

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
 Data File : VU055828.D
 Acq On : 20 Oct 2023 13:26
 Operator : MD/SY
 Sample : 04922-03
 Misc : 6.13g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EOAQ9

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	55	59	66	rVB2	5549	5704	0.27%	0.032%
2	1.596	86	95	117	rVB	171426	271886	12.83%	1.528%
3	1.811	136	162	163	rBV	25920	78155	3.69%	0.439%
4	1.875	178	182	198	rVB	53531	79563	3.75%	0.447%
5	2.541	376	389	406	rBV	413169	673418	31.77%	3.786%
6	2.628	412	416	417	rBV2	1460	976	0.05%	0.005%
7	2.763	454	458	459	rBV	821	592	0.03%	0.003%
8	2.811	470	473	475	rBV3	828	535	0.03%	0.003%
9	2.862	485	489	492	rBV4	484	436	0.02%	0.002%
10	2.894	496	499	501	rBV2	388	227	0.01%	0.001%
11	2.923	505	508	509	rBV2	536	287	0.01%	0.002%
12	2.952	509	517	518	rBV5	1555	1568	0.07%	0.009%
13	3.036	531	543	561	rVB4	9017	23191	1.09%	0.130%
14	3.107	561	565	569	rBV2	865	788	0.04%	0.004%
15	3.177	575	587	600	rVV3	5458	12273	0.58%	0.069%
16	3.338	631	637	642	rBV6	1880	2883	0.14%	0.016%
17	3.431	664	666	670	rVB2	503	355	0.02%	0.002%
18	3.464	670	676	679	rBV4	883	811	0.04%	0.005%
19	3.666	733	739	742	rBV4	1528	1726	0.08%	0.010%
20	3.824	786	788	793	rVB2	424	277	0.01%	0.002%
21	3.866	799	801	806	rVB2	490	365	0.02%	0.002%
22	3.997	840	842	845	rVB2	566	322	0.02%	0.002%
23	4.055	858	860	864	rVB2	653	396	0.02%	0.002%
24	4.091	868	871	876	rVB2	522	364	0.02%	0.002%
