

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135293.D
 Acq On : 15 Sep 2023 22:33
 Operator : CG\JU
 Sample : 04396-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHRT-24313

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: BF135293.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.387	558	561	576	rBV	1833894	1823039	42.31%	4.162%
2	6.404	730	734	746	rBV	1732227	1716428	39.84%	3.918%
3	6.757	791	794	798	rBV	680421	532104	12.35%	1.215%
4	7.322	886	890	893	rBV	1222571	1051202	24.40%	2.400%
5	7.798	967	971	973	rBV	61813	74637	1.73%	0.170%
6	7.957	987	998	999	rBV7	44417	126867	2.94%	0.290%
7	8.034	1006	1011	1015	rBV	703433	673914	15.64%	1.538%
8	8.086	1016	1020	1023	rVV2	78706	76377	1.77%	0.174%
9	8.139	1026	1029	1033	rVB3	65862	76513	1.78%	0.175%
10	8.263	1047	1050	1053	rVB2	157411	147450	3.42%	0.337%
11	8.328	1059	1061	1064	rVB	108917	82222	1.91%	0.188%
12	8.381	1068	1070	1074	rBV3	66551	81504	1.89%	0.186%
13	8.422	1074	1077	1078	rBV2	108281	111684	2.59%	0.255%
14	8.498	1088	1090	1093	rVB	254896	214821	4.99%	0.490%
15	8.581	1102	1104	1108	rVB3	105615	146233	3.39%	0.334%
16	8.722	1126	1128	1135	rVB6	147574	168819	3.92%	0.385%
17	8.781	1135	1138	1140	rBV	356803	292667	6.79%	0.668%
18	8.816	1140	1144	1146	rBV4	192960	248018	5.76%	0.566%
19	8.839	1146	1148	1151	rVV3	127183	124883	2.90%	0.285%
20	8.992	1171	1174	1176	rBV2	313061	354350	8.22%	0.809%
21	9.028	1178	1180	1183	rVV2	704061	674722	15.66%	1.540%
22	9.063	1183	1186	1190	rVB4	344632	472496	10.97%	1.079%
23	9.116	1190	1195	1199	rBV	1821312	2110942	49.00%	4.819%
24	9.192	1205	1208	1212	rBV	1567939	1670108	38.76%	3.813%
25	9.239	1214	1216	1218	rBV2	369357	398129	9.24%	0.909%
26	9.404	1241	1244	1245	rBV3	422879	422611	9.81%	0.965%
27	9.457	1251	1253	1257	rVB2	609450	626697	14.55%	1.431%
28	9.510	1258	1262	1265	rBV	3348518	3415309	79.27%	7.797%
29	9.563	1268	1271	1275	rVB3	1265269	1489198	34.56%	3.400%
30	9.669	1285	1289	1292	rBV3	2227246	2651206	61.54%	6.052%
31	9.722	1294	1298	1300	rVB	3709660	4308446	100.00%	9.835%
32	9.757	1300	1304	1306	rBV2	1274750	1730059	40.16%	3.949%
33	9.786	1306	1309	1315	rVB4	1794435	3003769	69.72%	6.857%
34	9.851	1317	1320	1324	rVV2	945633	1266649	29.40%	2.892%
35	10.080	1356	1359	1363	rBV5	844696	1244411	28.88%	2.841%
36	10.145	1366	1370	1373	rVV3	1398148	2149821	49.90%	4.908%

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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_F\Methods\8270-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.180	1374	1376	1379	rVV4	1019955	1149038	26.67%	2.623%
38	10.228	1380	1384	1387	rVV2	2281685	2784361	64.63%	6.356%
39	15.004	2193	2196	2204	rVB	503712	904993	21.01%	2.066%
40	15.304	2244	2247	2253	rVB	291893	314418	7.30%	0.718%
41	15.362	2254	2257	2263	rVB	365424	474781	11.02%	1.084%
42	15.427	2265	2268	2271	rBV	296651	338152	7.85%	0.772%
43	15.892	2344	2347	2351	rVB	121560	143955	3.34%	0.329%
44	16.904	2514	2519	2529	rVB3	138289	294455	6.83%	0.672%
45	17.345	2590	2594	2600	rVB	104745	183697	4.26%	0.419%
46	18.039	2706	2712	2723	rVB2	412855	1084906	25.18%	2.477%
47	18.521	2788	2794	2801	rVB3	160228	374499	8.69%	0.855%

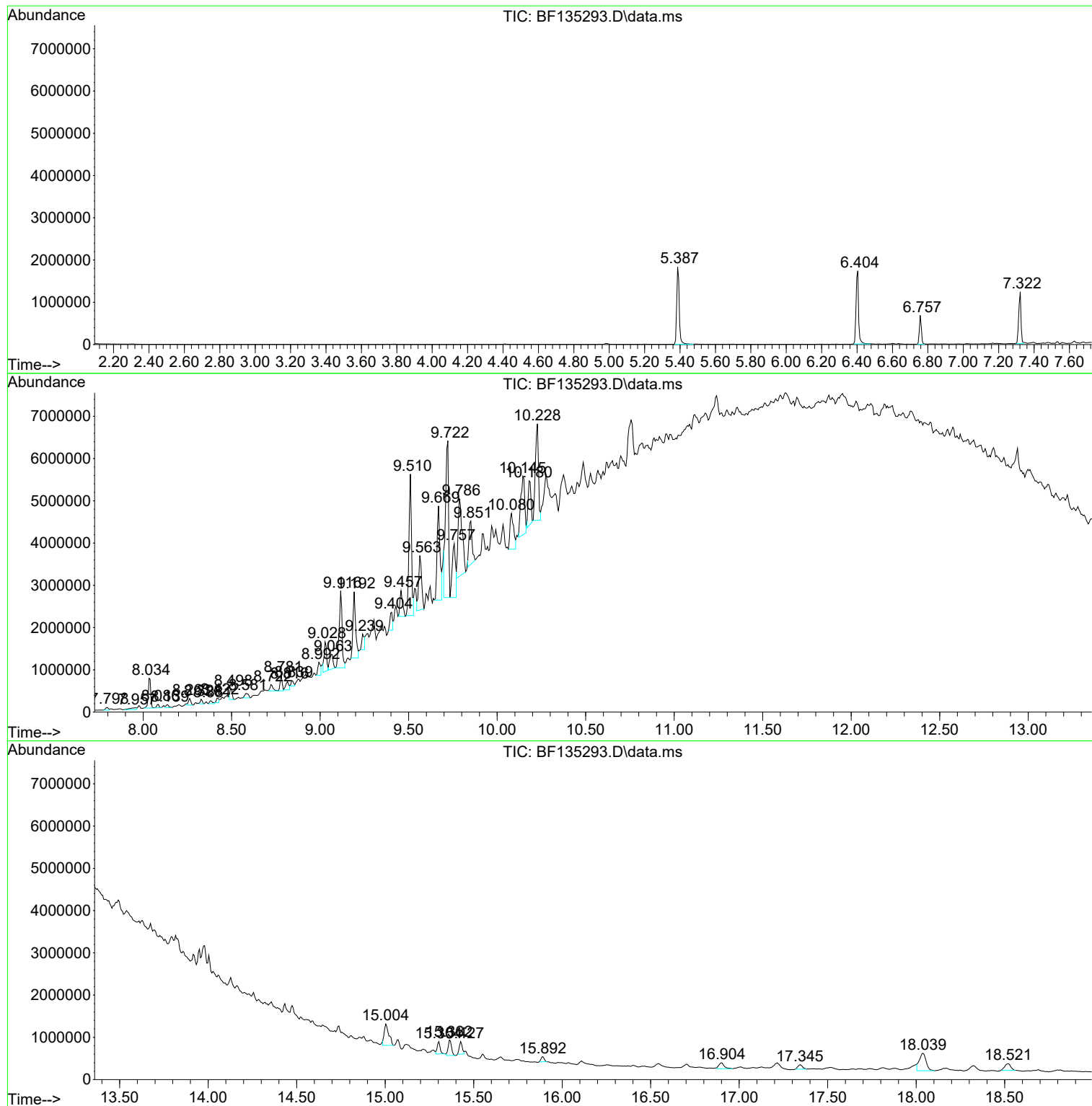
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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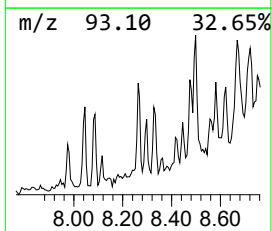
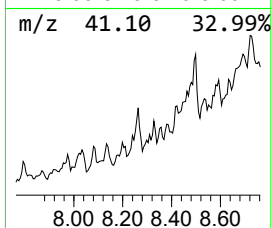
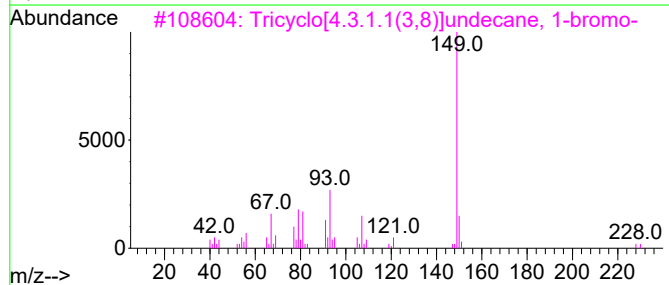
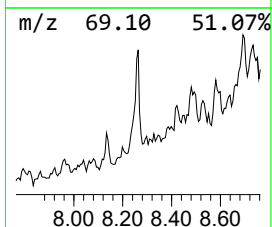
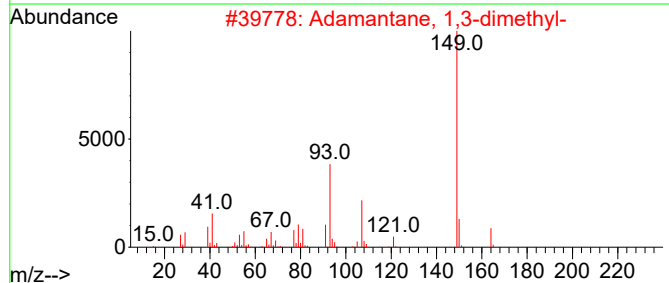
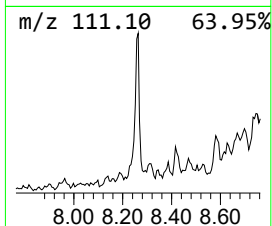
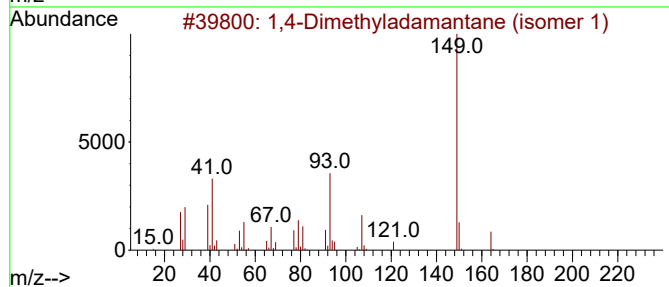
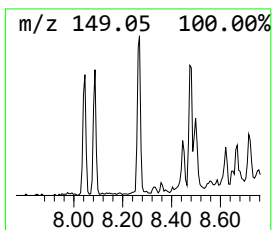
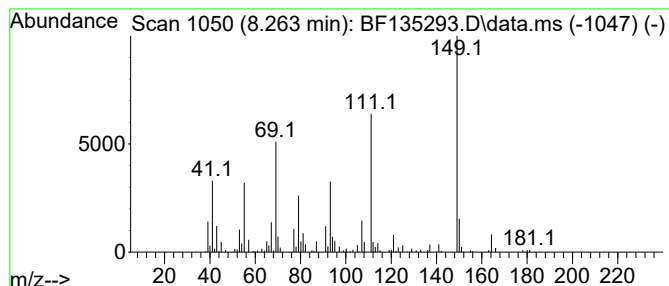
Instrument :
BNA_F
ClientSampleId :
CHRT-24313

