

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
 Data File : BF137032.D
 Acq On : 10 Jan 2024 21:37
 Operator : CG\JU
 Sample : P1086-02 5X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 332

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	19	rVB	120771	163665	18.41%	1.567%
2	5.434	565	569	585	rBV	136420	178468	20.07%	1.709%
3	6.440	737	740	750	rBV	127499	166432	18.72%	1.594%
4	6.787	795	799	804	rVB	303551	259317	29.16%	2.483%
5	7.322	883	890	892	rBV2	41190	61624	6.93%	0.590%
6	7.345	892	894	897	rVV	117764	112401	12.64%	1.076%
7	7.375	897	899	902	rVV	70744	56493	6.35%	0.541%
8	7.422	902	907	910	rVB5	51310	69360	7.80%	0.664%
9	7.804	969	972	978	rBV6	32975	61088	6.87%	0.585%
10	7.998	1003	1005	1010	rBV3	61370	88232	9.92%	0.845%
11	8.063	1013	1016	1019	rVV	426151	363987	40.93%	3.486%
12	8.110	1021	1024	1027	rVV2	96500	108467	12.20%	1.039%
13	8.140	1027	1029	1035	rVV5	31061	53886	6.06%	0.516%
14	8.257	1047	1049	1052	rVB2	59930	52922	5.95%	0.507%
15	8.292	1052	1055	1058	rBV2	74357	111754	12.57%	1.070%
16	8.351	1062	1065	1068	rVB3	107568	108208	12.17%	1.036%
17	8.445	1077	1081	1083	rBV3	73867	78863	8.87%	0.755%
18	8.481	1083	1087	1088	rBV3	62331	75621	8.50%	0.724%
19	8.498	1088	1090	1092	rVV3	122452	107247	12.06%	1.027%
20	8.522	1092	1094	1097	rVB2	126830	119422	13.43%	1.144%
21	8.563	1097	1101	1103	rBV2	127713	132159	14.86%	1.266%
22	8.604	1103	1108	1110	rBV2	53383	74860	8.42%	0.717%
23	8.687	1118	1122	1124	rBV4	78898	124532	14.00%	1.193%
24	8.745	1130	1132	1136	rVB4	89733	104928	11.80%	1.005%
25	8.804	1139	1142	1144	rBV3	90217	77175	8.68%	0.739%
26	8.834	1144	1147	1150	rBV3	92098	97385	10.95%	0.933%
27	8.887	1154	1156	1160	rBV3	193356	200322	22.53%	1.918%
28	8.922	1160	1162	1163	rBV	55968	52936	5.95%	0.507%
29	9.051	1182	1184	1187	rVB3	129502	114822	12.91%	1.100%
30	9.081	1187	1189	1192	rBV3	123556	131366	14.77%	1.258%
31	9.139	1194	1199	1203	rBV3	305409	361243	40.63%	3.459%
32	9.175	1203	1205	1208	rBV4	123000	103778	11.67%	0.994%
33	9.210	1208	1211	1215	rBV3	408094	526390	59.20%	5.041%
34	9.322	1228	1230	1234	rBV4	139894	130284	14.65%	1.248%
