

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
 Data File : VX042734.D
 Acq On : 30 Jul 2024 13:12
 Operator : JC/MD
 Sample : P3287-05
 Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 XB504

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\SFAMXML072624WMA.M

Title : VOC Analysis

Signal : TIC: VX042734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.203	17	19	20	rBV	540	317	0.01%	0.001%
2	1.264	26	29	31	rBV	7613	7195	0.19%	0.019%
3	1.300	31	35	43	rVB	54081	84461	2.28%	0.220%
4	1.374	43	47	48	rBV	11141	13131	0.35%	0.034%
5	2.282	189	196	205	rBV3	129291	283474	7.64%	0.737%
6	2.416	212	218	233	rBV2	83266	230667	6.21%	0.600%
7	2.721	264	268	271	rBV	6768	12864	0.35%	0.033%
8	2.776	271	277	317	rVB	332842	1055541	28.44%	2.744%
9	3.129	323	335	351	rBV	403423	961723	25.91%	2.500%
10	3.404	378	380	385	rVV3	921	1494	0.04%	0.004%
11	3.794	440	444	449	rBB	205	370	0.01%	0.001%
12	3.861	453	455	460	rVB2	197	282	0.01%	0.001%
13	4.166	502	505	506	rBV	257	293	0.01%	0.001%
14	4.483	546	557	567	rBV2	246223	740782	19.96%	1.926%
15	5.086	639	656	674	rBV4	141039	580502	15.64%	1.509%
16	5.385	703	705	707	rBV	337	387	0.01%	0.001%
17	5.489	720	722	727	rVB	254	316	0.01%	0.001%
18	5.537	727	730	731	rBV2	493	386	0.01%	0.001%
19	5.574	732	736	741	rVB2	580	858	0.02%	0.002%
20	5.617	741	743	747	rBV	260	357	0.01%	0.001%
21	5.678	752	753	758	rVB2	306	344	0.01%	0.001%
22	5.958	789	799	811	rBV3	171377	491942	13.25%	1.279%
23	6.086	811	820	837	rVB	363211	956705	25.78%	2.487%
24	6.330	858	860	865	rBV3	643	1086	0.03%	0.003%
25	6.495	884	887	889	rBV2	266	304	0.01%	0.001%
26	6.757	921	930	943	rBV2	163385	399484	10.76%	1.039%
27	7.123	981	990	1005	rBV	160494	351906	9.48%	0.915%
28	7.305	1012	1020	1031	rBV	100692	226452	6.10%	0.589%
29	7.427	1032	1040	1057	rVV	483163	1022988	27.56%	2.660%
30	7.580	1057	1065	1088	rVB	414934	828953	22.33%	2.155%
31	7.824	1098	1105	1118	rBV	124195	236642	6.38%	0.615%
32	7.964	1122	1128	1144	rBV	48994	97419	2.62%	0.253%
33	8.183	1158	1164	1167	rBV4	794	1468	0.04%	0.004%
34	8.324	1182	1187	1189	rBV	68964	99631	2.68%	0.259%
35	8.366	1189	1194	1211	rVV	641044	1054287	28.40%	2.741%
36	8.500	1212	1216	1224	rVV	15991	32522	0.88%	0.085%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
 Data File : VX042734.D
 Acq On : 30 Jul 2024 13:12
 Operator : JC/MD
 Sample : P3287-05
 Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 XB504

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\SFAMXML072624WMA.M
 Title : VOC Analysis

