

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091923\
 Data File : VW027157.D
 Acq On : 19 Sep 2023 19:03
 Operator : SY/MD
 Sample : VIBLK515
 Misc : 5.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VIBLK515

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\SFAMWLM091823SMA.M
 Title : SFAM01.0

Signal : TIC: VW027157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	39	52	53	rBV8	31756	90788	3.97%	0.509%
2	2.363	72	78	96	rVB	149001	384365	16.79%	2.153%
3	2.899	159	166	183	rVB	106769	302674	13.22%	1.696%
4	3.393	244	247	250	rVB4	986	1626	0.07%	0.009%
5	3.515	265	267	269	rBV3	1490	1603	0.07%	0.009%
6	3.558	272	274	278	rVB4	1561	1455	0.06%	0.008%
7	3.594	278	280	284	rBV5	1440	1900	0.08%	0.011%
8	3.673	289	293	294	rBV3	1176	1588	0.07%	0.009%
9	3.704	297	298	303	rVB5	1902	2101	0.09%	0.012%
10	3.801	311	314	315	rBV2	1734	1367	0.06%	0.008%
11	3.875	323	326	327	rBV2	1677	1314	0.06%	0.007%
12	3.893	327	329	331	rVB3	1730	1291	0.06%	0.007%
13	3.917	331	333	336	rVB4	1471	1614	0.07%	0.009%
14	4.021	336	350	367	rBV	212240	712108	31.11%	3.990%
15	4.216	379	382	385	rVB5	1941	2935	0.13%	0.016%
16	4.283	387	393	394	rBV6	1281	2041	0.09%	0.011%
17	4.326	397	400	402	rVB4	1388	1309	0.06%	0.007%
18	4.393	402	411	417	rBV2	8334	24095	1.05%	0.135%
19	4.442	417	419	420	rVB2	2301	1609	0.07%	0.009%
20	4.478	422	425	427	rVB4	1595	1904	0.08%	0.011%
21	4.509	427	430	431	rBV3	1106	1155	0.05%	0.006%
22	4.588	441	443	448	rVB6	1137	1531	0.07%	0.009%
23	4.704	458	462	464	rBV6	1118	1488	0.07%	0.008%
24	4.746	467	469	472	rVB4	1198	1315	0.06%	0.007%
25	4.813	478	480	484	rVB5	1414	1824	0.08%	0.010%
26	4.923	484	498	516	rBV2	49886	206101	9.00%	1.155%
27	5.155	532	536	540	rBV7	1131	2421	0.11%	0.014%
28	5.185	540	541	544	rVB3	1936	1675	0.07%	0.009%
29	5.216	544	546	551	rVB6	1181	1560	0.07%	0.009%
30	5.265	551	554	557	rBV5	1650	1971	0.09%	0.011%
31	5.319	561	563	564	rBV2	1308	962	0.04%	0.005%
32	5.380	570	573	575	rVB4	1280	1285	0.06%	0.007%
33	5.447	578	584	585	rBV5	1324	2086	0.09%	0.012%
34	5.575	603	605	607	rBV3	1002	1043	0.05%	0.006%
35	5.667	618	620	622	rBV2	1218	970	0.04%	0.005%
36	5.697	622	625	629	rVB6	1480	2105	0.09%	0.012%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091823SMA.M
 Title : SFAM01.0

