

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112321\
 Data File : BG051198.D
 Acq On : 24 Nov 2021 1:23
 Operator : CG/JU
 Sample : M4753-11
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A0018

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-BG112321.M
 Title : SVOA CALIBRATION

Signal : TIC: BG051198.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.543	4	9	13	rBV2	5229	9543	1.10%	0.092%
2	3.978	80	83	97	rVB	12075	23673	2.73%	0.228%
3	4.201	117	121	128	rVB3	3173	4503	0.52%	0.043%
4	4.501	169	172	178	rBV3	2086	3262	0.38%	0.031%
5	4.572	178	184	189	rVV	7069	11405	1.31%	0.110%
6	4.683	197	203	209	rVB6	1641	3020	0.35%	0.029%
7	5.993	423	426	433	rVV	5538	8882	1.02%	0.085%
8	6.217	460	464	473	rVB4	8635	14637	1.69%	0.141%
9	6.804	561	564	570	rVB2	3963	5850	0.67%	0.056%
10	6.887	573	578	582	rVB2	2541	4079	0.47%	0.039%
11	7.357	651	658	667	rBV	24094	46851	5.40%	0.450%
12	7.515	678	685	693	rBV	86517	154117	17.77%	1.482%
13	7.727	715	721	731	rBV	84849	149041	17.18%	1.433%
14	8.197	792	801	813	rBV	90656	155485	17.93%	1.495%
15	8.908	916	922	929	rBV	67906	125898	14.51%	1.210%
16	8.955	929	930	939	rVB3	2768	4039	0.47%	0.039%
17	9.372	995	1001	1015	rVV	109951	212144	24.46%	2.040%
18	9.724	1055	1061	1065	rBV2	4374	6487	0.75%	0.062%
19	10.100	1119	1125	1134	rVB	91177	169655	19.56%	1.631%
20	10.300	1153	1159	1165	rVB3	5616	9385	1.08%	0.090%
21	10.647	1211	1218	1234	rBV	121881	233924	26.97%	2.249%
22	10.776	1234	1240	1247	rBV3	6761	14156	1.63%	0.136%
23	11.023	1276	1282	1291	rVB	133803	245234	28.27%	2.358%
