

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091923\
 Data File : VW027151.D
 Acq On : 19 Sep 2023 16:39
 Operator : SY/MD
 Sample : VIBLK513
 Misc : 5.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VIBLK513

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: VW027151.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.052	26	27	30	rVB3	2916	2703	0.13%	0.015%
2	2.088	30	33	34	rBV3	1759	1643	0.08%	0.009%
3	2.168	42	46	47	rBV4	1624	2052	0.10%	0.012%
4	2.216	50	54	57	rBV6	6437	12435	0.60%	0.071%
5	2.247	57	59	60	rBV2	1838	1471	0.07%	0.008%
6	2.363	71	78	91	rBV	103249	255611	12.43%	1.465%
7	2.533	104	106	108	rVB3	2768	2157	0.10%	0.012%
8	2.594	109	116	118	rBV6	32786	69593	3.38%	0.399%
9	2.698	131	133	135	rBV3	8185	8086	0.39%	0.046%
10	2.899	159	166	178	rVB	118094	321405	15.62%	1.842%
11	3.210	216	217	220	rVB3	1538	1259	0.06%	0.007%
12	3.283	225	229	230	rBV3	1402	1957	0.10%	0.011%
13	3.320	230	235	236	rBV5	1187	1452	0.07%	0.008%
14	3.387	243	246	247	rBV3	2754	2758	0.13%	0.016%
15	3.527	264	269	271	rBV6	1782	2776	0.13%	0.016%
16	3.619	281	284	285	rBV3	1465	1290	0.06%	0.007%
17	3.795	309	313	316	rBV6	1650	2408	0.12%	0.014%
18	4.021	339	350	368	rBV	195918	648367	31.52%	3.715%
19	4.393	404	411	418	rVV3	5955	18105	0.88%	0.104%
20	4.442	418	419	424	rVV5	2015	1878	0.09%	0.011%
21	4.509	428	430	433	rVB3	1598	1546	0.08%	0.009%
22	4.545	433	436	438	rBV4	959	1456	0.07%	0.008%
23	4.564	438	439	444	rVV5	1360	1716	0.08%	0.010%
24	4.722	462	465	469	rBV6	1526	2558	0.12%	0.015%
25	4.814	477	480	482	rBV4	1109	1520	0.07%	0.009%
26	4.917	484	497	515	rBV2	50175	197606	9.61%	1.132%
27	5.039	515	517	519	rVV3	1668	1696	0.08%	0.010%
28	5.149	530	535	538	rBV6	2158	3877	0.19%	0.022%
29	5.259	551	553	559	rVB7	1986	3191	0.16%	0.018%
30	5.307	559	561	562	rBV2	1556	1564	0.08%	0.009%
31	5.515	593	595	597	rBV3	1507	1599	0.08%	0.009%
32	5.588	603	607	609	rVB5	1371	1584	0.08%	0.009%
33	5.637	609	615	617	rBV5	924	1481	0.07%	0.008%
34	5.752	630	634	635	rBV4	1688	2388	0.12%	0.014%
35	5.941	653	665	676	rVV2	35892	110075	5.35%	0.631%
36	6.118	692	694	696	rBV3	1353	1440	0.07%	0.008%

