

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
 Data File : BF141971.D
 Acq On : 14 Mar 2025 18:06
 Operator : RC/JU
 Sample : Q1553-01 5X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT2321

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-BF031025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141971.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	570	577	585	rBV	319457	443196	19.40%	4.005%
2	6.493	743	748	758	rVB	303758	390498	17.09%	3.529%
3	6.881	809	814	820	rBV	438526	562001	24.60%	5.079%
4	7.434	898	908	914	rBV	191860	259247	11.35%	2.343%
5	8.157	1026	1031	1037	rBV	528510	670917	29.36%	6.063%
6	9.228	1209	1213	1218	rBV	428663	601195	26.31%	5.433%
7	9.310	1224	1227	1231	rBV4	153828	223409	9.78%	2.019%
8	9.622	1277	1280	1285	rBV2	444316	712815	31.20%	6.441%
9	9.728	1294	1298	1302	rBV	704667	950664	41.61%	8.591%
10	9.781	1304	1307	1310	rBV2	497065	713889	31.24%	6.451%
11	9.828	1311	1315	1318	rVB	833160	1100748	48.17%	9.947%
12	9.910	1324	1329	1333	rBV3	872937	1568231	68.63%	14.171%
13	10.328	1397	1400	1405	rBV3	1614859	2284965	100.00%	20.648%
14	15.510	2277	2281	2293	rVB	340262	584412	25.58%	5.281%

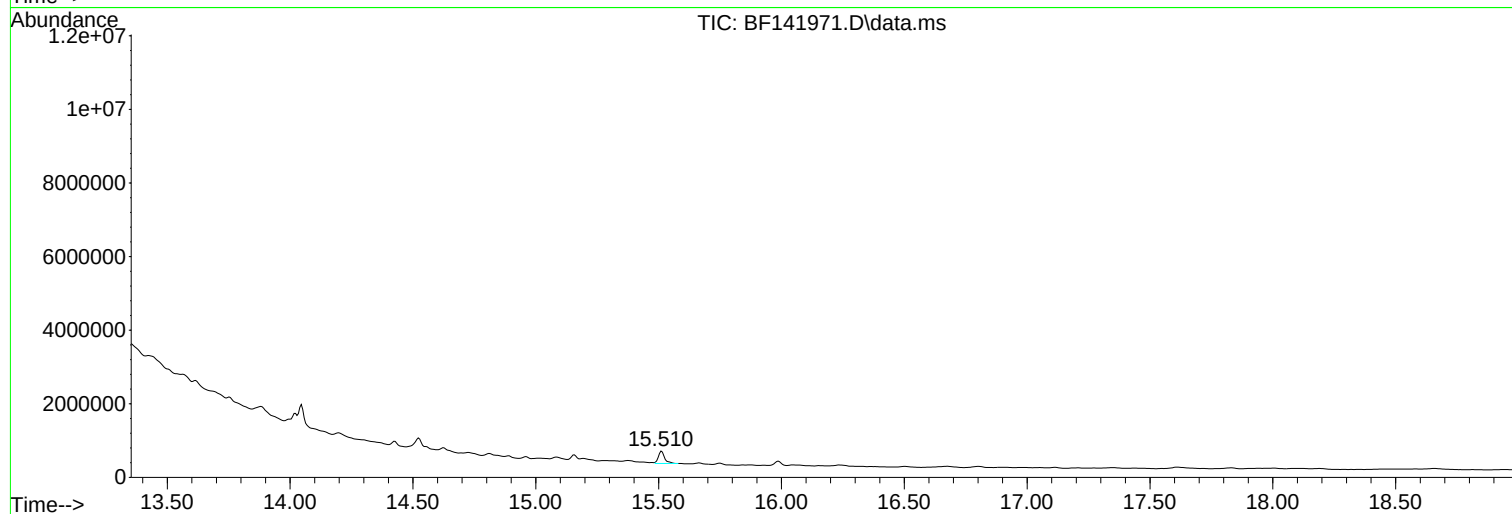
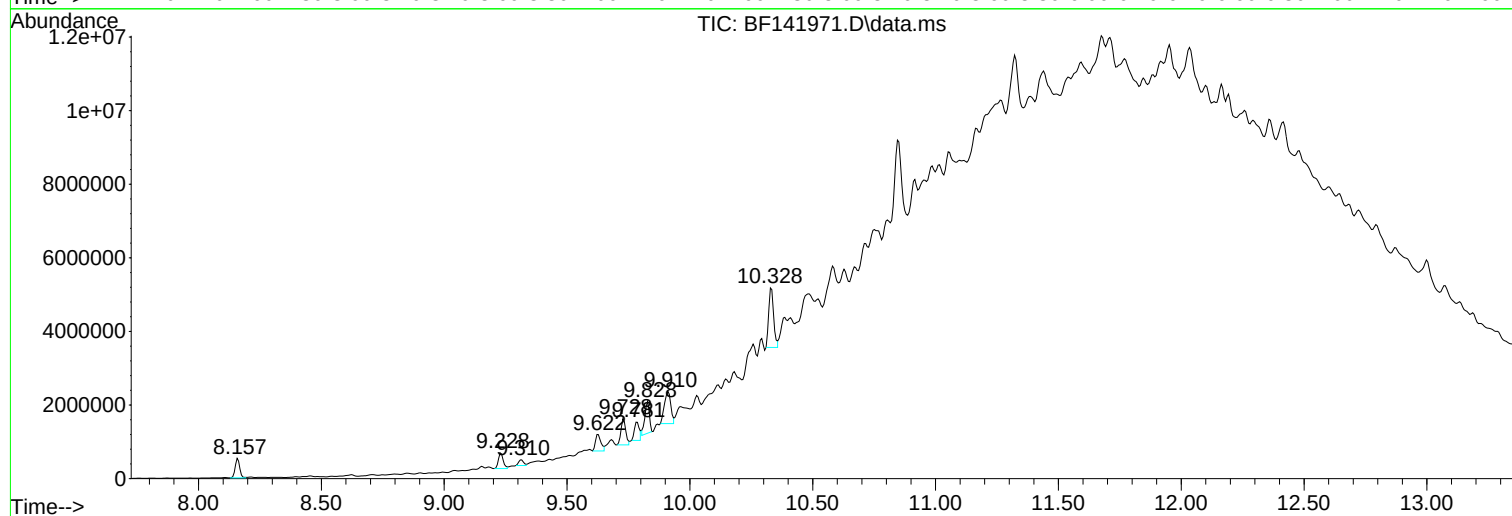
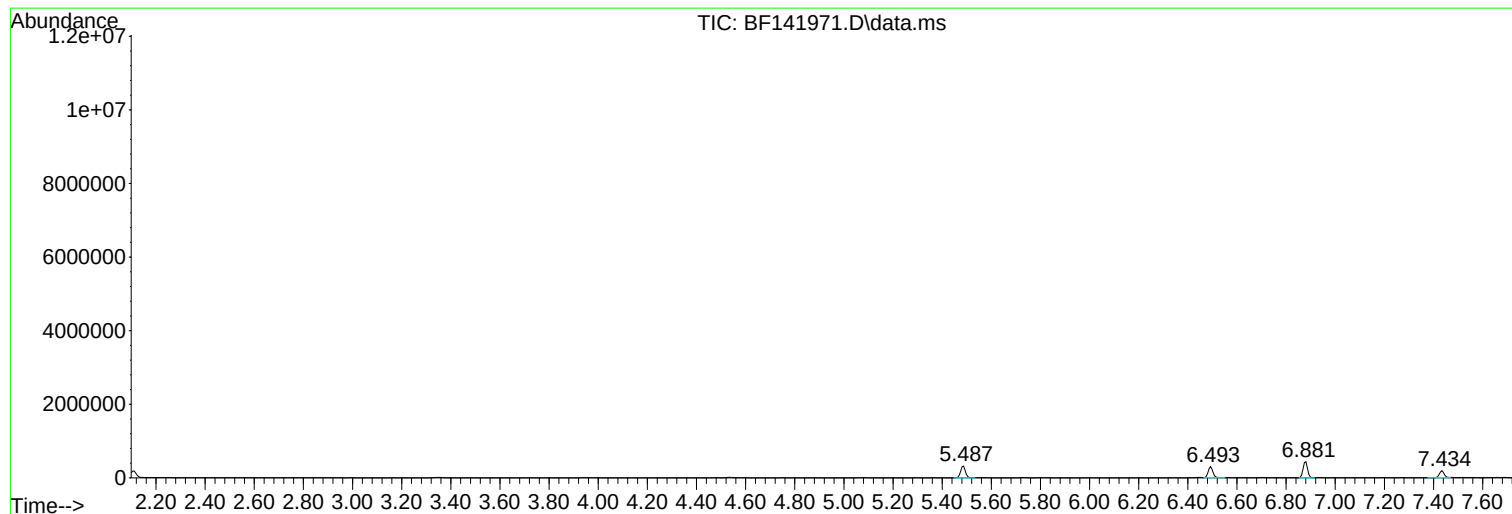
Sum of corrected areas: 11066187

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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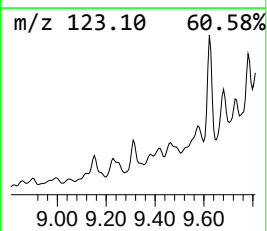
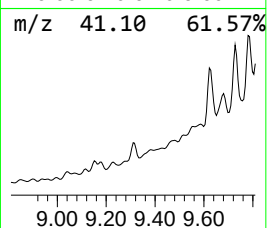
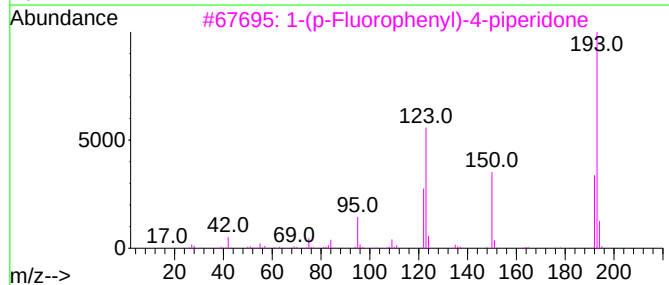
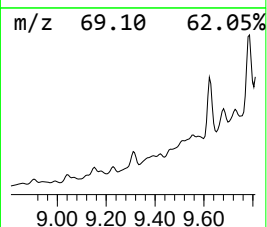
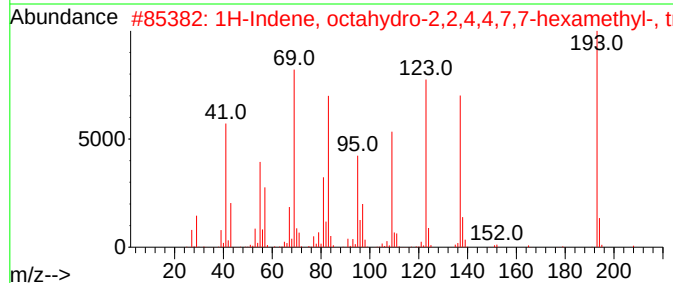
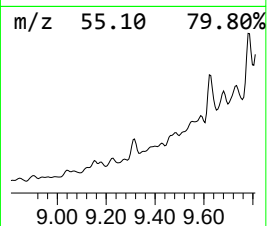
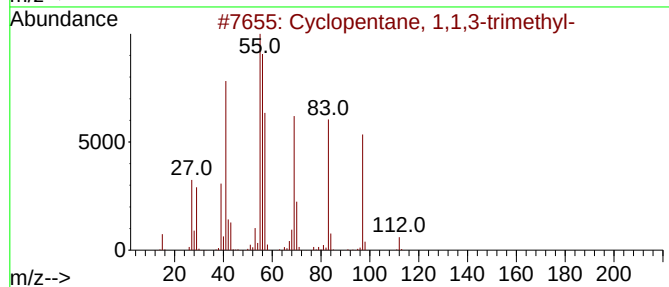
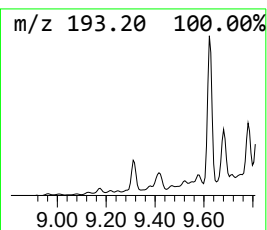
