

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
 Data File : BG056802.D
 Acq On : 2 Mar 2023 22:57
 Operator : CG/JU
 Sample : 01712-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DBAD7

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: BG056802.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.702	24	28	35	rVB5	2316	3942	0.29%	0.047%
2	4.143	100	103	111	rBV	13866	23765	1.77%	0.280%
3	4.384	141	144	145	rBV2	1736	1782	0.13%	0.021%
4	5.059	255	259	265	rBV5	1371	3445	0.26%	0.041%
5	6.088	432	434	440	rVB2	1251	1821	0.14%	0.021%
6	7.539	675	681	688	rBV2	20210	33883	2.52%	0.400%
7	7.721	705	712	721	rVB	51031	86003	6.40%	1.015%
8	7.938	743	749	756	rVB	53796	91301	6.79%	1.078%
9	8.414	824	830	837	rBV	57095	95420	7.10%	1.126%
10	9.102	942	947	954	rVB3	50927	87133	6.48%	1.028%
11	9.589	1023	1030	1040	rVB	71324	131826	9.81%	1.556%
12	10.318	1148	1154	1162	rVB3	61956	106678	7.94%	1.259%
13	10.859	1238	1246	1254	rBV	90940	157868	11.75%	1.863%
14	11.070	1279	1282	1285	rVB3	1476	1565	0.12%	0.018%
15	11.258	1306	1314	1325	rVB	85095	151418	11.27%	1.787%
16	11.376	1325	1334	1342	rBV	82438	147027	10.94%	1.735%
17	12.803	1574	1577	1583	rVB3	1229	2193	0.16%	0.026%
18	13.732	1732	1735	1740	rBV4	2629	3062	0.23%	0.036%
19	14.407	1843	1850	1857	rBV	215679	300029	22.33%	3.541%
20	14.719	1896	1903	1910	rBV	222502	344213	25.61%	4.063%
21	14.989	1943	1949	1953	rBV	934397	1343795	100.00%	15.861%
22	15.171	1976	1980	1986	rBV	23112	36460	2.71%	0.430%
23	15.718	2070	2073	2077	rBV3	3499	4391	0.33%	0.052%
24	15.759	2077	2080	2083	rVV4	2345	2763	0.21%	0.033%
25	15.794	2083	2086	2091	rVB3	928	1701	0.13%	0.020%
26	16.000	2115	2121	2129	rVB	279601	446795	33.25%	5.273%
27	16.099	2132	2138	2144	rBV	63298	89316	6.65%	1.054%
28	16.352	2177	2181	2184	rBV	1613	2221	0.17%	0.026%
29	17.756	2413	2420	2426	rBV	200779	315307	23.46%	3.722%
30	17.850	2430	2436	2444	rVV	352365	531176	39.53%	6.269%
31	18.220	2496	2499	2500	rBV	1405	1577	0.12%	0.019%
32	18.262	2503	2506	2508	rVV2	1329	1890	0.14%	0.022%
33	18.385	2523	2527	2532	rBV5	5092	9045	0.67%	0.107%
34	18.497	2544	2546	2551	rVB	1867	2204	0.16%	0.026%
35	18.673	2571	2576	2579	rBV	2472	3460	0.26%	0.041%
36	18.814	2595	2600	2609	rBV	73664	112470	8.37%	1.327%

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37	19.454	2705	2709	2713	rBV3	2030	2766	0.21%	0.033%
38	19.683	2743	2748	2751	rVB3	4427	7074	0.53%	0.083%
39	19.748	2754	2759	2762	rVV3	4228	6715	0.50%	0.079%
40	19.924	2779	2789	2791	rBV5	6321	12557	0.93%	0.148%

41	20.001	2791	2802	2803	rBV8	18645	44562	3.32%	0.526%
42	20.112	2815	2821	2829	rVB	437539	630943	46.95%	7.447%
43	20.218	2837	2839	2842	rVB3	2243	2498	0.19%	0.029%
44	20.259	2843	2846	2848	rVV4	1799	2065	0.15%	0.024%
45	20.588	2900	2902	2906	rVB5	2986	2634	0.20%	0.031%

46	20.624	2906	2908	2913	rBV3	1809	2950	0.22%	0.035%
47	20.859	2946	2948	2950	rBV2	2598	2675	0.20%	0.032%
48	21.035	2975	2978	2981	rVB3	1258	1662	0.12%	0.020%
49	21.235	3009	3012	3013	rBV3	1702	2040	0.15%	0.024%
50	21.352	3030	3032	3033	rBV	3074	2319	0.17%	0.027%

51	21.440	3045	3047	3049	rVB3	2354	1959	0.15%	0.023%
52	21.599	3072	3074	3075	rBV2	2117	1689	0.13%	0.020%
53	21.646	3075	3082	3088	rVV	753235	1004763	74.77%	11.859%
54	21.705	3091	3092	3097	rVB5	2002	1931	0.14%	0.023%
55	21.899	3122	3125	3126	rBV3	2417	2012	0.15%	0.024%

