

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020325\
 Data File : BF141394.D
 Acq On : 04 Feb 2025 02:35
 Operator : RC/JU
 Sample : Q1261-01 5X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHRT-20430

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-BF012925.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.798	794	800	806	rVB	362902	471432	2.40%	1.182%
2	7.969	993	999	1004	rVV9	79600	240655	1.23%	0.604%
3	8.022	1005	1008	1012	rVV4	124623	220052	1.12%	0.552%
4	8.081	1013	1018	1023	rVV	502011	796415	4.06%	1.998%
5	8.539	1090	1096	1100	rVB2	228578	491606	2.51%	1.233%
6	8.769	1132	1135	1141	rVB7	169944	269672	1.38%	0.676%
7	9.075	1184	1187	1190	rBV2	340039	393542	2.01%	0.987%
8	9.104	1190	1192	1196	rVB5	270253	292176	1.49%	0.733%
9	9.151	1196	1200	1204	rBV5	390307	560939	2.86%	1.407%
10	9.233	1210	1214	1219	rBV2	757996	1325365	6.76%	3.324%
11	9.551	1265	1268	1274	rBV3	1472569	2147084	10.95%	5.386%
12	9.710	1291	1295	1298	rBV3	1034767	1609070	8.21%	4.036%
13	9.757	1299	1303	1306	rVB	2001060	2647774	13.51%	6.641%
14	9.827	1311	1315	1321	rBV5	1442059	3230459	16.48%	8.103%
15	10.263	1385	1389	1394	rBV3	1974793	3088078	15.75%	7.746%
16	15.268	2236	2240	2253	rVB2	296861	531154	2.71%	1.332%
17	15.474	2261	2275	2281	rVB	7328672	19605435	100.00%	49.176%
18	15.621	2296	2300	2314	rVB	271057	567590	2.90%	1.424%