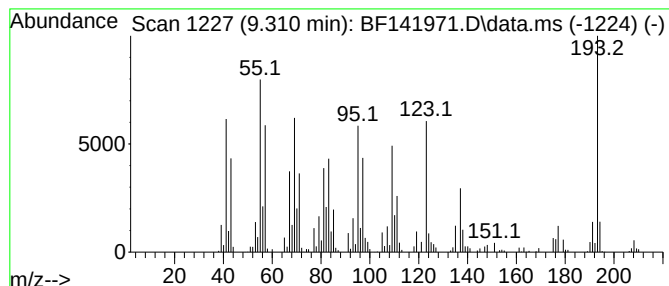
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown9.310 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.310	2.85 ng	223409	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	45
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	35
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	30
4			Octacosanol	410	C28H58O	000557-61-9	30
5			Toxoflavin	193	C7H7N5O2	000084-82-2	25



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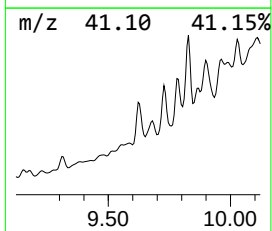
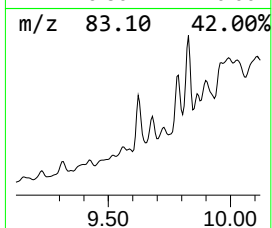
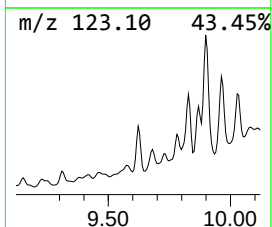
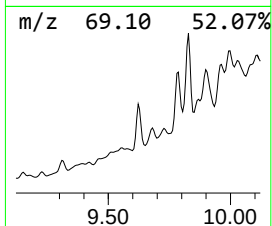
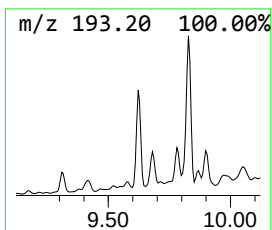
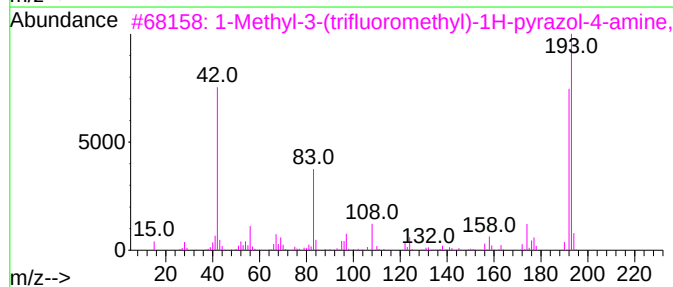
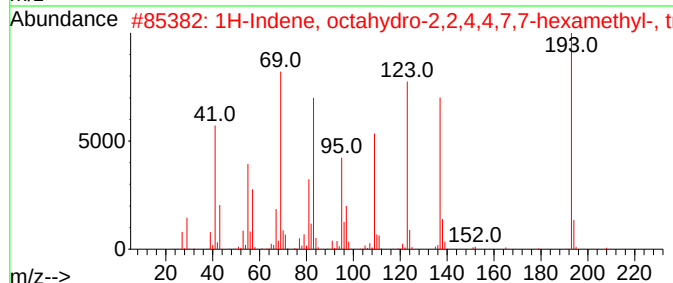
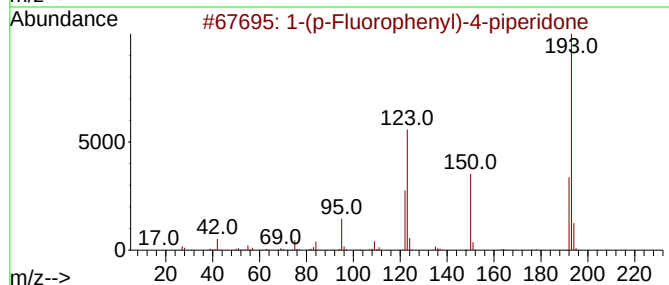
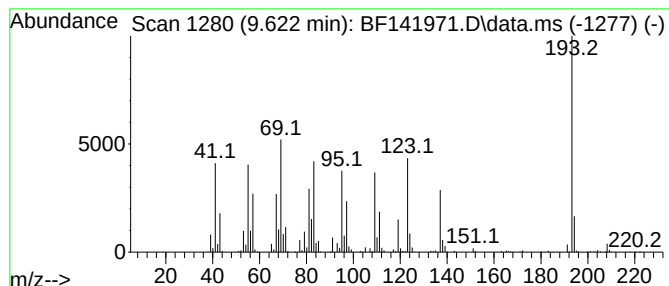