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

37	6.441	742	747	748	rBV5	1256	1434	0.07%	0.008%
38	6.795	802	805	809	rVB5	1423	1675	0.08%	0.010%
39	6.844	811	813	817	rBV4	1497	1948	0.09%	0.011%
40	6.911	819	824	825	rBV4	1914	2420	0.12%	0.014%
41	6.990	836	837	840	rBV3	1218	1213	0.06%	0.007%
42	7.081	843	852	854	rBV	41604	97187	4.72%	0.557%
43	7.136	854	861	876	rVB	92841	270659	13.16%	1.551%
44	7.319	889	891	894	rVB4	1637	1693	0.08%	0.010%
45	7.484	917	918	922	rVB4	1615	1863	0.09%	0.011%
46	7.520	922	924	927	rBV4	1732	2293	0.11%	0.013%
47	7.575	930	933	934	rVV3	1537	1255	0.06%	0.007%
48	7.648	934	945	957	rVV	311686	769248	37.39%	4.407%
49	7.746	959	961	962	rVV2	1693	1486	0.07%	0.009%
50	7.764	962	964	969	rVV6	2165	3143	0.15%	0.018%
51	7.825	971	974	977	rVB5	1617	2130	0.10%	0.012%
52	8.057	1011	1012	1015	rBV3	1275	1520	0.07%	0.009%
53	8.081	1015	1016	1020	rVB4	1054	1226	0.06%	0.007%
54	8.154	1025	1028	1032	rVB5	1282	1563	0.08%	0.009%
55	8.276	1035	1048	1063	rBV2	693232	2057202	100.00%	11.787%
56	8.380	1063	1065	1072	rVV8	2182	4582	0.22%	0.026%
57	8.520	1085	1088	1090	rBV4	812	1311	0.06%	0.008%
58	8.606	1099	1102	1105	rBV5	946	1329	0.06%	0.008%
59	8.691	1111	1116	1117	rBV4	1566	2276	0.11%	0.013%
60	8.843	1132	1141	1160	rBV	623927	1248561	60.69%	7.154%
61	9.057	1175	1176	1178	rBV2	1834	1772	0.09%	0.010%
62	9.087	1180	1181	1187	rVB6	3575	5085	0.25%	0.029%
63	9.148	1187	1191	1193	rVB5	1837	2828	0.14%	0.016%
64	9.179	1193	1196	1197	rBV2	1479	1875	0.09%	0.011%
65	9.221	1197	1203	1204	rBV6	14336	27506	1.34%	0.158%
66	9.270	1204	1211	1224	rVV	541720	1128577	54.86%	6.466%
67	9.538	1253	1255	1257	rBV3	4114	3763	0.18%	0.022%
68	9.648	1271	1273	1280	rBV8	4175	7680	0.37%	0.044%
69	9.788	1295	1296	1301	rBV5	4530	5851	0.28%	0.034%
70	10.032	1330	1336	1347	rVB	271818	499352	24.27%	2.861%
71	10.184	1360	1361	1363	rBV2	6293	5336	0.26%	0.031%
72	10.319	1376	1383	1393	rBV	1136948	2047737	99.54%	11.733%
73	10.575	1419	1425	1432	rVB	179363	320681	15.59%	1.837%
74	10.703	1440	1446	1455	rVB	105389	195620	9.51%	1.121%
75	10.849	1467	1470	1474	rVB5	11107	16209	0.79%	0.093%
76	10.922	1476	1482	1492	rBV	205414	365221	17.75%	2.093%

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 Title : SFAM01.0

77	11.062	1502	1505	1509	rVB2	21885	31352	1.52%	0.180%
78	11.166	1518	1522	1524	rBV5	18188	32528	1.58%	0.186%
79	11.434	1563	1566	1576	rVB	40194	86977	4.23%	0.498%
80	11.574	1586	1589	1591	rBV4	14826	19170	0.93%	0.110%
81	11.629	1591	1598	1606	rVB	1161574	1973964	95.95%	11.310%
82	11.843	1629	1633	1635	rBV5	6762	10518	0.51%	0.060%
83	11.934	1640	1648	1650	rBV9	16769	40680	1.98%	0.233%
84	12.105	1670	1676	1677	rBV6	16510	31301	1.52%	0.179%
85	12.471	1732	1736	1740	rBV6	11048	18670	0.91%	0.107%
86	12.605	1752	1758	1766	rBV	91892	182806	8.89%	1.047%
87	12.690	1766	1772	1782	rVB	410911	666657	32.41%	3.820%
88	12.897	1804	1806	1807	rBV2	14025	13742	0.67%	0.079%
89	13.099	1837	1839	1844	rBV6	8864	14474	0.70%	0.083%
90	13.556	1907	1914	1921	rVB	1078919	1698528	82.56%	9.732%
91	13.848	1956	1962	1968	rBV	1004127	1653212	80.36%	9.472%
92	14.062	1993	1997	2004	rVB	34571	64061	3.11%	0.367%
93	14.434	2056	2058	2065	rBV8	10196	14755	0.72%	0.085%
94	14.720	2102	2105	2107	rBV4	7690	10823	0.53%	0.062%
95	15.318	2198	2203	2208	rBV9	9937	23620	1.15%	0.135%
96	15.427	2217	2221	2226	rVB2	24065	38266	1.86%	0.219%
97	16.080	2326	2328	2329	rBV2	3017	1464	0.07%	0.008%
98	16.269	2356	2359	2365	rBV8	7284	13103	0.64%	0.075%
99	16.702	2428	2430	2432	rVB3	2493	1504	0.07%	0.009%
100	16.781	2441	2443	2444	rBV2	3170	2124	0.10%	0.012%

