

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
 Data File : BG059779.D
 Acq On : 20 Nov 2023 21:50
 Operator : MA/JU
 Sample : 05376-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 204

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\8270-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059779.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.754	58	62	65	rVB4	7808	12153	1.09%	0.094%
2	5.364	332	336	340	rVB4	9947	14026	1.26%	0.108%
3	5.822	408	414	421	rBV	280174	459877	41.18%	3.553%
4	7.456	684	692	700	rVB	338224	572644	51.28%	4.424%
5	8.331	835	841	847	rBV2	147525	249137	22.31%	1.925%
6	9.306	1005	1007	1012	rBV2	6444	12527	1.12%	0.097%
7	9.530	1038	1045	1052	rVB2	223464	412291	36.92%	3.185%
8	11.181	1318	1326	1332	rBV	189053	382549	34.26%	2.955%
9	11.234	1332	1335	1342	rVB3	23186	37679	3.37%	0.291%
10	11.527	1380	1385	1388	rBV	8520	13714	1.23%	0.106%
11	12.086	1477	1480	1484	rVB3	8403	12168	1.09%	0.094%
12	12.814	1597	1604	1610	rBV3	24318	49993	4.48%	0.386%
13	12.943	1621	1626	1629	rVB5	6749	12170	1.09%	0.094%
14	13.032	1636	1641	1644	rBV	23317	37093	3.32%	0.287%
15	13.584	1728	1735	1742	rVB2	583160	878425	78.67%	6.786%
16	13.789	1765	1770	1776	rVB2	141508	236419	21.17%	1.826%
17	13.989	1800	1804	1806	rBV4	9665	13259	1.19%	0.102%
18	14.124	1823	1827	1835	rVB7	18425	39868	3.57%	0.308%
19	14.283	1848	1854	1858	rBV5	19650	39684	3.55%	0.307%
20	14.336	1858	1863	1867	rBV8	13716	24072	2.16%	0.186%
21	14.518	1887	1894	1895	rBV5	18565	25568	2.29%	0.198%
22	14.694	1921	1924	1929	rVB5	15184	23796	2.13%	0.184%
23	14.777	1934	1938	1941	rVB5	12101	14858	1.33%	0.115%
24	14.965	1964	1970	1975	rVV	309663	480233	43.01%	3.710%
25	15.029	1976	1981	1986	rVB2	67609	101999	9.13%	0.788%
26	15.158	2000	2003	2006	rVB5	12345	13882	1.24%	0.107%
27	15.358	2028	2037	2041	rBV4	49871	100823	9.03%	0.779%
28	15.411	2044	2046	2050	rVV3	20120	16953	1.52%	0.131%
29	15.487	2053	2059	2062	rBV7	10223	17896	1.60%	0.138%
30	15.552	2064	2070	2073	rVB6	20112	27089	2.43%	0.209%