19	15.739	2316	2320	2328	rVB	126346	209125	1.07%	0.525%
20	16.062	2368	2375	2381	rBV3	130300	317214	1.62%	0.796%
21	16.551	2452	2458	2480	rVB	248599	617800	3.15%	1.550%
22	17.109	2547	2553	2561	rVB2	106969	234953	1.20%	0.589%

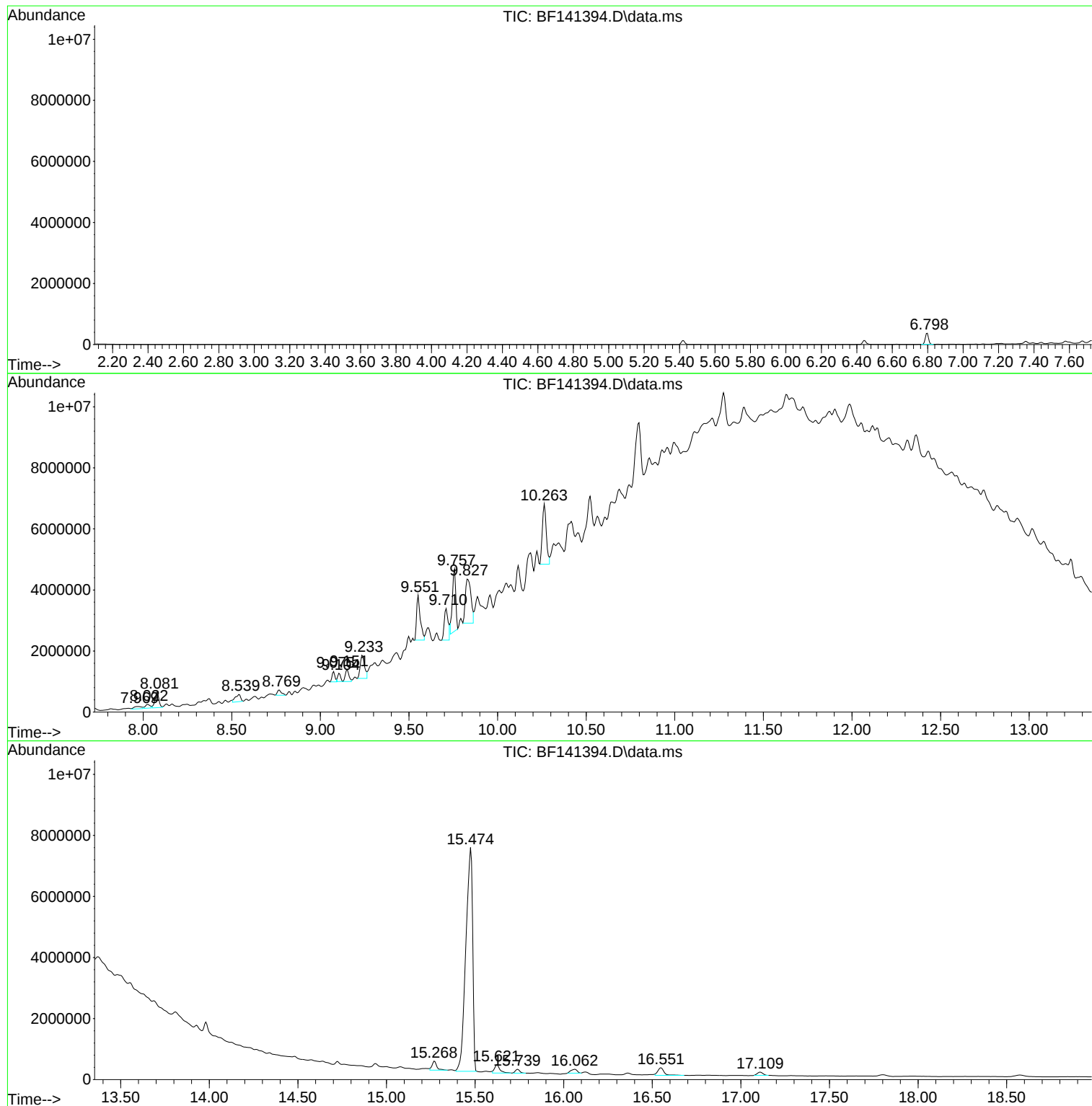
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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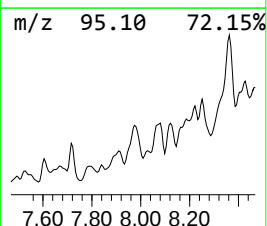
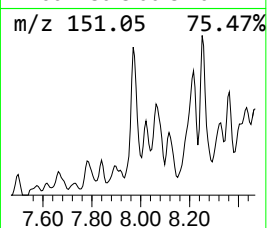
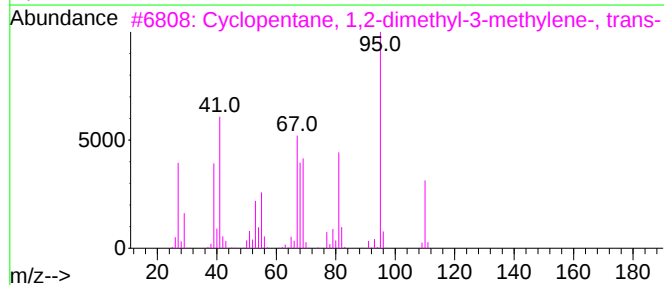
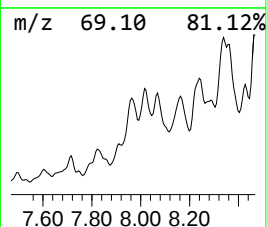
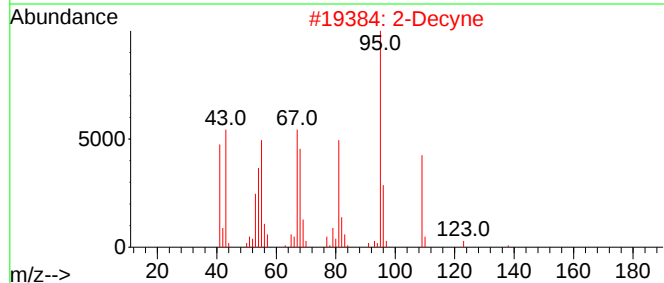
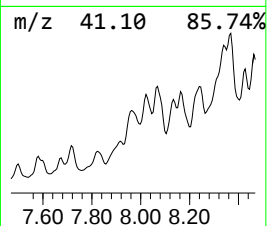
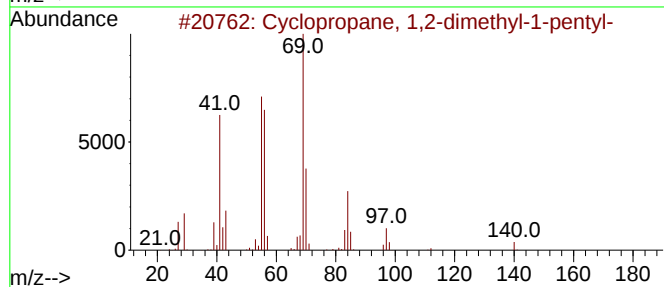
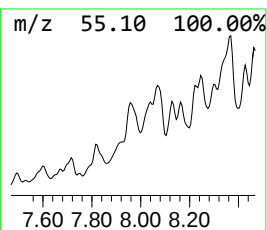
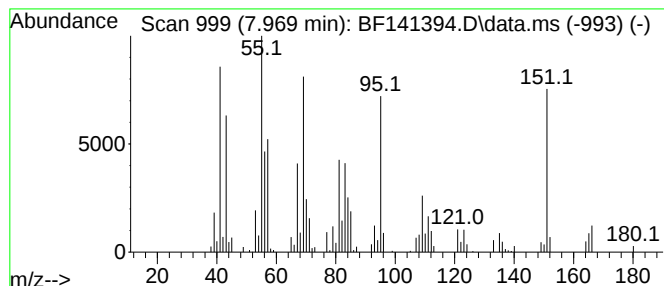
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.969 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	6.04 ng	240655	Naphthalene-d8	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	30
2			2-Decyne	138	C10H18	002384-70-5	25
3			Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	25
4			2-sec-Butyl-3-methyl-1-pentene	140	C10H20	075144-24-0	18
5			Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	15



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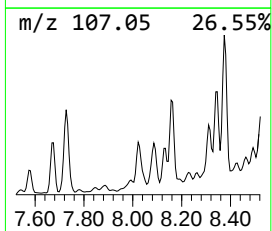
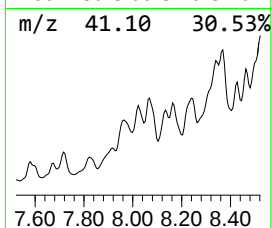
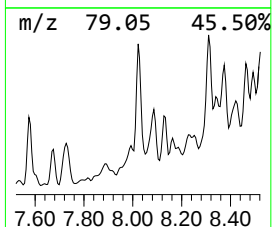
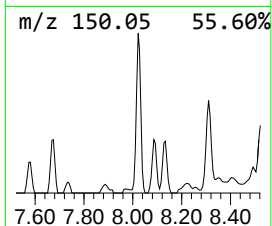
