

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091223\
 Data File : VW027069.D
 Acq On : 12 Sep 2023 15:29
 Operator : SY/MD
 Sample : 04387-14RE
 Misc : 3.56g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 C0AH1RE

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\SFAMWLM090523SMA.M
 Title : SFAM01.0

Signal : TIC: VW027069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	73	78	90	rVB	61008	160487	9.57%	1.469%
2	3.521	267	268	270	rBV2	3537	3177	0.19%	0.029%
3	3.655	289	290	293	rBV3	2104	1301	0.08%	0.012%
4	4.021	338	350	363	rBV2	121943	445680	26.57%	4.081%
5	4.387	404	410	418	rBV3	8280	21554	1.28%	0.197%
6	4.594	441	444	448	rBV5	3633	5413	0.32%	0.050%
7	4.795	472	477	481	rBV8	2216	5005	0.30%	0.046%
8	4.850	485	486	487	rBV	1237	688	0.04%	0.006%
9	4.923	489	498	512	rVV3	23041	95480	5.69%	0.874%
10	5.301	558	560	562	rVB3	1511	1456	0.09%	0.013%
11	5.374	570	572	574	rBV3	1196	1326	0.08%	0.012%
12	5.429	579	581	582	rVV2	1443	755	0.05%	0.007%
13	5.448	582	584	586	rVV4	1333	818	0.05%	0.007%
14	5.478	588	589	591	rBV2	1711	1321	0.08%	0.012%
15	5.612	610	611	613	rBV2	1065	804	0.05%	0.007%
16	5.807	641	643	645	rBV3	1092	896	0.05%	0.008%
17	5.935	655	664	675	rBV7	8661	30274	1.80%	0.277%
18	6.082	686	688	690	rVB3	1964	1819	0.11%	0.017%
19	6.118	690	694	695	rBV4	1807	1451	0.09%	0.013%
