

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW020323\
 Data File : VW025273.D
 Acq On : 03 Feb 2023 12:53
 Operator : SY/MD
 Sample : 01394-04
 Misc : 3.75g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 C1152

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\SFAMWLM020323SMA.M
 Title : SFAM01.0

Signal : TIC: VW025273.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.898	156	163	178	rBV	36992	103589	10.25%	1.751%
2	3.477	256	258	259	rBV2	308	243	0.02%	0.004%
3	3.520	264	265	267	rBV2	346	273	0.03%	0.005%
4	3.672	288	290	295	rVB	286	303	0.03%	0.005%
5	3.715	295	297	298	rBV	332	198	0.02%	0.003%
6	4.026	338	348	359	rBV	104153	283835	28.07%	4.799%
7	4.379	398	406	408	rBV3	2097	4141	0.41%	0.070%
8	4.605	438	443	444	rBV2	2034	2888	0.29%	0.049%
9	4.800	474	475	478	rBV	420	287	0.03%	0.005%
10	4.916	484	494	506	rBV2	27445	88712	8.77%	1.500%
11	5.105	524	525	526	rBV	281	151	0.01%	0.003%
12	5.361	566	567	571	rVB2	356	356	0.04%	0.006%
13	5.397	571	573	574	rBV2	297	240	0.02%	0.004%
14	5.446	579	581	583	rVV	316	209	0.02%	0.004%
15	5.464	583	584	587	rVV2	215	206	0.02%	0.003%
16	5.519	591	593	595	rVB2	335	249	0.02%	0.004%
17	5.544	595	597	601	rBV	293	413	0.04%	0.007%
18	5.574	601	602	605	rVB	438	283	0.03%	0.005%
19	5.605	605	607	609	rBV2	288	293	0.03%	0.005%
20	5.952	654	664	672	rBV5	2776	8810	0.87%	0.149%
21	6.135	692	694	697	rBV2	277	336	0.03%	0.006%
22	6.592	767	769	772	rVB2	278	181	0.02%	0.003%
23	6.946	825	827	828	rBV	209	145	0.01%	0.002%
24	7.080	839	849	854	rBV2	25361	76341	7.55%	1.291%
25	7.409	901	903	905	rVB	233	147	0.01%	0.002%
26	7.433	905	907	910	rBV2	302	273	0.03%	0.005%
27	7.488	915	916	920	rBV2	377	337	0.03%	0.006%
28	7.653	932	943	955	rBV	215559	534408	52.86%	9.035%
29	7.952	989	992	994	rBV2	317	282	0.03%	0.005%
30	7.970	994	995	998	rVV2	220	218	0.02%	0.004%
31	8.086	1010	1014	1016	rBV3	223	318	0.03%	0.005%
32	8.275	1034	1045	1062	rBV2	323360	1011067	100.00%	17.093%
33	8.427	1068	1070	1074	rBV	282	322	0.03%	0.005%
34	8.513	1082	1084	1088	rBV2	167	181	0.02%	0.003%
35	8.567	1091	1093	1095	rBV	266	343	0.03%	0.006%
36	8.842	1129	1138	1149	rBV	349247	697364	68.97%	11.790%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM020323SMA.M
 Title : SFAM01.0

