

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
 Data File : BF134078.D
 Acq On : 05 Jul 2023 21:34
 Operator : CG\JU
 Sample : 03474-01
 Misc :
 ALS Vial : 7 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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134078.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.916	301	311	318	rBV	362587	514273	31.10%	5.128%
2	5.475	572	576	590	rVB	1802551	1645648	99.52%	16.410%
3	6.481	743	747	755	rBV	1862040	1653642	100.00%	16.490%
4	6.845	806	809	816	rBV	722677	598604	36.20%	5.969%
5	7.404	901	904	908	rBV	1094474	995425	60.20%	9.926%
6	8.128	1020	1027	1030	rBV	873274	824233	49.84%	8.219%
7	8.181	1030	1036	1038	rBV6	121573	209533	12.67%	2.089%
8	8.298	1052	1056	1059	rBV4	182259	261544	15.82%	2.608%
9	8.369	1063	1068	1069	rBV3	149921	200123	12.10%	1.996%
10	8.445	1078	1081	1083	rBV2	225435	237246	14.35%	2.366%
11	8.475	1083	1086	1089	rVV3	139498	149623	9.05%	1.492%
12	8.510	1089	1092	1095	rBV2	268106	275828	16.68%	2.751%
13	8.569	1099	1102	1104	rBV3	266292	291418	17.62%	2.906%
14	8.628	1110	1112	1115	rVB2	172972	150796	9.12%	1.504%
15	8.663	1115	1118	1121	rBV4	253953	411307	24.87%	4.102%
16	14.839	2166	2168	2172	rVB	834065	856313	51.78%	8.539%
17	15.592	2292	2296	2304	rVB	488221	752544	45.51%	7.504%

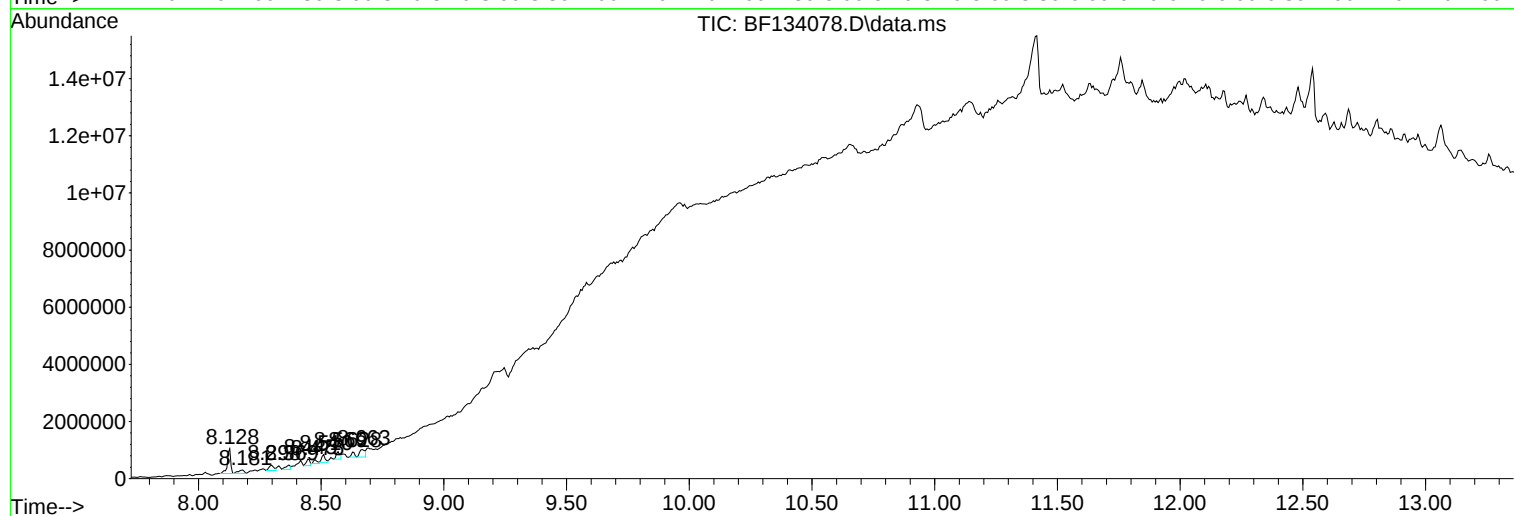
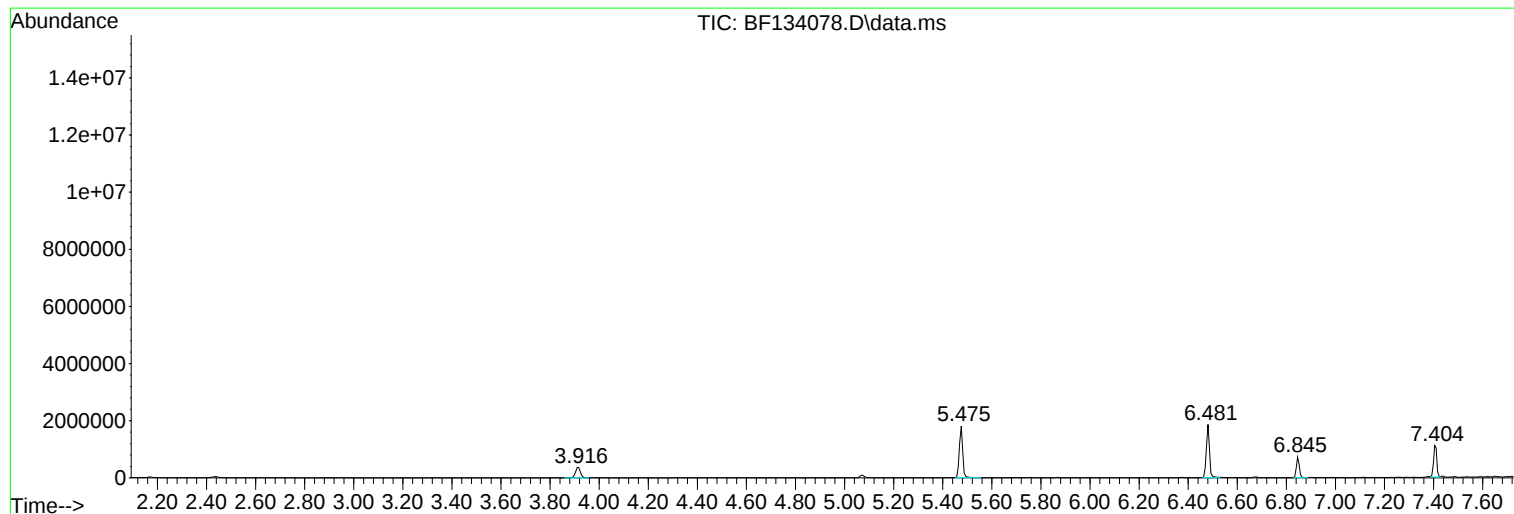
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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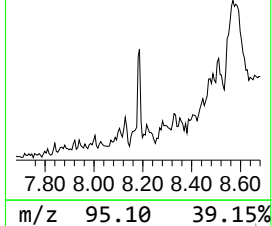
