

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
 Data File : VU055838.D
 Acq On : 20 Oct 2023 17:28
 Operator : MD/SY
 Sample : 04961-02ME
 Misc : 5.45g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EOLH9ME

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.483	55	60	65	rBV4	6366	6891	0.24%	0.037%
2	1.599	88	96	113	rVB	140953	226613	7.91%	1.206%
3	1.878	179	183	200	rVB	41930	66166	2.31%	0.352%
4	2.541	377	389	412	rVB	344473	574331	20.06%	3.057%
5	2.702	437	439	441	rBV2	683	398	0.01%	0.002%
6	2.898	495	500	505	rVB3	707	799	0.03%	0.004%
7	3.036	532	543	561	rVB6	7357	19821	0.69%	0.105%
8	3.100	561	563	565	rBV	564	368	0.01%	0.002%
9	3.174	571	586	606	rBV	37333	96217	3.36%	0.512%
10	3.338	632	637	643	rVB7	1356	1383	0.05%	0.007%
11	3.563	702	707	712	rBV3	545	647	0.02%	0.003%
12	3.673	729	741	743	rBV5	2628	3713	0.13%	0.020%
13	3.798	775	780	785	rVV3	416	416	0.01%	0.002%
14	3.962	826	831	834	rBV2	619	492	0.02%	0.003%
15	4.174	894	897	901	rBV	441	348	0.01%	0.002%
16	4.496	992	997	999	rBV3	948	865	0.03%	0.005%
17	4.518	999	1004	1007	rVV5	661	600	0.02%	0.003%
18	4.631	1027	1039	1090	rBV2	105176	416800	14.56%	2.218%
19	5.055	1154	1171	1203	rVV	309113	757865	26.47%	4.034%
20	5.290	1241	1244	1247	rBV4	574	455	0.02%	0.002%
21	5.328	1251	1256	1258	rBV4	647	571	0.02%	0.003%
