

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101123\
 Data File : VU055747.D
 Acq On : 11 Oct 2023 14:58
 Operator : MD/SY
 Sample : 04792-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY1B3

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: VU055747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.489	55	62	69	rBV2	18449	19653	0.83%	0.108%
2	1.602	87	97	111	rBV2	357866	463676	19.65%	2.559%
3	1.801	141	159	160	rBV3	30187	76848	3.26%	0.424%
4	1.888	178	186	204	rVB	166643	243024	10.30%	1.341%
5	1.975	206	213	226	rVB	48565	71827	3.04%	0.396%
6	2.267	301	304	306	rBV2	1439	906	0.04%	0.005%
7	2.560	382	395	421	rBV	369658	618629	26.22%	3.414%
8	2.679	428	432	435	rBV7	956	1006	0.04%	0.006%
9	2.782	461	464	465	rBV3	897	535	0.02%	0.003%
10	3.036	529	543	553	rBV4	14920	33795	1.43%	0.187%
11	3.123	565	570	571	rBV3	4498	3368	0.14%	0.019%
12	3.177	580	587	591	rBV3	6001	8696	0.37%	0.048%
13	3.354	625	642	672	rBV	317409	741376	31.42%	4.091%
14	3.621	722	725	731	rBV4	527	678	0.03%	0.004%
15	3.672	739	741	746	rVV4	705	480	0.02%	0.003%
16	3.859	794	799	807	rVB5	1675	2288	0.10%	0.013%
17	3.972	828	834	836	rBV5	949	831	0.04%	0.005%
18	4.277	921	929	931	rBV3	1260	1700	0.07%	0.009%
19	4.322	940	943	949	rVB4	785	799	0.03%	0.004%
