

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122324\
 Data File : BG063820.D
 Acq On : 24 Dec 2024 15:28
 Operator : RC/JU
 Sample : P5333-13
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E2915

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-BG121124.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG063820.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.666	94	98	109	rBV	272408	443785	17.69%	1.292%
2	5.387	387	391	394	rBV4	7152	11113	0.44%	0.032%
3	5.446	399	401	404	rBV3	11592	11352	0.45%	0.033%
4	5.822	460	465	468	rVB7	9999	16994	0.68%	0.049%
5	6.445	567	571	572	rBV4	6148	8403	0.33%	0.024%
6	6.609	595	599	604	rBV4	5076	11044	0.44%	0.032%
7	6.938	652	655	656	rVV2	8458	8369	0.33%	0.024%
8	6.985	657	663	676	rVB3	340017	685830	27.33%	1.997%
9	7.132	682	688	695	rBV	291811	492588	19.63%	1.435%
10	7.338	716	723	732	rVB	330169	556609	22.18%	1.621%
11	7.702	783	785	788	rBV3	5115	6831	0.27%	0.020%
12	7.796	795	801	809	rBV	432340	710401	28.31%	2.069%
13	7.861	810	812	816	rVV5	6498	7247	0.29%	0.021%
14	8.008	834	837	839	rBV3	4710	7230	0.29%	0.021%
15	8.049	841	844	845	rBV2	9574	9197	0.37%	0.027%
16	8.249	877	878	883	rBV	7894	10244	0.41%	0.030%
17	8.519	918	924	932	rBV2	289770	517911	20.64%	1.508%
18	8.619	938	941	946	rVB4	8288	12176	0.49%	0.035%
19	8.954	990	998	1006	rVV	363570	645445	25.72%	1.880%
20	9.024	1006	1010	1015	rVV3	21623	43121	1.72%	0.126%
21	9.118	1022	1026	1029	rVV4	11539	16781	0.67%	0.049%