37	5.734	629	631	633	rBV3	1432	1109	0.05%	0.006%
38	5.825	645	646	649	rVB3	1570	1398	0.06%	0.008%
39	5.856	649	651	653	rBV3	1484	1331	0.06%	0.007%
40	5.941	653	665	676	rBV2	27453	90841	3.97%	0.509%
41	6.057	681	684	686	rBV4	1269	1557	0.07%	0.009%
42	6.088	686	689	691	rVB4	1291	1356	0.06%	0.008%
43	6.155	695	700	703	rVB7	1240	2066	0.09%	0.012%
44	6.197	703	707	709	rBV5	1712	2806	0.12%	0.016%
45	6.277	718	720	722	rBV3	1437	1332	0.06%	0.007%
46	6.350	729	732	733	rBV3	13983	14479	0.63%	0.081%
47	6.368	733	735	736	rBV2	2136	1265	0.06%	0.007%
48	6.386	736	738	740	rBV3	2866	2278	0.10%	0.013%
49	6.502	755	757	759	rVB3	2723	1962	0.09%	0.011%
50	6.722	792	793	800	rBV7	3326	5594	0.24%	0.031%
51	6.862	813	816	818	rBV4	5927	8461	0.37%	0.047%
52	6.947	828	830	831	rBV2	3414	2477	0.11%	0.014%
53	7.081	843	852	855	rBV2	53410	134582	5.88%	0.754%
54	7.130	855	860	869	rVB	89074	247032	10.79%	1.384%
55	7.258	878	881	886	rVB7	4842	7712	0.34%	0.043%
56	7.301	886	888	889	rBV2	3215	2603	0.11%	0.015%
57	7.423	906	908	915	rVB8	1818	3278	0.14%	0.018%
58	7.478	915	917	918	rBV2	1445	1187	0.05%	0.007%
59	7.532	924	926	929	rVB4	2291	1768	0.08%	0.010%
60	7.648	935	945	960	rVB	327337	818225	35.75%	4.584%
61	7.758	960	963	966	rBV4	1742	2719	0.12%	0.015%
62	7.795	966	969	971	rVV4	1340	1672	0.07%	0.009%
63	7.813	971	972	976	rVB4	1368	1105	0.05%	0.006%
64	8.008	1002	1004	1005	rBV2	1044	963	0.04%	0.005%
65	8.166	1025	1030	1032	rBV6	1223	1645	0.07%	0.009%
66	8.191	1032	1034	1035	rVB2	1436	1021	0.04%	0.006%
67	8.276	1035	1048	1066	rBV2	724521	2122636	92.74%	11.893%
68	8.471	1077	1080	1083	rVB5	1470	1574	0.07%	0.009%
69	8.520	1085	1088	1089	rVB3	1443	1312	0.06%	0.007%
70	8.587	1096	1099	1100	rBV3	1491	1183	0.05%	0.007%
71	8.697	1114	1117	1121	rVB6	2929	3115	0.14%	0.017%
72	8.746	1123	1125	1126	rBV2	1245	1139	0.05%	0.006%
73	8.764	1126	1128	1130	rVB3	2230	1529	0.07%	0.009%
74	8.843	1130	1141	1152	rBV	707027	1416969	61.91%	7.939%
75	8.922	1152	1154	1158	rVB5	1743	2602	0.11%	0.015%
76	9.081	1178	1180	1184	rVB5	3518	3648	0.16%	0.020%

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 ClientSampleId :
 VIBLK515

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091823SMA.M
 Title : SFAM01.0

77	9.203	1195	1200	1203	rBV7	2573	5090	0.22%	0.029%
78	9.270	1203	1211	1222	rBV	436391	905804	39.58%	5.075%
79	9.422	1234	1236	1238	rBV3	2132	1851	0.08%	0.010%
80	9.666	1274	1276	1277	rBV2	2083	1308	0.06%	0.007%
81	9.764	1290	1292	1295	rBV4	2425	2651	0.12%	0.015%
82	9.819	1299	1301	1303	rBV3	1955	1228	0.05%	0.007%
83	9.904	1313	1315	1318	rBV3	2710	2371	0.10%	0.013%
84	9.934	1318	1320	1321	rVB2	2770	1226	0.05%	0.007%
85	9.959	1321	1324	1328	rBV6	4078	8485	0.37%	0.048%
86	10.032	1330	1336	1343	rVV	236968	432740	18.91%	2.425%
87	10.264	1371	1374	1375	rBV3	13401	14040	0.61%	0.079%
88	10.325	1376	1384	1395	rVV	1253037	2288801	100.00%	12.824%
89	10.575	1420	1425	1433	rVB	186743	327556	14.31%	1.835%
90	10.703	1440	1446	1453	rVB	96821	167162	7.30%	0.937%
91	10.922	1476	1482	1489	rBV	220907	393398	17.19%	2.204%
92	11.062	1502	1505	1510	rVB	30333	46059	2.01%	0.258%
93	11.629	1591	1598	1607	rVB	1057027	1831974	80.04%	10.264%
94	12.605	1750	1758	1766	rVB	160989	301826	13.19%	1.691%
95	12.690	1766	1772	1780	rVB	340332	560841	24.50%	3.142%
96	13.556	1908	1914	1926	rVB	1245969	2030154	88.70%	11.374%
97	13.848	1955	1962	1977	rBV	929335	1630953	71.26%	9.138%
98	14.062	1993	1997	2004	rVB2	52778	102026	4.46%	0.572%
99	15.433	2217	2222	2226	rVB	38874	63239	2.76%	0.354%
100	16.275	2356	2360	2366	rVB3	20902	36966	1.62%	0.207%