31	15.599	2073	2078	2083	rBV6	11631	25295	2.27%	0.195%
32	16.010	2140	2148	2153	rVB4	79612	147921	13.25%	1.143%
33	16.052	2153	2155	2159	rBV4	12462	15572	1.39%	0.120%
34	16.093	2159	2162	2164	rBV4	12437	14384	1.29%	0.111%
35	16.122	2164	2167	2169	rVV4	12613	13998	1.25%	0.108%
36	16.198	2178	2180	2184	rBV5	12249	16854	1.51%	0.130%

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37	16.281	2193	2194	2201	rVB5	26838	36745	3.29%	0.284%
38	16.445	2214	2222	2228	rBV2	565373	889771	79.68%	6.873%
39	16.698	2262	2265	2266	rBV3	13988	17115	1.53%	0.132%
40	16.862	2291	2293	2295	rBV3	16164	11360	1.02%	0.088%
41	16.980	2309	2313	2315	rBV5	21496	27252	2.44%	0.211%
42	17.150	2340	2342	2344	rBV3	12579	11861	1.06%	0.092%
43	17.221	2347	2354	2357	rBV9	26512	52202	4.67%	0.403%
44	17.362	2375	2378	2379	rBV3	25035	26782	2.40%	0.207%
45	17.420	2386	2388	2393	rVB6	20846	19189	1.72%	0.148%
46	17.532	2404	2407	2412	rVB2	48913	57717	5.17%	0.446%
47	17.714	2433	2438	2441	rBV	387691	572780	51.29%	4.425%
48	17.755	2441	2445	2452	rVB	695086	1077408	96.49%	8.323%
49	17.849	2456	2461	2465	rVB	180814	264853	23.72%	2.046%
50	18.014	2487	2489	2492	rVB4	22432	23525	2.11%	0.182%
51	18.049	2492	2495	2498	rBV5	20535	27404	2.45%	0.212%
52	18.120	2504	2507	2512	rVB3	66915	102776	9.20%	0.794%
53	18.225	2522	2525	2532	rVB9	28675	44753	4.01%	0.346%
54	18.578	2581	2585	2589	rVV2	63471	82810	7.42%	0.640%
55	18.625	2589	2593	2597	rVB	98573	141450	12.67%	1.093%
56	18.701	2603	2606	2612	rBV5	47466	85575	7.66%	0.661%
57	18.778	2612	2619	2622	rBV4	101032	237106	21.23%	1.832%
58	19.071	2664	2669	2672	rBV3	67175	97936	8.77%	0.757%
59	19.130	2674	2679	2683	rVB8	59687	108824	9.75%	0.841%
60	19.383	2720	2722	2723	rBV2	27501	26287	2.35%	0.203%
61	19.471	2734	2737	2741	rVB5	48760	64184	5.75%	0.496%
62	19.618	2760	2762	2763	rBV2	33360	21334	1.91%	0.165%
63	19.753	2780	2785	2789	rVB	669562	908778	81.38%	7.020%
64	20.076	2835	2840	2842	rBV3	101252	172428	15.44%	1.332%
65	20.117	2842	2847	2851	rVB	538627	743377	66.57%	5.743%
