

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082622\
 Data File : VW024411.D
 Acq On : 27 Aug 2022 19:24
 Operator : SY/VA
 Sample : N4363-02
 Misc : 5.25g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DBVV7

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\SFAMWLM082622SMA.M

Title : SFAM01.0

Signal : TIC: VW024411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.519	263	265	266	rBV2	1824	1495	0.15%	0.041%
2	4.001	331	344	356	rBV	30107	90064	8.88%	2.490%
3	4.123	361	364	370	rBV7	2758	4406	0.43%	0.122%
4	4.354	400	402	403	rBV2	1495	1045	0.10%	0.029%
5	4.531	428	431	433	rBV4	722	1002	0.10%	0.028%
6	4.586	438	440	443	rBV4	1446	1529	0.15%	0.042%
7	4.903	485	492	504	rVB4	8696	28612	2.82%	0.791%
8	5.031	512	513	515	rBV3	1266	934	0.09%	0.026%
9	5.244	547	548	550	rBV2	1442	970	0.10%	0.027%
10	5.269	550	552	553	rBV2	1056	894	0.09%	0.025%
11	5.391	569	572	575	rVB5	998	1292	0.13%	0.036%
12	5.513	589	592	597	rVB6	1630	3294	0.32%	0.091%
13	5.635	609	612	615	rVV5	1596	2236	0.22%	0.062%
14	5.726	623	627	629	rBV5	1106	1189	0.12%	0.033%
15	6.275	715	717	719	rVB2	1982	1183	0.12%	0.033%
16	6.311	719	723	727	rBV6	1681	2676	0.26%	0.074%
17	6.390	734	736	739	rVB4	1137	929	0.09%	0.026%
18	6.525	756	758	760	rVB3	1456	1370	0.14%	0.038%
19	6.555	760	763	764	rBV2	1297	1503	0.15%	0.042%
20	6.750	792	795	797	rBV4	1541	1831	0.18%	0.051%
21	6.842	808	810	812	rBV3	1306	1341	0.13%	0.037%
22	6.933	823	825	827	rBV3	1419	1367	0.13%	0.038%
23	7.037	840	842	843	rBV2	1529	1541	0.15%	0.043%
24	7.079	843	849	854	rBV2	13579	34576	3.41%	0.956%
25	7.268	878	880	882	rBV2	1328	1453	0.14%	0.040%
26	7.311	885	887	889	rVB3	1572	1247	0.12%	0.034%
27	7.531	922	923	925	rVB2	1725	1214	0.12%	0.034%
28	7.573	925	930	931	rBV5	1683	2815	0.28%	0.078%
29	7.646	934	942	956	rVB2	59106	146652	14.45%	4.055%
30	7.799	963	967	968	rBV5	1121	1339	0.13%	0.037%
31	7.939	986	990	993	rBV6	1773	2764	0.27%	0.076%
32	8.024	1000	1004	1007	rBV6	1145	1485	0.15%	0.041%
33	8.067	1009	1011	1013	rVB3	1380	1008	0.10%	0.028%
34	8.134	1021	1022	1023	rBV	1589	934	0.09%	0.026%
35	8.274	1036	1045	1061	rVV3	99256	334613	32.98%	9.251%
36	8.677	1109	1111	1115	rBV5	1759	2350	0.23%	0.065%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
 Title : SFAM01.0

