

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090823\
 Data File : BG058947.D
 Acq On : 9 Sep 2023 12:09
 Operator : MA/JU
 Sample : 04250-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BH4A1

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-BG090823.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG058947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.606	14	20	34	rVB	342486	568143	22.95%	2.524%
2	3.847	59	61	63	rBV	5691	5493	0.22%	0.024%
3	4.070	95	99	106	rBV	37806	64522	2.61%	0.287%
4	4.205	117	122	126	rBV6	4631	9837	0.40%	0.044%
5	4.287	132	136	141	rVB3	7450	11479	0.46%	0.051%
6	4.399	152	155	156	rBV3	5477	3682	0.15%	0.016%
7	4.411	156	157	162	rVB4	4991	5930	0.24%	0.026%
8	4.493	169	171	173	rVB2	5872	5413	0.22%	0.024%
9	4.634	192	195	196	rBV	3214	3705	0.15%	0.016%
10	4.793	218	222	227	rBV3	4992	7069	0.29%	0.031%
11	4.840	227	230	233	rVB3	4098	4926	0.20%	0.022%
12	4.892	238	239	241	rVB	5549	3770	0.15%	0.017%
13	4.945	246	248	250	rVB2	5927	5611	0.23%	0.025%
14	5.010	254	259	262	rBV3	4088	8077	0.33%	0.036%
15	5.233	294	297	302	rBV2	4142	6337	0.26%	0.028%
16	5.368	315	320	326	rBV2	39650	63245	2.55%	0.281%
17	5.586	354	357	362	rVB3	8381	11906	0.48%	0.053%
18	5.621	362	363	366	rBV2	4007	3693	0.15%	0.016%
19	5.739	382	383	388	rBV2	5608	5544	0.22%	0.025%
20	5.833	397	399	402	rVB4	3968	4034	0.16%	0.018%
21	5.874	402	406	408	rBV2	6807	7626	0.31%	0.034%
22	5.985	421	425	426	rBV3	7163	6804	0.27%	0.030%
23	6.379	490	492	496	rBV	3069	4063	0.16%	0.018%
24	6.861	570	574	577	rBV	3919	4541	0.18%	0.020%
25	7.102	613	615	619	rVB2	4323	5215	0.21%	0.023%
26	7.219	632	635	639	rVB3	3633	4548	0.18%	0.020%
27	7.372	658	661	664	rBV	3267	3767	0.15%	0.017%
28	7.437	664	672	682	rVB2	66891	117053	4.73%	0.520%
29	7.648	700	708	715	rBV	169660	288219	11.64%	1.280%
30	7.742	720	724	728	rVB	2940	4199	0.17%	0.019%
31	7.842	733	741	748	rBV	193496	320689	12.95%	1.425%
32	8.048	775	776	781	rVB2	3963	4677	0.19%	0.021%
33	8.206	800	803	808	rVB3	8735	12954	0.52%	0.058%
34	8.253	808	811	813	rBV	3755	4507	0.18%	0.020%
35	8.330	813	824	829	rBV	168522	302312	12.21%	1.343%
36	8.412	836	838	841	rVB	4403	3951	0.16%	0.018%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090823.MA.M
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37	8.476	844	849	851	rBV2	4314	5409	0.22%	0.024%
38	8.682	880	884	887	rVV3	10414	14944	0.60%	0.066%
39	8.747	892	895	897	rBV	2877	4140	0.17%	0.018%
40	8.911	921	923	928	rVB2	4191	4372	0.18%	0.019%

41	9.005	933	939	947	rVB3	170590	301493	12.18%	1.339%
42	9.434	1006	1012	1013	rBV	2518	4880	0.20%	0.022%
43	9.522	1019	1027	1034	rBV2	219105	380930	15.39%	1.692%
44	9.675	1051	1053	1058	rBV2	4611	5654	0.23%	0.025%
45	9.710	1058	1059	1062	rBV	3374	4117	0.17%	0.018%

46	9.851	1080	1083	1087	rBV	3806	5321	0.21%	0.024%
47	9.986	1105	1106	1110	rVB	4296	3995	0.16%	0.018%
48	10.110	1124	1127	1131	rVB2	3183	4078	0.16%	0.018%
49	10.245	1143	1150	1159	rVB3	169603	306116	12.36%	1.360%
50	10.703	1225	1228	1230	rBV	2927	3968	0.16%	0.018%