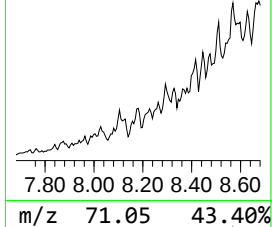
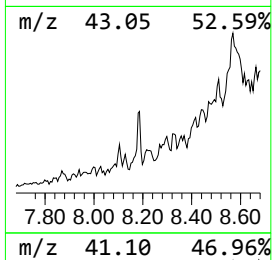
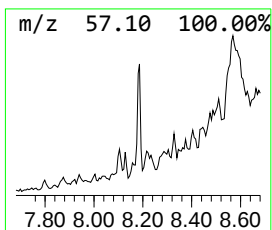
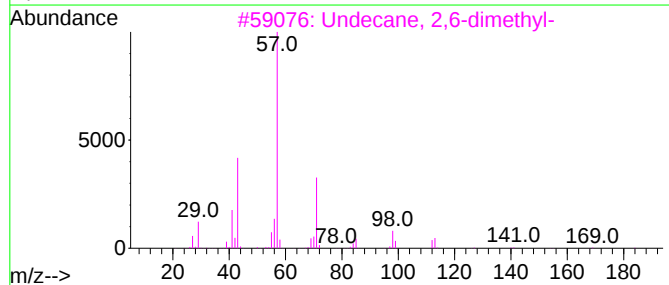
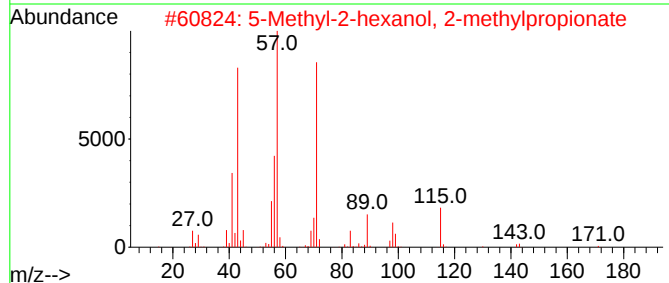
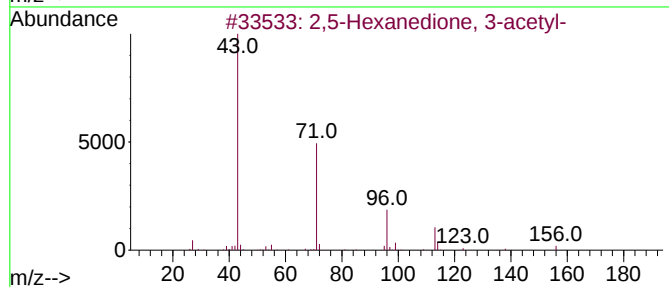
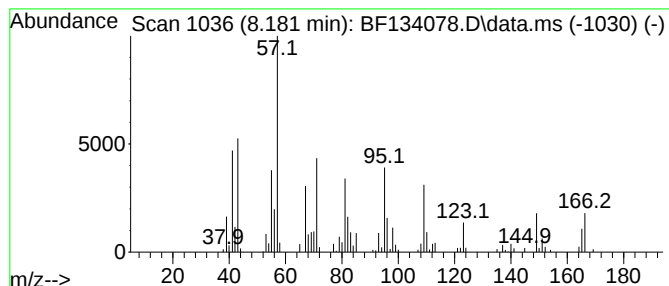
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Peak Number 2 unknown8.181 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.181	5.08 ng	209533	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Hexanedione, 3-acetyl-	156	C8H12O3	042781-07-7	14
2			5-Methyl-2-hexanol, 2-methylprop...	186	C11H22O2	1000447-34-4	14
3			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	14
4			Nonane, 3-methyl-	142	C10H22	005911-04-6	10
5			Sulfurous acid, octyl 2-propyl e...	236	C11H24O3S	1000309-11-9	10



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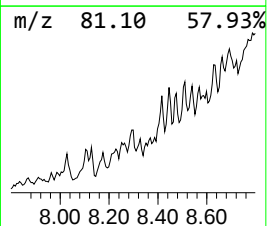
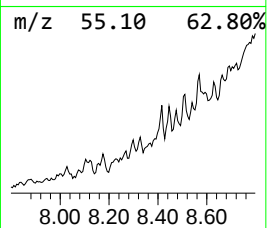
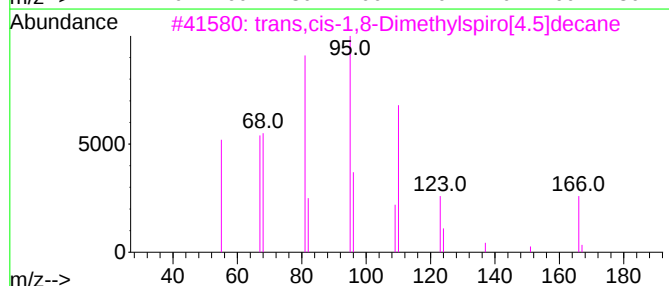
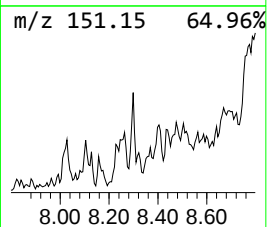
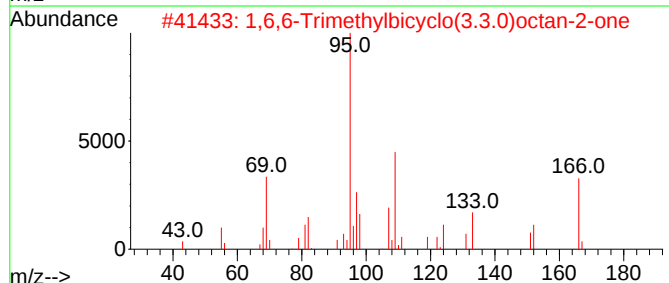
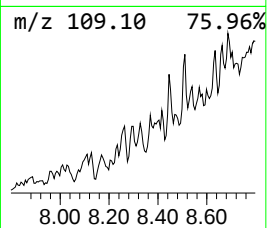
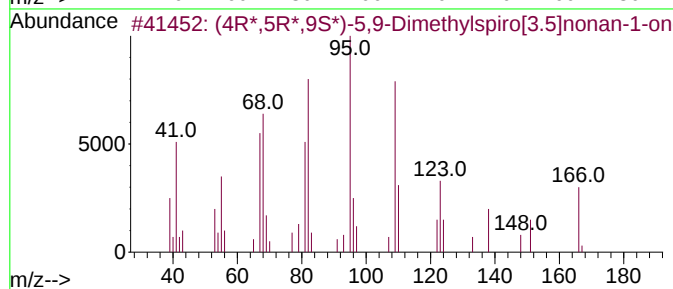
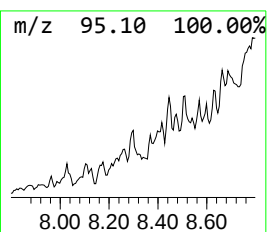
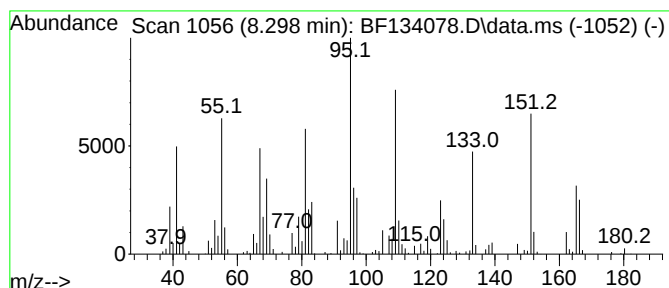
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Peak Number 3 (4R*,5R*,9S*)-5,9-Dimethyls... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	6.35 ng	261544	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4R*,5R*,9S*)-5,9-Dimethylspiro[...	166	C11H18O	063088-19-7	62		
