

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
 Data File : BG059540.D
 Acq On : 29 Oct 2023 4:14
 Operator : MA/JU
 Sample : 04925-09
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GCCX5

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: BG059540.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.517	21	22	25	rVB3	14172	9518	0.35%	0.058%
2	3.658	44	46	47	rVV	15413	11411	0.42%	0.070%
3	3.694	51	52	54	rVB2	11284	5809	0.21%	0.035%
4	3.840	75	77	79	rBV3	11544	9322	0.34%	0.057%
5	3.858	79	80	82	rVV3	12128	9686	0.35%	0.059%
6	3.882	82	84	86	rVV3	13666	14377	0.52%	0.088%
7	3.923	89	91	93	rVB2	15247	10548	0.38%	0.064%
8	4.052	110	113	114	rVB2	7349	6721	0.24%	0.041%
9	4.099	117	121	126	rVV5	11973	21055	0.77%	0.128%
10	4.310	151	157	161	rBV5	13847	23400	0.85%	0.143%
11	4.998	271	274	276	rBV2	4395	6527	0.24%	0.040%
12	5.151	296	300	303	rBV2	4945	5966	0.22%	0.036%
13	5.262	317	319	322	rVB	6884	6139	0.22%	0.037%
14	5.350	331	334	335	rVV2	6620	5838	0.21%	0.036%
15	5.374	335	338	344	rVB	23293	32460	1.18%	0.198%
16	6.373	505	508	512	rBV2	4595	8148	0.30%	0.050%
17	6.984	606	612	619	rVB4	22778	43064	1.57%	0.263%
18	7.090	627	630	633	rBV4	3398	6352	0.23%	0.039%
19	7.242	652	656	660	rBV3	6675	11352	0.41%	0.069%
20	7.471	688	695	705	rBV2	176761	351802	12.82%	2.147%
21	7.607	715	718	720	rBV3	7154	6163	0.22%	0.038%
22	7.677	723	730	737	rVB	103817	180434	6.57%	1.101%
23	7.765	741	745	746	rBV	6985	6862	0.25%	0.042%
24	7.877	755	764	771	rBV	158208	301205	10.97%	1.838%
25	7.977	780	781	783	rBV	7221	6151	0.22%	0.038%
26	8.041	790	792	795	rBV	5969	6059	0.22%	0.037%
27	8.206	819	820	824	rBV3	5854	6242	0.23%	0.038%
28	8.306	833	837	838	rBV3	6314	8095	0.29%	0.049%
29	8.364	841	847	855	rVB2	229376	399542	14.55%	2.438%
30	8.594	884	886	892	rVB6	7881	8810	0.32%	0.054%
31	9.005	952	956	957	rBV3	8227	9627	0.35%	0.059%
