

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050496.D
 Acq On : 29 Aug 2022 19:55
 Operator : SY/MD
 Sample : N4322-05ME
 Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY165ME

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: VU050496.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	39	43	48	rBV2	4149	4519	0.29%	0.037%
2	1.511	49	53	67	rVB2	5160	6880	0.45%	0.057%
3	1.591	71	78	87	rBV	85786	117083	7.62%	0.968%
4	2.520	354	367	383	rBV	288097	461311	30.03%	3.812%
5	2.652	397	408	409	rBV2	2170	2834	0.18%	0.023%
6	2.752	433	439	448	rVB4	830	1358	0.09%	0.011%
7	2.919	485	491	493	rBV2	545	633	0.04%	0.005%
8	3.025	513	524	538	rBV2	7754	15526	1.01%	0.128%
9	3.176	557	571	590	rVV2	12872	34122	2.22%	0.282%
10	3.379	631	634	640	rBB4	280	250	0.02%	0.002%
11	3.655	716	720	721	rBV2	802	602	0.04%	0.005%
12	4.491	976	980	985	rBV2	219	236	0.02%	0.002%
13	4.645	1015	1028	1078	rBV2	114439	426767	27.78%	3.527%
14	5.060	1140	1157	1184	rVV	247171	584169	38.03%	4.828%
15	5.285	1218	1227	1228	rBV2	1291	1397	0.09%	0.012%
16	5.369	1245	1253	1256	rBV2	885	1065	0.07%	0.009%
17	5.510	1292	1297	1302	rVB2	280	292	0.02%	0.002%
18	5.543	1303	1307	1316	rVB2	201	327	0.02%	0.003%
19	5.716	1338	1361	1384	rBV2	608164	1536173	100.00%	12.695%
20	5.877	1408	1411	1417	rVB3	322	266	0.02%	0.002%
21	5.980	1432	1443	1471	rBV4	11890	32256	2.10%	0.267%
22	6.118	1479	1486	1492	rBV3	403	547	0.04%	0.005%
23	6.247	1507	1526	1548	rBV	428172	863592	56.22%	7.137%
24	6.472	1593	1596	1600	rVB2	335	243	0.02%	0.002%
25	6.526	1605	1613	1624	rBV7	4281	8743	0.57%	0.072%
26	6.604	1628	1637	1649	rVV4	5919	12489	0.81%	0.103%
27	6.690	1649	1664	1691	rVB	336952	702587	45.74%	5.806%
28	6.800	1696	1698	1706	rVV5	1358	1472	0.10%	0.012%
29	6.829	1706	1707	1712	rVB2	403	231	0.02%	0.002%
30	6.854	1712	1715	1720	rVB3	695	385	0.03%	0.003%
31	6.983	1750	1755	1759	rBV2	204	218	0.01%	0.002%
32	7.160	1806	1810	1814	rBV	280	231	0.02%	0.002%
33	7.227	1814	1831	1841	rBV8	5122	13365	0.87%	0.110%
34	7.295	1850	1852	1853	rBV8	537	281	0.02%	0.002%
35	7.346	1865	1868	1871	rVB3	373	253	0.02%	0.002%
36	7.382	1876	1879	1886	rBV2	262	267	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\SFAMULM082422WMA.M
 Title : VOC Analysis