22	9.148	1029	1031	1033	rVB	8039	6735	0.27%	0.020%
23	9.512	1089	1093	1101	rVB4	40484	64675	2.58%	0.188%
24	9.676	1112	1121	1128	rBV2	310823	553094	22.04%	1.611%
25	9.988	1170	1174	1175	rBV	8735	11779	0.47%	0.034%
26	10.223	1207	1214	1224	rBV	414106	771375	30.74%	2.246%
27	10.440	1249	1251	1253	rBV4	7208	6759	0.27%	0.020%
28	10.587	1269	1276	1282	rBV	632440	1115417	44.45%	3.248%
29	10.728	1292	1300	1310	rBV	327753	632123	25.19%	1.841%
30	10.893	1325	1328	1331	rBV2	8322	6706	0.27%	0.020%
31	11.122	1362	1367	1370	rBV5	16797	28695	1.14%	0.084%
32	11.286	1392	1395	1397	rBV3	5950	7737	0.31%	0.023%
33	11.609	1447	1450	1453	rBV5	11134	12327	0.49%	0.036%
34	12.015	1514	1519	1524	rVV6	15948	28282	1.13%	0.082%
35	12.085	1528	1531	1536	rVB6	10066	10907	0.43%	0.032%
36	12.179	1544	1547	1550	rVV2	10887	12679	0.51%	0.037%

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37	12.256	1553	1560	1565	rVV	31411	60821	2.42%	0.177%
38	12.391	1579	1583	1585	rVV2	8716	10232	0.41%	0.030%
39	12.473	1592	1597	1600	rVV4	15762	24144	0.96%	0.070%
40	12.978	1678	1683	1687	rVB7	8860	17774	0.71%	0.052%
41	13.260	1724	1731	1738	rVV4	29384	54118	2.16%	0.158%
42	13.360	1744	1748	1752	rBV6	10845	15507	0.62%	0.045%
43	13.413	1752	1757	1763	rVV3	55517	99528	3.97%	0.290%
44	13.601	1785	1789	1792	rBV5	17029	28311	1.13%	0.082%
45	13.713	1805	1808	1811	rBV3	6894	9972	0.40%	0.029%
46	13.754	1811	1815	1821	rVV6	19696	34383	1.37%	0.100%