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown9.622 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.622	9.09 ng	712815	Acenaphthene-d10			9.916

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	42
3		1-Methyl-3-(trifluoromethyl)-1H...	193	C7H10F3N3	1000511-73-1	38
4		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38
5		S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	37



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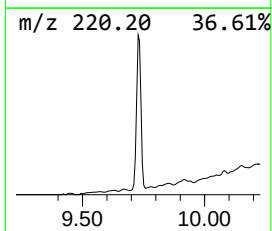
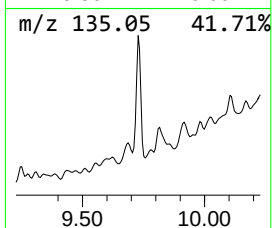
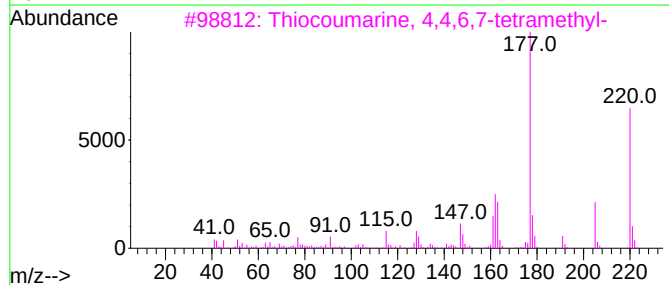
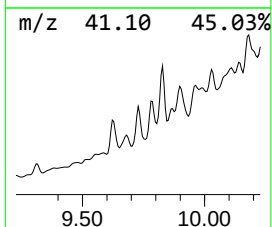
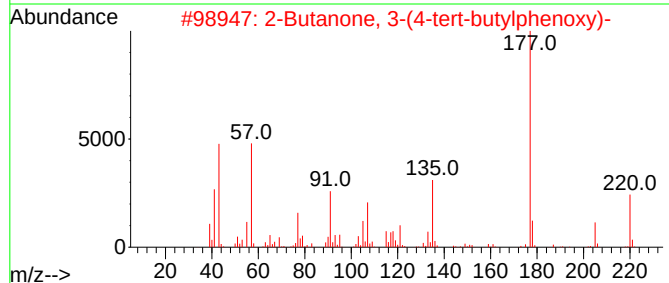
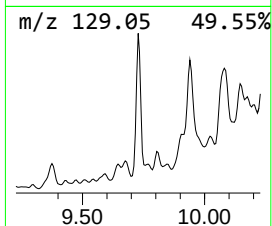
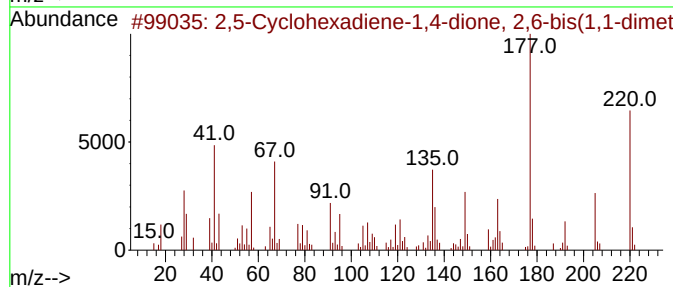
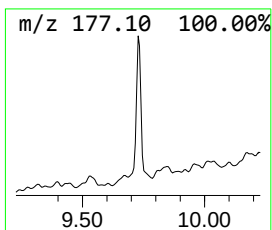
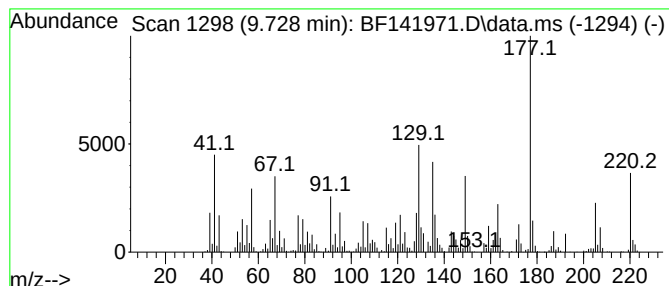
