

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
 Data File : VU050470.D
 Acq On : 26 Aug 2022 20:23
 Operator : SY/MD
 Sample : N4322-08ME
 Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY168ME

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: VU050470.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	37	43	47	rBV2	4914	6083	0.56%	0.059%
2	1.510	49	53	69	rVB	4558	7810	0.72%	0.076%
3	1.591	72	78	87	rBV	52477	70391	6.51%	0.684%
4	2.520	355	367	384	rVB	158503	261491	24.17%	2.540%
5	2.887	476	481	486	rBV2	372	325	0.03%	0.003%
6	2.951	498	501	502	rBV	674	359	0.03%	0.003%
7	3.025	513	524	542	rVB3	11079	22832	2.11%	0.222%
8	3.179	553	572	589	rBV	23411	61668	5.70%	0.599%
9	3.327	611	618	629	rVB4	2611	4515	0.42%	0.044%
10	3.658	713	721	722	rBV3	1013	925	0.09%	0.009%
11	3.986	821	823	831	rVB2	240	247	0.02%	0.002%
12	4.337	926	932	936	rBV2	224	234	0.02%	0.002%
13	4.385	943	947	956	rVB2	326	470	0.04%	0.005%
14	4.645	1014	1028	1075	rBV	155670	560341	51.79%	5.442%
15	4.941	1117	1120	1128	rBV3	193	248	0.02%	0.002%
16	5.060	1140	1157	1189	rBV	211036	494707	45.72%	4.805%
17	5.182	1193	1195	1201	rVB3	625	474	0.04%	0.005%
18	5.250	1211	1216	1220	rBV	768	720	0.07%	0.007%
19	5.288	1220	1228	1230	rBV	1060	1214	0.11%	0.012%
20	5.366	1244	1252	1255	rBV5	603	806	0.07%	0.008%
21	5.713	1341	1360	1383	rBV2	416727	1080298	99.85%	10.492%
22	5.902	1414	1419	1420	rBV2	309	258	0.02%	0.003%
23	5.983	1431	1444	1468	rBV4	11167	30124	2.78%	0.293%
24	6.111	1480	1484	1489	rBV2	442	501	0.05%	0.005%
25	6.247	1511	1526	1551	rBV	431230	868159	80.24%	8.432%
26	6.481	1596	1599	1603	rVV2	357	290	0.03%	0.003%
27	6.533	1603	1615	1628	rVV6	10380	21134	1.95%	0.205%
28	6.603	1628	1637	1649	rVV3	6165	12823	1.19%	0.125%
29	6.690	1650	1664	1688	rVB	266545	552808	51.09%	5.369%
30	7.041	1767	1773	1776	rVV2	343	311	0.03%	0.003%
31	7.185	1814	1818	1819	rBV	526	341	0.03%	0.003%
32	7.227	1819	1831	1846	rVV7	5230	13947	1.29%	0.135%
33	7.311	1850	1857	1864	rVV5	916	1512	0.14%	0.015%
34	7.497	1908	1915	1918	rBV4	898	1044	0.10%	0.010%
35	7.568	1924	1937	1959	rBV	106033	206520	19.09%	2.006%
36	7.706	1976	1980	1986	rBV3	362	450	0.04%	0.004%

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 Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY168ME