24	11.164	1298	1306	1316	rBV	95501	184150	21.23%	1.771%
25	11.534	1364	1369	1373	rBV3	3352	5874	0.68%	0.056%
26	11.593	1373	1379	1384	rVB4	4214	8115	0.94%	0.078%
27	11.687	1390	1395	1401	rVB	2595	4564	0.53%	0.044%
28	11.757	1401	1407	1412	rBV4	5497	11173	1.29%	0.107%
29	12.210	1479	1484	1487	rVV2	3234	6196	0.71%	0.060%
30	12.251	1487	1491	1498	rVV	7429	13695	1.58%	0.132%
31	12.398	1512	1516	1521	rVV3	2837	5031	0.58%	0.048%
32	12.492	1527	1532	1538	rVB5	3003	6391	0.74%	0.061%
33	12.668	1557	1562	1565	rBV4	3509	4668	0.54%	0.045%
34	13.056	1622	1628	1633	rVB5	2916	5682	0.66%	0.055%
35	13.173	1642	1648	1658	rBV	78320	135540	15.63%	1.303%
36	13.279	1663	1666	1669	rVV4	2868	4720	0.54%	0.045%

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37	13.361	1678	1680	1684	rVV3	2288	2850	0.33%	0.027%
38	13.420	1684	1690	1699	rVB	34381	52698	6.08%	0.507%
39	13.620	1718	1724	1726	rVV3	3519	6278	0.72%	0.060%
40	13.667	1726	1732	1749	rVB	359123	644753	74.33%	6.199%
41	14.225	1820	1827	1838	rVB	293072	443927	51.18%	4.268%
42	14.448	1858	1865	1866	rBV2	4753	5919	0.68%	0.057%
43	14.530	1870	1879	1885	rVB	322027	518993	59.83%	4.990%
44	14.677	1901	1904	1911	rVB4	2678	4368	0.50%	0.042%
45	14.807	1917	1926	1927	rVV	137660	186890	21.55%	1.797%
46	14.830	1927	1930	1936	rVV	226209	347853	40.10%	3.345%
47	14.883	1936	1939	1946	rVB4	4000	6202	0.72%	0.060%
48	15.059	1963	1969	1986	rBV3	15467	38532	4.44%	0.370%
49	15.189	1986	1991	1997	rVB5	1821	4319	0.50%	0.042%
50	15.553	2048	2053	2056	rBV	9104	12080	1.39%	0.116%
51	15.588	2056	2059	2062	rVV	7105	10029	1.16%	0.096%