37	8.841	1130	1138	1148	rBV	100131	204097	20.12%	5.643%
38	9.274	1202	1209	1217	rVB2	77929	163385	16.10%	4.517%
39	9.366	1222	1224	1228	rVB5	1717	1835	0.18%	0.051%
40	9.396	1228	1229	1231	rBV2	1315	1108	0.11%	0.031%
41	9.451	1236	1238	1241	rBV3	1138	1320	0.13%	0.036%
42	9.616	1263	1265	1266	rBV2	1096	1004	0.10%	0.028%
43	9.676	1273	1275	1276	rBV2	1310	890	0.09%	0.025%
44	9.914	1310	1314	1318	rVB7	1541	2777	0.27%	0.077%
45	9.957	1319	1321	1323	rBV	1028	1129	0.11%	0.031%
46	10.036	1325	1334	1343	rBV	36799	75557	7.45%	2.089%
47	10.219	1362	1364	1368	rVB5	1908	2110	0.21%	0.058%
48	10.323	1374	1381	1389	rBV	132506	231302	22.80%	6.395%
49	10.414	1394	1396	1398	rBV3	1144	949	0.09%	0.026%
50	10.579	1415	1423	1430	rBV	28669	51127	5.04%	1.414%
51	10.701	1436	1443	1450	rBV3	9154	18368	1.81%	0.508%
52	10.859	1460	1469	1475	rBV	601172	1014568	100.00%	28.051%
53	10.926	1475	1480	1491	rVB	52367	96837	9.54%	2.677%
54	11.060	1497	1502	1509	rBV2	15147	28065	2.77%	0.776%
55	11.182	1521	1522	1526	rVB4	1501	1195	0.12%	0.033%
56	11.432	1559	1563	1571	rVB10	3303	7408	0.73%	0.205%
57	11.627	1583	1595	1605	rBV	173699	304503	30.01%	8.419%
58	11.804	1623	1624	1626	rBV2	1470	1060	0.10%	0.029%
59	11.896	1637	1639	1643	rVB4	1225	1150	0.11%	0.032%
60	11.957	1644	1649	1653	rVB7	1630	3923	0.39%	0.108%
61	12.048	1661	1664	1667	rVB5	1604	2120	0.21%	0.059%
62	12.164	1679	1683	1684	rBV4	1526	1528	0.15%	0.042%
63	12.377	1717	1718	1721	rBV3	828	920	0.09%	0.025%
64	12.456	1726	1731	1733	rBV6	1840	3124	0.31%	0.086%
65	12.511	1738	1740	1744	rBV5	1120	1280	0.13%	0.035%
66	12.603	1749	1755	1762	rVB3	13522	22116	2.18%	0.611%
67	12.688	1762	1769	1775	rBV	88350	148512	14.64%	4.106%
68	12.816	1788	1790	1793	rVV4	1138	1274	0.13%	0.035%
69	13.005	1819	1821	1823	rBV3	816	1049	0.10%	0.029%
70	13.395	1884	1885	1886	rBV	1760	1038	0.10%	0.029%
71	13.505	1901	1903	1905	rVV3	1398	1218	0.12%	0.034%
72	13.554	1905	1911	1918	rVV	157903	254713	25.11%	7.042%
73	13.846	1953	1959	1967	rVB	129011	219552	21.64%	6.070%
74	13.944	1973	1975	1979	rBV5	1408	1558	0.15%	0.043%
75	14.023	1986	1988	1989	rBV2	1176	1149	0.11%	0.032%
76	14.060	1990	1994	2004	rVB2	8470	16042	1.58%	0.444%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
 Title : SFAM01.0

77	14.157	2006	2010	2012	rVB4	1594	1896	0.19%	0.052%
78	14.194	2012	2016	2020	rVB6	1454	1889	0.19%	0.052%
79	14.237	2020	2023	2025	rBV4	1630	1581	0.16%	0.044%
80	14.322	2034	2037	2038	rBV3	1795	1581	0.16%	0.044%
81	14.487	2061	2064	2065	rBV3	1007	1168	0.12%	0.032%
82	14.621	2084	2086	2089	rVB4	1295	982	0.10%	0.027%
83	14.712	2097	2101	2105	rBV7	2169	3811	0.38%	0.105%
84	14.834	2120	2121	2124	rBV3	1173	1196	0.12%	0.033%
85	15.011	2148	2150	2153	rVB4	901	908	0.09%	0.025%
86	15.096	2162	2164	2166	rBV3	1098	1293	0.13%	0.036%
87	15.224	2181	2185	2188	rBV5	1318	1893	0.19%	0.052%
88	15.279	2192	2194	2198	rVB4	1619	1747	0.17%	0.048%
89	15.334	2201	2203	2204	rBV2	1059	1128	0.11%	0.031%
90	15.425	2213	2218	2222	rBV6	4232	5954	0.59%	0.165%
91	15.493	2227	2229	2232	rVB4	1588	1523	0.15%	0.042%
92	15.535	2232	2236	2237	rBV3	1213	1836	0.18%	0.051%
93	15.669	2256	2258	2260	rBV3	1464	1008	0.10%	0.028%
94	16.151	2335	2337	2338	rBV2	1078	1066	0.11%	0.029%
95	16.303	2360	2362	2365	rBV4	905	876	0.09%	0.024%
96	16.346	2367	2369	2371	rBV3	1137	918	0.09%	0.025%
97	16.584	2407	2408	2411	rBV3	1373	1114	0.11%	0.031%
98	16.639	2415	2417	2419	rBV3	1198	947	0.09%	0.026%
99	16.675	2421	2423	2425	rBV3	1069	1290	0.13%	0.036%
100	16.724	2430	2431	2433	rBV2	1782	1291	0.13%	0.036%