51	10.768	1230	1239	1246	rVV	329367	592847	23.95%	2.633%
52	11.021	1275	1282	1287	rVB4	18461	34415	1.39%	0.153%
53	11.173	1298	1308	1315	rBV	235273	444485	17.95%	1.974%
54	11.314	1325	1332	1339	rBV	149598	288902	11.67%	1.283%
55	11.514	1363	1366	1367	rBV	4174	4273	0.17%	0.019%

56	11.544	1367	1371	1376	rVB4	11827	22567	0.91%	0.100%
57	11.690	1392	1396	1397	rBV	4899	4225	0.17%	0.019%
58	12.078	1459	1462	1465	rVB2	3422	4995	0.20%	0.022%
59	12.207	1481	1484	1487	rVB3	3803	4838	0.20%	0.021%
60	12.319	1500	1503	1504	rBV2	4323	3671	0.15%	0.016%

61	12.442	1522	1524	1525	rBV2	5976	4264	0.17%	0.019%
62	12.525	1535	1538	1540	rBV	3739	4311	0.17%	0.019%
63	12.648	1552	1559	1565	rBV	212283	352347	14.23%	1.565%
64	12.912	1602	1604	1607	rVB2	4703	4258	0.17%	0.019%
65	13.018	1620	1622	1627	rVB2	3699	5535	0.22%	0.025%

66	13.065	1627	1630	1631	rBV2	6112	5109	0.21%	0.023%
67	13.230	1655	1658	1661	rBV2	5539	7218	0.29%	0.032%
68	13.347	1677	1678	1680	rBV2	6317	5532	0.22%	0.025%
69	13.394	1684	1686	1688	rVV2	5473	5481	0.22%	0.024%
70	13.424	1688	1691	1695	rVV4	4018	6130	0.25%	0.027%

71	13.606	1720	1722	1724	rVB3	4374	3731	0.15%	0.017%
72	13.717	1736	1741	1742	rBV5	4188	4494	0.18%	0.020%
73	13.794	1749	1754	1757	rBV4	14769	24830	1.00%	0.110%
74	14.352	1842	1849	1857	rVV	682677	991915	40.06%	4.406%
75	14.411	1857	1859	1863	rVB4	4445	5246	0.21%	0.023%

76	14.499	1872	1874	1875	rBV2	5722	4222	0.17%	0.019%
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77	14.516	1875	1877	1882	rVB4	5050	6229	0.25%	0.028%
78	14.575	1885	1887	1893	rVB6	6168	8494	0.34%	0.038%
79	14.658	1893	1901	1908	rBV	704201	1139583	46.03%	5.062%
80	14.793	1922	1924	1926	rBV2	3392	3612	0.15%	0.016%
81	14.898	1940	1942	1943	rBV2	4767	4400	0.18%	0.020%
82	14.951	1944	1951	1958	rVB	480292	795796	32.14%	3.535%
83	15.110	1973	1978	1986	rBV4	64763	109138	4.41%	0.485%
84	15.216	1993	1996	1997	rBV3	5732	7216	0.29%	0.032%
85	15.445	2033	2035	2036	rBV2	5635	4273	0.17%	0.019%
86	15.633	2065	2067	2068	rBV2	5465	4215	0.17%	0.019%
87	15.703	2077	2079	2084	rVB6	6271	7151	0.29%	0.032%
88	15.821	2097	2099	2100	rBV2	7288	5404	0.22%	0.024%
89	15.938	2113	2119	2128	rBV	1008291	1532272	61.89%	6.806%
90	16.038	2131	2136	2141	rVV	249436	350386	14.15%	1.556%
91	17.090	2313	2315	2318	rBV4	10179	5273	0.21%	0.023%
92	17.501	2378	2385	2391	rVB	1405659	2014784	81.38%	8.950%
93	17.701	2414	2419	2425	rVB	714425	1122589	45.34%	4.987%
94	17.801	2430	2436	2442	rVV	1172842	1790463	72.32%	7.953%
95	18.529	2557	2560	2566	rBV8	45768	60486	2.44%	0.269%
96	20.075	2817	2823	2829	rBV	1502804	2202012	88.94%	9.781%
97	22.025	3150	3155	3162	rVB	757782	1337681	54.03%	5.942%
98	25.351	3710	3721	3733	rBV2	820765	2475769	100.00%	10.997%
99	25.603	3753	3764	3776	rVB	511479	1579703	63.81%	7.017%
100	26.144	3851	3856	3863	rVB4	62199	158641	6.41%	0.705%