2	1,6,6-Trimethylbicyclo(3.3.0)oct...	166	C11H18O	1000427-23-1	43		
3	trans,cis-1,8-Dimethylspiro[4.5]...	166	C12H22	1000111-72-9	43		
4	2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	43		
5	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	35		



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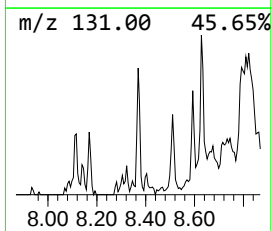
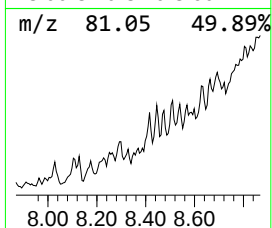
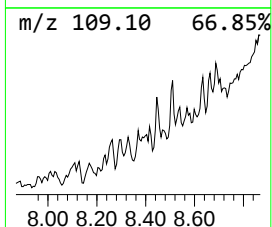
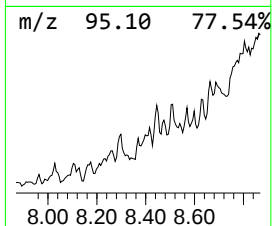
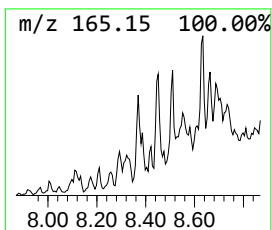
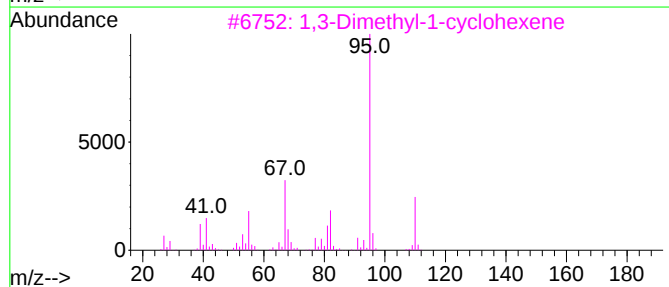
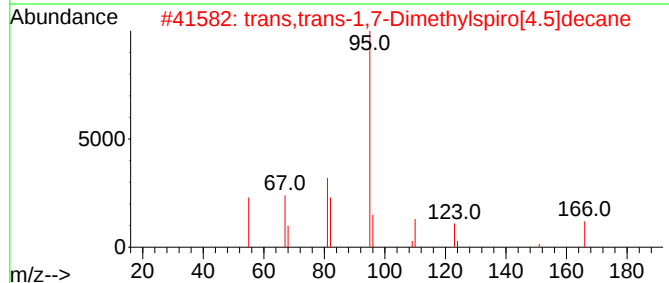
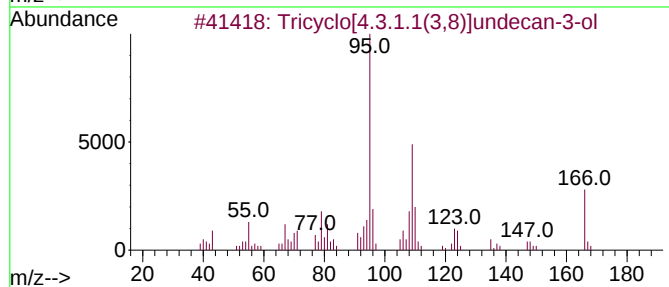
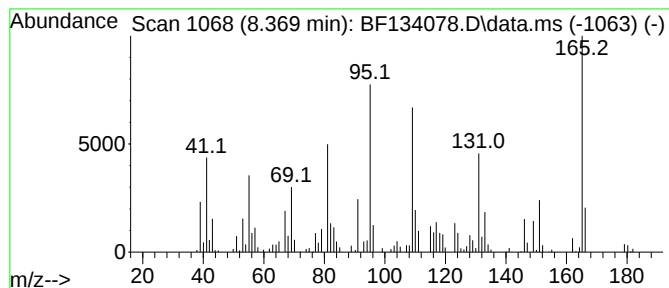
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Peak Number 4 unknown8.369 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.369	4.86 ng	200123	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[4.3.1.1(3,8)]undecan-3-ol	166	C11H18O	014504-80-4	30
2			trans,trans-1,7-Dimethylspiro[4....	166	C12H22	1000111-72-6	18
3			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	18
4			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	18
5			Cyclopentene, 5-hexyl-3,3-dimethyl-	180	C13H24	061142-66-3	18



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Misc :
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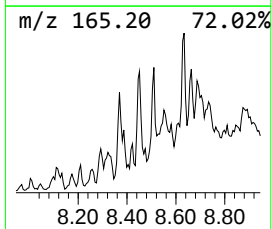
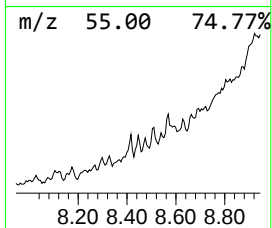
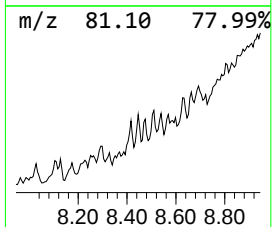
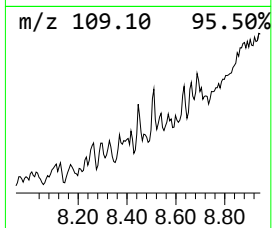
