

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
 Data File : VX030648.D
 Acq On : 16 Aug 2022 12:35
 Operator : JC/MD
 Sample : N4221-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KQ3

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: VX030648.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	57	rVB	157556	159924	13.14%	1.715%
2	1.666	90	95	101	rBV	117276	144786	11.89%	1.552%
3	2.307	192	200	209	rBV	268887	421199	34.59%	4.516%
4	2.392	209	214	218	rVB2	3795	6536	0.54%	0.070%
5	2.502	228	232	235	rBV2	643	1067	0.09%	0.011%
6	2.788	274	279	283	rBV5	1188	2580	0.21%	0.028%
7	2.874	291	293	294	rVB2	458	305	0.03%	0.003%
8	2.947	299	305	306	rBV2	1510	2718	0.22%	0.029%
9	3.044	319	321	323	rVV	540	353	0.03%	0.004%
10	3.203	344	347	348	rBV2	338	321	0.03%	0.003%
11	3.233	350	352	354	rVB2	417	342	0.03%	0.004%
12	3.264	354	357	359	rBV2	305	370	0.03%	0.004%
13	3.319	362	366	367	rBV2	469	495	0.04%	0.005%
14	3.867	452	456	459	rBV2	283	430	0.04%	0.005%
15	3.898	459	461	464	rVV2	451	363	0.03%	0.004%
16	4.172	503	506	508	rBV2	409	540	0.04%	0.006%
17	4.215	510	513	514	rBV3	324	343	0.03%	0.004%
18	4.349	533	535	538	rVB2	466	367	0.03%	0.004%
19	4.459	544	553	571	rBV	102006	291940	23.98%	3.130%
20	4.721	588	596	609	rVB2	29831	85535	7.03%	0.917%
21	4.898	623	625	627	rBV	505	575	0.05%	0.006%
22	5.056	637	651	668	rVV	161691	515372	42.33%	5.526%
23	5.251	681	683	684	rBV2	430	313	0.03%	0.003%
24	5.276	685	687	691	rVB	442	491	0.04%	0.005%
25	5.312	691	693	695	rBV	415	304	0.02%	0.003%
26	5.337	695	697	700	rBV2	370	474	0.04%	0.005%
27	5.714	758	759	761	rBV	447	305	0.03%	0.003%
28	5.971	788	801	816	rBV2	417155	1217523	100.00%	13.054%
29	6.257	847	848	852	rBV2	303	360	0.03%	0.004%
30	6.294	852	854	858	rVV2	368	490	0.04%	0.005%
31	6.367	864	866	867	rVV	429	307	0.03%	0.003%
32	6.403	871	872	875	rBV2	371	415	0.03%	0.004%
33	6.446	878	879	883	rBV	466	438	0.04%	0.005%
34	6.501	886	888	891	rVB2	486	570	0.05%	0.006%
35	6.525	891	892	893	rBV	434	280	0.02%	0.003%
36	6.690	916	919	920	rBV2	361	350	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
 Data File : VX030648.D
 Acq On : 16 Aug 2022 12:35
 Operator : JC/MD
 Sample : N4221-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KQ3

