

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121924\
Data File : BF140939.D
Acq On : 19 Dec 2024 20:52
Operator : RC/JU
Sample : P5342-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB21198

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF121624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140939.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.493	573	578	605	rBV	622660	986873	51.09%	8.555%
2	6.504	745	750	776	rBV	684206	1085698	56.21%	9.411%
3	6.851	804	809	816	rBV	211812	268703	13.91%	2.329%
4	7.416	900	905	914	rBV	438865	590607	30.58%	5.120%
5	8.128	1022	1026	1032	rBV	256701	322129	16.68%	2.792%
6	8.751	1128	1132	1137	rBV5	74447	181243	9.38%	1.571%
7	9.122	1191	1195	1196	rBV3	200039	267570	13.85%	2.319%
8	9.204	1204	1209	1213	rBV	833569	1180617	61.12%	10.234%
9	9.281	1218	1222	1225	rBV2	394840	581147	30.09%	5.038%
10	9.592	1271	1275	1280	rBV2	1253237	1917950	99.29%	16.626%
11	9.751	1299	1302	1305	rBV3	748201	1060983	54.93%	9.197%
12	9.798	1306	1310	1314	rVB	1443448	1931623	100.00%	16.744%
13	10.304	1393	1396	1400	rBV	965639	1160996	60.10%	10.064%

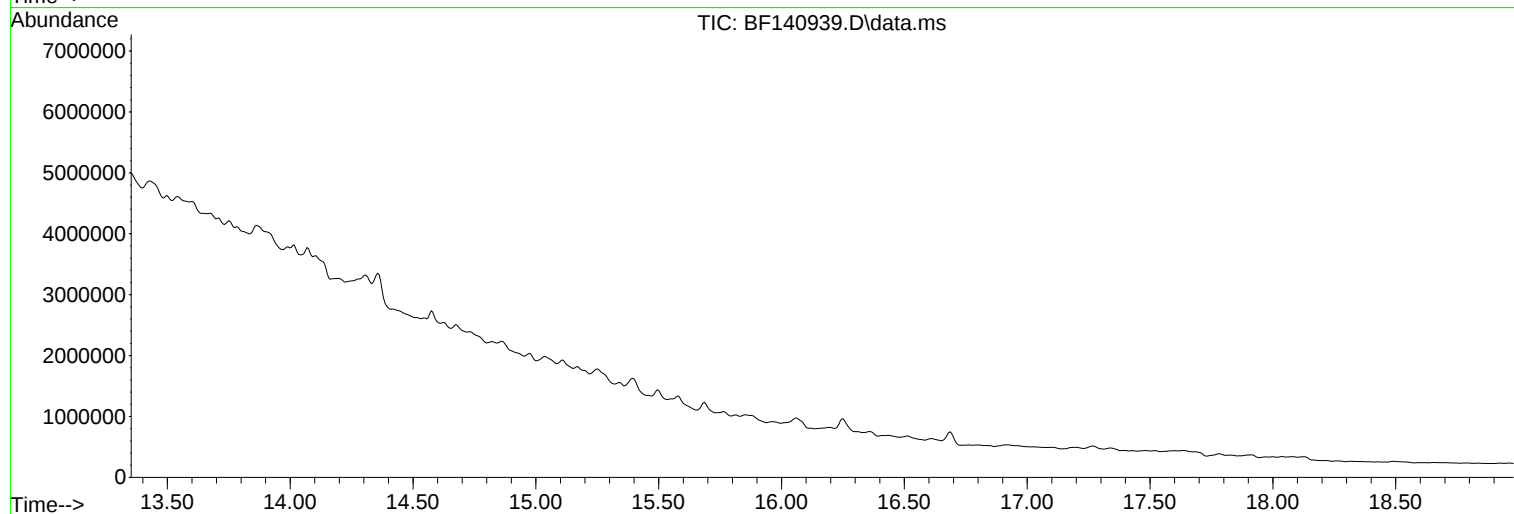
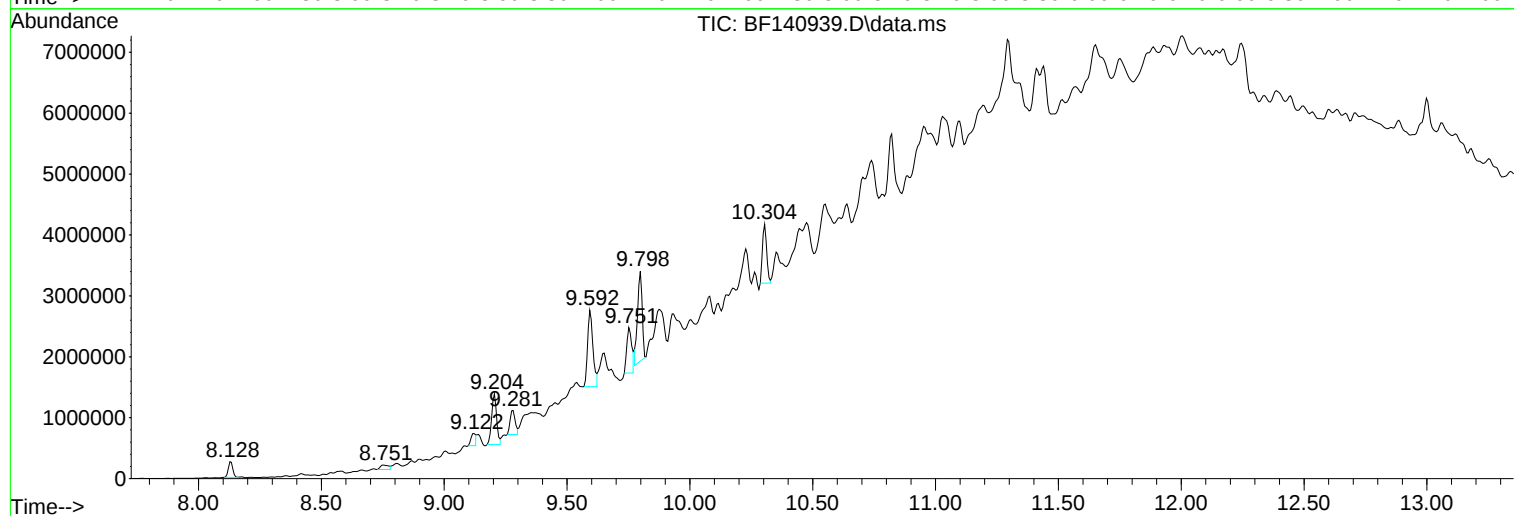
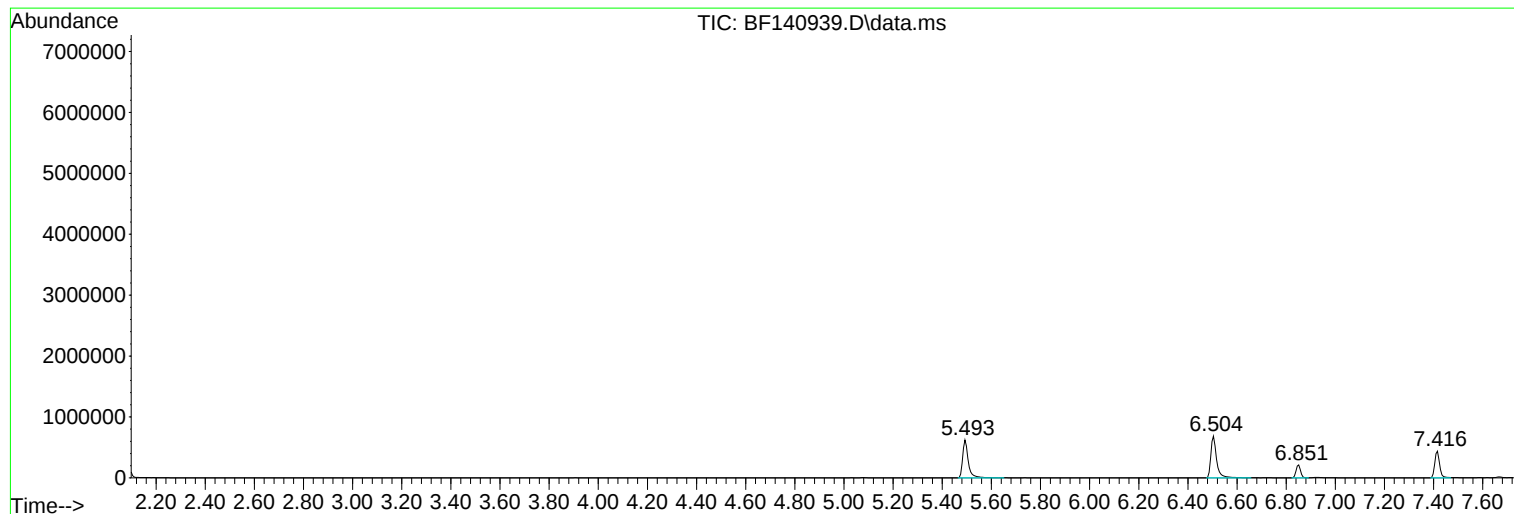
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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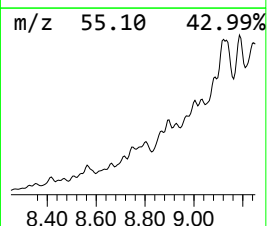
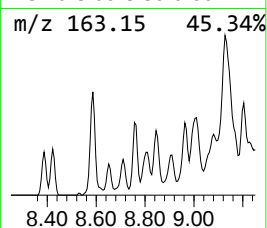
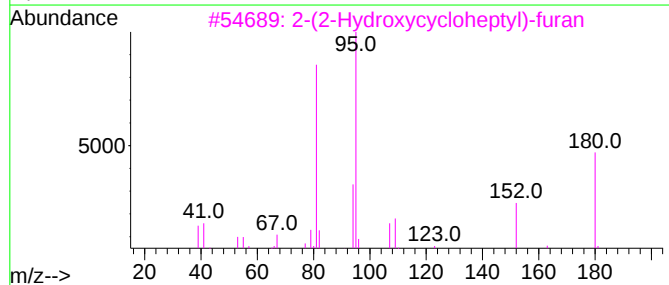
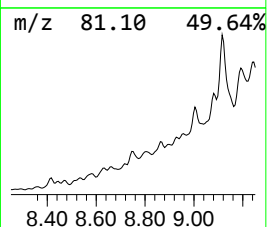
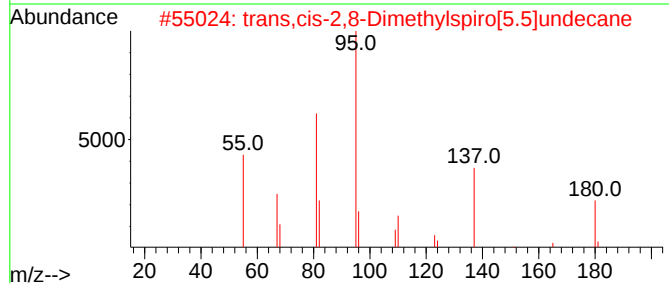
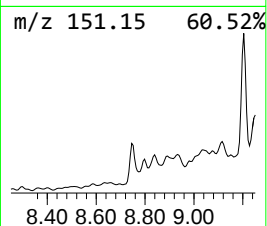
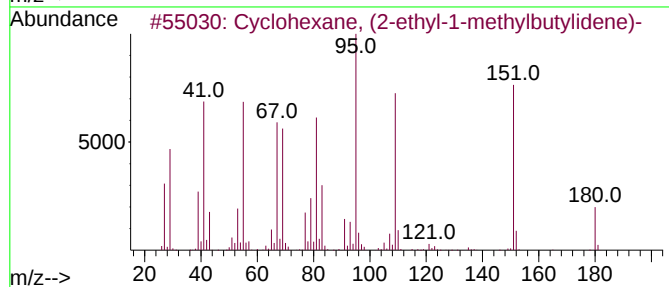
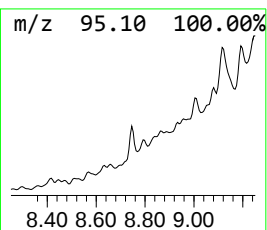
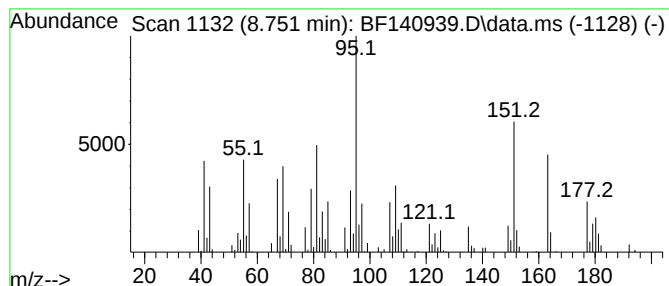
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown8.751 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.751	11.25 ng	181243	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	45
2			trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	38
3			2-(2-Hydroxycycloheptyl)-furan	180	C11H16O2	1000145-02-9	38
4			1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	27