66	20.288	2871	2876	2881	rBV	887319	1116645	100.00%	8.626%
67	21.533	3086	3088	3090	rBV3	54744	52858	4.73%	0.408%
68	22.033	3167	3173	3180	rBV2	292516	765387	68.54%	5.913%
69	22.097	3180	3184	3189	rVB2	198508	330978	29.64%	2.557%
70	25.446	3751	3754	3755	rBV3	69935	83516	7.48%	0.645%
71	25.617	3781	3783	3784	rBV2	67437	55505	4.97%	0.429%
72	26.762	3977	3978	3979	rBV	41930	19702	1.76%	0.152%

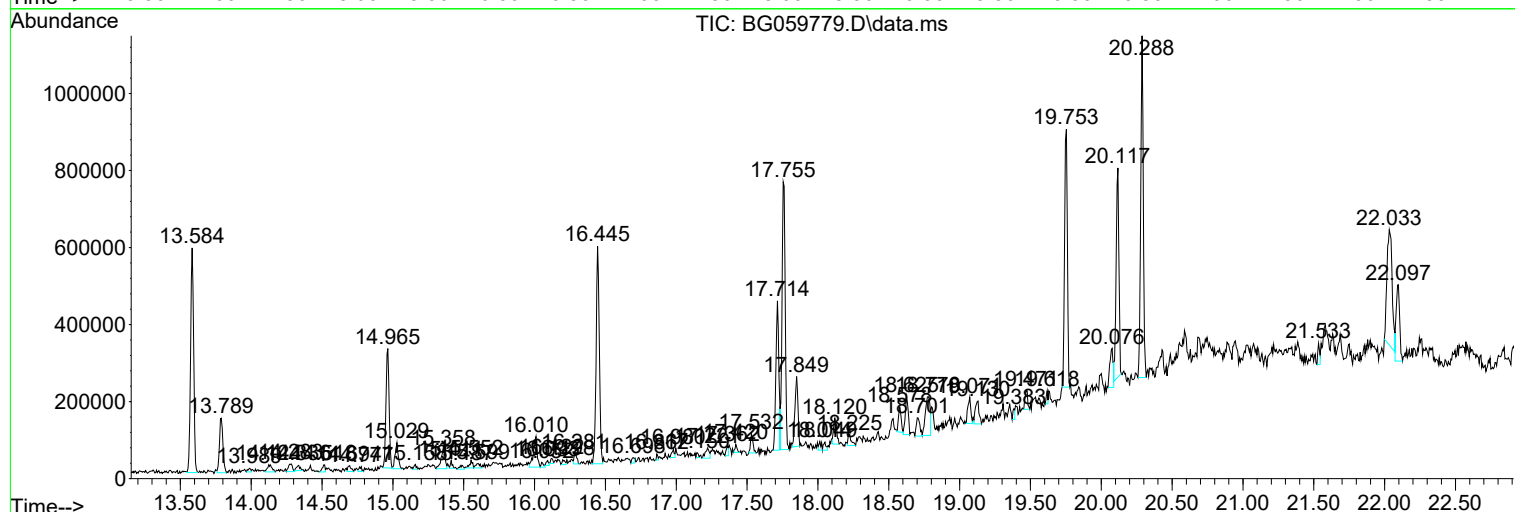
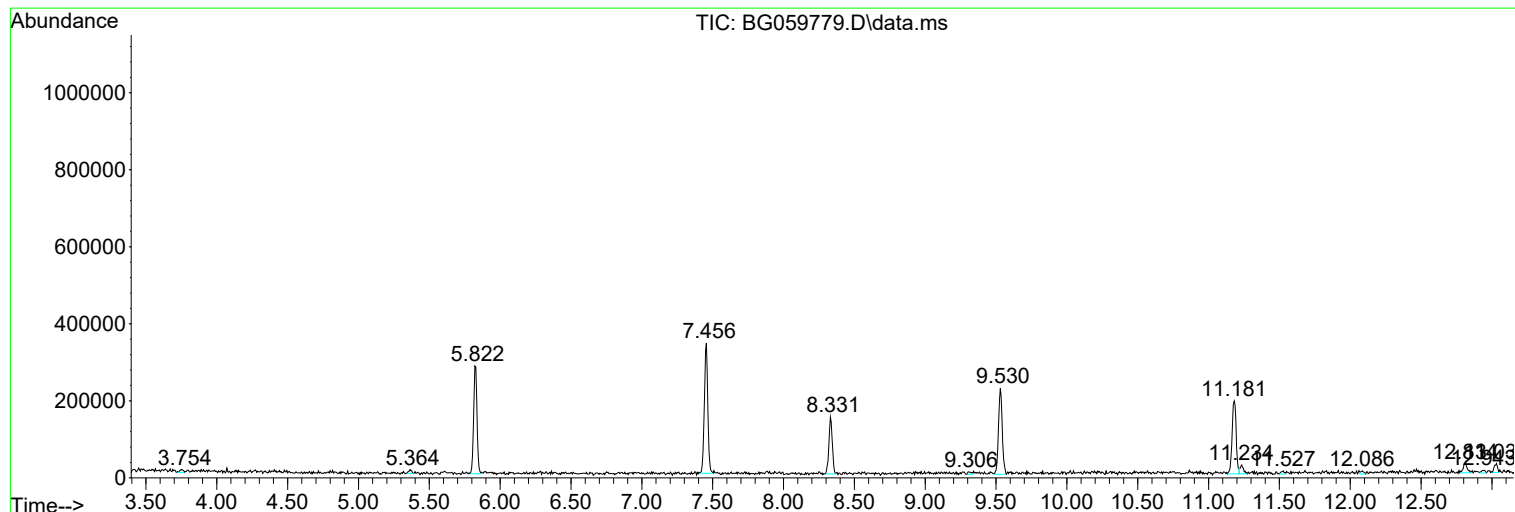
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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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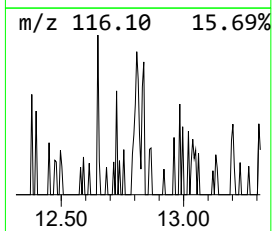
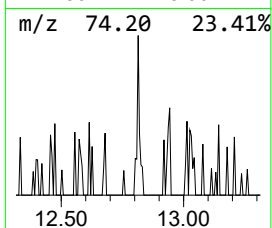
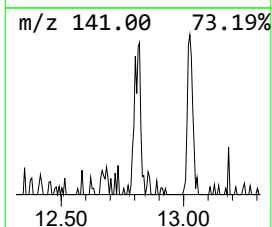
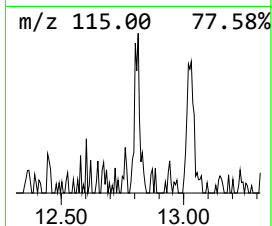
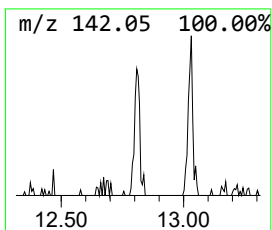
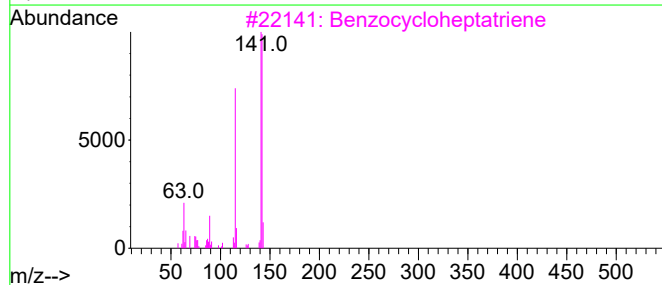
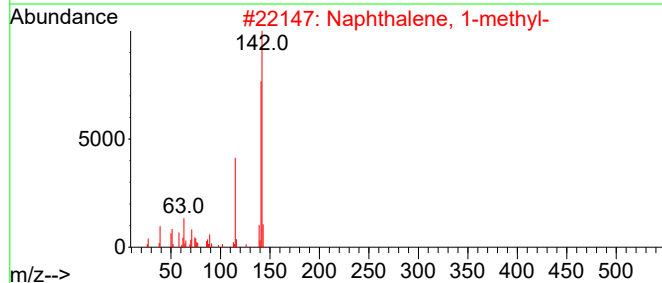
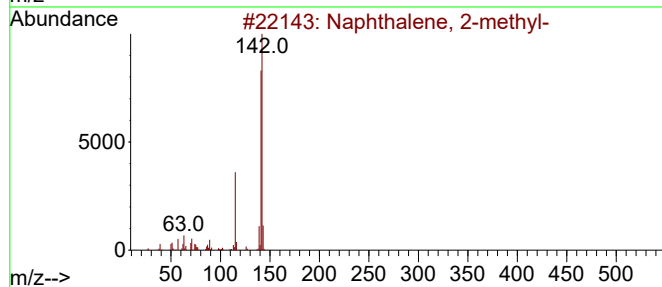
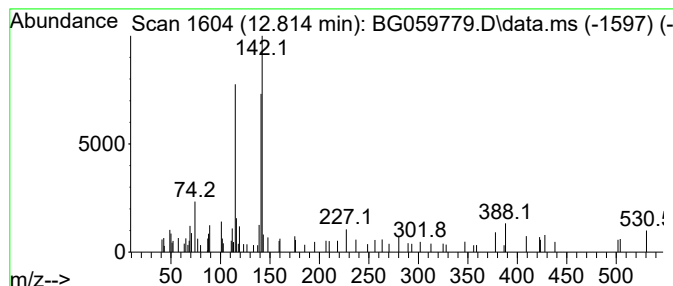
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Naphthalene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.814	2.61 ng	49993	Naphthalene-d8	11.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	83
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	83
3			Benzocycloheptatriene	142	C11H10	000264-09-5	72
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	53
5			5-Methylisophthalonitrile	142	C9H6N2	039718-07-5	49



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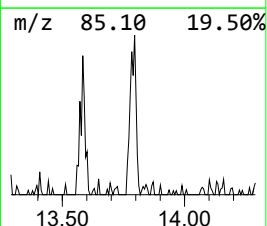
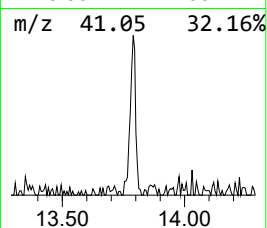
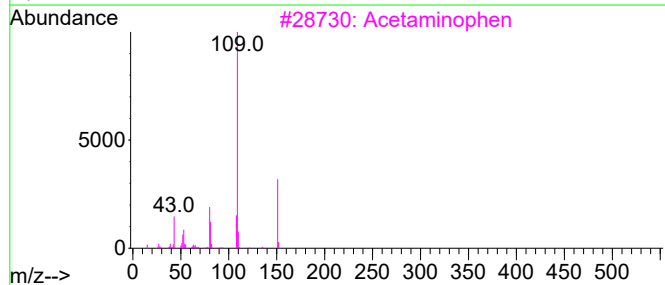
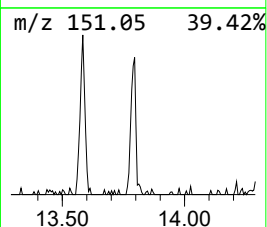
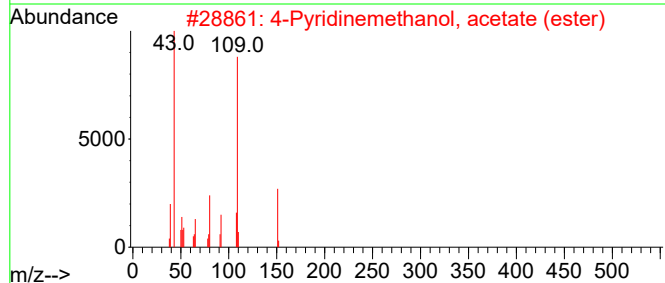
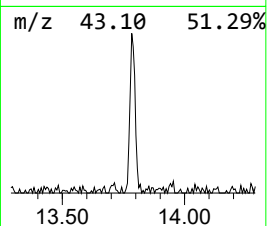
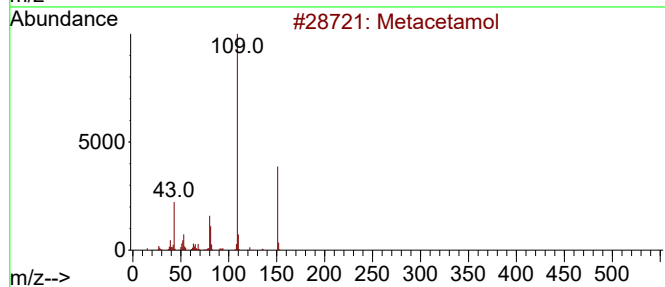
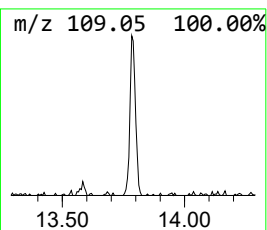
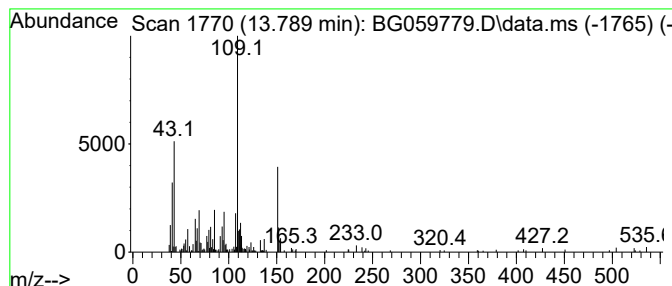
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Metacetamol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.789	9.85 ng	236419	Acenaphthene-d10	14.964