35	9.451	1249	1252	1254	rBV4	260281	261501	29.41%	2.504%
36	9.528	1263	1265	1267	rBV	489559	414361	46.60%	3.968%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.634	1281	1283	1287	rVB4	172148	145697	16.38%	1.395%
38	9.686	1289	1292	1294	rBV2	491820	520270	58.51%	4.982%
39	9.734	1297	1300	1303	rVB4	847114	804875	90.52%	7.708%
40	9.769	1304	1306	1309	rBV3	198769	169376	19.05%	1.622%
41	9.804	1309	1312	1314	rBV2	485734	683331	76.85%	6.544%
42	9.857	1319	1321	1324	rBV3	250631	262355	29.50%	2.512%
43	10.010	1345	1347	1349	rBV2	212522	152176	17.11%	1.457%
44	10.145	1367	1370	1371	rBV3	355123	363337	40.86%	3.479%
45	10.234	1382	1385	1388	rBV2	898392	889213	100.00%	8.515%
46	13.998	2023	2025	2028	rVB	410811	365384	41.09%	3.499%
47	14.474	2103	2106	2109	rBV	622922	528819	59.47%	5.064%
48	15.474	2273	2276	2281	rVB	206496	252252	28.37%	2.416%

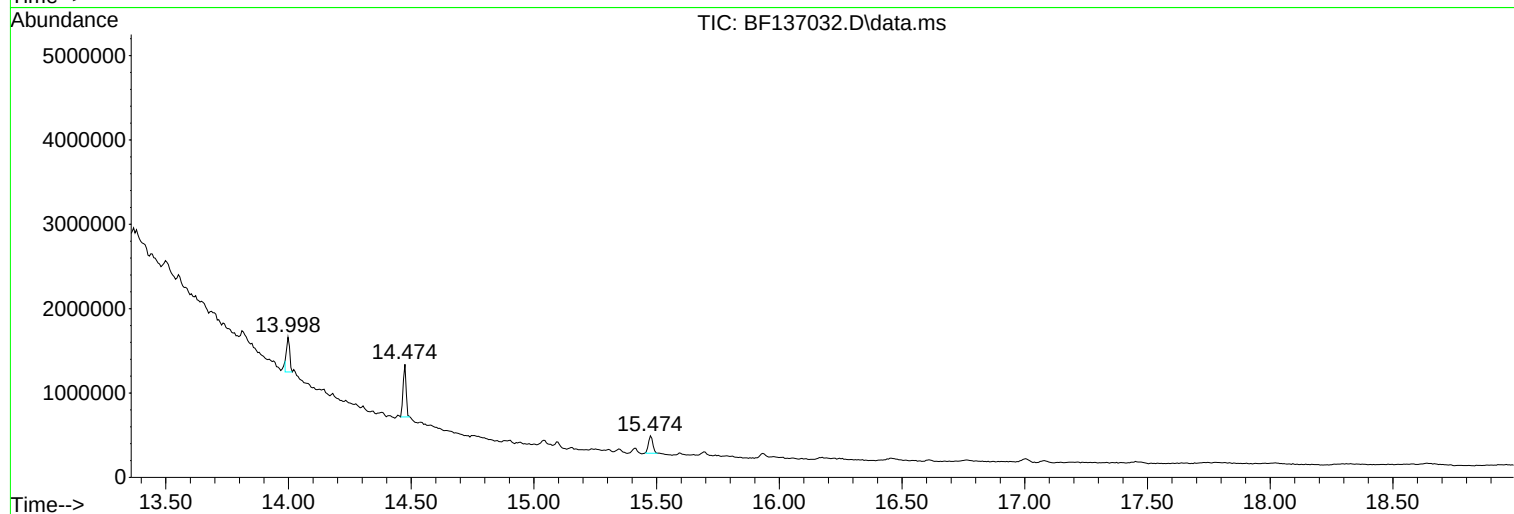
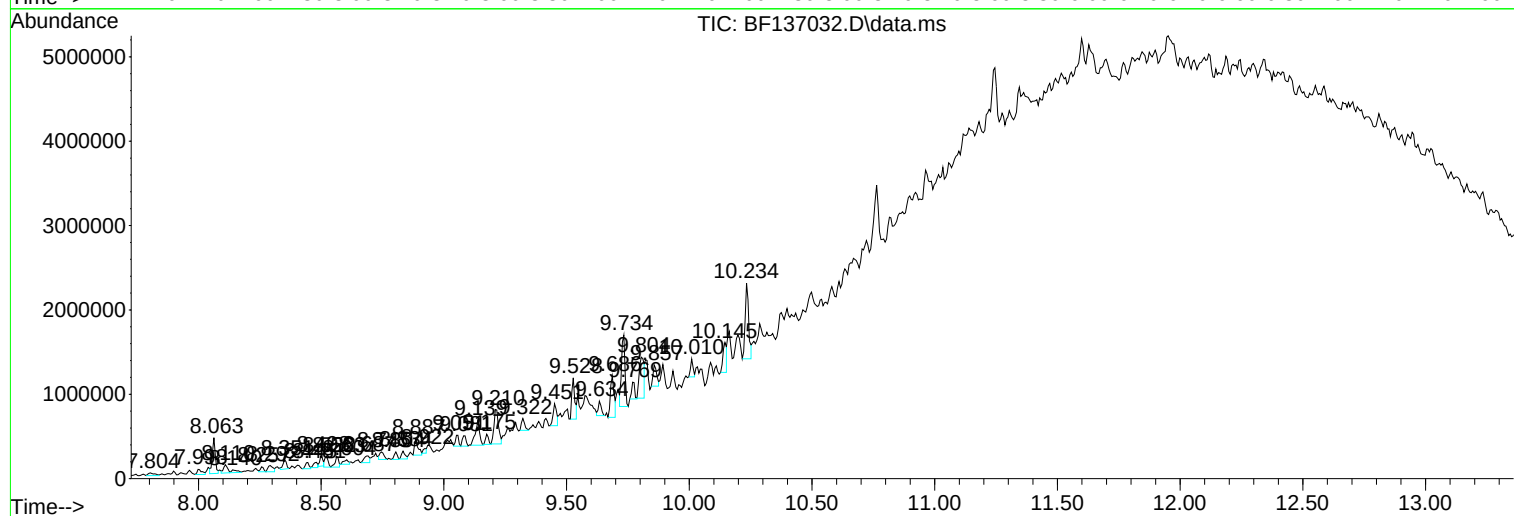
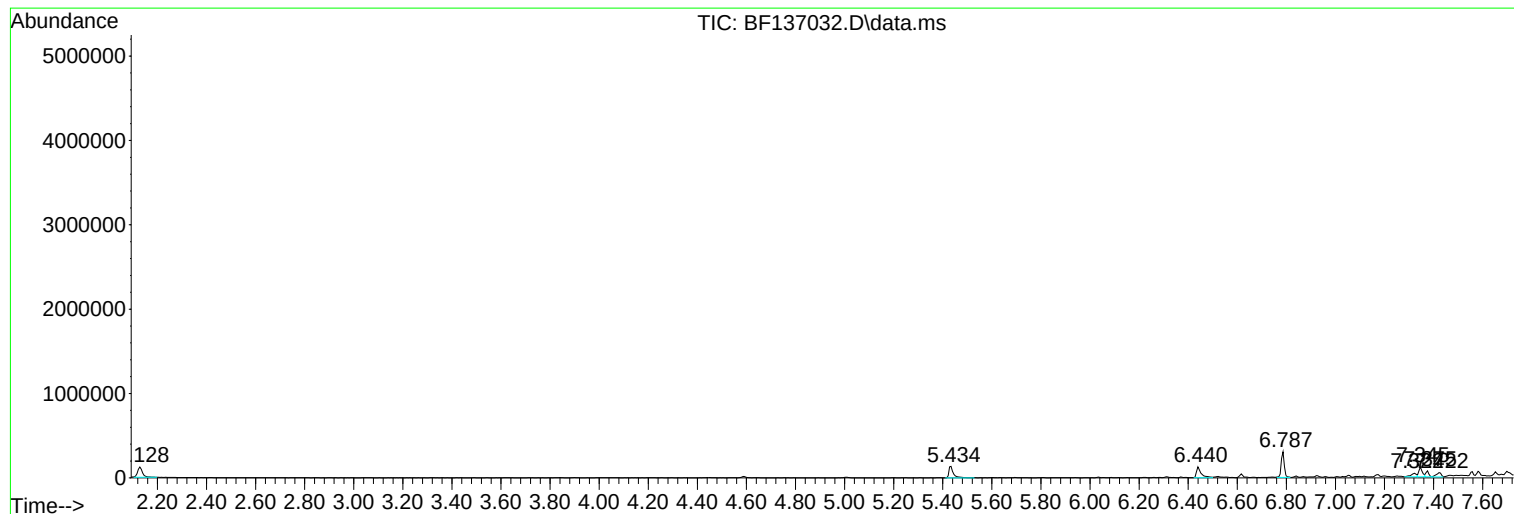
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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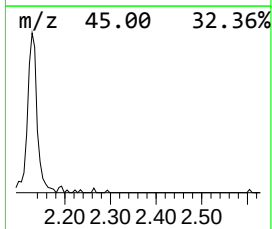
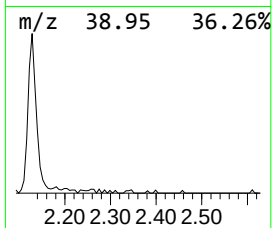
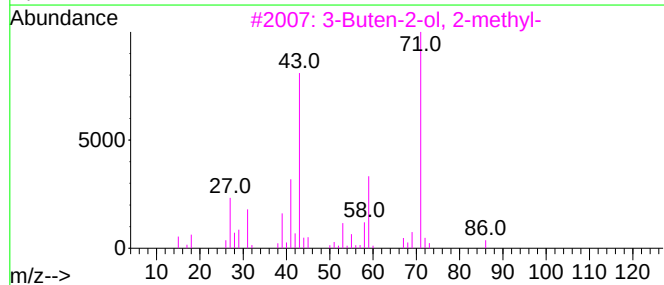
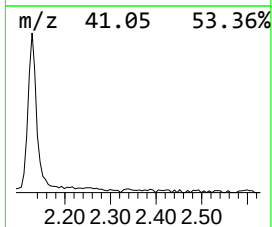
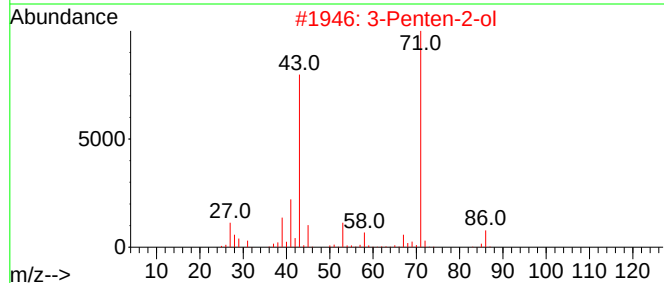
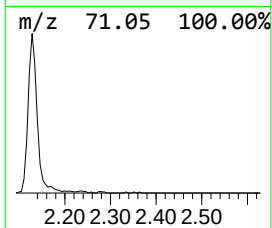
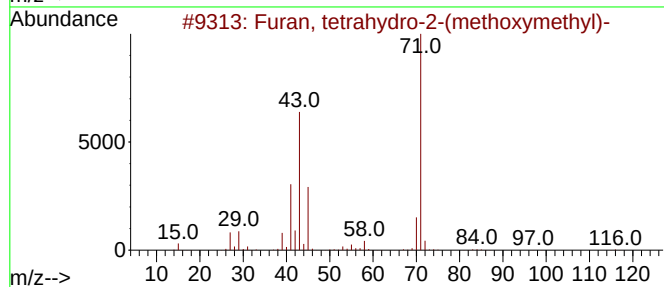
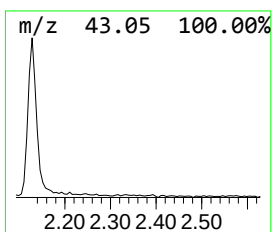
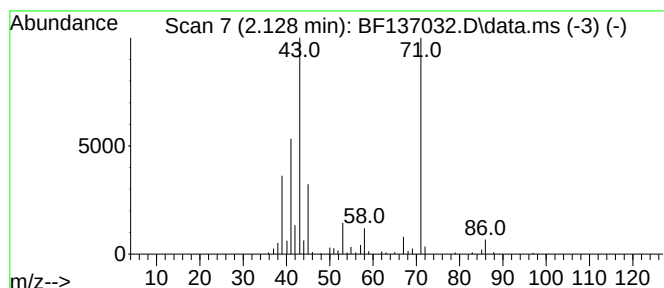
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Furan, tetrahydro-2-(methox... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	12.62 ng	163665	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
2			3-Penten-2-ol	86	C5H10O	001569-50-2	64
3			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	59
4			Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	50
5			1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	45



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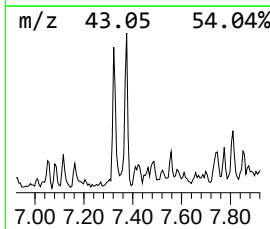
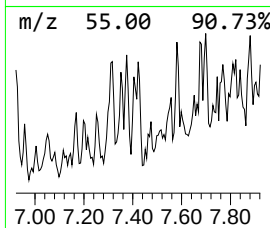
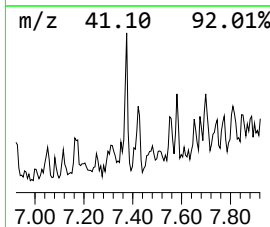
