

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW101124\
 Data File : VW030559.D
 Acq On : 11 Oct 2024 19:14
 Operator : SY/MD
 Sample : P4350-08
 Misc : 4.48g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EOAK9

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\SFAMWLM100924SMA.M
 Title : SFAM01.0

Signal : TIC: VW030559.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.058	26	28	30	rBV2	798	639	3.82%	0.383%
2	2.228	51	56	62	rBV9	2202	4441	26.52%	2.662%
3	2.363	76	78	83	rVV3	1090	1377	8.22%	0.825%
4	2.430	85	89	90	rBV3	499	546	3.26%	0.327%
5	2.722	135	137	139	rBV3	735	667	3.98%	0.400%
6	2.905	161	167	171	rBV5	2007	3865	23.08%	2.317%
7	3.070	192	194	198	rVB4	912	792	4.73%	0.475%
8	3.326	234	236	238	rVB	855	695	4.15%	0.417%
9	3.356	238	241	243	rBV4	562	723	4.32%	0.433%
10	3.393	245	247	250	rVV3	741	737	4.40%	0.442%
11	3.442	254	255	260	rVB3	649	633	3.78%	0.379%
12	3.795	311	313	315	rBV3	699	635	3.79%	0.381%
13	3.966	339	341	343	rBV2	705	691	4.13%	0.414%
14	4.131	366	368	370	rVV3	1178	1024	6.11%	0.614%
15	4.179	374	376	378	rBV3	711	581	3.47%	0.348%
16	4.222	381	383	385	rBV2	563	594	3.55%	0.356%
17	4.460	419	422	423	rBV3	763	779	4.65%	0.467%
18	4.728	461	466	469	rVV6	715	1169	6.98%	0.701%
19	4.758	469	471	473	rVB3	794	520	3.11%	0.312%
20	4.941	498	501	502	rBV2	709	717	4.28%	0.430%
21	4.996	505	510	511	rBV2	766	928	5.54%	0.556%
22	5.100	524	527	529	rBV3	747	835	4.99%	0.500%
23	5.307	559	561	562	rBV2	761	533	3.18%	0.319%
24	5.545	598	600	602	rBV2	678	809	4.83%	0.485%
25	5.588	605	607	610	rVV3	715	865	5.17%	0.518%
26	5.655	614	618	620	rBV4	799	1286	7.68%	0.771%
27	5.771	633	637	639	rBV3	575	615	3.67%	0.369%
28	6.051	681	683	687	rBV4	704	1002	5.98%	0.601%
29	6.088	687	689	691	rVB3	781	575	3.43%	0.345%
30	6.118	691	694	695	rVB3	830	735	4.39%	0.441%
31	6.216	708	710	712	rBV2	820	934	5.58%	0.560%
32	6.313	723	726	727	rBV3	570	527	3.15%	0.316%
33	6.374	734	736	739	rVV	557	568	3.39%	0.340%
34	6.661	779	783	786	rVB2	548	835	4.99%	0.500%
35	6.722	792	793	795	rBV2	847	533	3.18%	0.319%
36	6.746	795	797	799	rVV2	644	766	4.57%	0.459%

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37	7.008	837	840	841	rBV2	595	557	3.33%	0.334%
38	7.289	884	886	889	rBV3	680	631	3.77%	0.378%
39	7.319	889	891	893	rBV3	874	710	4.24%	0.426%
40	7.563	927	931	934	rBV4	463	601	3.59%	0.360%

41	7.654	939	946	950	rBV4	2827	6216	37.12%	3.726%
42	7.868	978	981	984	rVB2	677	755	4.51%	0.453%
43	7.898	984	986	989	rVB2	930	916	5.47%	0.549%
44	7.929	989	991	993	rBV2	549	563	3.36%	0.337%
45	7.953	993	995	1000	rVV4	642	1128	6.74%	0.676%

