

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
 Data File : BG057894.D
 Acq On : 28 Jun 2023 15:54
 Operator : CG/JU
 Sample : 03415-08
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ESII-TP1

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-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057894.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.030	324	330	339	rBV	52251	81328	3.35%	0.419%
2	5.494	402	409	422	rBV	948424	1535644	63.21%	7.918%
3	7.086	672	680	694	rBV	948413	1625703	66.92%	8.382%
4	7.920	815	822	830	rBV	223103	364324	15.00%	1.878%
5	9.084	1012	1020	1031	rBV	568902	999718	41.15%	5.154%
6	10.723	1292	1299	1306	rBV	298195	532788	21.93%	2.747%
7	13.185	1710	1718	1726	rVB	1286908	2008766	82.69%	10.357%
8	14.560	1944	1952	1958	rBV	430384	669944	27.58%	3.454%
9	14.618	1958	1962	1969	rVB	44131	69138	2.85%	0.356%
10	14.953	2013	2019	2025	rBV	35263	58033	2.39%	0.299%
11	15.605	2124	2130	2141	rVB	34942	55619	2.29%	0.287%
12	15.911	2175	2182	2188	rVB2	72566	119187	4.91%	0.615%
13	16.046	2198	2205	2215	rBV	1111999	1691142	69.61%	8.719%
14	16.957	2354	2360	2366	rVB	44602	68424	2.82%	0.353%
15	17.121	2382	2388	2393	rVB	28870	44152	1.82%	0.228%
16	17.303	2412	2419	2423	rBV	504869	814997	33.55%	4.202%
17	17.345	2423	2426	2432	rVV	571340	793465	32.66%	4.091%
18	17.433	2432	2441	2447	rVV	115366	181560	7.47%	0.936%
19	17.703	2480	2487	2493	rBV2	38332	66829	2.75%	0.345%
20	18.191	2563	2570	2573	rBV2	161505	296557	12.21%	1.529%
21	18.226	2573	2576	2581	rVB	101556	156703	6.45%	0.808%
22	18.308	2586	2590	2595	rVV	39669	65865	2.71%	0.340%
23	18.379	2596	2602	2605	rVV2	70855	144204	5.94%	0.743%
24	18.408	2605	2607	2614	rVB	43598	57686	2.37%	0.297%
25	18.678	2647	2653	2656	rBV	62311	92938	3.83%	0.479%
26	18.719	2656	2660	2665	rVB	40951	66670	2.74%	0.344%
27	19.090	2720	2723	2729	rBV2	22115	40410	1.66%	0.208%
28	19.231	2743	2747	2753	rBV	52743	94804	3.90%	0.489%
29	19.360	2763	2769	2774	rBV	619928	863376	35.54%	4.451%
30	19.460	2784	2786	2792	rVB7	22665	31597	1.30%	0.163%
31	19.689	2821	2825	2826	rBV	106314	129284	5.32%	0.667%
32	19.718	2826	2830	2838	rVB	498947	723748	29.79%	3.732%
33	19.789	2839	2842	2846	rVV2	25604	36948	1.52%	0.190%
34	19.918	2859	2864	2869	rVB	1902495	2429352	100.00%	12.525%
35	20.964	3039	3042	3049	rVB	74593	104098	4.29%	0.537%
36	21.205	3079	3083	3093	rVB4	159163	274761	11.31%	1.417%

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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-BG062723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.287	3095	3097	3107	rVB	84368	134146	5.52%	0.692%
38	21.557	3136	3143	3148	rBV3	497714	1127176	46.40%	5.812%
39	21.604	3148	3151	3158	rVB	200588	295035	12.14%	1.521%
40	24.718	3675	3681	3692	rVB	161015	449444	18.50%	2.317%