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Metacetamol	151	C8H9NO2	000621-42-1	64
2			4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	59
3			Acetaminophen	151	C8H9NO2	000103-90-2	59
4			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	47
5			Pyridine-2,4-diamine	109	C5H7N3	000461-88-1	43



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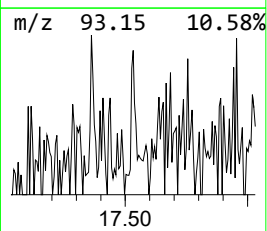
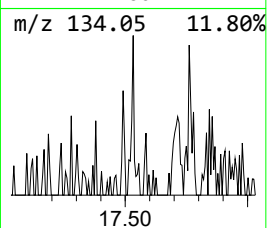
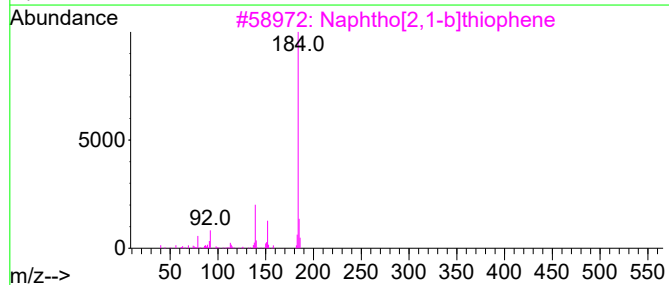
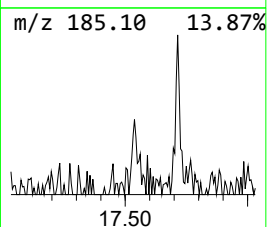
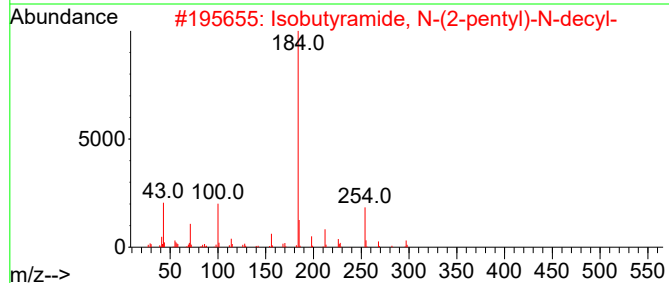
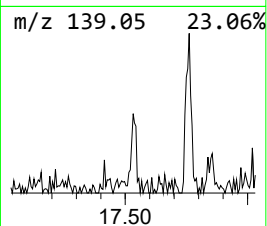
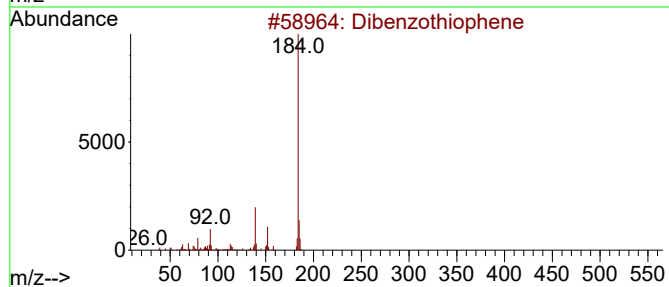
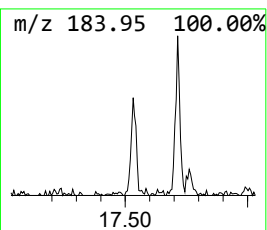
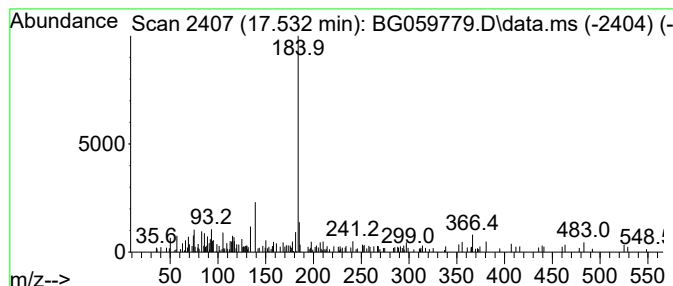
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Peak Number 3 Dibenzothiophene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.532	2.02 ng	57717	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzothiophene	184	C12H8S	000132-65-0	59
2			Isobutyramide, N-(2-pentyl)-N-decyl-	297	C19H39NO	1000464-58-2	53
3			Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	53
4			6-Methoxy-5-quinolinecarbonitrile	184	C11H8N2O	087299-97-6	49
5			l-Leucine, N-allyloxycarbonyl-N-	299	C16H29NO4	1000321-89-7	49



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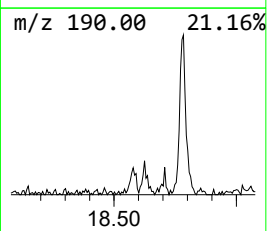
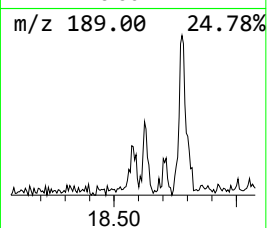
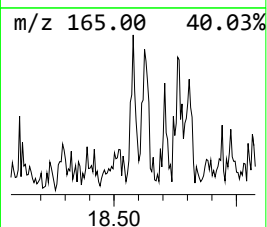
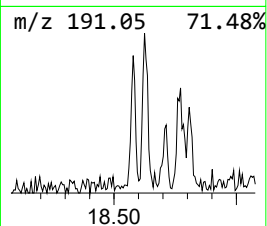
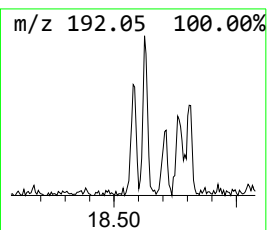
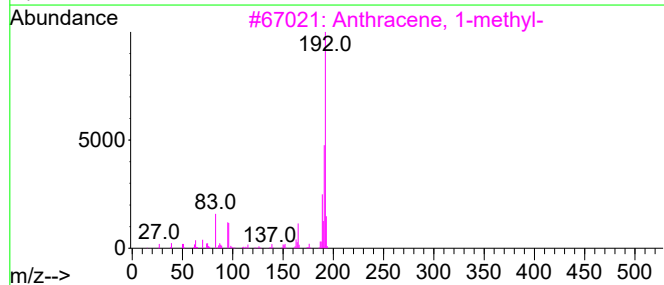
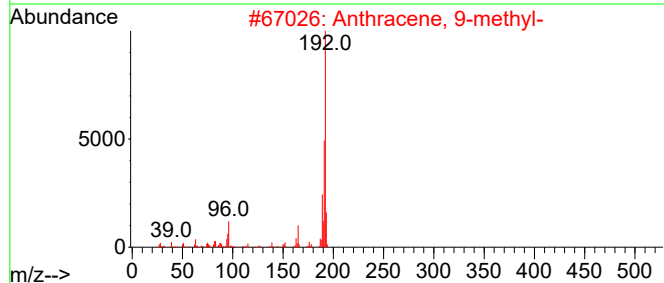
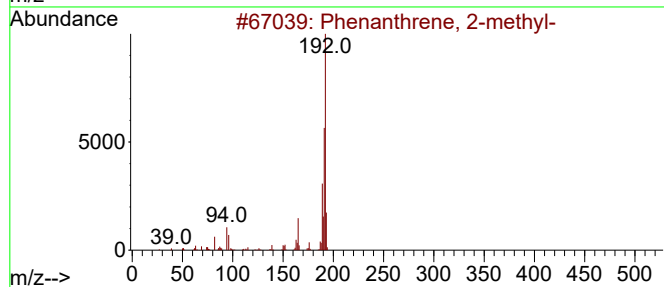
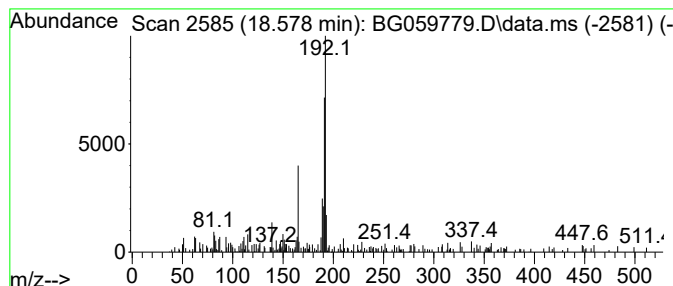
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.578	2.89 ng	82810	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	87
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	87
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	87



