

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090322\
 Data File : VU050621.D
 Acq On : 03 Sep 2022 18:44
 Operator : SY/MD
 Sample : N4440-08ME
 Misc : 4.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COZK3ME

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\SFAMULM090222WMA.M
 Title : VOC Analysis

Signal : TIC: VU050621.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	39	44	49	rBV2	5543	6400	0.17%	0.038%
2	1.594	71	79	90	rBV	102929	156177	4.24%	0.919%
3	1.893	167	172	183	rBV	35411	51820	1.41%	0.305%
4	2.527	357	369	385	rVB	273439	454042	12.31%	2.670%
5	2.646	401	406	407	rBV3	2734	2207	0.06%	0.013%
6	2.748	433	438	448	rVB4	1521	2162	0.06%	0.013%
7	2.909	482	488	492	rVB4	584	573	0.02%	0.003%
8	2.938	492	497	499	rBV5	737	701	0.02%	0.004%
9	2.957	500	503	507	rVV2	674	590	0.02%	0.003%
10	2.980	507	510	515	rVB4	753	615	0.02%	0.004%
11	3.031	515	526	541	rBV3	6401	13610	0.37%	0.080%
12	3.179	554	572	597	rBV	43345	129480	3.51%	0.762%
13	3.330	608	619	634	rVB2	57027	111777	3.03%	0.657%
14	3.459	655	659	663	rBV3	408	421	0.01%	0.002%
15	3.607	700	705	708	rBV	510	361	0.01%	0.002%
16	3.665	719	723	730	rVB4	708	753	0.02%	0.004%
17	3.726	738	742	745	rBV3	402	413	0.01%	0.002%
18	4.006	826	829	832	rBV2	540	441	0.01%	0.003%
19	4.076	847	851	859	rBV2	373	382	0.01%	0.002%
20	4.285	912	916	922	rBV2	831	974	0.03%	0.006%
21	4.658	1013	1032	1084	rBV2	1409946	3687502	100.00%	21.688%
22	5.060	1141	1157	1185	rVB	264334	636630	17.26%	3.744%
23	5.285	1219	1227	1228	rBV4	1341	1448	0.04%	0.009%
24	5.356	1246	1249	1250	rBV3	902	440	0.01%	0.003%
25	5.642	1333	1338	1340	rBV	412	351	0.01%	0.002%
26	5.716	1340	1361	1398	rBV2	638273	1636527	44.38%	9.625%
27	5.845	1398	1401	1410	rVB4	716	912	0.02%	0.005%
28	5.980	1431	1443	1469	rVV5	16220	42369	1.15%	0.249%
29	6.179	1493	1505	1509	rBV5	1729	2982	0.08%	0.018%
30	6.247	1511	1526	1558	rVB	518238	1057619	28.68%	6.220%
31	6.372	1563	1565	1570	rBV3	548	478	0.01%	0.003%
32	6.536	1588	1616	1632	rBV2	458415	965322	26.18%	5.677%
33	6.690	1650	1664	1687	rBV	360875	758032	20.56%	4.458%
34	6.800	1690	1698	1714	rVB3	19654	37835	1.03%	0.223%
35	6.887	1723	1725	1730	rVB2	486	434	0.01%	0.003%
36	6.948	1737	1744	1747	rBV2	1135	1519	0.04%	0.009%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

