

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
 Data File : BF134521.D
 Acq On : 28 Jul 2023 18:16
 Operator : CG\JU
 Sample : 03777-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	571	575	590	rBV	1817896	1735341	96.45%	12.776%
2	6.475	742	746	758	rBV	1878635	1799237	100.00%	13.246%
3	6.828	803	806	812	rBV	667469	591076	32.85%	4.352%
4	7.392	898	902	909	rBV	1255698	1089605	60.56%	8.022%
5	8.104	1020	1023	1027	rBV	767949	683020	37.96%	5.028%
6	8.728	1125	1129	1132	rBV5	55562	100160	5.57%	0.737%
7	8.981	1170	1172	1175	rVB4	84880	83162	4.62%	0.612%
8	9.098	1189	1192	1194	rBV3	87027	93289	5.18%	0.687%
9	9.122	1194	1196	1200	rBV3	90707	85212	4.74%	0.627%
10	9.186	1200	1207	1210	rBV	1700398	1641296	91.22%	12.083%
11	9.222	1210	1213	1215	rBV3	129047	133552	7.42%	0.983%
12	9.257	1216	1219	1222	rBV4	192998	269307	14.97%	1.983%
13	9.433	1246	1249	1251	rBV	194184	184910	10.28%	1.361%
14	9.492	1256	1259	1262	rBV2	320515	413180	22.96%	3.042%
15	9.569	1270	1272	1274	rBV2	247589	251891	14.00%	1.854%
16	9.680	1289	1291	1295	rBV	671833	622833	34.62%	4.585%
17	9.733	1297	1300	1302	rVV3	397461	527630	29.33%	3.884%
18	9.775	1305	1307	1310	rVB3	824850	796311	44.26%	5.862%
19	9.869	1321	1323	1327	rVB	794635	805911	44.79%	5.933%
20	9.910	1327	1330	1331	rBV3	373520	407277	22.64%	2.998%
21	10.286	1391	1394	1396	rBV	721131	745662	41.44%	5.490%
22	15.527	2281	2285	2289	rVB	416269	523307	29.08%	3.853%

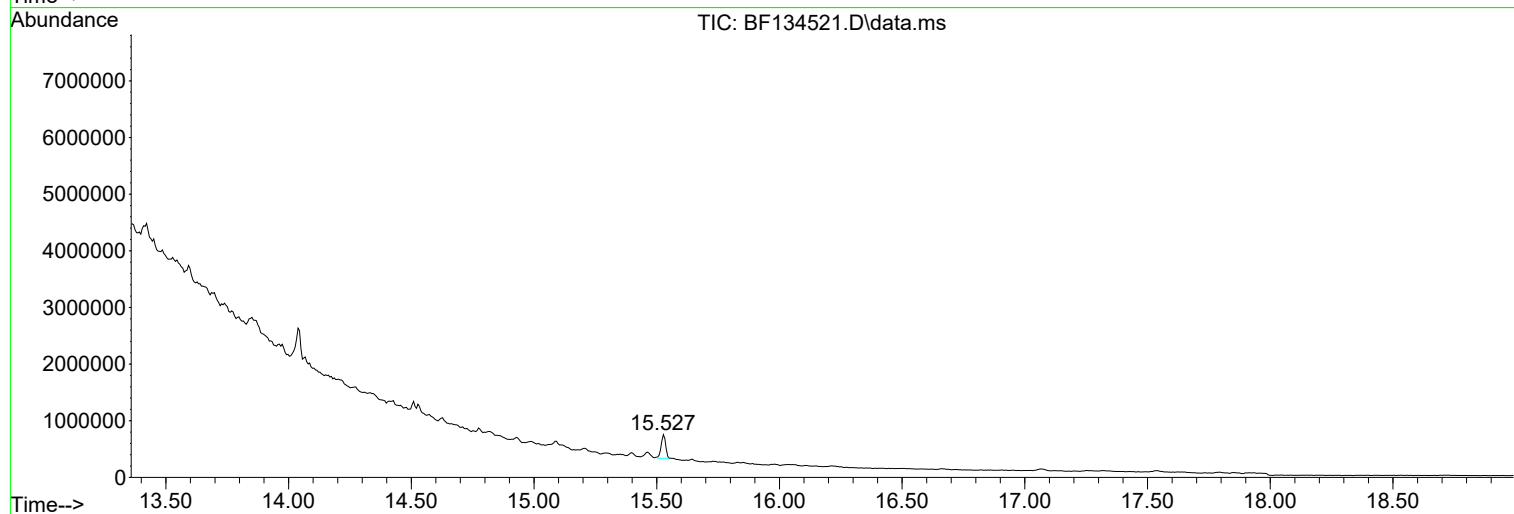
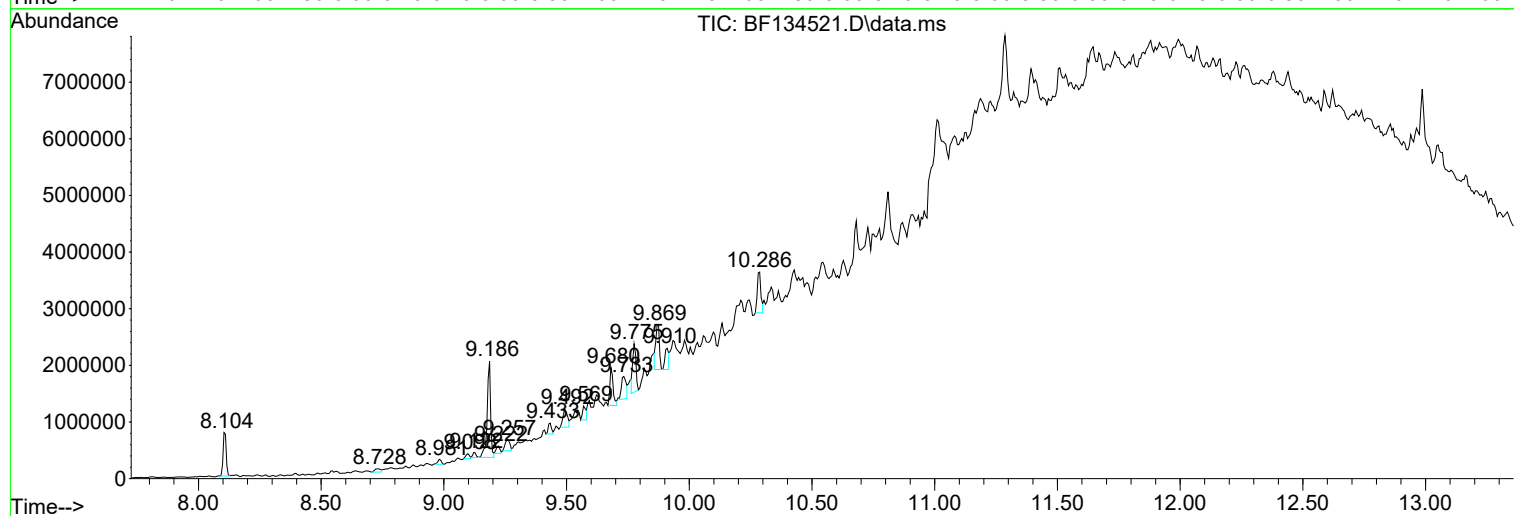
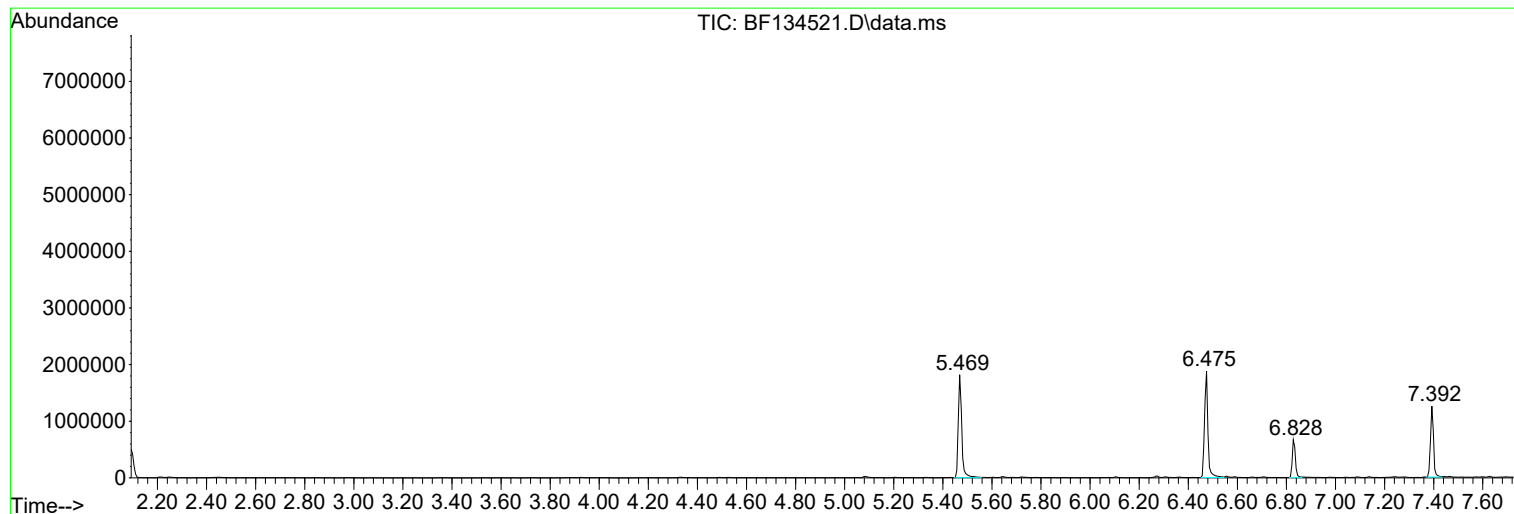
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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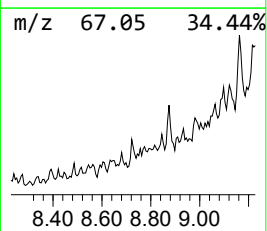
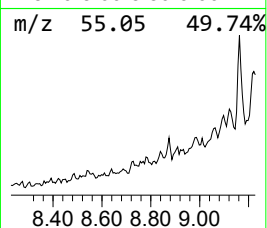
