

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051322\
 Data File : VU048567.D
 Acq On : 13 May 2022 16:54
 Operator : SY/MD
 Sample : N2766-11ME
 Misc : 6.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4G1ME

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\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048567.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	73	79	86	rBV	61446	82931	7.56%	0.887%
2	2.279	290	292	293	rBV	323	148	0.01%	0.002%
3	2.530	357	370	384	rBV	195215	317954	29.00%	3.402%
4	2.822	456	461	466	rBV3	581	644	0.06%	0.007%
5	2.864	472	474	476	rBV	415	164	0.01%	0.002%
6	2.922	489	492	493	rBV	587	313	0.03%	0.003%
7	3.012	518	520	522	rBV2	690	455	0.04%	0.005%
8	3.089	542	544	547	rVB	322	188	0.02%	0.002%
9	3.179	555	572	588	rBV	42433	109313	9.97%	1.170%
10	3.475	662	664	672	rVB	505	479	0.04%	0.005%
11	3.517	672	677	679	rBV2	273	282	0.03%	0.003%
12	3.645	713	717	720	rBV2	194	168	0.02%	0.002%
13	3.681	726	728	731	rBV2	280	151	0.01%	0.002%
14	3.703	733	735	739	rVB2	258	177	0.02%	0.002%
15	3.726	739	742	746	rVB2	395	317	0.03%	0.003%
16	3.748	746	749	752	rBV	225	209	0.02%	0.002%
17	3.851	776	781	785	rBV	347	395	0.04%	0.004%
18	3.896	789	795	801	rBB	273	388	0.04%	0.004%
19	3.935	802	807	812	rBB	323	311	0.03%	0.003%
20	3.977	817	820	823	rVB	235	134	0.01%	0.001%
21	4.034	834	838	839	rBV	195	170	0.02%	0.002%
22	4.128	863	867	874	rVB	266	318	0.03%	0.003%
23	4.160	875	877	882	rBB2	352	272	0.02%	0.003%
24	4.186	882	885	887	rBV	390	284	0.03%	0.003%
25	4.301	919	921	926	rVB2	317	279	0.03%	0.003%
26	4.330	927	930	931	rBV	221	132	0.01%	0.001%
27	4.385	944	947	950	rVV2	310	245	0.02%	0.003%
28	4.417	955	957	959	rVB	347	164	0.01%	0.002%
29	4.436	959	963	968	rBV2	317	407	0.04%	0.004%
30	4.632	1009	1024	1043	rBV	87493	270739	24.69%	2.897%
31	4.938	1115	1119	1121	rBV2	438	313	0.03%	0.003%
32	5.060	1140	1157	1179	rBV2	190566	454686	41.47%	4.865%
33	5.179	1191	1194	1196	rVB	361	181	0.02%	0.002%
34	5.195	1197	1199	1200	rBV2	284	156	0.01%	0.002%
35	5.292	1223	1229	1231	rBV3	625	735	0.07%	0.008%
36	5.459	1277	1281	1282	rBV	308	175	0.02%	0.002%

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 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4G1ME

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\SFAMULM050622WMA.M
 Title : VOC Analysis

