

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050501.D
 Acq On : 29 Aug 2022 22:17
 Operator : SY/MD
 Sample : N4322-11ME
 Misc : 3.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY171ME

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: VU050501.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	3673	3946	0.11%	0.016%
2	1.510	49	53	65	rVV2	4255	6752	0.18%	0.028%
3	1.591	71	78	87	rBV	202428	282079	7.55%	1.167%
4	1.880	163	168	177	rBV	77325	102728	2.75%	0.425%
5	2.526	355	369	397	rBV	708195	1157754	30.99%	4.791%
6	2.748	432	438	439	rBV3	1285	1221	0.03%	0.005%
7	2.899	481	485	487	rBV2	377	292	0.01%	0.001%
8	3.028	515	525	540	rVB2	8371	16066	0.43%	0.066%
9	3.176	558	571	586	rBV	10684	26903	0.72%	0.111%
10	3.321	614	616	621	rBV4	536	445	0.01%	0.002%
11	3.468	659	662	666	rVV2	420	296	0.01%	0.001%
12	3.559	687	690	695	rVB2	228	255	0.01%	0.001%
13	3.616	702	708	711	rBV2	273	252	0.01%	0.001%
14	3.661	715	722	724	rBV4	1256	1373	0.04%	0.006%
15	3.845	775	779	781	rBV2	331	279	0.01%	0.001%
16	3.874	786	788	792	rVB2	373	236	0.01%	0.001%
17	3.996	821	826	828	rVB2	269	204	0.01%	0.001%
18	4.102	850	859	861	rVV2	271	329	0.01%	0.001%
19	4.128	865	867	872	rVB2	339	249	0.01%	0.001%
20	4.153	872	875	878	rBV	266	196	0.01%	0.001%
21	4.227	893	898	902	rVB	237	211	0.01%	0.001%
22	4.263	902	909	911	rBV	199	222	0.01%	0.001%
23	4.282	911	915	919	rVB2	278	236	0.01%	0.001%
24	4.639	1009	1026	1098	rBV	295081	1056397	28.28%	4.372%
25	4.967	1126	1128	1136	rVB2	556	522	0.01%	0.002%
26	5.060	1138	1157	1182	rBV	615561	1424654	38.14%	5.896%
27	5.285	1222	1227	1230	rBV5	819	973	0.03%	0.004%
28	5.372	1243	1254	1264	rBV8	1840	3528	0.09%	0.015%
29	5.459	1275	1281	1286	rBV3	312	448	0.01%	0.002%
30	5.491	1286	1291	1293	rBV2	340	314	0.01%	0.001%
31	5.578	1310	1318	1320	rBV4	728	668	0.02%	0.003%
32	5.716	1337	1361	1395	rBV2	1470872	3735383	100.00%	15.458%
33	5.983	1433	1444	1466	rBV4	11938	29511	0.79%	0.122%
34	6.079	1471	1474	1476	rVB3	496	244	0.01%	0.001%
35	6.118	1478	1486	1498	rVB8	2203	4461	0.12%	0.018%
36	6.163	1498	1500	1502	rBV	421	207	0.01%	0.001%

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Instrument :
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 ClientSampleId :
 EY171ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Sampling : 1