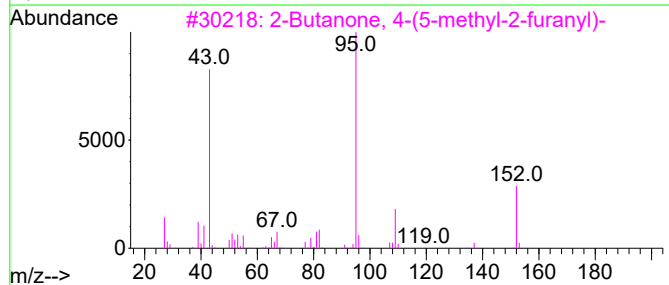
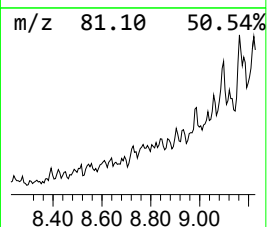
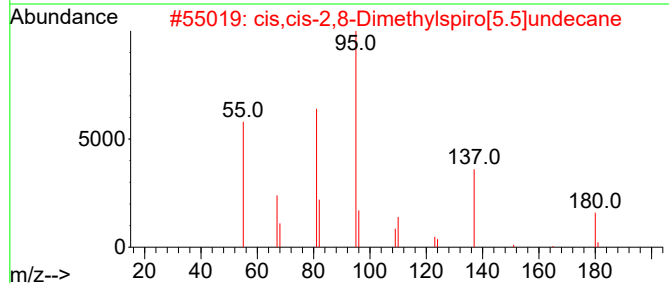
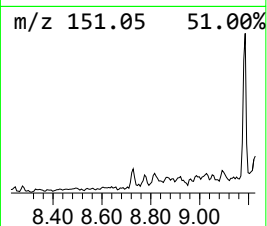
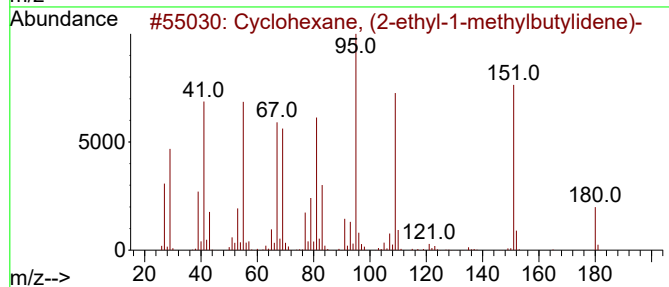
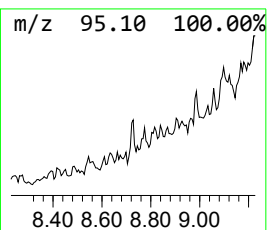
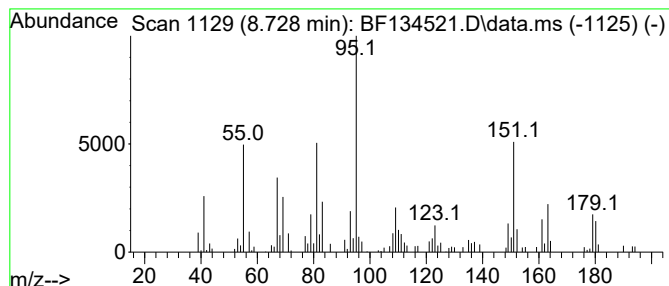
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown8.728 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.728	2.93 ng	100160	Naphthalene-d8	8.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	49
2			cis,cis-2,8-Dimethylspiro[5.5]un...	180	C13H24	095530-75-9	38
3			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	38
4			2-Furoic acid, tridec-2-ynyl ester	290	C18H26O3	1000299-24-1	35
5			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	30



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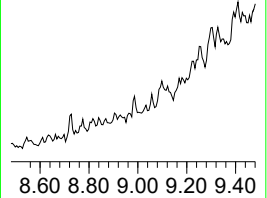
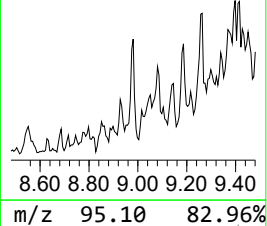
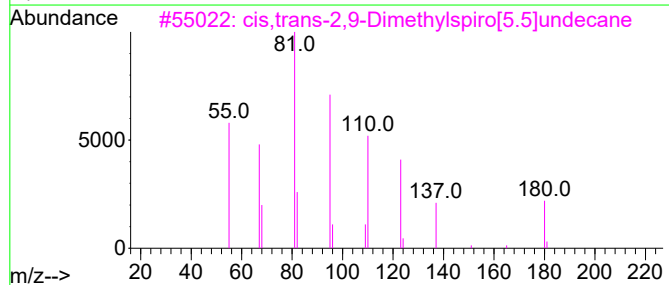
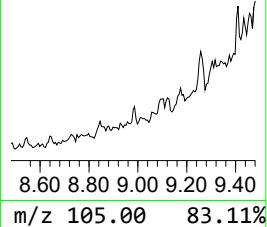
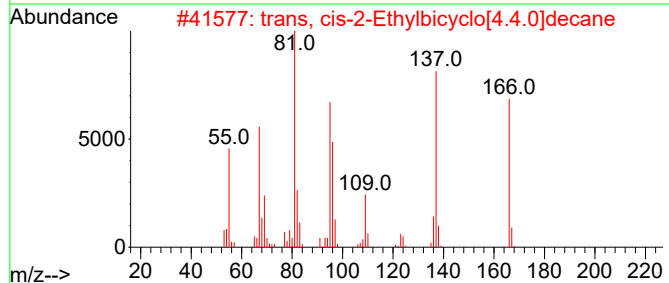
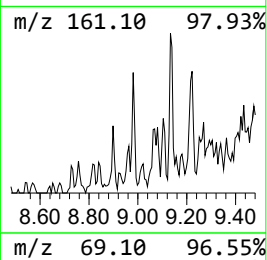
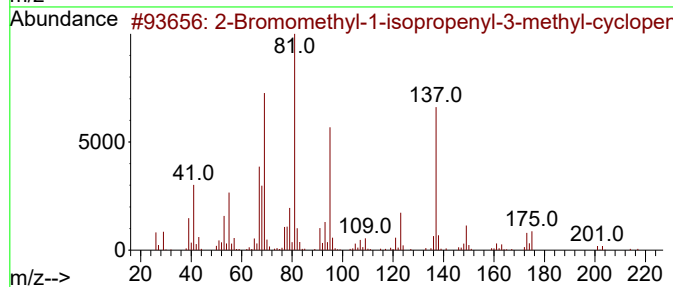
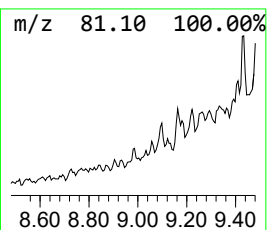
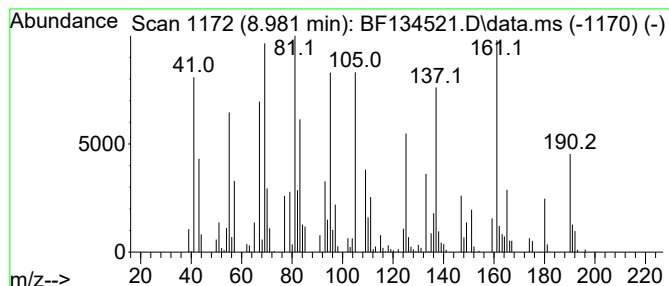
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown8.981 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.981	2.44 ng	83162	Naphthalene-d8	8.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromomethyl-1-isopropenyl-3-me...	216	C10H17Br	1000187-07-8	35		
2	trans, cis-2-Ethylbicyclo[4.4.0]...	166	C12H22	066660-39-7	35		
3	cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	22		
4	3-Hydroxypyridine monoacetate	137	C7H7NO2	017747-43-2	18		
5	3,7-Benzofurandiyl, 2,3-dihydro-...	180	C10H12O3	017781-15-6	15		



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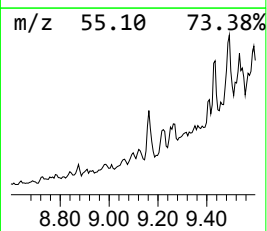