22	5.537	1316	1321	1325	rBV	483	483	0.02%	0.003%
23	5.714	1353	1376	1413	rBV2	695598	1868515	65.26%	9.945%
24	5.894	1429	1432	1437	rVB4	499	425	0.01%	0.002%
25	5.975	1449	1457	1461	rBV6	4675	7298	0.25%	0.039%
26	6.119	1495	1502	1503	rBV4	2331	1773	0.06%	0.009%
27	6.161	1513	1515	1517	rVB	827	412	0.01%	0.002%
28	6.184	1517	1522	1526	rBV2	497	439	0.02%	0.002%
29	6.242	1526	1540	1569	rBV	654500	1394088	48.69%	7.420%
30	6.393	1583	1587	1589	rBV2	623	460	0.02%	0.002%
31	6.534	1618	1631	1645	rBV6	46513	104406	3.65%	0.556%
32	6.685	1664	1678	1709	rVV2	396839	853235	29.80%	4.541%
33	6.811	1712	1717	1723	rVB9	2224	2636	0.09%	0.014%
34	6.888	1740	1741	1746	rVB2	496	350	0.01%	0.002%
35	6.975	1761	1768	1770	rBV5	1111	850	0.03%	0.005%
36	6.994	1772	1774	1777	rVB2	629	373	0.01%	0.002%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	7.052	1788	1792	1794	rBV2	611	445	0.02%	0.002%
38	7.193	1828	1836	1845	rBV7	6187	14959	0.52%	0.080%
39	7.306	1869	1871	1873	rBV4	659	344	0.01%	0.002%
40	7.422	1903	1907	1910	rVV4	457	381	0.01%	0.002%
41	7.496	1921	1930	1938	rBV6	2756	4640	0.16%	0.025%
42	7.563	1938	1951	1975	rBV	201201	414072	14.46%	2.204%
43	7.705	1986	1995	2001	rBV9	2802	4691	0.16%	0.025%
44	7.849	2034	2040	2041	rBV6	1409	1386	0.05%	0.007%
45	7.894	2041	2054	2074	rBV	781632	1464925	51.16%	7.797%