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Peak Location: TOP

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

37	6.246	1511	1526	1551	rBV	437373	867472	23.22%	3.590%
38	6.455	1589	1591	1596	rVB	421	360	0.01%	0.001%
39	6.529	1601	1614	1627	rBV9	7038	15521	0.42%	0.064%
40	6.603	1627	1637	1648	rBV4	5683	11584	0.31%	0.048%
41	6.690	1648	1664	1691	rBV	830976	1705529	45.66%	7.058%
42	6.925	1735	1737	1742	rVB2	506	312	0.01%	0.001%
43	6.973	1748	1752	1755	rBV2	471	456	0.01%	0.002%
44	7.034	1769	1771	1775	rVB3	304	234	0.01%	0.001%
45	7.060	1775	1779	1781	rBV2	908	790	0.02%	0.003%
46	7.224	1812	1830	1845	rBV2	6913	20086	0.54%	0.083%
47	7.304	1851	1855	1858	rBV5	569	502	0.01%	0.002%
48	7.324	1858	1861	1864	rVV3	821	520	0.01%	0.002%
49	7.420	1887	1891	1899	rVB4	917	985	0.03%	0.004%
50	7.494	1900	1914	1922	rBV4	6561	12479	0.33%	0.052%
51	7.568	1923	1937	1958	rVV	354220	676731	18.12%	2.801%
52	7.787	2000	2005	2006	rBV3	648	510	0.01%	0.002%
53	7.799	2006	2009	2012	rVV4	578	524	0.01%	0.002%
54	7.896	2025	2039	2060	rBV	1606512	2872647	76.90%	11.888%
55	8.127	2103	2111	2117	rBV4	9136	13906	0.37%	0.058%
56	8.182	2117	2128	2154	rVB	228892	462810	12.39%	1.915%
57	8.346	2172	2179	2180	rBV3	987	968	0.03%	0.004%
58	8.410	2193	2199	2202	rBV5	861	892	0.02%	0.004%
59	8.536	2229	2238	2240	rBV6	2841	3387	0.09%	0.014%
60	8.658	2258	2276	2314	rBV2	930129	2362437	63.24%	9.776%
61	8.925	2350	2359	2372	rBV5	9375	17301	0.46%	0.072%
62	9.073	2395	2405	2412	rBV7	3304	5733	0.15%	0.024%
63	9.121	2414	2420	2426	rVV5	2628	3583	0.10%	0.015%
64	9.169	2426	2435	2440	rVV5	4674	8204	0.22%	0.034%
65	9.211	2442	2448	2458	rVB4	8348	13384	0.36%	0.055%
66	9.333	2477	2486	2498	rBV4	8529	14223	0.38%	0.059%
67	9.420	2499	2513	2537	rBV	578273	1084156	29.02%	4.487%
68	9.552	2549	2554	2555	rBV3	995	736	0.02%	0.003%
69	9.661	2574	2588	2595	rBV9	3049	6507	0.17%	0.027%
70	9.745	2606	2614	2628	rVB3	20849	33160	0.89%	0.137%
71	9.870	2646	2653	2662	rBV8	2767	4173	0.11%	0.017%
72	9.954	2677	2679	2681	rBV2	584	368	0.01%	0.002%
73	10.018	2692	2699	2712	rBV9	2983	7043	0.19%	0.029%
74	10.118	2720	2730	2738	rBV10	4237	8760	0.23%	0.036%
75	10.250	2762	2771	2784	rBV4	11149	19727	0.53%	0.082%
76	10.394	2810	2816	2827	rVB4	11123	17989	0.48%	0.074%

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Instrument :
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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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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 Title : VOC Analysis

77	10.558	2854	2867	2874	rBV7	5186	11438	0.31%	0.047%
78	10.623	2882	2887	2893	rBV3	6460	8252	0.22%	0.034%
79	10.696	2907	2910	2913	rBV3	629	362	0.01%	0.001%
80	10.764	2913	2931	2959	rVV	1314533	2199296	58.88%	9.101%
81	10.941	2980	2986	2988	rBV4	2715	2843	0.08%	0.012%
82	11.063	3019	3024	3030	rBV6	3739	5597	0.15%	0.023%
83	11.114	3033	3040	3056	rVB2	44728	73919	1.98%	0.306%
84	11.317	3095	3103	3112	rBB9	3719	5689	0.15%	0.024%
85	11.378	3117	3122	3126	rBV4	2603	2966	0.08%	0.012%
86	11.417	3126	3134	3142	rVV2	24289	34383	0.92%	0.142%
87	11.606	3189	3193	3194	rBV2	2510	1694	0.05%	0.007%
88	11.716	3217	3227	3232	rBV10	5096	8876	0.24%	0.037%
89	11.815	3246	3258	3272	rBV	556094	898225	24.05%	3.717%
90	12.082	3335	3341	3343	rBV4	2317	2723	0.07%	0.011%
91	12.198	3364	3377	3396	rBV	1453827	2389641	63.97%	9.889%
92	12.327	3409	3417	3428	rVB2	73200	105670	2.83%	0.437%
93	12.667	3515	3523	3532	rBV5	9000	13711	0.37%	0.057%
94	12.928	3592	3604	3605	rBV5	12720	17024	0.46%	0.070%
95	13.005	3624	3628	3635	rBV6	4673	5731	0.15%	0.024%
96	13.047	3636	3641	3652	rVB7	9240	13269	0.36%	0.055%
97	13.433	3752	3761	3769	rBV2	62100	94764	2.54%	0.392%
98	13.587	3801	3809	3819	rBV	35867	56109	1.50%	0.232%
99	14.449	4070	4077	4087	rBV	44088	60692	1.62%	0.251%
100	15.976	4548	4552	4565	rVB5	10700	15068	0.40%	0.062%

