

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072624\
 Data File : VW029757.D
 Acq On : 26 Jul 2024 17:27
 Operator : SY/MD
 Sample : P3361-09
 Misc : 8.57g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 E20P1

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_W\Method\SFAMWLM072424SMA.M
 Title : SFAM01.0

Signal : TIC: VW029757.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.174	41	47	50	rBV3	3198	6185	0.00%	0.004%
2	2.375	71	80	98	rBV2	117069	344615	0.25%	0.220%
3	2.893	159	165	178	rVB	27022	79132	0.06%	0.051%
4	3.119	200	202	203	rBV2	1815	998	0.00%	0.001%
5	3.393	245	247	250	rVB4	672	785	0.00%	0.001%
6	3.466	257	259	263	rVB3	648	560	0.00%	0.000%
7	3.539	267	271	273	rBV5	683	1098	0.00%	0.001%
8	3.911	330	332	338	rVB4	592	986	0.00%	0.001%
9	4.039	338	353	386	rBV2	224234	890283	0.65%	0.569%
10	4.277	391	392	394	rVV2	855	622	0.00%	0.000%
11	4.295	394	395	398	rVV3	828	838	0.00%	0.001%
12	4.521	427	432	434	rBV5	475	708	0.00%	0.000%
13	4.917	488	497	521	rVB2	7468	35233	0.03%	0.022%
14	5.173	534	539	540	rBV3	496	849	0.00%	0.001%
15	5.326	561	564	568	rVB3	510	727	0.00%	0.000%
16	5.429	568	581	594	rBV	29472	93248	0.07%	0.060%
17	5.740	630	632	637	rBV4	798	1214	0.00%	0.001%
18	5.893	653	657	658	rVV5	546	705	0.00%	0.000%
19	5.947	658	666	675	rVV8	2268	5936	0.00%	0.004%
20	6.027	677	679	682	rVB3	614	613	0.00%	0.000%
21	6.338	728	730	733	rBV3	535	751	0.00%	0.000%
22	6.374	733	736	739	rVV4	530	783	0.00%	0.000%