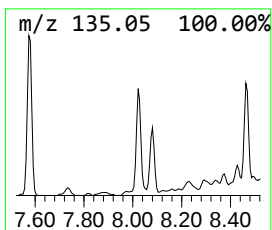
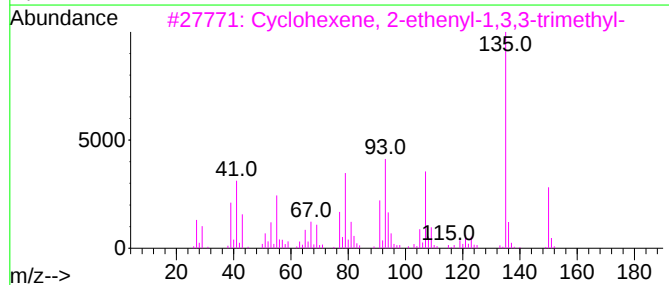
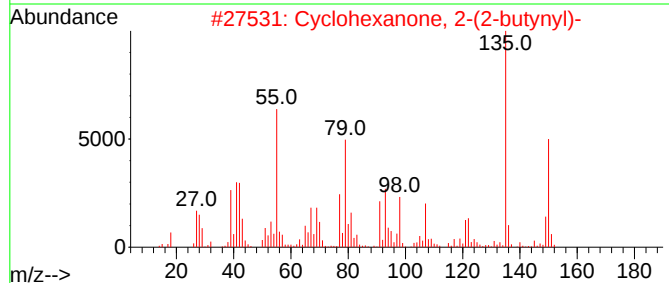
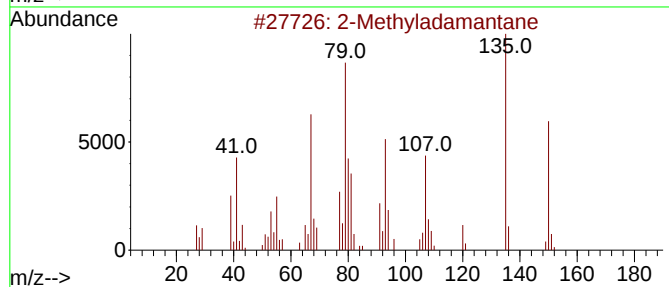
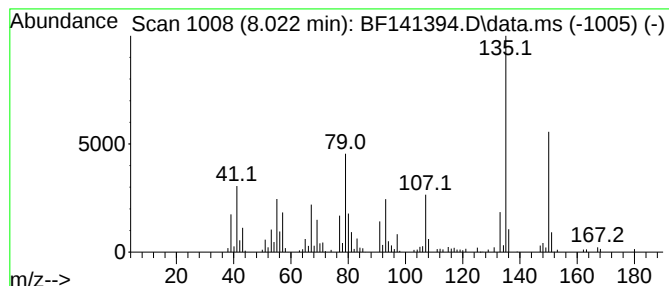
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Methyladamantane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	5.53 ng	220052	Naphthalene-d8	8.081

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methyladamantane	150	C11H18	000700-56-1	91
2		Cyclohexanone, 2-(2-butynyl)-	150	C10H14O	054166-48-2	83
3		Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	72
4		Adamantane-1-carboxylic acid	180	C11H16O2	000828-51-3	64
5		Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	64



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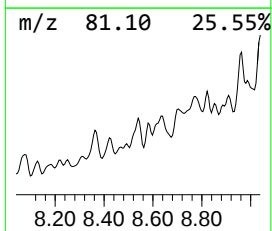
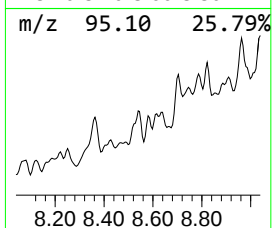
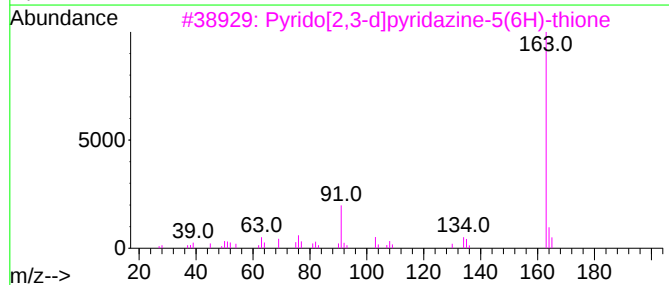
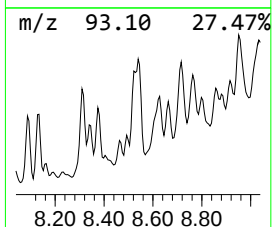
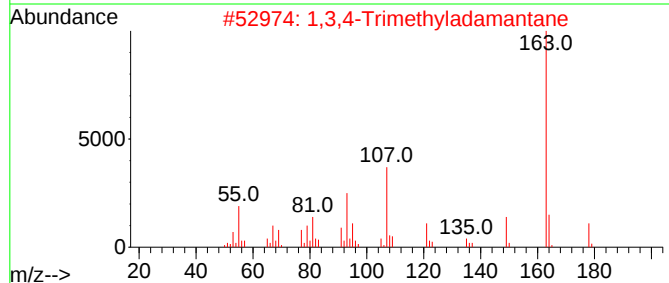
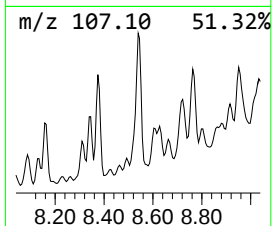
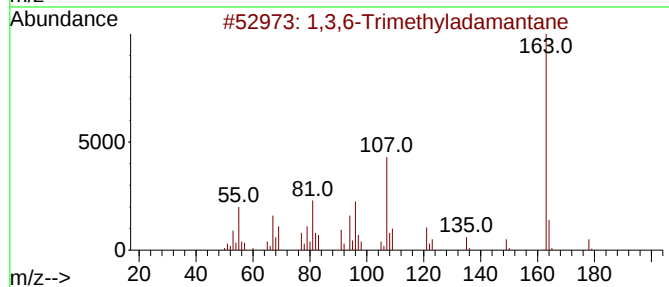
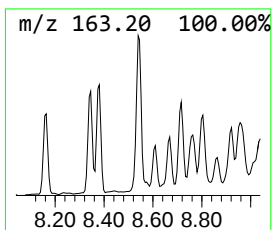
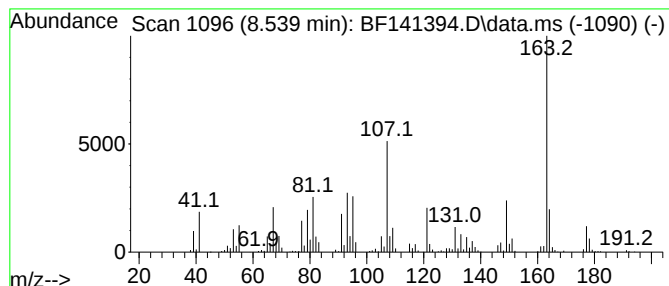
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Peak Number 3 unknown8.539 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	12.35 ng	491606	Naphthalene-d8	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	49
