

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021522\
 Data File : VX027030.D
 Acq On : 15 Feb 2022 14:48
 Operator : JC/MD
 Sample : N1486-06
 Misc : 5.00g/5.00mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 X3946

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\SFAMXML021422WMA.M
 Title : VOC Analysis

Signal : TIC: VX027030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	58	rVB	55788	62832	6.99%	0.459%
2	1.666	91	95	99	rBV	26774	31779	3.54%	0.232%
3	2.191	175	181	188	rVB	14793	22573	2.51%	0.165%
4	2.294	191	198	205	rBV	106244	172520	19.19%	1.260%
5	2.410	210	217	251	rVB	62189	218001	24.25%	1.592%
6	2.715	263	267	272	rBV3	1218	2278	0.25%	0.017%
7	2.788	272	279	297	rVB	325806	679233	75.57%	4.959%
8	3.081	325	327	334	rBV2	282	381	0.04%	0.003%
9	3.136	334	336	337	rBV2	128	103	0.01%	0.001%
10	3.306	362	364	366	rVV	147	130	0.01%	0.001%
11	3.361	370	373	375	rBV	95	101	0.01%	0.001%
12	3.605	403	413	429	rBV	194166	466809	51.93%	3.408%
13	3.879	455	458	461	rBV2	131	203	0.02%	0.001%
14	4.251	515	519	523	rBV2	141	275	0.03%	0.002%
15	4.294	523	526	527	rBV2	180	188	0.02%	0.001%
16	4.489	546	558	599	rBV2	98324	325097	36.17%	2.374%
17	4.904	614	626	641	rBV	155422	504843	56.17%	3.686%
18	5.068	642	653	675	rVB3	71419	311280	34.63%	2.273%
19	5.245	678	682	683	rBV2	161	191	0.02%	0.001%
20	5.379	692	704	722	rVB	88609	271984	30.26%	1.986%
21	5.513	724	726	729	rVV2	115	148	0.02%	0.001%
22	5.544	729	731	732	rVV2	320	289	0.03%	0.002%
23	5.672	735	752	767	rVB	97417	302597	33.66%	2.209%
24	5.971	789	801	811	rBV2	177611	508471	56.57%	3.713%
25	6.092	812	821	840	rVB	127587	354471	39.44%	2.588%
26	6.288	850	853	855	rBV	125	148	0.02%	0.001%
27	6.330	858	860	863	rVB2	110	118	0.01%	0.001%
28	6.434	875	877	878	rBV	148	110	0.01%	0.001%
29	6.507	885	889	890	rBV2	92	120	0.01%	0.001%
30	6.605	903	905	908	rVV3	347	297	0.03%	0.002%
31	6.666	913	915	918	rVV	147	132	0.01%	0.001%
32	6.763	921	931	948	rBV	118180	291801	32.46%	2.131%
33	6.952	959	962	965	rBV2	113	184	0.02%	0.001%
34	7.123	980	990	1005	rVV	160997	359903	40.04%	2.628%
35	7.312	1012	1021	1032	rBV	99353	226041	25.15%	1.650%