46	8.026	1003	1007	1009	rVB3	437	629	3.76%	0.377%
47	8.063	1009	1013	1015	rBV4	469	545	3.25%	0.327%
48	8.154	1026	1028	1031	rBV2	934	1030	6.15%	0.617%
49	8.294	1042	1051	1060	rBV5	4476	16746	100.00%	10.037%
50	8.380	1062	1065	1068	rVB2	582	699	4.17%	0.419%

51	8.435	1073	1074	1077	rBV3	500	556	3.32%	0.333%
52	8.471	1077	1080	1081	rVB3	817	677	4.04%	0.406%
53	8.630	1103	1106	1109	rVV4	616	909	5.43%	0.545%
54	8.843	1137	1141	1150	rVB4	3974	8694	51.92%	5.211%
55	9.008	1166	1168	1171	rVB2	1225	1076	6.43%	0.645%

56	9.124	1186	1187	1192	rVB3	703	753	4.50%	0.451%
57	9.197	1196	1199	1200	rBV3	656	793	4.74%	0.475%
58	9.270	1207	1211	1218	rVV7	4353	9357	55.88%	5.609%
59	9.325	1218	1220	1223	rVB4	667	721	4.31%	0.432%
60	9.416	1233	1235	1237	rVV2	555	574	3.43%	0.344%

61	9.532	1251	1254	1255	rBV2	1084	1150	6.87%	0.689%
62	9.593	1262	1264	1266	rVV3	596	546	3.26%	0.327%
63	9.764	1289	1292	1294	rBV3	690	588	3.51%	0.352%
64	9.812	1299	1300	1303	rBV2	810	928	5.54%	0.556%
65	9.940	1316	1321	1324	rBV4	786	1441	8.61%	0.864%

66	9.965	1324	1325	1328	rBV2	720	596	3.56%	0.357%
67	9.995	1328	1330	1332	rVB2	956	645	3.85%	0.387%
68	10.044	1332	1338	1340	rBV5	1667	3684	22.00%	2.208%
69	10.117	1346	1350	1352	rBV3	674	1040	6.21%	0.623%
70	10.166	1354	1358	1362	rBV6	808	1340	8.00%	0.803%

71	10.239	1367	1370	1373	rBV2	618	729	4.35%	0.437%
72	10.325	1379	1384	1390	rBV2	4383	8971	53.57%	5.377%
73	10.434	1400	1402	1405	rBV3	859	784	4.68%	0.470%
74	10.538	1416	1419	1420	rBV	525	528	3.15%	0.316%
75	10.556	1420	1422	1424	rBV3	521	562	3.36%	0.337%

76	10.703	1443	1446	1449	rBV3	656	872	5.21%	0.523%
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77	10.788	1458	1460	1463	rBV	471	517	3.09%	0.310%
78	10.867	1471	1473	1476	rVB3	839	1011	6.04%	0.606%
79	10.904	1476	1479	1482	rBV3	1150	1308	7.81%	0.784%
80	10.934	1482	1484	1486	rBV3	524	580	3.46%	0.348%
81	10.965	1486	1489	1490	rVB2	672	597	3.57%	0.358%
82	11.050	1501	1503	1507	rVB3	668	717	4.28%	0.430%
83	11.294	1540	1543	1544	rBV3	620	600	3.58%	0.360%
84	11.635	1592	1599	1604	rBV4	5481	11995	71.63%	7.190%
85	11.708	1610	1611	1613	rBV2	932	769	4.59%	0.461%
86	12.001	1656	1659	1662	rBV4	530	812	4.85%	0.487%
87	12.269	1699	1703	1707	rBV5	578	863	5.15%	0.517%
88	12.489	1736	1739	1742	rBV5	799	1063	6.35%	0.637%
89	12.568	1749	1752	1754	rBV2	740	996	5.95%	0.597%
90	12.690	1768	1772	1778	rVB5	3575	6269	37.44%	3.758%
91	12.952	1813	1815	1818	rBV4	850	766	4.57%	0.459%
92	13.153	1844	1848	1851	rBV3	1195	1315	7.85%	0.788%
93	13.184	1851	1853	1856	rBV4	798	850	5.08%	0.509%
94	13.562	1911	1915	1924	rVB9	3780	8985	53.65%	5.386%
95	13.678	1932	1934	1935	rBV2	834	712	4.25%	0.427%
96	13.854	1958	1963	1968	rBV6	4539	7815	46.67%	4.684%
97	13.989	1982	1985	1986	rBV2	1422	1360	8.12%	0.815%
98	14.153	2010	2012	2013	rBV2	1198	757	4.52%	0.454%
99	14.312	2036	2038	2042	rBV5	1059	1177	7.03%	0.705%
100	15.019	2153	2154	2156	rBV2	945	591	3.53%	0.354%