37	8.586	1224	1230	1236	rVV	174219	347804	9.37%	0.904%
38	8.647	1236	1240	1246	rVV	256979	422134	11.37%	1.097%
39	8.720	1246	1252	1280	rVB	1918772	3133157	84.41%	8.146%
40	8.976	1285	1294	1309	rVB2	260438	470595	12.68%	1.223%
41	9.153	1317	1323	1336	rVB	180951	271214	7.31%	0.705%
42	9.269	1336	1342	1357	rBV	519319	782428	21.08%	2.034%
43	9.397	1357	1363	1365	rBV	122550	198619	5.35%	0.516%
44	9.439	1365	1370	1379	rVV	875563	1656201	44.62%	4.306%
45	9.525	1379	1384	1391	rVV	207522	324230	8.74%	0.843%
46	9.610	1392	1398	1407	rVB	305074	436836	11.77%	1.136%
47	9.921	1446	1449	1452	rBV4	310	426	0.01%	0.001%
48	10.079	1465	1475	1483	rBV2	863458	1633494	44.01%	4.247%
49	10.165	1483	1489	1492	rBV	1251087	1867304	50.31%	4.855%
50	10.299	1506	1511	1530	rVB	1254207	1731388	46.65%	4.501%
51	10.652	1562	1569	1585	rVV3	2293412	3711709	100.00%	9.650%
52	10.799	1588	1593	1603	rVB	183301	259645	7.00%	0.675%
53	10.902	1608	1610	1612	rBV	431	405	0.01%	0.001%
54	10.963	1616	1620	1625	rVV3	3397	4637	0.12%	0.012%
55	11.085	1638	1640	1645	rVB	345	312	0.01%	0.001%
56	11.195	1652	1658	1661	rBV	196725	258336	6.96%	0.672%
57	11.238	1661	1665	1675	rVB	1081308	1466407	39.51%	3.812%
58	11.451	1694	1700	1709	rBV	266155	319308	8.60%	0.830%
59	11.616	1723	1727	1734	rBV2	1377	2029	0.05%	0.005%
60	11.683	1734	1738	1741	rVB3	921	1217	0.03%	0.003%
61	11.750	1741	1749	1759	rBV	237589	298498	8.04%	0.776%
62	11.890	1770	1772	1773	rBV2	514	315	0.01%	0.001%
63	11.969	1779	1785	1790	rBV	884805	1094290	29.48%	2.845%
64	12.042	1790	1797	1808	rVB2	974883	1672537	45.06%	4.348%
65	12.231	1826	1828	1831	rBV2	386	281	0.01%	0.001%
66	12.335	1837	1845	1857	rBV2	1778384	2487440	67.02%	6.467%
67	12.536	1874	1878	1884	rVB4	9414	12807	0.35%	0.033%
68	12.591	1884	1887	1890	rVB3	318	360	0.01%	0.001%
69	12.762	1911	1915	1921	rBV3	1679	2542	0.07%	0.007%
70	12.859	1928	1931	1937	rVV3	497	935	0.03%	0.002%
71	12.945	1939	1945	1954	rVV	347713	445953	12.01%	1.159%
72	13.115	1971	1973	1977	rVB2	518	553	0.01%	0.001%
73	13.231	1989	1992	1996	rVB3	954	1209	0.03%	0.003%
74	13.274	1996	1999	2000	rBV2	377	345	0.01%	0.001%
75	13.335	2005	2009	2010	rBV	357	301	0.01%	0.001%
76	13.481	2030	2033	2034	rBV2	560	466	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
 Data File : VX042734.D
 Acq On : 30 Jul 2024 13:12
 Operator : JC/MD
 Sample : P3287-05
 Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 XB504

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\SFAMXML072624WMA.M
 Title : VOC Analysis

77	13.585	2043	2050	2059	rBV	189293	244647	6.59%	0.636%
78	13.725	2067	2073	2077	rBV	1061331	1309196	35.27%	3.404%
79	13.774	2077	2081	2095	rVB	1516601	1797159	48.42%	4.672%
80	13.969	2108	2113	2118	rVB4	1265	1956	0.05%	0.005%
81	14.030	2122	2123	2125	rBV	499	373	0.01%	0.001%
82	14.127	2136	2139	2144	rBV2	1609	2311	0.06%	0.006%
83	14.329	2167	2172	2174	rBV3	469	830	0.02%	0.002%
84	14.432	2187	2189	2191	rVB	398	308	0.01%	0.001%
85	14.493	2196	2199	2201	rBV2	247	318	0.01%	0.001%
86	14.518	2201	2203	2206	rBV2	883	858	0.02%	0.002%
87	14.737	2236	2239	2245	rBV6	1465	2020	0.05%	0.005%
88	15.042	2288	2289	2292	rBV2	346	313	0.01%	0.001%
89	15.072	2292	2294	2299	rBV3	192	369	0.01%	0.001%
90	15.231	2316	2320	2323	rBV	573	724	0.02%	0.002%
91	15.280	2326	2328	2329	rBV	382	381	0.01%	0.001%
92	15.341	2336	2338	2342	rBV3	735	753	0.02%	0.002%
93	15.389	2344	2346	2352	rVB3	748	1031	0.03%	0.003%
94	15.615	2379	2383	2384	rBV2	263	358	0.01%	0.001%
95	15.786	2409	2411	2412	rBV2	442	333	0.01%	0.001%
96	15.932	2433	2435	2436	rBV2	321	285	0.01%	0.001%
97	15.962	2436	2440	2444	rVB2	782	1256	0.03%	0.003%
98	16.084	2459	2460	2462	rBV	411	295	0.01%	0.001%
99	16.200	2477	2479	2485	rVB2	543	877	0.02%	0.002%
100	16.651	2551	2553	2555	rVB2	446	347	0.01%	0.001%