32	9.046	957	963	970	rVB	213373	366691	13.36%	2.238%
33	9.211	983	991	1001	rBV	199515	372021	13.55%	2.270%
34	9.334	1006	1012	1016	rVB2	16757	29585	1.08%	0.181%
35	9.469	1031	1035	1037	rBV5	6448	7565	0.28%	0.046%
36	9.557	1043	1050	1058	rBV	145021	273507	9.96%	1.669%

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37	9.786	1084	1089	1090	rBV5	7001	10882	0.40%	0.066%
38	9.963	1117	1119	1122	rBV	8378	9233	0.34%	0.056%
39	10.280	1166	1173	1179	rBV2	133504	236902	8.63%	1.446%
40	10.374	1182	1189	1193	rBV3	49965	101807	3.71%	0.621%
41	10.480	1203	1207	1208	rBV4	8045	10640	0.39%	0.065%
42	10.509	1211	1212	1217	rVB3	8461	6895	0.25%	0.042%
43	10.632	1230	1233	1241	rVB3	21933	37384	1.36%	0.228%
44	10.744	1248	1252	1253	rBV3	5483	6326	0.23%	0.039%
45	10.803	1254	1262	1269	rVB2	233062	416709	15.18%	2.543%
46	11.208	1324	1331	1340	rBV	335213	611508	22.28%	3.732%
47	11.355	1348	1356	1366	rVB2	39603	83790	3.05%	0.511%
48	11.443	1369	1371	1373	rBV2	5726	6008	0.22%	0.037%
49	11.502	1377	1381	1384	rVV5	8750	14003	0.51%	0.085%
50	11.555	1387	1390	1393	rVV2	5777	9320	0.34%	0.057%
51	11.661	1404	1408	1411	rBV	6870	8652	0.32%	0.053%
52	11.731	1414	1420	1424	rBV4	24743	47805	1.74%	0.292%
53	11.855	1439	1441	1442	rBV	8836	6481	0.24%	0.040%
54	11.884	1442	1446	1448	rVV3	7336	11529	0.42%	0.070%
55	11.996	1459	1465	1471	rVB	25827	49053	1.79%	0.299%
56	12.201	1498	1500	1504	rVV3	6310	7888	0.29%	0.048%
57	12.254	1508	1509	1512	rBV2	8345	5872	0.21%	0.036%
58	12.483	1545	1548	1551	rBV2	5056	7305	0.27%	0.045%
59	12.524	1553	1555	1557	rVV3	9533	9436	0.34%	0.058%
60	12.560	1557	1561	1565	rVB4	14405	19478	0.71%	0.119%
61	12.683	1577	1582	1584	rBV3	9024	14995	0.55%	0.092%
62	12.753	1592	1594	1596	rBV2	10260	12688	0.46%	0.077%
63	12.847	1606	1610	1612	rBV4	6609	8286	0.30%	0.051%
64	13.024	1637	1640	1642	rVB	5953	6839	0.25%	0.042%
