

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
 Data File : BG051532.D
 Acq On : 15 Dec 2021 10:49
 Operator : CG/JU
 Sample : M4971-02
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
 Title : SVOA CALIBRATION

Signal : TIC: BG051532.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.605	16	20	25	rBV2	8890	11037	0.80%	0.096%
2	4.039	89	94	105	rBV2	19596	38687	2.81%	0.336%
3	4.216	121	124	127	rBV4	2092	2624	0.19%	0.023%
4	4.268	130	133	135	rBV2	1855	2023	0.15%	0.018%
5	4.386	149	153	159	rVB2	10239	14170	1.03%	0.123%
6	5.232	294	297	300	rVB2	1603	1882	0.14%	0.016%
7	5.320	310	312	320	rBV3	1833	3323	0.24%	0.029%
8	5.402	322	326	329	rBV	1111	1625	0.12%	0.014%
9	5.725	375	381	383	rBV3	3013	4412	0.32%	0.038%
10	5.755	383	386	394	rVB5	1635	3114	0.23%	0.027%
11	5.878	403	407	410	rBV2	1624	2651	0.19%	0.023%
12	6.072	437	440	442	rBV2	1578	1982	0.14%	0.017%
13	6.254	468	471	472	rBV2	1926	1470	0.11%	0.013%
14	6.325	481	483	488	rVB4	2430	2155	0.16%	0.019%
15	6.900	576	581	589	rVB2	11097	17477	1.27%	0.152%
16	7.123	615	619	620	rBV2	1714	2114	0.15%	0.018%
17	7.212	631	634	638	rBV3	2026	2084	0.15%	0.018%
18	7.347	655	657	661	rVV3	3311	4628	0.34%	0.040%
19	7.405	661	667	676	rVB2	48994	88551	6.43%	0.770%
20	7.582	691	697	706	rVB	120143	204486	14.85%	1.779%
21	7.799	727	734	743	rVV	129238	230517	16.74%	2.005%
22	7.893	746	750	751	rBV	1501	1664	0.12%	0.014%
23	7.922	751	755	759	rVB	2851	4242	0.31%	0.037%
24	8.281	809	816	821	rBV	108192	193402	14.05%	1.682%
