

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022024\
 Data File : VU057896.D
 Acq On : 20 Feb 2024 12:41
 Operator : MD/SY
 Sample : P1496-15
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHA06

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: VU057896.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	110	rVB	121597	148349	15.47%	1.921%
2	1.882	177	184	201	rVB	89885	132468	13.81%	1.715%
3	2.403	344	346	347	rBV	696	273	0.03%	0.004%
4	2.499	372	376	379	rBV2	284	274	0.03%	0.004%
5	2.554	380	393	405	rVV	200018	326969	34.10%	4.233%
6	2.612	406	411	428	rVB2	8693	15895	1.66%	0.206%
7	2.779	457	463	471	rVB2	650	999	0.10%	0.013%
8	2.882	489	495	501	rBV2	227	315	0.03%	0.004%
9	2.911	501	504	508	rBV	257	197	0.02%	0.003%
10	3.030	533	541	553	rVB2	3385	5484	0.57%	0.071%
11	3.175	575	586	594	rVV3	872	1959	0.20%	0.025%
12	3.300	623	625	631	rBV	259	248	0.03%	0.003%
13	3.345	631	639	645	rVV5	890	1281	0.13%	0.017%
14	3.393	649	654	658	rBV2	290	362	0.04%	0.005%
15	3.451	667	672	675	rBV	250	240	0.03%	0.003%
16	3.583	709	713	717	rBV2	338	331	0.03%	0.004%
17	3.911	810	815	821	rVB2	258	305	0.03%	0.004%
18	4.017	842	848	852	rBV2	286	362	0.04%	0.005%
19	4.049	852	858	863	rVB	165	242	0.03%	0.003%
20	4.297	931	935	938	rBV2	263	260	0.03%	0.003%