37	9.025	1164	1168	1172	rBV3	543	1095	0.11%	0.019%
38	9.086	1172	1178	1183	rVV8	2412	4738	0.47%	0.080%
39	9.275	1199	1209	1227	rBV	305639	614417	60.77%	10.388%
40	9.604	1260	1263	1266	rBV3	449	665	0.07%	0.011%
41	9.726	1281	1283	1285	rBV2	255	219	0.02%	0.004%
42	9.799	1292	1295	1296	rBV	350	290	0.03%	0.005%
43	9.921	1313	1315	1319	rVB2	264	267	0.03%	0.005%
44	9.976	1322	1324	1326	rBV2	229	230	0.02%	0.004%
45	10.037	1326	1334	1344	rBV	110293	203116	20.09%	3.434%
46	10.177	1355	1357	1358	rBV	247	189	0.02%	0.003%
47	10.207	1359	1362	1369	rVB4	652	1056	0.10%	0.018%
48	10.323	1373	1381	1389	rBV	371091	652686	64.55%	11.034%
49	10.451	1397	1402	1414	rBV	5947	13007	1.29%	0.220%
50	10.579	1416	1423	1432	rVB	62486	108514	10.73%	1.835%
51	10.701	1438	1443	1449	rVB2	11033	20188	2.00%	0.341%
52	10.866	1467	1470	1473	rVB3	846	927	0.09%	0.016%
53	10.921	1473	1479	1491	rBV	67554	127005	12.56%	2.147%
54	11.061	1497	1502	1511	rVB	16249	27856	2.76%	0.471%
55	11.152	1515	1517	1518	rBV	311	173	0.02%	0.003%
56	11.347	1546	1549	1551	rBV2	237	320	0.03%	0.005%
57	11.396	1555	1557	1558	rBV2	218	148	0.01%	0.003%
58	11.433	1558	1563	1572	rVB3	3958	6695	0.66%	0.113%
59	11.628	1588	1595	1605	rBV	326705	553702	54.76%	9.361%
60	11.725	1609	1611	1617	rVB4	678	1072	0.11%	0.018%
61	11.805	1622	1624	1625	rBV	268	148	0.01%	0.003%
62	12.012	1657	1658	1662	rBV2	310	326	0.03%	0.006%
63	12.170	1680	1684	1686	rVV3	720	970	0.10%	0.016%
64	12.347	1710	1713	1714	rBV	210	155	0.02%	0.003%
65	12.414	1723	1724	1726	rBV	307	177	0.02%	0.003%
66	12.457	1728	1731	1735	rBV2	383	637	0.06%	0.011%
67	12.524	1740	1742	1744	rVB2	238	181	0.02%	0.003%
68	12.554	1744	1747	1750	rBV2	313	481	0.05%	0.008%
69	12.603	1750	1755	1762	rVB2	10265	16821	1.66%	0.284%
70	12.689	1762	1769	1777	rBV	210232	341582	33.78%	5.775%
71	12.932	1804	1809	1815	rVB5	2150	3422	0.34%	0.058%
72	12.981	1815	1817	1821	rBV2	346	485	0.05%	0.008%
73	13.134	1840	1842	1845	rBV2	156	209	0.02%	0.004%
74	13.182	1848	1850	1851	rBV	246	188	0.02%	0.003%
75	13.359	1875	1879	1881	rBV2	187	254	0.03%	0.004%
76	13.377	1881	1882	1884	rBV	380	210	0.02%	0.004%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM020323SMA.M
 Title : SFAM01.0

77	13.420	1886	1889	1890	rBV	154	173	0.02%	0.003%
78	13.506	1897	1903	1904	rBV2	704	1111	0.11%	0.019%
79	13.554	1905	1911	1923	rVB	127763	210344	20.80%	3.556%
80	13.640	1923	1925	1929	rBV4	591	696	0.07%	0.012%
81	13.755	1942	1944	1948	rVB	271	260	0.03%	0.004%
82	13.847	1952	1959	1969	rBV	81034	139810	13.83%	2.364%
83	13.957	1975	1977	1980	rVB2	271	175	0.02%	0.003%
84	14.066	1987	1995	2000	rBV2	5287	8823	0.87%	0.149%
85	14.121	2002	2004	2005	rBV2	439	297	0.03%	0.005%
86	14.188	2011	2015	2016	rBV2	363	530	0.05%	0.009%
87	14.237	2019	2023	2026	rBV3	230	376	0.04%	0.006%
88	14.316	2029	2036	2041	rBV6	1907	3756	0.37%	0.063%
89	14.481	2060	2063	2064	rBV2	296	219	0.02%	0.004%
90	14.518	2067	2069	2072	rVB	431	281	0.03%	0.005%
91	14.548	2072	2074	2076	rBV2	207	208	0.02%	0.004%
92	14.621	2083	2086	2092	rBV5	1292	1680	0.17%	0.028%
93	14.725	2099	2103	2105	rBV3	1739	2199	0.22%	0.037%
94	14.749	2105	2107	2111	rVV2	420	467	0.05%	0.008%
95	14.792	2112	2114	2117	rVB	396	299	0.03%	0.005%
96	15.127	2166	2169	2175	rVB5	1798	2846	0.28%	0.048%
97	15.426	2214	2218	2223	rVB2	8860	12303	1.22%	0.208%
98	15.548	2234	2238	2241	rVB5	1876	2971	0.29%	0.050%
99	15.755	2268	2272	2275	rBV4	1019	1912	0.19%	0.032%
100	16.731	2430	2432	2434	rVB3	688	463	0.05%	0.008%

