

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040721\
 Data File : VU042980.D
 Acq On : 07 Apr 2021 14:49
 Operator : SY/MD
 Sample : M1906-07
 Misc : 5.0g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 X3312

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\SFAMULM040721WMA.M

Title : VOC Analysis

Signal : TIC: VU042980.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	101	rVB	53662	90317	4.78%	0.364%
2	2.540	361	373	395	rBV	143441	267795	14.18%	1.078%
3	2.649	398	407	453	rVB	107504	326526	17.29%	1.315%
4	2.916	488	490	493	rBV	433	312	0.02%	0.001%
5	3.041	514	529	572	rVB	288473	736157	38.99%	2.964%
6	3.340	608	622	642	rVB	158128	313724	16.62%	1.263%
7	3.517	673	677	680	rBV	236	253	0.01%	0.001%
8	3.601	701	703	706	rVB	163	54	0.00%	0.000%
9	3.694	730	732	734	rVB	245	115	0.01%	0.000%
10	3.781	756	759	763	rVB	205	118	0.01%	0.000%
11	3.868	769	786	810	rVB2	69421	176904	9.37%	0.712%
12	3.954	810	813	817	rBV2	314	316	0.02%	0.001%
13	4.067	846	848	851	rBV	171	135	0.01%	0.001%
14	4.099	856	858	862	rVB2	294	234	0.01%	0.001%
15	4.122	863	865	866	rBV	169	90	0.00%	0.000%
16	4.189	881	886	888	rBV	165	158	0.01%	0.001%
17	4.199	888	889	892	rVB	223	108	0.01%	0.000%
18	4.221	893	896	901	rBV	267	253	0.01%	0.001%
19	4.269	906	911	912	rBV	265	214	0.01%	0.001%
