

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
 Data File : BG056803.D
 Acq On : 2 Mar 2023 23:38
 Operator : CG/JU
 Sample : 01712-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DBAD8

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: BG056803.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.997	76	78	82	rVB2	1565	1567	0.13%	0.019%
2	4.138	100	102	113	rBV	20862	34271	2.74%	0.423%
3	4.385	142	144	150	rVB2	2261	3026	0.24%	0.037%
4	4.496	160	163	166	rBV2	1851	2506	0.20%	0.031%
5	7.540	676	681	686	rBV	21700	32403	2.59%	0.400%
6	7.722	706	712	718	rVB	54208	90373	7.22%	1.114%
7	7.939	741	749	758	rVB	56683	94872	7.58%	1.170%
8	8.415	823	830	839	rVB	54417	94482	7.54%	1.165%
9	9.103	941	947	958	rVB2	53805	89782	7.17%	1.107%
10	9.590	1023	1030	1037	rVB	79796	140440	11.22%	1.732%
11	10.319	1148	1154	1162	rVB	57141	100224	8.00%	1.236%
12	10.859	1239	1246	1253	rBV2	92298	164591	13.14%	2.030%
13	11.059	1279	1280	1286	rBV4	1739	1911	0.15%	0.024%
14	11.253	1307	1313	1322	rVB	76694	140415	11.21%	1.732%
15	11.376	1327	1334	1341	rBV	89255	152539	12.18%	1.881%
16	12.798	1573	1576	1581	rBV3	1409	2288	0.18%	0.028%
17	13.732	1733	1735	1737	rBV	2560	1999	0.16%	0.025%
18	14.408	1843	1850	1856	rVB	225446	316960	25.31%	3.909%
19	14.720	1896	1903	1910	rVB	230733	359925	28.74%	4.439%
20	14.925	1932	1938	1942	rVB2	1561	2341	0.19%	0.029%
21	14.990	1942	1949	1953	rBV	861678	1252249	100.00%	15.443%
22	15.019	1953	1954	1962	rVB	143430	143634	11.47%	1.771%
23	15.172	1975	1980	1988	rVB2	17717	26845	2.14%	0.331%
24	15.730	2069	2075	2077	rBV3	4405	5756	0.46%	0.071%
25	15.759	2077	2080	2083	rVV	2513	2650	0.21%	0.033%
26	16.000	2115	2121	2130	rVB	313170	475183	37.95%	5.860%
27	16.100	2133	2138	2143	rBV3	7952	10119	0.81%	0.125%
28	17.751	2413	2419	2426	rBV	200189	297315	23.74%	3.666%
29	17.851	2430	2436	2443	rVV	361500	542858	43.35%	6.694%
30	17.928	2446	2449	2454	rVB3	2040	3048	0.24%	0.038%
31	17.998	2458	2461	2465	rBV2	1158	1791	0.14%	0.022%
32	18.386	2523	2527	2531	rBV3	1844	2855	0.23%	0.035%
33	18.497	2541	2546	2550	rVB2	1719	2959	0.24%	0.036%
34	18.591	2558	2562	2565	rBV2	1847	1988	0.16%	0.025%
35	18.674	2572	2576	2580	rBV2	3159	4158	0.33%	0.051%
36	18.809	2595	2599	2608	rBV3	10139	18217	1.45%	0.225%

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37	19.009	2630	2633	2637	rVB5	1183	1907	0.15%	0.024%
38	19.461	2707	2710	2714	rVB5	1528	1806	0.14%	0.022%
39	19.678	2744	2747	2751	rVB5	5177	6296	0.50%	0.078%
40	19.749	2751	2759	2764	rVB5	4508	7572	0.60%	0.093%

41	20.113	2815	2821	2828	rVB	430853	628380	50.18%	7.749%
42	20.225	2835	2840	2842	rBV2	1001	1686	0.13%	0.021%
43	20.313	2851	2855	2860	rBV4	2043	4061	0.32%	0.050%
44	20.542	2891	2894	2897	rBV2	1725	2368	0.19%	0.029%
45	20.583	2899	2901	2903	rBV	2272	1594	0.13%	0.020%

46	20.942	2959	2962	2965	rBV2	1618	1815	0.14%	0.022%
47	21.024	2974	2976	2977	rBV2	1952	1863	0.15%	0.023%
48	21.188	3000	3004	3006	rBV4	1318	1879	0.15%	0.023%
49	21.447	3045	3048	3050	rVB3	1604	1922	0.15%	0.024%
50	21.641	3075	3081	3089	rVB	609424	820484	65.52%	10.118%

