

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
 Data File : BG059679.D
 Acq On : 6 Nov 2023 7:56
 Operator : MA/JU
 Sample : 04948-15
 Misc :
 ALS Vial : 71 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AL4

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-BG110323.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059679.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.011	103	106	109	rBV2	3841	6033	0.78%	0.103%
2	4.199	135	138	140	rBV3	5886	8415	1.08%	0.144%
3	4.293	150	154	161	rVB3	9366	19390	2.49%	0.331%
4	4.351	161	164	166	rBV	6178	5252	0.68%	0.090%
5	4.422	172	176	180	rVB2	22010	29248	3.76%	0.499%
6	4.745	226	231	232	rVV3	5562	7471	0.96%	0.128%
7	4.939	262	264	267	rBV3	4065	4673	0.60%	0.080%
8	5.045	279	282	285	rBV4	4143	5139	0.66%	0.088%
9	5.098	288	291	295	rVB3	3857	4267	0.55%	0.073%
10	5.356	332	335	337	rVV2	6960	7611	0.98%	0.130%
11	5.391	340	341	345	rVB2	4423	4046	0.52%	0.069%
12	5.427	345	347	350	rBV	3892	4728	0.61%	0.081%
13	5.450	350	351	355	rVB	6371	5143	0.66%	0.088%
14	5.597	374	376	378	rVB	5066	3912	0.50%	0.067%
15	5.626	378	381	386	rBV	5389	8744	1.12%	0.149%
16	5.738	398	400	404	rBV2	4194	4663	0.60%	0.080%
17	5.785	404	408	411	rBV3	11586	13699	1.76%	0.234%
18	5.914	425	430	440	rBV4	30851	81117	10.43%	1.385%
19	6.038	450	451	455	rVB	5887	5668	0.73%	0.097%
20	6.079	456	458	462	rBV	4753	6899	0.89%	0.118%
21	6.296	491	495	500	rVB3	19132	27889	3.58%	0.476%
22	6.631	550	552	555	rBV	3941	4040	0.52%	0.069%
23	6.972	609	610	615	rBV	3319	4732	0.61%	0.081%
24	7.131	635	637	641	rVB	5515	4599	0.59%	0.079%
25	7.160	641	642	646	rBV	4451	4464	0.57%	0.076%
26	7.389	677	681	686	rVB2	18276	29562	3.80%	0.505%
27	7.460	688	693	702	rBV4	53399	110410	14.19%	1.885%
28	7.665	722	728	738	rVV3	35074	66902	8.60%	1.142%
29	7.865	755	762	768	rBV2	50162	106109	13.64%	1.811%
30	7.959	773	778	783	rVB3	20264	32072	4.12%	0.547%
31	8.353	839	845	852	rVB2	106704	183927	23.64%	3.140%
32	8.429	856	858	864	rVB5	6850	10293	1.32%	0.176%
33	8.805	919	922	925	rBV	4844	7827	1.01%	0.134%
34	8.846	927	929	932	rBV	5566	8040	1.03%	0.137%
35	8.952	944	947	949	rBV2	8774	9501	1.22%	0.162%
36	9.028	954	960	967	rBV3	41642	78364	10.07%	1.338%

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
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37	9.116	974	975	978	rBV2	3714	4532	0.58%	0.077%
38	9.187	981	987	996	rBV2	48207	103296	13.28%	1.763%
39	9.275	1000	1002	1007	rVB2	9304	8147	1.05%	0.139%
40	9.545	1039	1048	1055	rBV2	54407	106325	13.67%	1.815%

41	9.675	1069	1070	1074	rVB2	4543	4548	0.58%	0.078%
42	9.751	1080	1083	1085	rVV2	3733	3922	0.50%	0.067%
43	9.845	1098	1099	1102	rVB2	7014	5182	0.67%	0.088%
44	9.968	1117	1120	1123	rVB2	4928	6554	0.84%	0.112%
45	10.021	1126	1129	1131	rBV	7791	5606	0.72%	0.096%

46	10.198	1156	1159	1162	rBV	4437	6032	0.78%	0.103%
47	10.268	1164	1171	1178	rVV3	49969	91859	11.81%	1.568%
48	10.409	1193	1195	1198	rVB	6014	5200	0.67%	0.089%
49	10.626	1226	1232	1236	rVB5	9595	17268	2.22%	0.295%
50	10.715	1243	1247	1249	rVB	3890	5806	0.75%	0.099%

51	10.791	1255	1260	1269	rVB3	76174	138203	17.76%	2.359%
52	10.867	1269	1273	1279	rVB5	8051	15524	2.00%	0.265%
53	10.985	1291	1293	1296	rBV2	4832	5099	0.66%	0.087%
54	11.196	1323	1329	1336	rBV	155568	271139	34.85%	4.628%
55	11.296	1343	1346	1347	rBV	5155	5644	0.73%	0.096%

