

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
 Data File : VU048375.D
 Acq On : 02 May 2022 17:55
 Operator : SY/MD
 Sample : N2639-15
 Misc : 5.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXL23

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\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	38	44	51	rBV	27697	39427	2.08%	0.267%
2	1.597	74	80	86	rBV	55997	83987	4.42%	0.568%
3	2.533	354	371	387	rBV	258855	479849	25.28%	3.244%
4	2.871	473	476	481	rBV2	609	537	0.03%	0.004%
5	2.964	491	505	510	rBV3	3321	6085	0.32%	0.041%
6	3.031	520	526	537	rBV5	2953	5551	0.29%	0.038%
7	3.118	549	553	557	rBV5	645	600	0.03%	0.004%
8	3.179	559	572	588	rBV	22021	55087	2.90%	0.372%
9	3.662	717	722	726	rVV3	1250	1304	0.07%	0.009%
10	3.697	730	733	737	rVB	754	582	0.03%	0.004%
11	3.916	794	801	803	rBV	745	844	0.04%	0.006%
12	4.247	900	904	907	rBV	550	456	0.02%	0.003%
13	4.308	920	923	927	rVB2	685	476	0.03%	0.003%
14	4.330	927	930	934	rBV	493	471	0.02%	0.003%
15	4.388	943	948	951	rBV	460	479	0.03%	0.003%
16	4.652	1015	1030	1046	rBV2	113141	426478	22.47%	2.883%
17	5.067	1142	1159	1192	rBV	292410	770330	40.58%	5.207%
18	5.208	1196	1203	1223	rVB	10569	25368	1.34%	0.171%
19	5.719	1342	1362	1392	rBV2	766693	1898254	100.00%	12.832%
