

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
 Data File : BG059539.D
 Acq On : 29 Oct 2023 3:32
 Operator : MA/JU
 Sample : 04925-19
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GCCY5

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-BG102723.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059539.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.658	42	46	52	rVB4	10403	17244	1.24%	0.116%
2	4.099	115	121	132	rVB	71966	128674	9.22%	0.864%
3	4.310	154	157	162	rBV2	14755	23178	1.66%	0.156%
4	4.404	171	173	176	rVB2	7367	7016	0.50%	0.047%
5	4.434	176	178	182	rVB4	5256	8160	0.58%	0.055%
6	4.810	240	242	243	rBV2	6288	5909	0.42%	0.040%
7	5.039	279	281	285	rBV4	3348	4854	0.35%	0.033%
8	5.092	288	290	291	rBV2	8015	4890	0.35%	0.033%
9	5.204	308	309	313	rBV2	5206	6069	0.43%	0.041%
10	5.368	334	337	346	rVB2	22167	40198	2.88%	0.270%
11	5.638	380	383	385	rBV3	7961	9778	0.70%	0.066%
12	5.668	385	388	389	rVB2	5986	6006	0.43%	0.040%
13	5.944	433	435	436	rVB	6877	4157	0.30%	0.028%
14	5.967	436	439	440	rBV3	8246	8303	0.59%	0.056%
15	6.014	444	447	449	rBV2	6177	5959	0.43%	0.040%
16	6.050	449	453	455	rVV2	8549	6844	0.49%	0.046%
17	6.255	485	488	489	rBV2	7009	6104	0.44%	0.041%
18	6.719	564	567	568	rBV	7671	6331	0.45%	0.043%
19	6.843	586	588	592	rVB3	5775	5883	0.42%	0.039%
20	6.890	592	596	598	rBV2	5034	7172	0.51%	0.048%
21	7.166	641	643	646	rBV2	3429	4518	0.32%	0.030%
22	7.471	689	695	704	rVB	235952	421980	30.24%	2.833%
23	7.560	709	710	713	rVB2	7061	5340	0.38%	0.036%
24	7.583	713	714	717	rBV2	3782	4293	0.31%	0.029%
25	7.683	725	731	739	rVB	162874	265624	19.03%	1.783%
26	7.742	739	741	745	rVB4	4134	4225	0.30%	0.028%
27	7.877	757	764	770	rBV	251963	430187	30.83%	2.888%
28	8.124	803	806	808	rBV2	5442	5002	0.36%	0.034%
29	8.306	834	837	838	rBV	5500	4367	0.31%	0.029%
30	8.318	838	839	841	rBV	5387	5262	0.38%	0.035%
31	8.365	841	847	857	rVB	235582	410841	29.44%	2.758%
32	8.564	879	881	884	rVB	4688	4177	0.30%	0.028%
33	8.605	886	888	891	rVB3	5128	5271	0.38%	0.035%
34	8.746	910	912	915	rVB2	6034	6290	0.45%	0.042%
35	8.793	918	920	922	rBV	5300	4831	0.35%	0.032%
36	8.840	925	928	933	rVB4	13094	19227	1.38%	0.129%

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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-BG102723.MA.M
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37	8.929	940	943	944	rBV2	5410	5897	0.42%	0.040%
38	9.040	956	962	969	rVB2	249457	427059	30.60%	2.867%
39	9.205	986	990	995	rVB4	19524	32788	2.35%	0.220%
40	9.334	1010	1012	1017	rBV5	4722	5173	0.37%	0.035%

41	9.557	1043	1050	1057	rBV2	215168	375697	26.92%	2.523%
42	9.745	1078	1082	1083	rBV3	4720	6068	0.43%	0.041%
43	9.892	1106	1107	1110	rVB3	8806	4459	0.32%	0.030%
44	9.933	1113	1114	1117	rBV	4301	5013	0.36%	0.034%
45	10.016	1125	1128	1130	rVB3	5582	4720	0.34%	0.032%

46	10.051	1130	1134	1135	rBV2	6698	7828	0.56%	0.053%
47	10.280	1165	1173	1181	rBV2	184423	360478	25.83%	2.420%
48	10.497	1208	1210	1214	rVB3	5653	4263	0.31%	0.029%
49	10.721	1246	1248	1251	rBV4	6628	5045	0.36%	0.034%
50	10.803	1254	1262	1271	rVB	338380	612668	43.90%	4.114%

51	10.867	1271	1273	1274	rBV	8964	5473	0.39%	0.037%
52	10.920	1279	1282	1284	rBV	8222	9098	0.65%	0.061%
53	10.961	1287	1289	1291	rBV2	4902	4299	0.31%	0.029%
54	11.003	1295	1296	1299	rBV	6580	6190	0.44%	0.042%
55	11.208	1324	1331	1338	rBV	333281	631561	45.26%	4.240%

