

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
 Data File : BF134630.D
 Acq On : 04 Aug 2023 13:49
 Operator : CG\JU
 Sample : 03864-01
 Misc :
 ALS Vial : 11 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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134630.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	562	567	570	rBV	3216669	2978502	100.00%	18.606%
2	6.428	733	738	741	rBV	2879167	2912527	97.78%	18.194%
3	6.798	797	801	804	rBV	1390963	1051035	35.29%	6.566%
4	7.357	892	896	899	rVB	2082640	1668348	56.01%	10.422%
5	8.075	1014	1018	1021	rBV	1564595	1228180	41.23%	7.672%
6	8.616	1107	1110	1112	rBV3	118364	161909	5.44%	1.011%
7	8.704	1121	1125	1128	rBV4	157344	252779	8.49%	1.579%
8	8.822	1142	1145	1147	rBV	216279	218646	7.34%	1.366%
9	8.963	1166	1169	1171	rBV4	279183	261697	8.79%	1.635%
10	9.034	1179	1181	1184	rBV3	230318	289039	9.70%	1.806%
11	9.069	1185	1187	1190	rVV2	380616	405914	13.63%	2.536%
12	9.157	1198	1202	1206	rBV	2451430	2448364	82.20%	15.294%
13	14.504	2109	2111	2113	rBV	1159593	972643	32.66%	6.076%