20	5.980	1433	1443	1466	rBV3	15036	40473	2.13%	0.274%
21	6.247	1512	1526	1558	rVB	496400	1050251	55.33%	7.099%
22	6.404	1564	1575	1593	rBV2	11139	25086	1.32%	0.170%
23	6.526	1604	1613	1623	rBV9	5531	11242	0.59%	0.076%
24	6.604	1630	1637	1650	rBV2	6758	11310	0.60%	0.076%
25	6.690	1650	1664	1687	rBV	395967	862618	45.44%	5.831%
26	6.941	1733	1742	1749	rBV2	6634	14486	0.76%	0.098%
27	7.192	1810	1820	1852	rBV9	21289	80134	4.22%	0.542%
28	7.440	1894	1897	1901	rBV2	933	665	0.04%	0.004%
29	7.568	1923	1937	1961	rBV	196907	425257	22.40%	2.875%
30	7.694	1970	1976	1982	rBV8	1571	2610	0.14%	0.018%
31	7.793	1996	2007	2018	rBV3	7241	14719	0.78%	0.099%
32	7.899	2026	2040	2057	rBV	808948	1516627	79.90%	10.252%
33	8.186	2115	2129	2156	rBV	130909	318061	16.76%	2.150%
34	8.353	2176	2181	2188	rBV7	2004	2506	0.13%	0.017%
35	8.552	2238	2243	2252	rBV6	1442	2560	0.13%	0.017%
36	8.674	2257	2281	2307	rBV	488620	1195155	62.96%	8.079%

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 Title : VOC Analysis

37	9.176	2434	2437	2440	rVB2	861	607	0.03%	0.004%
38	9.195	2440	2443	2447	rVB2	943	528	0.03%	0.004%
39	9.423	2500	2514	2542	rBV	601464	1310084	69.02%	8.856%
40	9.584	2558	2564	2569	rBV7	907	1166	0.06%	0.008%
41	9.694	2594	2598	2610	rVB6	1935	3192	0.17%	0.022%
42	9.893	2654	2660	2664	rVB2	702	782	0.04%	0.005%