65	13.053	1642	1645	1648	rBV2	6407	10011	0.36%	0.061%
66	13.376	1697	1700	1703	rVB3	7224	7368	0.27%	0.045%
67	13.500	1714	1721	1725	rVB2	29785	48668	1.77%	0.297%
68	13.694	1750	1754	1755	rBV3	4822	6457	0.24%	0.039%
69	13.823	1770	1776	1782	rVB5	31709	57431	2.09%	0.350%
70	13.929	1789	1794	1796	rVB5	5330	7440	0.27%	0.045%
71	14.234	1844	1846	1847	rBV2	10499	5960	0.22%	0.036%
72	14.281	1852	1854	1858	rVB4	30177	29579	1.08%	0.181%
73	14.316	1858	1860	1863	rVB	5533	6115	0.22%	0.037%
74	14.381	1863	1871	1877	rBV	439585	686630	25.01%	4.190%
75	14.692	1918	1924	1930	rVB2	471025	769982	28.05%	4.699%
76	14.822	1942	1946	1947	rBV4	9782	10285	0.37%	0.063%

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77	14.986	1966	1974	1983	rBV	529578	850878	30.99%	5.193%
78	15.057	1983	1986	1987	rBV3	9112	7911	0.29%	0.048%
79	15.068	1987	1988	1990	rVB2	12069	5981	0.22%	0.037%
80	15.110	1990	1995	1998	rBV	39752	63589	2.32%	0.388%
81	15.151	1998	2002	2008	rVB2	209791	307190	11.19%	1.875%
82	15.251	2011	2019	2028	rBV	1718955	2745225	100.00%	16.754%
83	15.533	2065	2067	2068	rBV2	7936	5954	0.22%	0.036%
84	15.685	2091	2093	2094	rBV2	10277	7378	0.27%	0.045%
85	15.773	2105	2108	2110	rBV4	7091	9000	0.33%	0.055%
86	15.973	2136	2142	2150	rVB2	652517	1038970	37.85%	6.341%
87	16.032	2150	2152	2154	rBV3	9439	11910	0.43%	0.073%
88	16.073	2154	2159	2164	rVB2	128796	193996	7.07%	1.184%
89	16.343	2200	2205	2210	rVB2	130406	183592	6.69%	1.120%
90	16.625	2248	2253	2258	rBV2	54158	90936	3.31%	0.555%
91	17.354	2373	2377	2383	rVB4	113287	175063	6.38%	1.068%
92	17.742	2437	2443	2451	rBV	624784	956877	34.86%	5.840%
93	17.842	2453	2460	2467	rBV	618691	983521	35.83%	6.002%
94	18.511	2571	2574	2578	rVB5	85240	103803	3.78%	0.634%
95	18.564	2579	2583	2590	rBV2	354112	491349	17.90%	2.999%
96	19.316	2707	2711	2715	rBV3	180445	221399	8.06%	1.351%