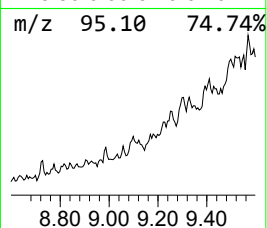
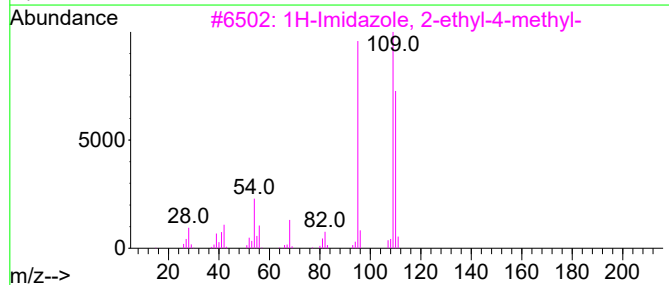
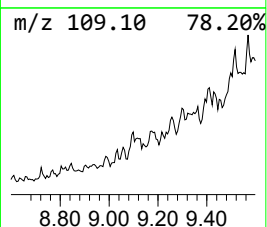
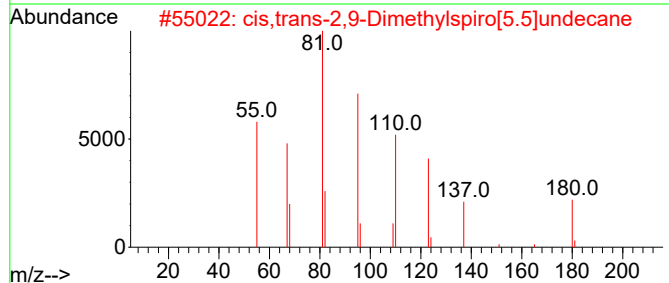
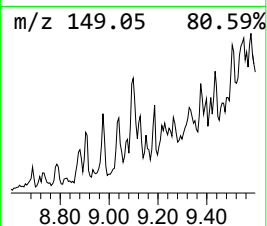
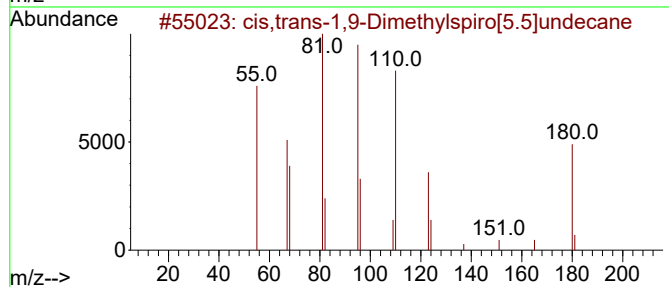
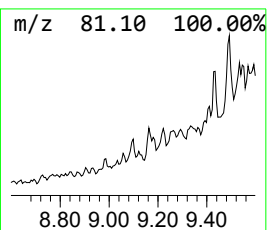
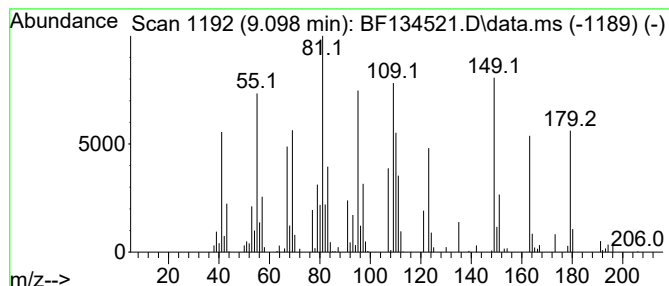
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.098 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.098	2.32 ng	93289	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,trans-1,9-Dimethylspiro[5.5]...	180	C13H24	1000111-73-3	38
2			cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	35
3			1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	30
4			1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	25
5			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	22



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ALS Vial : 5 Sample Multiplier: 1

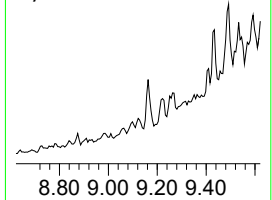
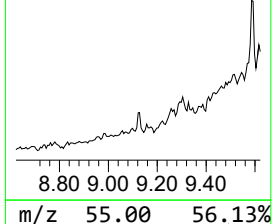
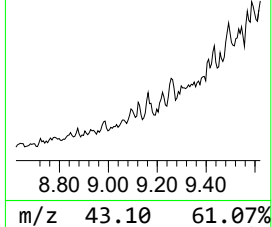
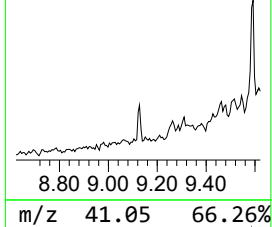
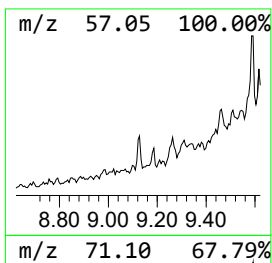
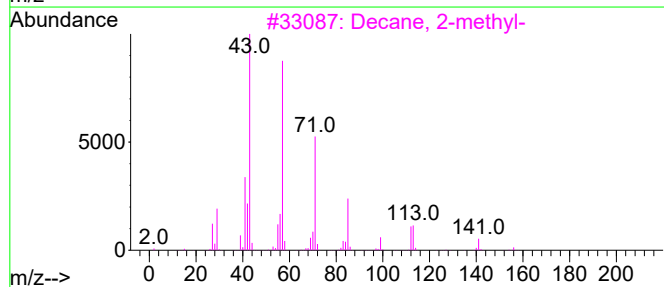
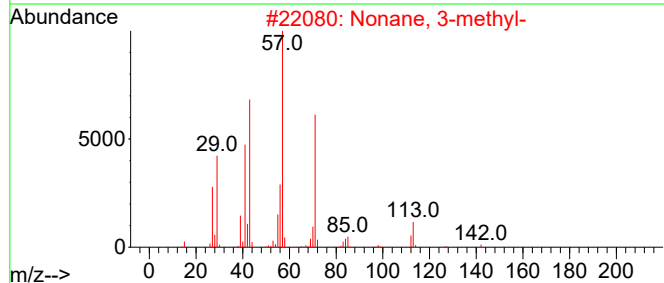
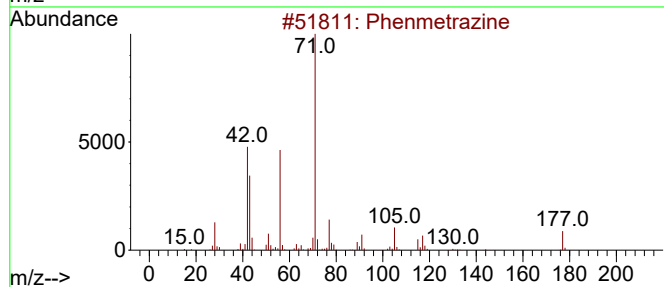
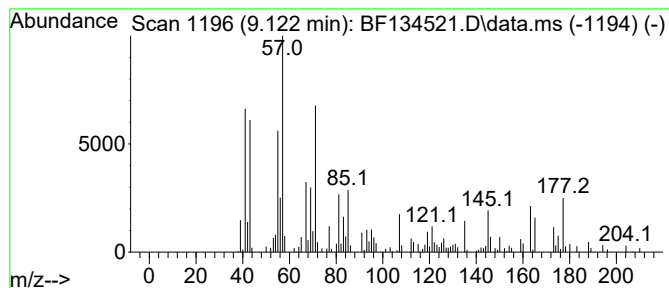
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown9.122 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.122	2.11 ng	85212	Acenaphthene-d10		9.875	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenmetrazine		177	C11H15NO	000134-49-6	25
2	Nonane, 3-methyl-		142	C10H22	005911-04-6	25
3	Decane, 2-methyl-		156	C11H24	006975-98-0	22
4	Tetradecane, 4-methyl-		212	C15H32	025117-24-2	22
5	Tetradecane		198	C14H30	000629-59-4	22



