

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022024\
 Data File : VU057899.D
 Acq On : 20 Feb 2024 13:53
 Operator : MD/SY
 Sample : P1496-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH9Y0

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\SFAMULM021924WMA.M
 Title : VOC Analysis

Signal : TIC: VU057899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	87	95	112	rVB	125040	148726	15.55%	1.925%
2	1.888	178	186	201	rVB	91746	130676	13.66%	1.692%
3	2.554	379	393	405	rBV	200274	324654	33.94%	4.203%
4	2.615	406	412	427	rVB	9986	18842	1.97%	0.244%
5	2.731	445	448	452	rBV2	277	237	0.02%	0.003%
6	2.779	457	463	473	rVB3	554	1011	0.11%	0.013%
7	2.843	479	483	485	rBV	173	154	0.02%	0.002%
8	2.914	501	505	509	rBV2	190	217	0.02%	0.003%
9	3.033	534	542	553	rVB4	3207	5161	0.54%	0.067%
10	3.161	576	582	585	rBV4	1085	1212	0.13%	0.016%
11	3.213	595	598	607	rVB4	532	629	0.07%	0.008%
12	3.345	632	639	642	rBV3	536	677	0.07%	0.009%
13	3.547	693	702	703	rBV	230	349	0.04%	0.005%
14	3.772	767	772	776	rBV2	213	222	0.02%	0.003%
15	3.837	789	792	797	rVB2	337	363	0.04%	0.005%
16	3.872	797	803	806	rBV	326	332	0.03%	0.004%
17	3.917	814	817	821	rBV2	191	161	0.02%	0.002%
18	4.075	862	866	871	rBV2	260	308	0.03%	0.004%
19	4.284	929	931	937	rVB2	169	155	0.02%	0.002%
20	4.467	984	988	990	rBV	285	289	0.03%	0.004%
21	4.557	1011	1016	1017	rBV2	201	180	0.02%	0.002%
22	4.608	1022	1032	1041	rBV	64484	146962	15.36%	1.902%
23	5.049	1153	1169	1197	rBV	163079	364165	38.07%	4.714%
24	5.171	1203	1207	1210	rBV2	284	265	0.03%	0.003%
25	5.283	1240	1242	1246	rVB2	272	180	0.02%	0.002%
26	5.322	1246	1254	1267	rBV5	1298	2791	0.29%	0.036%
27	5.412	1278	1282	1285	rBV	155	144	0.02%	0.002%
28	5.457	1294	1296	1301	rBV2	153	160	0.02%	0.002%
29	5.714	1351	1376	1411	rBV2	350617	956544	100.00%	12.383%
30	5.853	1416	1419	1424	rVB3	489	365	0.04%	0.005%
31	5.968	1453	1455	1456	rBV3	377	190	0.02%	0.002%
32	6.036	1473	1476	1482	rVB3	396	253	0.03%	0.003%
33	6.068	1482	1486	1493	rVB2	261	308	0.03%	0.004%
34	6.174	1515	1519	1525	rBV3	333	400	0.04%	0.005%
35	6.238	1526	1539	1569	rBV	361017	690736	72.21%	8.942%
36	6.541	1624	1633	1663	rBV4	18381	63197	6.61%	0.818%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
 Title : VOC Analysis

