

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030656.D
 Acq On : 17 Aug 2022 13:41
 Operator : JC/MD
 Sample : N4221-19
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KP1

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: VX030656.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	54	rVB	149873	155405	12.68%	1.644%
2	1.666	91	95	104	rVB	118347	143529	11.71%	1.518%
3	2.307	193	200	209	rBV	267900	416829	34.02%	4.408%
4	2.392	210	214	221	rVB	4032	7468	0.61%	0.079%
5	2.508	228	233	238	rBV2	1193	1857	0.15%	0.020%
6	2.550	238	240	242	rBV2	498	451	0.04%	0.005%
7	2.611	249	250	252	rVB2	691	385	0.03%	0.004%
8	2.666	255	259	261	rVB3	709	923	0.08%	0.010%
9	2.691	261	263	265	rBV2	507	499	0.04%	0.005%
10	2.794	275	280	283	rBV2	1561	2458	0.20%	0.026%
11	2.916	298	300	301	rBV2	490	418	0.03%	0.004%
12	2.947	302	305	308	rVB2	1286	1474	0.12%	0.016%
13	3.093	327	329	330	rVV	435	391	0.03%	0.004%
14	3.111	330	332	334	rVV	621	520	0.04%	0.005%
15	3.136	334	336	339	rVV2	544	596	0.05%	0.006%
16	3.733	431	434	435	rVV	886	759	0.06%	0.008%
17	3.776	439	441	442	rVV	765	533	0.04%	0.006%
18	4.465	545	554	569	rBV	101953	292283	23.85%	3.091%