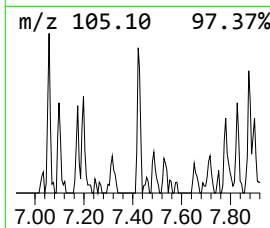
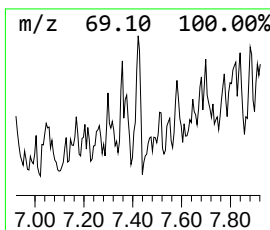
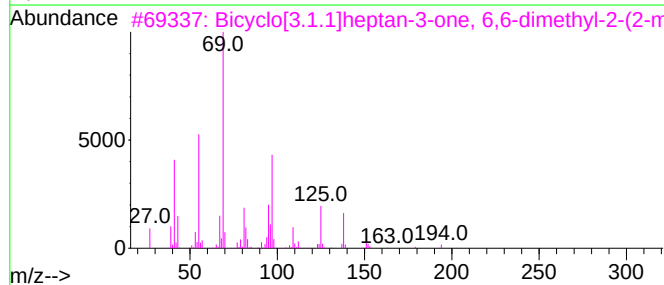
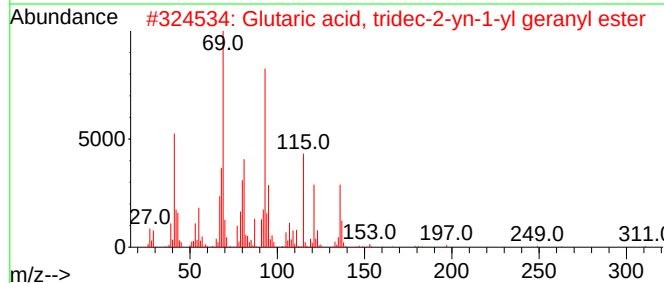
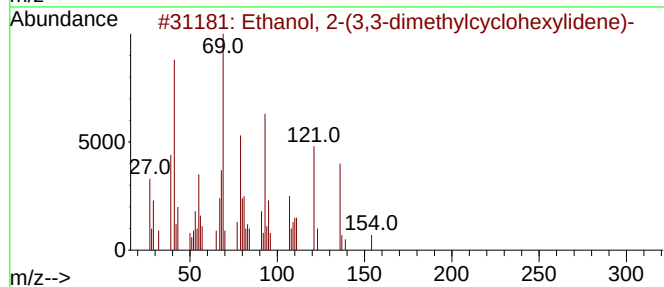
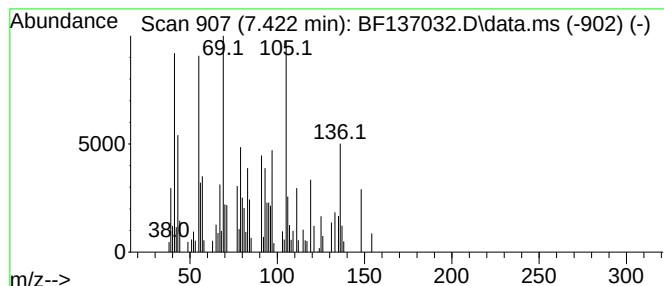
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.422 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.422	5.35 ng	69360	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(3,3-dimethylcyclohex...	154	C10H18O	041370-29-0	43
2			Glutaric acid, tridec-2-yn-1-yl ...	446	C28H46O4	1000405-02-9	38
3			Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	38
4			Butyric acid, 2-phenyl-, oct-3-e...	274	C18H26O2	1000406-91-7	27
5			Cyclooctane, methyl-	126	C9H18	001502-38-1	27



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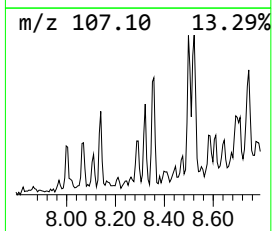
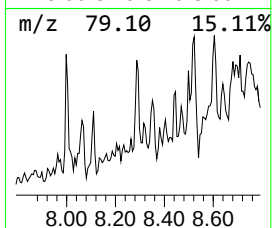
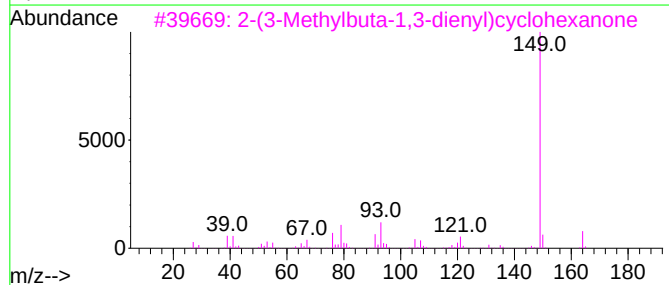
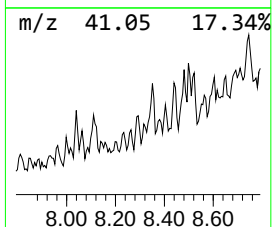
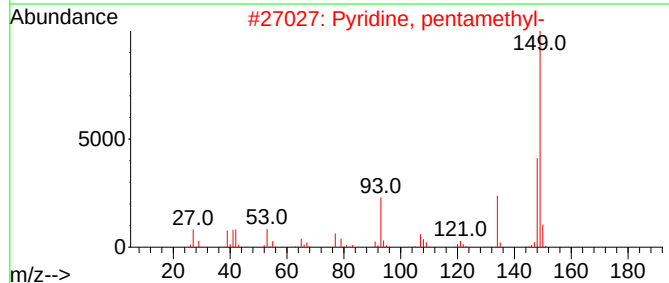
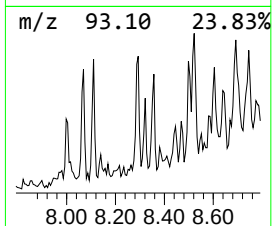
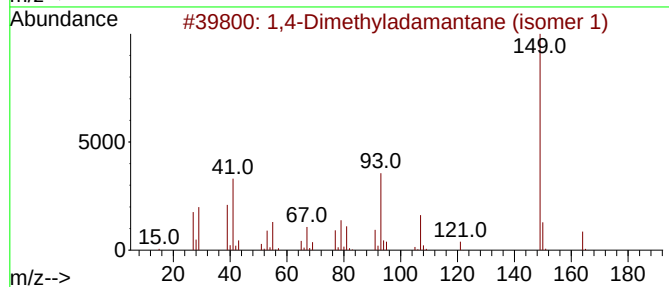
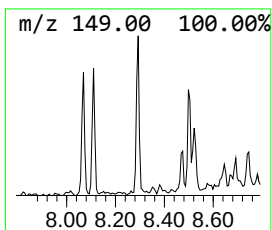
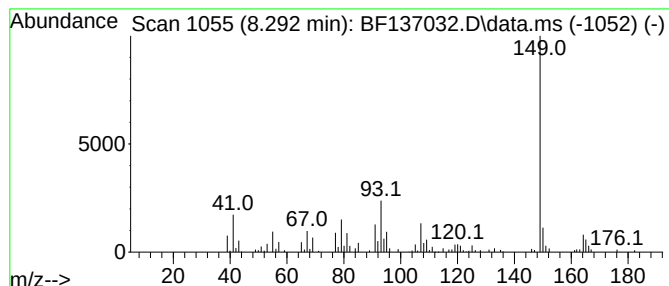
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,4-Dimethyladamantane (iso... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.292	6.14 ng	111754	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	81
2			Pyridine, pentamethyl-	149	C10H15N	003748-83-2	64
3			2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	59
4			Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	58
5			2'-Hydroxy-4',5'-dimethylacetoph...	164	C10H12O2	036436-65-4	53



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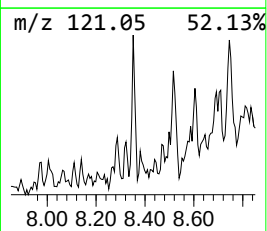
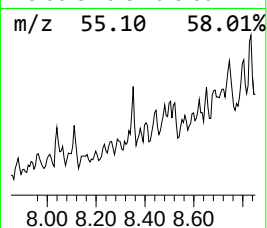
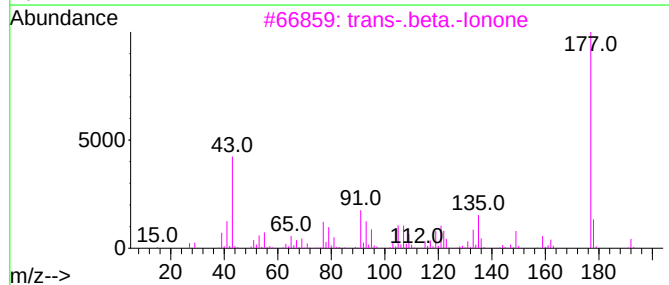
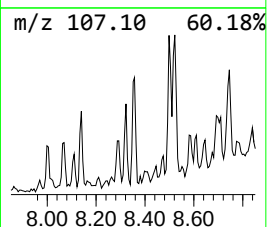
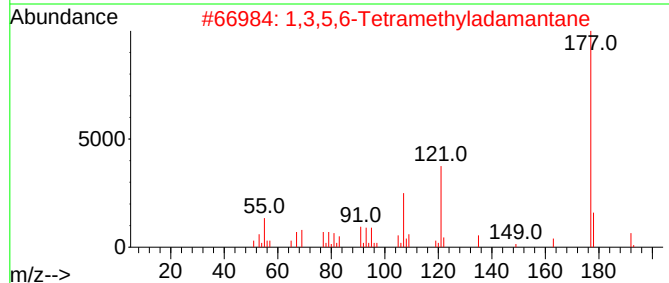
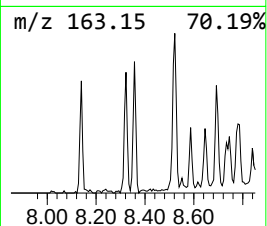
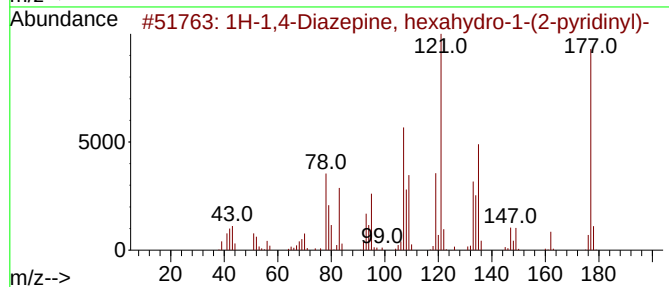
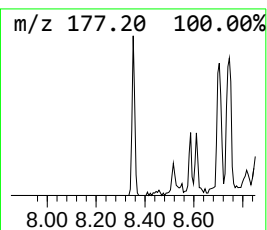
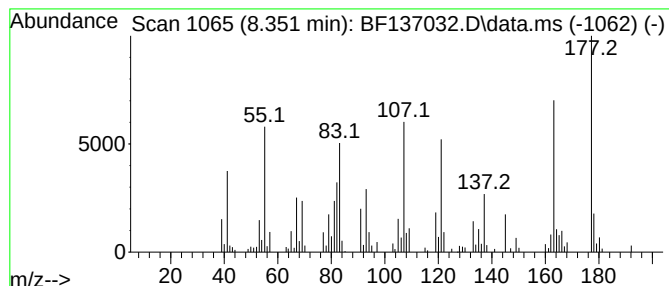