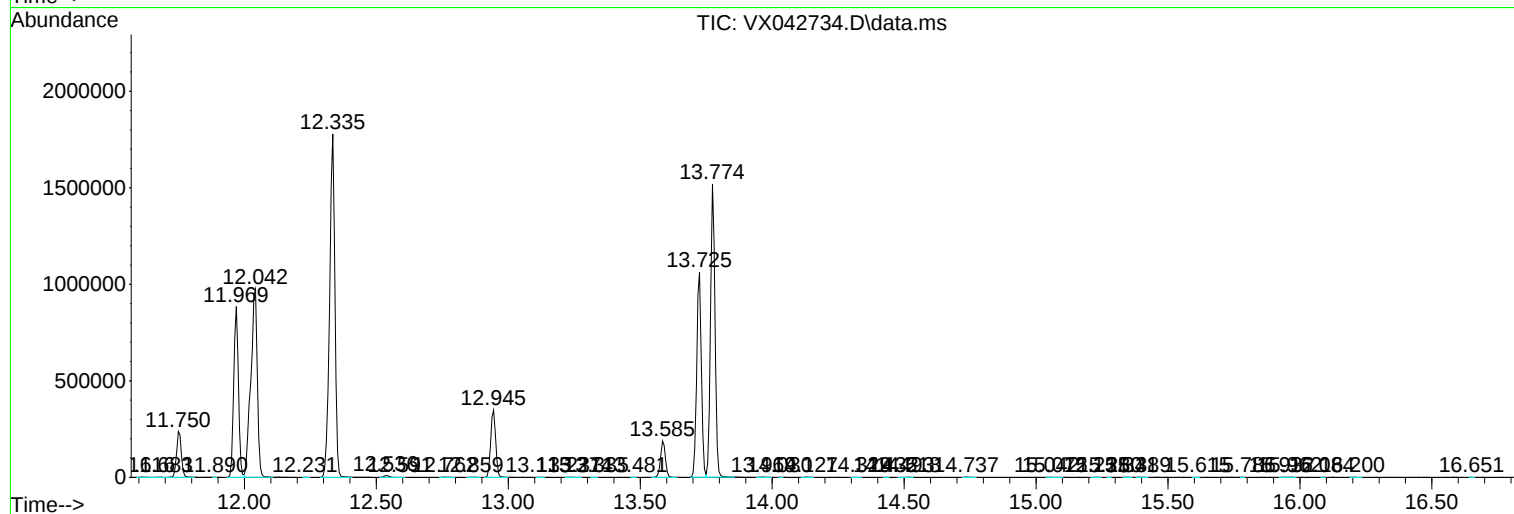
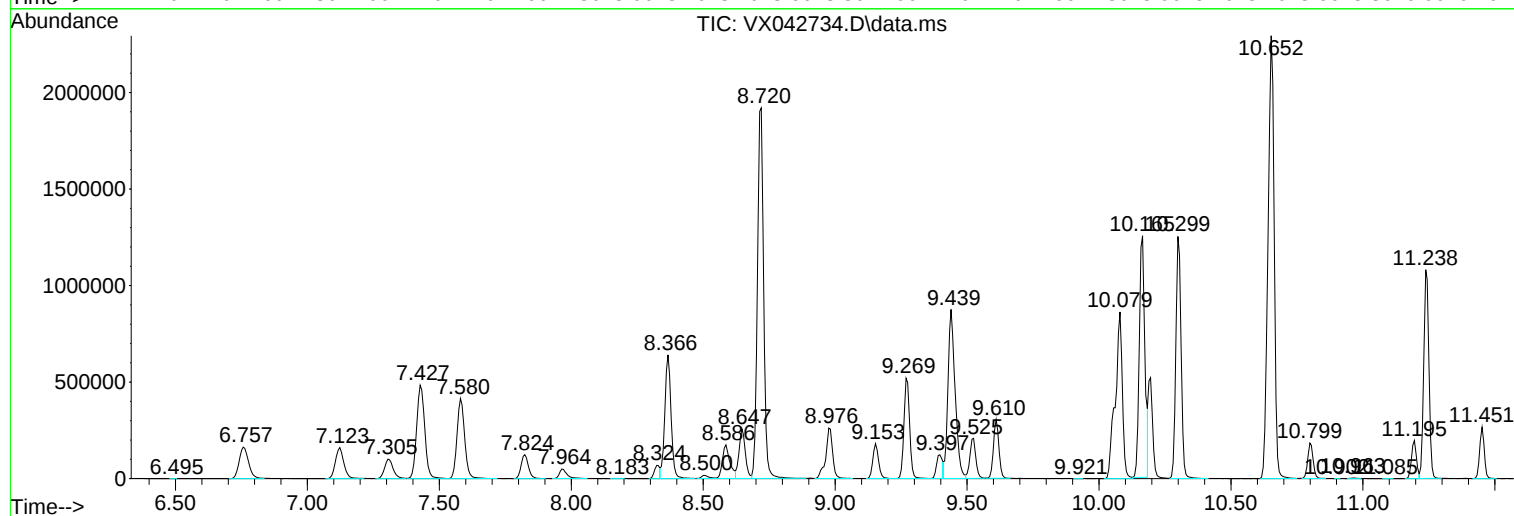