47	13.842	1821	1830	1835	rVV	879370	1311169	52.25%	3.818%
48	13.889	1835	1838	1842	rVV	109935	160027	6.38%	0.466%
49	13.924	1842	1844	1848	rVB3	19778	20770	0.83%	0.060%
50	14.001	1854	1857	1858	rVB2	8682	7442	0.30%	0.022%
51	14.130	1873	1879	1888	rVB2	1007937	1492257	59.47%	4.346%
52	14.259	1899	1901	1903	rBV	11033	6749	0.27%	0.020%
53	14.336	1911	1914	1920	rVB5	22420	30653	1.22%	0.089%
54	14.441	1924	1932	1938	rBV	1168015	1775349	70.75%	5.170%
55	14.494	1938	1941	1946	rVV6	23887	37249	1.48%	0.108%
56	14.559	1951	1952	1958	rVB2	9335	13336	0.53%	0.039%
57	14.676	1965	1972	1985	rBV2	209012	453260	18.06%	1.320%
58	14.841	1996	2000	2005	rVB5	22495	28257	1.13%	0.082%
59	15.158	2051	2054	2057	rBV4	7039	7276	0.29%	0.021%
60	15.235	2062	2067	2073	rBV	70633	107753	4.29%	0.314%
61	15.293	2075	2077	2081	rVB4	15437	14463	0.58%	0.042%
62	15.434	2094	2101	2108	rBV	1239759	1789140	71.30%	5.210%
63	15.534	2114	2118	2119	rBV4	7266	9032	0.36%	0.026%
64	15.569	2119	2124	2130	rVV2	198427	298430	11.89%	0.869%
65	15.799	2157	2163	2169	rVV	649184	884977	35.27%	2.577%
66	15.910	2178	2182	2185	rBV5	6608	10240	0.41%	0.030%
67	16.163	2220	2225	2226	rBV3	30187	44704	1.78%	0.130%
68	16.233	2235	2237	2240	rBV3	6691	8506	0.34%	0.025%
69	16.280	2244	2245	2248	rBV3	9222	9800	0.39%	0.029%
70	16.363	2257	2259	2263	rVB4	18974	20990	0.84%	0.061%
71	16.474	2275	2278	2279	rBV3	10555	12520	0.50%	0.036%