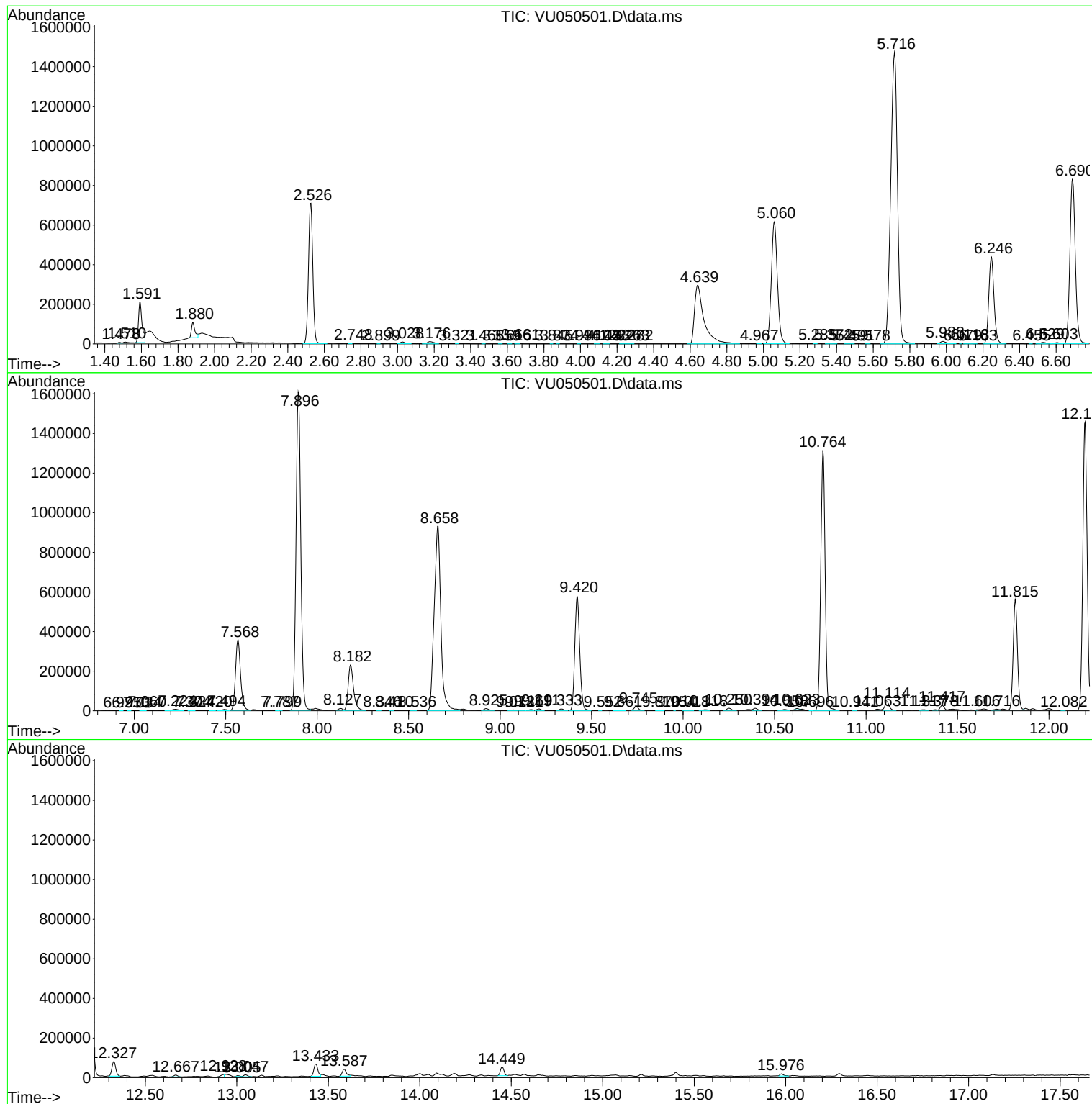
Sum of corrected areas: 24164465

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Instrument :
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ClientSampleId :
EY171ME