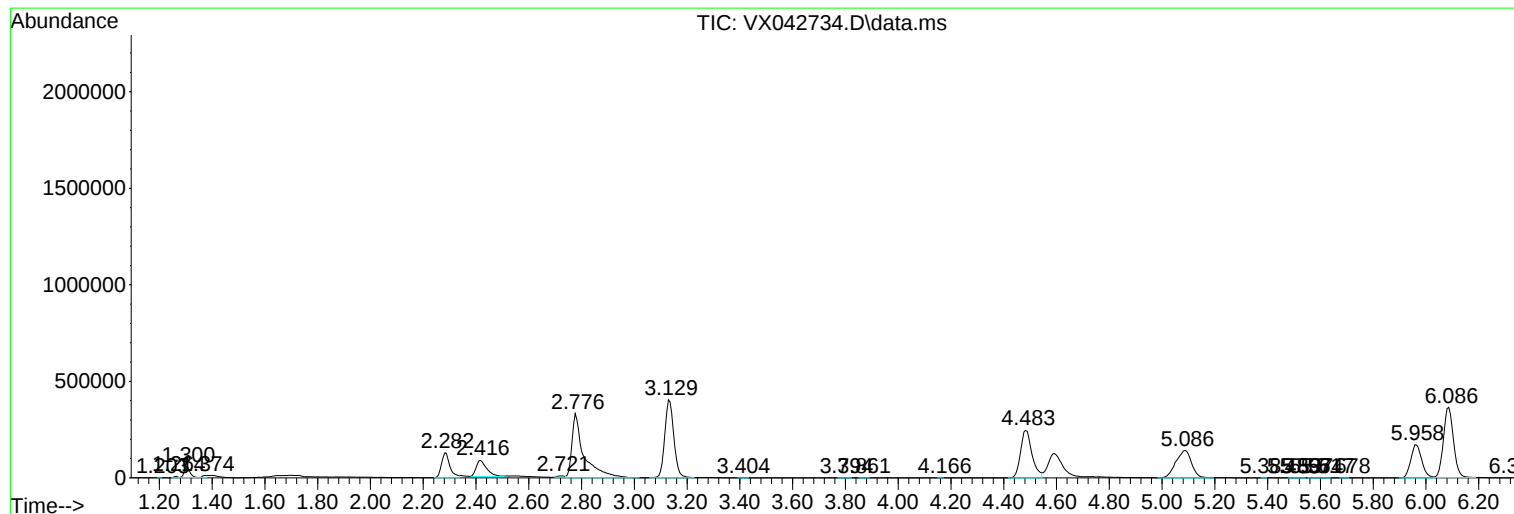
Sum of corrected areas: 38463498