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36	7.434	1032	1041	1053	rVB	145396	317205	35.29%	2.316%
37	7.629	1070	1073	1075	rBV	106	105	0.01%	0.001%
38	7.678	1075	1081	1084	rBV3	293	620	0.07%	0.005%
39	7.787	1097	1099	1101	rBV	112	103	0.01%	0.001%
40	7.830	1101	1106	1111	rVB3	479	938	0.10%	0.007%
41	7.940	1118	1124	1126	rBV2	329	587	0.07%	0.004%
42	8.104	1148	1151	1152	rBV	114	130	0.01%	0.001%
43	8.123	1152	1154	1155	rVV	137	111	0.01%	0.001%
44	8.171	1158	1162	1168	rBV3	396	722	0.08%	0.005%
45	8.251	1173	1175	1179	rVB2	172	143	0.02%	0.001%
46	8.330	1181	1188	1200	rBV	55424	102591	11.41%	0.749%
47	8.415	1200	1202	1204	rVB2	272	190	0.02%	0.001%
48	8.440	1204	1206	1208	rVB	126	99	0.01%	0.001%
49	8.494	1213	1215	1217	rBV	147	168	0.02%	0.001%
50	8.586	1222	1230	1232	rBV2	220802	399182	44.41%	2.915%
51	8.720	1249	1252	1267	rVB3	4599	10073	1.12%	0.074%
52	8.909	1277	1283	1288	rBV	236782	335449	37.32%	2.449%
53	8.958	1288	1291	1300	rVB	34938	57652	6.41%	0.421%
54	9.055	1305	1307	1309	rVB	156	121	0.01%	0.001%
55	9.159	1317	1324	1336	rBV	345056	659086	73.33%	4.812%
56	9.275	1336	1343	1356	rVB	506235	736911	81.98%	5.380%
57	9.415	1357	1366	1378	rBV	107640	229235	25.50%	1.674%
58	9.525	1378	1384	1393	rVV	245468	451516	50.23%	3.297%
59	9.610	1393	1398	1408	rVB	139665	231127	25.71%	1.688%
60	9.744	1418	1420	1422	rVB	214	159	0.02%	0.001%
61	10.055	1465	1471	1484	rBV	218577	352276	39.19%	2.572%
62	10.202	1492	1495	1500	rVB2	351	442	0.05%	0.003%
63	10.305	1509	1512	1518	rBV3	643	986	0.11%	0.007%
64	10.366	1518	1522	1523	rVB	266	309	0.03%	0.002%
65	10.378	1523	1524	1527	rBV	117	139	0.02%	0.001%
66	10.622	1561	1564	1565	rBV2	191	196	0.02%	0.001%
67	10.665	1565	1571	1585	rVV	319715	465767	51.82%	3.401%
68	10.817	1592	1596	1599	rVB2	300	376	0.04%	0.003%
69	10.964	1615	1620	1629	rVB	322030	434917	48.39%	3.175%
70	11.055	1631	1635	1636	rBV	83	99	0.01%	0.001%
71	11.122	1642	1646	1650	rVB	1874	2165	0.24%	0.016%
72	11.201	1653	1659	1669	rBV	527943	713588	79.39%	5.210%
73	11.476	1699	1704	1714	rBV	190272	220564	24.54%	1.610%
74	11.750	1744	1749	1754	rBV2	1702	2282	0.25%	0.017%
75	11.848	1762	1765	1772	rVB3	244	489	0.05%	0.004%

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76	11.933	1775	1779	1781	rBV2	935	1066	0.12%	0.008%
77	11.976	1781	1786	1790	rVV	227017	291852	32.47%	2.131%
78	12.043	1790	1797	1807	rVB2	442238	898848	100.00%	6.563%
79	12.146	1812	1814	1818	rVB2	1385	1610	0.18%	0.012%
80	12.232	1826	1828	1830	rBV2	155	100	0.01%	0.001%
81	12.262	1830	1833	1836	rBV2	122	209	0.02%	0.002%
82	12.323	1836	1843	1852	rVV	306317	381146	42.40%	2.783%
83	12.427	1858	1860	1866	rVB2	568	614	0.07%	0.004%
84	12.652	1896	1897	1902	rBV2	181	262	0.03%	0.002%
85	12.762	1911	1915	1920	rBV2	3468	4569	0.51%	0.033%
86	12.945	1940	1945	1953	rBV	113874	141585	15.75%	1.034%
87	13.055	1959	1963	1965	rVB2	208	253	0.03%	0.002%
88	13.116	1968	1973	1984	rVB	628968	770333	85.70%	5.624%
89	13.268	1996	1998	2001	rVV	392	339	0.04%	0.002%
90	13.420	2020	2023	2027	rBV2	159	359	0.04%	0.003%
91	13.524	2037	2040	2041	rVB2	159	137	0.02%	0.001%
92	13.591	2045	2051	2060	rBV	289650	355304	39.53%	2.594%
93	13.750	2075	2077	2080	rBV	417	361	0.04%	0.003%
94	13.780	2080	2082	2084	rVB	231	173	0.02%	0.001%
95	13.963	2109	2112	2115	rVB	713	832	0.09%	0.006%
96	14.134	2136	2140	2144	rVB3	455	594	0.07%	0.004%
97	14.365	2175	2178	2180	rBV2	146	161	0.02%	0.001%
98	14.573	2207	2212	2213	rBV2	209	315	0.04%	0.002%
99	14.756	2239	2242	2244	rVB3	534	511	0.06%	0.004%
100	14.957	2273	2275	2277	rBV2	149	190	0.02%	0.001%