72	16.545	2288	2290	2296	rVB7	18225	27348	1.09%	0.080%
73	16.592	2296	2298	2299	rBV	9285	8857	0.35%	0.026%
74	16.686	2312	2314	2315	rBV2	7216	6658	0.27%	0.019%
75	16.727	2318	2321	2325	rVV6	16015	23411	0.93%	0.068%
76	16.850	2337	2342	2347	rBV4	25164	46526	1.85%	0.135%

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77	16.915	2348	2353	2356	rBV3	34424	54505	2.17%	0.159%
78	16.950	2356	2359	2362	rVB5	25297	31613	1.26%	0.092%
79	17.191	2393	2400	2405	rBV	1561412	2322235	92.55%	6.763%
80	17.232	2405	2407	2411	rVV	126207	154757	6.17%	0.451%
81	17.291	2411	2417	2426	rVB2	1313320	1923691	76.67%	5.602%
82	17.467	2444	2447	2448	rBV3	12155	12038	0.48%	0.035%
83	17.849	2510	2512	2514	rBV3	10504	12529	0.50%	0.036%
84	18.037	2540	2544	2547	rBV5	110680	188772	7.52%	0.550%
85	18.096	2550	2554	2564	rVB3	224344	478611	19.07%	1.394%
86	18.255	2578	2581	2586	rVB4	48377	64268	2.56%	0.187%
87	18.995	2703	2707	2713	rBV4	61568	124149	4.95%	0.362%
88	19.118	2724	2728	2737	rVB	348594	483975	19.29%	1.409%
89	19.253	2747	2751	2759	rVB	197419	284015	11.32%	0.827%
90	19.588	2803	2808	2823	rBV2	1441606	2329816	92.85%	6.785%
91	20.934	3033	3037	3041	rBV	115770	143406	5.72%	0.418%
92	21.104	3063	3066	3070	rBV2	151881	244459	9.74%	0.712%
93	21.216	3082	3085	3091	rVB2	211839	282793	11.27%	0.824%
94	21.339	3101	3106	3116	rBV	664349	1123979	44.79%	3.273%
95	21.439	3117	3123	3129	rBV2	1527079	2484303	99.01%	7.235%
96	21.774	3175	3180	3187	rBV	416123	661065	26.35%	1.925%