56	11.349	1348	1355	1366	rBV	93089	216692	15.53%	1.455%
57	11.531	1385	1386	1387	rBV	7631	5078	0.36%	0.034%
58	11.896	1446	1448	1451	rVB2	11035	10498	0.75%	0.070%
59	12.054	1472	1475	1478	rVB2	5584	5245	0.38%	0.035%
60	12.137	1485	1489	1492	rBV3	6264	11095	0.80%	0.074%

61	12.201	1497	1500	1501	rVV3	6026	4365	0.31%	0.029%
62	12.325	1519	1521	1525	rBV2	4301	5683	0.41%	0.038%
63	12.460	1543	1544	1547	rBV3	8220	7106	0.51%	0.048%
64	12.701	1582	1585	1586	rBV	5364	5070	0.36%	0.034%
65	12.759	1591	1595	1601	rVV4	11872	20439	1.46%	0.137%

66	13.829	1773	1777	1784	rVB4	27486	44962	3.22%	0.302%
67	14.269	1850	1852	1855	rVB3	7781	5307	0.38%	0.036%
68	14.299	1855	1857	1858	rBV2	8788	6464	0.46%	0.043%
69	14.387	1865	1872	1879	rVB	600710	874040	62.63%	5.869%
70	14.452	1879	1883	1885	rBV4	6021	8582	0.61%	0.058%

71	14.692	1916	1924	1933	rBV2	683340	1089810	78.09%	7.317%
72	14.992	1969	1975	1984	rVB	536395	854465	61.23%	5.737%
73	15.151	1996	2002	2008	rBV	281141	437063	31.32%	2.935%
74	15.339	2030	2034	2039	rVB3	59721	92878	6.66%	0.624%
75	15.979	2137	2143	2149	rBV	832421	1280024	91.72%	8.594%

76	16.073	2155	2159	2165	rVB2	155915	230155	16.49%	1.545%
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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-BG102723.MA.M
Title : SVOA CALIBRATION

77	17.066	2324	2328	2332	rBV2	112471	150584	10.79%	1.011%
78	17.566	2410	2413	2418	rVB4	104964	146664	10.51%	0.985%
79	17.630	2421	2424	2429	rVB2	117005	144303	10.34%	0.969%
80	17.742	2438	2443	2450	rVB	683909	1052729	75.44%	7.068%
81	17.842	2454	2460	2467	rBV2	908147	1395515	100.00%	9.370%
82	18.570	2579	2584	2591	rBV	829069	1110837	79.60%	7.458%
83	20.110	2842	2846	2851	rVB	882461	1250133	89.58%	8.394%