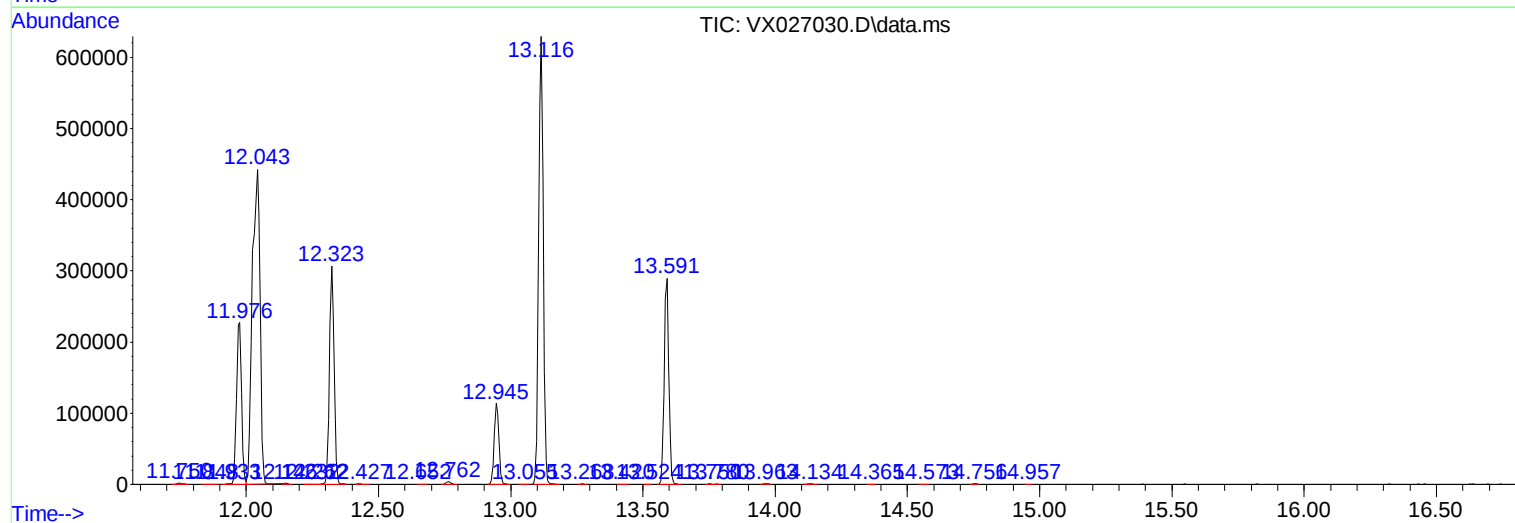
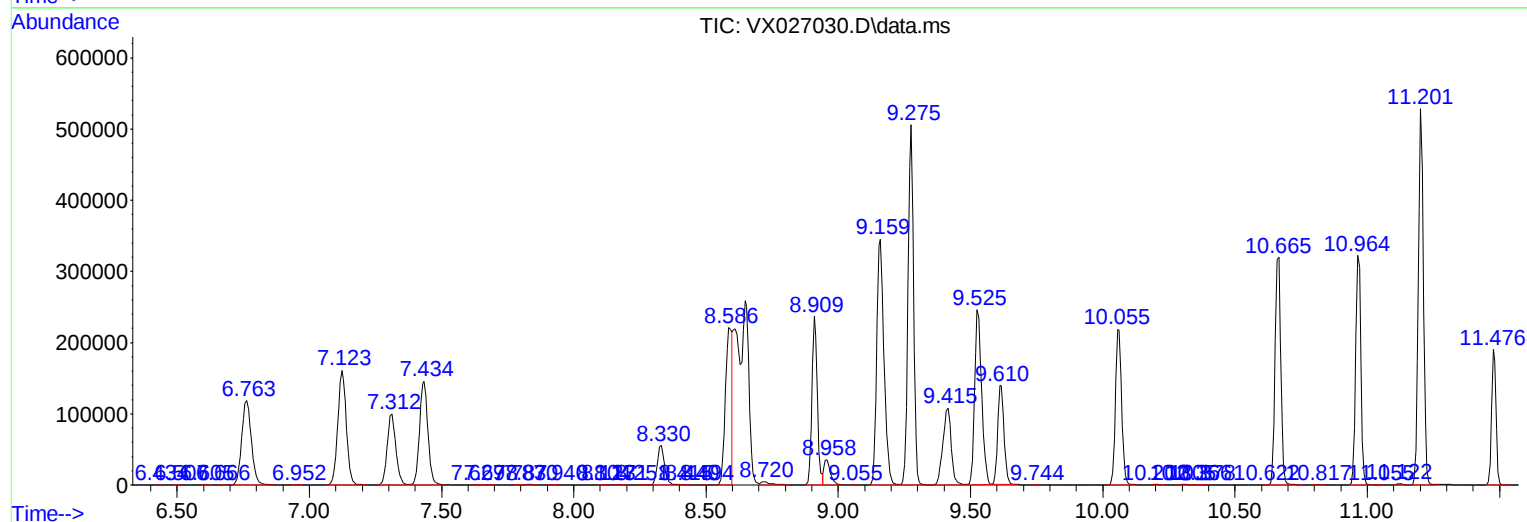