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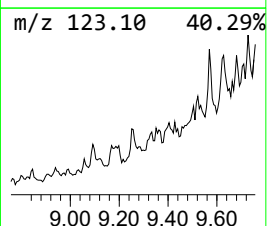
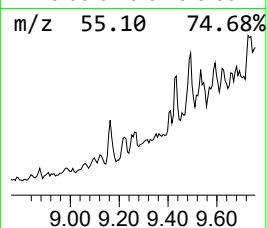
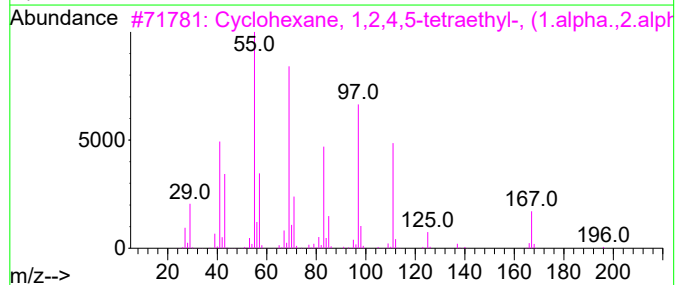
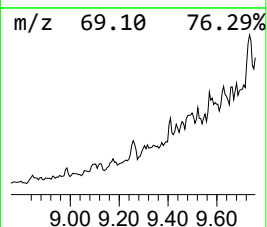
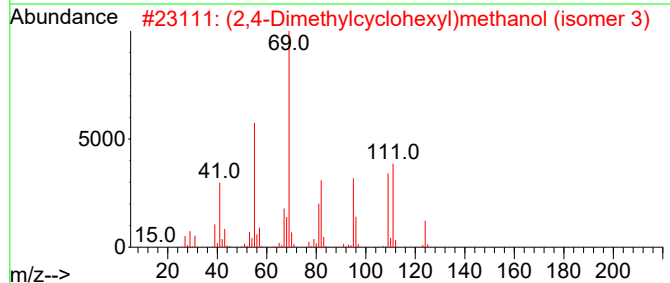
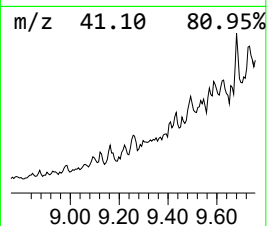
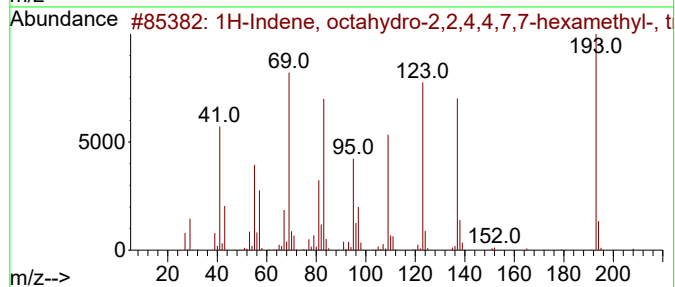
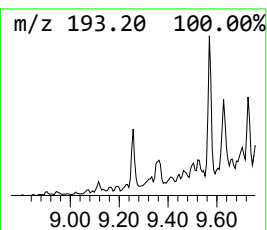
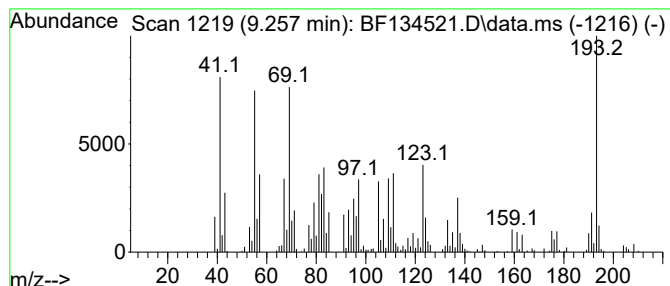
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown9.257 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	6.68 ng	269307	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	38
2			(2,4-Dimethylcyclohexyl)methanol...	142	C9H18O	1000499-02-8	30
3			Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	30
4			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	27
5			(2,4-Dimethylcyclohexyl)methanol...	142	C9H18O	1000499-02-6	22



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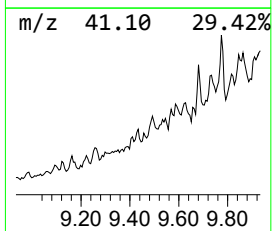
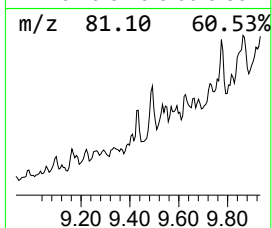
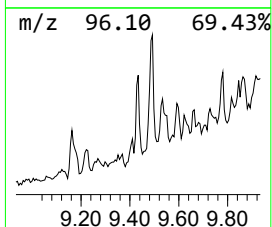
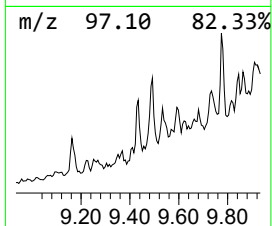
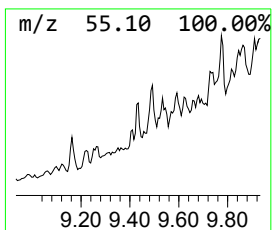
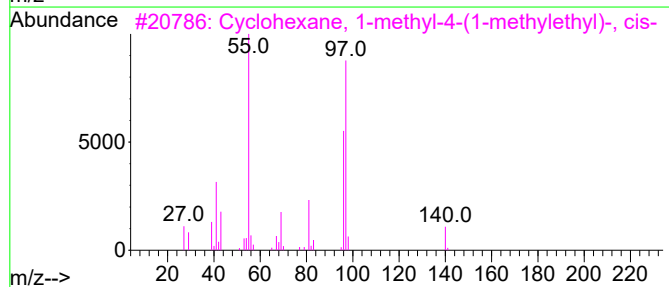
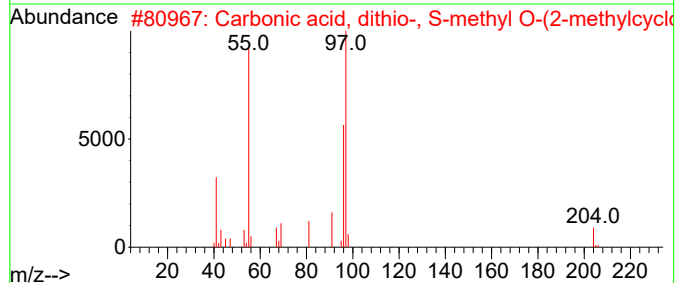
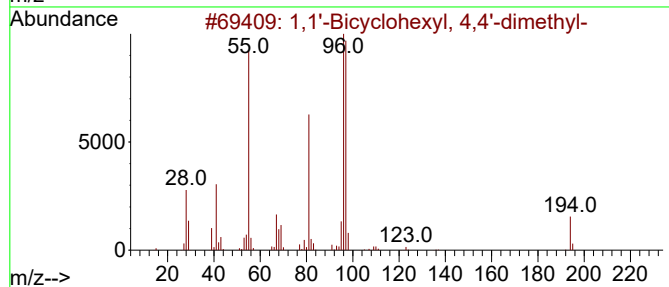
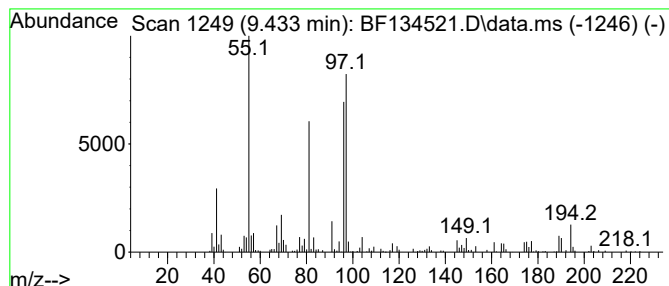
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,1'-Bicyclohexyl, 4,4'-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.433	4.59 ng	184910	Acenaphthene-d10	9.875	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Bicyclohexyl, 4,4'-dimethyl-	194	C14H26	054823-99-3	68
2	Carbonic acid, dithio-, S-methyl...	204	C9H16OS2	015288-13-8	59
3	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	59
