

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
 Data File : BG051579.D
 Acq On : 16 Dec 2021 20:54
 Operator : CG/JU
 Sample : M4971-10
 Misc :
 ALS Vial : 79 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: BG051579.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.601	16	19	25	rBV2	8766	12929	0.87%	0.103%
2	4.036	89	93	100	rBV	22098	41503	2.80%	0.331%
3	4.271	129	133	138	rBV4	2020	3903	0.26%	0.031%
4	4.306	138	139	144	rVB	2003	1806	0.12%	0.014%
5	4.389	148	153	159	rVB2	8690	14495	0.98%	0.116%
6	4.759	214	216	220	rVB3	1982	2152	0.15%	0.017%
7	5.323	309	312	314	rBV	1811	2228	0.15%	0.018%
8	5.499	339	342	345	rBV2	1287	1652	0.11%	0.013%
9	5.716	376	379	383	rBV4	2511	3283	0.22%	0.026%
10	5.875	403	406	407	rBV2	2598	2059	0.14%	0.016%
11	6.080	437	441	445	rVB4	1400	2016	0.14%	0.016%
12	6.157	450	454	458	rVB2	1207	1934	0.13%	0.015%
13	6.233	464	467	469	rBV3	1861	1547	0.10%	0.012%
14	6.262	469	472	476	rVB2	2382	3353	0.23%	0.027%
15	6.321	479	482	488	rVV4	1916	2995	0.20%	0.024%
16	6.891	575	579	587	rBV3	10744	17613	1.19%	0.140%
17	7.114	611	617	620	rBV	1423	2114	0.14%	0.017%
18	7.343	654	656	660	rBV4	2614	3482	0.24%	0.028%