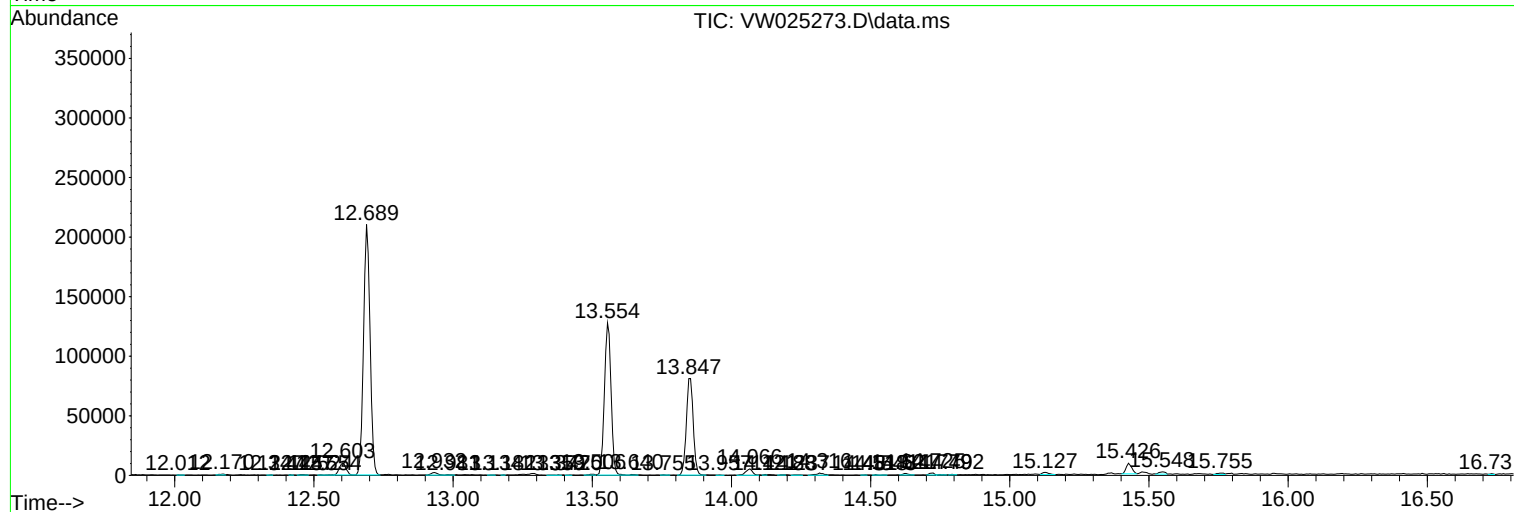
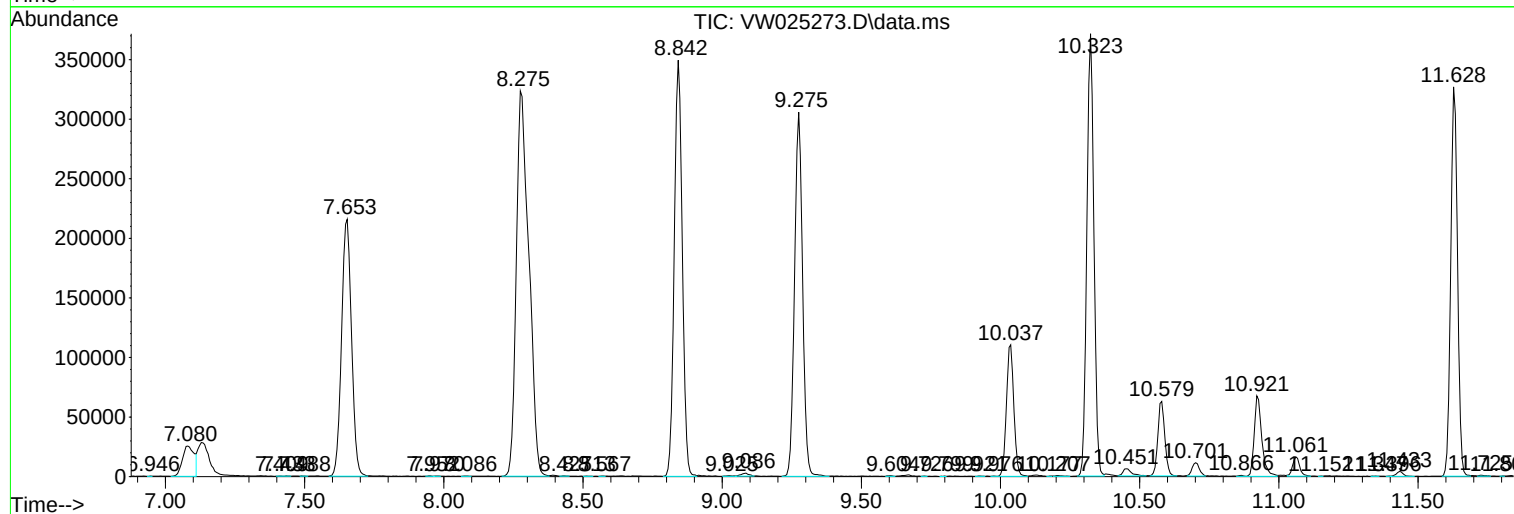