4	1-Bromo-1-methyl-1-silacyclohexane	192	C6H13BrSi	085125-32-2	50
5	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054824-04-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
Data File : BF134521.D
Acq On : 28 Jul 2023 18:16
Operator : CG\JU
Sample : 03777-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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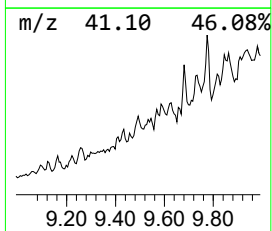
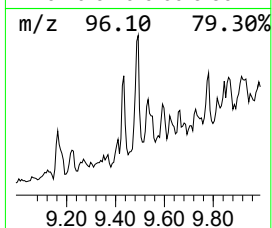
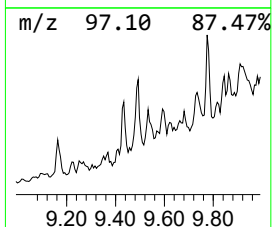
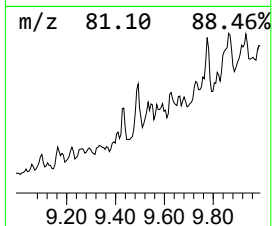
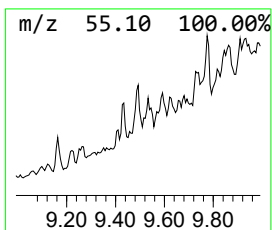
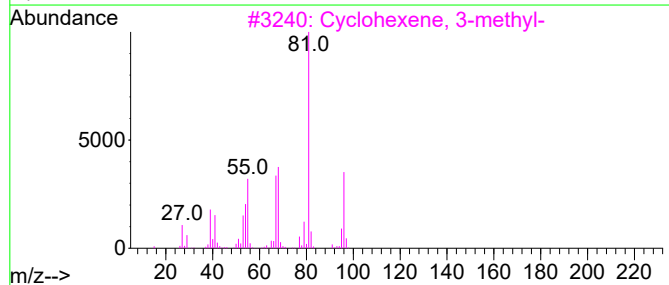
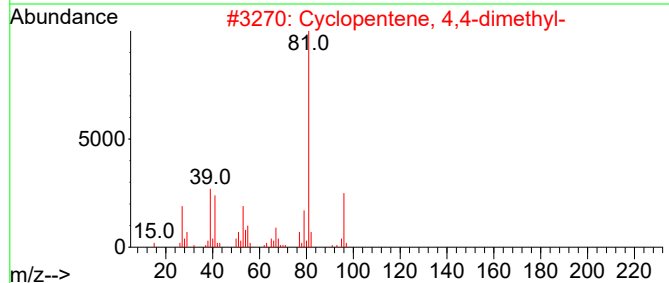
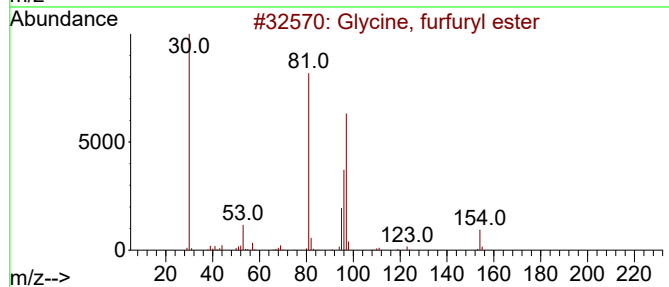
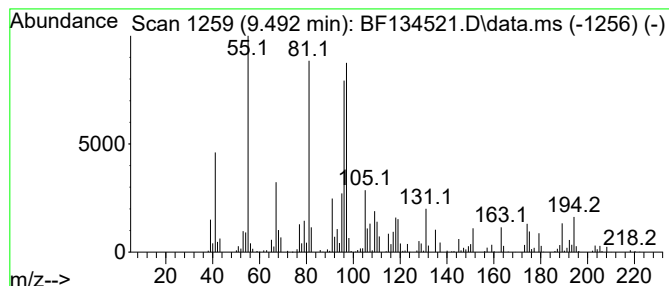
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Glycine, furfuryl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.492	10.25 ng	413180	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycine, furfuryl ester	155	C7H9NO3	1000306-78-7	50
2			Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	43
3			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	43
4			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	38
5			6-Methyl-bicyclo[4.2.0]octan-7-ol	140	C9H16O	1000193-87-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
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Acq On : 28 Jul 2023 18:16
Operator : CG\JU
Sample : 03777-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

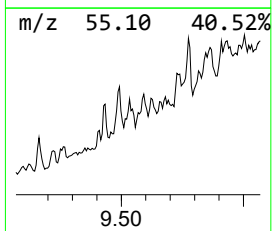
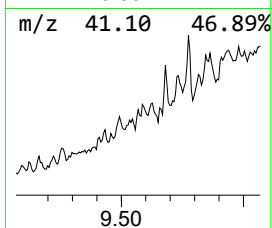
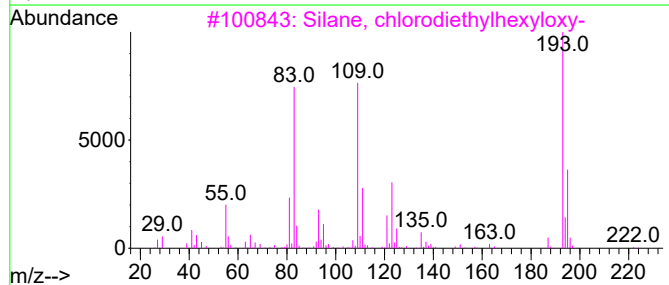
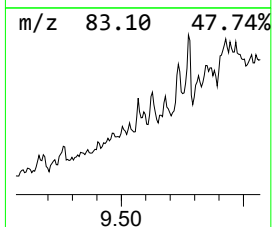
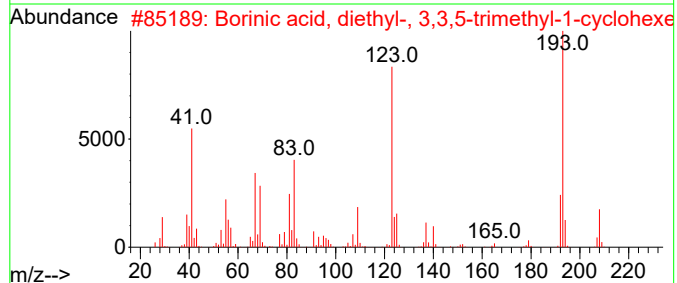
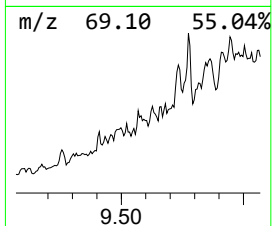
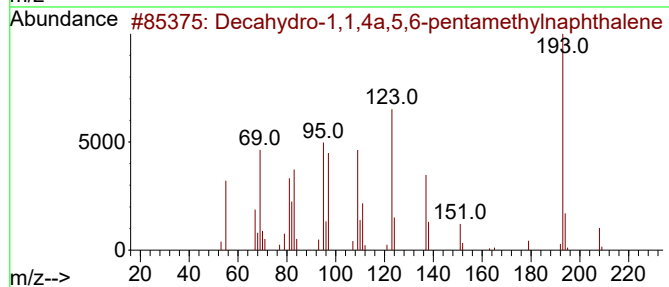
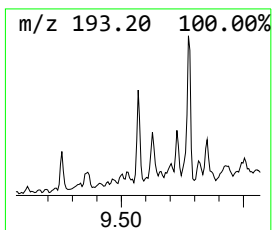