51	21.799	3106	3108	3112	rBV5	1112	1723	0.14%	0.021%
52	21.905	3121	3126	3127	rBV5	5723	6509	0.52%	0.080%
53	21.976	3127	3138	3139	rBV8	26605	61284	4.89%	0.756%
54	22.058	3146	3152	3167	rVB2	195610	393649	31.44%	4.854%
55	22.375	3203	3206	3209	rVB4	2063	2518	0.20%	0.031%

56	22.411	3209	3212	3215	rBV4	2027	3295	0.26%	0.041%
57	22.475	3220	3223	3226	rBV3	1452	2371	0.19%	0.029%
58	22.869	3285	3290	3298	rVV8	5439	11427	0.91%	0.141%
59	23.627	3417	3419	3421	rVV3	2057	1864	0.15%	0.023%
60	24.367	3543	3545	3547	rBV3	2228	1780	0.14%	0.022%

61	24.508	3567	3569	3570	rBV2	2088	1698	0.14%	0.021%
62	24.637	3590	3591	3596	rBV5	1859	2765	0.22%	0.034%
63	24.696	3600	3601	3603	rBV	2562	1878	0.15%	0.023%
64	24.761	3609	3612	3614	rBV4	2083	1995	0.16%	0.025%
65	24.890	3632	3634	3637	rBV3	1685	2396	0.19%	0.030%

66	25.178	3679	3683	3687	rBV6	2018	3346	0.27%	0.041%
67	25.342	3699	3711	3724	rVB2	202553	601547	48.04%	7.418%
68	25.472	3731	3733	3735	rVB3	2223	1835	0.15%	0.023%
69	25.583	3739	3752	3764	rBV3	104979	318648	25.45%	3.930%
70	25.848	3795	3797	3800	rBV4	1801	1632	0.13%	0.020%

71	25.901	3804	3806	3812	rBV5	1337	2216	0.18%	0.027%
72	26.359	3879	3884	3886	rBV6	1882	3146	0.25%	0.039%
73	26.964	3985	3987	3992	rBV6	1376	2598	0.21%	0.032%
74	27.164	4019	4021	4025	rBV4	1342	1693	0.14%	0.021%
75	27.211	4027	4029	4033	rBV5	2107	2669	0.21%	0.033%

76	27.346	4040	4052	4062	rVB3	55681	182253	14.55%	2.248%
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77	27.516	4077	4081	4082	rBV3	1541	1603	0.13%	0.020%
78	27.681	4107	4109	4114	rVB5	2296	3139	0.25%	0.039%
79	27.822	4132	4133	4137	rBV4	2424	1891	0.15%	0.023%
80	27.857	4137	4139	4142	rVV4	1787	1647	0.13%	0.020%
81	28.033	4166	4169	4170	rBV2	1992	2197	0.18%	0.027%
82	28.157	4189	4190	4193	rBV3	2294	1688	0.13%	0.021%
83	28.321	4215	4218	4219	rVV3	2257	2141	0.17%	0.026%
84	28.498	4246	4248	4251	rVB4	2152	1893	0.15%	0.023%
85	28.756	4289	4292	4293	rVB3	2693	1958	0.16%	0.024%
86	28.774	4293	4295	4297	rBV3	1790	1731	0.14%	0.021%
87	28.950	4321	4325	4326	rVV3	2555	2704	0.22%	0.033%
88	28.985	4329	4331	4333	rVV3	2240	1723	0.14%	0.021%
89	29.050	4341	4342	4350	rVB7	3687	4427	0.35%	0.055%
90	29.238	4373	4374	4378	rBV4	1297	2013	0.16%	0.025%
91	29.408	4401	4403	4407	rVB4	2169	1788	0.14%	0.022%
92	30.060	4512	4514	4516	rBV	2156	1918	0.15%	0.024%
93	30.278	4549	4551	4555	rBV4	1630	2522	0.20%	0.031%
94	30.360	4564	4565	4570	rBV4	2787	2772	0.22%	0.034%
95	30.460	4580	4582	4585	rVB4	1585	1632	0.13%	0.020%
96	30.654	4600	4615	4633	rVB4	75792	338567	27.04%	4.175%
97	31.576	4767	4772	4775	rBV4	1402	2700	0.22%	0.033%
98	31.876	4821	4823	4826	rVB3	1986	2025	0.16%	0.025%
99	32.305	4893	4896	4897	rBV3	2168	1574	0.13%	0.019%
100	32.581	4942	4943	4946	rBV2	2129	1901	0.15%	0.023%