56	21.940	3130	3132	3135	rVB3	2417	1708	0.13%	0.020%
57	22.063	3146	3153	3160	rVB	191349	338752	25.21%	3.998%
58	22.280	3187	3190	3191	rBV3	2071	2132	0.16%	0.025%
59	22.439	3216	3217	3220	rBV3	1965	1618	0.12%	0.019%
60	22.633	3249	3250	3252	rBV2	2046	1609	0.12%	0.019%

61	22.739	3265	3268	3271	rBV4	1798	2880	0.21%	0.034%
62	22.862	3285	3289	3294	rBV7	6832	14455	1.08%	0.171%
63	23.250	3354	3355	3357	rBV2	2189	1849	0.14%	0.022%
64	23.532	3402	3403	3406	rVB3	1847	1772	0.13%	0.021%
65	23.608	3414	3416	3417	rBV2	1966	1608	0.12%	0.019%

66	23.626	3417	3419	3422	rVV3	2806	2820	0.21%	0.033%
67	23.990	3477	3481	3484	rVB6	1539	1914	0.14%	0.023%
68	24.014	3484	3485	3487	rBV2	3202	2057	0.15%	0.024%
69	24.049	3489	3491	3493	rBV2	2162	2241	0.17%	0.026%
70	24.119	3501	3503	3506	rVB4	2450	2006	0.15%	0.024%

71	24.454	3558	3560	3562	rBV3	2037	1584	0.12%	0.019%
72	24.472	3562	3563	3568	rBV5	1173	1650	0.12%	0.019%
73	24.707	3598	3603	3607	rBV6	2663	6786	0.50%	0.080%
74	24.754	3607	3611	3612	rBV4	2934	3274	0.24%	0.039%
75	24.977	3647	3649	3652	rBV4	2176	2101	0.16%	0.025%

76	25.242	3692	3694	3696	rVB2	1607	1544	0.11%	0.018%
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77	25.342	3698	3711	3724	rVV2	204633	608310	45.27%	7.180%
78	25.588	3742	3753	3767	rVB3	106776	336495	25.04%	3.972%
79	26.105	3840	3841	3845	rVB3	2297	2156	0.16%	0.025%
80	26.810	3960	3961	3966	rVV5	2310	3258	0.24%	0.038%
81	27.216	4028	4030	4033	rVB2	2305	2046	0.15%	0.024%
82	27.345	4040	4052	4064	rVB3	67957	232151	17.28%	2.740%
83	27.939	4151	4153	4156	rVB3	2209	1951	0.15%	0.023%
84	27.997	4162	4163	4165	rBV2	2242	1595	0.12%	0.019%
85	28.038	4168	4170	4171	rBV2	1831	1554	0.12%	0.018%
86	28.103	4178	4181	4182	rBV2	1678	1641	0.12%	0.019%
87	28.344	4218	4222	4226	rVV4	2811	3734	0.28%	0.044%
88	28.432	4235	4237	4240	rVB2	2026	1855	0.14%	0.022%
89	28.984	4329	4331	4334	rBV3	1381	1764	0.13%	0.021%
90	29.096	4348	4350	4352	rBV3	2129	2016	0.15%	0.024%
91	29.842	4474	4477	4479	rBV3	1991	2734	0.20%	0.032%
92	30.506	4589	4590	4595	rVB4	1592	1626	0.12%	0.019%
93	30.665	4599	4617	4634	rVV6	91816	442862	32.96%	5.227%
94	31.575	4769	4772	4774	rVB5	2462	2083	0.16%	0.025%
95	31.593	4774	4775	4778	rBV3	1561	1801	0.13%	0.021%
96	32.010	4845	4846	4848	rBV2	2226	1548	0.12%	0.018%
97	32.028	4848	4849	4853	rVV3	1607	1962	0.15%	0.023%
98	32.169	4871	4873	4876	rVB4	2017	2056	0.15%	0.024%
99	32.410	4913	4914	4917	rBV3	1708	1821	0.14%	0.021%
100	32.545	4933	4937	4939	rBV5	2373	2325	0.17%	0.027%

