

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050502.D
 Acq On : 29 Aug 2022 22:41
 Operator : SY/MD
 Sample : N4322-07ME
 Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY167ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050502.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	38	43	48	rBV2	4539	5473	0.35%	0.047%
2	1.591	71	78	87	rBV	78053	106926	6.90%	0.927%
3	2.523	355	368	389	rVB	261674	422565	27.29%	3.662%
4	2.639	399	404	405	rBV6	996	880	0.06%	0.008%
5	2.983	507	511	514	rBV4	600	542	0.03%	0.005%
6	3.028	514	525	538	rVV3	7258	14550	0.94%	0.126%
7	3.176	559	571	591	rVV2	11361	29514	1.91%	0.256%
8	3.407	640	643	648	rVB	381	269	0.02%	0.002%
9	3.845	776	779	785	rVB2	358	306	0.02%	0.003%
10	4.022	829	834	837	rBV2	253	282	0.02%	0.002%
11	4.645	1014	1028	1080	rBV2	121083	447863	28.92%	3.881%
12	5.060	1140	1157	1181	rBV	248863	582263	37.60%	5.046%
13	5.288	1220	1228	1231	rBV2	963	1185	0.08%	0.010%
14	5.366	1243	1252	1264	rBV4	956	1624	0.10%	0.014%
15	5.417	1264	1268	1273	rVB2	337	325	0.02%	0.003%
16	5.452	1273	1279	1280	rBV2	291	252	0.02%	0.002%
17	5.716	1341	1361	1389	rVV2	609323	1548586	100.00%	13.420%
18	5.980	1430	1443	1464	rBV3	13157	32939	2.13%	0.285%
19	6.108	1479	1483	1485	rVV2	605	423	0.03%	0.004%
20	6.247	1511	1526	1551	rBV	437984	879516	56.79%	7.622%