46	8.061	2102	2106	2110	rBV5	753	818	0.03%	0.004%
47	8.129	2121	2127	2132	rBV5	3214	4128	0.14%	0.022%
48	8.180	2132	2143	2171	rVB	125599	281622	9.84%	1.499%
49	8.280	2171	2174	2179	rVB3	904	749	0.03%	0.004%
50	8.348	2190	2195	2197	rBV4	1367	1364	0.05%	0.007%
51	8.428	2216	2220	2222	rBV2	698	406	0.01%	0.002%
52	8.550	2244	2258	2276	rBV	1628837	2863180	100.00%	15.239%
53	8.656	2276	2291	2319	rVV2	310673	809336	28.27%	4.308%
54	8.920	2365	2373	2383	rBV2	4634	8798	0.31%	0.047%
55	8.984	2388	2393	2394	rBV4	795	629	0.02%	0.003%
56	9.068	2414	2419	2425	rVB6	1346	1658	0.06%	0.009%
57	9.113	2427	2433	2440	rBV7	3011	3952	0.14%	0.021%
58	9.171	2441	2451	2456	rVV8	4064	7716	0.27%	0.041%
59	9.209	2457	2463	2473	rVB6	6254	11210	0.39%	0.060%
60	9.335	2490	2502	2512	rBV4	7349	13502	0.47%	0.072%
61	9.418	2515	2528	2554	rBV	859676	1766565	61.70%	9.403%
62	9.630	2590	2594	2596	rBV2	773	654	0.02%	0.003%
63	9.650	2596	2600	2605	rVV6	1558	1632	0.06%	0.009%
64	9.672	2605	2607	2609	rBV2	876	436	0.02%	0.002%
65	9.743	2623	2629	2639	rVB5	12380	18822	0.66%	0.100%
66	9.868	2662	2668	2677	rBV4	1685	3017	0.11%	0.016%
67	9.955	2687	2695	2697	rBV4	1244	1582	0.06%	0.008%
68	10.016	2706	2714	2725	rBV10	4142	8229	0.29%	0.044%
69	10.090	2732	2737	2738	rBV3	973	595	0.02%	0.003%
70	10.110	2738	2743	2744	rBV2	3498	2325	0.08%	0.012%