23	6.563	765	767	771	rVB3	367	573	0.00%	0.000%
24	6.606	771	774	779	rBV5	595	815	0.00%	0.001%
25	6.819	806	809	812	rBV4	566	828	0.00%	0.001%
26	6.905	818	823	825	rBV5	551	686	0.00%	0.000%
27	6.966	830	833	836	rVB5	628	859	0.00%	0.001%
28	7.014	836	841	842	rVB3	579	784	0.00%	0.001%
29	7.081	842	852	856	rBV	28219	73524	0.05%	0.047%
30	7.167	856	866	893	rVB	3951446	10337856	7.56%	6.601%
31	7.648	935	945	956	rVV	147052	369311	0.27%	0.236%
32	7.752	959	962	963	rBV3	993	688	0.00%	0.000%
33	7.996	1000	1002	1004	rBV2	667	595	0.00%	0.000%
34	8.160	1022	1029	1031	rBV5	908	1536	0.00%	0.001%
35	8.276	1037	1048	1063	rBV2	266417	802249	0.59%	0.512%
36	8.630	1104	1106	1109	rBV3	683	885	0.00%	0.001%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
 Title : SFAM01.0

37	8.691	1113	1116	1120	rVV5	1388	2248	0.00%	0.001%
38	8.727	1120	1122	1126	rVB4	640	713	0.00%	0.000%
39	8.843	1132	1141	1157	rBV	491230	952512	0.70%	0.608%
40	8.983	1162	1164	1168	rVB3	745	694	0.00%	0.000%
41	9.093	1171	1182	1204	rBV2	47610322	136699164	100.00%	87.291%
42	9.276	1205	1212	1230	rVB	196517	422522	0.31%	0.270%
43	9.666	1272	1276	1283	rVB8	2382	4662	0.00%	0.003%
44	10.032	1327	1336	1346	rBV	96199	177180	0.13%	0.113%
45	10.215	1364	1366	1369	rBV4	748	886	0.00%	0.001%
46	10.319	1375	1383	1392	rBV	319874	571224	0.42%	0.365%
47	10.575	1419	1425	1437	rVB	59113	107198	0.08%	0.068%
48	10.703	1439	1446	1451	rVB2	3354	6363	0.00%	0.004%