19	7.402	660	666	674	rVB	48975	87930	5.94%	0.701%
20	7.584	690	697	705	rBV	122288	207877	14.05%	1.658%
21	7.802	728	734	742	rVB	137377	235144	15.89%	1.875%
22	7.919	753	754	761	rVB2	2944	3078	0.21%	0.025%
23	8.277	807	815	821	rBV2	119938	217299	14.69%	1.733%
24	8.324	821	823	830	rVB2	18917	25983	1.76%	0.207%
25	8.971	925	933	942	rVB	120432	208271	14.08%	1.661%
26	9.100	951	955	961	rVB	9360	12373	0.84%	0.099%
27	9.376	997	1002	1007	rBV3	13331	24060	1.63%	0.192%
28	9.446	1007	1014	1022	rVB	176085	308063	20.82%	2.457%
29	10.181	1128	1139	1146	rBV	130061	238471	16.12%	1.902%
30	10.721	1223	1231	1240	rBV	209164	375695	25.39%	2.997%
31	11.009	1273	1280	1284	rVB6	6214	11255	0.76%	0.090%
32	11.115	1290	1298	1310	rVB	168437	305473	20.65%	2.436%
33	11.232	1310	1318	1330	rVB	163165	298805	20.19%	2.383%
34	11.367	1338	1341	1345	rBV2	1212	1625	0.11%	0.013%
35	12.266	1489	1494	1496	rBV	2297	3068	0.21%	0.024%
36	12.360	1504	1510	1517	rBV2	38367	65461	4.42%	0.522%

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37	12.689	1561	1566	1569	rBV5	3350	5564	0.38%	0.044%
38	13.183	1647	1650	1653	rBV2	2206	2853	0.19%	0.023%