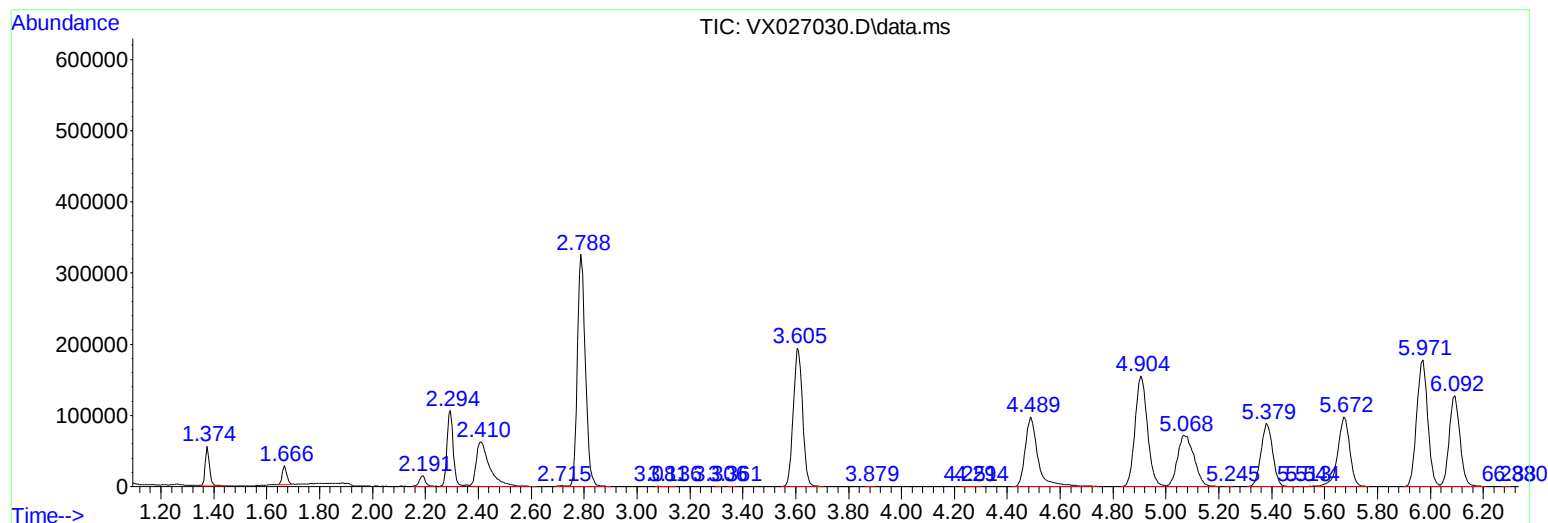
Sum of corrected areas: 13696172

