

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
 Data File : BF135713.D
 Acq On : 11 Oct 2023 15:10
 Operator : CG\JU
 Sample : 04656-15
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105S

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_F\Methods\8270-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135713.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.769	281	286	295	rVB3	36328	64025	2.12%	0.376%
2	5.040	498	502	515	rBV	111355	139969	4.63%	0.821%
3	5.375	556	559	577	rBV	1019869	1269043	42.00%	7.447%
4	6.386	729	731	748	rBV	649607	859550	28.45%	5.044%
5	6.739	788	791	798	rBV	628218	549927	18.20%	3.227%
6	7.310	883	888	902	rBV	1830936	1896817	62.78%	11.131%
7	8.016	1005	1008	1015	rBV	733065	670600	22.20%	3.935%
8	9.098	1187	1192	1195	rBV	3414477	3021303	100.00%	17.729%
9	9.774	1303	1307	1311	rBV	940660	796357	26.36%	4.673%
10	9.804	1311	1312	1320	rVB3	26870	33311	1.10%	0.195%
11	9.998	1342	1345	1348	rBV3	29054	33215	1.10%	0.195%
12	10.574	1439	1443	1454	rBV	1710807	1777898	58.85%	10.433%
13	10.669	1456	1459	1464	rVB	149730	131172	4.34%	0.770%
14	10.763	1472	1475	1479	rBV2	20206	38166	1.26%	0.224%
15	11.110	1531	1534	1537	rBV	84563	75158	2.49%	0.441%
16	11.269	1558	1561	1565	rBV	903060	775208	25.66%	4.549%
17	11.339	1569	1573	1576	rVV2	158240	143230	4.74%	0.840%
18	11.810	1650	1653	1657	rBV	405328	424086	14.04%	2.489%
19	12.598	1784	1787	1805	rVB	633457	709990	23.50%	4.166%
20	12.798	1817	1821	1829	rVB2	31973	58446	1.93%	0.343%
21	12.868	1829	1833	1836	rBV	2623493	2343208	77.56%	13.750%
22	13.904	2002	2009	2011	rBV3	49514	86019	2.85%	0.505%