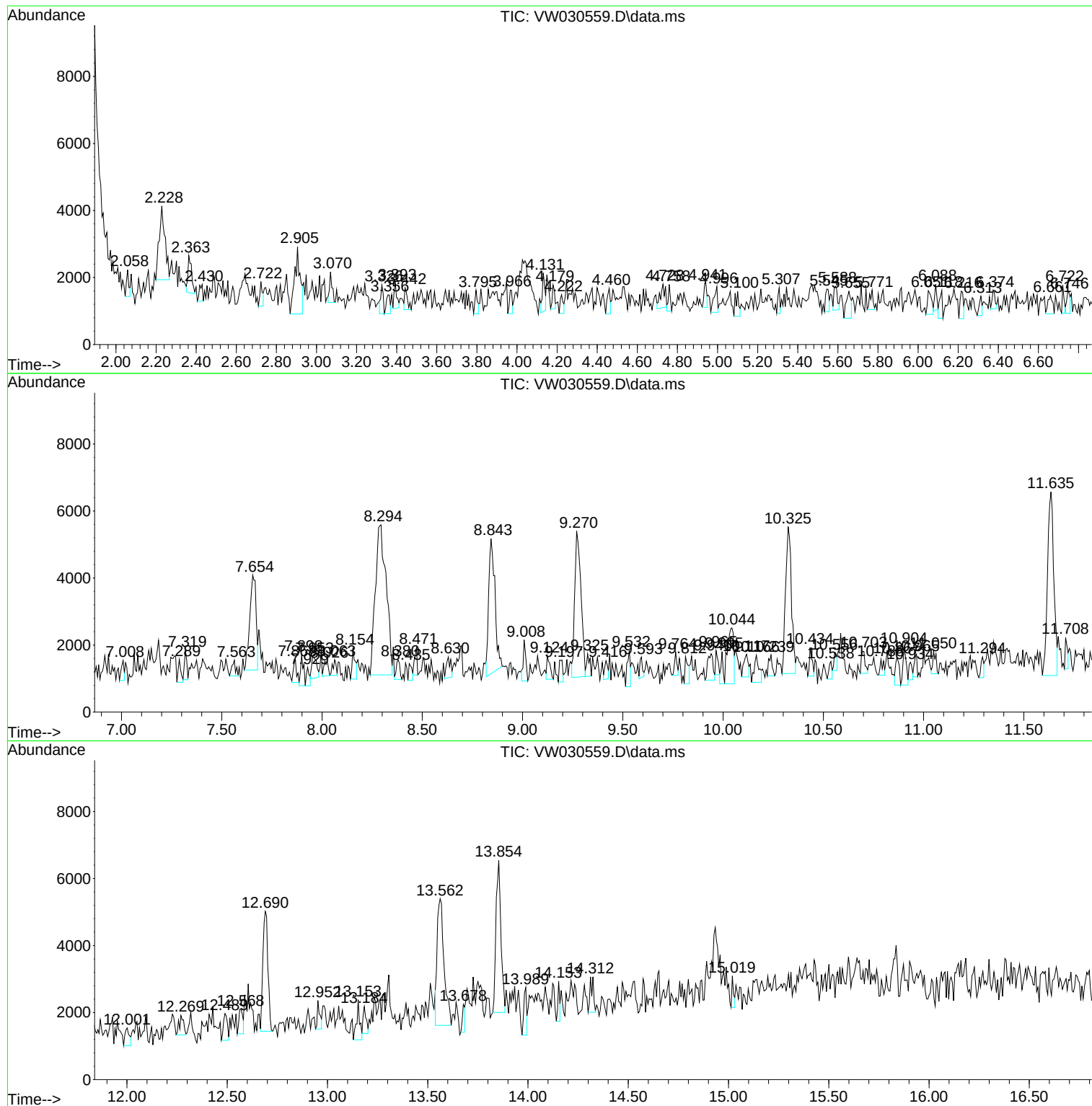
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100924SMA.M
Quant Title : SFAM01.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW101124\
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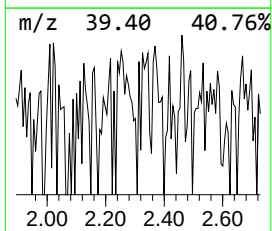
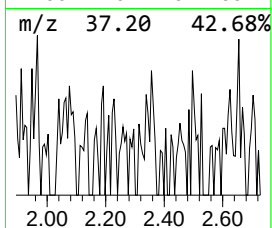
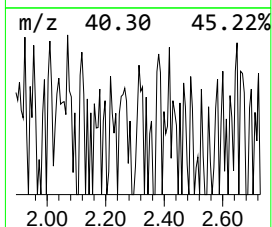
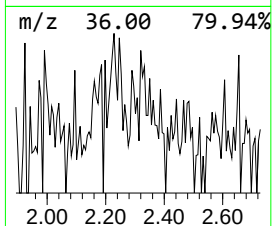
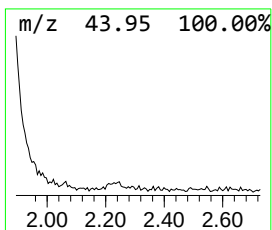
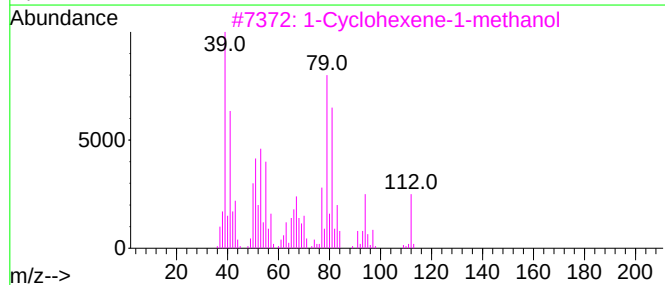
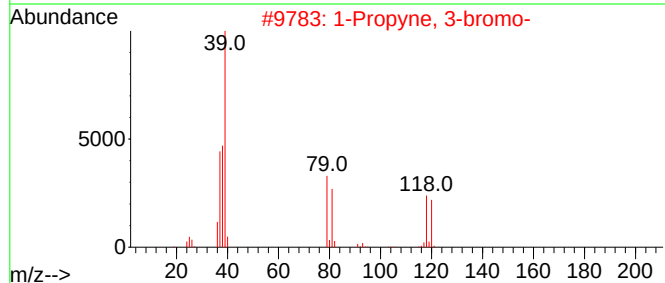
