

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
 Data File : VU053003.D
 Acq On : 08 Feb 2023 16:16
 Operator : JC/MD
 Sample : 01443-06
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 X3E95

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\SFAMULM020823WMA.M
 Title : VOC Analysis

Signal : TIC: VU053003.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.257	44	52	68	rVB	171751	244302	6.19%	0.449%
2	1.528	124	136	137	rBV7	16417	27422	0.69%	0.050%
3	1.598	152	158	181	rVB	139936	225601	5.71%	0.414%
4	2.547	443	453	468	rVB	298933	505047	12.79%	0.928%
5	2.656	474	487	517	rVB	99473	339295	8.59%	0.623%
6	3.036	599	605	624	rVB2	10079	20852	0.53%	0.038%
7	3.338	686	699	722	rVB	638752	1256568	31.83%	2.308%
8	3.614	783	785	790	rVB5	1902	1393	0.04%	0.003%
9	3.804	840	844	845	rBV4	981	825	0.02%	0.002%
10	3.843	849	856	857	rBV7	1640	1572	0.04%	0.003%
11	3.923	878	881	885	rVB4	1711	1224	0.03%	0.002%
12	3.987	897	901	904	rVB6	1737	1270	0.03%	0.002%
13	4.010	904	908	910	rBV5	1850	1331	0.03%	0.002%
14	4.042	916	918	924	rVB8	1902	1658	0.04%	0.003%
15	4.074	924	928	929	rBV4	1586	784	0.02%	0.001%
16	4.119	938	942	945	rVB6	1526	1138	0.03%	0.002%
17	4.351	1012	1014	1017	rBV4	1284	882	0.02%	0.002%
18	4.392	1024	1027	1031	rBV6	1646	1284	0.03%	0.002%
19	4.515	1059	1065	1069	rBV9	1737	2161	0.05%	0.004%
20	4.585	1083	1087	1091	rBV6	1381	1076	0.03%	0.002%
21	4.646	1091	1106	1139	rBV2	47774	202457	5.13%	0.372%
22	4.981	1208	1210	1217	rVB7	1401	1017	0.03%	0.002%
23	5.061	1220	1235	1262	rBV	226854	567182	14.37%	1.042%
24	5.164	1265	1267	1272	rBV5	2182	1925	0.05%	0.004%
25	5.232	1284	1288	1291	rVB5	1181	903	0.02%	0.002%
26	5.306	1291	1311	1332	rBV	997651	2283910	57.86%	4.195%
27	5.508	1370	1374	1376	rBV4	1740	1427	0.04%	0.003%
28	5.617	1406	1408	1414	rVB6	1763	1340	0.03%	0.002%
29	5.717	1418	1439	1446	rBV2	535698	1347364	34.13%	2.475%
30	5.765	1447	1454	1477	rVB	1133279	2250178	57.00%	4.133%
31	5.974	1513	1519	1523	rVV9	1649	2226	0.06%	0.004%
32	6.055	1540	1544	1545	rBV4	1302	880	0.02%	0.002%
33	6.190	1584	1586	1589	rVV5	1559	1230	0.03%	0.002%
34	6.244	1590	1603	1625	rVB	391930	781606	19.80%	1.435%
35	6.341	1631	1633	1637	rVB6	1712	870	0.02%	0.002%
36	6.537	1678	1694	1719	rBV	1559074	2922695	74.04%	5.368%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
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37	6.688	1727	1741	1757	rBV	293832	593366	15.03%	1.090%
38	6.788	1759	1772	1790	rVB	584881	1156554	29.30%	2.124%
39	6.891	1802	1804	1808	rBV4	983	790	0.02%	0.001%
40	6.949	1818	1822	1826	rVB7	2050	1882	0.05%	0.003%
41	7.006	1838	1840	1845	rVB5	1348	970	0.02%	0.002%
42	7.032	1845	1848	1850	rBV4	1636	927	0.02%	0.002%
43	7.103	1856	1870	1894	rBV	376897	782751	19.83%	1.438%
44	7.376	1951	1955	1957	rBV5	1123	1113	0.03%	0.002%
45	7.495	1986	1992	1996	rBV8	1210	1536	0.04%	0.003%
46	7.563	2001	2013	2037	rVB	189397	370683	9.39%	0.681%
47	7.707	2051	2058	2060	rVV7	1317	1400	0.04%	0.003%
48	7.897	2104	2117	2128	rVV	671852	1215928	30.80%	2.233%
49	7.968	2128	2139	2164	rVB	2003724	3570261	90.44%	6.557%
50	8.125	2176	2188	2198	rBV	605240	991033	25.10%	1.820%
51	8.180	2198	2205	2230	rVB2	123190	254872	6.46%	0.468%
52	8.305	2242	2244	2249	rVB6	1431	907	0.02%	0.002%
53	8.402	2259	2274	2298	rBV	460244	1065013	26.98%	1.956%
54	8.550	2306	2320	2335	rBV	943374	1611716	40.83%	2.960%
55	8.678	2338	2360	2366	rBV	200167	575792	14.59%	1.057%
56	8.923	2421	2436	2456	rBV	262466	528808	13.40%	0.971%
57	9.055	2475	2477	2479	rBV3	1510	929	0.02%	0.002%
58	9.109	2492	2494	2497	rVV3	1595	824	0.02%	0.002%
59	9.167	2509	2512	2515	rBV4	1331	1063	0.03%	0.002%
60	9.244	2533	2536	2541	rVB6	2274	1473	0.04%	0.003%
61	9.347	2566	2568	2574	rBV6	1508	1331	0.03%	0.002%
62	9.447	2577	2599	2621	rVV2	1266679	3366838	85.29%	6.183%
63	9.569	2624	2637	2657	rVB	1573569	2790791	70.70%	5.125%
64	9.698	2663	2677	2703	rVB	2056794	3595463	91.08%	6.603%
65	10.006	2770	2773	2775	rBV4	1671	959	0.02%	0.002%
66	10.116	2788	2807	2828	rVV2	1588097	3348330	84.82%	6.149%
67	10.267	2851	2854	2856	rBV5	1205	862	0.02%	0.002%
68	10.305	2861	2866	2869	rBV6	1670	1839	0.05%	0.003%
69	10.485	2907	2922	2940	rVV	2343236	3947636	100.00%	7.250%
70	10.601	2955	2958	2961	rBV4	1448	1029	0.03%	0.002%
71	10.633	2966	2968	2970	rBV2	1309	801	0.02%	0.001%
72	10.675	2979	2981	2985	rVB5	1714	1102	0.03%	0.002%
73	10.765	2995	3009	3023	rVB	411922	680972	17.25%	1.251%
74	10.871	3040	3042	3045	rBV4	1284	964	0.02%	0.002%
75	11.048	3094	3097	3100	rVV5	1542	1156	0.03%	0.002%
76	11.109	3103	3116	3135	rVV	507578	728319	18.45%	1.338%