21	6.526	1601	1613	1626	rBV9	5710	11414	0.74%	0.099%
22	6.603	1629	1637	1649	rBV4	5534	10773	0.70%	0.093%
23	6.690	1649	1664	1684	rBV	342774	703910	45.46%	6.100%
24	6.790	1693	1695	1699	rBV4	578	439	0.03%	0.004%
25	7.224	1816	1830	1839	rBV7	5487	12486	0.81%	0.108%
26	7.295	1848	1852	1855	rBV3	563	492	0.03%	0.004%
27	7.501	1902	1916	1922	rBV7	1656	3059	0.20%	0.027%
28	7.568	1922	1937	1959	rVV	135241	261640	16.90%	2.267%
29	7.655	1961	1964	1967	rVV3	1111	853	0.06%	0.007%
30	7.697	1971	1977	1978	rBV3	651	502	0.03%	0.004%
31	7.787	2001	2005	2011	rBV5	566	598	0.04%	0.005%
32	7.896	2025	2039	2058	rBV	617066	1109867	71.67%	9.618%
33	8.057	2085	2089	2091	rBV3	621	409	0.03%	0.004%
34	8.128	2104	2111	2116	rBV3	2360	3395	0.22%	0.029%
35	8.182	2116	2128	2152	rVV	85224	172641	11.15%	1.496%
36	8.285	2157	2160	2165	rVB3	407	352	0.02%	0.003%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

37	8.346	2173	2179	2181	rBV4	1314	1266	0.08%	0.011%
38	8.449	2205	2211	2216	rVB4	323	358	0.02%	0.003%
39	8.533	2232	2237	2241	rBV5	436	490	0.03%	0.004%
40	8.552	2241	2243	2247	rBV3	343	313	0.02%	0.003%
41	8.587	2251	2254	2259	rVB3	469	415	0.03%	0.004%
42	8.661	2259	2277	2312	rBV2	358116	950585	61.38%	8.238%
43	8.925	2349	2359	2373	rVB8	2706	5498	0.36%	0.048%