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1H-1,4-Diazepine, hexahydro... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.351	5.95 ng	108208	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,4-Diazepine, hexahydro-1-(2...	177	C10H15N3	1000337-93-1	53		
2	1,3,5,6-Tetramethyladamantane	192	C14H24	034694-70-7	38		
3	trans-.beta.-Ionone	192	C13H20O	000079-77-6	25		
4	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	25		
5	1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	25		



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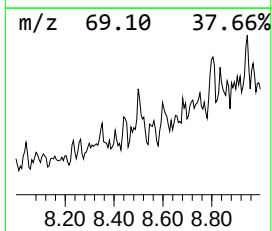
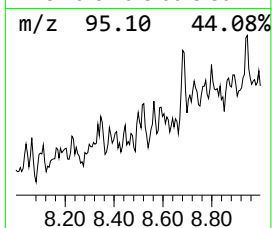
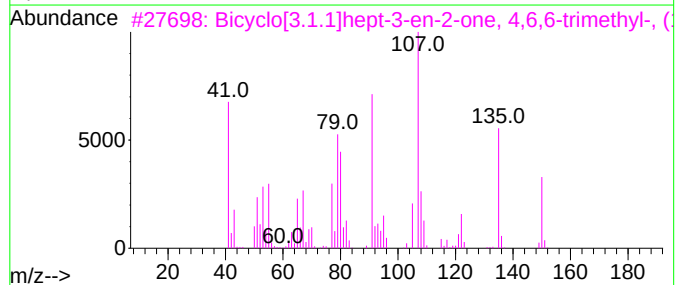
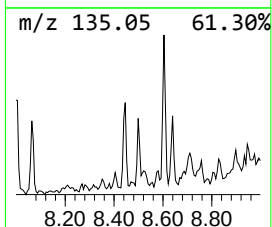
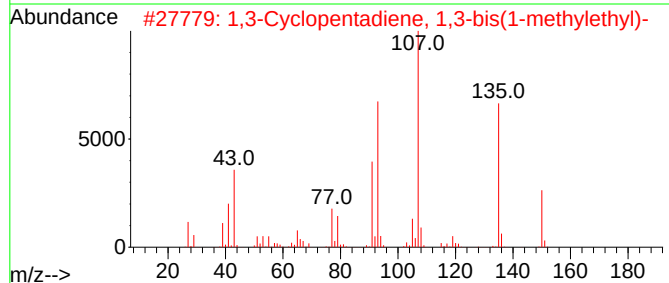
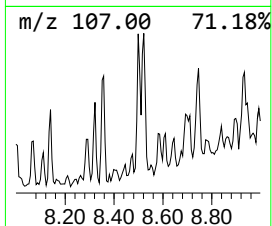
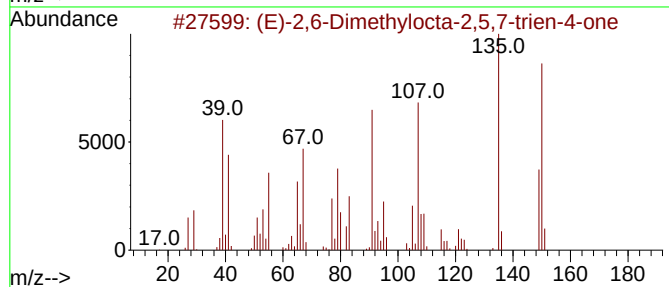
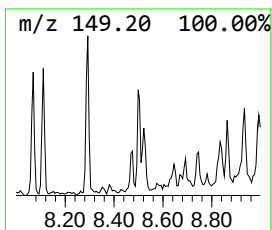
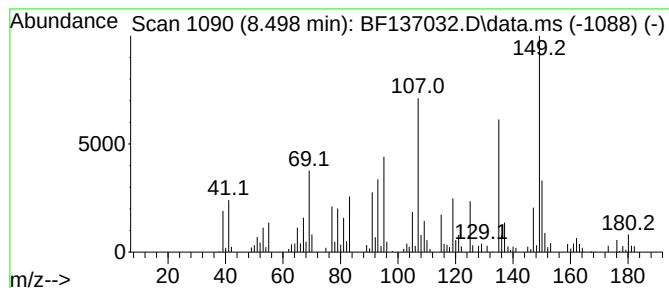
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.498 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.498	5.89 ng	107247	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-2,6-Dimethylocta-2,5,7-trien...	150	C10H14O	033746-72-4	42		
2	1,3-Cyclopentadiene, 1,3-bis(1-m...	150	C11H18	123278-27-3	38		
3	Bicyclo[3.1.1]hept-3-en-2-one, 4...	150	C10H14O	001196-01-6	30		
4	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	30		
5	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	30		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
Operator : CG\JU
Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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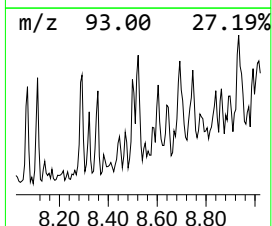
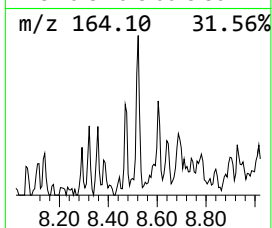
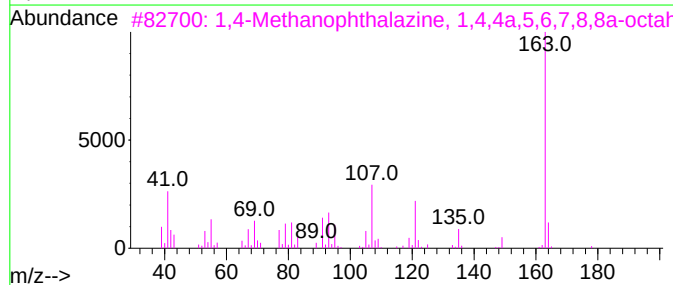
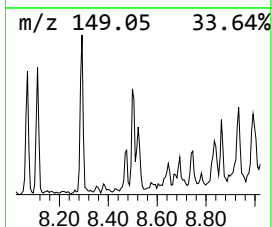
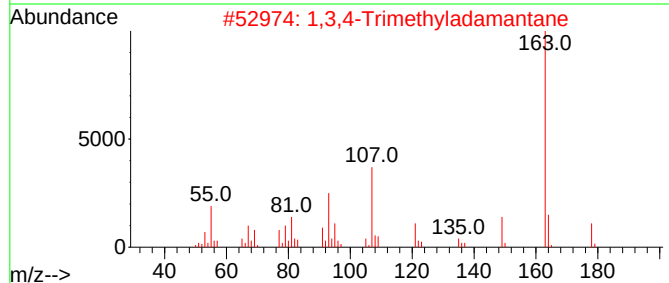
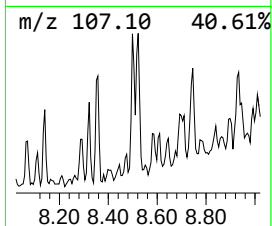
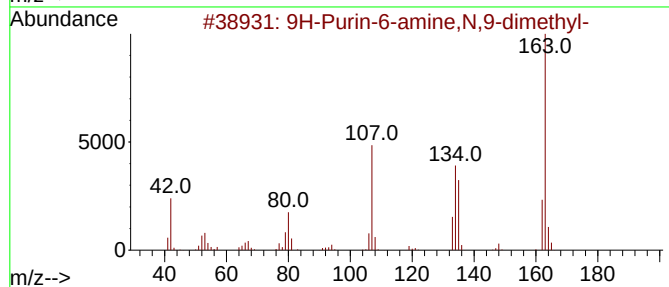
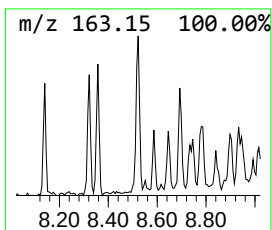
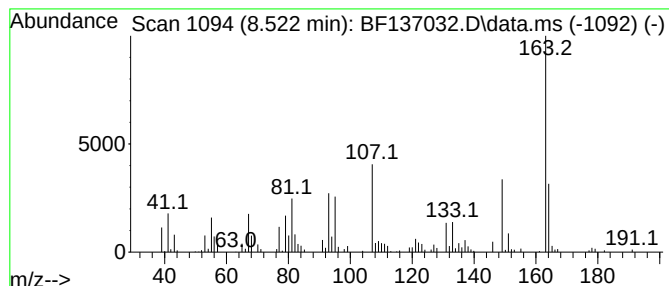
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.522 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	6.56 ng	119422	Naphthalene-d8	8.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9H-Purin-6-amine,N,9-dimethyl-	163	C7H9N5	002009-52-1	43
