

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
 Data File : BF135227.D
 Acq On : 13 Sep 2023 17:36
 Operator : CG\JU
 Sample : 04363-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11940

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: BF135227.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	557	561	583	rBV	1888632	1713398	100.00%	11.913%
2	6.398	729	733	742	rBV	1686941	1713002	99.98%	11.910%
3	6.763	791	795	798	rBV	861635	707509	41.29%	4.919%
4	7.322	886	890	893	rBV	1202952	1093667	63.83%	7.604%
5	8.040	1009	1012	1016	rVB	1110368	853892	49.84%	5.937%
6	8.922	1159	1162	1165	rBV2	111154	105440	6.15%	0.733%
7	8.969	1165	1170	1172	rBV5	53265	98065	5.72%	0.682%
8	9.034	1177	1181	1183	rBV2	137498	159689	9.32%	1.110%
9	9.063	1183	1186	1188	rBV4	61910	66905	3.90%	0.465%
10	9.122	1192	1196	1199	rVB	1934176	1627858	95.01%	11.318%
11	9.157	1199	1202	1204	rBV3	92846	99615	5.81%	0.693%
12	9.204	1206	1210	1212	rVV3	161537	202671	11.83%	1.409%
13	9.504	1259	1261	1263	rBV	372817	299956	17.51%	2.086%
14	9.557	1268	1270	1273	rVV3	198722	222748	13.00%	1.549%
15	9.622	1278	1281	1283	rBV	611657	628901	36.70%	4.373%
16	9.675	1286	1290	1292	rVV3	311523	545766	31.85%	3.795%
17	9.710	1294	1296	1299	rVB	716127	712292	41.57%	4.952%
18	9.781	1305	1308	1309	rBV2	607095	569843	33.26%	3.962%
19	9.804	1310	1312	1316	rVB	836716	803651	46.90%	5.588%
20	10.216	1380	1382	1385	rBV2	728307	622002	36.30%	4.325%
21	13.963	2017	2019	2026	rVB	587958	704708	41.13%	4.900%
22	15.421	2263	2267	2271	rBV	534181	604417	35.28%	4.202%
23	15.892	2343	2347	2355	rVB	131690	226686	13.23%	1.576%