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 1 1,4-Dimethyladamantane (iso... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.263	4.38 ng	147450	Naphthalene-d8	8.034	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	64
2	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	53
3	Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	50
4	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	47
5	Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	38



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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24313

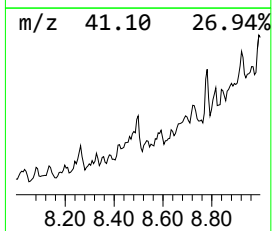
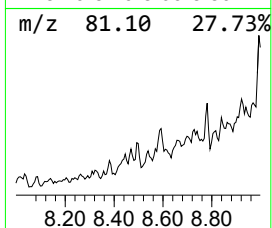
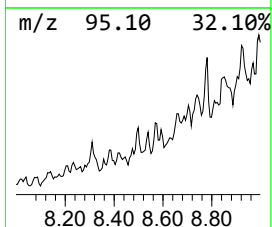
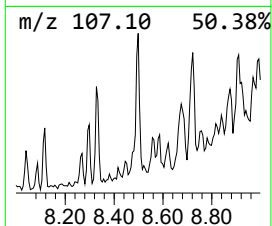
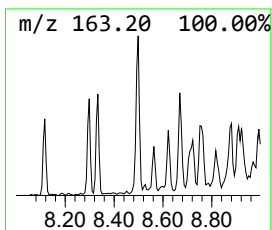
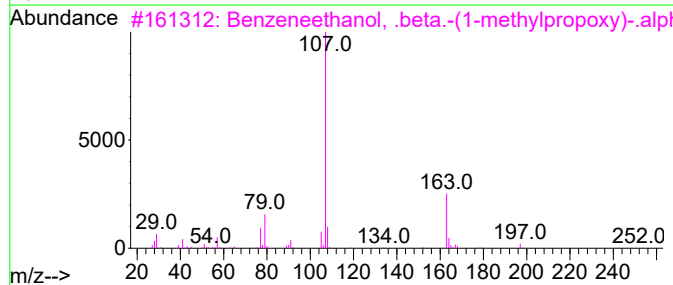
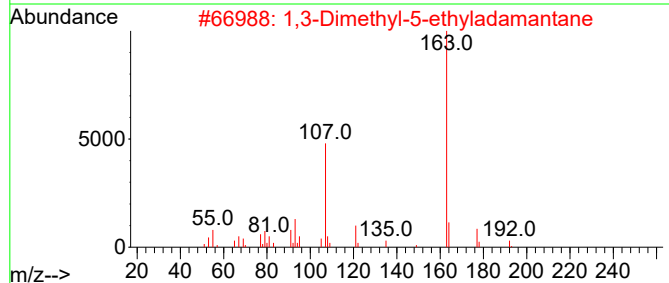
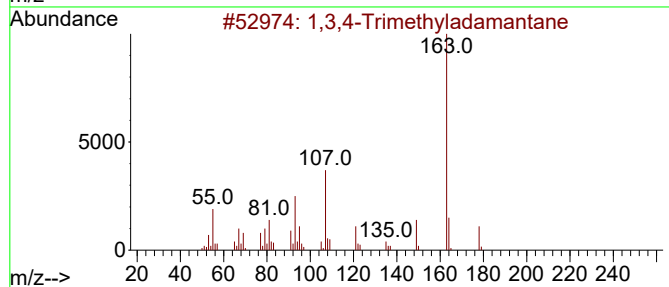
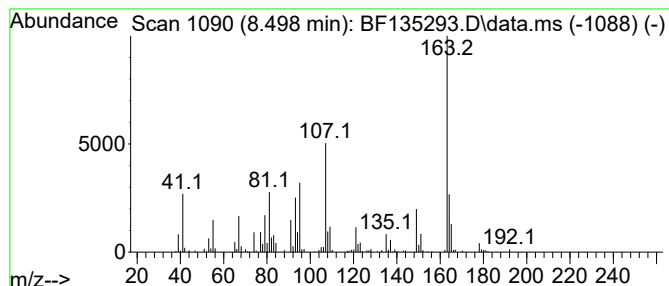
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3,4-Trimethyladamantane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.498	6.38 ng	214821	Naphthalene-d8	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	64		
2	1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	53		
3	Benzeneethanol, .beta.-(1-methyl...	270	C18H22O2	053288-15-6	50		
4	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	38		
5	4H-1,2,4-Triazole, 3-(3,5-dimeth...	163	C7H9N5	003310-78-9	38		



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Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

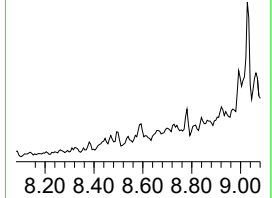
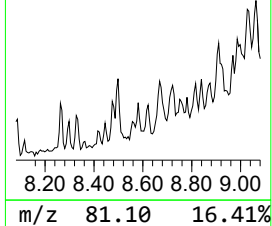
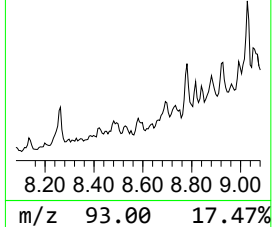
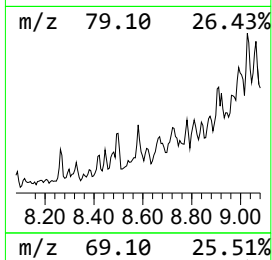
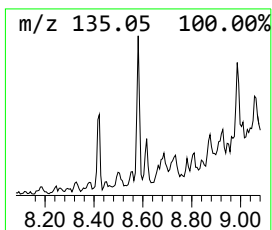
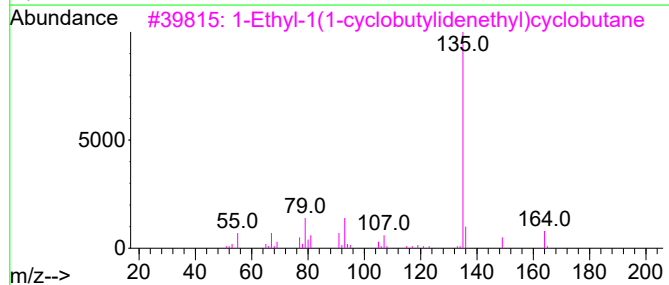
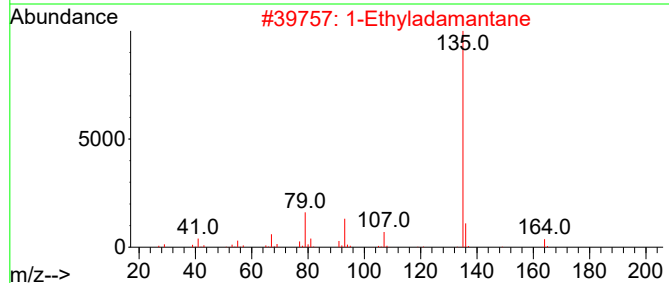
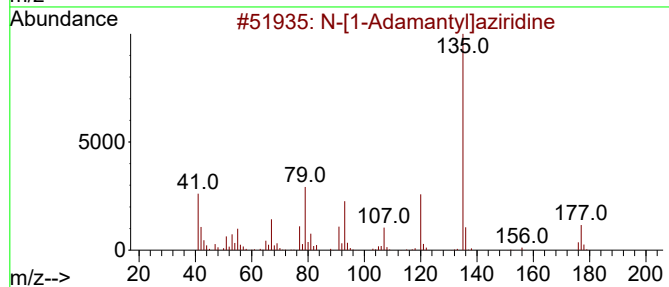
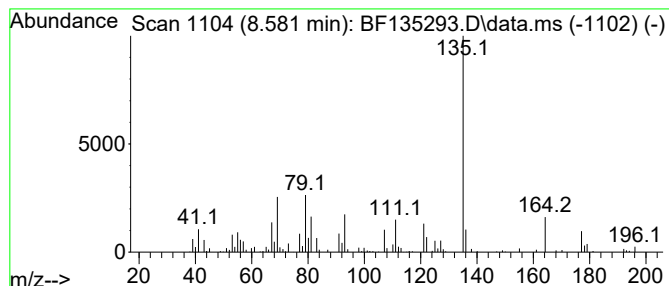
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 N-[1-Adamantyl]aziridine Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.581	4.34 ng	146233	Naphthalene-d8	8.034	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[1-Adamantyl]aziridine	177	C12H19N	1000256-62-9	76
2	1-Ethyladamantane	164	C12H20	000770-69-4	76
3	1-Ethyl-1(1-cyclobutylidenethyl)...	164	C12H20	1000215-13-7	64
4	Adamantane-1-carboxylic acid, 4-...	284	C18H20O3	1000276-61-1	59
5	Benzenesulfonamide, N-adamantan-...	384	C17H21ClN2O4S	1000303-35-0	59



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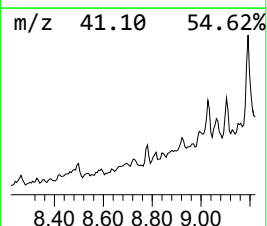
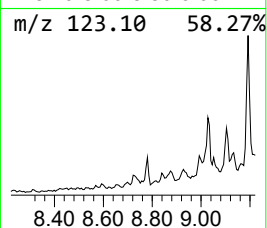
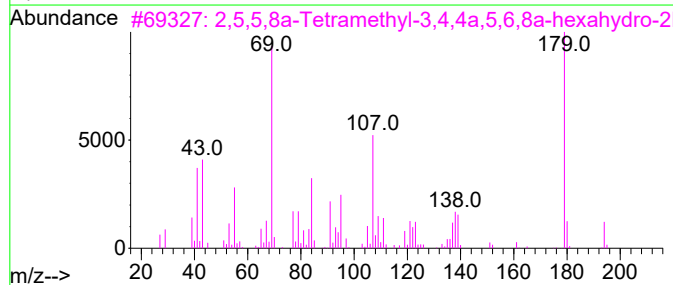
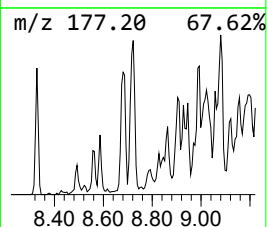
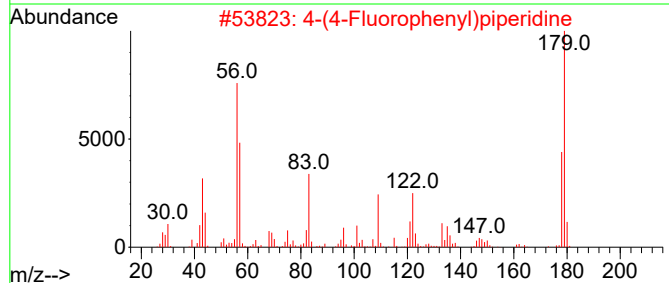
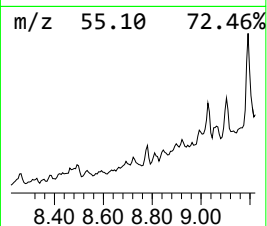
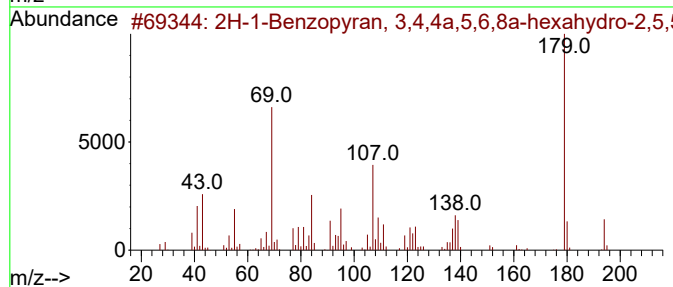
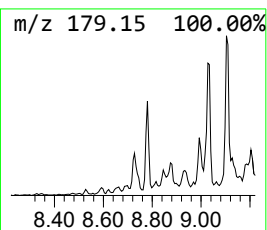
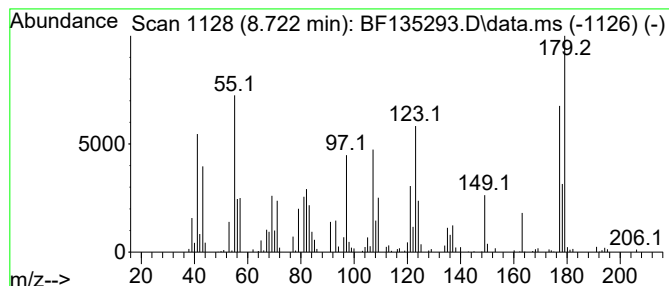
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown8.722 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.722	5.01 ng	168819	Naphthalene-d8	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-1-Benzopyran, 3,4,4a,5,6,8a-h...	194	C13H22O	041678-32-4	27
2			4-(4-Fluorophenyl)piperidine	179	C11H14FN	037656-48-7	22
3			2,5,5,8a-Tetramethyl-3,4,4a,5,6,...	194	C13H22O	072746-44-2	12
4			N,N'-Ethane-1,2-diylbis(3-bromop...	328	C8H14Br2N2O2	016044-35-2	12
5			1-Piperidineacetonitrile	124	C7H12N2	003010-03-5	11