21	4.464	984	987	992	rBV2	438	439	0.05%	0.006%
22	4.525	1003	1006	1014	rVB	217	308	0.03%	0.004%
23	4.567	1014	1019	1021	rBV2	216	217	0.02%	0.003%
24	4.609	1022	1032	1041	rBV	61832	144895	15.11%	1.876%
25	5.049	1151	1169	1193	rBV	163482	364754	38.04%	4.722%
26	5.203	1214	1217	1220	rBV2	238	216	0.02%	0.003%
27	5.525	1313	1317	1325	rVB	241	336	0.04%	0.004%
28	5.615	1339	1345	1348	rBV2	175	234	0.02%	0.003%
29	5.711	1355	1375	1403	rBV2	356107	958880	100.00%	12.415%
30	5.975	1454	1457	1460	rVB	427	307	0.03%	0.004%
31	6.036	1472	1476	1480	rBV2	349	258	0.03%	0.003%
32	6.084	1488	1491	1494	rVB2	235	194	0.02%	0.003%
33	6.239	1526	1539	1564	rBV	369757	705365	73.56%	9.132%
34	6.554	1621	1637	1663	rBV5	15554	56682	5.91%	0.734%
35	6.679	1663	1676	1696	rVB	216452	425463	44.37%	5.508%
36	6.882	1731	1739	1750	rBV4	3688	7935	0.83%	0.103%

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Integrator: RTE

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

37	7.158	1822	1825	1826	rBV	440	253	0.03%	0.003%
38	7.178	1829	1831	1833	rVV3	387	215	0.02%	0.003%
39	7.361	1883	1888	1890	rBV2	219	234	0.02%	0.003%
40	7.441	1909	1913	1918	rVB	262	270	0.03%	0.003%
41	7.557	1928	1949	1972	rBV	121423	218509	22.79%	2.829%
42	7.666	1980	1983	1985	rBV	444	268	0.03%	0.003%