43	10.012	2694	2697	2700	rBV	713	561	0.03%	0.004%
44	10.063	2706	2713	2718	rVB	654	950	0.05%	0.006%
45	10.102	2719	2725	2728	rBV2	1211	1421	0.07%	0.010%
46	10.234	2762	2766	2770	rVV	501	487	0.03%	0.003%
47	10.301	2781	2787	2790	rBV	817	867	0.05%	0.006%
48	10.327	2793	2795	2801	rVB	842	867	0.05%	0.006%
49	10.362	2801	2806	2809	rBV2	944	965	0.05%	0.007%
50	10.462	2834	2837	2839	rBV	721	532	0.03%	0.004%
51	10.520	2852	2855	2857	rBV	758	523	0.03%	0.004%
52	10.629	2886	2889	2895	rBV2	744	961	0.05%	0.006%
53	10.674	2895	2903	2909	rVV5	2308	3341	0.18%	0.023%
54	10.771	2919	2933	2948	rBV	701644	1161043	61.16%	7.848%
55	10.893	2967	2971	2980	rVB7	1610	2061	0.11%	0.014%
56	11.057	3013	3022	3029	rBV6	5236	7629	0.40%	0.052%
57	11.115	3029	3040	3059	rVV3	66546	100434	5.29%	0.679%
58	11.243	3077	3080	3086	rVB2	987	909	0.05%	0.006%
59	11.279	3086	3091	3095	rBV3	654	869	0.05%	0.006%
60	11.301	3095	3098	3103	rVV3	604	463	0.02%	0.003%
61	11.417	3131	3134	3135	rBV2	1269	635	0.03%	0.004%
62	11.481	3141	3154	3159	rVB6	1912	3754	0.20%	0.025%
63	11.504	3159	3161	3165	rVB2	886	576	0.03%	0.004%
64	11.639	3197	3203	3209	rBV3	606	702	0.04%	0.005%
65	11.697	3214	3221	3228	rBV6	1713	2623	0.14%	0.018%
66	11.732	3228	3232	3235	rBV3	602	457	0.02%	0.003%