20	4.372	939	943	945	rBV	179	181	0.01%	0.001%
21	4.417	954	957	960	rBV	127	134	0.01%	0.001%
22	4.501	981	983	984	rBV	165	87	0.00%	0.000%
23	4.511	984	986	988	rVV	212	92	0.00%	0.000%
24	4.575	1003	1006	1008	rBB	164	112	0.01%	0.000%
25	4.665	1008	1034	1079	rBV2	299985	867646	45.96%	3.493%
26	4.887	1100	1103	1107	rBV3	149	119	0.01%	0.000%
27	4.986	1117	1134	1148	rBV	122814	335145	17.75%	1.349%
28	5.202	1198	1201	1203	rBV	169	100	0.01%	0.000%
29	5.298	1226	1231	1236	rVB2	854	913	0.05%	0.004%
30	5.347	1241	1246	1248	rBV	195	221	0.01%	0.001%
31	5.372	1251	1254	1256	rBV	364	282	0.01%	0.001%
32	5.440	1266	1275	1285	rBV5	1573	2904	0.15%	0.012%
33	5.523	1285	1301	1319	rVV2	100132	221352	11.72%	0.891%
34	5.626	1331	1333	1335	rBV	139	95	0.01%	0.000%
35	5.726	1344	1364	1370	rBV2	330082	811470	42.98%	3.267%
36	5.986	1444	1445	1451	rVB2	249	215	0.01%	0.001%

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37	6.019	1451	1455	1456	rBV	282	174	0.01%	0.001%
38	6.044	1461	1463	1467	rVB	425	231	0.01%	0.001%
39	6.131	1483	1490	1495	rBV5	1003	1312	0.07%	0.005%
40	6.253	1514	1528	1551	rVB	266154	551741	29.22%	2.221%
41	6.546	1604	1619	1643	rBV	607331	1174191	62.19%	4.727%
42	6.700	1650	1667	1687	rBV	185242	398944	21.13%	1.606%
43	6.887	1723	1725	1726	rBV	194	89	0.00%	0.000%