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

37	6.763	921	931	946	rVV	293291	701338	57.60%	7.520%
38	6.903	953	954	958	rBV2	450	426	0.03%	0.005%
39	7.111	980	988	996	rBV2	9762	22527	1.85%	0.242%
40	7.196	1000	1002	1003	rBV	578	388	0.03%	0.004%
41	7.312	1013	1021	1035	rVB	253611	555890	45.66%	5.960%
42	7.464	1043	1046	1047	rBV	796	744	0.06%	0.008%
43	7.586	1059	1066	1076	rBV4	1393	3767	0.31%	0.040%
44	7.665	1076	1079	1081	rBV2	382	405	0.03%	0.004%
45	7.873	1111	1113	1116	rVB2	538	514	0.04%	0.006%
46	7.940	1116	1124	1128	rBV4	1517	3566	0.29%	0.038%
47	8.324	1181	1187	1196	rBV	166791	273799	22.49%	2.936%
48	8.458	1207	1209	1210	rBV	492	346	0.03%	0.004%
49	8.476	1210	1212	1215	rVV4	727	938	0.08%	0.010%
50	8.647	1234	1240	1249	rBV	608656	956303	78.54%	10.253%
51	8.805	1264	1266	1267	rBV2	639	391	0.03%	0.004%
52	8.952	1284	1290	1303	rVV	125123	181635	14.92%	1.947%
53	9.281	1339	1344	1350	rVB3	5392	7914	0.65%	0.085%
54	9.385	1356	1361	1375	rVV	447509	639461	52.52%	6.856%
55	9.525	1379	1384	1391	rVV	24727	36301	2.98%	0.389%
56	9.811	1430	1431	1432	rBV	553	298	0.02%	0.003%
57	9.891	1442	1444	1446	rBV	424	312	0.03%	0.003%
58	10.055	1465	1471	1479	rBV	617097	820684	67.41%	8.799%
59	10.305	1510	1512	1514	rBV2	673	642	0.05%	0.007%
60	10.397	1525	1527	1529	rVB2	504	436	0.04%	0.005%
61	10.647	1564	1568	1572	rBV	9251	12316	1.01%	0.132%
62	10.775	1582	1589	1592	rBV4	1741	3149	0.26%	0.034%
63	10.860	1599	1603	1610	rVB3	2755	4700	0.39%	0.050%
64	10.915	1610	1612	1615	rBV	496	571	0.05%	0.006%
65	10.970	1619	1621	1622	rVB	689	318	0.03%	0.003%
66	11.195	1652	1658	1669	rVB	423365	556177	45.68%	5.963%
67	11.317	1674	1678	1682	rVB3	3971	5724	0.47%	0.061%
68	11.354	1682	1684	1685	rBV2	466	322	0.03%	0.003%
69	11.451	1698	1700	1704	rBV3	621	1055	0.09%	0.011%
70	11.616	1725	1727	1731	rVV4	804	1060	0.09%	0.011%
71	11.756	1747	1750	1757	rVB3	3260	5846	0.48%	0.063%
72	11.811	1757	1759	1761	rVB2	645	473	0.04%	0.005%
73	11.835	1761	1763	1764	rBV	462	384	0.03%	0.004%
74	11.927	1773	1778	1782	rVB4	2389	2949	0.24%	0.032%
75	11.963	1782	1784	1786	rBV	614	638	0.05%	0.007%
76	12.024	1788	1794	1802	rBV	614908	755914	62.09%	8.105%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
 Data File : VX030648.D
 Acq On : 16 Aug 2022 12:35
 Operator : JC/MD
 Sample : N4221-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KQ3

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

77	12.219	1821	1826	1837	rBV	29270	52043	4.27%	0.558%
78	12.323	1837	1843	1848	rVV	630397	804952	66.11%	8.631%
79	12.597	1883	1888	1897	rVB6	2650	6245	0.51%	0.067%
80	12.671	1897	1900	1901	rBV2	650	539	0.04%	0.006%
81	12.853	1927	1930	1936	rVB4	7680	10293	0.85%	0.110%
82	13.103	1966	1971	1974	rBV2	15657	20146	1.65%	0.216%
83	13.170	1980	1982	1983	rBV	668	401	0.03%	0.004%
84	13.469	2028	2031	2035	rVB3	793	1070	0.09%	0.011%
85	13.536	2041	2042	2044	rBV2	675	461	0.04%	0.005%
86	13.561	2044	2046	2049	rBV	746	1011	0.08%	0.011%
87	13.597	2050	2052	2054	rVB	790	508	0.04%	0.005%
88	13.658	2060	2062	2064	rVV	477	297	0.02%	0.003%
89	13.689	2065	2067	2069	rVB	1152	852	0.07%	0.009%
90	13.829	2088	2090	2096	rVB3	638	868	0.07%	0.009%
91	13.939	2107	2108	2109	rBV	513	295	0.02%	0.003%
92	14.000	2116	2118	2120	rBV	766	436	0.04%	0.005%
93	14.030	2120	2123	2125	rBV2	360	391	0.03%	0.004%
94	14.128	2136	2139	2147	rVB2	2151	2919	0.24%	0.031%
95	14.329	2169	2172	2174	rBV3	530	463	0.04%	0.005%
96	14.640	2221	2223	2225	rBV2	704	825	0.07%	0.009%
97	15.042	2287	2289	2290	rBV2	672	321	0.03%	0.003%
98	15.304	2328	2332	2335	rBV3	610	911	0.07%	0.010%
99	15.640	2386	2387	2388	rBV	704	363	0.03%	0.004%
100	16.578	2539	2541	2542	rBV	733	392	0.03%	0.004%