37	7.494	1907	1914	1919	rBV4	1866	2555	0.17%	0.021%
38	7.568	1924	1937	1959	rBV	133453	258433	16.82%	2.136%
39	7.649	1959	1962	1965	rBV3	866	654	0.04%	0.005%
40	7.896	2025	2039	2060	rBV	614894	1105201	71.95%	9.134%
41	7.993	2062	2069	2083	rVB5	5995	14311	0.93%	0.118%
42	8.124	2103	2110	2117	rBV5	3219	4488	0.29%	0.037%
43	8.182	2117	2128	2157	rVB	85591	174433	11.36%	1.442%
44	8.288	2157	2161	2167	rBV3	655	612	0.04%	0.005%
45	8.350	2172	2180	2182	rBV4	1903	1673	0.11%	0.014%
46	8.430	2200	2205	2209	rBV2	373	305	0.02%	0.003%
47	8.456	2209	2213	2215	rBV2	353	256	0.02%	0.002%
48	8.491	2221	2224	2230	rVB3	456	396	0.03%	0.003%
49	8.552	2230	2243	2259	rBV	151082	261164	17.00%	2.158%
50	8.661	2259	2277	2310	rBV2	349395	902468	58.75%	7.458%
51	8.874	2340	2343	2346	rVB2	615	382	0.02%	0.003%
52	8.925	2349	2359	2368	rVV6	5178	9570	0.62%	0.079%
53	8.980	2372	2376	2378	rBV3	627	496	0.03%	0.004%
54	9.070	2396	2404	2409	rBV4	1574	2206	0.14%	0.018%
55	9.115	2414	2418	2426	rVV3	1265	1597	0.10%	0.013%
56	9.173	2426	2436	2441	rVV6	2585	4525	0.29%	0.037%
57	9.208	2443	2447	2458	rVB5	4161	6780	0.44%	0.056%
58	9.333	2476	2486	2498	rBV7	4439	7512	0.49%	0.062%
59	9.420	2499	2513	2537	rBV	567389	1072041	69.79%	8.860%
60	9.555	2551	2555	2556	rBV2	382	292	0.02%	0.002%
61	9.600	2567	2569	2573	rVB	596	370	0.02%	0.003%
62	9.642	2573	2582	2584	rBV5	1040	1071	0.07%	0.009%
63	9.665	2584	2589	2593	rBV5	960	1160	0.08%	0.010%
64	9.742	2604	2613	2629	rVB2	12647	20277	1.32%	0.168%
65	9.867	2647	2652	2653	rBV4	1160	886	0.06%	0.007%
66	9.954	2672	2679	2690	rBV5	752	1317	0.09%	0.011%
67	10.018	2691	2699	2710	rBV6	2626	4418	0.29%	0.037%
68	10.108	2722	2727	2728	rBV3	1303	931	0.06%	0.008%
69	10.208	2754	2758	2761	rBV3	433	389	0.03%	0.003%
70	10.250	2761	2771	2784	rBV2	9813	16159	1.05%	0.134%
71	10.314	2784	2791	2793	rBV3	2187	2401	0.16%	0.020%
72	10.394	2809	2816	2829	rVB3	12386	21224	1.38%	0.175%
73	10.456	2829	2835	2836	rBV4	1288	1310	0.09%	0.011%
74	10.555	2851	2866	2875	rBV7	5980	12178	0.79%	0.101%
75	10.623	2882	2887	2893	rBV3	6427	8413	0.55%	0.070%
76	10.764	2912	2931	2955	rBV	527303	901135	58.66%	7.447%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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	10.944	2980	2987	2994	rBV8	1943	3371	0.22%	0.028%
78	11.012	3006	3008	3013	rBV5	631	545	0.04%	0.005%
79	11.060	3017	3023	3031	rVV8	5039	9079	0.59%	0.075%
80	11.115	3031	3040	3056	rVB2	45593	74184	4.83%	0.613%
81	11.240	3077	3079	3082	rBV3	607	441	0.03%	0.004%
82	11.256	3082	3084	3089	rVB4	1083	769	0.05%	0.006%
83	11.314	3094	3102	3114	rBV7	4672	8134	0.53%	0.067%
84	11.378	3116	3122	3125	rBV5	3695	4457	0.29%	0.037%
85	11.417	3126	3134	3141	rVV2	23696	34439	2.24%	0.285%
86	11.459	3142	3147	3155	rVB6	4835	6620	0.43%	0.055%
87	11.574	3174	3183	3189	rBV6	3274	6438	0.42%	0.053%
88	11.816	3247	3258	3271	rBV	544025	865688	56.35%	7.154%
89	11.912	3283	3288	3299	rVB9	8114	11094	0.72%	0.092%
90	12.082	3338	3341	3344	rBV5	1453	1434	0.09%	0.012%
91	12.198	3364	3377	3392	rBV	571098	924293	60.17%	7.639%
92	12.327	3409	3417	3427	rVB	81402	116264	7.57%	0.961%
93	12.668	3517	3523	3532	rVB5	10337	14593	0.95%	0.121%
94	12.935	3593	3606	3610	rBV6	14805	33104	2.15%	0.274%
95	13.009	3623	3629	3635	rBV6	6946	9688	0.63%	0.080%
96	13.433	3752	3761	3769	rBV	77653	118865	7.74%	0.982%
97	13.587	3801	3809	3818	rBV	43391	66327	4.32%	0.548%
98	14.449	4070	4077	4086	rBV	60715	82285	5.36%	0.680%
99	15.211	4308	4314	4326	rVB4	14489	22577	1.47%	0.187%
100	16.295	4646	4651	4665	rVB2	20194	26633	1.73%	0.220%