37	6.993	1753	1758	1760	rBV5	672	624	0.02%	0.004%
38	7.054	1772	1777	1782	rBV5	447	506	0.01%	0.003%
39	7.147	1801	1806	1809	rBV3	1051	1069	0.03%	0.006%
40	7.227	1817	1831	1848	rBV3	7367	19578	0.53%	0.115%
41	7.333	1862	1864	1872	rVB6	1142	1453	0.04%	0.009%
42	7.372	1872	1876	1880	rBV2	396	387	0.01%	0.002%
43	7.430	1884	1894	1906	rBV4	5991	11058	0.30%	0.065%
44	7.494	1911	1914	1920	rVB4	1141	1095	0.03%	0.006%
45	7.565	1924	1936	1960	rVV	144726	288525	7.82%	1.697%
46	7.687	1964	1974	1980	rVV8	1630	2890	0.08%	0.017%
47	7.896	2016	2039	2055	rBV	632682	1149553	31.17%	6.761%
48	8.099	2099	2102	2107	rVB4	1298	1122	0.03%	0.007%
49	8.182	2116	2128	2155	rVV2	91755	199561	5.41%	1.174%
50	8.362	2172	2184	2195	rVV2	3787	7785	0.21%	0.046%
51	8.549	2229	2242	2252	rVB10	5137	10231	0.28%	0.060%
52	8.668	2257	2279	2312	rBV3	304261	941075	25.52%	5.535%
53	8.922	2349	2358	2369	rBV5	8821	15348	0.42%	0.090%
54	8.967	2369	2372	2375	rBV4	789	647	0.02%	0.004%
55	9.073	2400	2405	2409	rVV5	1030	1174	0.03%	0.007%
56	9.118	2410	2419	2426	rVV6	3545	5490	0.15%	0.032%
57	9.163	2426	2433	2442	rVV6	5068	9941	0.27%	0.058%
58	9.211	2443	2448	2457	rVB8	5077	7526	0.20%	0.044%
59	9.266	2463	2465	2468	rBV2	516	401	0.01%	0.002%
60	9.333	2477	2486	2493	rBV4	4747	7246	0.20%	0.043%
61	9.420	2499	2513	2535	rBV	652949	1297233	35.18%	7.630%
62	9.568	2549	2559	2570	rVB10	3253	7008	0.19%	0.041%
63	9.629	2575	2578	2579	rBV3	731	361	0.01%	0.002%
64	9.668	2585	2590	2591	rBV4	2038	1826	0.05%	0.011%
65	9.716	2599	2605	2611	rBV5	5167	8740	0.24%	0.051%
66	9.886	2651	2658	2659	rBV5	1794	1940	0.05%	0.011%
67	9.951	2672	2678	2681	rBV5	1431	1805	0.05%	0.011%
68	10.018	2688	2699	2703	rBV5	13037	20417	0.55%	0.120%
69	10.118	2725	2730	2741	rVB8	7499	10748	0.29%	0.063%
70	10.250	2752	2771	2784	rBV6	17081	46256	1.25%	0.272%
71	10.356	2795	2804	2810	rBV5	16848	31612	0.86%	0.186%
72	10.465	2830	2838	2851	rVB5	6110	12756	0.35%	0.075%
73	10.555	2851	2866	2874	rBV6	21792	49405	1.34%	0.291%
74	10.764	2919	2931	2966	rVB	544988	1006527	27.30%	5.920%
75	10.954	2981	2990	3001	rBV8	12304	27538	0.75%	0.162%
76	11.015	3002	3009	3016	rVV8	13091	25852	0.70%	0.152%

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Instrument :
 MSVOA_U
 ClientSampleId :
 C0ZK3ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

77	11.066	3018	3025	3031	rVV3	27018	46573	1.26%	0.274%
78	11.115	3032	3040	3055	rVB3	91133	153594	4.17%	0.903%
79	11.417	3128	3134	3141	rVB3	38310	50342	1.37%	0.296%
80	11.571	3179	3182	3187	rBV6	5827	7137	0.19%	0.042%
81	11.816	3247	3258	3271	rBV	599395	958033	25.98%	5.635%
82	12.083	3337	3341	3342	rBV3	2414	1633	0.04%	0.010%
83	12.195	3363	3376	3392	rBV	417005	701108	19.01%	4.123%
84	12.327	3410	3417	3426	rVB2	32117	43603	1.18%	0.256%
85	12.594	3496	3500	3501	rBV2	1259	841	0.02%	0.005%
86	12.703	3531	3534	3535	rBV3	1563	913	0.02%	0.005%
87	12.925	3592	3603	3604	rBV8	4005	4886	0.13%	0.029%
88	13.012	3626	3630	3633	rBV6	1114	1146	0.03%	0.007%
89	13.176	3676	3681	3683	rBV4	661	477	0.01%	0.003%
90	13.282	3711	3714	3718	rVB2	845	558	0.02%	0.003%
91	13.391	3742	3748	3754	rBV8	3621	5615	0.15%	0.033%
92	13.433	3755	3761	3769	rVV6	5712	8608	0.23%	0.051%
93	13.552	3794	3798	3801	rBV5	1169	1131	0.03%	0.007%
94	13.587	3802	3809	3812	rBV6	2817	3101	0.08%	0.018%
95	13.722	3848	3851	3854	rBV3	872	741	0.02%	0.004%
96	13.803	3873	3876	3882	rVB3	1106	865	0.02%	0.005%
97	13.848	3883	3890	3894	rBV7	2047	2931	0.08%	0.017%
98	14.089	3962	3965	3966	rBV3	1504	912	0.02%	0.005%
99	14.169	3987	3990	3991	rBV2	974	468	0.01%	0.003%
100	14.414	4059	4066	4072	rBV9	5669	8923	0.24%	0.052%