49	10.782	1453	1459	1466	rBV	65788	118611	0.09%	0.076%
50	10.861	1466	1472	1477	rVV	62174	105298	0.08%	0.067%
51	10.922	1477	1482	1496	rVB	96099	167630	0.12%	0.107%
52	11.160	1520	1521	1524	rBV3	804	933	0.00%	0.001%
53	11.215	1528	1530	1531	rBV	741	571	0.00%	0.000%
54	11.379	1555	1557	1559	rVV2	901	851	0.00%	0.001%
55	11.428	1563	1565	1570	rVV4	585	823	0.00%	0.001%
56	11.629	1590	1598	1608	rBV	619539	1031959	0.75%	0.659%
57	11.727	1609	1614	1622	rVV5	7661	15486	0.01%	0.010%
58	11.830	1625	1631	1637	rVV5	3008	6358	0.00%	0.004%
59	11.873	1637	1638	1640	rVV2	996	787	0.00%	0.001%
60	11.916	1640	1645	1651	rVB8	2849	5154	0.00%	0.003%
61	12.056	1666	1668	1671	rVB3	624	630	0.00%	0.000%
62	12.154	1678	1684	1685	rBV4	1653	2916	0.00%	0.002%
63	12.355	1710	1717	1721	rBV9	1941	4271	0.00%	0.003%
64	12.471	1730	1736	1739	rBV6	1406	2572	0.00%	0.002%
65	12.605	1750	1758	1764	rVV2	6062	13713	0.01%	0.009%
66	12.690	1766	1772	1781	rVB	152569	252262	0.18%	0.161%
67	12.769	1781	1785	1790	rBV6	2179	4503	0.00%	0.003%
68	12.855	1795	1799	1804	rBV4	6605	10704	0.01%	0.007%
69	13.038	1823	1829	1831	rBV6	1699	3652	0.00%	0.002%
70	13.080	1834	1836	1838	rVV3	846	635	0.00%	0.000%
71	13.099	1838	1839	1843	rVB4	1220	1164	0.00%	0.001%
72	13.184	1848	1853	1854	rBV4	977	1580	0.00%	0.001%
73	13.202	1854	1856	1858	rBV3	898	724	0.00%	0.000%
74	13.251	1858	1864	1870	rVB4	3390	5482	0.00%	0.004%
75	13.342	1874	1879	1885	rVB7	2053	3716	0.00%	0.002%