43	7.750	2002	2009	2013	rBV2	488	660	0.07%	0.009%
44	7.843	2033	2038	2040	rBV2	282	299	0.03%	0.004%
45	7.888	2040	2052	2073	rBV	432264	756213	78.86%	9.791%
46	8.071	2106	2109	2112	rBV	329	241	0.03%	0.003%
47	8.171	2128	2140	2166	rBV	80530	140573	14.66%	1.820%
48	8.303	2178	2181	2185	rVB3	365	230	0.02%	0.003%
49	8.451	2224	2227	2228	rBV	478	271	0.03%	0.004%
50	8.467	2230	2232	2241	rVV	665	697	0.07%	0.009%
51	8.628	2271	2282	2315	rBV	207652	426317	44.46%	5.520%
52	8.785	2321	2331	2353	rVB2	35591	74046	7.72%	0.959%
53	8.933	2376	2377	2382	rVB3	522	397	0.04%	0.005%
54	8.981	2385	2392	2395	rBV2	267	351	0.04%	0.005%
55	9.030	2402	2407	2411	rVB2	372	443	0.05%	0.006%
56	9.052	2411	2414	2417	rBV2	248	199	0.02%	0.003%
57	9.100	2426	2429	2434	rVB	369	284	0.03%	0.004%
58	9.216	2459	2465	2470	rBV2	255	332	0.03%	0.004%
59	9.409	2513	2525	2557	rBV	503284	848841	88.52%	10.990%
60	9.698	2606	2615	2619	rBV3	1085	1585	0.17%	0.021%
61	9.843	2656	2660	2663	rBV2	224	206	0.02%	0.003%
62	10.251	2782	2787	2790	rVB3	289	306	0.03%	0.004%
63	10.351	2811	2818	2833	rBV5	3293	6198	0.65%	0.080%
64	10.483	2855	2859	2864	rVB2	352	372	0.04%	0.005%
65	10.515	2864	2869	2872	rBV2	318	356	0.04%	0.005%
66	10.750	2930	2942	2961	rBV	258370	426768	44.51%	5.525%