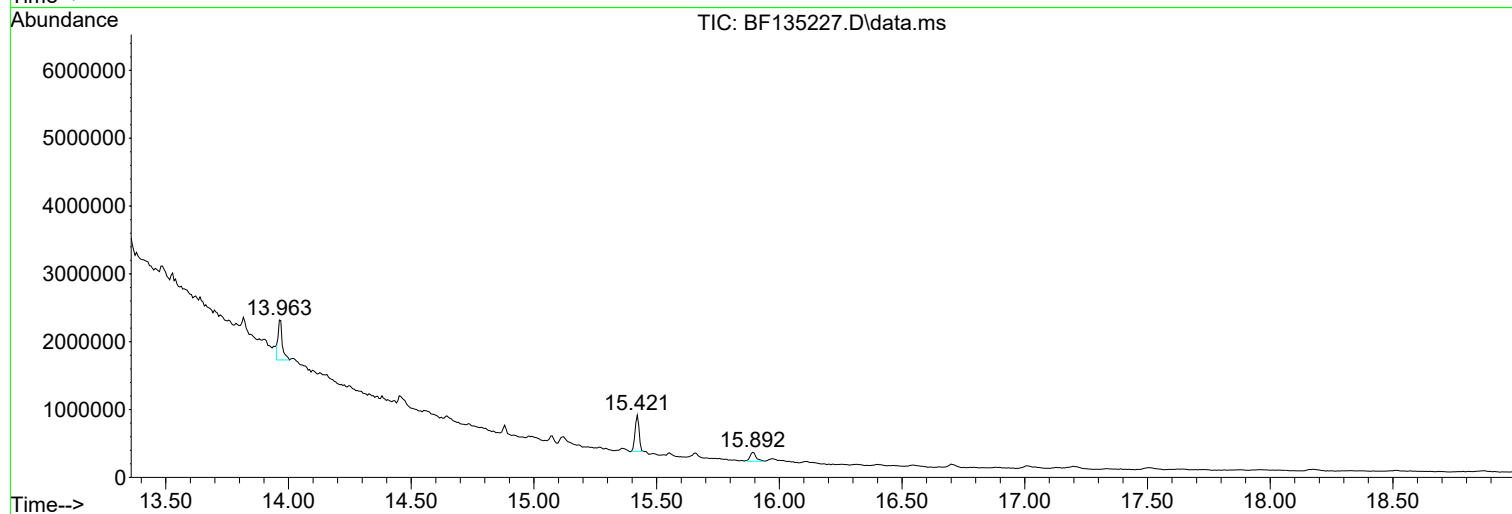
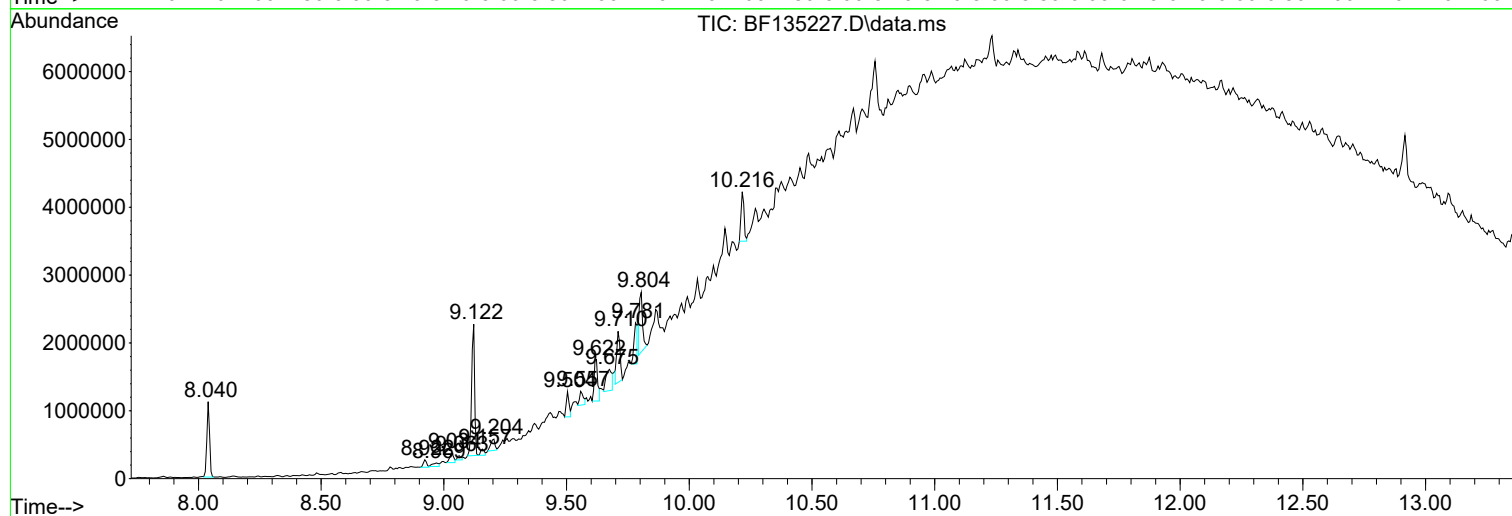
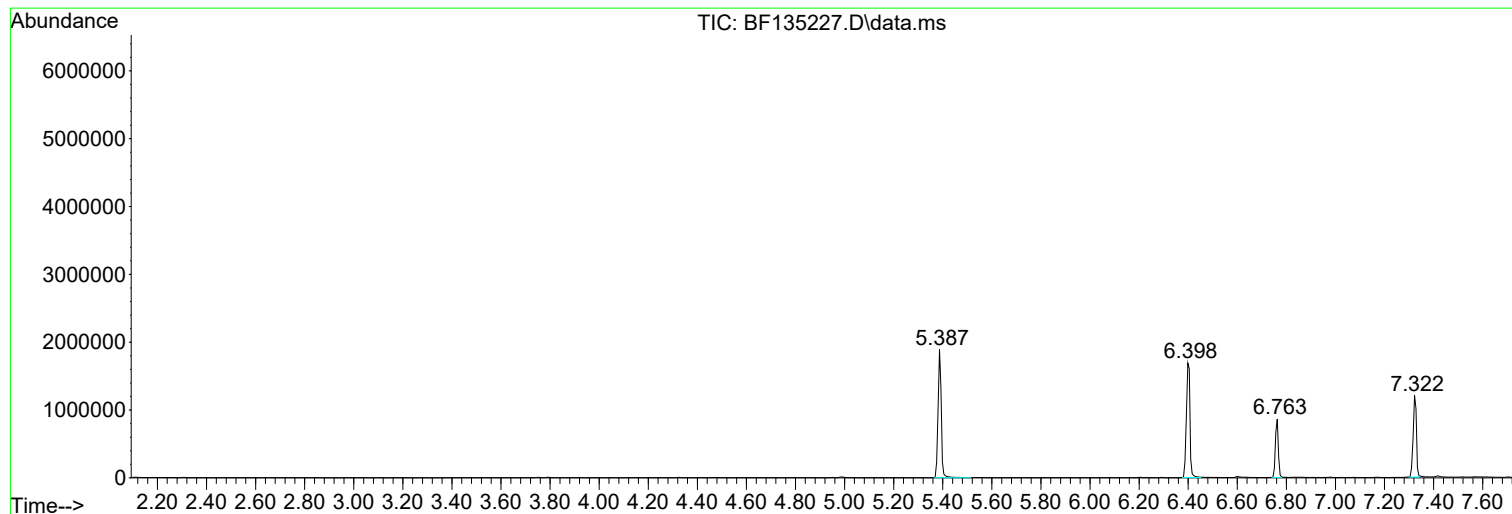
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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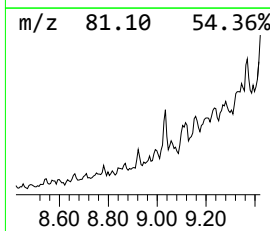
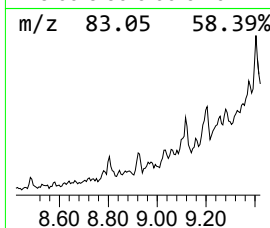
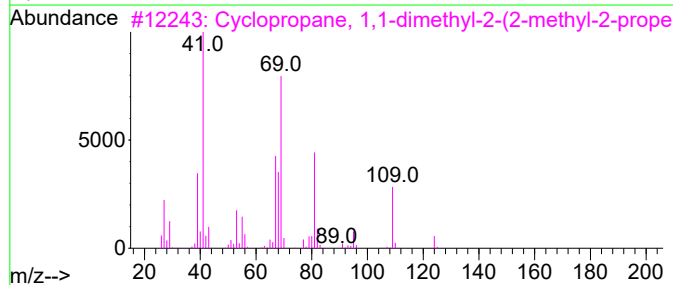
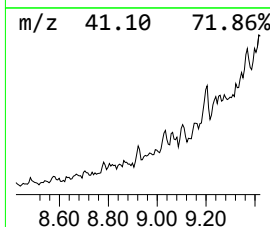
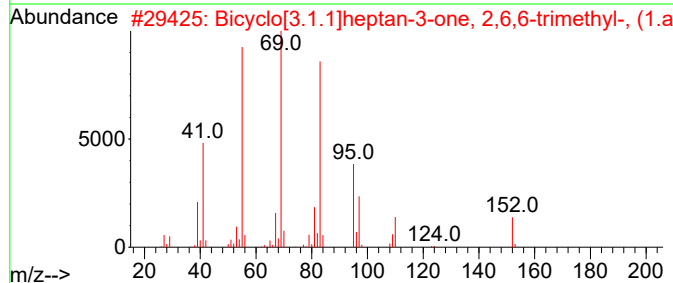
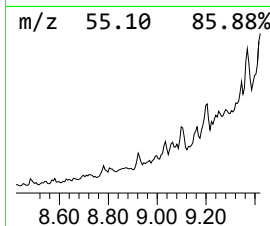
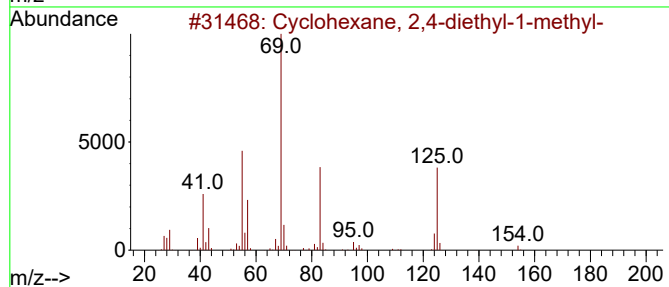
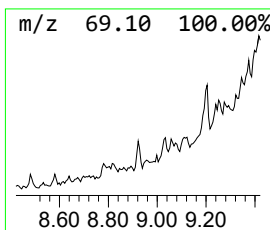
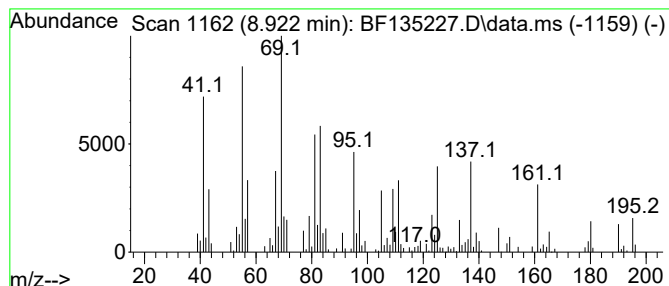
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown8.922 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.922	2.47 ng	105440	Naphthalene-d8	8.040

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	43
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	38
3		Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	18
4		6-Octen-1-ol, 7-methyl-3-methylene-	154	C10H18O	013066-51-8	14
5		1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	14