14	15.404	2261	2264	2271	rVB	407732	606476	20.36%	3.789%
15	15.468	2272	2275	2278	rVB	508903	552125	18.54%	3.449%

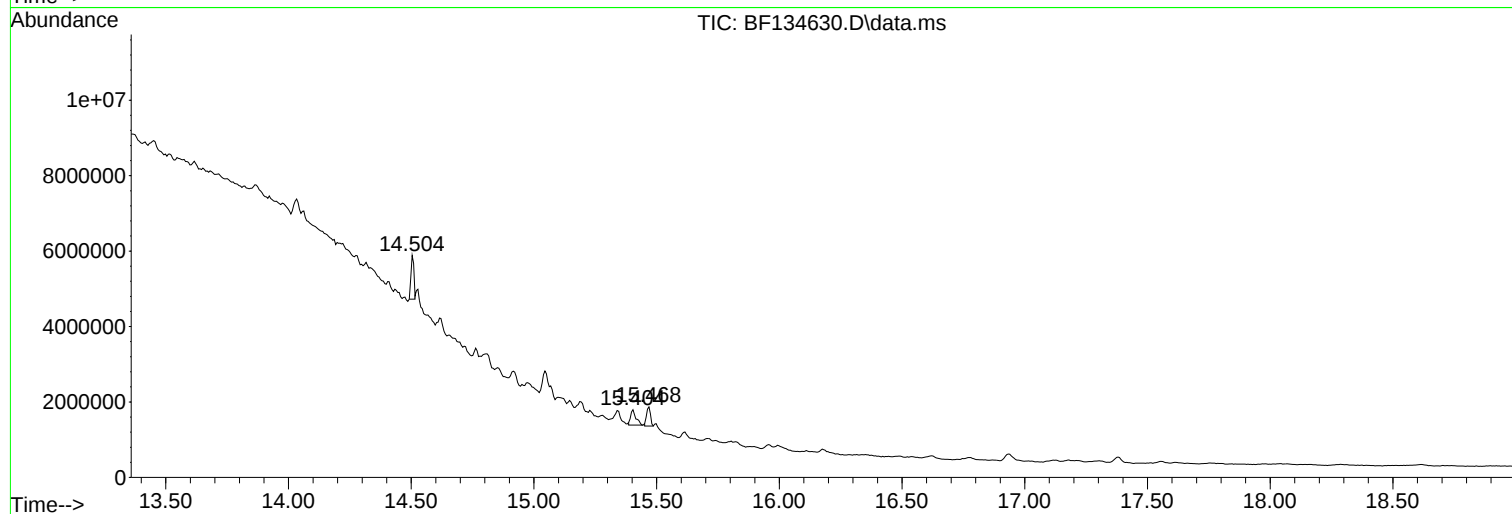
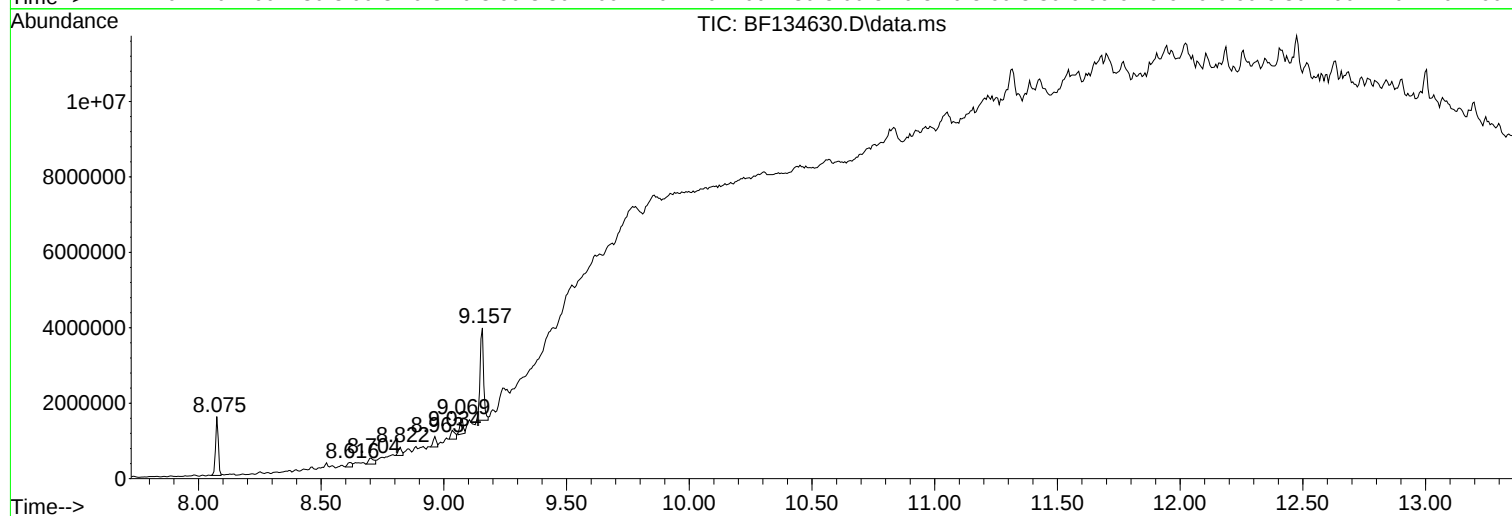
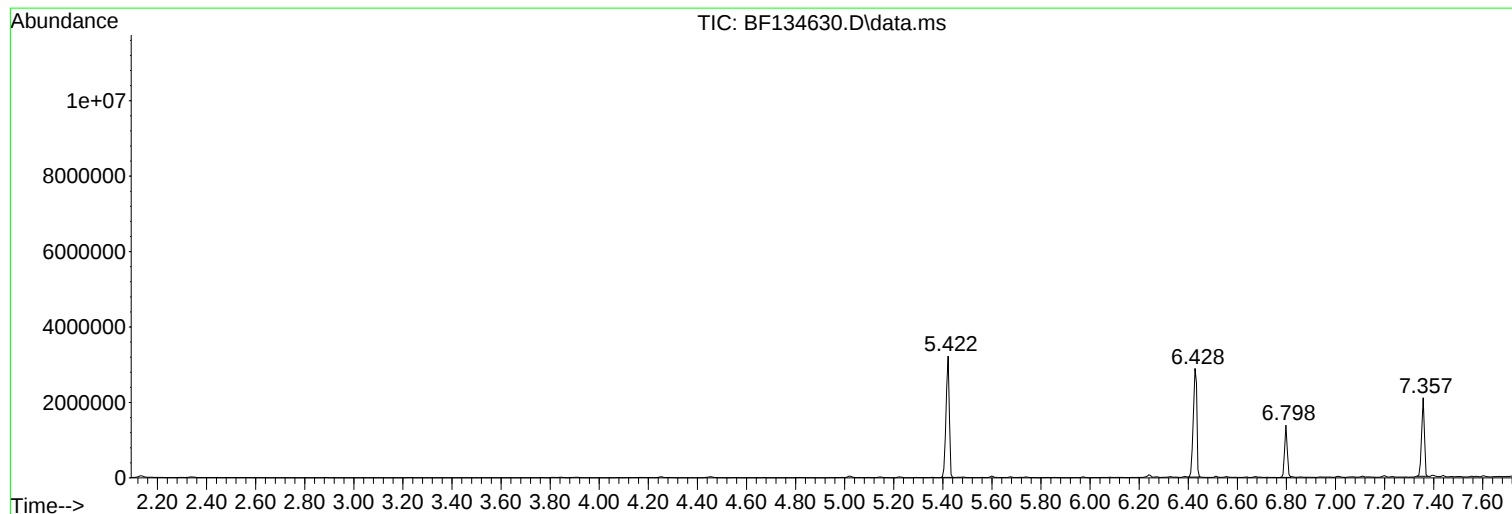
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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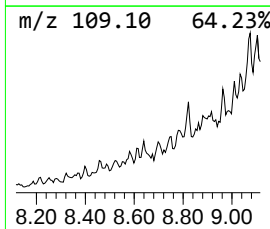
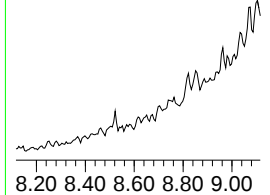
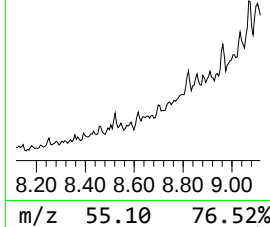
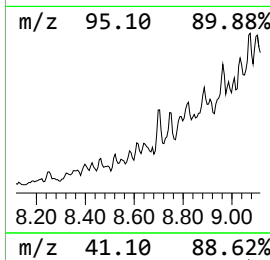
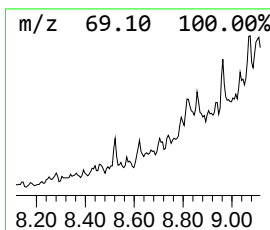
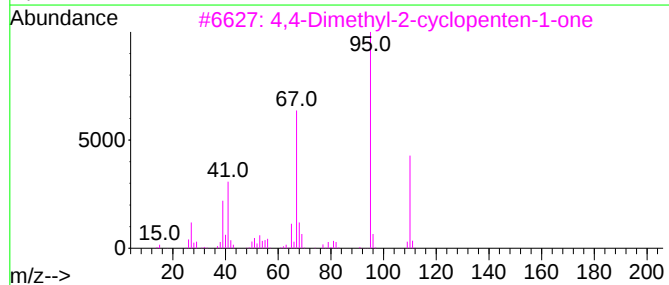
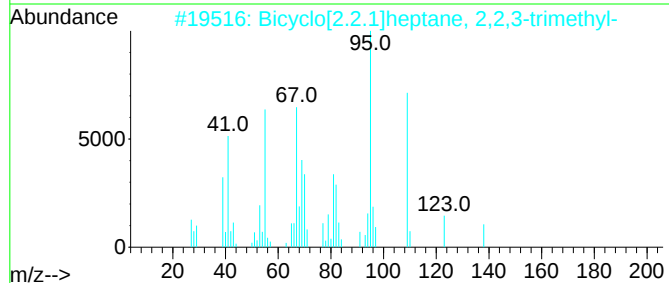
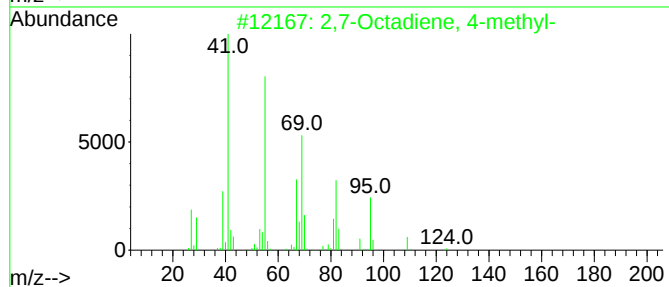
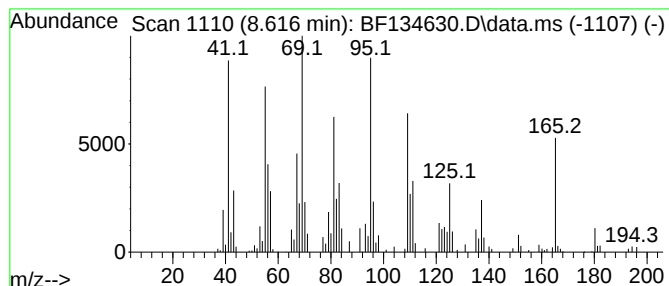
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,7-Octadiene, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	2.64 ng	161909	Naphthalene-d8	8.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,7-Octadiene, 4-methyl-			124	C9H16	1000061-78-0	78
2	Bicyclo[2.2.1]heptane, 2,2,3-tri...			138	C10H18	000473-19-8	38
3	4,4-Dimethyl-2-cyclopenten-1-one			110	C7H10O	022748-16-9	30
