

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030623\
 Data File : BG056853.D
 Acq On : 6 Mar 2023 22:56
 Operator : CG/JU
 Sample : 01712-12
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DBZX4

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-BG022323.M
 Title : SVOA CALIBRATION

Signal : TIC: BG056853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.139	99	102	115	rBV2	45883	75686	15.69%	1.245%
2	7.083	599	603	608	rVB3	6798	9841	2.04%	0.162%
3	7.541	675	681	689	rBV	83680	143432	29.74%	2.359%
4	7.717	705	711	719	rBV	53660	89152	18.49%	1.466%
5	7.941	743	749	757	rVB	72468	123865	25.68%	2.037%
6	8.417	824	830	837	rVB	72356	120143	24.91%	1.976%
7	8.728	878	883	887	rBV2	5957	8084	1.68%	0.133%
8	9.104	941	947	955	rVB	96913	162787	33.75%	2.677%
9	9.592	1023	1030	1038	rVB	82710	142189	29.48%	2.338%
10	9.715	1049	1051	1054	rBV	797	677	0.14%	0.011%
11	9.968	1090	1094	1096	rBV3	1168	1297	0.27%	0.021%
12	10.132	1120	1122	1124	rBV	827	661	0.14%	0.011%
13	10.320	1147	1154	1161	rBV	71042	121645	25.22%	2.000%
14	10.861	1239	1246	1255	rVB	105182	184447	38.24%	3.033%
15	11.254	1306	1313	1322	rVB	105865	184483	38.25%	3.034%
16	11.378	1326	1334	1340	rBV2	80063	144623	29.99%	2.378%
17	12.805	1573	1577	1580	rBV2	1286	1758	0.36%	0.029%