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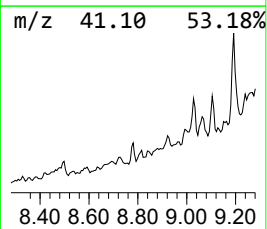
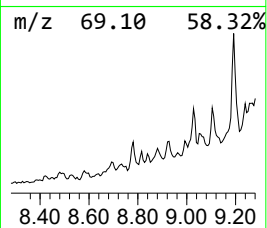
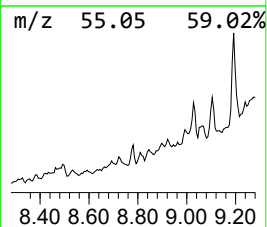
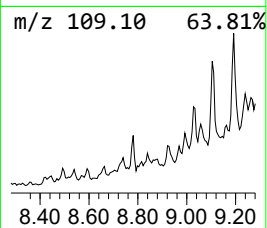
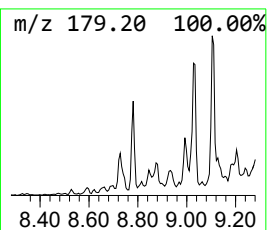
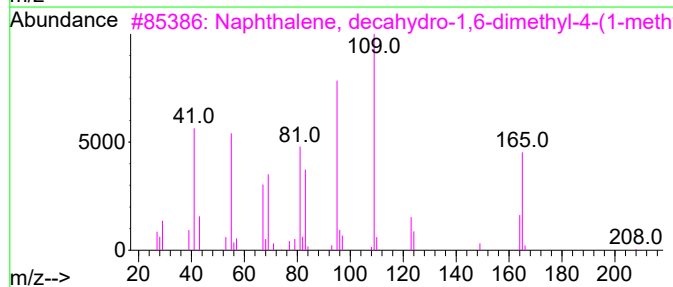
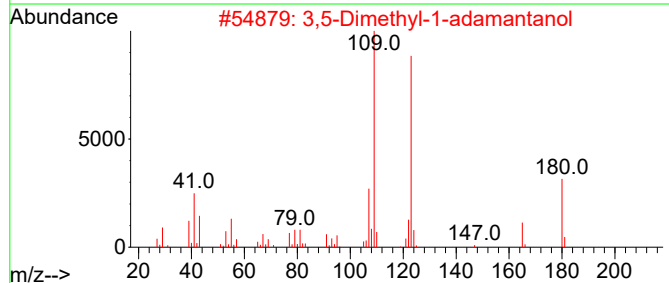
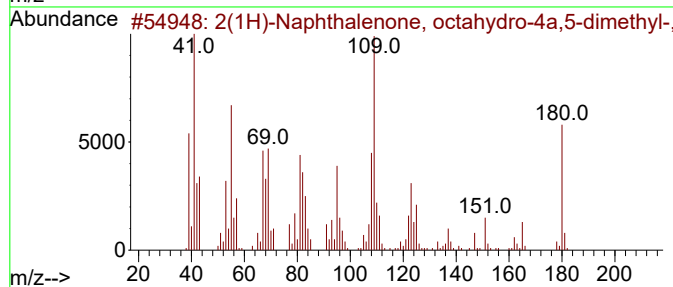
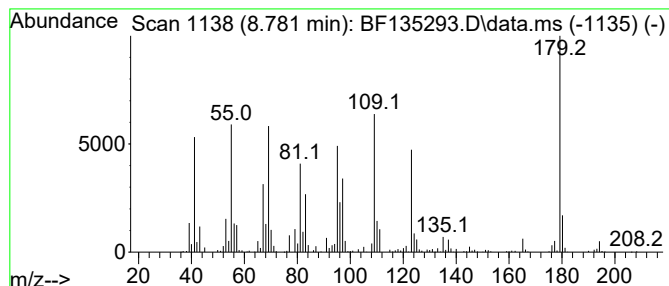
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.781 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.781	8.69 ng	292667	Naphthalene-d8	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-4...	180	C12H20O	051557-64-3	30		
2	3,5-Dimethyl-1-adamantanol	180	C12H20O	000707-37-9	25		
3	Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	22		
4	2H-Benzocyclohepten-2-one, decah...	180	C12H20O	055103-64-5	18		
5	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24313

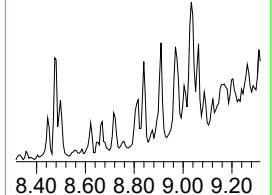
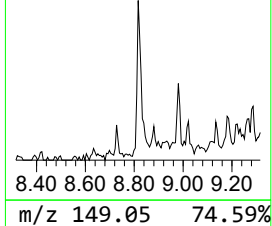
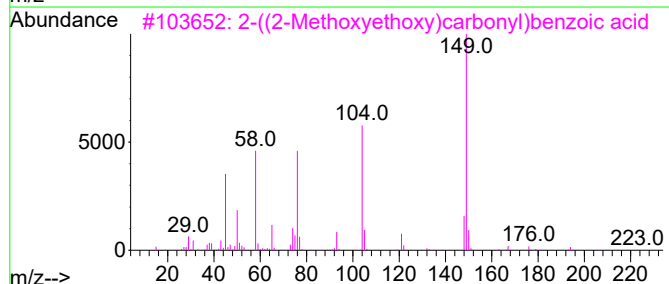
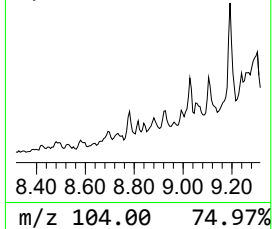
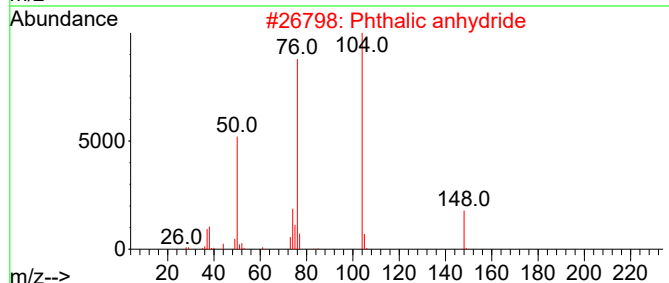
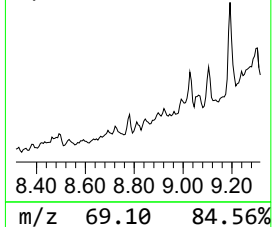
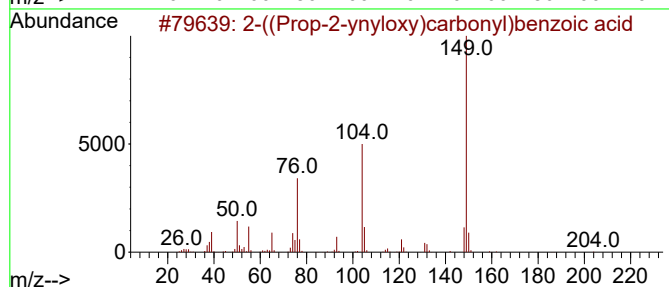
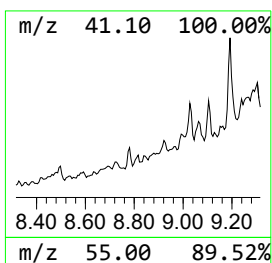
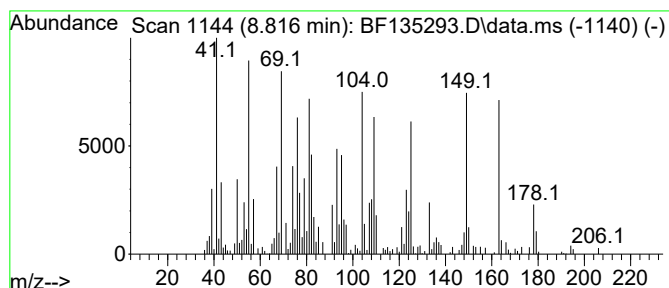
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.816 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.816	7.36 ng	248018	Naphthalene-d8	8.034

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-((Prop-2-ynyloxy)carbonyl)benz...	204	C11H8O4	006139-61-3	27	
2	Phthalic anhydride	148	C8H4O3	000085-44-9	25	
3	2-((2-Methoxyethoxy)carbonyl)ben...	224	C11H12O5	016501-01-2	22	
4	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	22	
5	1H-Isindole-1,3(2H)-dione, 2-hy...	163	C8H5NO3	000524-38-9	14	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
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Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