25	8.328	821	824	830	rVB3	18673	30301	2.20%	0.264%
26	8.527	854	858	863	rVB3	1281	2323	0.17%	0.020%
27	8.886	915	919	923	rBV4	1841	3079	0.22%	0.027%
28	8.968	926	933	943	rVB2	120757	205808	14.95%	1.790%
29	9.103	951	956	962	rVB2	7661	12679	0.92%	0.110%
30	9.379	995	1003	1008	rBV3	13403	23443	1.70%	0.204%
31	9.444	1008	1014	1022	rVB	165646	292374	21.24%	2.543%
32	10.178	1130	1139	1149	rVB	127643	229535	16.67%	1.996%
33	10.719	1224	1231	1240	rBV	209829	374895	27.23%	3.261%
34	11.006	1274	1280	1288	rVB5	6096	11357	0.82%	0.099%
35	11.118	1290	1299	1305	rBV	146727	261615	19.00%	2.275%
36	11.165	1305	1307	1312	rVB3	3319	3441	0.25%	0.030%

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37	11.236	1312	1319	1327	rBV	160343	288038	20.92%	2.505%
38	12.264	1490	1494	1498	rBV4	2552	3522	0.26%	0.031%
39	12.358	1504	1510	1516	rBV2	40257	65646	4.77%	0.571%
40	12.675	1561	1564	1565	rBV	3053	3075	0.22%	0.027%
41	12.687	1565	1566	1571	rVB2	4374	4004	0.29%	0.035%
42	13.192	1648	1652	1654	rVB3	2071	1869	0.14%	0.016%
43	13.286	1664	1668	1671	rBV4	2115	3092	0.22%	0.027%
44	13.527	1701	1709	1712	rVB4	4597	5302	0.39%	0.046%
45	13.744	1742	1746	1751	rVV2	3210	4245	0.31%	0.037%
46	13.814	1751	1758	1764	rBV2	39761	61852	4.49%	0.538%
47	14.132	1806	1812	1818	rVB2	1173	3033	0.22%	0.026%
48	14.302	1835	1841	1848	rVB	458583	654701	47.56%	5.694%
49	14.437	1861	1864	1868	rBV3	1240	1897	0.14%	0.016%
50	14.607	1886	1893	1901	rVB	453967	726527	52.77%	6.319%