97	19.828	2795	2798	2804	rVB7	99768	131010	4.77%	0.800%
98	20.110	2841	2846	2852	rVB	644086	868346	31.63%	5.299%
99	21.631	3102	3105	3109	rBV4	125454	154650	5.63%	0.944%
100	22.072	3176	3180	3187	rVB2	420195	765381	27.88%	4.671%

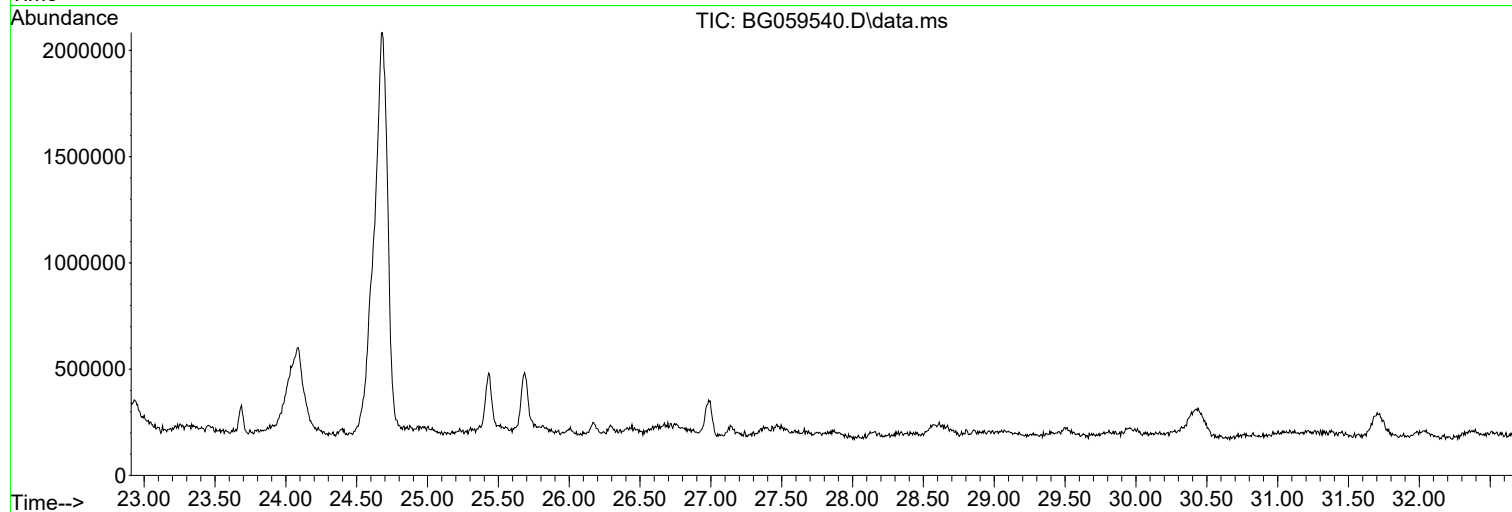
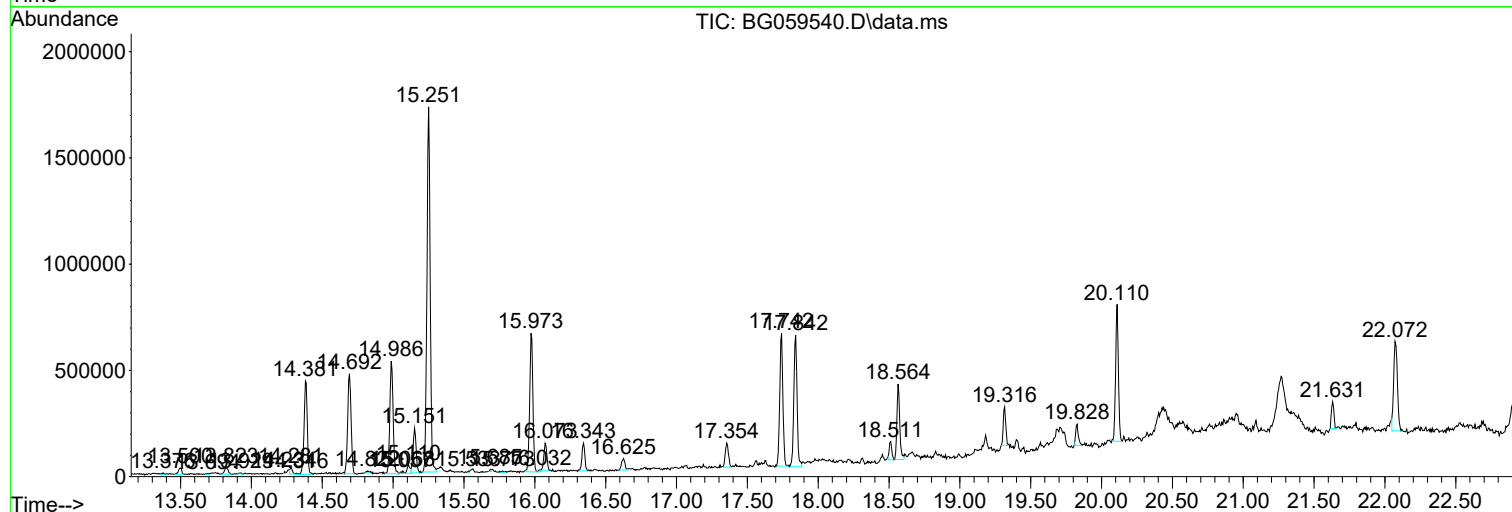
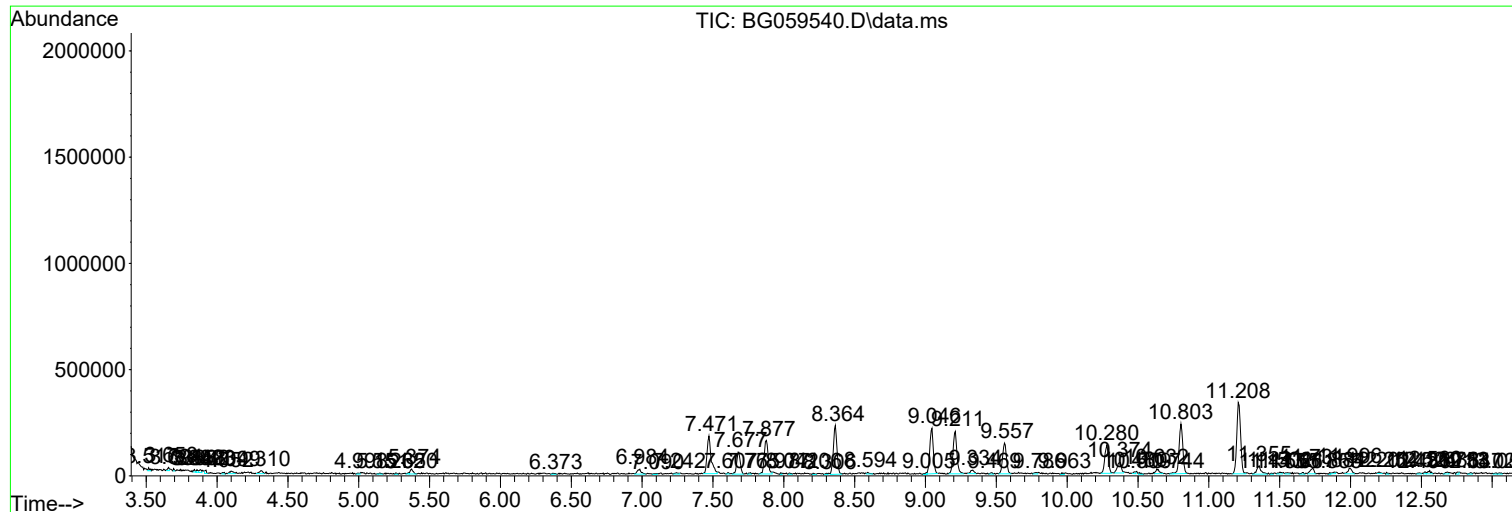
Sum of corrected areas: 16385603

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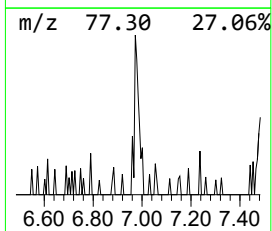
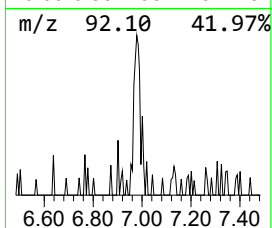
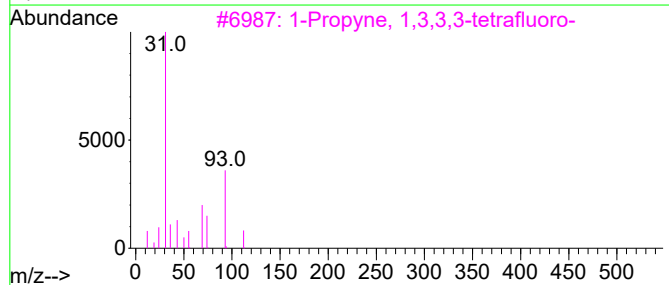
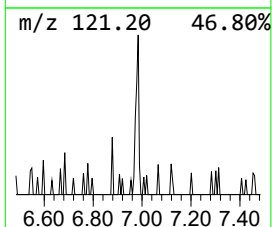
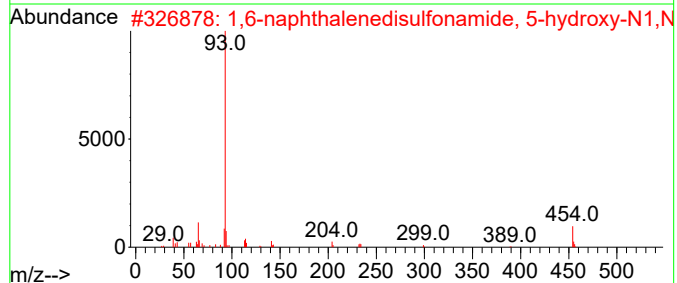
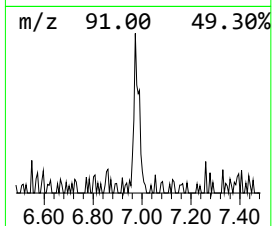
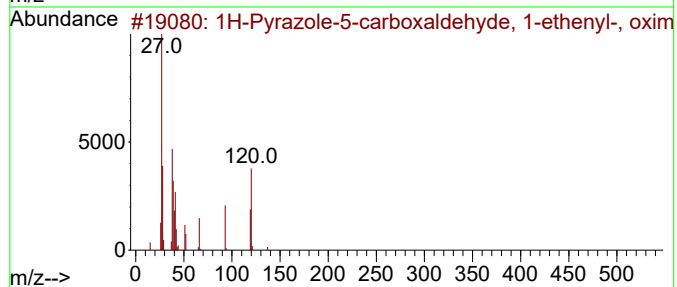
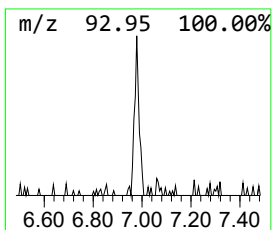
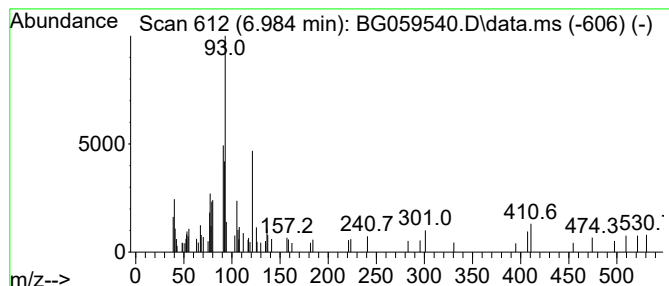
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.984	2.16 ng/ul	43064	1,4-Dichlorobenzene-d4	8.364

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrazole-5-carboxaldehyde, 1-...	137	C6H7N3O	1000460-67-6	4
2			1,6-naphthalenedisulfonamide, 5-...	454	C22H18N2O5S2	1000399-40-8	3
3			1-Propyne, 1,3,3,3-tetrafluoro-	112	C3F4	020174-11-2	2
4			1,4-benzenediol, 2-(4-aminopheno...	495	C27H39Cl2NO3	1000399-60-7	2
5			1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	2



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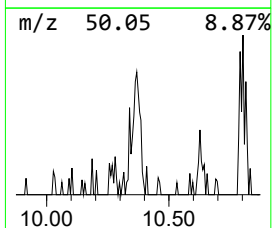
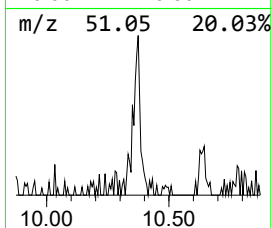
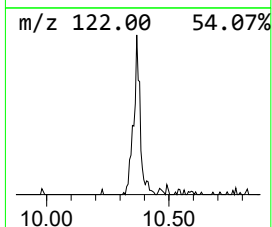
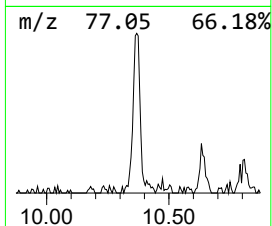
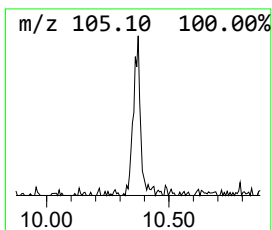
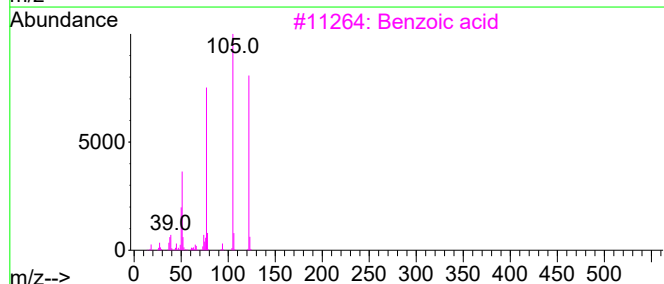
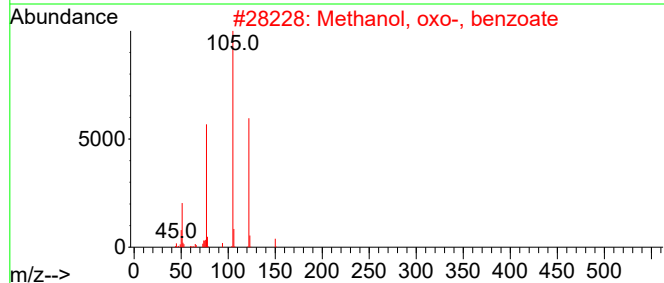
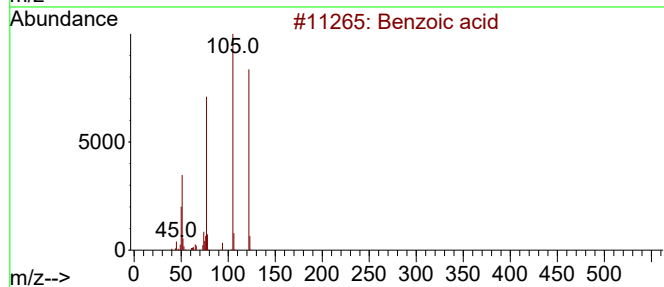
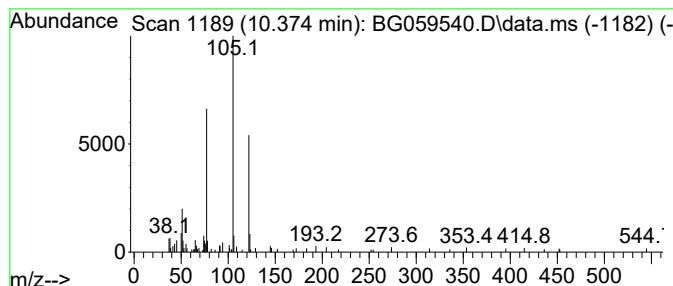
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.374	3.33 ng/ul	101807	Naphthalene-d8	11.208