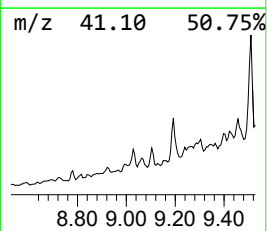
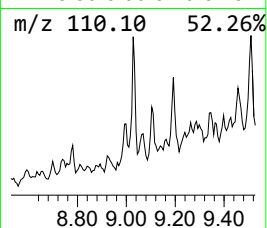
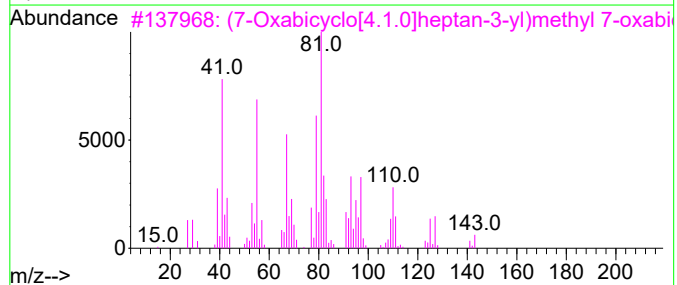
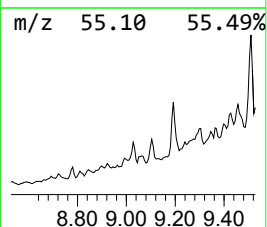
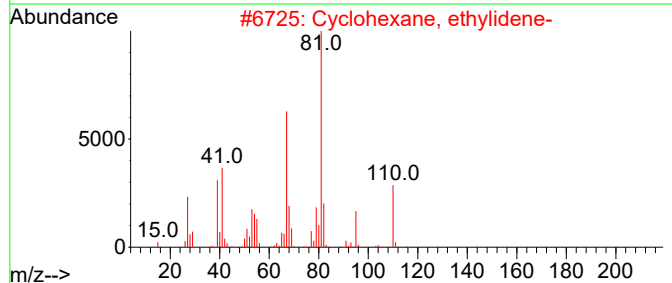
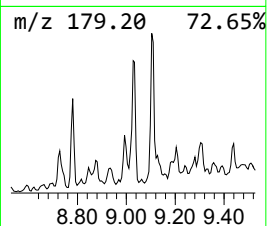
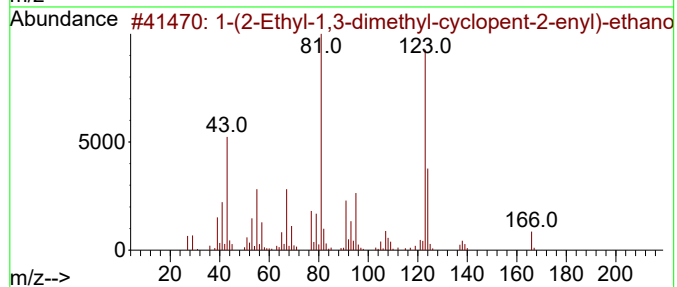
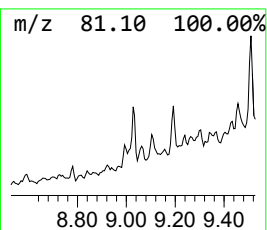
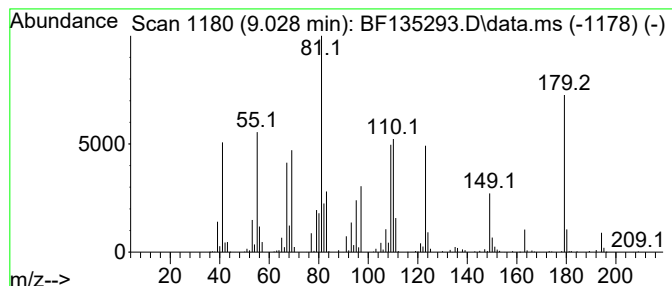
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-(2-Ethyl-1,3-dimethyl-cyc... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.028	4.49 ng	674722	Acenaphthene-d10	9.810	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Ethyl-1,3-dimethyl-cyclopent-2-en-1-yl)ethanol	166	C11H18O	1010185-18-1	50
2	Cyclohexane, ethylidene-	110	C8H14	001003-64-1	43
3	(7-Oxabicyclo[4.1.0]heptan-3-yl)methyl 7-oxabicyclo[4.1.0]heptan-3-ylmethoxy	252	C14H20O4	1000473-40-7	38
4	trans-(2-Ethylcyclopentyl)methyl 7-oxabicyclo[4.1.0]heptan-3-ylmethoxy	170	C10H18O2	1000099-13-9	35
5	2-Propenyl-3-vinylloxirane	110	C7H10O	070597-49-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
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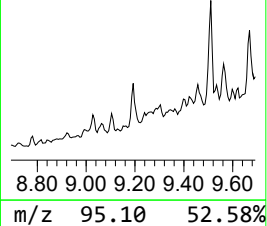
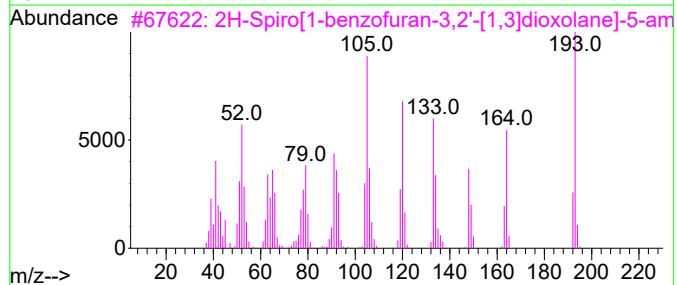
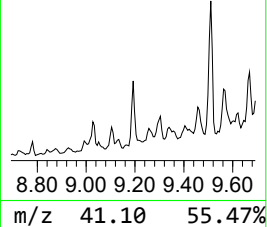
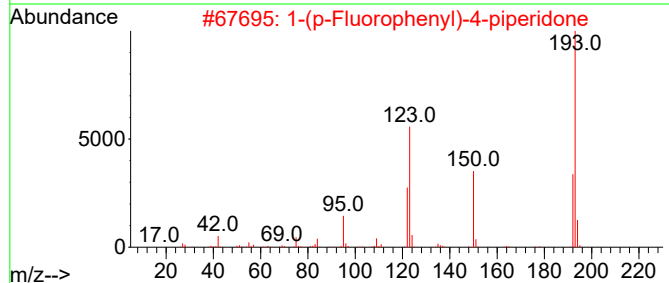
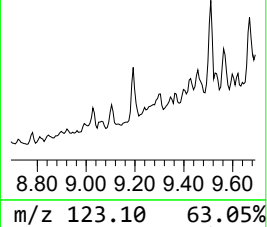
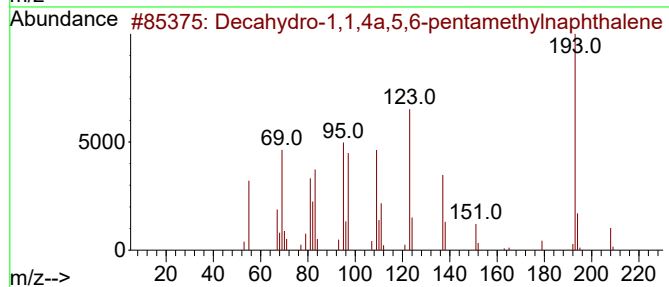
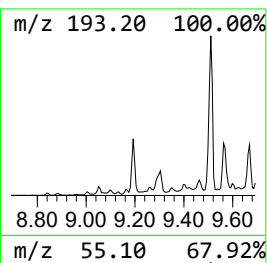
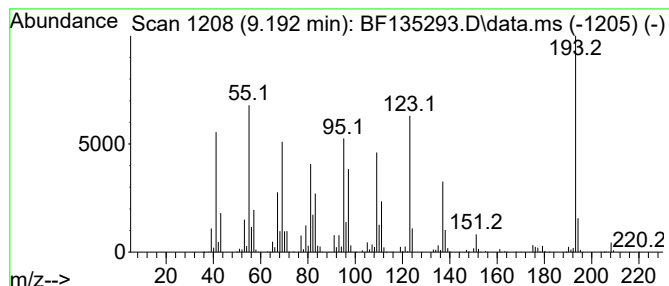
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.192	11.12 ng	1670110	Acenaphthene-d10	9.810	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	52
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
3	2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	35
4	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	27
5	1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
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Sample : 04396-01
Misc :
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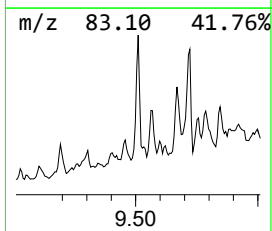
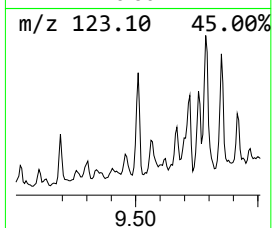
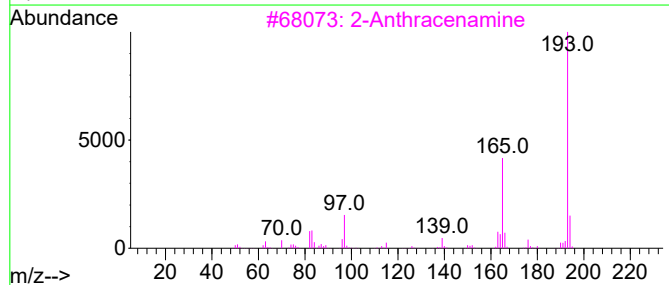
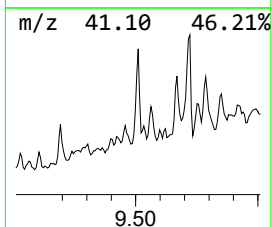
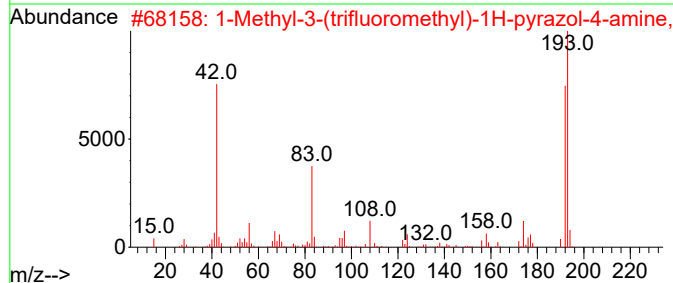
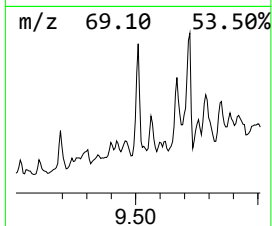
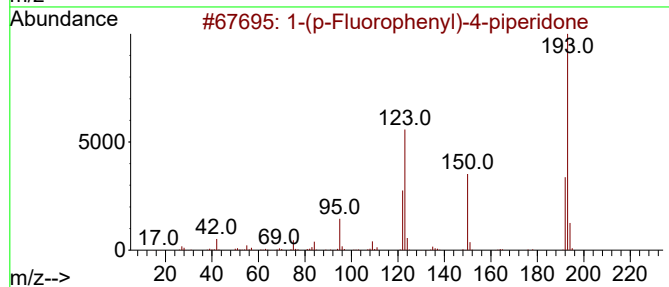
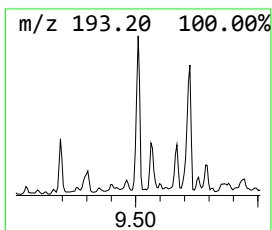
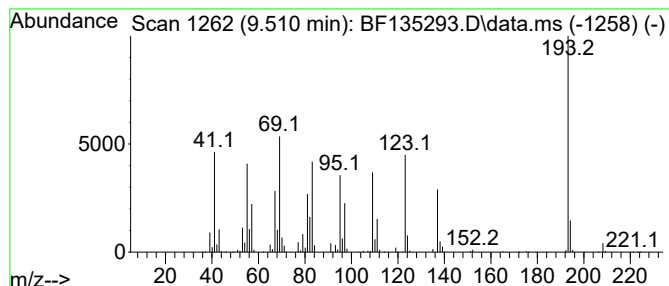
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.510 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.510	22.74 ng	3415310	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43		
2	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	38		
3	2-Anthracenamine	193	C14H11N	000613-13-8	30		
4	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	27		
5	9-Phenanthrenamine	193	C14H11N	000947-73-9	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
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Misc :
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ClientSampleId :
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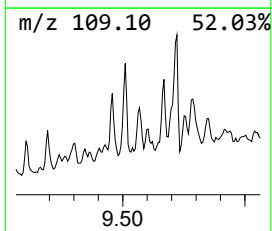
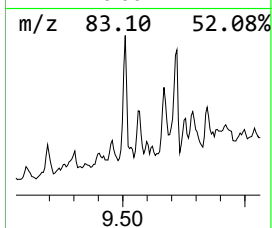
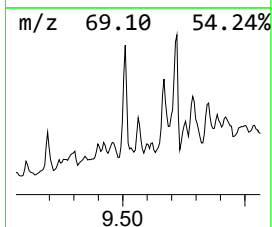
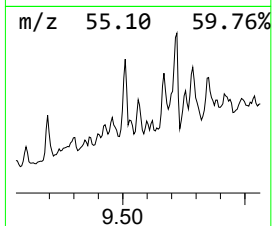
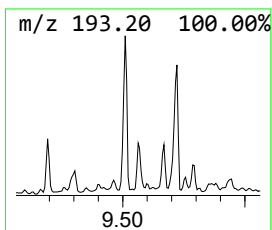
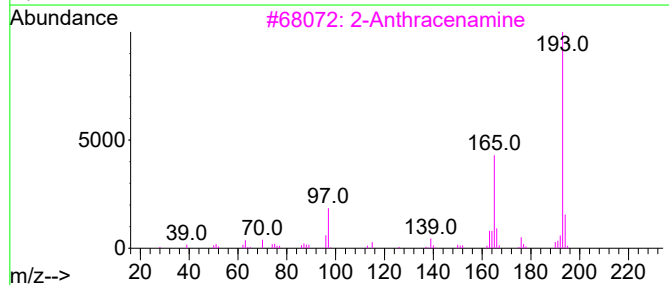
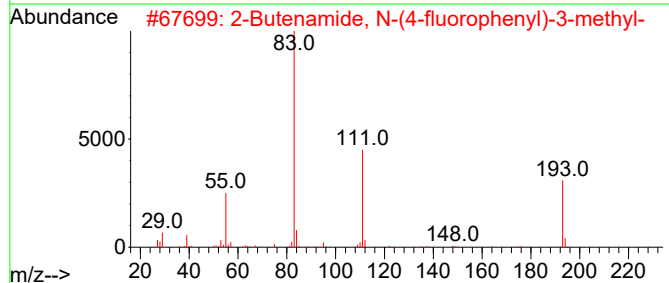
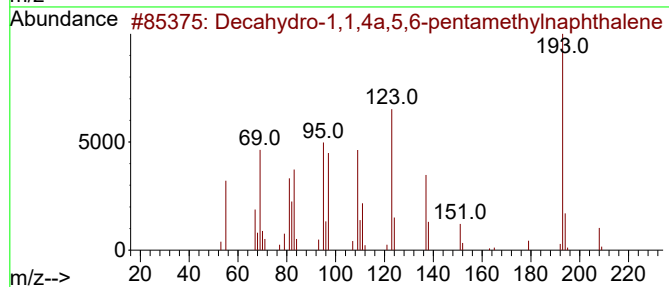
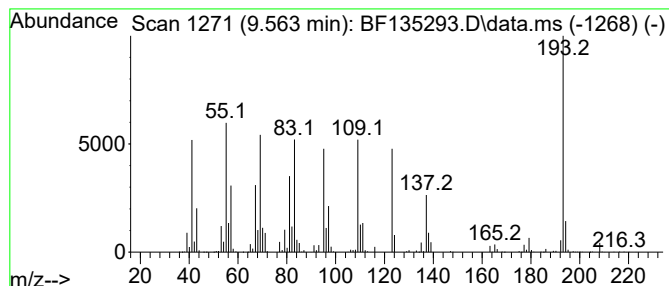
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.563 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.563	9.92 ng	1489200	Acenaphthene-d10	9.810