44	9.063	2396	2402	2403	rBV3	823	759	0.05%	0.007%
45	9.111	2409	2417	2419	rBV4	740	1012	0.07%	0.009%
46	9.169	2429	2435	2439	rVV5	1579	1750	0.11%	0.015%
47	9.208	2443	2447	2454	rVB4	1940	2649	0.17%	0.023%
48	9.336	2478	2487	2493	rBV5	2135	3276	0.21%	0.028%
49	9.420	2499	2513	2540	rBV	576176	1100352	71.06%	9.536%
50	9.562	2554	2557	2560	rBV2	769	582	0.04%	0.005%
51	9.655	2583	2586	2589	rBV	588	528	0.03%	0.005%
52	9.745	2607	2614	2623	rVB5	5507	7722	0.50%	0.067%
53	9.870	2649	2653	2660	rVB3	1022	1136	0.07%	0.010%
54	9.951	2675	2678	2680	rBV3	381	272	0.02%	0.002%
55	10.015	2694	2698	2701	rBV3	735	597	0.04%	0.005%
56	10.057	2709	2711	2717	rVB2	312	293	0.02%	0.003%
57	10.118	2723	2730	2743	rVB7	1356	2445	0.16%	0.021%
58	10.250	2764	2771	2781	rVV4	3999	5851	0.38%	0.051%
59	10.301	2782	2787	2789	rVV3	386	361	0.02%	0.003%
60	10.320	2791	2793	2796	rVV4	621	391	0.03%	0.003%
61	10.356	2797	2804	2806	rVV6	1139	1465	0.09%	0.013%
62	10.391	2810	2815	2826	rVB5	3761	6217	0.40%	0.054%
63	10.462	2831	2837	2843	rBV5	645	889	0.06%	0.008%
64	10.491	2843	2846	2850	rVB4	317	264	0.02%	0.002%
65	10.555	2857	2866	2873	rBV6	1945	3303	0.21%	0.029%
66	10.623	2883	2887	2893	rBV5	1721	1926	0.12%	0.017%
67	10.764	2914	2931	2954	rBV	529474	897815	57.98%	7.781%