39	13.271	1663	1665	1671	rVB3	1847	3047	0.21%	0.024%
40	13.517	1702	1707	1715	rVB4	3143	5251	0.35%	0.042%
41	13.746	1741	1746	1749	rBV3	2721	4131	0.28%	0.033%
42	13.817	1751	1758	1764	rVV	39094	64560	4.36%	0.515%
43	14.305	1834	1841	1847	rBV	458040	685004	46.30%	5.464%
44	14.604	1885	1892	1902	rVB	465727	756188	51.11%	6.031%
45	14.910	1937	1944	1952	rBV	290351	462737	31.27%	3.691%
46	14.980	1952	1956	1961	rVB3	7444	9637	0.65%	0.077%
47	15.068	1963	1971	1977	rBV2	51856	84759	5.73%	0.676%
48	15.309	2009	2012	2013	rBV2	1747	1643	0.11%	0.013%
49	15.568	2052	2056	2063	rBV2	7047	11295	0.76%	0.090%
50	15.632	2063	2067	2073	rVB2	9915	15008	1.01%	0.120%
51	15.703	2073	2079	2082	rBV3	1694	3342	0.23%	0.027%
52	15.902	2105	2113	2121	rBV	664607	1005790	67.98%	8.022%
53	15.996	2123	2129	2137	rBV	206696	299152	20.22%	2.386%
54	16.137	2149	2153	2158	rVB4	2657	4244	0.29%	0.034%
55	16.249	2167	2172	2178	rVB3	5379	8633	0.58%	0.069%
56	16.590	2224	2230	2232	rVB	1067	2193	0.15%	0.017%
57	16.678	2242	2245	2250	rBV3	2972	3798	0.26%	0.030%
58	16.889	2278	2281	2285	rBV2	1468	1808	0.12%	0.014%
59	17.248	2336	2342	2345	rVB4	2223	3097	0.21%	0.025%