4	Pyridine, 2-butoxy-			151	C9H13NO	027361-16-6	30
5	trans,trans-3,5-Heptadien-2-one			110	C7H10O	018402-90-9	30



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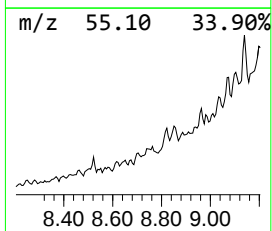
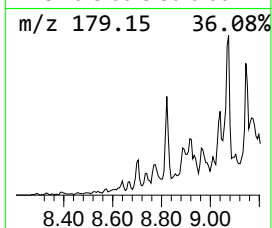
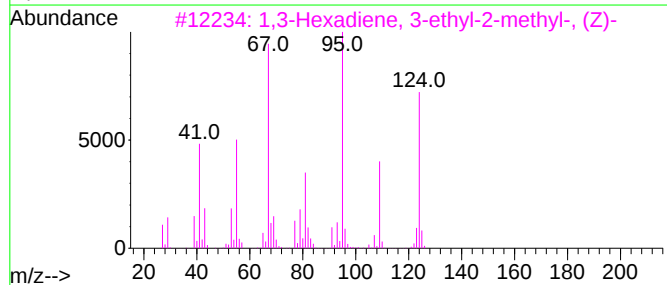
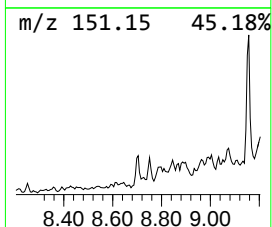
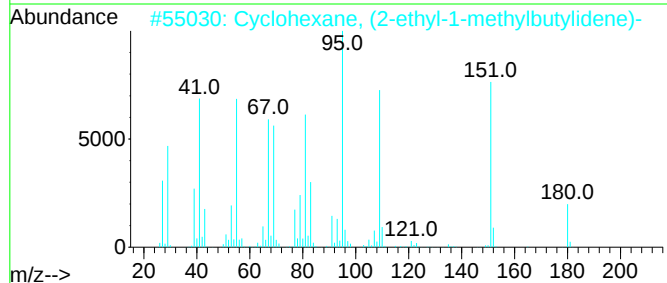
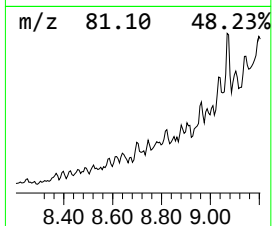
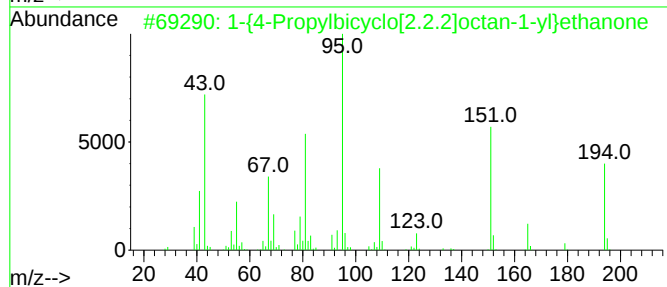
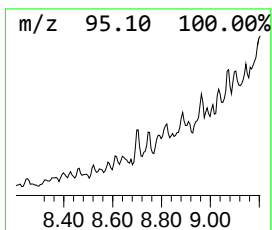
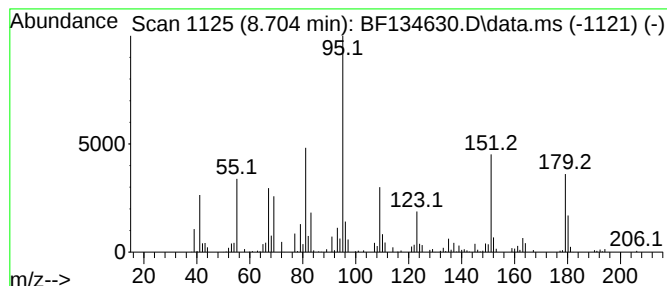
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 1-{4-Propylbicyclo[2.2.2]oc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.704	4.12 ng	252779	Naphthalene-d8	8.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1		1-{4-Propylbicyclo[2.2.2]octan-1...	194	C13H22O	1000435-24-0	72
2	Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	60		
3	1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	60		
4	2-(2-Hydroxycycloheptyl)-furan	180	C11H16O2	1000145-02-9	49		