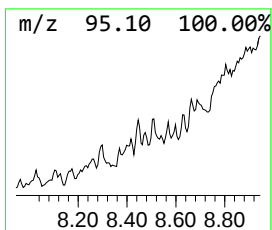
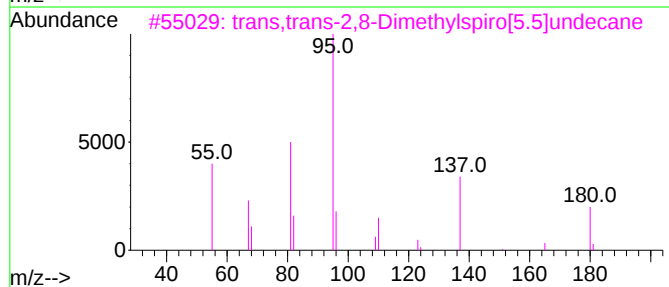
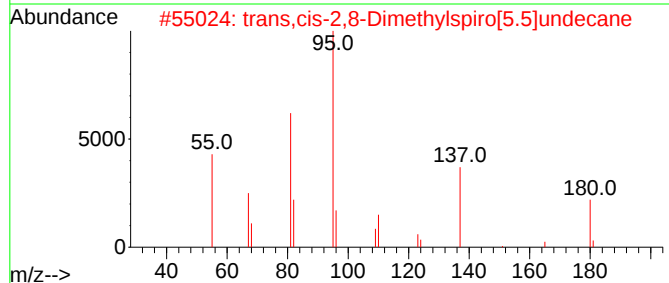
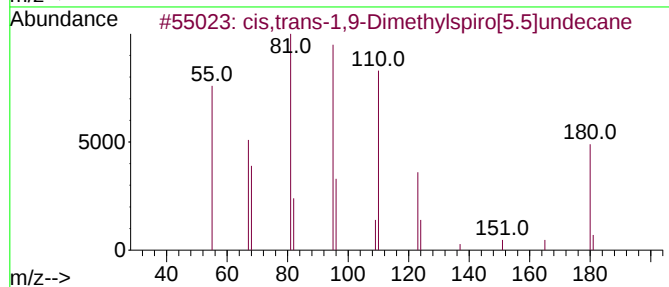
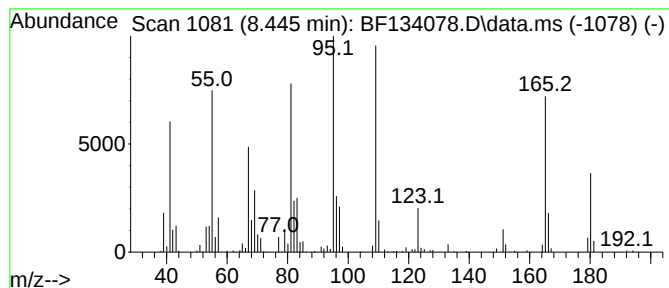
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Peak Number 5 cis,trans-1,9-Dimethylspiro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	5.76 ng	237246	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,trans-1,9-Dimethylspiro[5.5]...	180	C13H24	1000111-73-3	53
2			trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	49
3			trans,trans-2,8-Dimethylspiro[5.5]...	180	C13H24	095530-76-0	49
4			cis,cis-1,9-Dimethylspiro[5.5]un...	180	C13H24	1000111-73-4	46
5			trans,trans- and trans,cis-1,8-D...	180	C13H24	1000111-73-2	38



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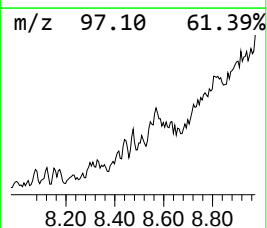
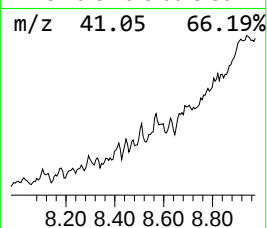
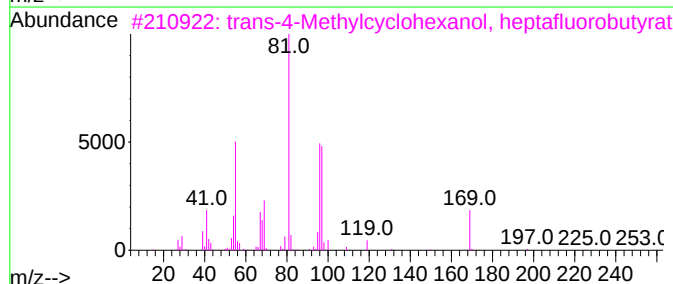
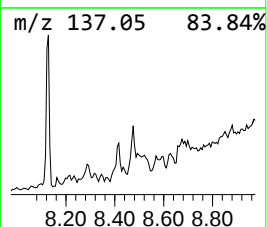
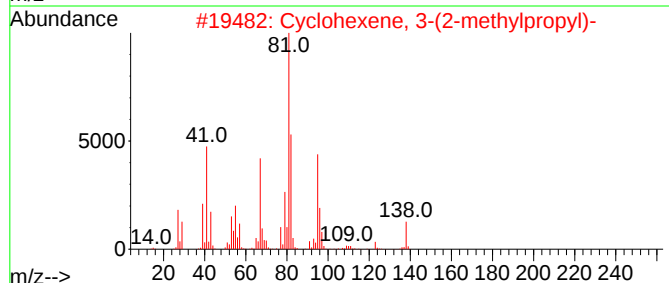
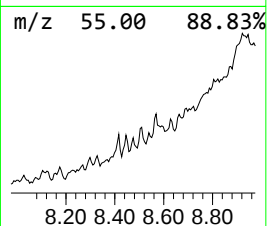
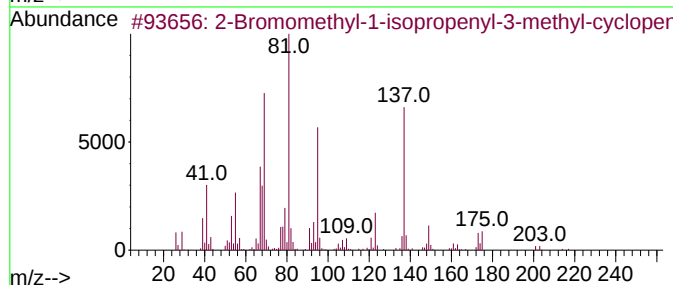
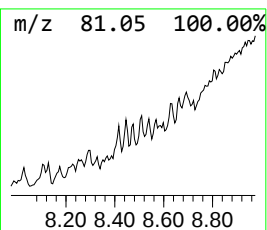
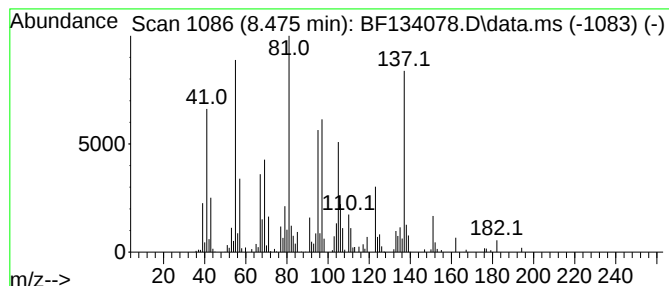
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Peak Number 6 2-Bromomethyl-1-isopropenyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	3.63 ng	149623	Naphthalene-d8	8.128

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Bromomethyl-1-isopropenyl-3-me...	216	C10H17Br	1000187-07-8	50