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Peak Number 3 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	12.12 ng	950664	Acenaphthene-d10	9.916

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	45		
3	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	45		
4	N-[4-(Ethyl-methyl-amino)-phenyl...	192	C11H16N2O	099981-45-0	43		
5	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	41		



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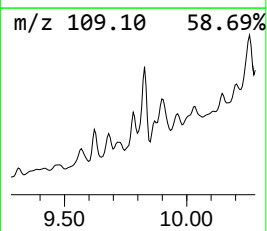
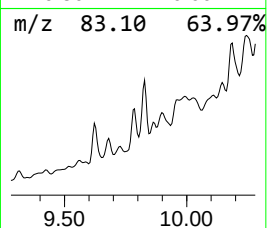
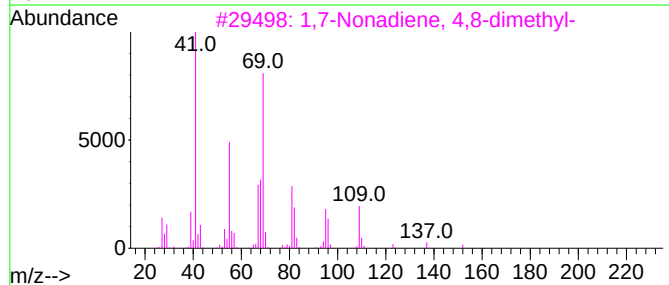
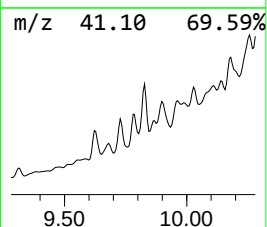
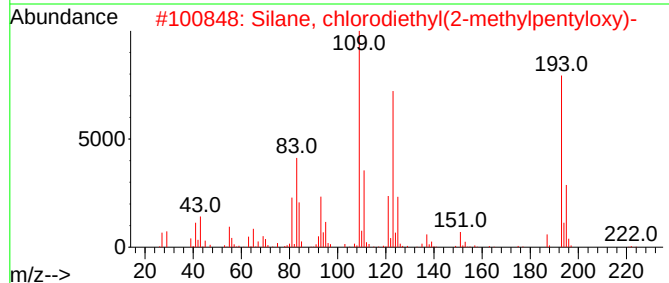
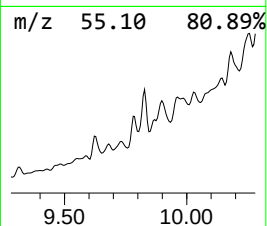
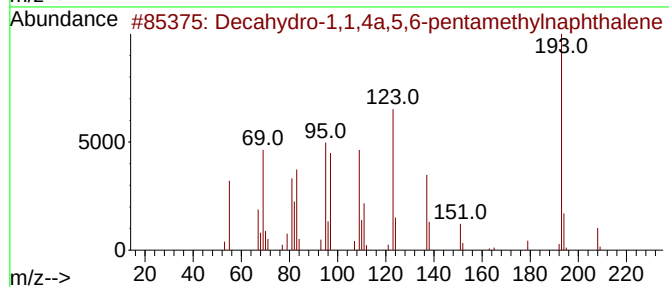
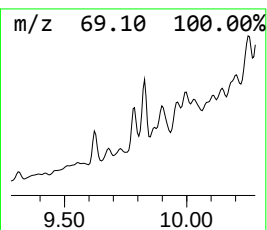
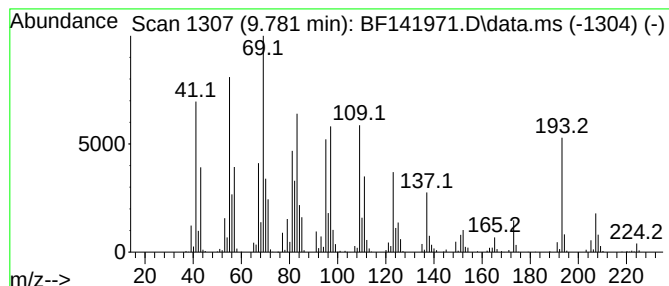