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77	11.254	3155	3161	3162	rBV6	1190	953	0.02%	0.002%
78	11.469	3222	3228	3238	rVB	12293	18584	0.47%	0.034%
79	11.662	3283	3288	3289	rBV3	1091	882	0.02%	0.002%
80	11.746	3301	3314	3325	rBV	1055433	1688543	42.77%	3.101%
81	11.817	3325	3336	3337	rBV	753777	923468	23.39%	1.696%
82	11.987	3386	3389	3391	rBV4	1174	872	0.02%	0.002%
83	12.019	3395	3399	3402	rBV4	2194	1859	0.05%	0.003%
84	12.199	3438	3455	3476	rBV2	852684	1983007	50.23%	3.642%
85	12.337	3494	3498	3502	rVB7	1793	1363	0.03%	0.003%
86	12.598	3575	3579	3584	rBV7	1692	1558	0.04%	0.003%
87	12.630	3586	3589	3591	rBV4	1204	803	0.02%	0.001%
88	12.672	3599	3602	3605	rBV4	1563	1358	0.03%	0.002%
89	12.704	3610	3612	3617	rVB6	2137	1416	0.04%	0.003%
90	12.768	3630	3632	3634	rBV3	1745	865	0.02%	0.002%
91	12.977	3692	3697	3700	rBV7	1876	2077	0.05%	0.004%
92	13.215	3758	3771	3796	rVB	1278251	2044505	51.79%	3.755%
93	13.771	3941	3944	3947	rBV6	2041	1408	0.04%	0.003%
94	13.836	3951	3964	3983	rVV	1321968	2083014	52.77%	3.826%
95	14.087	4034	4042	4052	rVB	9936	15736	0.40%	0.029%
96	14.202	4075	4078	4079	rBV3	1372	843	0.02%	0.002%
97	14.324	4103	4116	4134	rBV	933959	1471154	37.27%	2.702%
98	14.617	4204	4207	4208	rBV3	1855	944	0.02%	0.002%
99	14.730	4238	4242	4245	rBV3	1740	1423	0.04%	0.003%
100	14.775	4253	4256	4259	rBV6	1368	1146	0.03%	0.002%