23	13.933	2011	2014	2022	rVB	525679	524753	17.37%	3.079%
24	15.033	2198	2201	2205	rVB2	31441	34036	1.13%	0.200%
25	15.404	2260	2264	2274	rBV	397753	586074	19.40%	3.439%

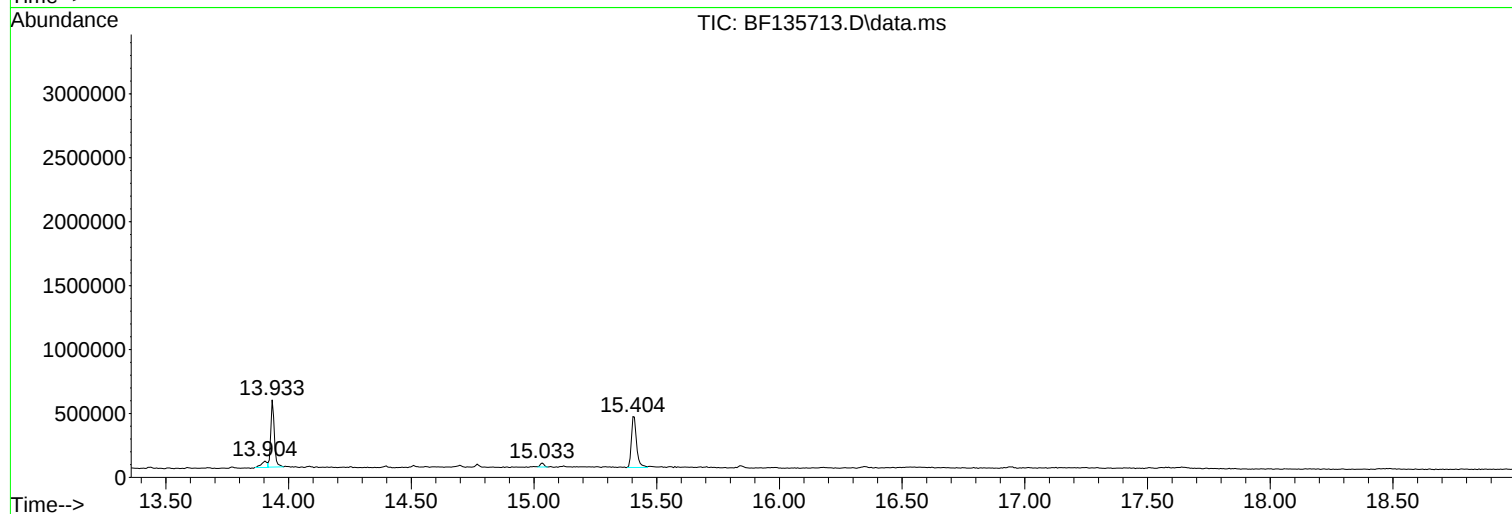
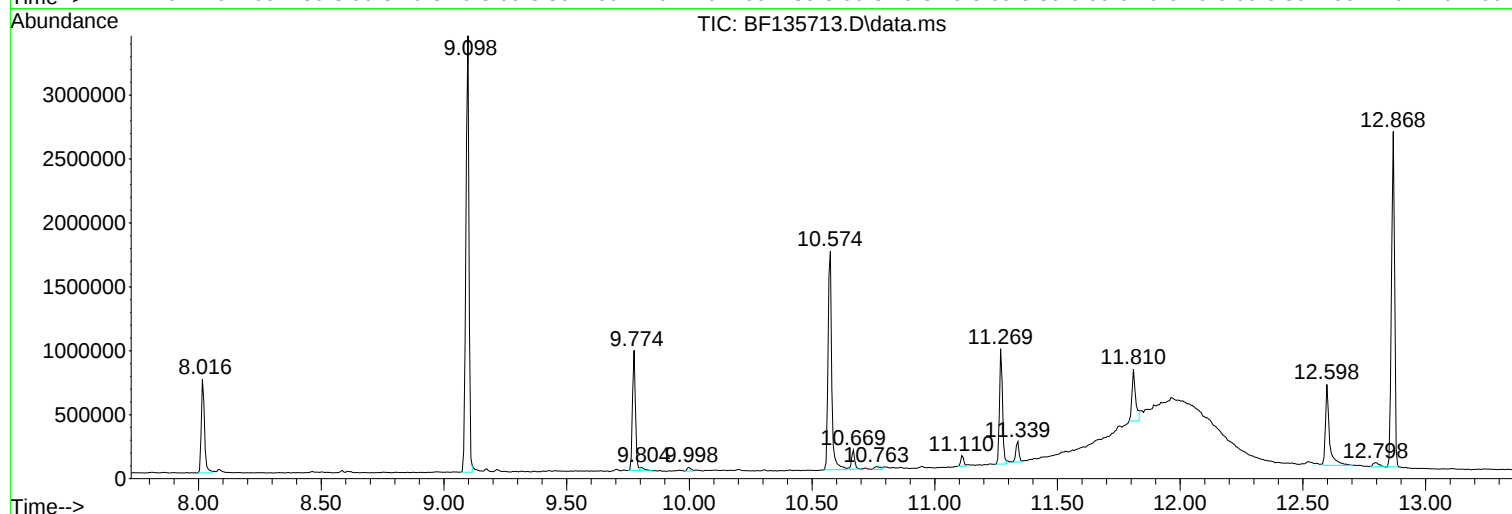
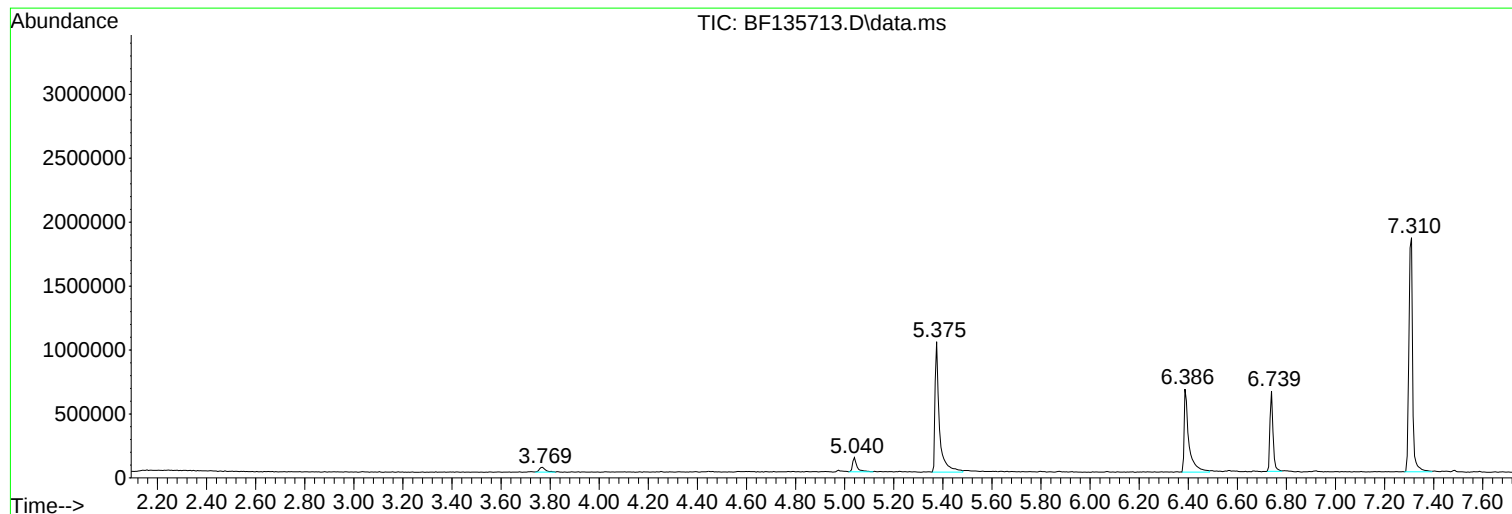
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Instrument :
BNA_F
ClientSampleId :
MW-105S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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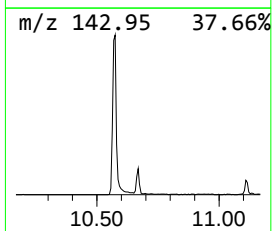
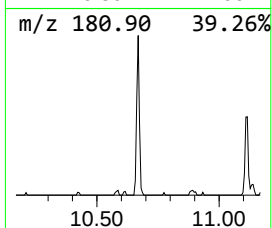
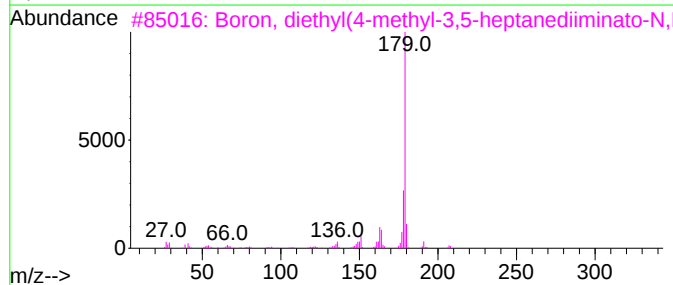
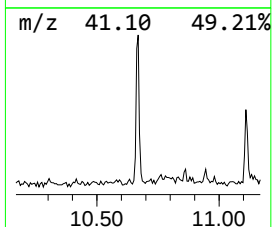
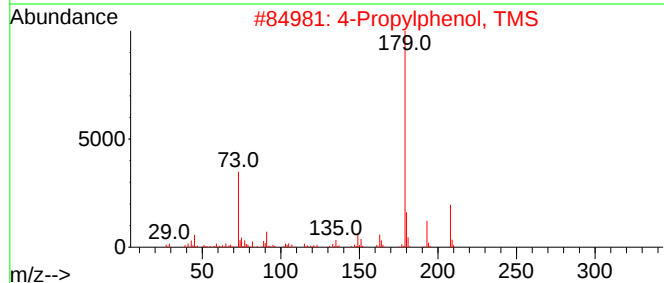
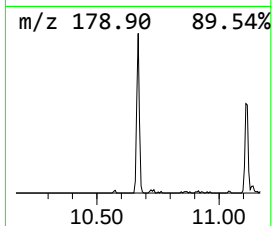
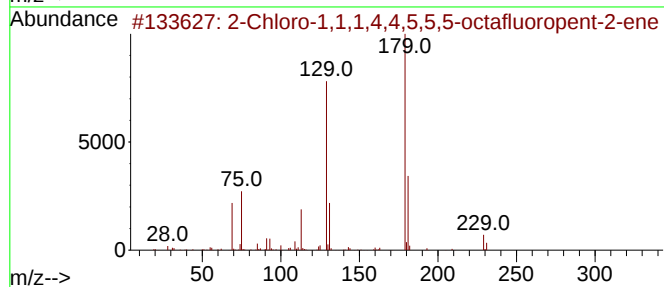