20	6.295	720	723	725	rBV3	1196	1276	0.08%	0.012%
21	6.356	731	733	736	rBV4	2215	2305	0.14%	0.021%
22	6.380	736	737	739	rVV2	1272	965	0.06%	0.009%
23	6.447	743	748	749	rBV5	903	1407	0.08%	0.013%
24	6.508	756	758	760	rBV3	1946	1870	0.11%	0.017%
25	6.575	766	769	770	rBV3	2046	2035	0.12%	0.019%
26	6.594	770	772	773	rVV2	1436	1294	0.08%	0.012%
27	6.630	776	778	779	rBV2	1022	595	0.04%	0.005%
28	6.691	786	788	790	rVB3	1393	988	0.06%	0.009%
29	6.740	790	796	799	rBV8	2155	4233	0.25%	0.039%
30	6.813	806	808	809	rVB2	884	598	0.04%	0.005%
31	6.832	809	811	813	rBV3	1138	1026	0.06%	0.009%
32	6.862	813	816	818	rBV5	1457	1600	0.10%	0.015%
33	6.886	818	820	822	rVB3	1566	1358	0.08%	0.012%
34	6.911	822	824	825	rBV2	2394	1821	0.11%	0.017%
35	7.136	846	861	875	rBV	143081	446165	26.59%	4.085%
36	7.356	895	897	899	rVB3	2224	1715	0.10%	0.016%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM090523SMA.M
 Title : SFAM01.0

37	7.648	935	945	955	rVB	351448	873128	52.04%	7.994%
38	7.746	959	961	963	rBV3	2025	1409	0.08%	0.013%
39	7.886	982	984	985	rBV2	1796	908	0.05%	0.008%
40	7.996	1000	1002	1004	rVB3	2202	1384	0.08%	0.013%
41	8.045	1008	1010	1011	rBV2	1455	1150	0.07%	0.011%
42	8.100	1016	1019	1021	rBV4	1237	1403	0.08%	0.013%
43	8.276	1035	1048	1064	rBV2	514772	1677657	100.00%	15.360%
44	8.569	1093	1096	1098	rBV4	1540	1662	0.10%	0.015%