51	14.678	1901	1905	1906	rBV3	1214	1470	0.11%	0.013%
52	14.748	1914	1917	1923	rVB3	1653	2648	0.19%	0.023%
53	14.837	1927	1932	1935	rBV3	935	1578	0.11%	0.014%
54	14.913	1938	1945	1952	rVB	252274	403957	29.34%	3.513%
55	14.983	1952	1957	1961	rBV5	6712	10743	0.78%	0.093%
56	15.066	1964	1971	1982	rBV2	42036	76183	5.53%	0.663%
57	15.494	2041	2044	2047	rBV2	1776	2686	0.20%	0.023%
58	15.571	2050	2057	2063	rVV4	7520	13582	0.99%	0.118%
59	15.635	2063	2068	2072	rVV3	10222	14292	1.04%	0.124%
60	15.700	2075	2079	2081	rVV3	1855	1698	0.12%	0.015%
61	15.900	2106	2113	2120	rVB	626393	963616	69.99%	8.381%
62	15.994	2123	2129	2136	rBV	93745	140753	10.22%	1.224%
63	16.141	2150	2154	2159	rBV2	1958	3007	0.22%	0.026%
64	16.252	2170	2173	2181	rVB2	4718	6692	0.49%	0.058%
65	16.423	2197	2202	2203	rBV3	1705	2239	0.16%	0.019%
66	16.575	2223	2228	2232	rVV4	1376	2887	0.21%	0.025%
67	16.681	2242	2246	2250	rBV4	2267	3344	0.24%	0.029%
68	16.775	2260	2262	2268	rBV2	1388	1995	0.14%	0.017%
69	16.893	2278	2282	2284	rBV4	1609	2263	0.16%	0.020%
70	16.998	2298	2300	2303	rVB2	1789	1402	0.10%	0.012%
71	17.034	2303	2306	2307	rBV3	1346	1534	0.11%	0.013%
72	17.245	2339	2342	2347	rVB4	3174	3498	0.25%	0.030%
73	17.451	2373	2377	2381	rVV3	1552	2506	0.18%	0.022%
74	17.539	2390	2392	2396	rVB4	1433	1453	0.11%	0.013%
75	17.603	2401	2403	2405	rVV2	1583	1602	0.12%	0.014%
76	17.656	2405	2412	2420	rVV	336981	534328	38.81%	4.647%

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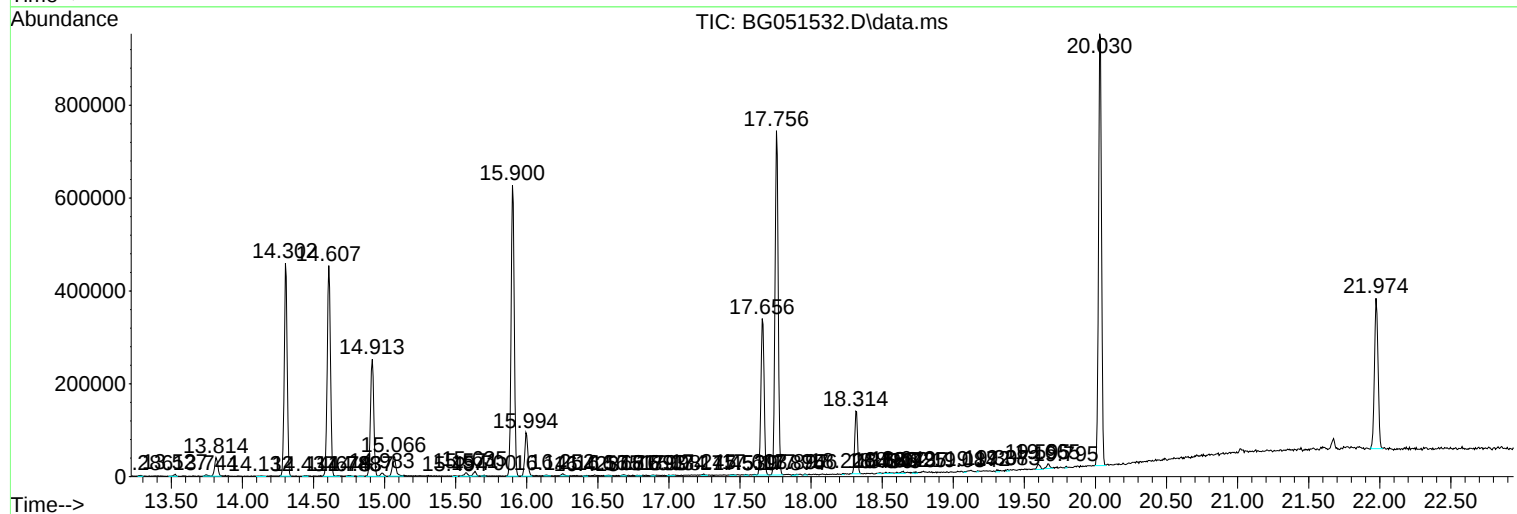