60	17.394	2364	2367	2368	rBV	1090	1497	0.10%	0.012%
61	17.594	2399	2401	2405	rVV4	2116	2592	0.18%	0.021%
62	17.659	2405	2412	2419	rVV	399799	622460	42.07%	4.965%
63	17.759	2422	2429	2437	rVV	817576	1227952	82.99%	9.794%
64	17.917	2454	2456	2460	rVB2	1854	2040	0.14%	0.016%
65	18.029	2469	2475	2477	rBV5	1554	2899	0.20%	0.023%
66	18.317	2519	2524	2529	rBV	148728	187918	12.70%	1.499%
67	18.464	2547	2549	2551	rBV2	1669	1758	0.12%	0.014%
68	18.599	2570	2572	2575	rBV	2747	2086	0.14%	0.017%
69	18.640	2577	2579	2582	rVV3	4666	5183	0.35%	0.041%
70	18.693	2585	2588	2591	rVV	2103	2786	0.19%	0.022%
71	18.793	2602	2605	2608	rVB4	2622	3086	0.21%	0.025%
72	18.928	2626	2628	2629	rBV2	2119	1553	0.10%	0.012%
73	19.116	2658	2660	2664	rBV5	2703	4009	0.27%	0.032%
74	19.151	2664	2666	2669	rVV4	2649	2631	0.18%	0.021%
75	19.192	2671	2673	2675	rBV3	2402	1795	0.12%	0.014%
76	19.427	2711	2713	2715	rBV3	2201	1793	0.12%	0.014%

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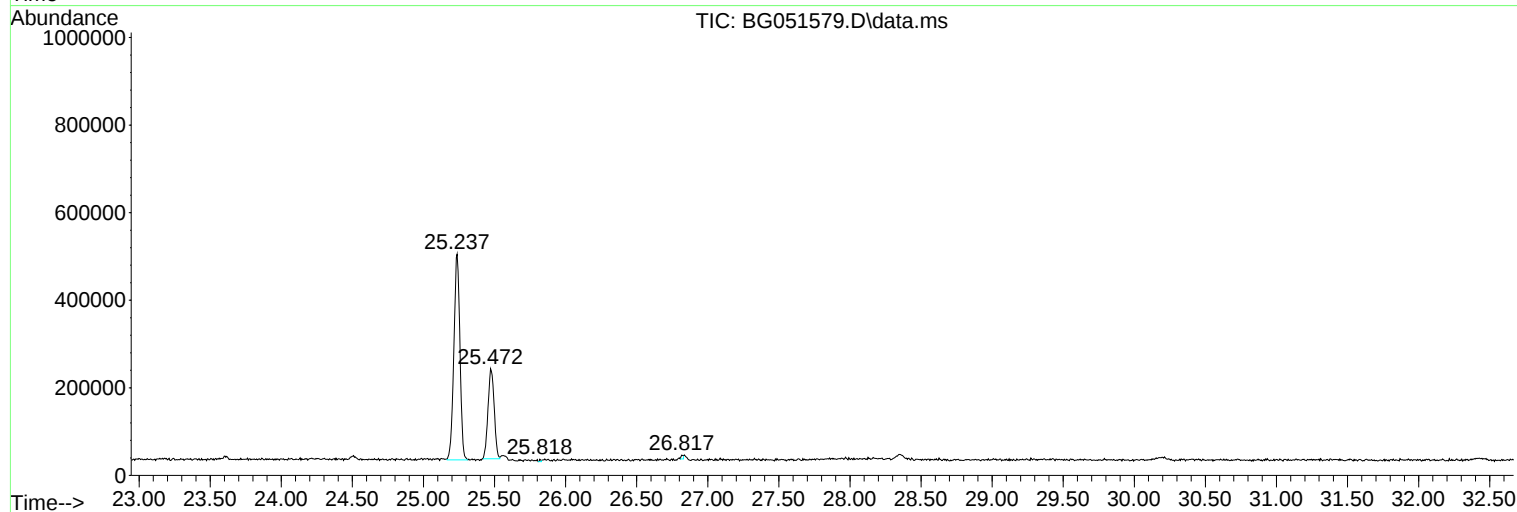
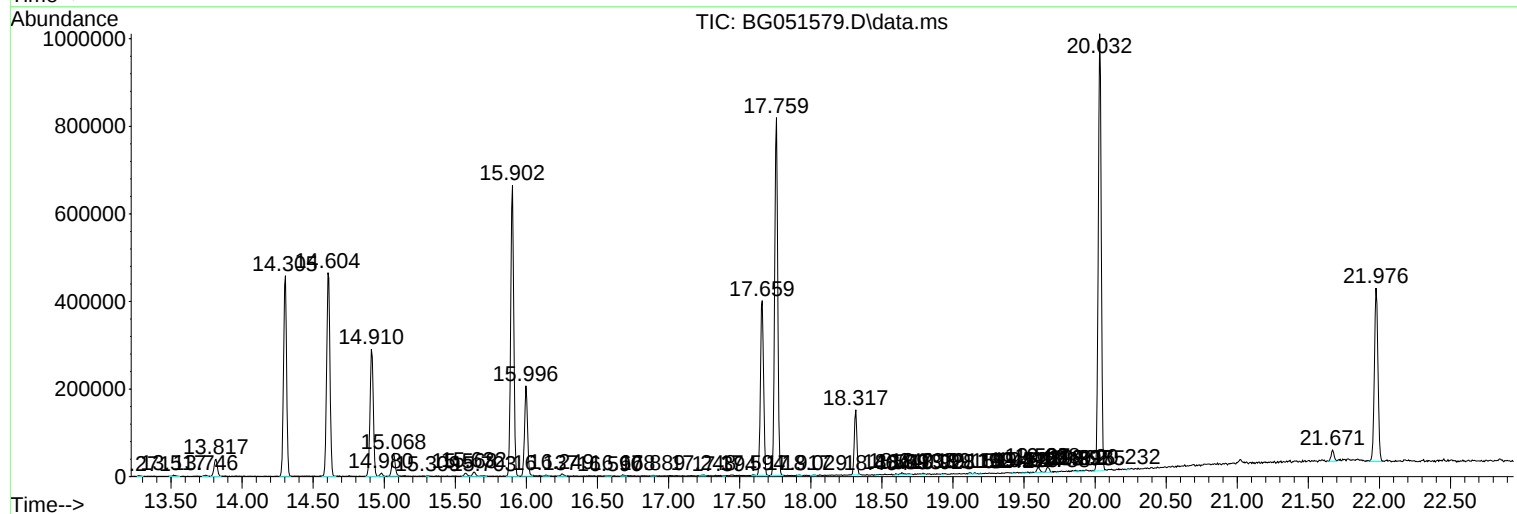
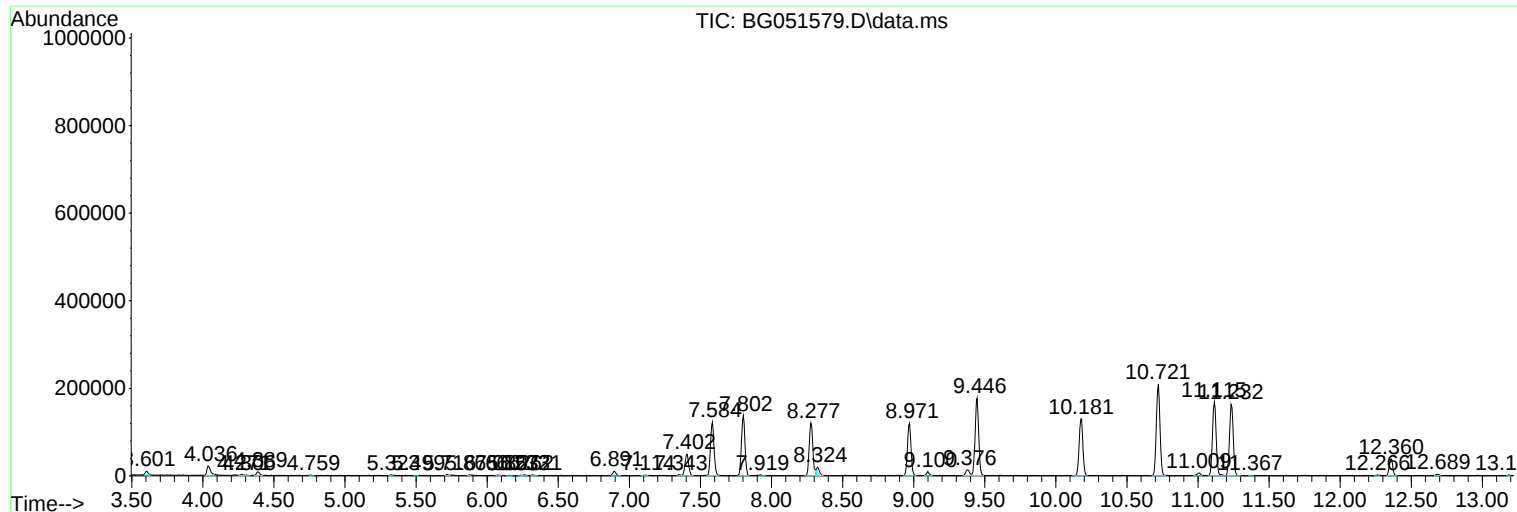
77	19.492	2722	2724	2726	rBV3	2060	1815	0.12%	0.014%
