

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030659.D
 Acq On : 17 Aug 2022 14:51
 Operator : JC/MD
 Sample : N4221-17
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KN9

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_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030659.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	26	30	42	rBV3	7728	20950	1.57%	0.209%
2	1.367	42	46	57	rVB	191600	194572	14.54%	1.937%
3	1.666	91	95	105	rVB	135213	167360	12.50%	1.666%
4	2.013	151	152	155	rBV2	1186	1026	0.08%	0.010%
5	2.306	193	200	210	rBV	319966	494362	36.93%	4.921%
6	2.391	210	214	219	rVB2	4265	6315	0.47%	0.063%
7	2.660	253	258	260	rBV2	783	1175	0.09%	0.012%
8	2.708	265	266	269	rBV	414	533	0.04%	0.005%
9	2.794	275	280	283	rVB4	897	1294	0.10%	0.013%
10	2.885	293	295	297	rVB	439	376	0.03%	0.004%
11	3.129	332	335	338	rBV	458	585	0.04%	0.006%
12	3.428	383	384	387	rVB2	443	412	0.03%	0.004%
13	3.471	389	391	394	rBV2	292	376	0.03%	0.004%
14	3.592	409	411	415	rVB2	559	646	0.05%	0.006%
15	3.635	415	418	419	rBV	530	459	0.03%	0.005%
16	3.727	431	433	434	rBV2	562	532	0.04%	0.005%
17	3.989	473	476	479	rBV2	403	427	0.03%	0.004%
18	4.117	496	497	502	rVB2	382	573	0.04%	0.006%
19	4.159	502	504	506	rBV	428	412	0.03%	0.004%