45	8.776	1126	1130	1131	rBV4	1407	1569	0.09%	0.014%
46	8.843	1132	1141	1153	rBV	793276	1558038	92.87%	14.265%
47	9.166	1192	1194	1197	rVB3	2859	2366	0.14%	0.022%
48	9.270	1204	1211	1221	rBV	449441	925338	55.16%	8.472%
49	9.727	1284	1286	1288	rVB3	2045	1365	0.08%	0.012%
50	9.929	1318	1319	1322	rBV3	1608	1136	0.07%	0.010%
51	10.032	1331	1336	1346	rVB	37705	72822	4.34%	0.667%
52	10.203	1362	1364	1367	rBV4	2909	2672	0.16%	0.024%
53	10.325	1376	1384	1393	rBV	532477	953836	56.86%	8.733%
54	10.581	1420	1426	1434	rVB2	28521	52852	3.15%	0.484%
55	10.703	1441	1446	1453	rVB2	28870	57809	3.45%	0.529%
56	10.928	1478	1483	1493	rBV2	7873	17069	1.02%	0.156%
57	11.020	1497	1498	1499	rBV	1063	643	0.04%	0.006%
58	11.062	1501	1505	1509	rVV2	12593	18598	1.11%	0.170%
59	11.233	1531	1533	1536	rBV4	1171	1461	0.09%	0.013%
60	11.434	1562	1566	1573	rVB2	12183	22694	1.35%	0.208%
61	11.489	1573	1575	1576	rBV2	1490	1002	0.06%	0.009%
62	11.544	1582	1584	1586	rBV3	1269	1174	0.07%	0.011%
63	11.629	1590	1598	1609	rVV	807718	1360618	81.10%	12.457%
64	11.733	1613	1615	1617	rBV3	2382	2114	0.13%	0.019%
65	11.831	1629	1631	1632	rBV2	2713	1755	0.10%	0.016%
66	12.050	1665	1667	1668	rBV2	1550	964	0.06%	0.009%
67	12.123	1677	1679	1682	rVB4	1578	1560	0.09%	0.014%
68	12.154	1682	1684	1685	rBV2	1435	1309	0.08%	0.012%
69	12.233	1695	1697	1699	rBV3	1154	1002	0.06%	0.009%