5			5-Octen-2-yn-4-ol	124	C8H12O	1010196-87-1	25



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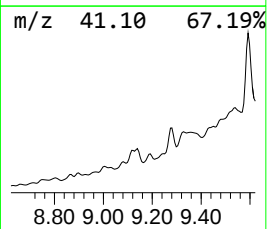
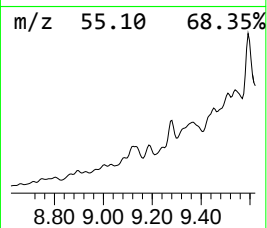
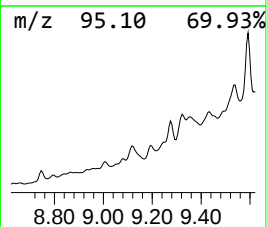
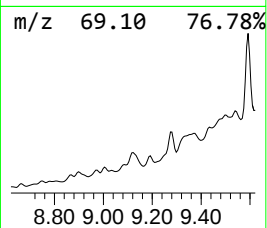
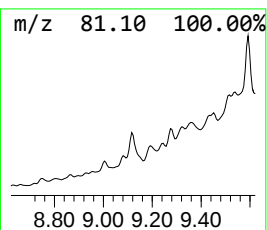
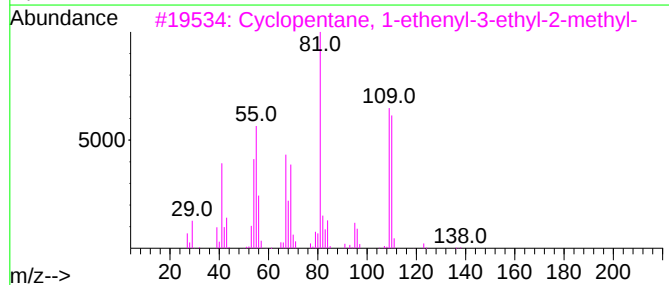
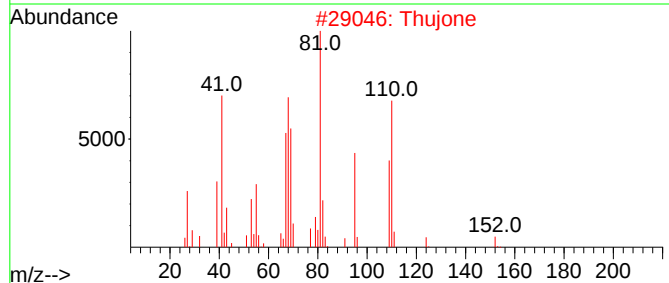
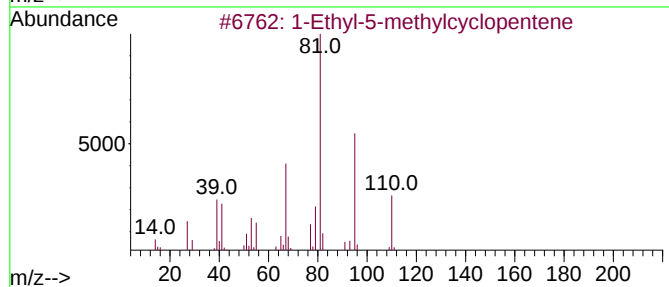
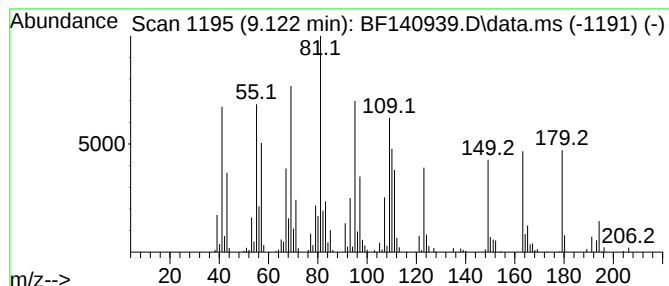
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Peak Number 2 unknown9.122 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.122	2.77 ng	267570	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	30
2			Thujone	152	C10H16O	000546-80-5	25
3			Cyclopentane, 1-ethenyl-3-ethyl-...	138	C10H18	055170-98-4	22
4			1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	18
5			3,4,5-Trimethylpyrazole	110	C6H10N2	005519-42-6	18



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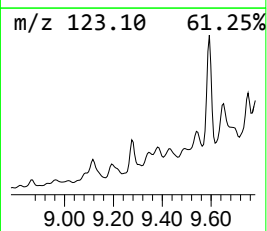
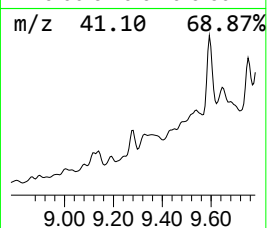