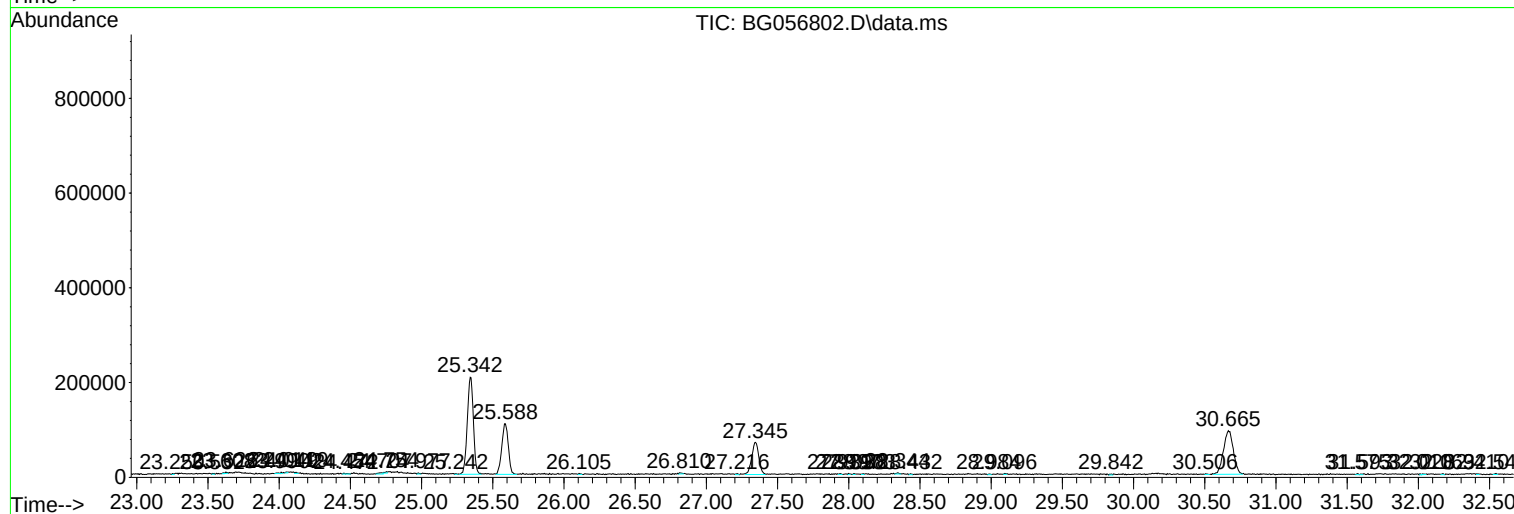
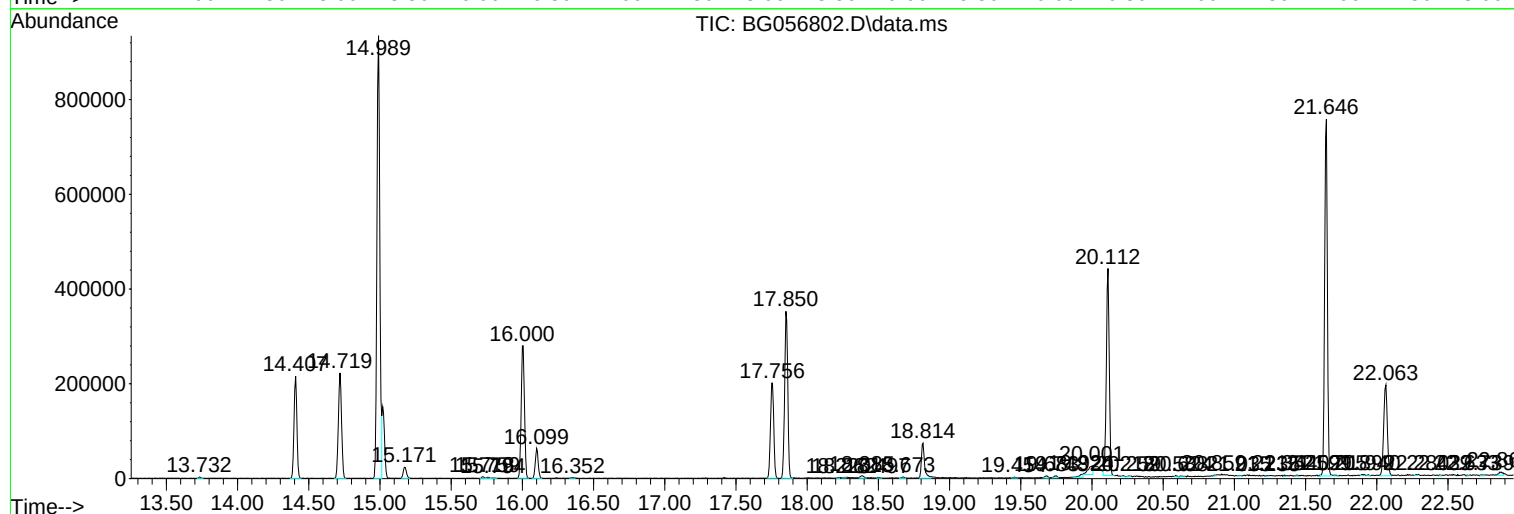
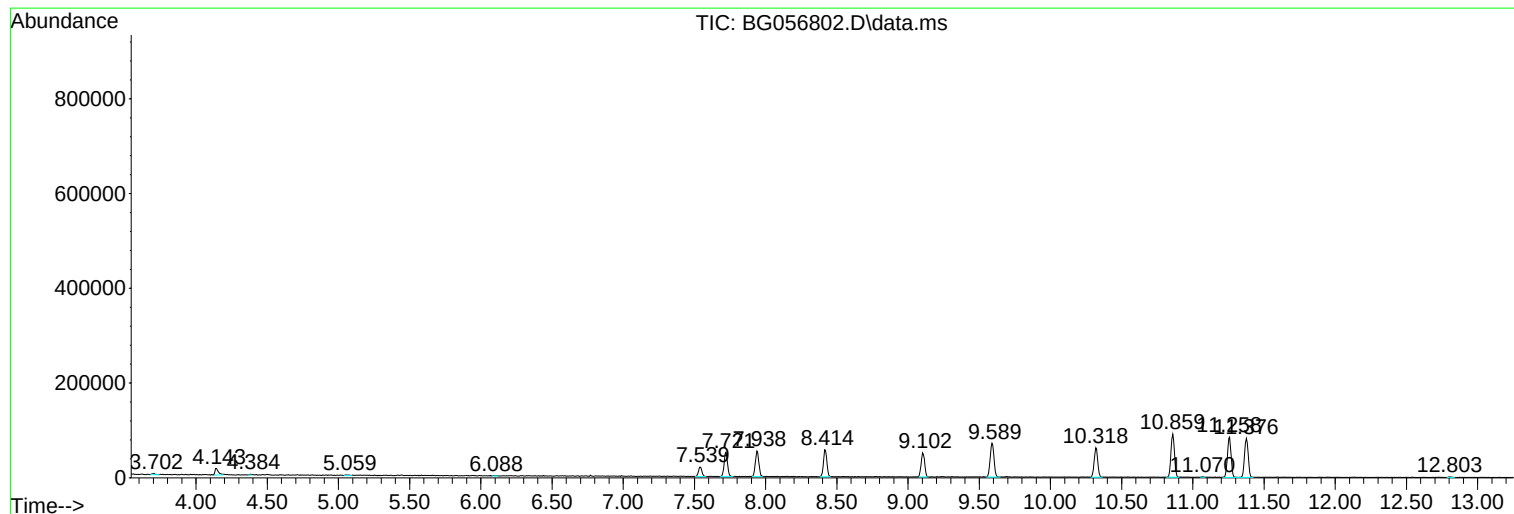
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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