37	5.488	1287	1290	1291	rBV	234	134	0.01%	0.001%
38	5.571	1312	1316	1319	rVB2	242	161	0.01%	0.002%
39	5.716	1339	1361	1384	rBV2	425726	1096432	100.00%	11.732%
40	5.883	1410	1413	1417	rBV3	353	243	0.02%	0.003%
41	5.902	1417	1419	1421	rVB	446	222	0.02%	0.002%
42	5.922	1422	1425	1427	rBV	325	186	0.02%	0.002%
43	5.970	1431	1440	1457	rBV4	9377	22367	2.04%	0.239%
44	6.124	1486	1488	1492	rVB	338	215	0.02%	0.002%
45	6.166	1492	1501	1509	rBV2	985	1760	0.16%	0.019%
46	6.247	1512	1526	1550	rVB	336635	670483	61.15%	7.174%
47	6.407	1573	1576	1579	rBV	411	178	0.02%	0.002%
48	6.481	1597	1599	1600	rBV	309	149	0.01%	0.002%
49	6.526	1603	1613	1622	rBV6	4906	9274	0.85%	0.099%
50	6.594	1625	1634	1636	rBV2	3586	4395	0.40%	0.047%
51	6.690	1649	1664	1686	rVB	238065	493232	44.99%	5.278%
52	6.800	1695	1698	1701	rVB2	806	441	0.04%	0.005%
53	6.861	1715	1717	1721	rVB2	447	206	0.02%	0.002%
54	6.883	1721	1724	1726	rVV	223	146	0.01%	0.002%
55	6.935	1735	1740	1742	rBV2	482	459	0.04%	0.005%
56	7.009	1760	1763	1768	rVB2	512	561	0.05%	0.006%
57	7.050	1769	1776	1778	rBV2	754	810	0.07%	0.009%
58	7.365	1870	1874	1879	rBV2	212	196	0.02%	0.002%
59	7.407	1884	1887	1893	rBV2	362	553	0.05%	0.006%
60	7.494	1912	1914	1918	rVV4	425	307	0.03%	0.003%
61	7.565	1923	1936	1959	rVV2	131754	260198	23.73%	2.784%
62	7.690	1971	1975	1977	rBV4	531	338	0.03%	0.004%
63	7.790	1996	2006	2017	rBV4	7235	14486	1.32%	0.155%
64	7.896	2026	2039	2056	rBV	492480	881751	80.42%	9.435%
65	8.076	2093	2095	2099	rBV3	632	440	0.04%	0.005%
66	8.111	2103	2106	2110	rBV2	459	326	0.03%	0.003%
67	8.182	2116	2128	2148	rBV	89247	184144	16.79%	1.970%
68	8.304	2164	2166	2170	rVV	377	245	0.02%	0.003%
69	8.343	2175	2178	2181	rBV3	875	687	0.06%	0.007%
70	8.655	2256	2275	2309	rBV	291881	728140	66.41%	7.791%
71	9.102	2412	2414	2416	rBV	262	156	0.01%	0.002%
72	9.124	2419	2421	2423	rBV2	288	143	0.01%	0.002%
73	9.195	2440	2443	2445	rBV2	371	238	0.02%	0.003%
74	9.420	2500	2513	2541	rVB	470413	882026	80.45%	9.438%
75	9.565	2554	2558	2560	rBV2	492	368	0.03%	0.004%
76	9.693	2596	2598	2599	rBV	526	214	0.02%	0.002%

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 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4G1ME

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

77	9.735	2609	2611	2613	rBV2	603	292	0.03%	0.003%
78	9.774	2621	2623	2627	rVB	267	149	0.01%	0.002%
79	9.793	2627	2629	2631	rBV	256	162	0.01%	0.002%
80	9.861	2644	2650	2652	rBV2	385	380	0.03%	0.004%
81	9.873	2652	2654	2658	rVB3	838	560	0.05%	0.006%
82	9.944	2673	2676	2678	rBV	305	179	0.02%	0.002%
83	10.063	2711	2713	2717	rBV	218	134	0.01%	0.001%
84	10.246	2762	2770	2783	rBV5	2196	4232	0.39%	0.045%
85	10.317	2789	2792	2793	rBV5	505	263	0.02%	0.003%
86	10.352	2798	2803	2807	rVV5	606	736	0.07%	0.008%
87	10.623	2881	2887	2888	rBV3	1068	831	0.08%	0.009%
88	10.764	2918	2931	2956	rBV	419449	700082	63.85%	7.491%
89	10.915	2976	2978	2980	rBV2	559	349	0.03%	0.004%
90	10.947	2985	2988	2989	rVV	917	637	0.06%	0.007%
91	10.979	2993	2998	3001	rVV3	580	607	0.06%	0.006%
92	11.115	3033	3040	3057	rVB5	10399	17913	1.63%	0.192%
93	11.246	3079	3081	3082	rBV5	550	224	0.02%	0.002%
94	11.417	3127	3134	3141	rBV4	6527	8883	0.81%	0.095%
95	11.568	3177	3181	3183	rBV4	896	833	0.08%	0.009%
96	11.815	3246	3258	3273	rBV	627760	996013	90.84%	10.657%
97	12.198	3364	3377	3392	rBV	606947	978530	89.25%	10.470%
98	13.005	3624	3628	3634	rBV7	3154	4165	0.38%	0.045%
99	13.430	3753	3760	3769	rBV2	38683	58143	5.30%	0.622%
100	14.449	4071	4077	4086	rVB2	51552	70115	6.39%	0.750%