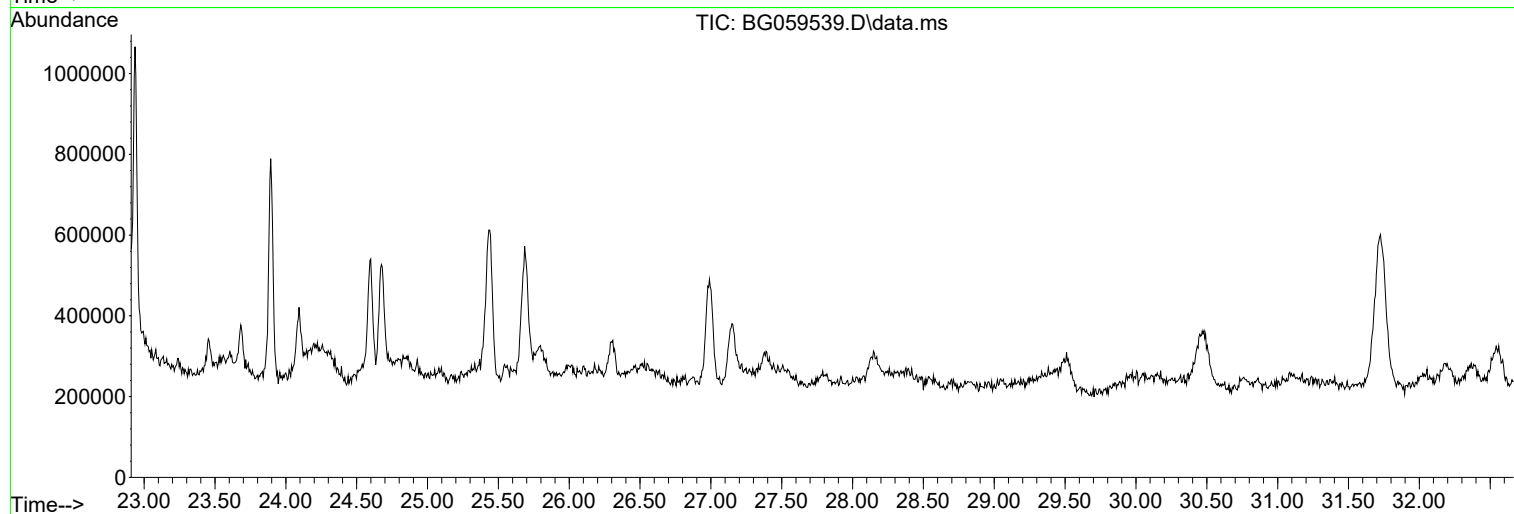
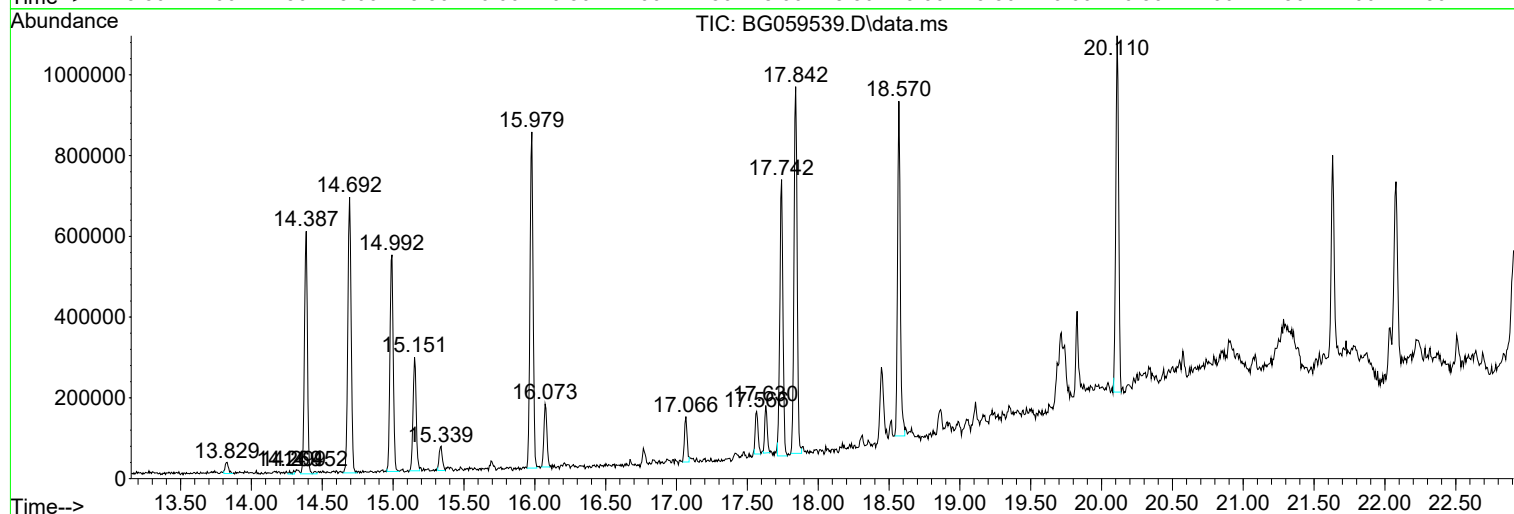
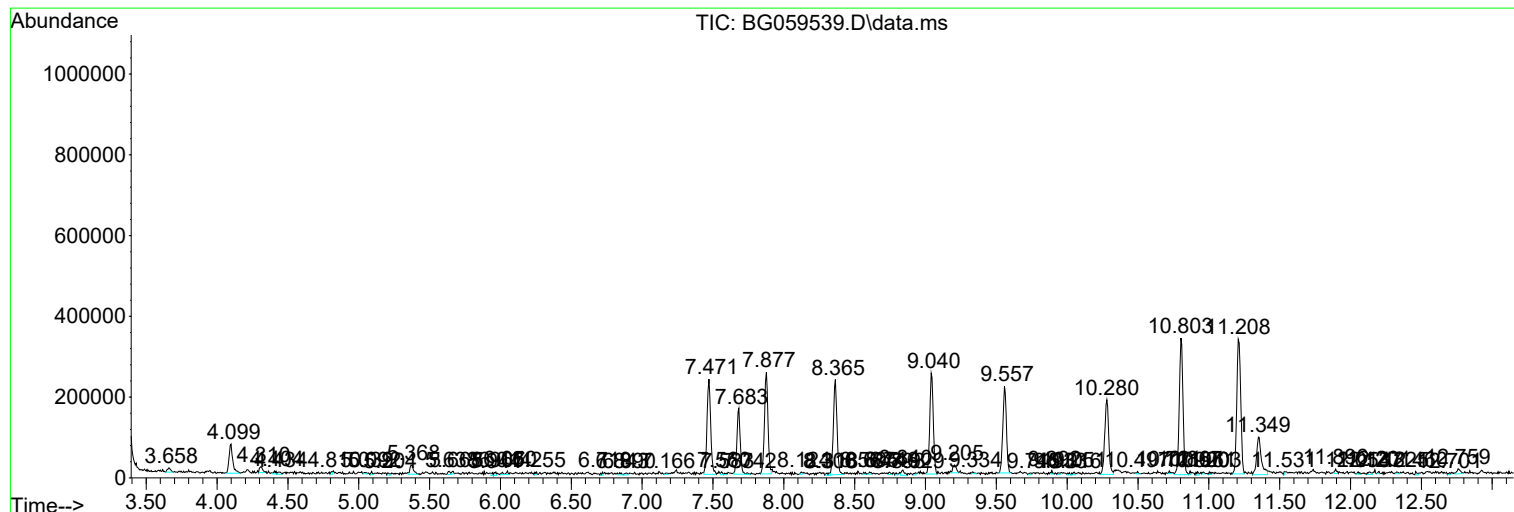
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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