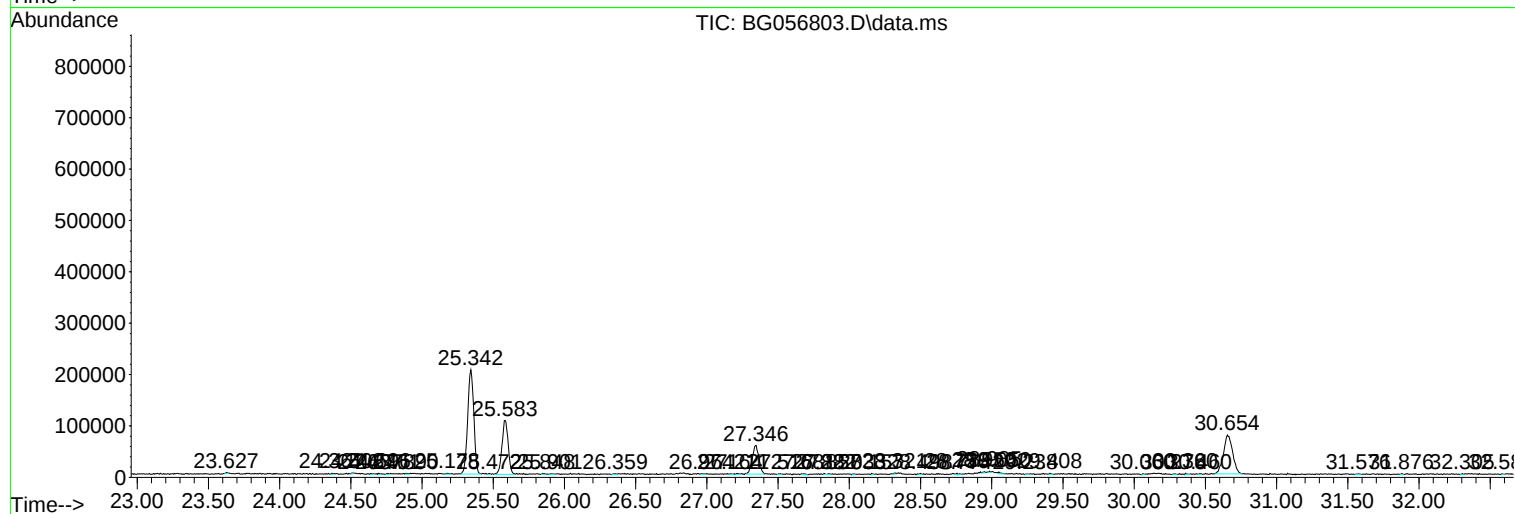
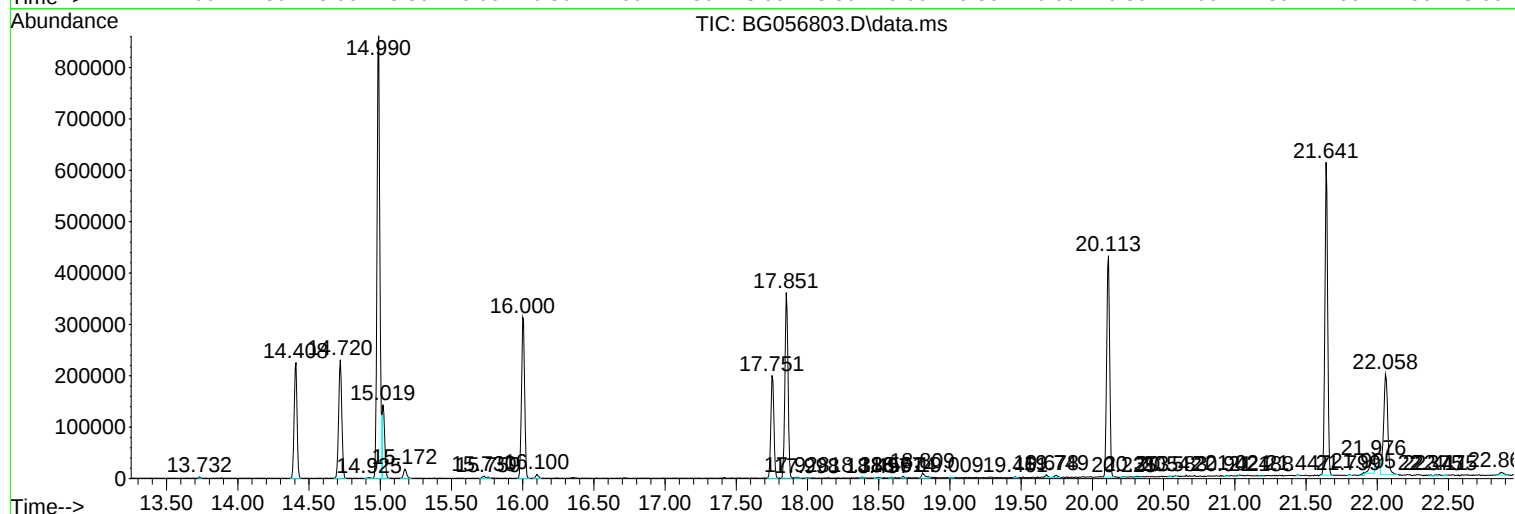
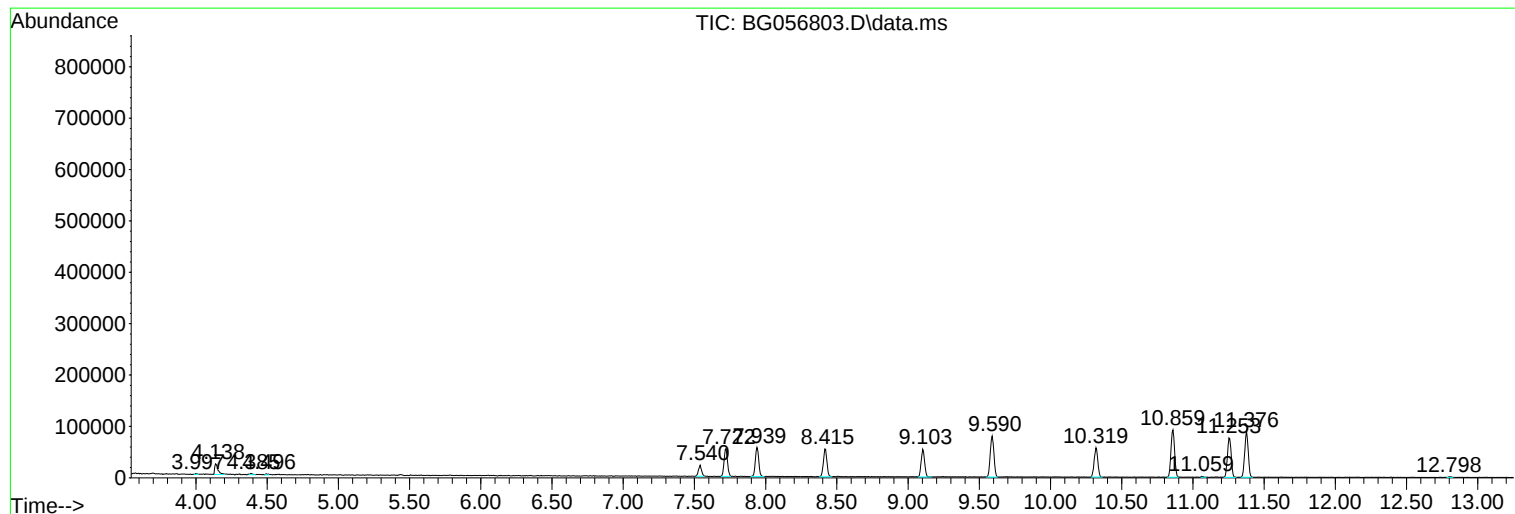
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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