67	11.819	3244	3259	3272	rBV	792394	1253988	66.06%	8.477%
68	11.915	3282	3289	3295	rVB7	3968	5730	0.30%	0.039%
69	12.002	3312	3316	3325	rVB5	3868	5054	0.27%	0.034%
70	12.066	3328	3336	3349	rBV5	8801	18539	0.98%	0.125%
71	12.198	3363	3377	3394	rBV	875119	1422760	74.95%	9.617%
72	12.330	3409	3418	3429	rVB2	15695	23233	1.22%	0.157%
73	12.497	3466	3470	3475	rBV2	537	629	0.03%	0.004%
74	12.600	3499	3502	3506	rVV2	834	671	0.04%	0.005%
75	12.706	3531	3535	3539	rBV2	928	790	0.04%	0.005%
76	12.777	3543	3557	3565	rVV4	3061	5741	0.30%	0.039%

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 Title : VOC Analysis

77	12.819	3565	3570	3575	rVB4	528	637	0.03%	0.004%
78	12.893	3582	3593	3603	rBV7	3096	6317	0.33%	0.043%
79	12.996	3619	3625	3629	rBV2	961	1330	0.07%	0.009%
80	13.115	3658	3662	3664	rBV	716	656	0.03%	0.004%
81	13.214	3683	3693	3705	rBV2	16188	25150	1.32%	0.170%
82	13.324	3722	3727	3731	rBV	1001	998	0.05%	0.007%
83	13.391	3740	3748	3755	rVV5	8112	11461	0.60%	0.077%
84	13.433	3755	3761	3769	rVB4	3956	5169	0.27%	0.035%
85	13.497	3774	3781	3786	rBV4	705	791	0.04%	0.005%
86	13.848	3887	3890	3895	rVB3	630	553	0.03%	0.004%
87	13.951	3919	3922	3929	rVB3	672	631	0.03%	0.004%
88	13.992	3929	3935	3937	rBV	939	971	0.05%	0.007%
89	14.060	3953	3956	3961	rVB4	501	520	0.03%	0.004%