18	13.422	1680	1682	1686	rBV2	448	751	0.16%	0.012%
19	13.816	1746	1749	1751	rVB3	1625	1342	0.28%	0.022%
20	13.898	1757	1763	1768	rBV5	4627	6642	1.38%	0.109%
21	14.274	1823	1827	1828	rBV	672	813	0.17%	0.013%
22	14.345	1833	1839	1844	rVV2	69204	99388	20.61%	1.634%
23	14.404	1844	1849	1856	rVB	183867	270010	55.99%	4.440%
24	14.721	1896	1903	1912	rVB	208538	325537	67.50%	5.353%
25	14.850	1920	1925	1927	rBV2	970	1272	0.26%	0.021%
26	14.968	1939	1945	1949	rBV3	17939	25548	5.30%	0.420%
27	15.021	1949	1954	1960	rVV	172072	262457	54.42%	4.316%
28	15.073	1960	1963	1966	rVB3	1712	1789	0.37%	0.029%
29	15.179	1974	1981	1989	rBV	79648	126415	26.21%	2.079%
30	15.250	1990	1993	1997	rVB2	2766	3472	0.72%	0.057%
31	15.314	2001	2004	2005	rBV2	941	1130	0.23%	0.019%
32	15.585	2049	2050	2055	rBV2	514	731	0.15%	0.012%
33	15.820	2087	2090	2093	rBV2	767	953	0.20%	0.016%
34	15.884	2097	2101	2103	rBV	753	722	0.15%	0.012%
35	16.002	2115	2121	2128	rBV	265240	408579	84.72%	6.719%
36	16.102	2132	2138	2146	rBV2	70031	103868	21.54%	1.708%

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37	16.243	2158	2162	2167	rBV3	693	1489	0.31%	0.024%
38	16.354	2173	2181	2187	rBV	91244	131110	27.19%	2.156%
39	16.466	2194	2200	2204	rBV3	5177	7150	1.48%	0.118%