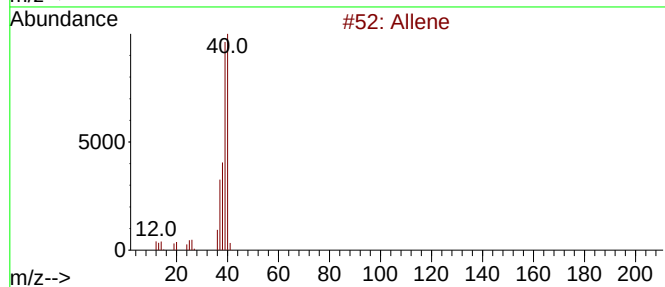
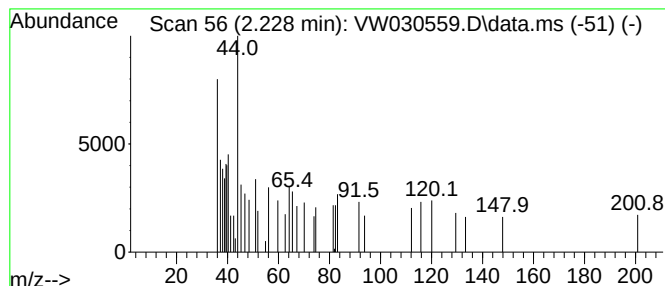
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100924SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	12.77 ug/L	4441	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allene			40	C3H4	000463-49-0	43
2	1-Propyne, 3-bromo-			118	C3H3Br	000106-96-7	40
3	1-Cyclohexene-1-methanol			112	C7H12O	004845-04-9	30
4	Phenol, 3-(4H-1,2,4-triazol-4-yl)-			161	C8H7N3O	1000410-77-9	25
5	1H-Pyrazole-3-acetic acid, 2,5-d...			142	C5H6N2O3	1000362-41-0	23