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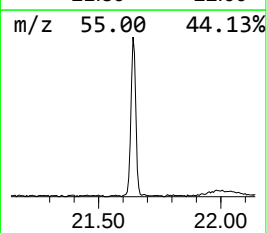
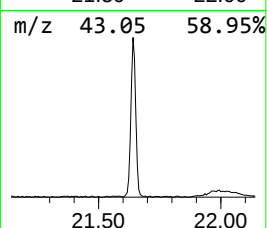
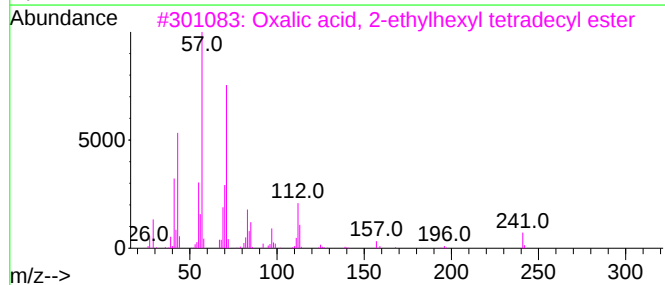
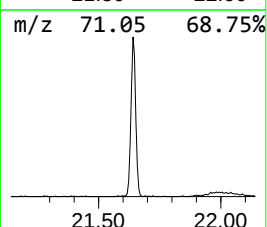
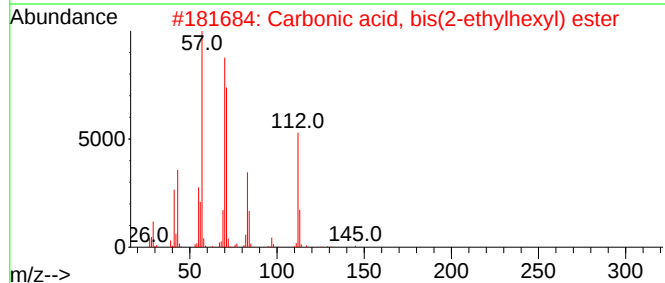
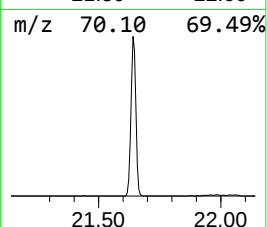
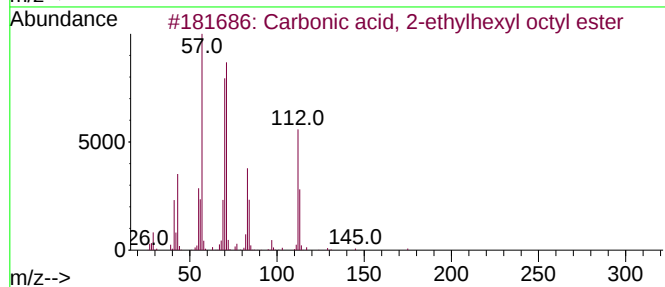
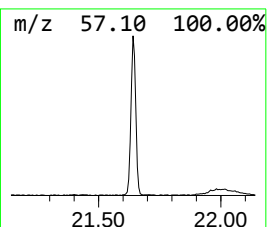
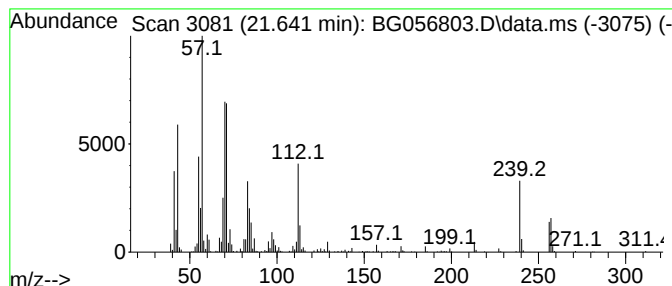
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Carbonic acid, 2-ethylhexyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.641	41.69 ng/ul	820484	Chrysene-d12	22.058