19	4.721	589	596	609	rVB2	25928	74080	6.05%	0.783%
20	5.062	636	652	671	rBV	158615	521771	42.58%	5.518%
21	5.294	689	690	693	rBV	579	448	0.04%	0.005%
22	5.385	701	705	706	rBV3	1046	1311	0.11%	0.014%
23	5.538	724	730	731	rBV3	1182	1678	0.14%	0.018%
24	5.629	743	745	747	rVB2	676	509	0.04%	0.005%
25	5.654	747	749	751	rBV2	333	356	0.03%	0.004%
26	5.733	760	762	765	rBV2	288	344	0.03%	0.004%
27	5.806	771	774	777	rVB2	343	398	0.03%	0.004%
28	5.873	777	785	787	rVB2	310	526	0.04%	0.006%
29	5.971	787	801	820	rBV2	414683	1225369	100.00%	12.960%
30	6.099	820	822	827	rVV4	1377	2004	0.16%	0.021%
31	6.178	831	835	836	rBV2	385	438	0.04%	0.005%
32	6.251	845	847	849	rVV2	651	566	0.05%	0.006%
33	6.324	852	859	861	rBV2	737	841	0.07%	0.009%
34	6.355	861	864	866	rBV2	757	790	0.06%	0.008%
35	6.702	918	921	922	rBV	581	482	0.04%	0.005%
36	6.763	922	931	947	rVV2	280723	676401	55.20%	7.154%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXMLM080422WMA.M
 Title : VOC Analysis

37	7.031	972	975	980	rVB2	404	689	0.06%	0.007%
38	7.111	980	988	998	rBV2	12882	30083	2.46%	0.318%
39	7.214	1002	1005	1008	rVB2	393	542	0.04%	0.006%
40	7.312	1011	1021	1036	rBV	256692	560635	45.75%	5.929%