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
2		2-Butenamide, N-(4-fluorophenyl)...	193	C11H12FNO	1000307-26-7	30
3		2-Anthracenamine	193	C14H11N	000613-13-8	25
4		Heptadienyl angelate, 2E, 4E-	194	C12H18O2	1000383-64-8	25
5		Acridine, 9-methyl-	193	C14H11N	000611-64-3	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
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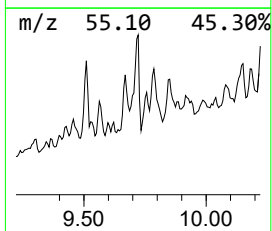
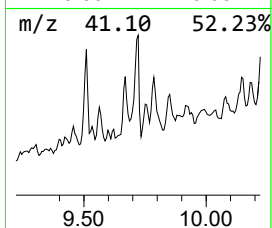
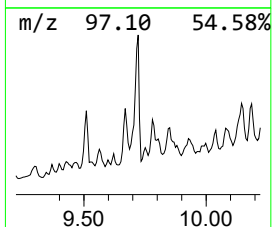
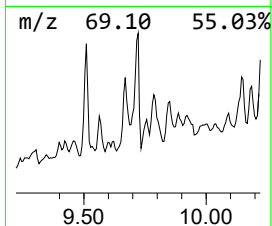
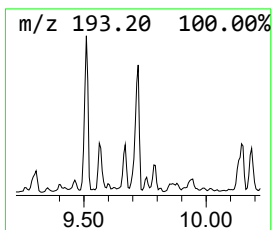
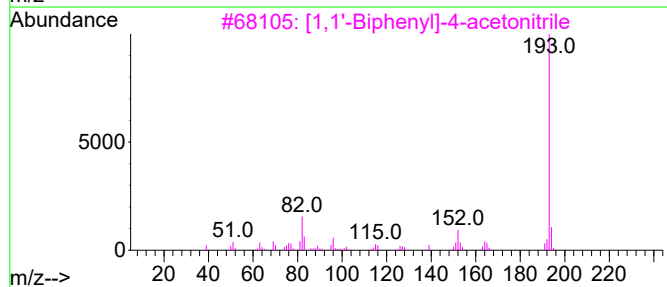
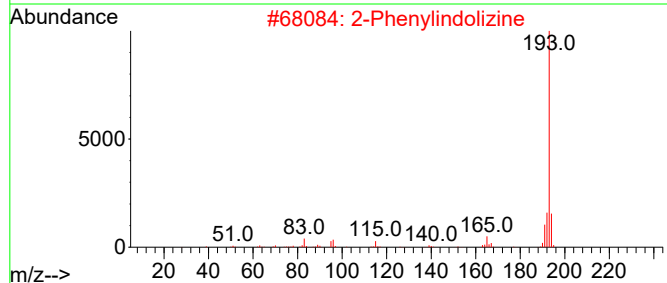
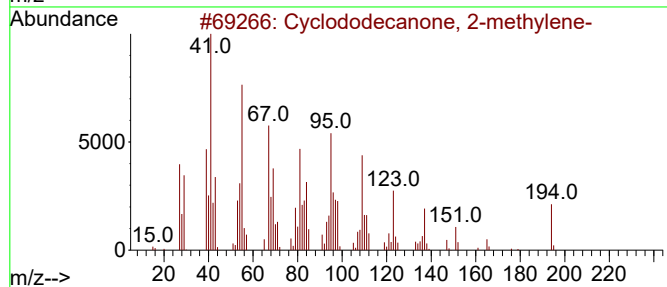
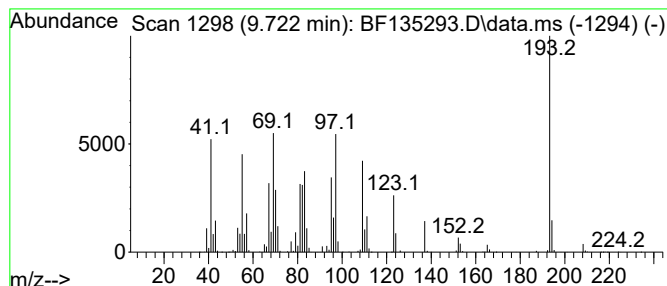
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown9.722 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.722	28.69 ng	4308450	Acenaphthene-d10	9.810

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	38
2		2-Phenylindolizine	193	C14H11N	025379-20-8	27
3		[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	22
4		9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	22
5		6-Methylphenanthridine	193	C14H11N	003955-65-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHRT-24313

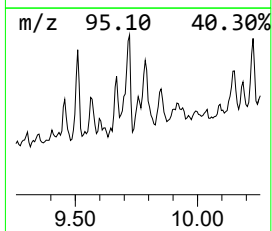
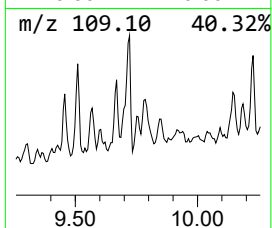
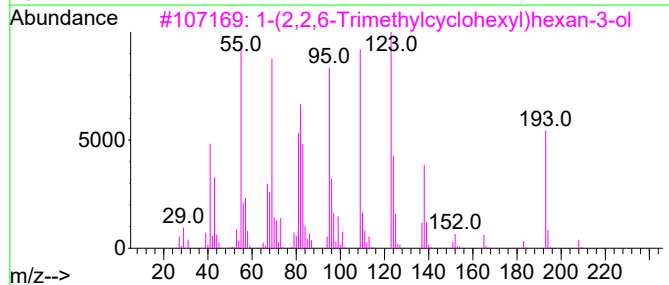
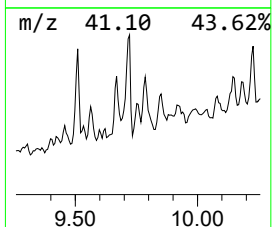
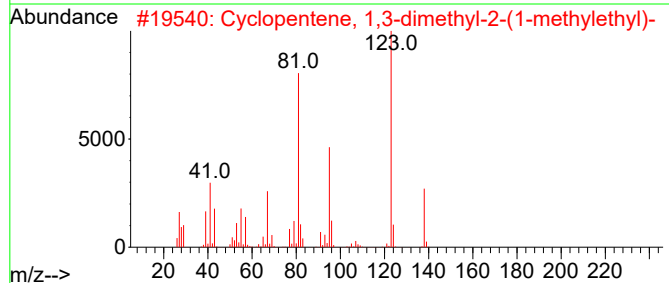
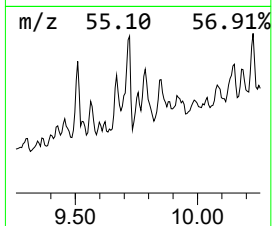
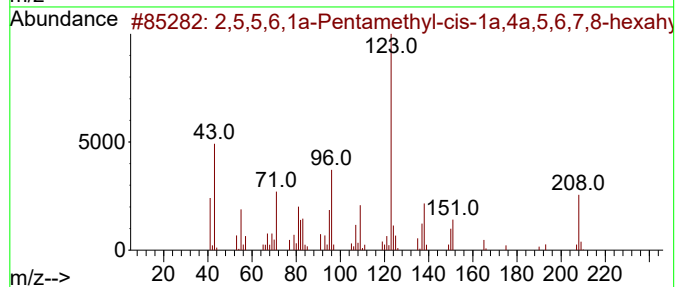
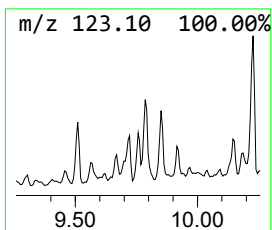
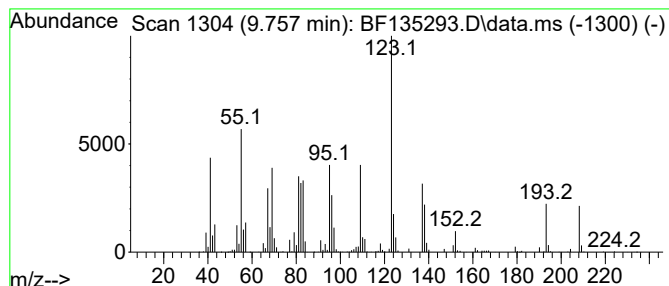
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown9.757 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	11.52 ng	1730060	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1010215-77-9	49		
2	Cyclopentene, 1,3-dimethyl-2-(1-...	138	C10H18	061142-32-3	49		
3	1-(2,2,6-Trimethylcyclohexyl)hex...	226	C15H30O	070788-30-6	46		
4	Imidazolidin-2-one, 1-(2-fluorob...	208	C10H9FN2O2	1010310-62-2	43		
5	Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24313