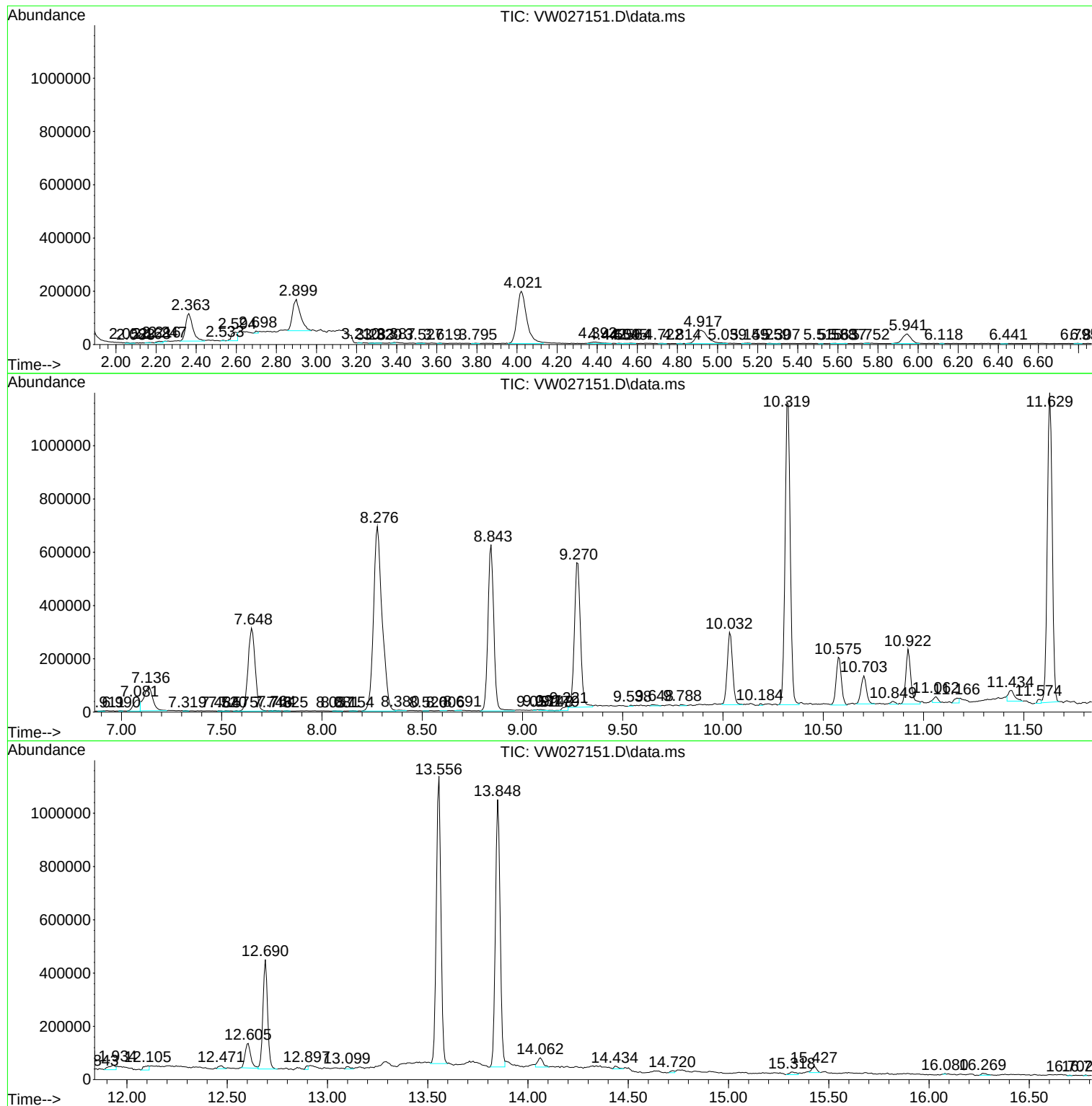
Sum of corrected areas: 17453312

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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



