

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072222\
 Data File : VW024052.D
 Acq On : 23 Jul 2022 13:33
 Operator : SY/VA
 Sample : N3790-21
 Misc : 5.95g/10mL/MSVOA_W/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DBUL7

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\SFAMWLM071322SMA.M
 Title : SFAM01.0

Signal : TIC: VW024052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.343	68	72	80	rVB	88369	146224	19.23%	2.440%
2	2.873	154	159	172	rVB	62909	147013	19.33%	2.453%
3	3.635	282	284	288	rBV3	846	1276	0.17%	0.021%
4	3.775	304	307	308	rBV3	2042	1808	0.24%	0.030%
5	4.001	335	344	360	rBV2	59985	197619	25.99%	3.298%
6	4.391	402	408	411	rBV6	2010	4113	0.54%	0.069%
7	4.416	411	412	416	rVV4	1230	1116	0.15%	0.019%
8	4.538	431	432	435	rVB3	1393	868	0.11%	0.014%
9	4.653	448	451	453	rBV3	1213	1348	0.18%	0.022%
10	5.037	512	514	517	rBV4	1253	1424	0.19%	0.024%
11	5.208	540	542	545	rVB3	1337	797	0.10%	0.013%
12	5.531	591	595	598	rBV6	1041	1609	0.21%	0.027%
13	5.586	601	604	605	rVV3	1007	748	0.10%	0.012%
14	5.757	630	632	634	rBV2	1035	667	0.09%	0.011%
15	5.934	652	661	671	rBV4	10577	34195	4.50%	0.571%
16	6.068	681	683	688	rBV5	1608	1455	0.19%	0.024%
17	6.123	689	692	693	rVV3	896	703	0.09%	0.012%
18	6.208	704	706	709	rBV4	729	899	0.12%	0.015%
19	6.671	779	782	785	rVB5	938	999	0.13%	0.017%
20	6.702	785	787	790	rBV4	1210	1397	0.18%	0.023%
21	6.757	790	796	797	rBV5	835	1406	0.18%	0.023%
22	6.769	797	798	801	rVB3	1541	1101	0.14%	0.018%
23	6.811	801	805	807	rBV4	518	680	0.09%	0.011%
24	7.080	842	849	858	rBV2	22099	63766	8.39%	1.064%
25	7.244	874	876	877	rVB2	1441	870	0.11%	0.015%
26	7.647	933	942	952	rVB	145507	357440	47.01%	5.965%
27	8.031	1004	1005	1007	rBV2	1030	668	0.09%	0.011%
28	8.128	1019	1021	1023	rBV3	1336	1095	0.14%	0.018%
29	8.275	1036	1045	1059	rBV2	238924	760372	100.00%	12.688%
30	8.744	1121	1122	1125	rVB3	1198	749	0.10%	0.012%
31	8.842	1128	1138	1152	rBV	299140	594694	78.21%	9.924%
32	9.177	1189	1193	1196	rBV4	1338	1487	0.20%	0.025%
33	9.274	1201	1209	1218	rBV	194717	393708	51.78%	6.570%
34	9.476	1240	1242	1246	rBV4	977	1543	0.20%	0.026%
35	9.665	1268	1273	1275	rBV3	1951	3410	0.45%	0.057%
36	9.756	1285	1288	1290	rBV3	1080	1525	0.20%	0.025%