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Acq On : 20 Nov 2023 21:50
Operator : MA/JU
Sample : 05376-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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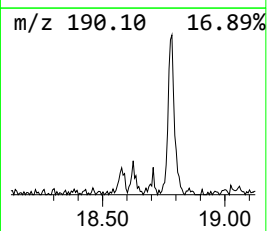
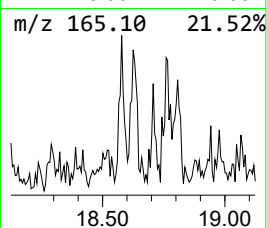
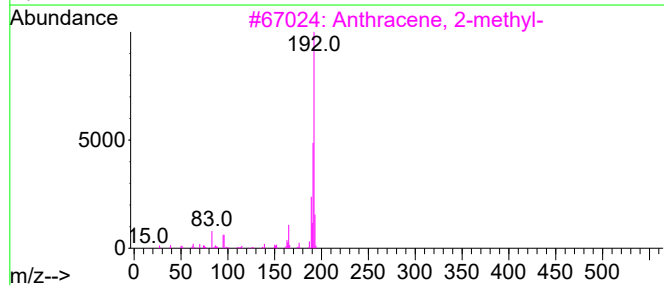
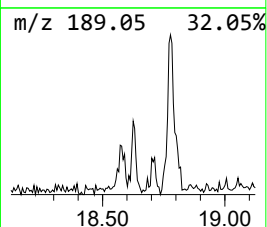
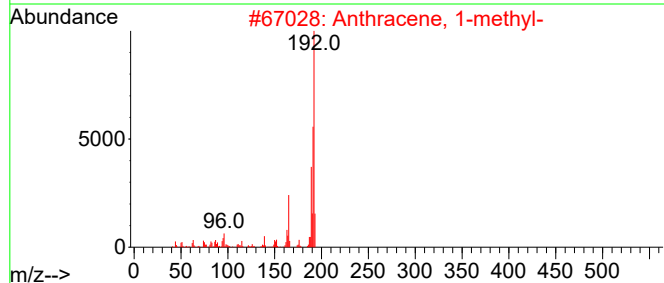
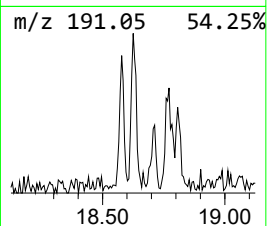
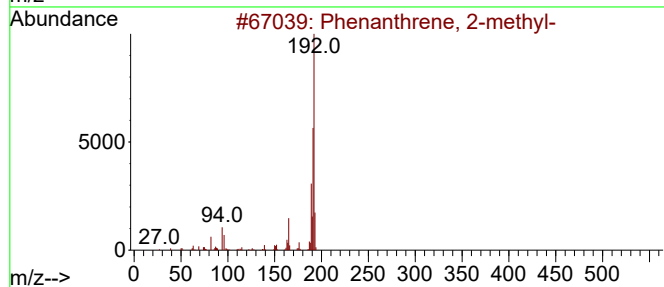
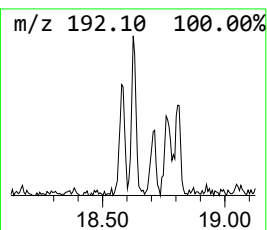
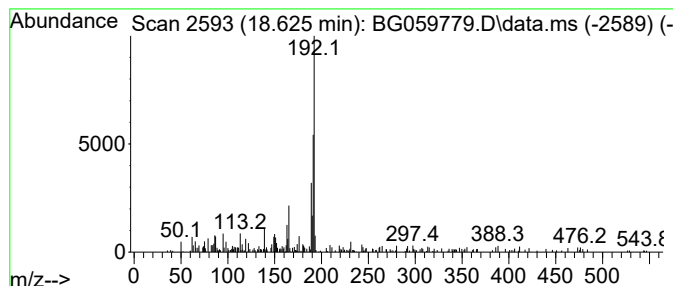
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.625	4.94 ng	141450	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	74
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	72
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	72
4			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	64
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059779.D
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Sample : 05376-01
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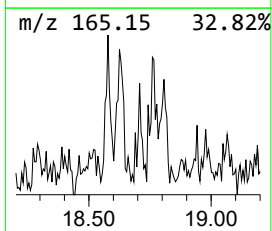
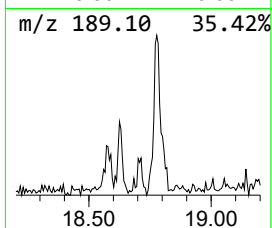
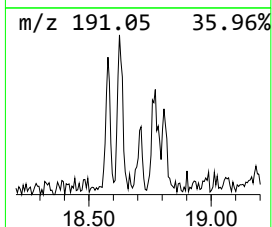
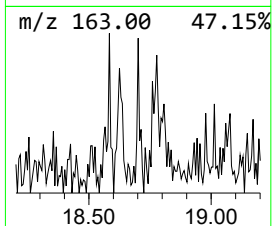
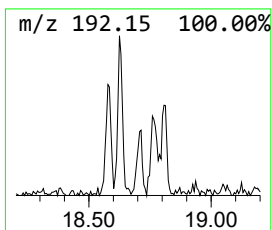
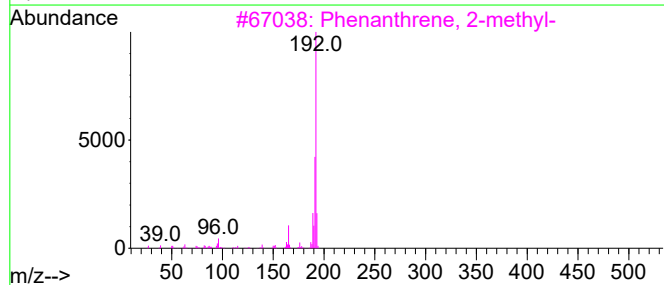
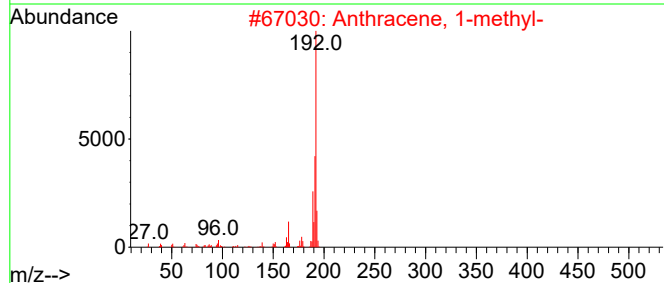
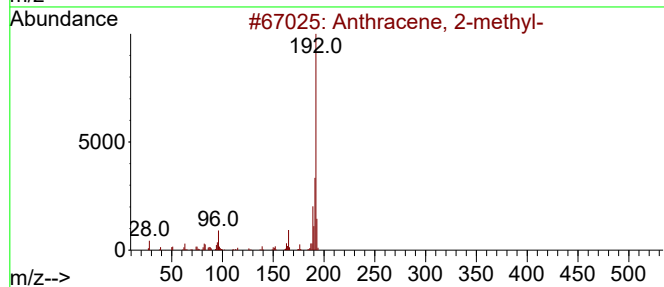
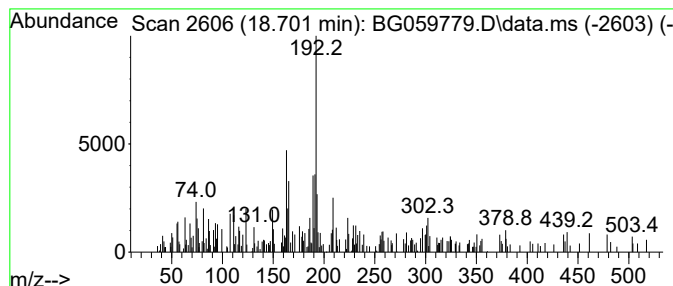
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown18.701 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.701	2.99 ng	85575	Phenanthrene-d10	17.714

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 2-methyl-	192	C15H12	000613-12-7	45
2		Anthracene, 1-methyl-	192	C15H12	000610-48-0	45
3		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	43
4		Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	43
5		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059779.D
Acq On : 20 Nov 2023 21:50
Operator : MA/JU