2			1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	43
3			Pyrido[2,3-d]pyridazine-5(6H)-th...	163	C7H5N3S	015370-85-1	25
4			2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	22
5			Fenipentol	164	C11H16O	000583-03-9	14



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Instrument :
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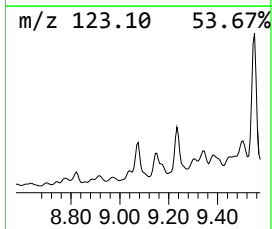
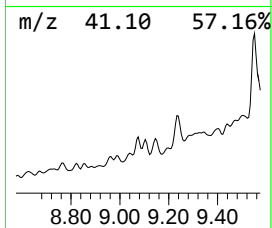
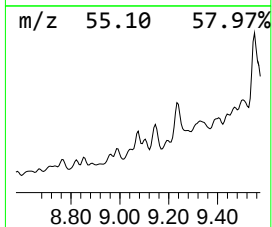
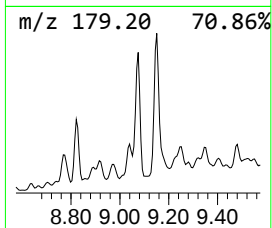
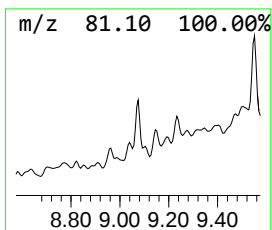
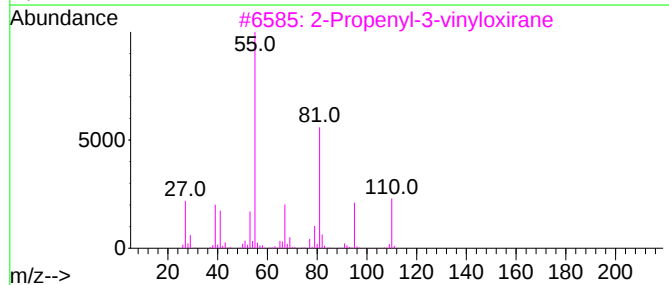
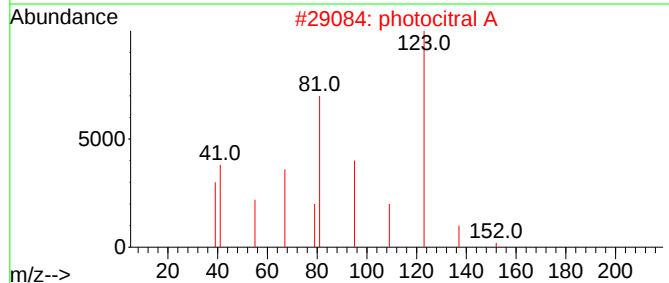
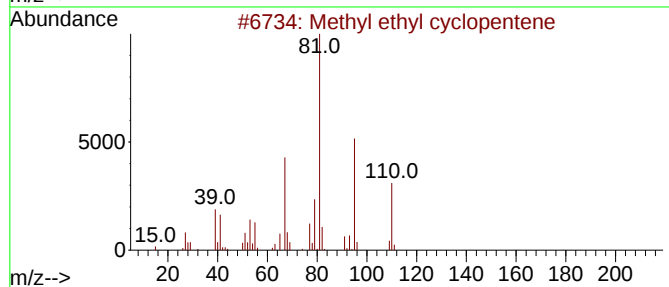
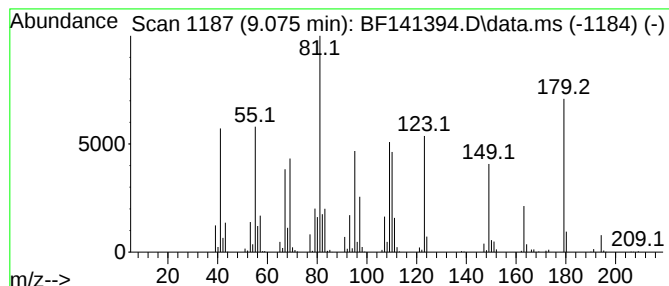
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Peak Number 4 Methyl ethyl cyclopentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.075	2.44 ng	393542	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	50
2			photocitral A	152	C10H16O	055253-28-6	38
3			2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	38
4			3-Heptyne, 5-methyl-	110	C8H14	061228-09-9	35
5			2-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	35



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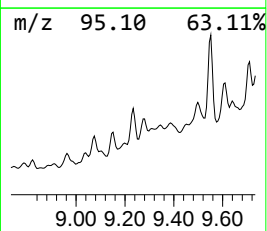
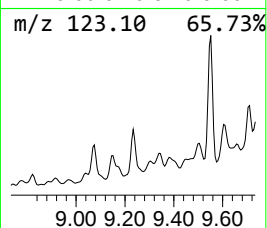
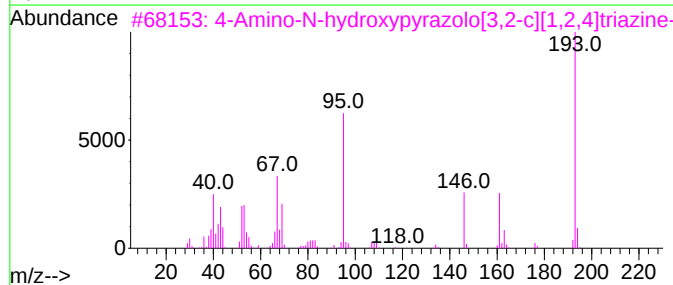