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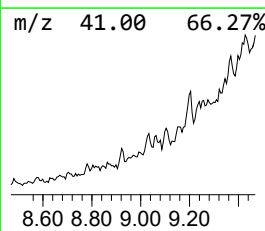
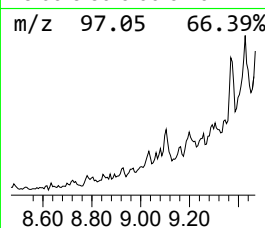
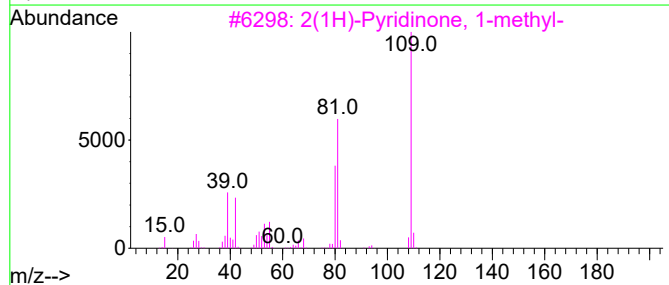
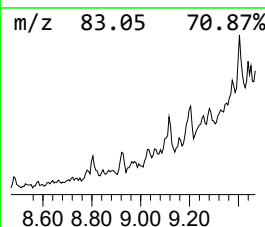
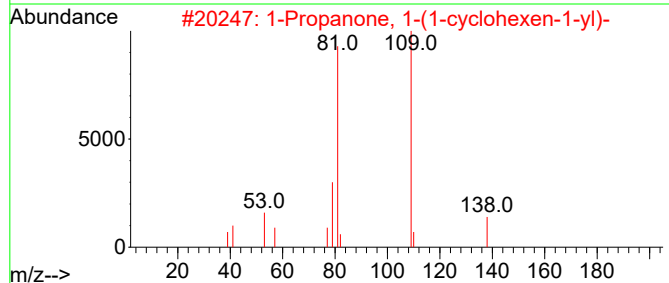
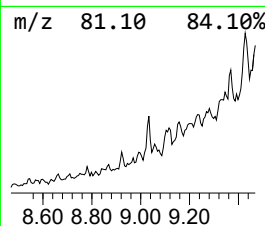
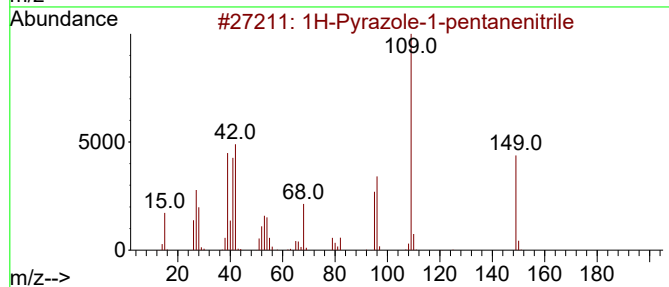
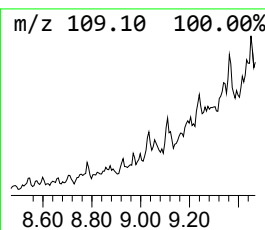
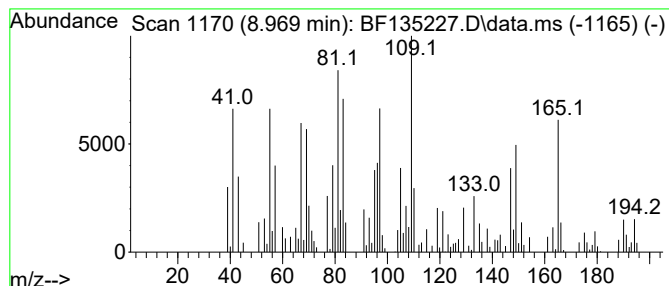
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Peak Number 2 unknown8.969 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.969	2.44 ng	98065	Acenaphthene-d10	9.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrazole-1-pentanenitrile	149	C8H11N3	1000460-75-9	30
2			1-Propanone, 1-(1-cyclohexen-1-yl)-	138	C9H14O	001655-03-4	27
3			2(1H)-Pyridinone, 1-methyl-	109	C6H7NO	000694-85-9	27
4			2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	18
5			9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	18



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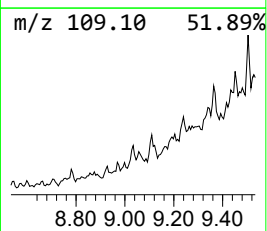
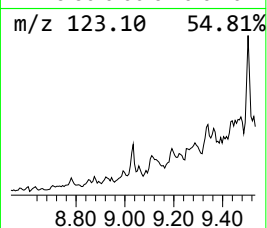
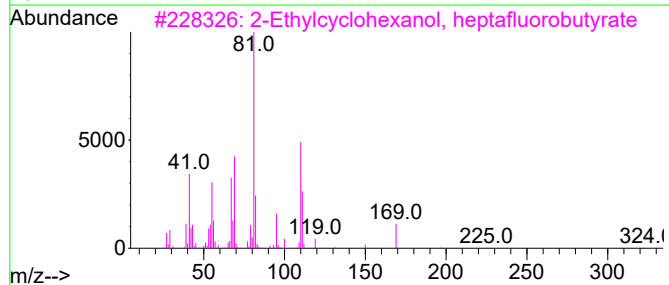
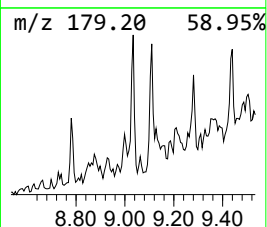
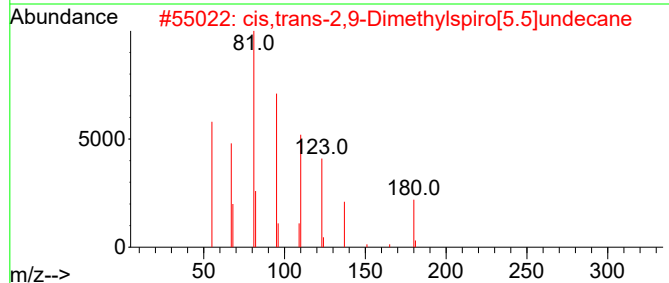
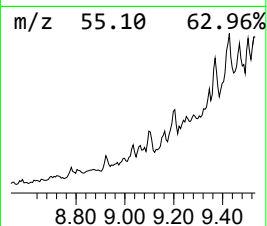
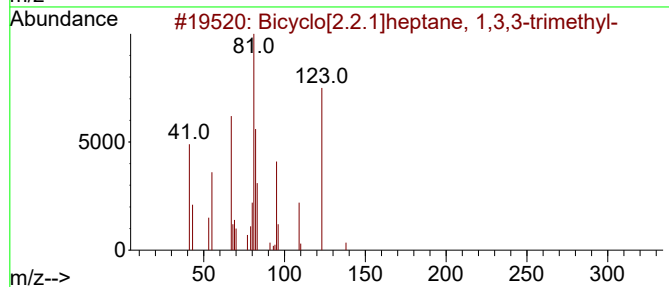
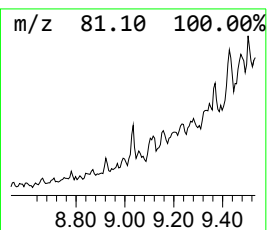
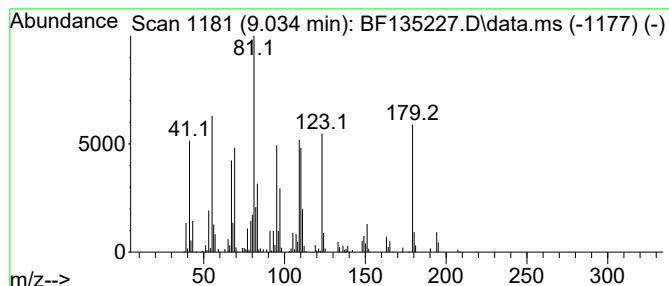
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Peak Number 3 Bicyclo[2.2.1]heptane, 1,3,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.034	3.97 ng	159689	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	55
2	cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	49
3	2-Ethylcyclohexanol, heptafluoro...	324	C12H15F7O2	959079-92-6	38
4	Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	38
5	2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	38