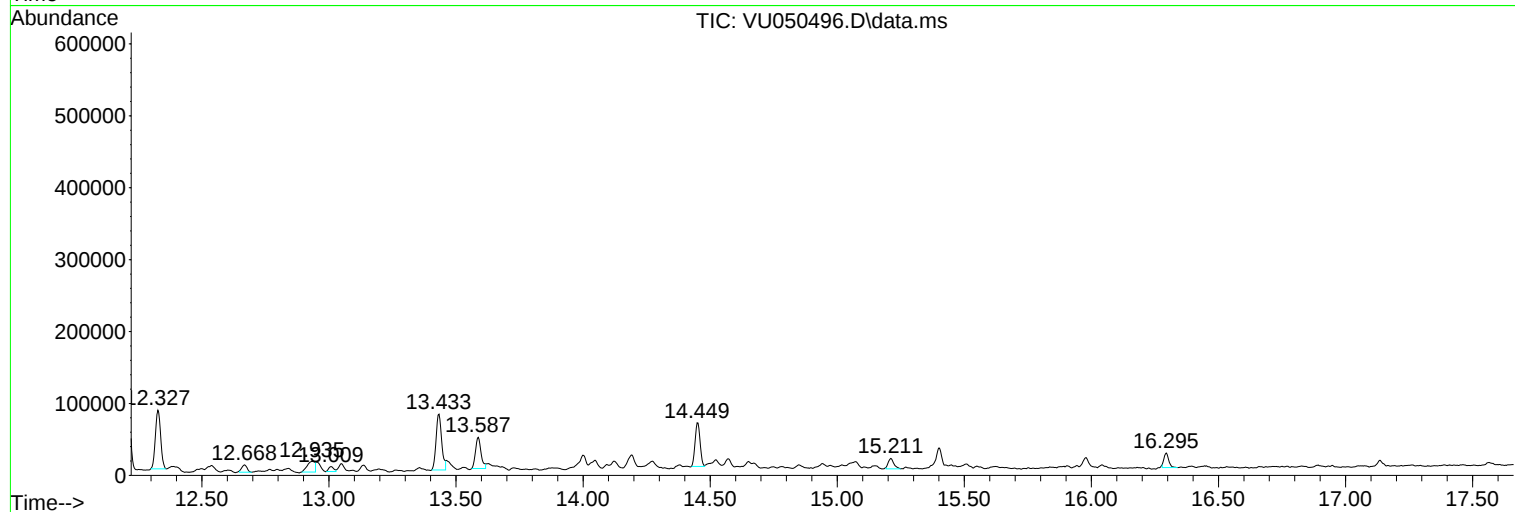
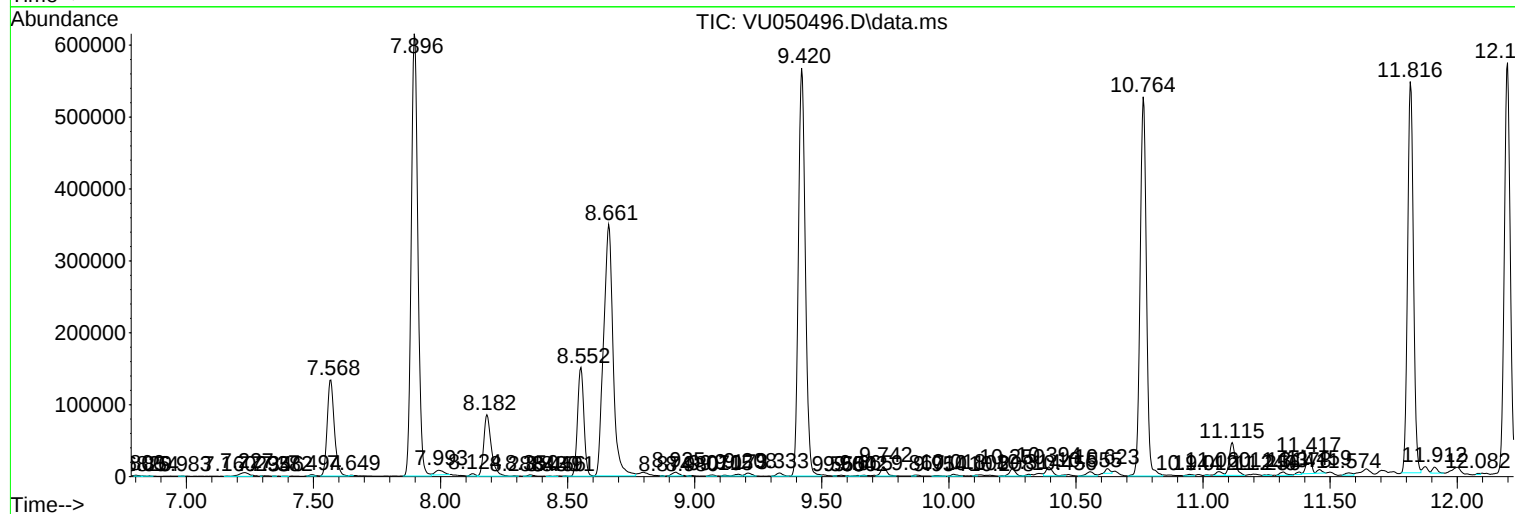
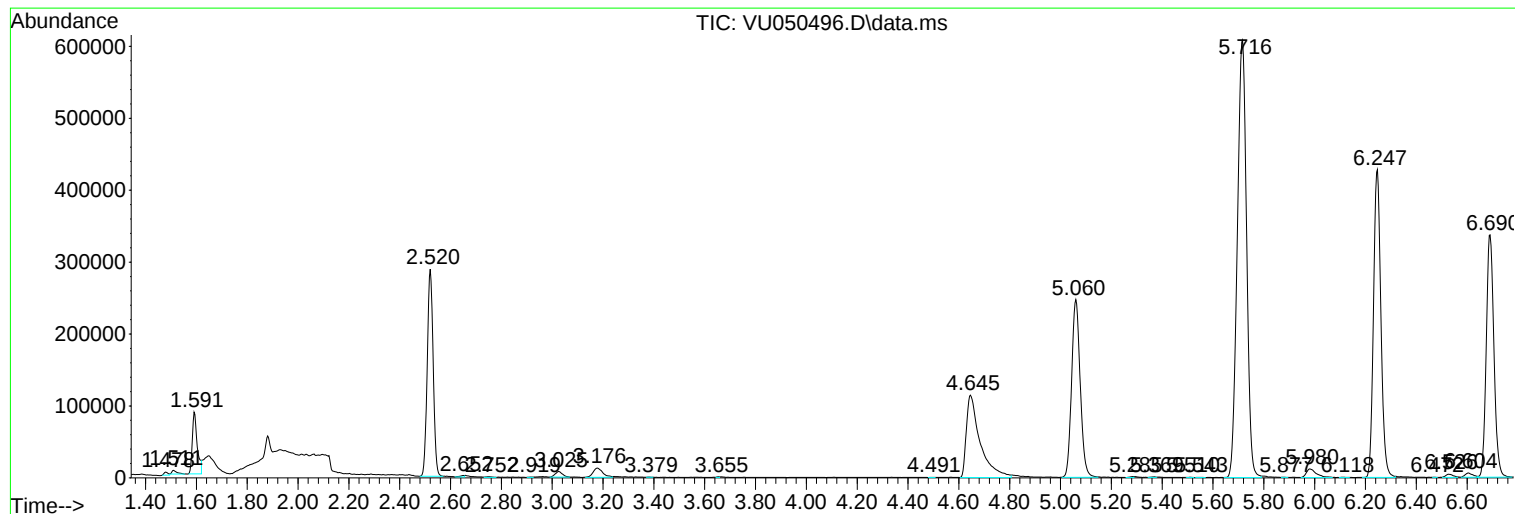
Sum of corrected areas: 12100281