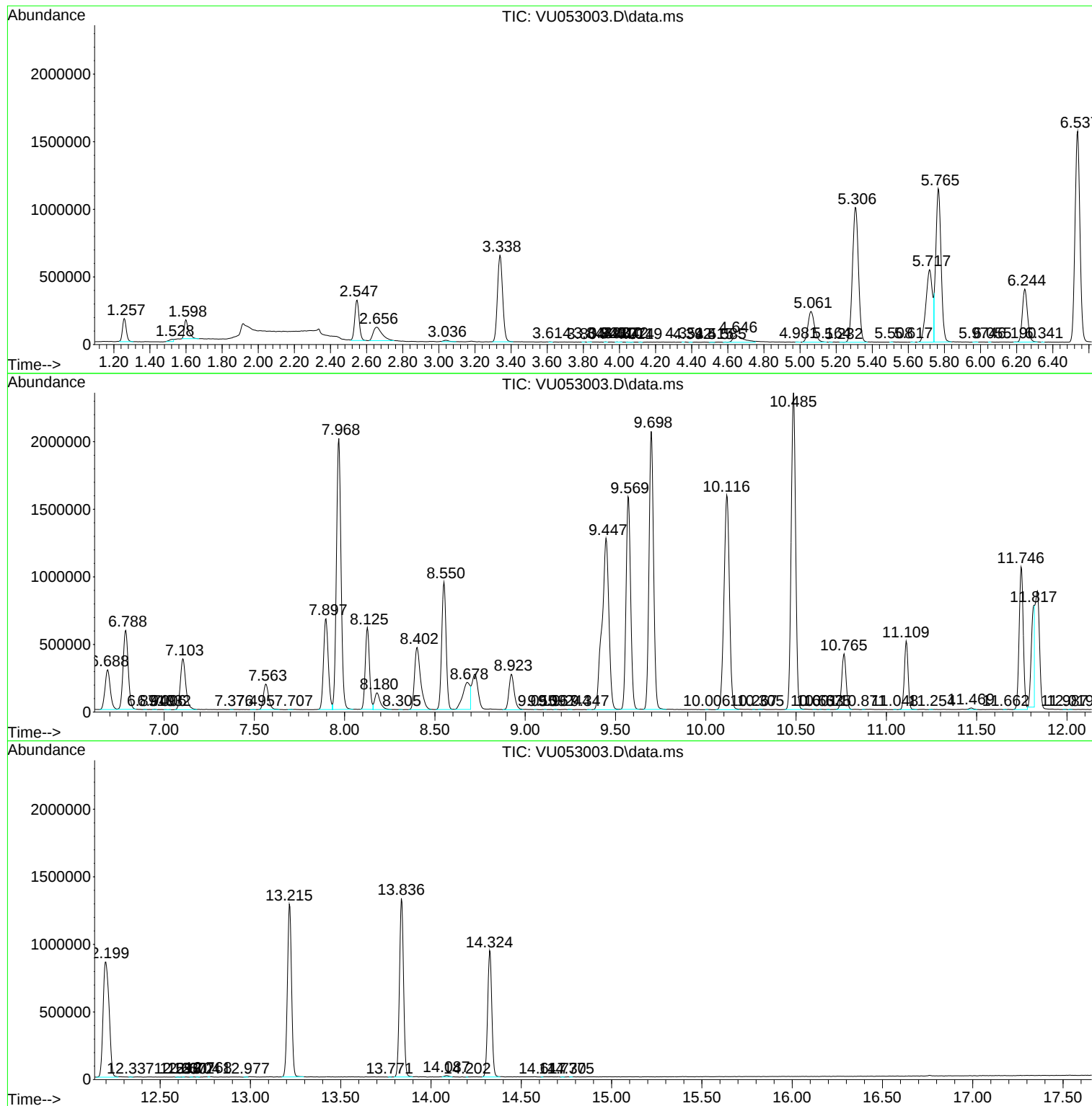
Sum of corrected areas: 54449659

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
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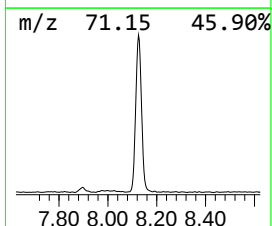
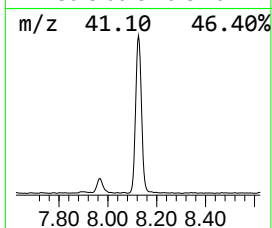
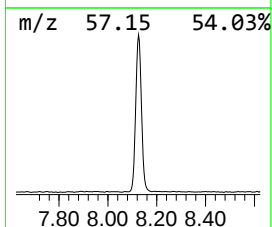
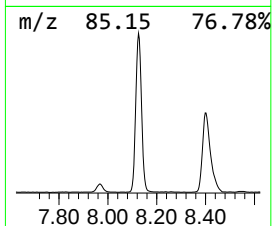
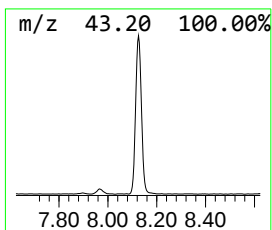
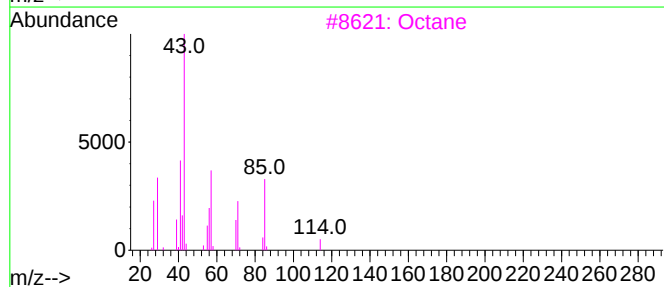
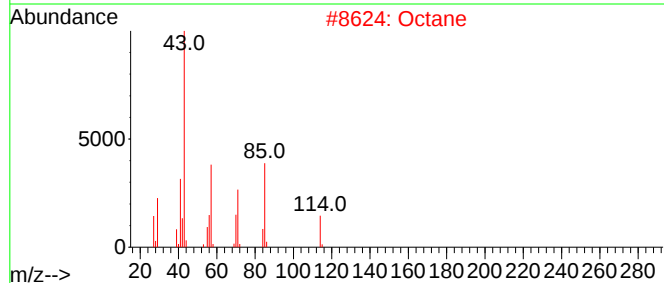