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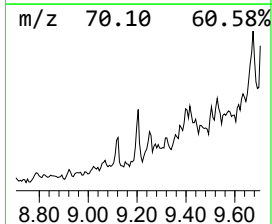
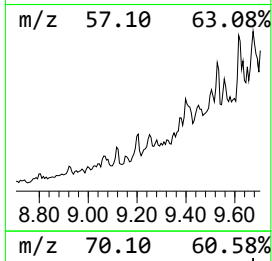
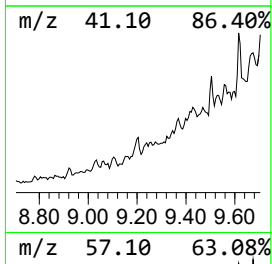
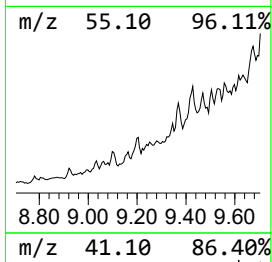
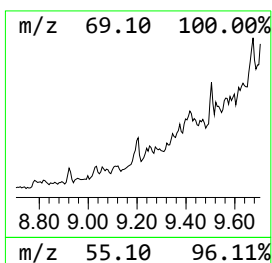
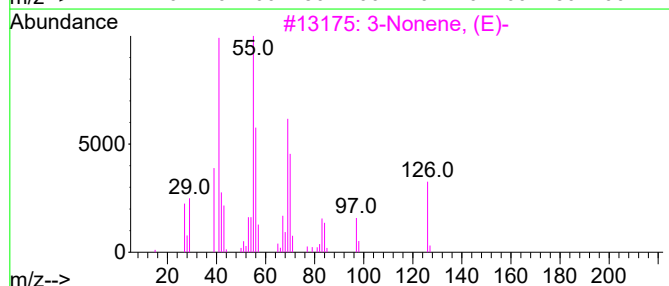
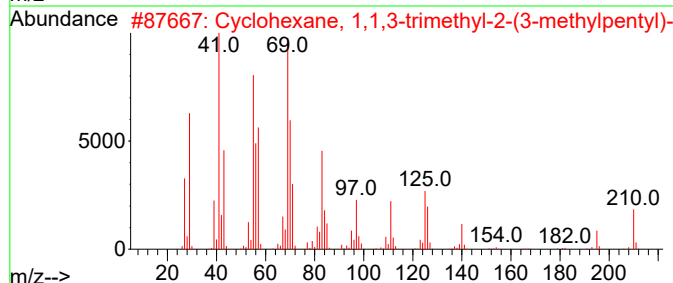
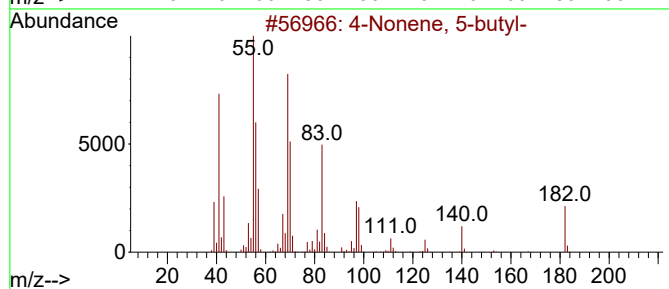
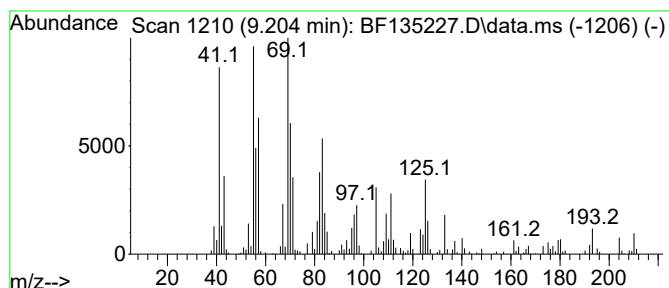
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Peak Number 4 4-Nonene, 5-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.204	5.04 ng	202671	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonene, 5-butyl-	182	C13H26	007367-38-6	81
2	Cyclohexane, 1,1,3-trimethyl-2-(...	210	C15H30	054965-05-8	80
3	3-Nonene, (E)-	126	C9H18	020063-92-7	70
4	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	58
5	9-Undecenal, 2,6,10-trimethyl-	210	C14H26O	000141-13-9	55



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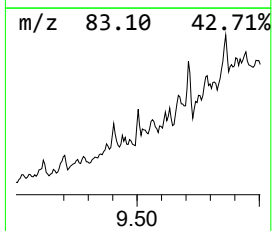
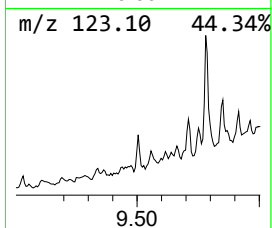
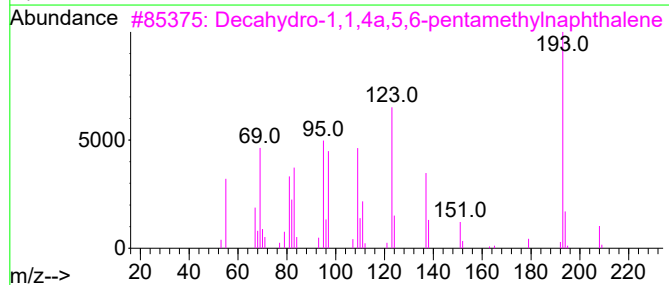
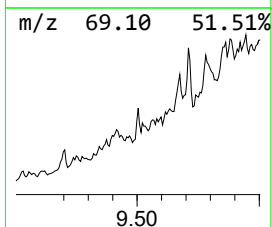
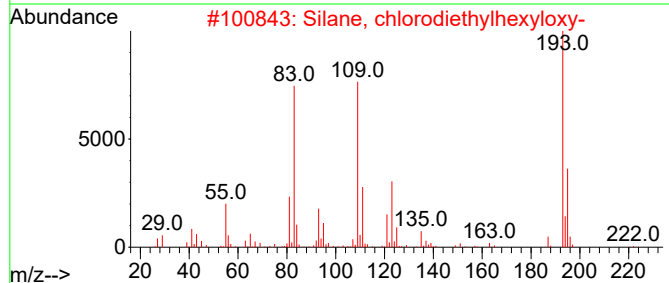
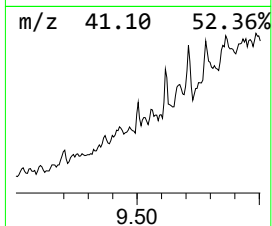
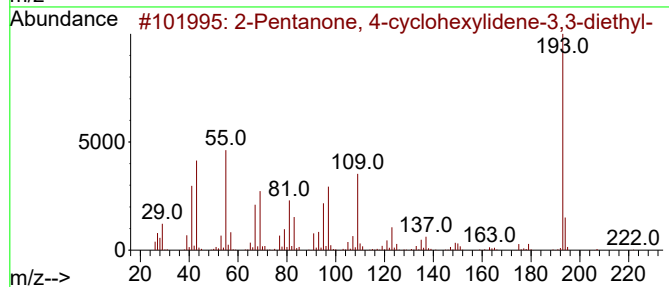
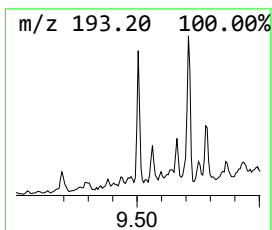
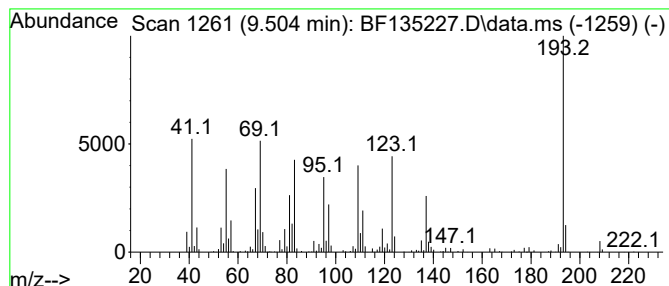
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Peak Number 5 2-Pentanone, 4-cyclohexylidene... Concentration Rank 6