Sample : 05376-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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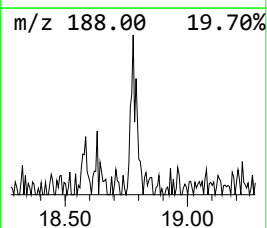
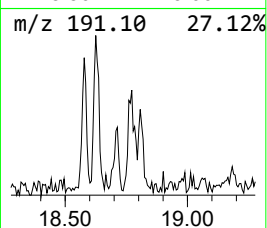
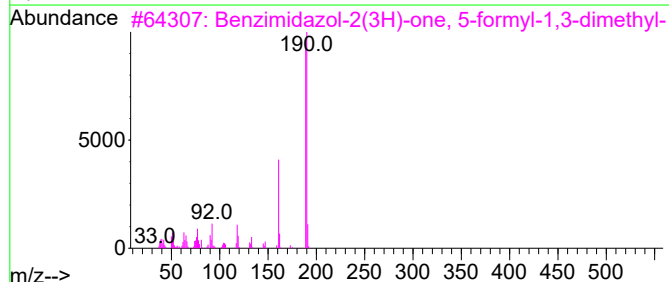
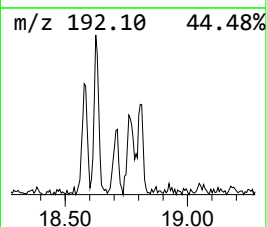
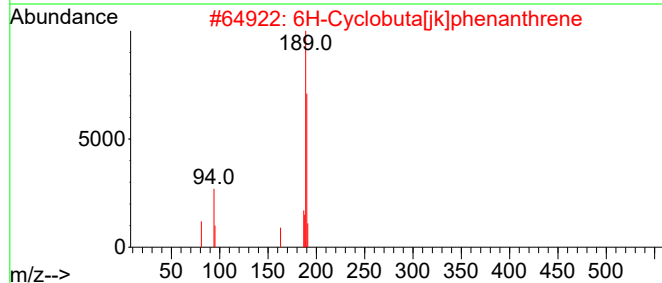
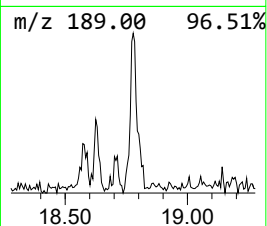
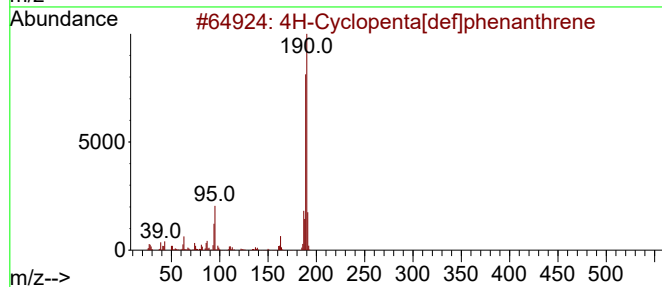
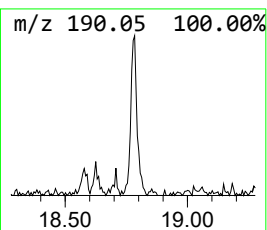
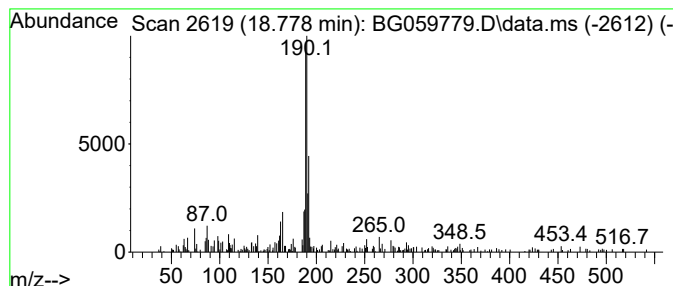
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.778	8.28 ng	237106	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	59
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3			Benzimidazol-2(3H)-one, 5-formyl...	190	C10H10N2O2	055241-49-1	40
4			1-Aminocyclopentanecarboxylic ac...	347	C17H30ClNO4	1000329-16-9	38
5			Carbonic acid, 2-formyl-4,6-dich...	276	C11H10Cl2O4	1000331-39-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059779.D
Acq On : 20 Nov 2023 21:50
Operator : MA/JU
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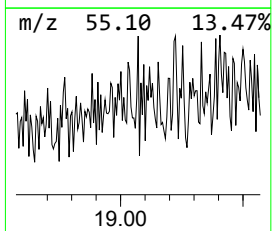
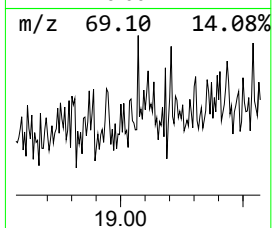
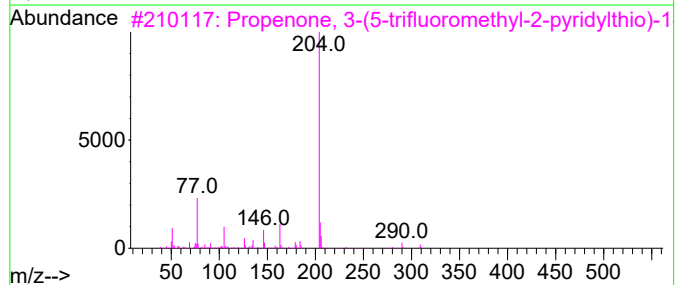
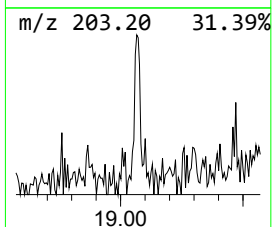
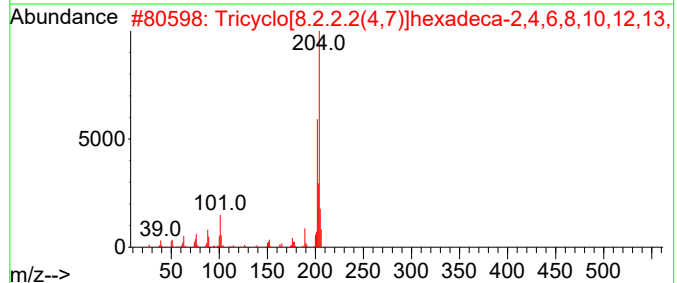
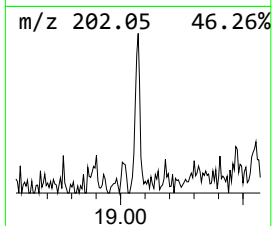
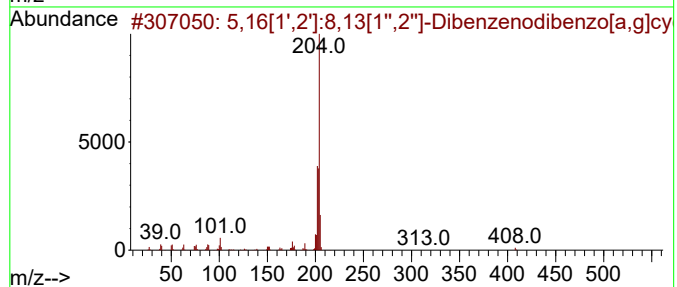
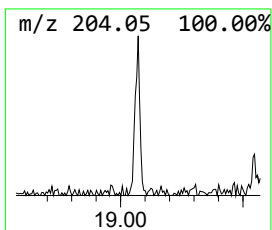
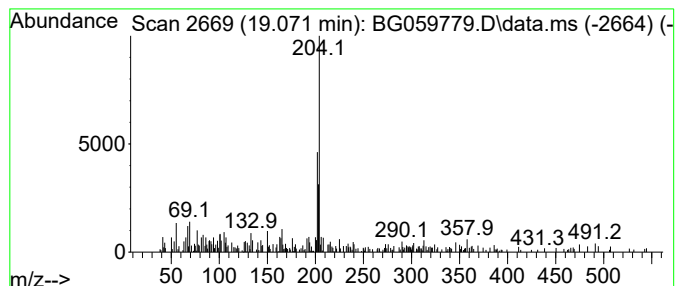
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5,16[1',2']:8,13[1'',2'']-D... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.072	3.42 ng	97936	Phenanthrene-d10	17.714	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	50
2	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	49
3	Propenone, 3-(5-trifluoromethyl-...	309	C15H10F3NOS	284496-12-4	46
4	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	46
5	Sulfamic acid, [[(5-methyl-3-iso...	297	C11H11N3O5S	1000327-58-4	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059779.D
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Sample : 05376-01