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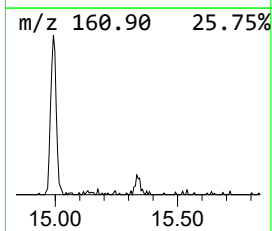
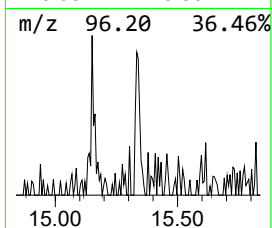
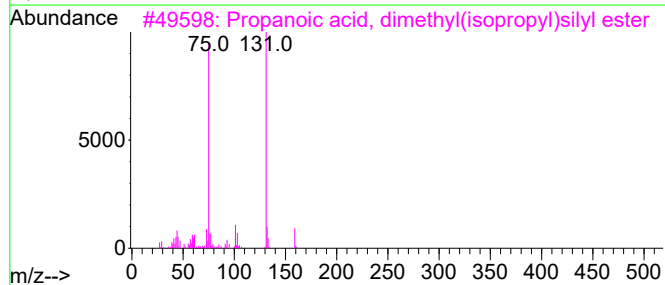
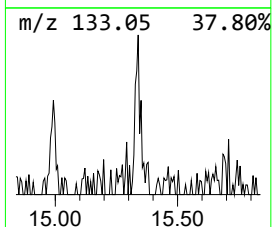
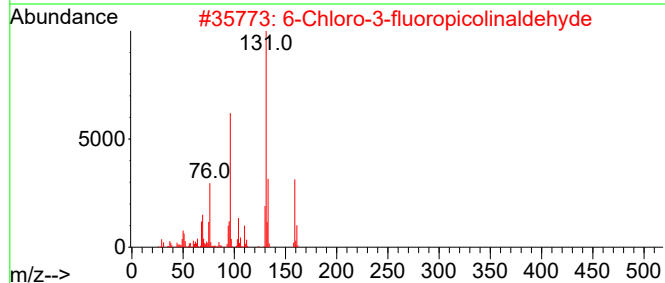
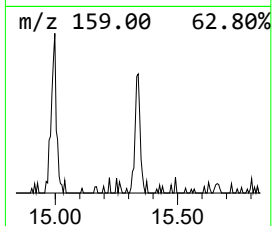
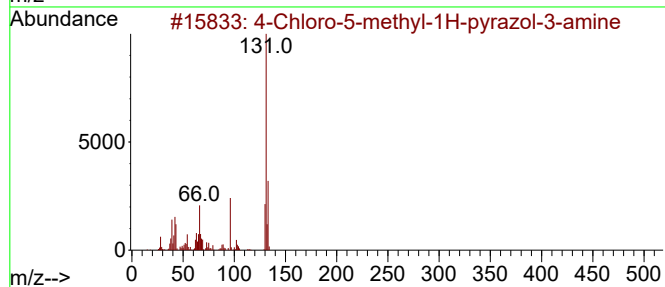
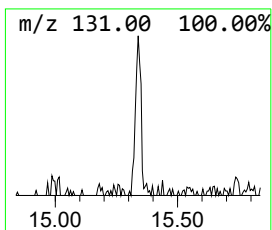
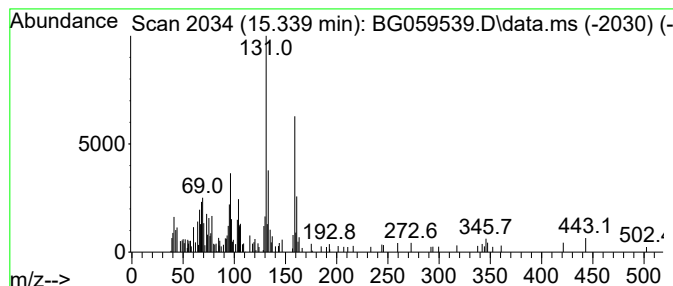
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 4-Chloro-5-methyl-1H-pyrazo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	2.17 ng/ul	92878	Acenaphthene-d10	14.986