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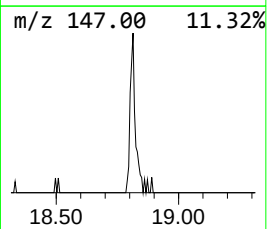
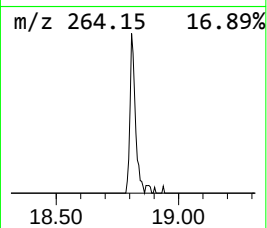
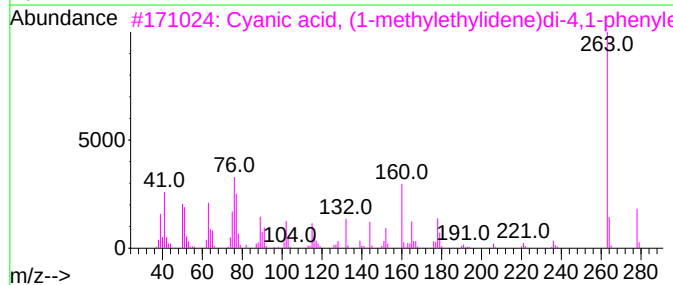
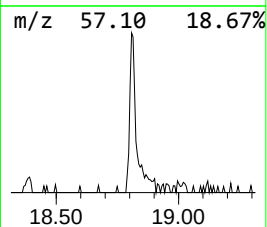
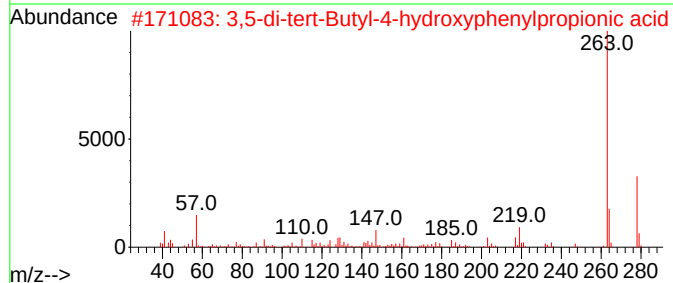
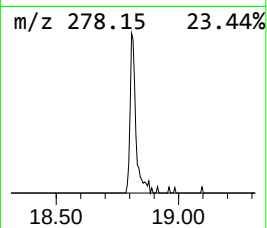
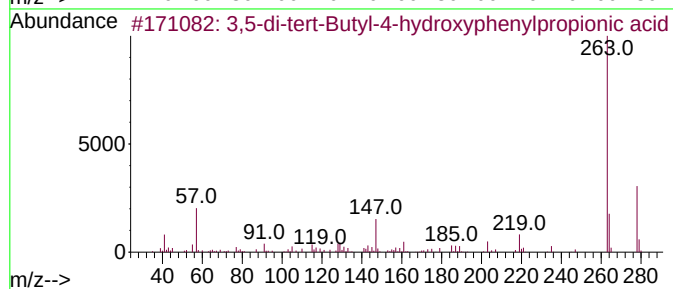
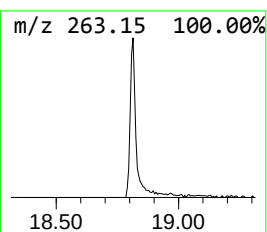
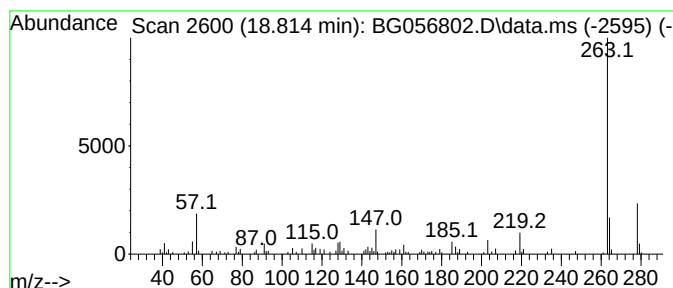
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.814	7.13 ng/ul	112470	Phenanthrene-d10	17.750	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	98
2	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	95
3	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	72
4	5-(2,3-Difluorophenyl)-2-pyridin...	278	C14H16F2N2Si	1000504-49-4	64
5	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	64