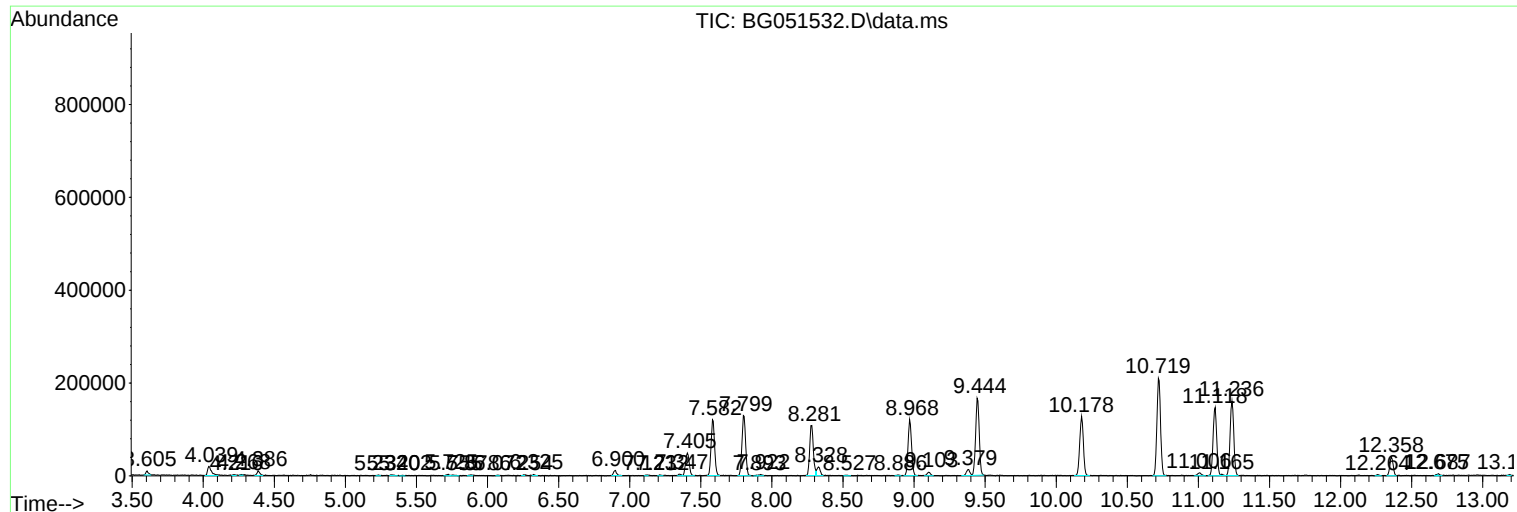
77	17.756	2422	2429	2437	rVB2	741617	1156330	83.99%	10.057%
78	17.874	2447	2449	2451	rBV2	1842	1974	0.14%	0.017%
79	17.897	2451	2453	2455	rBV3	1492	1578	0.11%	0.014%
80	17.956	2461	2463	2466	rBV3	2704	2785	0.20%	0.024%
81	18.226	2507	2509	2510	rBV	2408	1728	0.13%	0.015%
82	18.314	2519	2524	2530	rVB2	135116	185140	13.45%	1.610%
83	18.490	2550	2554	2555	rVB4	1934	2055	0.15%	0.018%
84	18.526	2558	2560	2562	rVB3	2861	1797	0.13%	0.016%
85	18.549	2562	2564	2568	rBV4	2187	2555	0.19%	0.022%
86	18.602	2571	2573	2575	rVB3	2747	1993	0.14%	0.017%
87	18.649	2575	2581	2583	rBV5	4859	6960	0.51%	0.061%
88	18.725	2592	2594	2595	rVB2	2549	1574	0.11%	0.014%
89	18.737	2595	2596	2598	rBV2	3278	2192	0.16%	0.019%
90	19.084	2653	2655	2656	rBV2	1722	1412	0.10%	0.012%
91	19.172	2668	2670	2671	rBV	2448	1713	0.12%	0.015%
92	19.307	2691	2693	2696	rBV4	4800	5354	0.39%	0.047%
93	19.383	2704	2706	2708	rBV3	3268	2887	0.21%	0.025%
94	19.595	2739	2742	2748	rBV6	11471	18341	1.33%	0.160%
95	19.665	2751	2754	2760	rVV4	9477	14287	1.04%	0.124%
96	19.795	2774	2776	2777	rBV2	3801	2588	0.19%	0.023%
97	20.030	2810	2816	2823	rBV	930245	1376694	100.00%	11.974%
98	21.974	3141	3147	3155	rVB	324024	555701	40.36%	4.833%
99	25.234	3691	3702	3714	rVB2	425430	1289341	93.65%	11.214%
100	25.475	3733	3743	3754	rVB	181537	540731	39.28%	4.703%

Sum of corrected areas: 11497639