44	7.047	1772	1775	1776	rBV	300	198	0.01%	0.001%
45	7.118	1782	1797	1831	rBV	273509	659280	34.92%	2.654%
46	7.330	1862	1863	1865	rBV	143	77	0.00%	0.000%
47	7.363	1870	1873	1875	rBV	294	205	0.01%	0.001%
48	7.417	1888	1890	1892	rVB2	180	93	0.00%	0.000%
49	7.430	1892	1894	1897	rBV	184	88	0.00%	0.000%
50	7.491	1911	1913	1914	rBV	200	62	0.00%	0.000%
51	7.578	1925	1940	1964	rBV2	104468	227235	12.04%	0.915%
52	7.691	1972	1975	1977	rBV	244	138	0.01%	0.001%
53	7.716	1977	1983	1990	rVB3	343	409	0.02%	0.002%
54	7.845	1997	2023	2033	rBV2	344936	1265347	67.02%	5.094%
55	7.977	2055	2064	2082	rVB	270579	511019	27.07%	2.057%
56	8.076	2093	2095	2099	rVB2	420	224	0.01%	0.001%
57	8.134	2099	2113	2123	rBV	636474	1018834	53.96%	4.102%
58	8.282	2157	2159	2161	rVB2	408	164	0.01%	0.001%
59	8.340	2175	2177	2179	rVB	231	88	0.00%	0.000%
60	8.353	2179	2181	2182	rBV	217	86	0.00%	0.000%
61	8.366	2183	2185	2188	rVB2	368	146	0.01%	0.001%
62	8.465	2214	2216	2220	rBV2	195	148	0.01%	0.001%
63	8.559	2231	2245	2262	rBV	1079555	1888024	100.00%	7.601%
64	8.671	2262	2280	2287	rBV	250737	602368	31.90%	2.425%
65	8.826	2316	2328	2350	rVB3	153565	428181	22.68%	1.724%
66	8.970	2370	2373	2377	rBV4	631	634	0.03%	0.003%
67	9.025	2388	2390	2393	rVB	211	80	0.00%	0.000%
68	9.128	2420	2422	2425	rVB2	413	186	0.01%	0.001%