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

37	7.748	1989	1993	1996	rVB	278	238	0.02%	0.002%
38	7.790	2001	2006	2007	rBV2	487	374	0.03%	0.004%
39	7.896	2026	2039	2057	rBV	320641	585969	54.16%	5.691%
40	7.999	2060	2071	2081	rVB4	6443	14588	1.35%	0.142%
41	8.063	2088	2091	2096	rVB5	539	584	0.05%	0.006%
42	8.082	2096	2097	2103	rVB3	354	277	0.03%	0.003%
43	8.182	2116	2128	2147	rBV2	69012	139458	12.89%	1.354%
44	8.343	2175	2178	2180	rBV2	668	454	0.04%	0.004%
45	8.465	2213	2216	2218	rBV2	385	283	0.03%	0.003%
46	8.552	2234	2243	2253	rVB2	15512	26093	2.41%	0.253%
47	8.661	2258	2277	2307	rBV2	418817	1072402	99.12%	10.415%
48	8.841	2331	2333	2338	rVB4	650	448	0.04%	0.004%
49	8.922	2350	2358	2366	rBV7	3007	4633	0.43%	0.045%
50	8.973	2371	2374	2376	rBV2	641	420	0.04%	0.004%
51	9.098	2410	2413	2415	rBV	510	268	0.02%	0.003%
52	9.115	2416	2418	2419	rVV2	540	239	0.02%	0.002%
53	9.124	2419	2421	2425	rVB3	817	452	0.04%	0.004%
54	9.169	2427	2435	2439	rVV5	1265	1573	0.15%	0.015%
55	9.211	2441	2448	2456	rVB5	2403	3428	0.32%	0.033%
56	9.330	2478	2485	2494	rVB4	2049	3002	0.28%	0.029%
57	9.420	2500	2513	2545	rBV	583930	1081931	100.00%	10.508%
58	9.658	2584	2587	2591	rVB4	634	543	0.05%	0.005%
59	9.690	2591	2597	2599	rBV2	754	839	0.08%	0.008%
60	9.706	2599	2602	2607	rVV3	1066	971	0.09%	0.009%
61	9.745	2607	2614	2622	rVB5	3699	5535	0.51%	0.054%
62	10.025	2692	2701	2704	rBV2	1006	1342	0.12%	0.013%
63	10.105	2722	2726	2727	rBV2	328	229	0.02%	0.002%
64	10.118	2727	2730	2733	rBV3	823	632	0.06%	0.006%
65	10.166	2742	2745	2751	rVB4	431	431	0.04%	0.004%
66	10.250	2761	2771	2780	rBV5	3999	6436	0.59%	0.063%
67	10.317	2790	2792	2795	rVV2	481	276	0.03%	0.003%
68	10.356	2796	2804	2807	rVV5	1271	1843	0.17%	0.018%
69	10.394	2807	2816	2828	rVB4	4388	8118	0.75%	0.079%
70	10.452	2829	2834	2836	rBV3	551	460	0.04%	0.004%
71	10.558	2856	2867	2873	rBV8	2465	4246	0.39%	0.041%
72	10.626	2882	2888	2893	rBV4	2938	3773	0.35%	0.037%
73	10.764	2912	2931	2960	rBV	591135	988926	91.40%	9.604%
74	10.860	2960	2961	2964	rVV3	496	268	0.02%	0.003%
75	10.883	2965	2968	2971	rVB2	471	293	0.03%	0.003%
76	10.947	2982	2988	2991	rBV4	651	836	0.08%	0.008%

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 Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY168ME

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

77	10.976	2995	2997	3002	rVB4	641	563	0.05%	0.005%
78	11.066	3019	3025	3031	rVB7	1747	2252	0.21%	0.022%
79	11.115	3031	3040	3053	rVB3	16166	25374	2.35%	0.246%
80	11.188	3060	3063	3065	rBV2	939	663	0.06%	0.006%
81	11.243	3076	3080	3081	rBV	530	348	0.03%	0.003%
82	11.314	3094	3102	3114	rVV8	2605	4638	0.43%	0.045%
83	11.375	3114	3121	3126	rBV6	2617	3788	0.35%	0.037%
84	11.417	3126	3134	3142	rVB3	12599	17508	1.62%	0.170%
85	11.455	3143	3146	3149	rBV5	1116	1110	0.10%	0.011%
86	11.578	3176	3184	3187	rBV5	1386	2050	0.19%	0.020%
87	11.616	3193	3196	3198	rBV4	849	650	0.06%	0.006%
88	11.815	3246	3258	3272	rBV	538580	857552	79.26%	8.329%
89	12.089	3339	3343	3351	rBV9	1447	1905	0.18%	0.019%
90	12.198	3365	3377	3395	rBV	477157	788507	72.88%	7.658%
91	12.327	3409	3417	3428	rVB2	38056	53809	4.97%	0.523%
92	12.494	3461	3469	3472	rBV7	2079	3287	0.30%	0.032%
93	12.667	3514	3523	3530	rBV8	6385	10182	0.94%	0.099%
94	12.954	3592	3612	3622	rBV8	9655	31900	2.95%	0.310%
95	13.005	3623	3628	3634	rBV7	4118	5176	0.48%	0.050%
96	13.433	3752	3761	3769	rBV2	51535	75422	6.97%	0.732%
97	13.587	3802	3809	3820	rBV	29719	45314	4.19%	0.440%
98	14.452	4070	4078	4087	rBV2	44870	63336	5.85%	0.615%
99	15.401	4369	4373	4382	rVB2	22621	26838	2.48%	0.261%
100	16.294	4645	4651	4664	rVB3	16929	24898	2.30%	0.242%