2		Cyclohexene, 3-(2-methylpropyl)-	138	C10H18	004104-56-7	30
3		trans-4-Methylcyclohexanol, hept...	310	C11H13F7O2	1000364-14-0	27
4		Cyclohexene,3-butyl-	138	C10H18	003983-07-1	22
5		Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	22



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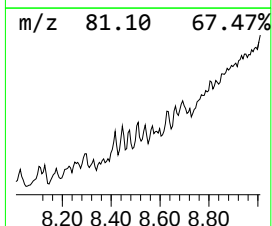
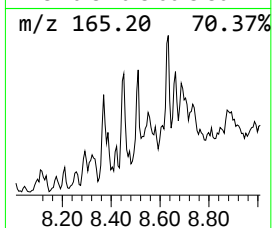
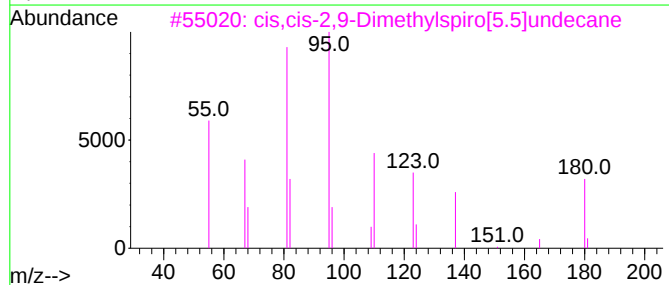
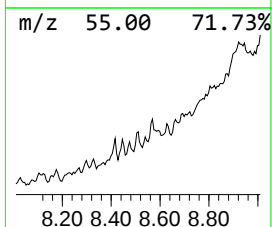
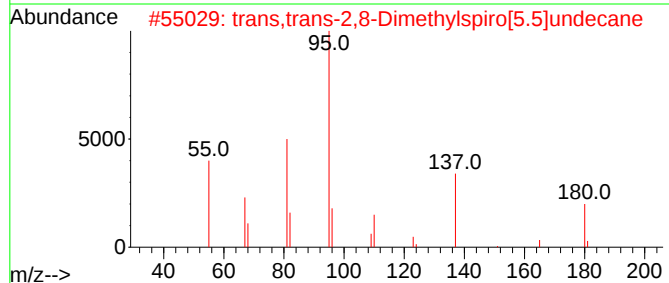
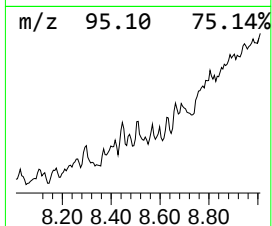
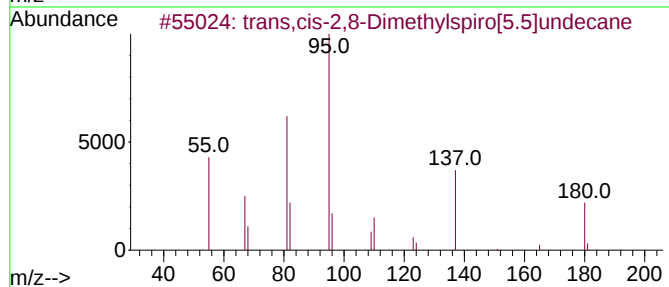
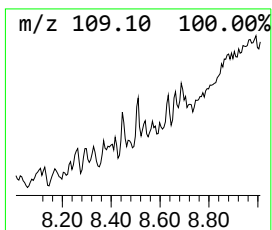
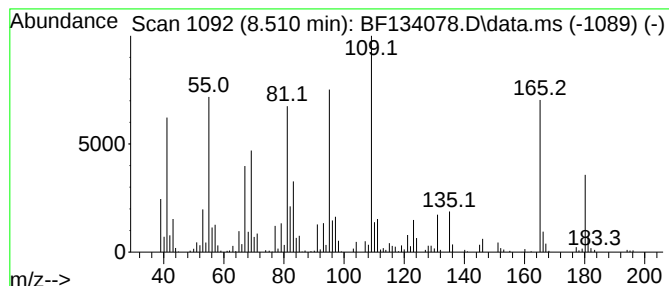
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.510 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	6.69 ng	275828	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans,cis-2,8-Dimethylspiro[5.5]undecane	180	C13H24	095472-52-9	46
2			trans,trans-2,8-Dimethylspiro[5.5]undecane	180	C13H24	095530-76-0	45
3			cis,cis-2,9-Dimethylspiro[5.5]undecane	180	C13H24	095472-51-8	45
4			2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	42
5			cis,trans-1,7-Dimethylspiro[5.5]undecane	180	C13H24	1000111-73-1	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134078.D
Acq On : 05 Jul 2023 21:34
Operator : CG\JU
Sample : 03474-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

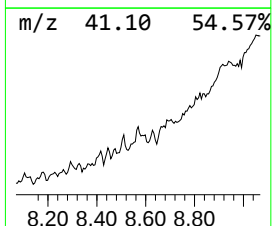
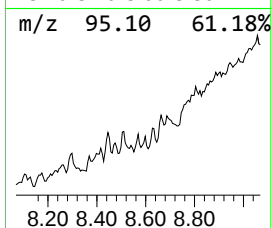
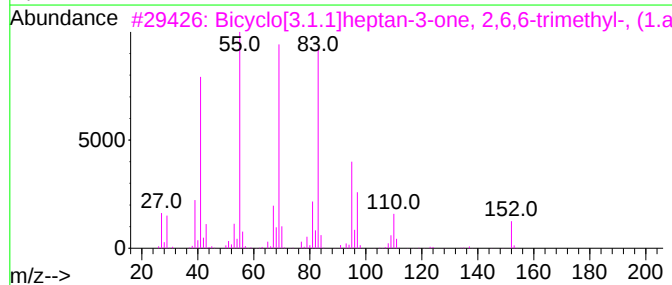