25	4.123	876	881	886	rBV3	480	435	0.02%	0.002%
26	4.200	901	905	908	rVB2	443	309	0.01%	0.002%
27	4.296	929	935	938	rBV3	306	297	0.01%	0.002%
28	4.470	987	989	992	rBV2	363	320	0.02%	0.002%
29	4.505	995	1000	1003	rVV4	769	775	0.04%	0.004%
30	4.521	1003	1005	1009	rVB3	848	590	0.03%	0.003%
31	4.628	1026	1038	1086	rBV	126510	466532	22.01%	2.623%
32	4.965	1141	1143	1146	rBV3	364	232	0.01%	0.001%
33	5.055	1155	1171	1197	rBV	359041	841093	39.68%	4.728%
34	5.258	1231	1234	1237	rVB2	506	277	0.01%	0.002%
35	5.290	1242	1244	1246	rVB3	513	234	0.01%	0.001%
36	5.328	1246	1256	1258	rBV4	1503	1994	0.09%	0.011%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	5.541	1319	1322	1324	rBV	607	404	0.02%	0.002%
38	5.576	1327	1333	1337	rBV4	1141	1209	0.06%	0.007%
39	5.714	1356	1376	1405	rBV2	792773	2119487	100.00%	11.915%
40	5.981	1448	1459	1461	rBV6	4379	6417	0.30%	0.036%
41	6.039	1474	1477	1480	rVB4	1480	1025	0.05%	0.006%
42	6.062	1480	1484	1486	rVB	330	235	0.01%	0.001%
43	6.103	1493	1497	1499	rBV3	709	517	0.02%	0.003%
44	6.119	1499	1502	1503	rBV	867	496	0.02%	0.003%
45	6.242	1526	1540	1572	rBV	629852	1297602	61.22%	7.295%
46	6.428	1594	1598	1600	rBV4	392	275	0.01%	0.002%
47	6.463	1607	1609	1613	rBV4	416	301	0.01%	0.002%
48	6.531	1616	1630	1643	rBV9	26377	61050	2.88%	0.343%
49	6.595	1644	1650	1652	rBV4	3641	4133	0.20%	0.023%
50	6.685	1663	1678	1706	rBV	449377	946148	44.64%	5.319%
51	6.910	1744	1748	1750	rBV4	398	306	0.01%	0.002%