20	4.425	961	975	994	rBV4	7258	18286	0.78%	0.101%
21	4.521	997	1005	1017	rVB7	1846	4113	0.17%	0.023%
22	4.660	1022	1048	1073	rBV2	848186	2359252	100.00%	13.020%
23	5.055	1155	1171	1198	rBV	340436	768815	32.59%	4.243%
24	5.306	1246	1249	1250	rBV2	1018	619	0.03%	0.003%
25	5.370	1266	1269	1272	rBV3	778	663	0.03%	0.004%
26	5.457	1283	1296	1315	rBV5	19846	43861	1.86%	0.242%
27	5.624	1340	1348	1350	rBV6	2737	3024	0.13%	0.017%
28	5.721	1357	1378	1389	rBV2	686287	1881570	79.75%	10.384%
29	6.116	1493	1501	1502	rBV4	911	872	0.04%	0.005%
30	6.180	1518	1521	1526	rVB3	579	452	0.02%	0.002%
31	6.242	1526	1540	1566	rBV	512450	1005195	42.61%	5.547%
32	6.463	1605	1609	1614	rVB5	934	927	0.04%	0.005%
33	6.534	1618	1631	1646	rBV5	28705	62367	2.64%	0.344%
34	6.685	1664	1678	1707	rBV	423611	856961	36.32%	4.729%
35	6.859	1724	1732	1734	rBV6	3227	3961	0.17%	0.022%
36	6.917	1745	1750	1762	rVB6	2637	4344	0.18%	0.024%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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

37	7.065	1785	1796	1807	rBV9	4072	8603	0.36%	0.047%
38	7.200	1826	1838	1842	rVV10	2558	5113	0.22%	0.028%
39	7.254	1845	1855	1872	rVB5	16302	35391	1.50%	0.195%
40	7.377	1876	1893	1907	rBV4	26240	57570	2.44%	0.318%
41	7.560	1937	1950	1964	rBV	229363	418659	17.75%	2.310%