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

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



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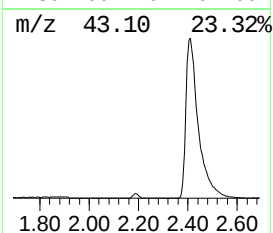
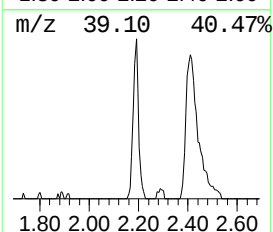
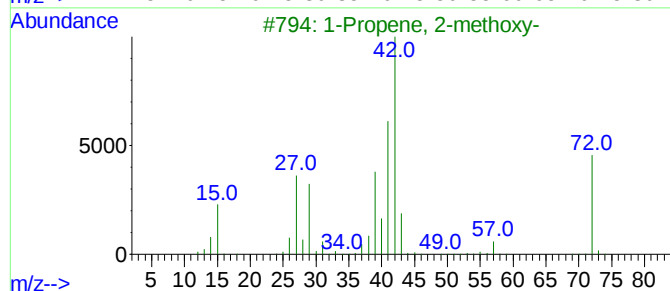
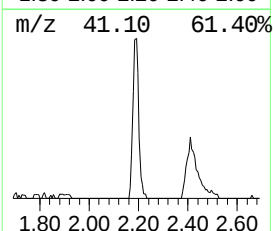
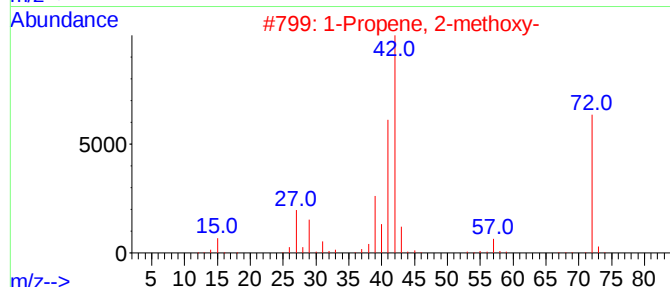
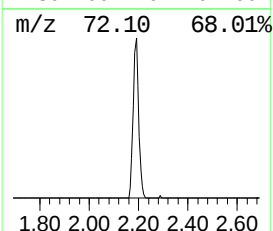
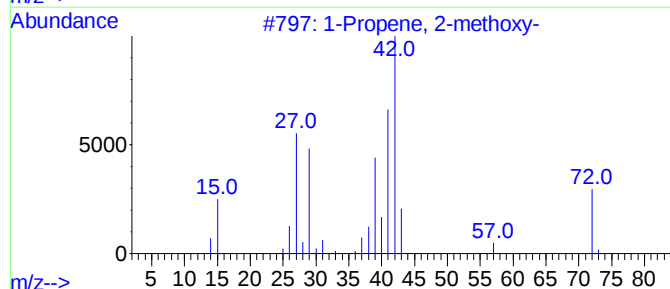
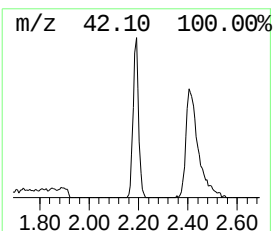
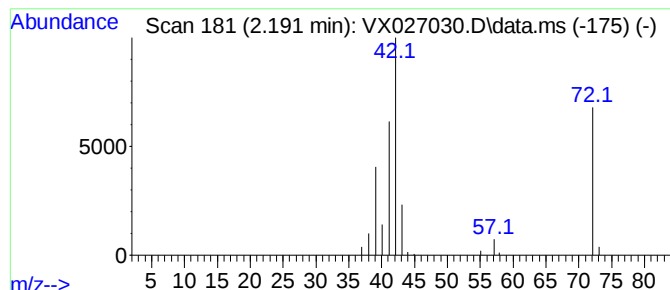
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 1-Propene, 2-methoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.191	3.87 ug/L	22573	1,4-Difluorobenzene	6.763

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	83	
2	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	64	
3	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	59	
4	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	59	
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47	