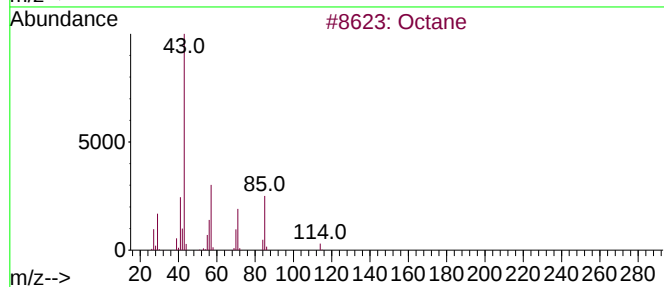
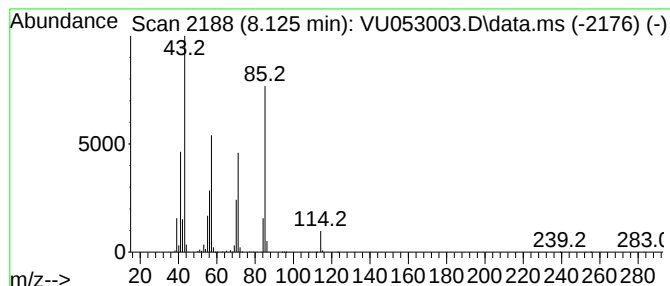
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

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.
8.125	14.72 ug/L	991033	Chlorobenzene-d5	9.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane			114	C8H18	000111-65-9	91
2	Octane			114	C8H18	000111-65-9	91
3	Octane			114	C8H18	000111-65-9	91
4	Heptane, 2,4-dimethyl-			128	C9H20	002213-23-2	72
5	Heptane, 2,4-dimethyl-			128	C9H20	002213-23-2	64