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	58
2			Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	58
3			Oxalic acid, 2-ethylhexyl tetrad...	398	C24H46O4	1000309-39-7	38
4			Oxalic acid, 2-ethylhexyl pentad...	412	C25H48O4	1000309-39-8	38
5			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	35



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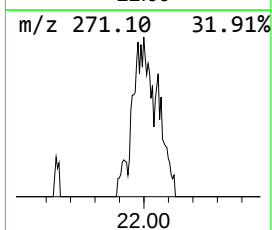
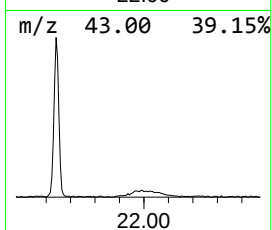
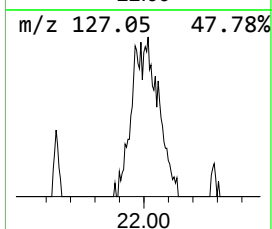
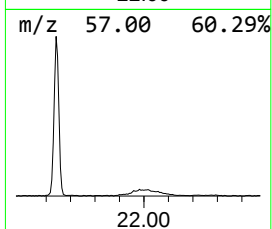
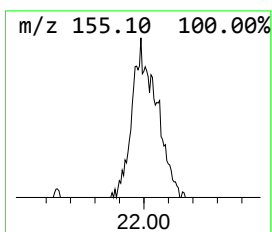
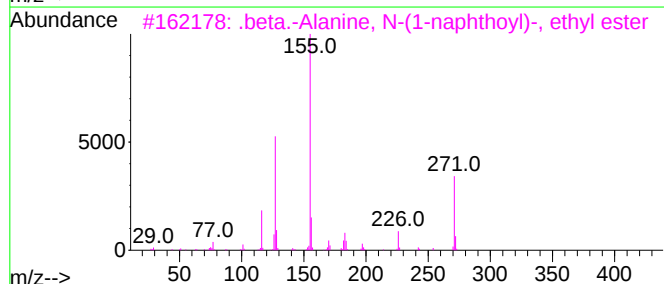
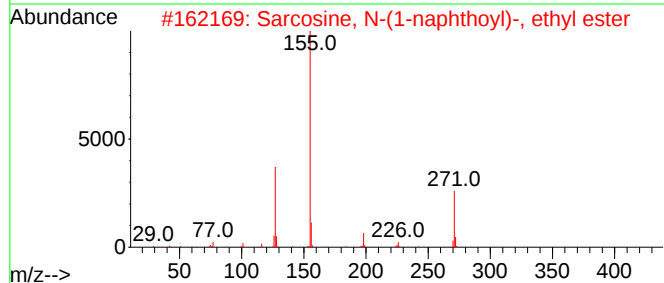
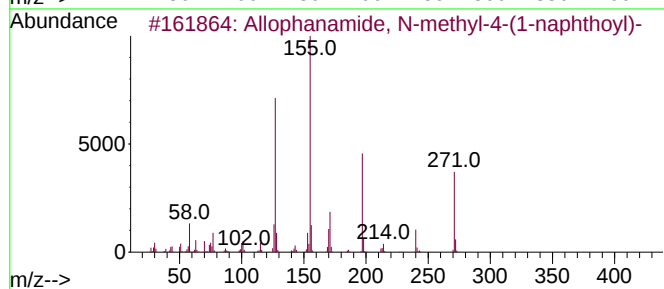
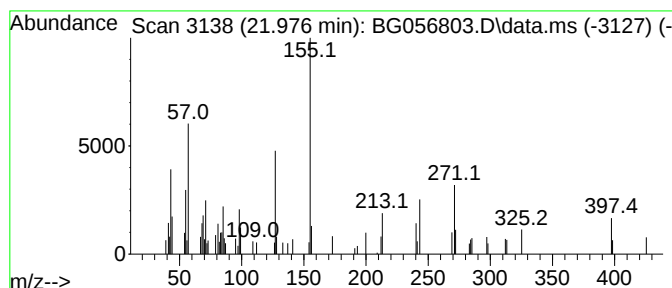
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Allophanamide, N-methyl-4-(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.976	3.11 ng/ul	61284	Chrysene-d12	22.058

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Allophanamide, N-methyl-4-(1-nap...	271	C14H13N3O3	1000160-42-1	64
2			Sarcosine, N-(1-naphthoyl)-, eth...	271	C16H17NO3	1000321-39-8	58
3			.beta.-Alanine, N-(1-naphthoyl)-...	271	C16H17NO3	1000321-94-4	58
4			Sarcosine, N-(1-naphthoyl)-, und...	397	C25H35NO3	1000321-40-9	50
5			5-Oxazolidinone, 2-(1,1-dimethyl...	297	C18H19NO3	119215-56-4	49