68	10.877	2963	2966	2970	rBV4	372	418	0.03%	0.004%
69	10.947	2980	2988	2996	rBV5	1128	1649	0.11%	0.014%
70	10.983	2996	2999	3006	rVB4	853	793	0.05%	0.007%
71	11.012	3006	3008	3010	rBV2	417	271	0.02%	0.002%
72	11.066	3017	3025	3030	rBV4	1270	1726	0.11%	0.015%
73	11.115	3030	3040	3056	rVB2	17266	29849	1.93%	0.259%
74	11.182	3056	3061	3063	rBV2	865	685	0.04%	0.006%
75	11.253	3080	3083	3088	rVB3	473	352	0.02%	0.003%
76	11.314	3094	3102	3109	rVB6	2251	3044	0.20%	0.026%

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Instrument :
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 ClientSampleId :
 EY167ME

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

77	11.352	3112	3114	3116	rBV3	406	246	0.02%	0.002%
78	11.375	3116	3121	3126	rBV5	1731	2089	0.13%	0.018%
79	11.417	3126	3134	3142	rVB3	10237	14154	0.91%	0.123%
80	11.459	3143	3147	3148	rBV3	1018	739	0.05%	0.006%
81	11.571	3176	3182	3188	rBV5	1374	2089	0.13%	0.018%
82	11.716	3218	3227	3233	rBV9	1760	2819	0.18%	0.024%
83	11.754	3233	3239	3245	rVB7	1936	2780	0.18%	0.024%
84	11.815	3245	3258	3273	rBV	550676	885670	57.19%	7.675%
85	11.999	3307	3315	3324	rVB10	3631	6934	0.45%	0.060%
86	12.041	3324	3328	3333	rVB6	862	754	0.05%	0.007%
87	12.086	3334	3342	3345	rBV5	1108	1551	0.10%	0.013%
88	12.102	3345	3347	3351	rVB2	652	344	0.02%	0.003%