69	9.337	2484	2487	2491	rBV	232	248	0.01%	0.001%
70	9.459	2501	2525	2549	rBV2	593731	1859106	98.47%	7.485%
71	9.581	2550	2563	2586	rVB	259127	490747	25.99%	1.976%
72	9.710	2589	2603	2622	rVV	741310	1377384	72.95%	5.546%
73	9.822	2634	2638	2639	rBV	154	88	0.00%	0.000%
74	10.018	2697	2699	2703	rBV	195	123	0.01%	0.000%
75	10.115	2714	2729	2749	rBV	505093	926177	49.06%	3.729%
76	10.311	2785	2790	2799	rVB2	755	984	0.05%	0.004%

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77	10.543	2857	2862	2864	rBV2	798	824	0.04%	0.003%
78	10.678	2897	2904	2912	rVB3	2777	4301	0.23%	0.017%
79	10.797	2921	2941	2960	rBV2	479180	1265275	67.02%	5.094%
80	10.874	2962	2965	2968	rBV2	460	347	0.02%	0.001%
81	10.925	2977	2981	2985	rBV2	492	321	0.02%	0.001%
82	11.121	3030	3042	3055	rBV	556293	804173	42.59%	3.238%
83	11.208	3068	3069	3071	rBV	193	62	0.00%	0.000%
84	11.385	3121	3124	3129	rBV2	393	367	0.02%	0.001%
85	11.475	3142	3152	3162	rVB7	5155	10037	0.53%	0.040%
86	11.703	3216	3223	3228	rBV4	1466	2162	0.11%	0.009%
87	11.758	3228	3240	3251	rVV	963050	1534431	81.27%	6.178%
88	11.825	3251	3261	3279	rVB	472799	764371	40.49%	3.077%
89	11.951	3294	3300	3304	rBV4	1414	1830	0.10%	0.007%
90	12.025	3321	3323	3325	rBV	247	122	0.01%	0.000%
91	12.057	3331	3333	3338	rVB	327	215	0.01%	0.001%