97	22.191	3248	3251	3256	rBV3	129171	205106	8.17%	0.597%
98	22.250	3256	3261	3271	rVB2	356438	740726	29.52%	2.157%
99	24.242	3594	3600	3608	rBV	410878	954207	38.03%	2.779%
100	24.453	3628	3636	3649	rVB	959151	2509177	100.00%	7.307%

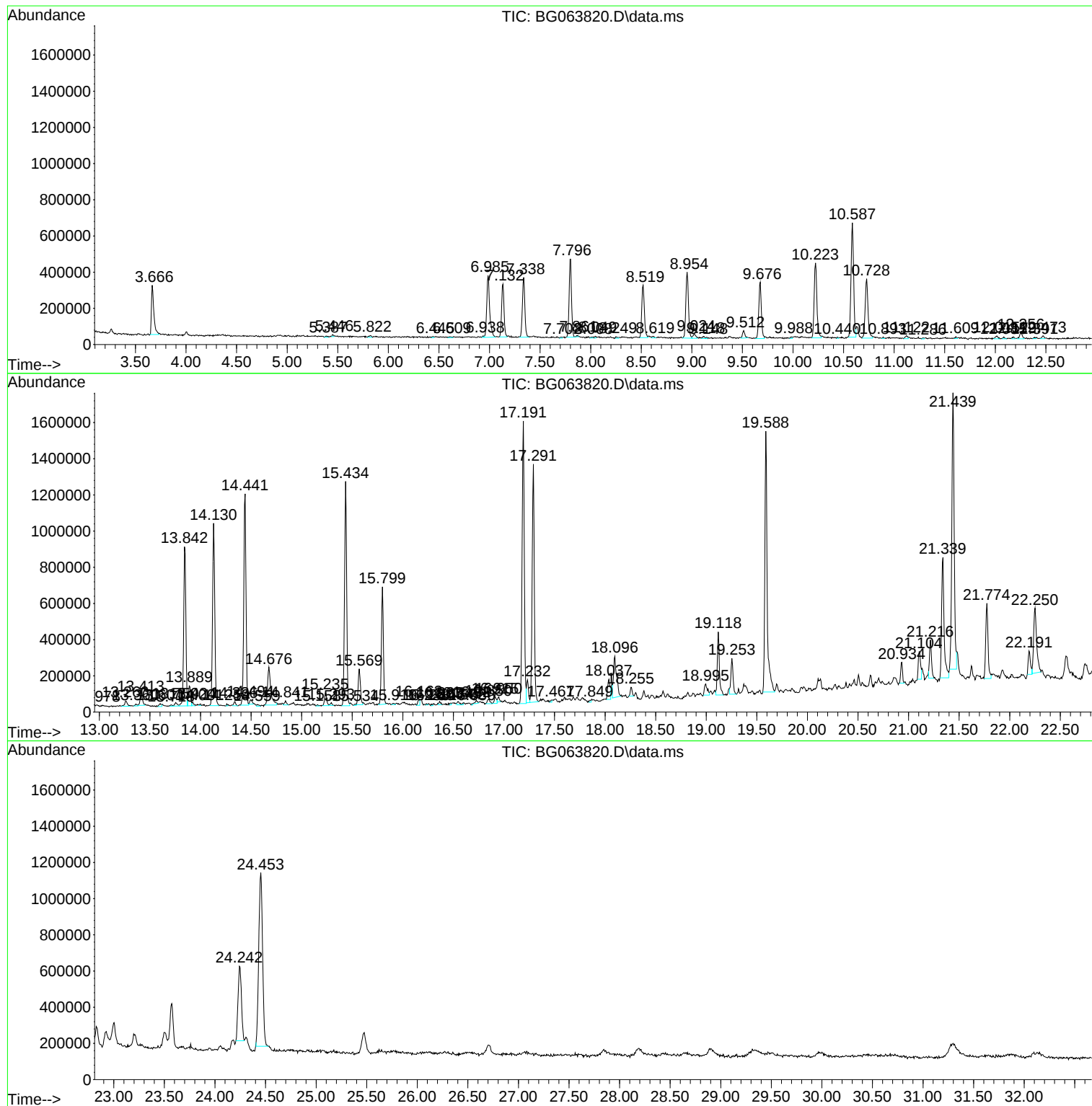
Sum of corrected areas: 34338095

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121124.MA.M
Quant Title : SVOA CALIBRATION

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



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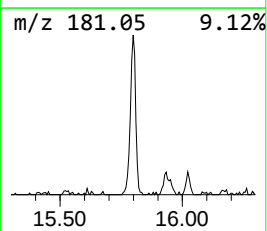
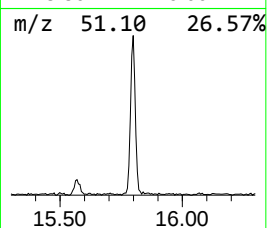
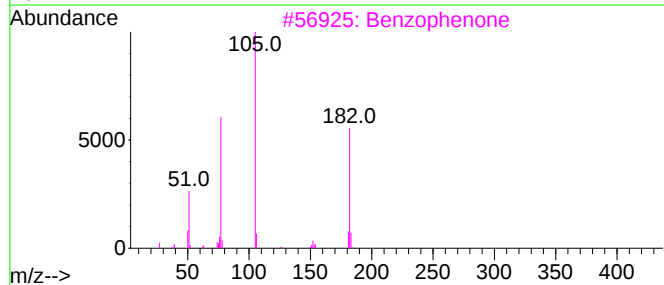
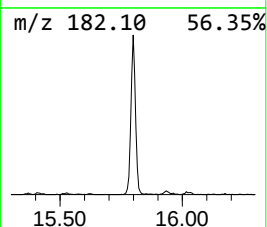
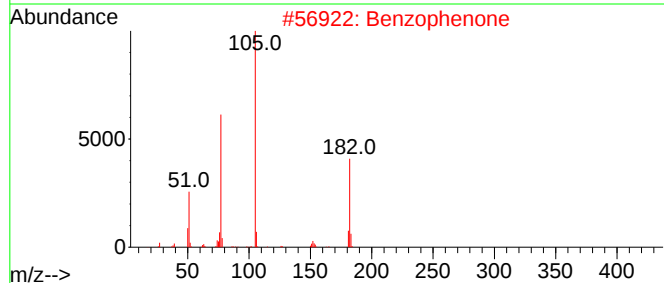
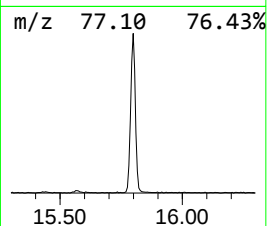
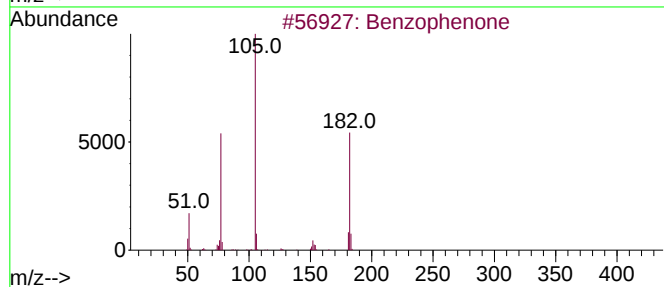
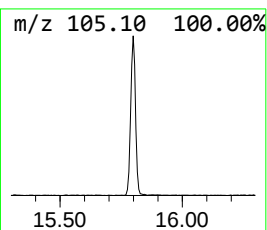
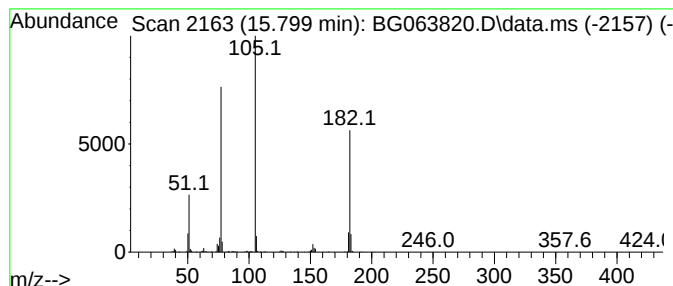
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.799	9.97 ng/ul	884977	Acenaphthene-d10	14.441

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	95
4			Benzophenone	182	C13H10O	000119-61-9	91
5			Azobenzene	182	C12H10N2	000103-33-3	72



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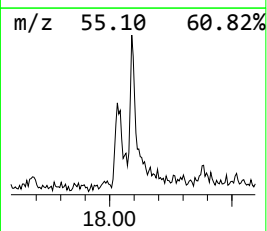
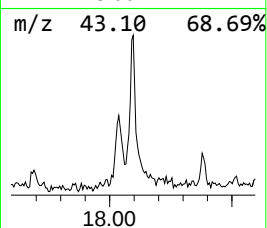
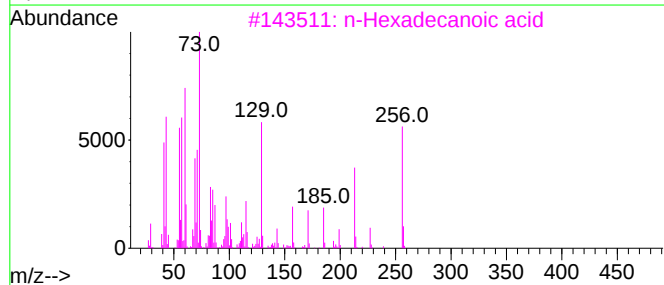
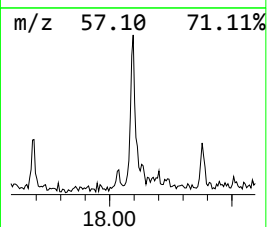
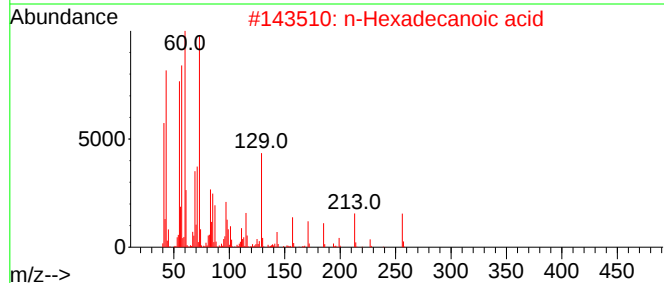