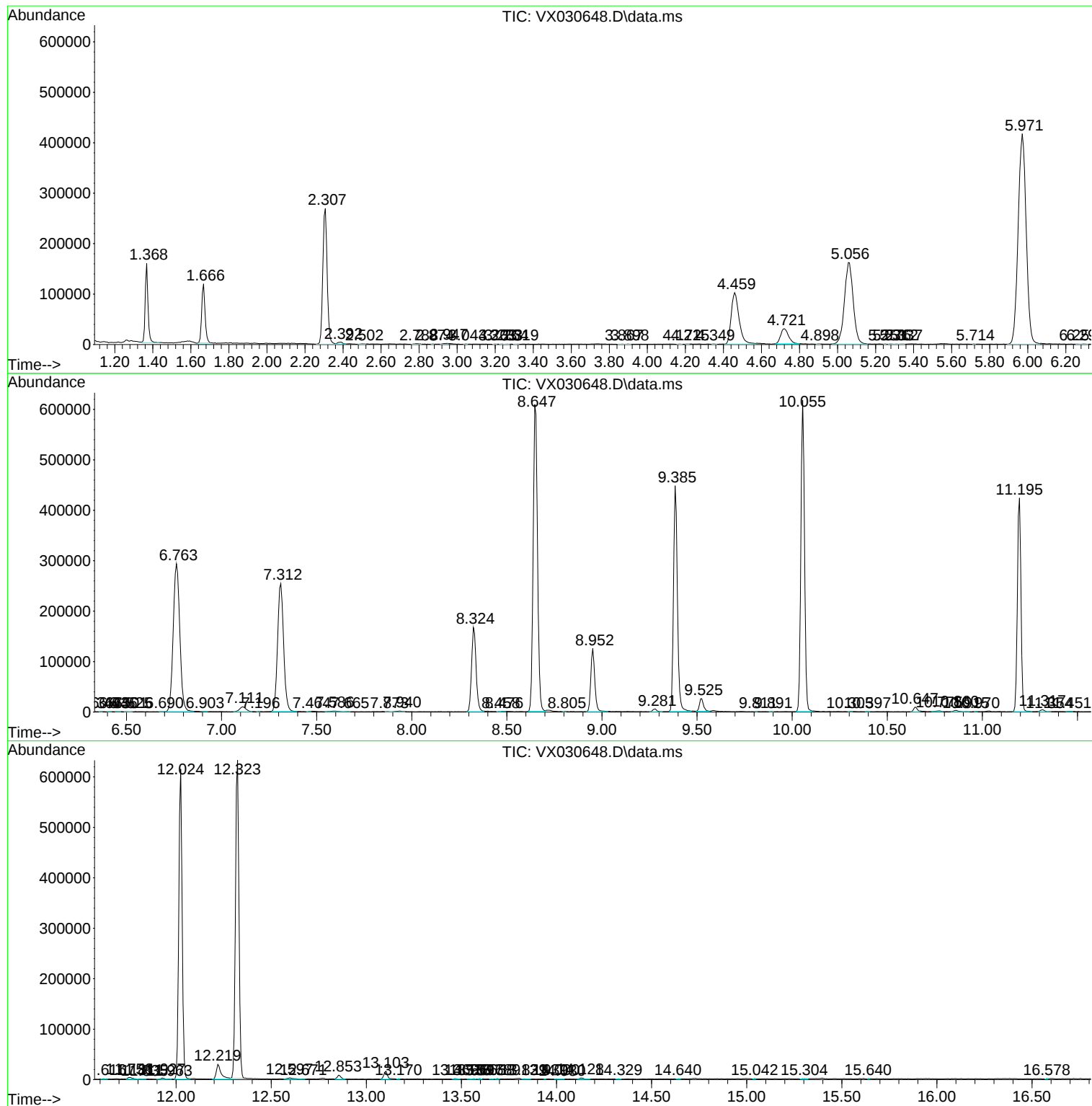
Sum of corrected areas: 9326704

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
Data File : VX030648.D
Acq On : 16 Aug 2022 12:35
Operator : JC/MD
Sample : N4221-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KQ3