42	7.843	2029	2038	2039	rBV6	2811	3267	0.14%	0.018%
43	7.894	2042	2054	2076	rVV	821699	1425582	60.43%	7.867%
44	8.177	2130	2142	2157	rBV2	158591	281509	11.93%	1.554%
45	8.360	2192	2199	2206	rBV8	3506	6076	0.26%	0.034%
46	8.402	2208	2212	2220	rVB5	3340	4819	0.20%	0.027%
47	8.457	2224	2229	2230	rBV2	876	626	0.03%	0.003%
48	8.479	2231	2236	2246	rVB5	3226	5509	0.23%	0.030%
49	8.550	2246	2258	2272	rBV	128692	219886	9.32%	1.213%
50	8.634	2272	2284	2327	rBV3	527273	1223759	51.87%	6.753%
51	8.997	2394	2397	2400	rVB5	587	436	0.02%	0.002%
52	9.058	2410	2416	2418	rBV6	1199	1065	0.05%	0.006%
53	9.209	2460	2463	2467	rBV4	538	440	0.02%	0.002%
54	9.274	2471	2483	2493	rBV3	3464	6362	0.27%	0.035%
55	9.322	2494	2498	2500	rBV2	714	503	0.02%	0.003%
56	9.338	2500	2503	2504	rBV2	1002	685	0.03%	0.004%
57	9.415	2514	2527	2549	rBV	761069	1286397	54.53%	7.099%
58	9.601	2582	2585	2588	rBV5	658	651	0.03%	0.004%
59	9.692	2605	2613	2618	rBV9	2302	3193	0.14%	0.018%
60	9.762	2633	2635	2638	rBV3	758	420	0.02%	0.002%
61	9.827	2650	2655	2658	rBV6	879	837	0.04%	0.005%
62	9.888	2671	2674	2677	rVV3	774	584	0.02%	0.003%
63	9.984	2700	2704	2707	rVB2	800	444	0.02%	0.002%
64	10.016	2711	2714	2715	rBV	1153	535	0.02%	0.003%
65	10.100	2734	2740	2743	rVV4	1145	1154	0.05%	0.006%