89	12.195	3363	3376	3395	rBV	573171	965191	62.33%	8.365%
90	12.327	3409	3417	3428	rVB	33679	50508	3.26%	0.438%
91	12.369	3428	3430	3431	rBV2	1033	413	0.03%	0.004%
92	12.471	3458	3462	3464	rBV2	1196	973	0.06%	0.008%
93	12.664	3516	3522	3532	rVB5	4924	6952	0.45%	0.060%
94	12.931	3591	3605	3606	rBV7	6326	9986	0.64%	0.087%
95	13.005	3623	3628	3635	rBV8	3149	3954	0.26%	0.034%
96	13.134	3662	3668	3676	rBV6	4231	5626	0.36%	0.049%
97	13.433	3752	3761	3770	rBV	40110	59461	3.84%	0.515%
98	13.587	3801	3809	3827	rBV2	23715	38702	2.50%	0.335%
99	14.449	4070	4077	4087	rBV	32751	45774	2.96%	0.397%
100	15.401	4368	4373	4384	rVB3	16760	22709	1.47%	0.197%

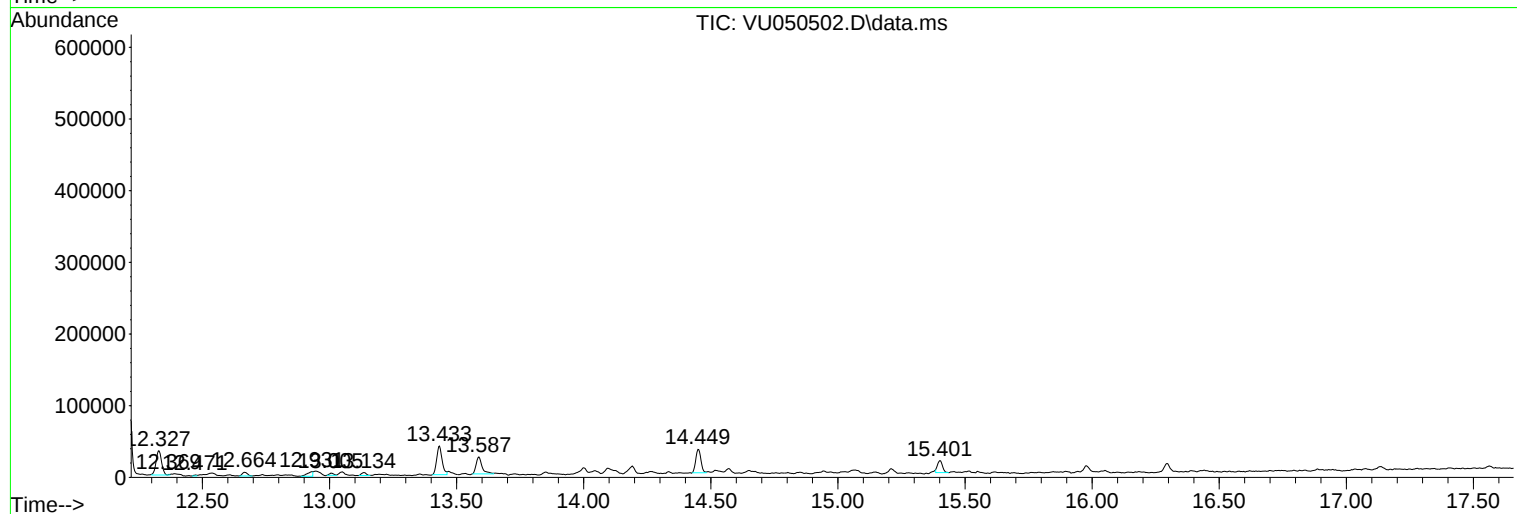
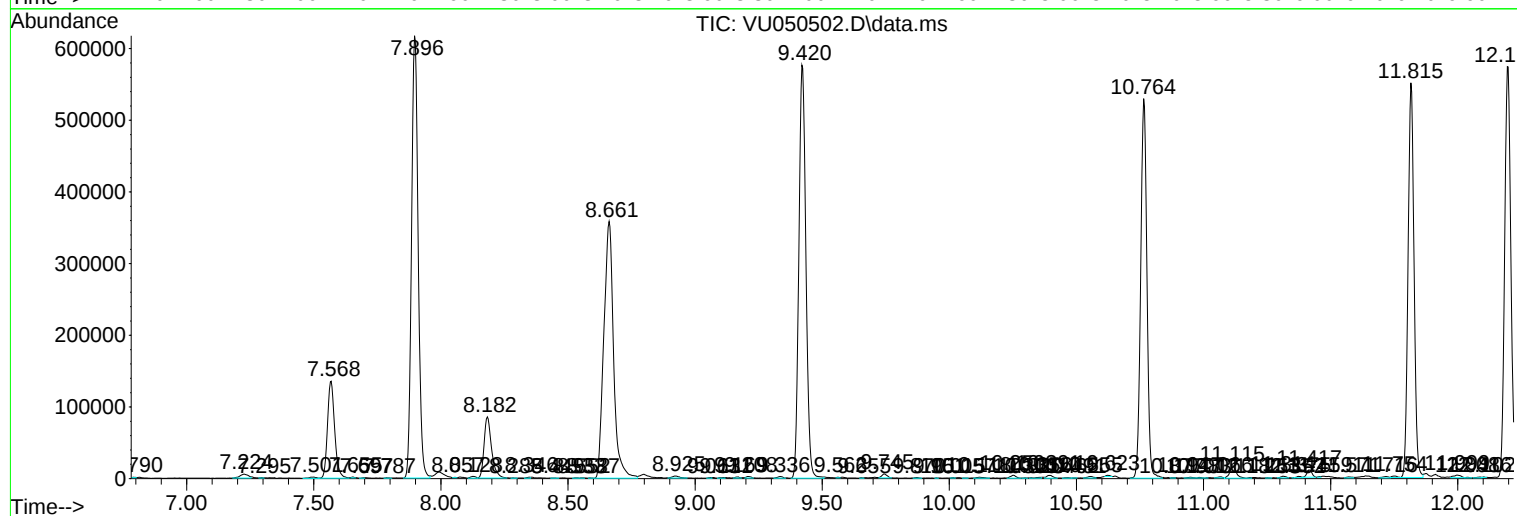
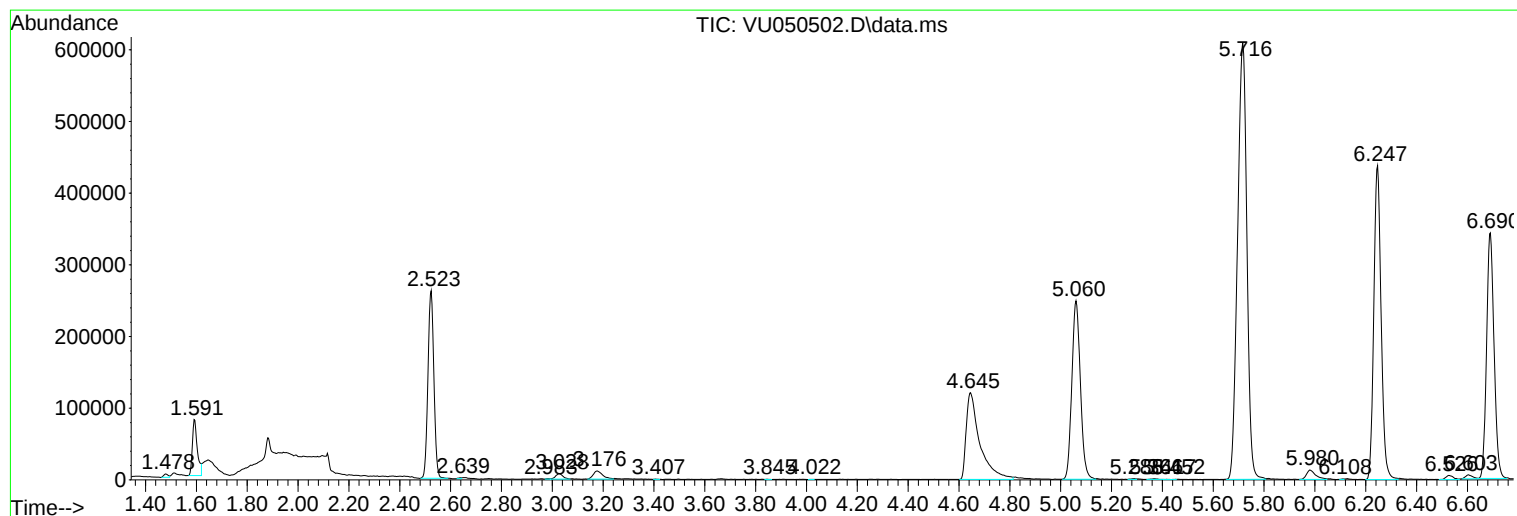
Sum of corrected areas: 11539098

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ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY167ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY167ME

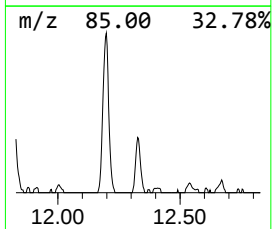
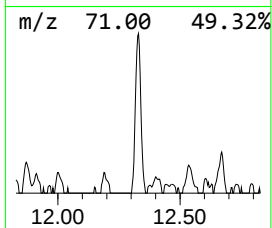
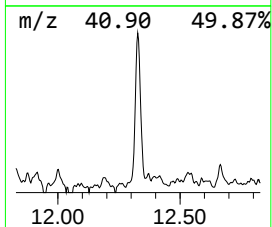
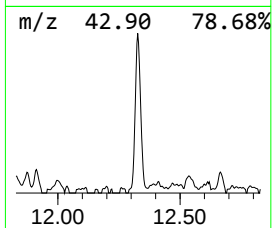
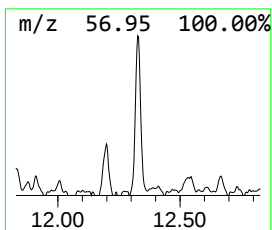
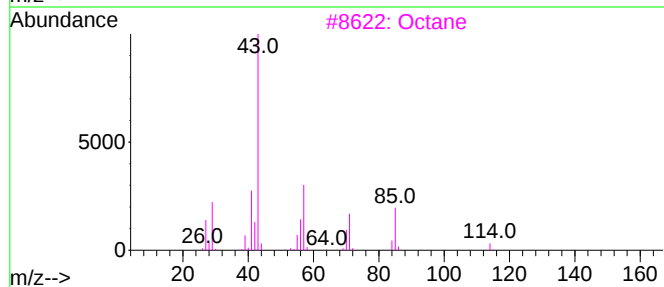
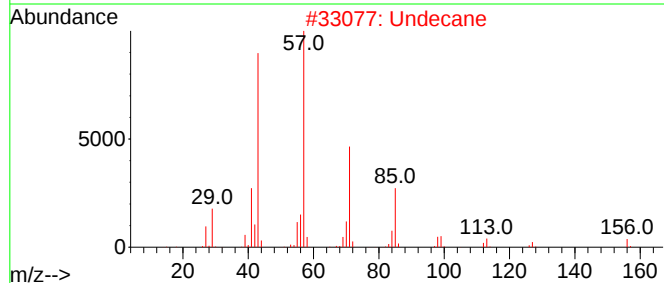