56	11.337	1348	1353	1362	rVV3	44350	91712	11.79%	1.566%
57	11.549	1388	1389	1394	rVB3	4549	4246	0.55%	0.072%
58	11.725	1416	1419	1422	rVB3	8591	9345	1.20%	0.160%
59	12.201	1497	1500	1503	rVB2	7239	8094	1.04%	0.138%
60	12.236	1504	1506	1509	rBV	3618	3884	0.50%	0.066%

61	12.371	1528	1529	1532	rBV	4416	4590	0.59%	0.078%
62	12.565	1560	1562	1570	rVB3	6479	10322	1.33%	0.176%
63	12.818	1600	1605	1606	rBV2	8697	9069	1.17%	0.155%
64	12.894	1616	1618	1621	rBV2	4277	5817	0.75%	0.099%
65	12.947	1625	1627	1630	rBV2	3315	4379	0.56%	0.075%

66	13.041	1640	1643	1648	rBV3	8927	14562	1.87%	0.249%
67	13.359	1695	1697	1698	rBV3	5201	4005	0.51%	0.068%
68	13.441	1707	1711	1712	rBV	5691	5702	0.73%	0.097%
69	13.635	1740	1744	1745	rBV	4670	4106	0.53%	0.070%
70	13.717	1755	1758	1761	rBV	5721	6213	0.80%	0.106%

71	13.770	1764	1767	1768	rBV	6140	6277	0.81%	0.107%
72	13.870	1781	1784	1785	rBV	4286	4998	0.64%	0.085%
73	14.287	1852	1855	1859	rVV3	8976	11491	1.48%	0.196%
74	14.369	1862	1869	1875	rVB	158289	235472	30.27%	4.019%
75	14.516	1892	1894	1897	rBV3	6833	5540	0.71%	0.095%

76	14.680	1915	1922	1931	rVB	172029	271114	34.85%	4.628%
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 Title : SVOA CALIBRATION

77	14.751	1931	1934	1935	rBV2	5007	4837	0.62%	0.083%
78	14.892	1954	1958	1960	rBV	5656	7849	1.01%	0.134%
79	14.980	1966	1973	1981	rBV2	263415	434288	55.82%	7.413%
80	15.151	1995	2002	2006	rBV3	74382	120075	15.43%	2.050%
81	15.239	2014	2017	2018	rBV3	4916	5265	0.68%	0.090%
82	15.380	2039	2041	2045	rVB3	6520	7759	1.00%	0.132%
83	15.421	2047	2048	2051	rVB	6819	4353	0.56%	0.074%
84	15.703	2094	2096	2099	rBV2	5052	4210	0.54%	0.072%
85	15.891	2125	2128	2129	rBV2	5697	6439	0.83%	0.110%
86	15.961	2135	2140	2148	rBV	206181	308125	39.61%	5.260%
87	16.067	2153	2158	2165	rVB3	62996	102643	13.19%	1.752%
88	16.220	2178	2184	2185	rBV	6143	12445	1.60%	0.212%
89	16.355	2205	2207	2210	rBV	4221	5816	0.75%	0.099%
90	16.502	2230	2232	2235	rBV2	4333	4533	0.58%	0.077%
91	16.784	2279	2280	2285	rBV2	6966	10186	1.31%	0.174%
92	17.042	2322	2324	2327	rVB3	6442	5478	0.70%	0.094%
93	17.236	2354	2357	2360	rVB4	10971	11428	1.47%	0.195%
94	17.730	2433	2441	2447	rBV	366319	554632	71.29%	9.467%
95	17.830	2452	2458	2464	rBV2	208150	330473	42.48%	5.641%
96	17.935	2475	2476	2479	rBV2	6079	6601	0.85%	0.113%
97	18.547	2576	2580	2585	rVB3	71328	94536	12.15%	1.614%
98	19.798	2791	2793	2800	rVB7	48946	73688	9.47%	1.258%
99	20.098	2839	2844	2849	rVB	363543	509018	65.43%	8.689%
100	22.060	3172	3178	3188	rVB	435321	777970	100.00%	13.280%