67	10.885	2982	2984	2990	rVB2	504	542	0.06%	0.007%
68	11.001	3017	3020	3025	rVB2	305	349	0.04%	0.005%
69	11.055	3032	3037	3041	rBV3	399	494	0.05%	0.006%
70	11.110	3050	3054	3060	rVV3	654	751	0.08%	0.010%
71	11.258	3094	3100	3110	rBV3	694	1134	0.12%	0.015%
72	11.329	3118	3122	3124	rBV	232	202	0.02%	0.003%
73	11.579	3196	3200	3205	rBV	272	326	0.03%	0.004%
74	11.647	3218	3221	3223	rBV2	223	190	0.02%	0.002%
75	11.666	3224	3227	3230	rVB	345	232	0.02%	0.003%
76	11.695	3230	3236	3246	rBV4	3205	5314	0.55%	0.069%

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77	11.804	3258	3270	3300	rBV	510132	829346	86.49%	10.738%
78	11.939	3310	3312	3318	rVB2	446	276	0.03%	0.004%
79	12.068	3344	3352	3365	rBV5	5031	11270	1.18%	0.146%
80	12.145	3373	3376	3377	rBV2	409	257	0.03%	0.003%
81	12.187	3377	3389	3407	rVV	395318	650183	67.81%	8.418%
82	12.377	3445	3448	3451	rBV3	294	219	0.02%	0.003%
83	12.554	3499	3503	3505	rBV2	204	210	0.02%	0.003%
84	12.669	3535	3539	3543	rBV2	262	282	0.03%	0.004%
85	12.734	3554	3559	3562	rBV	350	355	0.04%	0.005%
86	12.759	3562	3567	3570	rBV3	452	426	0.04%	0.006%
87	12.853	3593	3596	3602	rVB	324	245	0.03%	0.003%
88	12.891	3602	3608	3618	rBV5	3244	5739	0.60%	0.074%
89	12.946	3622	3625	3628	rVB2	309	204	0.02%	0.003%