2		1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	42
3		1,4-Methanophthalazine, 1,4,4a,5...	206	C13H22N2	109746-14-7	40
4		Tricyclo[3.3.1.1(3,7)-]decane, 1...	242	C12H19Br	000941-37-7	37
5		l-Tyrophanamide	180	C9H12N2O2	1000131-25-3	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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Sample : P1086-02 5X
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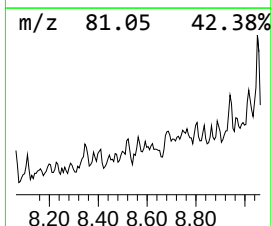
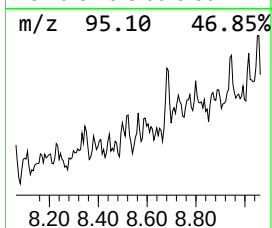
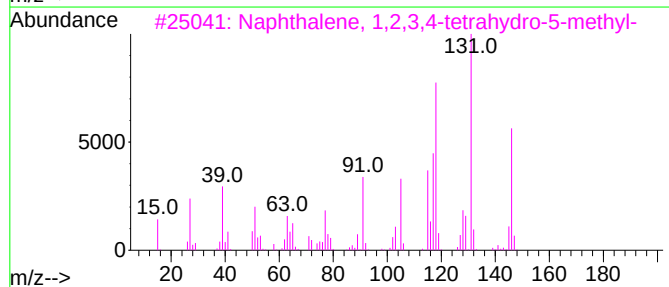
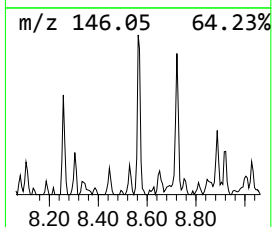
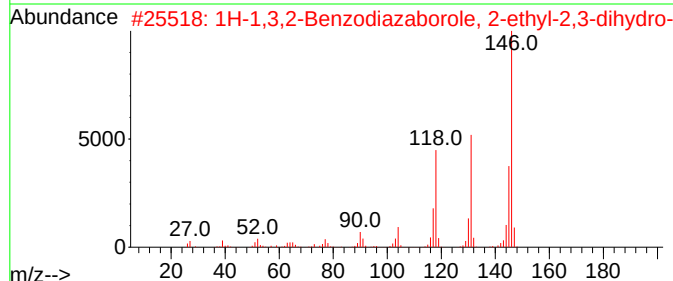
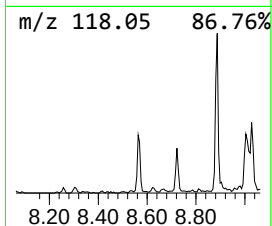
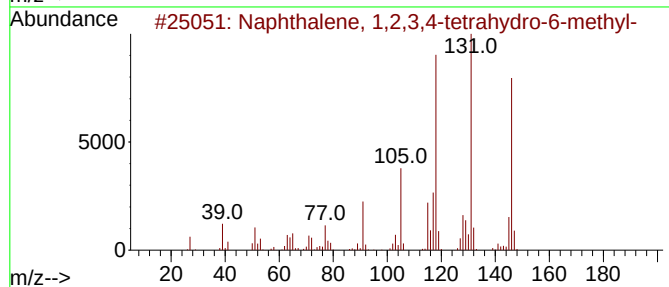
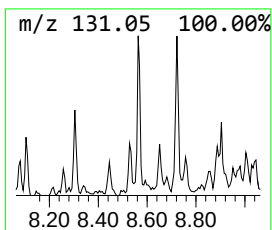
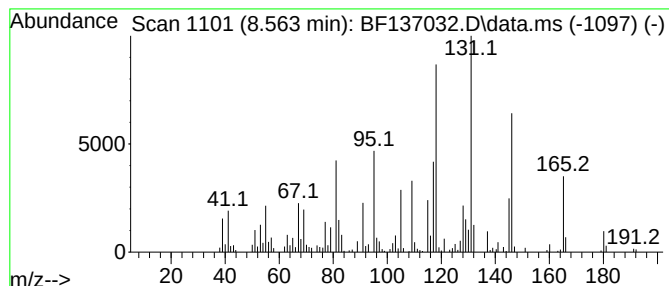
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.563	7.26 ng	132159	Naphthalene-d8	8.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	83
2	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	70
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	70
4	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	58
5	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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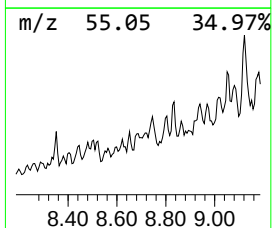
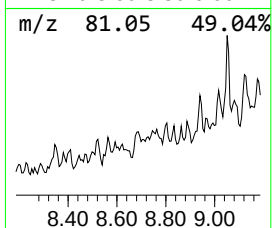
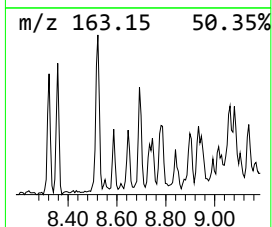
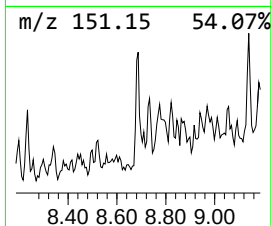
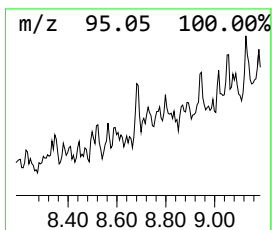
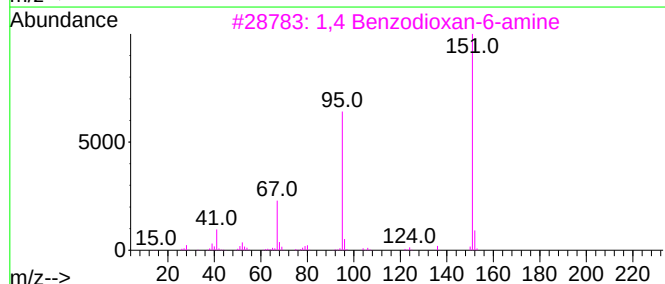
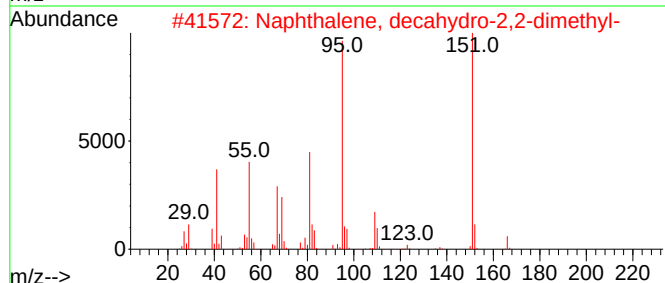
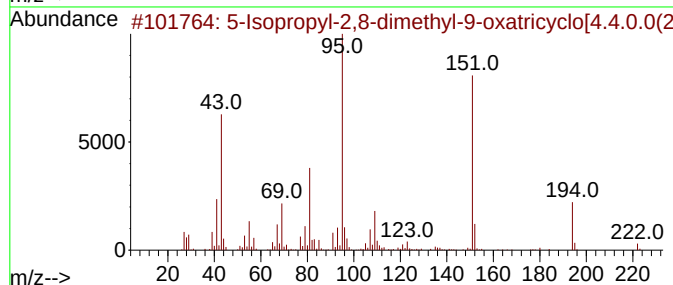
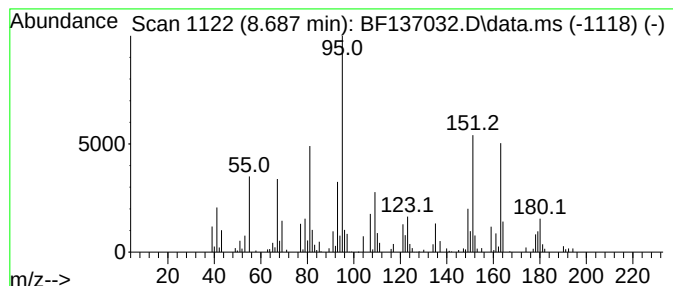
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.687 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.687	6.84 ng	124532	Naphthalene-d8	8.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Isopropyl-2,8-dimethyl-9-oxatr...	222	C14H22O2	1010185-23-8	38
2	Naphthalene, decahydro-2,2-dimet...	166	C12H22	031124-85-3	38
3	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	35