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 : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY171ME

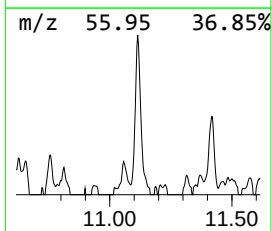
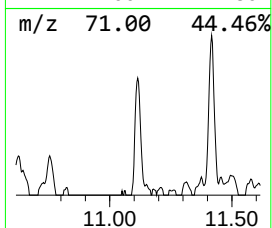
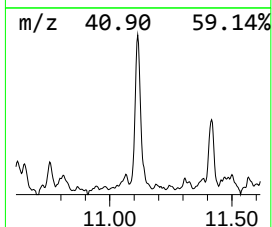
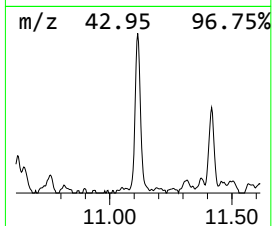
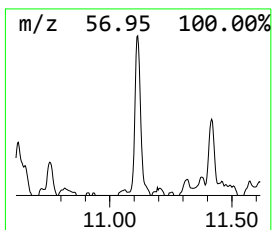
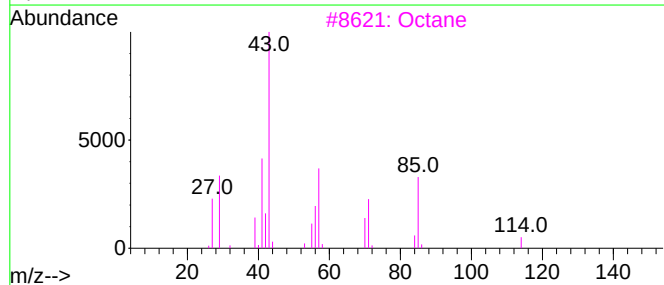
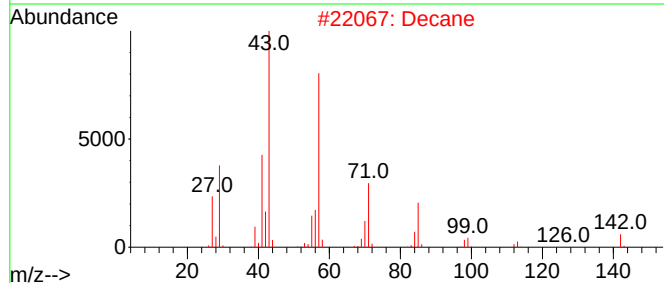
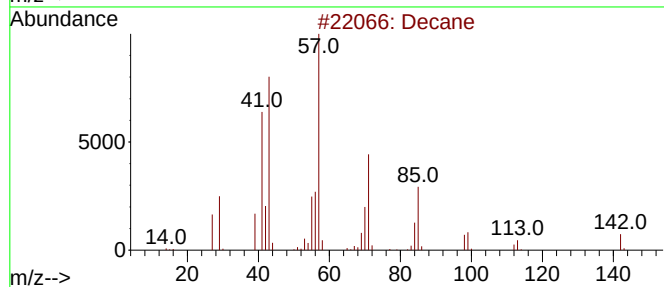
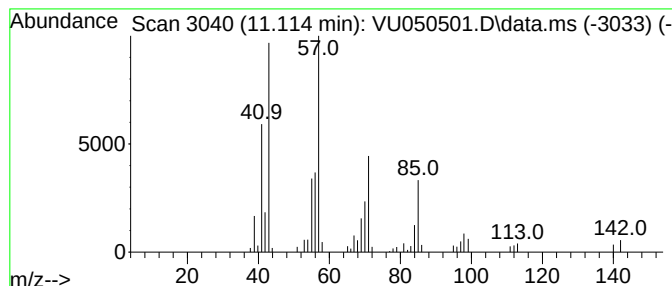
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	4.11 ug/L	73919	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane			142	C10H22	000124-18-5	94
2	Decane			142	C10H22	000124-18-5	91
3	Octane			114	C8H18	000111-65-9	72
4	Decane			142	C10H22	000124-18-5	68
5	Octane			114	C8H18	000111-65-9	64



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Misc : 3.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
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Instrument :
MSVOA_U
ClientSampleId :
EY171ME