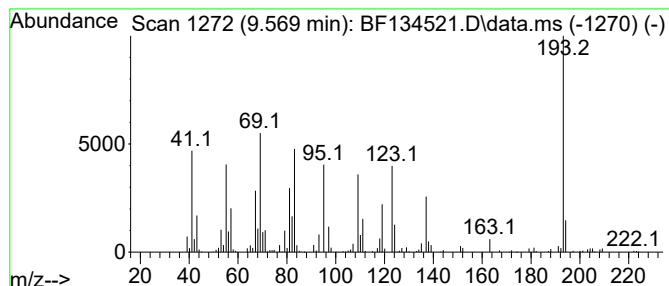
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.569	6.25 ng	251891	Acenaphthene-d10	9.875	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	58
2	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	47
3	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	47
4	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45
5	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
Data File : BF134521.D
Acq On : 28 Jul 2023 18:16
Operator : CG\JU
Sample : 03777-01
Misc :
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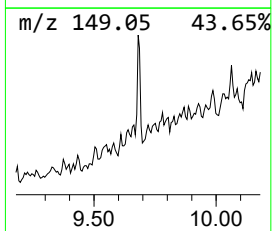
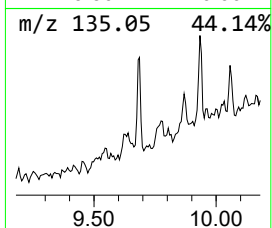
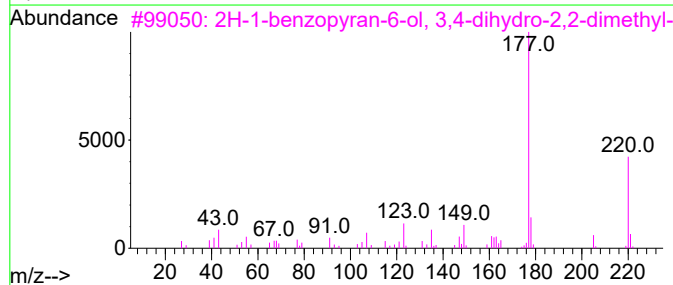
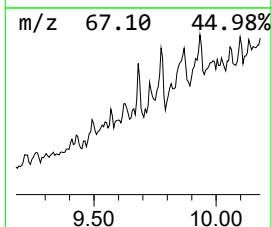
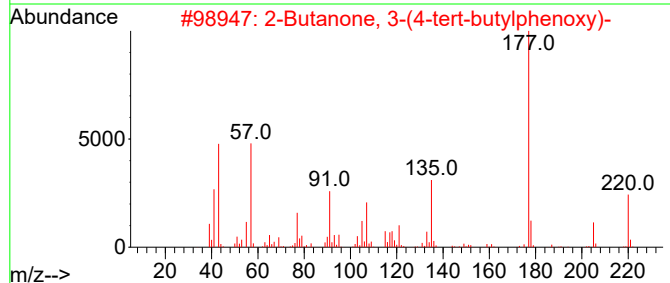
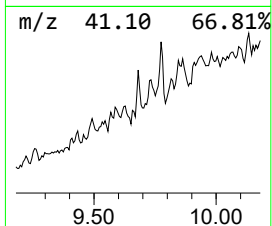
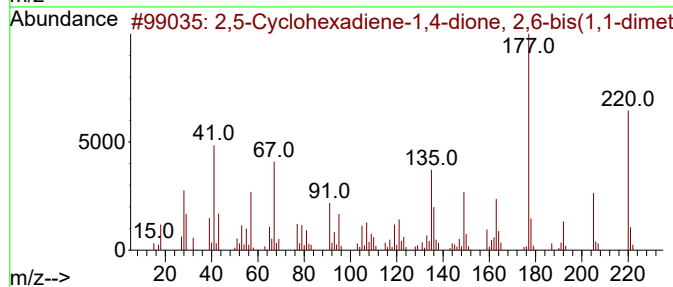
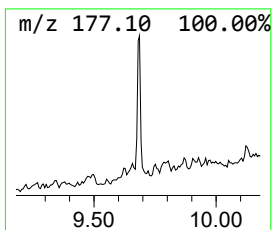
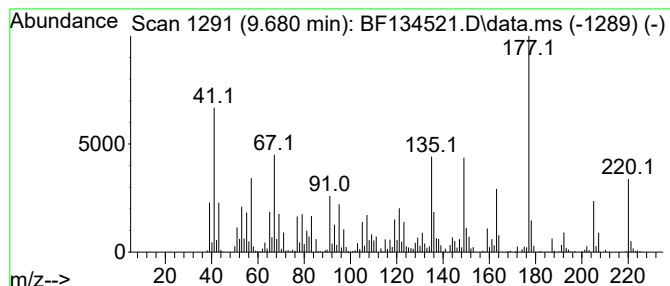
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.680	15.46 ng	622833	Acenaphthene-d10	9.875	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	45
3	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	41
4	1,3-Benzenedicarboxylic acid, di...	222	C12H14O4	000636-53-3	35
5	1-(4-Fluorophenyl)-1H-pyrazol-5-...	177	C9H8FN3	727967-95-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
Data File : BF134521.D
Acq On : 28 Jul 2023 18:16
Operator : CG\JU
Sample : 03777-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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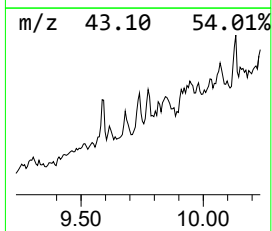
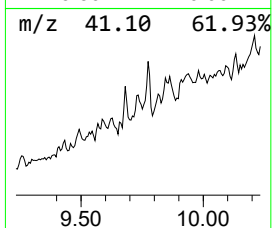
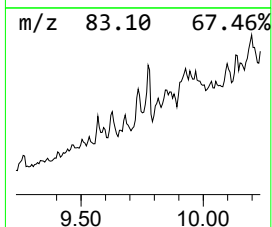
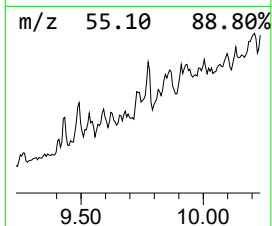
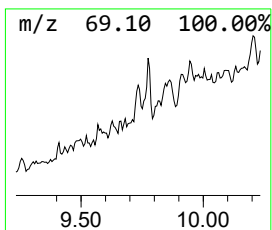