71	10.219	2769	2777	2778	rBV4	1376	1345	0.05%	0.007%
72	10.248	2778	2786	2798	rVB4	11184	19157	0.67%	0.102%
73	10.296	2798	2801	2802	rBV3	635	372	0.01%	0.002%
74	10.309	2802	2805	2808	rBV5	1190	1058	0.04%	0.006%
75	10.393	2824	2831	2844	rVB4	16211	26964	0.94%	0.144%
76	10.557	2870	2882	2892	rBV9	7520	16907	0.59%	0.090%

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Instrument :
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 ClientSampleId :
 E0LH9ME

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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 Title : VOC Analysis

77	10.621	2898	2902	2909	rVB3	6717	6597	0.23%	0.035%
78	10.759	2928	2945	2978	rBV	607968	1044550	36.48%	5.560%
79	10.897	2985	2988	2989	rBV2	1009	572	0.02%	0.003%
80	11.007	3018	3022	3023	rBV3	1608	1173	0.04%	0.006%
81	11.065	3031	3040	3046	rBV7	6696	11386	0.40%	0.061%
82	11.113	3047	3055	3072	rVB2	39999	67347	2.35%	0.358%
83	11.187	3072	3078	3079	rBV4	1772	1653	0.06%	0.009%
84	11.309	3110	3116	3117	rBV4	3716	3612	0.13%	0.019%
85	11.376	3129	3137	3141	rBV6	4937	7578	0.26%	0.040%
86	11.415	3142	3149	3157	rVB3	22681	34429	1.20%	0.183%
87	11.576	3190	3199	3202	rBV7	3291	5461	0.19%	0.029%
88	11.711	3236	3241	3246	rBV7	4571	5627	0.20%	0.030%
89	11.814	3261	3273	3287	rBV	1016686	1643835	57.41%	8.749%
90	12.142	3373	3375	3378	rBV4	1104	847	0.03%	0.005%