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-5-methyl-1H-pyrazol-3-a...	131	C4H6ClN3	110580-44-4	53
2		6-Chloro-3-fluoropicolinaldehyde	159	C6H3ClFNO	884494-77-3	53
3		Propanoic acid, dimethyl(isoprop...)	174	C8H18O2Si	1000279-45-8	27
4		8-Quinololinol, 2-methyl-	159	C10H9NO	000826-81-3	27
5		4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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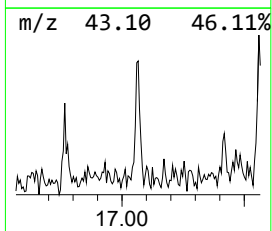
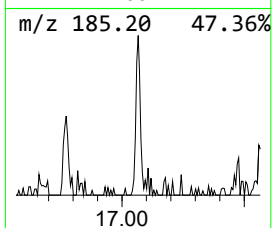
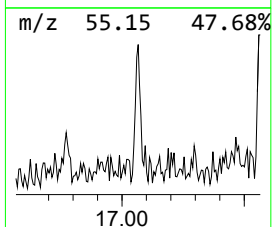
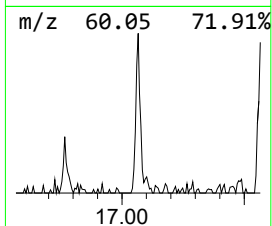
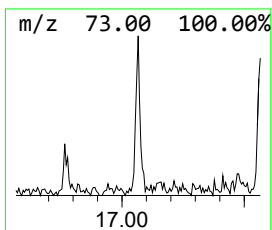
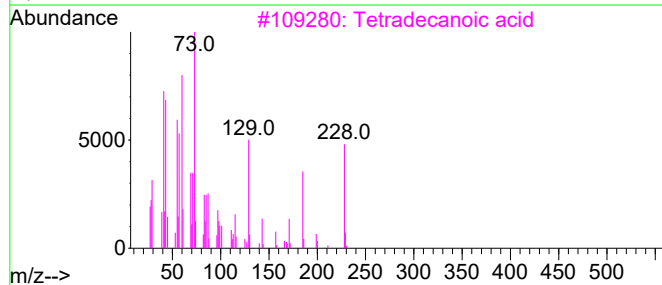
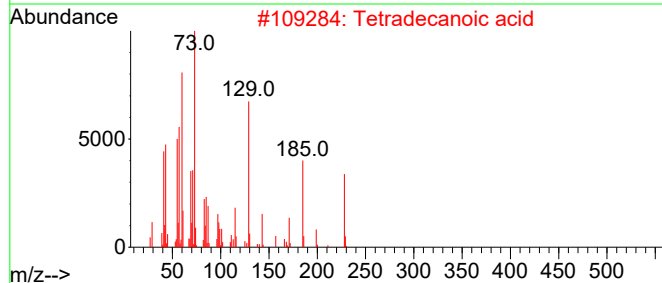
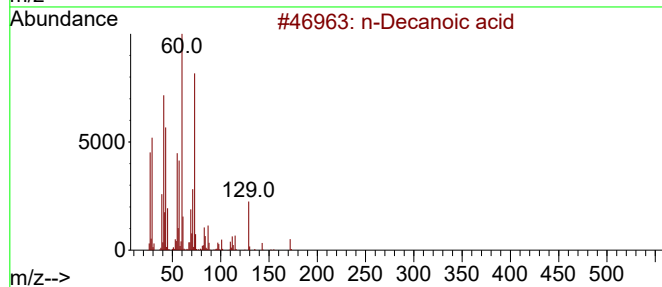
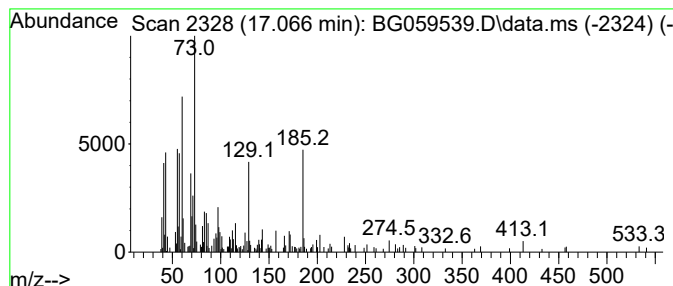
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Decanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.066	2.86 ng/ul	150584	Phenanthrene-d10	17.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	60
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			n-Decanoic acid	172	C10H20O2	000334-48-5	49
5			Dodecanoic acid	200	C12H24O2	000143-07-7	47