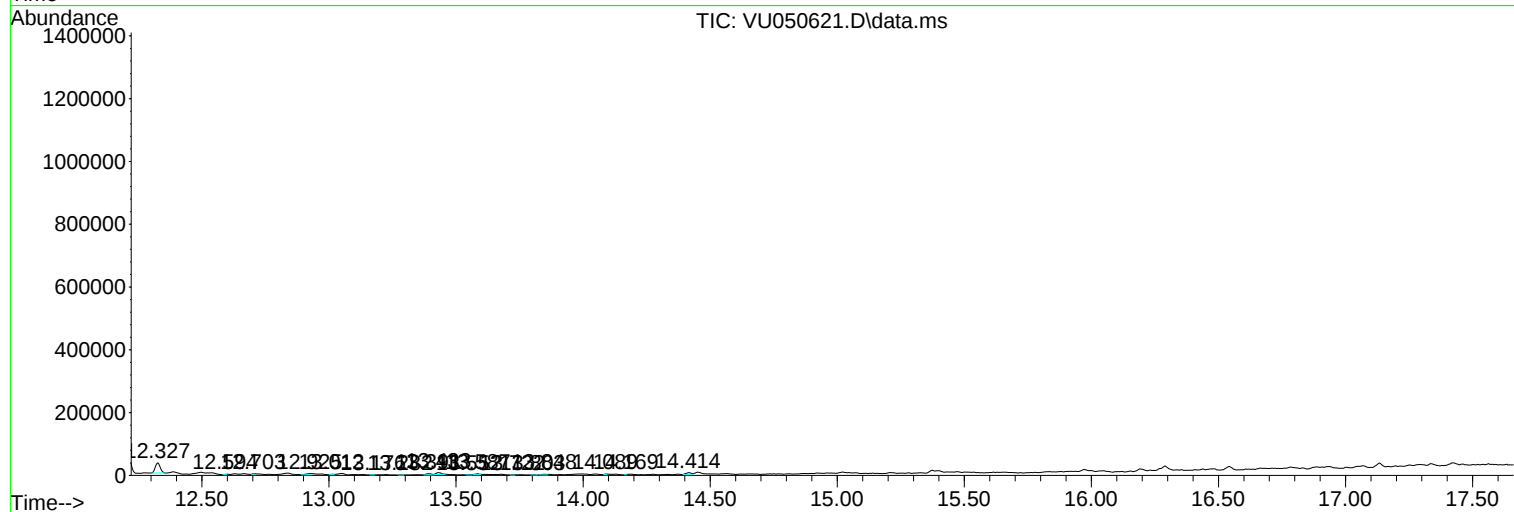
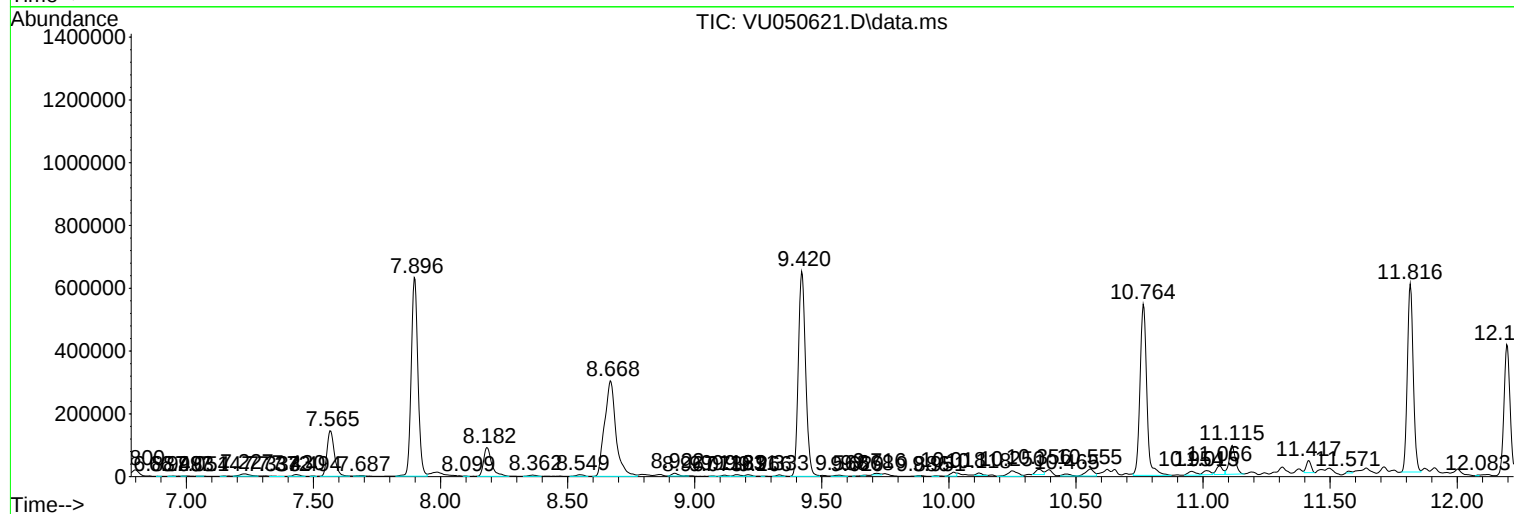