40	16.695	2237	2239	2243	rBV2	989	1368	0.28%	0.022%
41	16.912	2273	2276	2280	rVB2	2203	2639	0.55%	0.043%
42	17.189	2320	2323	2326	rVB	646	829	0.17%	0.014%
43	17.347	2348	2350	2356	rVB2	906	1229	0.25%	0.020%
44	17.447	2363	2367	2368	rBV	1704	1930	0.40%	0.032%
45	17.612	2392	2395	2398	rBV	1022	1273	0.26%	0.021%
46	17.753	2412	2419	2425	rBV	212965	314076	65.12%	5.165%
47	17.852	2429	2436	2443	rVB	275828	406372	84.26%	6.682%
48	17.911	2443	2446	2447	rBV	1893	1623	0.34%	0.027%
49	17.929	2447	2449	2455	rVB3	1647	2859	0.59%	0.047%
50	17.982	2455	2458	2459	rBV	844	673	0.14%	0.011%
51	18.099	2475	2478	2483	rBV3	934	1383	0.29%	0.023%
52	18.199	2492	2495	2501	rVB	1150	1770	0.37%	0.029%
53	18.246	2501	2503	2504	rBV	1115	832	0.17%	0.014%
54	18.293	2509	2511	2515	rVB	867	967	0.20%	0.016%
55	18.340	2517	2519	2521	rBV	698	678	0.14%	0.011%
56	18.358	2521	2522	2525	rVB	757	687	0.14%	0.011%
57	18.387	2525	2527	2528	rBV	887	760	0.16%	0.012%
58	18.487	2542	2544	2550	rVB3	3770	5135	1.06%	0.084%
59	18.552	2553	2555	2557	rBV2	890	798	0.17%	0.013%
60	18.593	2557	2562	2573	rBV	46248	76545	15.87%	1.259%
61	18.693	2578	2579	2582	rVB2	1720	847	0.18%	0.014%
62	18.746	2586	2588	2589	rBV	1243	907	0.19%	0.015%
63	18.834	2601	2603	2607	rBV3	885	1114	0.23%	0.018%