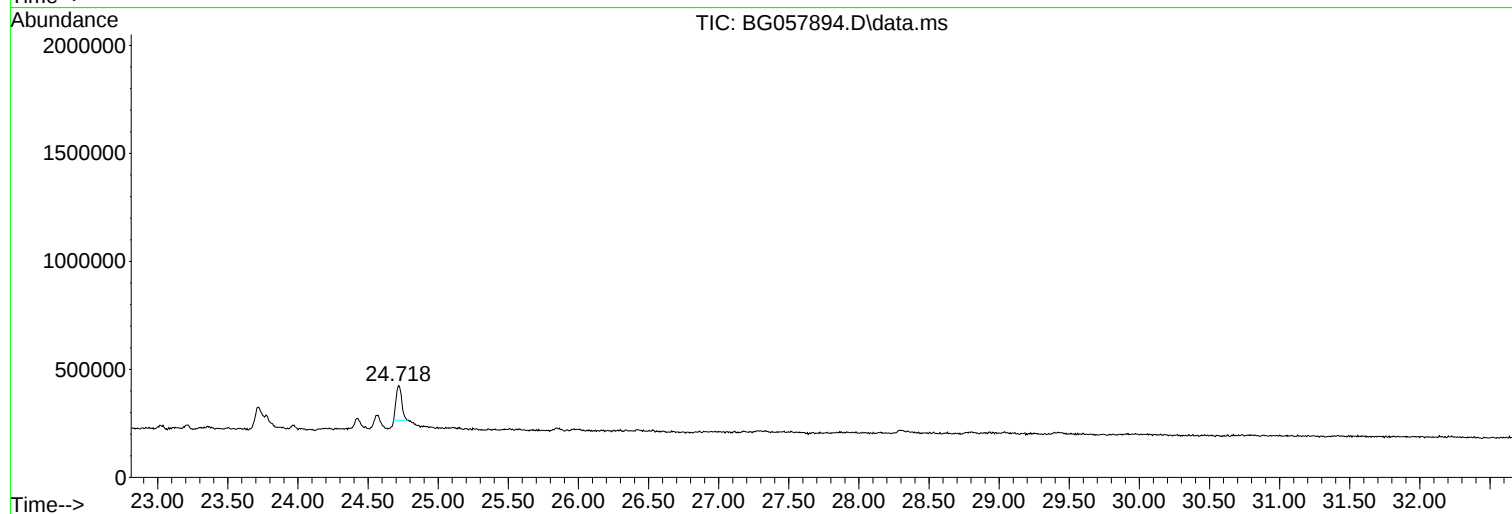
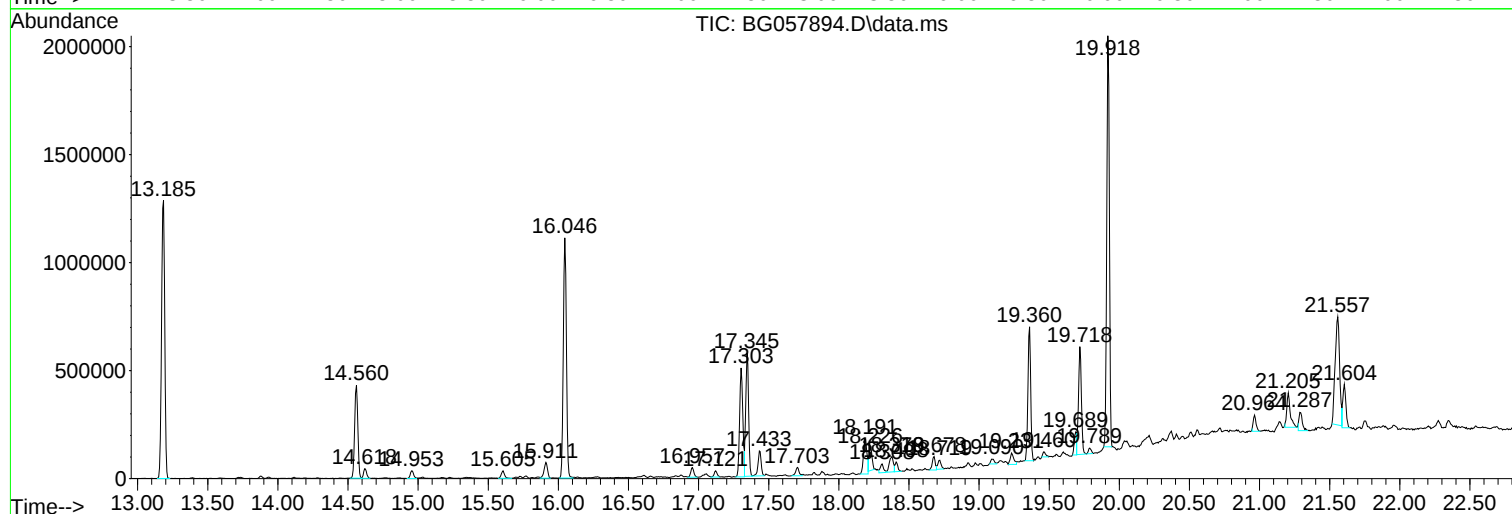
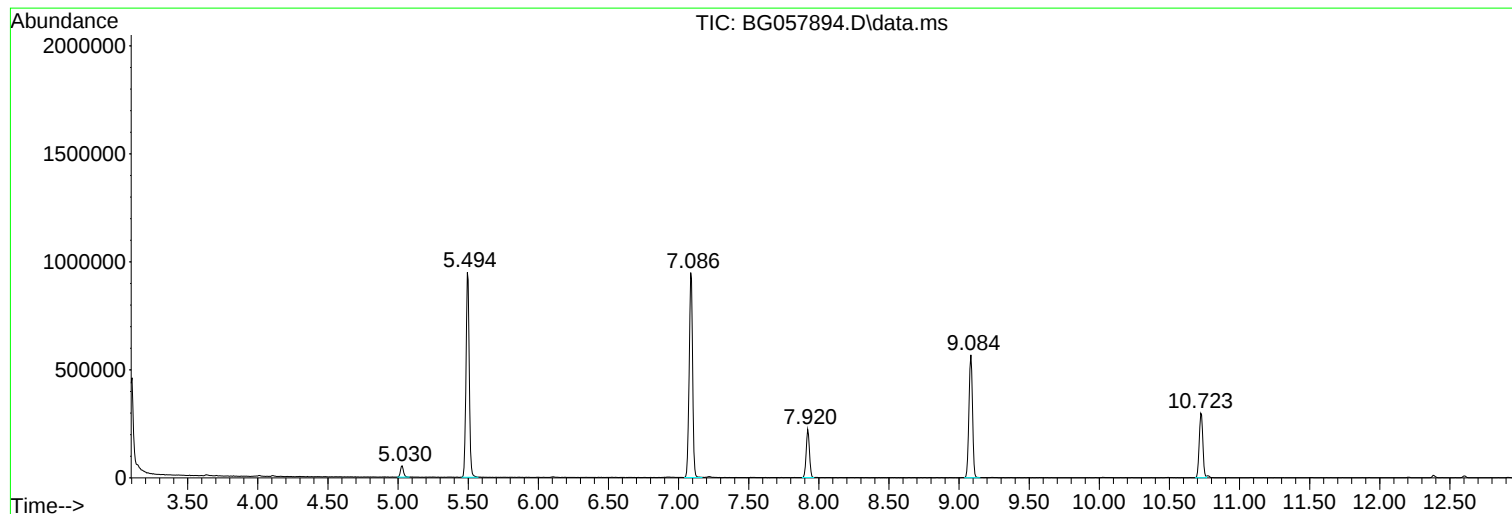
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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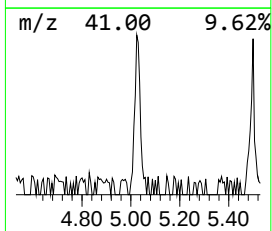
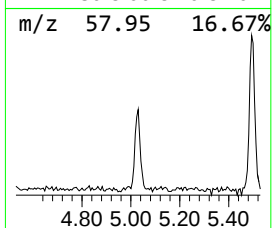
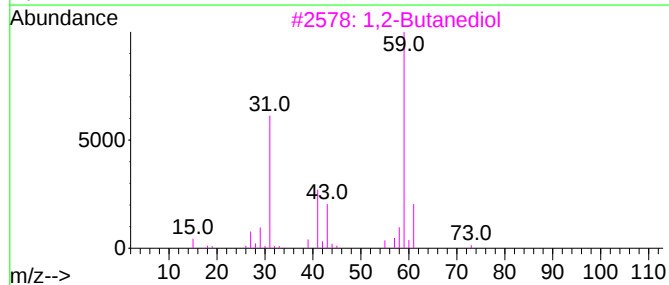
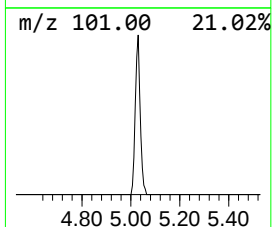
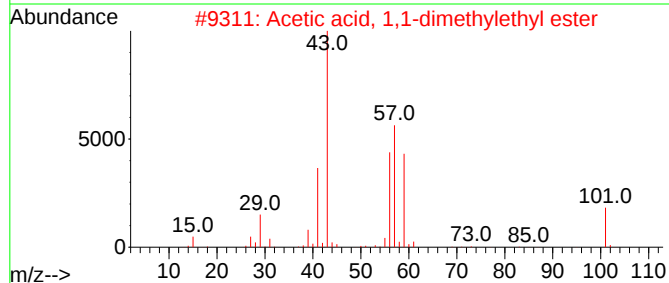
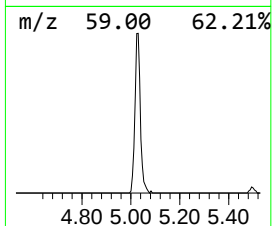
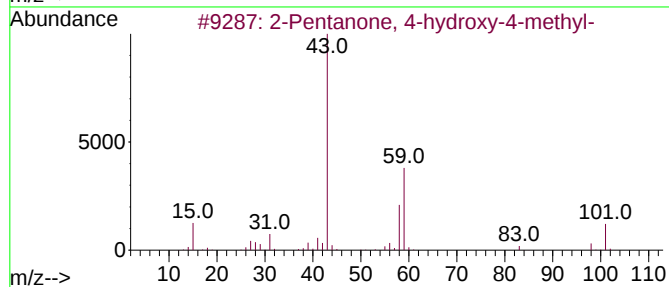
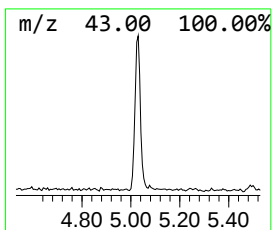
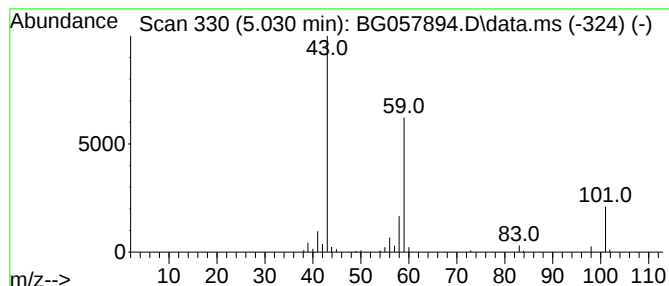
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.030	4.46 ng	81328	1,4-Dichlorobenzene-d4	7.920