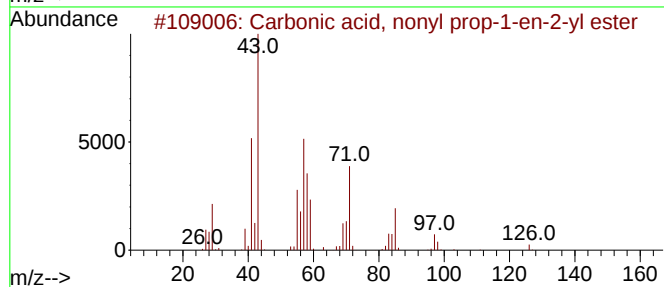
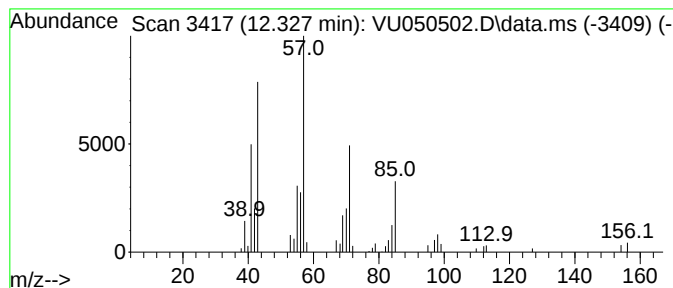
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Carbonic acid, nonyl prop-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	2.85 ug/L	50508	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	72
2			Undecane	156	C11H24	001120-21-4	64
3			Octane	114	C8H18	000111-65-9	59
4			Octane	114	C8H18	000111-65-9	59
5			Undecane	156	C11H24	001120-21-4	52



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Instrument :
MSVOA_U
ClientSampleId :
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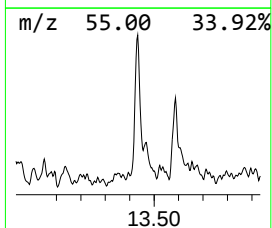
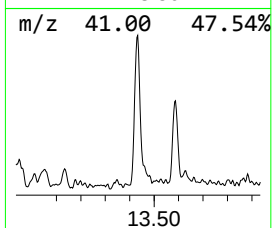
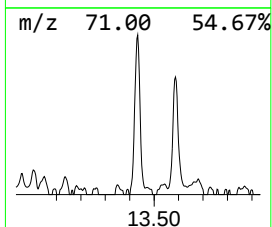
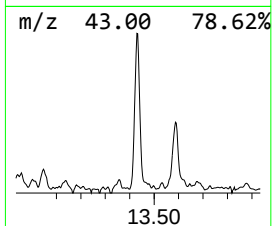
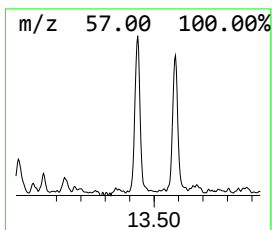
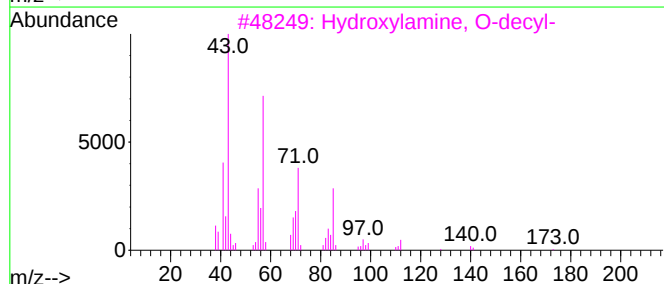
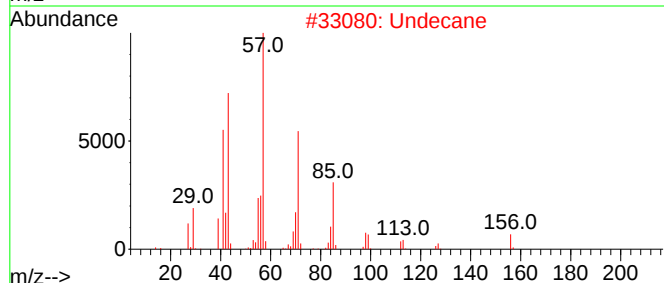
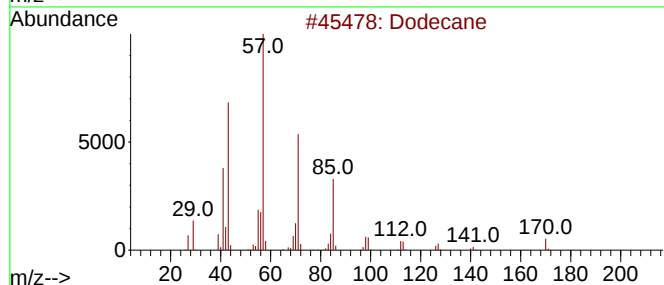
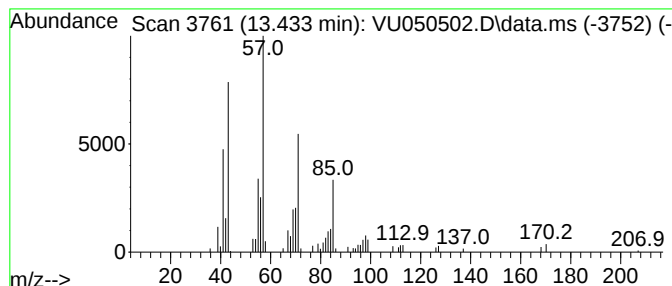
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	3.36 ug/L	59461	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	81
2			Undecane	156	C11H24	001120-21-4	80
3			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	78
4			Dodecane	170	C12H26	000112-40-3	74
5			Undecane	156	C11H24	001120-21-4	64