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Instrument :
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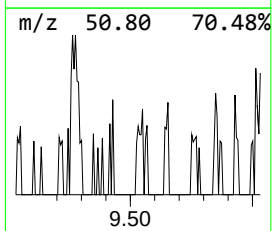
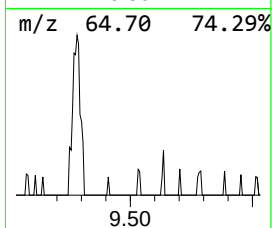
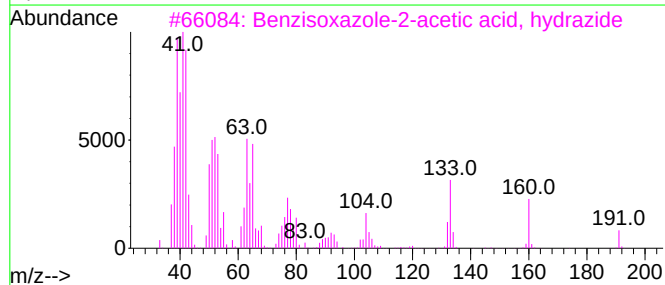
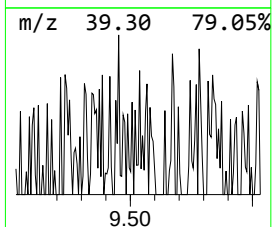
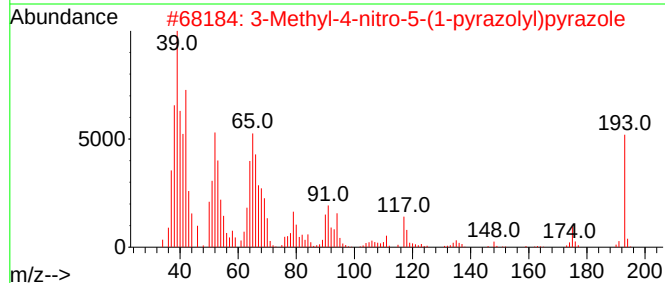
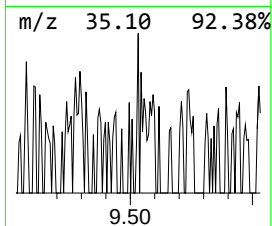
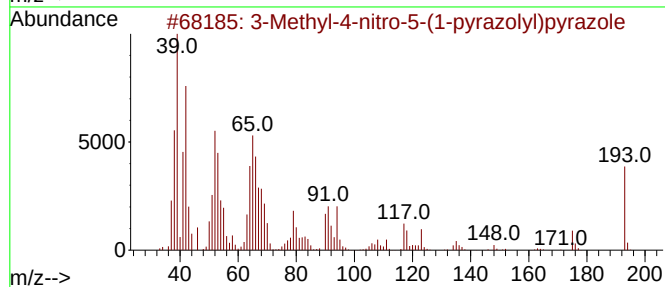
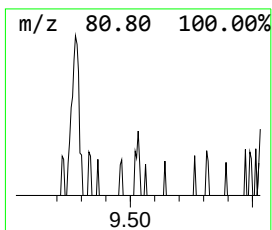
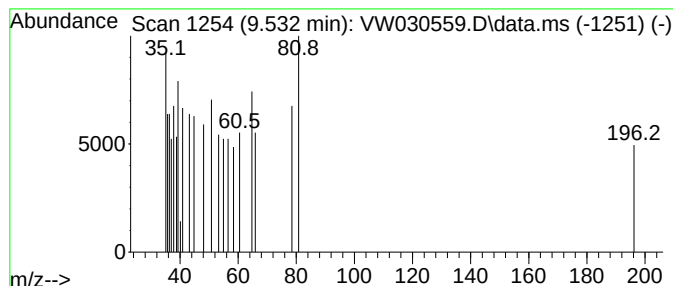
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100924SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 3-Methyl-4-nitro-5-(1-pyrazolyl)pyrazole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.532	3.31 ug/L	1150	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-nitro-5-(1-pyrazolyl)...	193	C7H7N5O2	292855-42-6	50		
2	3-Methyl-4-nitro-5-(1-pyrazolyl)...	193	C7H7N5O2	292855-42-6	42		
3	Benzisoxazole-2-acetic acid, hyd...	191	C9H9N3O2	055244-10-5	38		
4	Carbamic acid, N-(4-chlorophenyl...	292	C13H9ClN2O4	003848-41-7	37		
5	1,2-Benzenediol, 3-(1H-1,2,3,4-t...	178	C7H6N4O2	1000362-63-3	33		