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042734.D
Acq On : 30 Jul 2024 13:12
Operator : JC/MD
Sample : P3287-05
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042734.D
Acq On : 30 Jul 2024 13:12
Operator : JC/MD
Sample : P3287-05
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504

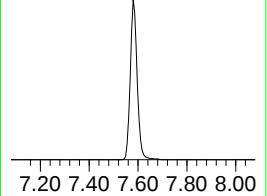
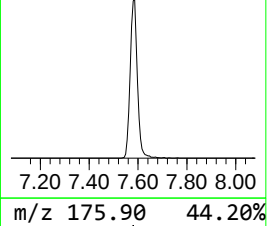
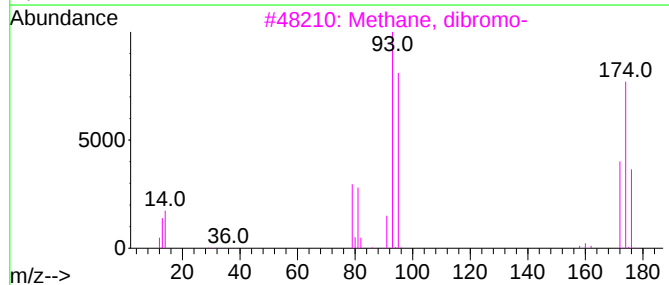
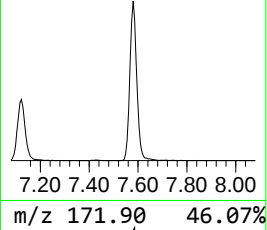
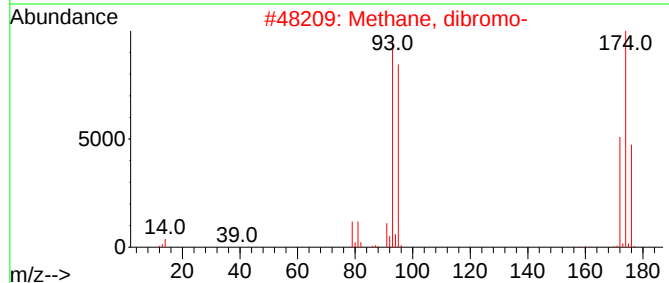
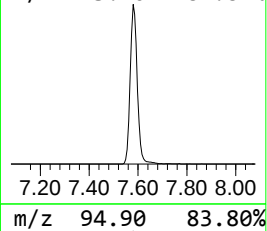
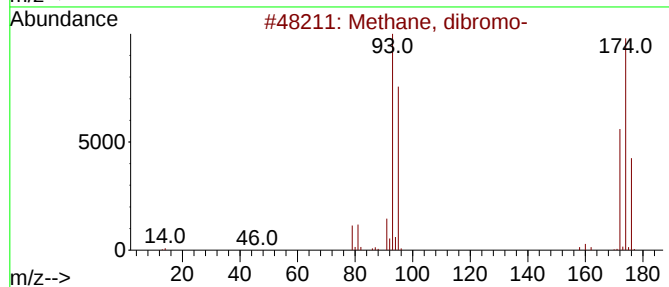
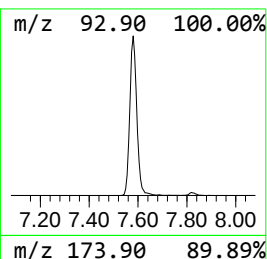
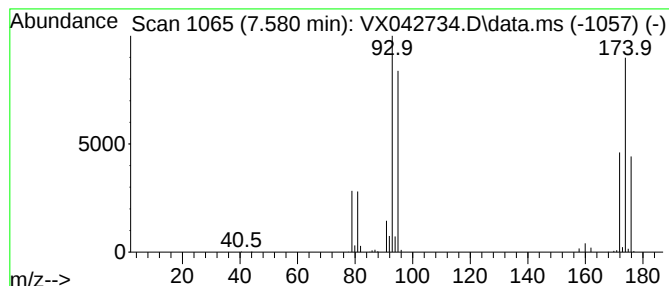
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methane, dibromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.580	103.75 ug/L	828953	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, dibromo-	172	CH2Br2	000074-95-3	96
2			Methane, dibromo-	172	CH2Br2	000074-95-3	96
3			Methane, dibromo-	172	CH2Br2	000074-95-3	94
4			Methane, dibromo-	172	CH2Br2	000074-95-3	91
5			Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042734.D
Acq On : 30 Jul 2024 13:12
Operator : JC/MD
Sample : P3287-05
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504