90	13.203	3694	3705	3706	rBV2	281	516	0.05%	0.007%
91	13.428	3771	3775	3783	rVV2	259	448	0.05%	0.006%
92	13.695	3855	3858	3862	rBV2	286	325	0.03%	0.004%
93	13.853	3899	3907	3912	rBV4	1504	1726	0.18%	0.022%
94	13.920	3924	3928	3930	rBV	331	247	0.03%	0.003%
95	14.107	3981	3986	3990	rBV3	1047	933	0.10%	0.012%
96	14.219	4018	4021	4024	rVB	357	249	0.03%	0.003%
97	14.309	4047	4049	4052	rBV2	326	260	0.03%	0.003%
98	15.193	4321	4324	4328	rVB2	438	342	0.04%	0.004%
99	15.840	4522	4525	4528	rBV2	616	397	0.04%	0.005%
100	15.991	4569	4572	4575	rBV4	661	571	0.06%	0.007%

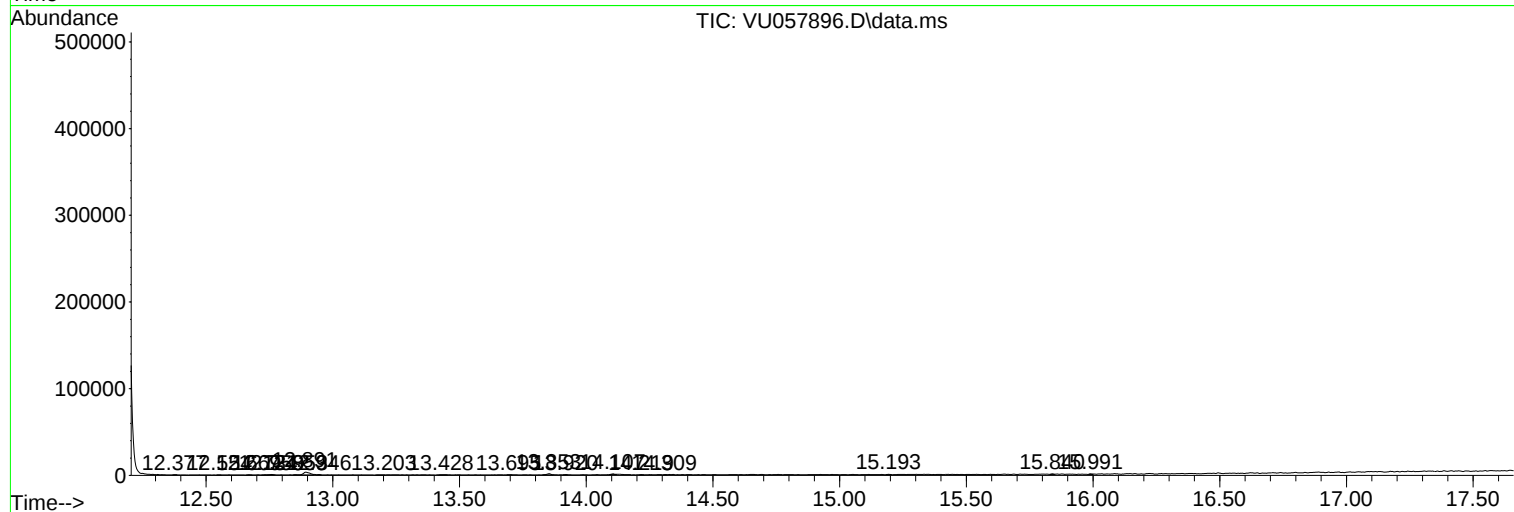
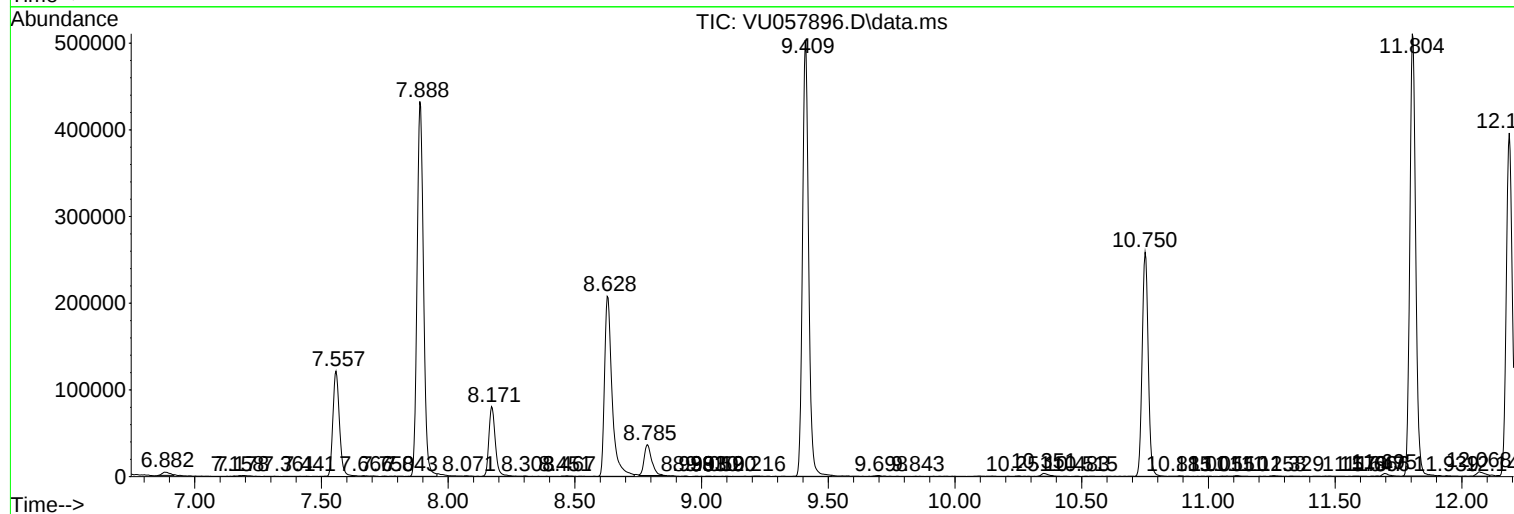
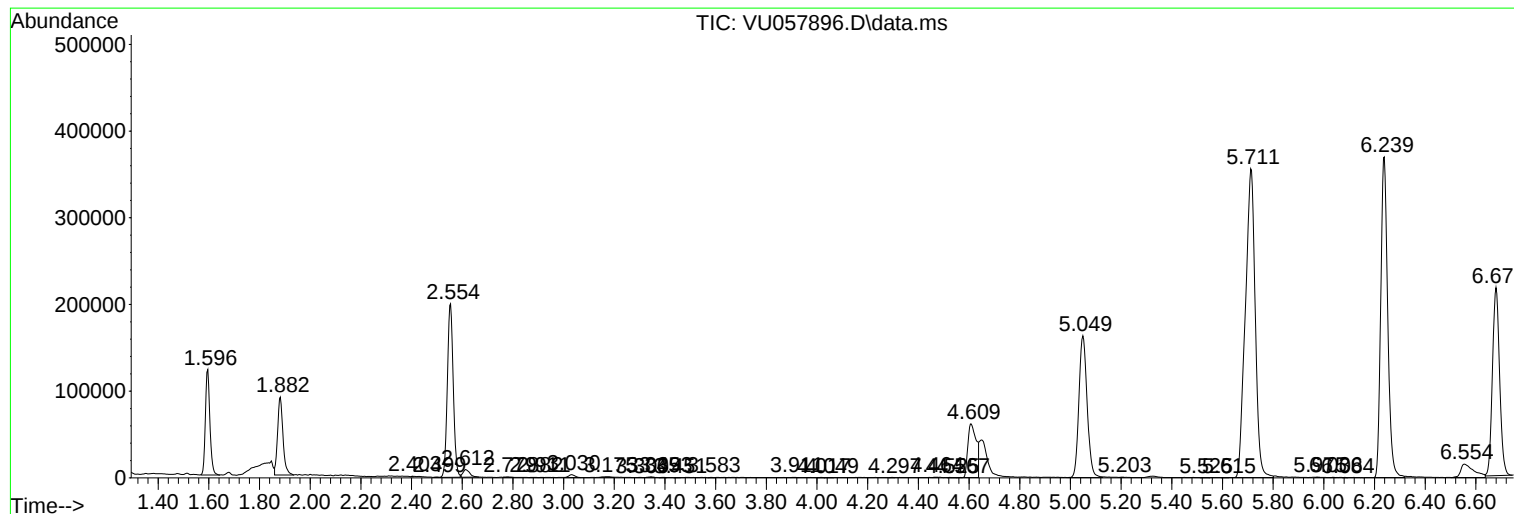
Sum of corrected areas: 7723790

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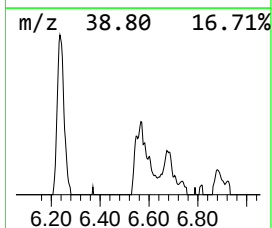
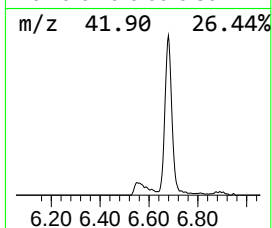
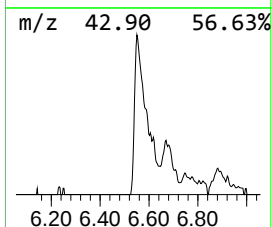
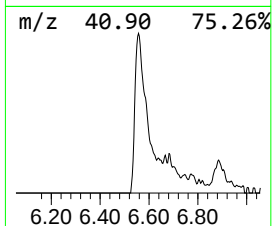
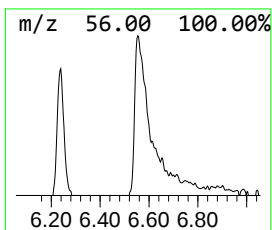
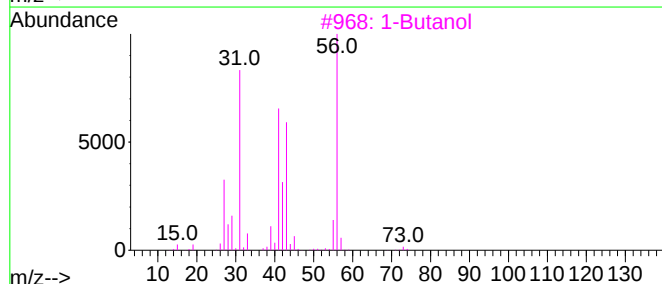
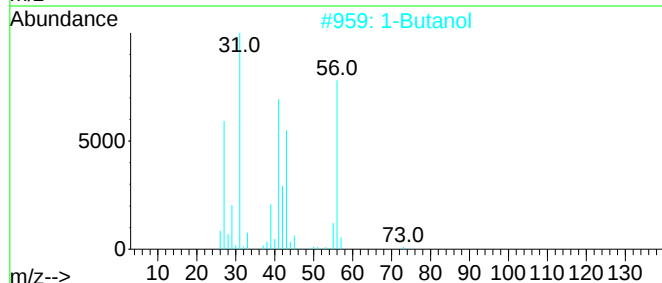
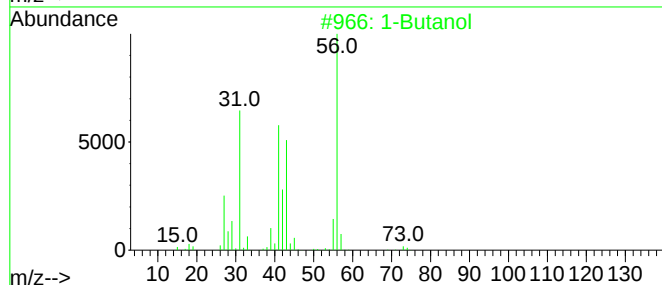
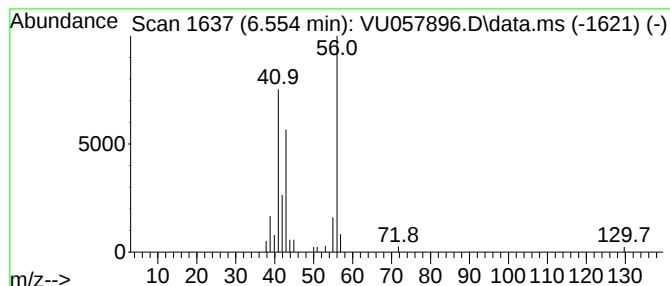
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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.