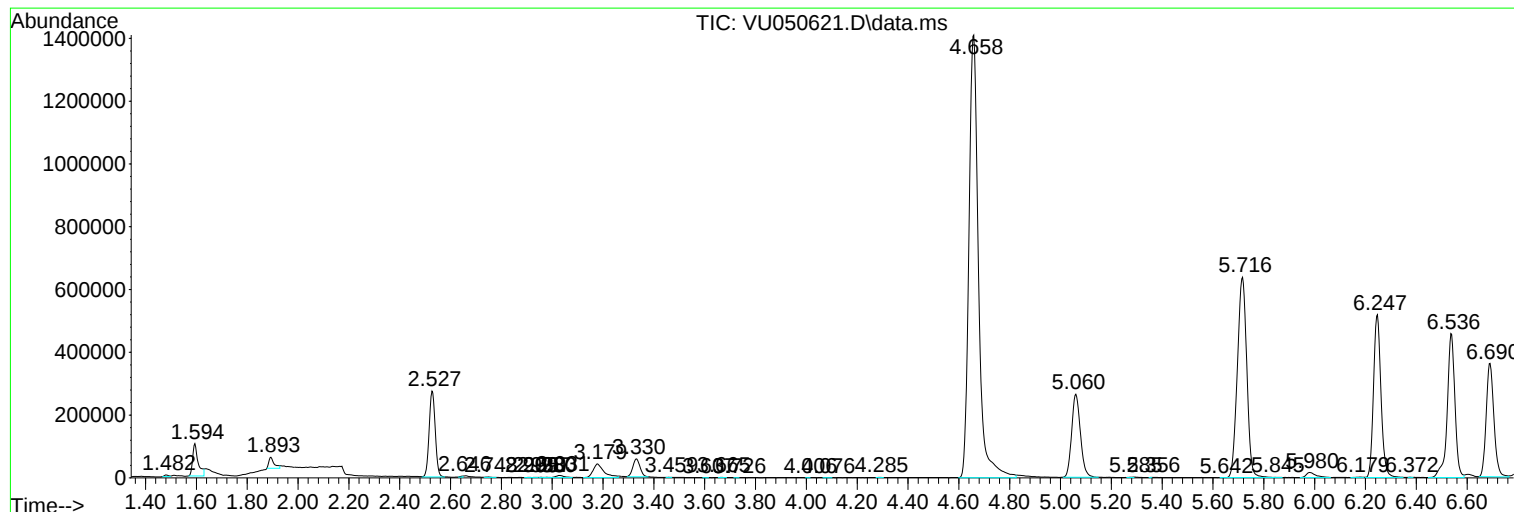
Sum of corrected areas: 17002747