41	7.415	1036	1038	1039	rBV	733	445	0.04%	0.005%
42	7.476	1045	1048	1057	rVB4	893	2247	0.18%	0.024%
43	7.586	1063	1066	1071	rVB5	1163	1857	0.15%	0.020%
44	7.678	1078	1081	1083	rBV	416	423	0.03%	0.004%
45	7.708	1083	1086	1089	rVV2	509	633	0.05%	0.007%
46	7.860	1108	1111	1112	rBV	545	488	0.04%	0.005%
47	7.940	1120	1124	1125	rBV2	1206	1356	0.11%	0.014%
48	8.068	1143	1145	1148	rVB	755	451	0.04%	0.005%
49	8.165	1159	1161	1166	rBV2	360	387	0.03%	0.004%
50	8.330	1179	1188	1197	rBV	165929	281299	22.96%	2.975%
51	8.433	1203	1205	1208	rVB3	854	909	0.07%	0.010%
52	8.476	1210	1212	1213	rBV	1208	883	0.07%	0.009%
53	8.653	1234	1241	1250	rBV	614364	974207	79.50%	10.303%
54	8.952	1284	1290	1301	rBV	127108	187915	15.34%	1.987%
55	9.275	1340	1343	1348	rVB3	3901	4998	0.41%	0.053%
56	9.317	1348	1350	1352	rVB	639	427	0.03%	0.005%
57	9.385	1356	1361	1376	rVV	453086	645826	52.70%	6.830%
58	9.525	1379	1384	1390	rVV2	27330	41069	3.35%	0.434%
59	9.586	1392	1394	1401	rVB3	2311	2948	0.24%	0.031%
60	10.055	1465	1471	1483	rBV	598466	784838	64.05%	8.301%
61	10.189	1491	1493	1498	rVB4	781	852	0.07%	0.009%
62	10.238	1498	1501	1505	rVB3	757	1109	0.09%	0.012%