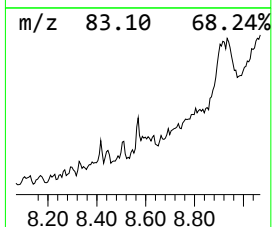
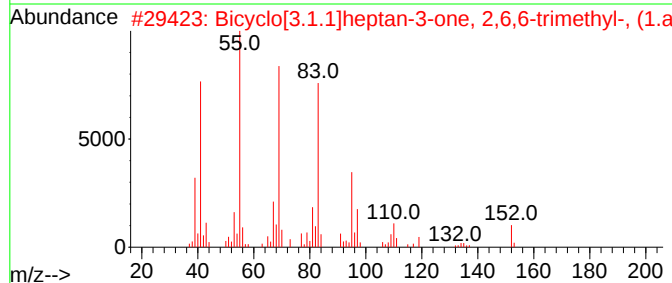
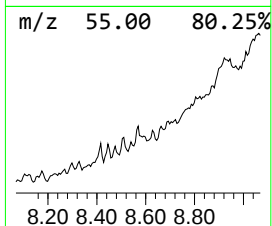
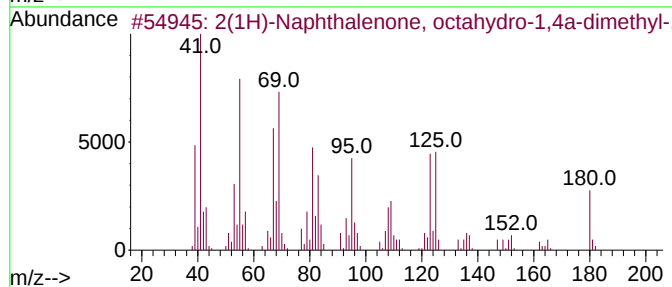
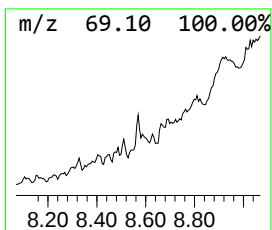
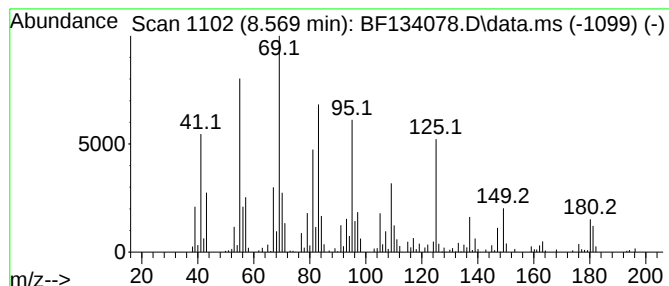
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2(1H)-Naphthalenone, octahy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	7.07 ng	291418	Naphthalene-d8	8.128

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(1H)-Naphthalenone, octahydro-1...	180	C12H20O	022738-31-4	53
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	38
3		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	38
4		Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	38
5		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134078.D
Acq On : 05 Jul 2023 21:34
Operator : CG\JU
Sample : 03474-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

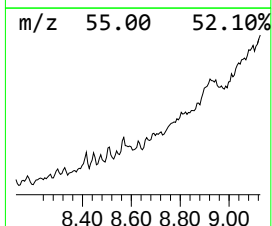
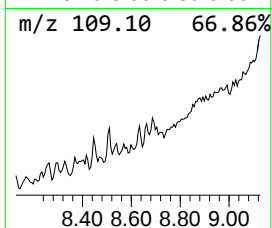
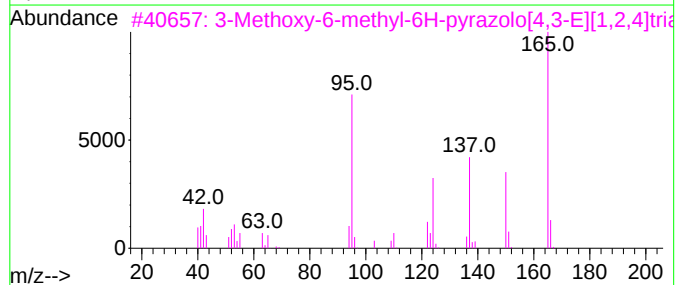
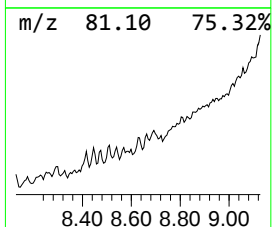
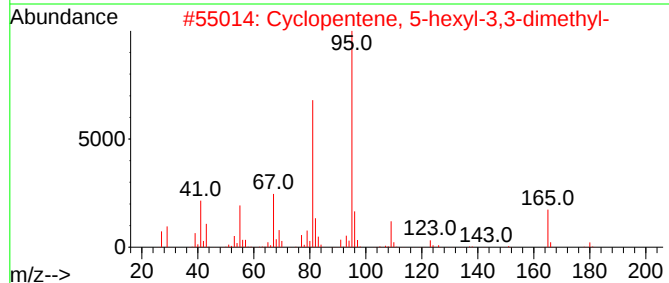
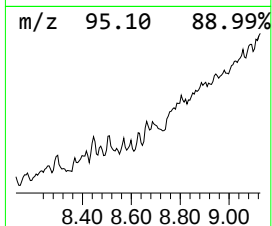
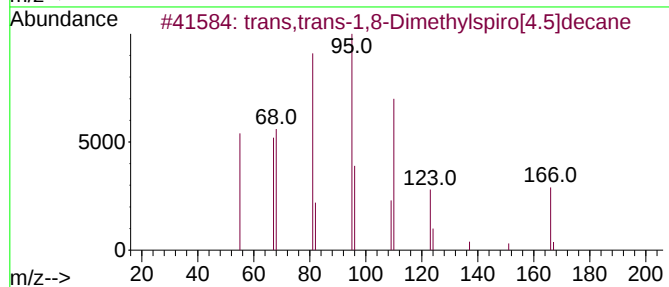
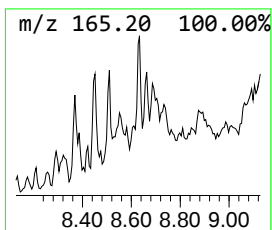
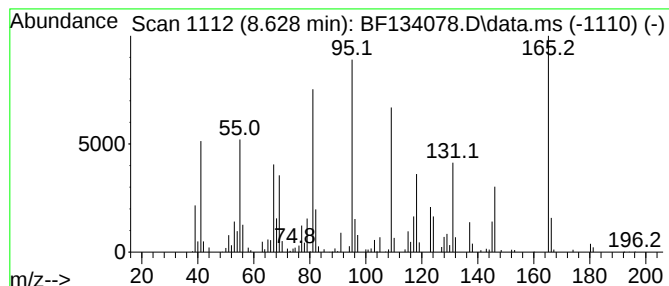
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.628 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.628	3.66 ng	150796	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans,trans-1,8-Dimethylspiro[4...	166	C12H22	1000111-72-8	46