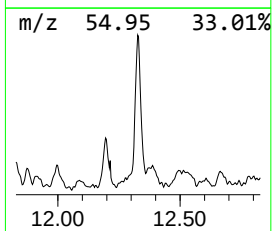
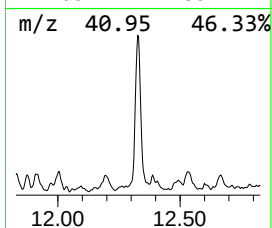
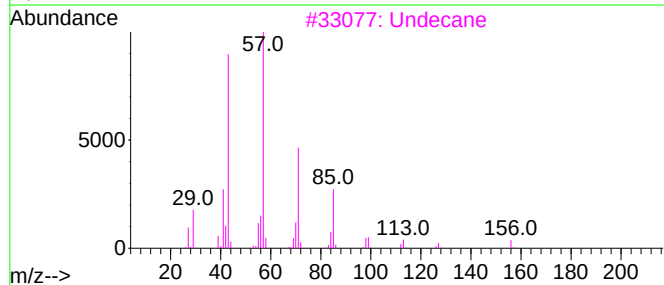
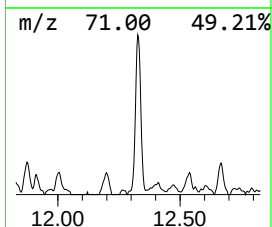
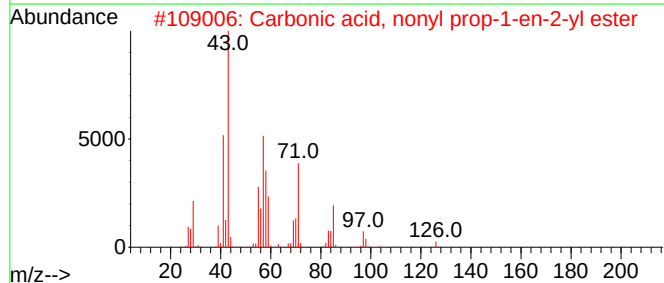
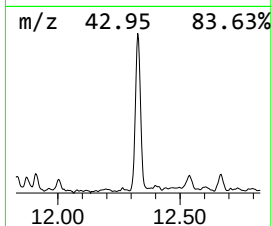
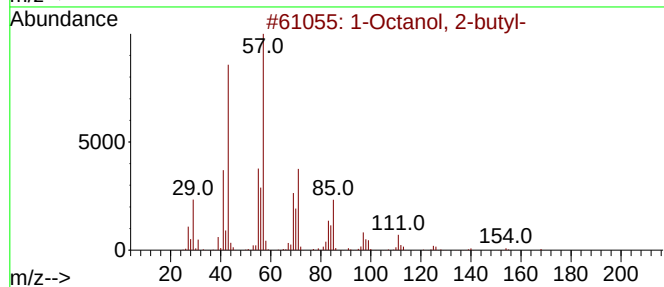
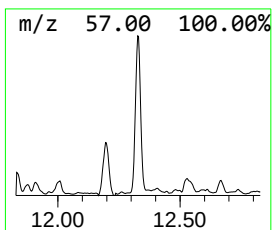
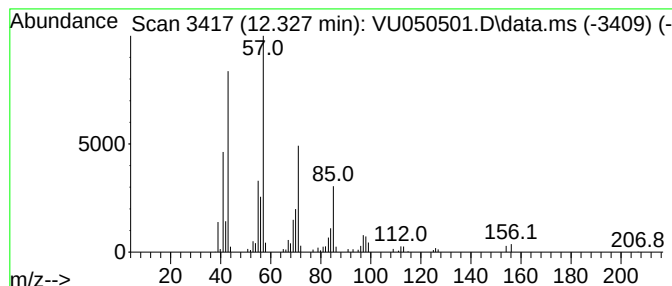
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Octanol, 2-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	5.88 ug/L	105670	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-butyl-			186	C12H26O	003913-02-8	90
2	Carbonic acid, nonyl prop-1-en-2...			228	C13H24O3	1000382-53-9	80
3	Undecane			156	C11H24	001120-21-4	72
4	Octane			114	C8H18	000111-65-9	72
5	Nonane			128	C9H20	000111-84-2	64



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Misc : 3.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY171ME