63	10.269	1505	1506	1509	rBV2	493	499	0.04%	0.005%
64	10.311	1509	1513	1516	rBV2	1082	1360	0.11%	0.014%
65	10.543	1549	1551	1553	rBV2	461	369	0.03%	0.004%
66	10.647	1564	1568	1573	rBV2	9271	11855	0.97%	0.125%
67	10.768	1583	1588	1592	rVV6	1512	2857	0.23%	0.030%
68	10.860	1599	1603	1610	rVB3	3990	4902	0.40%	0.052%
69	10.957	1617	1619	1623	rVB2	777	830	0.07%	0.009%
70	11.031	1627	1631	1634	rBV	1715	1927	0.16%	0.020%
71	11.104	1642	1643	1646	rBV3	418	441	0.04%	0.005%
72	11.153	1649	1651	1652	rBV	382	349	0.03%	0.004%
73	11.195	1652	1658	1669	rBV	450410	566711	46.25%	5.994%
74	11.317	1674	1678	1681	rVB2	2801	3316	0.27%	0.035%
75	11.390	1687	1690	1692	rVB3	816	768	0.06%	0.008%
76	11.451	1698	1700	1702	rBV	1035	829	0.07%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

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77	11.555	1714	1717	1719	rBV2	408	595	0.05%	0.006%
78	11.622	1722	1728	1731	rVV2	1254	1774	0.14%	0.019%
79	11.683	1733	1738	1741	rVB5	852	1322	0.11%	0.014%
80	11.756	1747	1750	1756	rVB2	4095	5721	0.47%	0.061%
81	11.841	1762	1764	1769	rVB3	927	1363	0.11%	0.014%
82	11.933	1775	1779	1783	rVB3	2336	2968	0.24%	0.031%