37	6.679	1664	1676	1696	rVB	216228	424195	44.35%	5.491%
38	6.881	1726	1739	1752	rBV5	5032	12107	1.27%	0.157%
39	7.013	1776	1780	1783	rBV2	329	259	0.03%	0.003%
40	7.055	1791	1793	1796	rVB	355	183	0.02%	0.002%
41	7.078	1796	1800	1801	rBV	222	150	0.02%	0.002%
42	7.090	1801	1804	1808	rVB	285	196	0.02%	0.003%
43	7.136	1815	1818	1821	rVB2	354	199	0.02%	0.003%
44	7.200	1836	1838	1842	rVB3	353	201	0.02%	0.003%
45	7.557	1936	1949	1973	rBV	120725	216511	22.63%	2.803%
46	7.734	2002	2004	2007	rVV	307	190	0.02%	0.002%
47	7.804	2019	2026	2029	rBV3	326	410	0.04%	0.005%
48	7.888	2040	2052	2083	rBV	425000	758746	79.32%	9.822%
49	8.074	2108	2110	2115	rVB2	384	254	0.03%	0.003%
50	8.171	2130	2140	2171	rBV2	80034	139919	14.63%	1.811%
51	8.476	2224	2235	2239	rVB2	530	861	0.09%	0.011%
52	8.502	2239	2243	2248	rVB2	191	155	0.02%	0.002%
53	8.553	2257	2259	2264	rVB	209	152	0.02%	0.002%
54	8.627	2271	2282	2315	rBV2	221096	437990	45.79%	5.670%
55	8.785	2321	2331	2355	rVB3	39503	77750	8.13%	1.006%
56	8.917	2369	2372	2375	rVB	350	177	0.02%	0.002%
57	8.936	2375	2378	2382	rBV	220	188	0.02%	0.002%
58	9.058	2412	2416	2419	rBV2	393	268	0.03%	0.003%
59	9.409	2512	2525	2553	rBV	500056	839775	87.79%	10.871%
60	9.566	2572	2574	2579	rBV	233	256	0.03%	0.003%
61	9.695	2602	2614	2621	rBV3	914	1635	0.17%	0.021%
62	9.750	2627	2631	2634	rBV2	188	159	0.02%	0.002%
63	9.933	2685	2688	2692	rVB	239	206	0.02%	0.003%
64	9.955	2692	2695	2697	rBV	248	165	0.02%	0.002%
65	10.049	2721	2724	2728	rBV2	202	154	0.02%	0.002%
66	10.235	2775	2782	2783	rBV2	287	333	0.03%	0.004%
67	10.248	2783	2786	2788	rVV	196	154	0.02%	0.002%
68	10.351	2806	2818	2840	rBV7	3871	8141	0.85%	0.105%
69	10.534	2873	2875	2879	rVB	284	201	0.02%	0.003%
70	10.650	2907	2911	2916	rBV2	220	224	0.02%	0.003%
71	10.750	2925	2942	2963	rBV	263303	437312	45.72%	5.661%
72	10.888	2980	2985	2993	rVB2	744	901	0.09%	0.012%
73	10.981	3011	3014	3017	rBV	186	169	0.02%	0.002%
74	11.061	3037	3039	3042	rVB	393	232	0.02%	0.003%
75	11.213	3080	3086	3089	rBV	365	447	0.05%	0.006%
76	11.267	3094	3103	3107	rBV4	737	1205	0.13%	0.016%

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77	11.454	3157	3161	3164	rBV2	270	266	0.03%	0.003%
78	11.473	3164	3167	3168	rBV	214	149	0.02%	0.002%
79	11.582	3199	3201	3205	rBV	156	149	0.02%	0.002%
80	11.627	3212	3215	3217	rBV2	223	168	0.02%	0.002%
81	11.669	3225	3228	3230	rBV	324	156	0.02%	0.002%
82	11.695	3230	3236	3246	rBV5	3641	6101	0.64%	0.079%
83	11.804	3258	3270	3295	rBV	500413	817930	85.51%	10.588%
84	12.071	3343	3353	3368	rBV3	6704	15920	1.66%	0.206%
85	12.187	3377	3389	3412	rVB	397488	650032	67.96%	8.415%
86	12.299	3421	3424	3429	rVB4	376	271	0.03%	0.004%
87	12.518	3490	3492	3495	rVV	375	248	0.03%	0.003%
88	12.582	3507	3512	3513	rBV	218	192	0.02%	0.002%
89	12.766	3562	3569	3572	rBV2	614	865	0.09%	0.011%
90	12.894	3602	3609	3618	rBV7	3369	5593	0.58%	0.072%
91	13.280	3726	3729	3733	rVB2	341	259	0.03%	0.003%
92	13.737	3868	3871	3874	rBV2	215	190	0.02%	0.002%
93	13.852	3903	3907	3918	rVB3	487	673	0.07%	0.009%
94	14.119	3988	3990	3994	rBV	320	271	0.03%	0.004%
95	14.450	4091	4093	4096	rVB	398	194	0.02%	0.003%
96	14.470	4096	4099	4100	rBV	249	146	0.02%	0.002%
97	14.521	4112	4115	4120	rBV2	395	392	0.04%	0.005%
98	14.576	4129	4132	4138	rBV2	288	251	0.03%	0.003%
99	15.354	4372	4374	4378	rBV2	425	201	0.02%	0.003%
100	15.830	4520	4522	4526	rBV2	591	356	0.04%	0.005%