52	15.623	2062	2065	2071	rVB2	12422	18565	2.14%	0.179%
53	15.817	2090	2098	2109	rVB	434536	684808	78.95%	6.584%
54	15.946	2114	2120	2130	rBV	128273	205186	23.66%	1.973%
55	16.158	2151	2156	2158	rBV3	2640	4248	0.49%	0.041%
56	16.187	2158	2161	2171	rVB6	2742	5074	0.58%	0.049%
57	16.346	2182	2188	2191	rBV6	1980	4356	0.50%	0.042%
58	16.422	2198	2201	2207	rBV6	4413	7556	0.87%	0.073%
59	16.511	2211	2216	2221	rVB6	6117	10191	1.17%	0.098%
60	16.687	2242	2246	2250	rVB7	3560	5792	0.67%	0.056%
61	17.216	2333	2336	2342	rBV5	2882	4843	0.56%	0.047%
62	17.286	2342	2348	2354	rVV4	5850	7957	0.92%	0.077%
63	17.374	2360	2363	2366	rVB4	3567	3910	0.45%	0.038%
64	17.451	2372	2376	2380	rVB2	13017	15286	1.76%	0.147%
65	17.515	2383	2387	2392	rBV	24010	34361	3.96%	0.330%
66	17.580	2392	2398	2408	rVB	275740	438408	50.54%	4.215%
67	17.680	2408	2415	2424	rBV	502384	783445	90.32%	7.533%
68	17.827	2435	2440	2444	rBV	5398	9586	1.11%	0.092%
69	18.203	2499	2504	2510	rVB3	9550	13115	1.51%	0.126%
70	18.338	2524	2527	2531	rVV5	2233	3272	0.38%	0.031%
71	18.414	2531	2540	2545	rBV2	20346	34377	3.96%	0.331%
72	18.543	2553	2562	2569	rBV	510775	749227	86.38%	7.204%
73	18.696	2580	2588	2589	rBV5	5122	8728	1.01%	0.084%
74	18.737	2590	2595	2600	rVB	51658	73349	8.46%	0.705%
75	18.849	2611	2614	2618	rVB7	2463	3059	0.35%	0.029%
76	18.955	2627	2632	2637	rBV	83621	106235	12.25%	1.021%

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77	18.996	2637	2639	2643	rVB5	3990	5127	0.59%	0.049%
78	19.190	2669	2672	2676	rVB4	4178	5369	0.62%	0.052%
79	19.272	2682	2686	2688	rBV3	9345	9637	1.11%	0.093%