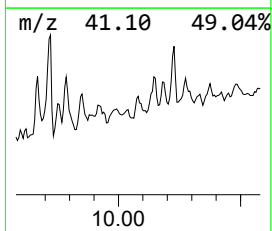
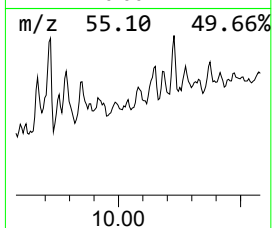
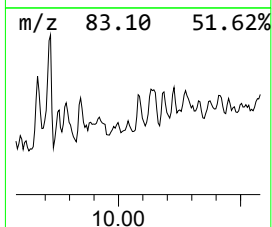
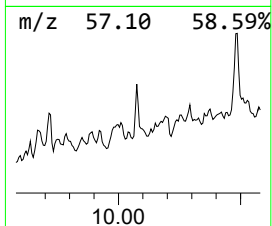
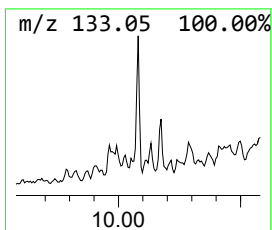
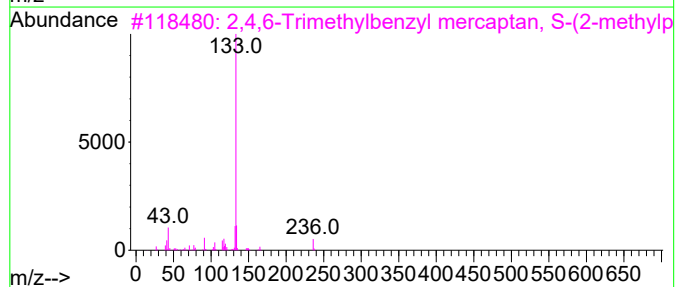
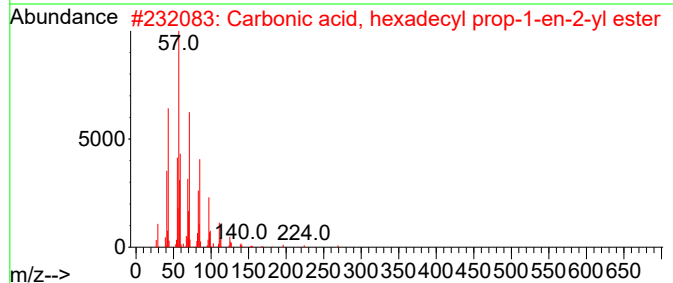
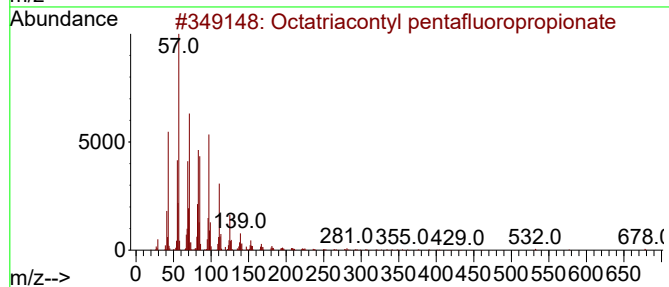
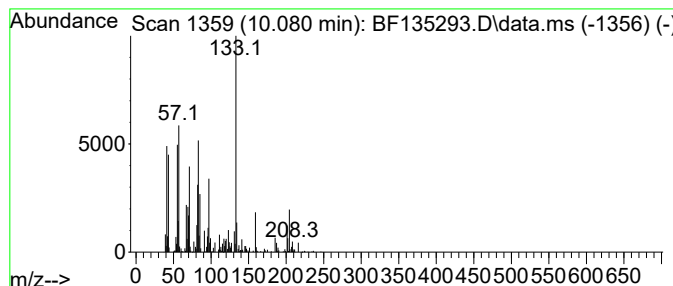
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown10.081 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.081	8.29 ng	1244410	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	27
2			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	18
3			2,4,6-Trimethylbenzyl mercaptan,...	236	C14H20OS	1010469-60-2	18
4			Tetradecane	198	C14H30	000629-59-4	15
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

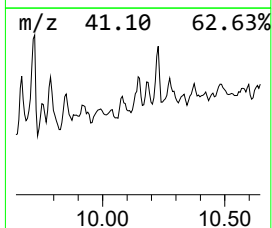
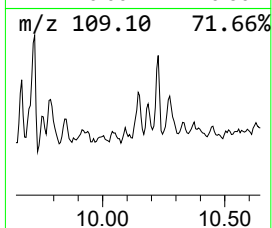
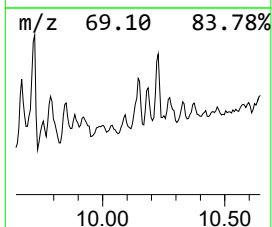
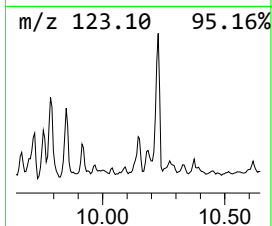
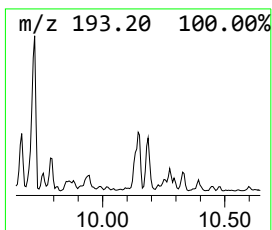
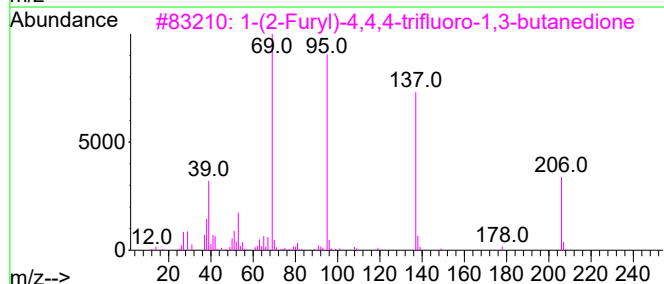
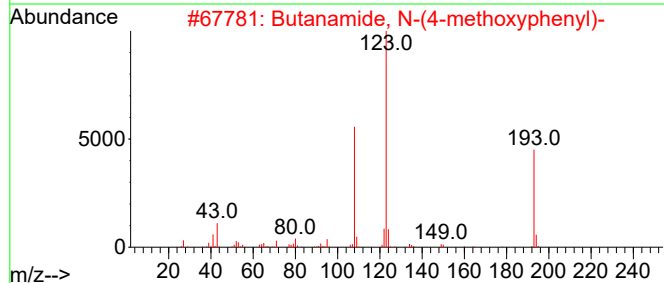
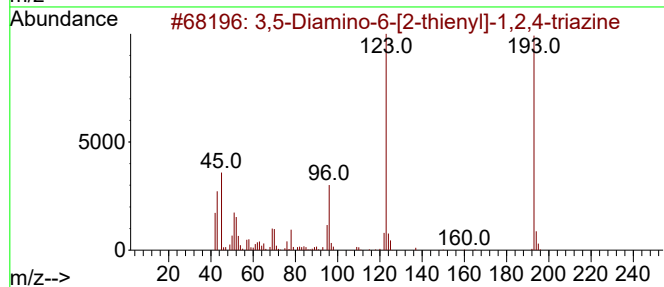
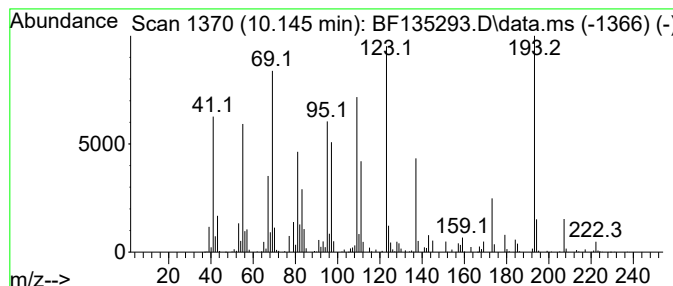
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown10.145 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.145	14.31 ng	2149820	Acenaphthene-d10			9.810
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Diamino-6-[2-thienyl]-1,2,4-...	193	C7H7N5S		058848-66-1	27
2	Butanamide, N-(4-methoxyphenyl)-	193	C11H15NO2		1000306-91-5	25
3	1-(2-Furyl)-4,4,4-trifluoro-1,3-...	206	C8H5F3O3		000326-90-9	22
4	2-Octene, 2-methyl-6-methylene-	138	C10H18		010054-09-8	22
5	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18		062238-28-2	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

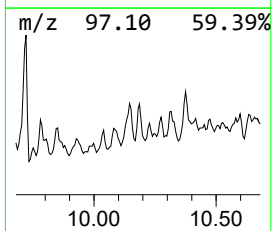
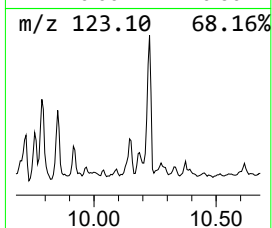
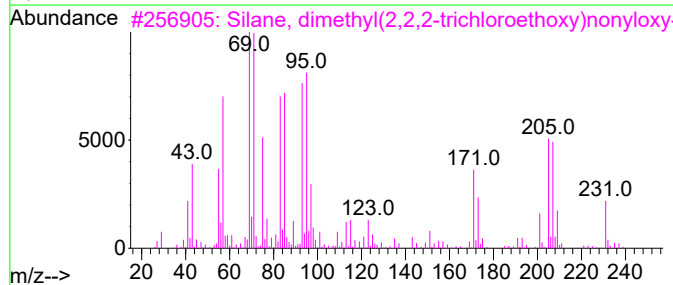
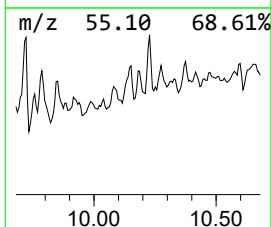
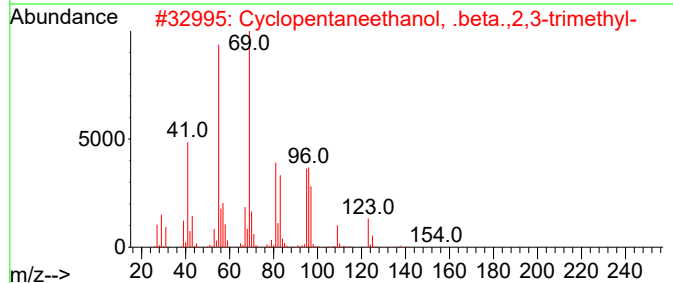
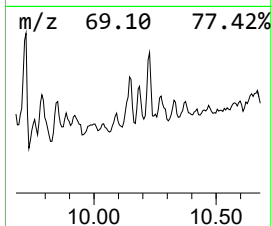
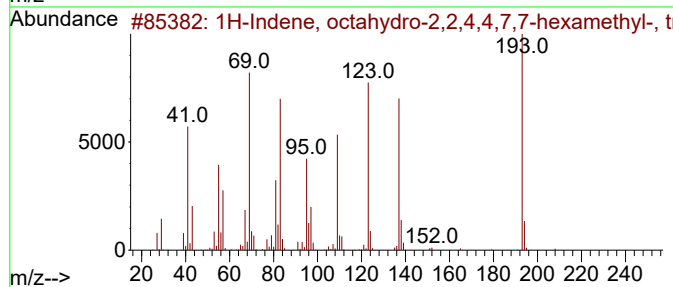
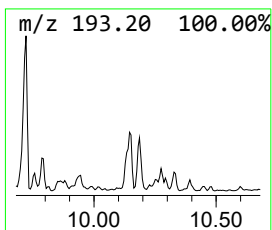
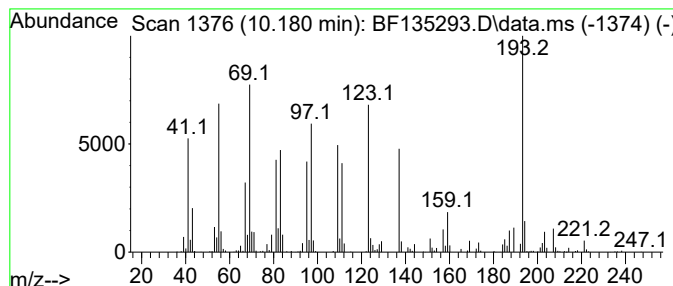
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1H-Indene, octahydro-2,2,4,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.181	7.65 ng	1149040	Acenaphthene-d10	9.810	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	72
2	Cyclopentaneethanol, .beta.,2,3-...	156	C10H20O	021721-18-6	27
3	Silane, dimethyl(2,2,2-trichloro...	348	C13H27Cl3O2Si	1010347-56-7	22
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	18
5	3,5-Diamino-6-[2-thienyl]-1,2,4-...	193	C7H7N5S	058848-66-1	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
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Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHRT-24313