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Instrument :
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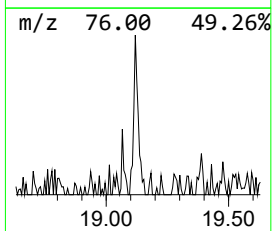
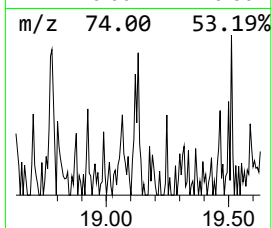
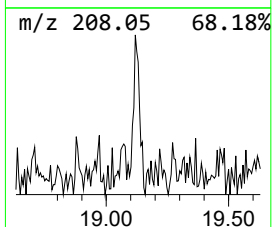
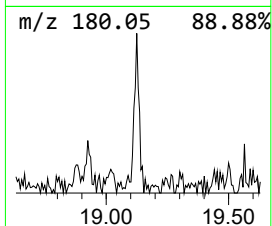
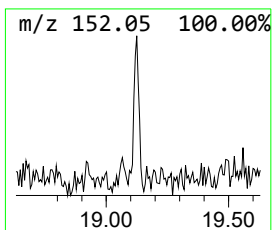
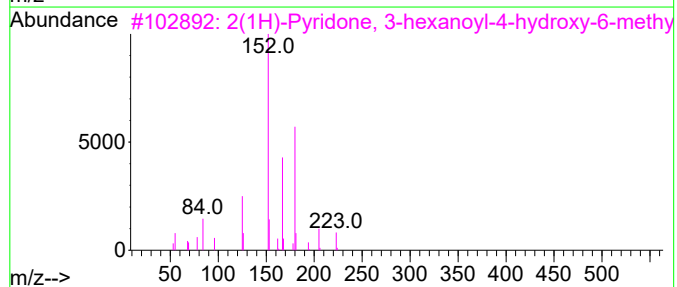
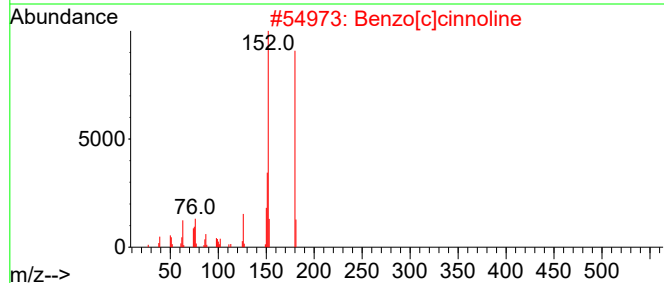
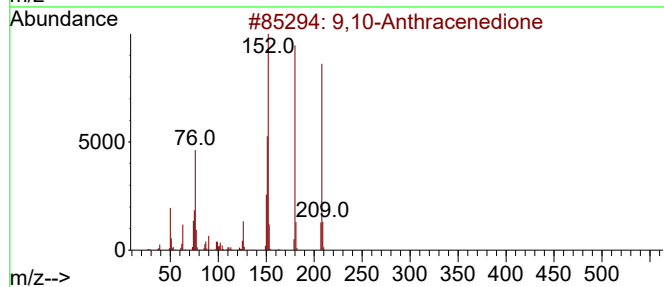
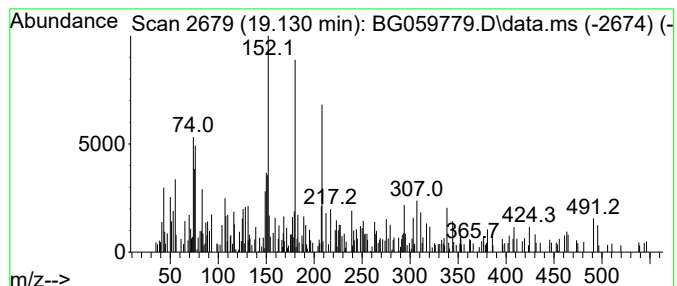
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9,10-Anthracenedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.130	3.80 ng	108824	Phenanthrene-d10	17.714

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	81	
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	60	
3	2(1H)-Pyridone, 3-hexanoyl-4-hyd...	223	C12H17NO3	007164-95-6	60	
4	9-Propyl-acridan	223	C16H17N	065753-73-3	46	
5	4-Quinolinol,4-ethenyl-1-ethylde...	223	C14H25NO	038463-57-9	45	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
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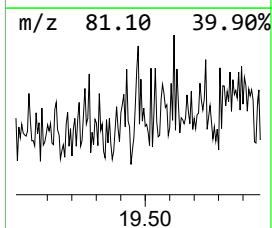
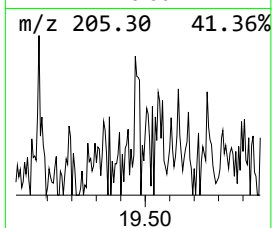
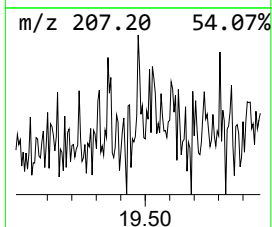
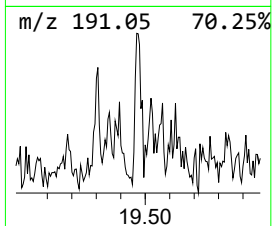
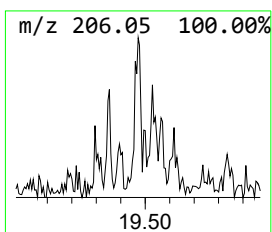
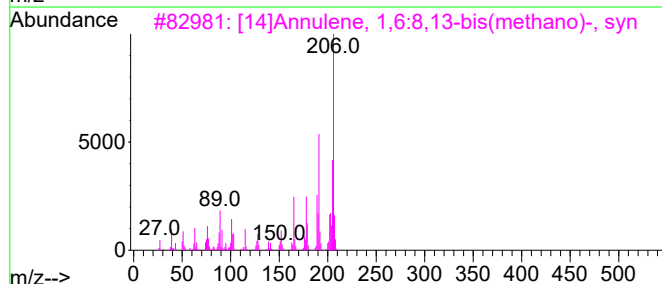
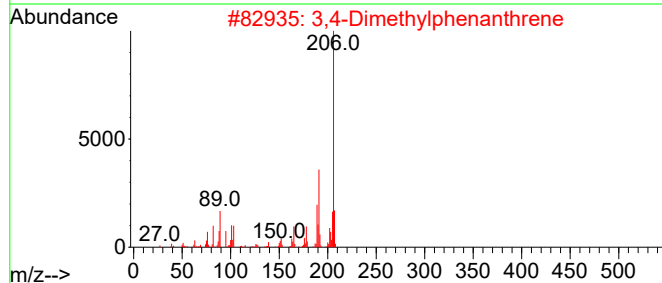
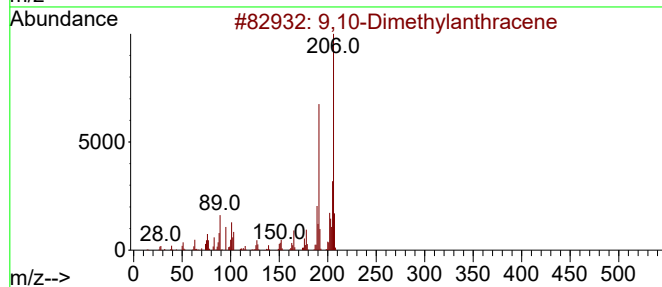
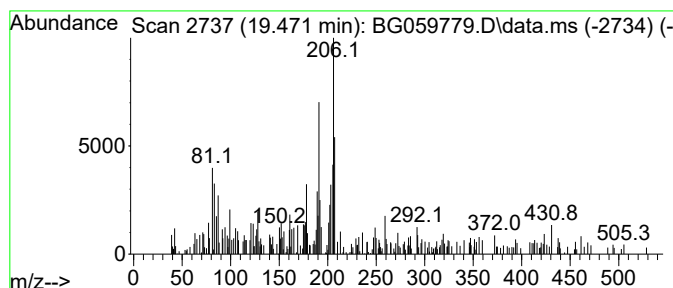
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9,10-Dimethylantracene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
19.471	2.24 ng	64184	Phenanthrene-d10			17.714
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylantracene	206	C16H14	000781-43-1	58	
2	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	55	
3	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	52	
4	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	49	
5	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	49	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059779.D