80	19.337	2694	2697	2701	rVB5	4317	6425	0.74%	0.062%
81	19.472	2716	2720	2722	rBV5	5404	8582	0.99%	0.083%
82	19.525	2724	2729	2734	rVV7	8694	20752	2.39%	0.200%
83	19.589	2736	2740	2746	rVV	9243	14469	1.67%	0.139%
84	19.813	2775	2778	2784	rBV4	7652	11309	1.30%	0.109%
85	19.877	2787	2789	2792	rBV4	2881	3292	0.38%	0.032%
86	19.959	2797	2803	2809	rBV	589663	867390	100.00%	8.340%
87	20.006	2809	2811	2817	rVV6	6425	10691	1.23%	0.103%
88	20.048	2817	2818	2822	rVB3	3948	4988	0.58%	0.048%
89	20.694	2925	2928	2931	rBV2	9329	11061	1.28%	0.106%
90	21.252	3020	3023	3024	rBV3	2591	3279	0.38%	0.032%
91	21.481	3057	3062	3073	rVB3	11587	38827	4.48%	0.373%
92	21.881	3123	3130	3139	rVB	258865	439986	50.73%	4.230%
93	23.379	3381	3385	3393	rVB5	11385	22916	2.64%	0.220%
94	24.225	3525	3529	3534	rBV4	10721	18197	2.10%	0.175%
95	25.042	3657	3668	3681	rVB2	282093	816555	94.14%	7.851%
96	25.277	3694	3708	3719	rVV2	145501	462978	53.38%	4.451%
97	25.753	3786	3789	3790	rBV3	3085	3722	0.43%	0.036%
98	26.182	3860	3862	3865	rBV4	3624	4046	0.47%	0.039%
99	26.411	3894	3901	3910	rVB5	14143	40818	4.71%	0.392%
100	27.838	4138	4144	4155	rVB8	12819	38449	4.43%	0.370%

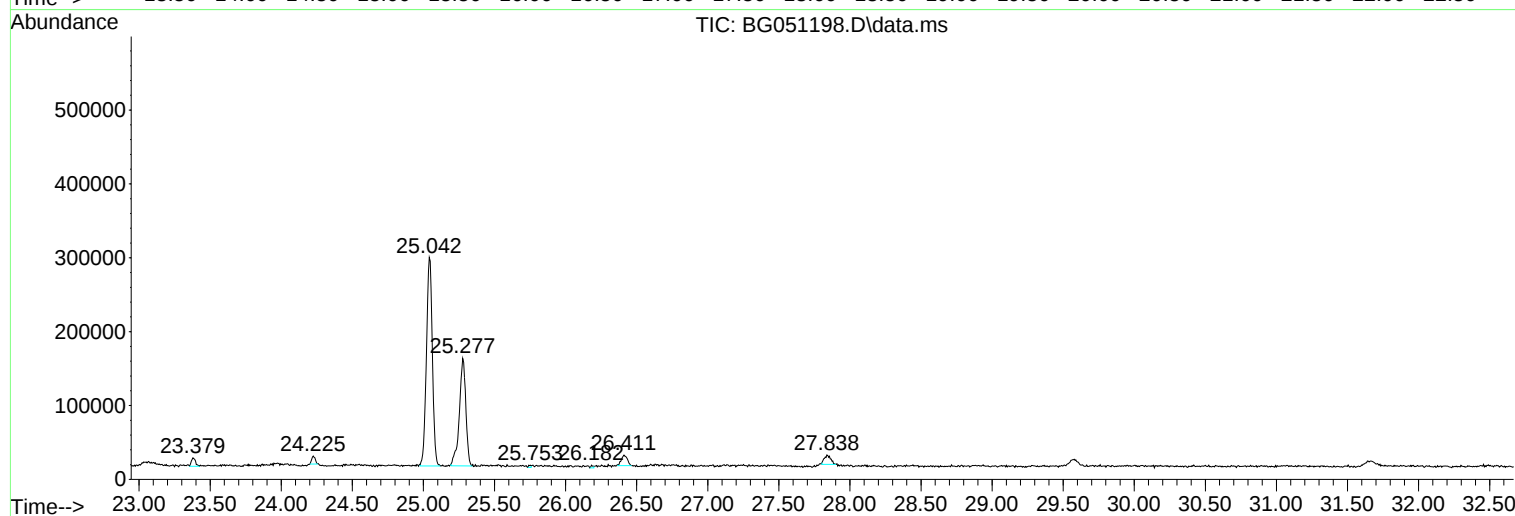
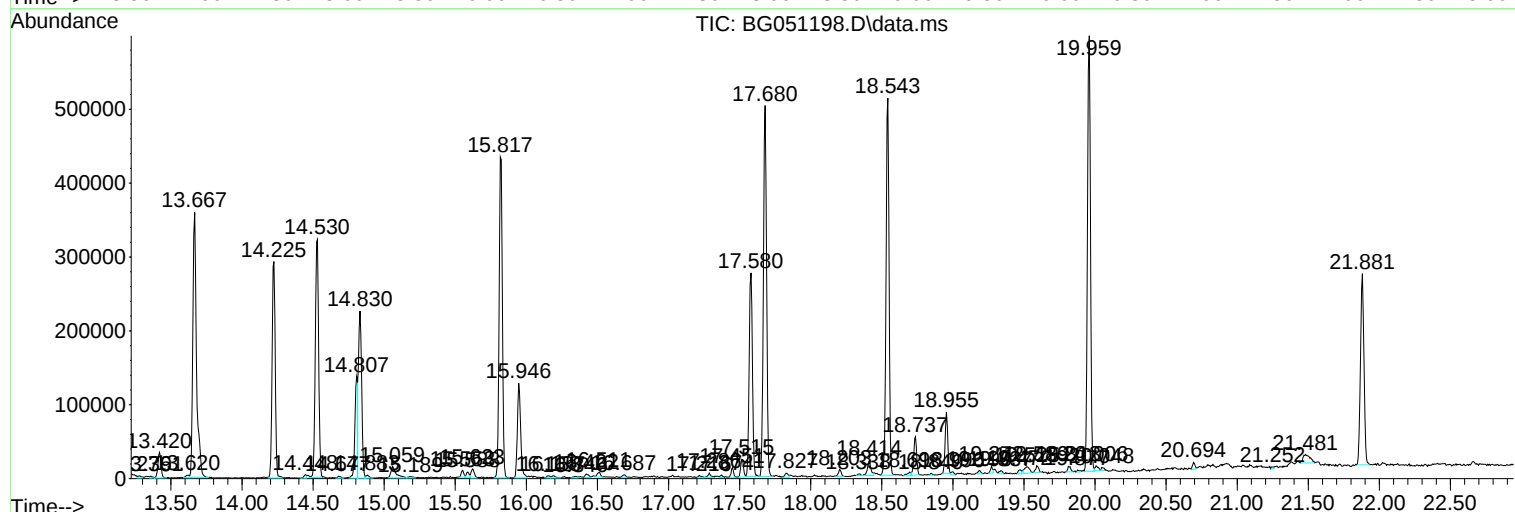
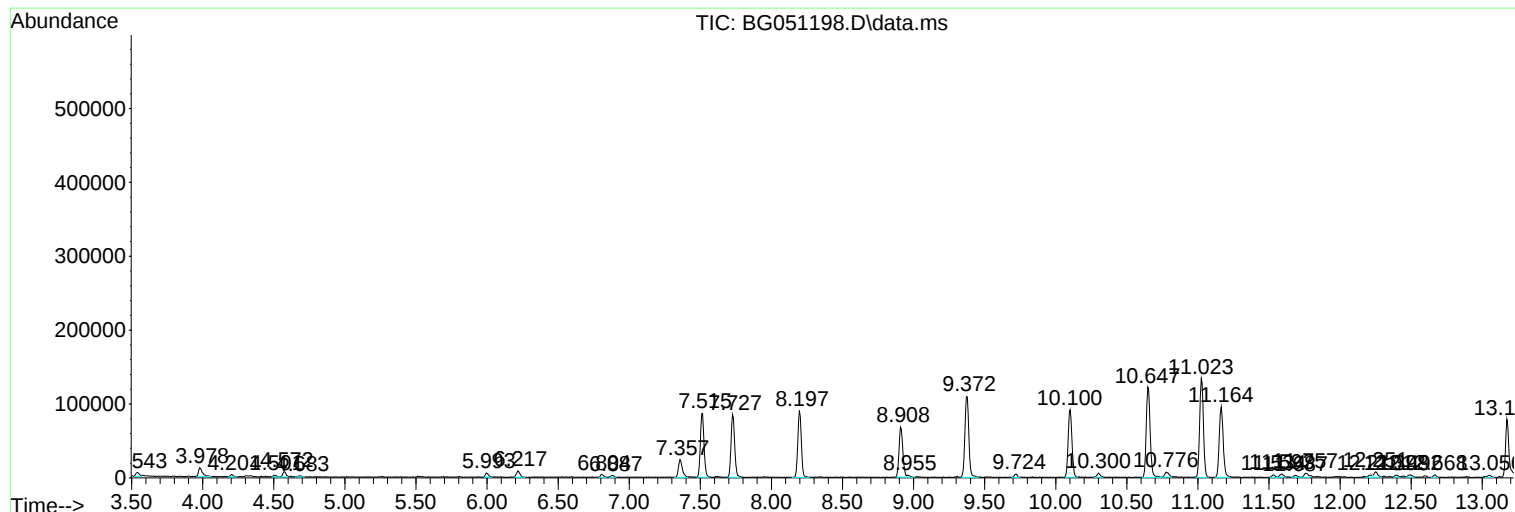
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

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



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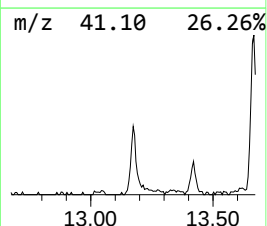
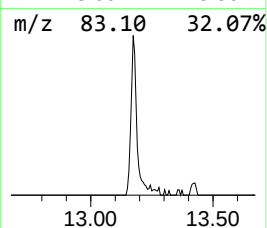
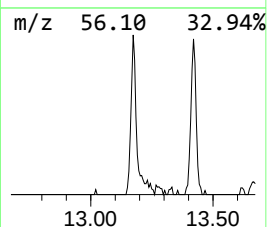