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9.504	7.46 ng	299956	Acenaphthene-d10			9.804
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...		222	C15H26O	313253-65-5	55
2	Silane, chlorodiethylhexyloxy-		222	C10H23ClOSi	1000363-74-4	46
3	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	38
4	1-(p-Fluorophenyl)-4-piperidone		193	C11H12FNO	1000238-56-7	38
5	2-Anthracenamine		193	C14H11N	000613-13-8	22



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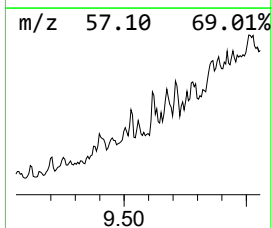
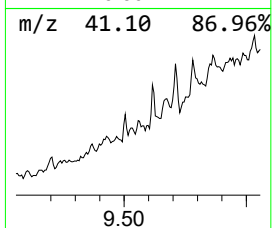
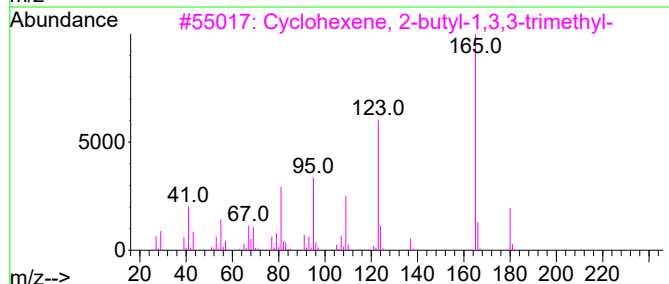
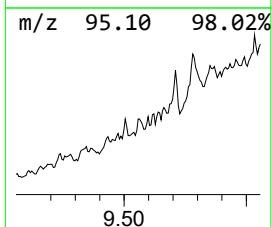
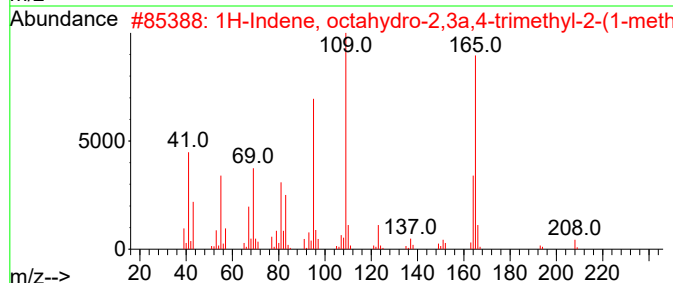
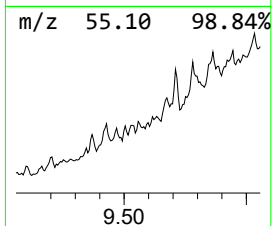
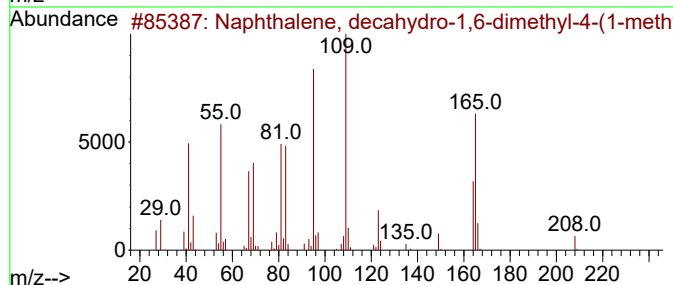
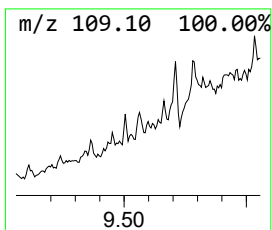
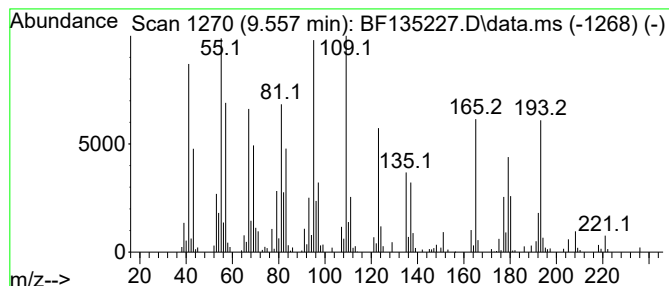
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BNA_F
ClientSampleId :
72-11940

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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, decahydro-1,6-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.557	5.54 ng	222748	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	55
2	1H-Indene, octahydro-2,3a,4-trim...	208	C15H28	031230-13-4	55
3	Cyclohexene, 2-butyl-1,3,3-trime...	180	C13H24	003293-50-3	46
4	Silane, chlorodiisopropylisoprop...	208	C9H21ClOSi	1000305-87-8	41
5	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135227.D
Acq On : 13 Sep 2023 17:36
Operator : CG\JU
Sample : 04363-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