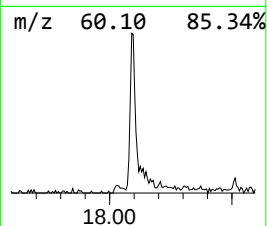
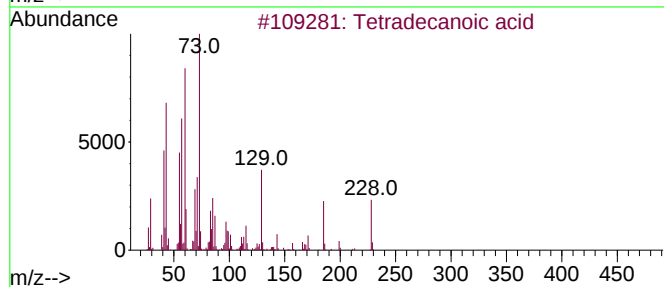
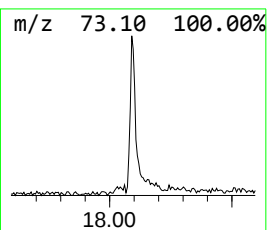
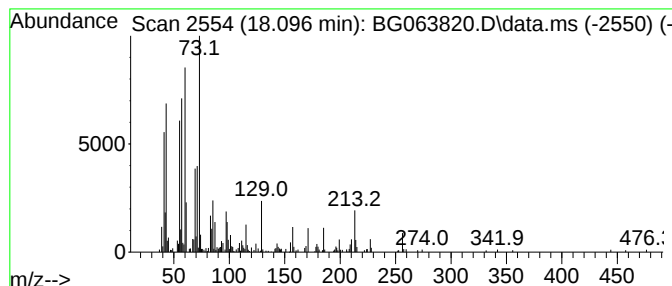
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121124.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
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Peak Number 2 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.096	4.12 ng/ul	478611	Phenanthrene-d10	17.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	92
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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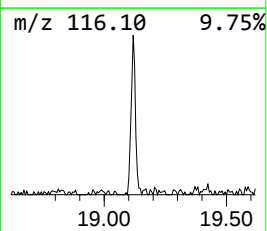
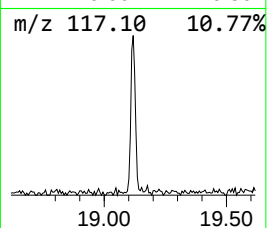
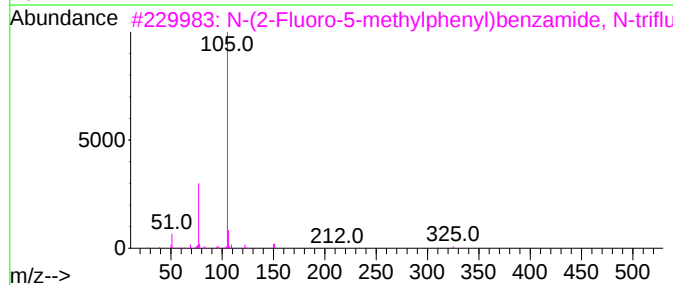
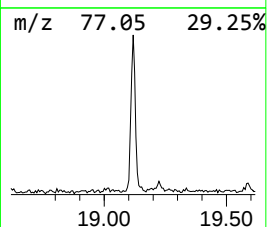
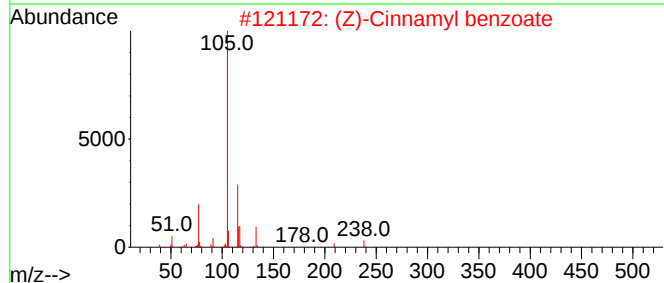
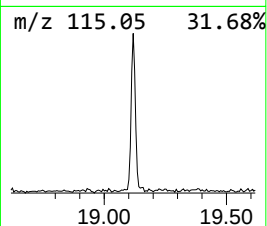
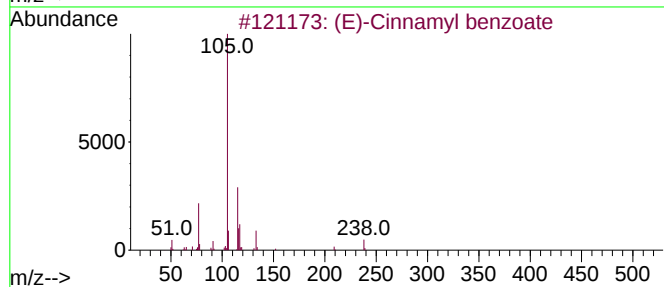
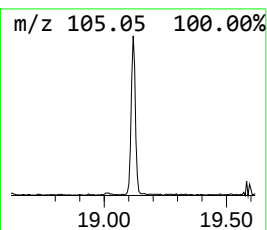
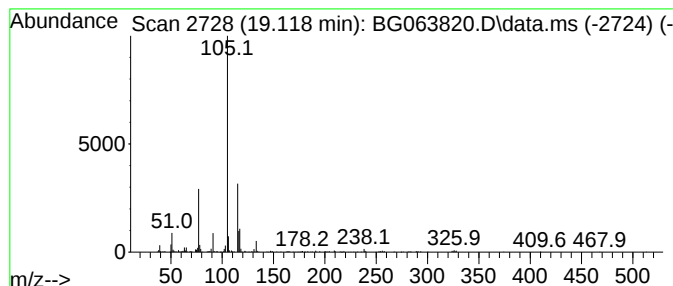
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (E)-Cinnamyl benzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.118	4.17 ng/ul	483975	Phenanthrene-d10	17.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Cinnamyl benzoate		238	C16H14O2	050555-04-9	90	
2	(Z)-Cinnamyl benzoate		238	C16H14O2	117204-78-1	90	
3	N-(2-Fluoro-5-methylphenyl)benza...		325	C16H11F4NO2	1000492-40-0	38	
4	Oxazol-5(4H)-one, 4-methylaminom...		202	C11H10N2O2	313527-71-8	38	