20	4.464	545	554	572	rBV	102064	303206	22.65%	3.018%
21	4.726	587	597	610	rBV	32340	90101	6.73%	0.897%
22	5.062	639	652	674	rVB	175672	558580	41.73%	5.560%
23	5.232	676	680	682	rVB2	674	884	0.07%	0.009%
24	5.562	726	734	743	rVB4	2162	5295	0.40%	0.053%
25	5.732	760	762	766	rBV2	477	686	0.05%	0.007%
26	5.976	789	802	820	rBV2	458410	1338565	100.00%	13.325%
27	6.177	834	835	839	rVB3	446	394	0.03%	0.004%
28	6.220	839	842	843	rBV	408	386	0.03%	0.004%
29	6.354	862	864	867	rVB2	519	540	0.04%	0.005%
30	6.440	874	878	879	rBV2	433	519	0.04%	0.005%
31	6.641	906	911	913	rBV2	395	542	0.04%	0.005%
32	6.769	922	932	944	rBV	296899	710837	53.10%	7.076%
33	6.958	961	963	965	rBV2	351	369	0.03%	0.004%
34	7.116	981	989	997	rBV4	11799	28155	2.10%	0.280%
35	7.220	1005	1006	1009	rBV2	376	383	0.03%	0.004%
36	7.311	1012	1021	1034	rVV	275938	595887	44.52%	5.932%

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 Title : VOC Analysis

37	7.427	1038	1040	1042	rBV	738	504	0.04%	0.005%
38	7.580	1064	1065	1066	rBV	758	534	0.04%	0.005%
39	7.683	1080	1082	1087	rBV2	440	578	0.04%	0.006%
40	7.933	1118	1123	1130	rVV3	1552	3107	0.23%	0.031%
41	7.994	1130	1133	1135	rVV2	377	375	0.03%	0.004%
42	8.329	1179	1188	1205	rBV	182133	301836	22.55%	3.005%