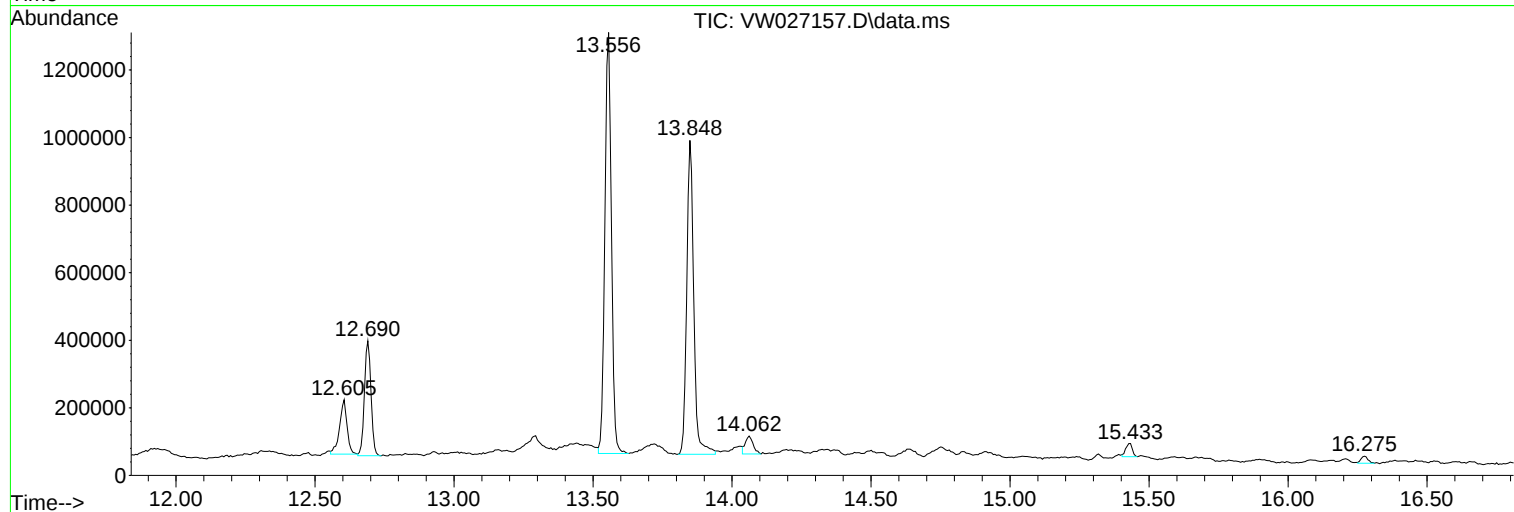
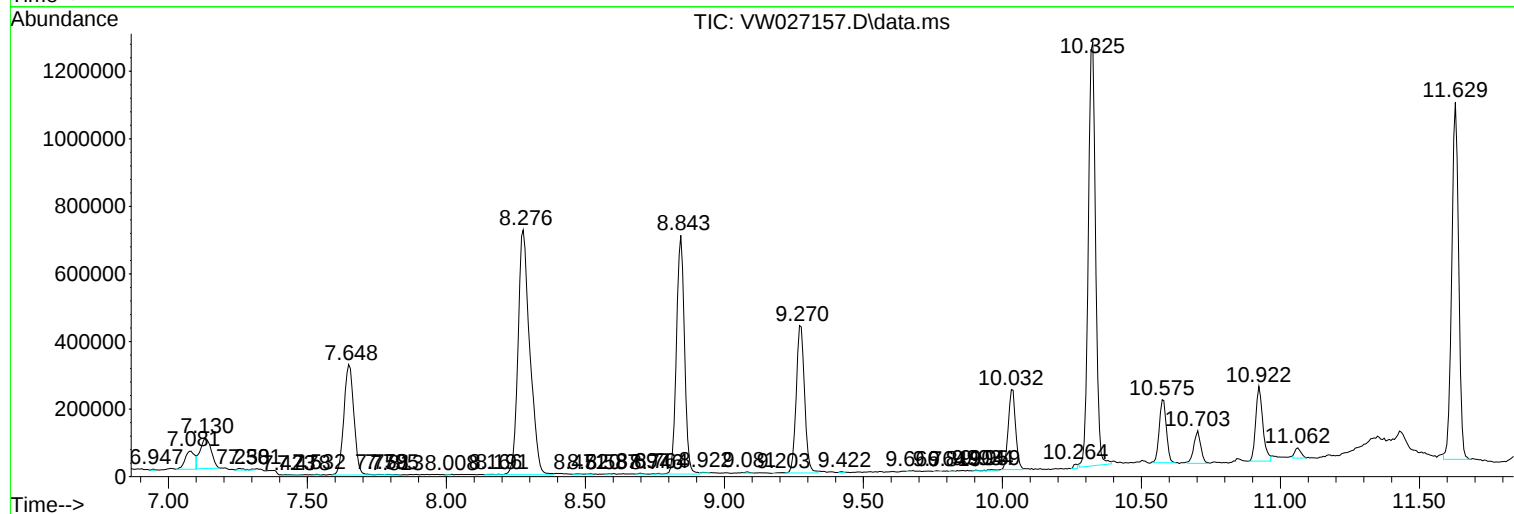
