

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050494.D
 Acq On : 29 Aug 2022 19:07
 Operator : SY/MD
 Sample : N4322-10ME
 Misc : 5.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY170ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050494.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	39	44	49	rBV3	4267	5217	0.33%	0.044%
2	1.594	71	79	86	rBV	97568	129346	8.13%	1.089%
3	1.887	165	170	179	rBV	37372	52938	3.33%	0.446%
4	2.523	356	368	392	rVB	315790	517059	32.50%	4.355%
5	2.941	494	498	501	rBV2	436	419	0.03%	0.004%
6	3.028	515	525	543	rVB2	7937	16379	1.03%	0.138%
7	3.182	558	573	596	rBV	10297	30158	1.90%	0.254%
8	3.375	631	633	639	rVB3	418	389	0.02%	0.003%
9	3.514	673	676	681	rVB2	376	305	0.02%	0.003%
10	3.542	681	685	690	rBV2	247	304	0.02%	0.003%
11	3.665	713	723	733	rVB5	1503	2638	0.17%	0.022%
12	3.726	736	742	750	rBV	290	356	0.02%	0.003%
13	3.819	765	771	773	rBV2	257	283	0.02%	0.002%
14	4.234	893	900	902	rBV2	252	266	0.02%	0.002%
15	4.591	1006	1011	1014	rBV2	273	286	0.02%	0.002%
16	4.649	1015	1029	1074	rBV	112074	416726	26.19%	3.510%
17	5.060	1140	1157	1184	rBV	266661	649237	40.81%	5.468%
18	5.285	1220	1227	1238	rBV5	1388	2557	0.16%	0.022%
19	5.356	1238	1249	1253	rBV4	2037	3127	0.20%	0.026%
20	5.443	1273	1276	1280	rBV3	529	494	0.03%	0.004%
21	5.578	1308	1318	1327	rVB7	3044	5658	0.36%	0.048%