5	Butyrophenone, 2-phenyl-		224	C16H16O	016282-16-9	38	



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Acq On : 24 Dec 2024 15:28
Operator : RC/JU
Sample : P5333-13
Misc :
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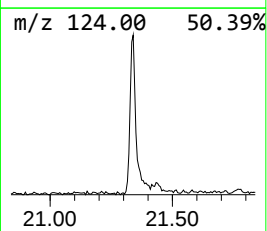
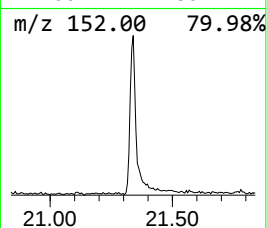
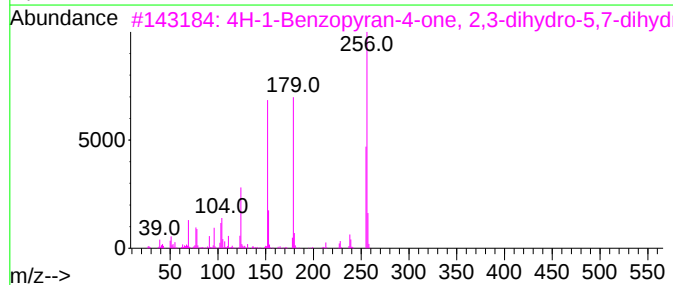
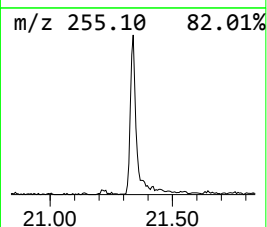
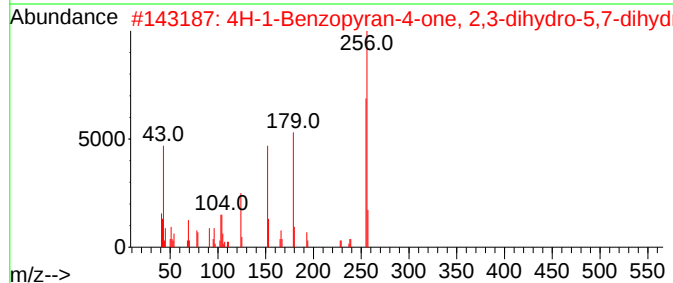
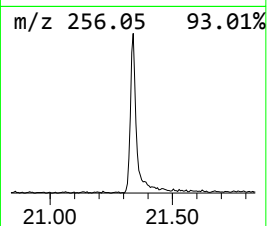
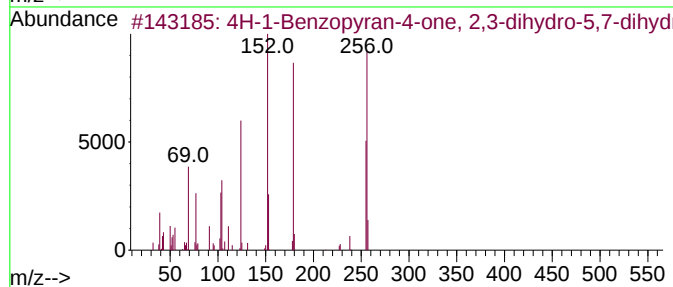
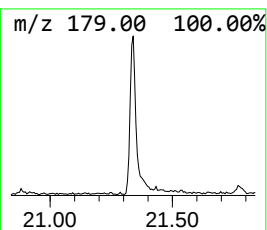
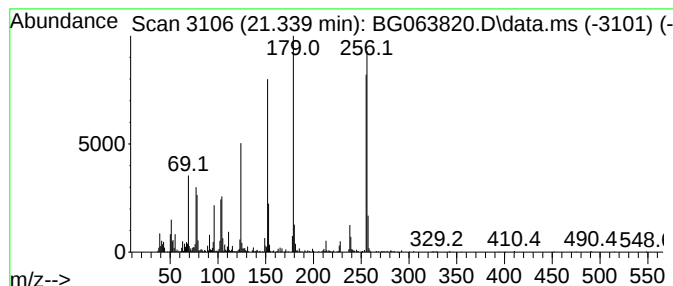
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 4H-1-Benzopyran-4-one, 2,3-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.339	9.05 ng/ul	1123980	Chrysene-d12	21.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1-Benzopyran-4-one, 2,3-dihyd...	256	C15H12O4	000480-39-7	98
2	4H-1-Benzopyran-4-one, 2,3-dihyd...	256	C15H12O4	000480-39-7	94
3	4H-1-Benzopyran-4-one, 2,3-dihyd...	256	C15H12O4	000480-39-7	93
4	4H-1-Benzopyran-4-one, 2,3-dihyd...	256	C15H12O4	000480-39-7	90
5	2,2'-Biquinoline	256	C18H12N2	000119-91-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122324\
Data File : BG063820.D
Acq On : 24 Dec 2024 15:28
Operator : RC/JU
Sample : P5333-13
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E2915

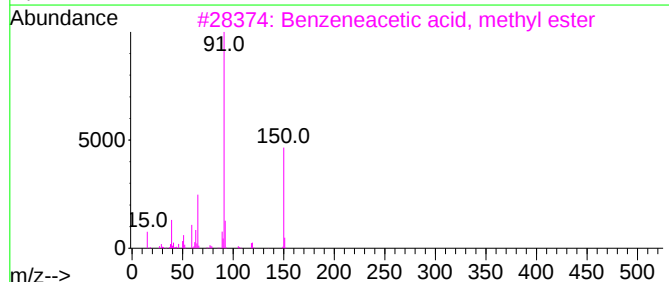
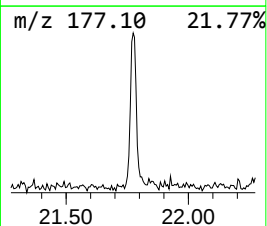