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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

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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Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

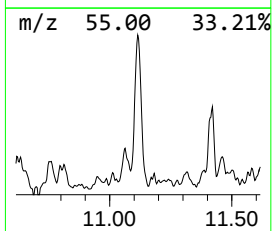
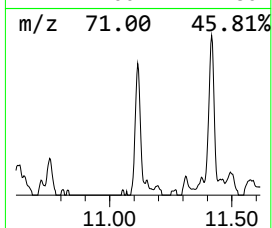
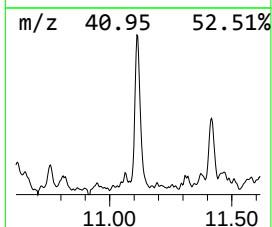
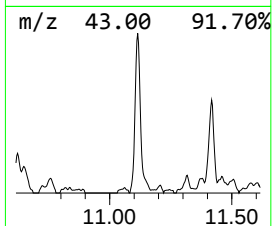
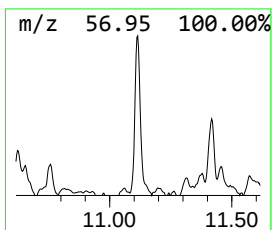
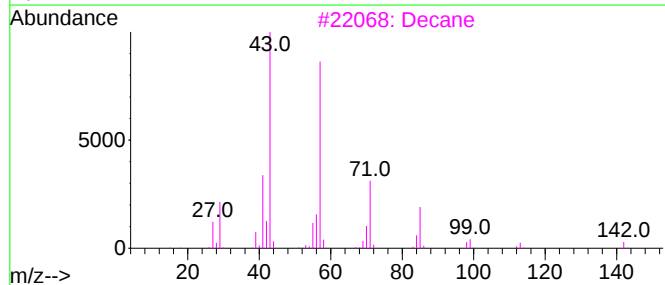
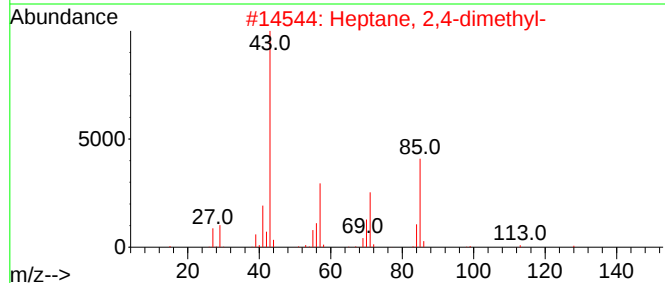
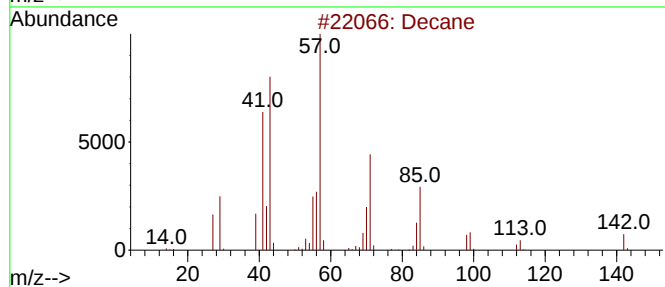
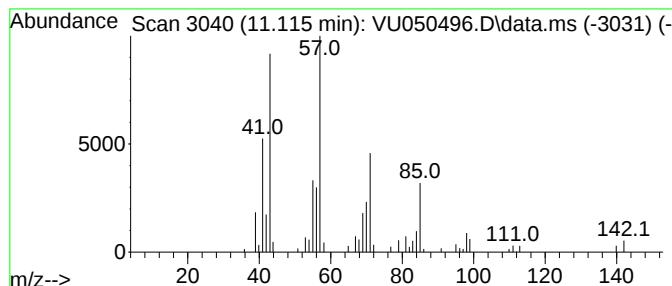
Instrument :
MSVOA_U
ClientSampleId :
EY165ME