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
Data File : VX030648.D
Acq On : 16 Aug 2022 12:35
Operator : JC/MD
Sample : N4221-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KQ3

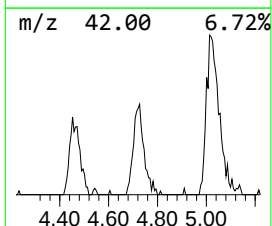
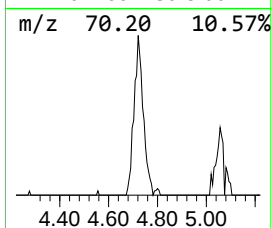
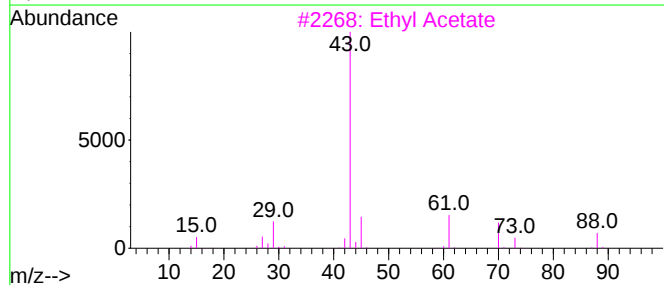
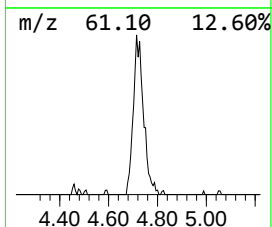
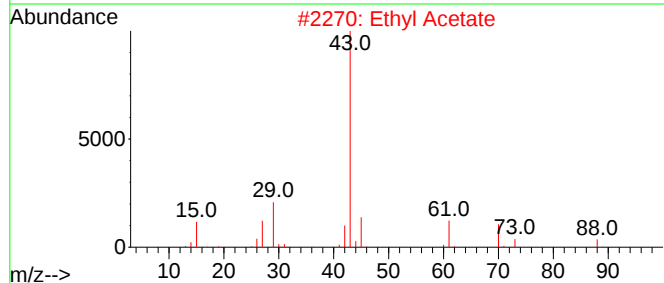
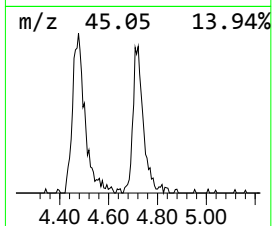
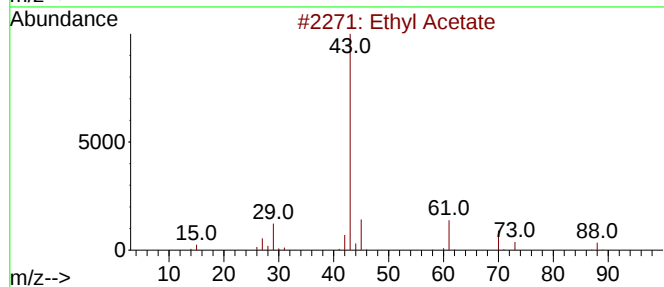
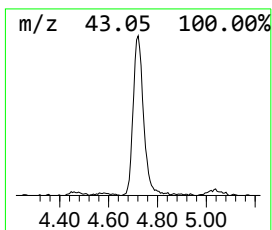
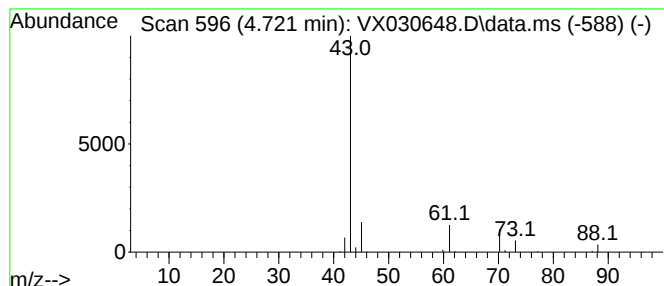
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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.
4.721	6.10 ug/L	85535	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	86
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	56
4			Ethyl Acetate	88	C4H8O2	000141-78-6	53
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
Data File : VX030648.D
Acq On : 16 Aug 2022 12:35
Operator : JC/MD
Sample : N4221-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KQ3