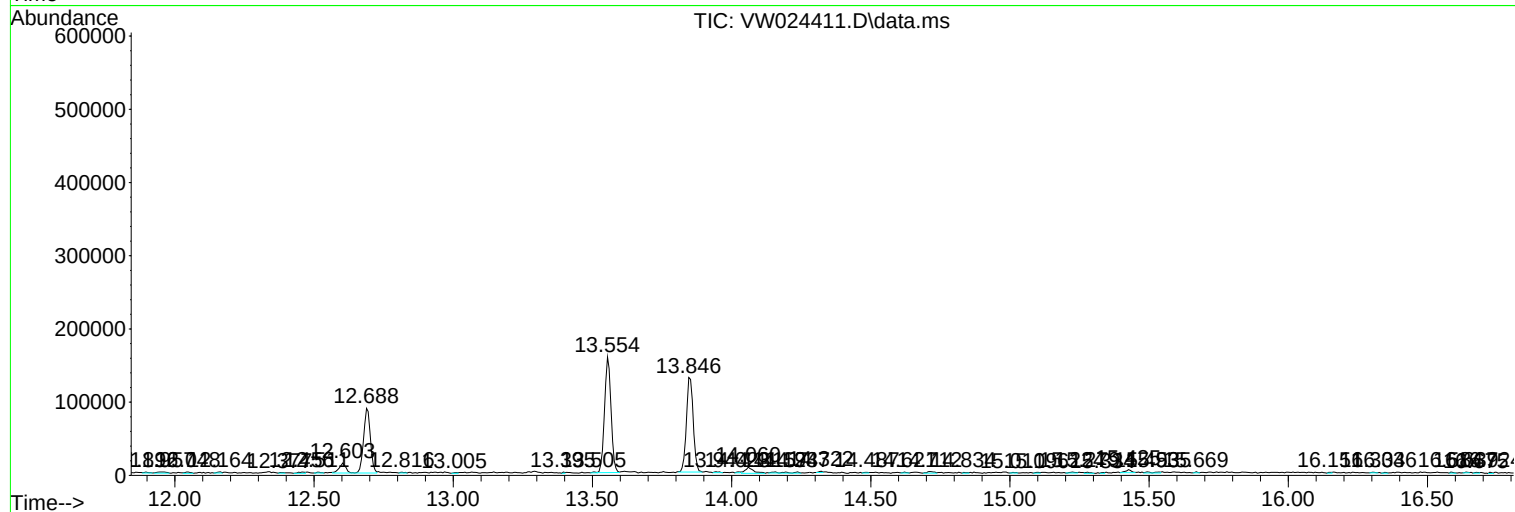
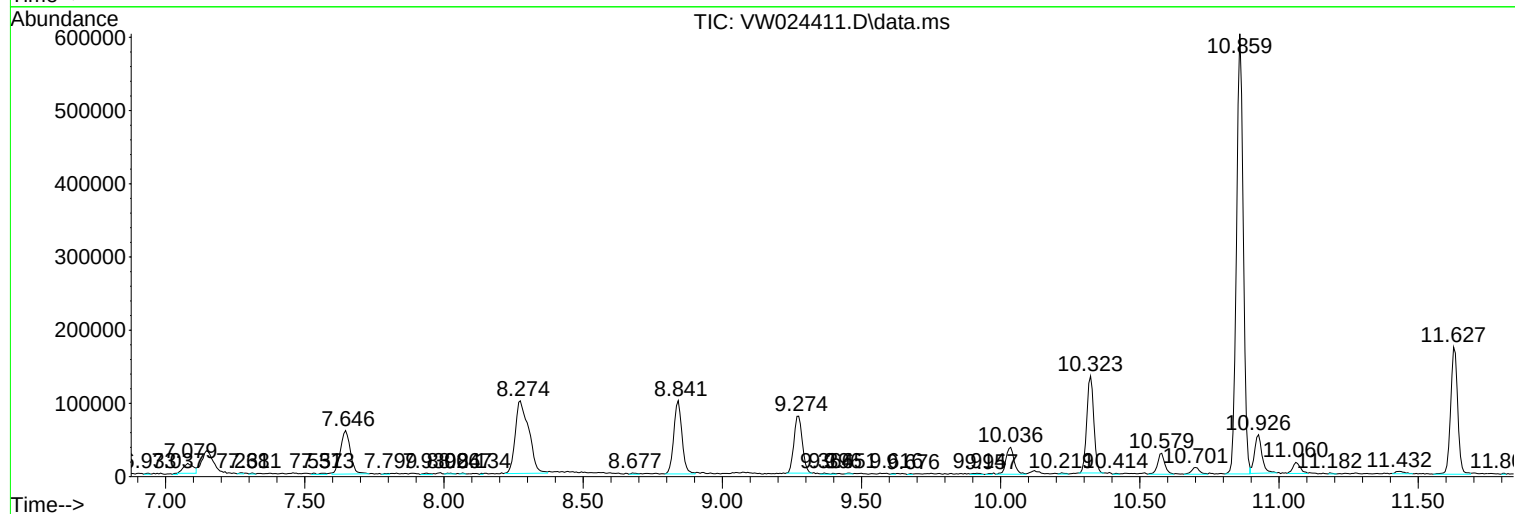