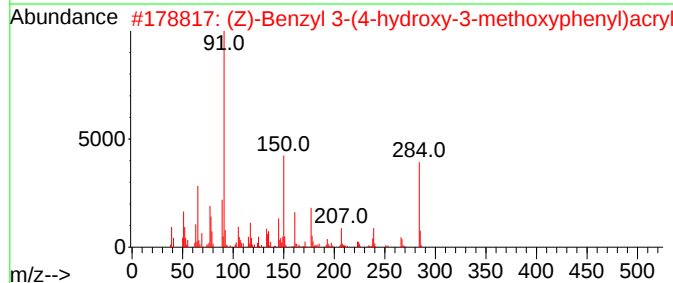
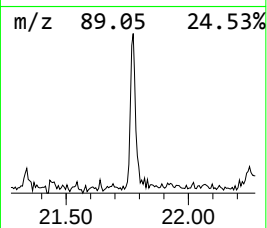
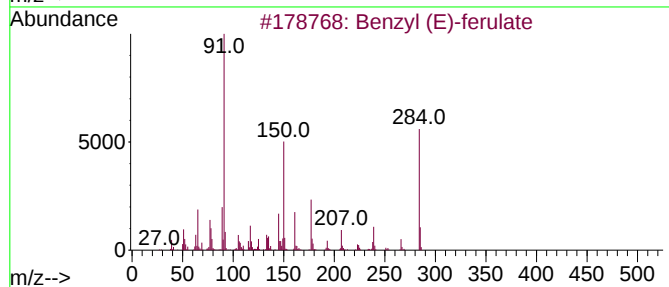
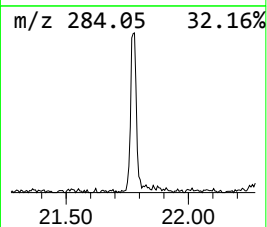
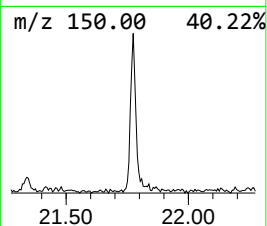
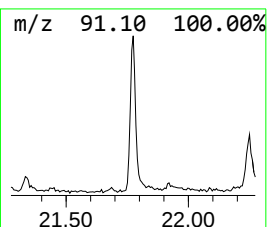
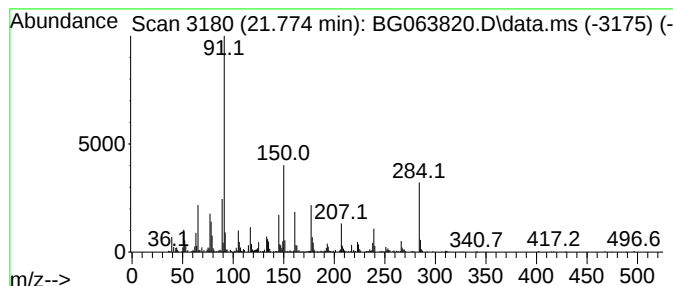
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Benzyl (E)-ferulate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.774	5.32 ng/ul	661065	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl (E)-ferulate	284	C17H16O4	132335-97-8	98
2			(Z)-Benzyl 3-(4-hydroxy-3-methox...	284	C17H16O4	132336-01-7	86
3			Benzeneacetic acid, methyl ester	150	C9H10O2	000101-41-7	20
4			Benzeneacetic acid, methyl ester	150	C9H10O2	000101-41-7	18
5			Benzeneacetic acid, methyl ester	150	C9H10O2	000101-41-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122324\
Data File : BG063820.D
Acq On : 24 Dec 2024 15:28
Operator : RC/JU
Sample : P5333-13
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E2915

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121124.MA.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
Benzophenone	15.799	10.0	ng/ul	884977	3	14.441	1775350	20.0
Tetradecanoic acid	18.096	4.1	ng/ul	478611	4	17.191	2322240	20.0
(E)-Cinnamyl be...	19.118	4.2	ng/ul	483975	4	17.191	2322240	20.0
4H-1-Benzopyran...	21.339	9.1	ng/ul	1123980	5	21.439	2484300	20.0
Benzyl (E)-feru...	21.774	5.3	ng/ul	661065	5	21.439	2484300	20.0