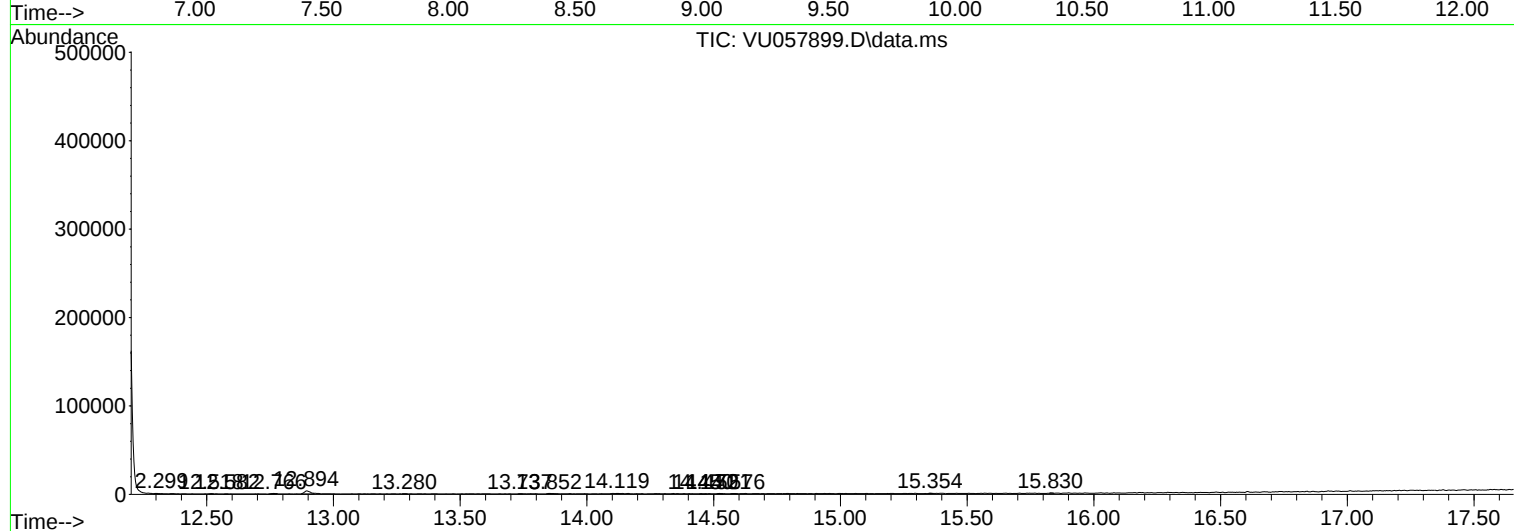
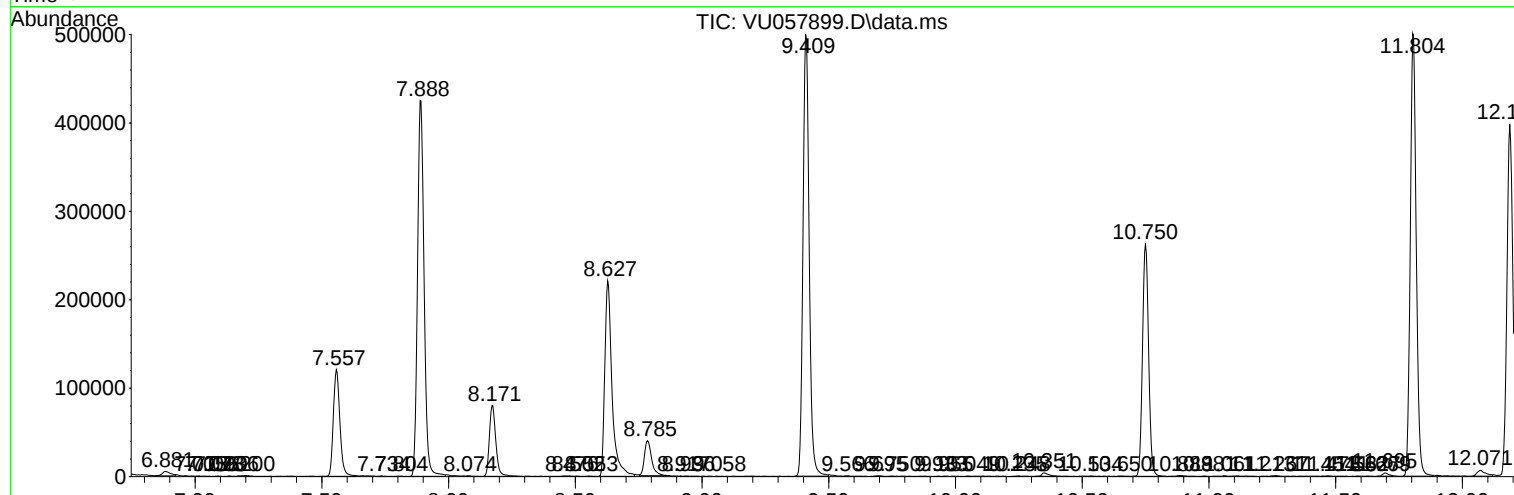