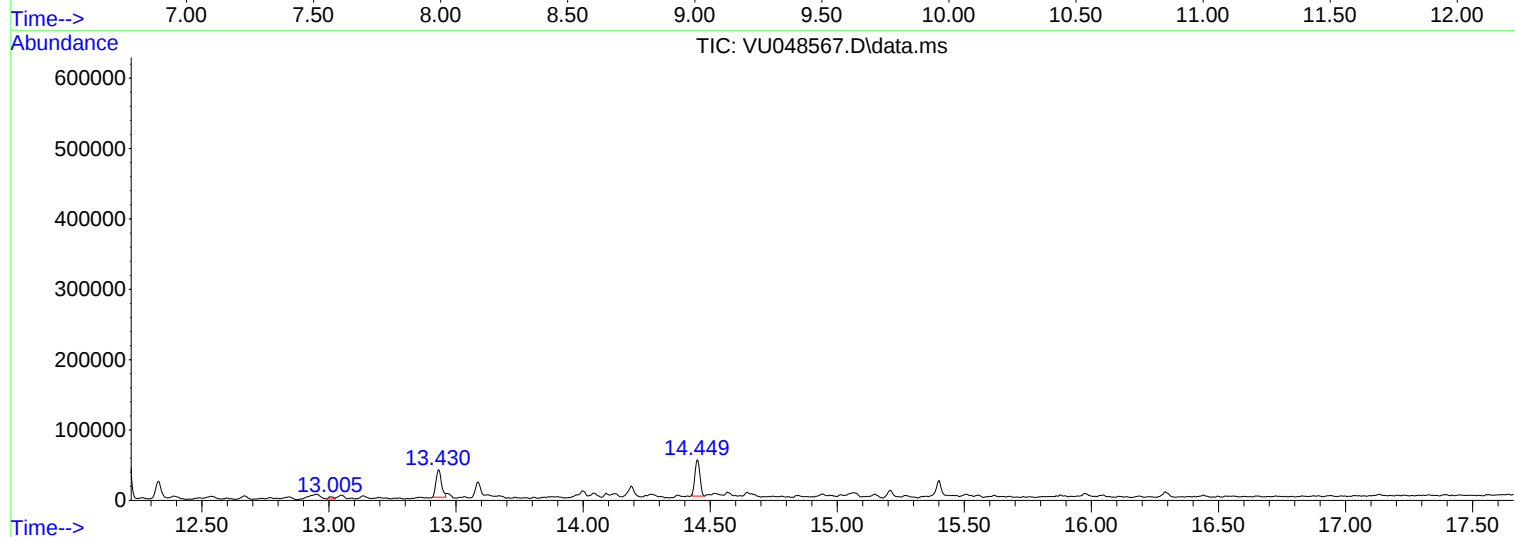
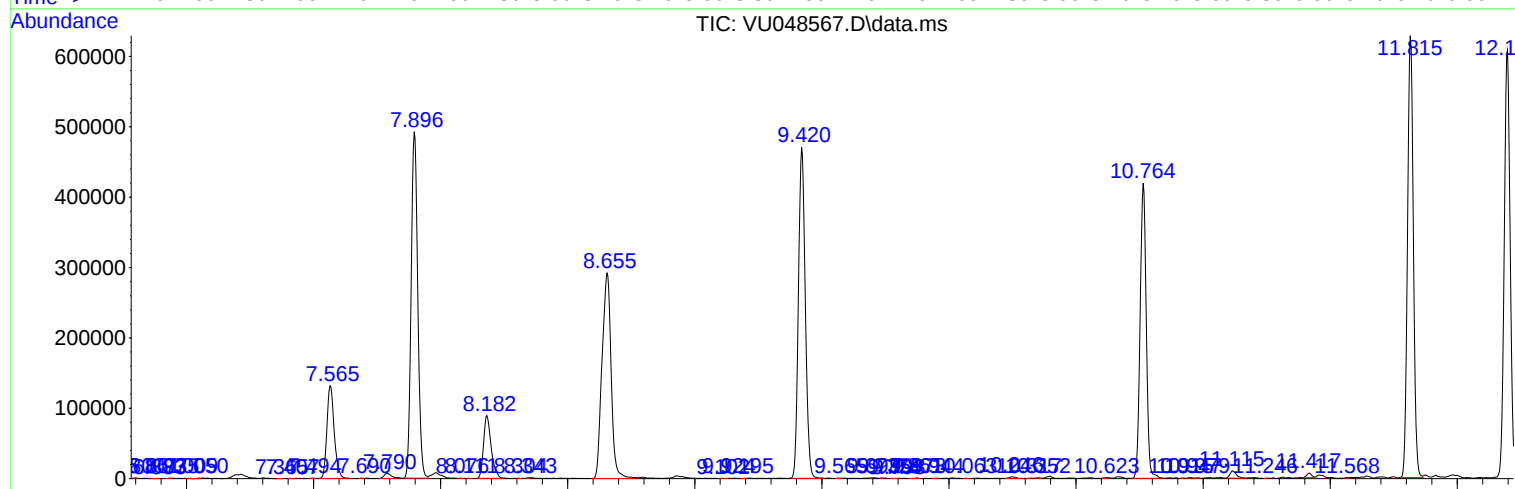