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Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.781	9.10 ng	713889	Acenaphthene-d10	9.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	91
2	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	45
3	1,7-Nonadiene, 4,8-dimethyl-	152	C11H20	062108-28-5	43
4	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	43
5	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	38



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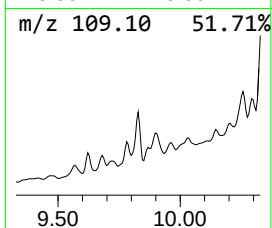
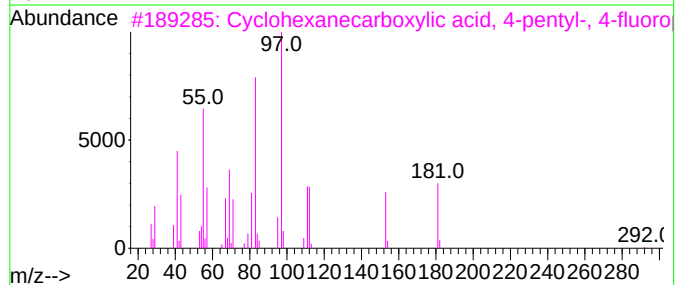
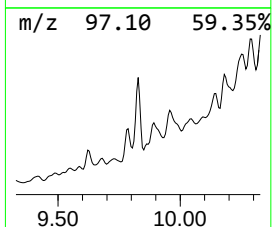
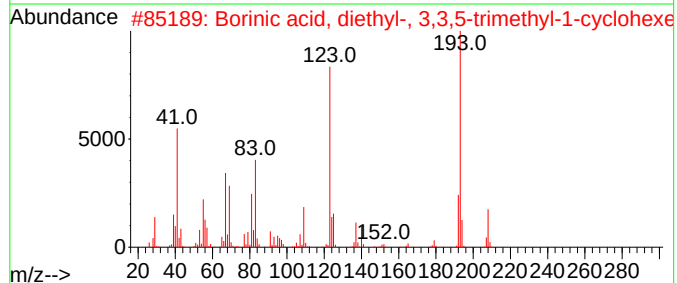
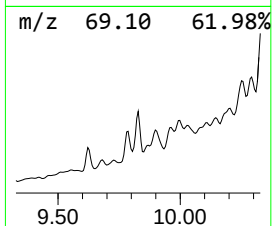
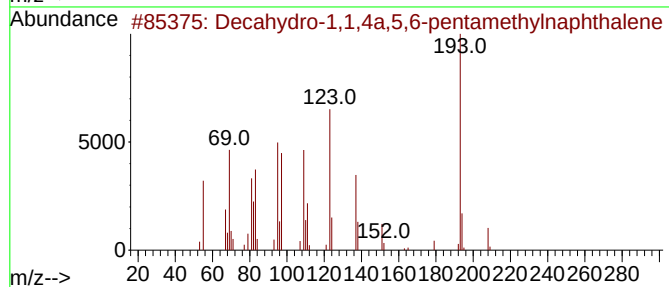
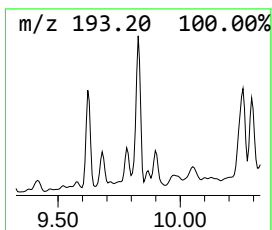
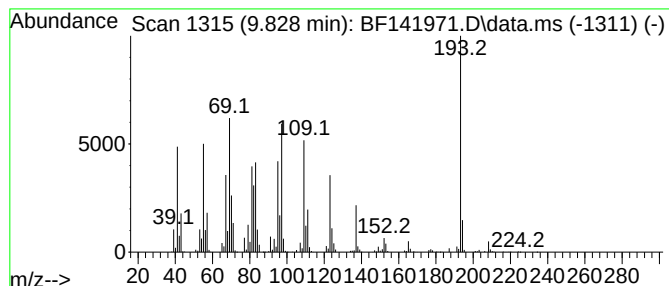
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.828 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.828	14.04 ng	1100750	Acenaphthene-d10	9.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