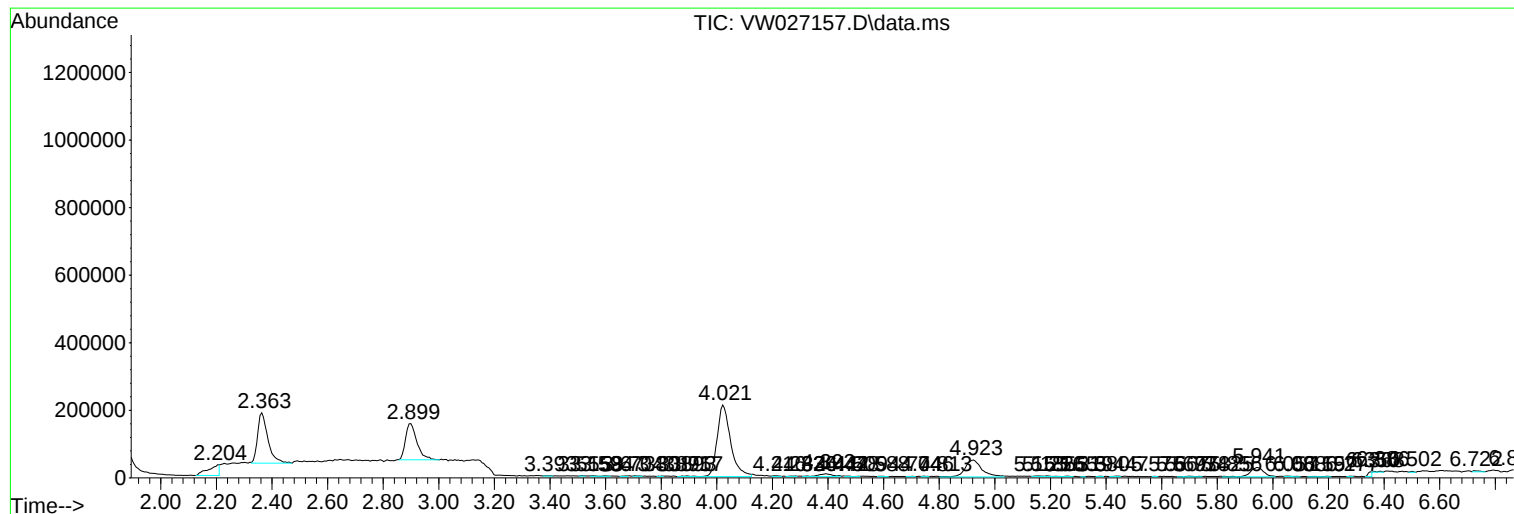
Sum of corrected areas: 17848459