5	2-Furoic acid, 3-chloroprop-2-en...	186	C8H7ClO3	1000299-24-2	47		



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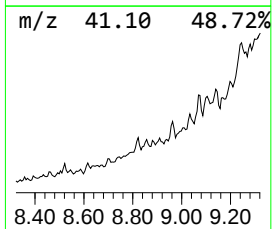
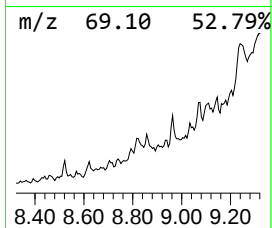
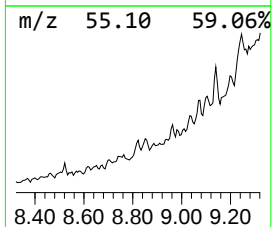
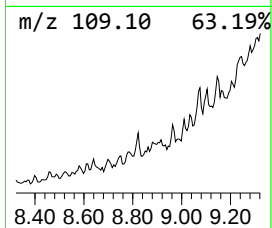
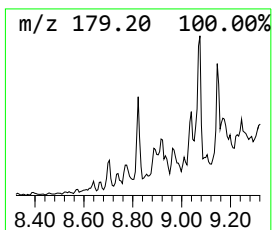
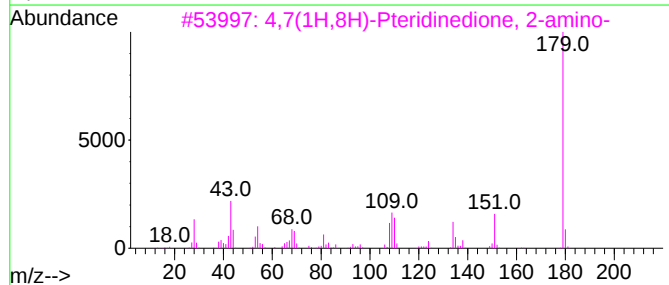
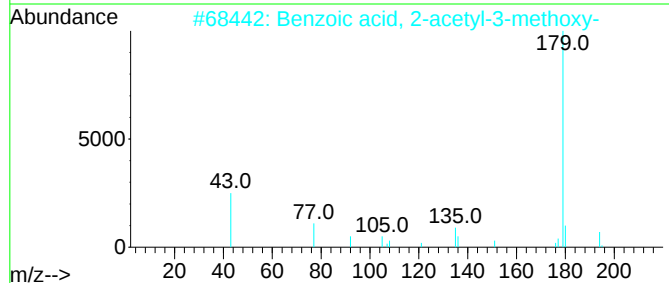
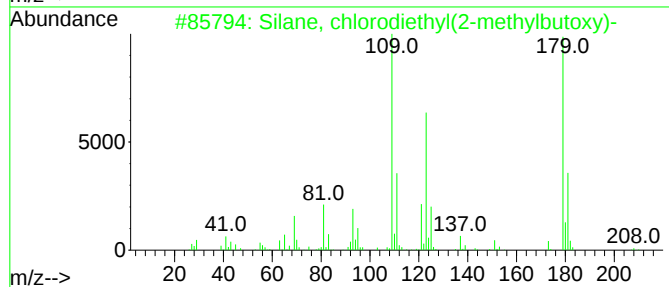
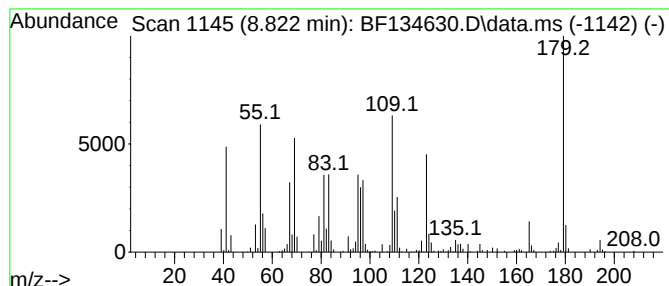
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Peak Number 3 unknown8.822 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.822	3.56 ng	218646	Naphthalene-d8	8.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, chlorodiethyl(2-methylbu...	208	C9H21ClOSi	1000363-11-1	46
2			Benzoic acid, 2-acetyl-3-methoxy-	194	C10H10O4	120714-42-3	30
3			4,7(1H,8H)-Pteridinedione, 2-amino-	179	C6H5N5O2	000529-69-1	27
4			3,5-Dimethyl-1-hexylpyrazole	180	C11H20N2	024475-41-0	22
5			1-Dimethyl(phenyl)silyloxypropane	194	C11H18OSi	013360-21-9	22



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WC-1