70	12.373	1719	1720	1724	rVB4	1853	1859	0.11%	0.017%
71	12.410	1724	1726	1728	rVB3	1785	1749	0.10%	0.016%
72	12.465	1728	1735	1741	rBV10	7190	14428	0.86%	0.132%
73	12.550	1748	1749	1751	rBV2	1686	1279	0.08%	0.012%
74	12.605	1751	1758	1765	rVV2	54762	92772	5.53%	0.849%
75	12.690	1765	1772	1781	rVV	313652	502966	29.98%	4.605%
76	12.843	1794	1797	1799	rBV4	2085	2497	0.15%	0.023%

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 Title : SFAM01.0

77	12.922	1808	1810	1815	rVB6	3671	4840	0.29%	0.044%
78	13.147	1846	1847	1849	rBV2	1111	1078	0.06%	0.010%
79	13.196	1852	1855	1857	rBV4	2225	2840	0.17%	0.026%
80	13.288	1866	1870	1878	rVB9	5826	11837	0.71%	0.108%
81	13.397	1885	1888	1894	rVB7	3988	6969	0.42%	0.064%
82	13.471	1895	1900	1901	rBV5	4470	6044	0.36%	0.055%
83	13.556	1908	1914	1926	rVB	469658	748186	44.60%	6.850%
84	13.849	1956	1962	1968	rBV	291954	491000	29.27%	4.495%
85	14.068	1993	1998	2007	rVB2	21417	41915	2.50%	0.384%
86	14.141	2007	2010	2012	rBV4	1665	1606	0.10%	0.015%
87	14.233	2022	2025	2027	rBV4	1554	2271	0.14%	0.021%
88	14.324	2033	2040	2044	rBV9	4766	11657	0.69%	0.107%
89	14.623	2084	2089	2092	rBV7	2136	3841	0.23%	0.035%
90	14.714	2101	2104	2107	rVV4	7216	9672	0.58%	0.089%
91	14.775	2111	2114	2117	rVB5	2152	3194	0.19%	0.029%
92	15.025	2153	2155	2157	rBV3	1630	1674	0.10%	0.015%