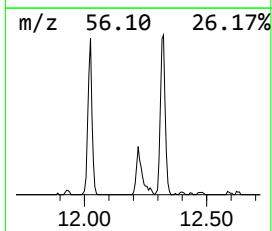
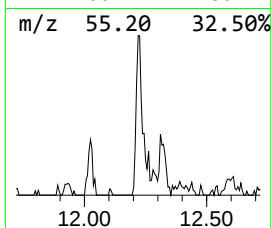
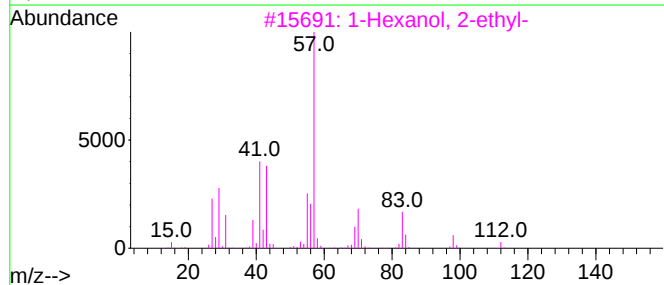
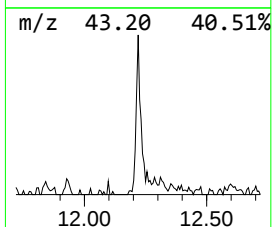
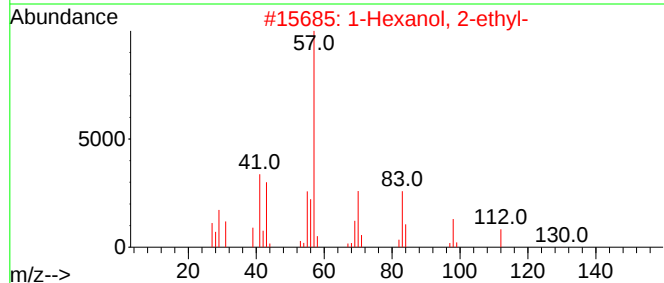
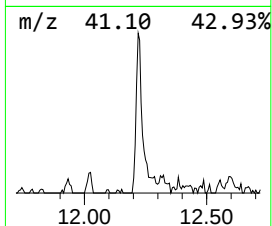
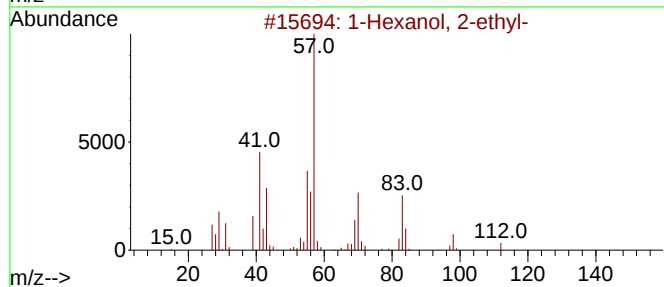
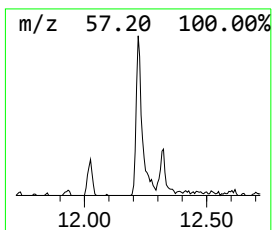
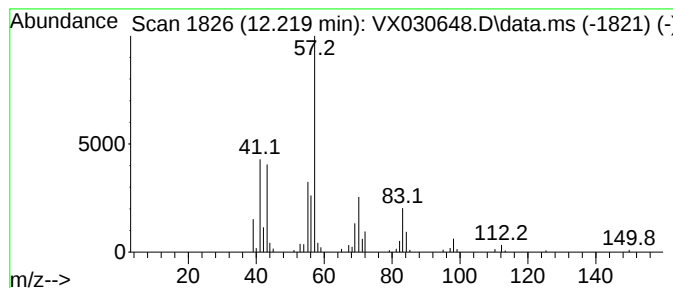
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	3.44 ug/L	52043	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	64
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
Data File : VX030648.D
Acq On : 16 Aug 2022 12:35
Operator : JC/MD
Sample : N4221-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KQ3

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	6.1	ug/L	85535	1	6.763	701338	50.0
1-Hexanol, 2-et...	12.219	3.4	ug/L	52043	3	12.024	755914	50.0