66	10.113	2743	2744	2747	rVV	1079	527	0.02%	0.003%
67	10.261	2785	2790	2791	rBV2	971	775	0.03%	0.004%
68	10.293	2798	2800	2805	rVB4	821	550	0.02%	0.003%
69	10.399	2830	2833	2836	rVB2	780	509	0.02%	0.003%
70	10.486	2857	2860	2864	rBV2	803	518	0.02%	0.003%
71	10.753	2930	2943	2966	rBV	686921	1133597	48.05%	6.256%
72	10.843	2969	2971	2974	rVB3	995	551	0.02%	0.003%
73	10.878	2979	2982	2985	rBV3	1202	1028	0.04%	0.006%
74	11.019	3023	3026	3029	rVB3	819	567	0.02%	0.003%
75	11.415	3146	3149	3153	rBV5	666	544	0.02%	0.003%
76	11.470	3162	3166	3168	rBV2	1059	808	0.03%	0.004%

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 Title : VOC Analysis

77	11.643	3216	3220	3227	rVB4	1339	1300	0.06%	0.007%
78	11.810	3259	3272	3296	rBV	790541	1268734	53.78%	7.002%
79	12.003	3327	3332	3341	rVB6	1798	2589	0.11%	0.014%
80	12.190	3376	3390	3411	rBV	835411	1385102	58.71%	7.644%
81	12.338	3434	3436	3442	rVV4	810	476	0.02%	0.003%
82	12.486	3480	3482	3487	rBV4	596	444	0.02%	0.002%
83	12.762	3560	3568	3570	rBV5	1360	1659	0.07%	0.009%
84	12.913	3610	3615	3618	rBV	677	553	0.02%	0.003%
85	12.936	3620	3622	3626	rVV3	671	628	0.03%	0.003%
86	13.113	3672	3677	3685	rVB4	1386	1779	0.08%	0.010%
87	13.151	3685	3689	3691	rBV	559	443	0.02%	0.002%
88	13.232	3710	3714	3715	rBV3	1164	787	0.03%	0.004%