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	83
2			Methanol, oxo-, benzoate	150	C8H6O3	1000305-65-2	80
3			Benzoic acid	122	C7H6O2	000065-85-0	80
4			Cyclobutane-1,1-dicarboxamide, N...	382	C20H18N2O6	1000253-25-3	72
5			Cyclopropanecarboxamide, N-benzo...	205	C11H11NO3	1000253-25-4	72



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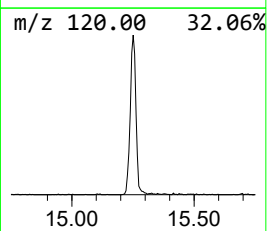
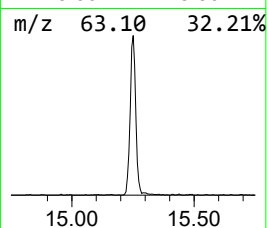
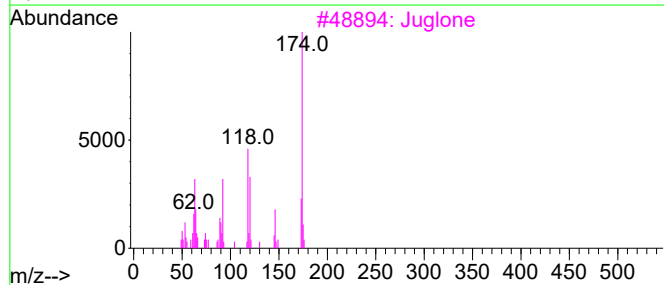
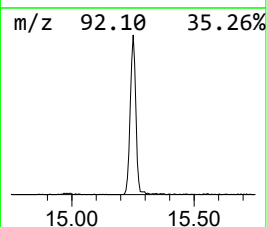
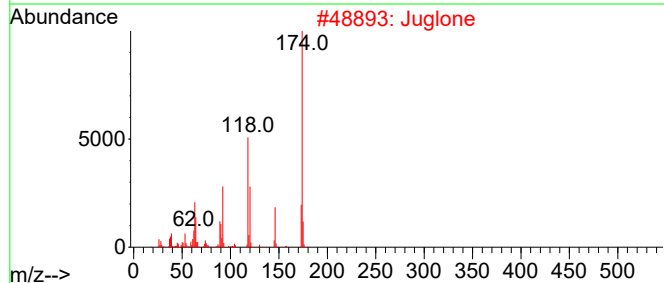
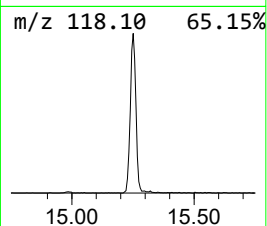
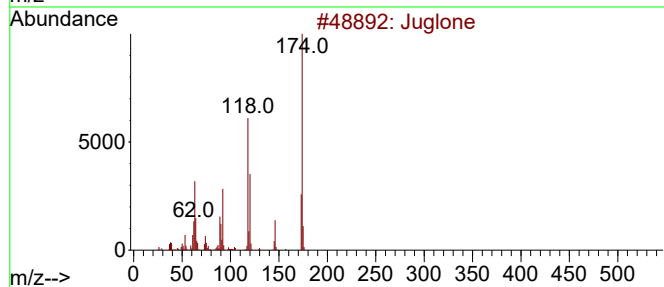
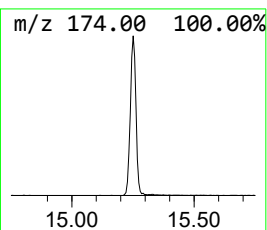
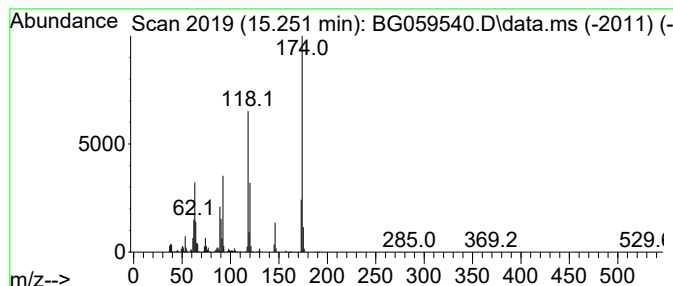
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Juglone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.251	64.53 ng/ul	2745230	Acenaphthene-d10	14.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone			174	C10H6O3	000481-39-0	98
2	Juglone			174	C10H6O3	000481-39-0	93
3	Juglone			174	C10H6O3	000481-39-0	74
4	Juglone			174	C10H6O3	000481-39-0	70
5	1-Methyl-5-(4-methylphenyl)tetra...			174	C9H10N4	068826-33-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059540.D
Acq On : 29 Oct 2023 4:14
Operator : MA/JU
Sample : 04925-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCX5

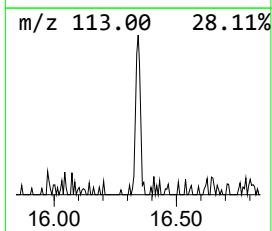
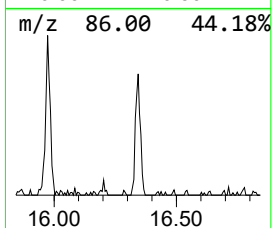
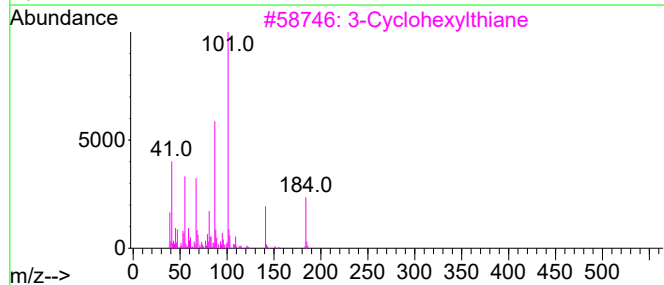
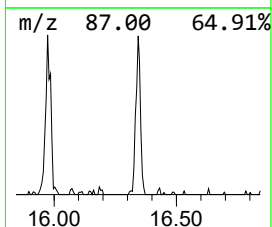
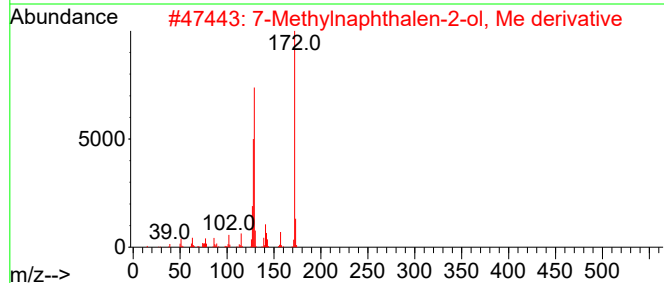
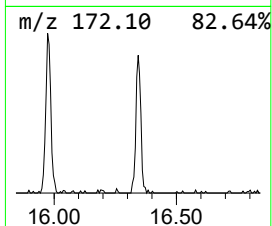
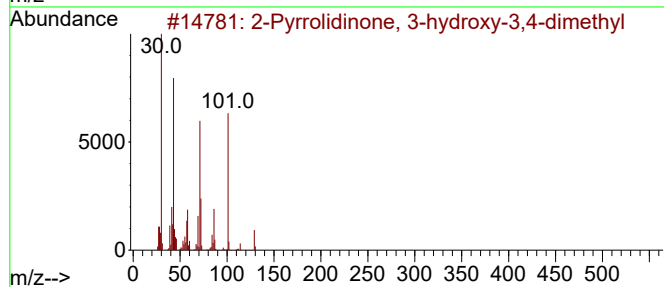
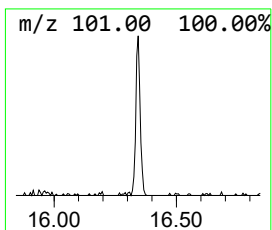
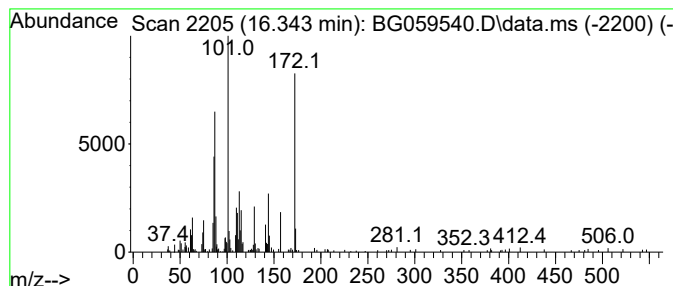
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Quant Title : SVOA CALIBRATION

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.