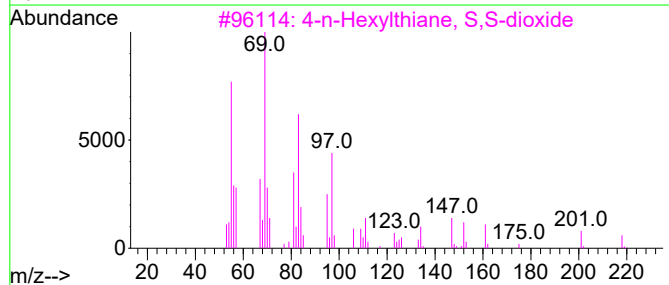
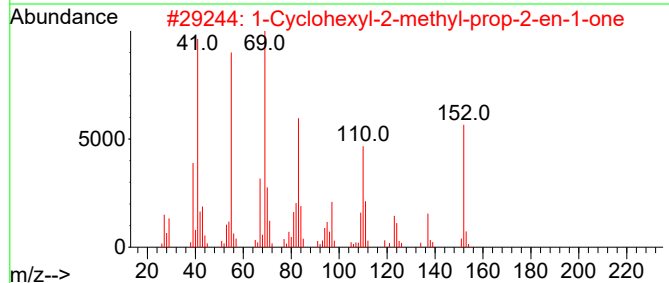
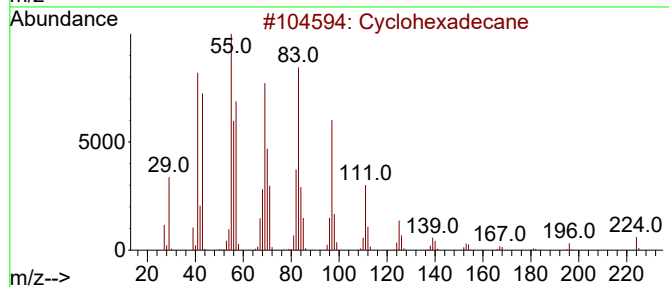
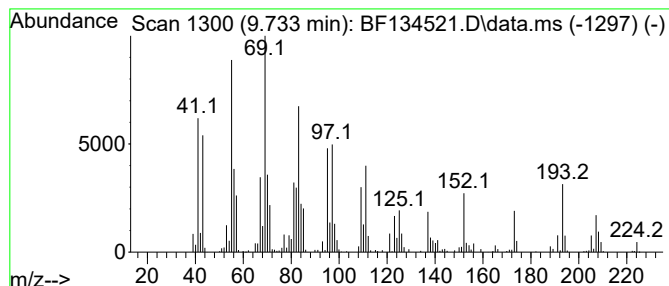
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	13.09 ng	527630	Acenaphthene-d10	9.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	55
2		1-Cyclohexyl-2-methyl-prop-2-en-...	152	C10H16O	025183-82-8	55
3		4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	38
4		Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	38
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
Data File : BF134521.D
Acq On : 28 Jul 2023 18:16
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Sample : 03777-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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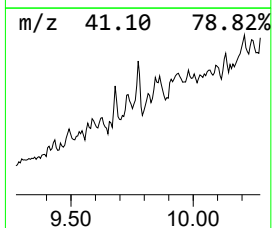
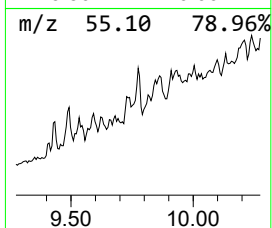
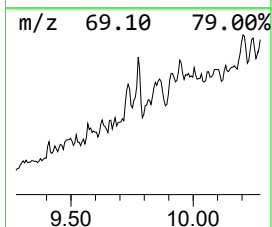
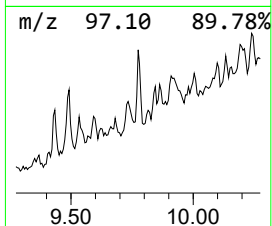
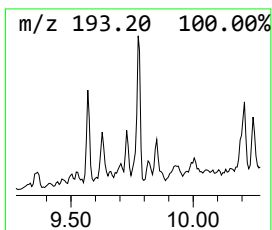
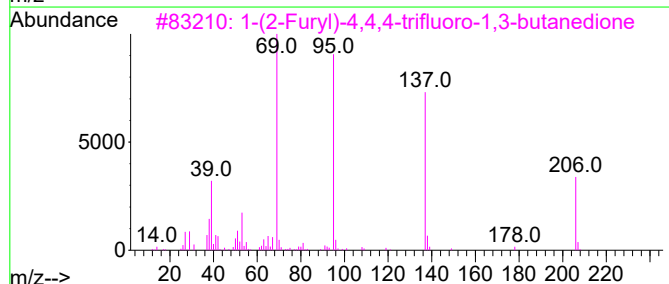
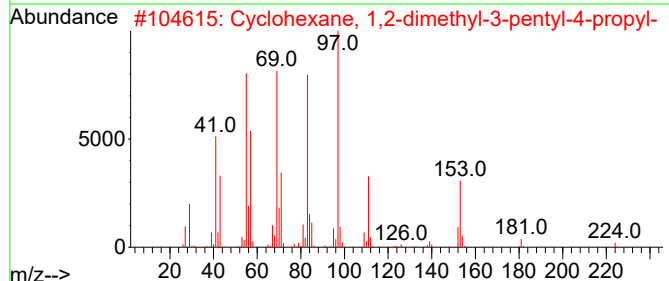
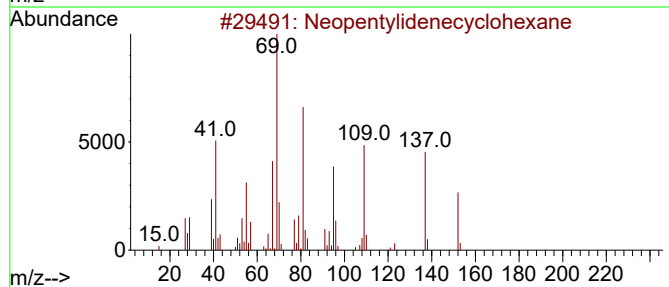
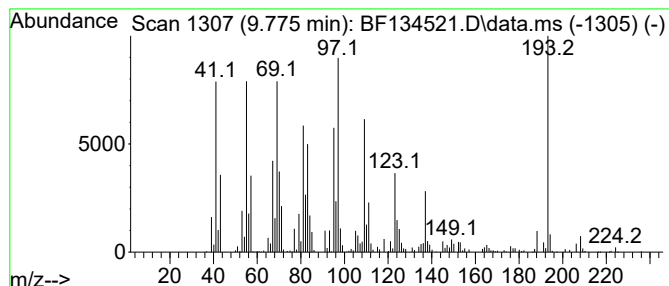
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown9.775 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.775	19.76 ng	796311	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentylidenecyclohexane	152	C11H20	039546-80-0	42
2			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	30
3			1-(2-Furyl)-4,4,4-trifluoro-1,3-...	206	C8H5F3O3	000326-90-9	25
4			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	25
5			Citronellyl valerate	240	C15H28O2	007540-53-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
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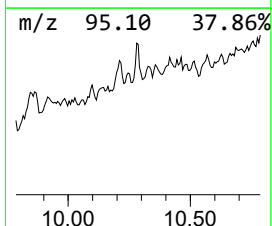