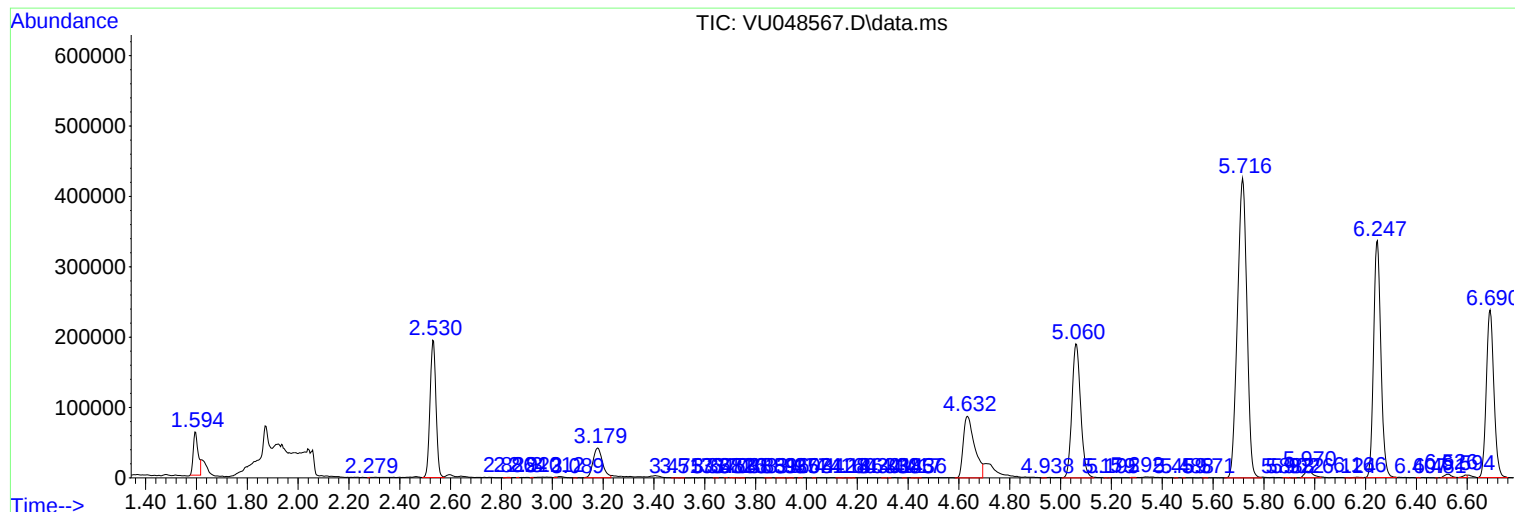
Sum of corrected areas: 9345799

