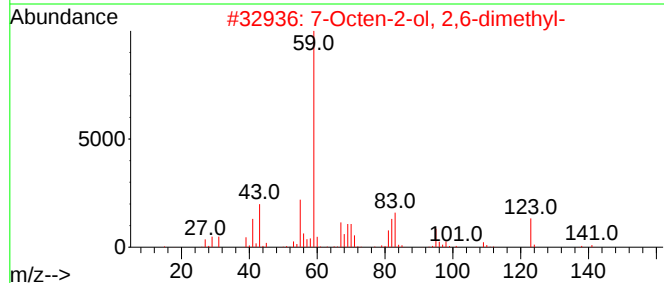
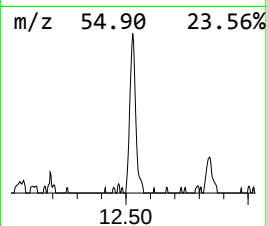
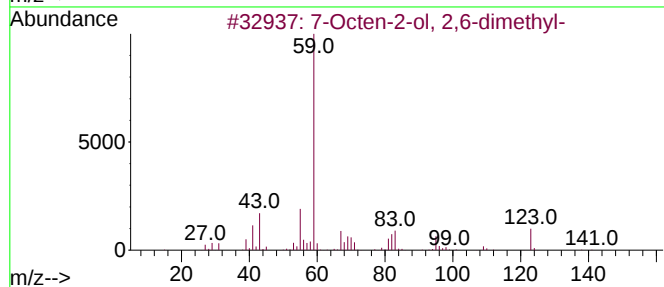
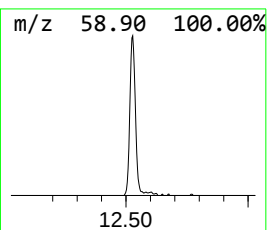
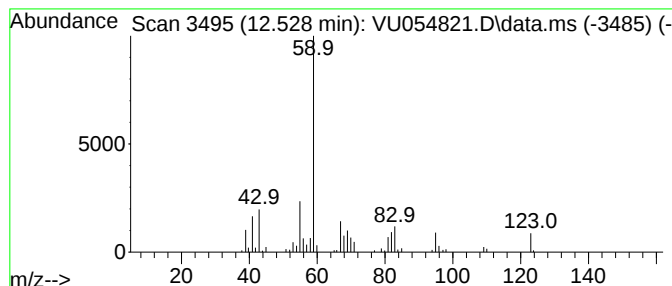
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.528	8.30 ug/L	73828	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	90
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	83
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
5			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071923\
Data File : VU054821.D
Acq On : 19 Jul 2023 15:45
Operator : MD/SY
Sample : 03656-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2X9

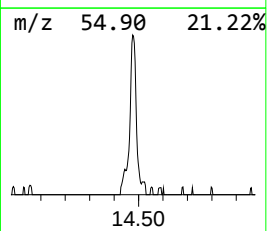
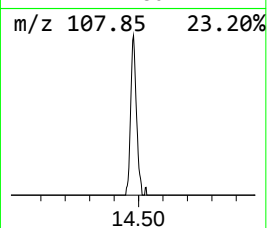
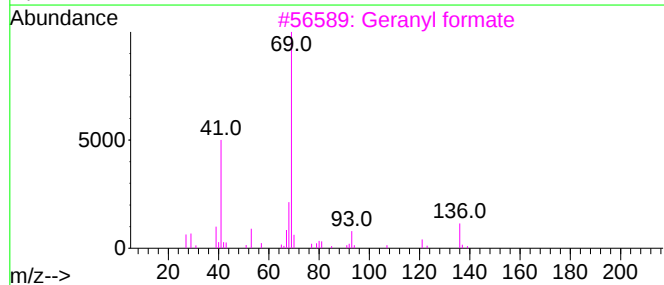
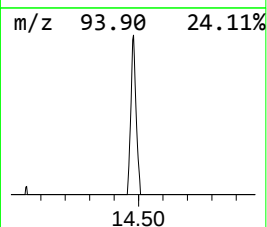
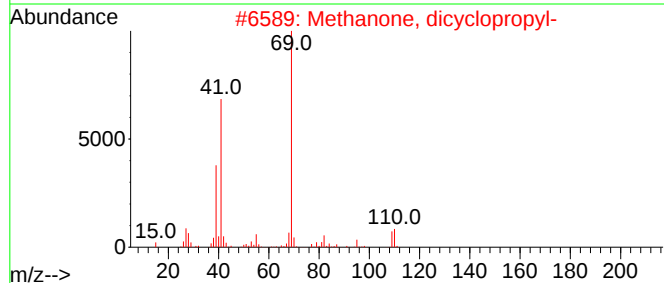
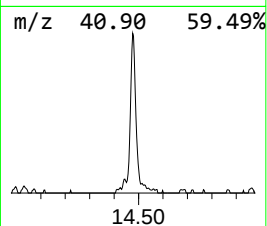
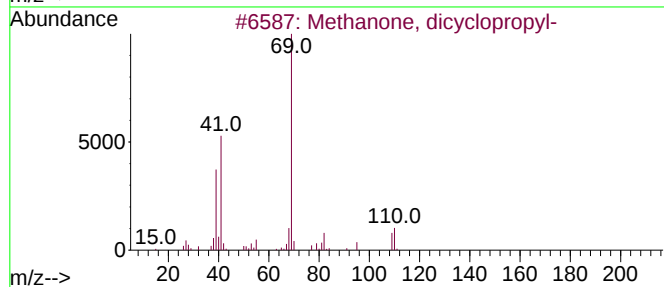
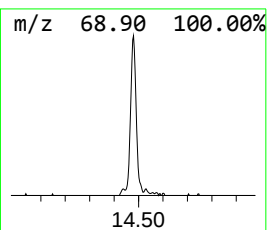
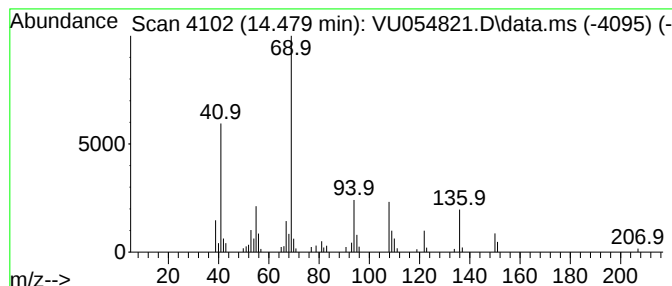
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.479	7.42 ug/L	66046	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	46
2			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	43
3			Geranyl formate	182	C11H18O2	000105-86-2	43
4			(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	42
5			3-Ethyl-1,5-octadiene	138	C10H18	1000114-87-7	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071923\
Data File : VU054821.D
Acq On : 19 Jul 2023 15:45
Operator : MD/SY
Sample : 03656-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 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
2-Propanol, 2-m...	3.181	13.2	ug/L	85437	1	6.245	324674	50.0
2-Butanone, 3,3...	7.161	8.8	ug/L	57245	1	6.245	324674	50.0
7-Octen-2-ol, 2...	12.528	8.3	ug/L	73828	3	11.811	444971	50.0
unknown-01	14.479	7.4	ug/L	66046	3	11.811	444971	50.0