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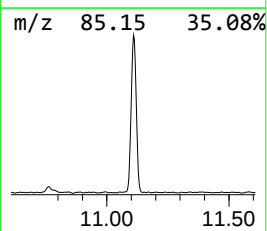
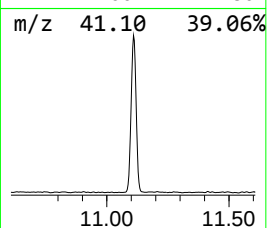
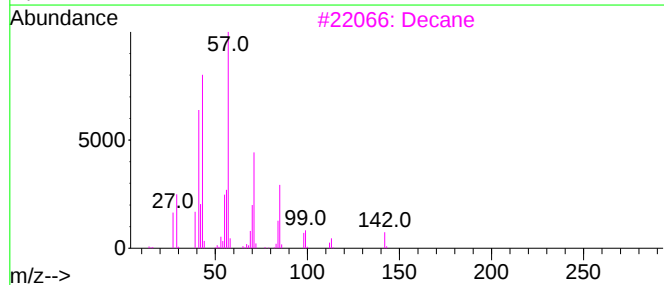
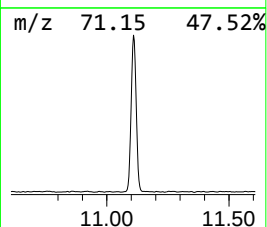
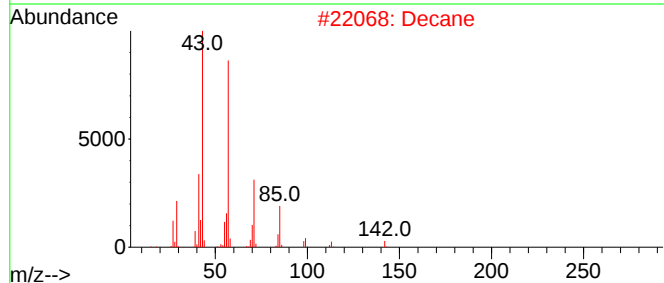
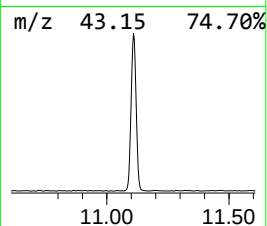
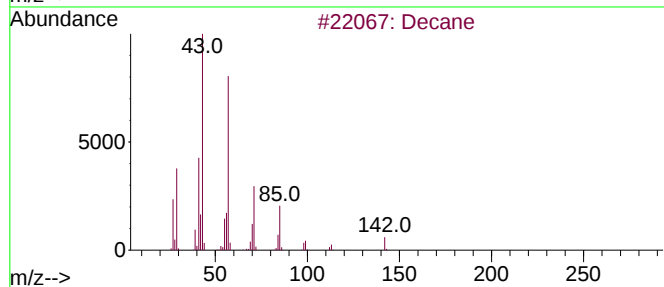
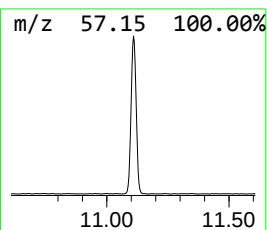
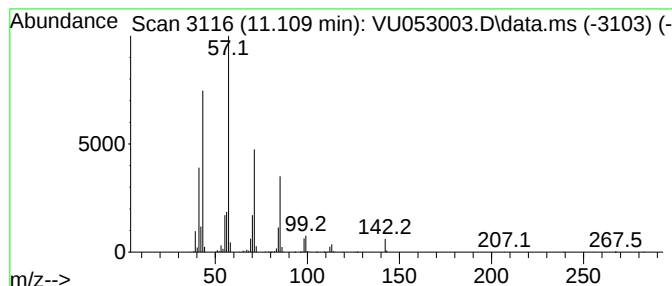
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

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.
11.109	39.43 ug/L	728319	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	95
2			Decane	142	C10H22	000124-18-5	91
3			Decane	142	C10H22	000124-18-5	91
4			Decane	142	C10H22	000124-18-5	91
5			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	83