4	Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	30
5	2-naphthalenemethanol, decahydro...	182	C12H22O	1000404-89-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
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Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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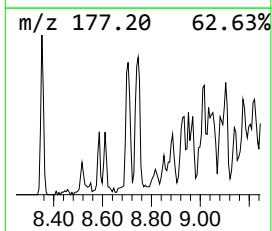
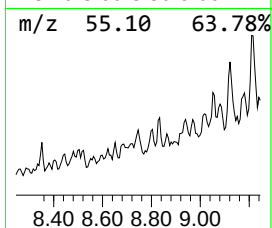
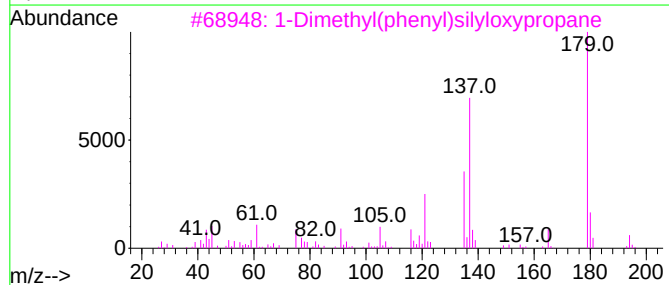
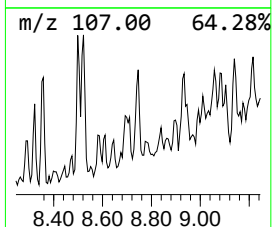
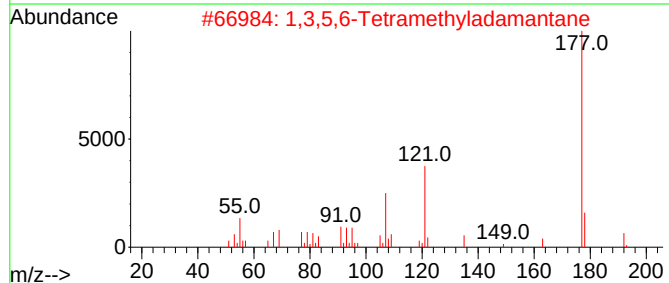
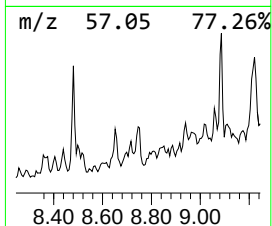
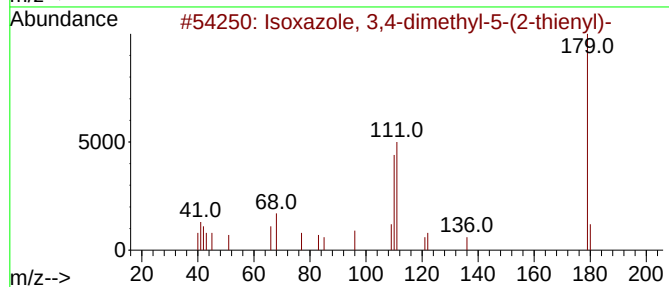
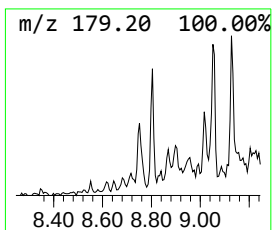
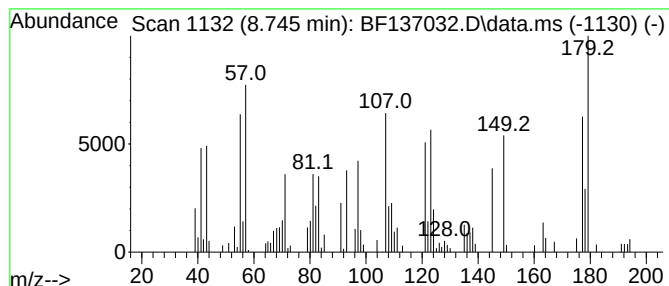
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.745 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.745	5.77 ng	104928	Naphthalene-d8	8.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isoxazole, 3,4-dimethyl-5-(2-thi...	179	C9H9NOS	056421-65-9	10
2		1,3,5,6-Tetramethyladamantane	192	C14H24	034694-70-7	10
3		1-Dimethyl(phenyl)silyloxypropane	194	C11H18OSi	013360-21-9	10
4		p-Phenylbenzonitrile	179	C13H9N	002920-38-9	10
5		Phenanthridine	179	C13H9N	000229-87-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
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Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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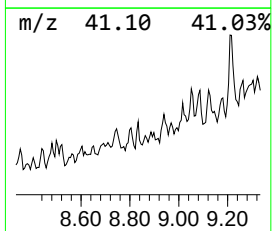
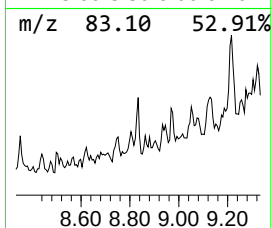
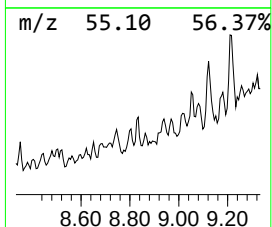
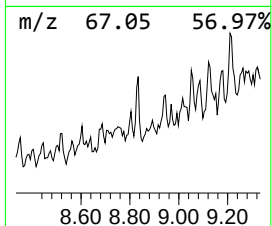
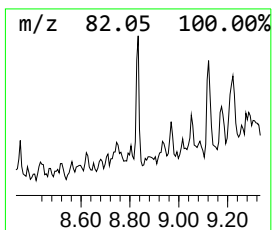
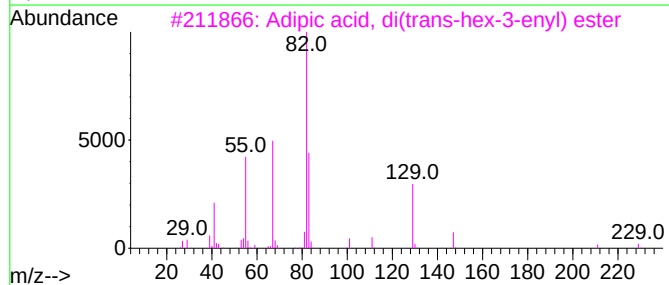
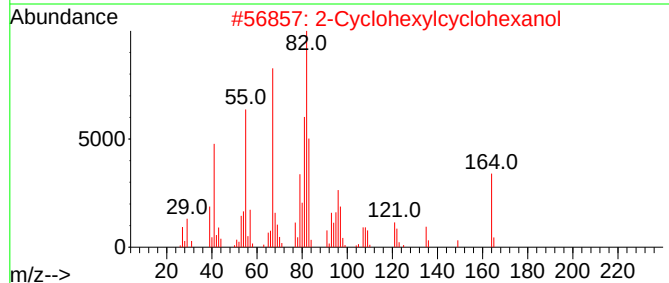
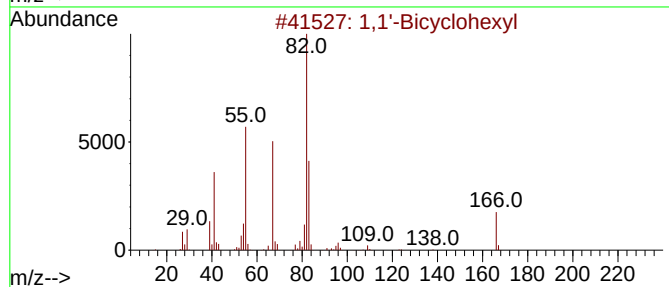
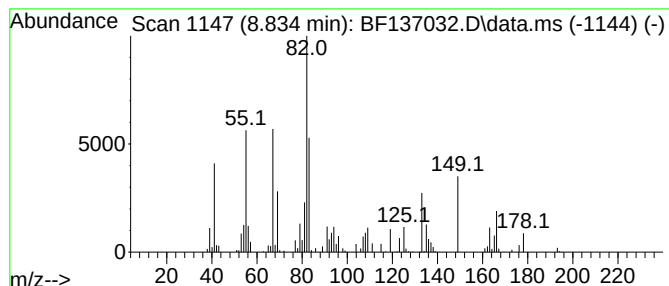
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,1'-Bicyclohexyl Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.834	5.35 ng	97385	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Bicyclohexyl			166	C12H22	000092-51-3	58
2	2-Cyclohexylcyclohexanol			182	C12H22O	006531-86-8	50
3	Adipic acid, di(trans-hex-3-enyl...			310	C18H30O4	1000354-02-3	47