2	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	27
3	Cyclohexanecarboxylic acid, 4-pe...	292	C18H25FO2	079912-83-7	22
4	(Cyclopropyl)trivinylsilane	150	C9H14Si	1000109-93-8	22
5	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	18



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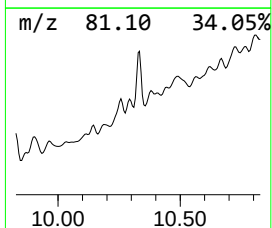
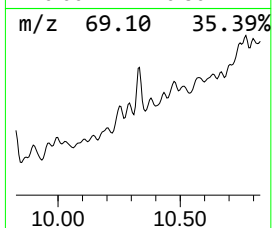
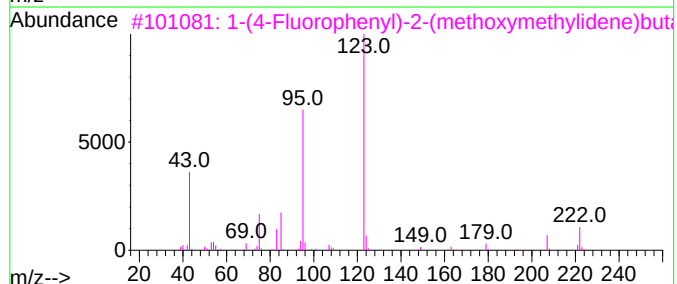
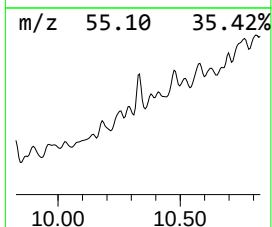
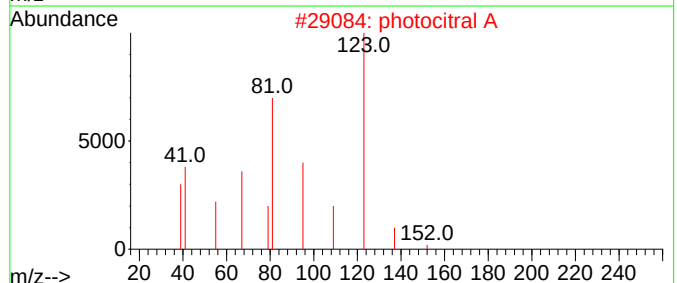
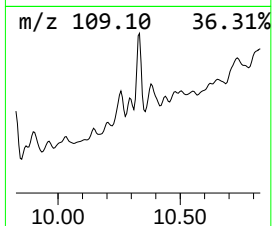
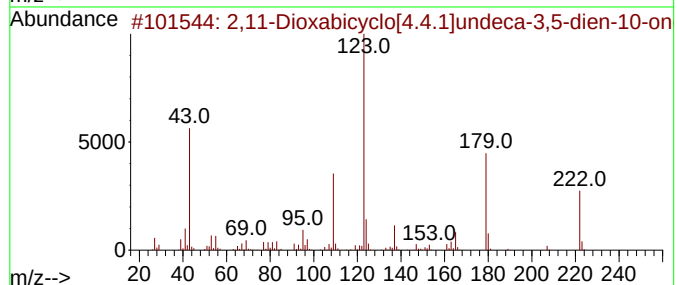
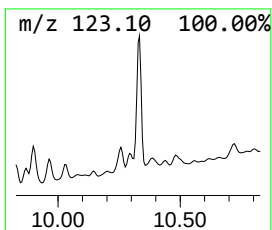
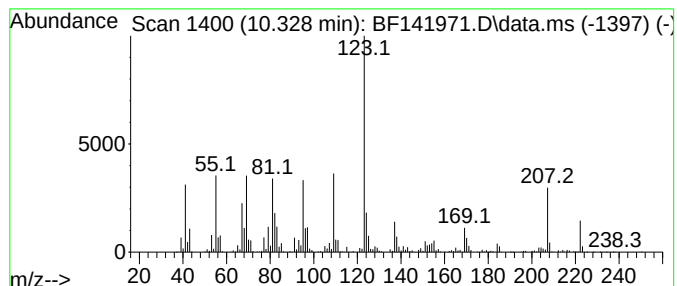
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ClientSampleId :
RT2321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.328	29.14 ng	2284970	Acenaphthene-d10		9.916
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	50
2	photocitral A	152	C10H16O	055253-28-6	50
3	1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	50
4	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	49
5	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141971.D
Acq On : 14 Mar 2025 18:06
Operator : RC/JU
Sample : Q1553-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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
unknown9.310	9.310	2.9	ng	223409	3	9.916	1568230	20.0
unknown9.622	9.622	9.1	ng	712815	3	9.916	1568230	20.0
2,5-Cyclohexadi...	9.728	12.1	ng	950664	3	9.916	1568230	20.0
Decahydro-1,1,4...	9.781	9.1	ng	713889	3	9.916	1568230	20.0
unknown9.828	9.828	14.0	ng	1100750	3	9.916	1568230	20.0
2,11-Dioxabicyc...	10.328	29.1	ng	2284970	3	9.916	1568230	20.0