22	5.716	1340	1361	1391	rBV2	629312	1590895	100.00%	13.398%
23	5.983	1432	1444	1466	rBV2	12456	30424	1.91%	0.256%
24	6.124	1478	1488	1499	rVB6	5080	9634	0.61%	0.081%
25	6.169	1499	1502	1510	rVB2	294	288	0.02%	0.002%
26	6.247	1510	1526	1550	rBV	446229	903159	56.77%	7.606%
27	6.443	1581	1587	1591	rVB3	428	483	0.03%	0.004%
28	6.529	1603	1614	1628	rBV7	5175	10731	0.67%	0.090%
29	6.610	1628	1639	1649	rVV5	5755	13099	0.82%	0.110%
30	6.690	1649	1664	1690	rVV	354596	731711	45.99%	6.162%
31	6.800	1693	1698	1709	rVV7	2142	3882	0.24%	0.033%
32	6.861	1711	1717	1724	rVB6	1502	1927	0.12%	0.016%
33	6.976	1750	1753	1761	rVB3	575	624	0.04%	0.005%
34	7.066	1773	1781	1791	rVB6	2362	3763	0.24%	0.032%
35	7.230	1815	1832	1846	rBV9	9261	21323	1.34%	0.180%
36	7.423	1885	1892	1899	rVB5	1086	1552	0.10%	0.013%

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Integration Parameters: LSCINT.P

Integrator: RTE

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

37	7.494	1899	1914	1921	rBV3	7684	14683	0.92%	0.124%
38	7.568	1925	1937	1957	rVV	146171	282579	17.76%	2.380%
39	7.655	1957	1964	1973	rVB6	4606	7155	0.45%	0.060%
40	7.899	2017	2040	2061	rBV	640963	1162573	73.08%	9.791%
41	7.992	2062	2069	2070	rBV3	5787	5824	0.37%	0.049%
42	8.127	2105	2111	2118	rVV3	8757	12101	0.76%	0.102%