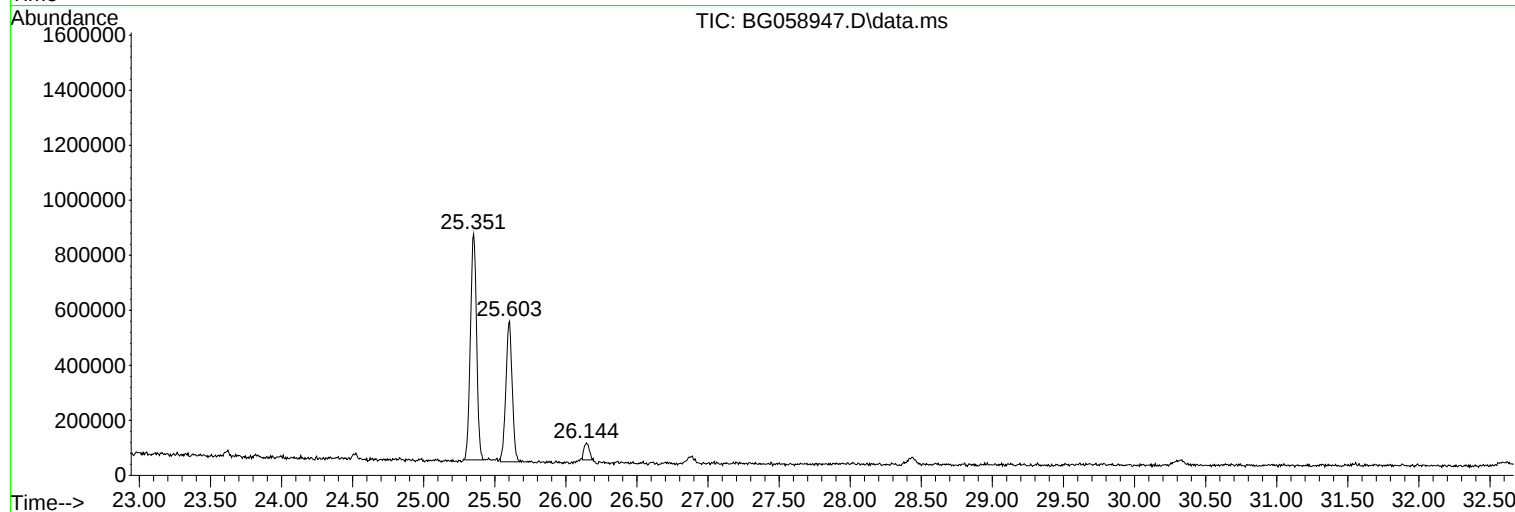
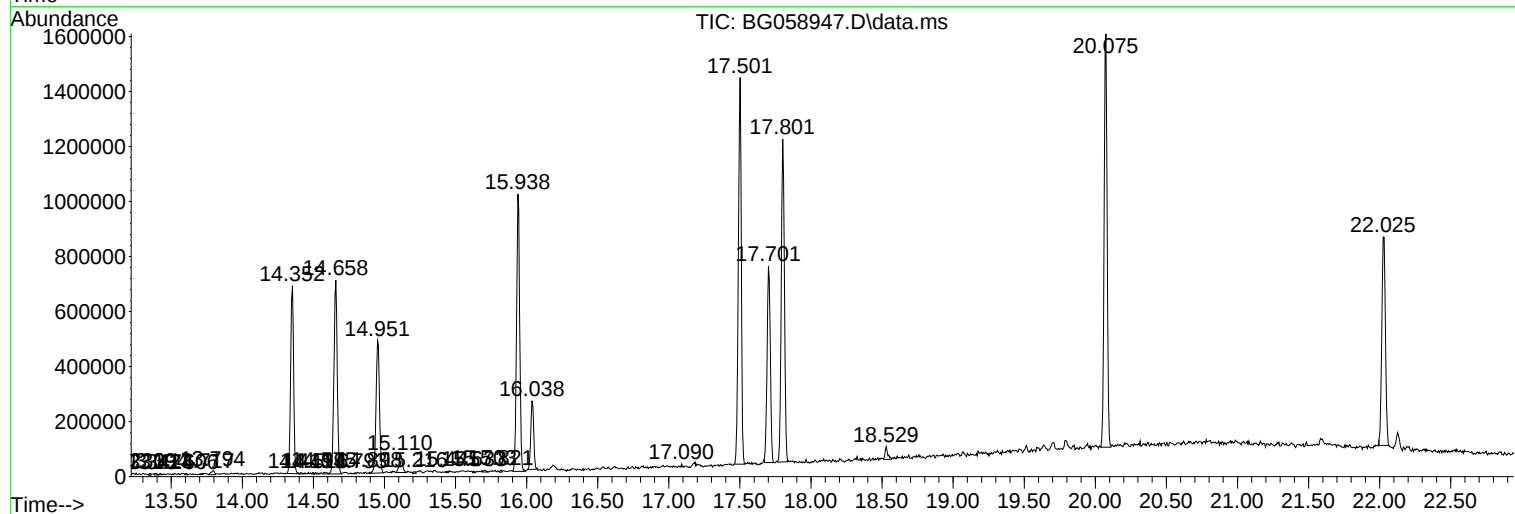