64	18.904	2613	2615	2619	rBV4	1617	1903	0.39%	0.031%
65	18.963	2621	2625	2628	rVV3	3048	4596	0.95%	0.076%
66	19.004	2628	2632	2637	rVB2	12707	15687	3.25%	0.258%
67	19.157	2655	2658	2659	rBV	805	868	0.18%	0.014%
68	19.204	2661	2666	2671	rVV4	4856	6988	1.45%	0.115%
69	19.251	2671	2674	2676	rVV4	1316	1179	0.24%	0.019%
70	19.445	2705	2707	2711	rVB3	1324	1385	0.29%	0.023%
71	19.515	2717	2719	2720	rBV2	1086	911	0.19%	0.015%
72	19.580	2728	2730	2731	rBV2	1511	1053	0.22%	0.017%
73	19.686	2741	2748	2750	rBV5	4721	8378	1.74%	0.138%
74	19.744	2755	2758	2762	rVB3	3847	6241	1.29%	0.103%
75	19.844	2771	2775	2780	rBV4	11858	15378	3.19%	0.253%
76	19.979	2796	2798	2803	rBV5	1814	2781	0.58%	0.046%

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77	20.115	2814	2821	2827	rBV	337570	482285	100.00%	7.931%
78	20.467	2879	2881	2886	rVB	16688	18803	3.90%	0.309%
79	20.538	2889	2893	2895	rBV3	8831	11155	2.31%	0.183%
80	20.855	2945	2947	2949	rBV3	2990	3141	0.65%	0.052%
81	21.025	2973	2976	2980	rBV6	5045	9267	1.92%	0.152%
82	21.278	3016	3019	3024	rVB5	7854	11018	2.28%	0.181%
83	21.460	3045	3050	3056	rVB	152758	206293	42.77%	3.392%
84	21.636	3076	3080	3091	rVB6	29505	53281	11.05%	0.876%
85	22.065	3146	3153	3159	rVB2	182687	323788	67.14%	5.324%