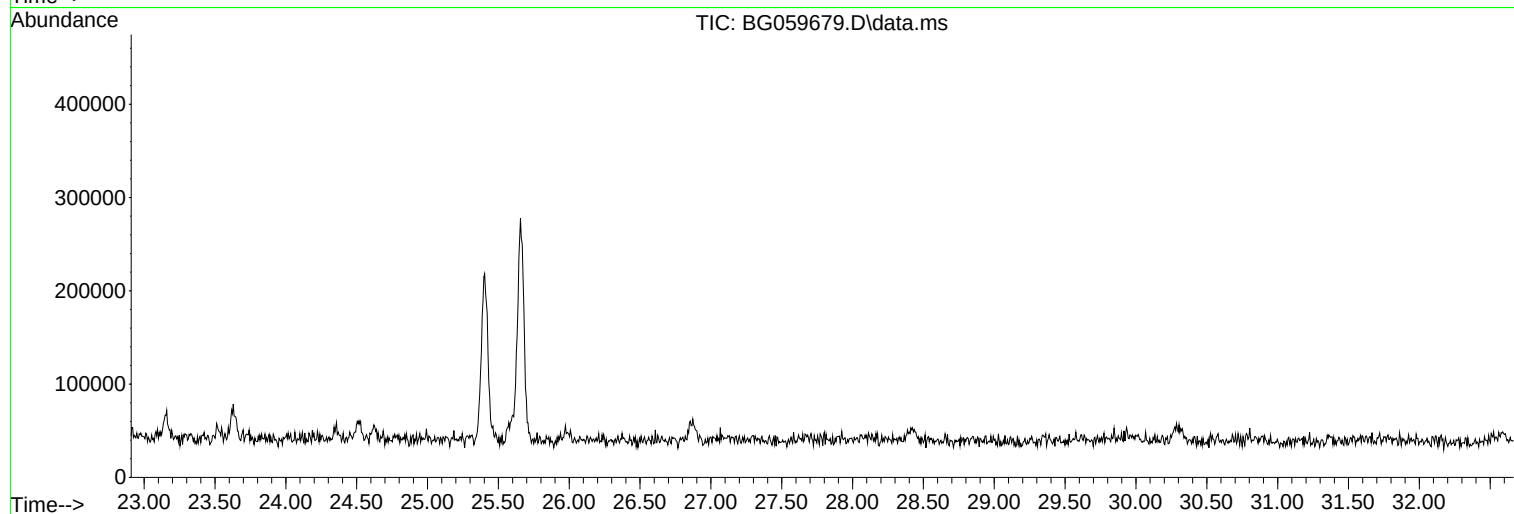
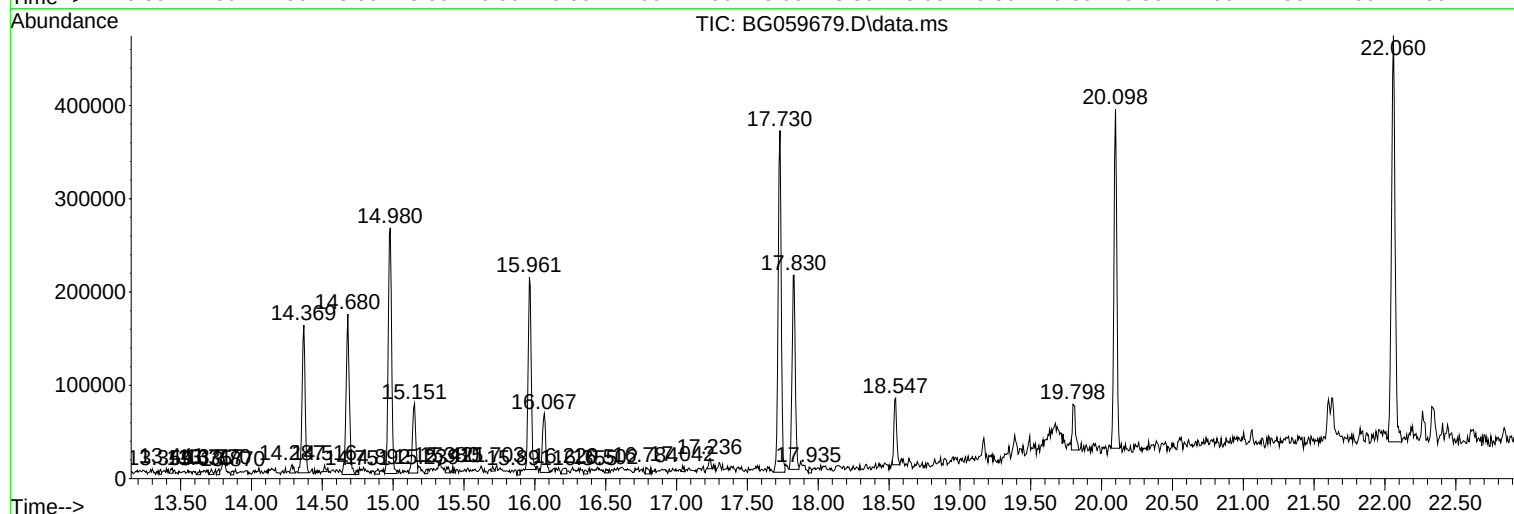
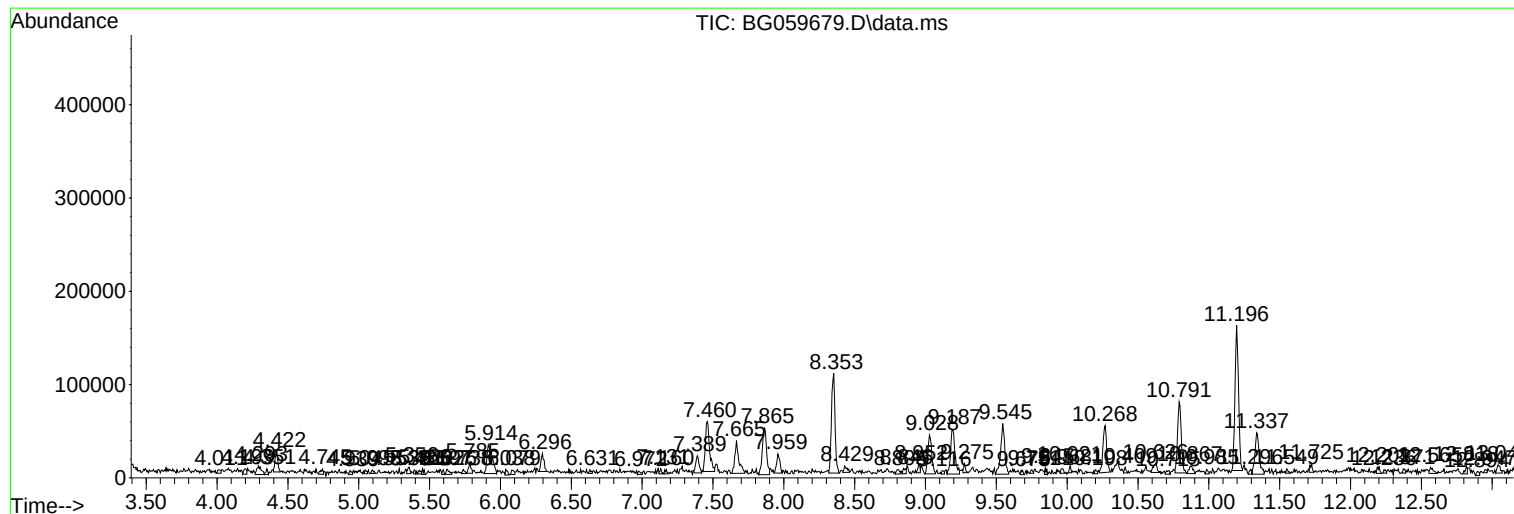
Sum of corrected areas: 5858320