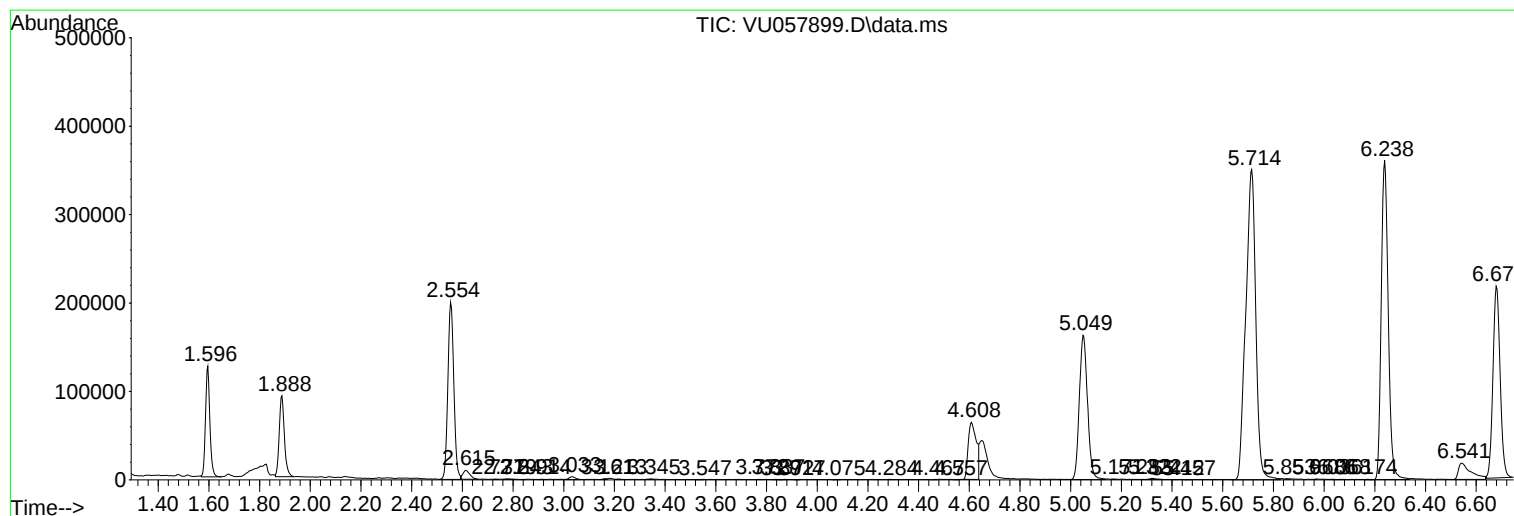
Sum of corrected areas: 7724918