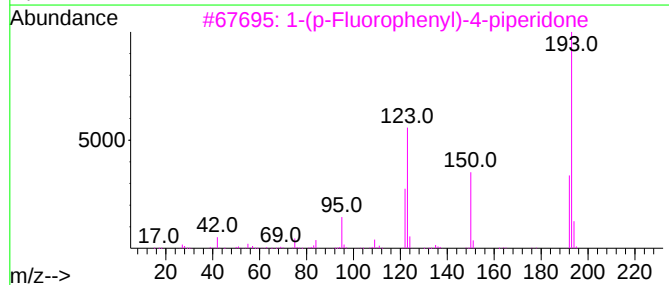
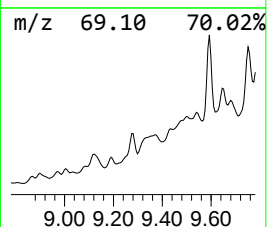
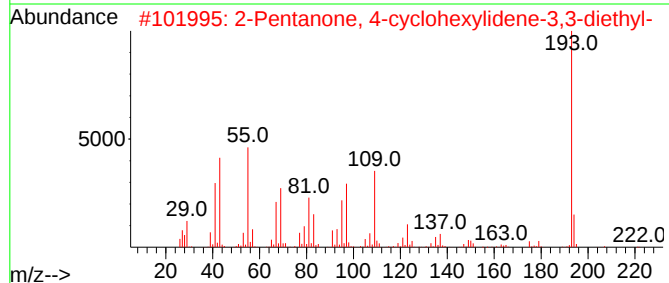
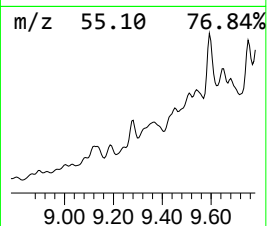
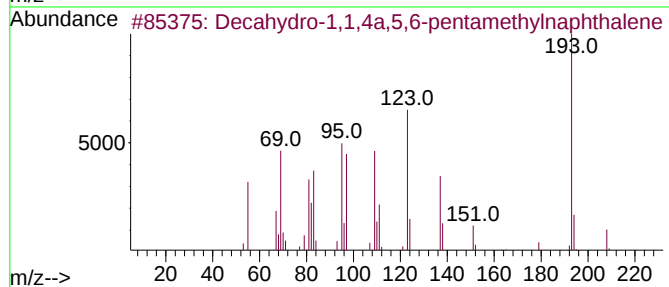
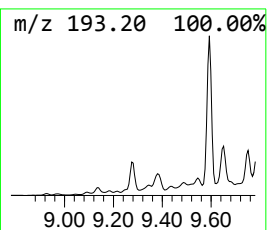
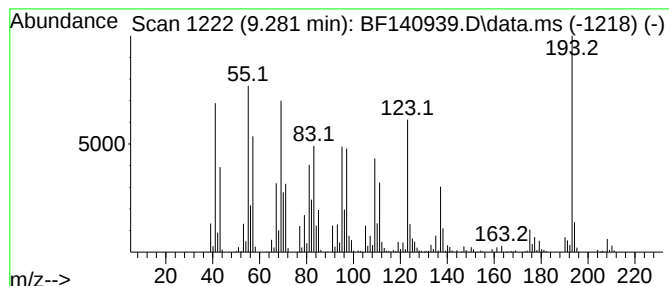
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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.281	6.02 ng	581147	Acenaphthene-d10			9.892
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	80
2	2-Pentanone, 4-cyclohexylidene-3...		222	C15H26O	313253-65-5	43
3	1-(p-Fluorophenyl)-4-piperidone		193	C11H12FNO	1000238-56-7	43
4	2-Anthracenamine		193	C14H11N	000613-13-8	30
5	Bicyclo[3.1.1]heptan-3-one, 2-(b...		192	C13H20O	1010163-96-1	25



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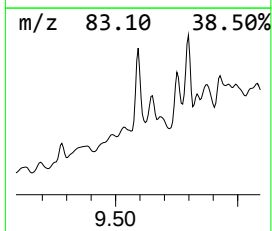
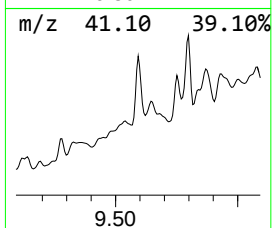
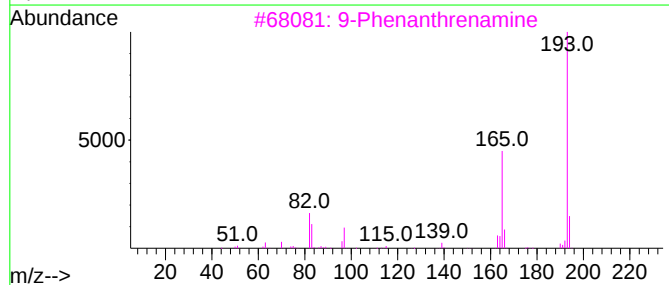
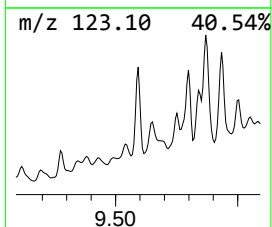
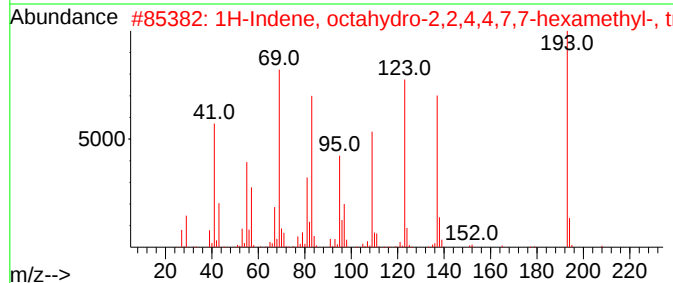
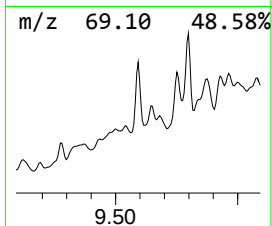