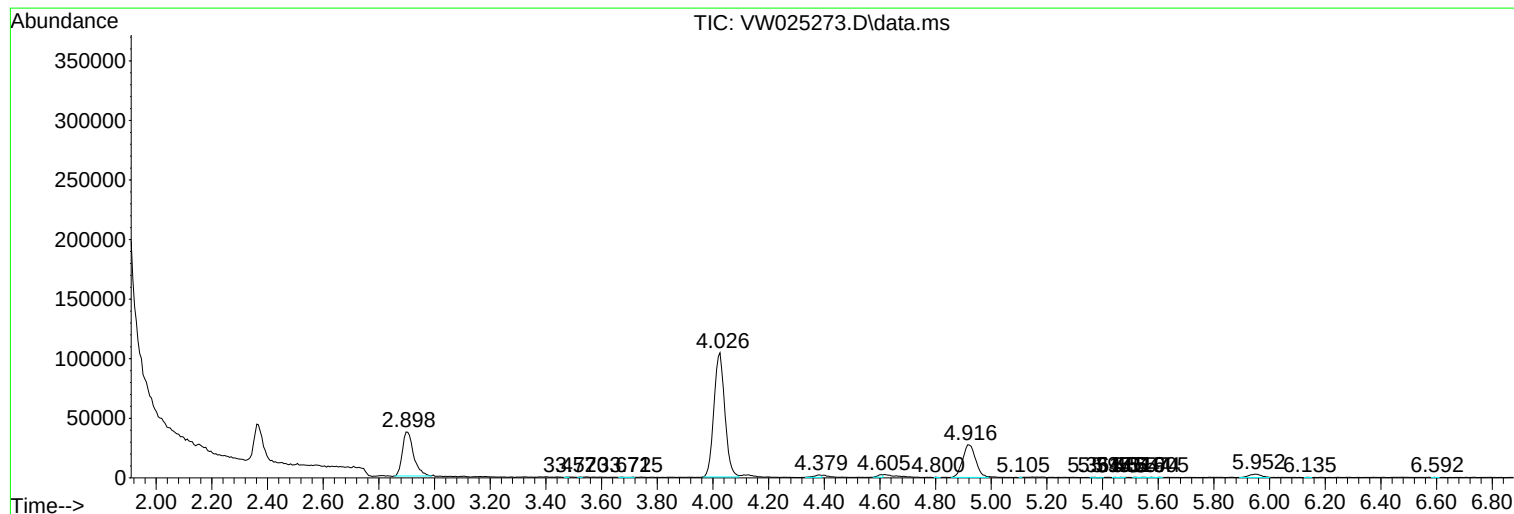
Sum of corrected areas: 5914962