92	12.221	3362	3384	3399	rBV2	695022	1626622	86.15%	6.549%
93	12.314	3410	3413	3415	rBV2	504	361	0.02%	0.001%
94	12.478	3461	3464	3472	rBV2	195	228	0.01%	0.001%
95	12.777	3549	3557	3565	rBV	1174	2104	0.11%	0.008%
96	13.009	3615	3629	3648	rVB	479191	766295	40.59%	3.085%
97	13.160	3673	3676	3680	rVB2	560	327	0.02%	0.001%
98	13.218	3684	3694	3708	rBV2	11608	19109	1.01%	0.077%
99	13.440	3761	3763	3765	rBV3	427	188	0.01%	0.001%
100	14.340	4030	4043	4063	rBV	308362	493798	26.15%	1.988%

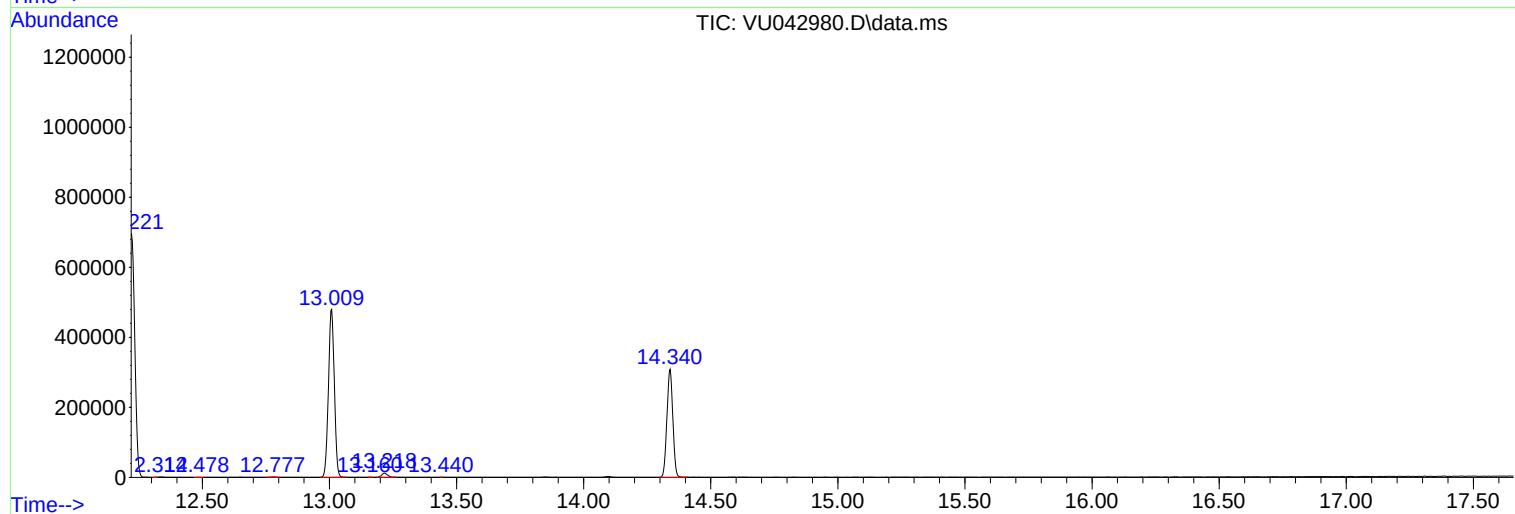
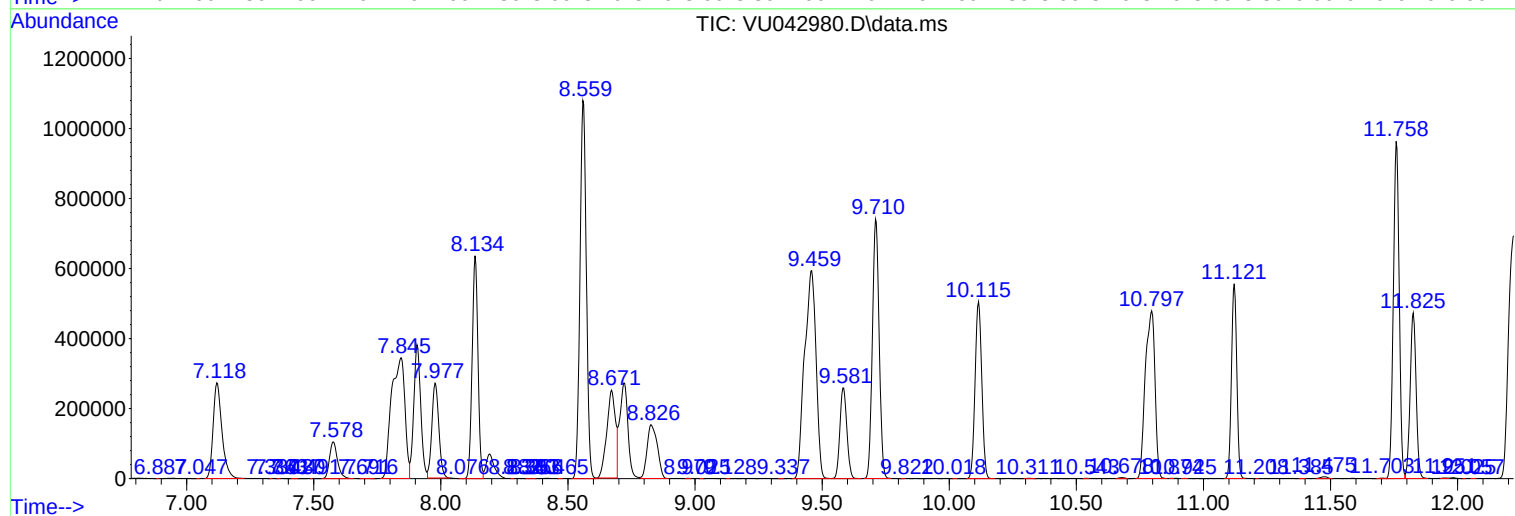
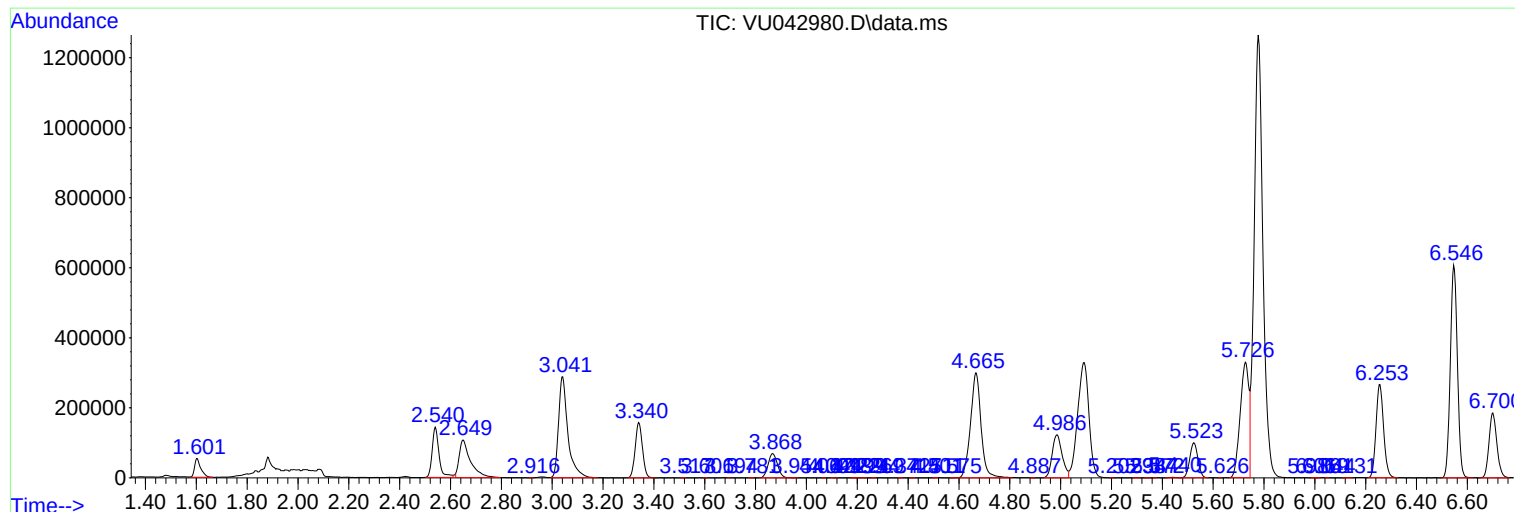
Sum of corrected areas: 24837574

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM040721WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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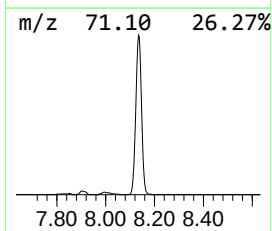
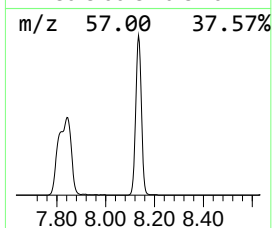
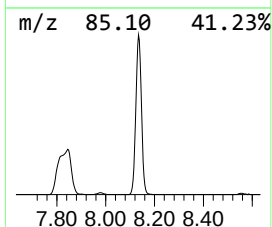
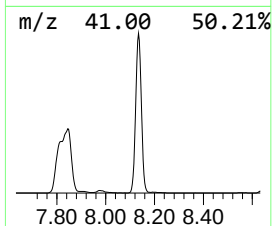
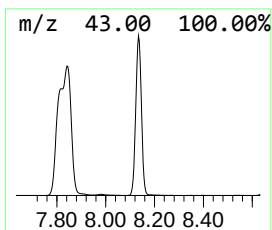
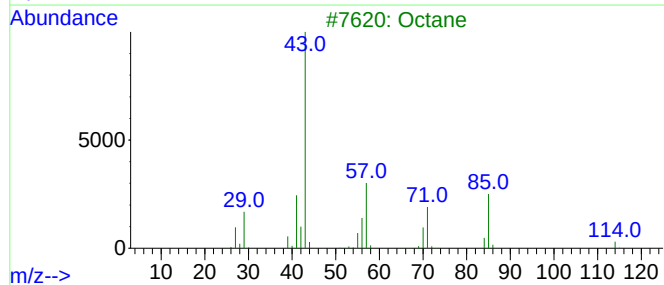
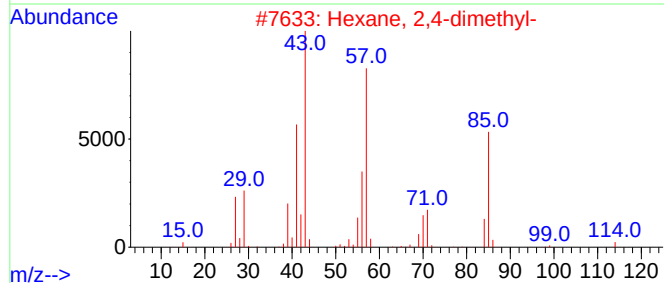
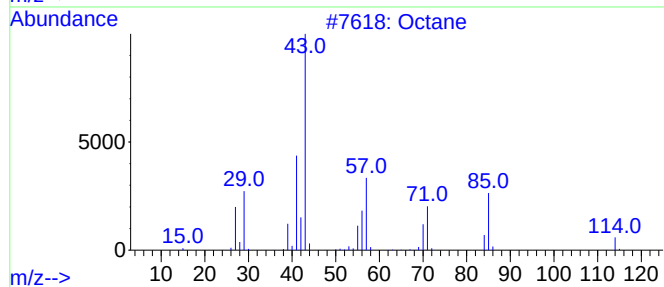
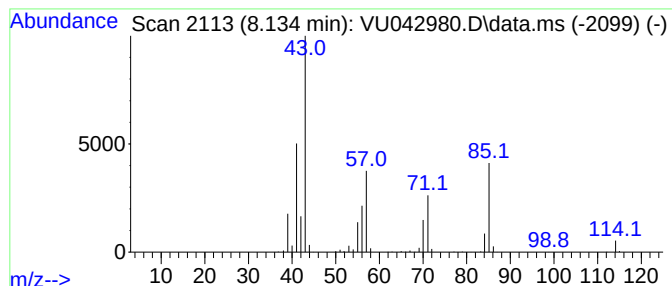