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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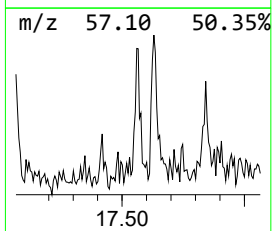
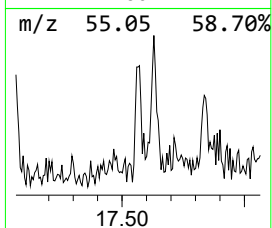
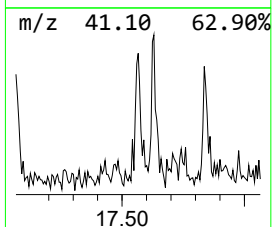
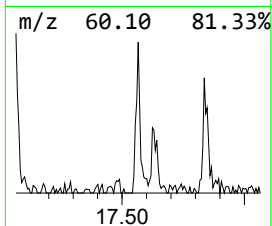
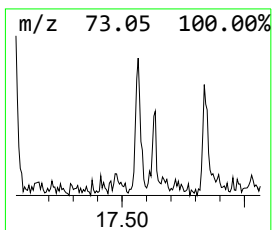
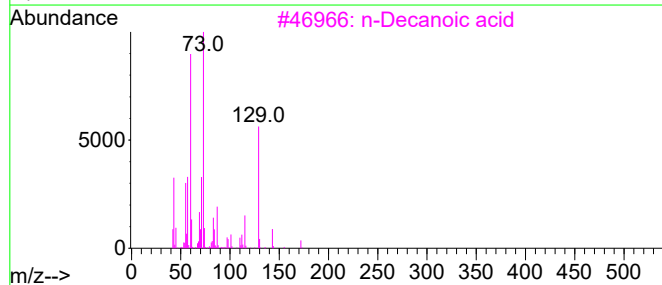
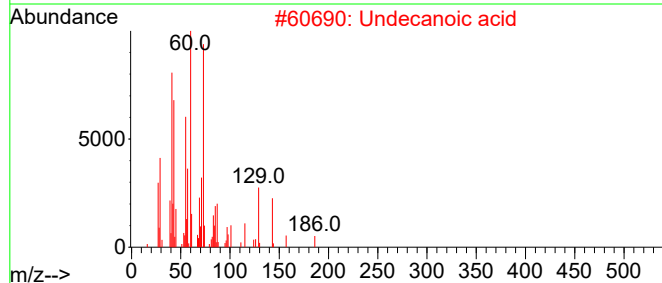
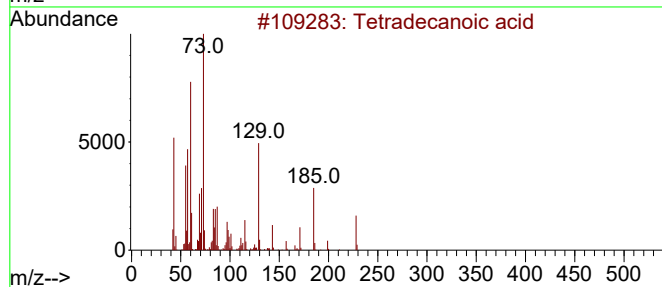
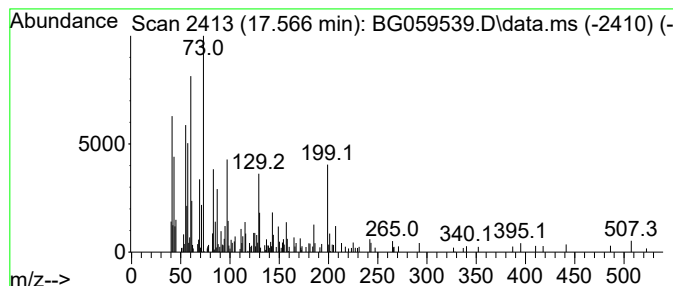
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.566	2.79 ng/ul	146664	Phenanthrene-d10	17.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
2			Undecanoic acid	186	C11H22O2	000112-37-8	38
3			n-Decanoic acid	172	C10H20O2	000334-48-5	38
4			n-Decanoic acid	172	C10H20O2	000334-48-5	38
5			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	35