78	19.515	2726	2728	2729	rVV	1756	1500	0.10%	0.012%
79	19.544	2732	2733	2735	rBV2	2379	2097	0.14%	0.017%
80	19.597	2738	2742	2749	rVV4	11850	18377	1.24%	0.147%
81	19.668	2750	2754	2759	rVB3	11069	17335	1.17%	0.138%
82	19.738	2764	2766	2767	rBV2	1926	1636	0.11%	0.013%
83	19.862	2785	2787	2790	rVB4	3199	2921	0.20%	0.023%
84	19.897	2790	2793	2794	rBV3	3024	2547	0.17%	0.020%
85	19.915	2794	2796	2798	rBV3	2675	2530	0.17%	0.020%
86	19.985	2806	2808	2809	rBV2	2288	1761	0.12%	0.014%
87	20.032	2809	2816	2822	rVV	998328	1479643	100.00%	11.802%
88	20.232	2848	2850	2851	rBV2	2623	1892	0.13%	0.015%
89	21.671	3090	3095	3100	rBV	25556	36782	2.49%	0.293%
90	21.976	3140	3147	3154	rVB	396111	675675	45.66%	5.389%
91	25.237	3690	3702	3715	rVB	470094	1388653	93.85%	11.076%
92	25.472	3733	3742	3753	rBV2	205785	619915	41.90%	4.944%
93	25.818	3799	3801	3803	rBV2	5299	3964	0.27%	0.032%
94	26.817	3969	3971	3973	rBV3	8749	9884	0.67%	0.079%

Sum of corrected areas: 12537694

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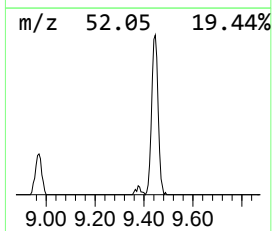
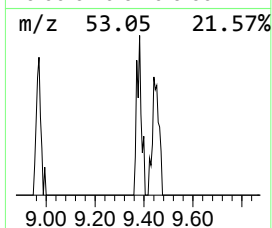
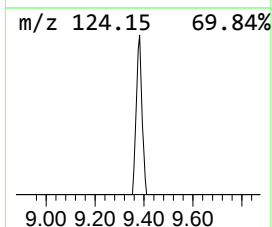