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM040721WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.134	27.40 ug/L	1018830	Chlorobenzene-d5	9.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane			114	C8H18	000111-65-9	95
2	Hexane, 2,4-dimethyl-			114	C8H18	000589-43-5	86
3	Octane			114	C8H18	000111-65-9	81
4	Heptane, 2,4-dimethyl-			128	C9H20	002213-23-2	72
5	Ether, hexyl pentyl			172	C11H24O	032357-83-8	64



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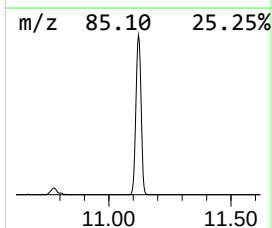
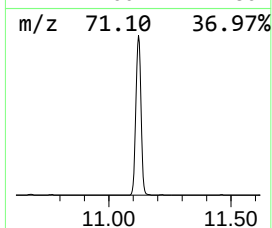
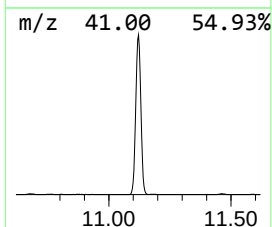
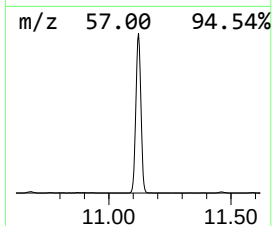
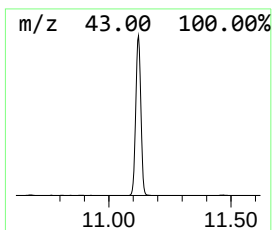
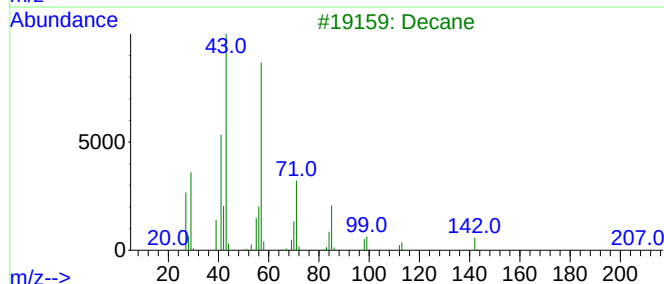
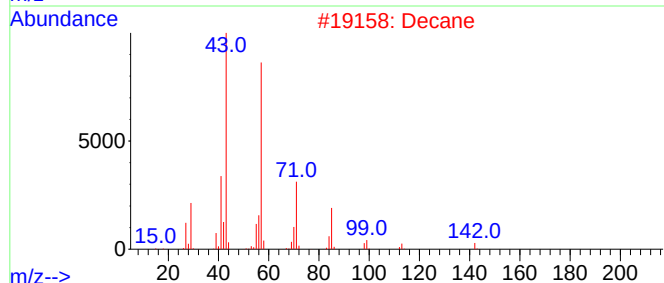
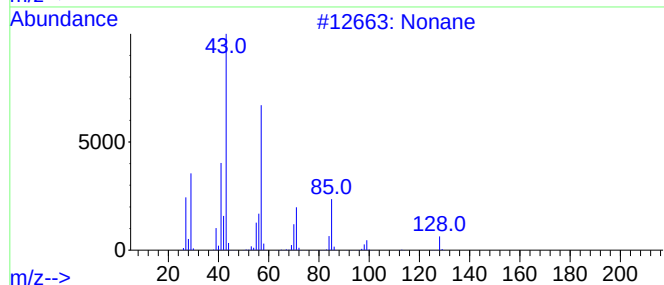
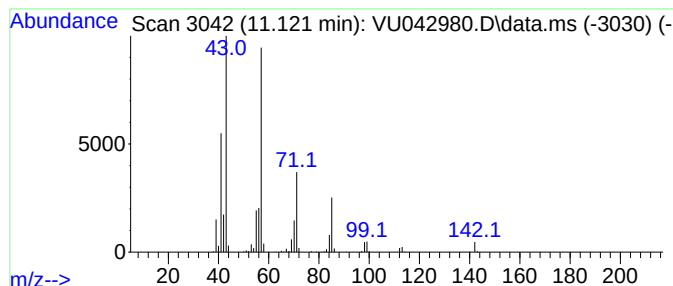
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 TIC Integration Parameters: LSCINT.P

 Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.121	52.60 ug/L	804173	1,4-Dichlorobenzene-d4			11.825
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonane		128	C9H20	000111-84-2	90
2	Decane		142	C10H22	000124-18-5	87
3	Decane		142	C10H22	000124-18-5	83
4	Nonane		128	C9H20	000111-84-2	83
5	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	83



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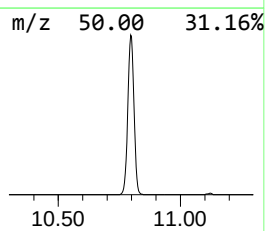