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4G1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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



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Sample : N2766-11ME
Misc : 6.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4G1ME

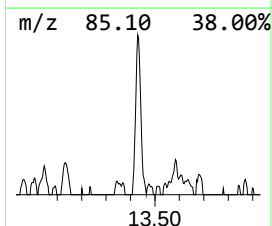
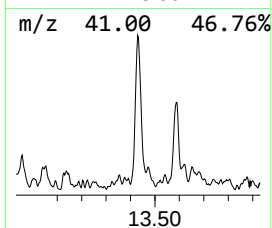
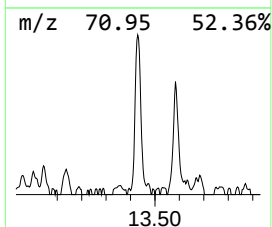
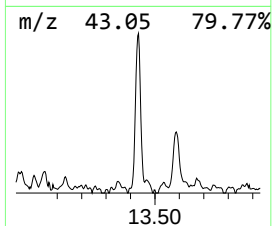
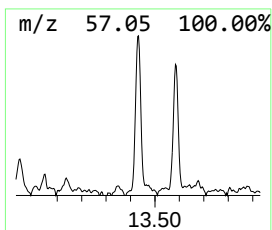
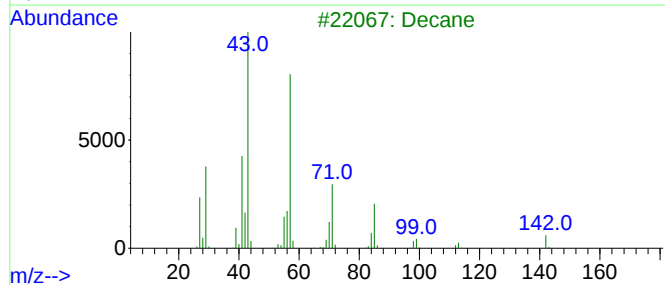
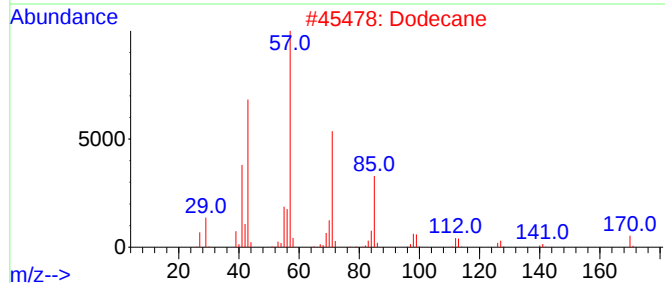
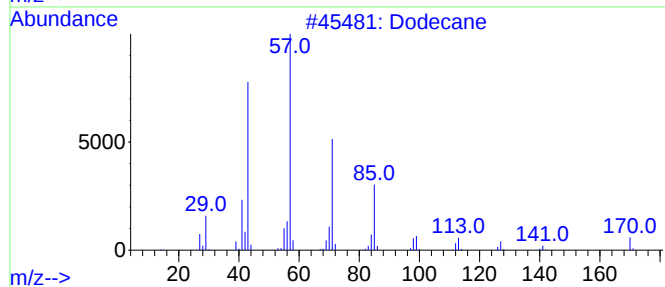
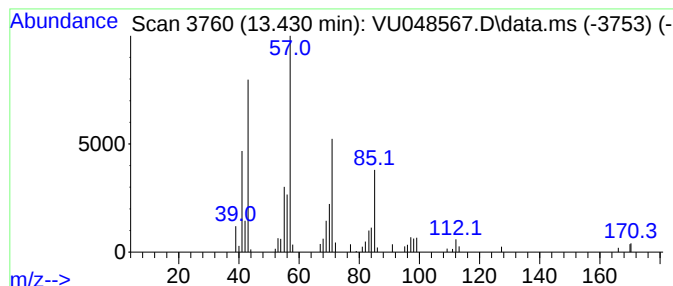
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.430	2.92 ug/L	58143	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	83
3			Decane	142	C10H22	000124-18-5	83
4			Dodecane	170	C12H26	000112-40-3	74
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72



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Misc : 6.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4G1ME