43	8.182	2118	2128	2157	rVB	93861	195234	12.27%	1.644%
44	8.353	2173	2181	2187	rBV	1550	2309	0.15%	0.019%
45	8.433	2201	2206	2210	rBV3	922	652	0.04%	0.005%
46	8.468	2214	2217	2218	rBV3	503	273	0.02%	0.002%
47	8.539	2229	2239	2250	rVB3	2686	4967	0.31%	0.042%
48	8.661	2259	2277	2306	rBV2	339119	892070	56.07%	7.513%
49	8.861	2336	2339	2349	rVB5	3465	4198	0.26%	0.035%
50	8.925	2349	2359	2371	rBV2	13931	25737	1.62%	0.217%
51	9.031	2388	2392	2394	rBV2	653	418	0.03%	0.004%
52	9.070	2394	2404	2414	rVV8	5230	9613	0.60%	0.081%
53	9.118	2414	2419	2426	rVV6	2443	3180	0.20%	0.027%
54	9.166	2426	2434	2441	rVV8	5604	10197	0.64%	0.086%
55	9.214	2443	2449	2458	rVB2	6297	10350	0.65%	0.087%
56	9.336	2477	2487	2494	rBV3	7224	11781	0.74%	0.099%
57	9.420	2500	2513	2538	rBV	596171	1109095	69.72%	9.341%
58	9.542	2547	2551	2552	rBV3	412	278	0.02%	0.002%
59	9.661	2574	2588	2595	rBV6	2849	7017	0.44%	0.059%
60	9.745	2600	2614	2625	rVB3	13097	23785	1.50%	0.200%
61	9.822	2633	2638	2641	rBV2	513	450	0.03%	0.004%
62	9.870	2647	2653	2661	rBV3	2386	3301	0.21%	0.028%
63	9.957	2674	2680	2683	rBV3	309	341	0.02%	0.003%
64	10.018	2691	2699	2700	rBV4	2815	2508	0.16%	0.021%
65	10.118	2722	2730	2733	rBV5	2012	2546	0.16%	0.021%
66	10.250	2762	2771	2786	rVV5	7694	19025	1.20%	0.160%
67	10.307	2787	2789	2792	rVB4	946	581	0.04%	0.005%