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 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.115	4.28 ug/L	74184	1,4-Dichlorobenzene-d4			11.816
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decane		142	C10H22	000124-18-5	94
2	Heptane, 2,4-dimethyl-		128	C9H20	002213-23-2	64
3	Decane		142	C10H22	000124-18-5	64
4	Octane		114	C8H18	000111-65-9	64
5	Sulfurous acid, hexyl octyl ester		278	C14H30O3S	1000309-13-0	53



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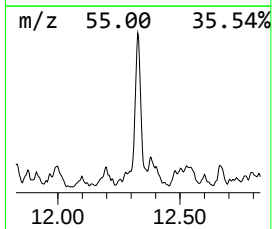
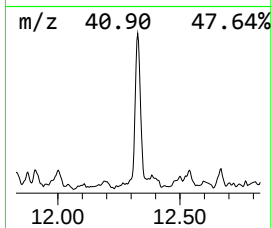
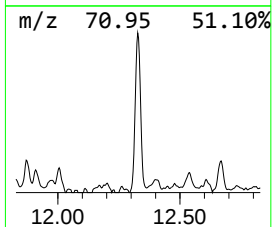
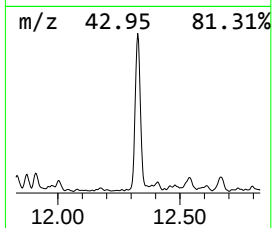
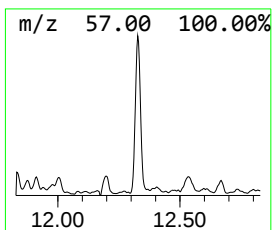
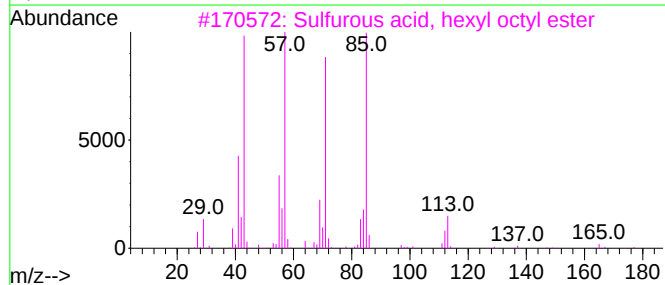
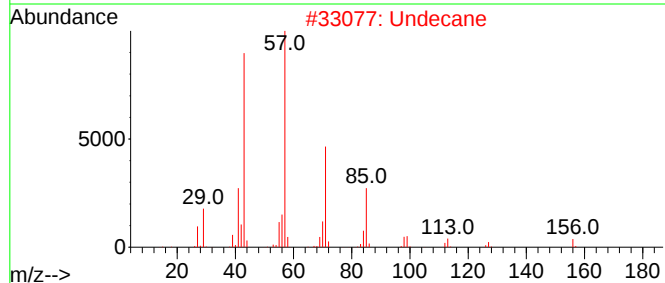
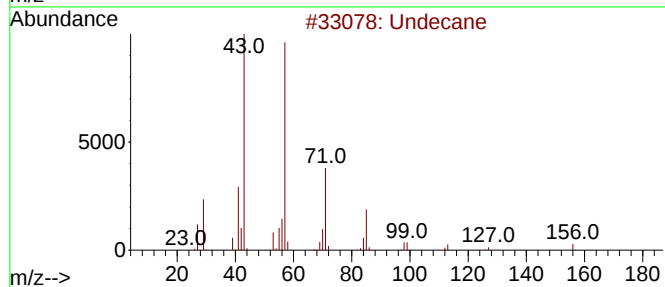
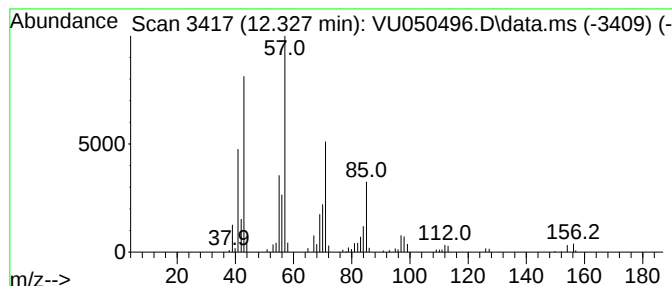
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	6.72 ug/L	116264	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	72
2			Undecane	156	C11H24	001120-21-4	72
3			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	53
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53
5			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	50