43	8.445	1205	1207	1209	rBV2	583	437	0.03%	0.004%
44	8.573	1226	1228	1231	rBV2	651	713	0.05%	0.007%
45	8.653	1234	1241	1250	rBV	703990	1075434	80.34%	10.705%
46	8.951	1284	1290	1300	rBV	130854	192191	14.36%	1.913%
47	9.031	1302	1303	1304	rVV	1046	405	0.03%	0.004%
48	9.079	1307	1311	1315	rBV	508	871	0.07%	0.009%
49	9.146	1320	1322	1325	rBV	491	394	0.03%	0.004%
50	9.280	1340	1344	1348	rVB4	2574	3595	0.27%	0.036%
51	9.390	1356	1362	1374	rBV	460525	674691	50.40%	6.716%
52	9.524	1379	1384	1391	rVV	29295	42259	3.16%	0.421%
53	9.585	1391	1394	1402	rVV5	2408	4620	0.35%	0.046%
54	9.683	1407	1410	1411	rVV2	570	406	0.03%	0.004%
55	9.719	1414	1416	1418	rVB2	556	444	0.03%	0.004%
56	9.780	1424	1426	1428	rVB2	531	417	0.03%	0.004%
57	9.817	1428	1432	1434	rBV3	376	514	0.04%	0.005%
58	10.055	1465	1471	1486	rVV	620665	835734	62.44%	8.319%
59	10.250	1501	1503	1506	rVB3	604	402	0.03%	0.004%
60	10.457	1534	1537	1538	rVB2	473	389	0.03%	0.004%
61	10.597	1558	1560	1562	rVB2	490	411	0.03%	0.004%
62	10.646	1564	1568	1573	rBV	7686	11443	0.85%	0.114%
63	10.768	1584	1588	1594	rVB6	1683	3215	0.24%	0.032%
64	10.817	1594	1596	1597	rBV6	359	370	0.03%	0.004%
65	10.866	1599	1604	1607	rBV2	2906	3689	0.28%	0.037%
66	11.030	1626	1631	1635	rBV2	2664	3150	0.24%	0.031%