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50		
3	1,2-Butanediol	90	C4H10O2	000584-03-2	32		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25		



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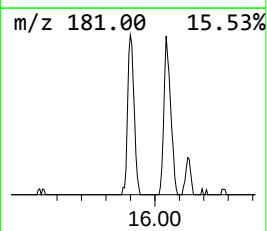
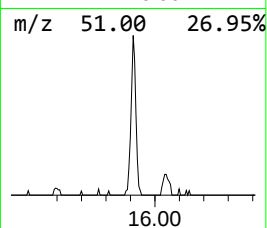
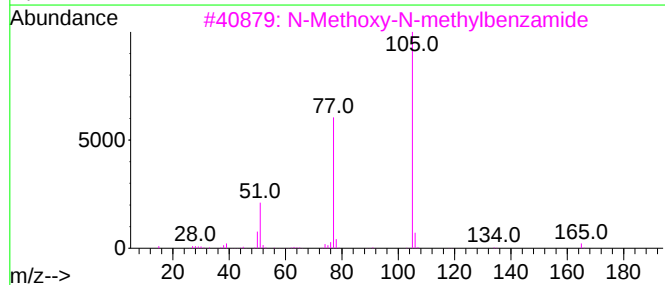
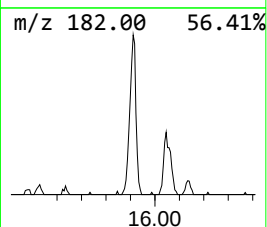
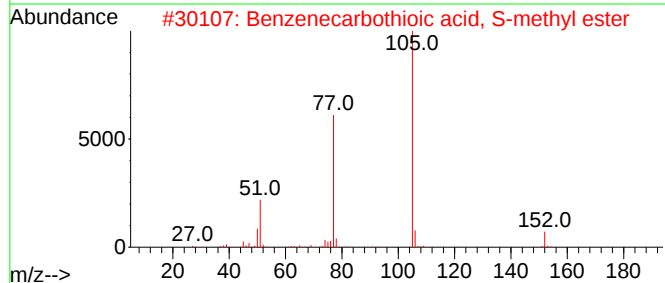
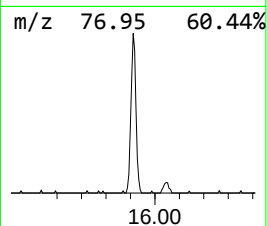
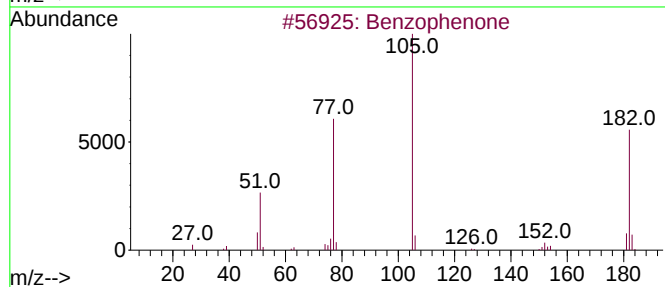
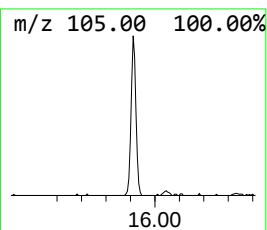
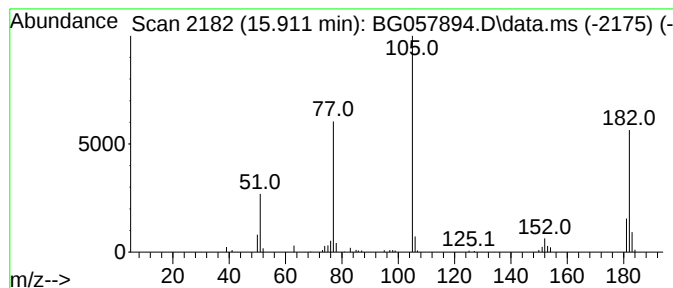
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.911	3.56 ng	119187	Acenaphthene-d10	14.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43
4			Benzoylformic acid	150	C8H6O3	000611-73-4	43
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	43