86	25.191	3683	3685	3686	rBV	3294	1656	0.34%	0.027%
87	25.350	3701	3712	3725	rVB3	141643	440741	91.39%	7.248%
88	25.590	3743	3753	3768	rVB2	105133	326979	67.80%	5.377%
89	25.773	3782	3784	3787	rBV3	2617	2199	0.46%	0.036%

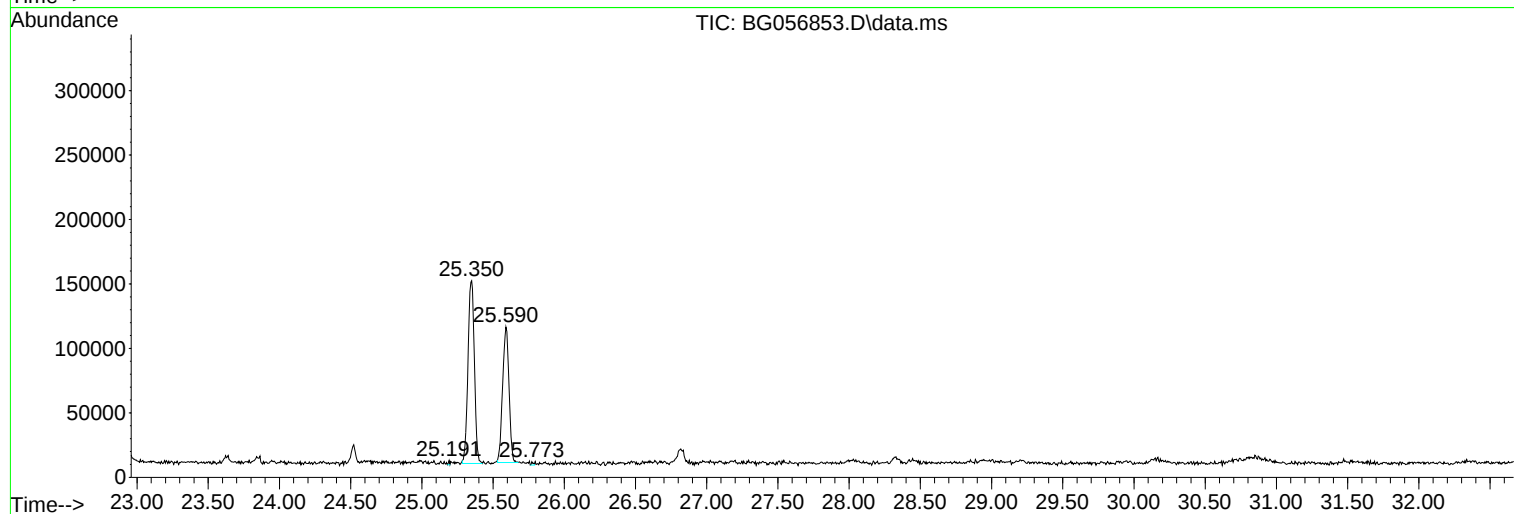
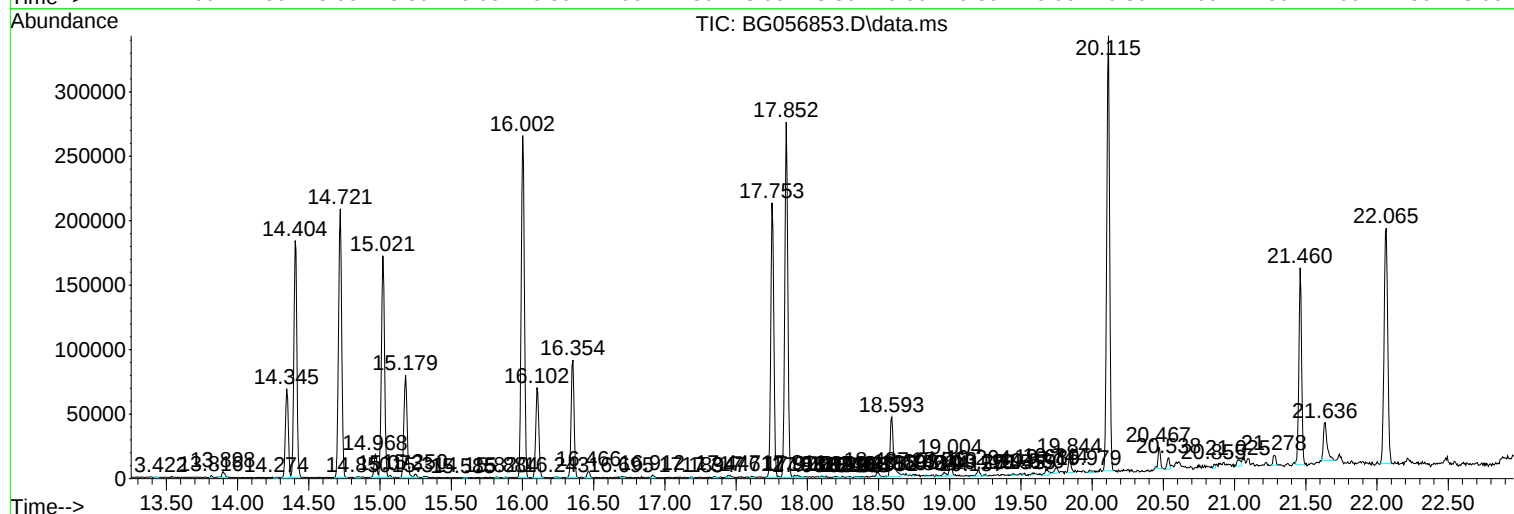
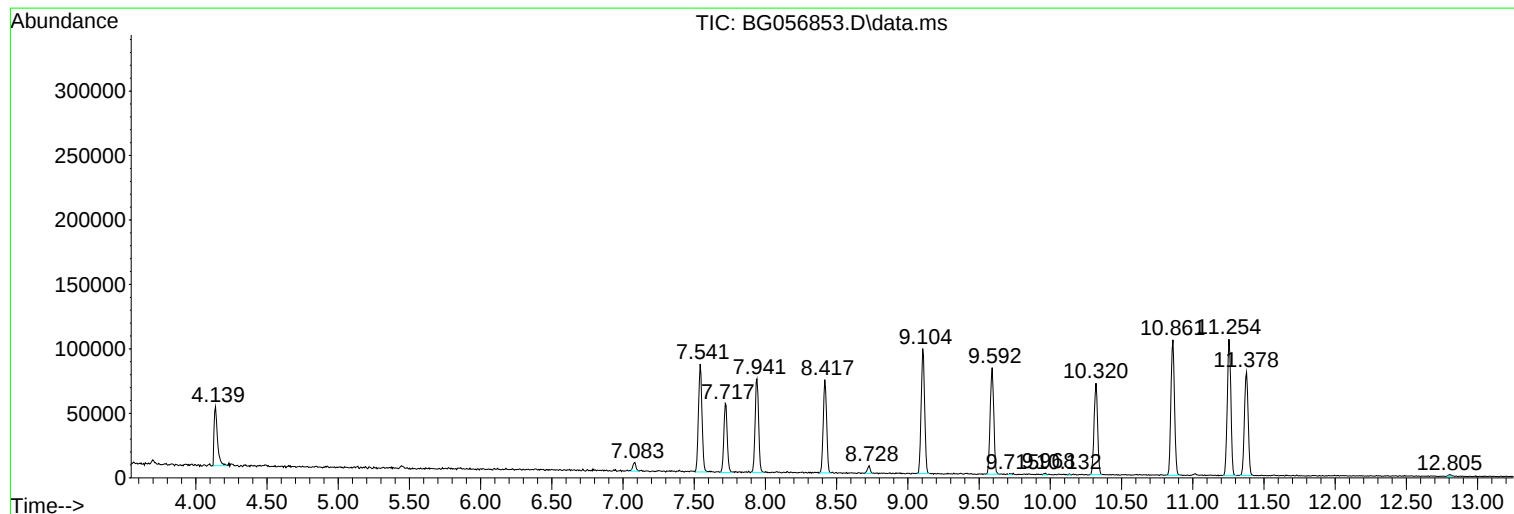
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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



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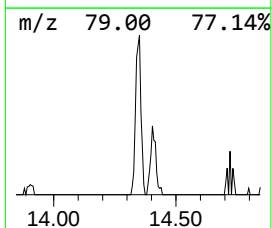
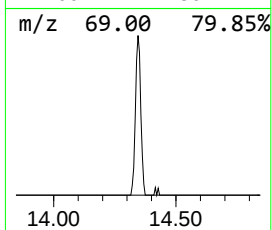
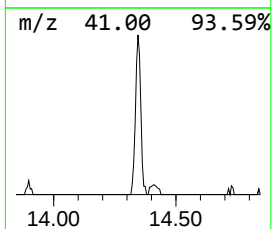
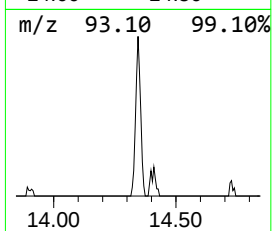
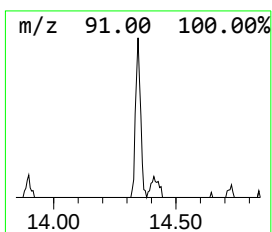
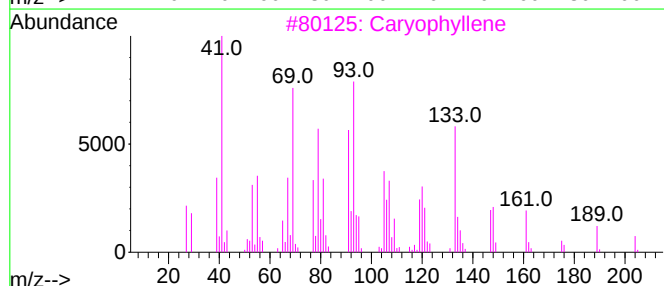
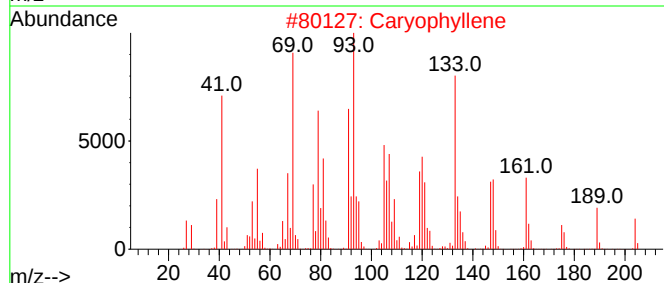
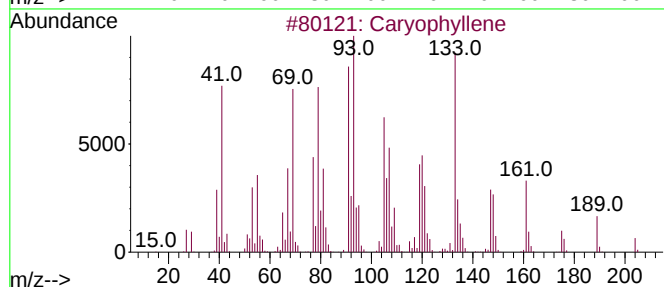
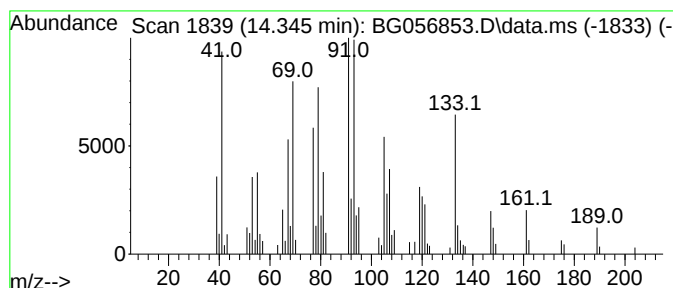
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Caryophyllene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	7.57 ng/ul	99388	Acenaphthene-d10	15.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	93
2			Caryophyllene	204	C15H24	000087-44-5	91
3			Caryophyllene	204	C15H24	000087-44-5	91
4			Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	87