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Misc : 5.00g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
VIBLK515

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091823SMA.M
Quant Title : SFAM01.0

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



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ALS Vial : 1 Sample Multiplier: 1

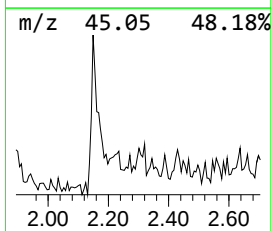
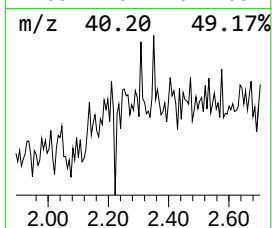
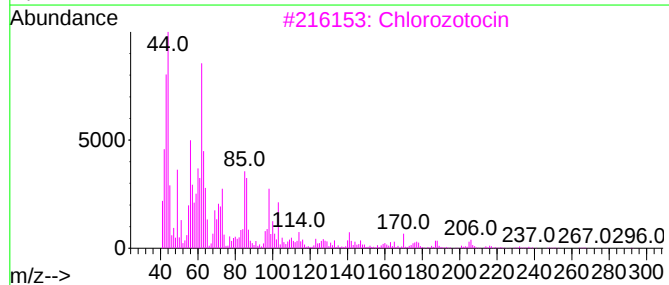
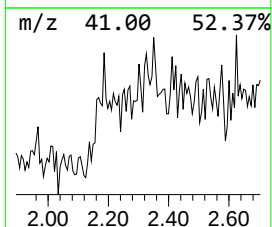
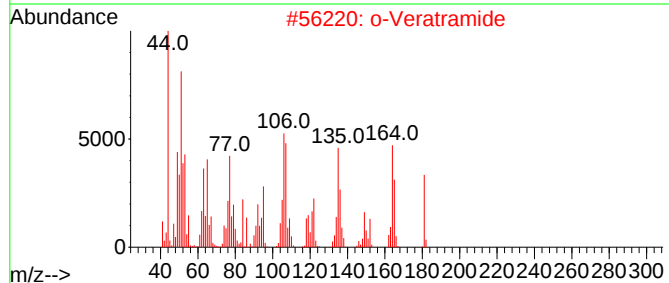
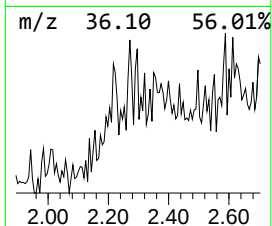
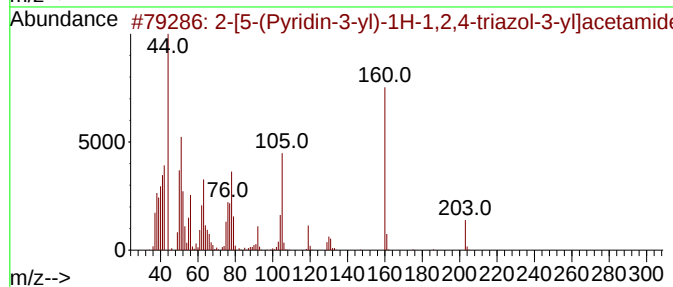
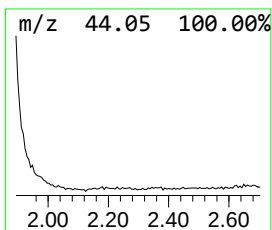
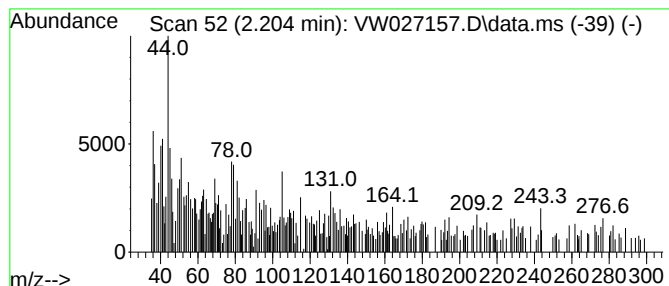
Instrument :
MSVOA_W
ClientSampleId :
VIBLK515

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091823SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 2-[5-(Pyridin-3-yl)-1H-1,2,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.204	1.60 ug/L	90788	1,4-Difluorobenzene	8.843	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[5-(Pyridin-3-yl)-1H-1,2,4-tri...	203	C9H9N5O	1000410-33-9	56
2	o-Veratramide	181	C9H11NO3	001521-39-7	27
3	Chlorozotocin	313	C9H16ClN3O7	054749-90-5	25
4	Ethyl allophanate	132	C4H8N2O3	000626-36-8	18
5	N,N'-Dicarbethoxy-N-[2,4-diamino...	300	C10H16N6O5	049810-02-8	16