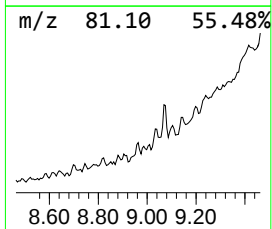
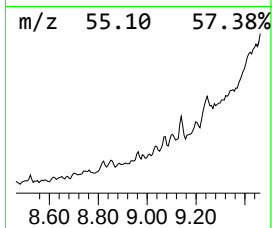
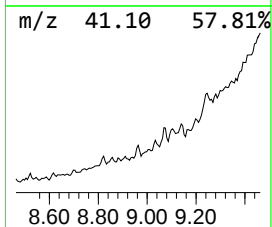
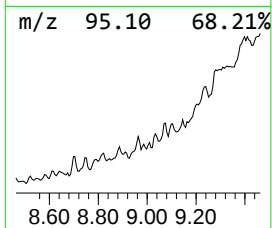
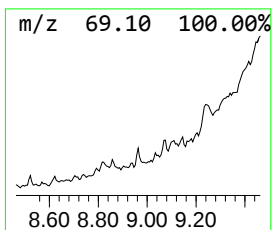
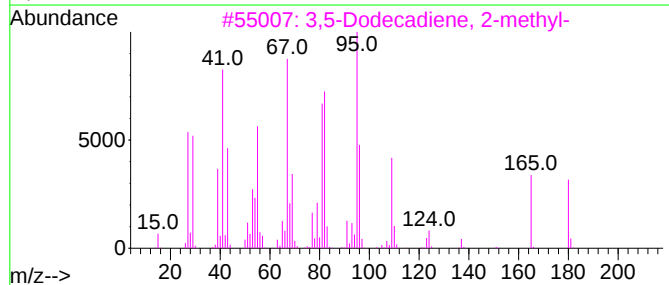
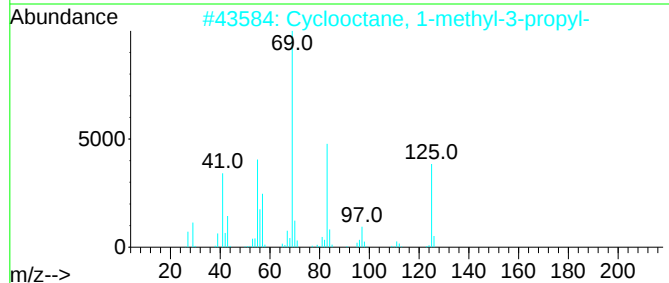
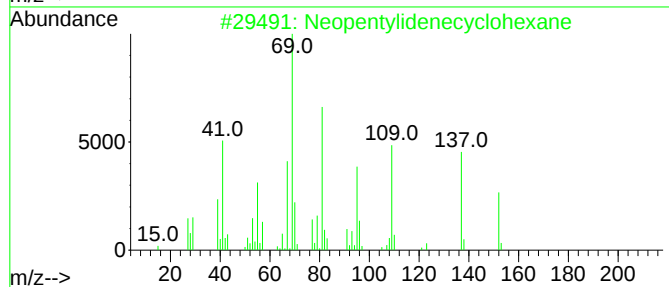
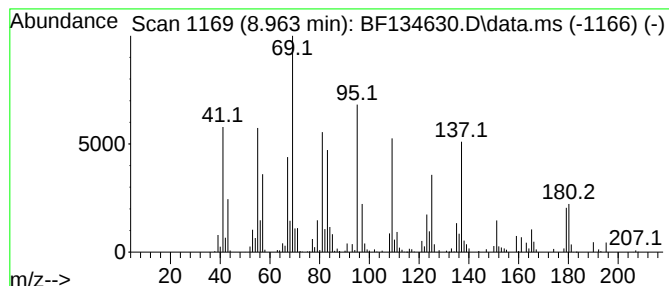
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Peak Number 4 unknown8.963 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.963	4.26 ng	261697	Naphthalene-d8	8.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentylidenecyclohexane	152	C11H20	039546-80-0	47
2			Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	27
3			3,5-Dodecadiene, 2-methyl-	180	C13H24	055638-51-2	25
4			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	006876-13-7	25
5			1b,5,5,6a-Tetramethyl-octahydro-...	208	C13H20O2	1000194-13-1	25



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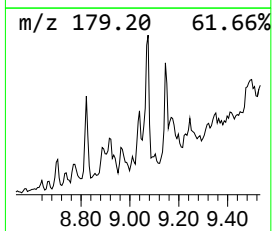
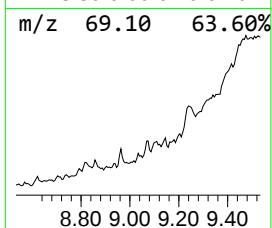
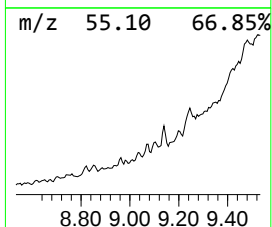