91	12.193	3379	3391	3411	rVV	783168	1297953	45.33%	6.908%
92	12.325	3424	3432	3443	rVB	79279	113812	3.98%	0.606%
93	12.666	3530	3538	3549	rVB6	12454	19647	0.69%	0.105%
94	12.933	3610	3621	3622	rBV8	15798	23105	0.81%	0.123%
95	13.003	3638	3643	3650	rBV7	8016	10217	0.36%	0.054%
96	13.045	3652	3656	3665	rVB3	12342	15632	0.55%	0.083%
97	13.132	3678	3683	3693	rVB5	10274	13380	0.47%	0.071%
98	13.428	3767	3775	3799	rVB2	87178	151111	5.28%	0.804%
99	13.582	3816	3823	3832	rBV	37589	57471	2.01%	0.306%
100	14.447	4085	4092	4100	rBV2	40525	55005	1.92%	0.293%

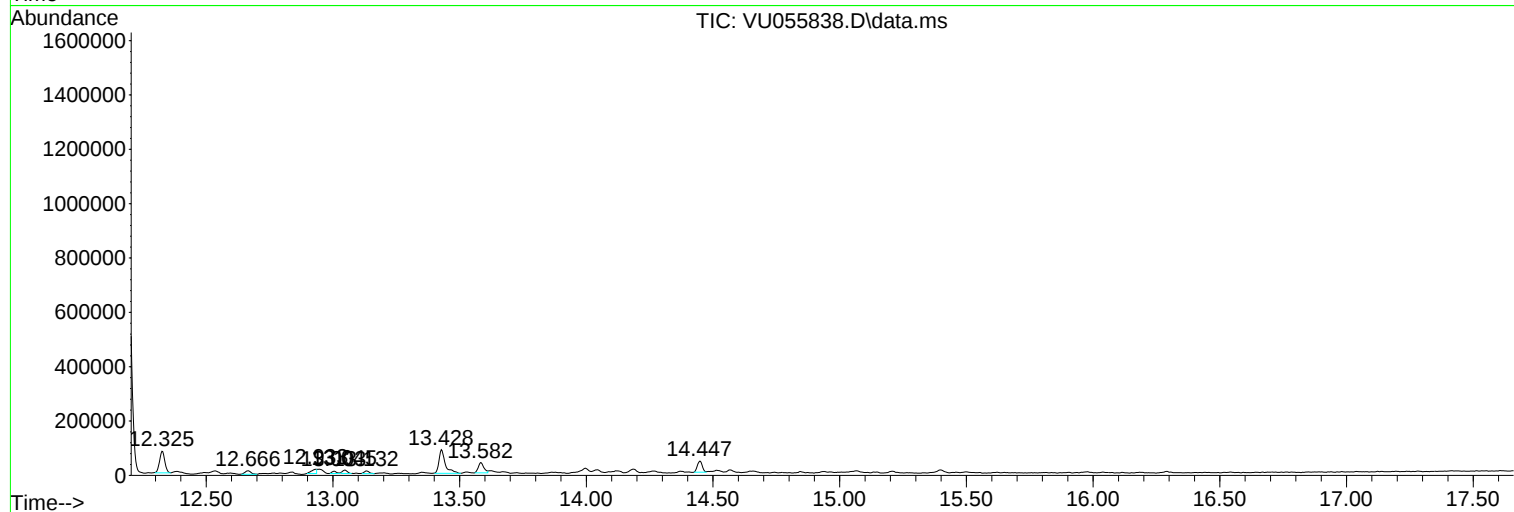
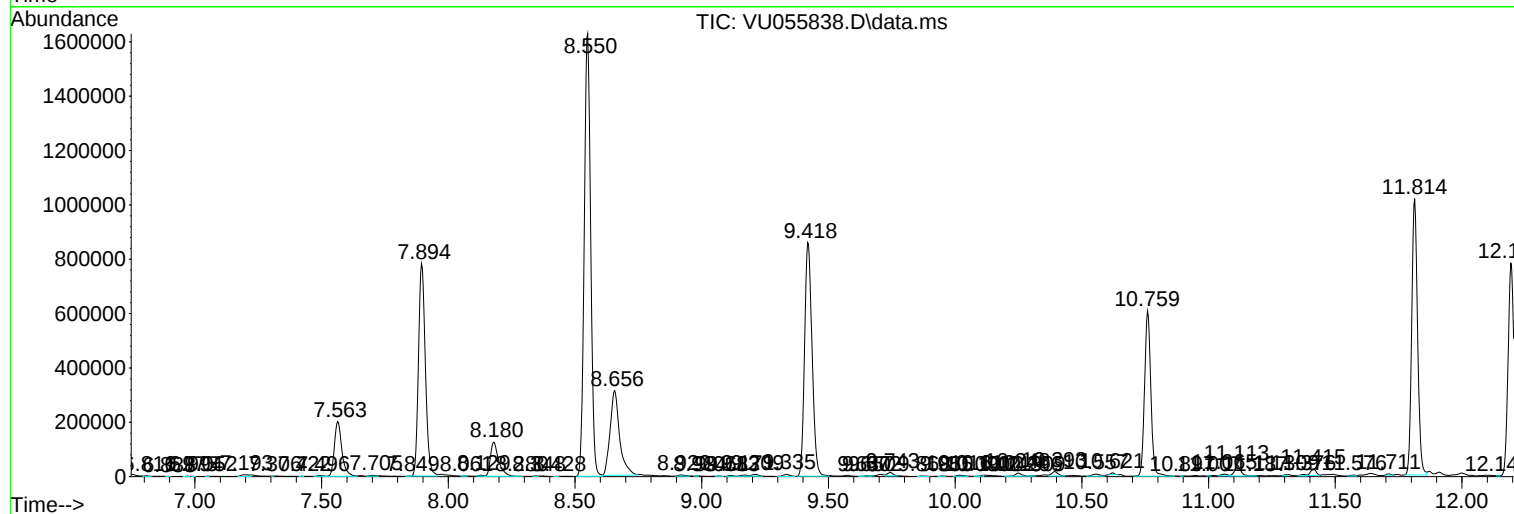
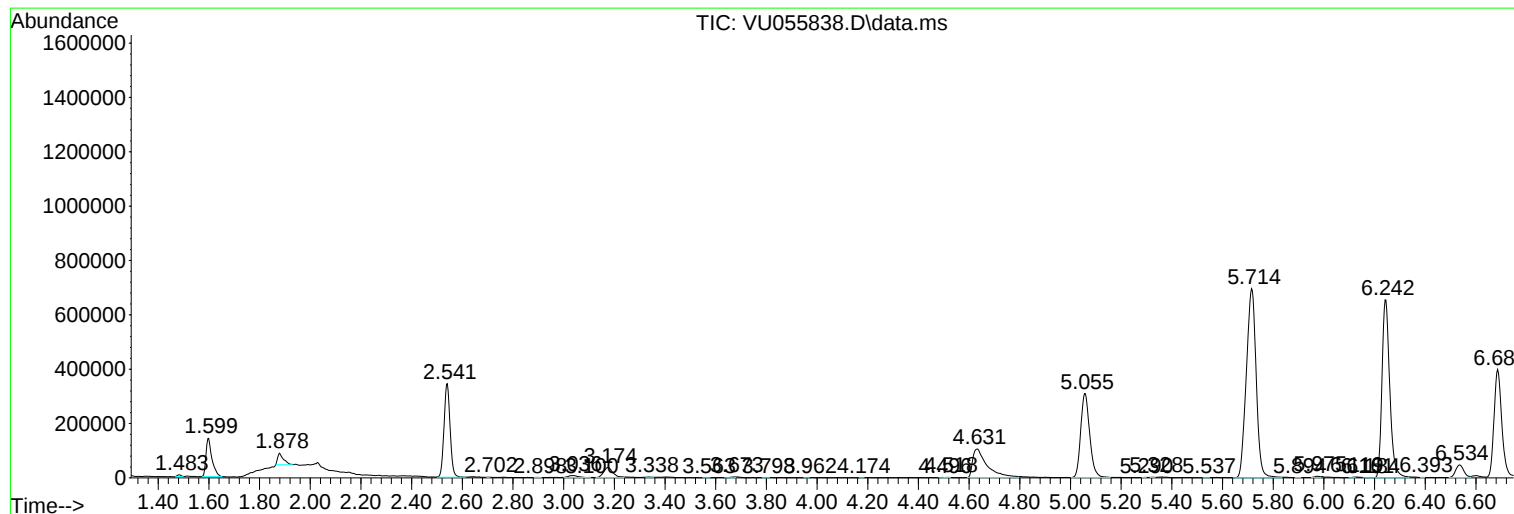
Sum of corrected areas: 18788073

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Instrument :
MSVOA_U
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E0LH9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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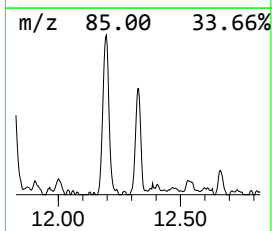
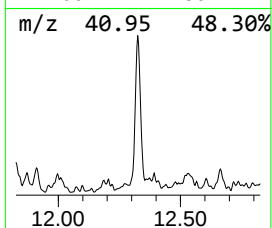
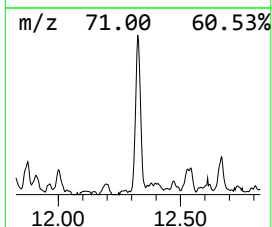
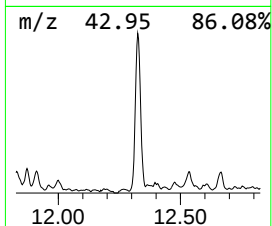
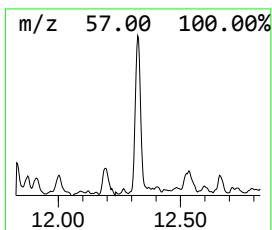
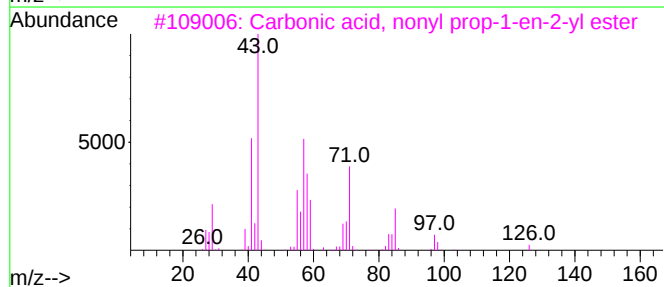
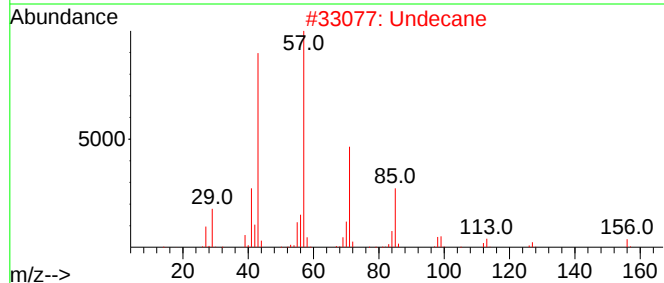
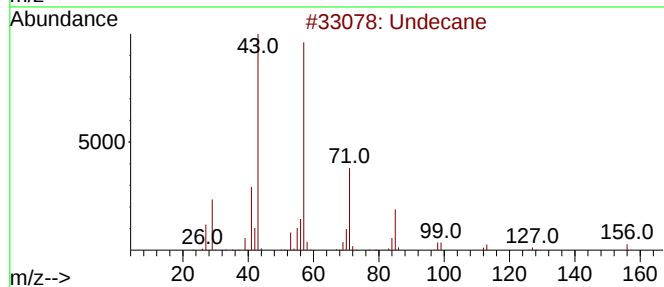