93	15.196	2181	2183	2186	rVB3	2469	1661	0.10%	0.015%
94	15.336	2203	2206	2207	rBV3	3285	3178	0.19%	0.029%
95	15.428	2216	2221	2226	rBV2	46146	76406	4.55%	0.700%
96	16.171	2341	2343	2344	rBV2	2169	1250	0.07%	0.011%
97	16.403	2379	2381	2384	rBV4	1817	2057	0.12%	0.019%

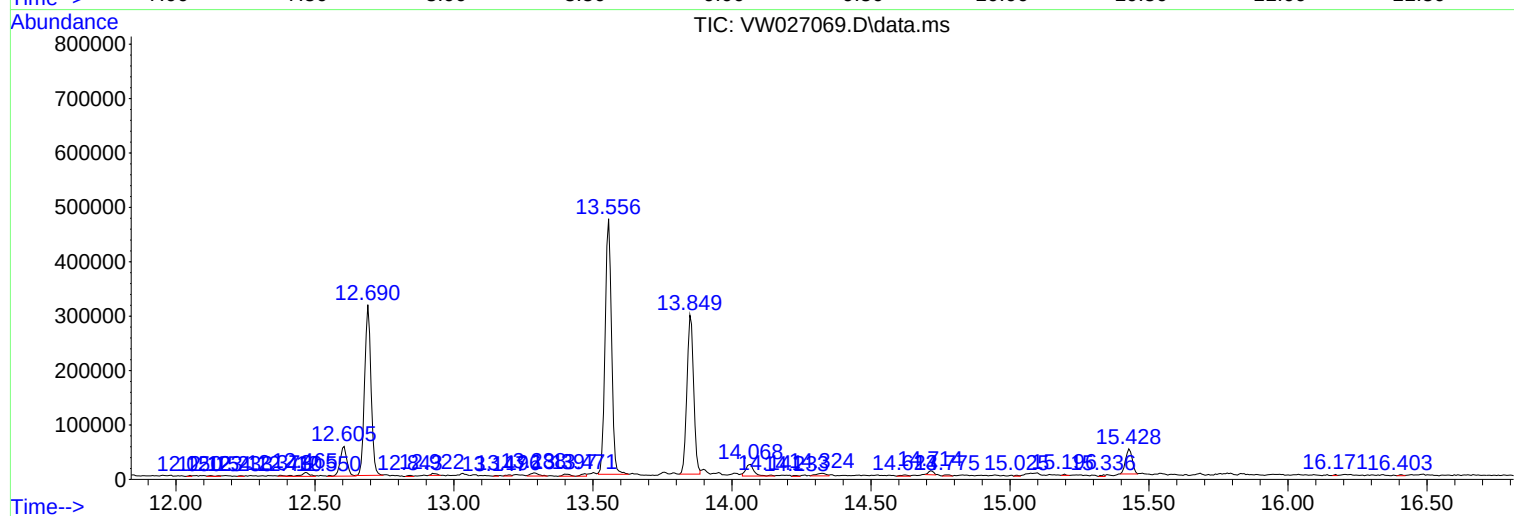
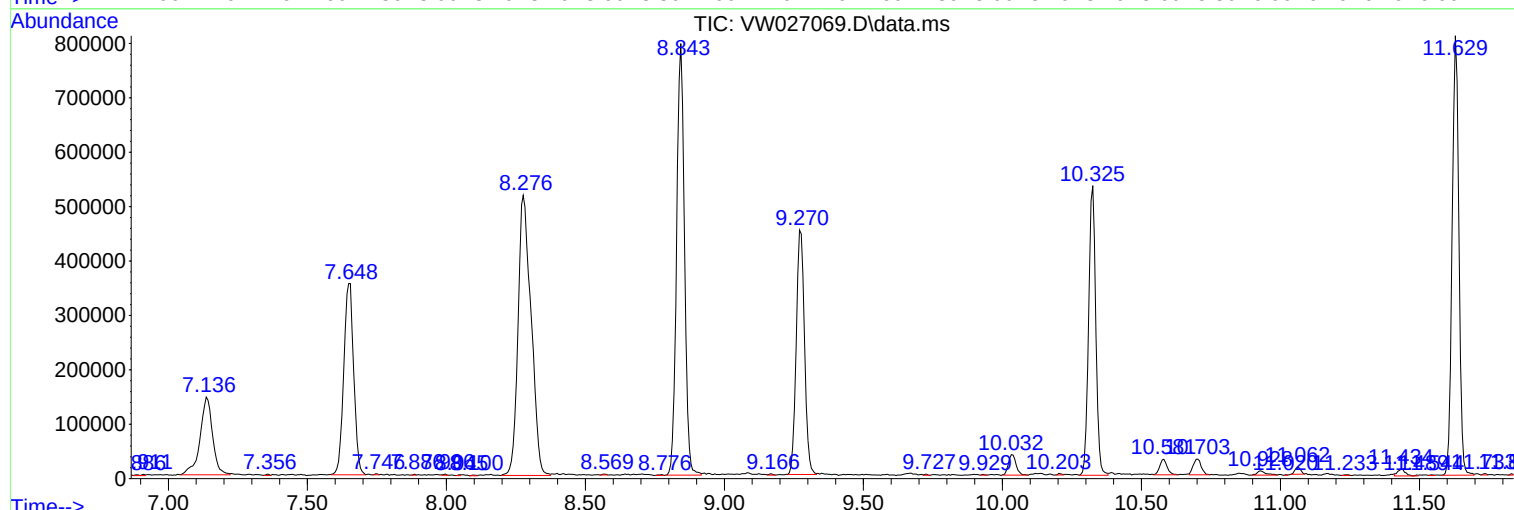
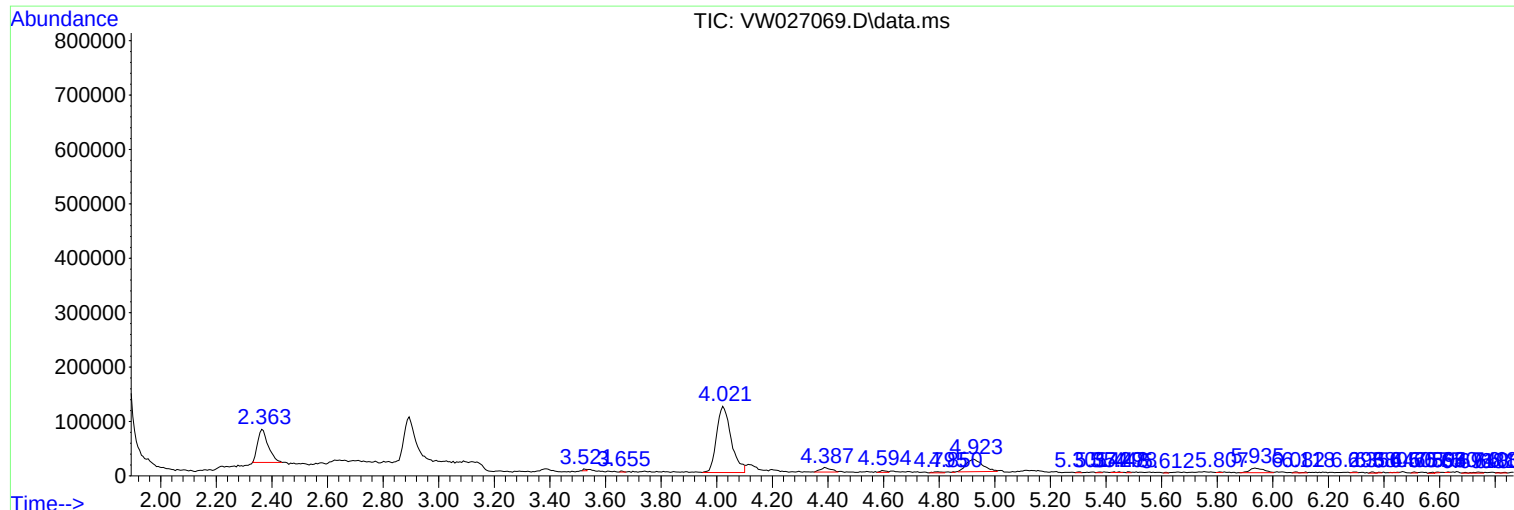
Sum of corrected areas: 10922149

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM090523SMA.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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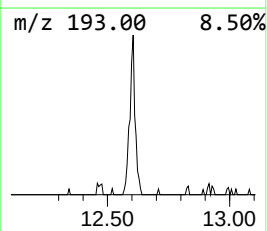
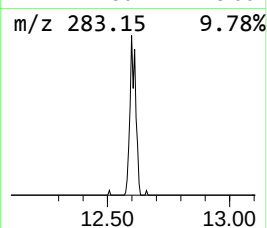
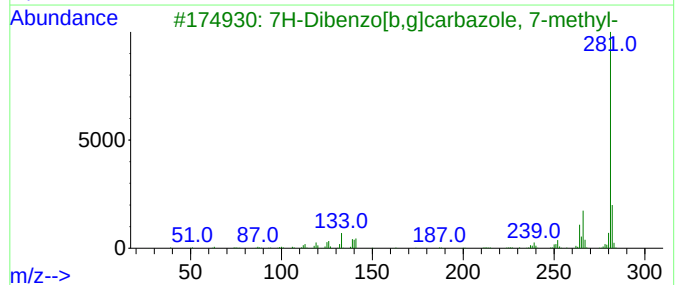
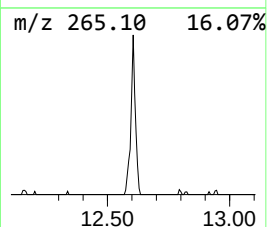
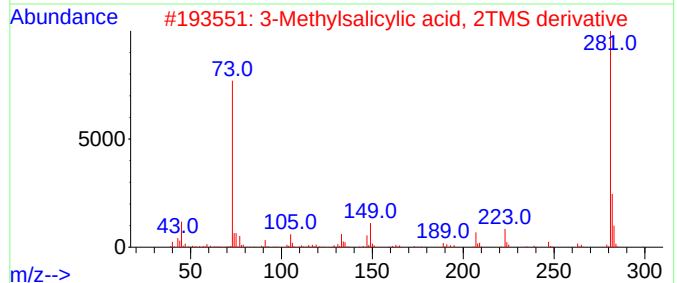
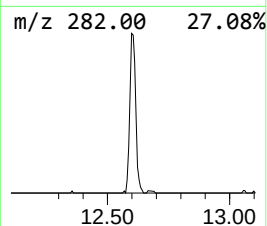
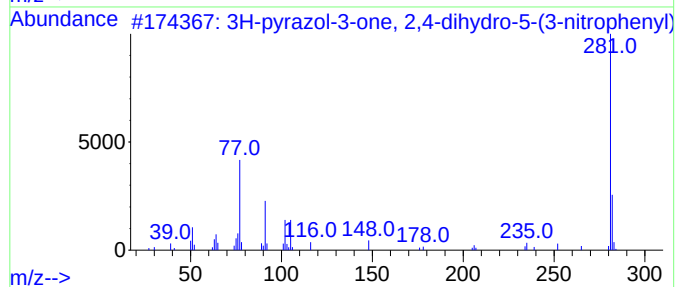
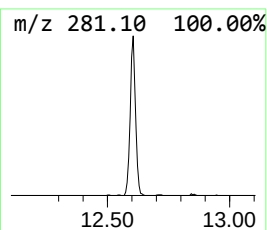
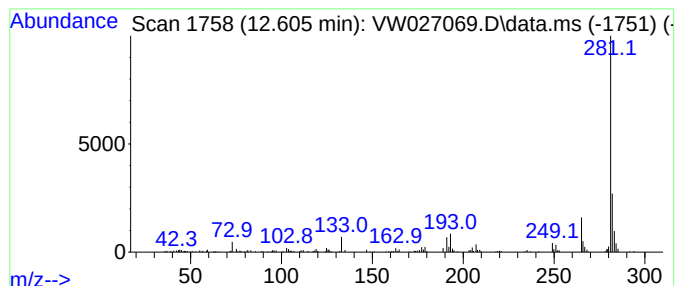
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM090523SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 3H-pyrazol-3-one, 2,4-dihyd... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.605	3.10 ug/L	92772	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3H-pyrazol-3-one, 2,4-dihydro-5-...	281	C15H11N3O3	1000401-91-2	59