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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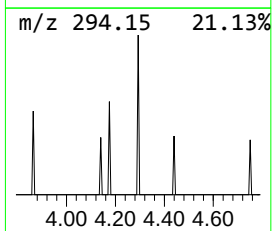
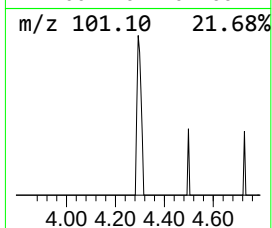
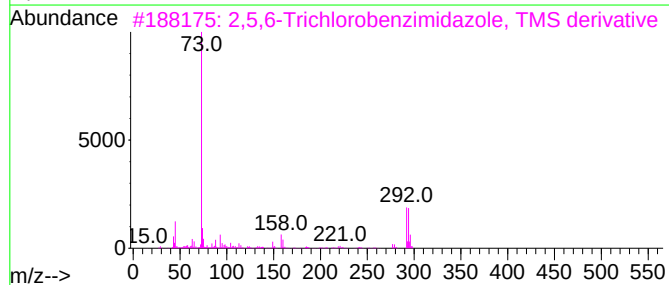
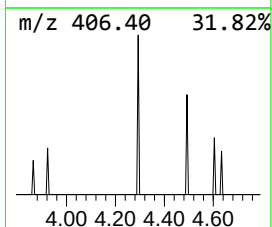
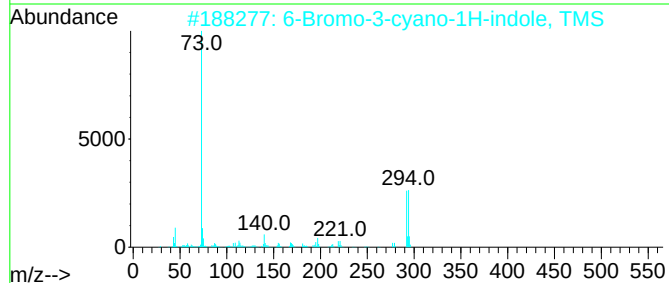
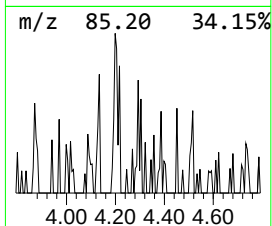
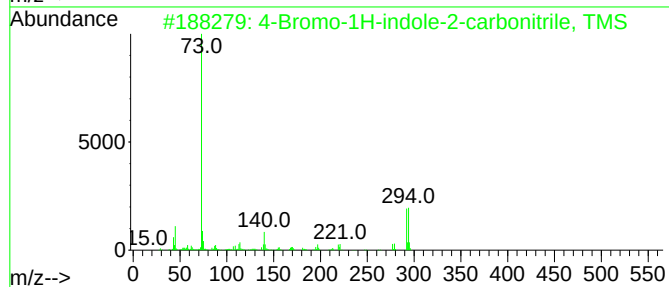
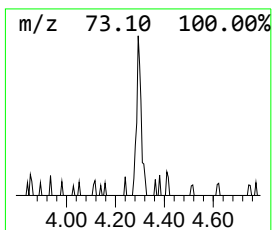
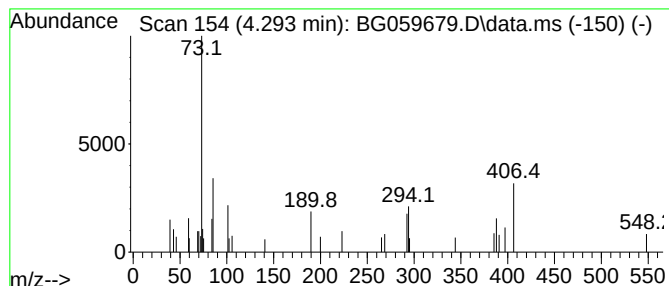
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.293	2.11 ng/ul	19390	1,4-Dichlorobenzene-d4	8.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Bromo-1H-indole-2-carbonitrile...	292	C12H13BrN2Si	1000499-35-9	22
2			6-Bromo-3-cyano-1H-indole, TMS	292	C12H13BrN2Si	1000499-30-3	22
3			2,5,6-Trichlorobenzimidazole, TM...	292	C10H11Cl3N2Si	1000508-95-7	12
4			3-Bromo-4-cyanoindole, TMS	292	C12H13BrN2Si	1000508-62-4	9
5			4-Bromo-1H-indole-6-carbonitrile	292	C12H13BrN2Si	1000501-02-6	9