16.343	4.32 ng/ul	183592	Acenaphthene-d10	14.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 3-hydroxy-3,4-d...	129	C6H11N02	1000196-87-3	38		
2	7-Methylnaphthalen-2-ol, Me deri...	172	C12H12O	1000504-28-7	27		
3	3-Cyclohexylthiane	184	C11H20S	061639-13-2	22		
4	cis-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-76-1	22		
5	Myo-Inositol, 1,2,3,4,5,6-hexa-O...	264	C12H24O6	002075-22-1	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059540.D
Acq On : 29 Oct 2023 4:14
Operator : MA/JU
Sample : 04925-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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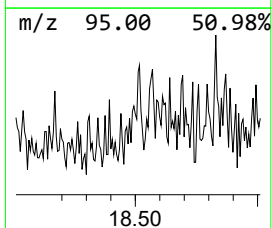
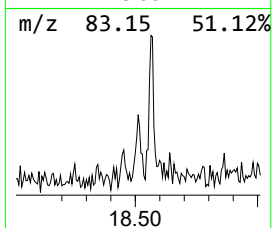
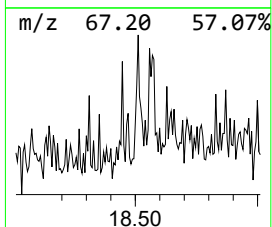
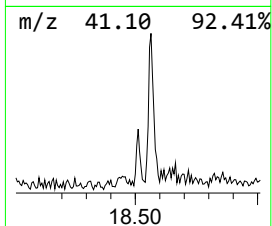
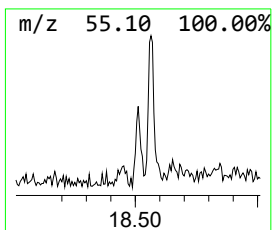
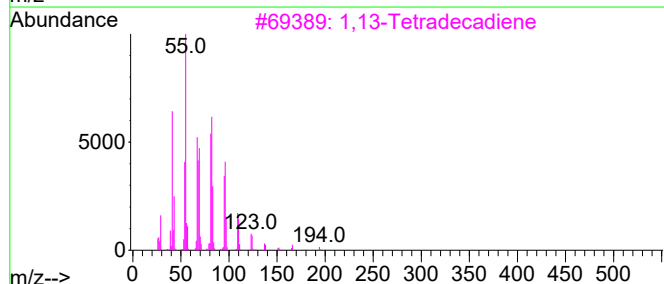
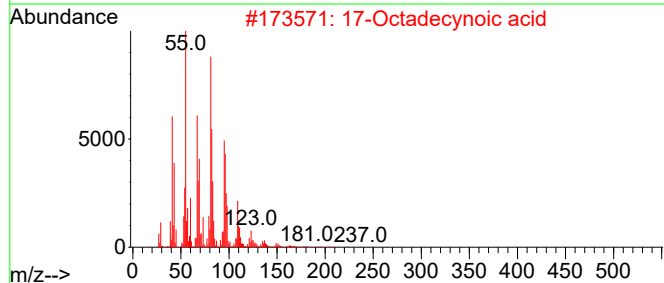
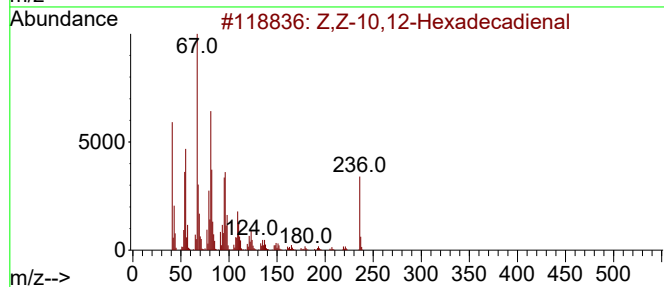
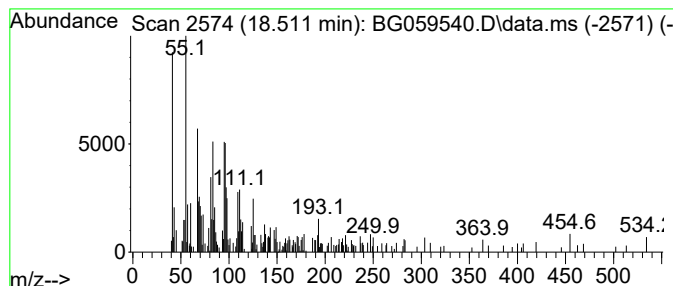
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Z,Z-10,12-Hexadecadienal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	2.17 ng/ul	103803	Phenanthrene-d10	17.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z,Z-10,12-Hexadecadienal	236	C16H28O	1000130-86-6	64
2			17-Octadecynoic acid	280	C18H32O2	034450-18-5	58
3			1,13-Tetradecadiene	194	C14H26	021964-49-8	52
4			1,13-Tetradecadiene	194	C14H26	021964-49-8	52
5			2(1H)-Naphthalenone, octahydro-4...	166	C11H18O	000938-06-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059540.D
Acq On : 29 Oct 2023 4:14
Operator : MA/JU
Sample : 04925-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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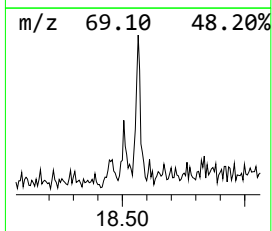
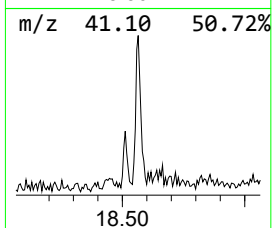
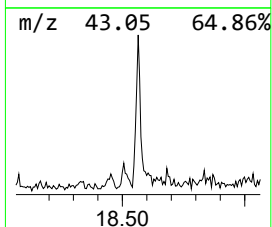
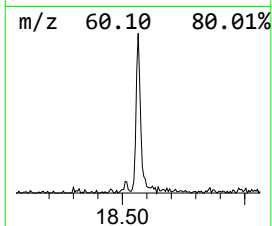
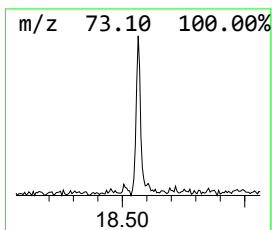
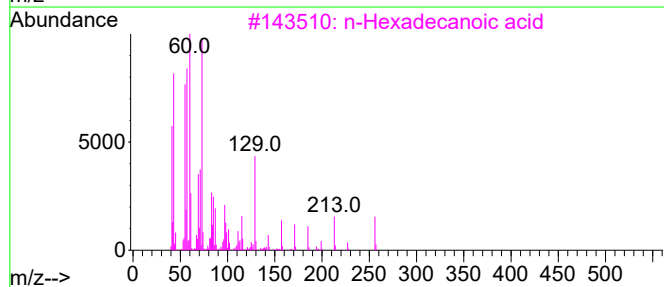