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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZK3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZK3ME

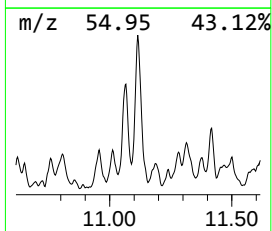
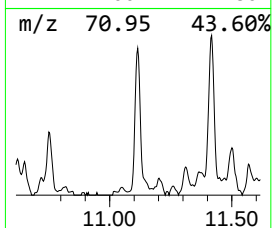
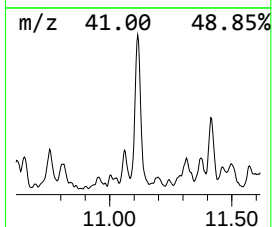
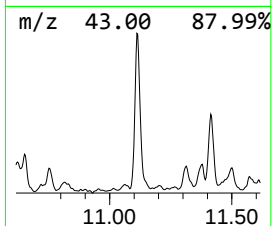
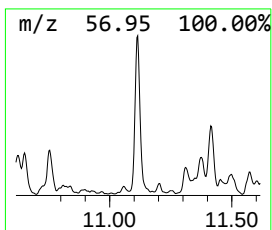
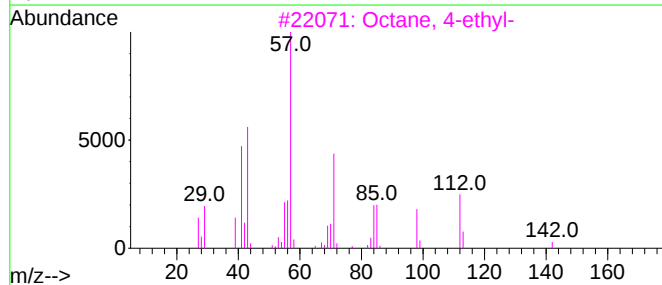
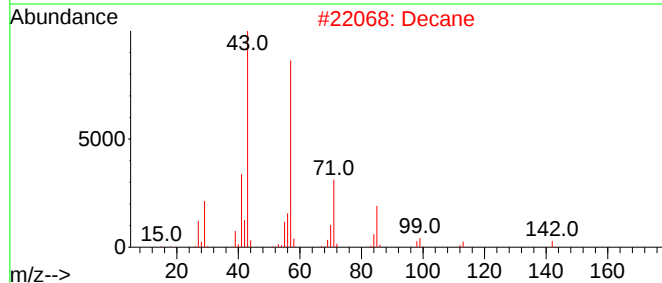
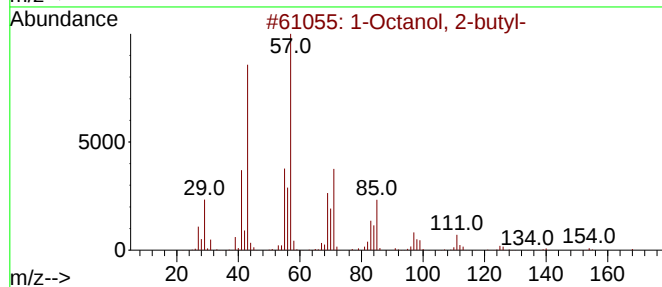
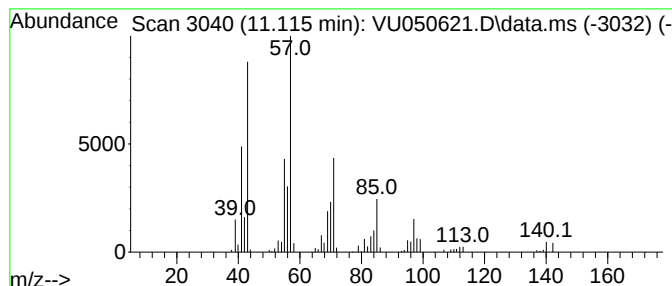
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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.
11.115	8.02 ug/L	153594	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	78
2			Decane	142	C10H22	000124-18-5	68
3			Octane, 4-ethyl-	142	C10H22	015869-86-0	64
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	59
5			Hydroxylamine, 0-decyl-	173	C10H23NO	029812-79-1	53