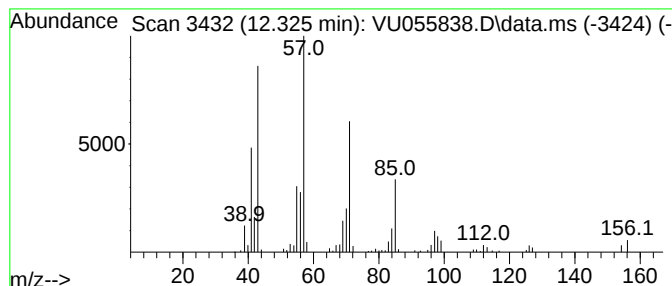
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.325	3.46 ug/L	113812	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	81
2	Undecane			156	C11H24	001120-21-4	74
3	Carbonic acid, nonyl prop-1-en-2...			228	C13H24O3	1000382-53-9	72
4	Undecane			156	C11H24	001120-21-4	68
5	Ether, heptyl hexyl			200	C13H28O	007289-40-9	58



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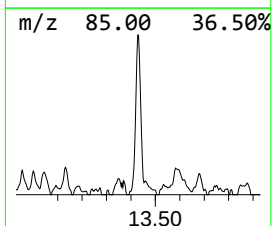
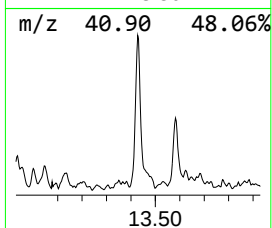
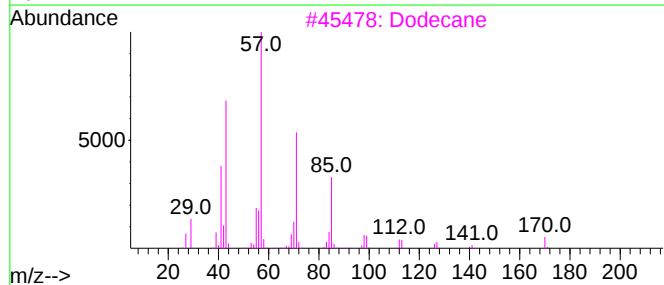
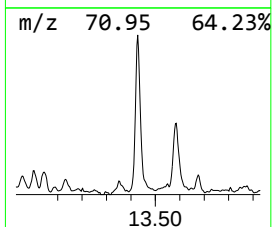
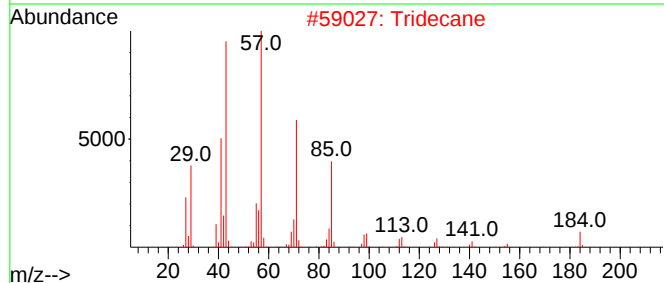
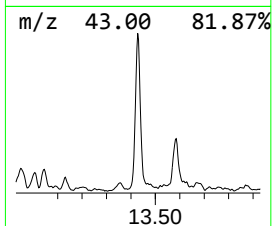
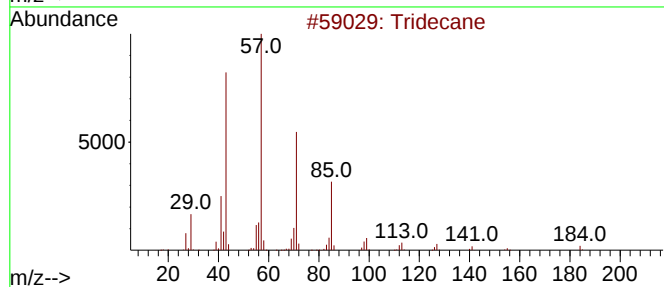
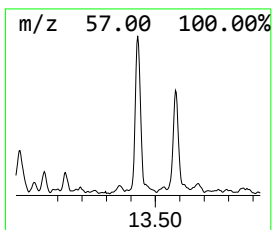
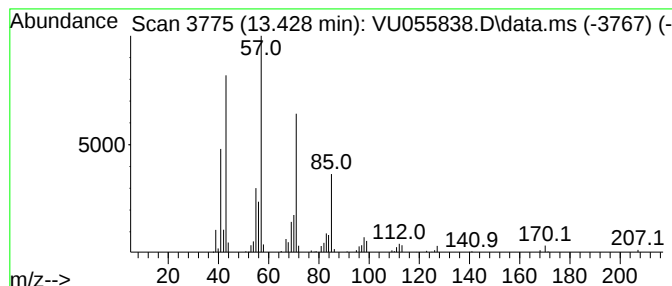
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
13.428	4.60 ug/L	151111	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	80
2			Tridecane	184	C13H28	000629-50-5	80
3			Dodecane	170	C12H26	000112-40-3	76
4			Hexadecane	226	C16H34	000544-76-3	72
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64



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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	12.325	3.5	ug/L	113812	3	11.814	1643840	50.0
(DEL) Alkane: S...	13.428	4.6	ug/L	151111	3	11.814	1643840	50.0