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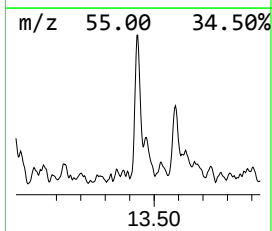
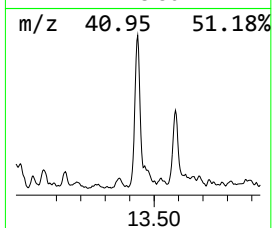
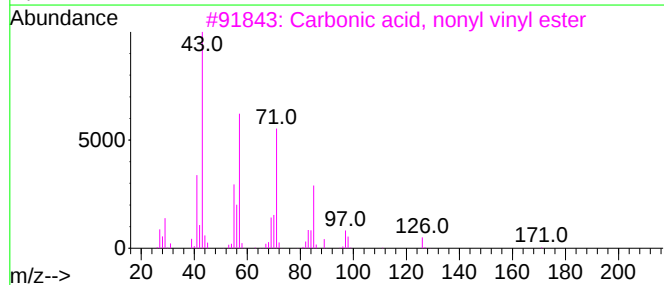
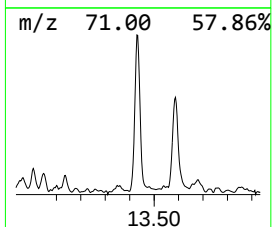
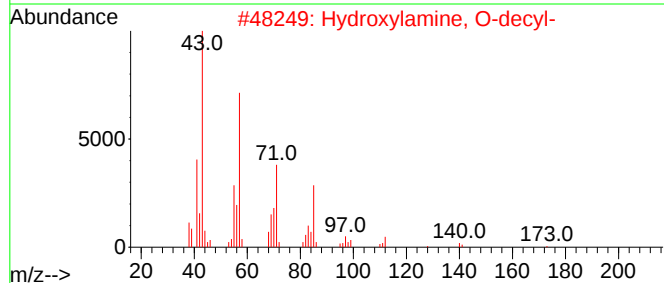
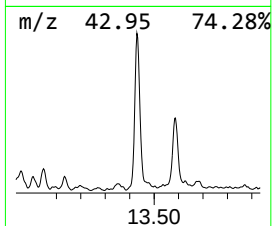
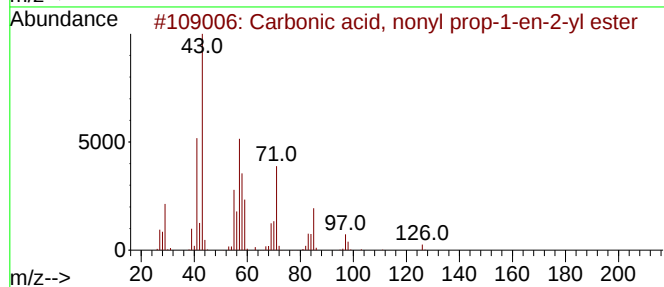
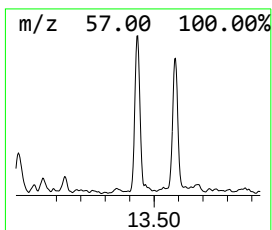
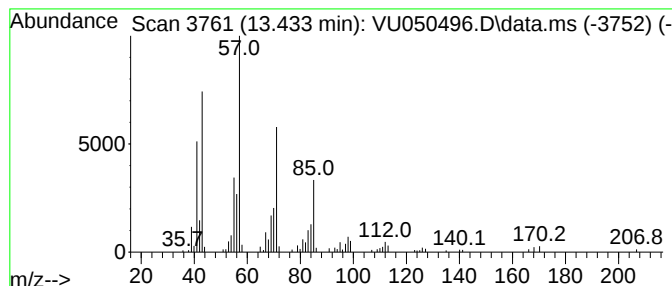
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Quant Title : VOC Analysis