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 Title : SFAM01.0

37	9.866	1305	1306	1308	rBV2	1037	689	0.09%	0.011%
38	10.037	1326	1334	1342	rBV	71512	134921	17.74%	2.251%
39	10.323	1373	1381	1388	rBV	350205	603109	79.32%	10.064%
40	10.573	1416	1422	1431	rVB	52272	92819	12.21%	1.549%
41	10.695	1439	1442	1445	rBV5	1224	1567	0.21%	0.026%
42	10.780	1454	1456	1459	rBV3	1200	1356	0.18%	0.023%
43	10.860	1467	1469	1472	rVB4	1451	1747	0.23%	0.029%
44	10.921	1473	1479	1491	rVV	90688	167405	22.02%	2.793%
45	11.164	1518	1519	1523	rBV4	1040	879	0.12%	0.015%
46	11.195	1523	1524	1528	rBV3	958	1372	0.18%	0.023%
47	11.341	1546	1548	1551	rVB4	1186	1282	0.17%	0.021%
48	11.579	1585	1587	1588	rBV2	924	764	0.10%	0.013%
49	11.628	1588	1595	1604	rVV	434200	741784	97.56%	12.378%
50	11.920	1639	1643	1645	rBV4	1041	1692	0.22%	0.028%
51	12.054	1661	1665	1666	rBV3	758	907	0.12%	0.015%
52	12.097	1670	1672	1674	rBV2	706	873	0.11%	0.015%
53	12.280	1700	1702	1706	rVB5	1168	1588	0.21%	0.026%
54	12.329	1706	1710	1711	rBV4	973	1218	0.16%	0.020%
55	12.445	1726	1729	1730	rBV2	755	930	0.12%	0.016%
56	12.536	1742	1744	1748	rBV5	1286	2290	0.30%	0.038%
57	12.597	1752	1754	1759	rVV6	2504	4150	0.55%	0.069%
58	12.688	1762	1769	1778	rVV	187655	310729	40.87%	5.185%
59	12.786	1784	1785	1787	rVB2	1362	863	0.11%	0.014%
60	12.817	1787	1790	1792	rBV4	1401	1404	0.18%	0.023%
61	12.865	1796	1798	1800	rBV3	1118	879	0.12%	0.015%
62	13.134	1839	1842	1844	rBV3	1208	1437	0.19%	0.024%
63	13.176	1847	1849	1851	rBV4	748	785	0.10%	0.013%
64	13.219	1853	1856	1857	rBV3	599	705	0.09%	0.012%
65	13.487	1898	1900	1903	rBV4	1356	1677	0.22%	0.028%
66	13.554	1904	1911	1923	rVV	389055	616997	81.14%	10.296%
67	13.688	1931	1933	1935	rBV3	982	761	0.10%	0.013%
68	13.847	1952	1959	1970	rBV	322295	528020	69.44%	8.811%
69	13.987	1980	1982	1984	rBV3	967	894	0.12%	0.015%
70	14.060	1992	1994	1998	rBV4	1018	1470	0.19%	0.025%
71	14.121	2002	2004	2005	rBV2	798	710	0.09%	0.012%
72	14.328	2036	2038	2040	rVB3	1790	1031	0.14%	0.017%
73	14.572	2076	2078	2079	rBV2	1277	872	0.11%	0.015%
74	14.609	2082	2084	2087	rBV4	1314	1684	0.22%	0.028%
75	14.694	2096	2098	2099	rBV2	889	730	0.10%	0.012%
76	14.719	2099	2102	2106	rVB5	1746	2903	0.38%	0.048%

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 Title : SFAM01.0

77	14.853	2122	2124	2126	rBV2	720	660	0.09%	0.011%
78	14.877	2126	2128	2129	rVV	1298	727	0.10%	0.012%
79	14.932	2133	2137	2139	rVV3	1012	1406	0.18%	0.023%
80	14.981	2143	2145	2148	rVB4	876	746	0.10%	0.012%
81	15.017	2148	2151	2155	rBV5	895	1335	0.18%	0.022%
82	15.048	2155	2156	2158	rBV2	1264	908	0.12%	0.015%
83	15.127	2165	2169	2173	rBV5	1180	1748	0.23%	0.029%
84	15.158	2173	2174	2177	rBV3	951	1010	0.13%	0.017%
85	15.225	2181	2185	2187	rBV4	1431	1723	0.23%	0.029%
86	15.420	2215	2217	2218	rBV2	1105	763	0.10%	0.013%
87	15.481	2222	2227	2228	rBV4	768	1441	0.19%	0.024%
88	15.529	2233	2235	2238	rBV4	945	1095	0.14%	0.018%
89	15.627	2250	2251	2254	rVB3	1313	863	0.11%	0.014%
90	15.938	2300	2302	2306	rVB4	844	799	0.11%	0.013%
91	16.151	2336	2337	2338	rBV	1172	665	0.09%	0.011%
92	16.170	2338	2340	2341	rVV2	1180	787	0.10%	0.013%
93	16.206	2345	2346	2349	rVV2	810	773	0.10%	0.013%
94	16.359	2369	2371	2373	rBV3	839	712	0.09%	0.012%
95	16.377	2373	2374	2377	rVB3	1199	795	0.10%	0.013%
96	16.407	2377	2379	2382	rVB4	1058	1049	0.14%	0.018%
97	16.584	2406	2408	2411	rBV3	1011	977	0.13%	0.016%
98	16.627	2413	2415	2420	rVB5	1120	1104	0.15%	0.018%
99	16.706	2426	2428	2431	rVV3	1061	1129	0.15%	0.019%
100	16.737	2431	2433	2435	rVB3	1077	872	0.11%	0.015%