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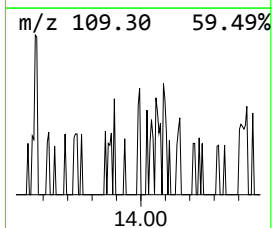
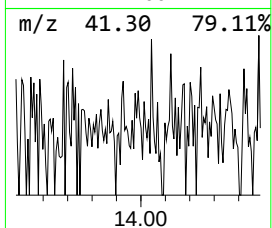
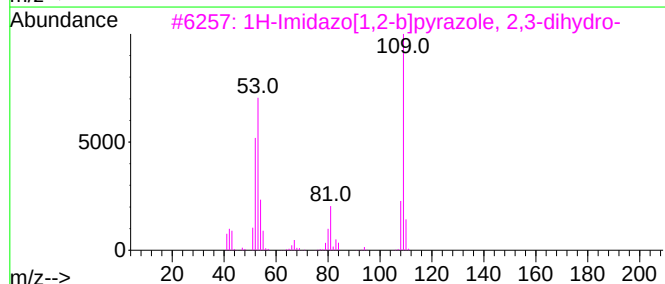
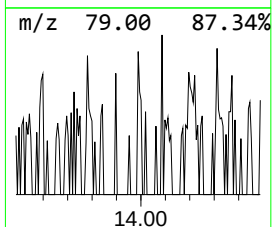
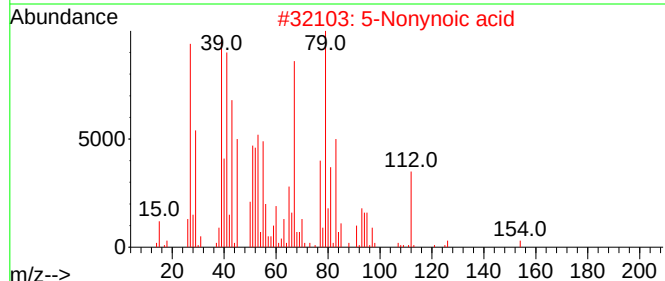
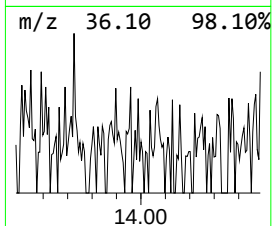
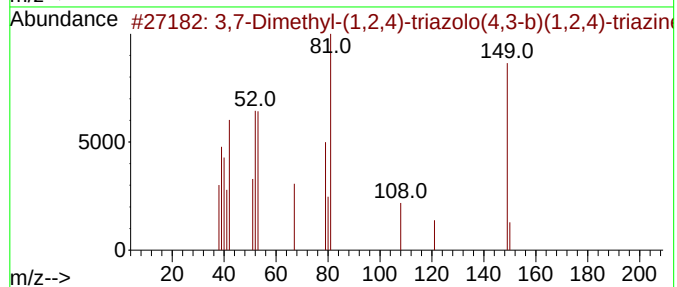
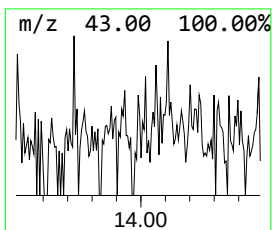
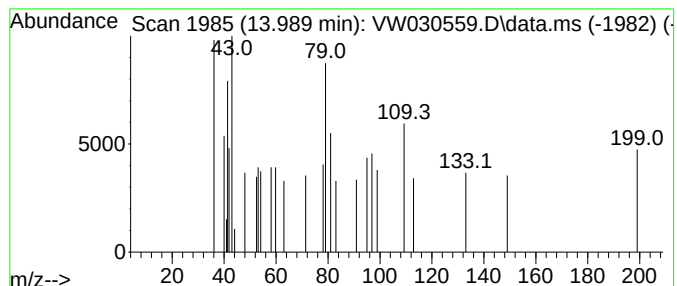
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100924SMA.M
Quant Title : SFAM01.0