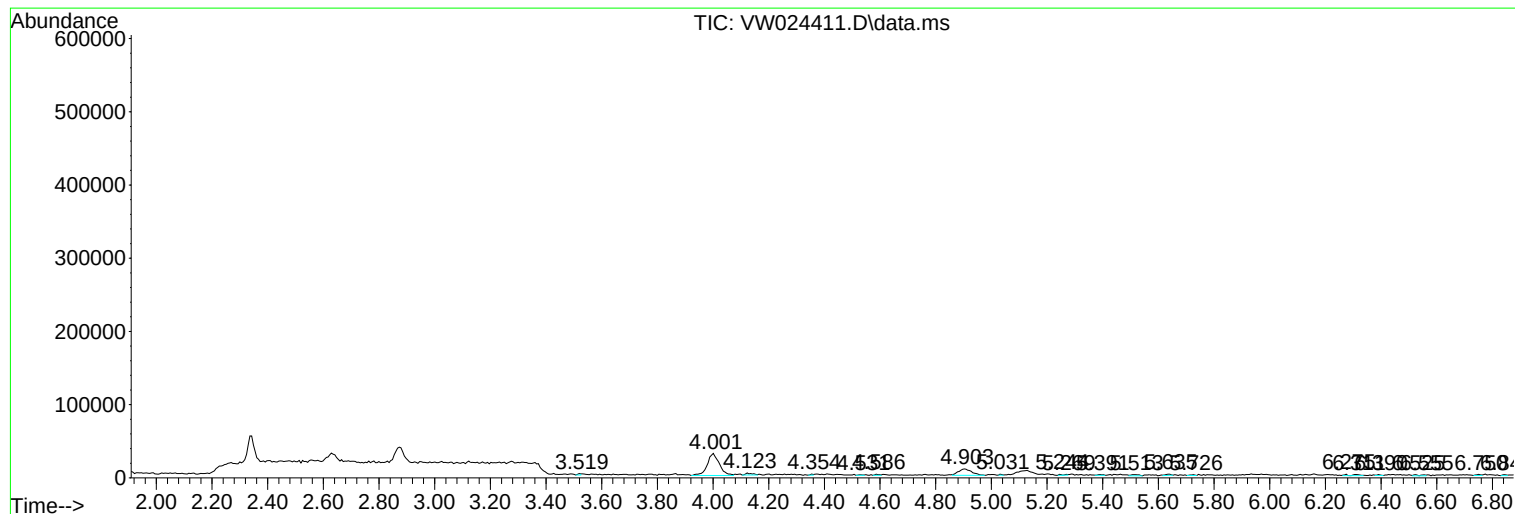
Sum of corrected areas: 3616909