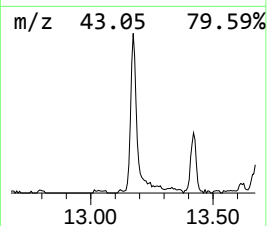
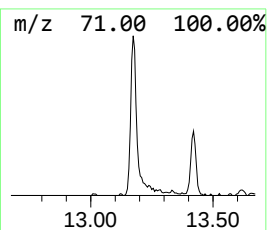
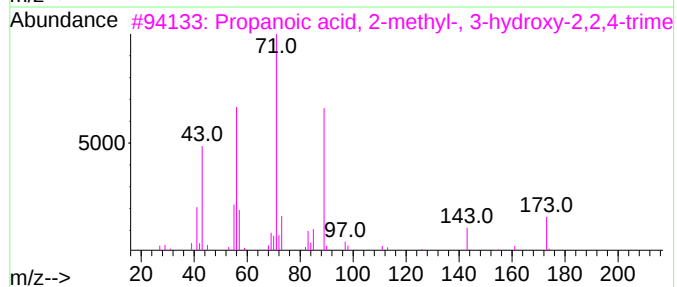
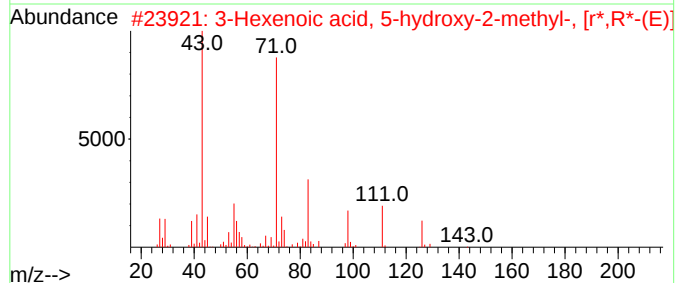
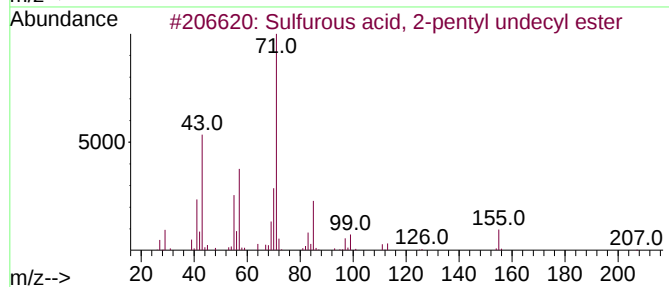
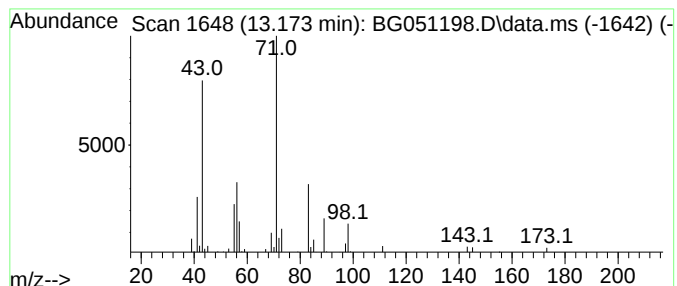
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.173	7.79 ng/ul	135540	Acenaphthene-d10	14.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-pentyl undecyl...	306	C16H34O3S	1000309-16-0	47
2			3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	45
3			Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	000077-68-9	40
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	40
5			Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	38



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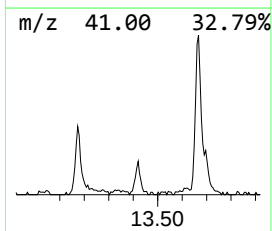
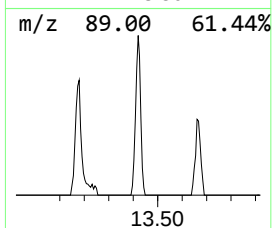
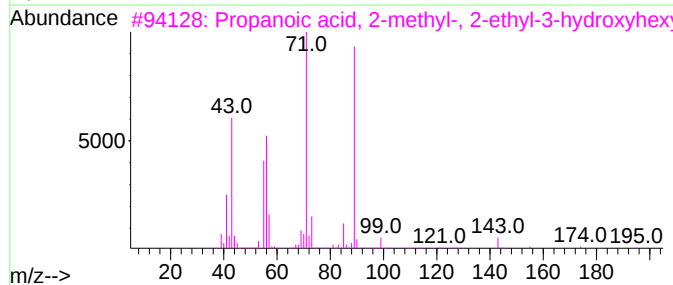
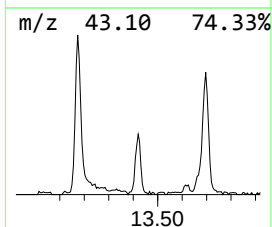
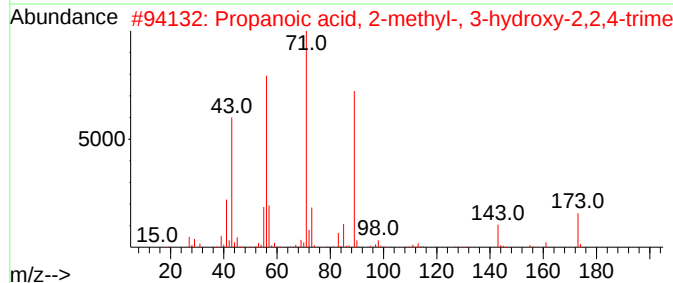
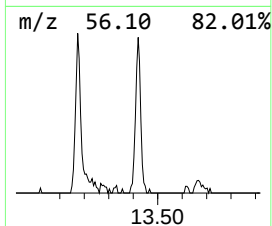
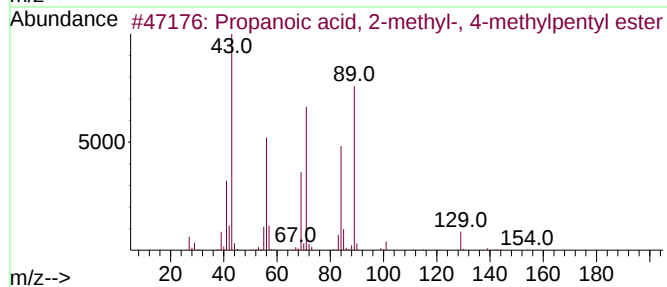
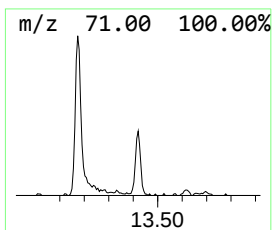
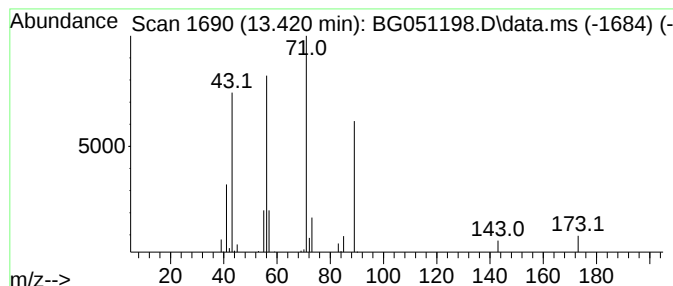
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	3.03 ng/ul	52698	Acenaphthene-d10	14.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 4-met...	172	C10H20O2	035852-44-9	78
2			Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	000077-68-9	78
3			Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	72
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
5			Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	000077-68-9	64