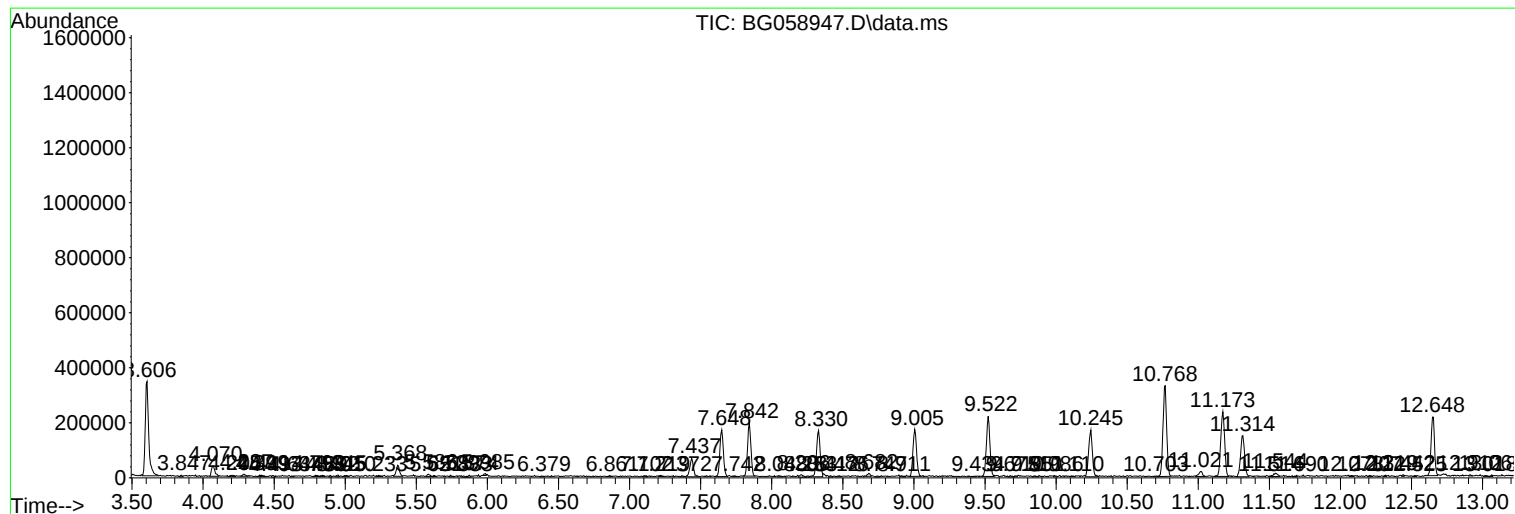
Sum of corrected areas: 22512369