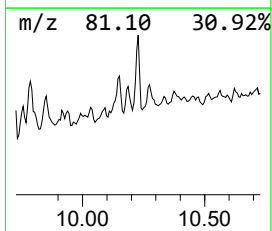
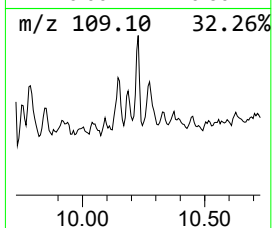
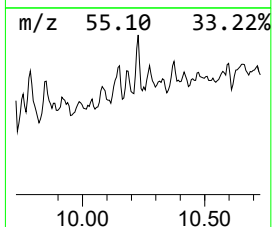
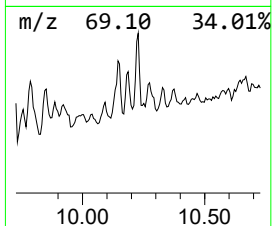
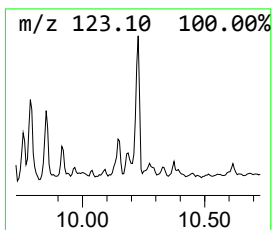
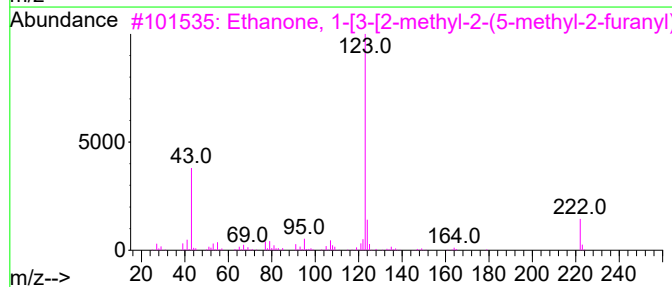
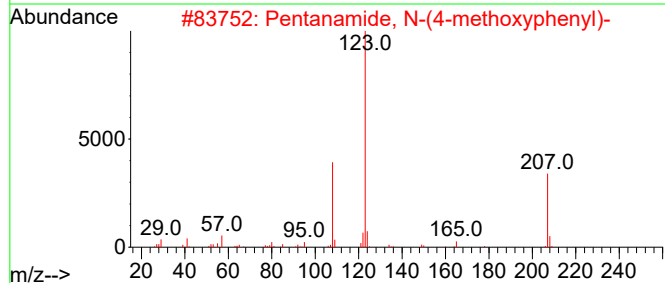
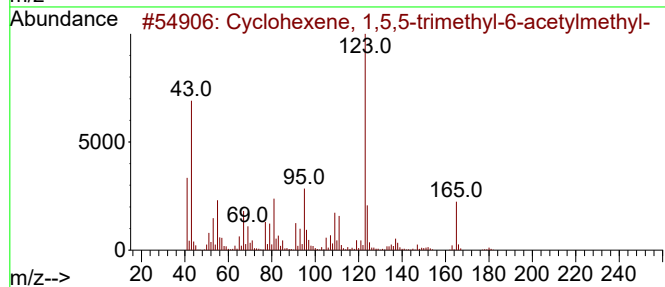
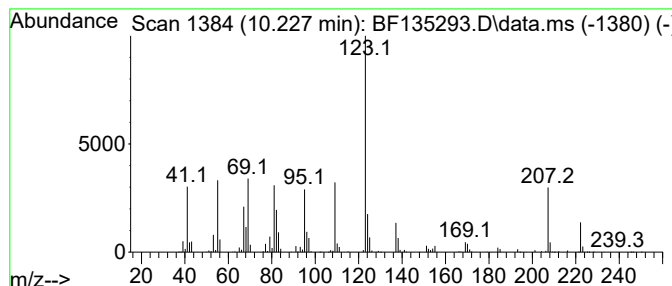
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Cyclohexene, 1,5,5-trimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.227	18.54 ng	2784360	Acenaphthene-d10	9.810

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	53
2		Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	47
3		Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	47
4		1H-Purine-2,6-dione, 1,3-diethyl...	222	C10H14N4O2	054965-57-0	43
5		3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

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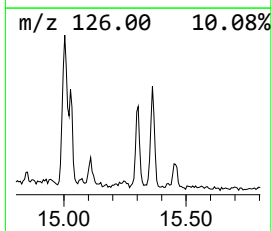
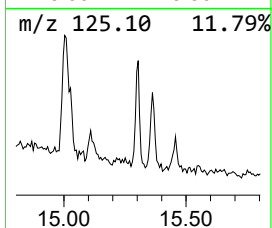
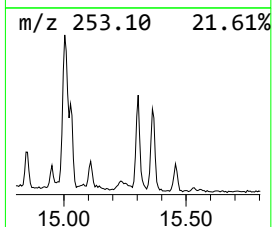
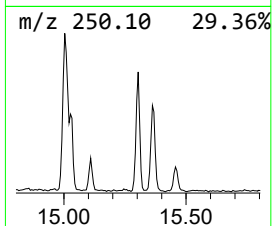
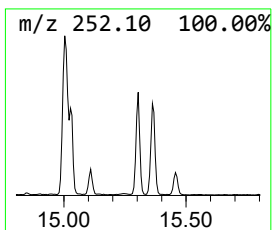
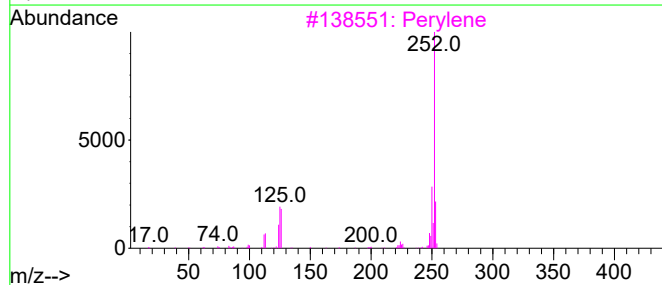
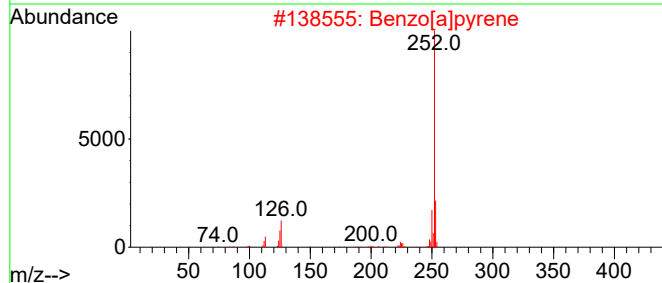
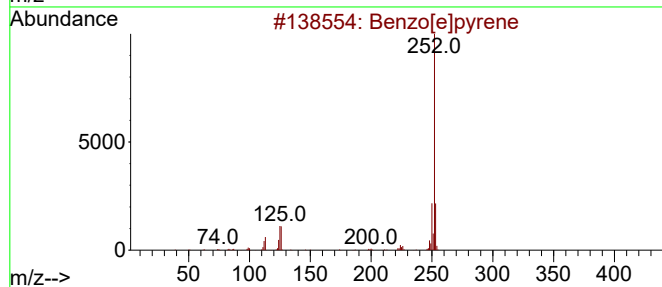
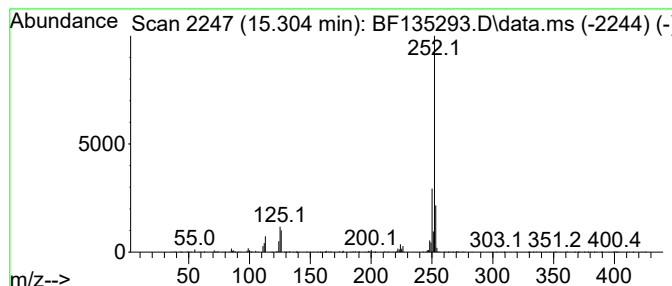
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	18.60 ng	314418	Perylene-d12	15.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[a]pyrene	252	C20H12	000050-32-8	97
3		Perylene	252	C20H12	000198-55-0	94
4		Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
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Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId :
CHRT-24313

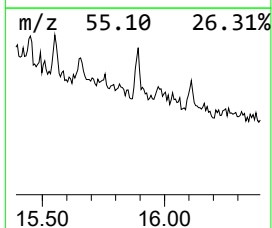
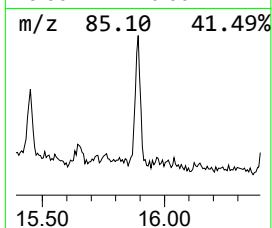
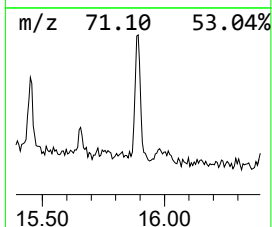
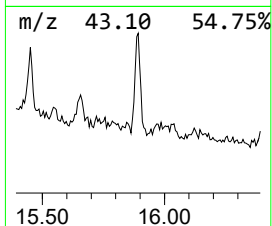
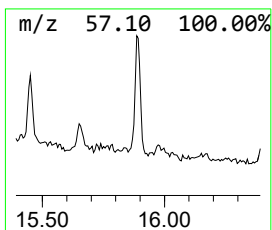
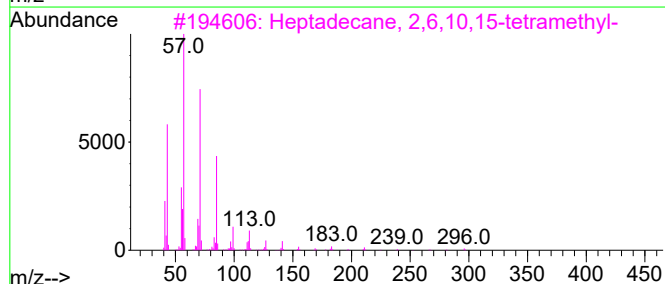
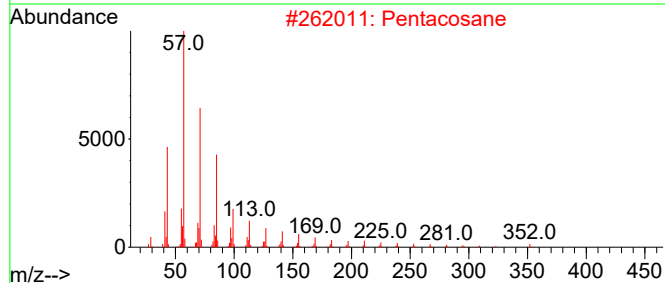
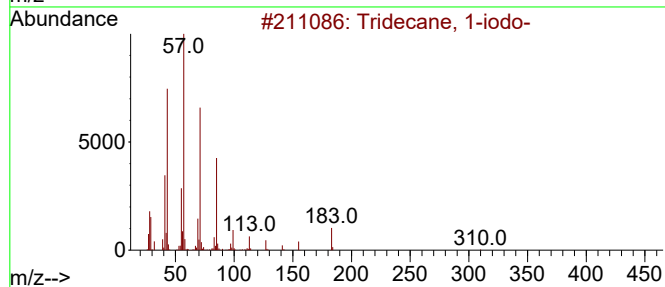
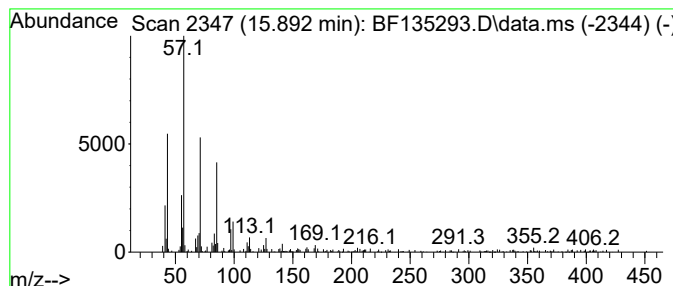
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Tridecane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	8.51 ng	143955	Perylene-d12	15.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
2		Pentacosane	352	C25H52	000629-99-2	89
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4		Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24313