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

Peak Number 9 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.989	3.78 ug/L	1360	1,4-Dichlorobenzene-d4	13.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,7-Dimethyl-(1,2,4)-triazolo(4,...	149	C6H7N5	061139-72-8	35
2			5-Nonynoic acid	154	C9H14O2	056630-34-3	32
3			1H-Imidazo[1,2-b]pyrazole, 2,3-d...	109	C5H7N3	006714-29-0	32
4			1,8-Cyclopentadecadiyne	202	C15H22	004722-42-3	23
5			5-Hexyn-1-ol	98	C6H10O	000928-90-5	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW101124\
Data File : VW030559.D
Acq On : 11 Oct 2024 19:14
Operator : SY/MD
Sample : P4350-08
Misc : 4.48g/10mL/MSVOA_W/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EOAK9

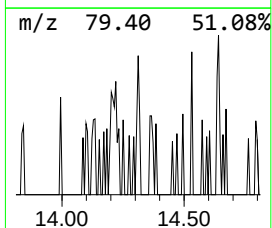
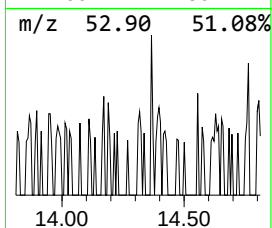
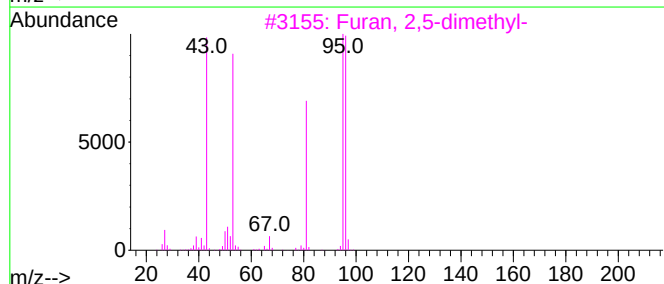
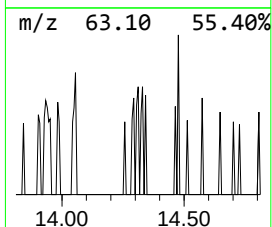
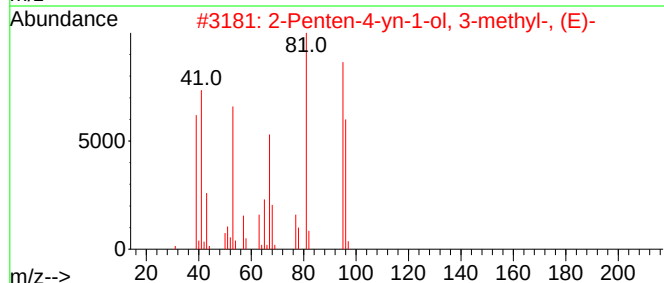
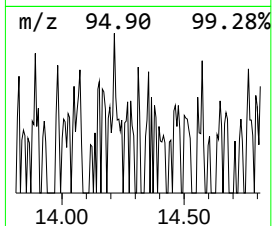
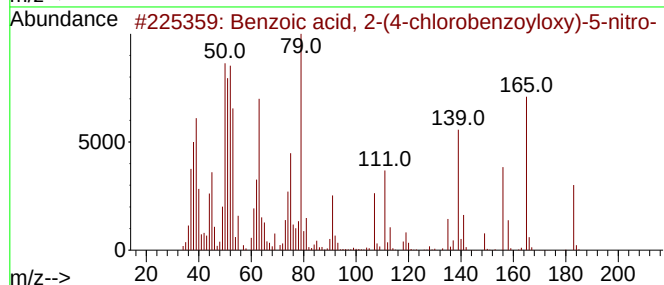
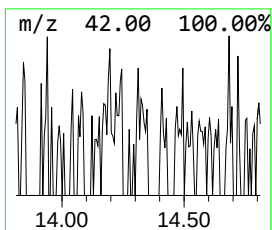