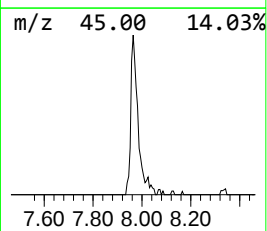
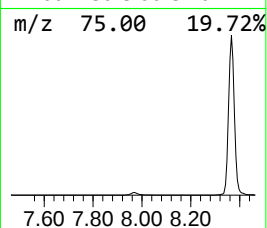
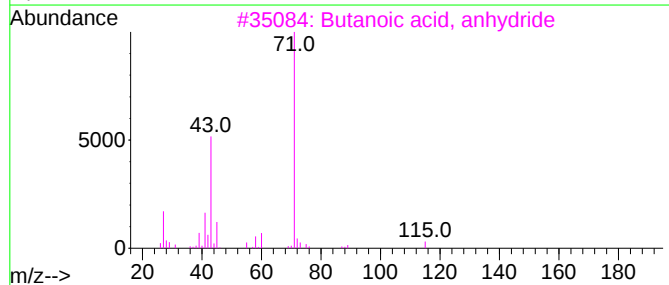
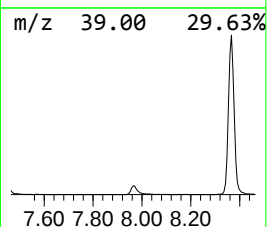
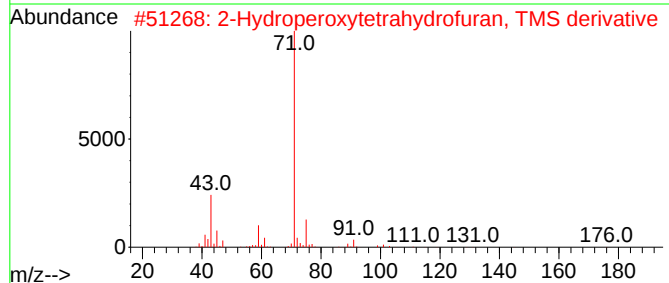
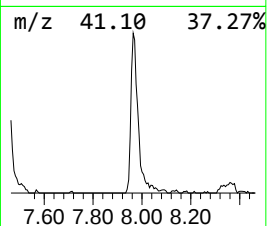
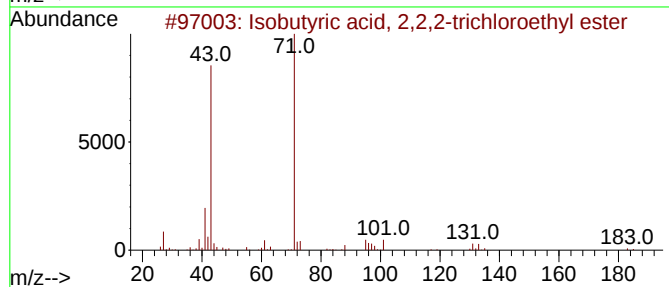
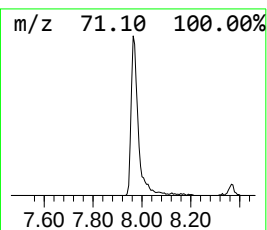
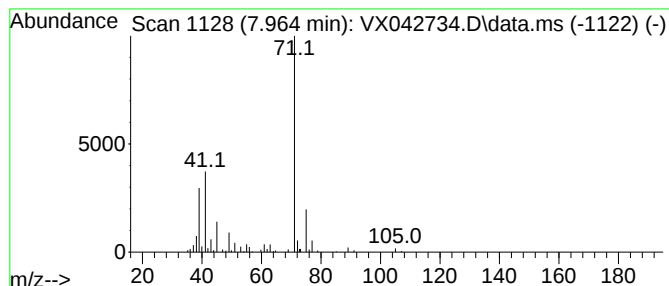
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isobutyric acid, 2,2,2-tric... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.964	12.19 ug/L	97419	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyric acid, 2,2,2-trichloro...	218	C6H9Cl3O2	1000354-63-4	42
2			2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	39
3			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38
4			Tetrahydrofurfuryl chloride	120	C5H9ClO	003003-84-7	33
5			Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042734.D
Acq On : 30 Jul 2024 13:12
Operator : JC/MD
Sample : P3287-05
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504