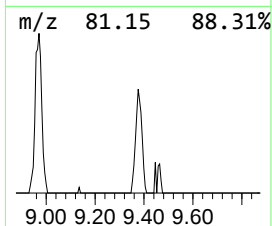
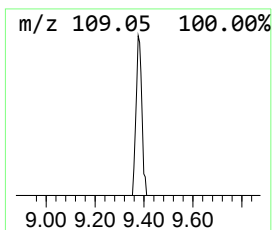
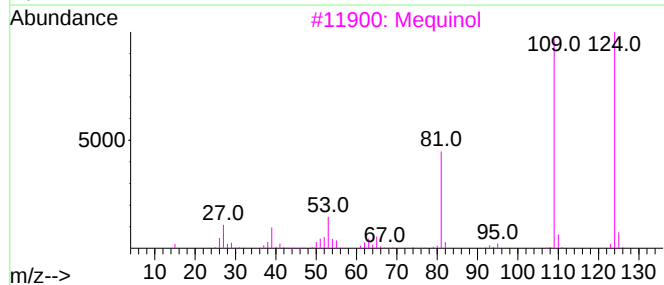
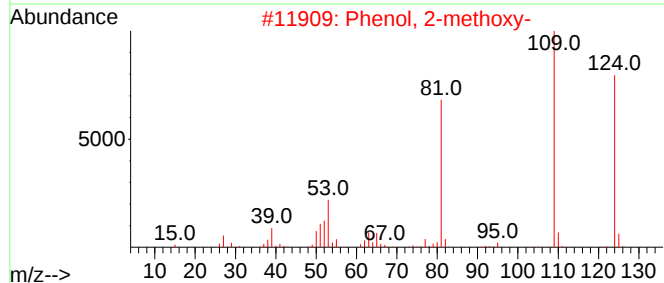
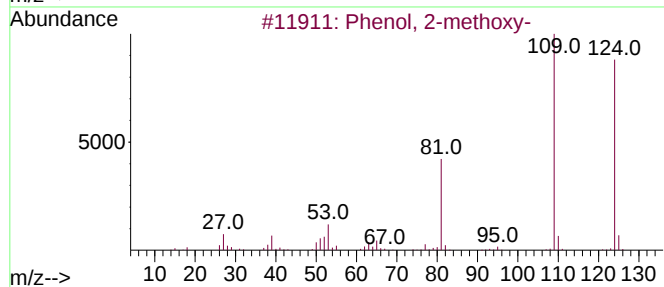
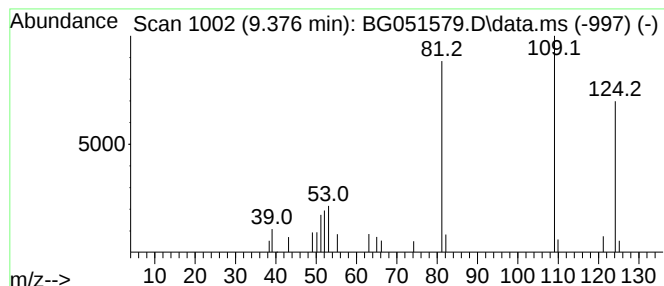
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.376	2.21 ng/ul	24060	1,4-Dichlorobenzene-d4	8.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	80
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	64
3			Mequinol	124	C7H8O2	000150-76-5	58
4			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	58
5			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	49



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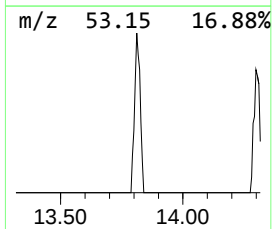
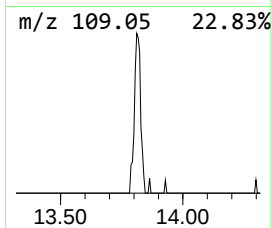
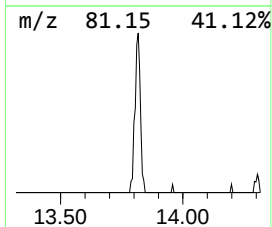
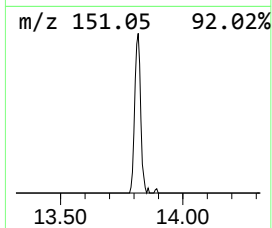
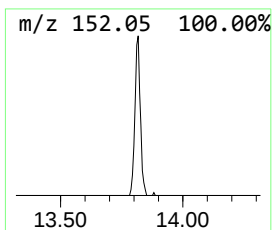
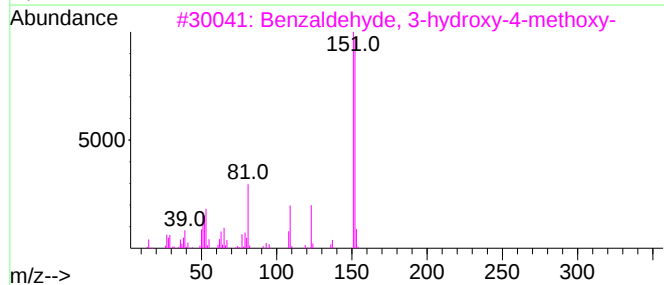
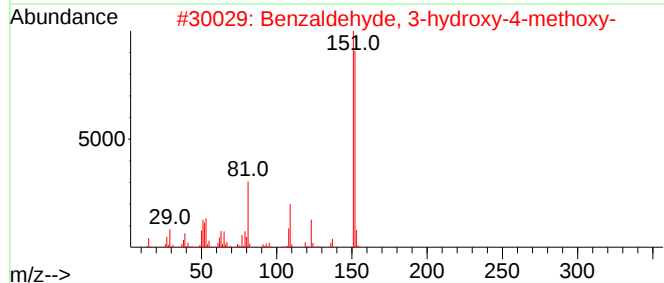
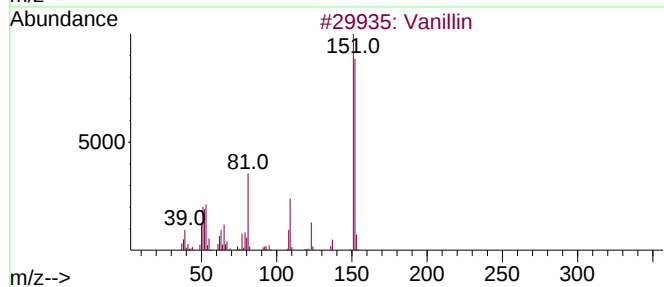
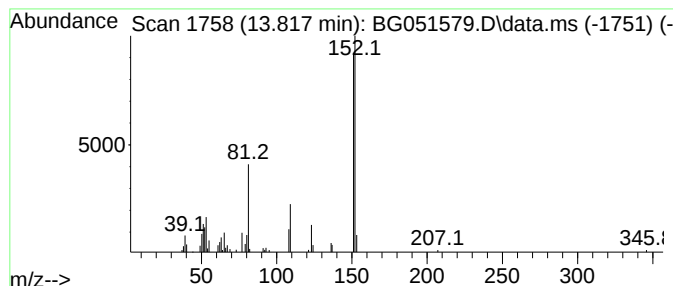
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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.