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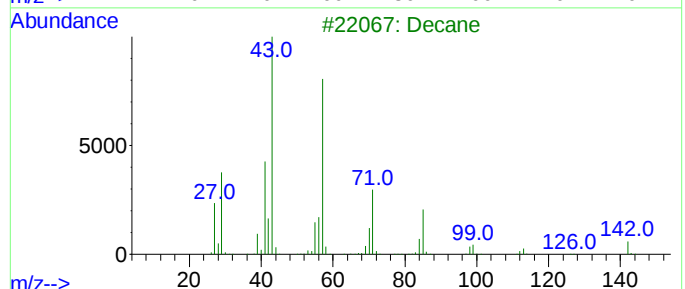
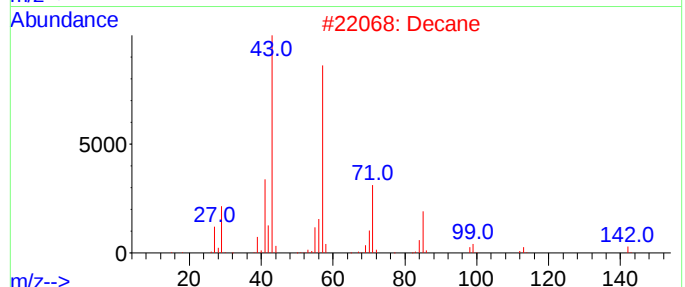
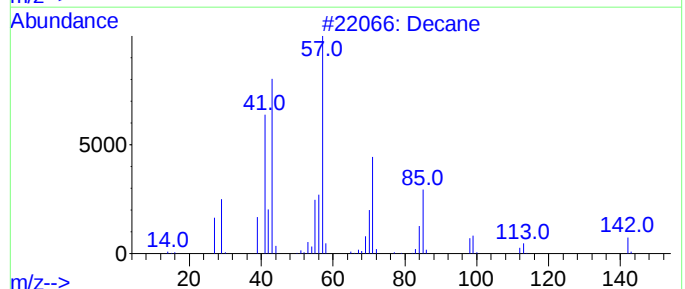
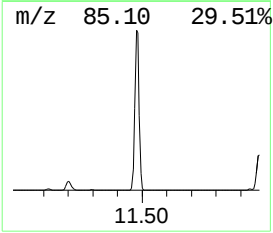
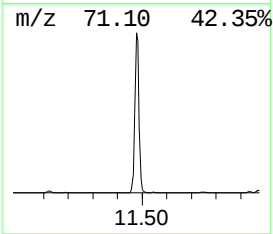
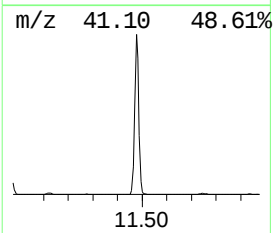
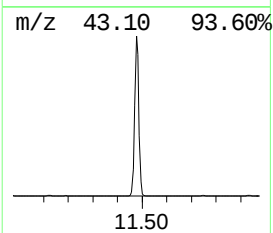
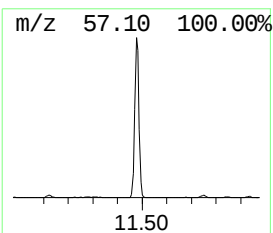
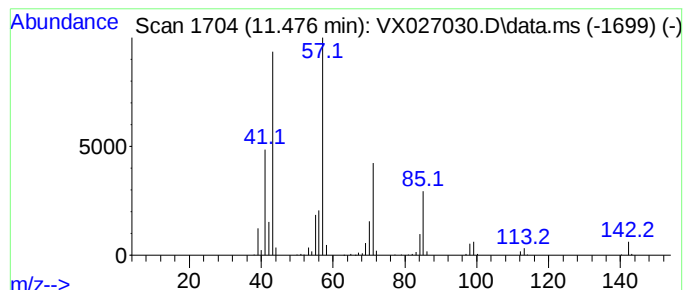
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.476	12.27 ug/L	220564	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	95
2			Decane	142	C10H22	000124-18-5	91
3			Decane	142	C10H22	000124-18-5	87
4			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	83
5			Nonane	128	C9H20	000111-84-2	72