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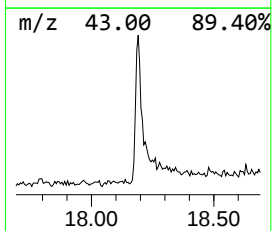
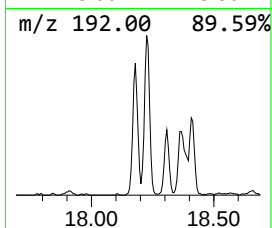
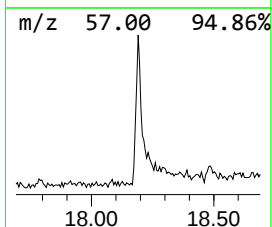
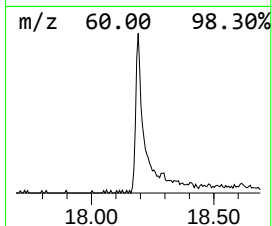
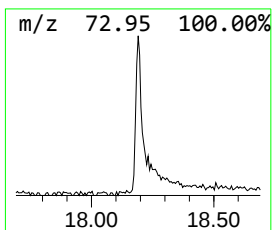
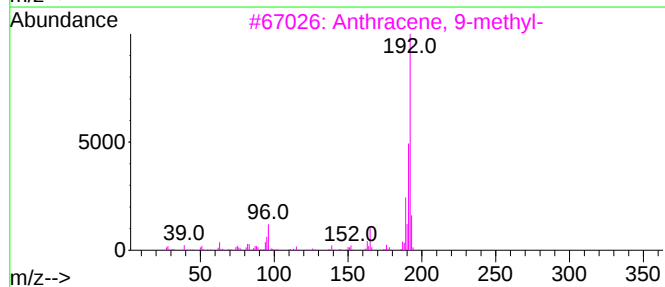
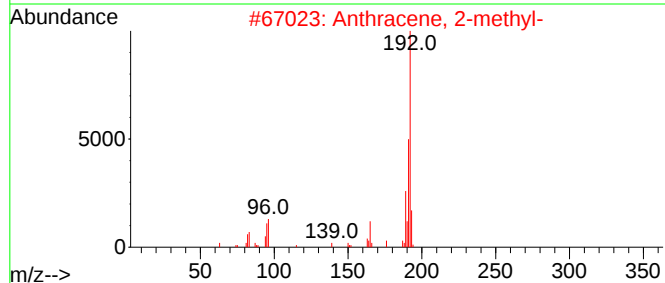
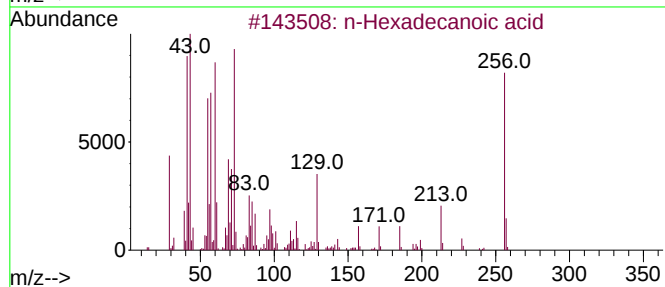
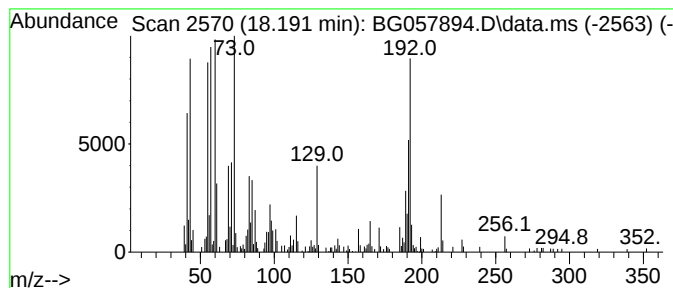
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.191	7.28 ng	296557	Phenanthrene-d10		17.303	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	95
2	Anthracene, 2-methyl-		192	C15H12	000613-12-7	93
3	Anthracene, 9-methyl-		192	C15H12	000779-02-2	64
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
5	Anthracene, 1-methyl-		192	C15H12	000610-48-0	60