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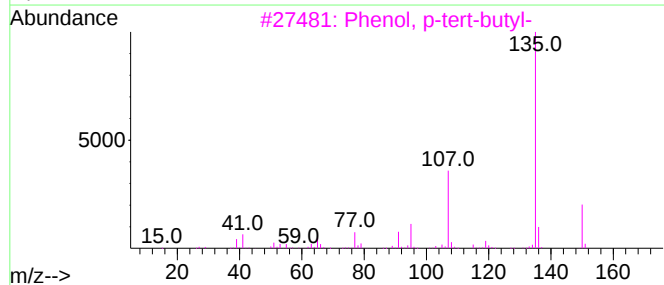
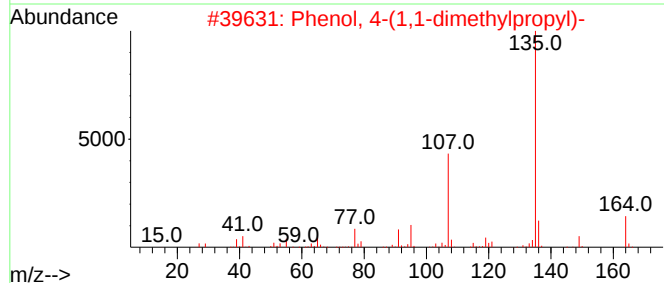
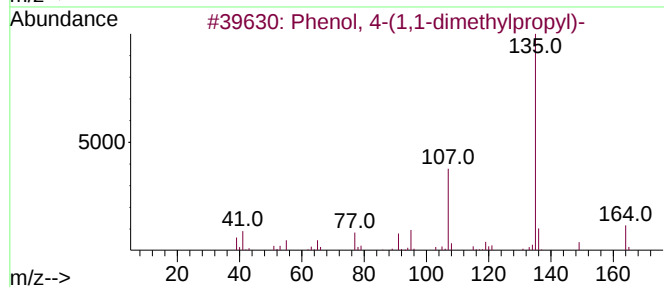
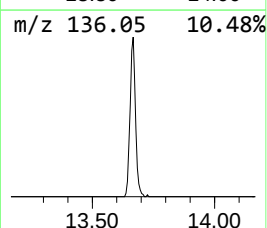
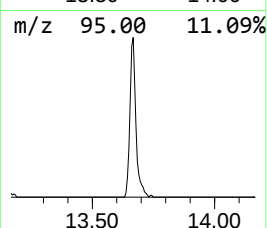
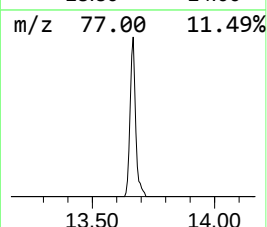
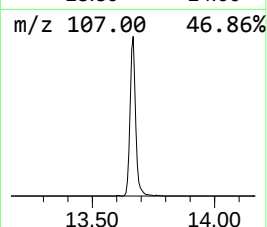
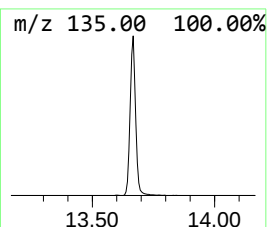
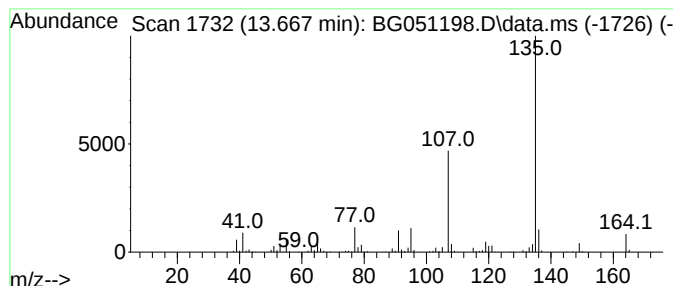
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.667	37.07 ng/ul	644753	Acenaphthene-d10	14.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
3			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
4			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
5			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112321\
Data File : BG051198.D
Acq On : 24 Nov 2021 1:23
Operator : CG/JU
Sample : M4753-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A0018

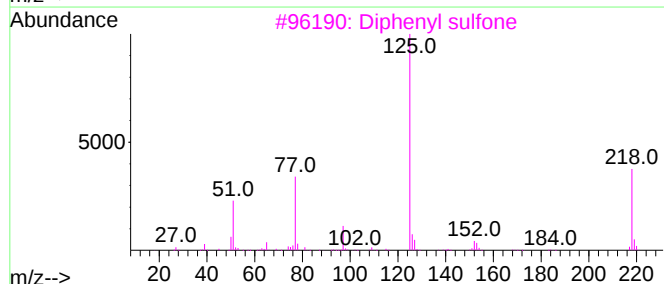
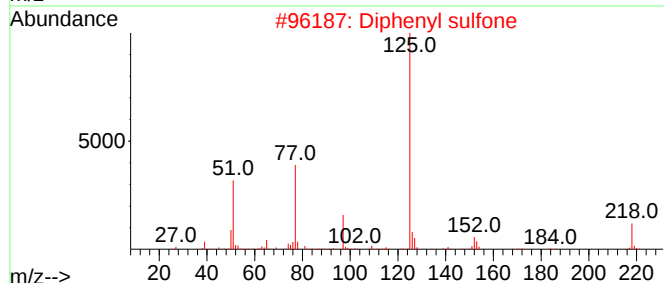
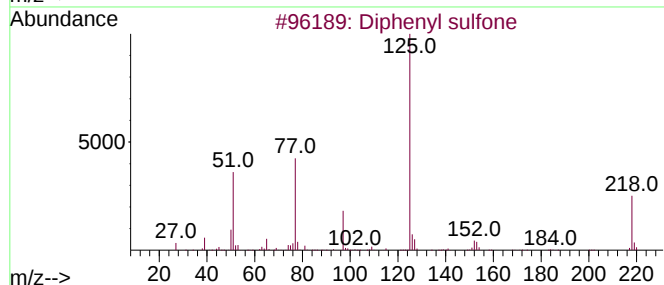
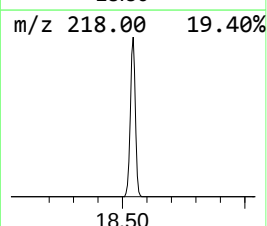
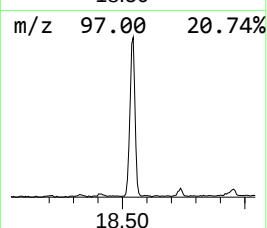
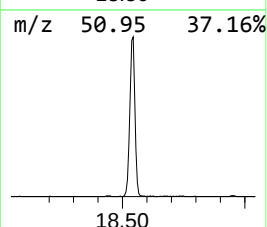
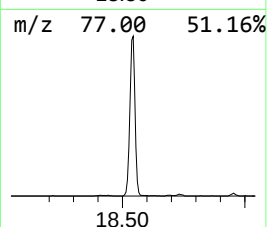
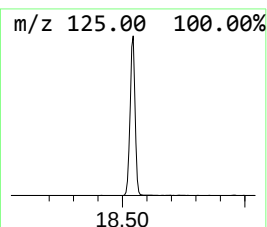
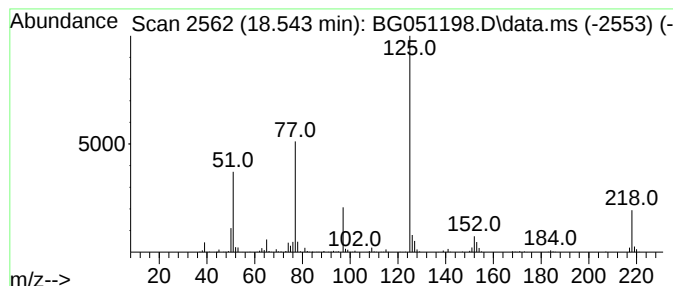
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Diphenyl sulfone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.543	34.18 ng/ul	749227	Phenanthrene-d10	17.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diphenyl sulfone	218	C12H10O2S	000127-63-9	97
2			Diphenyl sulfone	218	C12H10O2S	000127-63-9	96