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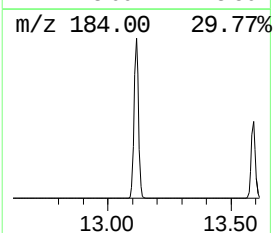
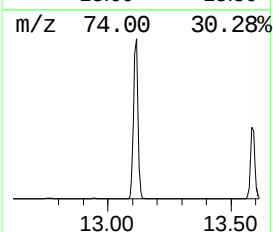
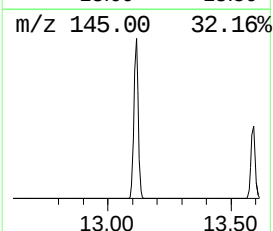
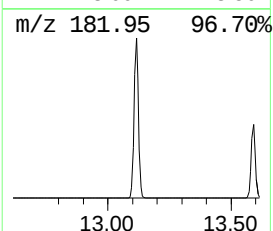
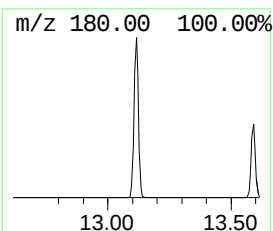
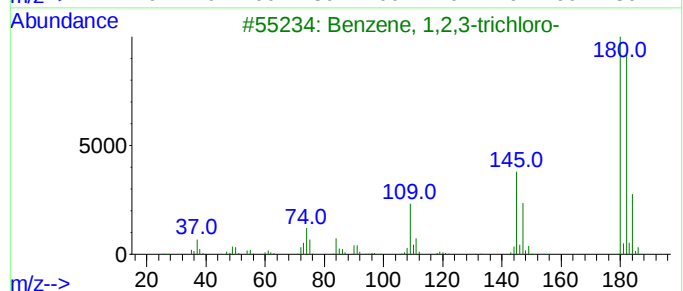
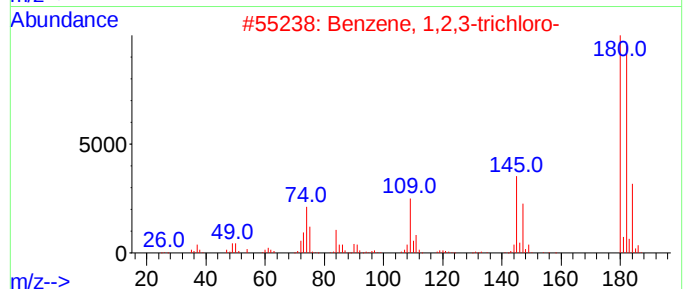
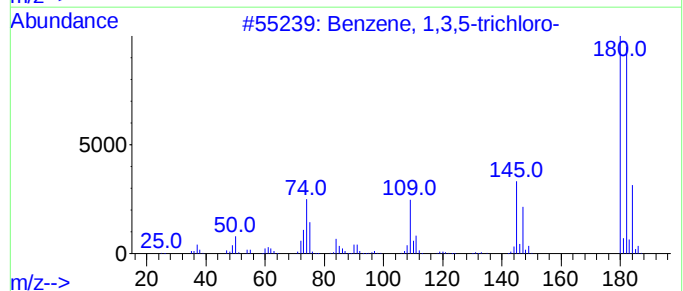
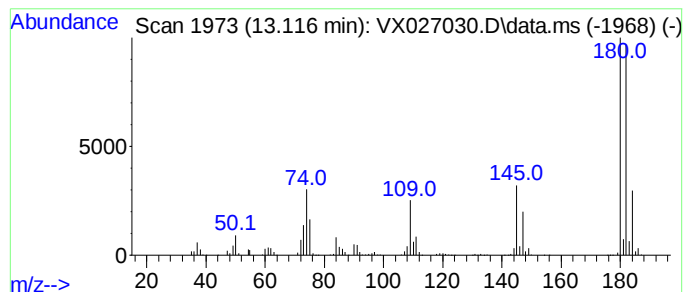
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Benzene, 1,3,5-trichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.116	42.85 ug/L	770333	1,4-Dichlorobenzene-d4	12.024

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
2		Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
3		Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
4		Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
5		Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	98



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021522\
Data File : VX027030.D
Acq On : 15 Feb 2022 14:48
Operator : JC/MD
Sample : N1486-06
Misc : 5.00g/5.00mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3946