52	6.959	1761	1763	1766	rBV2	356	256	0.01%	0.001%
53	7.000	1774	1776	1780	rVB2	555	348	0.02%	0.002%
54	7.042	1786	1789	1790	rBV	753	407	0.02%	0.002%
55	7.065	1792	1796	1805	rVB7	1467	1843	0.09%	0.010%
56	7.193	1824	1836	1840	rBV5	7084	11980	0.57%	0.067%
57	7.296	1866	1868	1870	rVB3	686	267	0.01%	0.002%
58	7.344	1880	1883	1885	rBV3	488	344	0.02%	0.002%
59	7.370	1885	1891	1893	rBV3	1823	1977	0.09%	0.011%
60	7.463	1917	1920	1922	rBV2	675	349	0.02%	0.002%
61	7.496	1922	1930	1935	rVV6	3006	4031	0.19%	0.023%
62	7.563	1939	1951	1972	rVV	227886	454675	21.45%	2.556%
63	7.775	2016	2017	2020	rVB	626	245	0.01%	0.001%
64	7.894	2031	2054	2075	rBV	901625	1665636	78.59%	9.364%
65	8.126	2123	2126	2131	rVB5	2541	2272	0.11%	0.013%
66	8.180	2131	2143	2173	rVB	146130	318941	15.05%	1.793%
67	8.315	2182	2185	2187	rBV2	638	418	0.02%	0.002%
68	8.361	2189	2199	2210	rVB2	2932	6588	0.31%	0.037%
69	8.402	2210	2212	2214	rBV	579	264	0.01%	0.001%
70	8.415	2214	2216	2217	rBV2	488	251	0.01%	0.001%
71	8.444	2221	2225	2230	rBV6	703	765	0.04%	0.004%
72	8.470	2230	2233	2235	rBV3	1202	720	0.03%	0.004%
73	8.550	2243	2258	2272	rVB3	42167	78055	3.68%	0.439%
74	8.653	2272	2290	2322	rBV3	381697	979133	46.20%	5.505%
75	8.920	2364	2373	2383	rBV5	10615	21657	1.02%	0.122%
76	9.049	2409	2413	2414	rBV3	1117	814	0.04%	0.005%

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 Title : VOC Analysis

77	9.065	2414	2418	2426	rVB6	3472	5008	0.24%	0.028%