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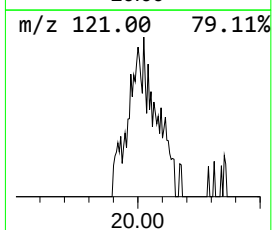
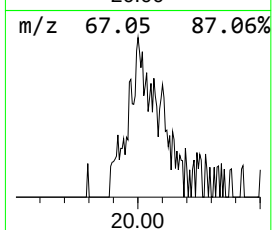
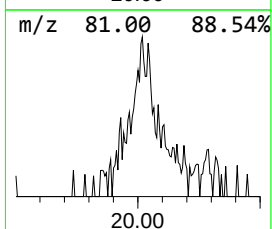
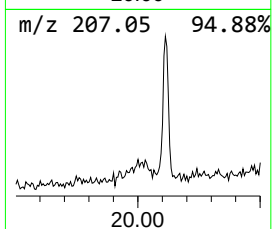
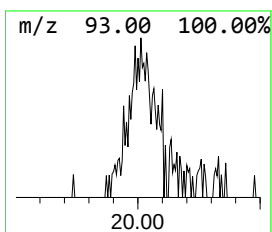
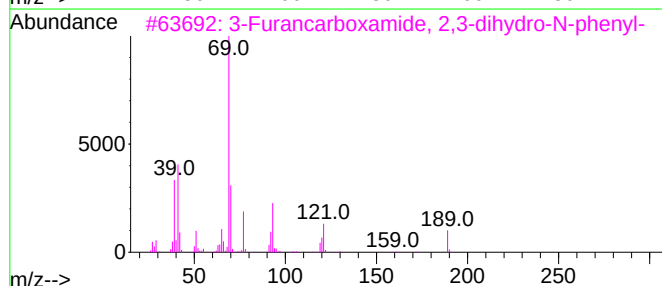
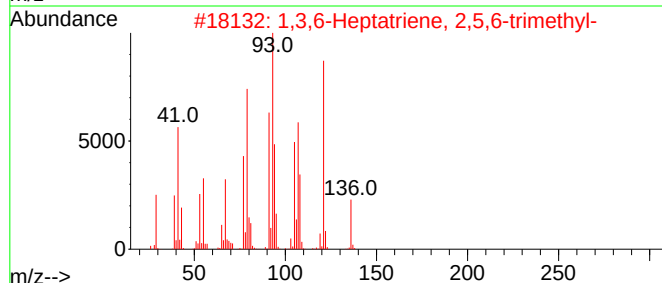
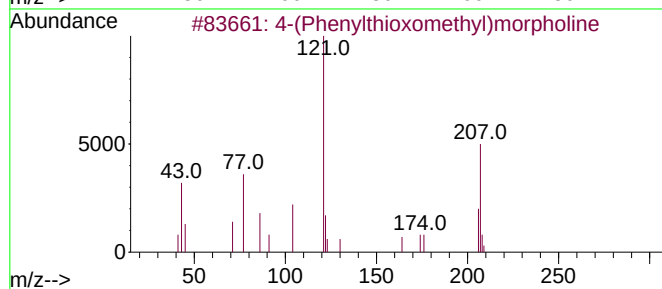
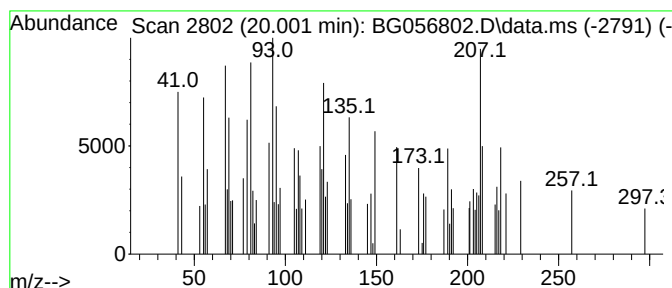
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.001	2.63 ng/ul	44562	Chrysene-d12	22.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(Phenylthioxomethyl)morpholine	207	C11H13NOS	002032-36-2	38
2	1,3,6-Heptatriene, 2,5,6-trimethyl-	136	C10H16	042123-66-0	25
3	3-Furancarboxamide, 2,3-dihydro-...	189	C11H11NO2	136309-88-1	18
4	1,1,2,2-Tetramethyl-5-methyliden...	218	C16H26	1010387-38-1	15
5	N-(2-Acetylcyclopentylidene)cycl...	207	C13H21NO	1000100-48-5	14