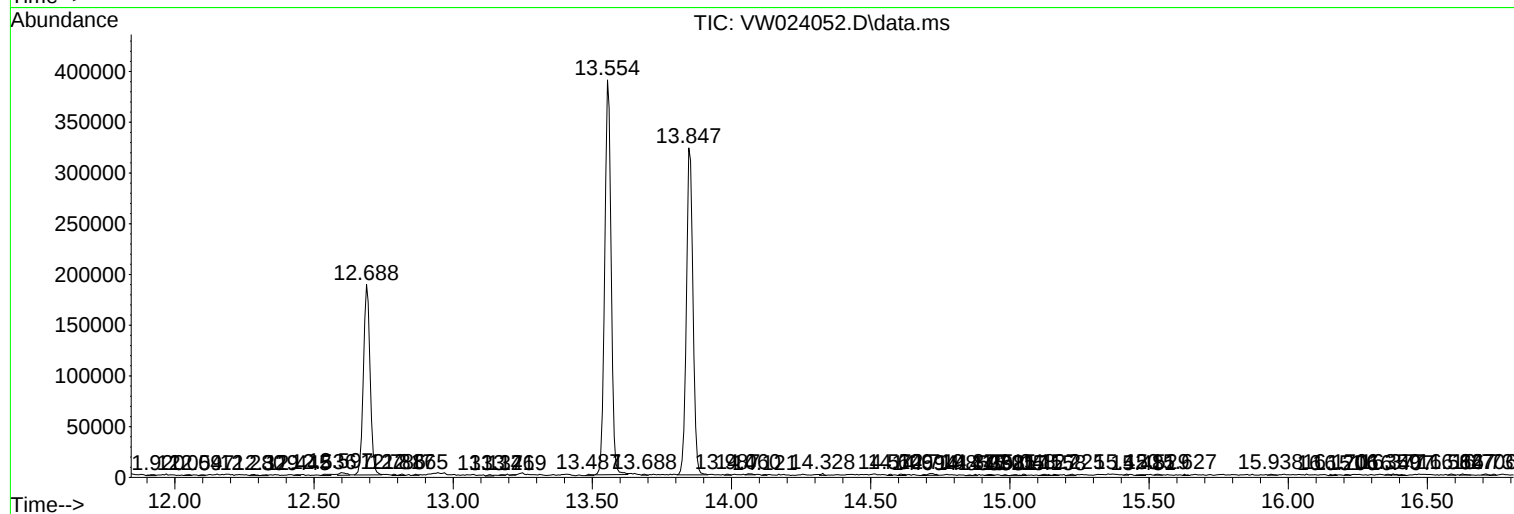
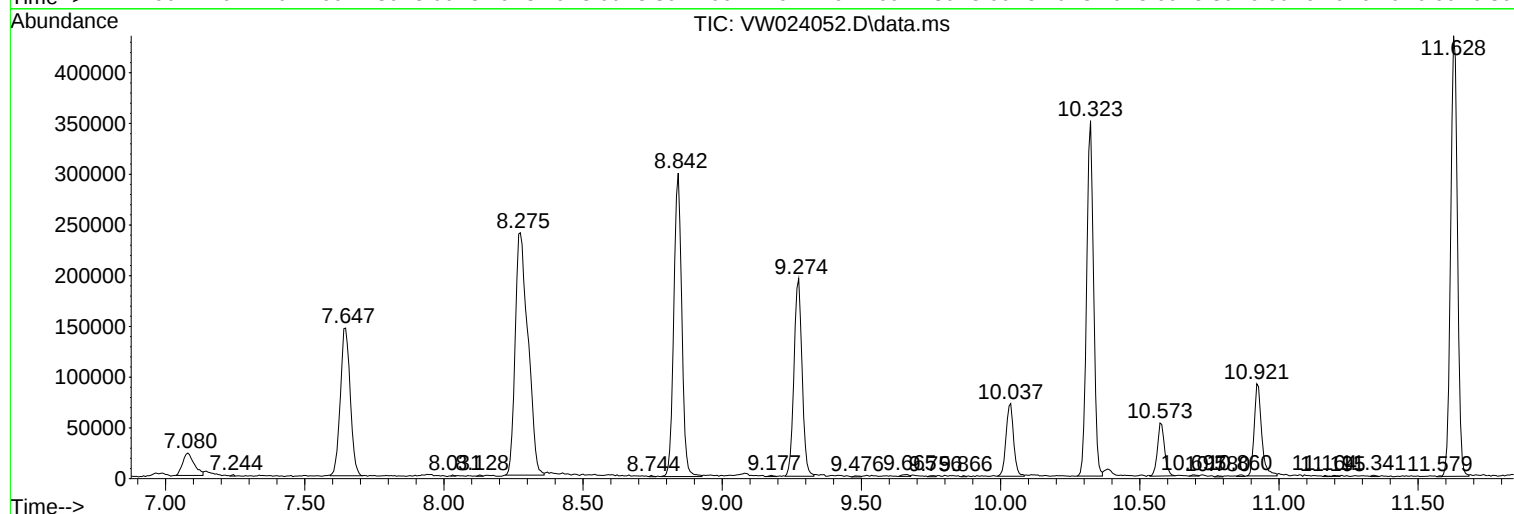