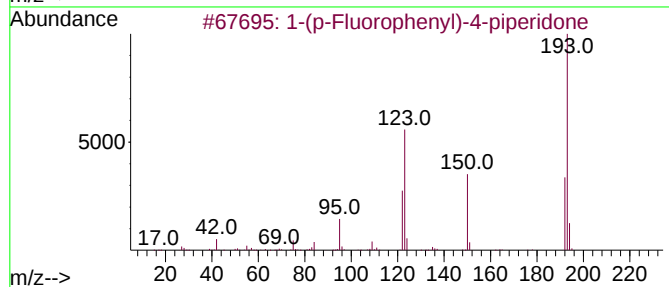
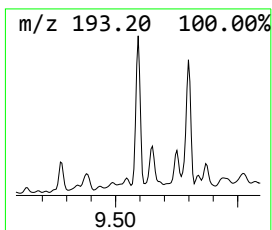
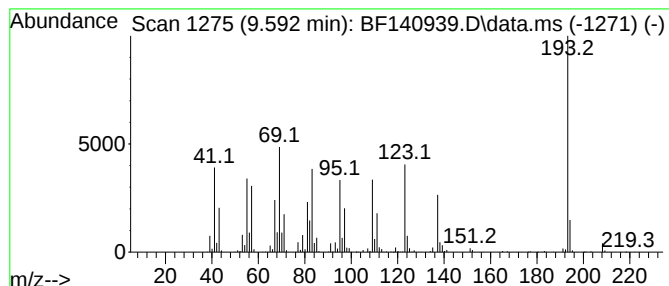
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Peak Number 4 unknown9.592 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	19.86 ng	1917950	Acenaphthene-d10	9.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	47	
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	40	
3	9-Phenanthrenamine	193	C14H11N	000947-73-9	38	
4	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	38	
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38	



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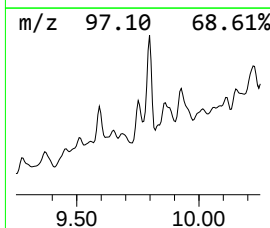
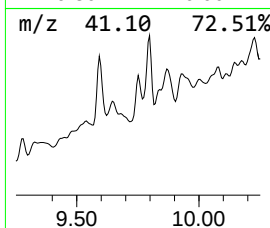
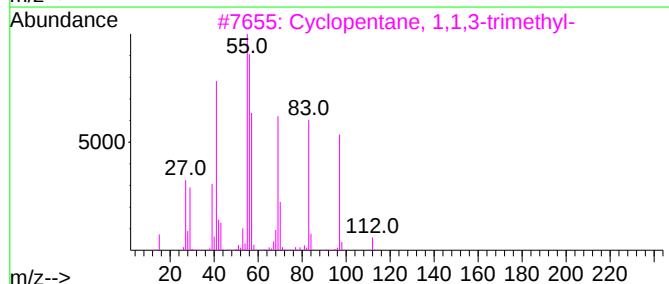
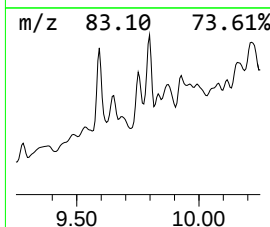
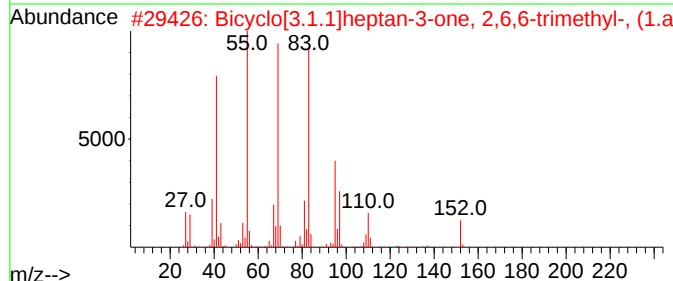
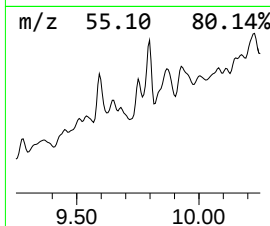
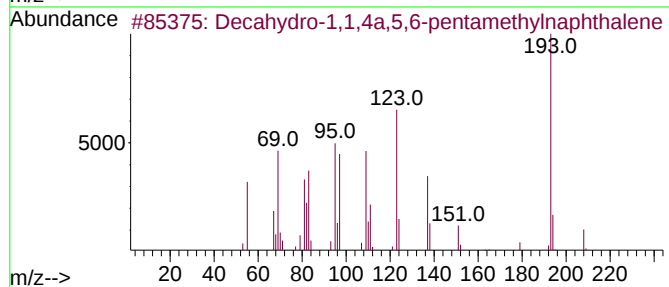
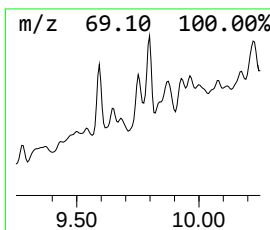
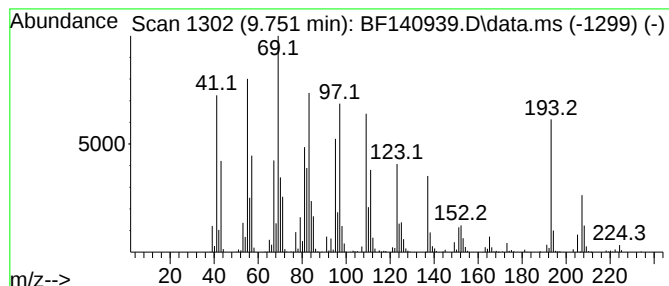