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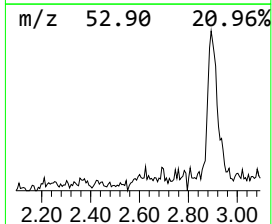
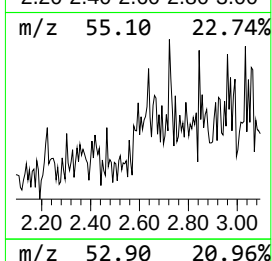
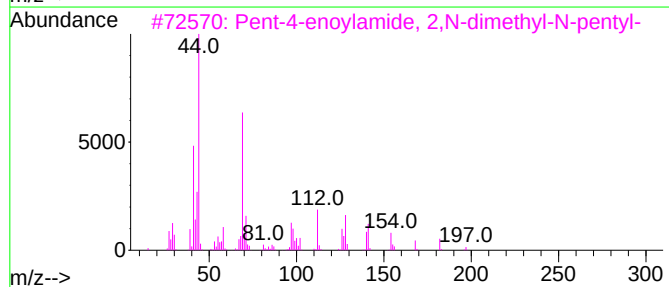
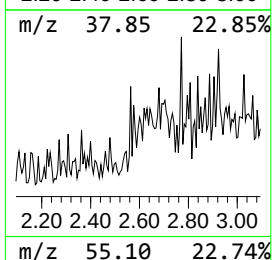
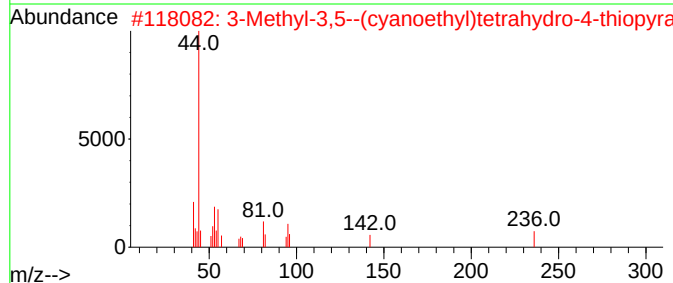
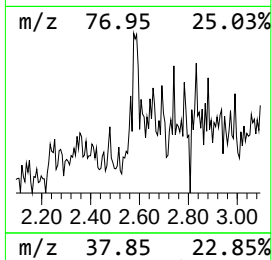
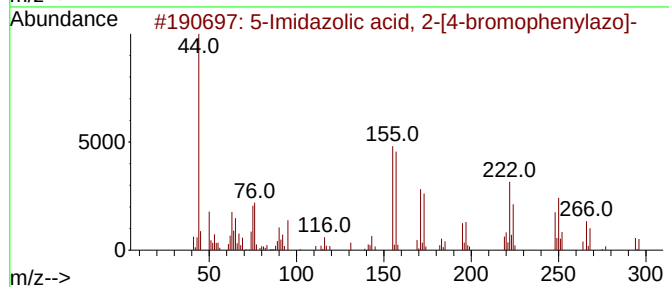
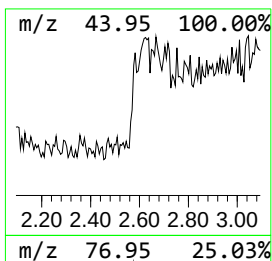
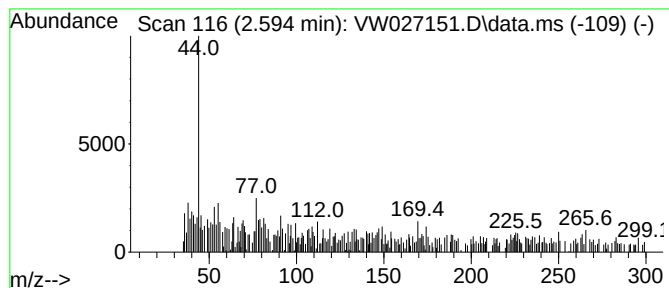
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091823SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 5-Imidazolic acid, 2-[4-bro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.594	1.39 ug/L	69593	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Imidazolic acid, 2-[4-bromophe...	294	C10H7BrN4O2	1000128-05-9	53
2			3-Methyl-3,5--(cyanoethyl)tetrah...	236	C12H16N2OS	1000140-32-3	50
3			Pent-4-enoylamide, 2,N-dimethyl-...	197	C12H23NO	1010437-40-0	47
4			Pterin-6-carboxylic acid	207	C7H5N5O3	000948-60-7	45
5			2-Dimethylaminomethyl-4-chloro-1...	235	C13H14ClNO	167163-22-6	43