76	13.434	1890	1894	1901	rVB2	13777	22787	0.02%	0.015%

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 Title : SFAM01.0

77	13.495	1901	1904	1905	rBV3	1104	1133	0.00%	0.001%
78	13.556	1906	1914	1923	rBV	475182	819746	0.60%	0.523%
79	13.647	1925	1929	1936	rVB2	4879	9415	0.01%	0.006%
80	13.848	1955	1962	1976	rVB	268037	449919	0.33%	0.287%
81	14.001	1982	1987	1990	rBV6	2379	4792	0.00%	0.003%
82	14.062	1992	1997	2008	rVB	6477	14965	0.01%	0.010%
83	14.208	2014	2021	2027	rBV10	3624	8362	0.01%	0.005%
84	14.281	2027	2033	2038	rBV3	19973	35792	0.03%	0.023%
85	14.440	2058	2059	2062	rBV3	824	764	0.00%	0.000%
86	14.556	2065	2078	2084	rVV	53240	93729	0.07%	0.060%
87	14.623	2084	2089	2094	rVB8	4700	8385	0.01%	0.005%
88	14.812	2113	2120	2127	rBV2	492688	749497	0.55%	0.479%
89	14.952	2136	2143	2151	rVB2	291430	538769	0.39%	0.344%
90	15.226	2182	2188	2195	rVB2	28241	50386	0.04%	0.032%
91	15.360	2207	2210	2216	rVB3	2806	3846	0.00%	0.002%
92	15.476	2223	2229	2237	rBV	3469	7772	0.01%	0.005%
93	15.592	2246	2248	2250	rVB3	947	691	0.00%	0.000%
94	15.714	2265	2268	2271	rVB5	1026	969	0.00%	0.001%
95	15.763	2274	2276	2277	rBV2	767	617	0.00%	0.000%
96	15.848	2287	2290	2293	rBV5	1173	1615	0.00%	0.001%
97	15.933	2302	2304	2308	rBV4	929	1234	0.00%	0.001%
98	16.159	2339	2341	2346	rVB5	1448	1755	0.00%	0.001%
99	16.439	2381	2387	2390	rBV6	2659	5797	0.00%	0.004%
100	16.634	2416	2419	2422	rBV5	1455	1820	0.00%	0.001%