5			Caryophyllene	204	C15H24	000087-44-5	86



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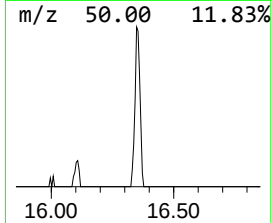
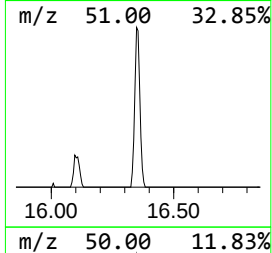
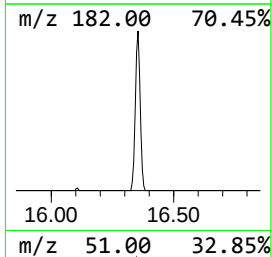
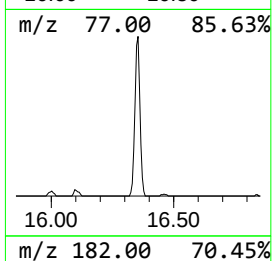
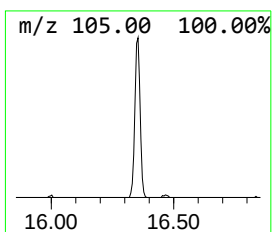
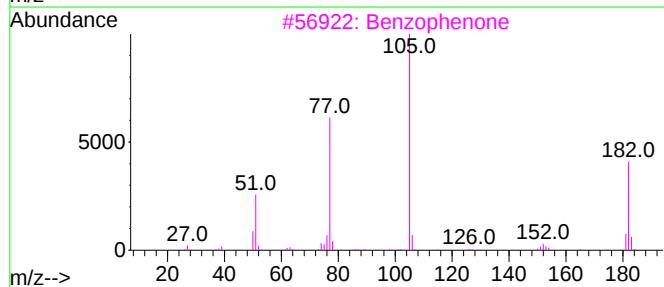
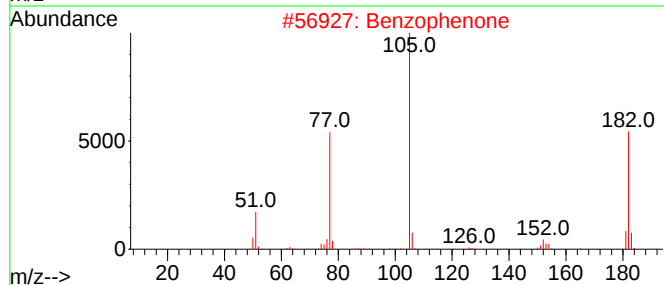
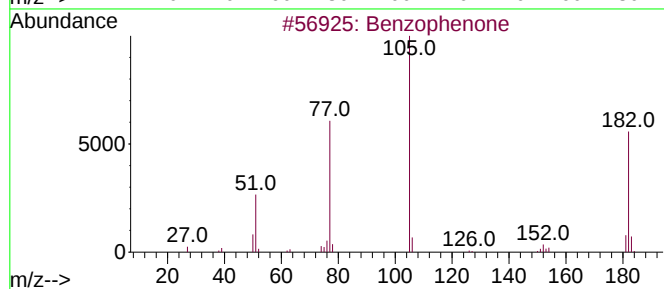
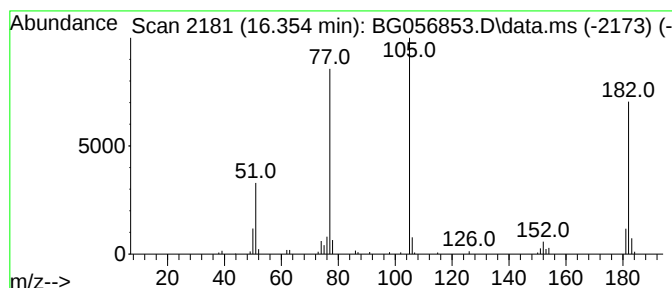
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	9.99 ng/ul	131110	Acenaphthene-d10	15.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	95
3			Benzophenone	182	C13H10O	000119-61-9	91
4			Benzophenone	182	C13H10O	000119-61-9	90
5			Benzophenone	182	C13H10O	000119-61-9	62



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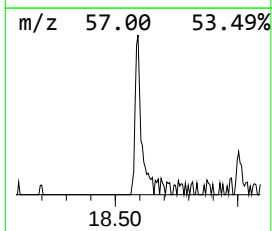
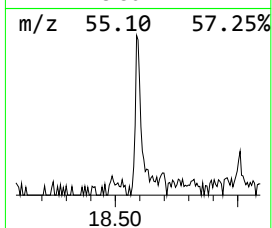
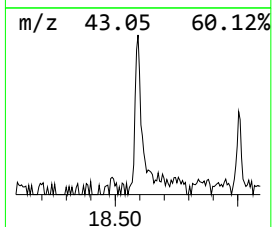
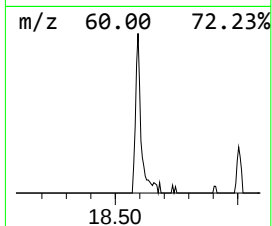
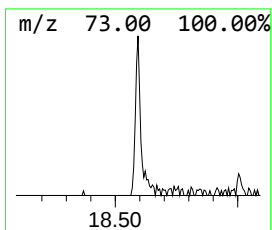
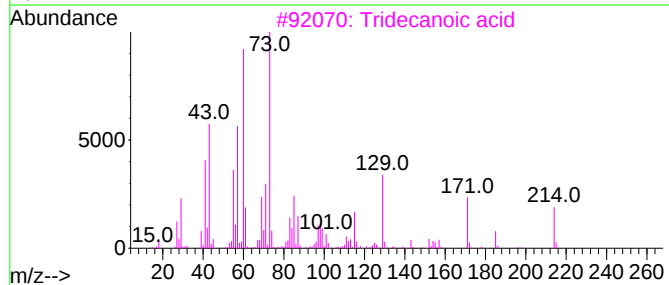
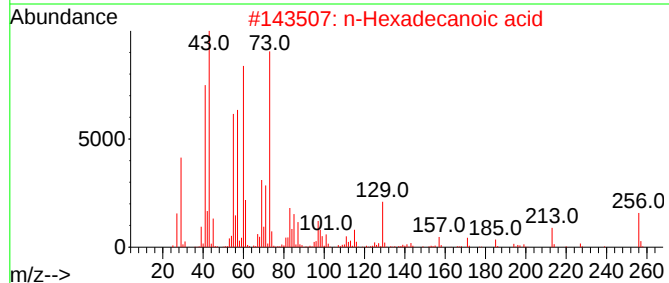
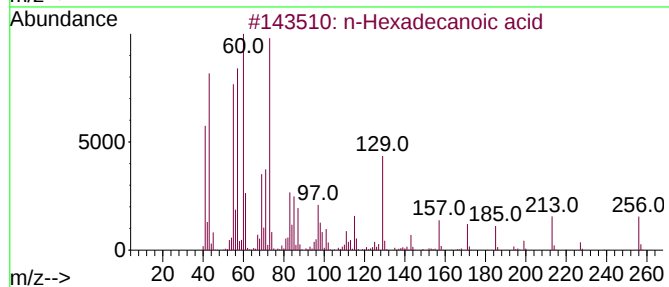
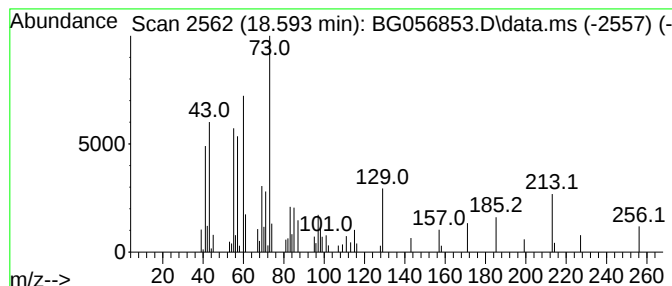
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.593	4.87 ng/ul	76545	Phenanthrene-d10	17.753