2			Cyclopentene, 5-hexyl-3,3-dimethyl-	180	C13H24	061142-66-3	35
3			3-Methoxy-6-methyl-6H-pyrazolo[4...	165	C6H7N5O	037526-57-1	27
4			Cyclohexene,1-propyl-	124	C9H16	002539-75-5	18
5			5-Hepten-2-ol, 6-methyl-	128	C8H16O	001569-60-4	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134078.D
Acq On : 05 Jul 2023 21:34
Operator : CG\JU
Sample : 03474-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

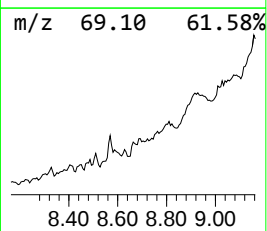
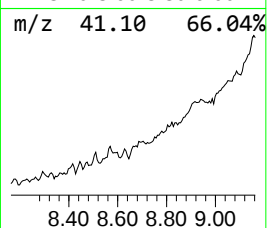
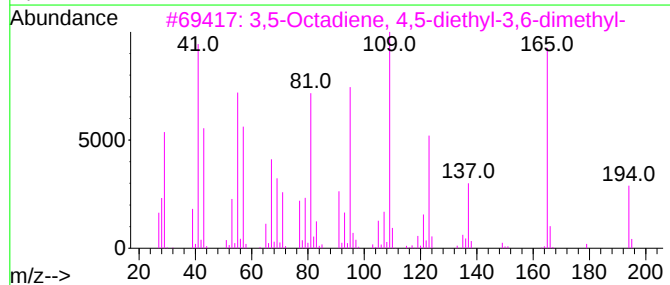
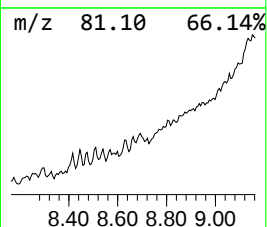
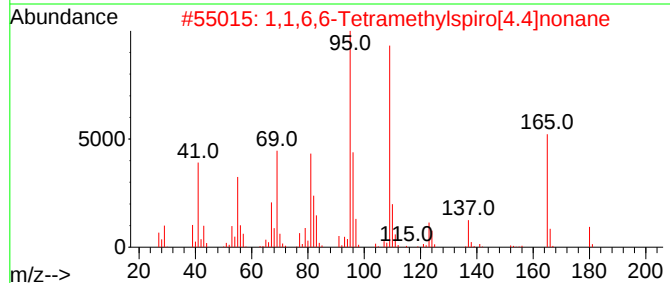
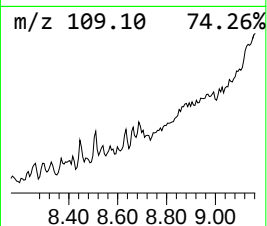
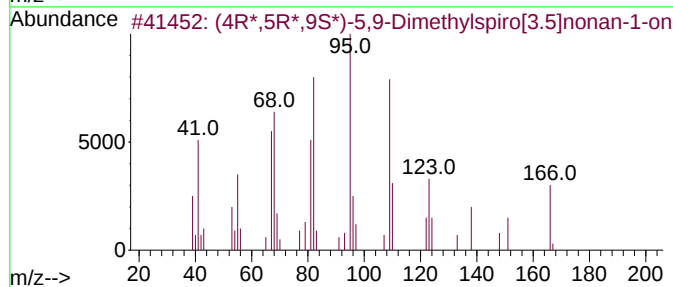
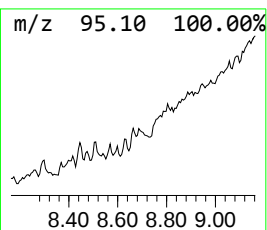
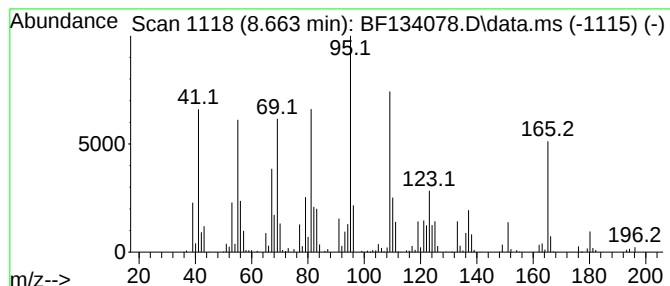
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,1,6,6-Tetramethylspiro[4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.663	9.98 ng	411307	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4R*,5R*,9S*)-5,9-Dimethylspiro[...	166	C11H18O	063088-19-7	72		
2	1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	58		
3	3,5-Octadiene, 4,5-diethyl-3,6-d...	194	C14H26	061233-79-2	50		
4	trans,trans-2,8-Dimethylspiro[5...	180	C13H24	095530-76-0	49		
5	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134078.D
Acq On : 05 Jul 2023 21:34
Operator : CG\JU
Sample : 03474-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

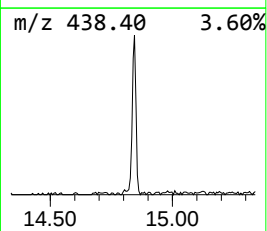
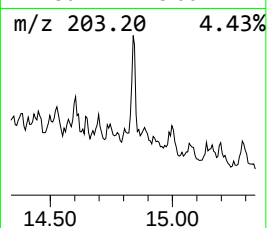