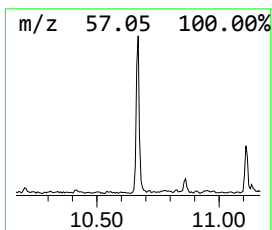
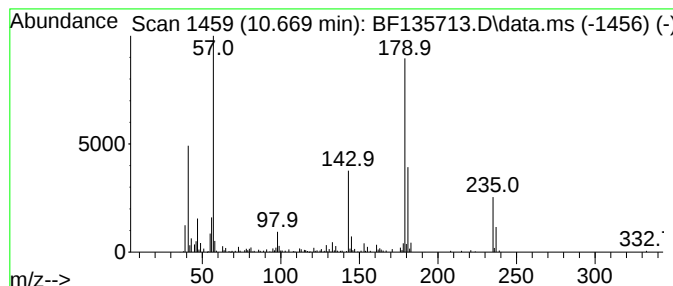
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown10.669 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.669	3.38 ng	131172	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-1,1,1,4,4,5,5,5-octaflu...	248	C5HClF8	1000461-23-0	25		
2	4-Propylphenol, TMS	208	C12H20OSi	959006-64-5	10		
3	Boron, diethyl(4-methyl-3,5-hept...	208	C12H25BN2	136705-02-7	9		
4	Phenanthridine	179	C13H9N	000229-87-8	9		
5	2-Chloro-6-quinolinol	179	C9H6ClNO	577967-89-6	9		



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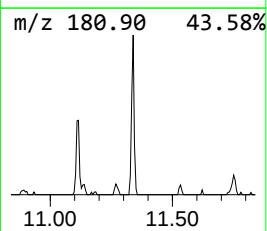
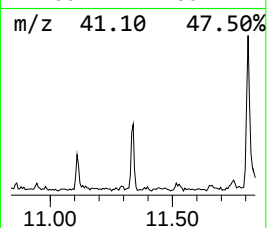
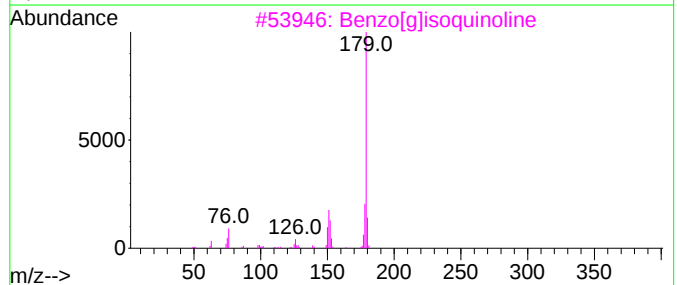
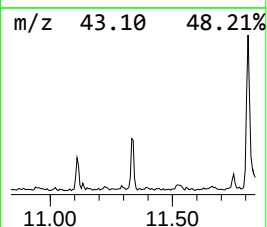
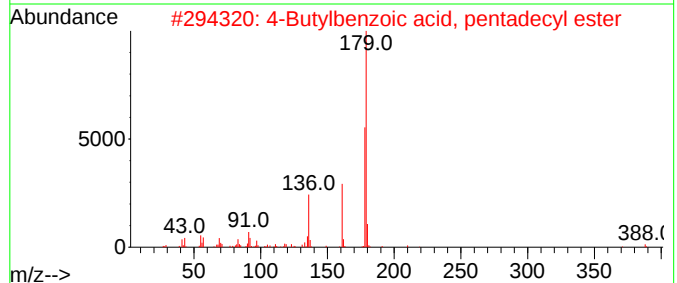