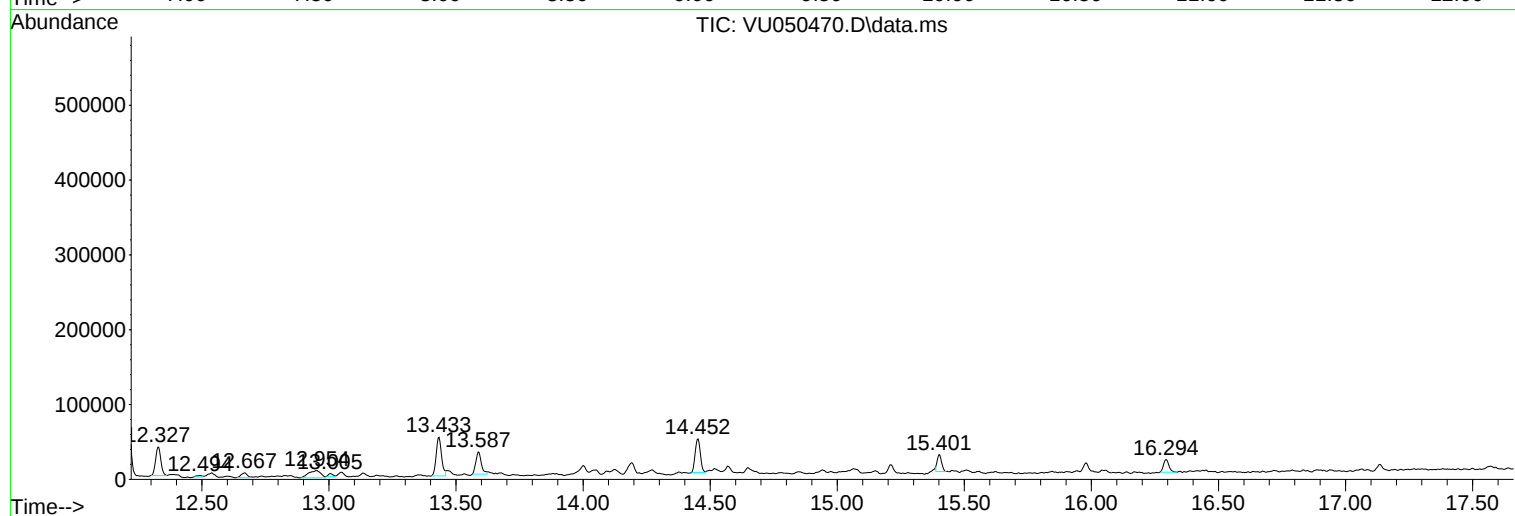
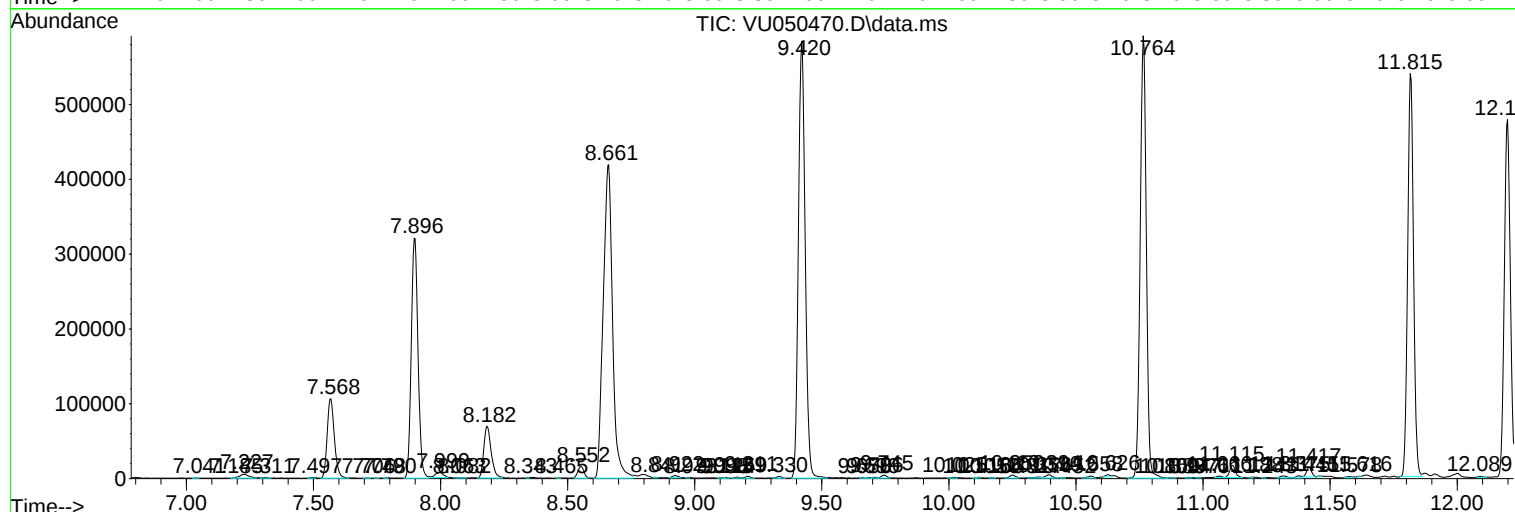
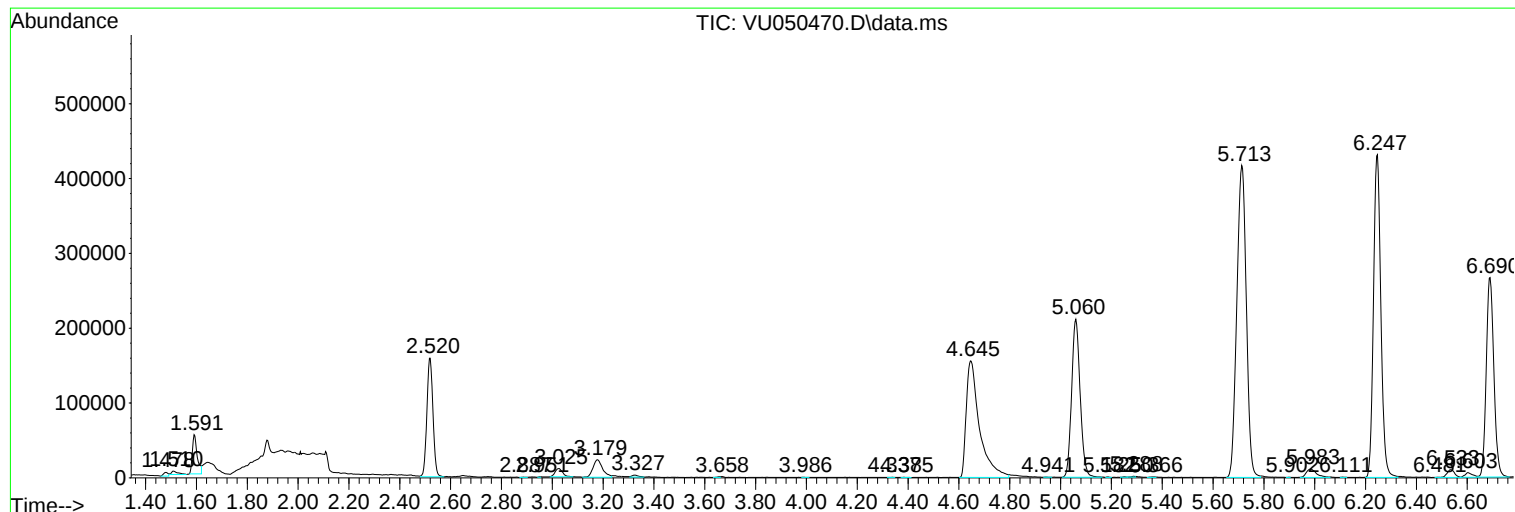
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050470.D
Acq On : 26 Aug 2022 20:23
Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050470.D
Acq On : 26 Aug 2022 20:23
Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