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Peak Number 5 unknown9.751 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.751	10.99 ng	1060980	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	60
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	43
3			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	43
4			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	38
5			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	38



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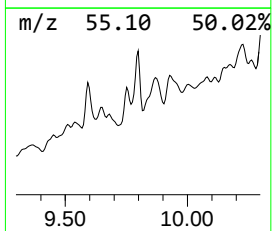
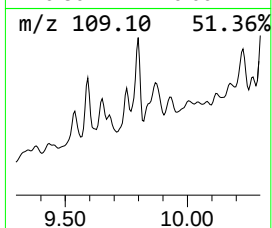
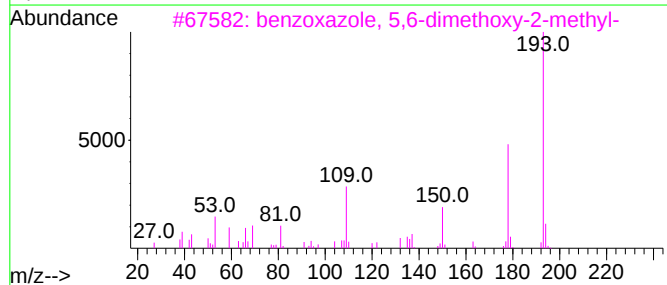
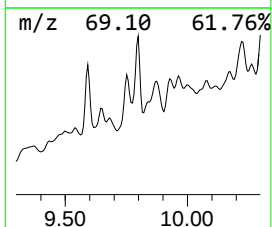
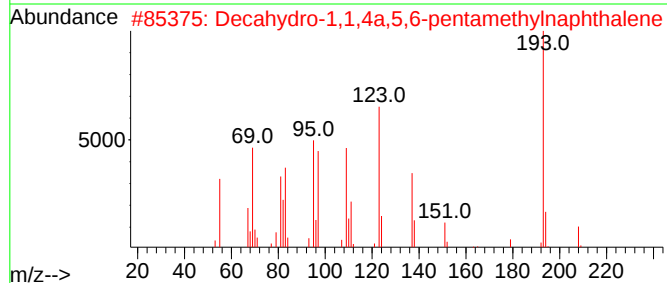
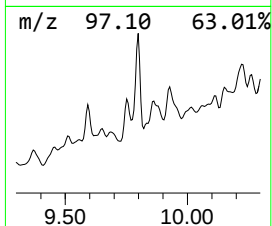
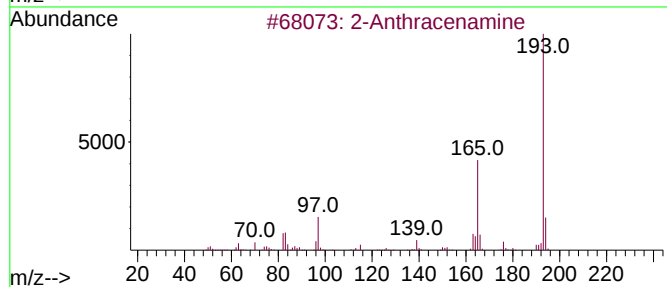
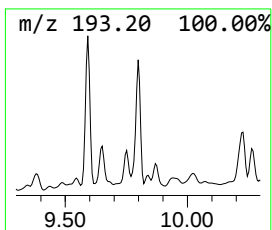
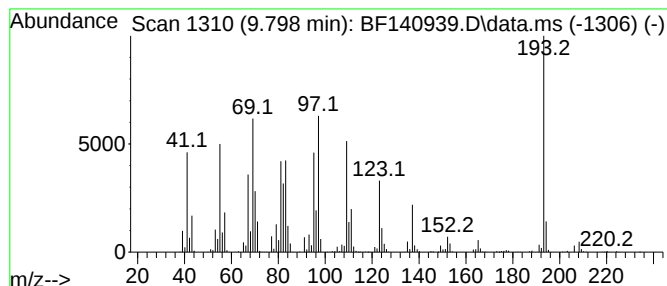
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.798 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.798	20.00 ng	1931620	Acenaphthene-d10	9.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Anthracenamine		193	C14H11N	000613-13-8	41