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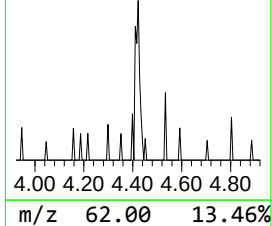
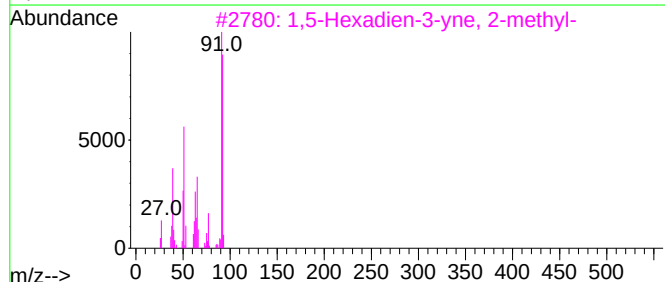
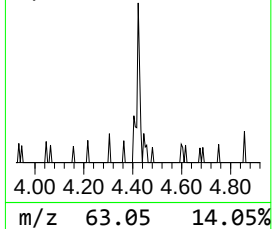
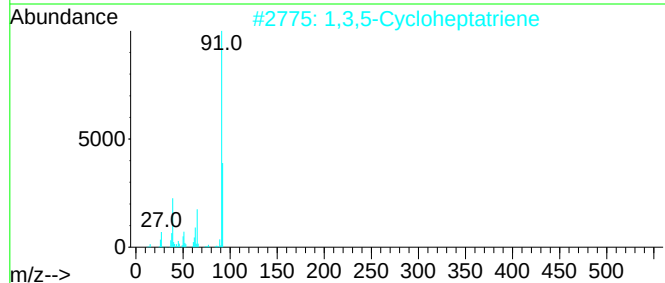
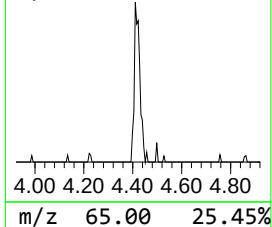
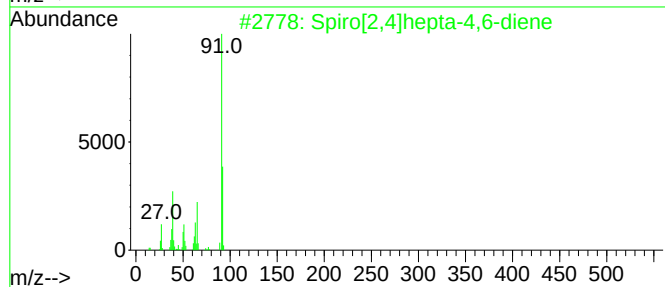
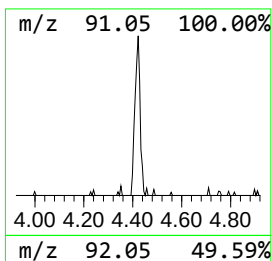
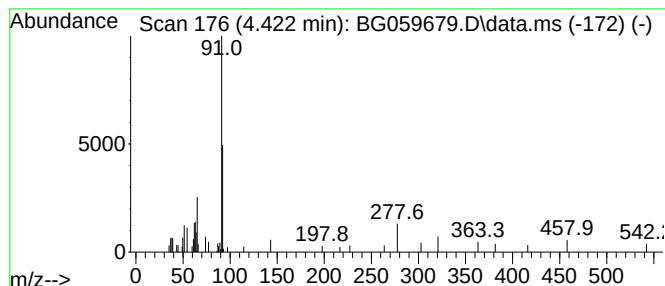
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Spiro[2,4]hepta-4,6-diene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.422	3.18 ng/ul	29248	1,4-Dichlorobenzene-d4	8.353