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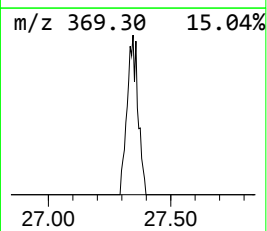
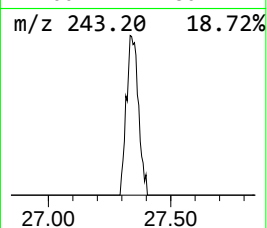
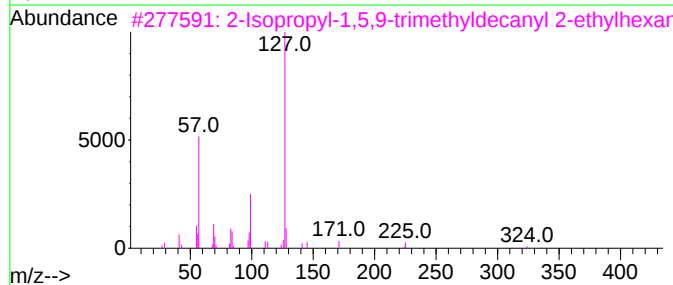
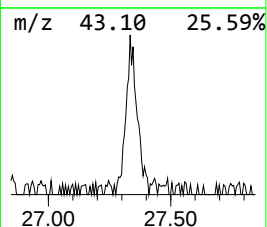
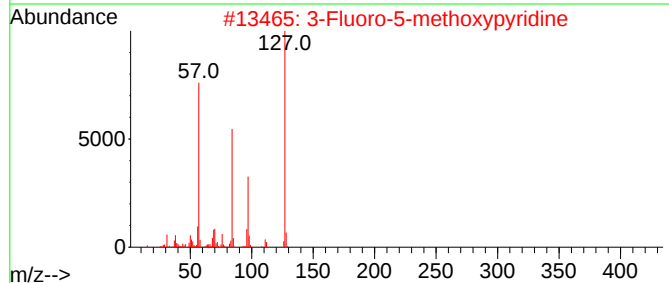
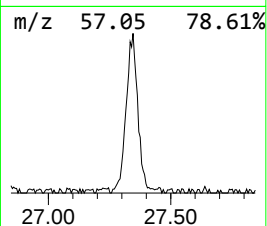
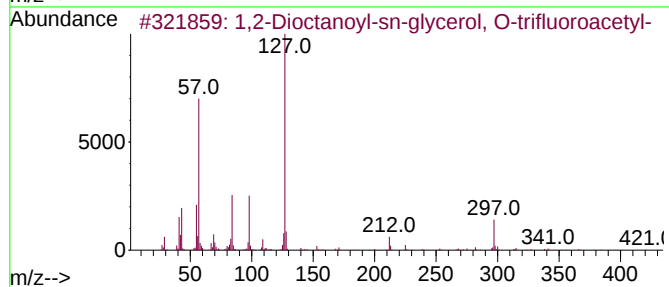
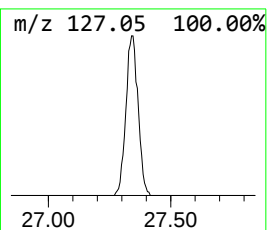
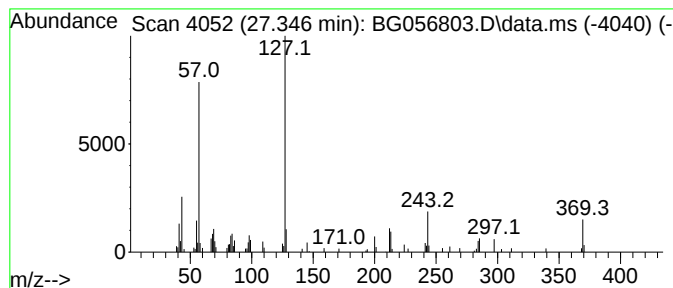
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 1,2-Dioctanoyl-sn-glycerol,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.346	11.44 ng/ul	182253	Perylene-d12	25.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dioctanoyl-sn-glycerol, O-tr...	440	C21H35F3O6	1000452-09-0	53
2			3-Fluoro-5-methoxypyridine	127	C6H6FNO	1060801-62-8	50
3			2-Isopropyl-1,5,9-trimethyldecan...	368	C24H48O2	1010432-40-5	50
4			Octanethioic acid, S-hexyl ester	244	C14H28O5	055590-85-7	50
5			1,2-Benzenediol, O-valeryl-O'-oc...	320	C19H28O4	1000329-77-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056803.D
Acq On : 2 Mar 2023 23:38
Operator : CG/JU
Sample : 01712-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAD8