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

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



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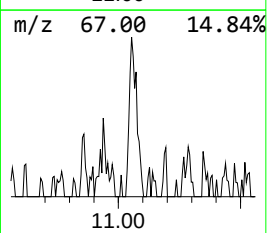
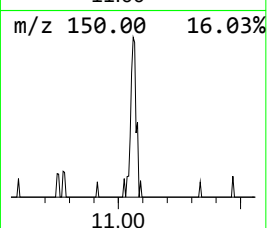
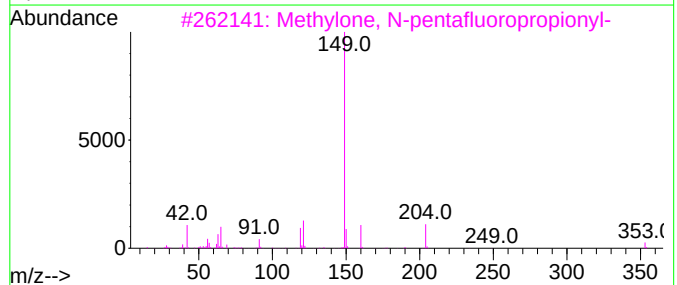
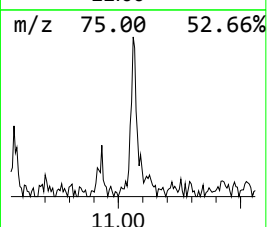
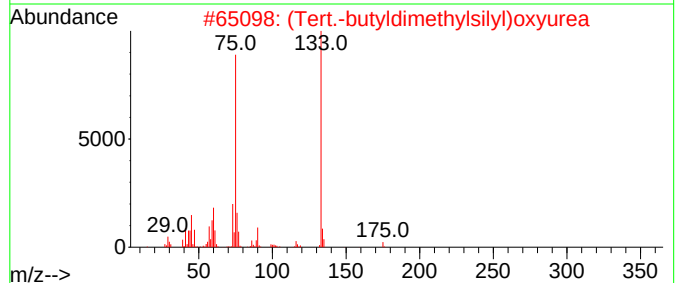
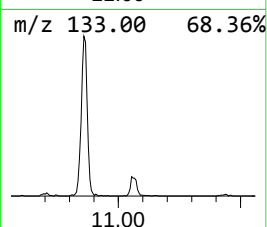
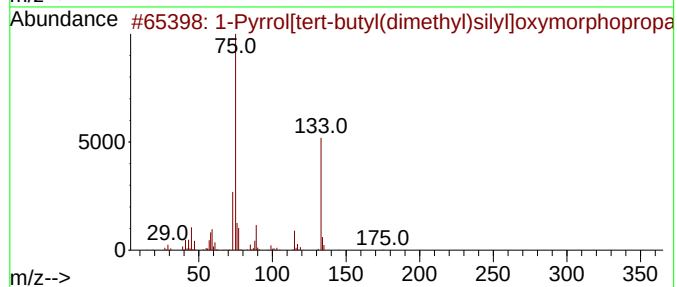
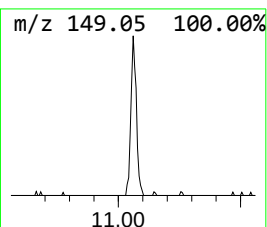
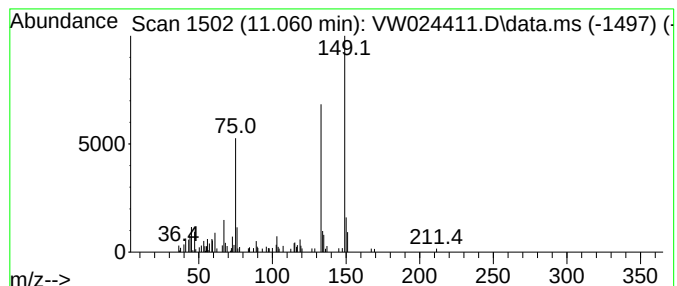
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.060	2.30 ug/L	28065	Chlorobenzene-d5	11.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pyrrol[tert-butyl(dimethyl)sil...	190	C9H22O2Si	1000333-03-5	32		
2	(Tert.-butyldimethylsilyl)oxyurea	190	C7H18N2O2Si	1000453-67-1	32		
3	Methylone, N-pentafluoropropionyl-	353	C14H12F5NO4	1000448-29-0	27		
4	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	27		
5	Benzenemethanol, 4-(1,1-dimethyl...	164	C11H16O	000877-65-6	27		