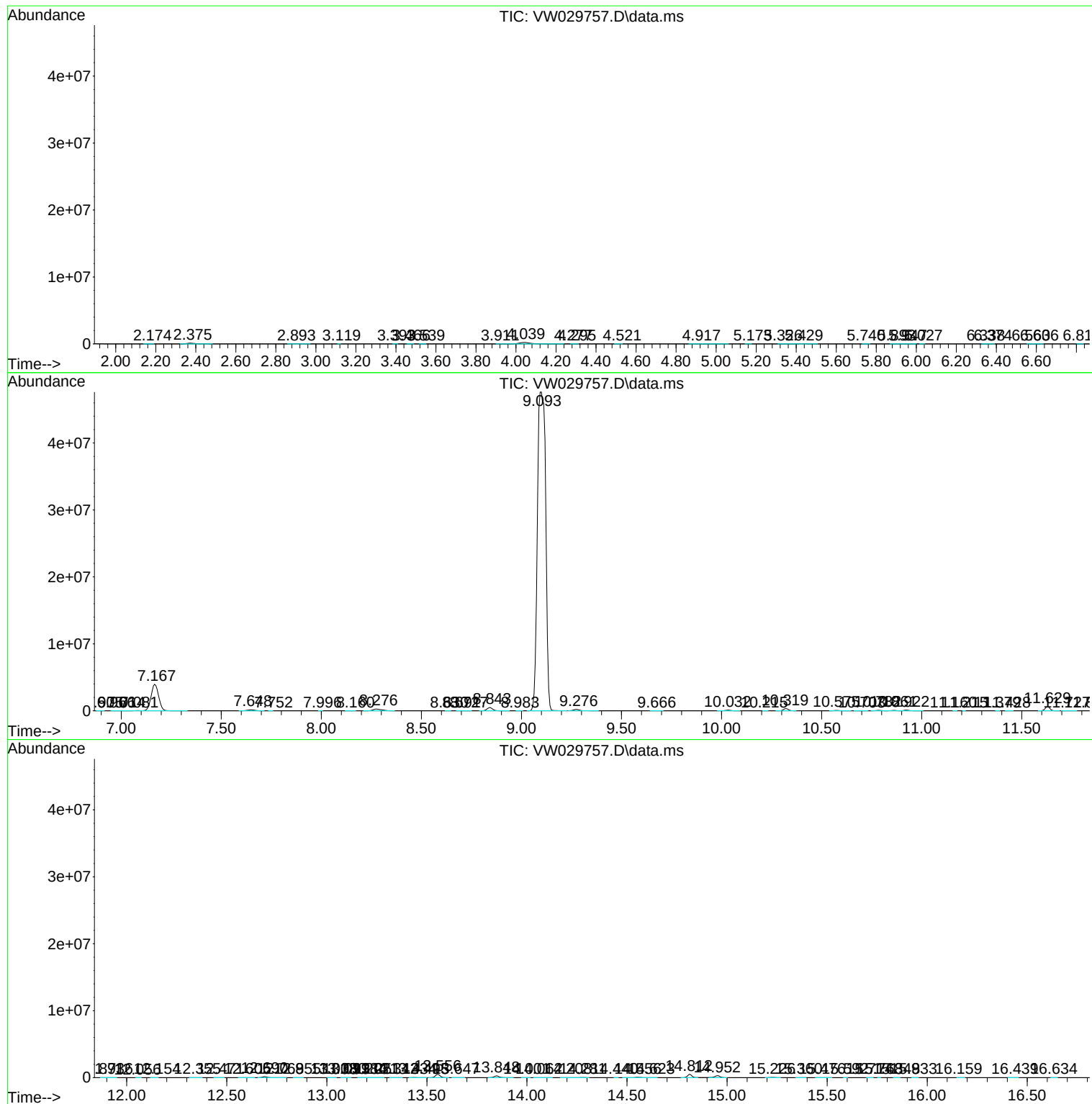
Sum of corrected areas: 156600966

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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



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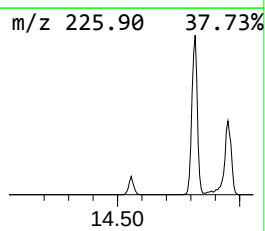
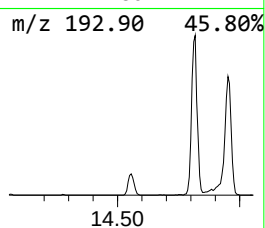
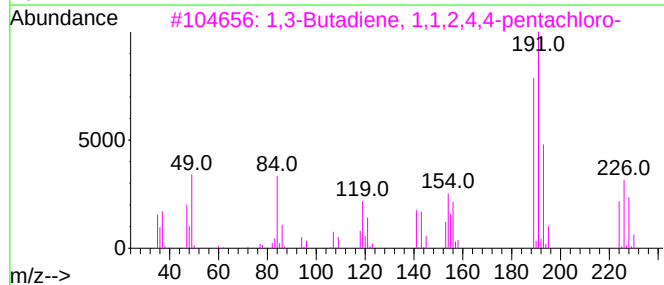
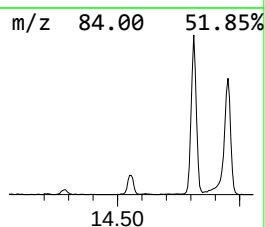
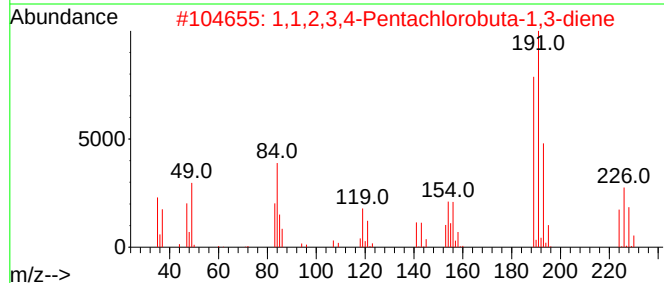
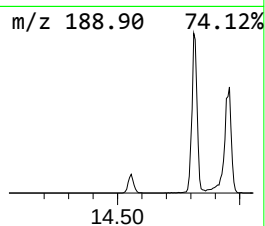
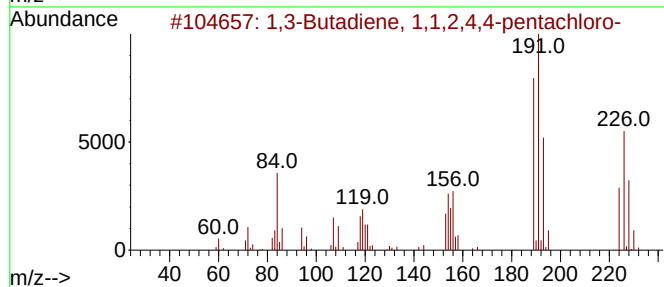
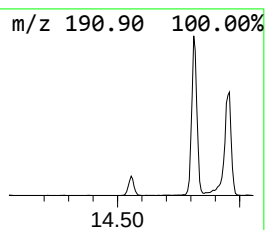
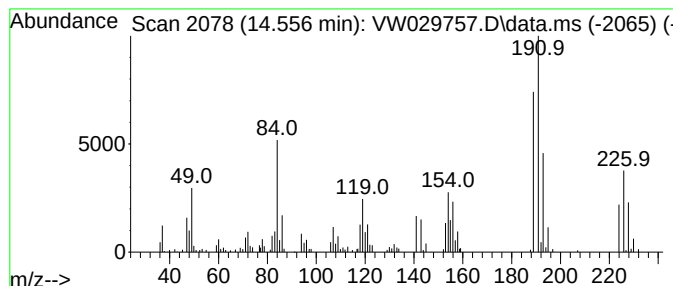
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.556	2.86 ug/L	93729	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	99		
2	1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HCl5	1010487-10-4	93		
3	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	91		
4	2-Thiophenecarbonyl chloride, 5-...	224	C5H2BrClOS	031555-60-9	38		
5	Thiophene-3-carbonyl chloride, 4...	224	C5H2BrClOS	072899-51-5	17		



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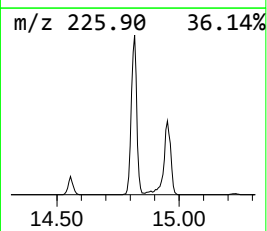
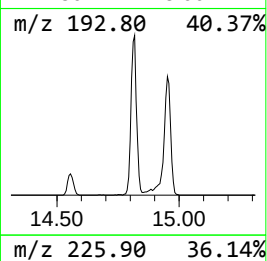
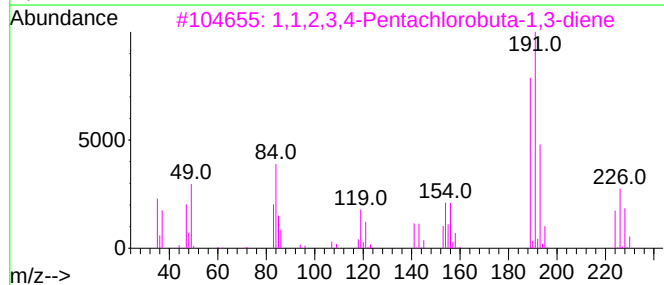
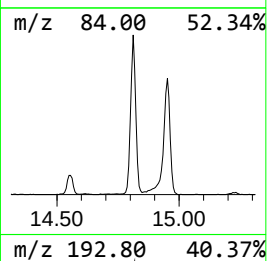
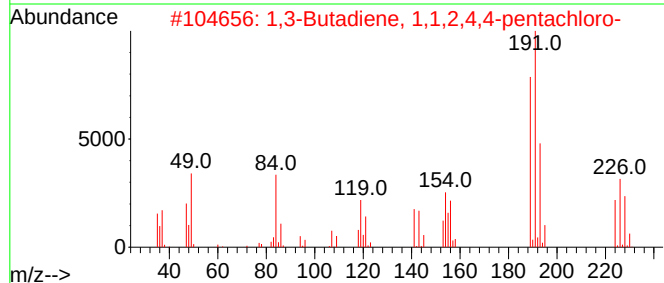
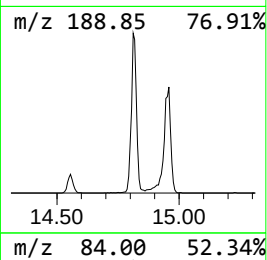
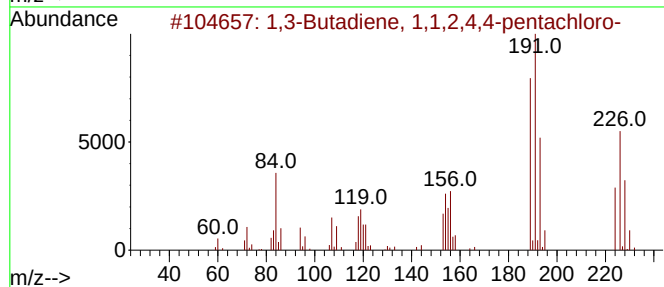
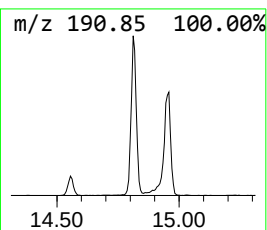