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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



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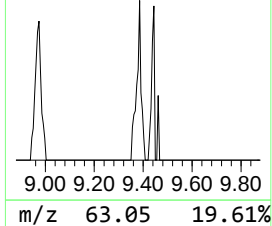
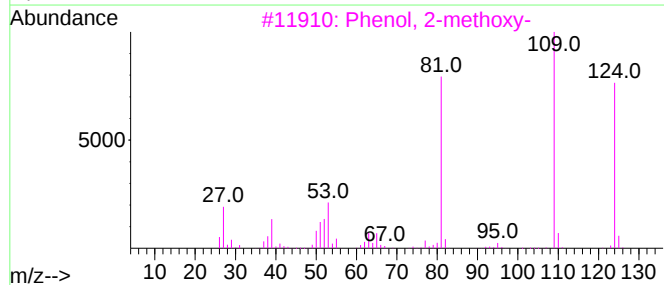
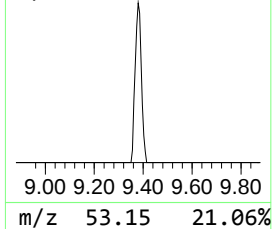
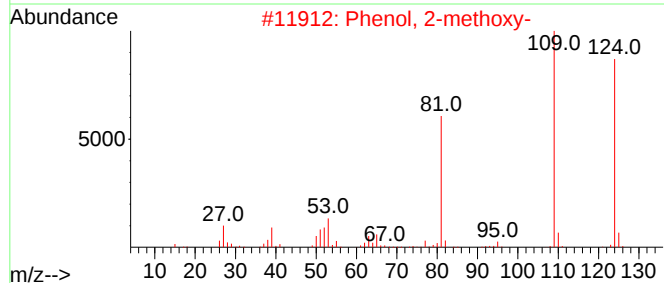
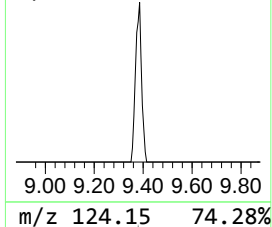
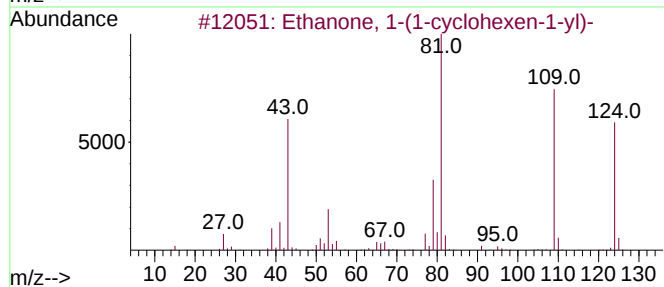
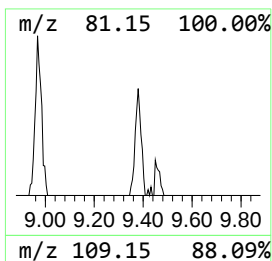
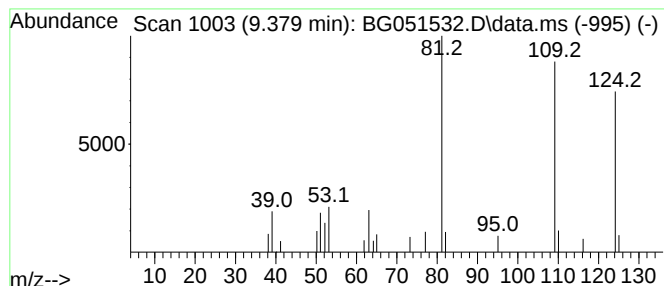
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Ethanone, 1-(1-cyclohexen-1-yl) Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.379	2.42 ng/ul	23443	1,4-Dichlorobenzene-d4	8.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	87
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	87
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	86
4			2-Cyclopenten-1-one, 2,3,4-trime...	124	C8H12O	028790-86-5	72
5			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	72



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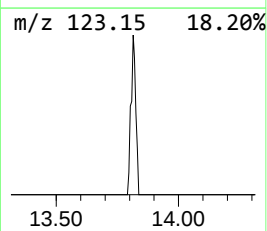
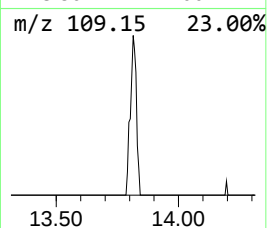
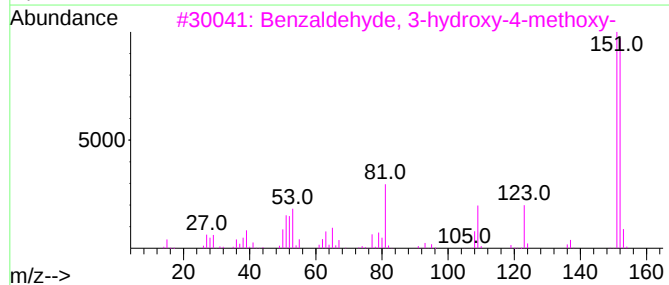
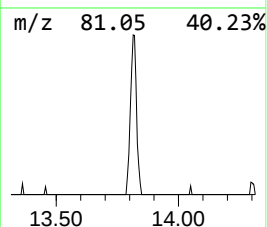
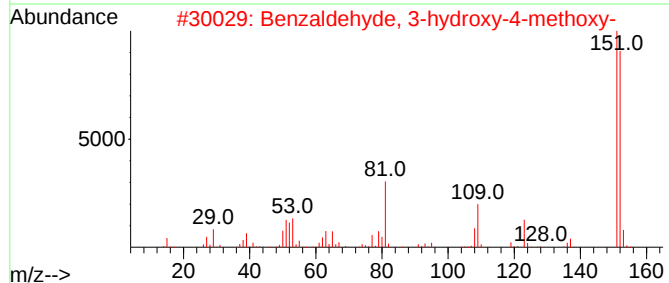
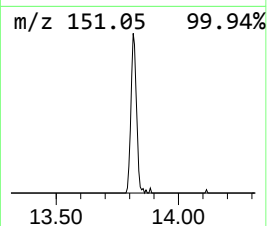
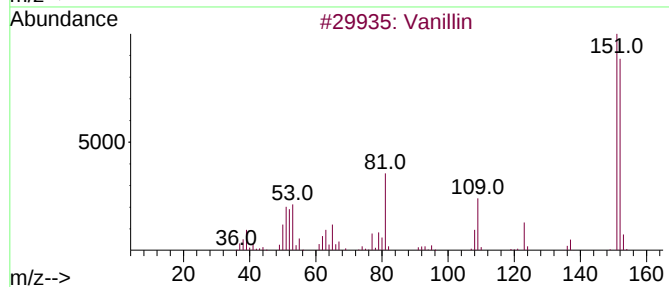
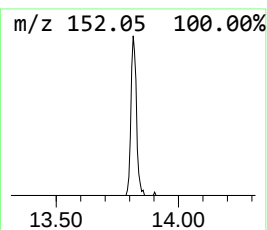
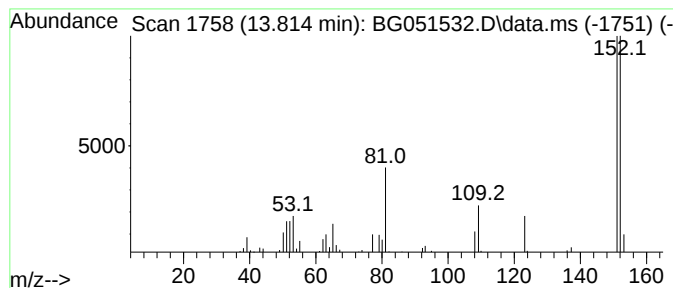