68	10.365	2797	2807	2810	rBV8	4206	7088	0.45%	0.060%
69	10.449	2827	2833	2834	rBV2	783	648	0.04%	0.005%
70	10.545	2852	2863	2864	rBV5	2562	3346	0.21%	0.028%
71	10.623	2884	2887	2893	rVB2	2918	2435	0.15%	0.021%
72	10.703	2904	2912	2914	rBV4	828	1069	0.07%	0.009%
73	10.764	2917	2931	2958	rVB	510544	867018	54.50%	7.302%
74	10.915	2974	2978	2979	rBV3	476	313	0.02%	0.003%
75	10.947	2983	2988	2995	rVB6	1726	2158	0.14%	0.018%
76	11.018	3004	3010	3017	rBV7	1592	2714	0.17%	0.023%

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Instrument :
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 ClientSampleId :
 EY170ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

77	11.063	3019	3024	3030	rVV7	3621	5602	0.35%	0.047%
78	11.115	3032	3040	3056	rVB2	21378	35355	2.22%	0.298%
79	11.176	3056	3059	3060	rBV2	794	443	0.03%	0.004%
80	11.188	3060	3063	3072	rVB6	1604	1926	0.12%	0.016%
81	11.307	3094	3100	3112	rBV8	3277	5316	0.33%	0.045%
82	11.375	3118	3121	3124	rBV4	1149	913	0.06%	0.008%
83	11.417	3127	3134	3142	rBV2	9654	12452	0.78%	0.105%
84	11.465	3143	3149	3154	rBV8	2221	3290	0.21%	0.028%
85	11.571	3176	3182	3186	rBV6	1370	1844	0.12%	0.016%
86	11.713	3220	3226	3233	rBV7	2943	3328	0.21%	0.028%
87	11.815	3246	3258	3272	rBV	515838	836333	52.57%	7.043%
88	11.992	3309	3313	3322	rVB9	3990	6384	0.40%	0.054%