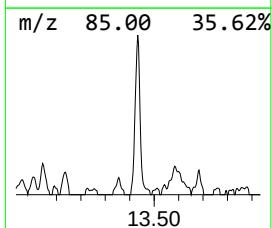
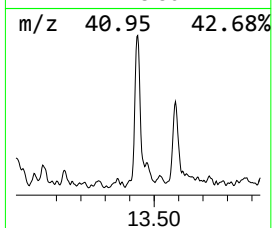
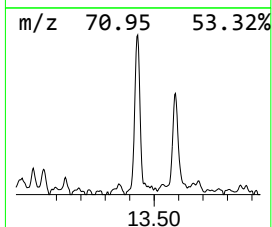
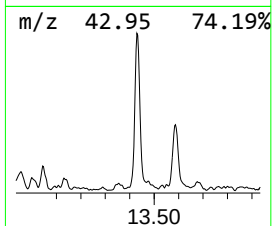
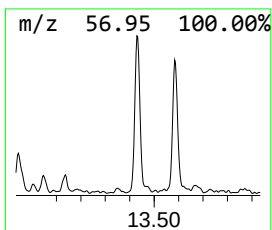
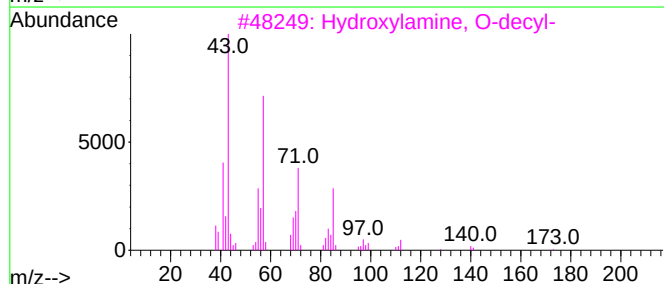
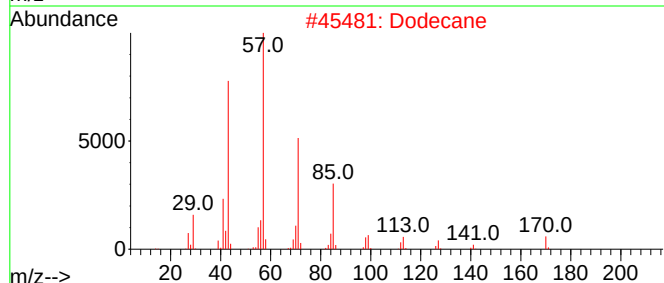
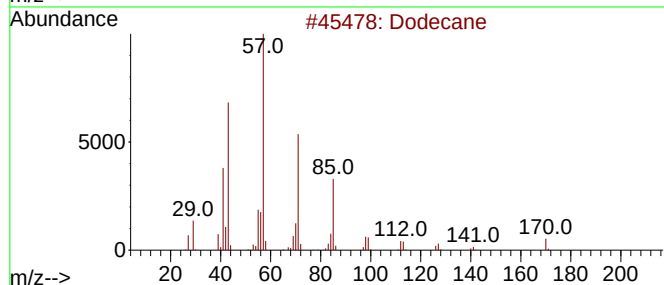
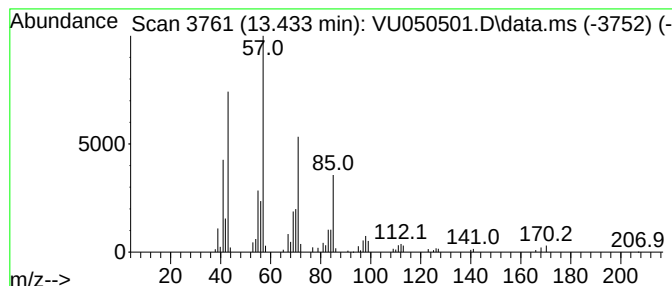
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	5.28 ug/L	94764	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	83
2			Dodecane	170	C12H26	000112-40-3	74
3			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	72
4			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	72
5			Nonadecane	268	C19H40	000629-92-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050501.D
Acq On : 29 Aug 2022 22:17
Operator : SY/MD
Sample : N4322-11ME
Misc : 3.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY171ME