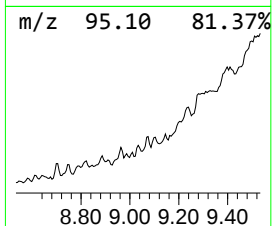
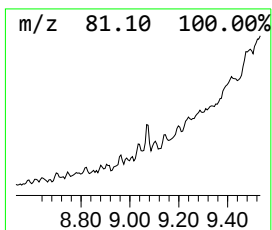
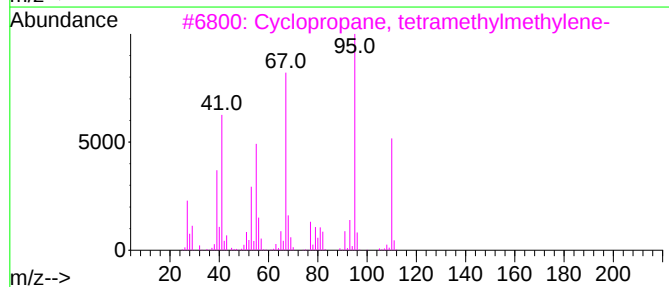
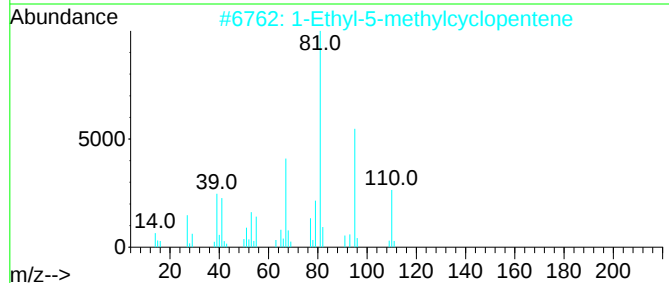
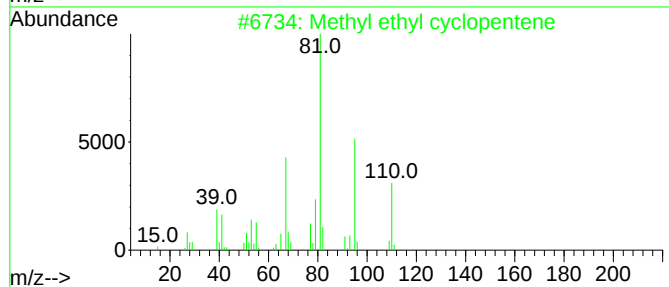
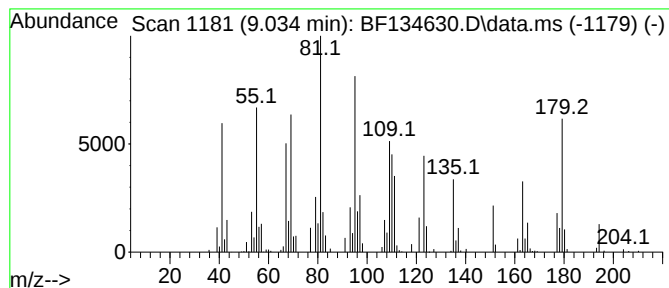
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown9.034 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.034	2.36 ng	289039	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	45
2			1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	38
3			Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	20
4			2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	18
5			2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	18



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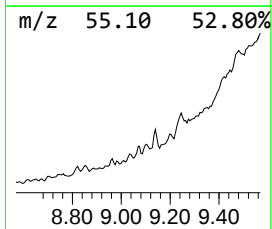
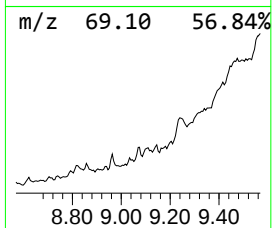
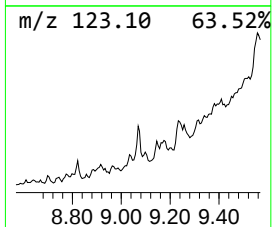
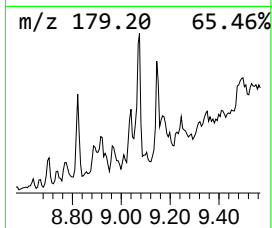
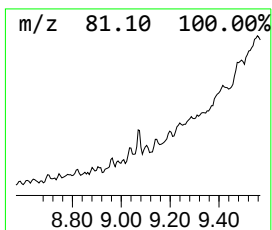
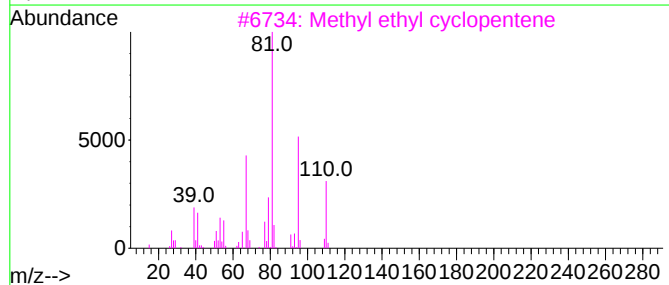
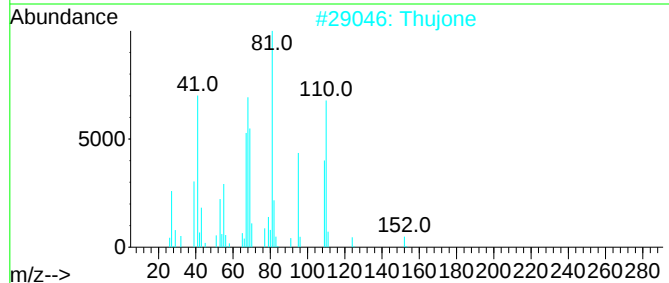
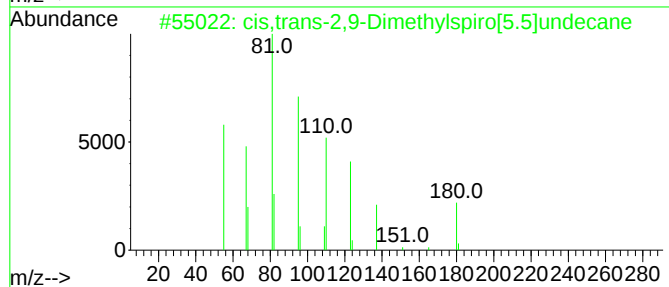