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090823.MA.M
Quant Title : SVOA CALIBRATION

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



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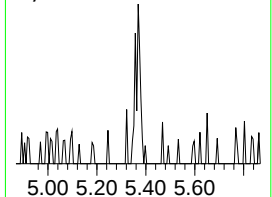
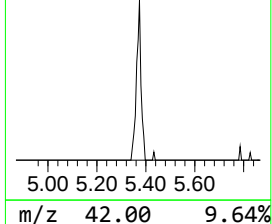
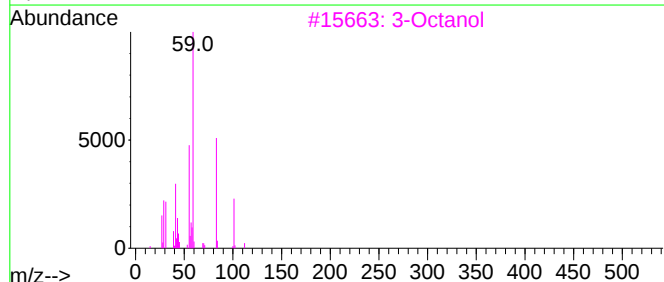
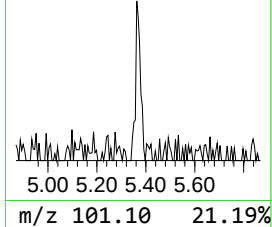
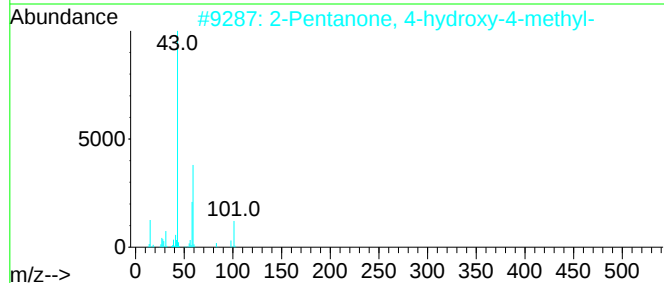
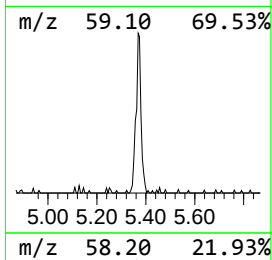
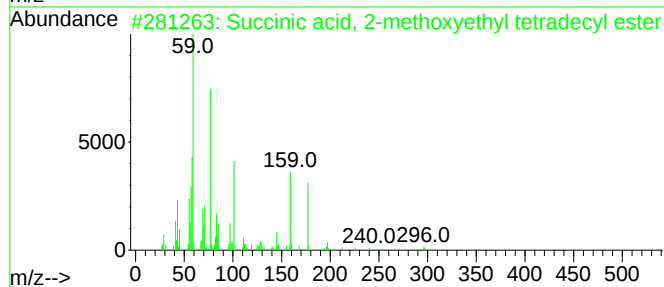
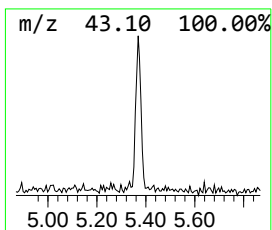
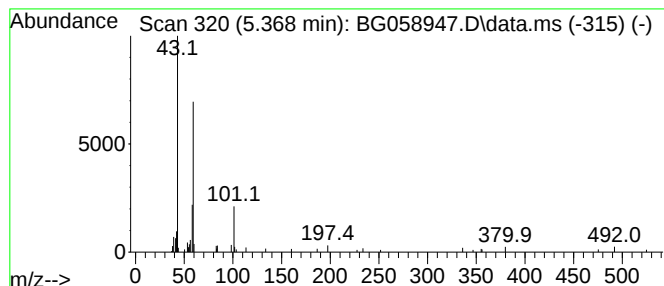
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Succinic acid, 2-methoxyeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.368	4.18 ng/ul	63245	1,4-Dichlorobenzene-d4	8.330

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-methoxyethyl te...	372	C21H40O5	1000325-81-3	50
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3			3-Octanol	130	C8H18O	000589-98-0	33
4			2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	33
5			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28