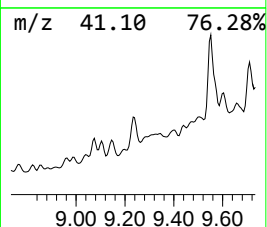
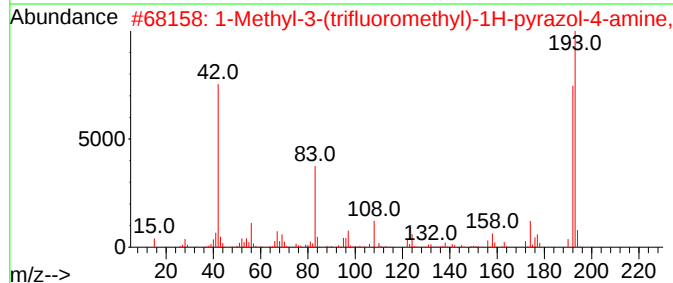
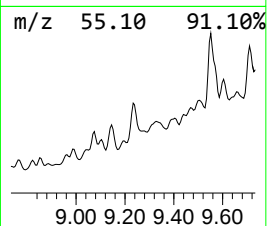
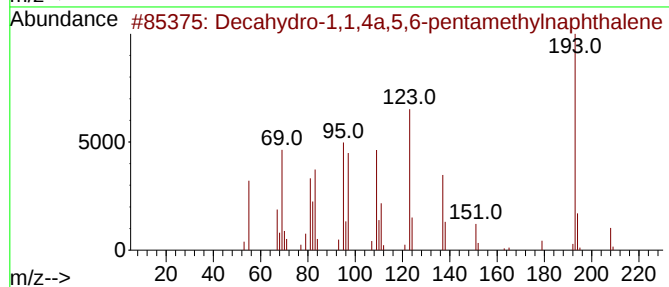
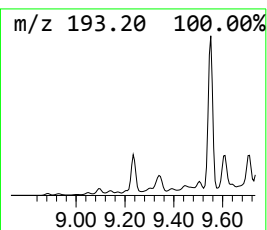
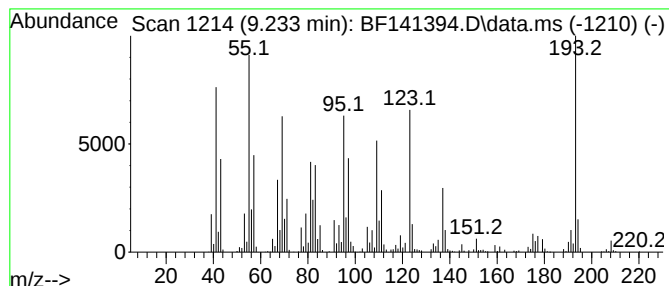
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Peak Number 5 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.233	8.21 ng	1325370	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	90
2			1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	27
3			4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	25
4			1-Anthracenamine	193	C14H11N	000610-49-1	22
5			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	15



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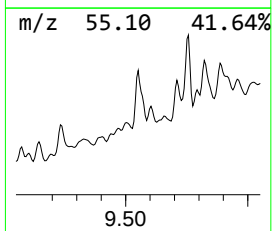
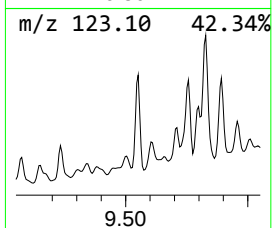
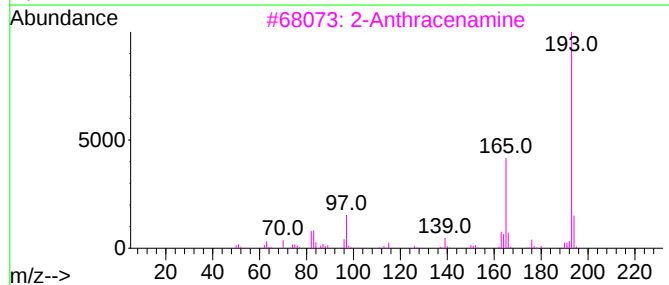
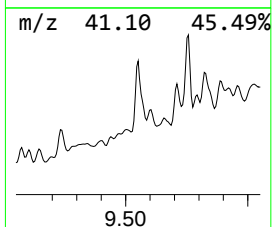
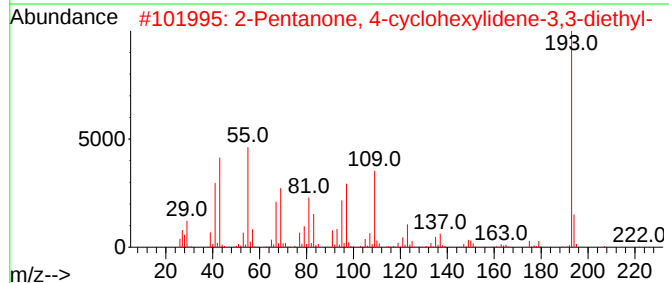
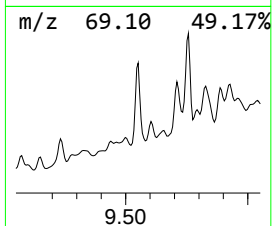
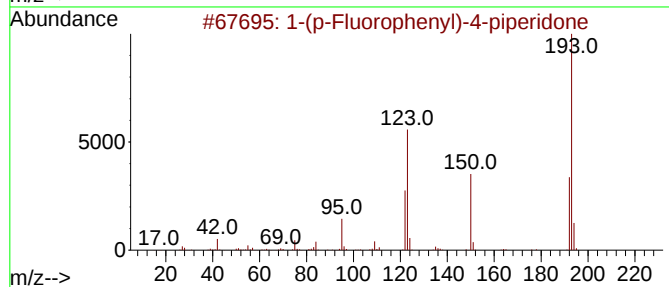
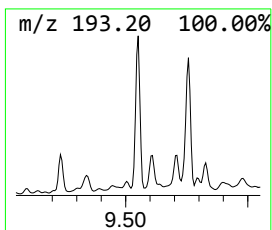
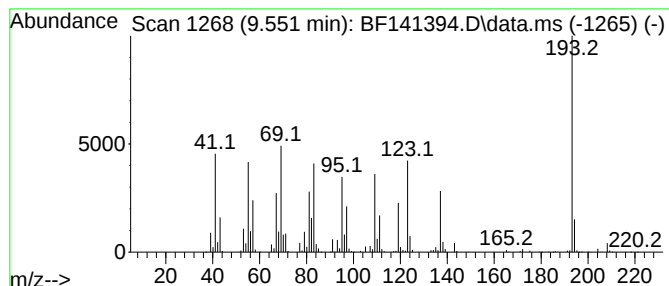
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ClientSampleId :
CHRT-20430

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.551 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.551	13.29 ng	2147080	Acenaphthene-d10			9.839