13.817	2.79 ng/ul	64560	Acenaphthene-d10	14.910

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	93
4			Vanillin	152	C8H8O3	000121-33-5	91
5			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	90



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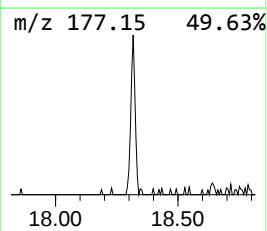
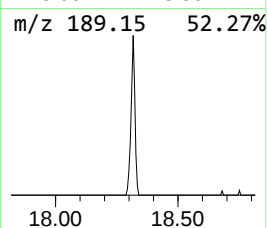
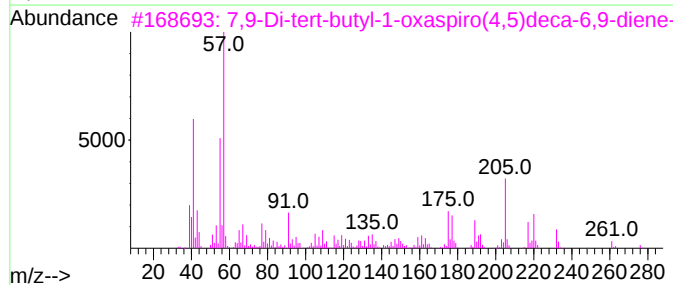
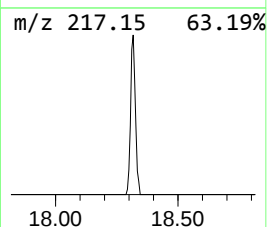
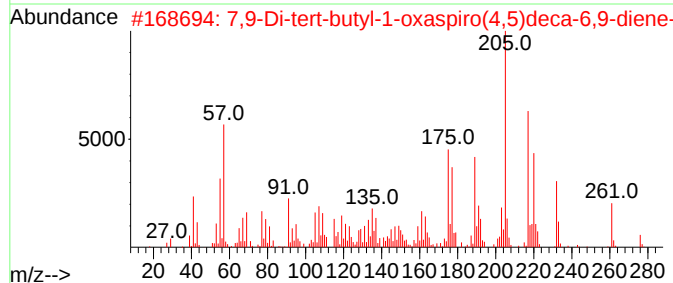
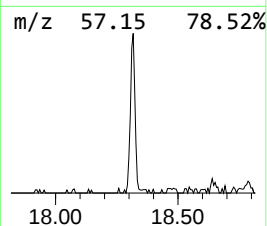
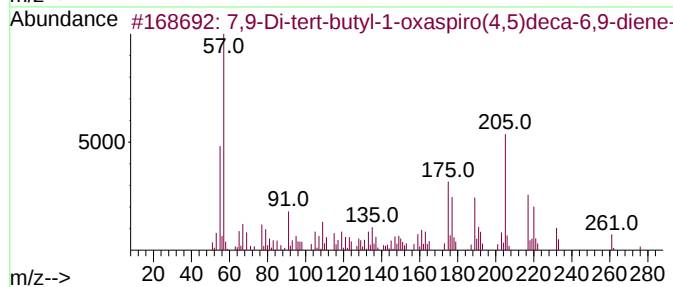
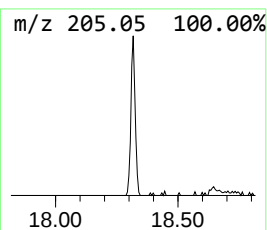
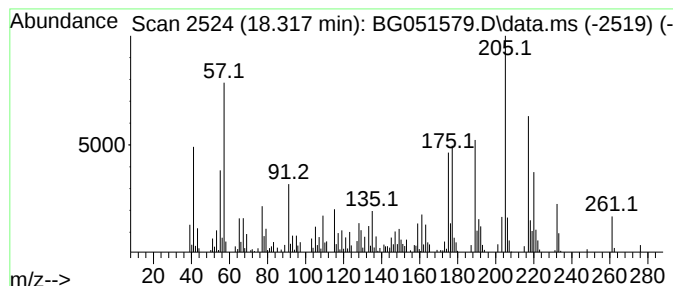
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Quant Title : SVOA CALIBRATION

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.
18.317	6.04 ng/ul	187918	Phenanthrene-d10	17.659

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	95		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	93		
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	66		
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
Data File : BG051579.D
Acq On : 16 Dec 2021 20:54
Operator : CG/JU
Sample : M4971-10
Misc :
ALS Vial : 79 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Phenol, 2-methoxy-	9.376	2.2	ng/ul	24060	1	8.277	217299	20.0
Vanillin	13.817	2.8	ng/ul	64560	3	14.910	462737	20.0
7,9-Di-tert-but...	18.317	6.0	ng/ul	187918	4	17.659	622460	20.0