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	64
2		1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	64
3		1,5-Hexadien-3-yne, 2-methyl-	92	C7H8	000820-54-2	58
4		1,6-Heptadien-3-yne	92	C7H8	005150-80-1	58
5		1,6-Heptadien-3-yne	92	C7H8	005150-80-1	52



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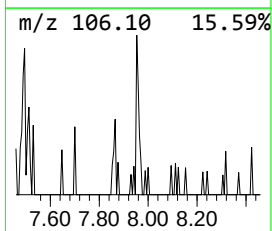
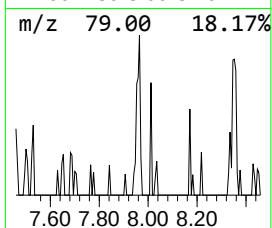
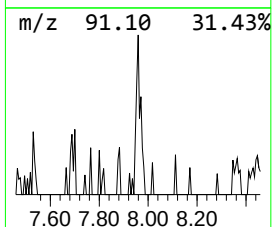
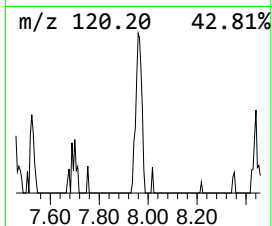
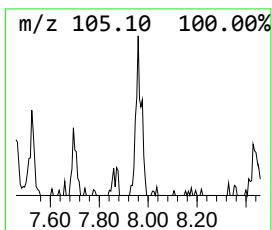
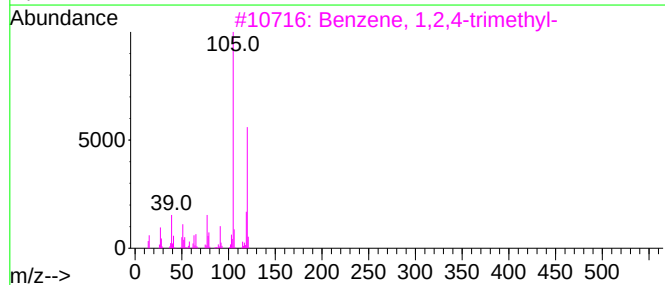
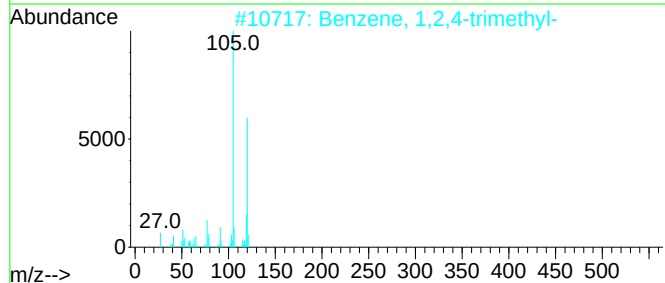
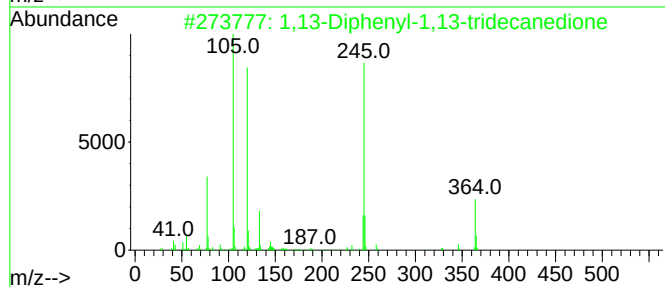
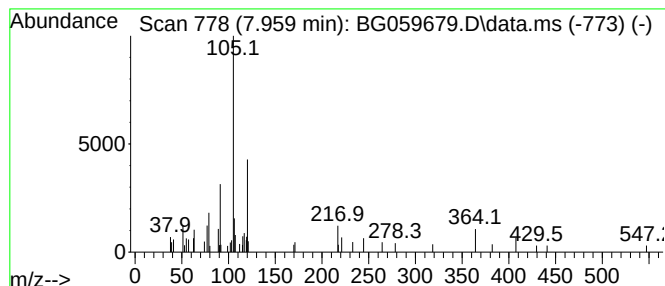
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.959	3.49 ng/ul	32072	1,4-Dichlorobenzene-d4	8.353