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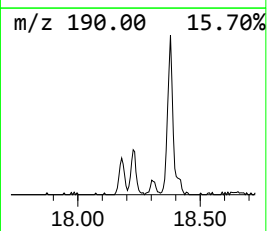
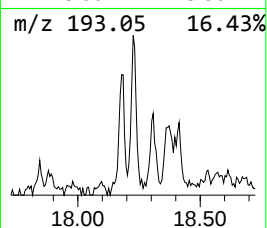
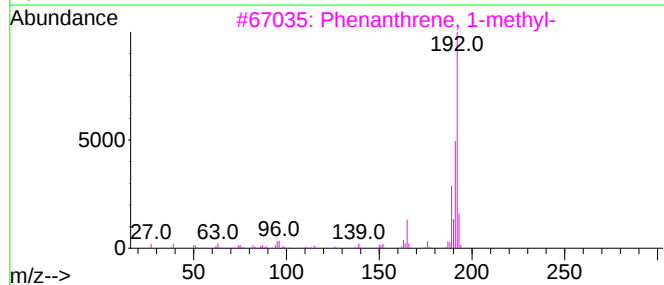
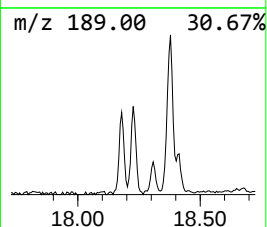
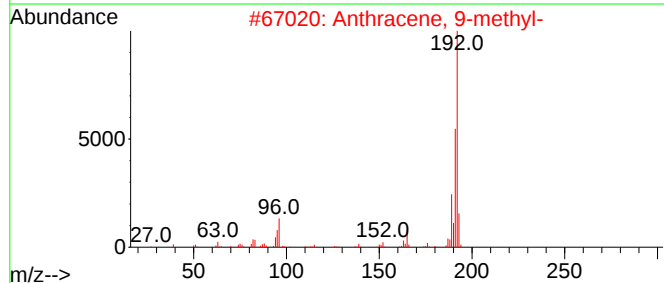
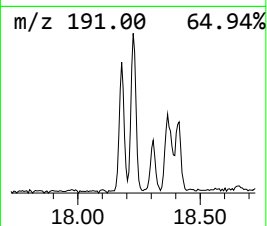
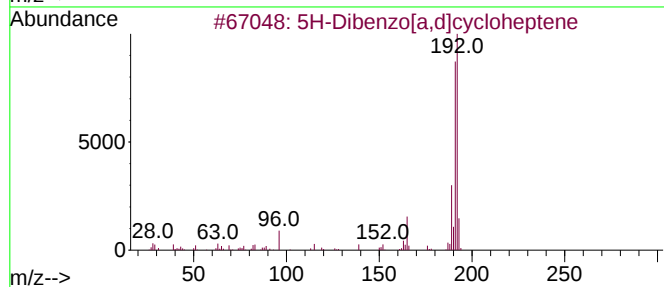
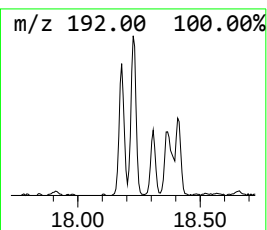
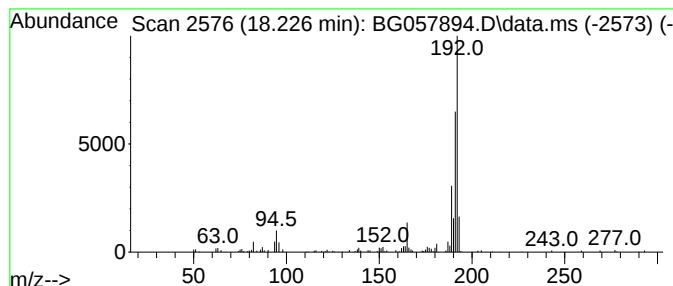
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 5H-Dibenzo[a,d]cycloheptene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.226	3.85 ng	156703	Phenanthrene-d10	17.303

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	93
2		Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
4		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90
5		Anthracene, 1-methyl-	192	C15H12	000610-48-0	90



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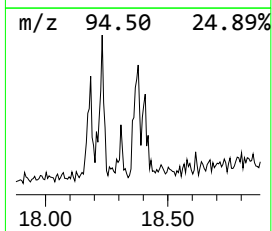
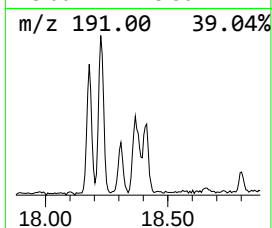
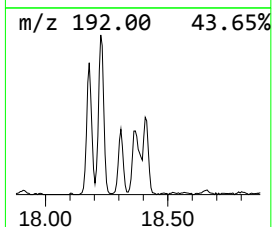
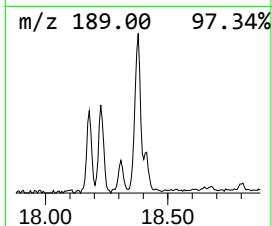
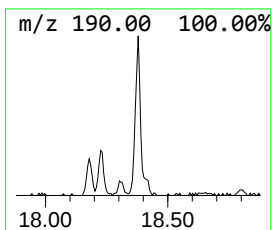
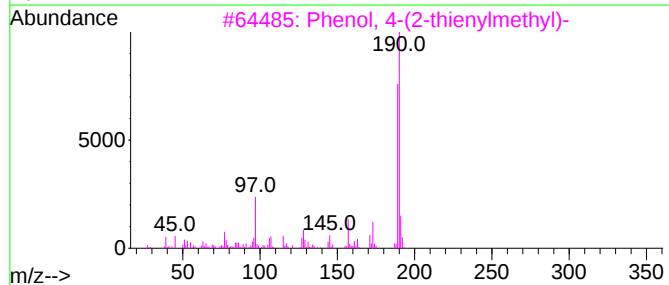
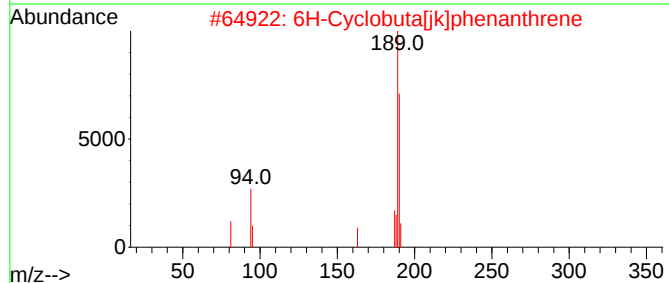
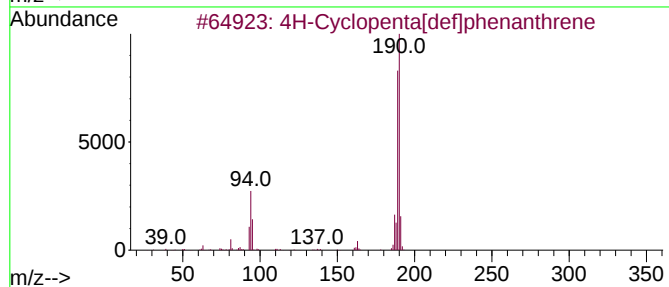
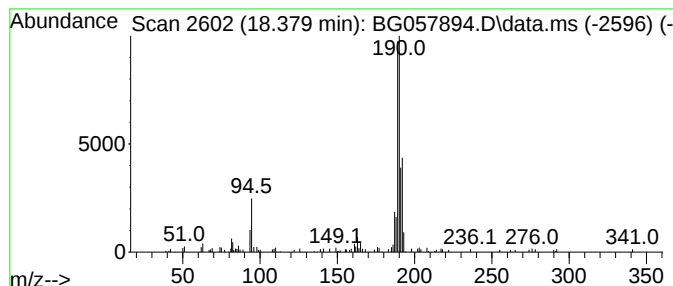
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.379	3.54 ng	144204	Phenanthrene-d10	17.303