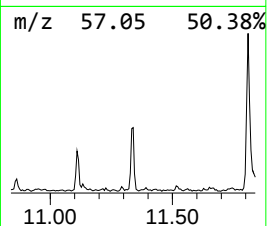
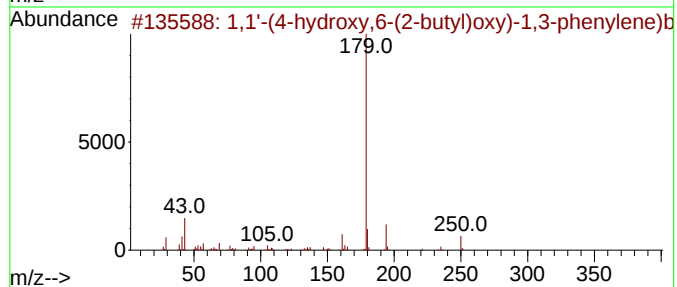
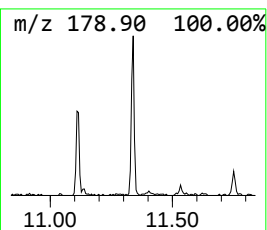
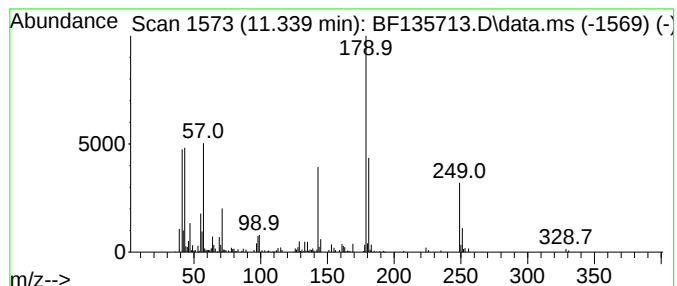
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.339 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.339	3.70 ng	143230	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-(4-hydroxy,6-(2-butyl)oxy)-...	250	C14H18O4	1000454-72-2	12		
2	4-Butylbenzoic acid, pentadecyl ...	388	C26H44O2	1000292-32-8	10		
3	Benzo[g]isoquinoline	179	C13H9N	000260-32-2	10		
4	4-Butylbenzoic acid, hexadecyl e...	402	C27H46O2	1010292-32-9	10		
5	5-Isobenzofurancarboxylic acid, ...	304	C18H24O4	054699-44-4	10		



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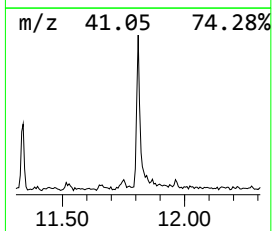
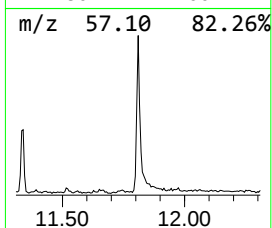