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,13-Diphenyl-1,13-tridecanedione	364	C25H32O2	116223-42-8	47
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	38
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	38
4			1,3-Cyclopentadiene, 5-(1-methyl...	120	C9H12	003141-02-4	38
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059679.D
Acq On : 6 Nov 2023 7:56
Operator : MA/JU
Sample : 04948-15
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AL4

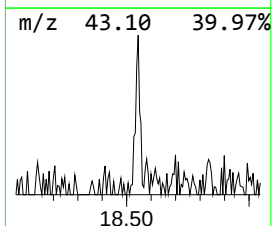
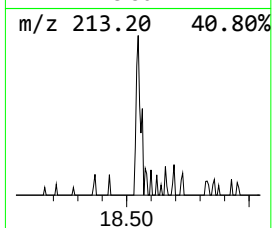
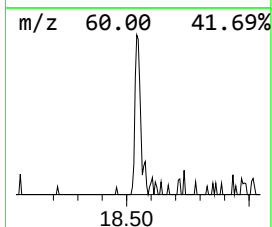
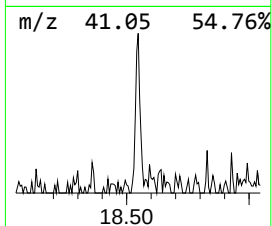
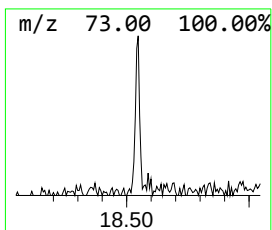
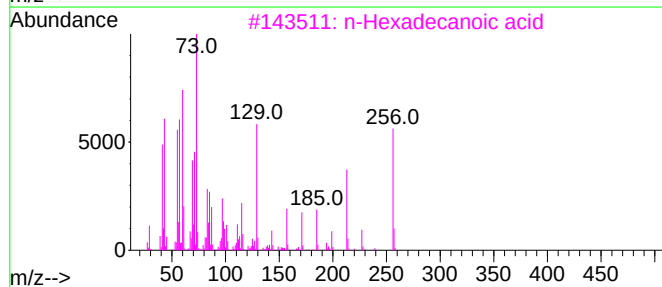
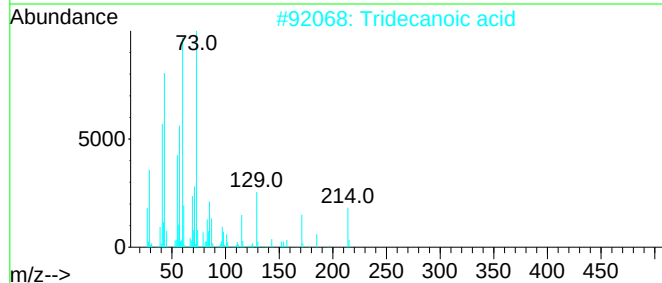
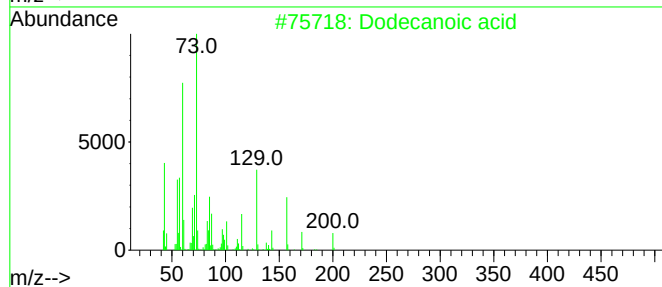
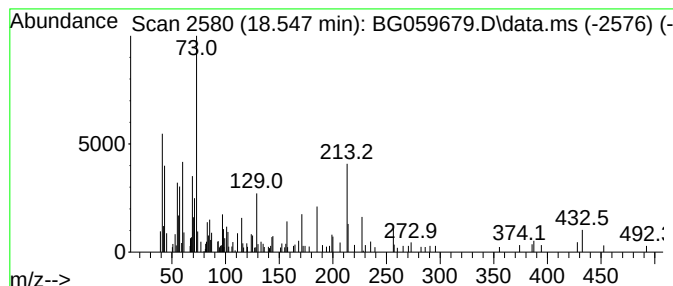
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.547	3.41 ng/ul	94536	Phenanthrene-d10	17.730

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	80
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45
4			Tridecanoic acid	214	C13H26O2	000638-53-9	43
5			Tridecanoic acid	214	C13H26O2	000638-53-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059679.D
Acq On : 6 Nov 2023 7:56
Operator : MA/JU
Sample : 04948-15
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COAL4