Acq On : 20 Nov 2023 21:50
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Sample : 05376-01
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ALS Vial : 13 Sample Multiplier: 1

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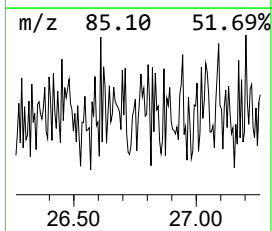
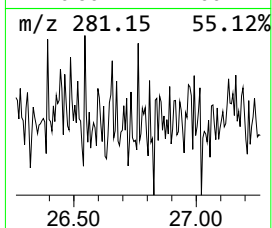
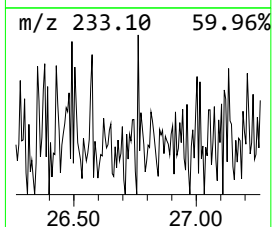
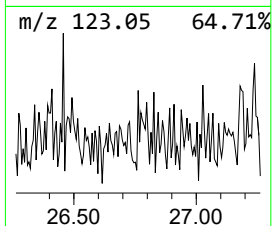
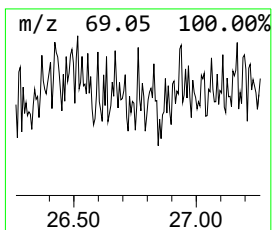
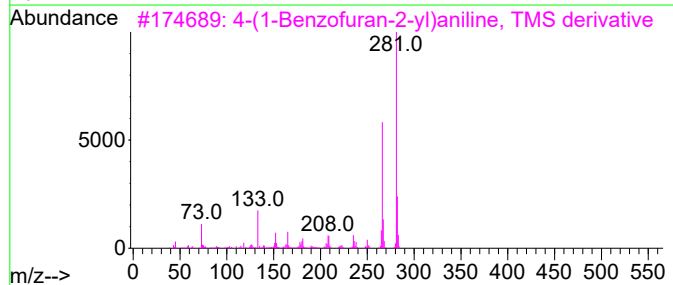
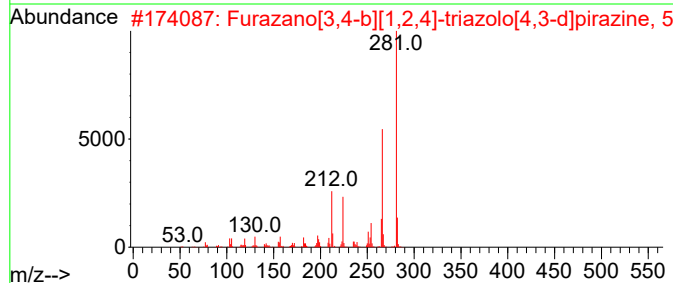
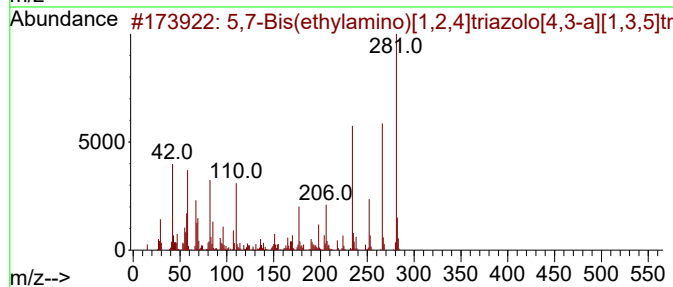
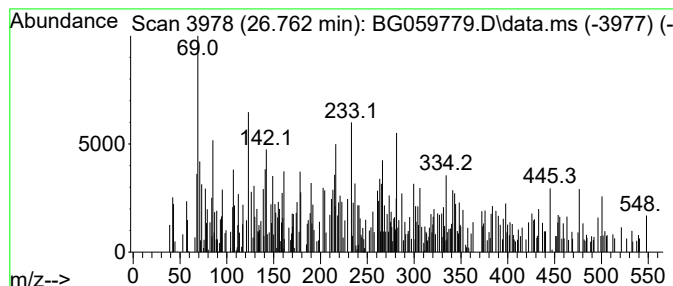
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown26.762 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.762	7.10 ng	19702	Perylene-d12	25.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,7-Bis(ethylamino)[1,2,4]triazolo...	281	C11H19N7S	1000510-86-9	43		
2	Furazano[3,4-b][1,2,4]-triazolo[...	281	C13H11N7O	311783-53-6	43		
3	4-(1-Benzofuran-2-yl)aniline, TM...	281	C17H19NOSi	1000477-09-8	38		
4	2-(Benzthiazol-2-yl)-6-methoxybe...	281	C16H11NO2S	1000284-45-0	38		
5	6-Chloro-3-ethyl-2-methyl-4-phen...	281	C18H16ClN	022609-09-2	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059779.D
Acq On : 20 Nov 2023 21:50
Operator : MA/JU
Sample : 05376-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Naphthalene, 2-...	12.814	2.6	ng	49993	2	11.175	382549	20.0
Metacetamol	13.789	9.8	ng	236419	3	14.964	480233	20.0
Dibenzothiophene	17.532	2.0	ng	57717	4	17.714	572780	20.0
Phenanthrene, 2...	18.578	2.9	ng	82810	4	17.714	572780	20.0
Anthracene, 1-m...	18.625	4.9	ng	141450	4	17.714	572780	20.0
unknown18.701	18.701	3.0	ng	85575	4	17.714	572780	20.0
4H-Cyclopenta[d...	18.778	8.3	ng	237106	4	17.714	572780	20.0
5,16[1',2']:8,1...	19.072	3.4	ng	97936	4	17.714	572780	20.0
9,10-Anthracene...	19.130	3.8	ng	108824	4	17.714	572780	20.0
9,10-Dimethylan...	19.471	2.2	ng	64184	4	17.714	572780	20.0
unknown26.762	26.762	7.1	ng	19702	6	25.628	55505	20.0