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	43
3			Phenol, 4-(2-thienylmethyl)-	190	C11H10O5	091680-55-6	28
4			Cyclohexanone, 2-(2-furanylmethyl)-	190	C12H14O2	056053-07-7	27
5			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057894.D
Acq On : 28 Jun 2023 15:54
Operator : CG/JU
Sample : 03415-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ESI-TP1

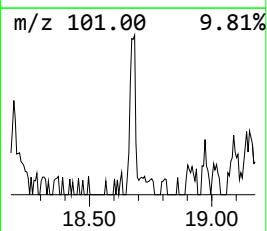
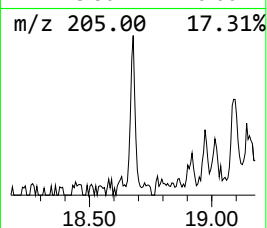
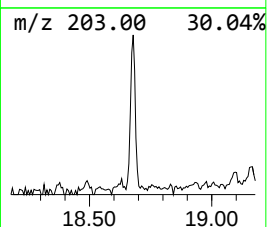
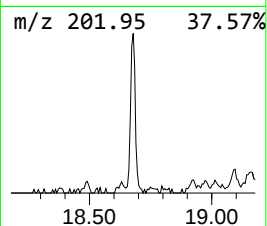
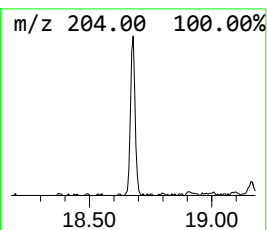
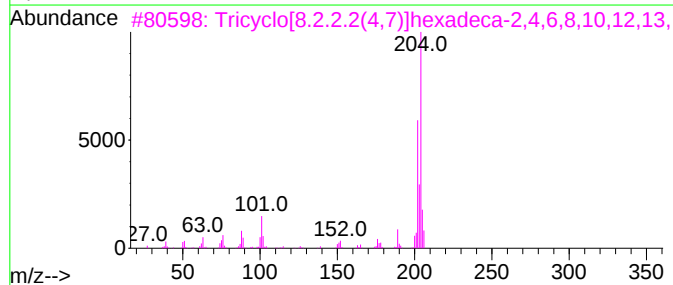
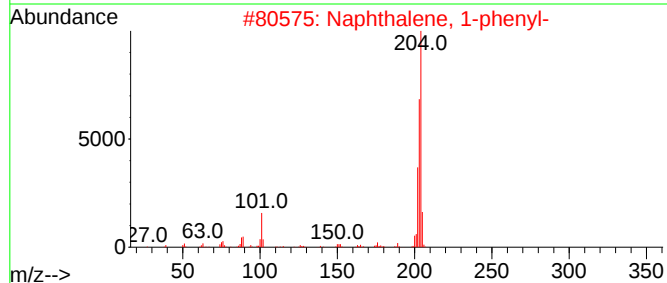
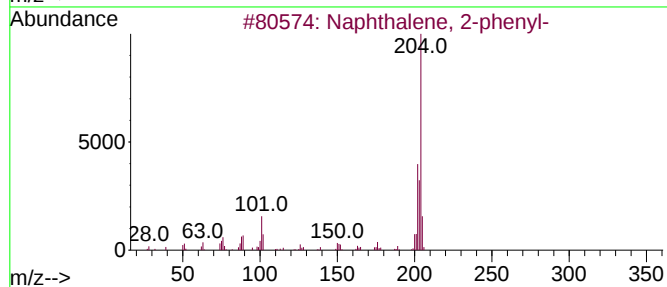
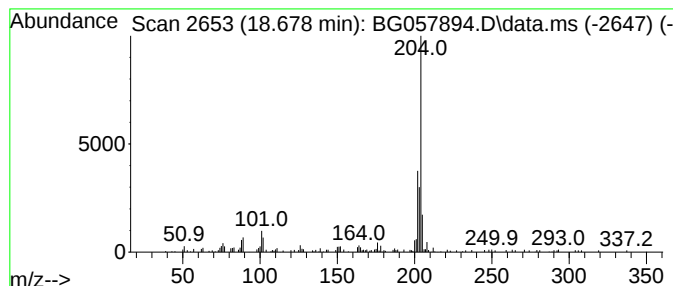
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Naphthalene, 2-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.678	2.28 ng	92938	Phenanthrene-d10	17.303

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	89
2			Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	70
3			Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	64
4			9-Acridinecarbonitrile	204	C14H8N2	005326-19-2	64
5			Acephenanthrylene, 4,5-dihydro-	204	C16H12	006232-48-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057894.D
Acq On : 28 Jun 2023 15:54
Operator : CG/JU
Sample : 03415-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