3			Diphenyl sulfone	218	C12H10O2S	000127-63-9	95
4			2-Propenenitrile, 3-(phenylsulfo...	193	C9H7N02S	001424-51-7	64
5			Benzene, (1-propenylsulfonyl)-, ...	182	C9H10O2S	028691-72-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112321\
Data File : BG051198.D
Acq On : 24 Nov 2021 1:23
Operator : CG/JU
Sample : M4753-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A0018

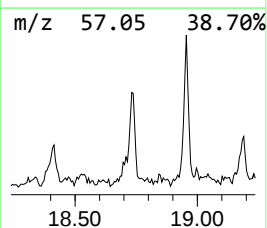
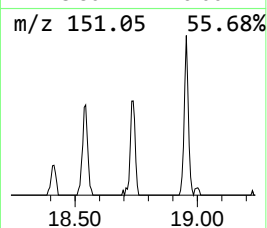
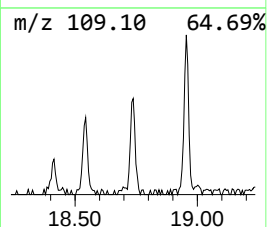
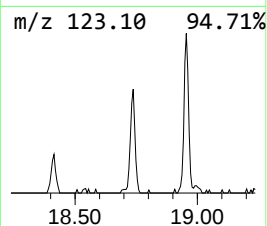
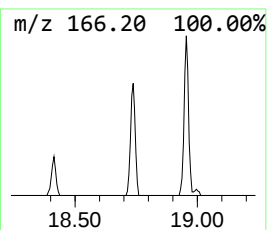
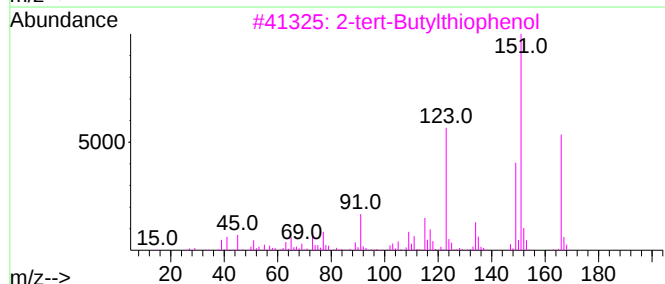
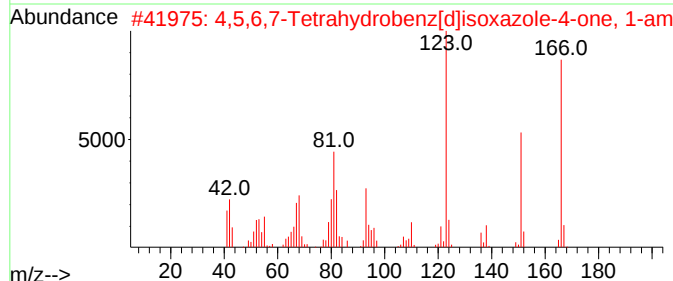
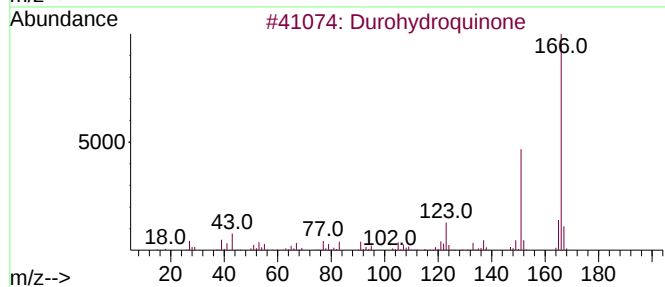
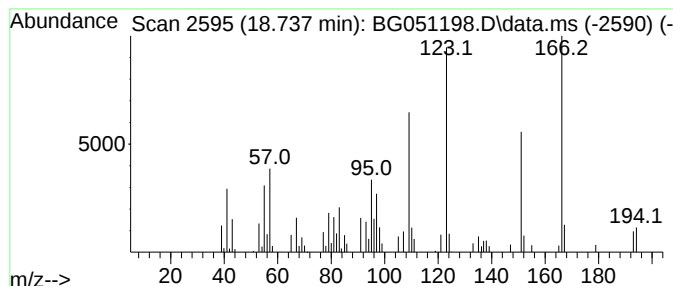
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Durohydroquinone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.737	3.35 ng/ul	73349	Phenanthrene-d10	17.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Durohydroquinone	166	C10H14O2	000527-18-4	58
2			4,5,6,7-Tetrahydrobenz[d]isoxazo...	166	C8H10N2O2	1000131-45-3	52
3			2-tert-Butylthiophenol	166	C10H14S	019728-41-7	50
4			7a-Methyl-3-methylenhexahydrobe...	166	C10H14O2	067498-53-7	49
5			Phenol, 5-methoxy-2,3,4-trimethyl-	166	C10H14O2	034883-02-8	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112321\
Data File : BG051198.D
Acq On : 24 Nov 2021 1:23
Operator : CG/JU
Sample : M4753-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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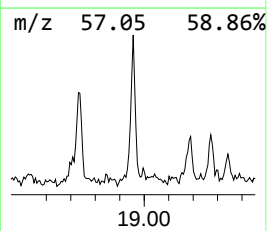