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99		
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95		
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93		
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89		
5	Tridecanoic acid	214	C13H26O2	000638-53-9	86		



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DBZX4

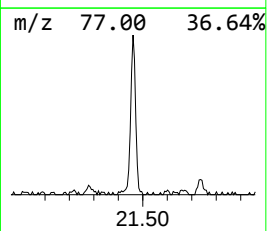
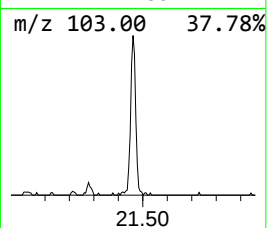
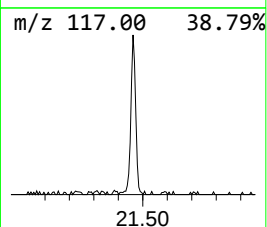
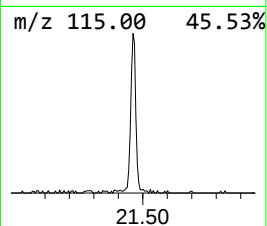
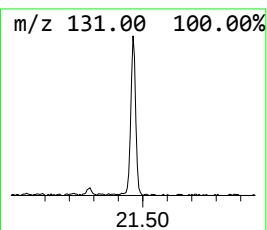
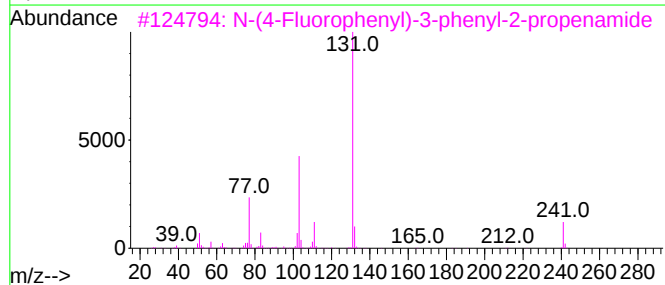
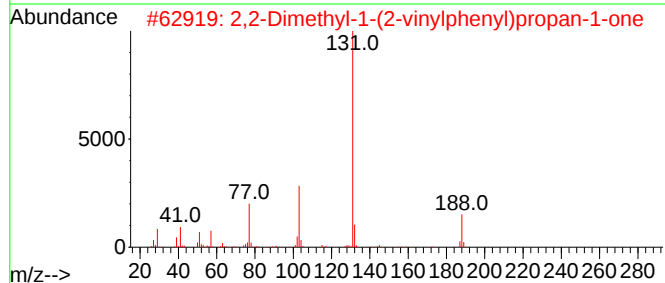
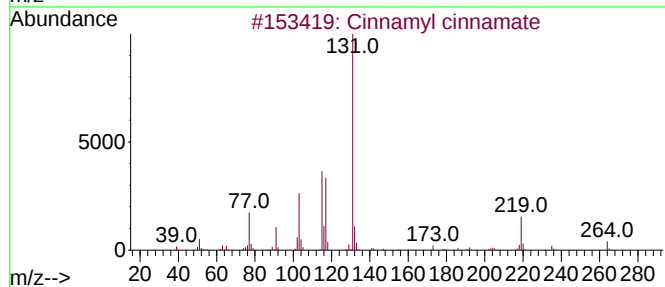
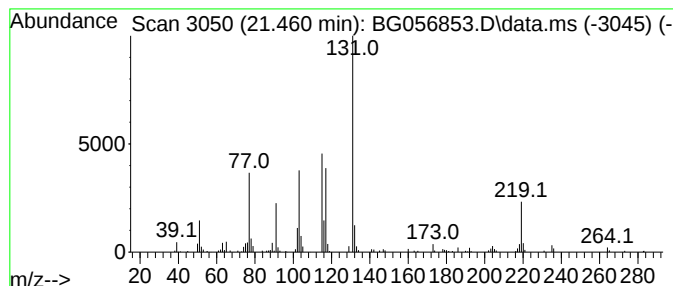
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.460	12.74 ng/ul	206293	Chrysene-d12	22.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	46
3			N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	43
4			(2E)-N-(4-Methylphenyl)-3-phenyl...	237	C16H15NO	134430-88-9	43
5			(2E)-N-(2-Fluorophenyl)-3-phenyl...	241	C15H12FNO	025893-50-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030623\
Data File : BG056853.D
Acq On : 6 Mar 2023 22:56
Operator : CG/JU
Sample : 01712-12