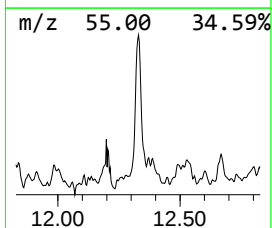
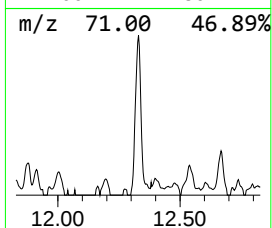
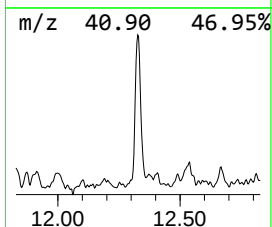
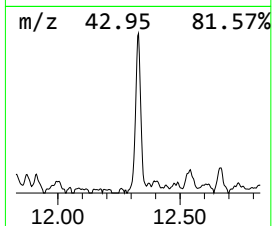
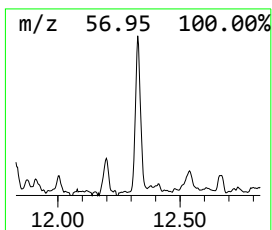
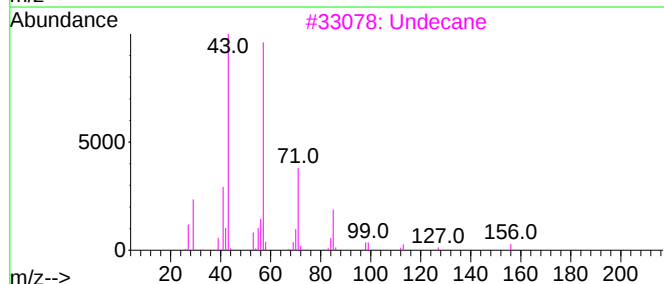
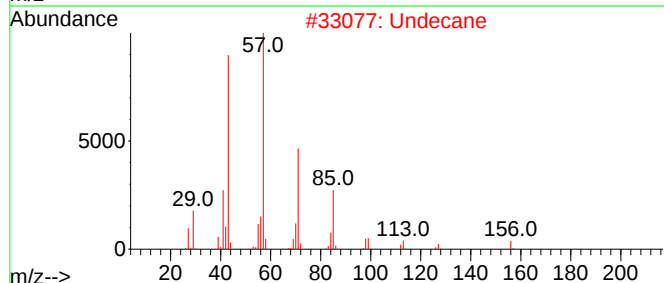
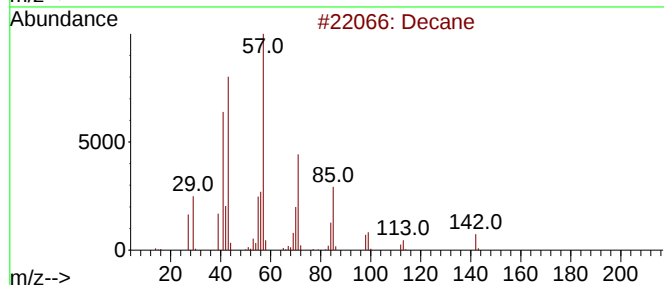
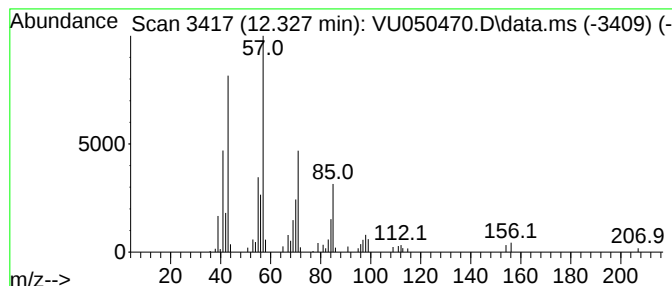
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	3.14 ug/L	53809	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	86
2			Undecane	156	C11H24	001120-21-4	72
3			Undecane	156	C11H24	001120-21-4	64
4			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
5			Undecane, 3-methyl-	170	C12H26	001002-43-3	59