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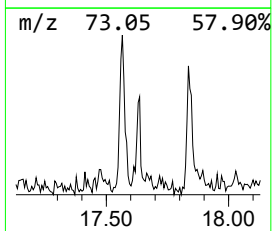
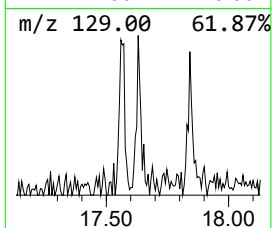
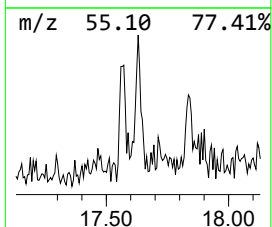
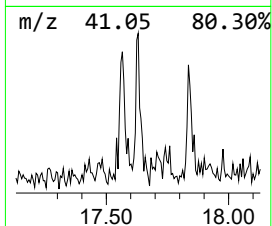
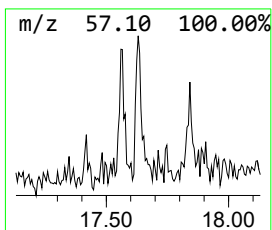
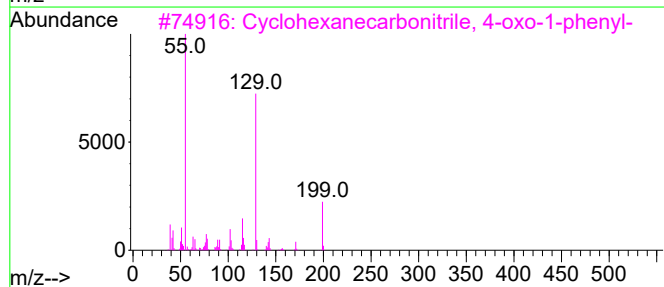
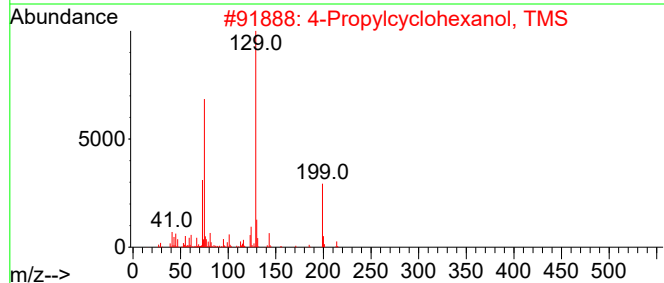
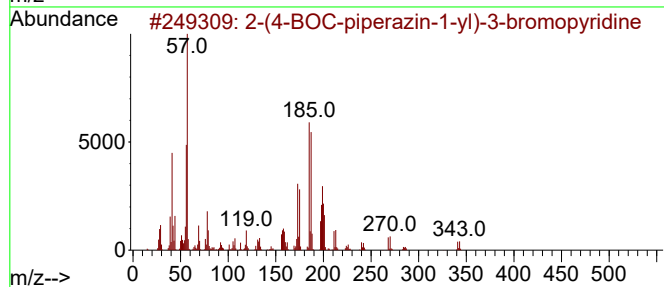
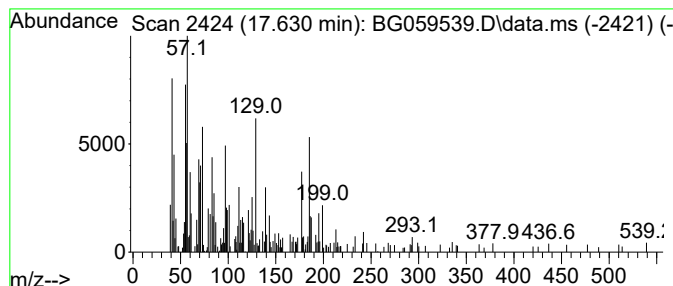
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.630	2.74 ng/ul	144303	Phenanthrene-d10	17.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-BOC-piperazin-1-yl)-3-bromo...	341	C14H20BrN3O2	1187386-01-1	30		
2	4-Propylcyclohexanol, TMS	214	C12H26OSi	1000506-69-6	25		
3	Cyclohexanecarbonitrile, 4-oxo-1...	199	C13H13NO	025115-74-6	25		
4	Hexan-1-one, 1-(2,6-dimethylmorp...	241	C14H27NO2	1000310-24-8	25		
5	Adipic acid, cyclopentylmethyl p...	298	C17H30O4	1010324-77-5	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059539.D
Acq On : 29 Oct 2023 3:32
Operator : MA/JU
Sample : 04925-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCY5