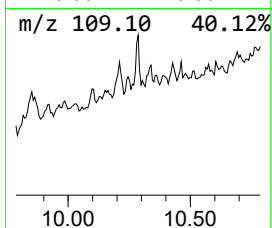
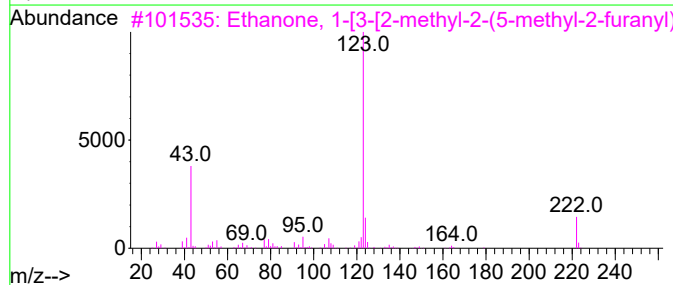
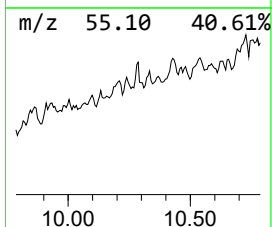
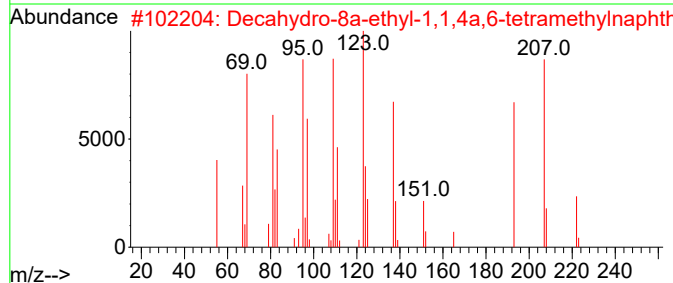
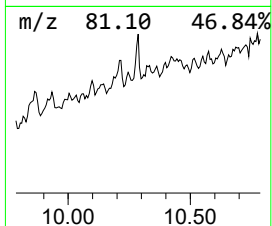
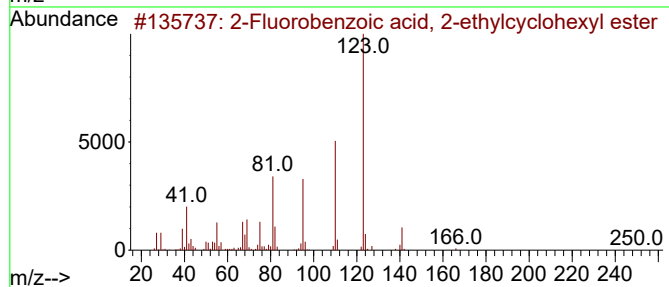
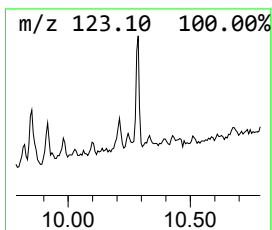
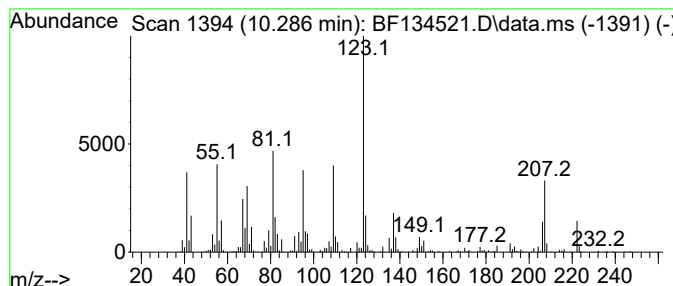
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.286 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.286	18.50 ng	745662	Acenaphthene-d10	9.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19F02	1000278-98-1	43
2		Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	43
3		Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	43
4		3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19F02	1000279-04-9	43
5		4-Fluorobenzoic acid, 4-tridecyl...	322	C20H31F02	1000280-68-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
Data File : BF134521.D
Acq On : 28 Jul 2023 18:16
Operator : CG\JU
Sample : 03777-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.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
unknown8.728	8.728	2.9	ng	100160	2	8.104	683020	20.0
unknown8.981	8.981	2.4	ng	83162	2	8.104	683020	20.0
unknown9.098	9.098	2.3	ng	93289	3	9.875	805911	20.0
unknown9.122	9.122	2.1	ng	85212	3	9.875	805911	20.0
unknown9.257	9.257	6.7	ng	269307	3	9.875	805911	20.0
1,1'-Bicyclohex...	9.433	4.6	ng	184910	3	9.875	805911	20.0
Glycine, furfur...	9.492	10.3	ng	413180	3	9.875	805911	20.0
Decahydro-1,1,4...	9.569	6.3	ng	251891	3	9.875	805911	20.0
2,5-Cyclohexadi...	9.680	15.5	ng	622833	3	9.875	805911	20.0
Cyclohexadecane	9.733	13.1	ng	527630	3	9.875	805911	20.0
unknown9.775	9.775	19.8	ng	796311	3	9.875	805911	20.0
unknown10.286	10.286	18.5	ng	745662	3	9.875	805911	20.0