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Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

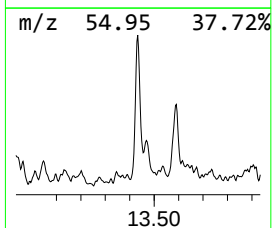
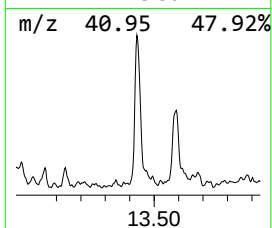
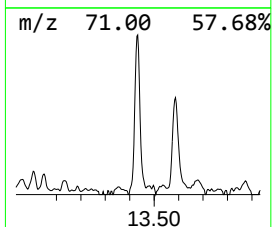
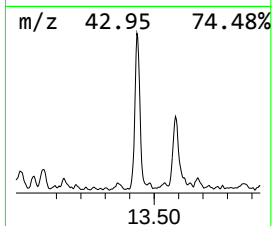
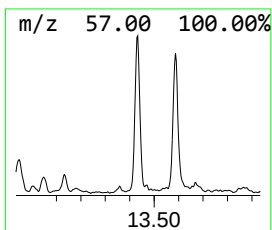
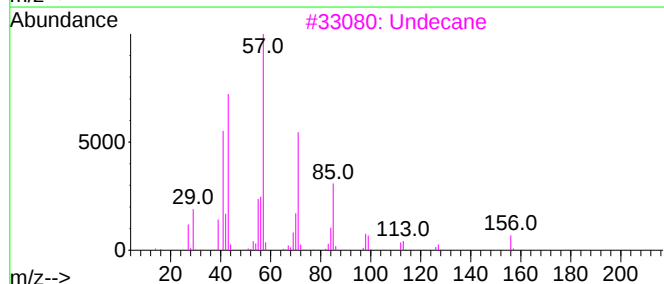
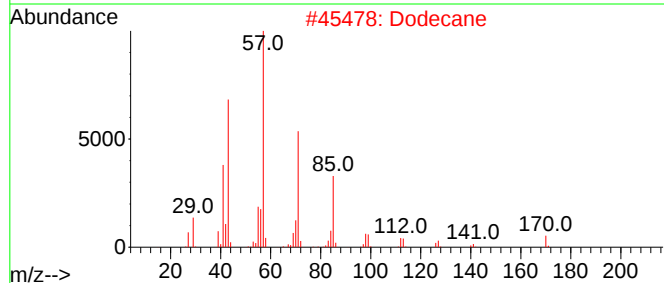
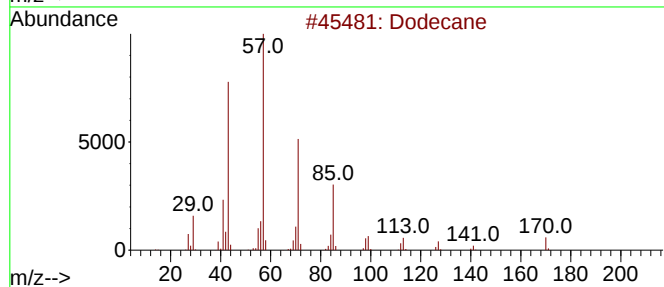
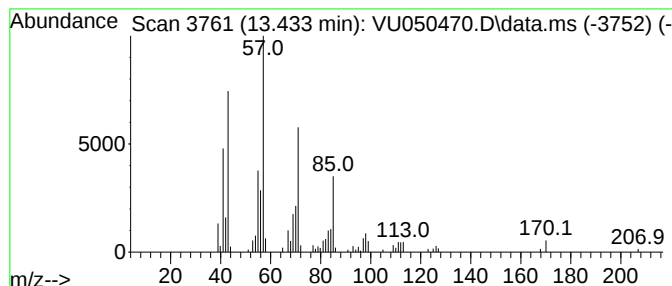
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	4.40 ug/L	75422	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	81
2			Dodecane	170	C12H26	000112-40-3	81
3			Undecane	156	C11H24	001120-21-4	78
4			Dodecane	170	C12H26	000112-40-3	76
5			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	72



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Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