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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



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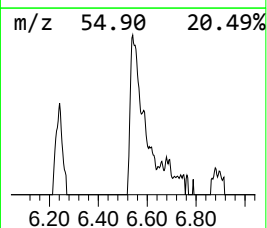
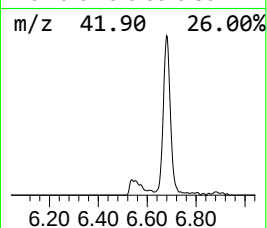
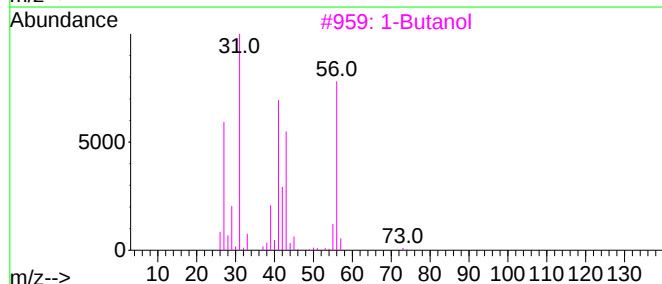
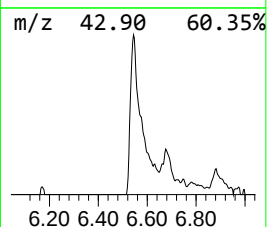
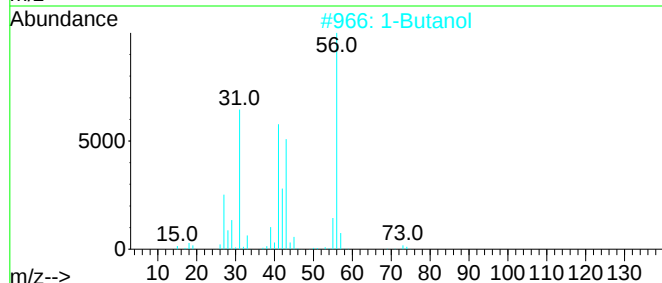
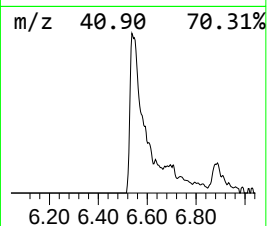
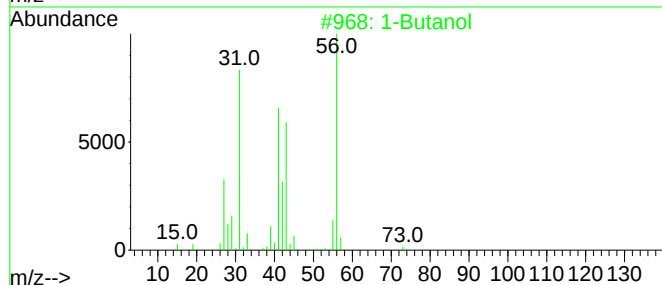
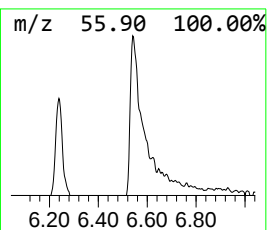
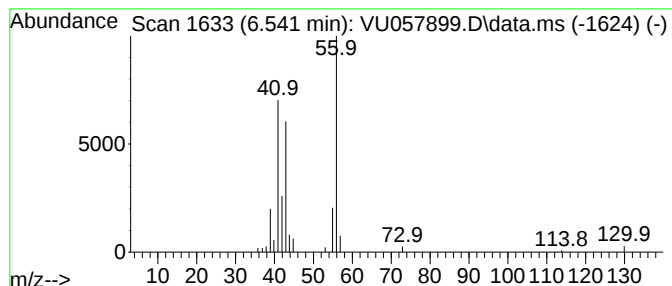
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.541	4.57 ug/L	63197	1,4-Difluorobenzene	6.238

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	78
2	1-Butanol			74	C4H10O	000071-36-3	78
3	1-Butanol			74	C4H10O	000071-36-3	56
4	1-Butanol			74	C4H10O	000071-36-3	38
5	1-Pentene, 2,4-dimethyl-			98	C7H14	002213-32-3	38