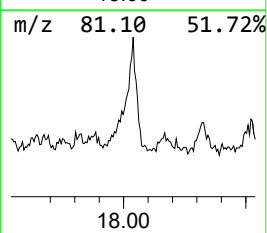
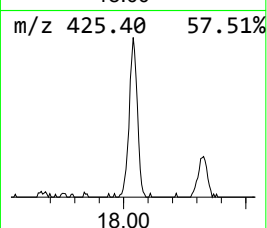
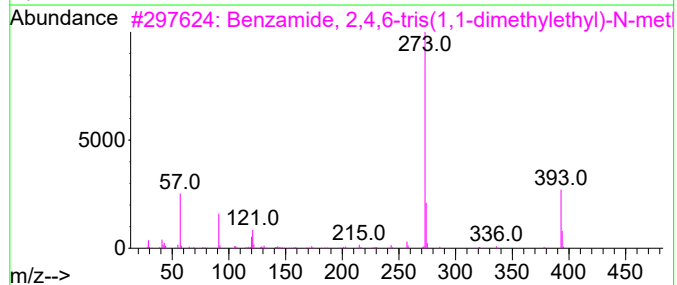
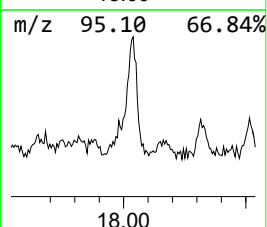
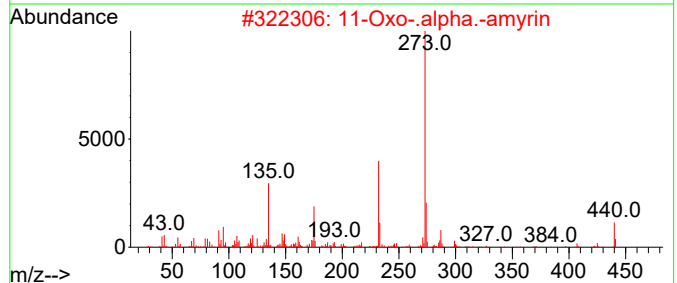
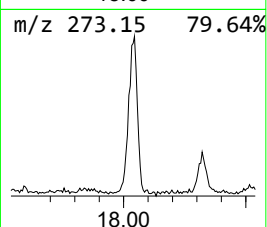
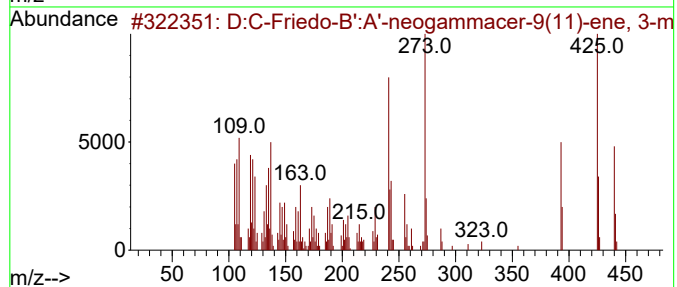
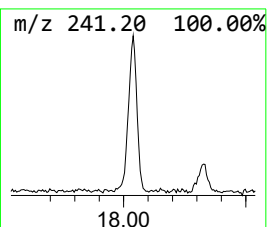
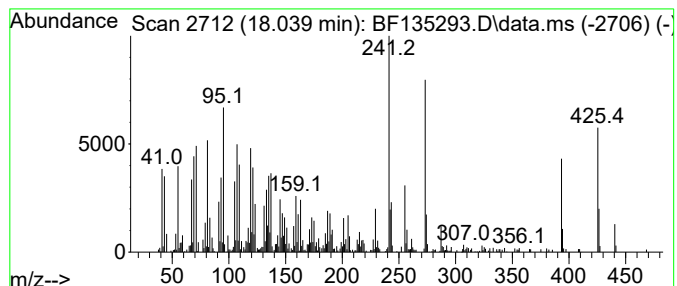
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	64.17 ng	1084910	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	50		
2	11-Oxo-.alpha.-amyrrin	440	C30H48O2	002118-90-3	25		
3	Benzamide, 2,4,6-tris(1,1-dimeth...	393	C27H39NO	016420-52-3	25		
4	1-Phenanthrenecarboxylic acid, 7...	316	C21H32O2	001686-62-0	12		
5	2-Methyl-4,6-bis(4-methylphenyl)...	273	C20H19N	130505-64-5	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24313

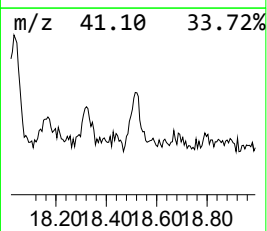
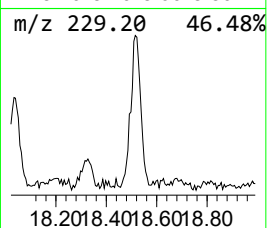
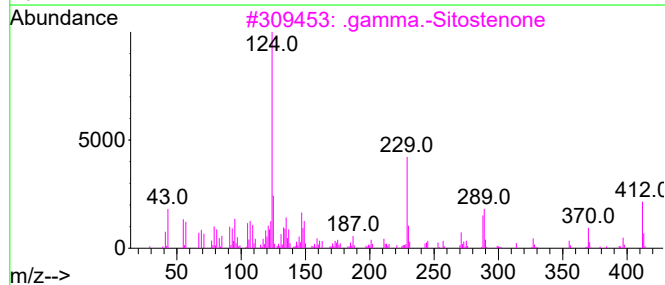
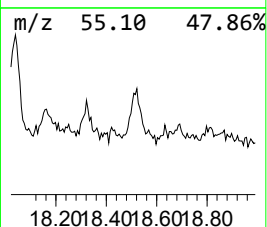
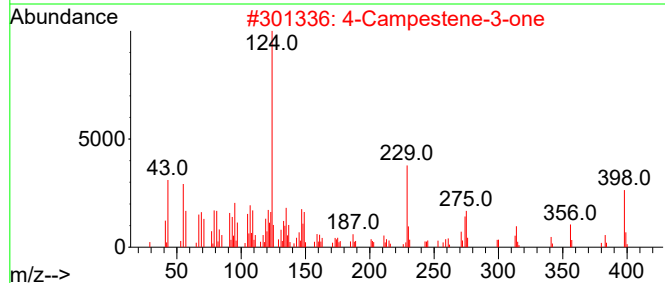
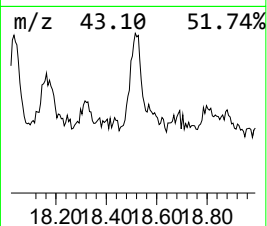
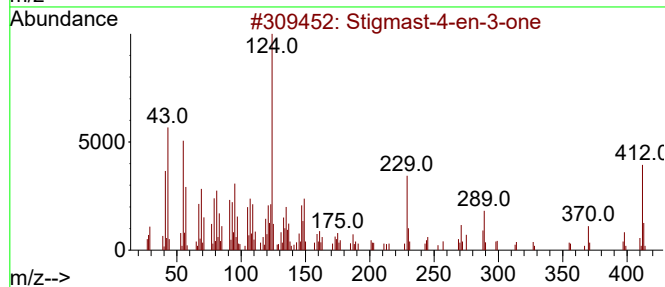
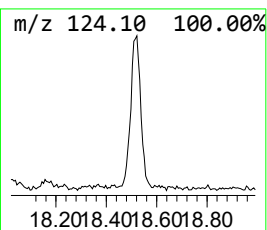
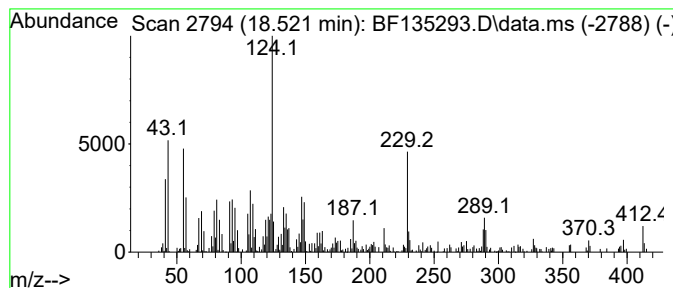
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Stigmast-4-en-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.521	22.15 ng	374499	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stigmast-4-en-3-one	412	C29H48O	001058-61-3	96
2			4-Campestene-3-one	398	C28H46O	051014-22-3	72
3			.gamma.-Sitostenone	412	C29H48O	084924-96-9	55
4			Testosterone	288	C19H28O2	000058-22-0	45
5			Pregn-4-en-3-one, 20-hydroxy-, (...)	316	C21H32O2	000145-14-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135293.D
Acq On : 15 Sep 2023 22:33
Operator : CG\JU
Sample : 04396-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24313

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
1,4-Dimethylada...	8.263	4.4	ng	147450	2	8.034	673914	20.0
1,3,4-Trimethyl...	8.498	6.4	ng	214821	2	8.034	673914	20.0
N-[1-Adamantyl]...	8.581	4.3	ng	146233	2	8.034	673914	20.0
unknown8.722	8.722	5.0	ng	168819	2	8.034	673914	20.0
unknown8.781	8.781	8.7	ng	292667	2	8.034	673914	20.0
unknown8.816	8.816	7.4	ng	248018	2	8.034	673914	20.0
1-(2-Ethyl-1,3-...	9.028	4.5	ng	674722	3	9.810	3003770	20.0
Decahydro-1,1,4...	9.192	11.1	ng	1670110	3	9.810	3003770	20.0
unknown9.510	9.510	22.7	ng	3415310	3	9.810	3003770	20.0
unknown9.563	9.563	9.9	ng	1489200	3	9.810	3003770	20.0
unknown9.722	9.722	28.7	ng	4308450	3	9.810	3003770	20.0
unknown9.757	9.757	11.5	ng	1730060	3	9.810	3003770	20.0
unknown10.081	10.081	8.3	ng	1244410	3	9.810	3003770	20.0
unknown10.145	10.145	14.3	ng	2149820	3	9.810	3003770	20.0
1H-Indene, octa...	10.181	7.7	ng	1149040	3	9.810	3003770	20.0
Cyclohexene, 1,...	10.227	18.5	ng	2784360	3	9.810	3003770	20.0
Benzo[e]pyrene	15.304	18.6	ng	314418	6	15.427	338152	20.0
Tridecane, 1-iodo-	15.892	8.5	ng	143955	6	15.427	338152	20.0
D:C-Friedo-B':A...	18.039	64.2	ng	1084910	6	15.427	338152	20.0
Stigmast-4-en-3...	18.521	22.1	ng	374499	6	15.427	338152	20.0