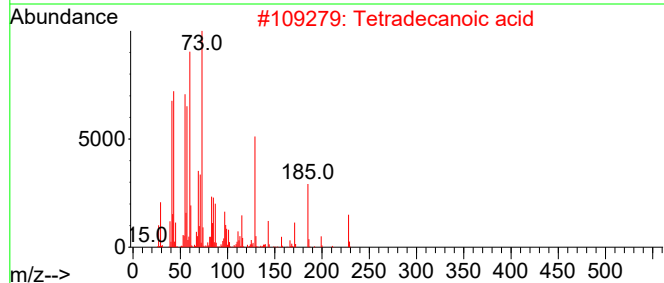
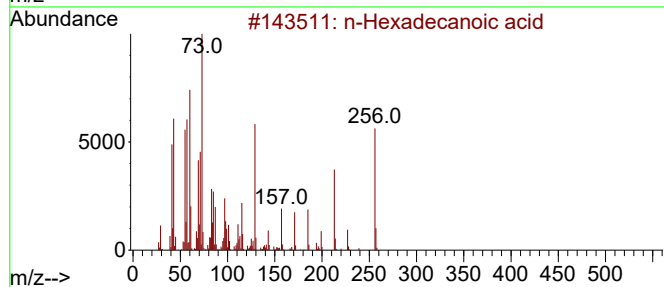
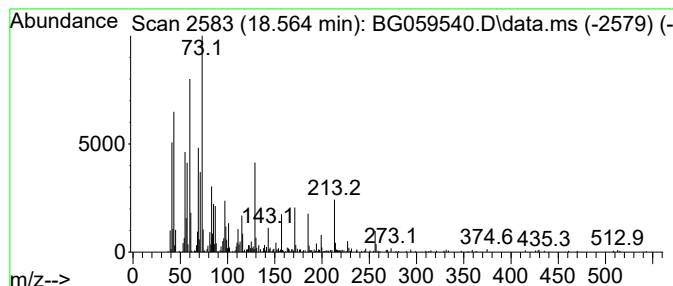
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.564	10.27 ng/ul	491349	Phenanthrene-d10	17.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059540.D
Acq On : 29 Oct 2023 4:14
Operator : MA/JU
Sample : 04925-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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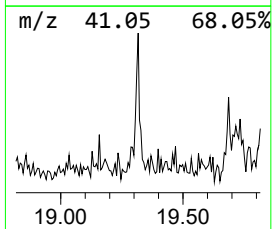
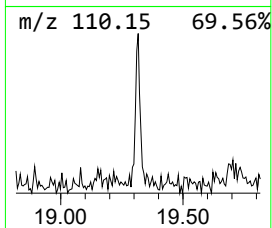
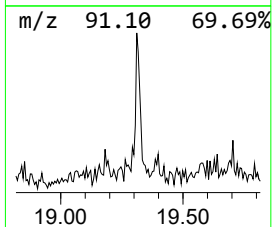
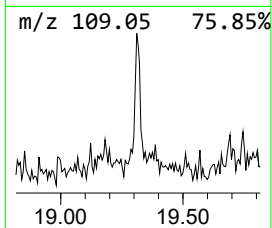
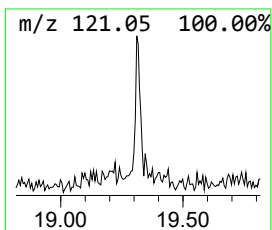
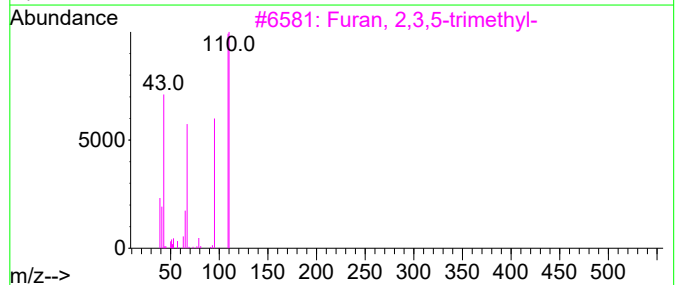
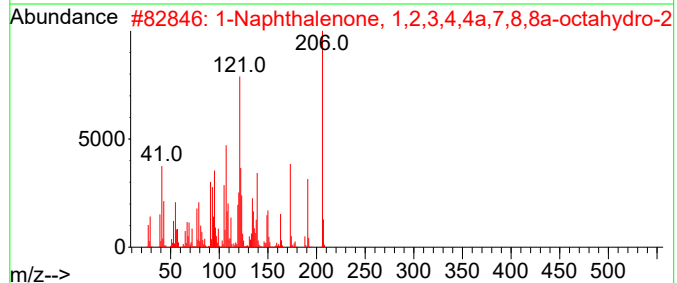
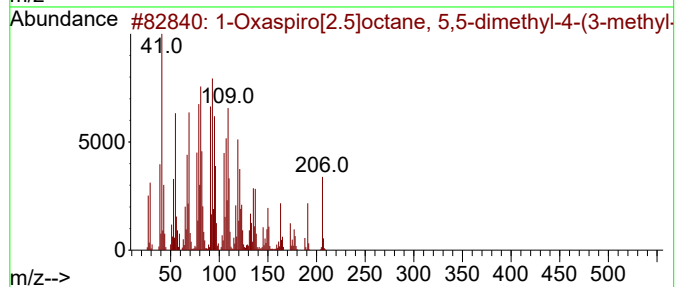
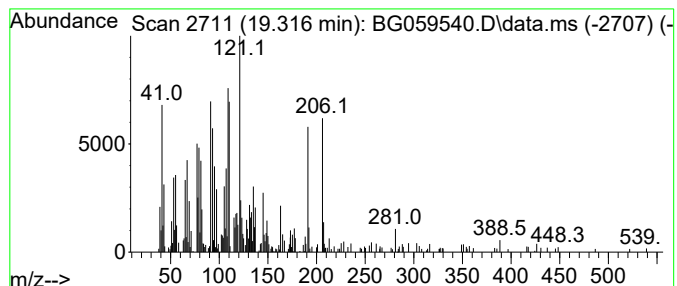
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Oxaspiro[2.5]octane, 5,5-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.316	4.63 ng/ul	221399	Phenanthrene-d10	17.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	70
2			1-Naphthalenone, 1,2,3,4,4a,7,8,...	206	C14H22O	020454-85-7	30
3			Furan, 2,3,5-trimethyl-	110	C7H10O	010504-04-8	30
4			Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	30
5			2,4,4-Trimethyl-3-(3-methylbuta...	206	C14H22O	097452-05-6	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059540.D
Acq On : 29 Oct 2023 4:14
Operator : MA/JU
Sample : 04925-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

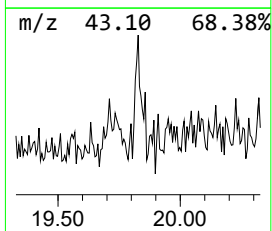
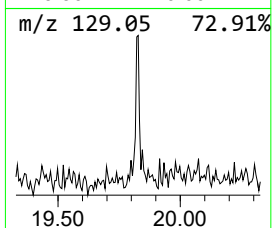
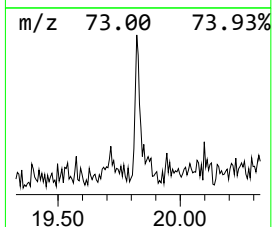
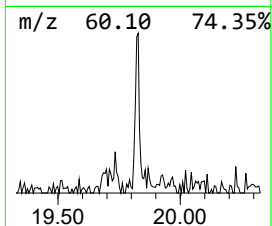
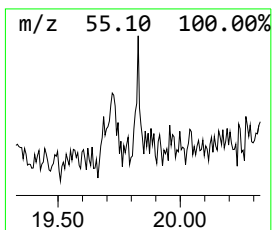
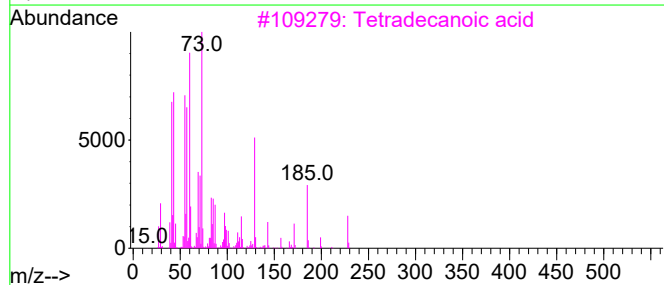
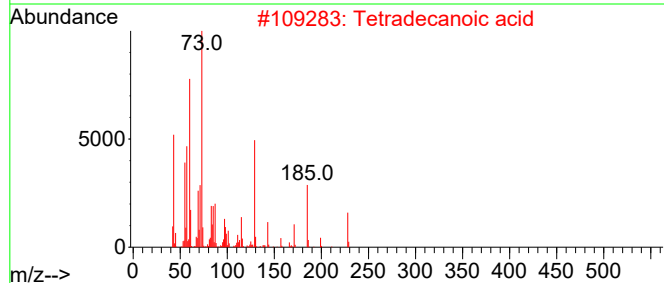
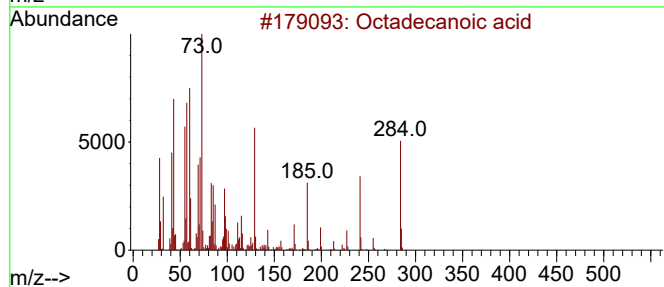
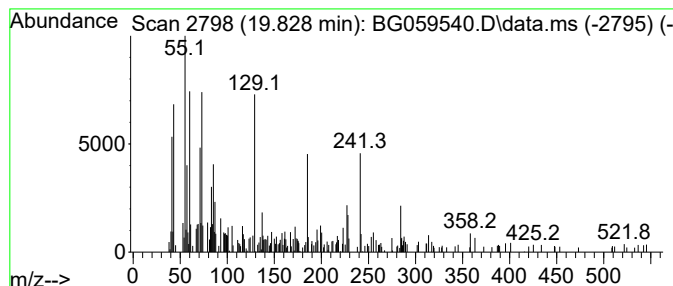
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.828	2.74 ng/ul	131010	Phenanthrene-d10		17.742	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	80