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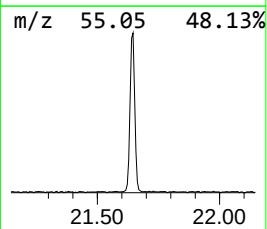
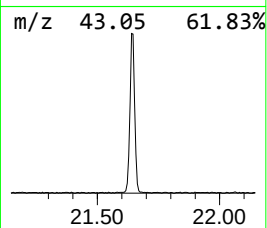
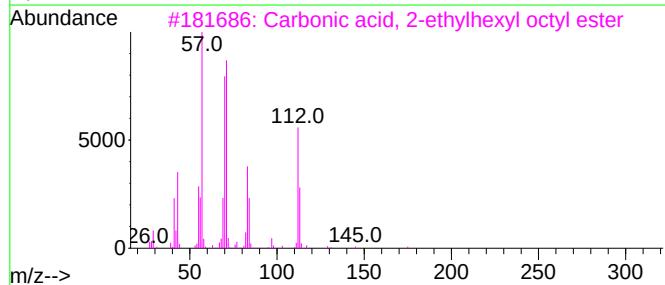
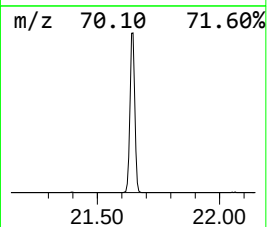
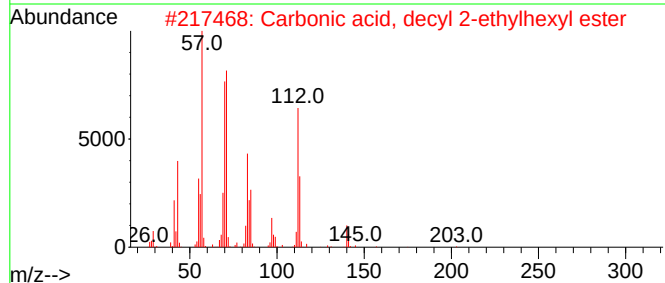
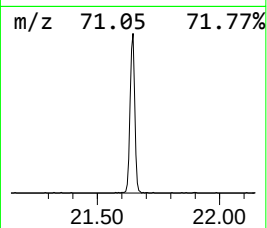
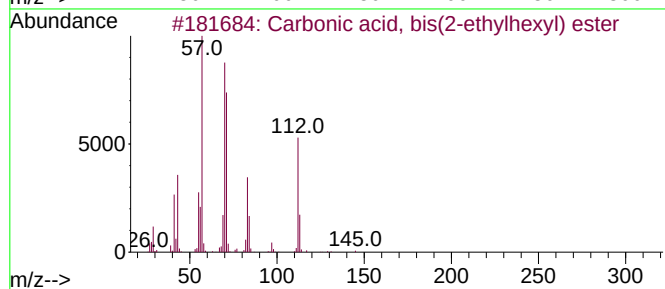
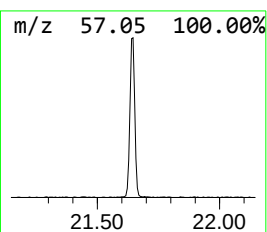
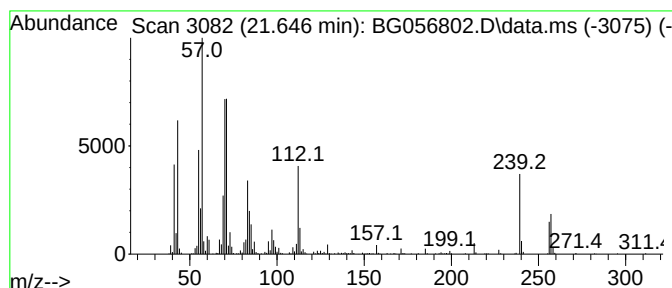
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ClientSampleId :
DBAD7

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 Carbonic acid, bis(2-ethylh... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.646	59.32 ng/ul	1004760	Chrysene-d12	22.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	58
2	Carbonic acid, decyl 2-ethylhexy...	314	C19H38O3	1000383-13-7	53
3	Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	53
4	Carbonic acid, 2-ethylhexyl nony...	300	C18H36O3	1000383-13-6	50
5	Oxalic acid, 2-ethylhexyl tetrad...	398	C24H46O4	1000309-39-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056802.D
Acq On : 2 Mar 2023 22:57
Operator : CG/JU
Sample : 01712-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAD7