83	11.969	1783	1785	1788	rBV2	1008	1037	0.08%	0.011%
84	12.024	1789	1794	1802	rBV	621645	754590	61.58%	7.981%
85	12.219	1822	1826	1837	rBV	67098	105433	8.60%	1.115%
86	12.323	1837	1843	1854	rVB	683890	874294	71.35%	9.247%
87	12.853	1927	1930	1936	rVB3	8492	11133	0.91%	0.118%
88	12.975	1948	1950	1953	rBV4	336	393	0.03%	0.004%
89	13.103	1966	1971	1977	rVV	16860	22403	1.83%	0.237%
90	13.207	1983	1988	1990	rBV3	576	725	0.06%	0.008%
91	13.256	1994	1996	1997	rBV2	731	539	0.04%	0.006%
92	13.469	2028	2031	2034	rBV4	797	1071	0.09%	0.011%
93	13.597	2049	2052	2054	rVB3	1119	1107	0.09%	0.012%
94	13.731	2073	2074	2078	rBV	685	646	0.05%	0.007%
95	13.786	2078	2083	2089	rVB6	1391	3479	0.28%	0.037%
96	13.835	2089	2091	2094	rBV2	484	606	0.05%	0.006%
97	14.134	2136	2140	2145	rVB2	2175	2511	0.20%	0.027%
98	14.884	2261	2263	2265	rBV2	596	523	0.04%	0.006%
99	15.981	2442	2443	2444	rBV	1250	598	0.05%	0.006%
100	16.335	2499	2501	2504	rBV2	841	718	0.06%	0.008%

Sum of corrected areas: 9455168

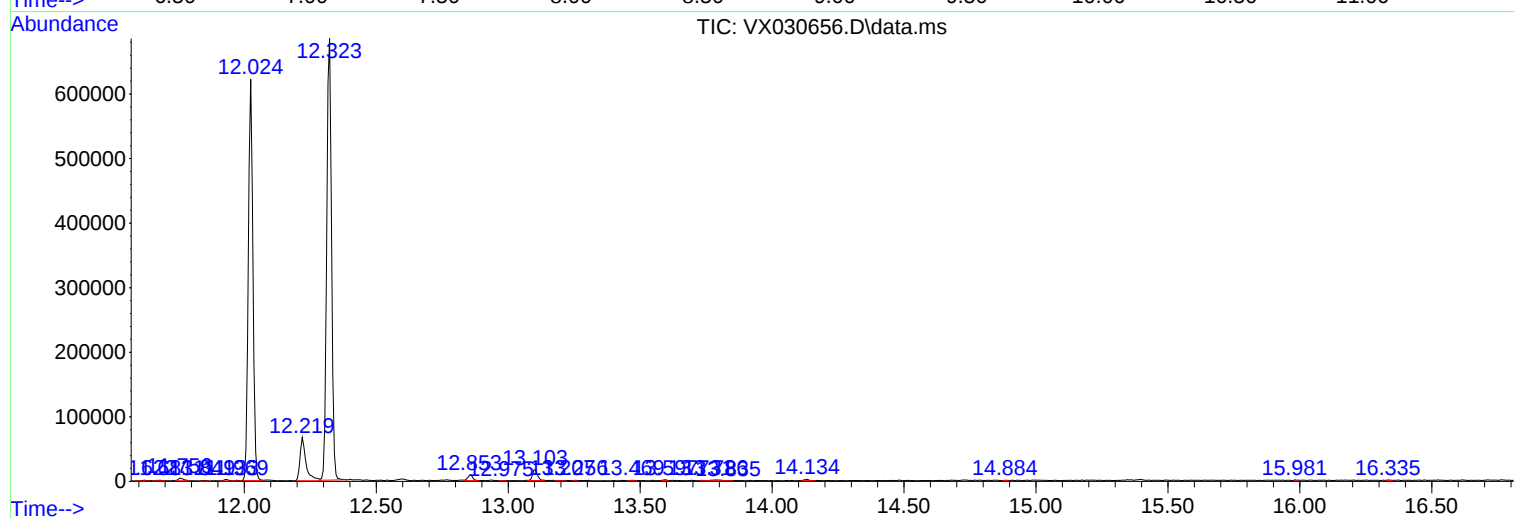
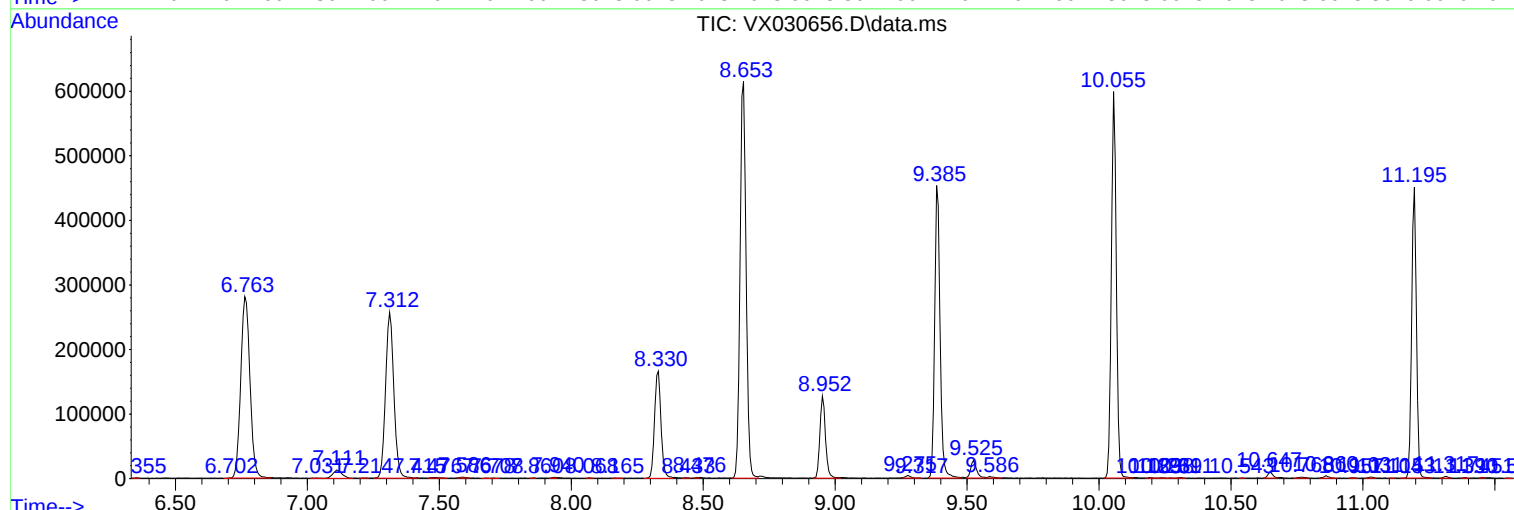
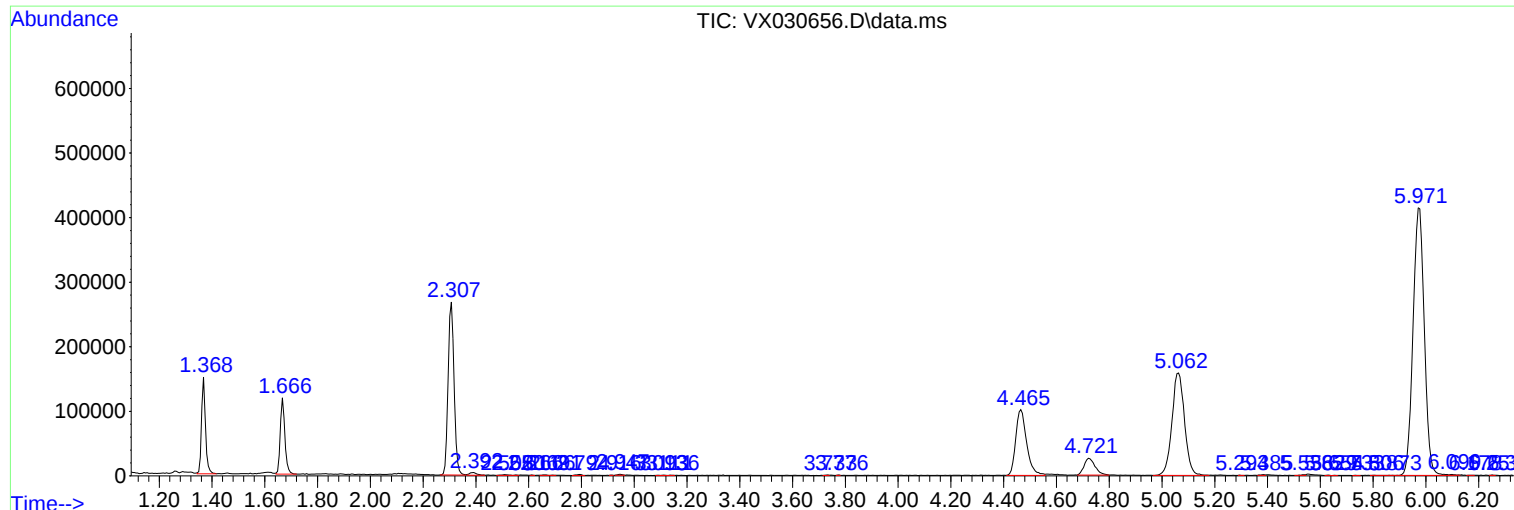
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Instrument :