67	11.146	1648	1650	1652	rBV	415	410	0.03%	0.004%
68	11.195	1652	1658	1664	rVV	469542	588651	43.98%	5.860%
69	11.317	1675	1678	1681	rVB3	1468	1802	0.13%	0.018%
70	11.384	1687	1689	1691	rBV	565	470	0.04%	0.005%
71	11.463	1698	1702	1703	rVB2	730	802	0.06%	0.008%
72	11.719	1741	1744	1746	rBV2	684	581	0.04%	0.006%
73	11.756	1746	1750	1757	rVV4	3590	5766	0.43%	0.057%
74	11.932	1775	1779	1783	rVV2	2038	2491	0.19%	0.025%
75	12.024	1789	1794	1802	rBV	637161	777160	58.06%	7.736%
76	12.219	1821	1826	1837	rBV2	17585	31143	2.33%	0.310%

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77	12.323	1837	1843	1850	rVV	726585	893177	66.73%	8.891%
78	12.597	1883	1888	1892	rBV6	2531	4429	0.33%	0.044%
79	12.859	1927	1931	1937	rVB	8788	11126	0.83%	0.111%
80	12.938	1940	1944	1946	rBV4	1929	2135	0.16%	0.021%
81	13.103	1966	1971	1978	rVB	15632	20159	1.51%	0.201%
82	13.164	1978	1981	1982	rBV2	607	825	0.06%	0.008%
83	13.365	2012	2014	2015	rBV2	775	373	0.03%	0.004%
84	13.469	2029	2031	2033	rBV2	646	549	0.04%	0.005%
85	13.542	2040	2043	2044	rVB2	574	368	0.03%	0.004%
86	13.639	2057	2059	2062	rBV2	607	465	0.03%	0.005%
87	13.749	2075	2077	2081	rBV2	521	749	0.06%	0.007%
88	13.786	2081	2083	2084	rBV2	811	767	0.06%	0.008%
89	13.889	2098	2100	2103	rVB	539	452	0.03%	0.004%