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM020323SMA.M
Quant Title : SFAM01.0

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



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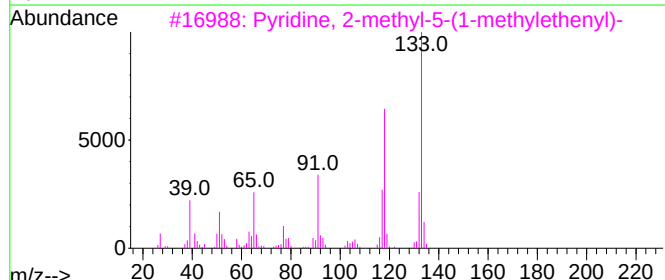
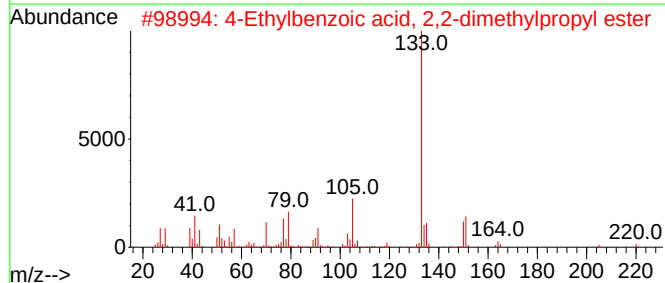
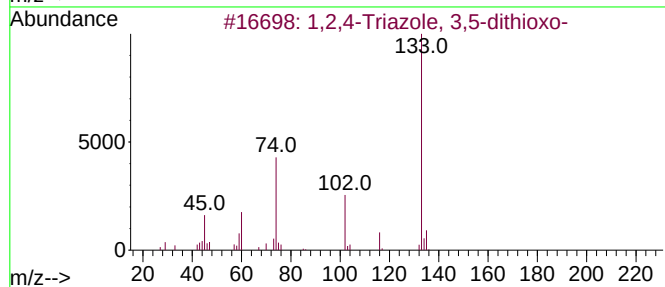
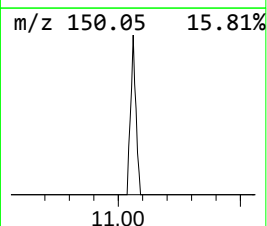
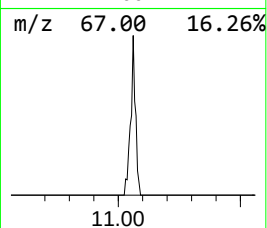
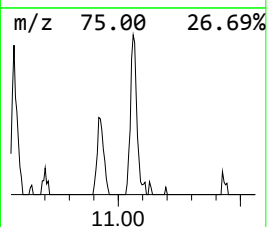
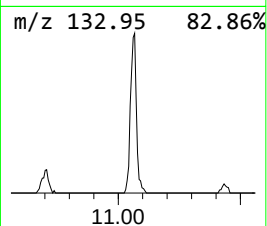
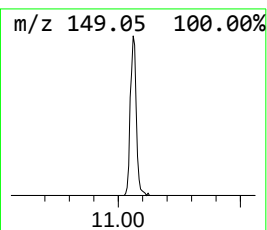
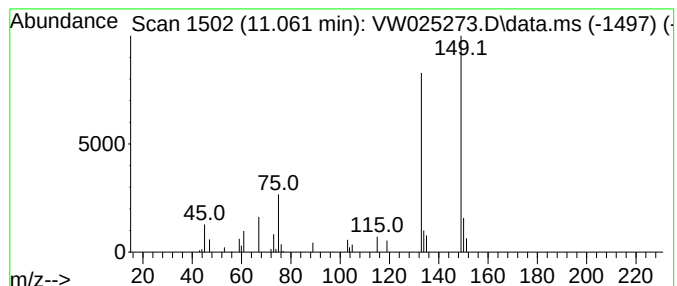
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM020323SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.061	1.26 ug/L	27856	Chlorobenzene-d5	11.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	27
2			4-Ethylbenzoic acid, 2,2-dimethy...	220	C14H20O2	1000293-49-5	17
3			Pyridine, 2-methyl-5-(1-methylet...	133	C9H11N	056057-93-3	16
4			1,2-Benzisothiazole, 3-methyl-	149	C8H7NS	006187-89-9	16
5			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	12