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone		193	C11H12FNO	1000238-56-7	43
2	2-Pentanone, 4-cyclohexylidene-3...		222	C15H26O	313253-65-5	37
3	2-Anthracenamine		193	C14H11N	000613-13-8	30
4	Butan-2-one, 1-[3-(3,3-dimethyl-...		278	C16H26N2O2	1000303-34-2	27
5	Pyrazole, 5-methyl-3-(5-nitro-2-...		193	C8H7N3O3	016239-90-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020325\
Data File : BF141394.D
Acq On : 04 Feb 2025 02:35
Operator : RC/JU
Sample : Q1261-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20430

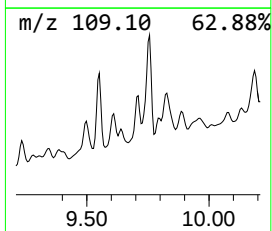
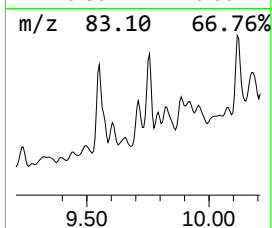
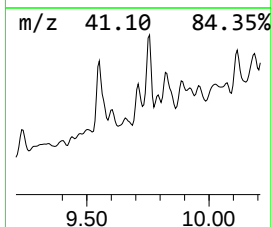
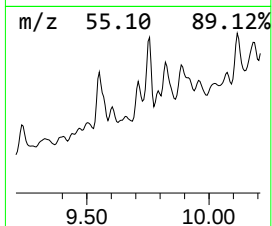
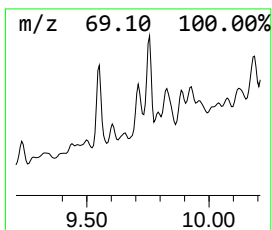
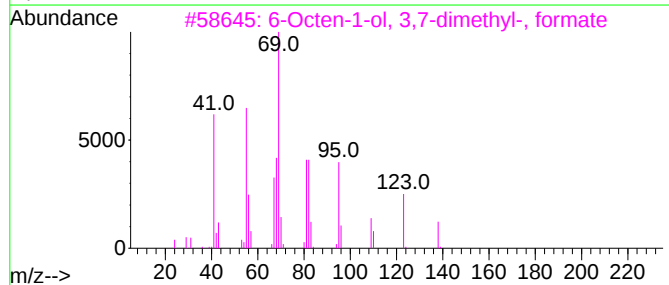
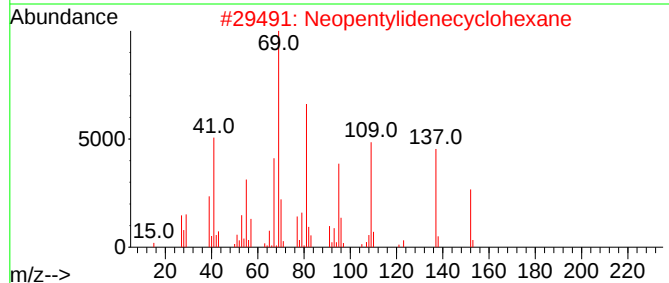
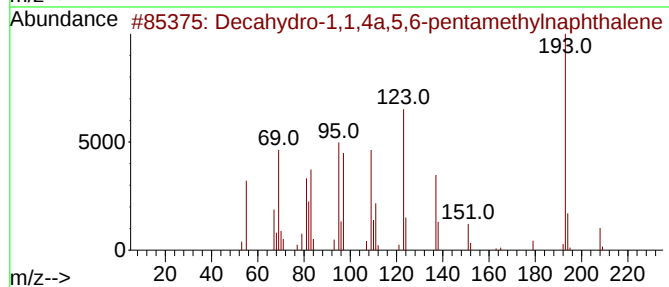
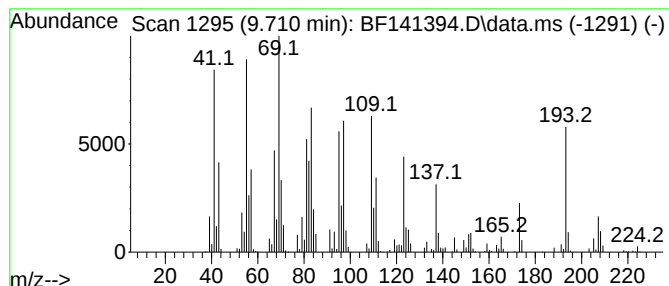
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.710 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	9.96 ng	1609070	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	96
2			Neopentylidenecyclohexane	152	C11H20	039546-80-0	45
3			6-Octen-1-ol, 3,7-dimethyl-, for...	184	C11H20O2	000105-85-1	38
4			Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	27
5			(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020325\
Data File : BF141394.D
Acq On : 04 Feb 2025 02:35