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

Peak Number 4 Carbonic acid, nonyl prop-1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	6.87 ug/L	118865	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	80
2			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	72
3			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	64
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	59
5			Tetradecane	198	C14H30	000629-59-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050496.D
Acq On : 29 Aug 2022 19:55
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

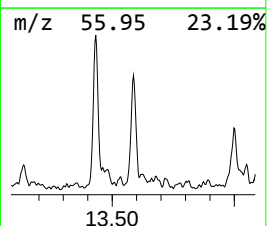
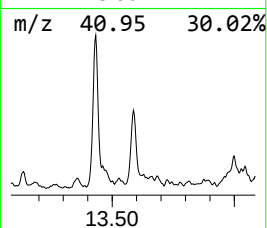
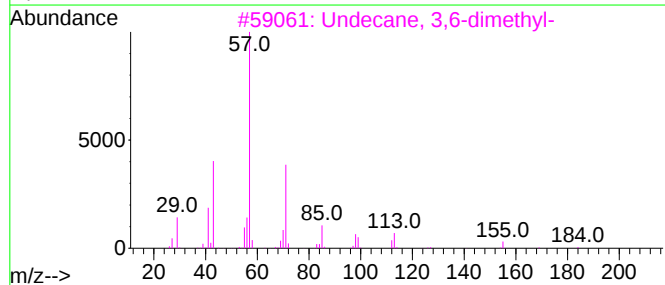
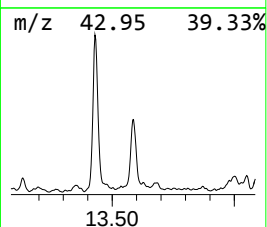
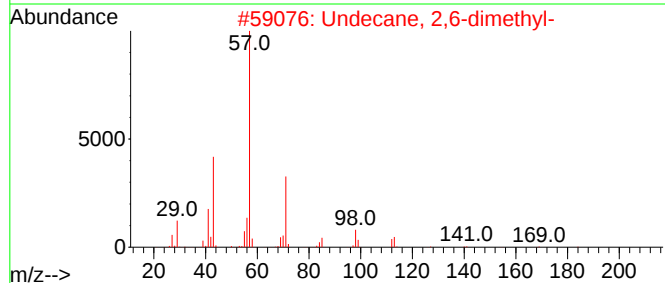
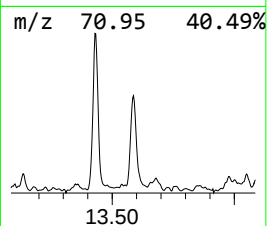
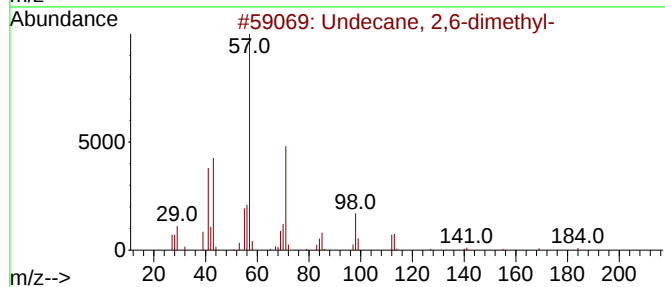
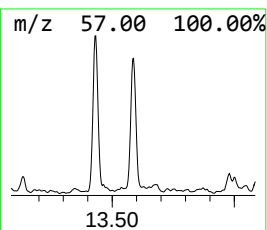
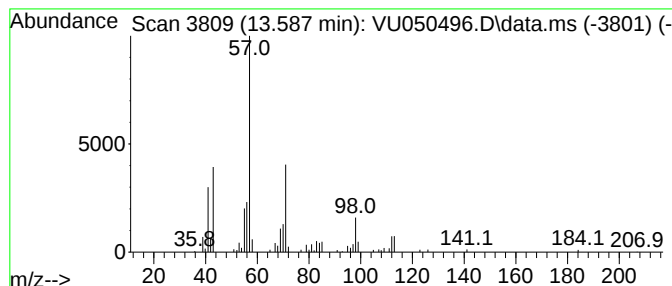
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	3.83 ug/L	66327	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	81
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	80
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	72
4	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
5	Dodecane, 6-methyl-	184	C13H28	006044-71-9	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050496.D
Acq On : 29 Aug 2022 19:55
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