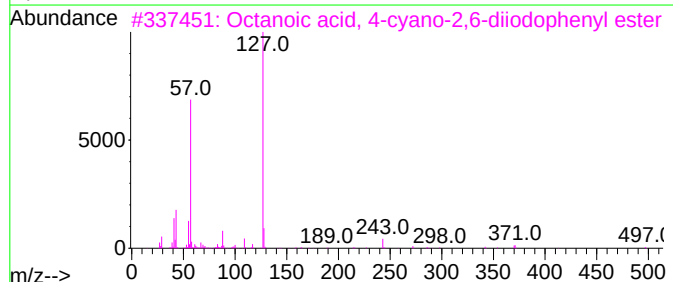
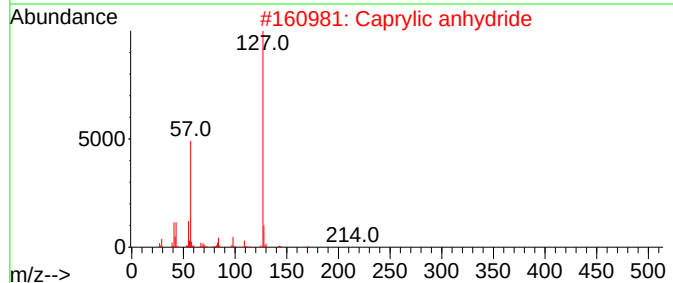
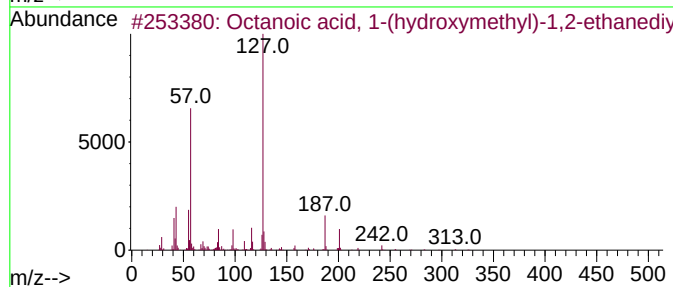
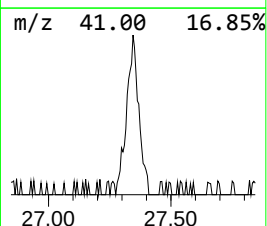
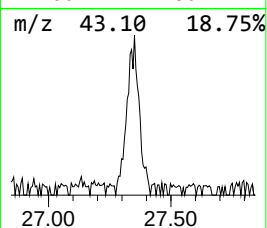
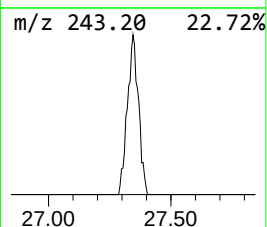
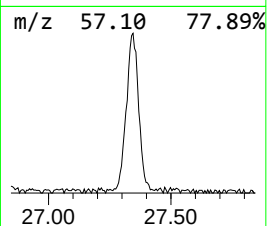
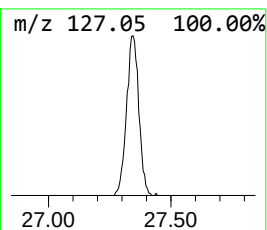
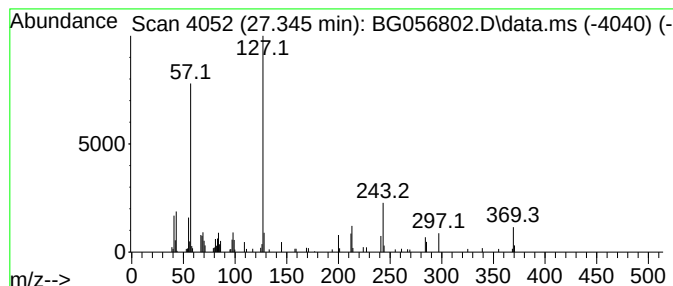
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octanoic acid, 1-(hydroxyme... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.345	13.80 ng/ul	232151	Perylene-d12	25.588

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid, 1-(hydroxymethyl)...	344	C19H36O5	060514-48-9	50
2			Caprylic anhydride	270	C16H30O3	000623-66-5	47
3			Octanoic acid, 4-cyano-2,6-diiod...	497	C15H17I2NO2	003861-47-0	47
4			3-Fluoro-5-methoxypyridine	127	C6H6FNO	1060801-62-8	47
5			2-Fluoro-5-methoxypyridine	127	C6H6FNO	136888-79-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056802.D
Acq On : 2 Mar 2023 22:57
Operator : CG/JU
Sample : 01712-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAD7