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	60
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	53
4	Octadecanoic acid		284	C18H36O2	000057-11-4	52
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059540.D
Acq On : 29 Oct 2023 4:14
Operator : MA/JU
Sample : 04925-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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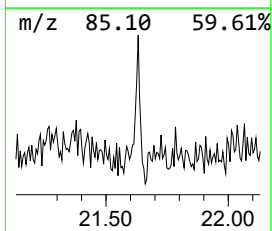
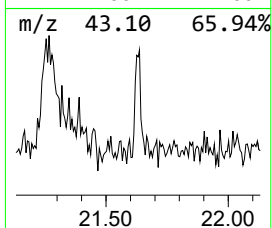
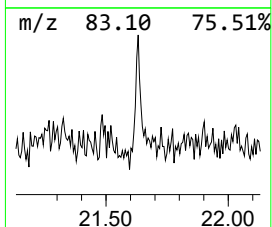
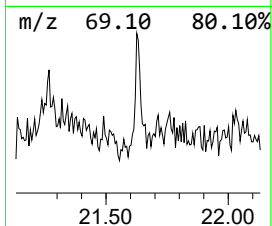
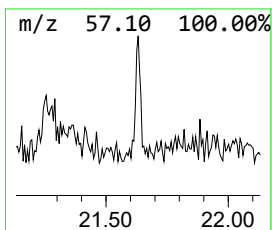
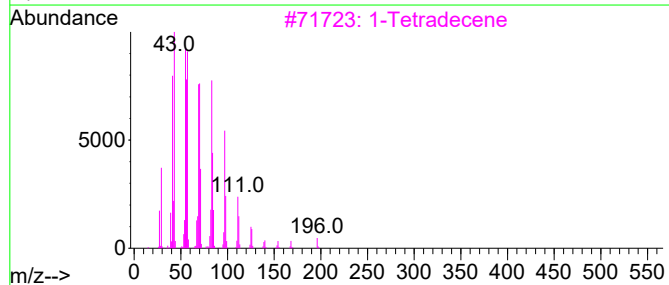
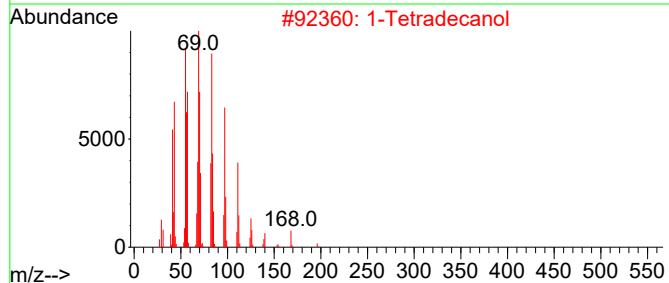
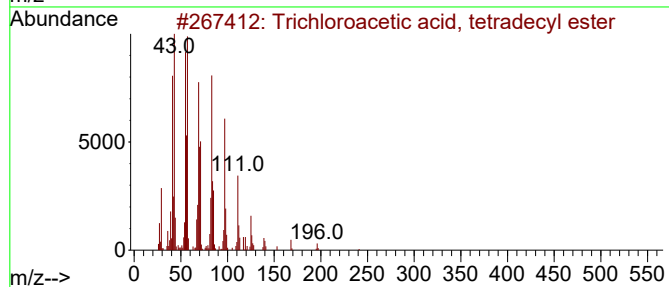
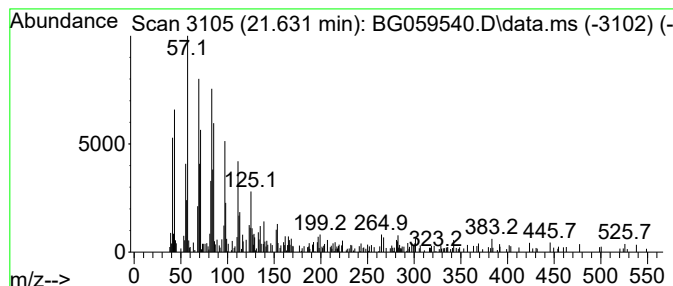
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Trichloroacetic acid, tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.631	4.04 ng/ul	154650	Chrysene-d12	22.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
2			1-Tetradecanol	214	C14H30O	000112-72-1	83
3			1-Tetradecene	196	C14H28	001120-36-1	74
4			Ether, dodecyl isopropyl	228	C15H32O	029379-42-8	74
5			1-Pentadecene	210	C15H30	013360-61-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
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Operator : MA/JU
Sample : 04925-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCX5

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
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Benzoic acid	10.374	3.3	ng/ul	101807	2	11.208	611508	20.0
Juglone	15.251	64.5	ng/ul	2745230	3	14.986	850878	20.0
unknown-02	16.343	4.3	ng/ul	183592	3	14.986	850878	20.0
Z,Z-10,12-Hexad...	18.511	2.2	ng/ul	103803	4	17.742	956877	20.0
n-Hexadecanoic ...	18.564	10.3	ng/ul	491349	4	17.742	956877	20.0
1-Oxaspiro[2.5]...	19.316	4.6	ng/ul	221399	4	17.742	956877	20.0
Octadecanoic acid	19.828	2.7	ng/ul	131010	4	17.742	956877	20.0
Trichloroacetic...	21.631	4.0	ng/ul	154650	5	22.072	765381	20.0