4	Succinic acid, cyclohexylmethyl ...			296	C17H28O4	1000391-08-5	43
5	4-Methyl-1,3-pentadiene			82	C6H10	000926-56-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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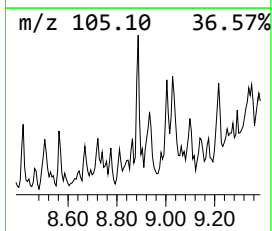
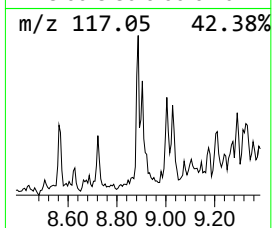
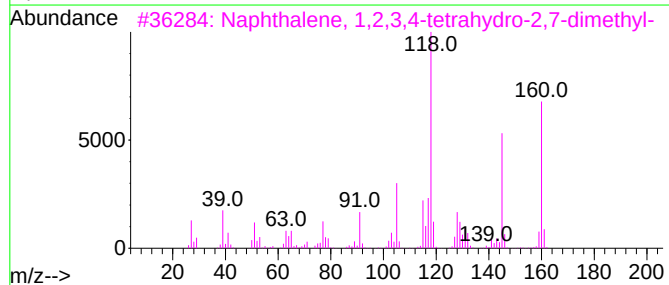
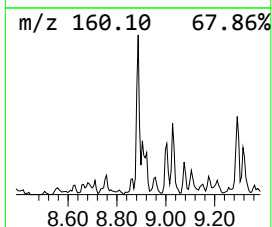
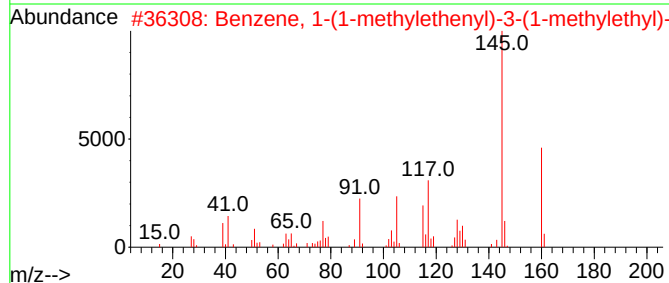
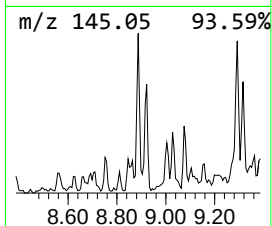
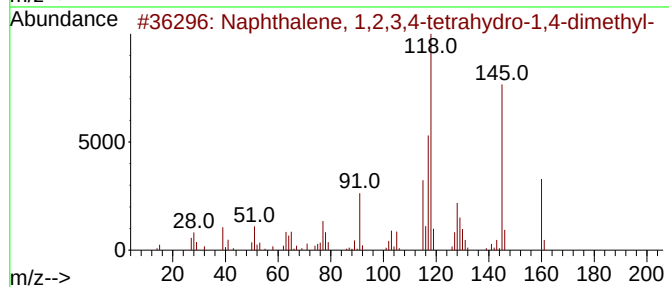
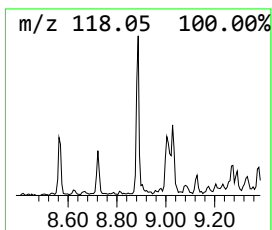
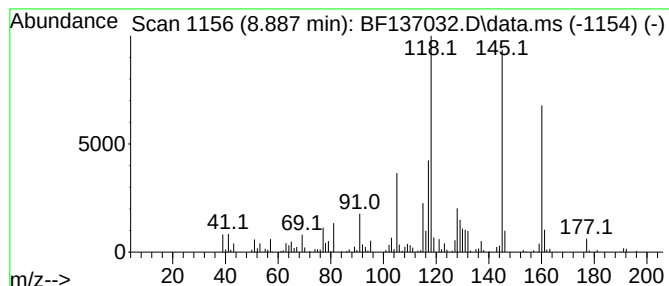
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.887	11.01 ng	200322	Naphthalene-d8	8.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	94
2	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	91
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	74
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	64
5	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
Operator : CG\JU
Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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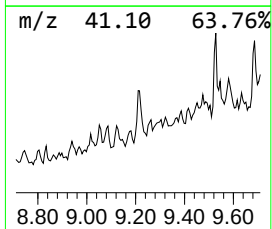
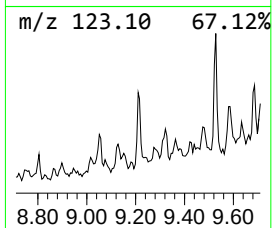
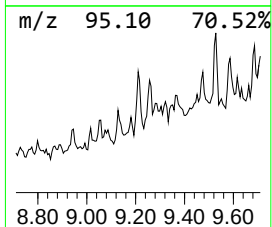
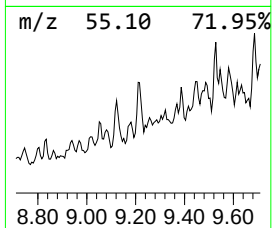
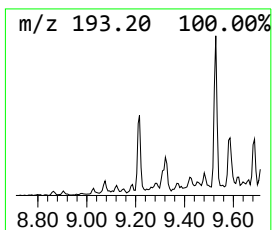
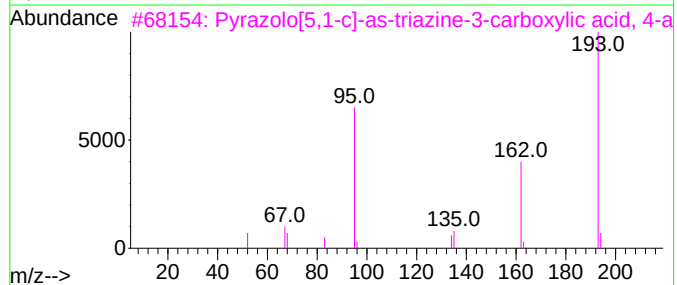
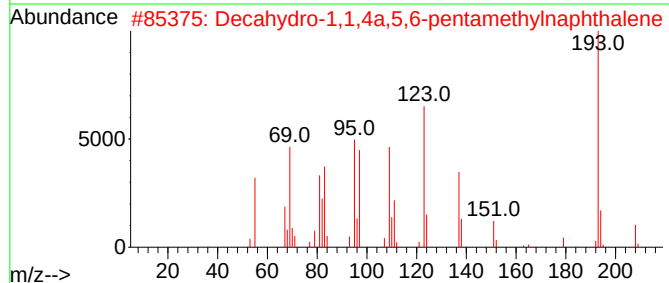
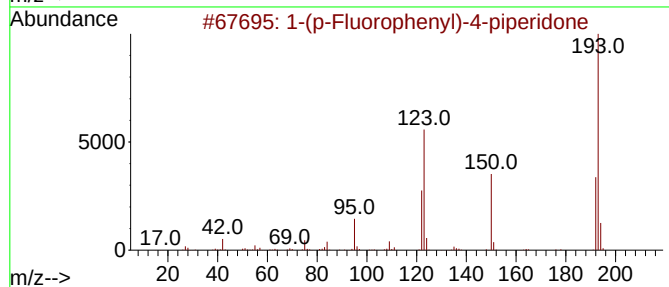
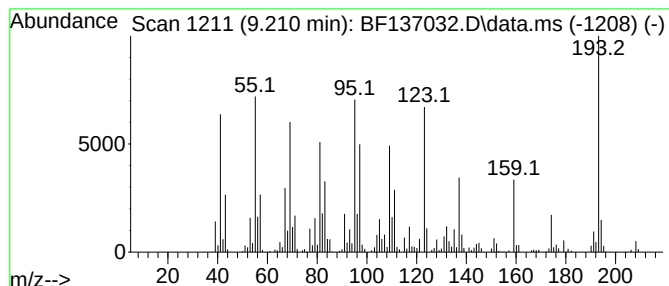
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown9.210 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.210	15.41 ng	526390	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38		
3	Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	27		
4	1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	27		
5	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
Operator : CG\JU
Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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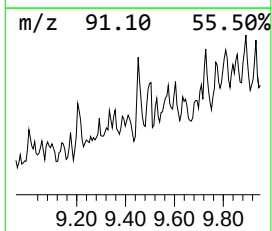
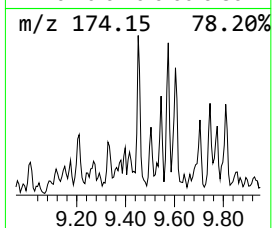