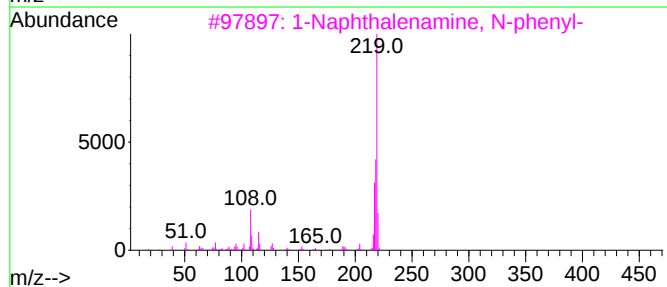
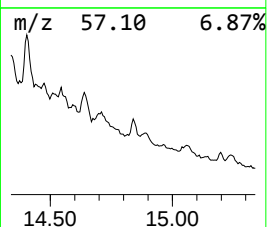
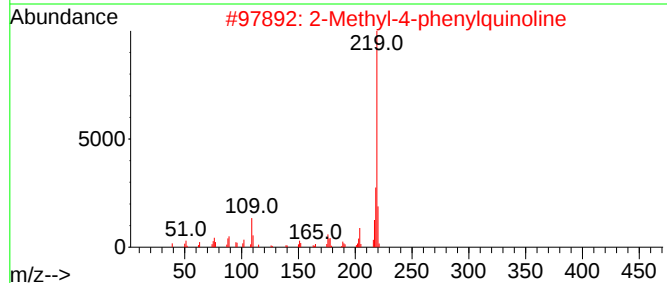
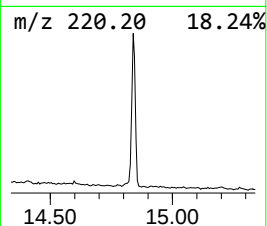
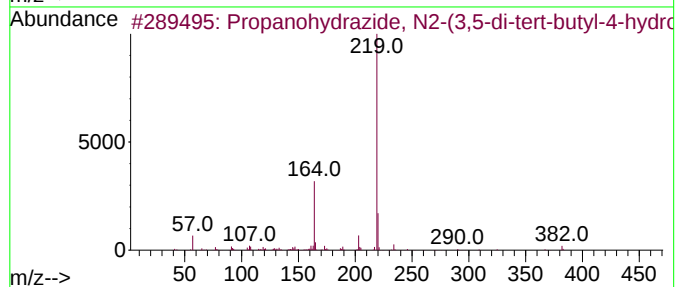
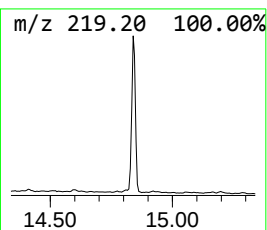
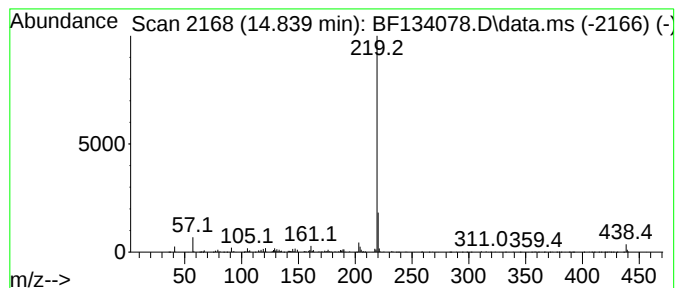
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Propanohydrazide, N2-(3,5-d... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	20.00 ng	856313	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanohydrazide, N2-(3,5-di-ter...	382	C24H34N2O2	304870-86-8	72
2			2-Methyl-4-phenylquinoline	219	C16H13N	001721-92-2	72
3			1-Naphthalenamine, N-phenyl-	219	C16H13N	000090-30-2	64
4			Quinoline, 2-(3-tolyl)-	219	C16H13N	024641-30-3	64
5			3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134078.D
Acq On : 05 Jul 2023 21:34
Operator : CG\JU
Sample : 03474-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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(4R*,5R*,9S*)-5...	8.298	6.3	ng	261544	2	8.128	824233	20.0
unknown8.369	8.369	4.9	ng	200123	2	8.128	824233	20.0
cis,trans-1,9-D...	8.445	5.8	ng	237246	2	8.128	824233	20.0
2-Bromomethyl-1...	8.475	3.6	ng	149623	2	8.128	824233	20.0
unknown8.510	8.510	6.7	ng	275828	2	8.128	824233	20.0
2(1H)-Naphthale...	8.569	7.1	ng	291418	2	8.128	824233	20.0
unknown8.628	8.628	3.7	ng	150796	2	8.128	824233	20.0
1,1,6,6-Tetrame...	8.663	10.0	ng	411307	2	8.128	824233	20.0
Propanohydrazid...	14.839	20.0	ng	856313	5	14.110	856313	20.0