78	9.116	2426	2434	2439	rBV5	3570	5251	0.25%	0.030%
79	9.164	2444	2449	2456	rVV8	6744	11484	0.54%	0.065%
80	9.213	2458	2464	2479	rVB7	9094	16633	0.78%	0.094%
81	9.335	2489	2502	2514	rBV5	9767	18921	0.89%	0.106%
82	9.418	2514	2528	2551	rBV	839895	1651150	77.90%	9.283%
83	9.627	2590	2593	2594	rBV3	1591	923	0.04%	0.005%
84	9.868	2658	2668	2680	rBV9	4977	10758	0.51%	0.060%
85	9.939	2685	2690	2691	rBV2	1035	853	0.04%	0.005%
86	9.949	2691	2693	2694	rBV2	713	316	0.01%	0.002%
87	10.026	2707	2717	2733	rVB10	13504	30260	1.43%	0.170%
88	10.110	2735	2743	2755	rVV5	14786	30033	1.42%	0.169%
89	10.251	2770	2787	2800	rBV8	30932	80016	3.78%	0.450%
90	10.354	2813	2819	2825	rBV7	18112	28238	1.33%	0.159%
91	10.560	2869	2883	2891	rBV9	14732	35519	1.68%	0.200%
92	10.759	2933	2945	2956	rBV	719564	1191570	56.22%	6.699%
93	11.113	3050	3055	3071	rVB2	117662	188584	8.90%	1.060%
94	11.299	3103	3113	3127	rVB8	37236	76396	3.60%	0.429%
95	11.415	3142	3149	3156	rVB3	52543	69723	3.29%	0.392%
96	11.811	3261	3272	3285	rBV	976393	1613041	76.11%	9.068%
97	12.097	3354	3361	3366	rBV3	32320	51274	2.42%	0.288%
98	12.193	3379	3391	3408	rBV	1000620	1716173	80.97%	9.648%
99	12.325	3425	3432	3441	rVB	142628	198804	9.38%	1.118%
100	13.450	3770	3782	3797	rVB7	101360	294814	13.91%	1.657%

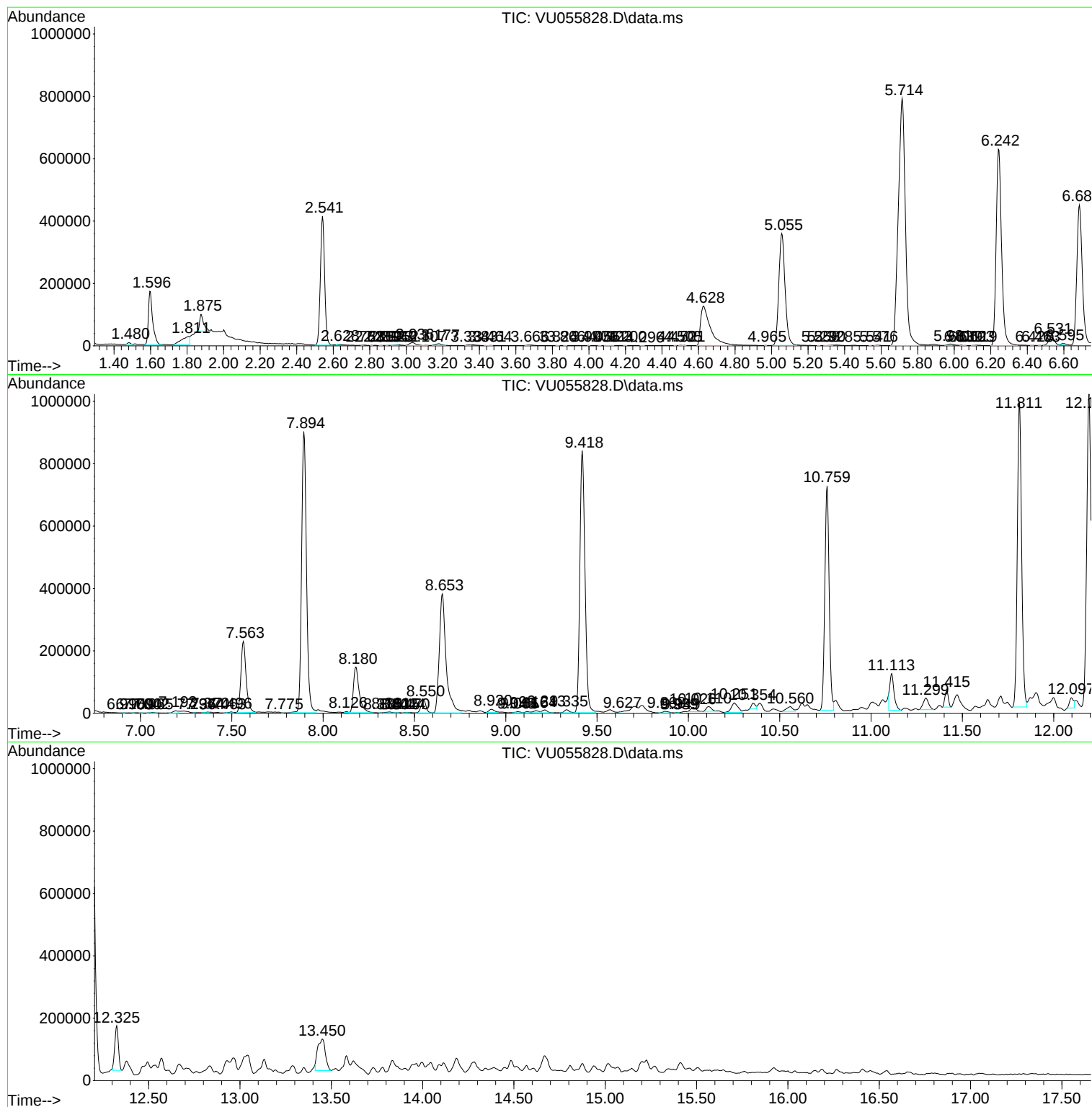
Sum of corrected areas: 17787769

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