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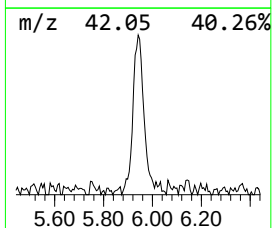
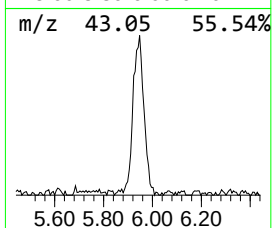
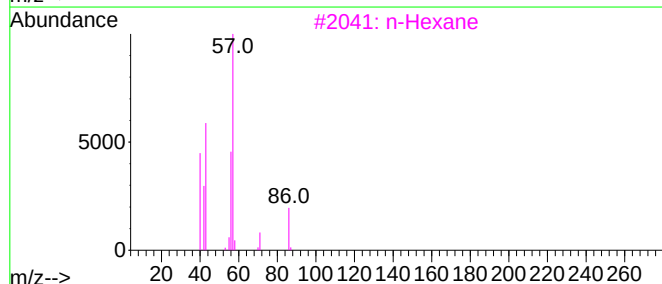
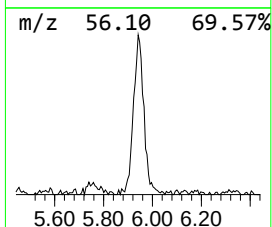
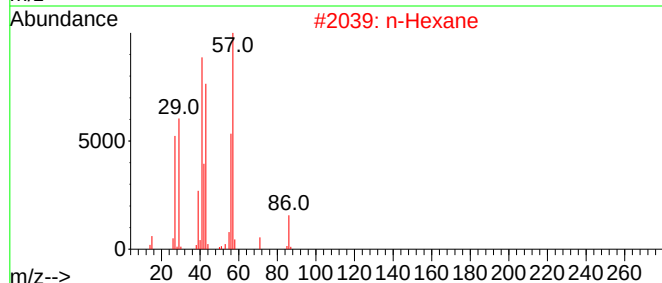
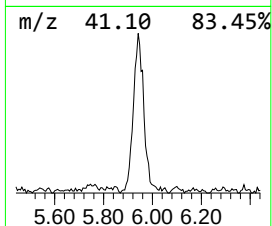
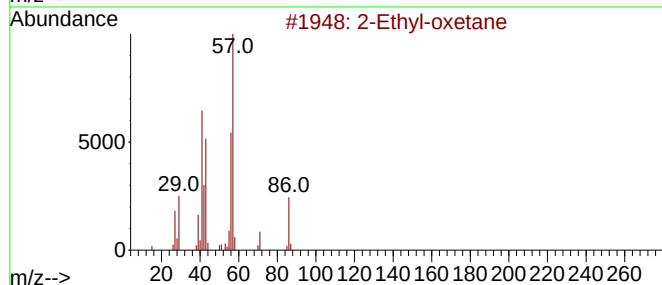
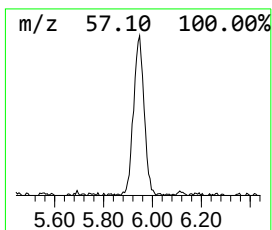
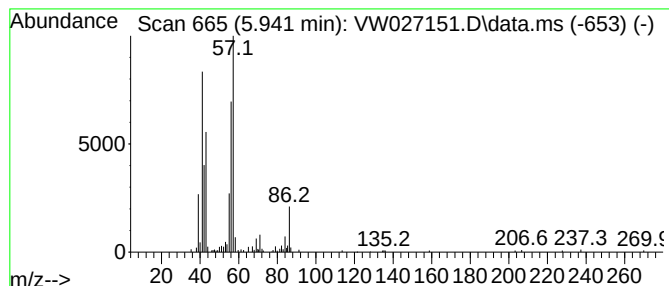
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091823SMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Ethyl-oxetane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.941	2.20 ug/L	110075	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			n-Hexane	86	C6H14	000110-54-3	80
4			n-Hexane	86	C6H14	000110-54-3	56
5			Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	43



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
5-Imidazolic ac...	2.594	1.4	ug/L	69593	1	8.843	1248560	25.0
2-Ethyl-oxetane	5.941	2.2	ug/L	110075	1	8.843	1248560	25.0