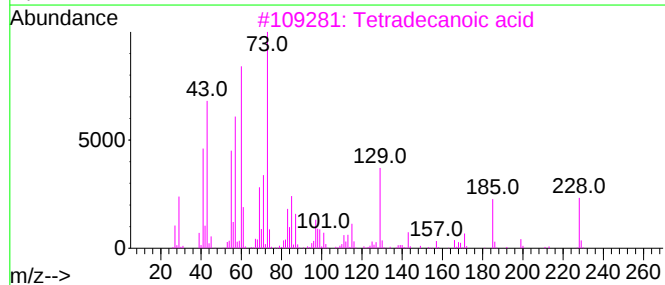
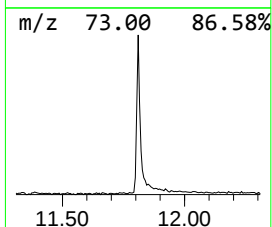
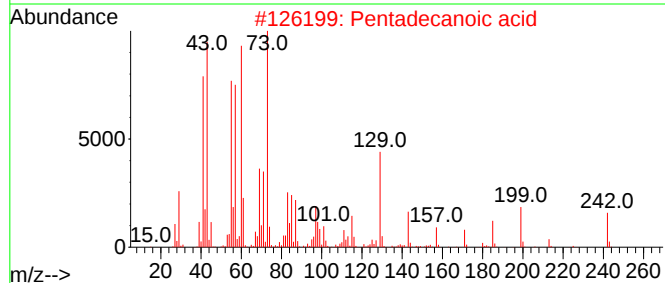
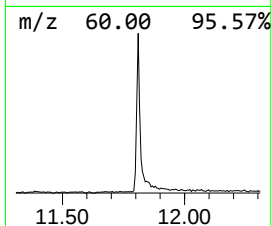
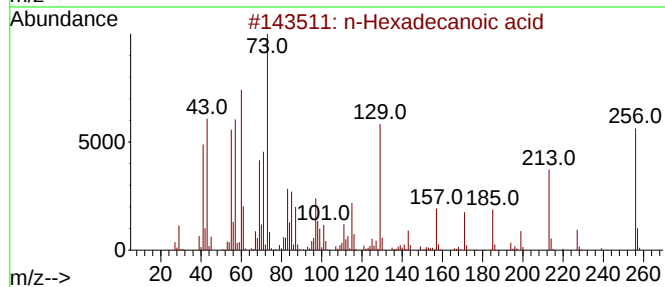
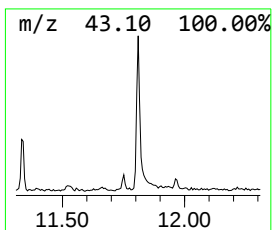
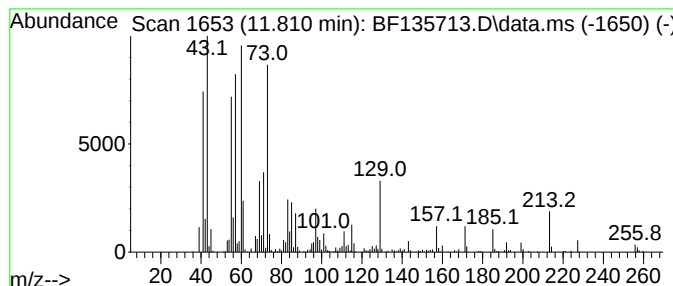
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.810	10.94 ng	424086	Phenanthrene-d10		11.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
4	Tridecanoic acid		214	C13H26O2	000638-53-9	64
5	n-Decanoic acid		172	C10H20O2	000334-48-5	53



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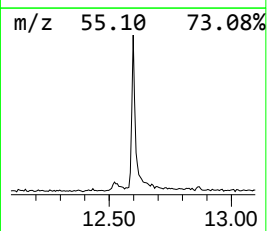
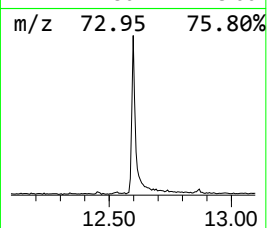
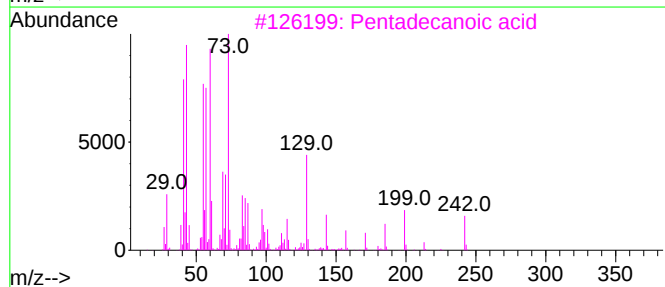
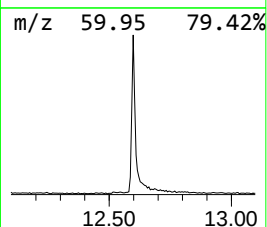
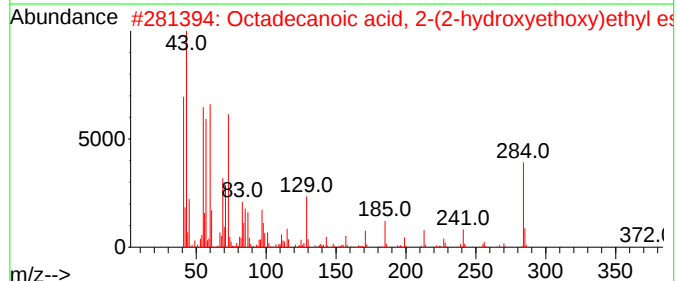