89	13.325	3739	3743	3752	rVB6	1926	2282	0.10%	0.013%
90	13.396	3759	3765	3767	rBV3	757	752	0.03%	0.004%
91	13.441	3770	3779	3784	rBV3	532	880	0.04%	0.005%
92	13.511	3797	3801	3802	rBV3	702	466	0.02%	0.003%
93	13.521	3802	3804	3810	rVB3	547	514	0.02%	0.003%
94	13.752	3874	3876	3880	rVB2	689	456	0.02%	0.003%
95	14.119	3982	3990	3991	rBV3	1692	1937	0.08%	0.011%
96	14.392	4072	4075	4080	rBV3	509	544	0.02%	0.003%
97	15.331	4364	4367	4368	rBV2	726	460	0.02%	0.003%
98	15.527	4426	4428	4433	rVB4	1082	750	0.03%	0.004%
99	15.556	4433	4437	4439	rBV2	877	668	0.03%	0.004%
100	16.379	4691	4693	4697	rBV5	1801	906	0.04%	0.005%

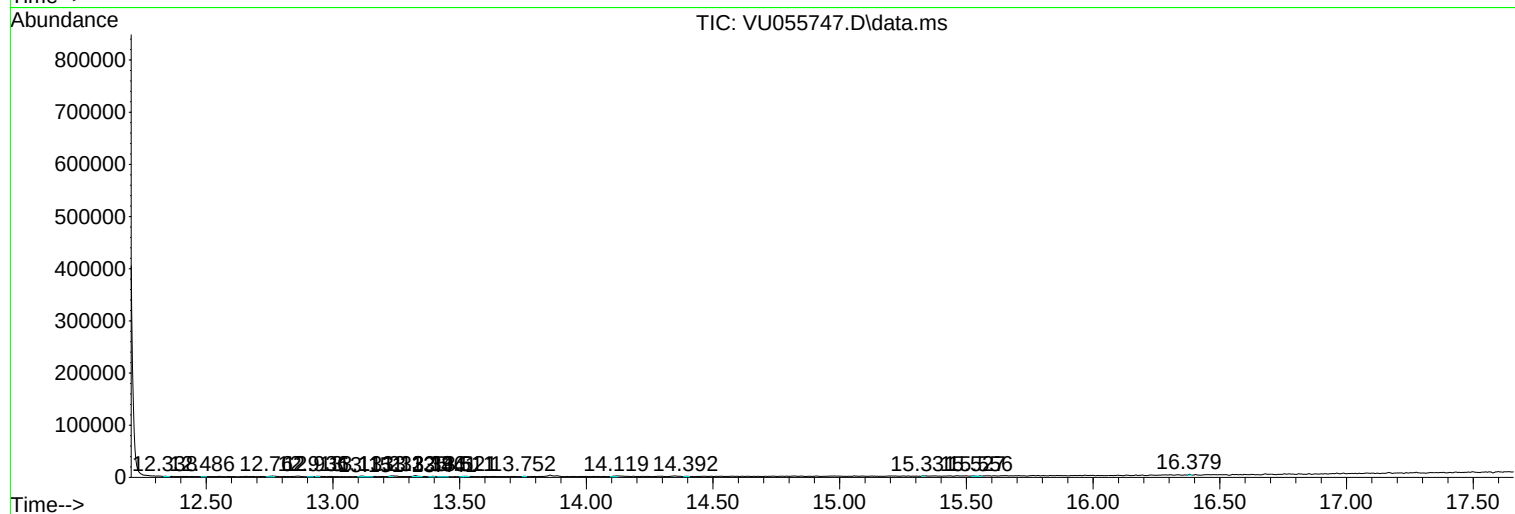
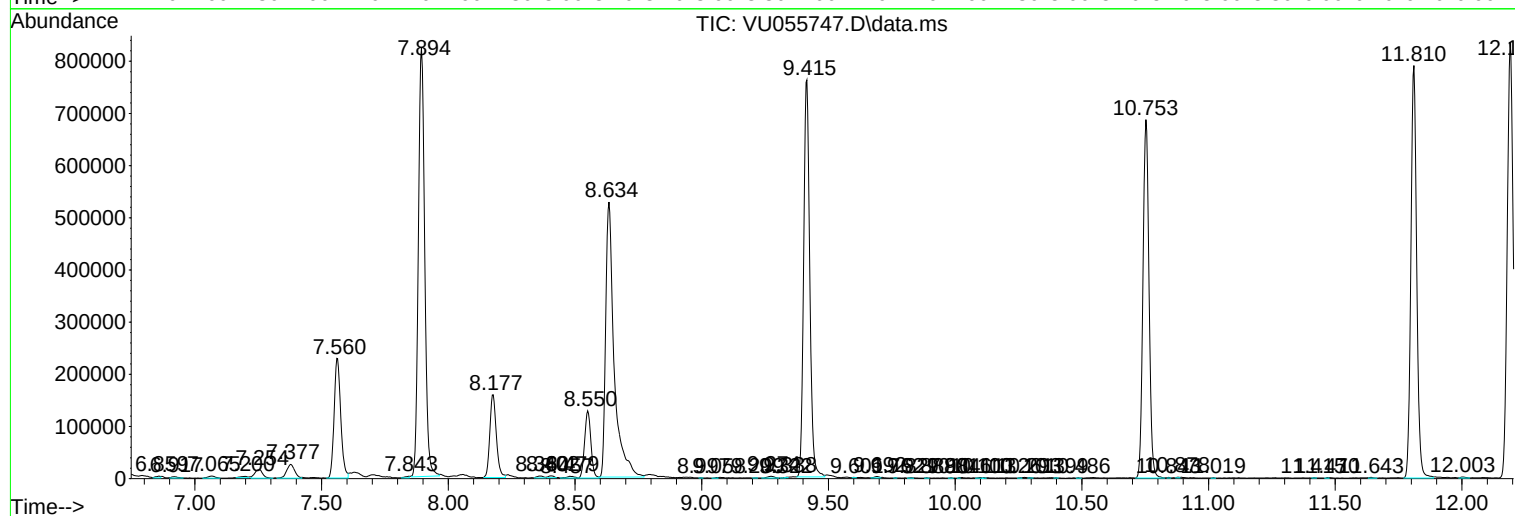
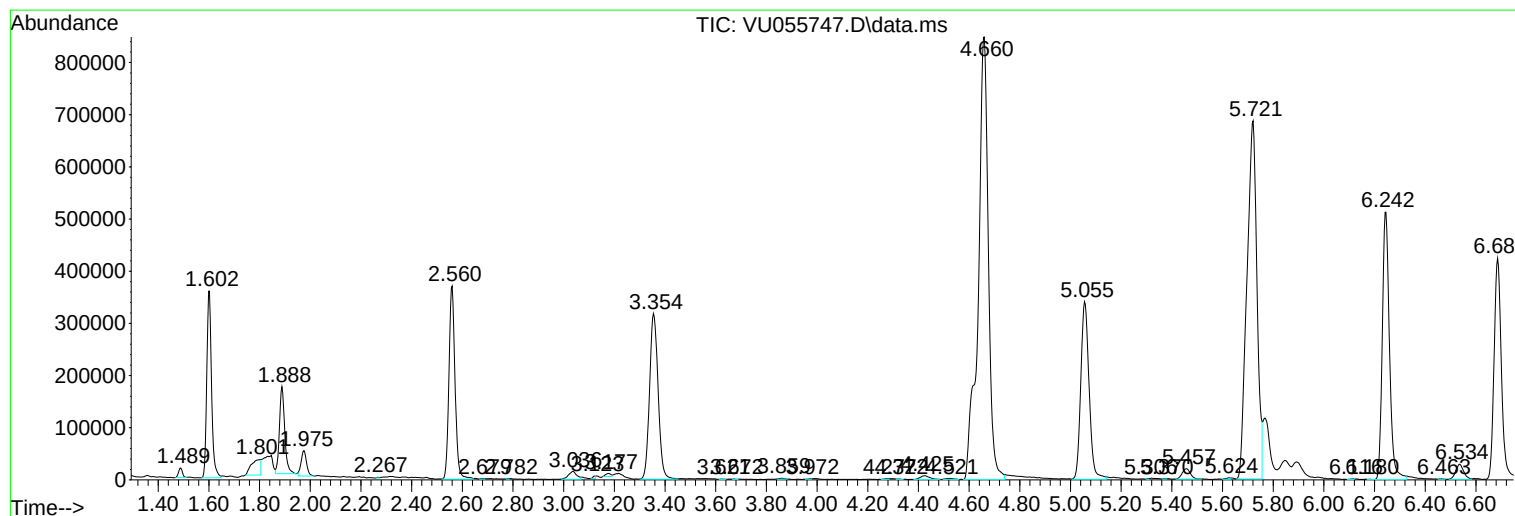
Sum of corrected areas: 18120555

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Instrument :
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ClientSampleId :
EY1B3

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101123\
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Instrument :
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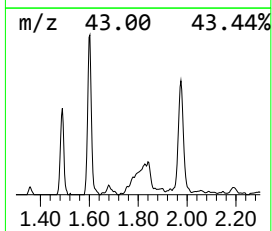
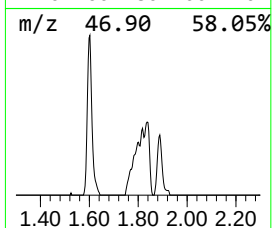
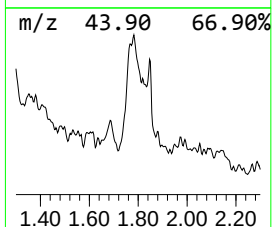
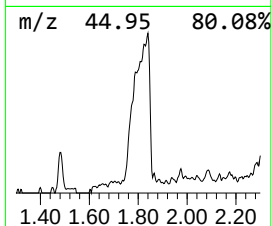