Operator : RC/JU
Sample : Q1261-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20430

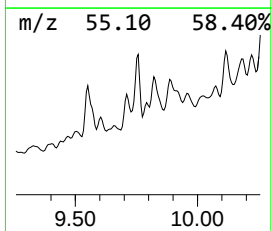
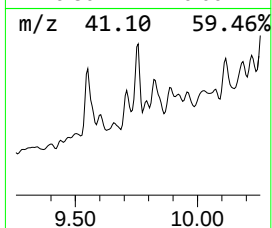
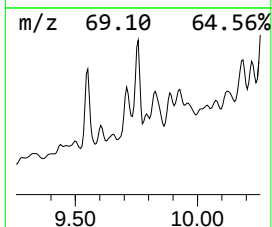
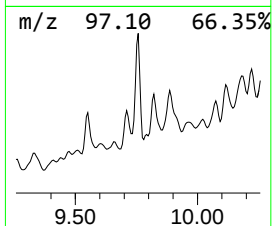
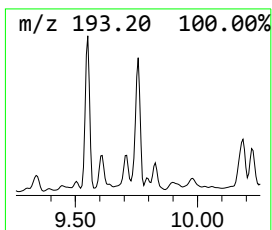
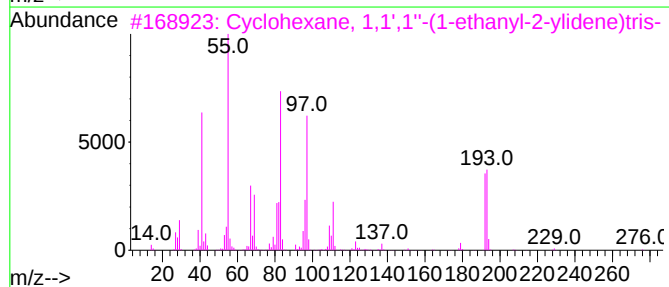
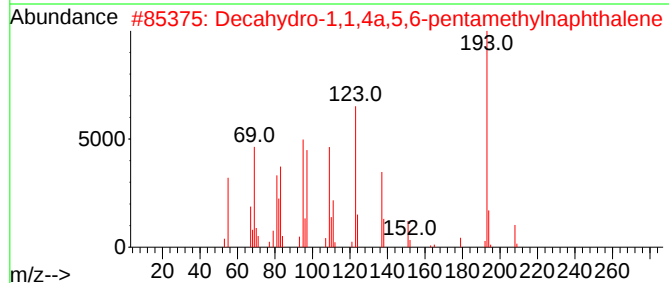
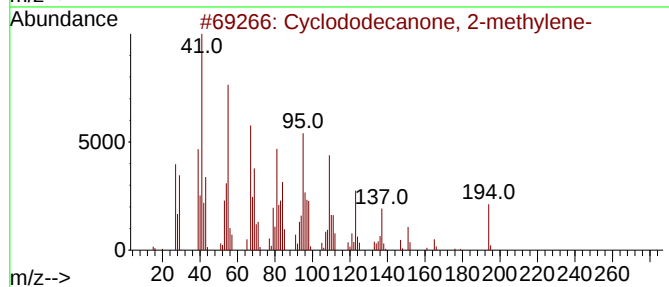
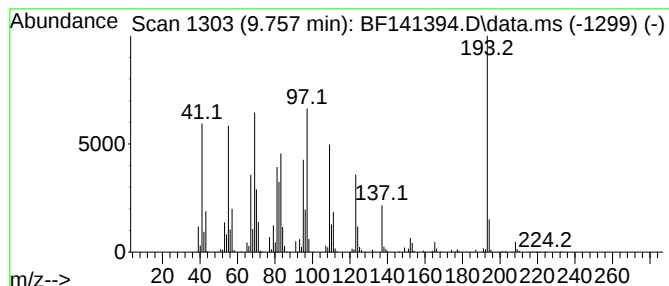
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.757 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	16.39 ng	2647770	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	43
2			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38
3			Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	22
4			Hexadecanedinitrile	248	C16H28N2	006812-44-8	14
5			3a,7a-Epoxy-1H-inden-4(5H)-one, ...	152	C9H12O2	039746-31-1	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020325\
Data File : BF141394.D
Acq On : 04 Feb 2025 02:35
Operator : RC/JU
Sample : Q1261-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20430

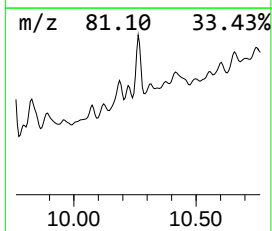
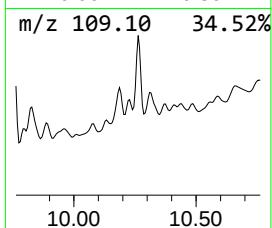
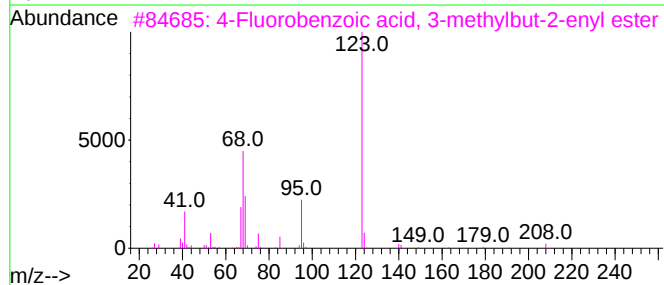
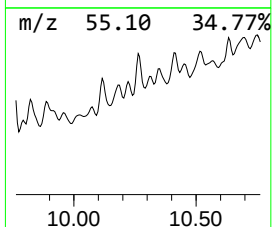
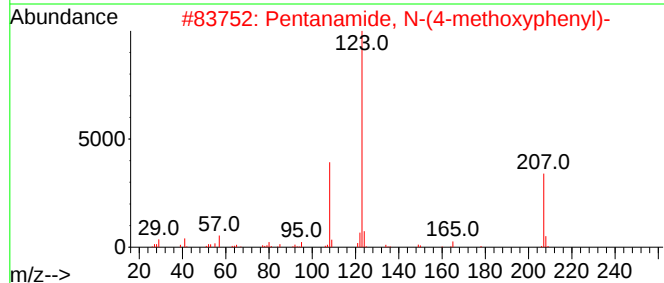
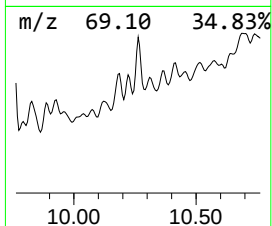