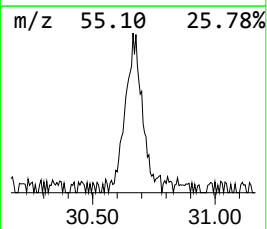
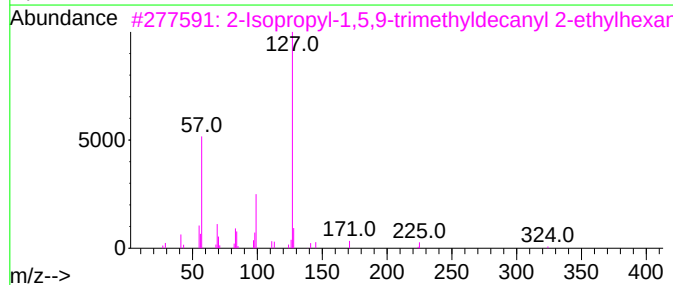
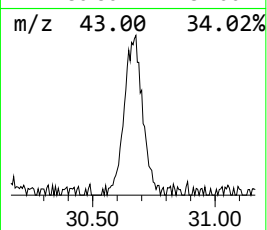
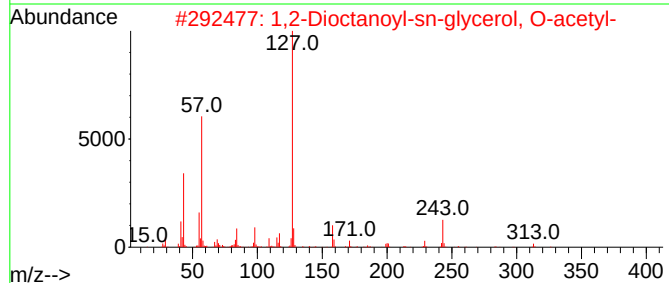
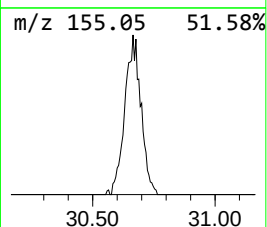
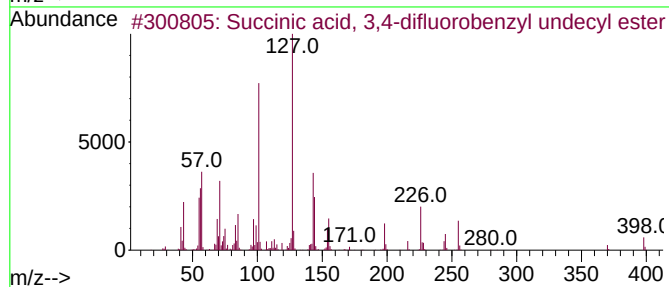
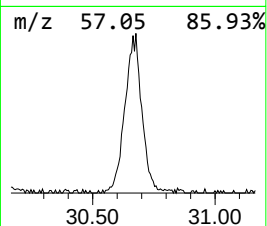
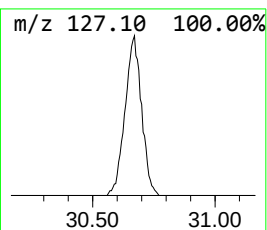
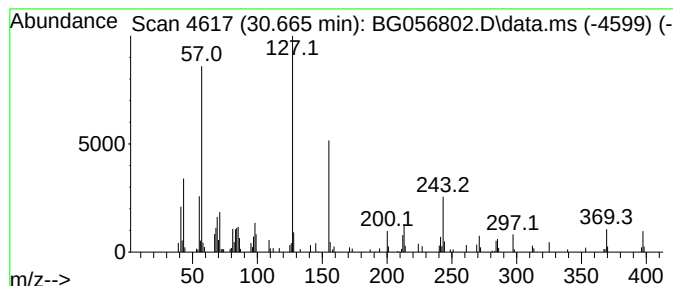
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.665	26.32 ng/ul	442862	Perylene-d12	25.588

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 3,4-difluorobenzy...	398	C22H32F2O4	1000381-74-9	38
2			1,2-Dioctanoyl-sn-glycerol, O-ac...	386	C21H38O6	1000452-09-1	38
3			2-Isopropyl-1,5,9-trimethyldecan...	368	C24H48O2	1010432-40-5	35
4			Octanoic acid, 4-cyano-2,6-diiod...	497	C15H17I2NO2	003861-47-0	35
5			Spiro[bicyclo[2.2.1]heptane-2,2'...	212	C12H20O3	035972-92-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056802.D
Acq On : 2 Mar 2023 22:57
Operator : CG/JU
Sample : 01712-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAD7

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
3,5-di-tert-But...	18.814	7.1	ng/u1	112470	4	17.750	315307	20.0
unknown-01	20.001	2.6	ng/u1	44562	5	22.063	338752	20.0
Carbonic acid, ...	21.646	59.3	ng/u1	1004760	5	22.063	338752	20.0
Octanoic acid, ...	27.345	13.8	ng/u1	232151	6	25.588	336495	20.0
unknown-02	30.665	26.3	ng/u1	442862	6	25.588	336495	20.0