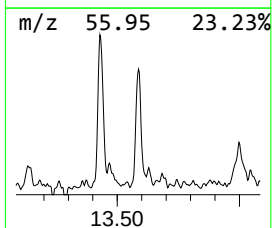
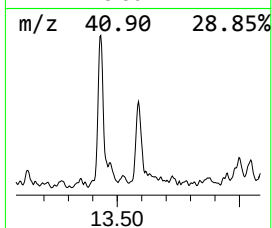
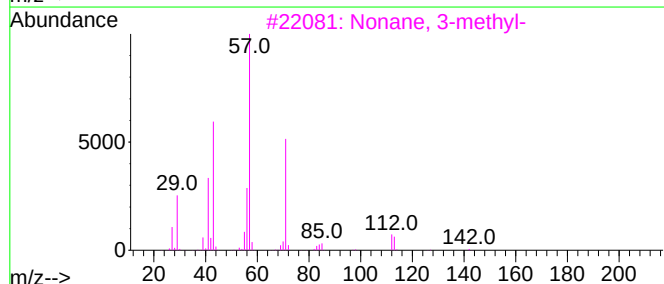
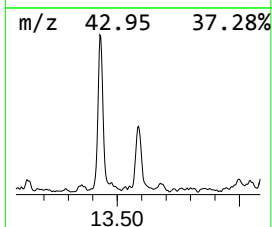
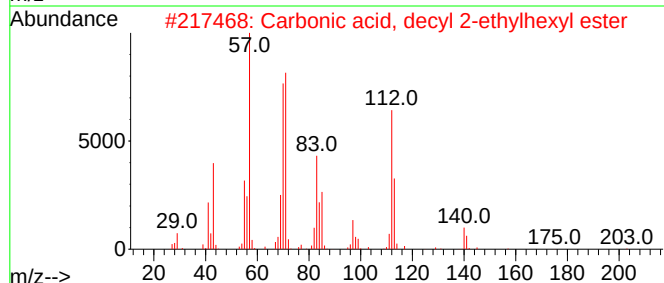
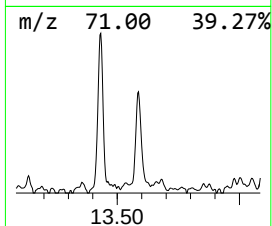
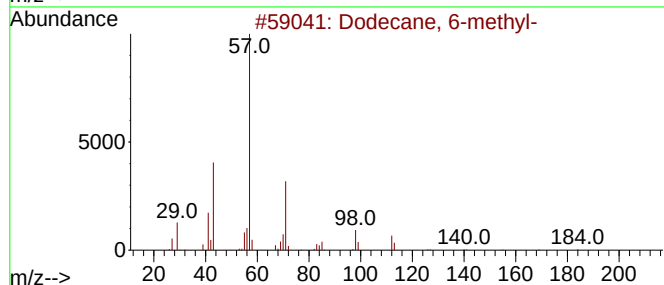
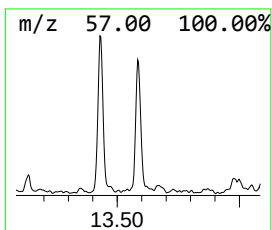
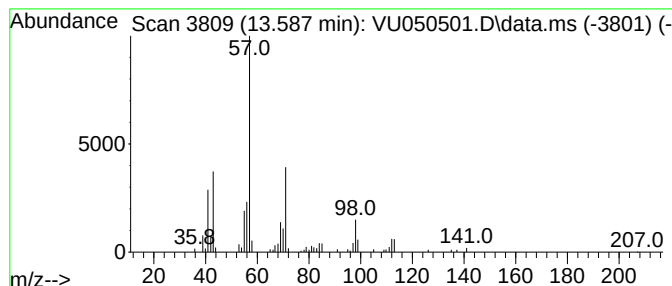
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Quant Title : VOC Analysis

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	3.12 ug/L	56109	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 6-methyl-	184	C13H28	006044-71-9	72
2			Carbonic acid, decyl 2-ethylhexy...	314	C19H38O3	1000383-13-7	64
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	59
4			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	59
5			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050501.D
Acq On : 29 Aug 2022 22:17
Operator : SY/MD
Sample : N4322-11ME
Misc : 3.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY171ME