6.554	4.02 ug/L	56682	1,4-Difluorobenzene	6.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	83
2	1-Butanol			74	C4H10O	000071-36-3	64
3	1-Butanol			74	C4H10O	000071-36-3	64
4	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	42
5	1-Butanol			74	C4H10O	000071-36-3	40



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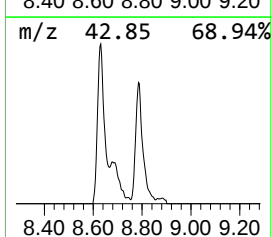
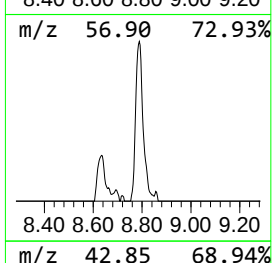
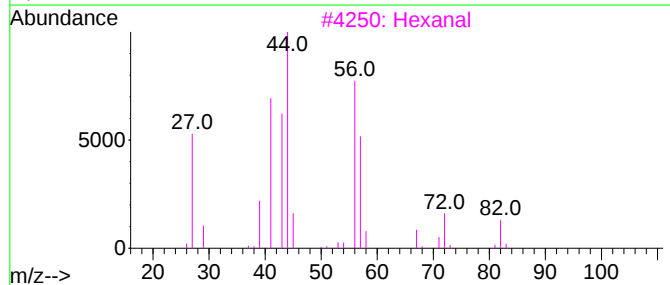
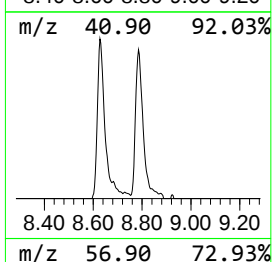
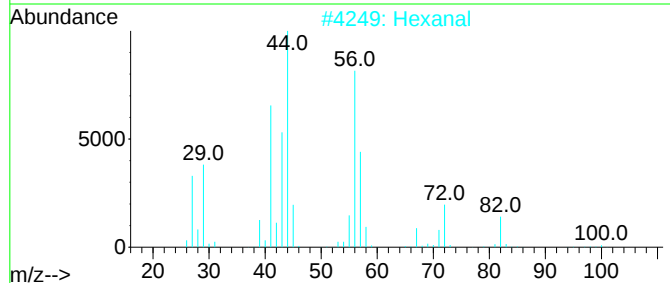
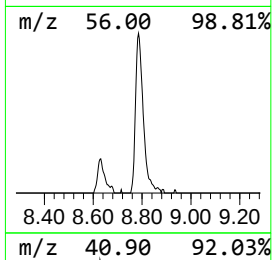
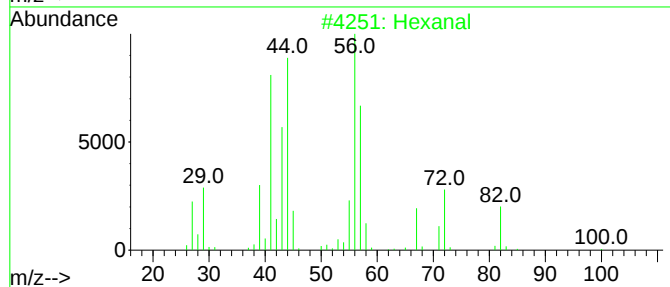
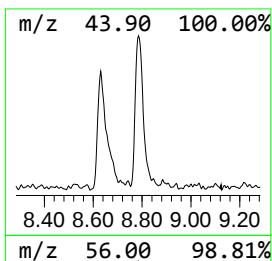
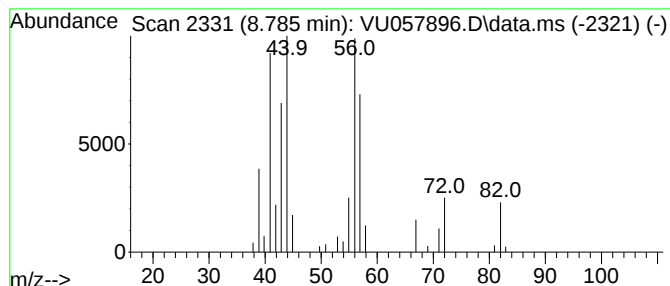
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	4.36 ug/L	74046	Chlorobenzene-d5	9.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	59
5	Hexanal			100	C6H12O	000066-25-1	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Butanol	6.554	4.0	ug/L	56682	1	6.239	705365	50.0
Hexanal	8.785	4.4	ug/L	74046	2	9.409	848841	50.0