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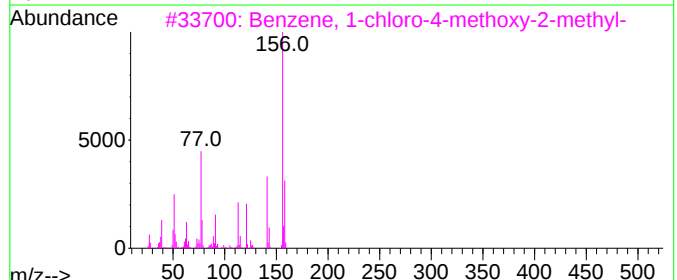
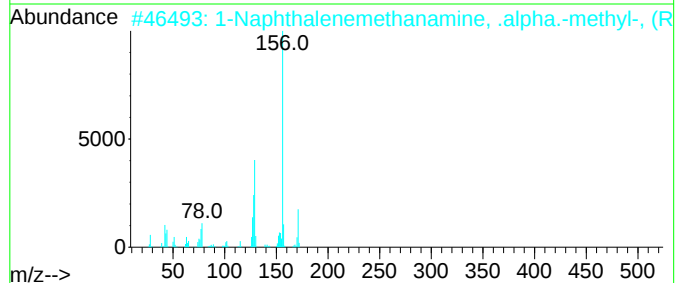
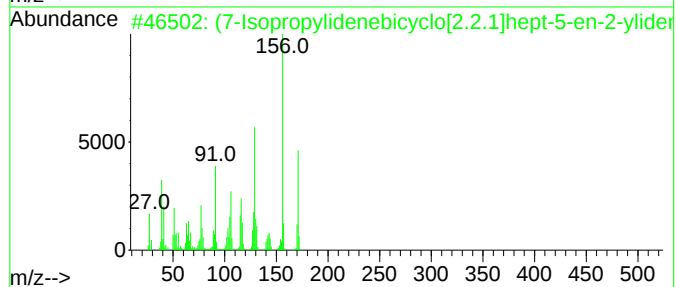
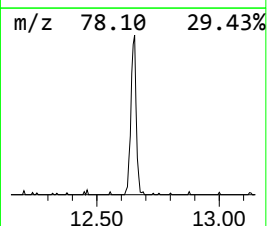
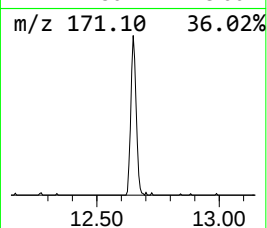
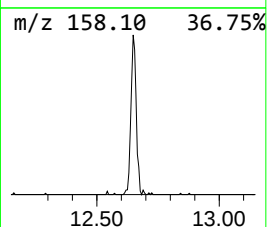
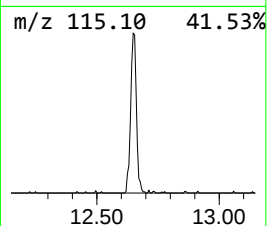
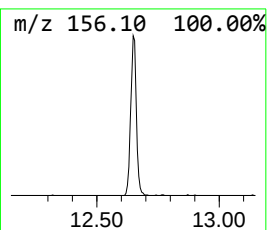
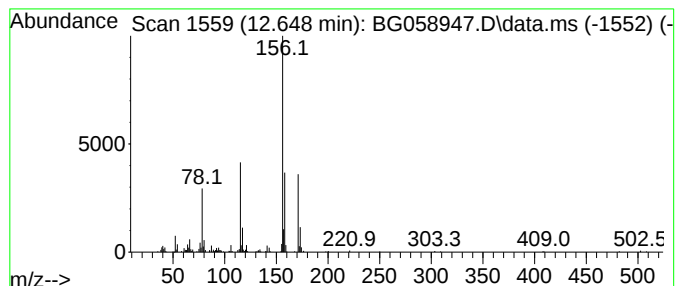
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.648	15.85 ng/ul	352347	Naphthalene-d8	11.173

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(7-Isopropylidenebicyclo[2.2.1]h...	171	C12H13N	1000211-01-9	43
2			1-Naphthalenemethanamine, .alpha...	171	C12H13N	003886-70-2	38
3			Benzene, 1-chloro-4-methoxy-2-me...	156	C8H9ClO	013334-71-9	38
4			1,2,3,3a-Tetrahydropentalene, 1,...	171	C12H13N	1000217-17-0	38
5			4-Chloro-3,5-dimethylphenol, O-(...	242	C12H15ClO3	1000487-35-2	38