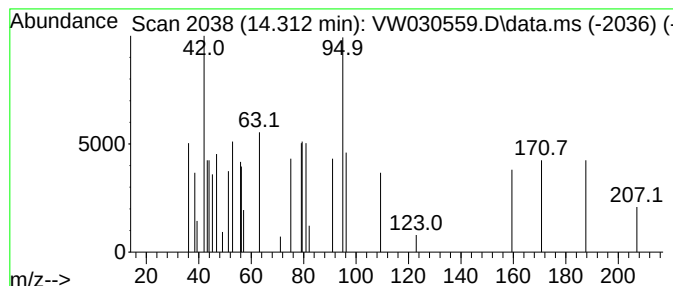
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Quant Title : SFAM01.0

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

Peak Number 10 unknown-03 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.312	3.27 ug/L	1177	1,4-Dichlorobenzene-d4	13.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-chlorobenzoyl...	321	C14H8ClNO6	306743-49-7	20
2			2-Penten-4-yn-1-ol, 3-methyl-, (E)-	96	C6H8O	006153-06-6	10
3			Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	9
4			1-Cyclopropanecarbonitrile, 1-amino	82	C4H6N2	196311-65-6	9
5			2,2-Dimethylhex-4-enylamine	127	C8H17N	133885-74-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW101124\
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EOAK9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100924SMA.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
unknown-01	2.228	12.8	ug/L	4441	1	8.843	8694	25.0
3-Methyl-4-nitr...	9.532	3.3	ug/L	1150	1	8.843	8694	25.0
unknown-02	13.989	3.8	ug/L	1360	3	13.562	8985	25.0
unknown-03	14.312	3.3	ug/L	1177	3	13.562	8985	25.0