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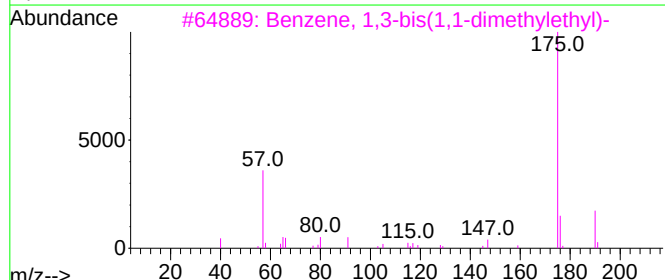
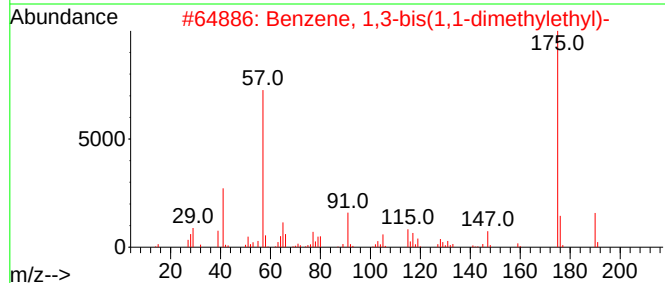
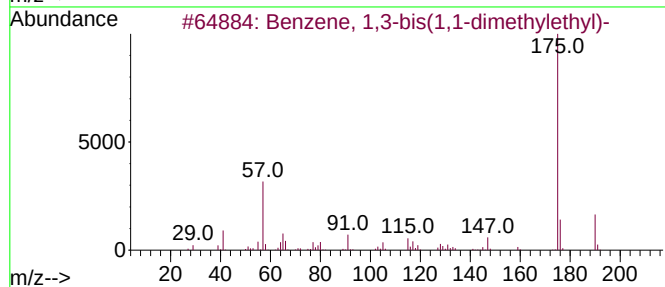
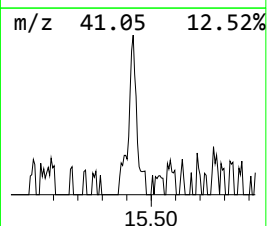
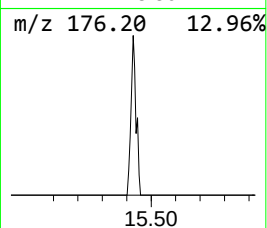
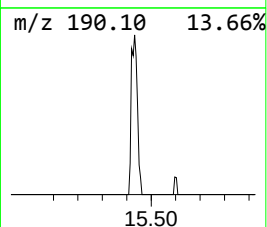
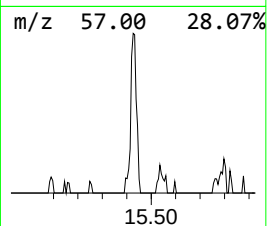
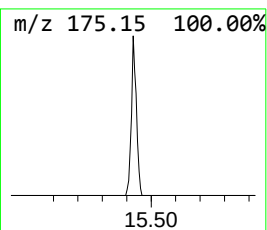
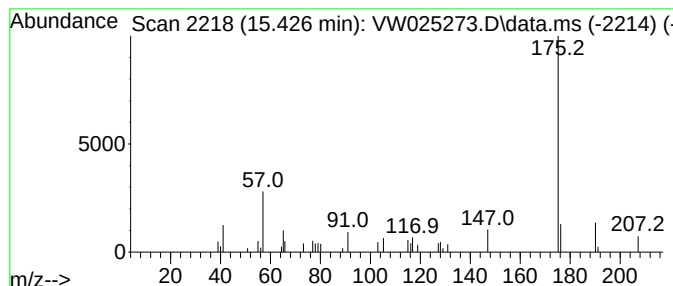
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM020323SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Benzene, 1,3-bis(1,1-dimeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.426	1.46 ug/L	12303	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	90
2			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	83
3			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	81
4			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	74
5			Benzenepropanal, 4-(1,1-dimethyl...	190	C13H18O	018127-01-0	72



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Quant Title : SFAM01.0

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	11.061	1.3	ug/L	27856	2	11.628	553702	25.0
Benzene, 1,3-bi...	15.426	1.5	ug/L	12303	3	13.554	210344	25.0