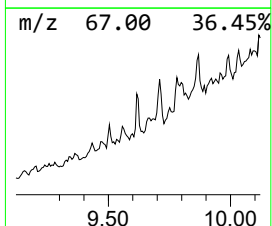
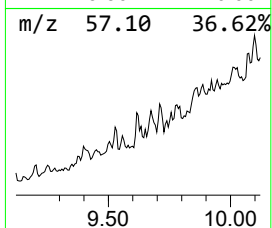
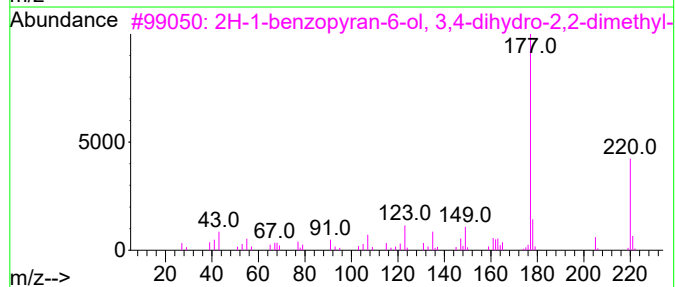
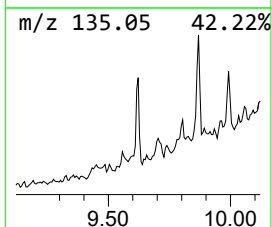
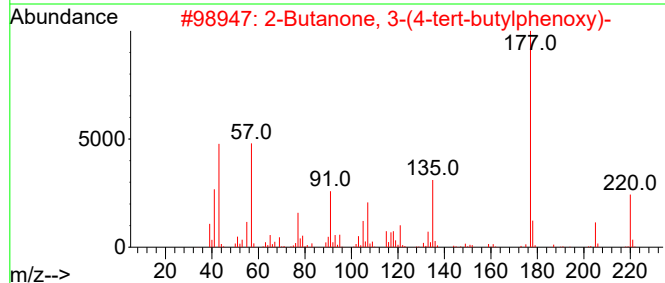
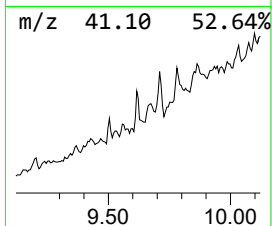
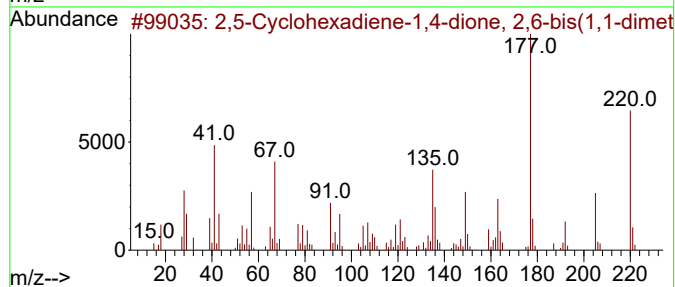
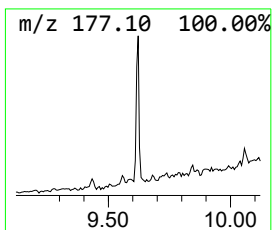
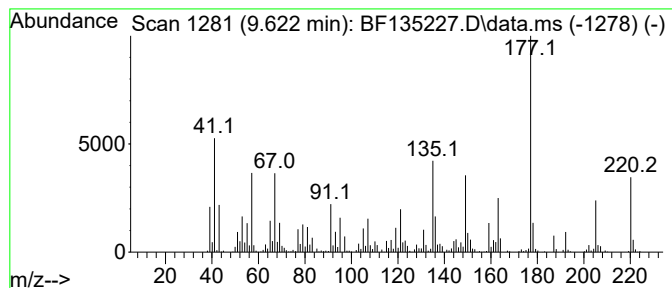
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.622	15.65 ng	628901	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	97
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	55
3	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	49
4	trans-.beta.-Ionone	192	C13H20O	000079-77-6	49
5	N-[4-(Ethyl-methyl-amino)-phenyl...	192	C11H16N2O	099981-45-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135227.D
Acq On : 13 Sep 2023 17:36
Operator : CG\JU
Sample : 04363-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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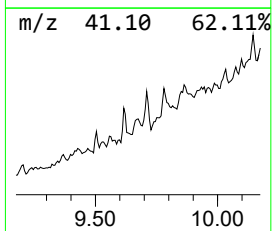
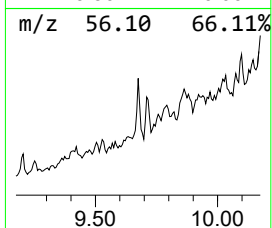
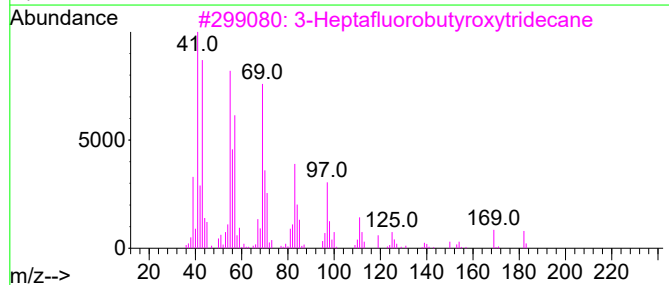
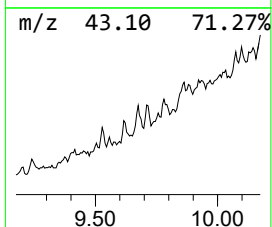
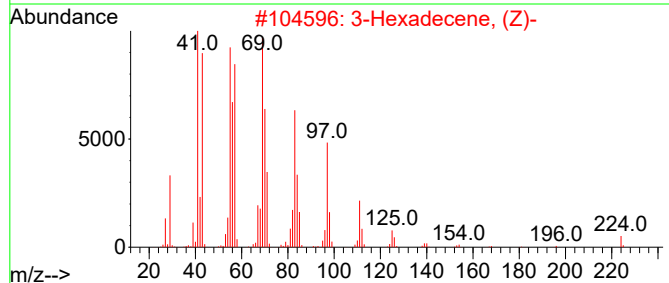
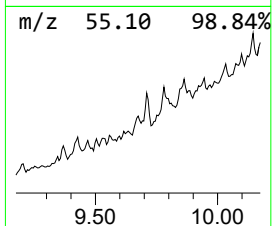
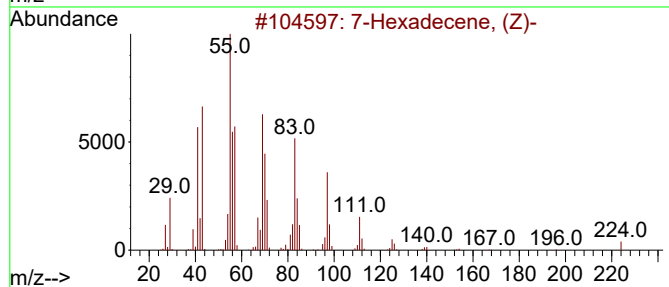
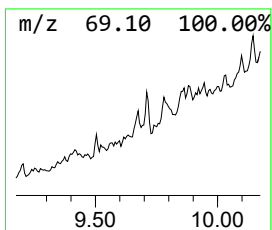
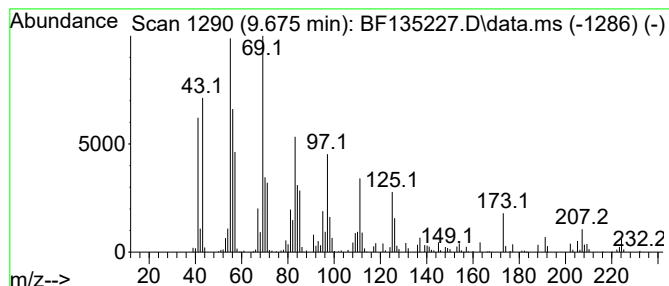
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 7-Hexadecene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.675	13.58 ng	545766	Acenaphthene-d10	9.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Hexadecene, (Z)-	224	C16H32	035507-09-6	90
2		3-Hexadecene, (Z)-	224	C16H32	034303-81-6	83
3		3-Heptafluorobutyroxytridecane	396	C17H27F7O2	1000245-49-5	80
4		Z-8-Hexadecene	224	C16H32	1000130-87-5	64
5		Cetene	224	C16H32	000629-73-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135227.D
Acq On : 13 Sep 2023 17:36
Operator : CG\JU
Sample : 04363-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