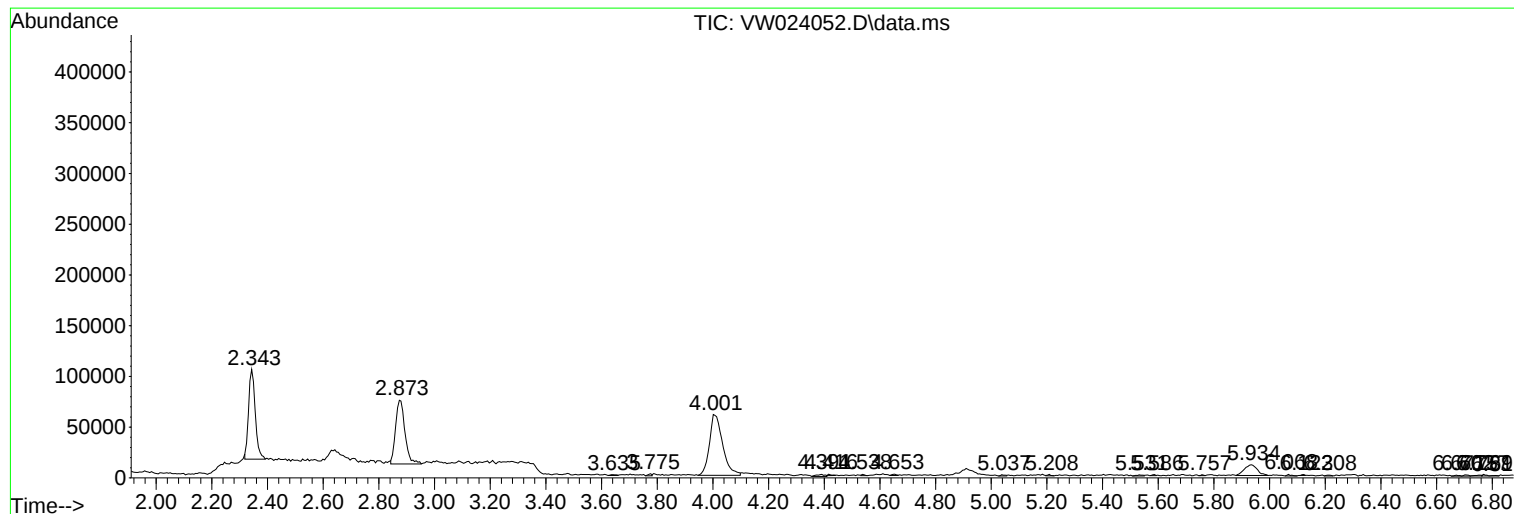
Sum of corrected areas: 5992772