2			3-Methylsalicylic acid, 2TMS der...	296	C14H24O3Si2	1000423-36-2	59
3			7H-Dibenzo[b,g]carbazole, 7-methyl-	281	C21H15N	003557-49-1	59
4			N-Ethyl-2-methyl-5-(5-methyl-1,2...	281	C12H15N3O3S	1000459-23-1	58
5			1-(2,4-Dihydroxyphenyl)-2-(4-flu...	406	C20H27F04Si2	1000474-42-3	50



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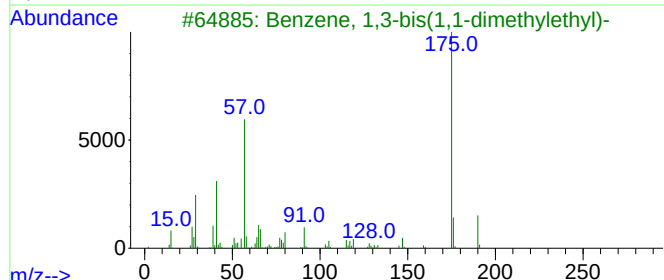
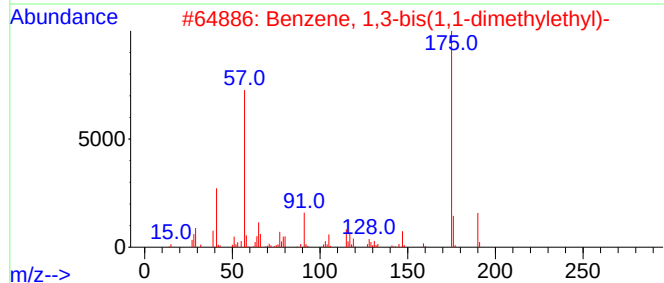
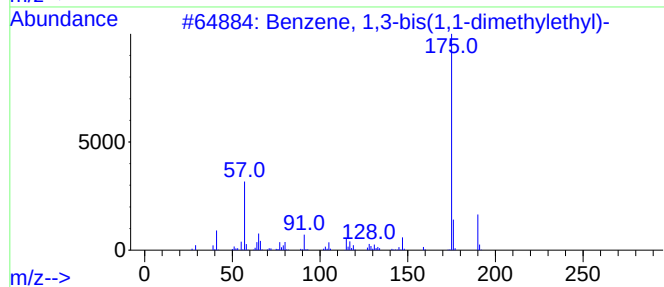
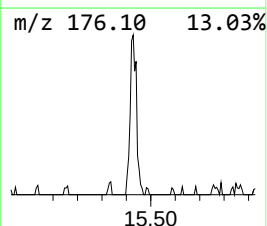
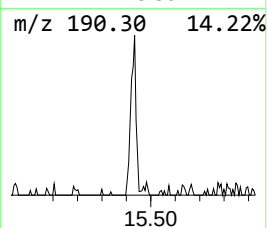
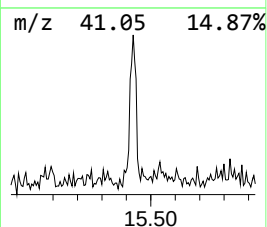
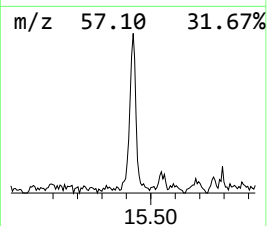
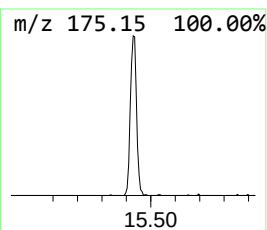
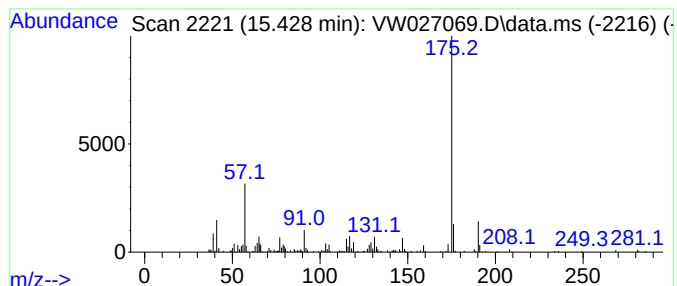
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1,3-bis(1,1-dimeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.428	2.55 ug/L	76406	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	87
2			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	81
3			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	81
4			m-Cymene, 5-tert-butyl-	190	C14H22	029577-19-3	80
5			Precocene I	190	C12H14O2	017598-02-6	74



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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
3H-pyrazol-3-on...	12.605	3.1	ug/L	92772	3	13.556	748186	25.0
Benzene, 1,3-bi...	15.428	2.5	ug/L	76406	3	13.556	748186	25.0