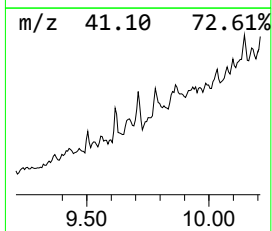
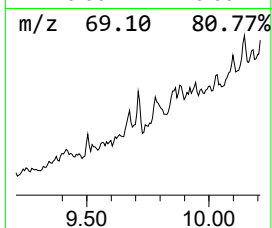
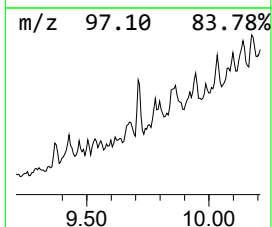
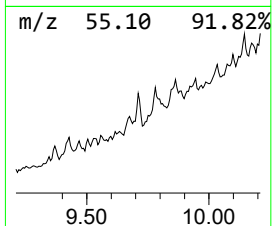
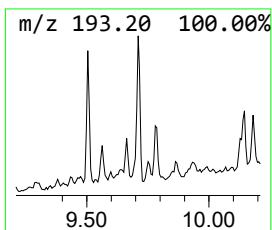
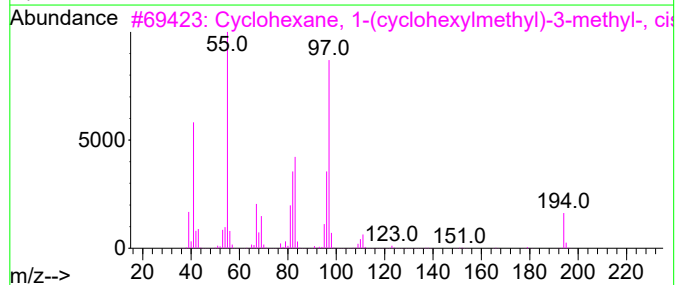
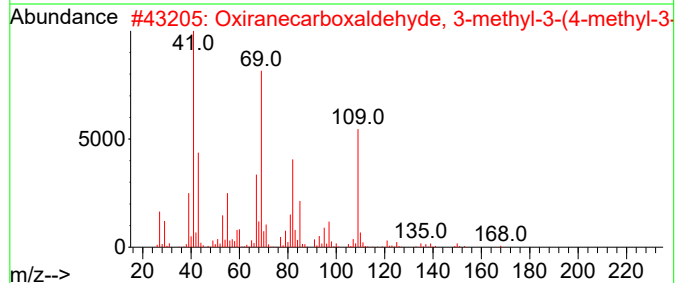
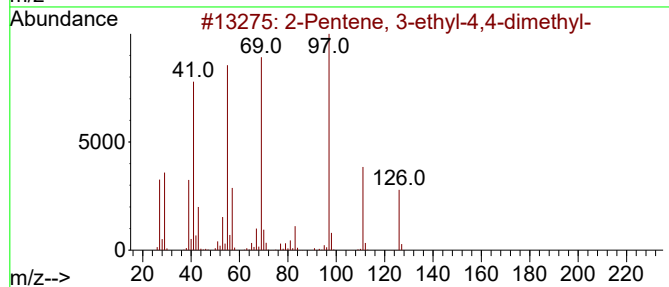
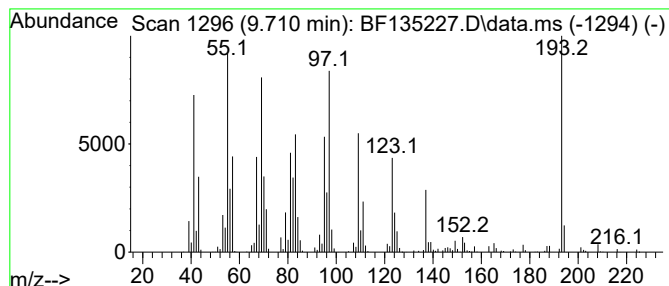
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.710 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	17.73 ng	712292	Acenaphthene-d10	9.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18		053907-59-8	30
2	Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2		016996-12-6	20
3	Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26		054823-96-0	18
4	Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26		054824-04-3	18
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18		004863-59-6	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135227.D
Acq On : 13 Sep 2023 17:36
Operator : CG\JU
Sample : 04363-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