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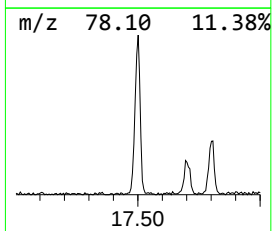
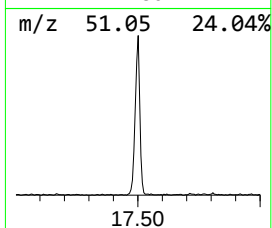
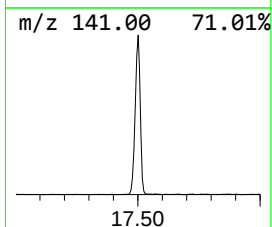
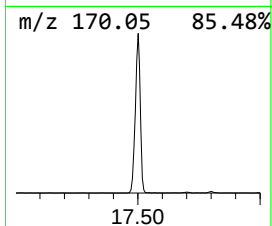
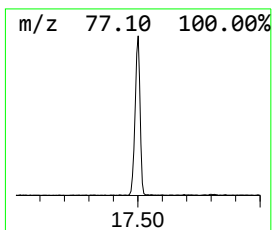
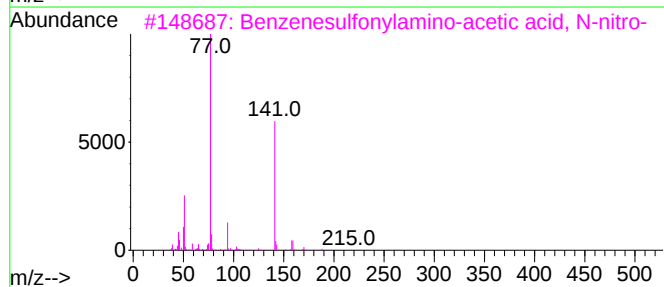
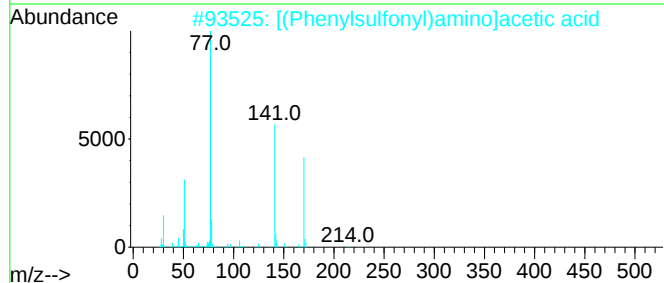
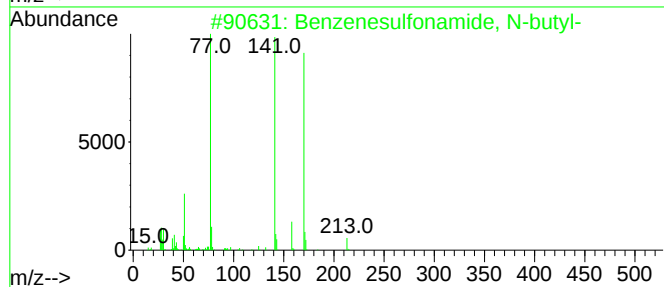
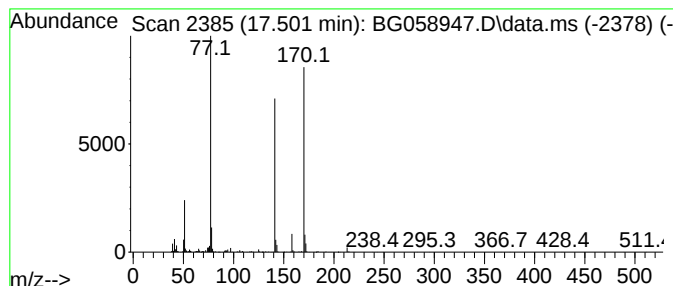
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzenesulfonamide, N-butyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.501	35.90 ng/ul	2014780	Phenanthrene-d10	17.701

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	72
2			[(Phenylsulfonyl)amino]acetic acid	215	C8H9NO4S	005398-96-9	58
3			Benzenesulfonylamino-acetic acid...	260	C8H8N2O6S	1000301-09-0	50
4			(Phenylsulfonyl)acetonitrile	181	C8H7NO2S	007605-28-9	47
5			Difluoromethyl phenyl sulfone	192	C7H6F2O2S	001535-65-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090823\
Data File : BG058947.D
Acq On : 9 Sep 2023 12:09
Operator : MA/JU
Sample : 04250-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BH4A1