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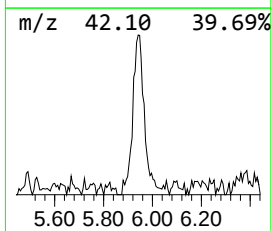
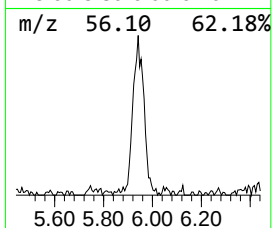
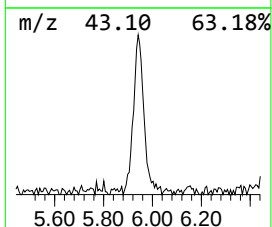
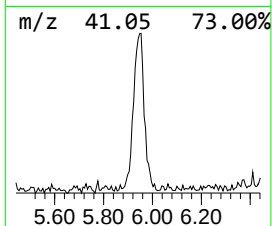
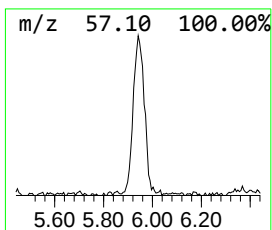
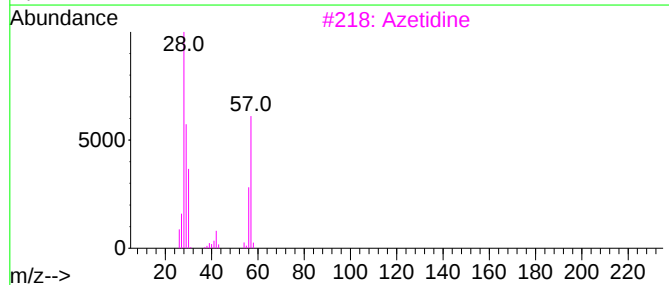
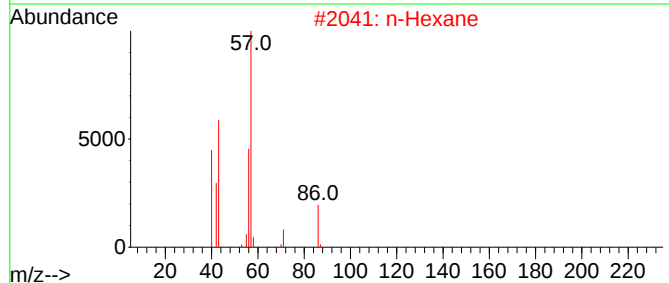
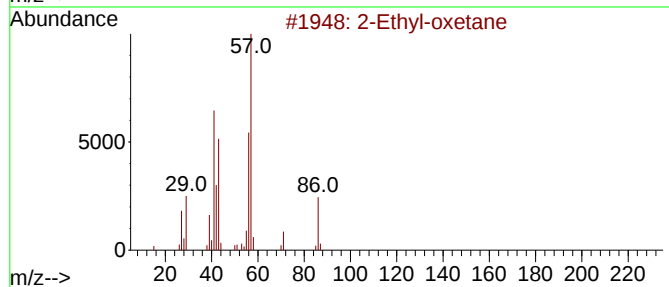
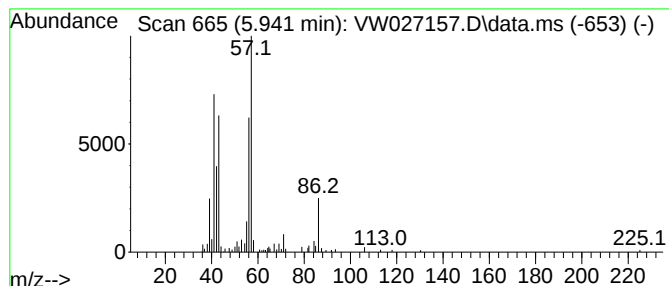
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091823SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 2-Ethyl-oxetane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.941	1.60 ug/L	90841	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	83
2			n-Hexane	86	C6H14	000110-54-3	80
3			Azetidine	57	C3H7N	000503-29-7	58
4			n-Hexane	86	C6H14	000110-54-3	50
5			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	47



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-[5-(Pyridin-3...	2.204	1.6	ug/L	90788	1	8.843	1416970	25.0
2-Ethyl-oxetane	5.941	1.6	ug/L	90841	1	8.843	1416970	25.0