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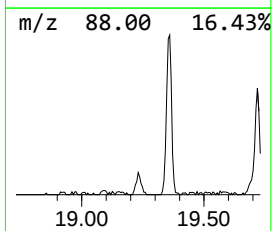
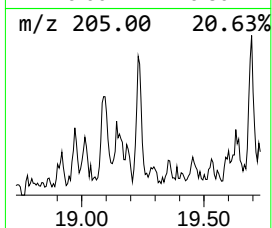
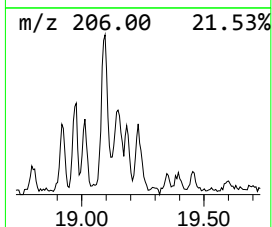
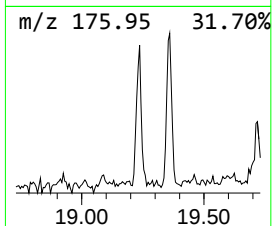
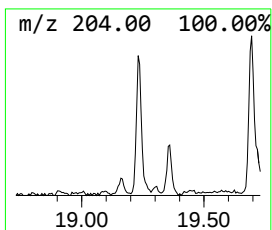
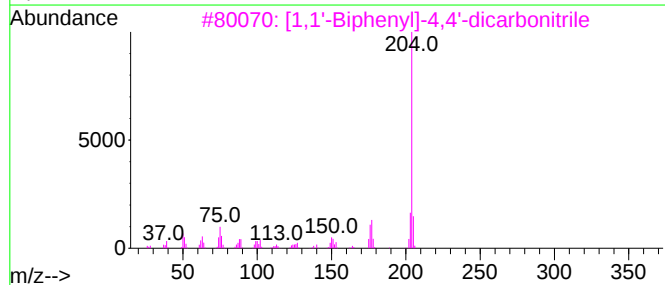
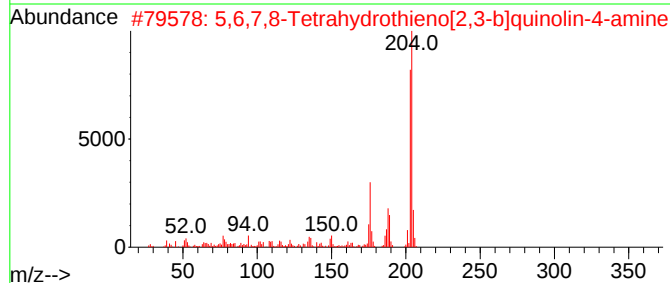
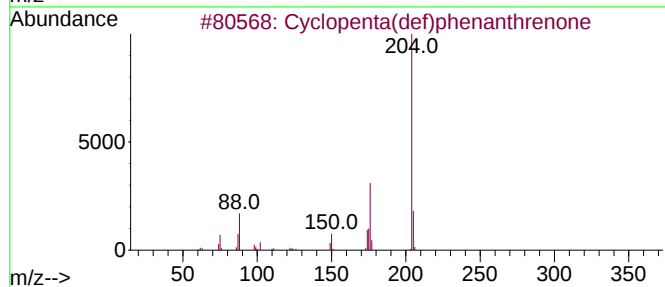
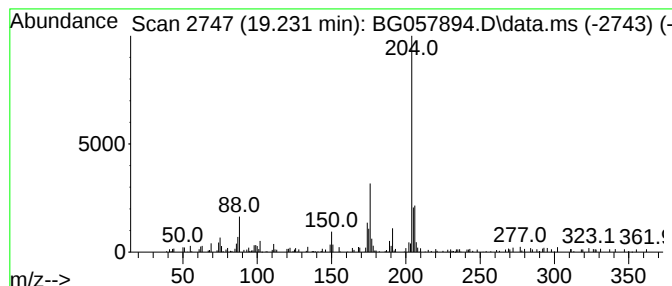
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopenta(def)phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.231	2.33 ng	94804	Phenanthrene-d10	17.303

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta(def)phenanthrene	204	C15H8O	005737-13-3	95
2			5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	64
3			[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	53
4			N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1010296-34-3	50
5			9-Acridinecarbonitrile	204	C14H8N2	005326-19-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057894.D
Acq On : 28 Jun 2023 15:54
Operator : CG/JU
Sample : 03415-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ESI-TP1

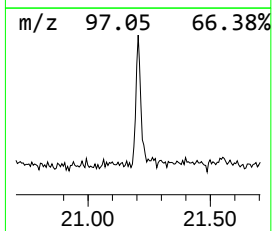
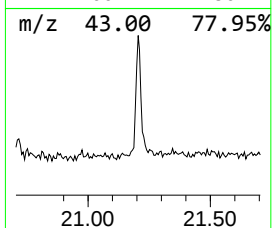
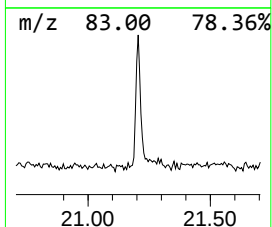
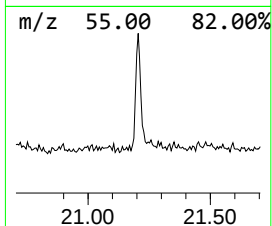
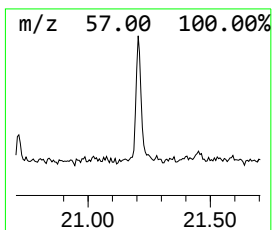
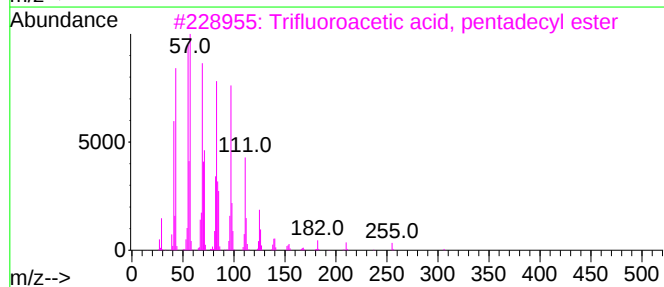
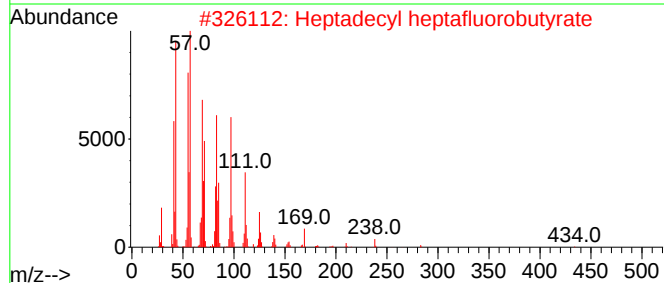
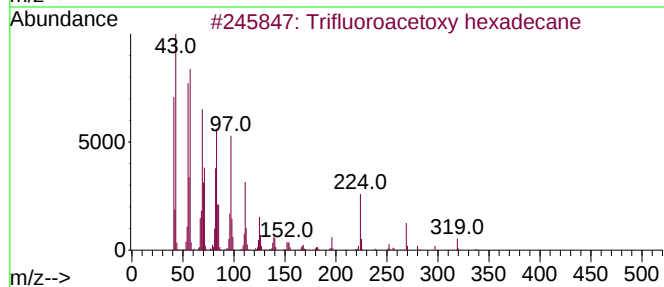
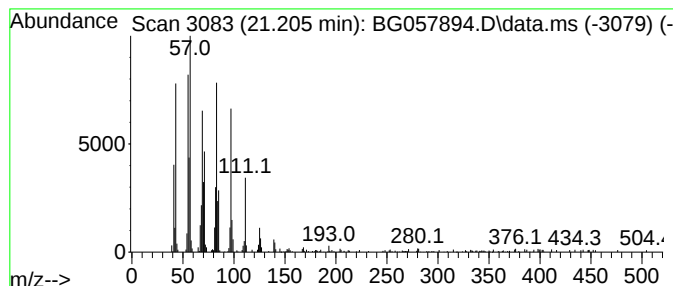
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.205	4.88 ng	274761	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			Cyclotetracosane	336	C24H48	000297-03-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
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Operator : CG/JU
Sample : 03415-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ESI-TP1