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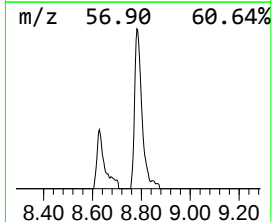
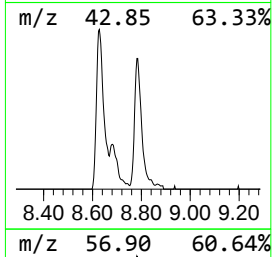
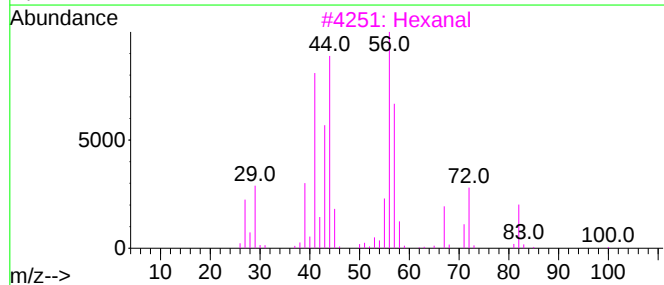
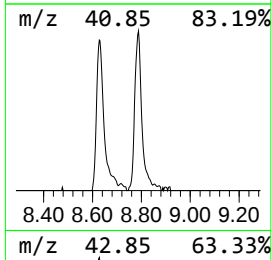
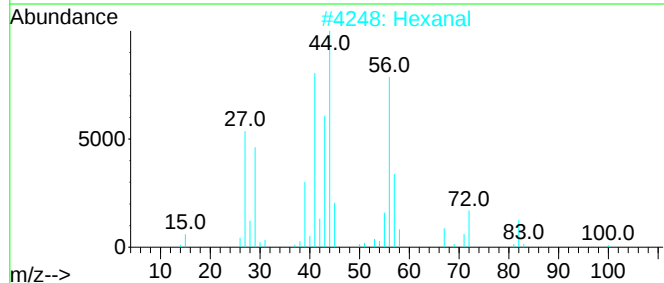
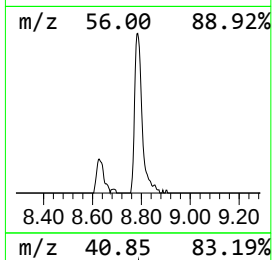
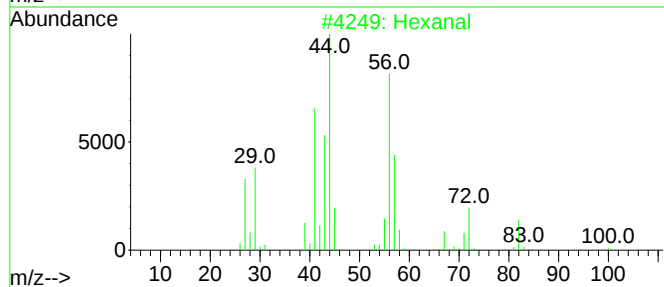
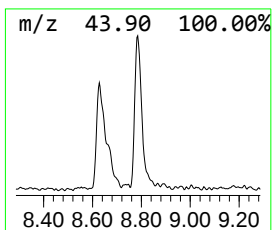
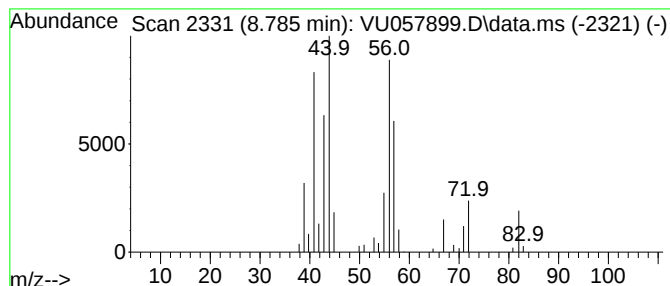
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Quant Title : VOC Analysis

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

Peak Number 3 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	4.63 ug/L	77750	Chlorobenzene-d5	9.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	90
3	Hexanal			100	C6H12O	000066-25-1	90
4	Hexanal			100	C6H12O	000066-25-1	90
5	Hexanal			100	C6H12O	000066-25-1	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Butanol	6.541	4.6	ug/L	63197	1	6.238	690736	50.0
Hexanal	8.785	4.6	ug/L	77750	2	9.409	839775	50.0