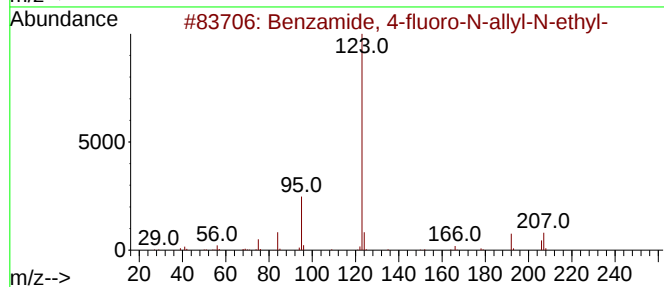
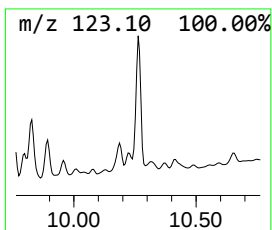
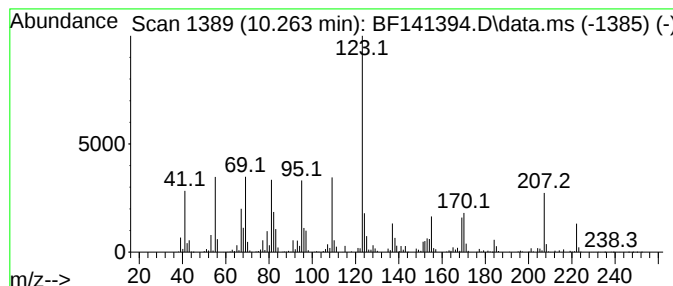
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.263 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.263	19.12 ng	3088080	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, 4-fluoro-N-allyl-N-et...	207	C12H14FNO	1000446-42-7	47
2			Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	46
3			4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	46
4			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	43
5			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020325\
Data File : BF141394.D
Acq On : 04 Feb 2025 02:35
Operator : RC/JU
Sample : Q1261-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-20430

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.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
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2-Methyladamantane	8.022	5.5	ng	220052	2	8.081	796415	20.0
unknown8.539	8.539	12.4	ng	491606	2	8.081	796415	20.0
Methyl ethyl cy...	9.075	2.4	ng	393542	3	9.839	3230460	20.0
Decahydro-1,1,4...	9.233	8.2	ng	1325370	3	9.839	3230460	20.0
unknown9.551	9.551	13.3	ng	2147080	3	9.839	3230460	20.0
unknown9.710	9.710	10.0	ng	1609070	3	9.839	3230460	20.0
unknown9.757	9.757	16.4	ng	2647770	3	9.839	3230460	20.0
unknown10.263	10.263	19.1	ng	3088080	3	9.839	3230460	20.0