90	14.095	3964	3967	3973	rBV3	949	1169	0.06%	0.008%
91	14.189	3994	3996	4003	rVB4	1889	1474	0.08%	0.010%
92	14.404	4060	4063	4067	rBV3	726	466	0.02%	0.003%
93	14.446	4070	4076	4083	rBV5	4956	7127	0.38%	0.048%
94	14.526	4096	4101	4103	rVB2	835	617	0.03%	0.004%
95	14.542	4103	4106	4109	rBV2	882	742	0.04%	0.005%
96	14.578	4111	4117	4122	rBV2	2376	2467	0.13%	0.017%
97	14.883	4210	4212	4216	rVB2	876	504	0.03%	0.003%
98	15.211	4308	4314	4317	rBV5	1676	2029	0.11%	0.014%
99	15.375	4360	4365	4369	rBV5	3530	4214	0.22%	0.028%
100	15.478	4395	4397	4400	rBV3	918	584	0.03%	0.004%

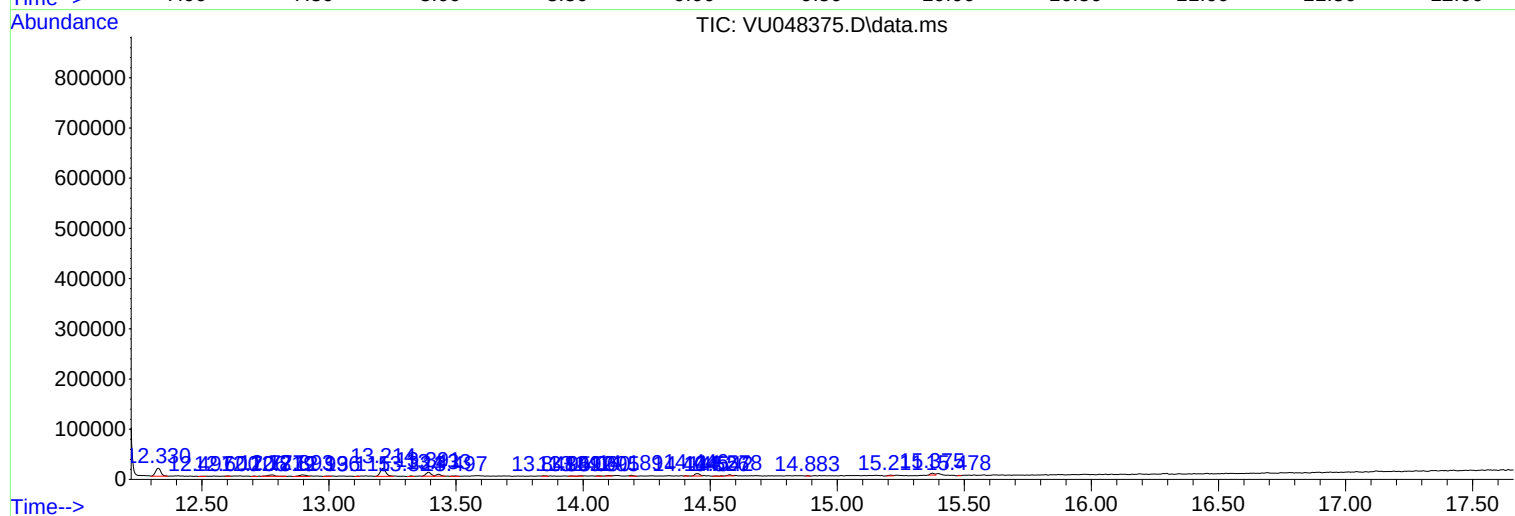
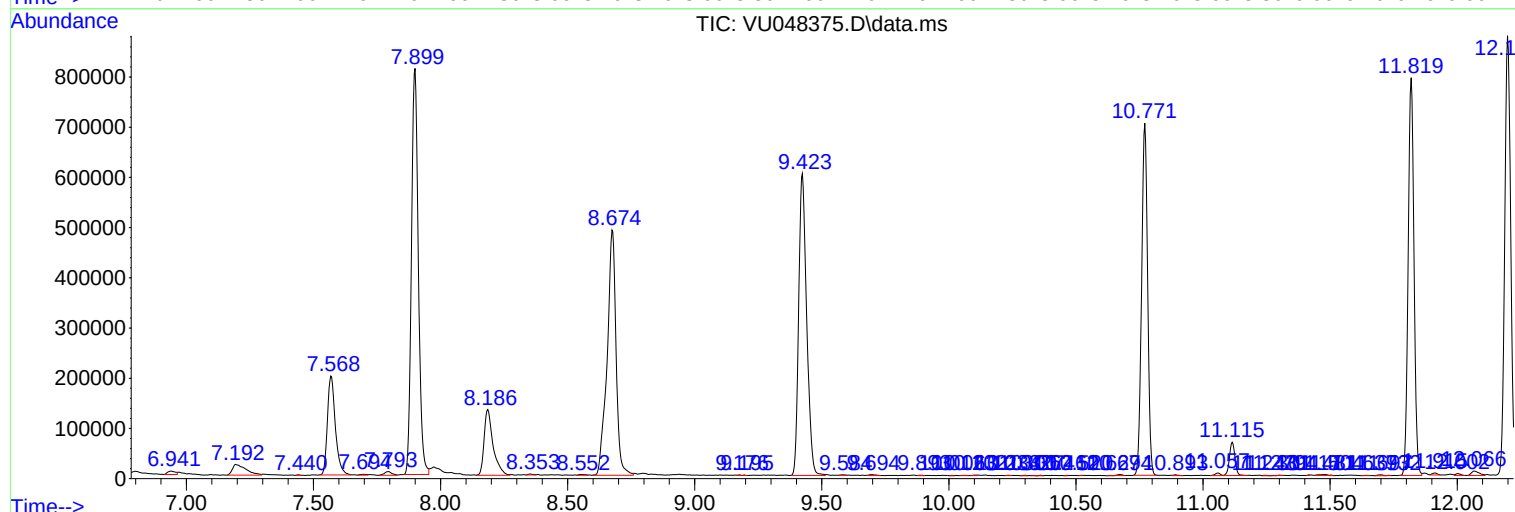
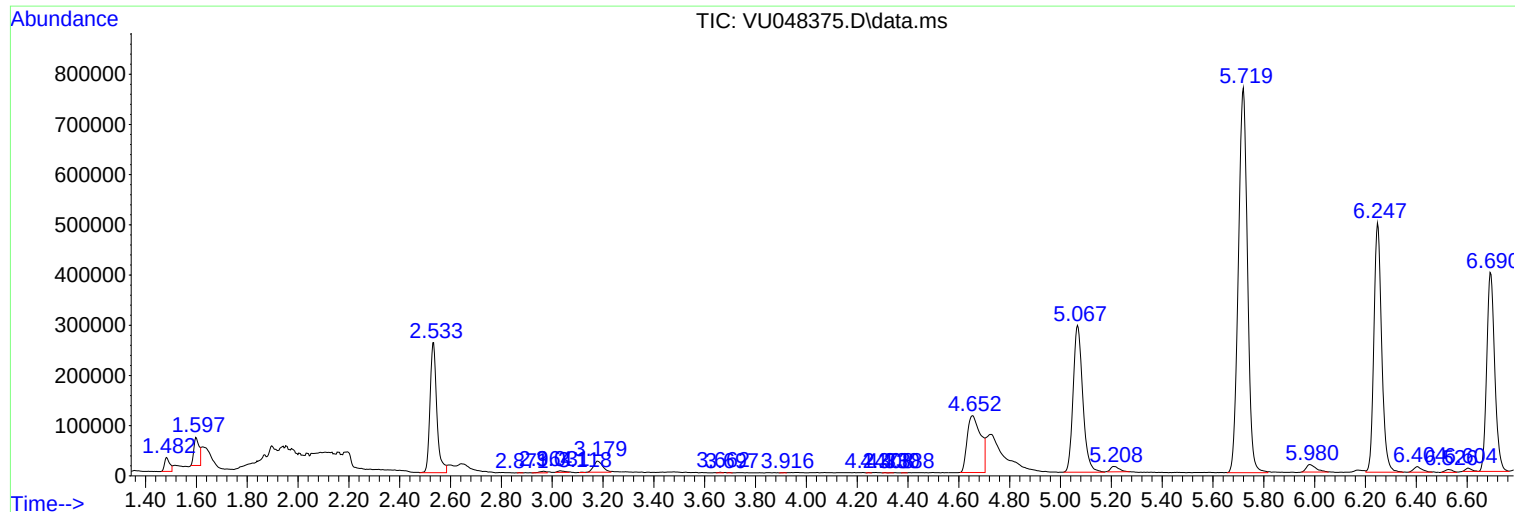
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



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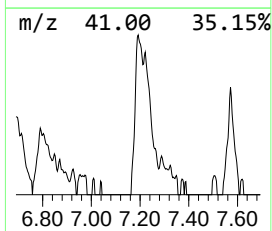
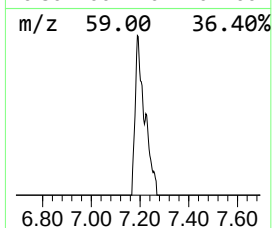
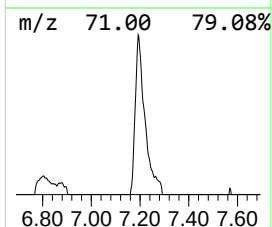
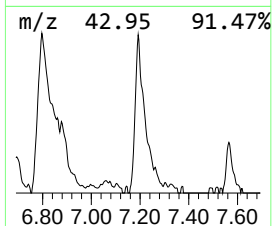
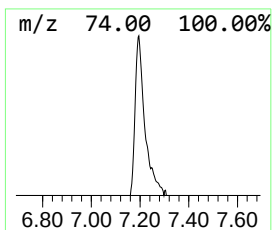
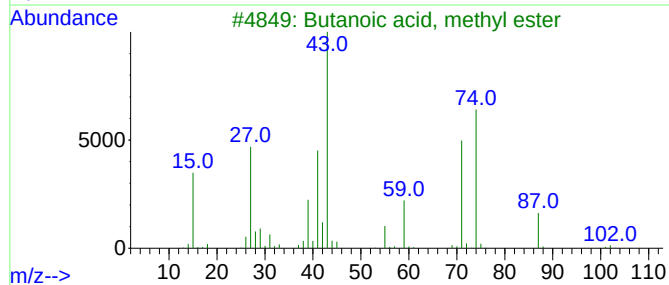
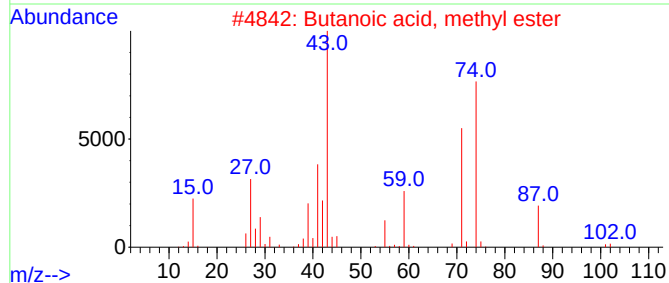
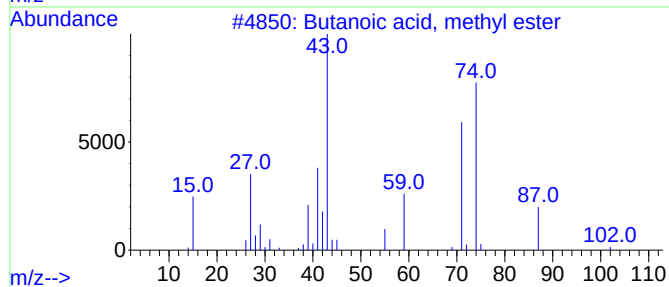
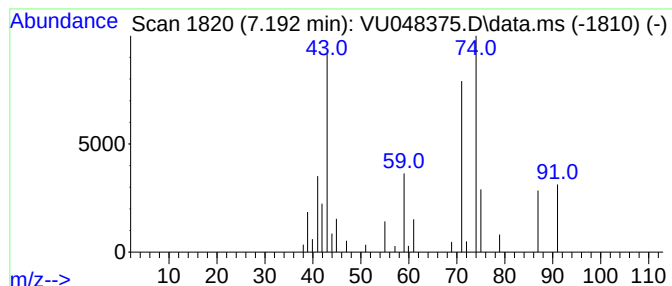