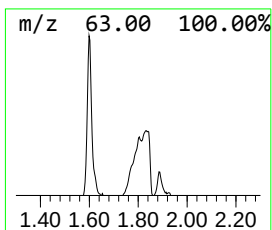
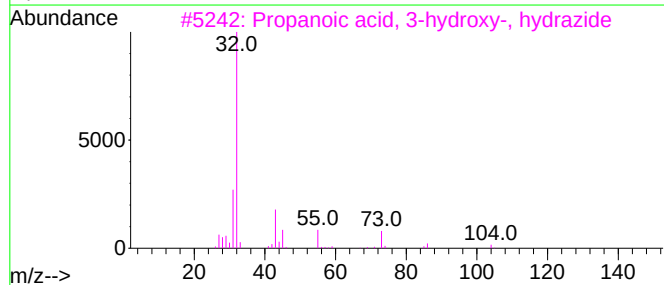
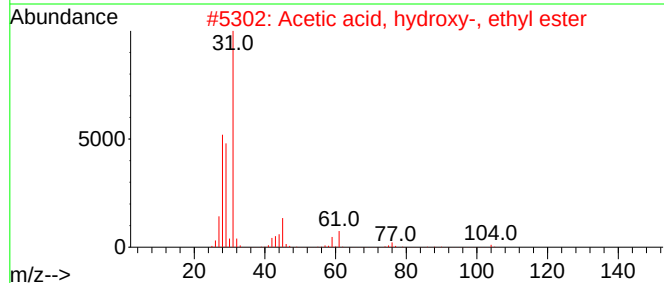
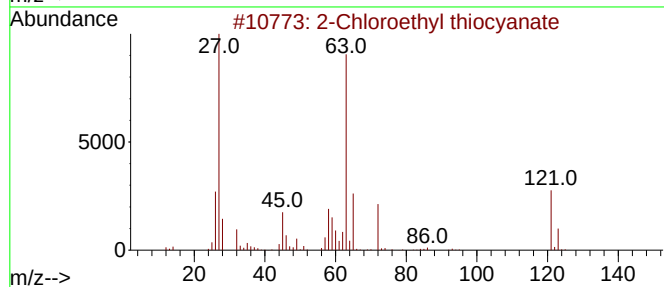
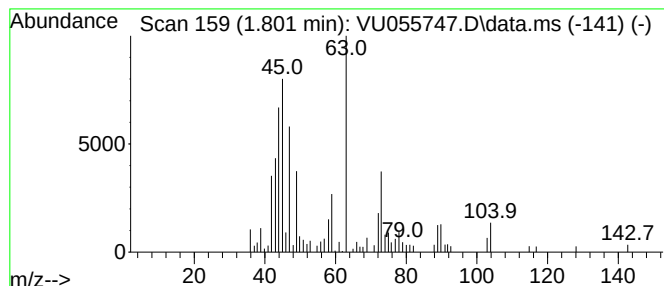
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.801	3.82 ug/L	76848	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloroethyl thiocyanate	121	C3H4ClNS	1000342-25-2	25
2			Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	10
3			Propanoic acid, 3-hydroxy-, hydr...	104	C3H8N2O2	024535-11-3	9
4			Ethylamine	45	C2H7N	000075-04-7	9
5			Ethylamine	45	C2H7N	000075-04-7	9



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Instrument :
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ClientSampleId :
EY1B3

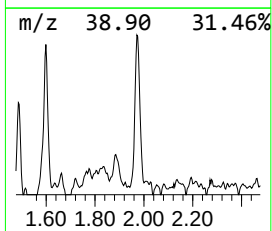
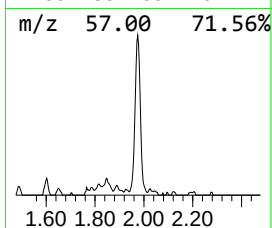
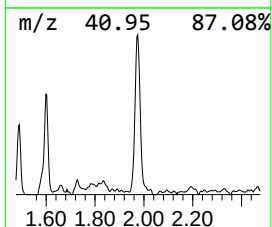
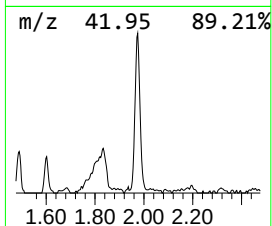
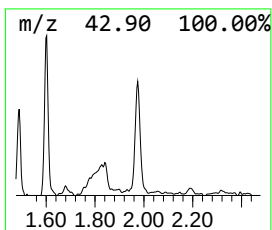
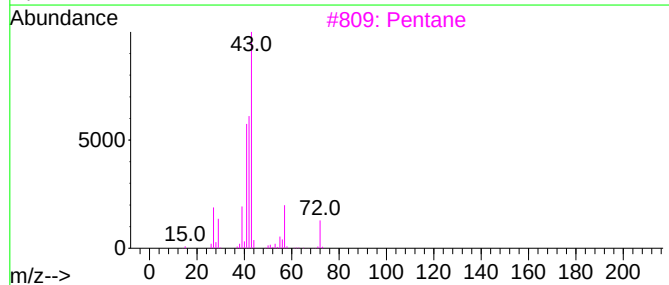
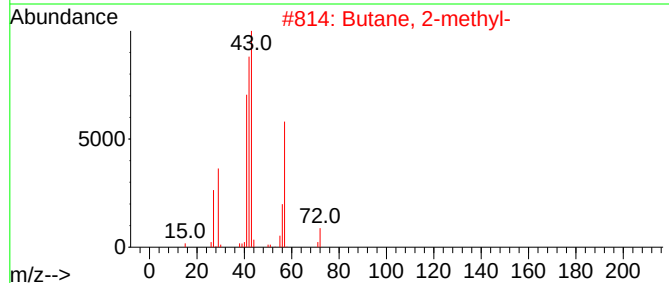
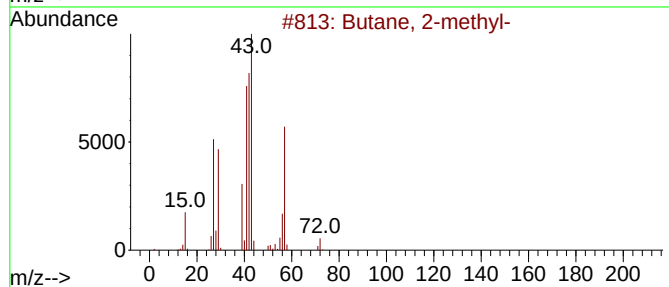
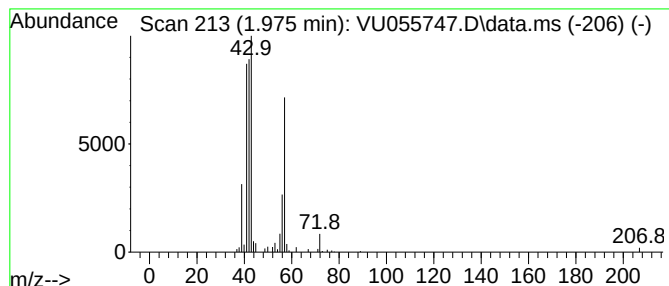
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.975	3.57 ug/L	71827	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	86
2	Butane, 2-methyl-			72	C5H12	000078-78-4	86