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EOAQ9

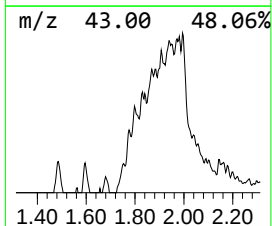
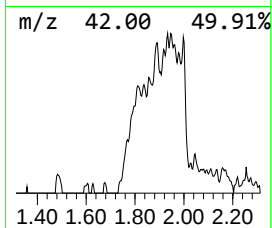
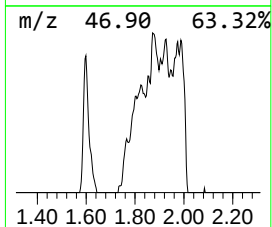
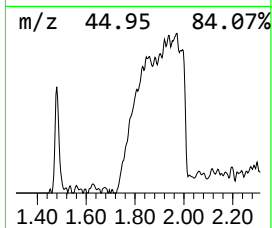
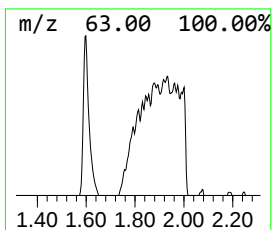
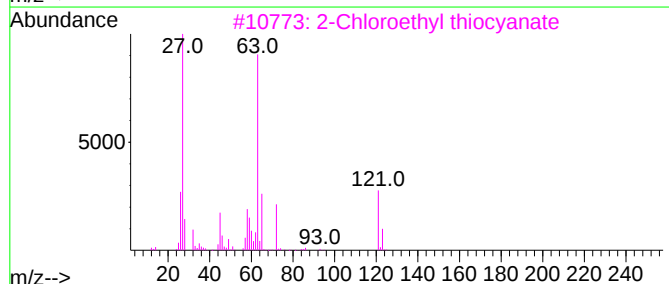
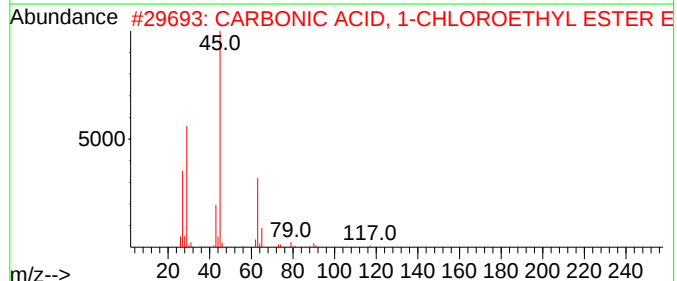
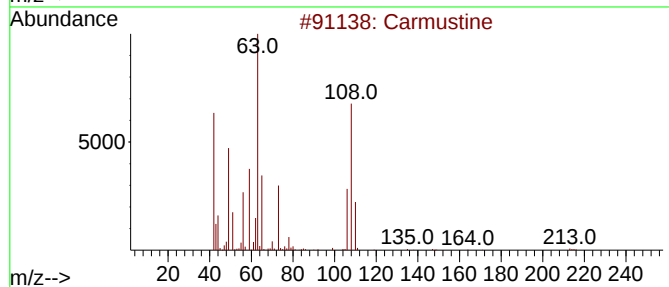
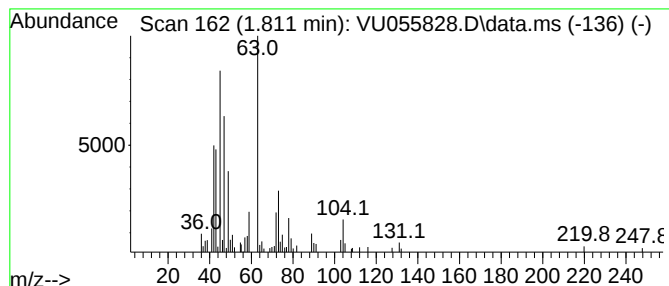
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.811	3.01 ug/L	78155	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carmustine	213	C5H9Cl2N3O2	000154-93-8	45
2			CARBONIC ACID, 1-CHLOROETHYL EST...	152	C5H9ClO3	050893-36-2	25
3			2-Chloroethyl thiocyanate	121	C3H4ClNS	1000342-25-2	23
4			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	17
5			Methyl 2,2,4-trichloro-3-oxopent...	232	C6H7Cl3O3	1000112-41-1	17



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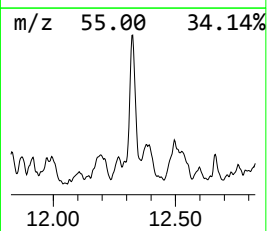
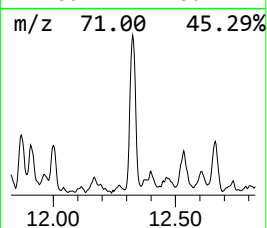
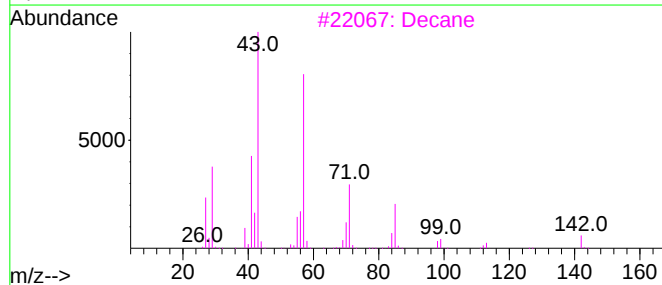
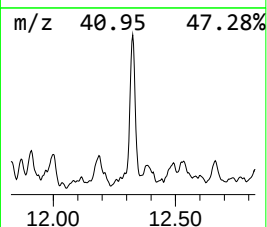
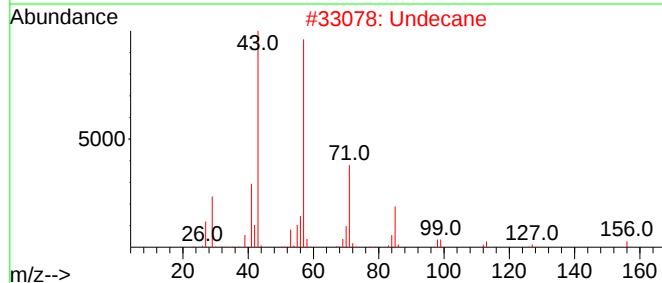
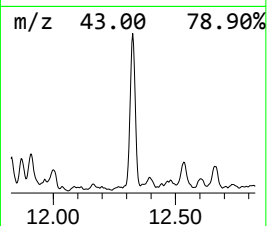
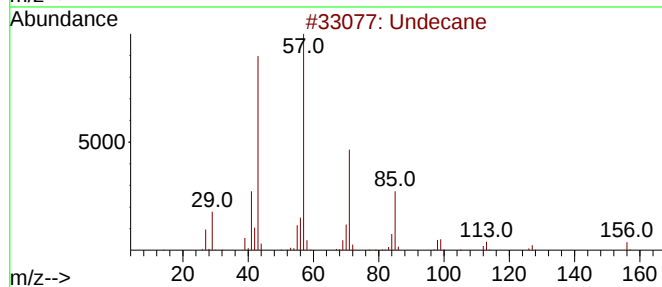
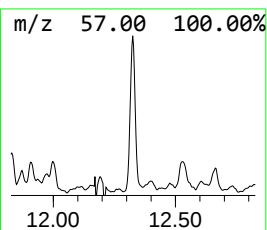
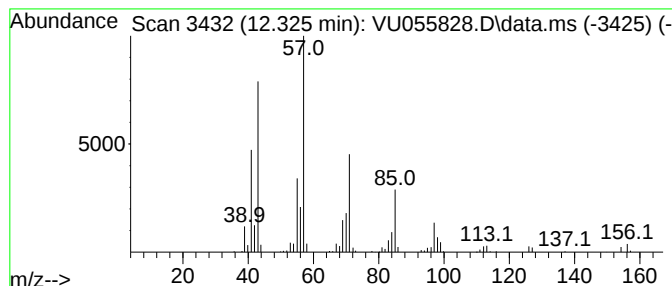
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.325	6.16 ug/L	198804	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Undecane			156	C11H24	001120-21-4	90