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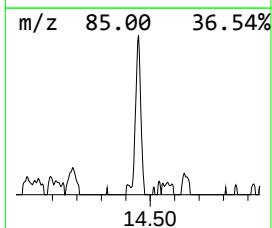
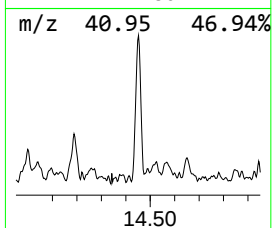
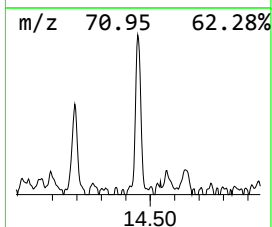
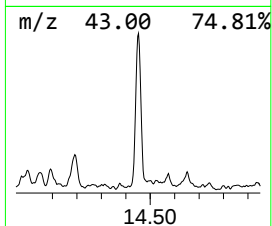
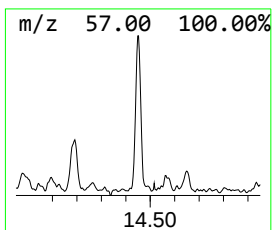
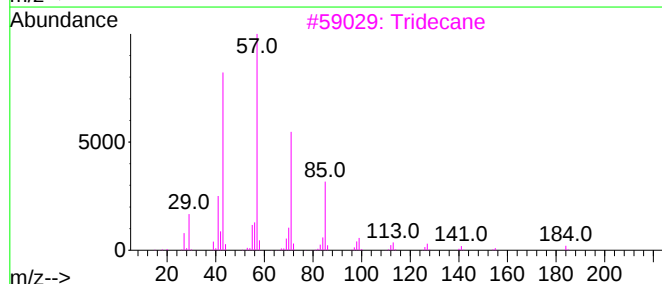
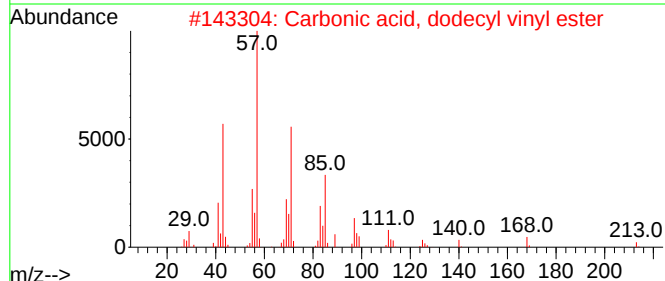
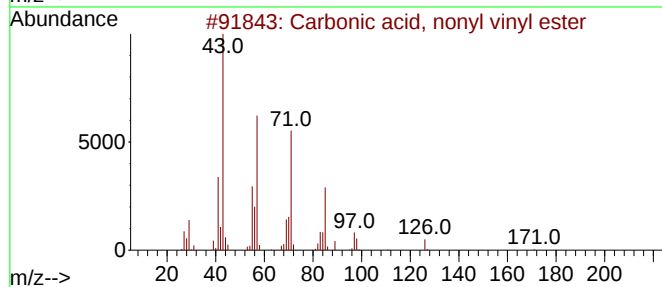
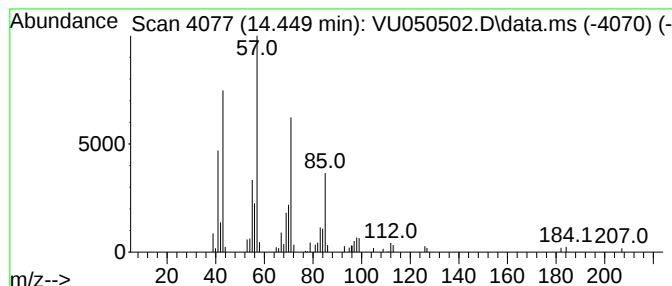
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Carbonic acid, nonyl vinyl ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.449	2.58 ug/L	45774	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	86
2			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	83
3			Tridecane	184	C13H28	000629-50-5	80
4			Nonadecane	268	C19H40	000629-92-5	80
5			Tetradecane	198	C14H30	000629-59-4	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050502.D
Acq On : 29 Aug 2022 22:41
Operator : SY/MD
Sample : N4322-07ME
Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY167ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.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
Carbonic acid, ...	12.327	2.9	ug/L	50508	3	11.816	885670	50.0
(DEL) Alkane: S...	13.433	3.4	ug/L	59461	3	11.816	885670	50.0
Carbonic acid, ...	14.449	2.6	ug/L	45774	3	11.816	885670	50.0