89	12.089	3335	3343	3349	rBV6	1767	3356	0.21%	0.028%
90	12.198	3364	3377	3391	rBV	544650	893376	56.16%	7.524%
91	12.330	3410	3418	3429	rVB2	30568	43399	2.73%	0.365%
92	12.667	3515	3523	3531	rVB8	4740	7102	0.45%	0.060%
93	12.706	3531	3535	3539	rBV6	1050	984	0.06%	0.008%
94	12.928	3594	3604	3607	rBV8	6183	9909	0.62%	0.083%
95	13.012	3622	3630	3634	rBV5	2728	4145	0.26%	0.035%
96	13.137	3661	3669	3673	rBV7	3675	4948	0.31%	0.042%
97	13.433	3753	3761	3783	rVB2	28517	50175	3.15%	0.423%
98	13.587	3802	3809	3817	rBV2	17006	24550	1.54%	0.207%
99	14.452	4070	4078	4086	rBV2	23148	31502	1.98%	0.265%
100	15.401	4368	4373	4383	rVB4	13904	18121	1.14%	0.153%

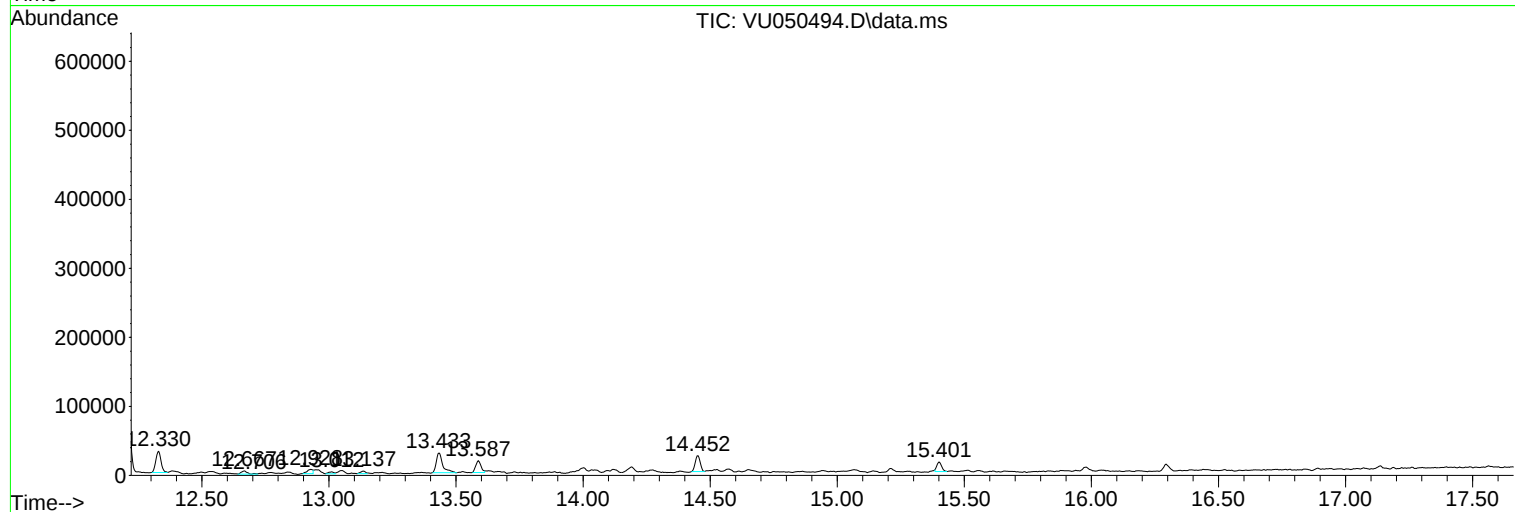
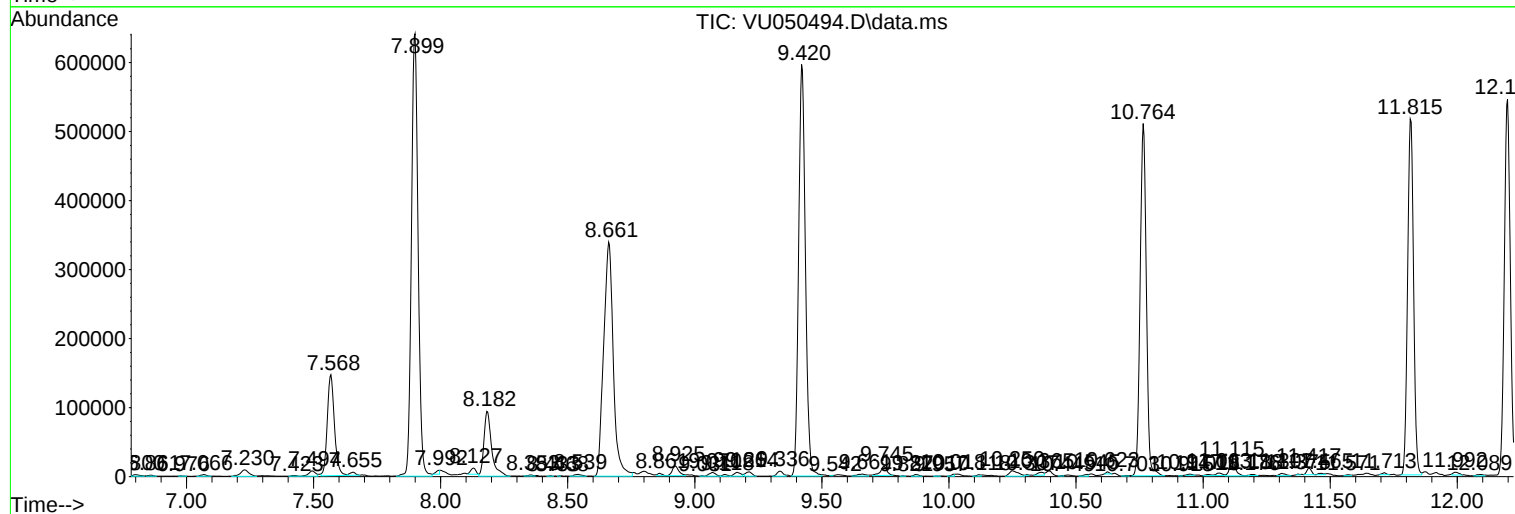
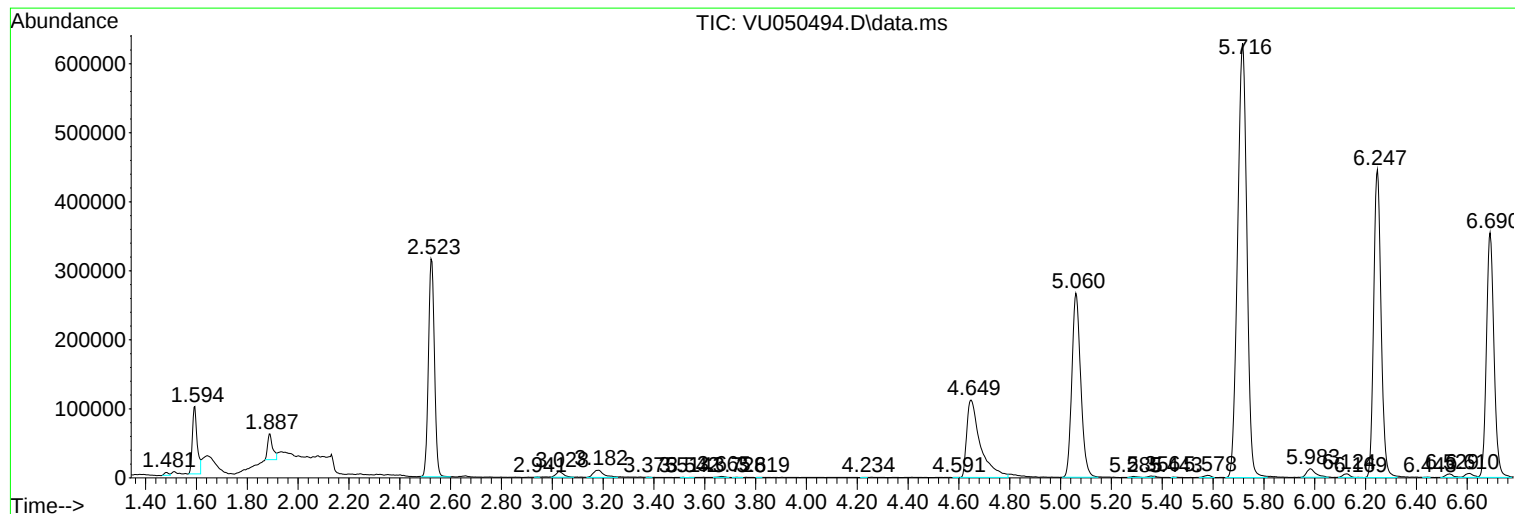
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY170ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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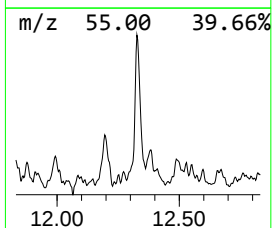
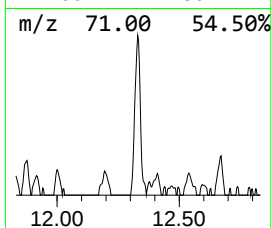
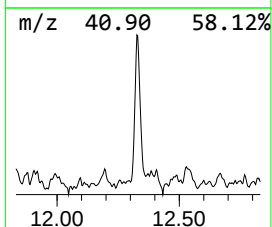
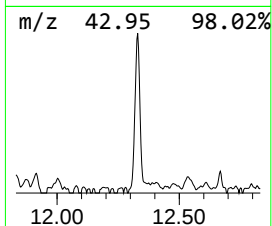
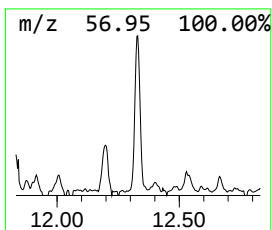
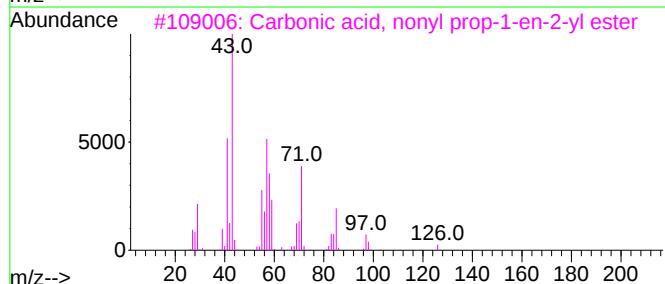
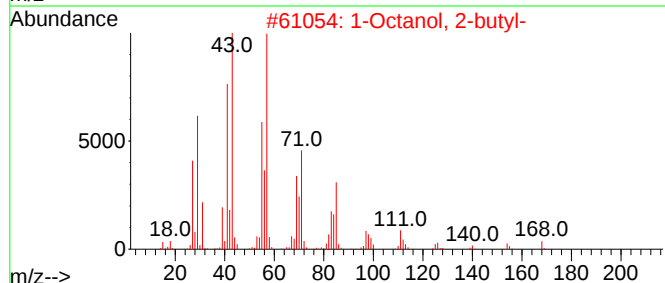
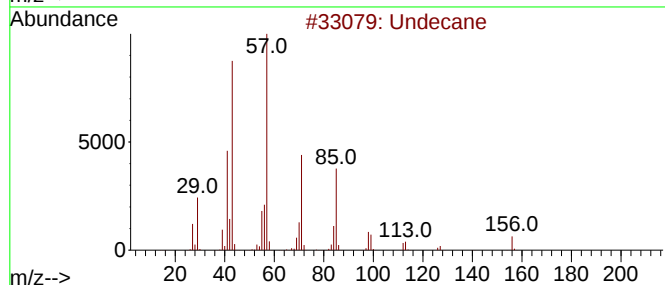
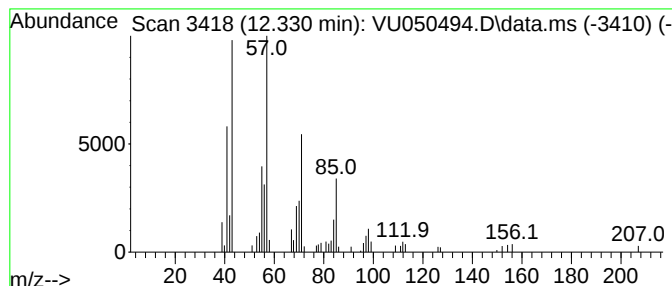