MSVOA_X
ClientSampleId :
C0KP1

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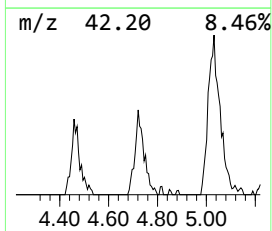
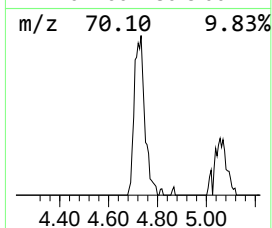
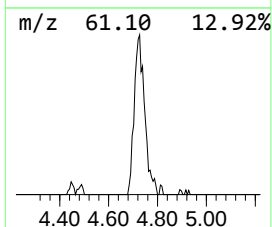
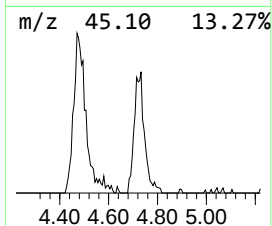
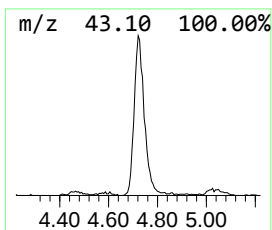
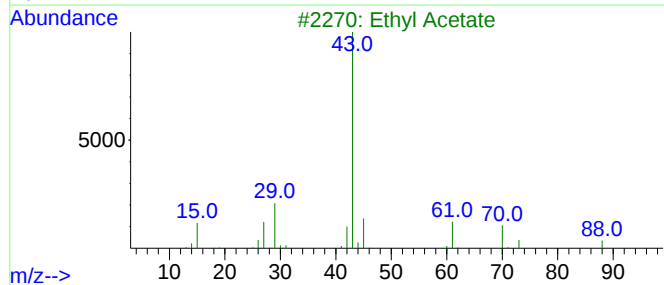
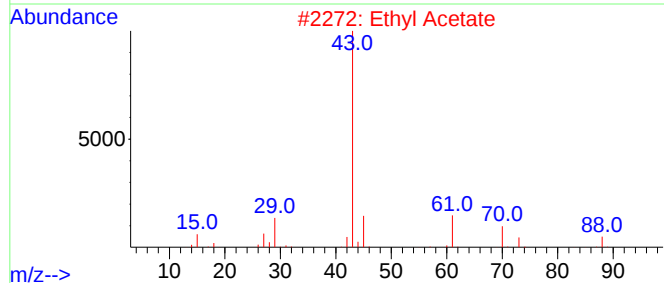
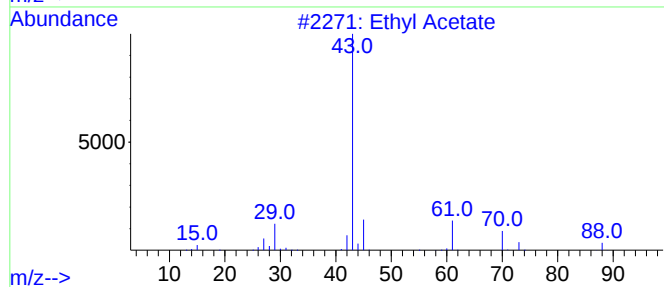
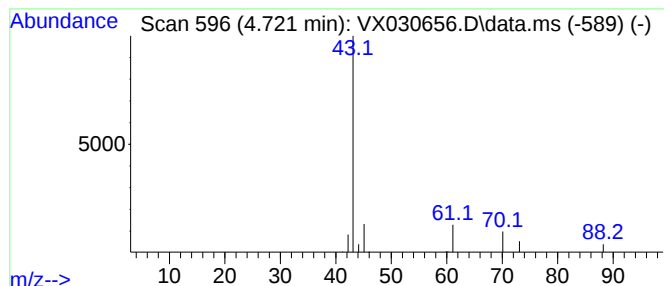
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.721	5.48 ug/L	74080	1,4-Difluorobenzene	6.763

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	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	90
4			Ethyl Acetate	88	C4H8O2	000141-78-6	64
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	50



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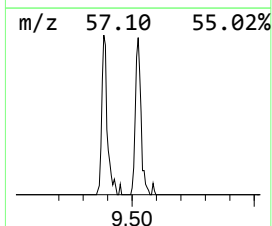
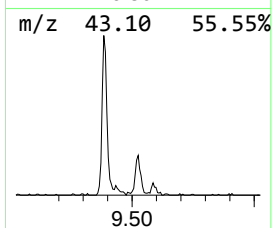
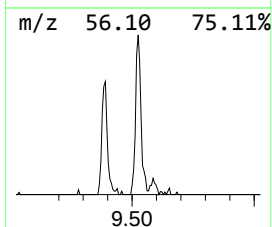
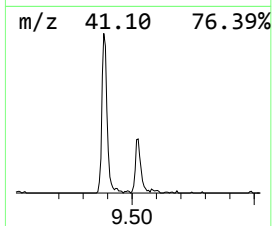
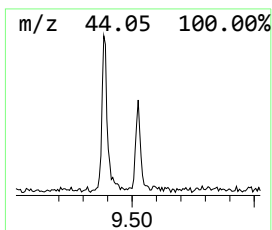
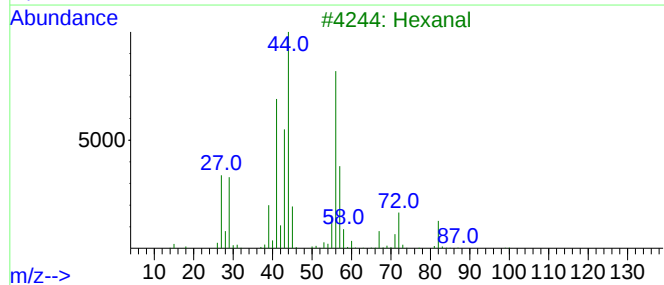
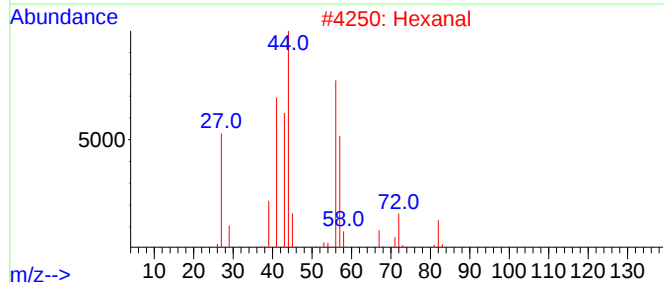