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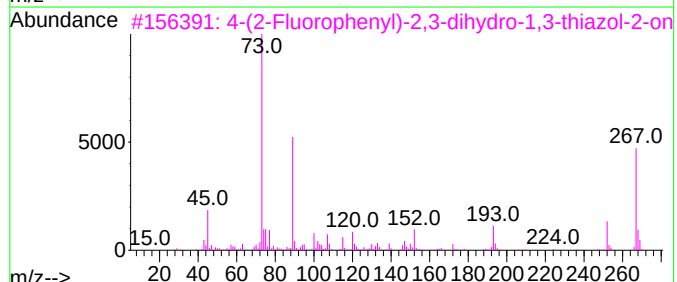
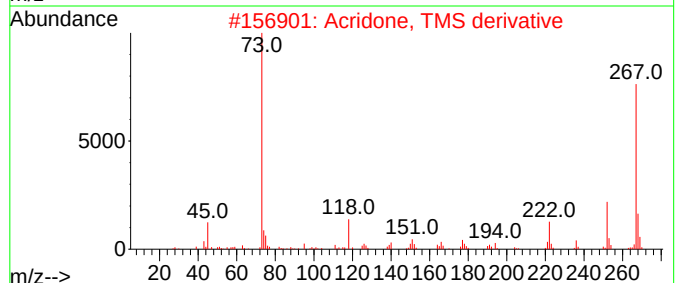
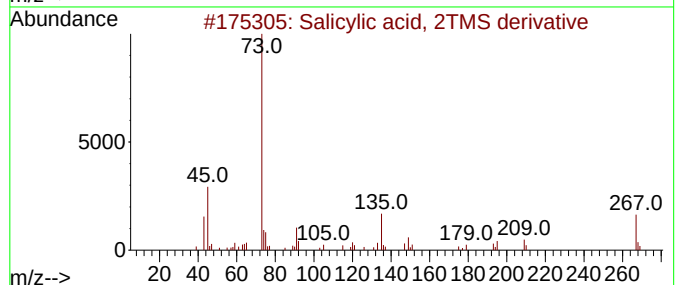
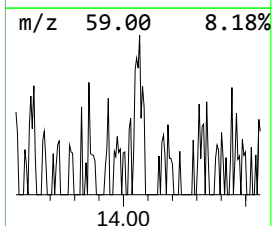
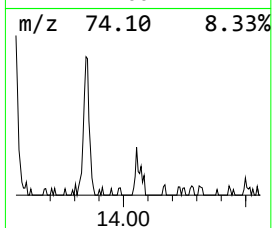
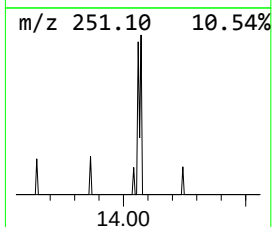
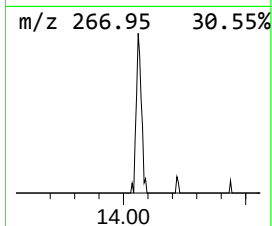
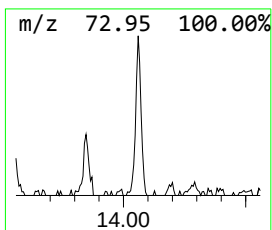
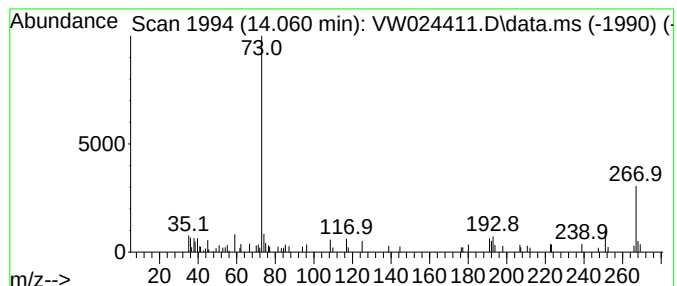
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 Salicylic acid, 2TMS deriva... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.060	1.57 ug/L	16042	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	50
2			Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	40
3			4-(2-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSi	1000504-37-6	38
4			6-Ethoxybenzo[d]thiazol-2-amine,...	266	C12H18N2OSSi	1000488-43-0	25
5			(1E)-N-(3-Chlorophenyl)-2-cyano...	266	C12H15ClN2OSi	1000487-54-5	17



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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	11.060	2.3	ug/L	28065	2	11.627	304503	25.0
Salicylic acid,...	14.060	1.6	ug/L	16042	3	13.554	254713	25.0