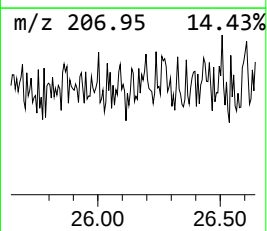
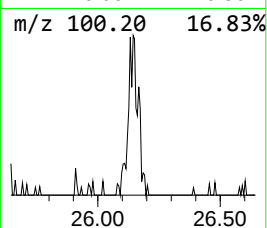
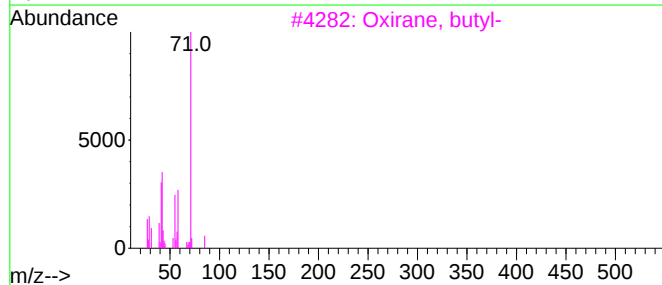
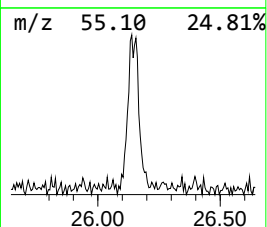
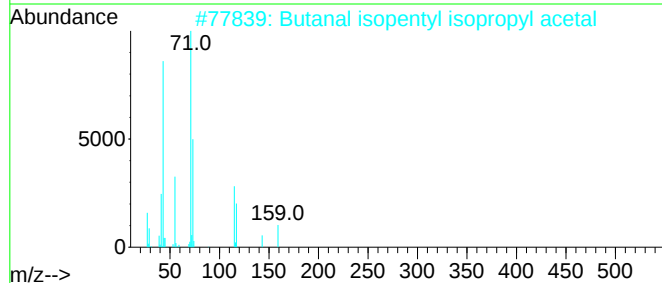
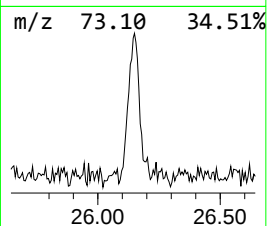
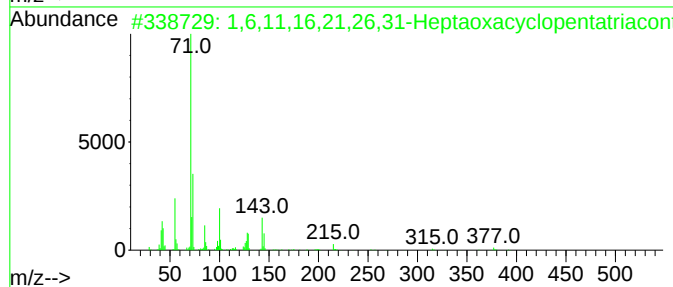
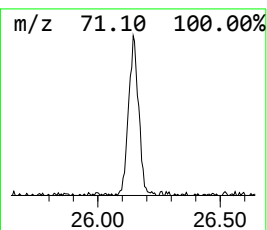
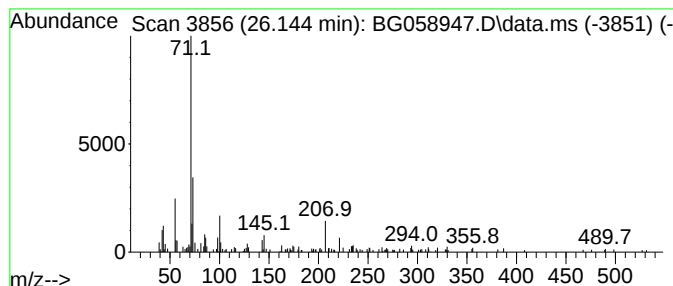
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 1,6,11,16,21,26,31-Heptaoxa... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.144	2.01 ng/ul	158641	Perylene-d12	25.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	72		
2	Butanal isopentyl isopropyl acetal	202	C12H26O2	1000431-61-0	50		
3	Oxirane, butyl-	100	C6H12O	001436-34-6	38		
4	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	35		
5	2-[Dimethyl(pentafluorophenyl)si...	326	C13H15F5O2Si	1000216-80-8	33		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090823\
Data File : BG058947.D
Acq On : 9 Sep 2023 12:09
Operator : MA/JU
Sample : 04250-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BH4A1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090823.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
Succinic acid, ...	5.368	4.2	ng/ul	63245	1	8.330	302312	20.0
unknown-01	12.648	15.9	ng/ul	352347	2	11.173	444485	20.0
Benzenesulfonam...	17.501	35.9	ng/ul	2014780	4	17.701	1122590	20.0
1,6,11,16,21,26...	26.144	2.0	ng/ul	158641	6	25.598	1579700	20.0