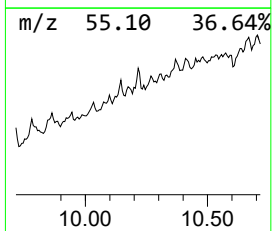
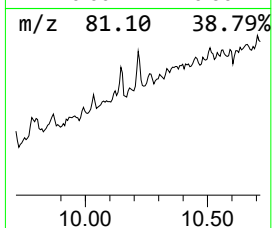
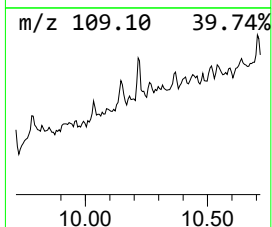
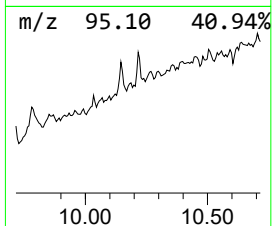
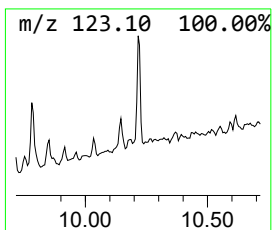
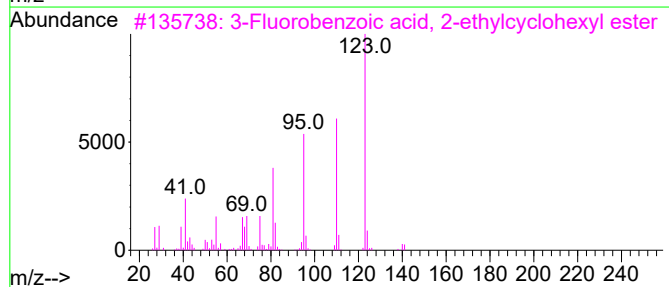
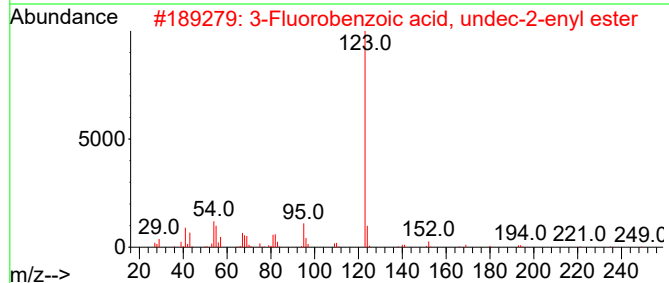
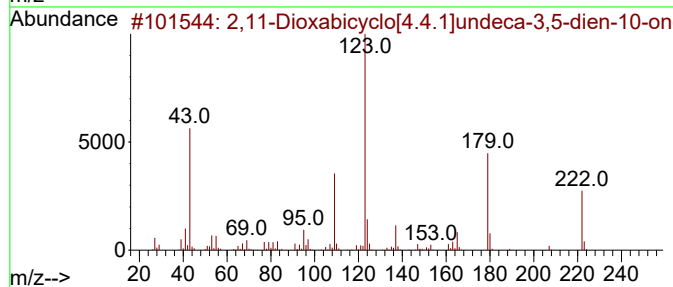
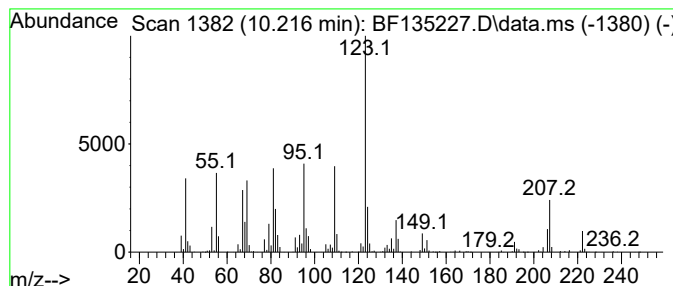
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.216 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.216	15.48 ng	622002	Acenaphthene-d10	9.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	47		
2	3-Fluorobenzoic acid, undec-2-en...	292	C18H25FO2	1000292-60-8	47		
3	3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	43		
4	2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	43		
5	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135227.D
Acq On : 13 Sep 2023 17:36
Operator : CG\JU
Sample : 04363-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

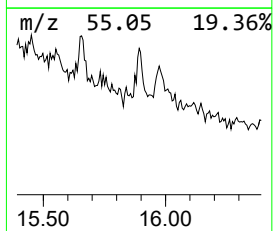
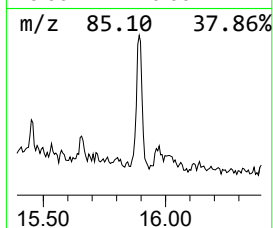
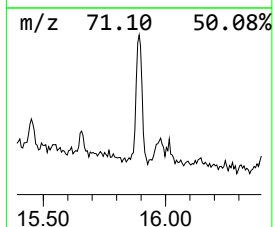
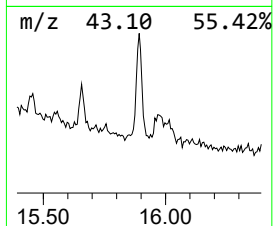
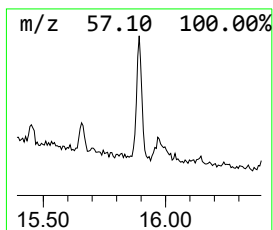
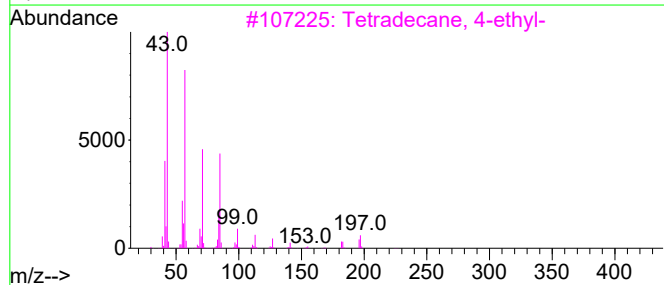
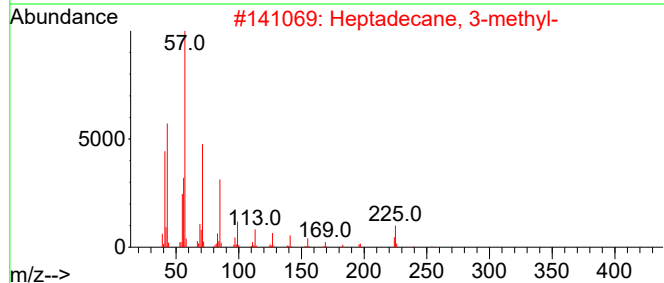
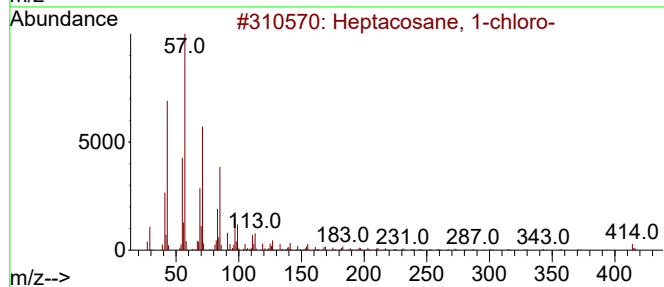
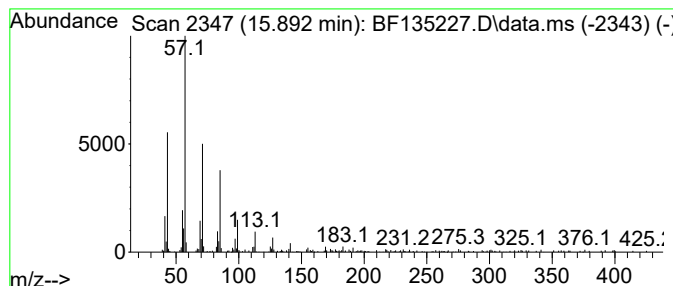
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.892	7.50 ng	226686	Perylene-d12	15.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87
2	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	87
3	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	87
4	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
5	Eicosane	282	C20H42	000112-95-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135227.D
Acq On : 13 Sep 2023 17:36
Operator : CG\JU
Sample : 04363-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown8.969	8.969	2.4	ng	98065	3	9.804	803651	20.0
Bicyclo[2.2.1]h...	9.034	4.0	ng	159689	3	9.804	803651	20.0
4-Nonene, 5-butyl-	9.204	5.0	ng	202671	3	9.804	803651	20.0
2-Pentanone, 4-...	9.504	7.5	ng	299956	3	9.804	803651	20.0
Naphthalene, de...	9.557	5.5	ng	222748	3	9.804	803651	20.0
2,5-Cyclohexadi...	9.622	15.7	ng	628901	3	9.804	803651	20.0
7-Hexadecene, (Z)-	9.675	13.6	ng	545766	3	9.804	803651	20.0
unknown9.710	9.710	17.7	ng	712292	3	9.804	803651	20.0
unknown10.216	10.216	15.5	ng	622002	3	9.804	803651	20.0
Heptacosane, 1-...	15.892	7.5	ng	226686	6	15.421	604417	20.0