3	Decane			142	C10H22	000124-18-5	86
4	Tritetracontane			605	C43H88	007098-21-7	83
5	Undecane			156	C11H24	001120-21-4	81



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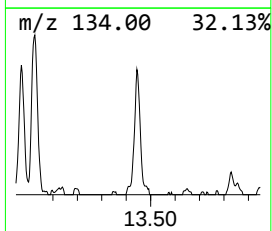
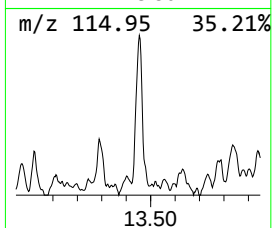
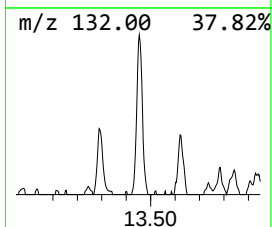
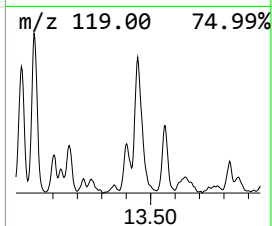
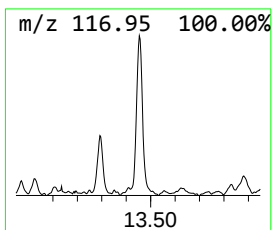
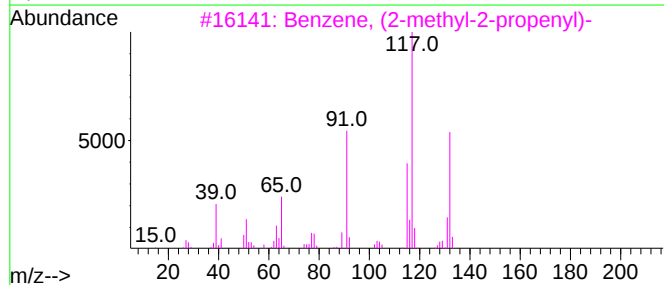
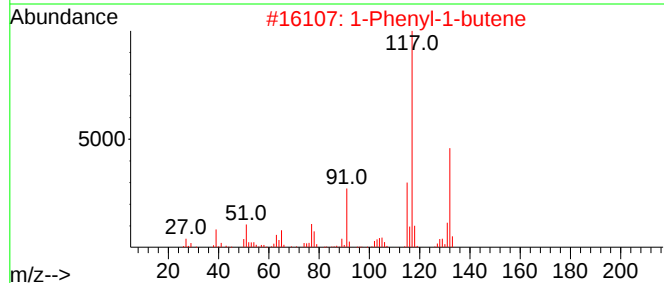
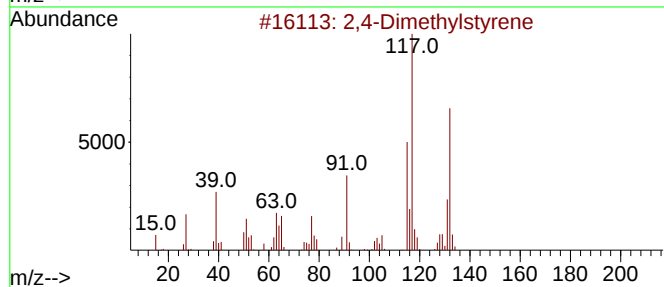
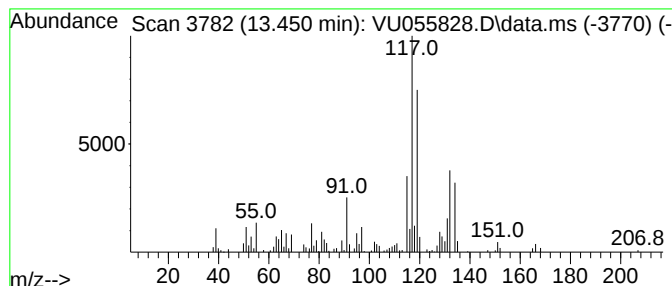
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 2,4-Dimethylstyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.450	9.14 ug/L	294814	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	74
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	55
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	55
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	55
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055828.D
Acq On : 20 Oct 2023 13:26
Operator : MD/SY
Sample : 04922-03
Misc : 6.13g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EOAQ9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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	1.811	3.0	ug/L	78155	1	6.242	1297600	50.0
(DEL) Alkane: S...	12.325	6.2	ug/L	198804	3	11.814	1613040	50.0
2,4-Dimethylsty...	13.450	9.1	ug/L	294814	3	11.814	1613040	50.0