90	13.975	2112	2114	2115	rVB	700	455	0.03%	0.005%
91	13.993	2115	2117	2122	rBV2	488	791	0.06%	0.008%
92	14.127	2136	2139	2140	rBV	913	918	0.07%	0.009%
93	14.347	2174	2175	2179	rVB2	546	553	0.04%	0.006%
94	14.615	2217	2219	2220	rBV	612	504	0.04%	0.005%
95	14.719	2234	2236	2241	rBV3	1243	1923	0.14%	0.019%
96	14.944	2271	2273	2277	rBV	538	667	0.05%	0.007%
97	15.255	2321	2324	2325	rBV2	998	1069	0.08%	0.011%
98	15.359	2336	2341	2343	rBV4	1574	2116	0.16%	0.021%
99	15.688	2394	2395	2397	rBV	827	392	0.03%	0.004%
100	15.706	2397	2398	2400	rBV2	650	589	0.04%	0.006%

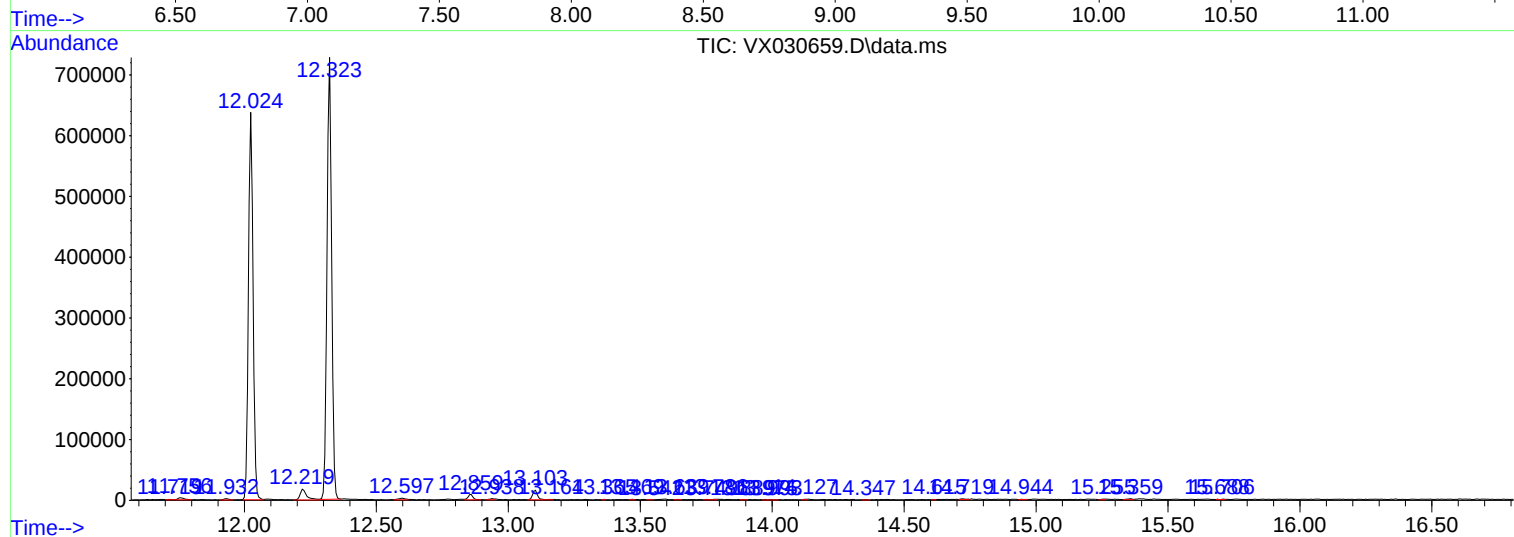
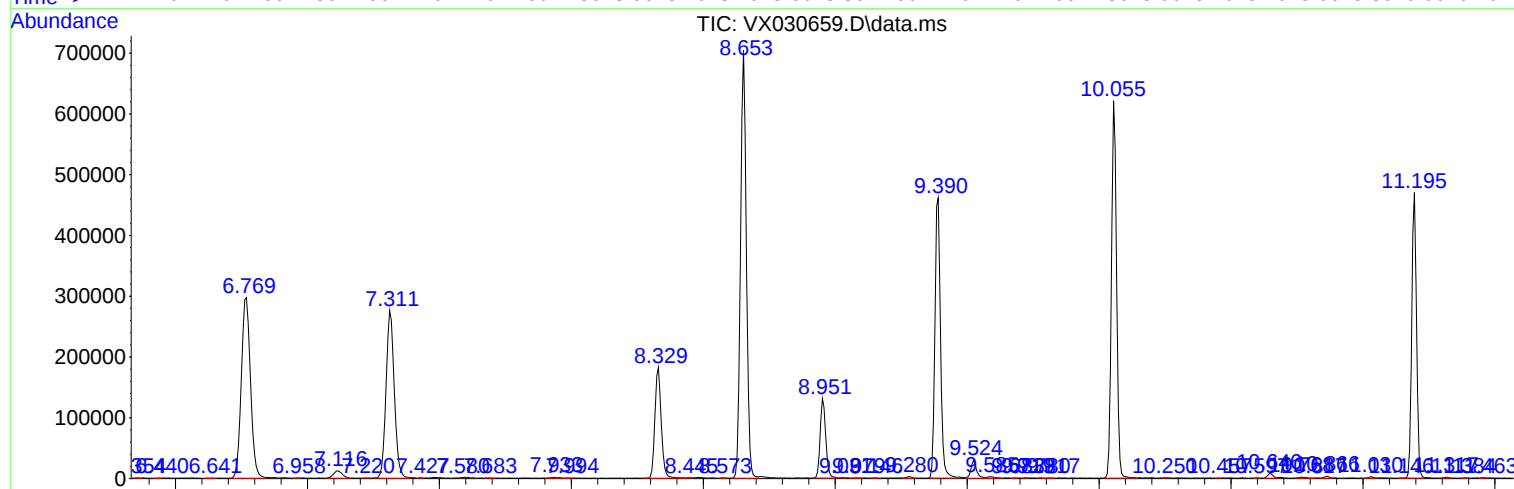
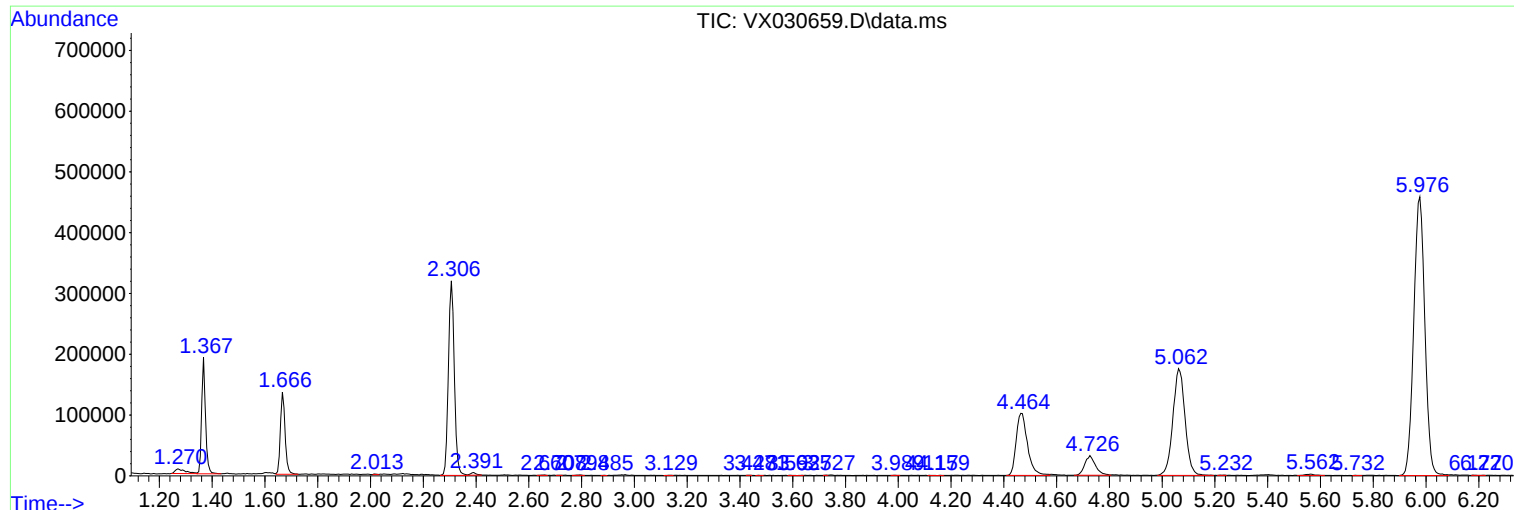
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Instrument :
MSVOA_X
ClientSampleId :
COKN9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.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_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

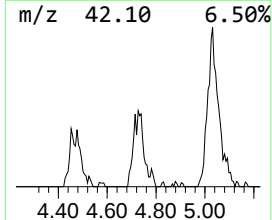
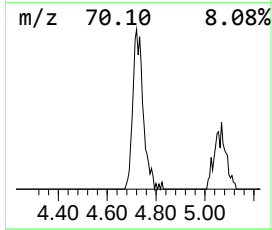
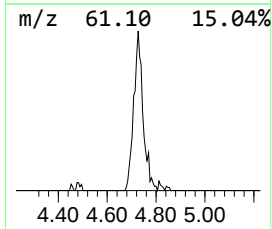
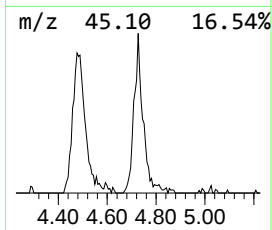
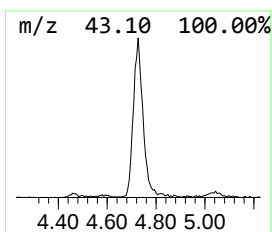
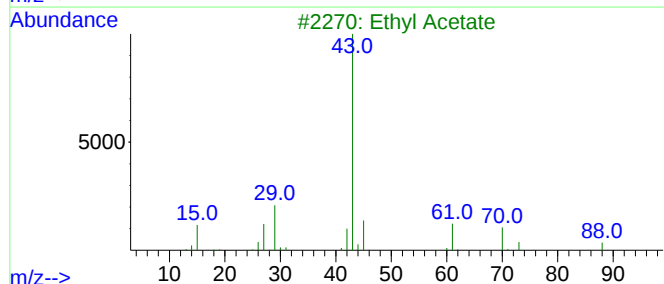
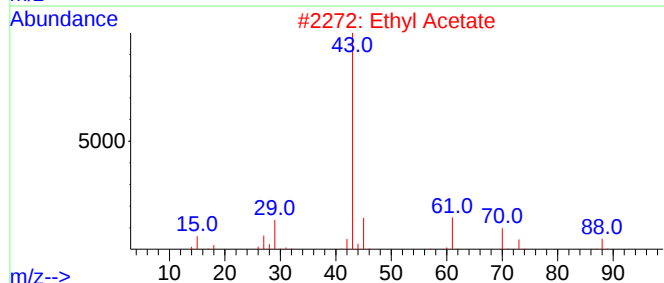
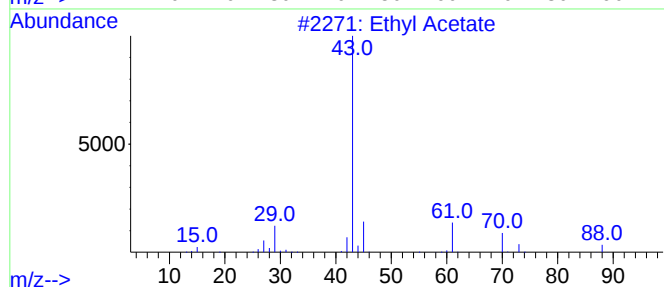