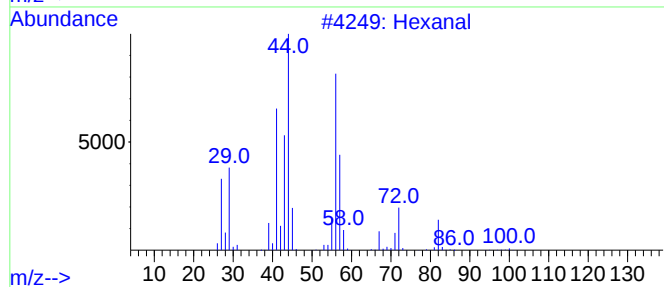
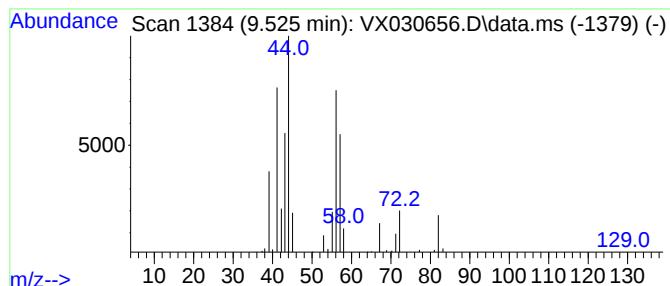
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.525	2.62 ug/L	41069	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	72
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	53



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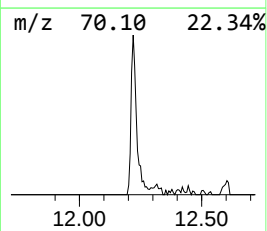
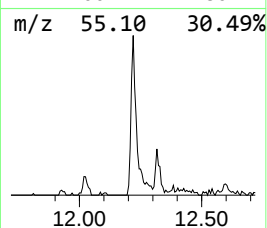
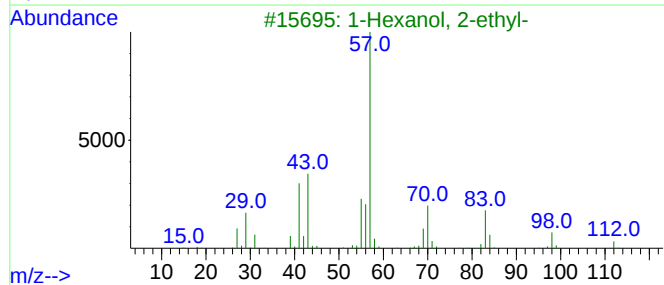
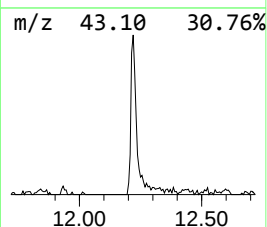
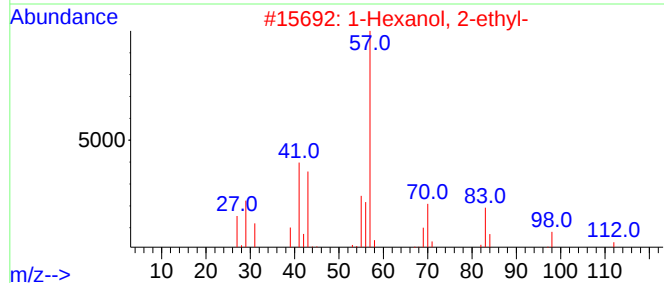
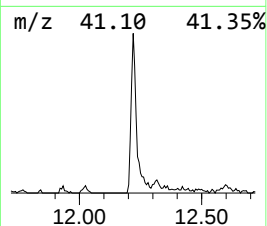
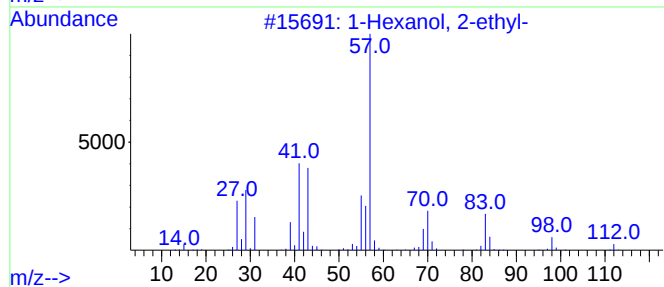
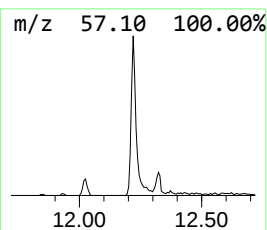
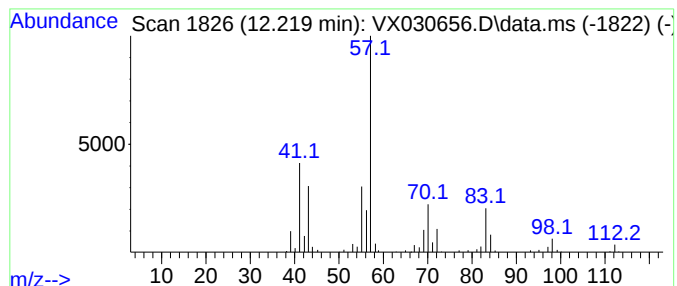
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	6.99 ug/L	105433	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
Data File : VX030656.D
Acq On : 17 Aug 2022 13:41
Operator : JC/MD
Sample : N4221-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KP1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.721	5.5	ug/L	74080	1	6.763	676401	50.0
Hexanal	9.525	2.6	ug/L	41069	2	10.055	784838	50.0
1-Hexanol, 2-et...	12.219	7.0	ug/L	105433	3	12.024	754590	50.0