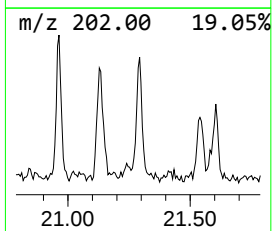
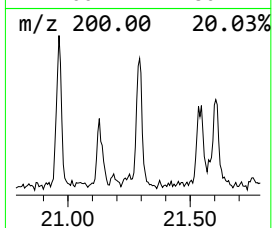
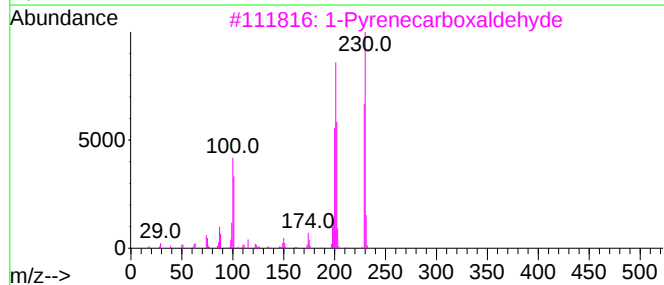
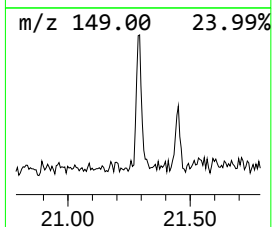
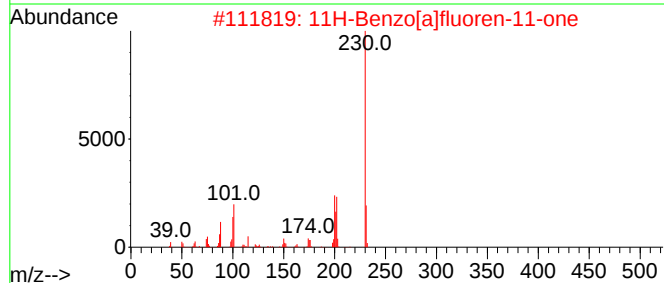
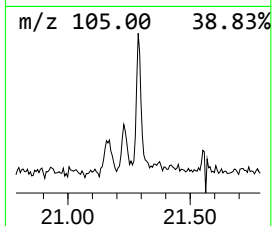
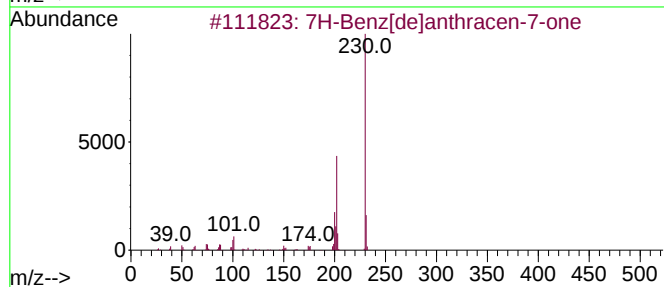
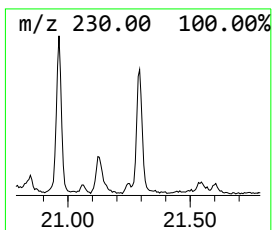
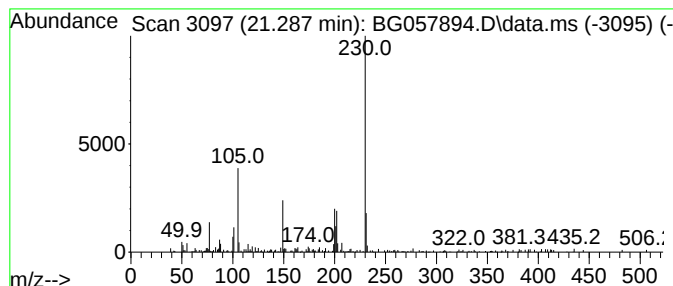
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 7H-Benz[de]anthracen-7-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.287	2.38 ng	134146	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	64
2			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	64
3			1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	59
4			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	52
5			o-Terphenyl	230	C18H14	000084-15-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
2-Pentanone, 4-...	5.030	4.5	ng	81328	1	7.920	364324	20.0
Benzophenone	15.911	3.6	ng	119187	3	14.560	669944	20.0
n-Hexadecanoic ...	18.191	7.3	ng	296557	4	17.303	814997	20.0
5H-Dibenzo[a,d]...	18.226	3.9	ng	156703	4	17.303	814997	20.0
4H-Cyclopenta[d]...	18.379	3.5	ng	144204	4	17.303	814997	20.0
Naphthalene, 2-...	18.678	2.3	ng	92938	4	17.303	814997	20.0
Cyclopenta(def)...	19.231	2.3	ng	94804	4	17.303	814997	20.0
Trifluoroacetox...	21.205	4.9	ng	274761	5	21.557	1127180	20.0
7H-Benz[de]anth...	21.287	2.4	ng	134146	5	21.557	1127180	20.0