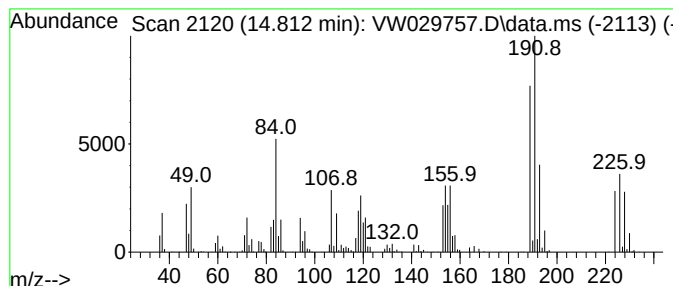
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.812	22.86 ug/L	749497	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	99		
2	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	99		
3	1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HC15	1010487-10-4	38		
4	2-Chloro-N-(5-propyl-1,3,4-thiad...	219	C7H10ClN3OS	015777-38-5	35		
5	5-Bromopyridine-2,3-diol	189	C5H4BrNO2	034206-49-0	22		



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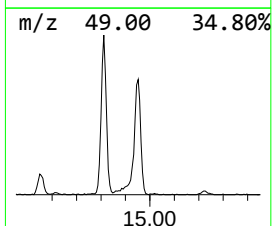
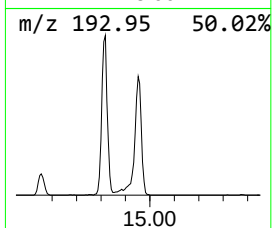
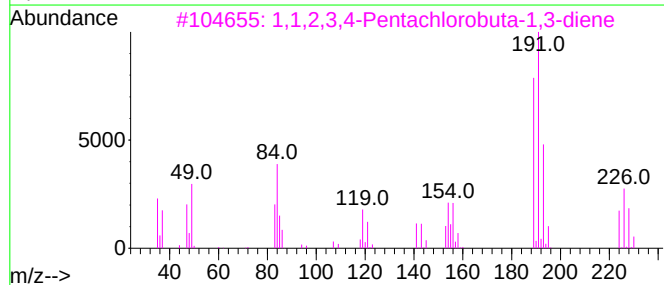
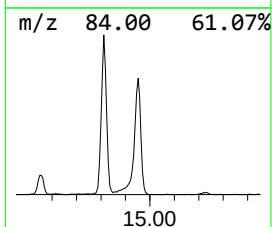
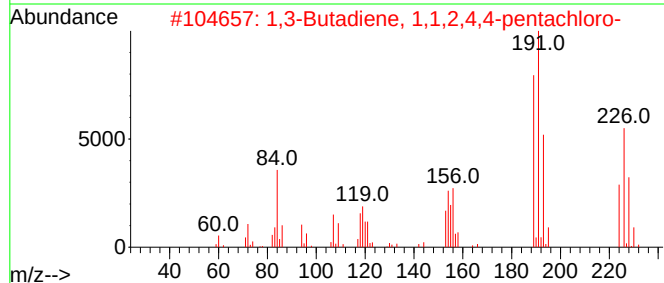
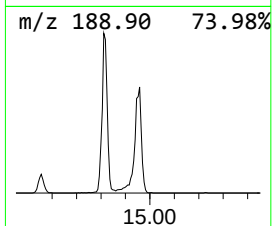
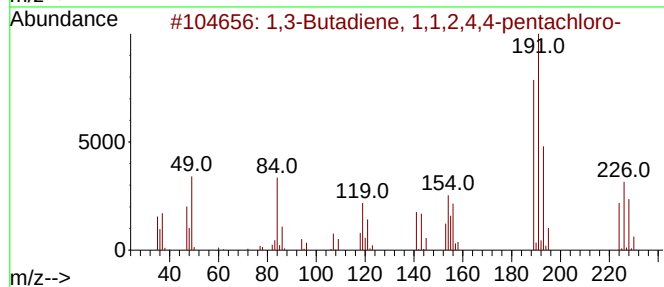
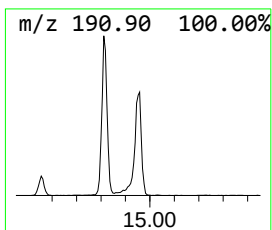
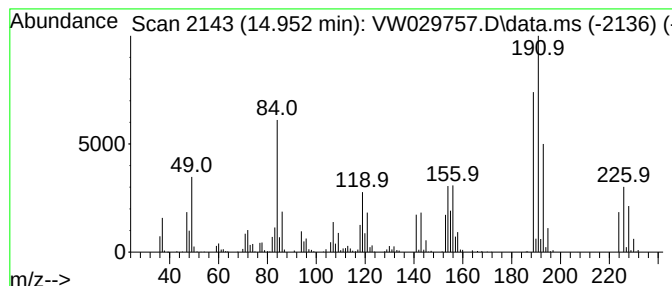
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.952	16.43 ug/L	538769	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	99		
2	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	99		
3	1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HC15	1010487-10-4	98		
4	Thiophene-3-carbonyl chloride, 4...	224	C5H2BrClOS	072899-51-5	38		
5	4-Bromo-2-fluoroaniline	189	C6H5BrFN	000367-24-8	25		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072624\
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Acq On : 26 Jul 2024 17:27
Operator : SY/MD