3	Pentane			72	C5H12	000109-66-0	59
4	1-Propanol, 2-methyl-			74	C4H10O	000078-83-1	38
5	3-Buten-1-ol			72	C4H8O	000627-27-0	37



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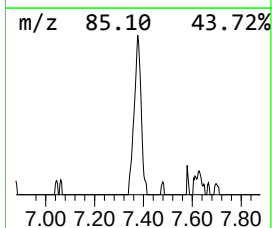
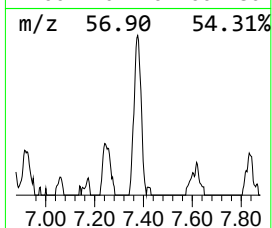
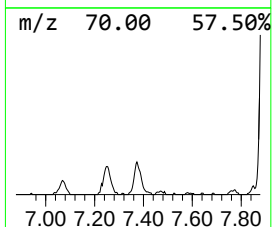
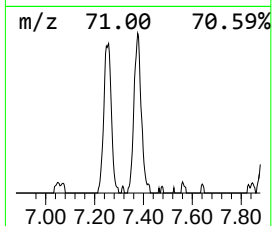
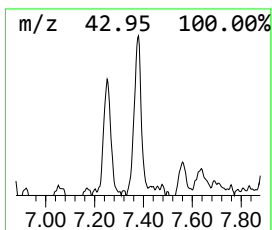
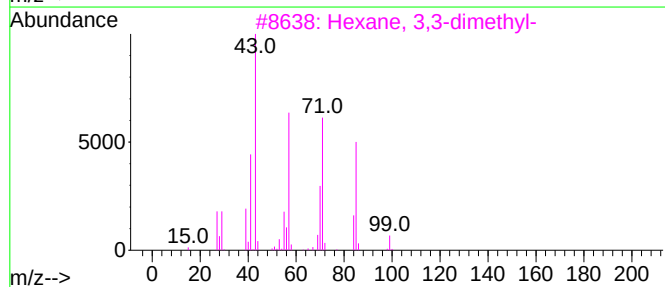
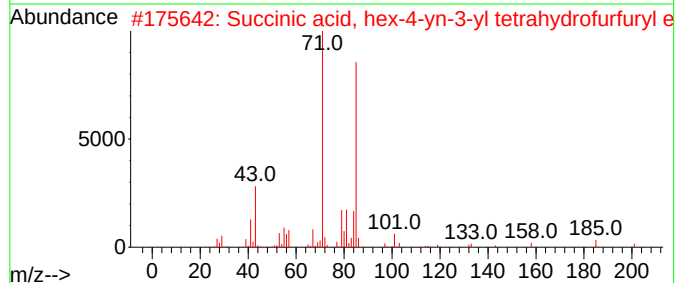
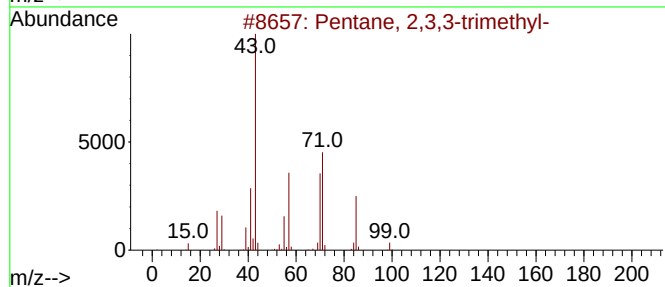
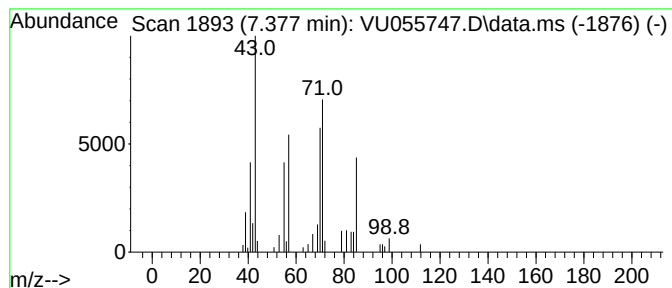
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.377	2.86 ug/L	57570	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
2		Succinic acid, hex-4-yn-3-yl tet...	282	C15H22O5	1000390-71-7	47
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
4		1-Hexene, 4-ethyl-	112	C8H16	016746-85-3	43
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101123\
Data File : VU055747.D
Acq On : 11 Oct 2023 14:58
Operator : MD/SY
Sample : 04792-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B3

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	1.801	3.8	ug/L	76848	1	6.245	1005200	50.0
(DEL) Alkane: S...	1.975	3.6	ug/L	71827	1	6.245	1005200	50.0
(DEL) Alkane: S...	7.377	2.9	ug/L	57570	1	6.245	1005200	50.0