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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



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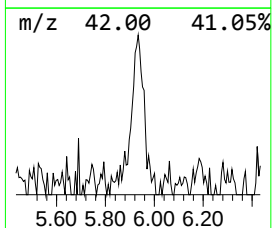
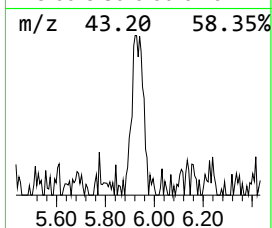
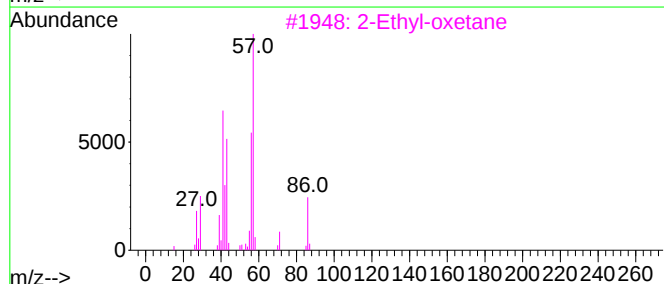
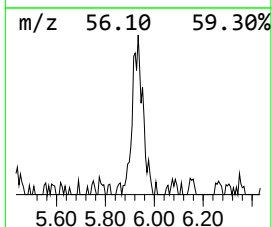
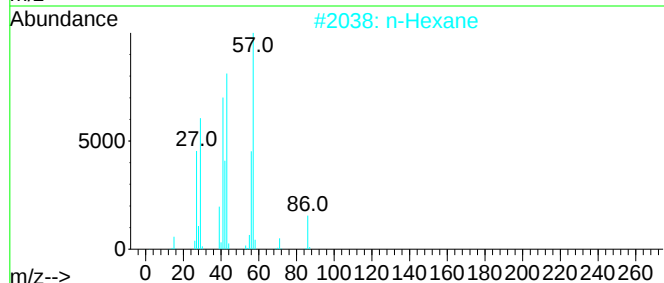
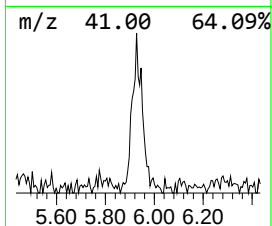
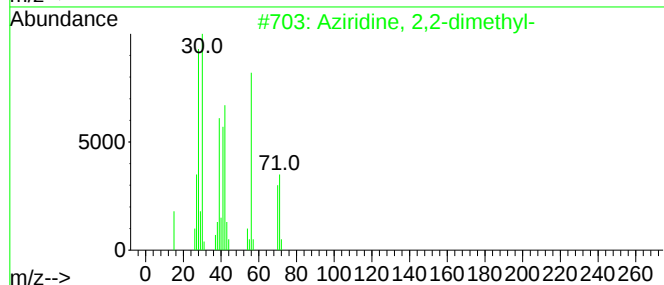
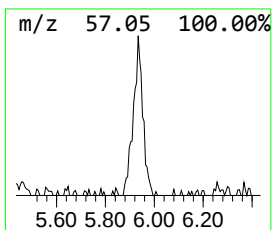
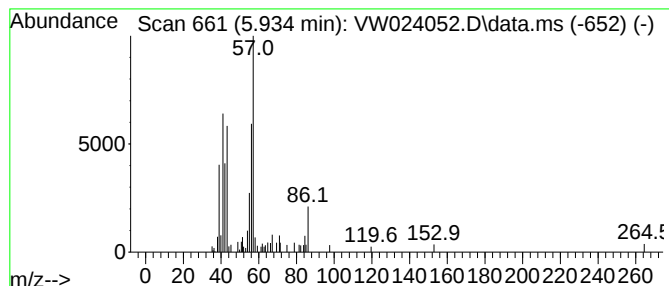
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Aziridine, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.934	1.44 ug/L	34195	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	50
2			n-Hexane	86	C6H14	000110-54-3	47
3			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	47
4			2H-Pyran-2-one, tetrahydro-6,6-d...	128	C7H12O2	002610-95-9	40
5			n-Hexane	86	C6H14	000110-54-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aziridine, 2,2-...	5.934	1.4	ug/L	34195	1	8.842	594694	25.0