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Butanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.192	3.81 ug/L	80134	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	56
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	50
4			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	16
5			3-Methylbutan-2-yl propyl carbonate	174	C9H18O3	1000372-83-4	12



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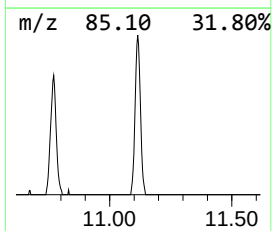
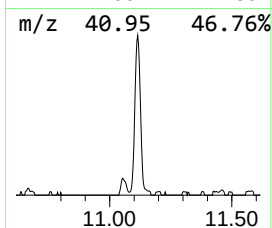
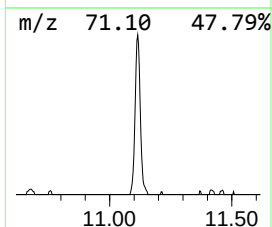
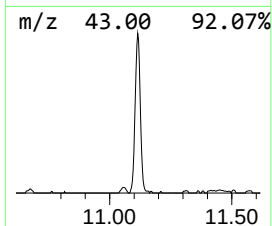
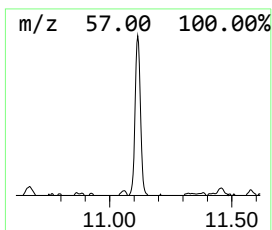
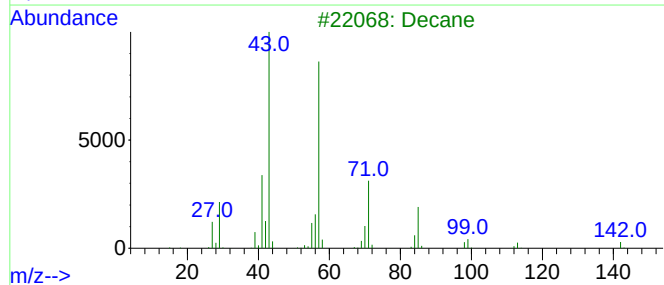
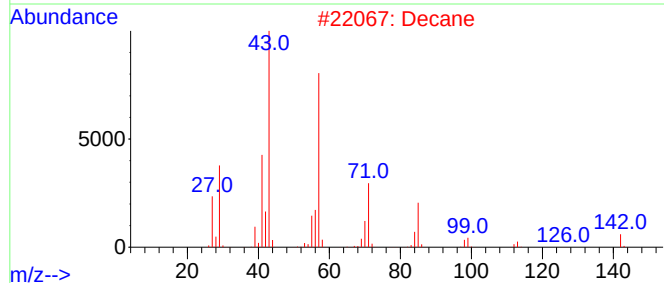
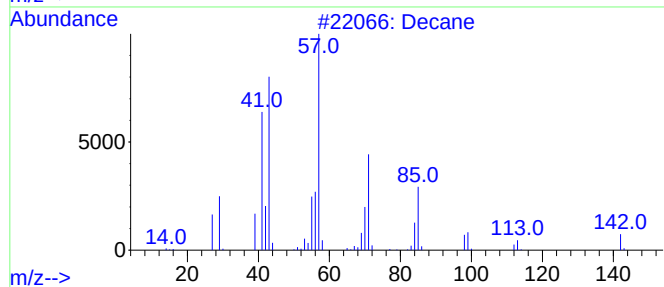
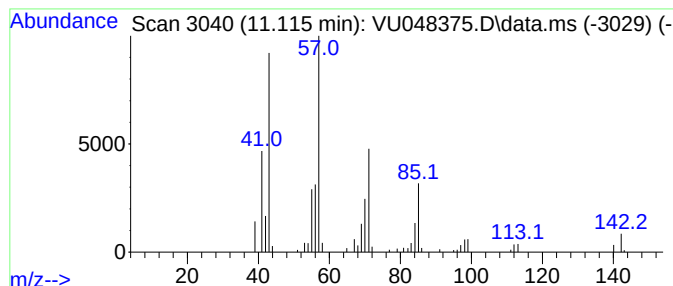
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	4.00 ug/L	100434	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	90
2			Decane	142	C10H22	000124-18-5	87
3			Decane	142	C10H22	000124-18-5	74
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
5			Tetradecane	198	C14H30	000629-59-4	64



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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
Butanoic acid, ...	7.192	3.8	ug/L	80134	1	6.247	1050250	50.0
(DEL) Alkane: S...	11.115	4.0	ug/L	100434	3	11.819	1253990	50.0