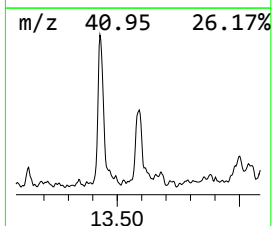
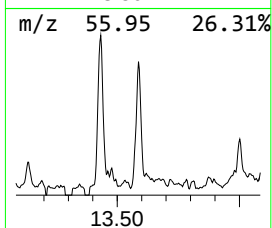
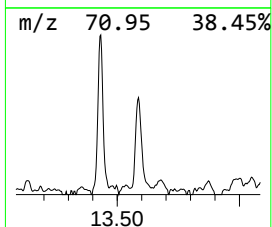
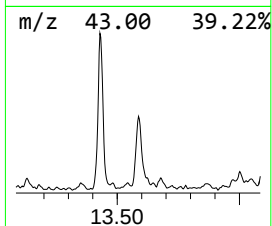
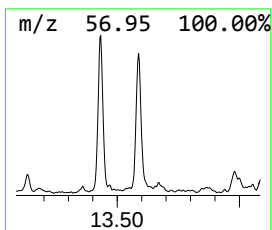
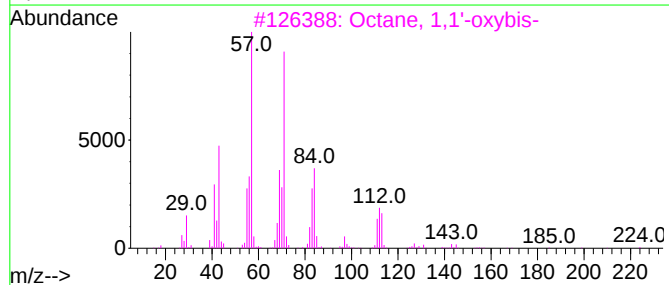
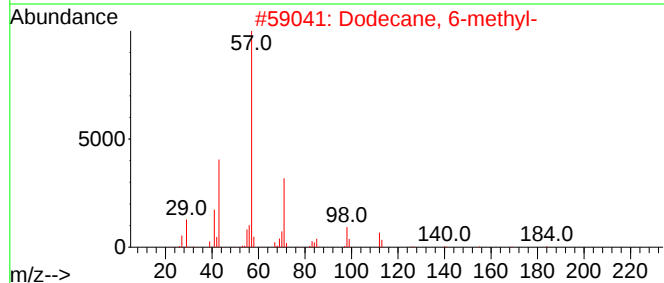
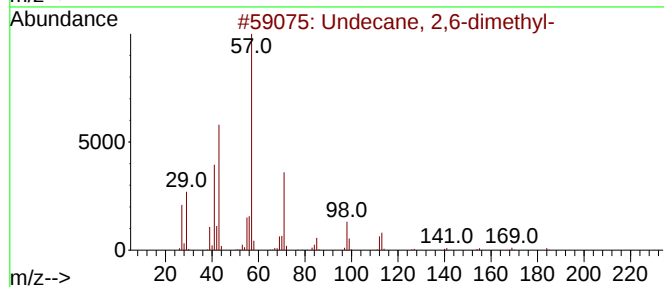
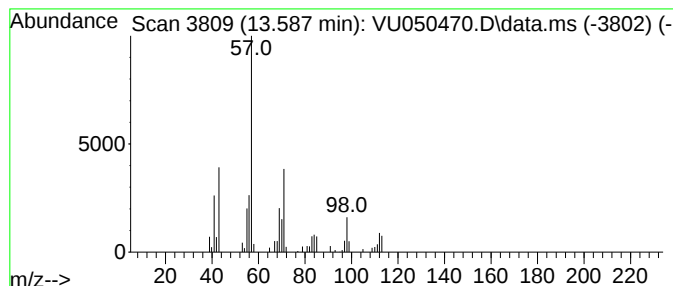
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Quant Title : VOC Analysis

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	2.64 ug/L	45314	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
2			Dodecane, 6-methyl-	184	C13H28	006044-71-9	64
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
4			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	59
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050470.D
Acq On : 26 Aug 2022 20:23
Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