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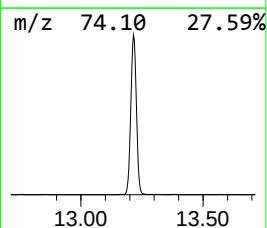
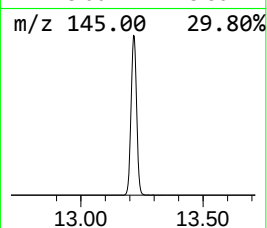
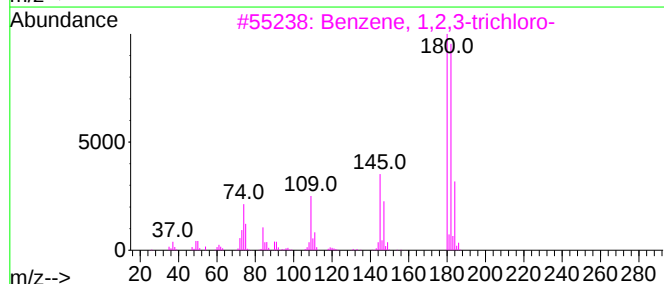
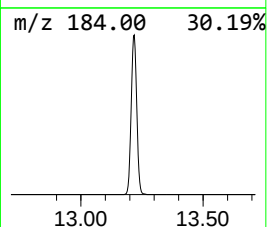
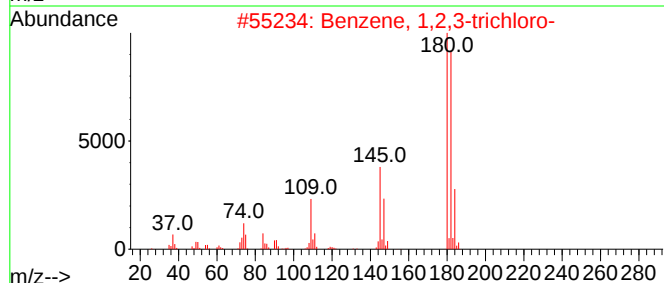
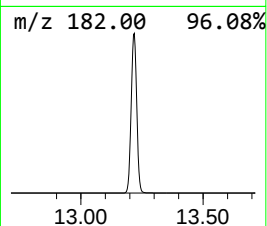
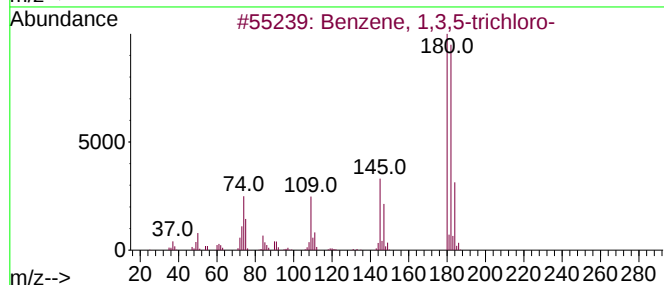
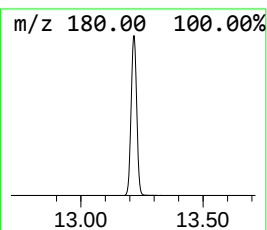
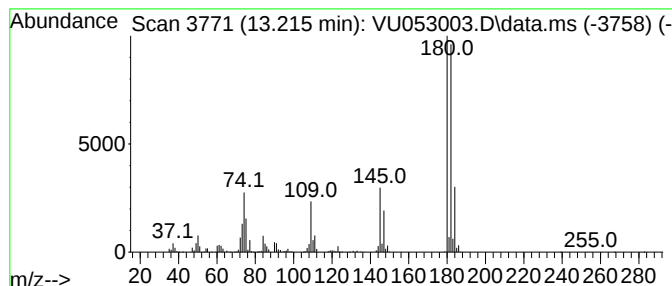
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Benzene, 1,3,5-trichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.215	110.70 ug/L	2044510	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
2			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
3			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
4			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
5			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053003.D
Acq On : 08 Feb 2023 16:16
Operator : JC/MD
Sample : 01443-06
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X3E95

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.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...	8.125	14.7	ug/L	991033	2	9.421	3366840	50.0
(DEL) Alkane: S...	11.109	39.4	ug/L	728319	3	11.813	923468	50.0
Benzene, 1,3,5-...	13.215	110.7	ug/L	2044510	3	11.813	923468	50.0