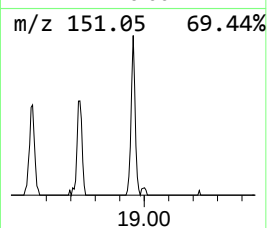
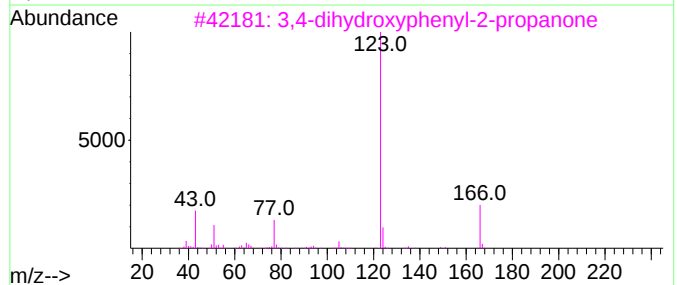
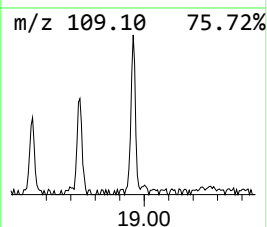
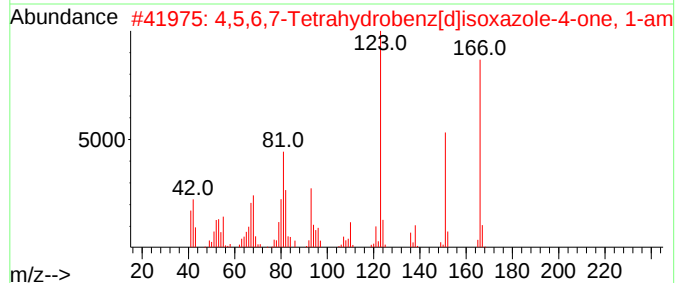
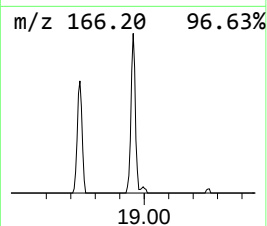
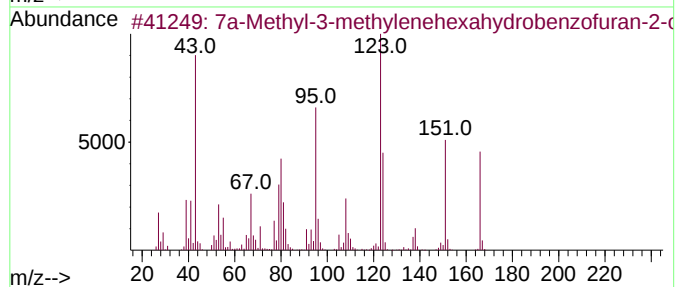
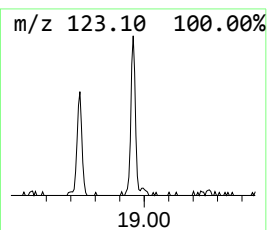
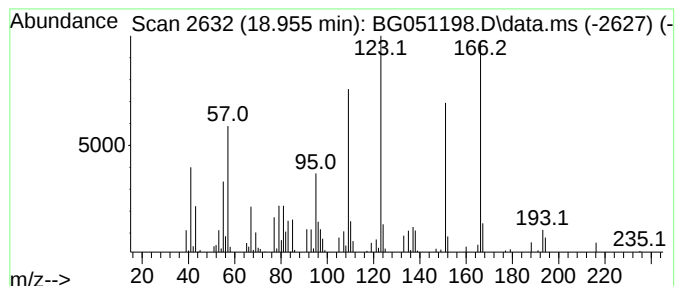
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 7a-Methyl-3-methylenehexahy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.955	4.85 ng/ul	106235	Phenanthrene-d10	17.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7a-Methyl-3-methylenehexahydrobe...	166	C10H14O2	067498-53-7	64
2			4,5,6,7-Tetrahydrobenz[d]isoxazo...	166	C8H10N2O2	1000131-45-3	60
3			3,4-dihydroxyphenyl-2-propanone	166	C9H10O3	1000378-94-2	43
4			Phenol, 5-methoxy-2,3,4-trimethyl-	166	C10H14O2	034883-02-8	42
5			Phenol, 3-methoxy-2,4,6-trimethyl-	166	C10H14O2	034883-05-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112321\
Data File : BG051198.D
Acq On : 24 Nov 2021 1:23
Operator : CG/JU
Sample : M4753-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A0018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.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
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Propanoic acid,...	13.420	3.0	ng/ul	52698	3	14.830	347853	20.0
Phenol, 4-(1,1-...	13.667	37.1	ng/ul	644753	3	14.830	347853	20.0
Diphenyl sulfone	18.543	34.2	ng/ul	749227	4	17.580	438408	20.0
Durohydroquinone	18.737	3.4	ng/ul	73349	4	17.580	438408	20.0
7a-Methyl-3-met...	18.955	4.8	ng/ul	106235	4	17.580	438408	20.0