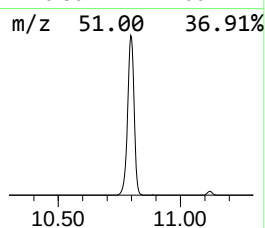
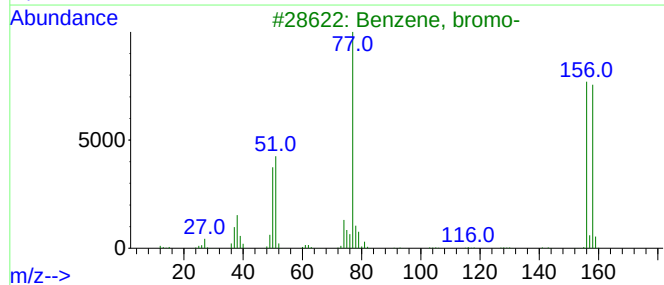
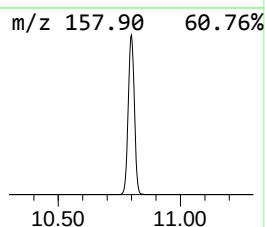
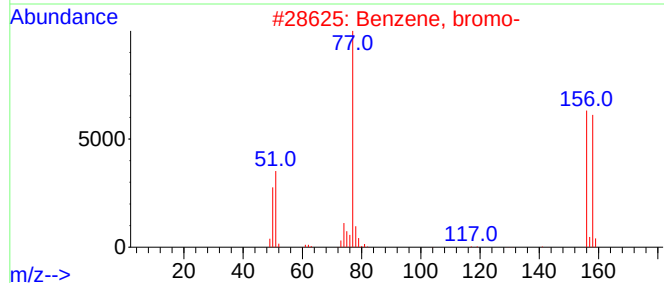
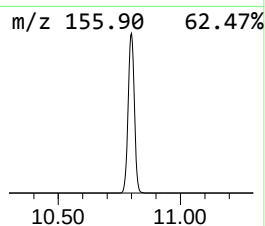
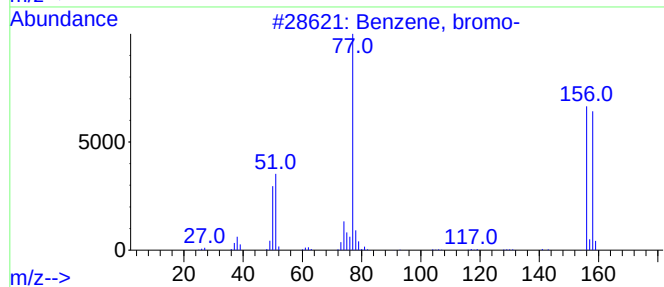
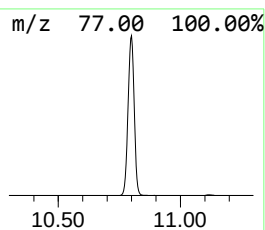
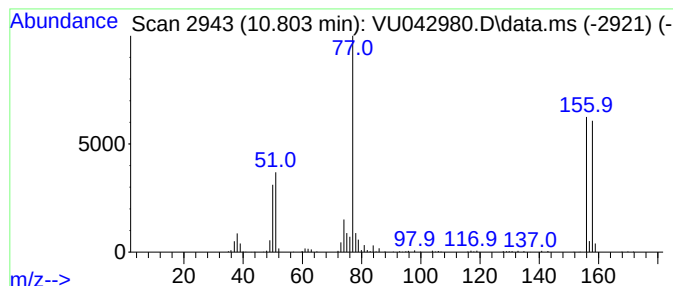
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, bromo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.797	82.77 ug/L	1265280	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, bromo-	156	C6H5Br	000108-86-1	97
2			Benzene, bromo-	156	C6H5Br	000108-86-1	96
3			Benzene, bromo-	156	C6H5Br	000108-86-1	94
4			Benzene, bromo-	156	C6H5Br	000108-86-1	93
5			Benzene, bromo-	156	C6H5Br	000108-86-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040721\
Data File : VU042980.D
Acq On : 07 Apr 2021 14:49
Operator : SY/MD
Sample : M1906-07
Misc : 5.0g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X3312

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM040721WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	8.134	27.4	ug/L	1018830	2	9.433	1859110	50.0
(DEL) Alkane: S...	11.121	52.6	ug/L	804173	3	11.825	764371	50.0
Benzene, bromo-	10.797	82.8	ug/L	1265280	3	11.825	764371	50.0