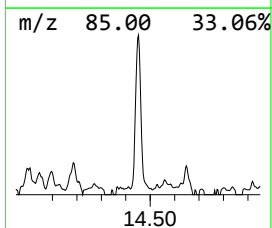
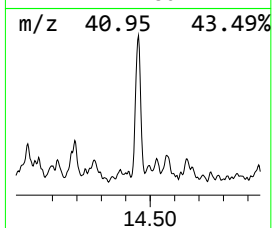
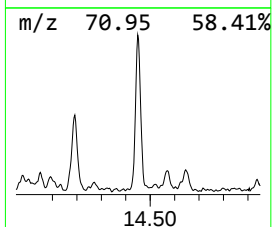
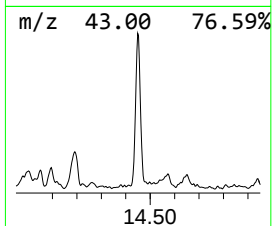
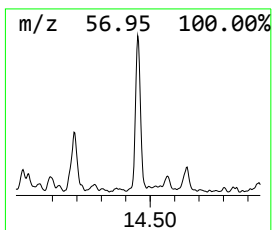
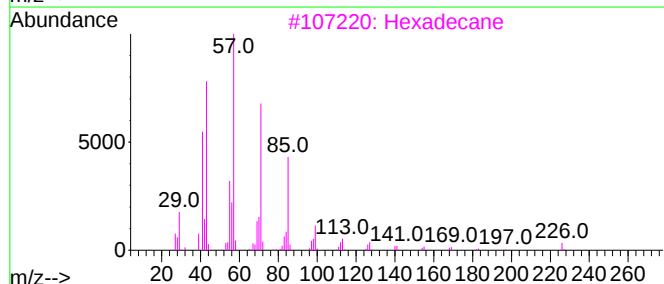
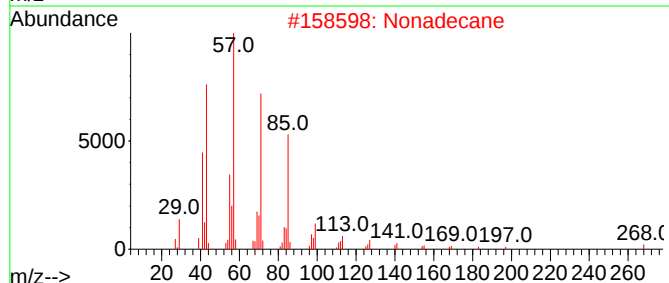
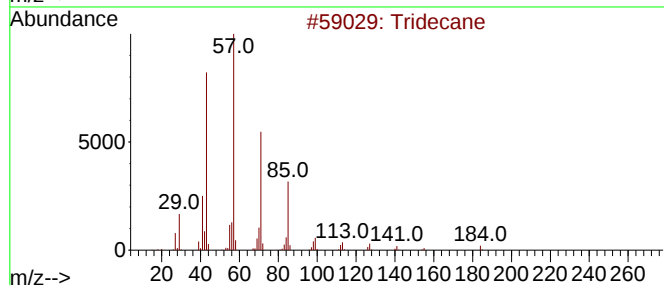
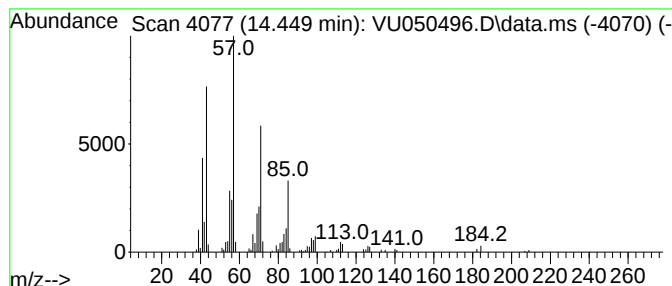
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.449	4.75 ug/L	82285	1,4-Dichlorobenzene-d4	11.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	87
2		Nonadecane	268	C19H40	000629-92-5	86
3		Hexadecane	226	C16H34	000544-76-3	86
4		Tetradecane	198	C14H30	000629-59-4	86
5		Undecane	156	C11H24	001120-21-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050496.D
Acq On : 29 Aug 2022 19:55
Operator : SY/MD
Sample : N4322-05ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY165ME

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
(DEL) Alkane: S...	11.115	4.3	ug/L	74184	3	11.816	865688	50.0
(DEL) Alkane: S...	12.327	6.7	ug/L	116264	3	11.816	865688	50.0
Carbonic acid, ...	13.433	6.9	ug/L	118865	3	11.816	865688	50.0
(DEL) Alkane: S...	13.587	3.8	ug/L	66327	3	11.816	865688	50.0
(DEL) Alkane: S...	14.449	4.8	ug/L	82285	3	11.816	865688	50.0