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Vanillin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.814	3.06 ng/ul	61852	Acenaphthene-d10	14.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	96
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
3			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
4			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
5			Vanillin	152	C8H8O3	000121-33-5	93



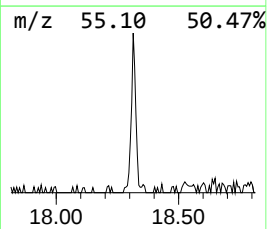
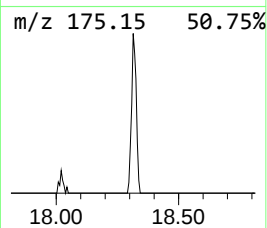
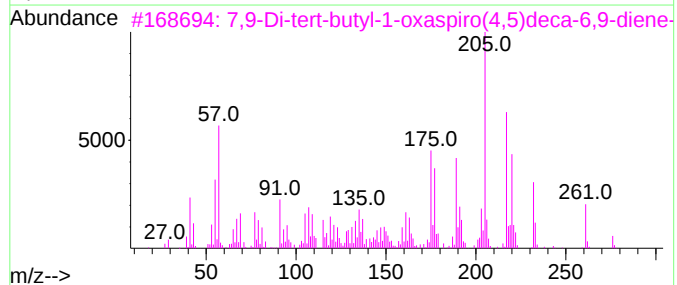
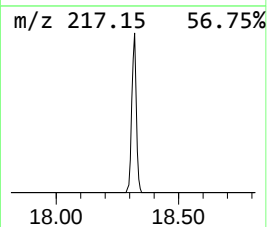
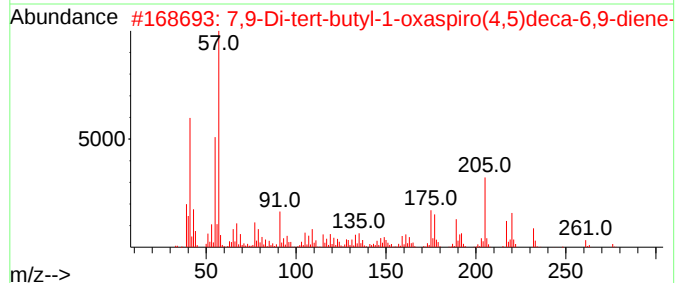
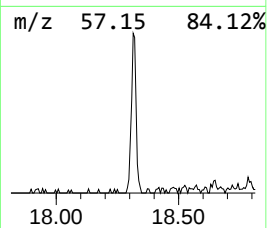
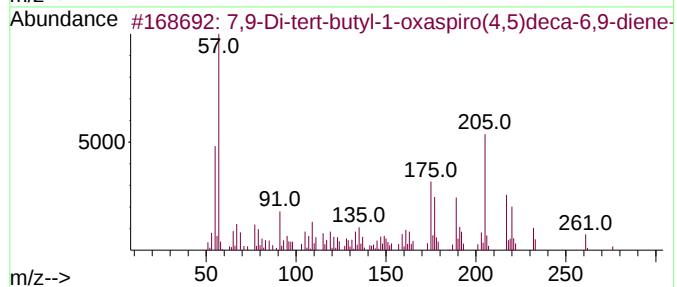
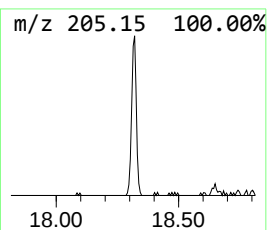
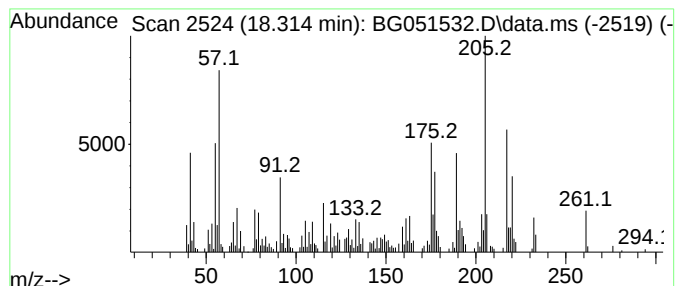
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.314	6.93 ng/ul	185140	Phenanthrene-d10	17.656	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	94
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	89
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	55
4	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	46
5	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	44



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
Data File : BG051532.D
Acq On : 15 Dec 2021 10:49
Operator : CG/JU
Sample : M4971-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanone, 1-(1-...	9.379	2.4	ng/ul	23443	1	8.281	193402	20.0
Vanillin	13.814	3.1	ng/ul	61852	3	14.913	403957	20.0
7,9-Di-tert-but...	18.314	6.9	ng/ul	185140	4	17.656	534328	20.0