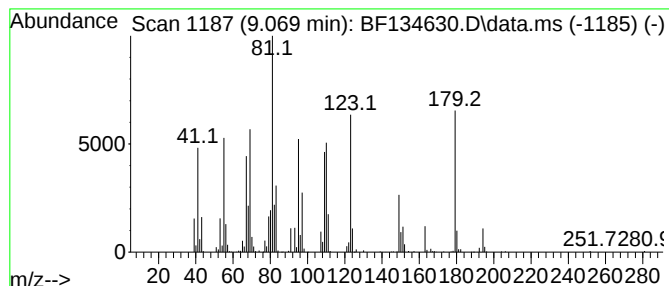
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.069 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.069	3.32 ng	405914	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	45
2			Thujone	152	C10H16O	000546-80-5	41
3			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	38
4			2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	35
5			Cyclopropane, tetramethylpropyli...	138	C10H18	024519-04-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
Data File : BF134630.D
Acq On : 04 Aug 2023 13:49
Operator : CG\JU
Sample : 03864-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

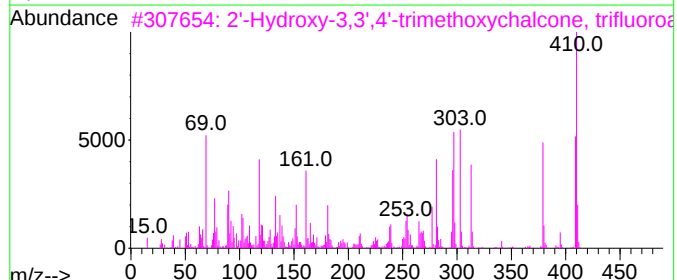
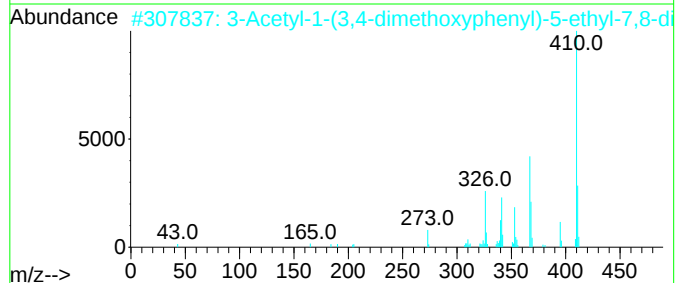
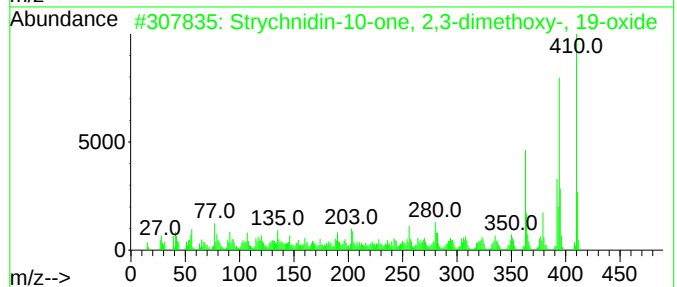
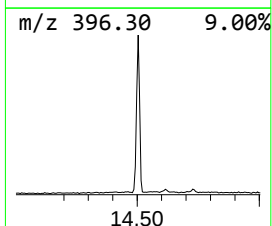
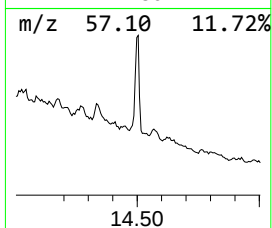
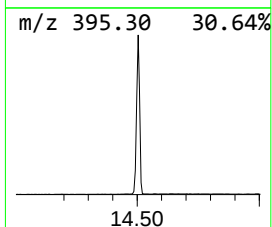
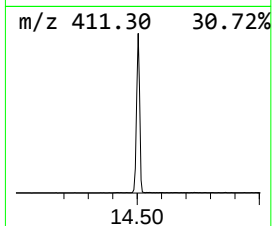
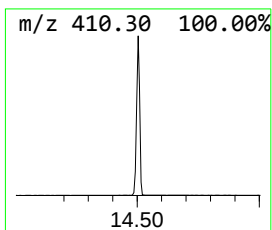
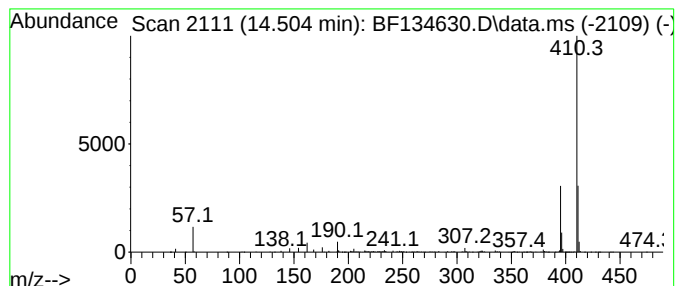
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Strychnidin-10-one, 2,3-dim... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	20.00 ng	972643	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Strychnidin-10-one, 2,3-dimethox...	410	C23H26N2O5	017301-81-4	86
2			3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	72
3			2'-Hydroxy-3,3',4'-trimethoxycha...	410	C20H17F3O6	1010453-84-8	53
4			6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	42
5			Ajmaline diacetate	410	C24H30N2O4	019775-56-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
Data File : BF134630.D
Acq On : 04 Aug 2023 13:49
Operator : CG\JU
Sample : 03864-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
2,7-Octadiene, ...	8.616	2.6	ng	161909	2	8.075	1228180	20.0
1-{4-Propylbicy...	8.704	4.1	ng	252779	2	8.075	1228180	20.0
unknown8.822	8.822	3.6	ng	218646	2	8.075	1228180	20.0
unknown8.963	8.963	4.3	ng	261697	2	8.075	1228180	20.0
unknown9.034	9.034	2.4	ng	289039	3	9.857	2448360	20.0
unknown9.069	9.069	3.3	ng	405914	3	9.857	2448360	20.0
Strychnidin-10-...	14.504	20.0	ng	972643	5	14.033	972643	20.0