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZX4

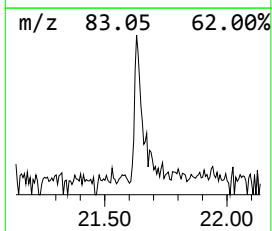
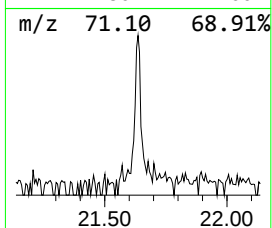
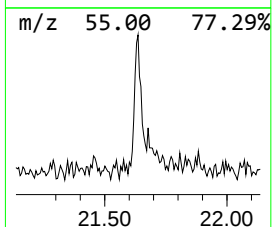
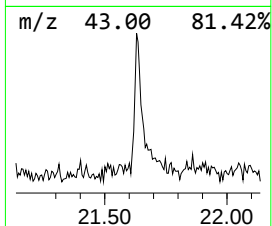
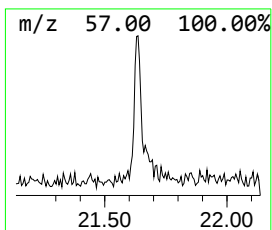
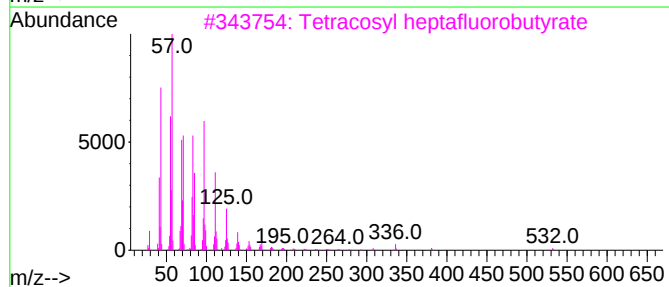
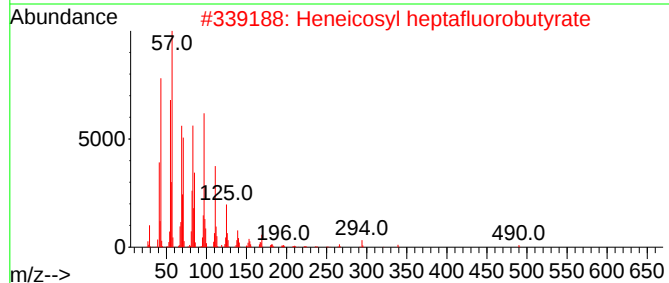
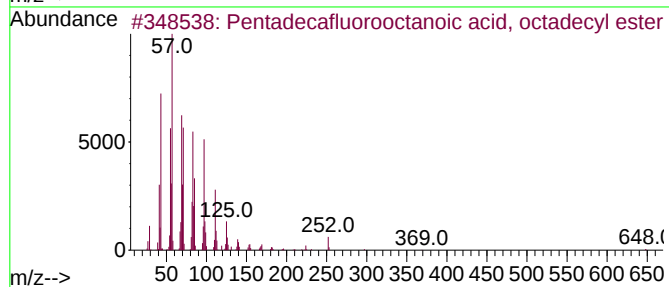
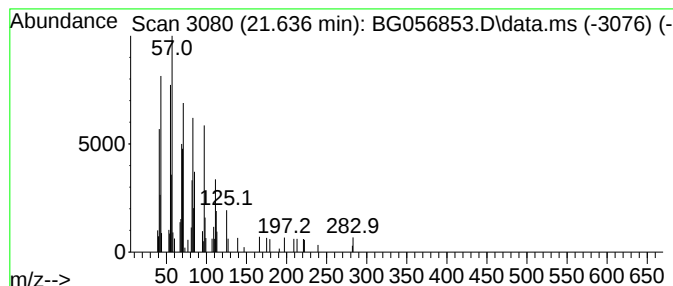
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.636	3.29 ng/ul	53281	Chrysene-d12	22.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
3			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	86
5			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030623\
Data File : BG056853.D
Acq On : 6 Mar 2023 22:56
Operator : CG/JU
Sample : 01712-12
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZX4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.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
Caryophyllene	14.345	7.6	ng/u1	99388	3	15.021	262457	20.0
Benzophenone	16.354	10.0	ng/u1	131110	3	15.021	262457	20.0
n-Hexadecanoic ...	18.593	4.9	ng/u1	76545	4	17.753	314076	20.0
Cinnamyl cinnamate	21.460	12.7	ng/u1	206293	5	22.065	323788	20.0
Pentadecafluoro...	21.636	3.3	ng/u1	53281	5	22.065	323788	20.0