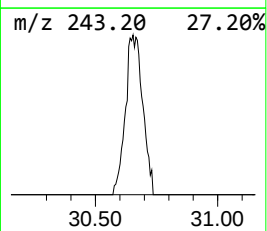
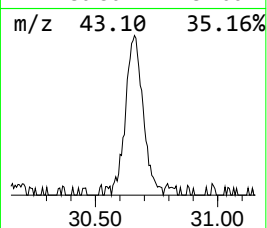
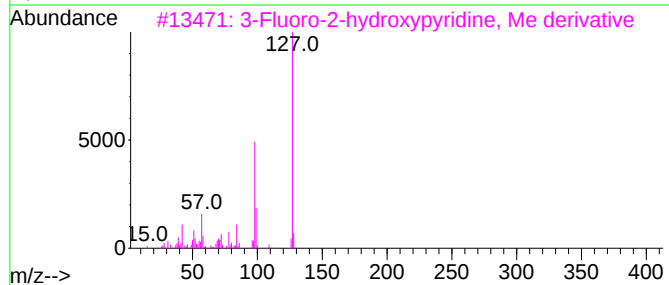
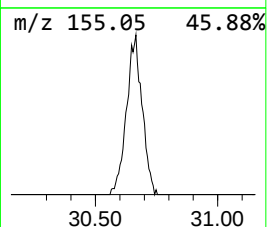
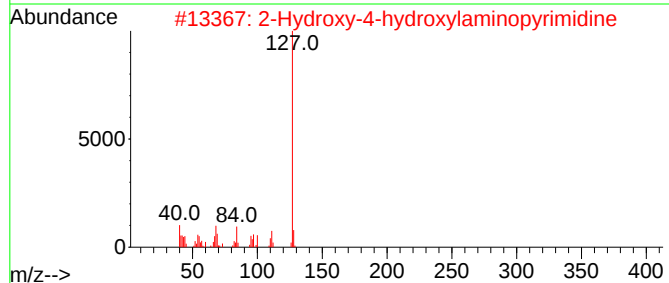
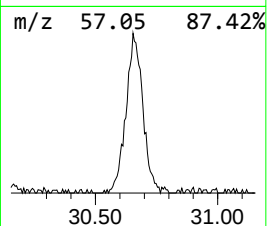
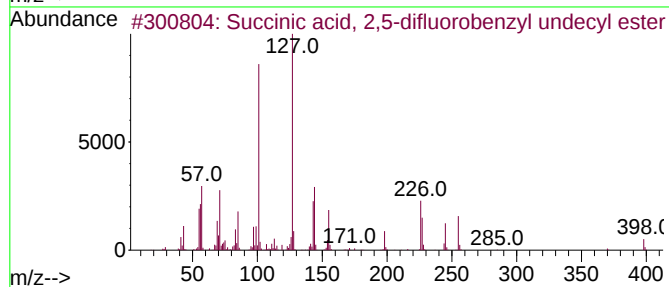
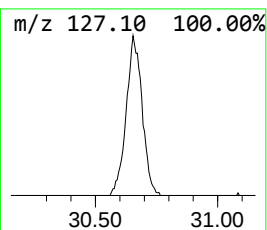
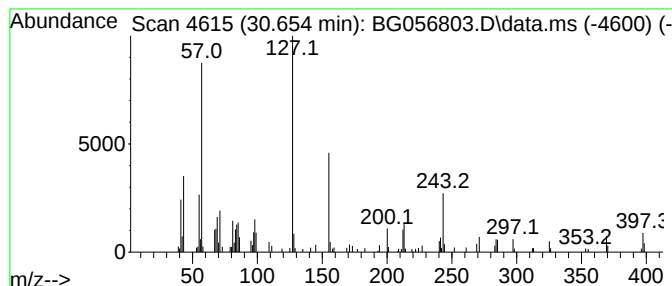
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.654	21.25 ng/ul	338567	Perylene-d12	25.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2,5-difluorobenzy...	398	C22H32F2O4	1000381-22-6	43
2			2-Hydroxy-4-hydroxylaminopyrimidine	127	C4H5N3O2	020555-88-8	38
3			3-Fluoro-2-hydroxypyridine, Me d...	127	C6H6FN0	1000496-78-9	38
4			cis-2-Methyl-2-butenedioic acid,...	158	C7H10O4	000617-54-9	35
5			1-Ethyl-2-methylpropyl isopropyl...	210	C9H20F02P	1000510-36-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056803.D
Acq On : 2 Mar 2023 23:38
Operator : CG/JU
Sample : 01712-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAD8

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
Carbonic acid, ...	21.641	41.7	ng/ul	820484	5	22.058	393649	20.0
Allophanamide, ...	21.976	3.1	ng/ul	61284	5	22.058	393649	20.0
1,2-Dioctanoyl-...	27.346	11.4	ng/ul	182253	6	25.583	318648	20.0
unknown-01	30.654	21.3	ng/ul	338567	6	25.583	318648	20.0