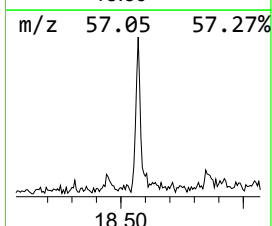
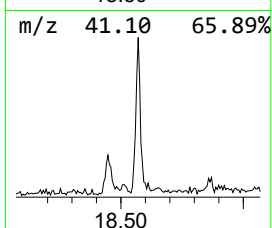
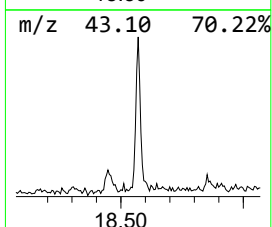
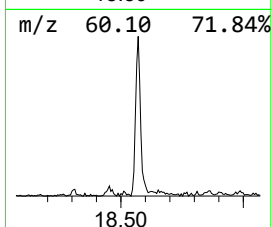
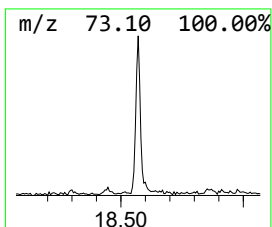
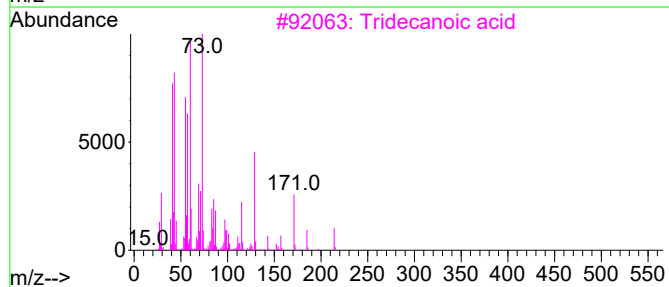
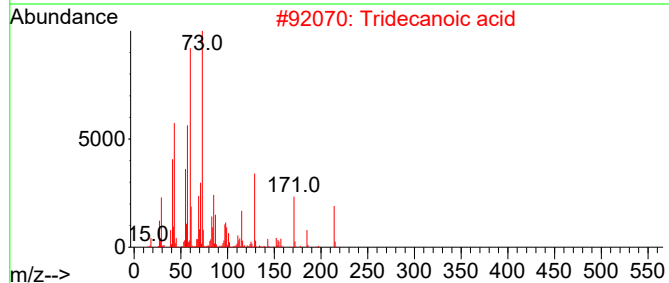
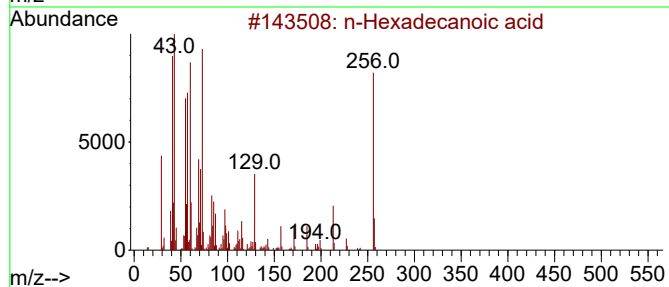
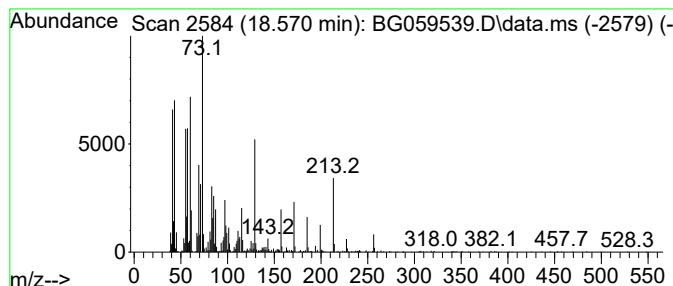
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.570	21.10 ng/ul	1110840	Phenanthrene-d10	17.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059539.D
Acq On : 29 Oct 2023 3:32
Operator : MA/JU
Sample : 04925-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCY5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.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
4-Chloro-5-meth...	15.339	2.2	ng/ul	92878	3	14.986	854465	20.0
n-Decanoic acid	17.066	2.9	ng/ul	150584	4	17.742	1052730	20.0
unknown-01	17.566	2.8	ng/ul	146664	4	17.742	1052730	20.0
unknown-02	17.630	2.7	ng/ul	144303	4	17.742	1052730	20.0
n-Hexadecanoic ...	18.570	21.1	ng/ul	1110840	4	17.742	1052730	20.0