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	2.59 ug/L	43399	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	86
2			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	86
3			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	78
4			Undecane	156	C11H24	001120-21-4	74
5			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	72



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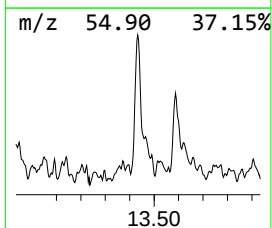
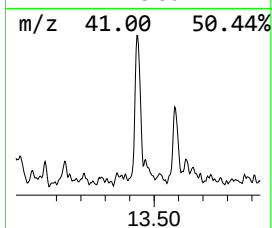
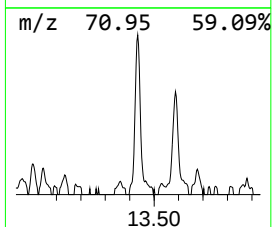
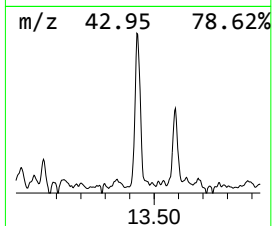
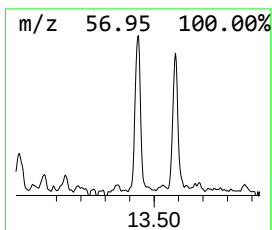
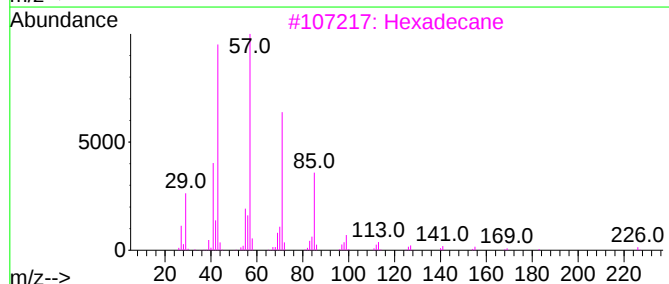
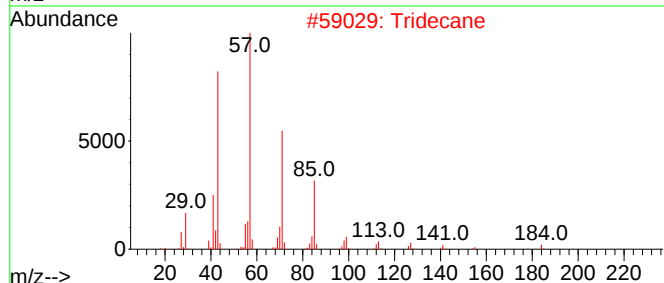
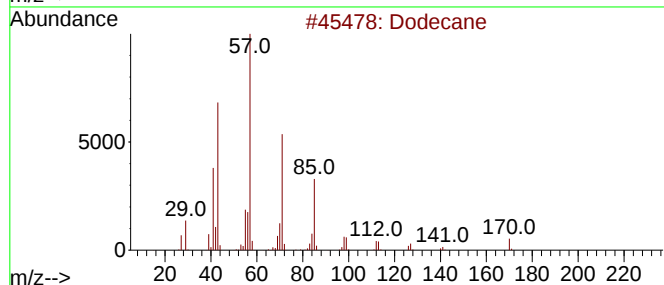
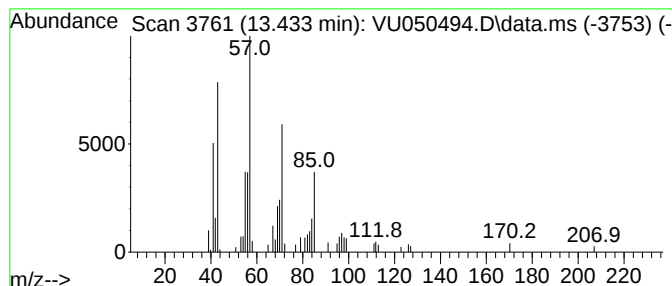
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Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	3.00 ug/L	50175	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	81
2			Tridecane	184	C13H28	000629-50-5	59
3			Hexadecane	226	C16H34	000544-76-3	59
4			Tetradecane	198	C14H30	000629-59-4	59
5			Hexadecane	226	C16H34	000544-76-3	59



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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...	12.330	2.6	ug/L	43399	3	11.819	836333 50.0
(DEL)	Alkane: S...	13.433	3.0	ug/L	50175	3	11.819	836333 50.0