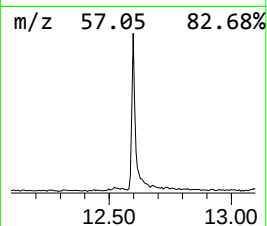
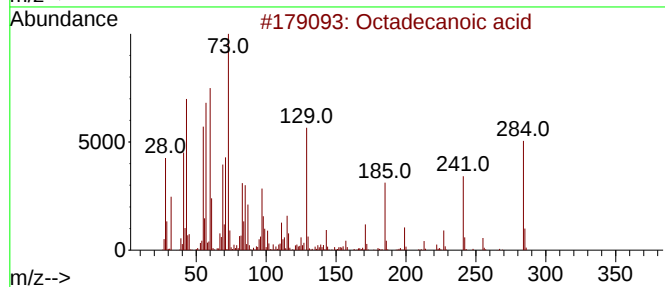
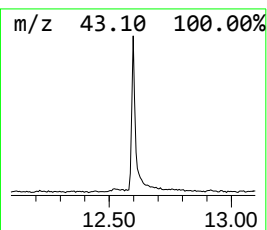
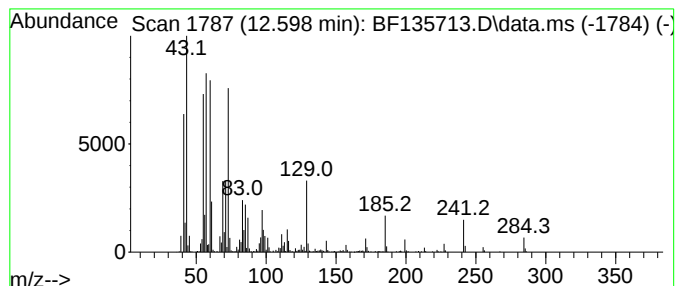
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.598	18.32 ng	709990	Phenanthrene-d10		11.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
5	Tridecanoic acid		214	C13H26O2	000638-53-9	72



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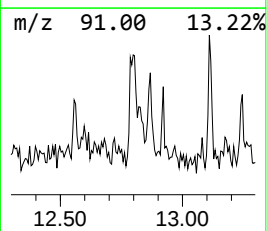
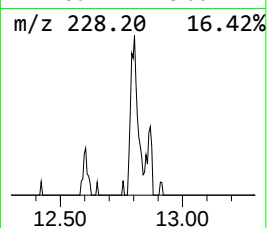
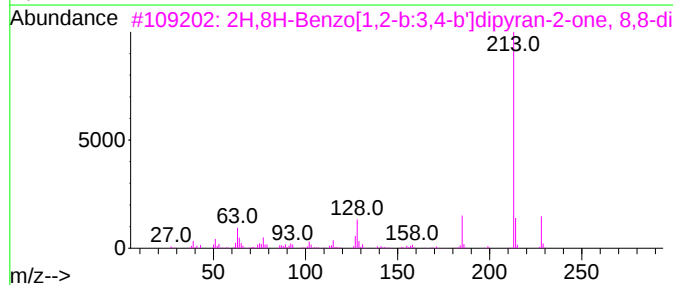
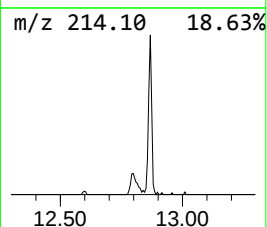
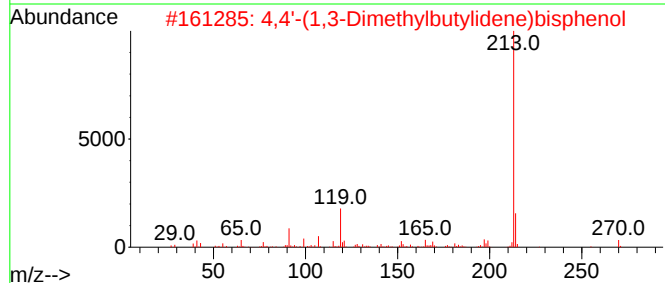
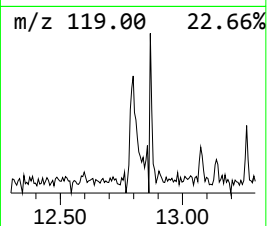
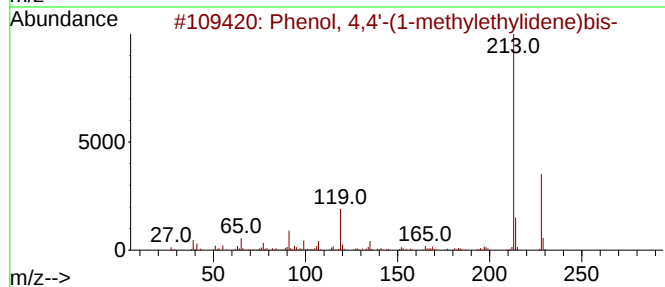
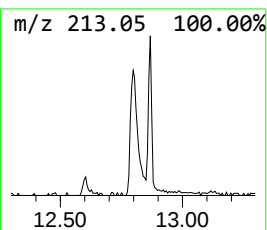
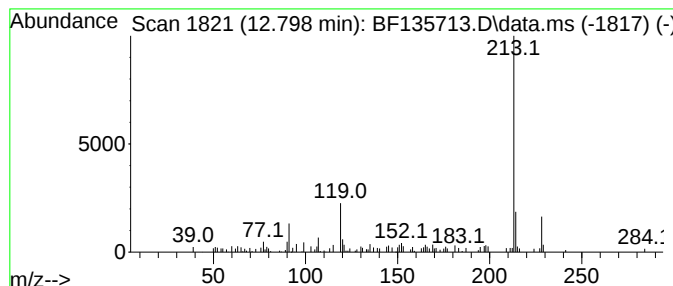
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TIC Library : C:\Database\NIST20.L
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Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.798	2.23 ng	58446	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	94
2			4,4'-(1,3-Dimethylbutylidene)bis-	270	C18H22O2	006807-17-6	72
3			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	64
4			3-Chloro-N,N-diethyl-4-nitroaniline	228	C10H13ClN2O2	1010110-36-0	59
5			2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown10.669	10.669	3.4	ng	131172	4	11.269	775208	20.0
unknown11.339	11.339	3.7	ng	143230	4	11.269	775208	20.0
n-Hexadecanoic ...	11.810	10.9	ng	424086	4	11.269	775208	20.0
Octadecanoic acid	12.598	18.3	ng	709990	4	11.269	775208	20.0
Phenol, 4,4'-(1...	12.798	2.2	ng	58446	5	13.933	524753	20.0