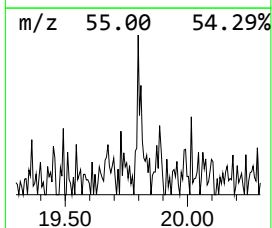
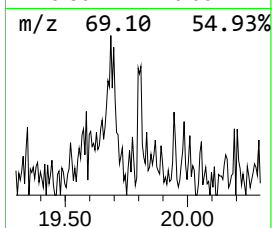
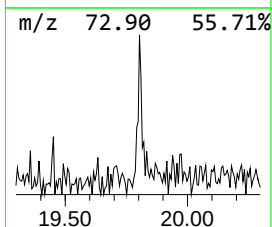
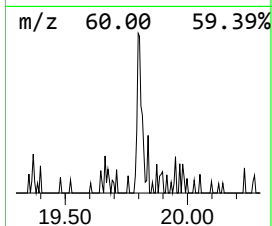
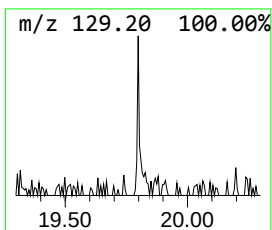
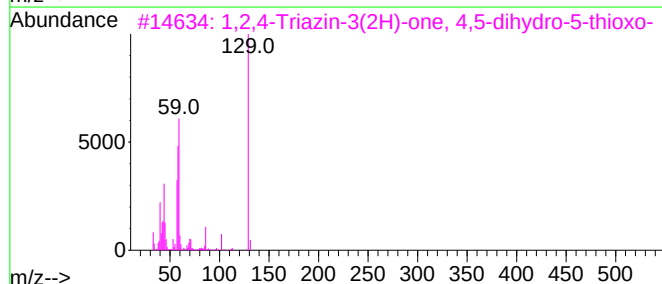
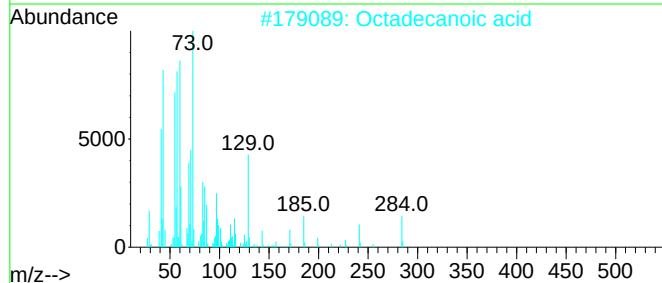
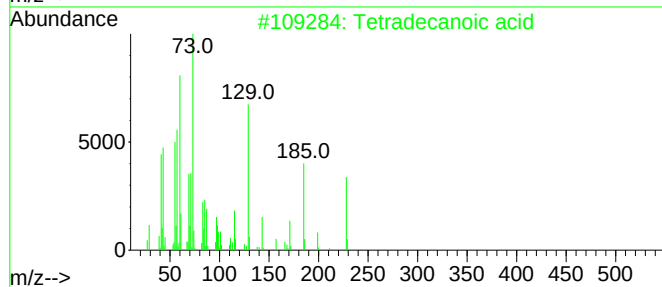
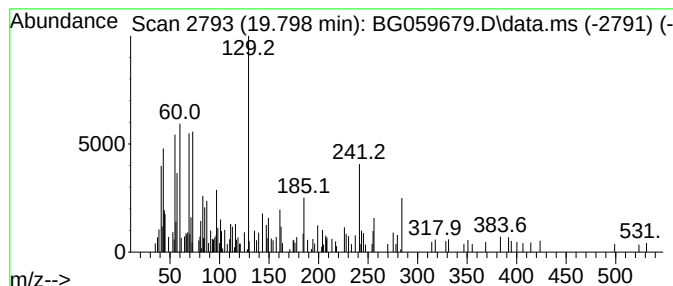
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.798	2.66 ng/ul	73688	Phenanthrene-d10	17.730

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	46
2			Octadecanoic acid	284	C18H36O2	000057-11-4	43
3			1,2,4-Triazin-3(2H)-one, 4,5-dih...	129	C3H3N3OS	001627-37-8	27
4			Malonic acid, 3-heptyl propyl ester	244	C13H24O4	1000349-14-7	27
5			Cyanuric acid	129	C3H3N3O3	000108-80-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059679.D
Acq On : 6 Nov 2023 7:56
Operator : MA/JU
Sample : 04948-15
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AL4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.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
unknown-01	4.293	2.1	ng/ul	19390	1	8.353	183927	20.0
Spiro[2,4]hepta...	4.422	3.2	ng/ul	29248	1	8.353	183927	20.0
unknown-02	7.959	3.5	ng/ul	32072	1	8.353	183927	20.0
Dodecanoic acid	18.547	3.4	ng/ul	94536	4	17.730	554632	20.0
unknown-03	19.798	2.7	ng/ul	73688	4	17.730	554632	20.0