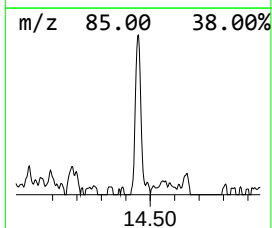
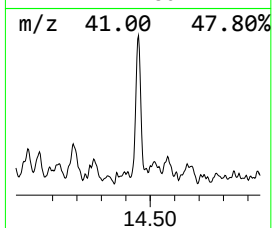
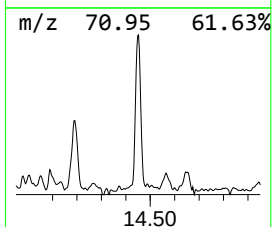
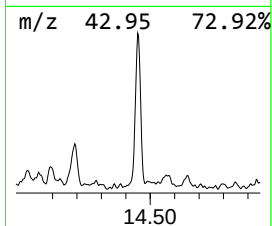
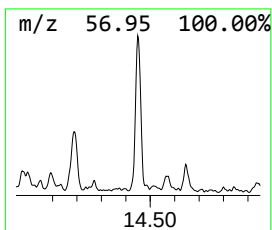
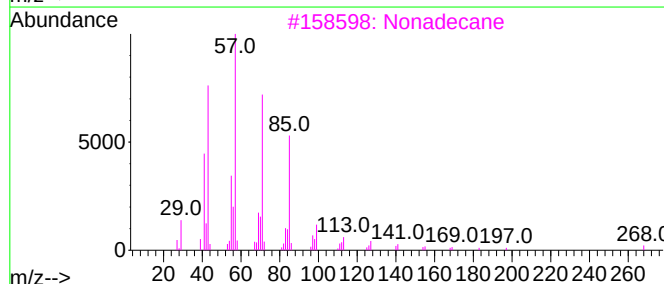
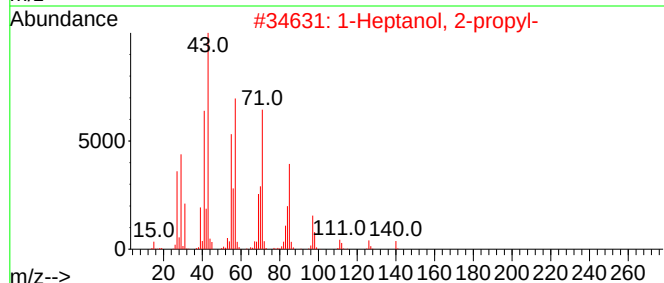
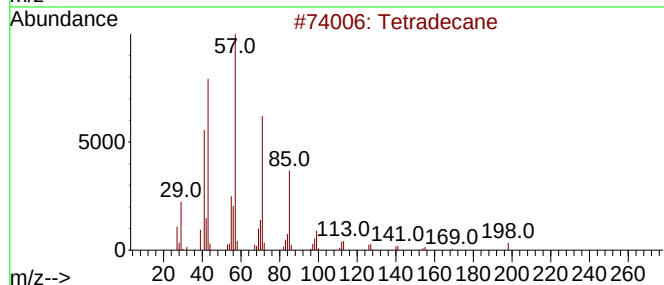
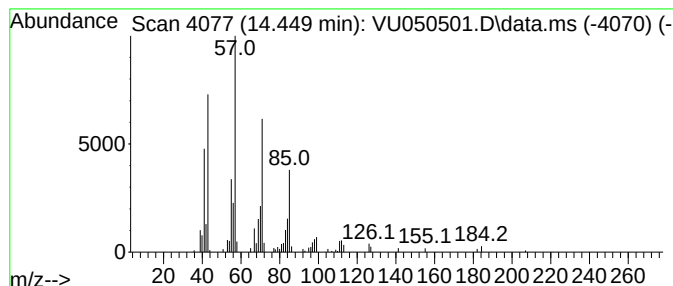
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.449	3.38 ug/L	60692	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	72
2			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	72
3			Nonadecane	268	C19H40	000629-92-5	72
4			Tridecane	184	C13H28	000629-50-5	70
5			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050501.D
Acq On : 29 Aug 2022 22:17
Operator : SY/MD
Sample : N4322-11ME
Misc : 3.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY171ME

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	4.1	ug/L	73919	3	11.815	898225	50.0
1-Octanol, 2-bu...	12.327	5.9	ug/L	105670	3	11.815	898225	50.0
(DEL) Alkane: S...	13.433	5.3	ug/L	94764	3	11.815	898225	50.0
(DEL) Alkane: S...	13.587	3.1	ug/L	56109	3	11.815	898225	50.0
(DEL) Alkane: S...	14.449	3.4	ug/L	60692	3	11.815	898225	50.0