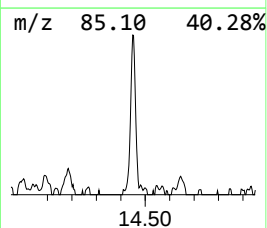
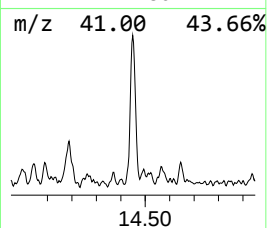
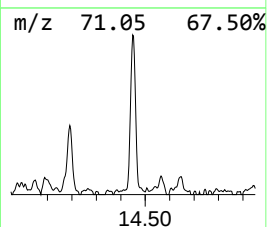
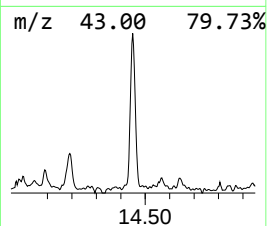
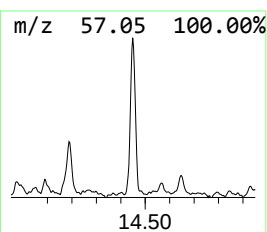
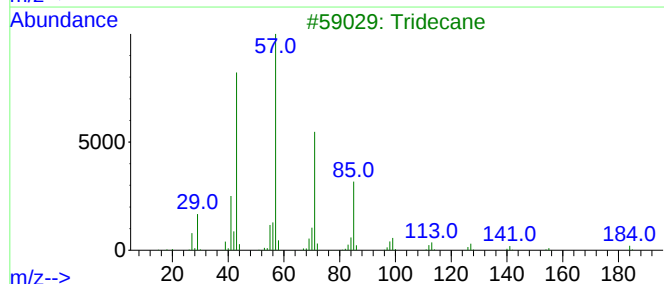
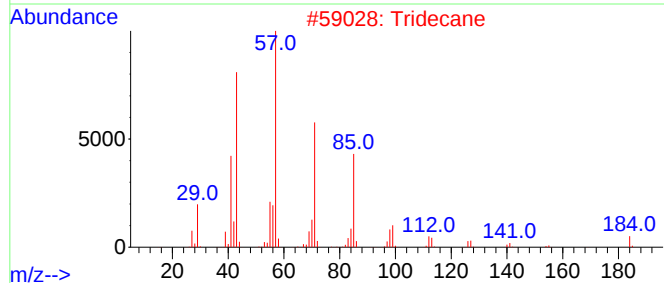
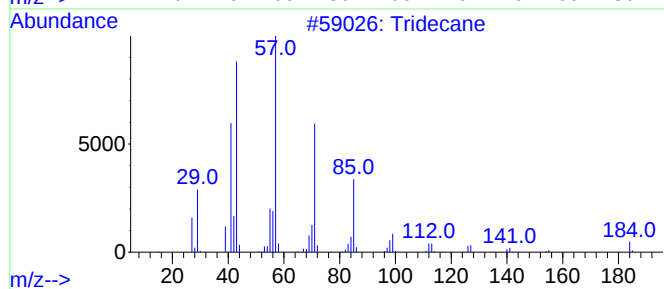
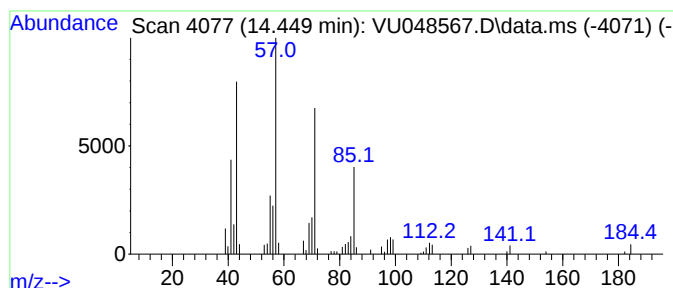
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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.
14.449	3.52 ug/L	70115	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Tridecane	184	C13H28	000629-50-5	94
3			Tridecane	184	C13H28	000629-50-5	93
4			Dodecane	170	C12H26	000112-40-3	90
5			Tetradecane	198	C14H30	000629-59-4	86



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ClientSampleId :
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Quant Title : VOC Analysis

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

					--Internal Standard--			
TIC Top	Hit name	RT	EstConc	Units	Response	#	RT	Resp Conc
(DEL)	Alkane: S...	13.430	2.9	ug/L	58143	3	11.815	996013 50.0
(DEL)	Alkane: S...	14.449	3.5	ug/L	70115	3	11.815	996013 50.0