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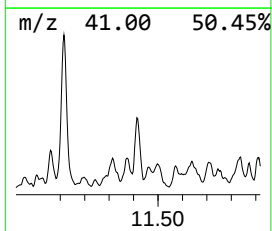
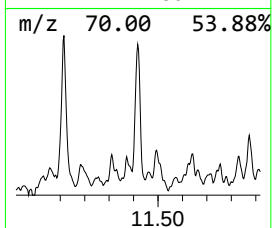
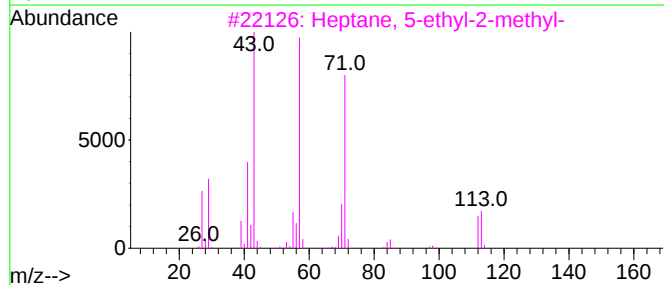
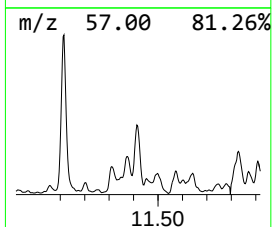
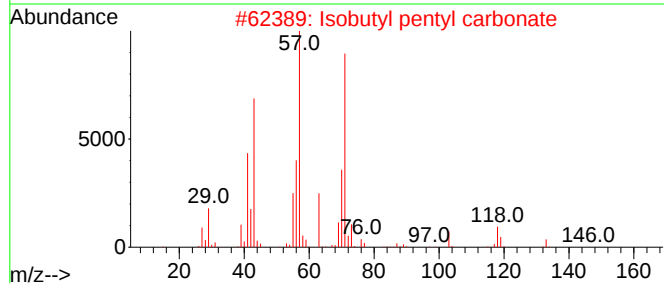
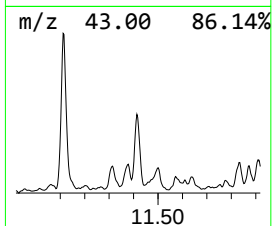
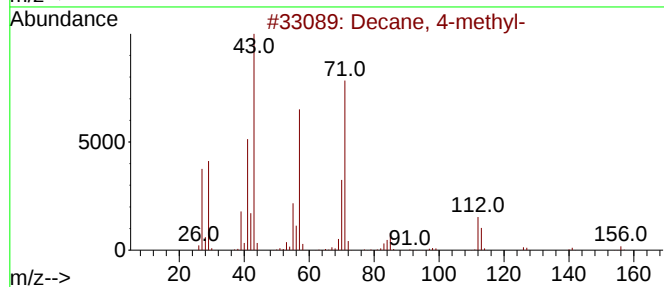
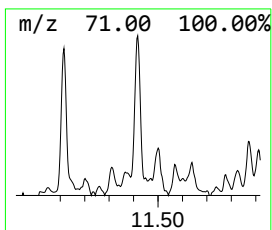
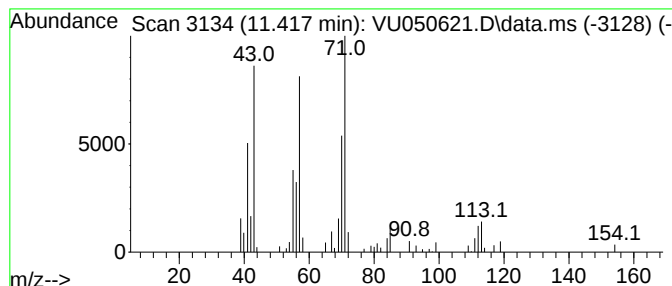
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.417	2.63 ug/L	50342	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	78
2			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	64
3			Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	59
4			Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	59
5			Decane, 4-methyl-	156	C11H24	002847-72-5	59



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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
1-Octanol, 2-bu...	11.115	8.0	ug/L	153594	3	11.816	958033	50.0
(DEL) Alkane: S...	11.417	2.6	ug/L	50342	3	11.816	958033	50.0