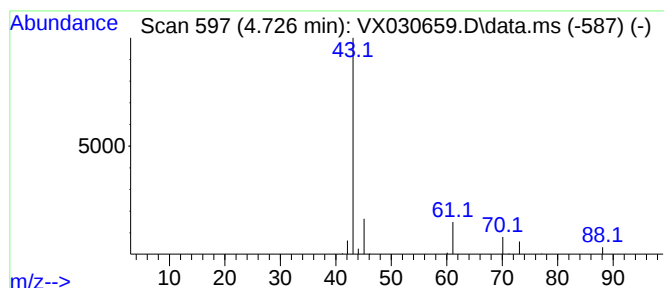
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.726	6.34 ug/L	90101	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	78
3			Ethyl Acetate	88	C4H8O2	000141-78-6	59
4			Ethyl Acetate	88	C4H8O2	000141-78-6	56
5			Isopropyl acetate	102	C5H10O2	000108-21-4	9



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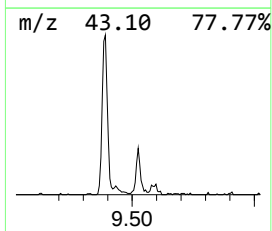
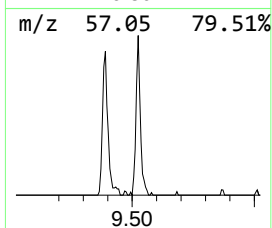
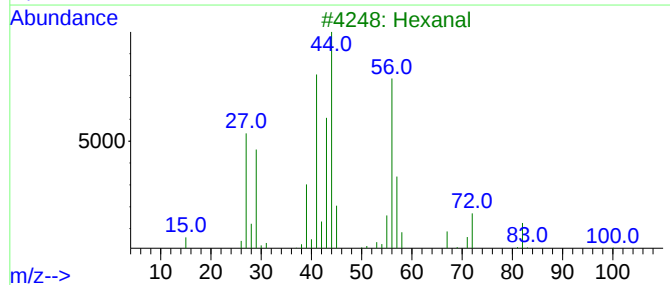
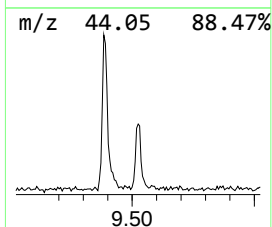
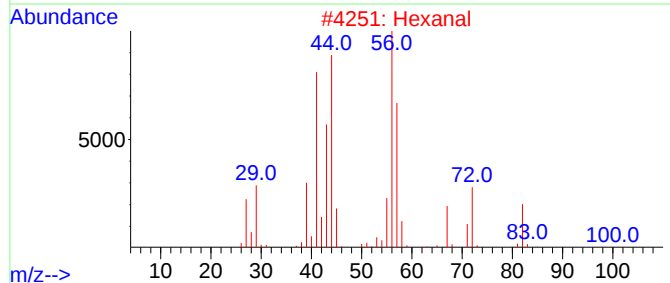
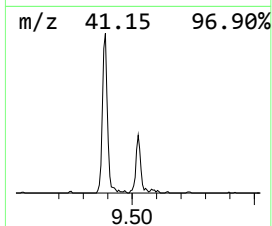
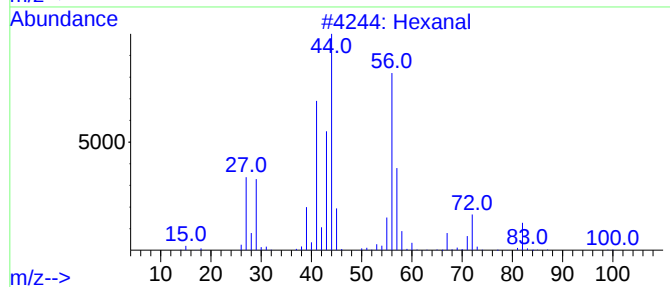
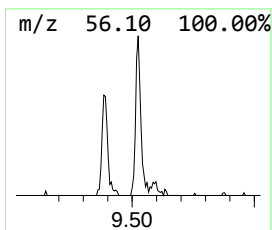
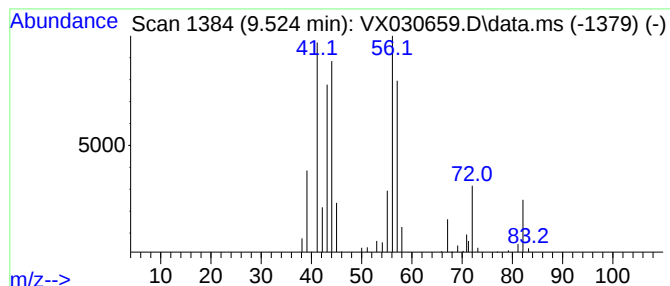
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.524	2.53 ug/L	42259	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	64
2	Hexanal			100	C6H12O	000066-25-1	59
3	Hexanal			100	C6H12O	000066-25-1	53
4	Hexanal			100	C6H12O	000066-25-1	53
5	Hexanal			100	C6H12O	000066-25-1	45



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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
Ethyl Acetate	4.726	6.3	ug/L	90101	1	6.769	710837	50.0
Hexanal	9.524	2.5	ug/L	42259	2	10.055	835734	50.0