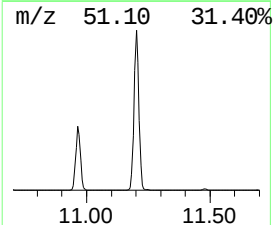
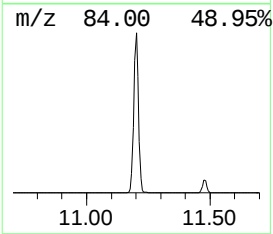
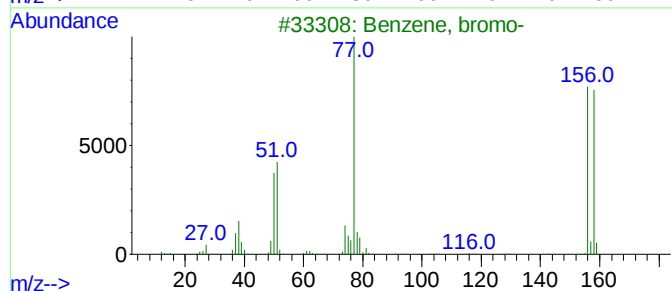
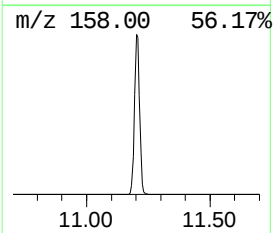
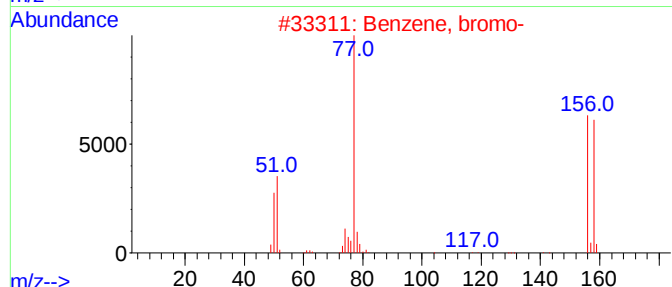
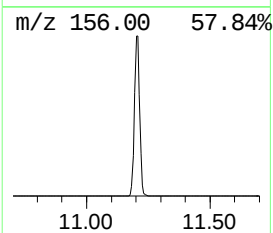
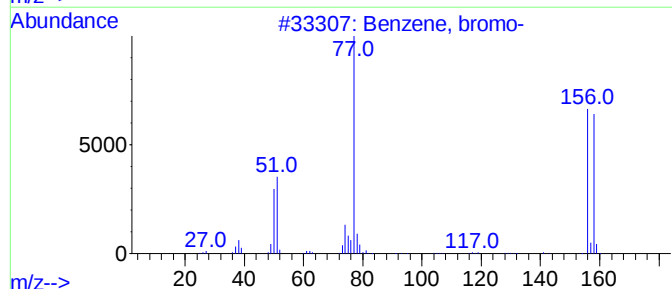
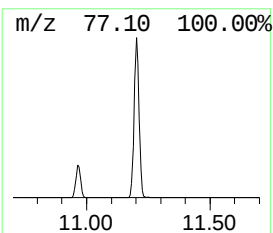
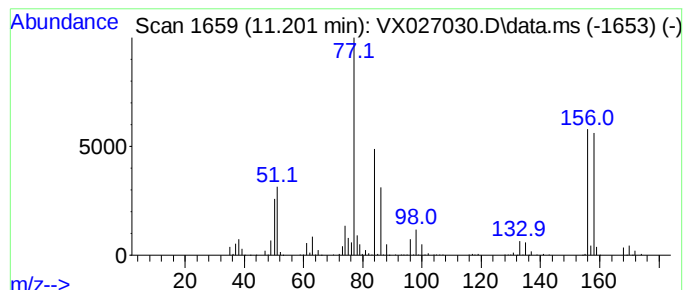
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Quant Title : VOC Analysis

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

Peak Number 6 Benzene, bromo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.201	39.69 ug/L	713588	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, bromo-	156	C6H5Br	000108-86-1	97
2	Benzene, bromo-	156	C6H5Br	000108-86-1	96
3	Benzene, bromo-	156	C6H5Br	000108-86-1	94
4	Benzene, bromo-	156	C6H5Br	000108-86-1	86
5	Benzene, bromo-	156	C6H5Br	000108-86-1	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021522\
Data File : VX027030.D
Acq On : 15 Feb 2022 14:48
Operator : JC/MD
Sample : N1486-06
Misc : 5.00g/5.00mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3946

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML021422WMA.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
1-Propene, 2-me...	2.191	3.9	ug/L	22573	1	6.763	291801	50.0
(DEL) Alkane: S...	11.476	12.3	ug/L	220564	3	12.024	898848	50.0
Benzene, 1,3,5-...	13.116	42.9	ug/L	770333	3	12.024	898848	50.0
Benzene, bromo-	11.201	39.7	ug/L	713588	3	12.024	898848	50.0