2	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	38
3	benzoxazole, 5,6-dimethoxy-2-met...		193	C10H11NO3	1000395-98-9	22
4	2,6-Heptadienal, 2,4-dimethyl-		138	C9H14O	085136-08-9	22
5	Hexadecanedinitrile		248	C16H28N2	006812-44-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121924\
Data File : BF140939.D
Acq On : 19 Dec 2024 20:52
Operator : RC/JU
Sample : P5342-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB21198

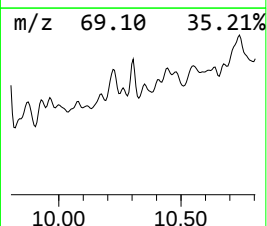
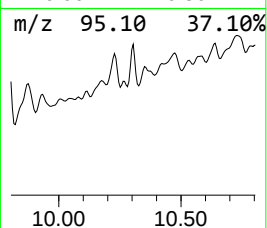
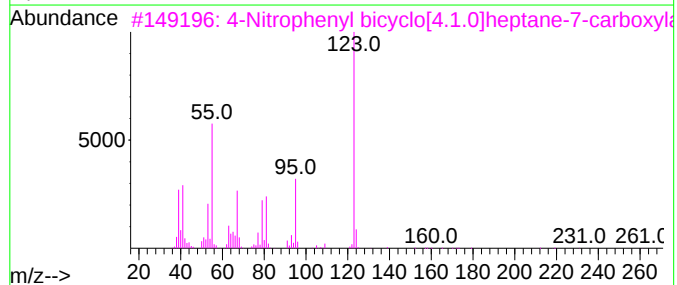
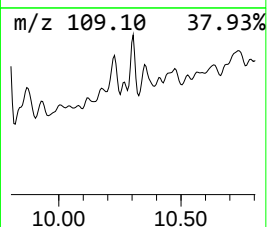
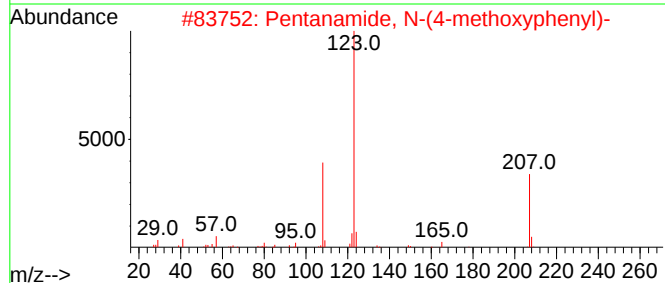
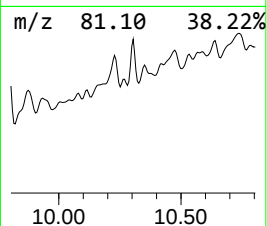
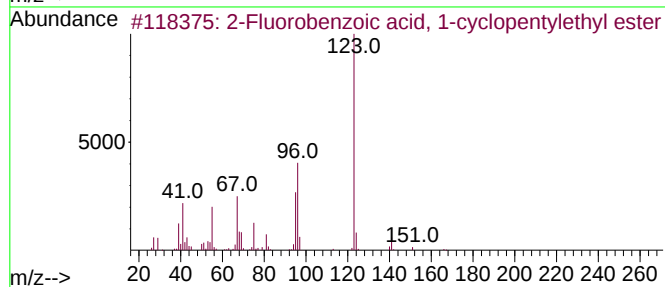
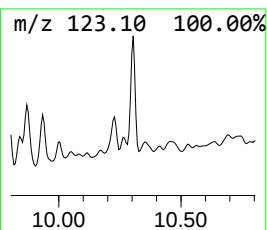
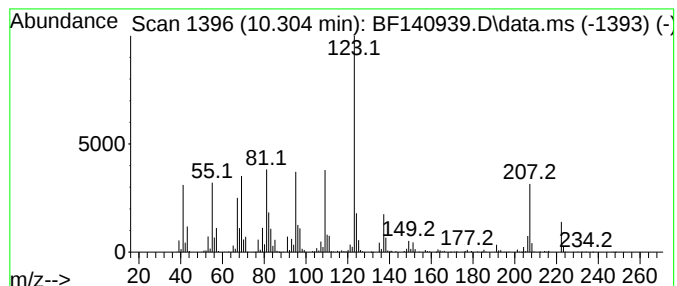
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.304 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.304	12.02 ng	1161000	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Fluorobenzoic acid, 1-cyclopentylethyl ester	236	C14H17FO2	1000278-98-2	47
2			Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	47
3			4-Nitrophenyl bicyclo[4.1.0]heptane-7-carboxamide	261	C14H15NO4	328938-65-4	47
4			Bicyclo[4.1.0]heptane-7-carboxamide	222	C11H14N2OS	329912-72-3	47
5			4-Fluorobenzoic acid, 3-pentadecyl ester	350	C22H35FO2	1000280-68-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121924\
Data File : BF140939.D
Acq On : 19 Dec 2024 20:52
Operator : RC/JU
Sample : P5342-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB21198

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121624.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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unknown9.122	9.122	2.8	ng	267570	3	9.892	1931620	20.0
Decahydro-1,1,4...	9.281	6.0	ng	581147	3	9.892	1931620	20.0
unknown9.592	9.592	19.9	ng	1917950	3	9.892	1931620	20.0
unknown9.751	9.751	11.0	ng	1060980	3	9.892	1931620	20.0
unknown9.798	9.798	20.0	ng	1931620	3	9.892	1931620	20.0
unknown10.304	10.304	12.0	ng	1161000	3	9.892	1931620	20.0