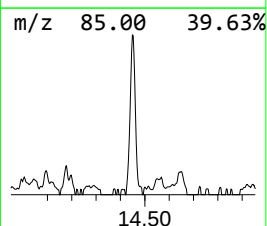
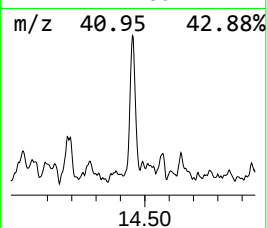
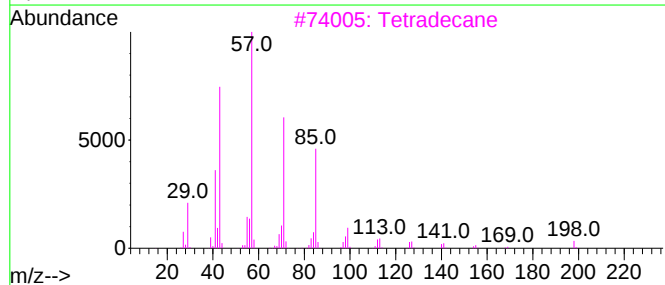
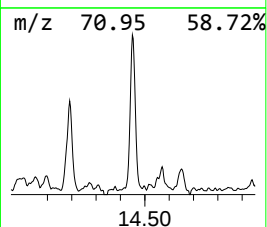
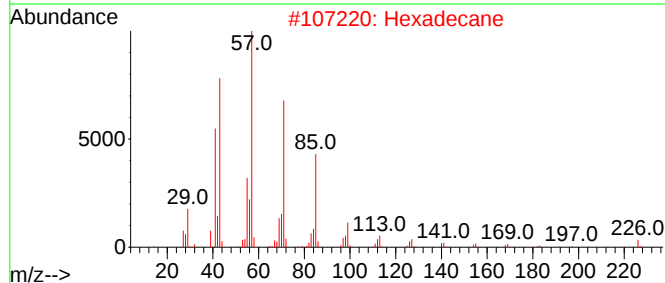
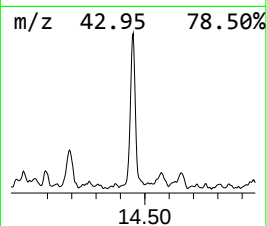
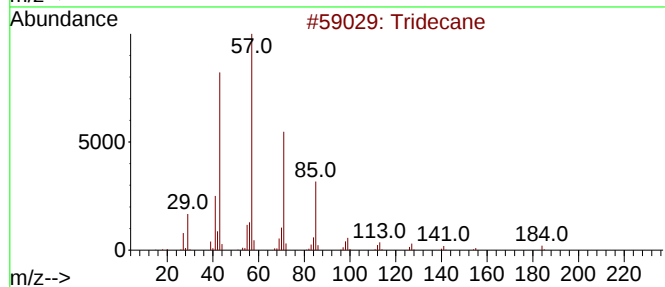
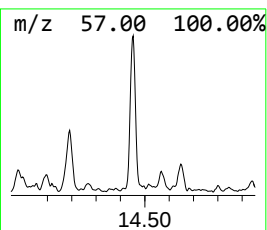
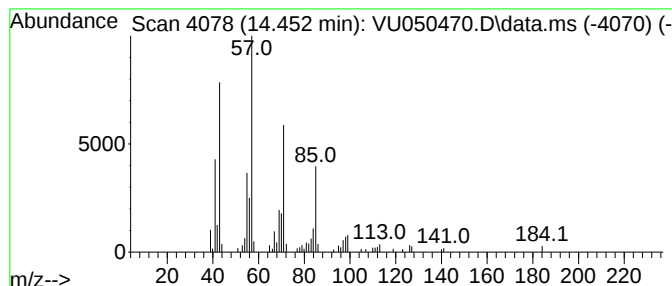
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.452	3.69 ug/L	63336	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	90
2			Hexadecane	226	C16H34	000544-76-3	90
3			Tetradecane	198	C14H30	000629-59-4	80
4			Tridecane	184	C13H28	000629-50-5	80
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
Data File : VU050470.D
Acq On : 26 Aug 2022 20:23
Operator : SY/MD
Sample : N4322-08ME
Misc : 4.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY168ME

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...	12.327	3.1	ug/L	53809	3	11.819	857552	50.0
(DEL) Alkane: S...	13.433	4.4	ug/L	75422	3	11.819	857552	50.0
(DEL) Alkane: S...	13.587	2.6	ug/L	45314	3	11.819	857552	50.0
(DEL) Alkane: S...	14.452	3.7	ug/L	63336	3	11.819	857552	50.0