Sample : P3361-09
Misc : 8.57g/10mL/MSVOA_W/SOIL/A
ALS Vial : 16 Sample Multiplier: 1

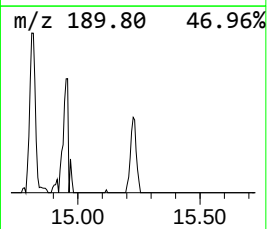
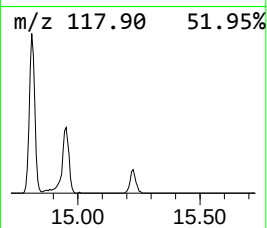
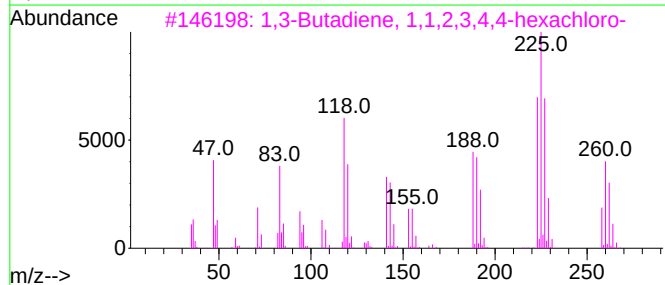
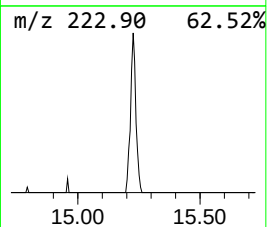
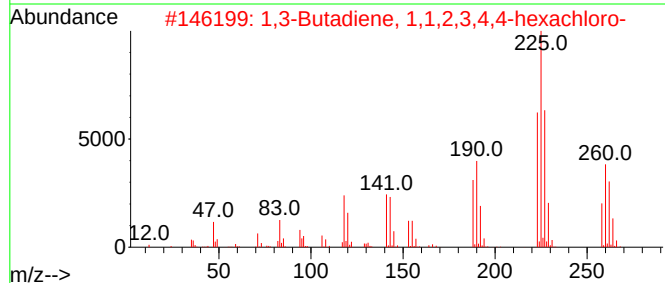
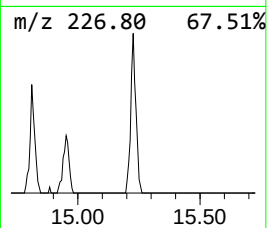
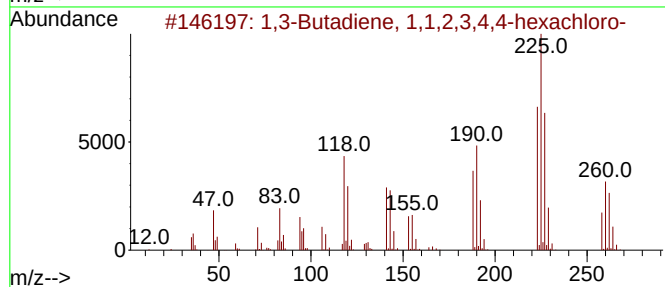
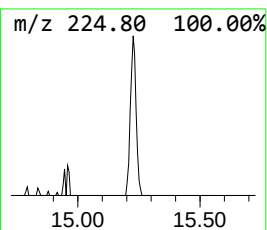
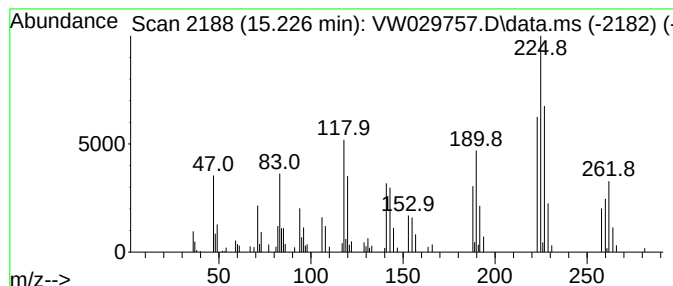
Instrument :
MSVOA_W
ClientSampleId :
E20P1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 1,3-Butadiene, 1,1,2,3,4,4-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.226	1.54 ug/L	50386	1,4-Dichlorobenzene-d4	13.556	
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	97
3	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	94
4	1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	93
5	Tin(IV) chloride	260	Cl4Sn	007646-78-8	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072624\
Data File : VW029757.D
Acq On : 26 Jul 2024 17:27
Operator : SY/MD
Sample : P3361-09
Misc : 8.57g/10mL/MSVOA_W/SOIL/A
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E20P1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Butadiene, ...	14.556	2.9	ug/L	93729	3	13.556	819746	25.0
unknown-01	14.812	22.9	ug/L	749497	3	13.556	819746	25.0
1,1,2,3,4-Penta...	14.952	16.4	ug/L	538769	3	13.556	819746	25.0
1,3-Butadiene, ...	15.226	1.5	ug/L	50386	3	13.556	819746	25.0