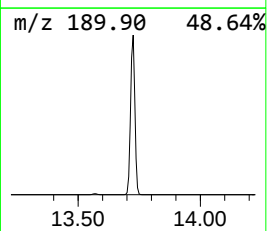
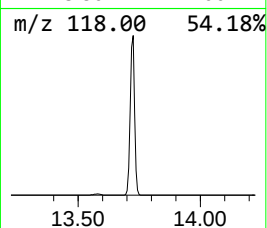
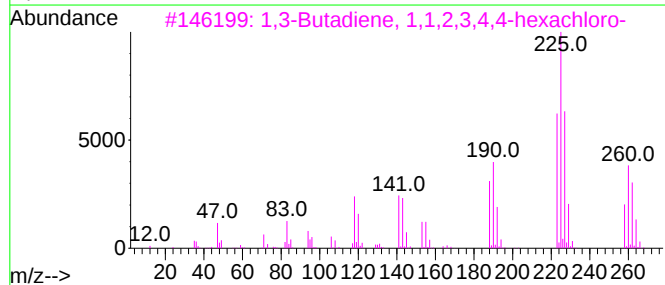
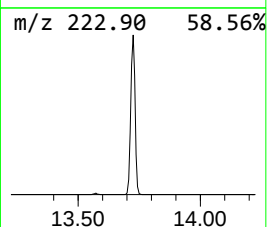
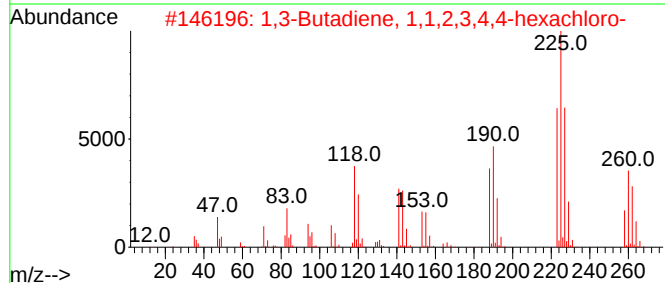
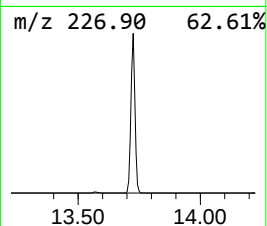
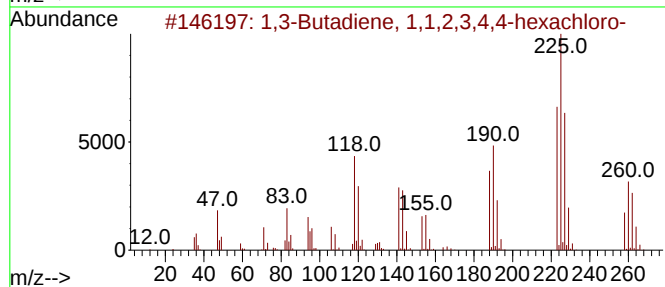
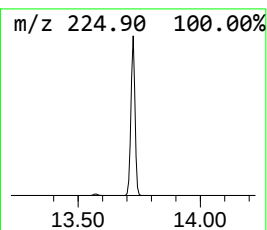
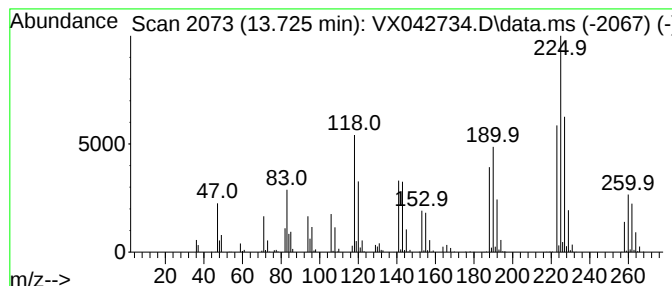
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1,3-Butadiene, 1,1,2,3,4,4-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.725	39.14 ug/L	1309200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99		
2	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99		
3	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99		
4	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99		
5	Tin(IV) chloride	260	Cl4Sn	007646-78-8	38		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042734.D
Acq On : 30 Jul 2024 13:12
Operator : JC/MD
Sample : P3287-05
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.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
Methane, dibromo-	7.580	103.8	ug/L	828953	1	6.757	399484	50.0
Isobutyric acid...	7.964	12.2	ug/L	97419	1	6.757	399484	50.0
1,3-Butadiene, ...	13.725	39.1	ug/L	1309200	3	12.024	1672540	50.0