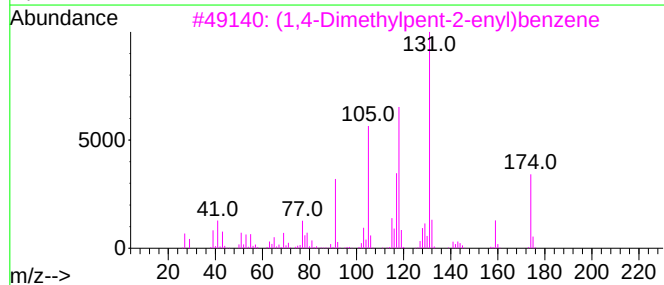
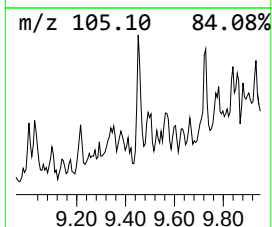
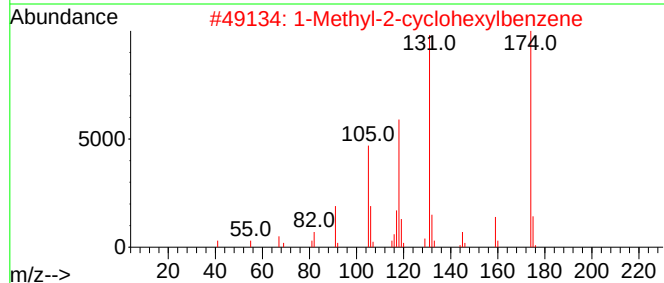
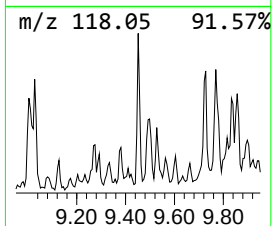
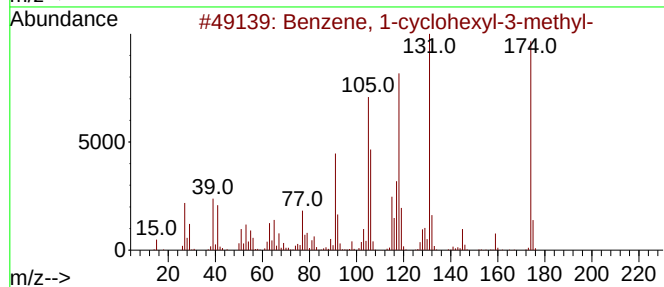
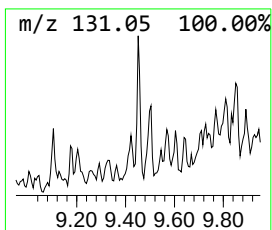
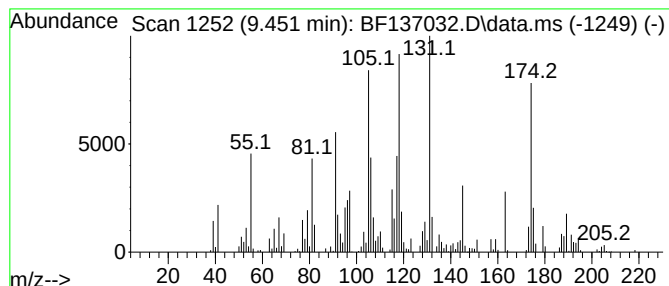
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzene, 1-cyclohexyl-3-met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.451	7.65 ng	261501	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	96
2			1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	76
3			(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	70
4			N-Benzyl-2-cyano-acetamide	174	C10H10N2O	1000300-42-1	25
5			Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
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Sample : P1086-02 5X
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Instrument :
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ClientSampleId :
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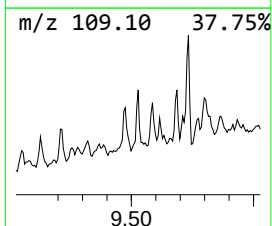
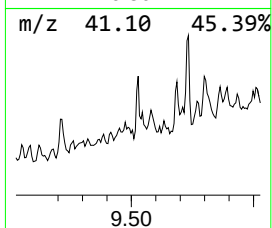
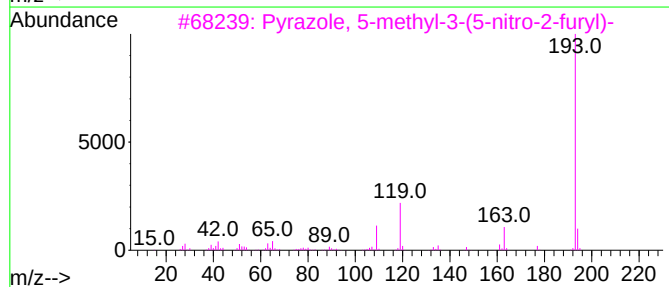
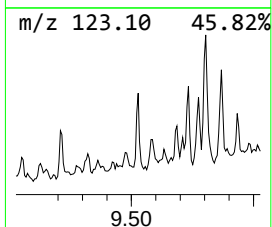
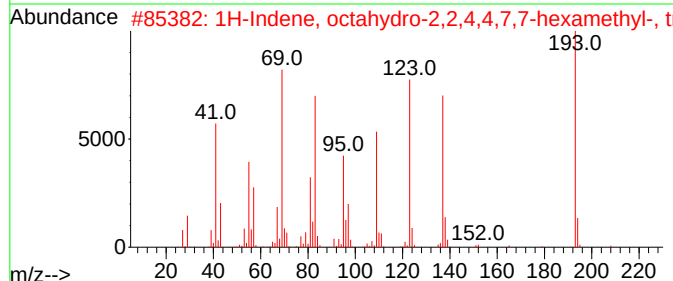
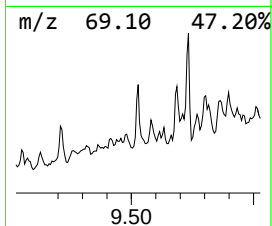
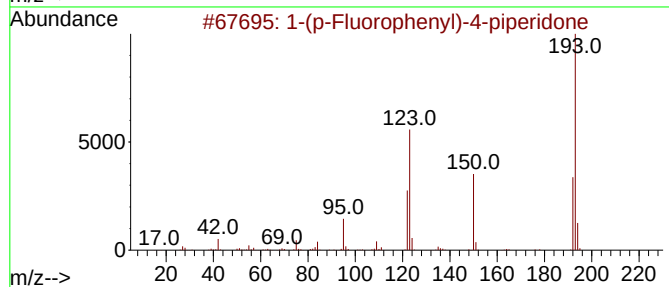
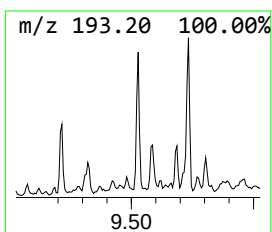
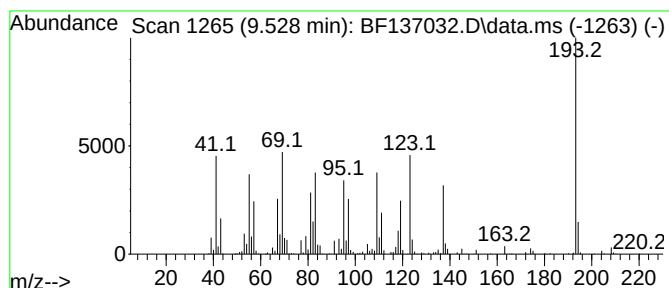
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown9.528 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	12.13 ng	414361	Acenaphthene-d10	9.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
2		1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	37
3		Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	35
4		3,4-Diethoxy-N-(4,5,6,7-tetrahyd...	346	C18H22N2O3S	1000311-37-1	25
5		[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
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Operator : CG\JU
Sample : P1086-02 5X
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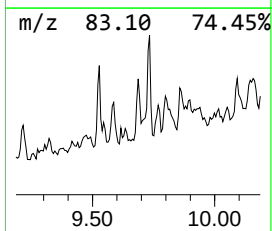
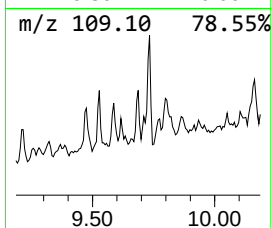
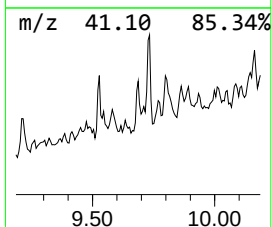
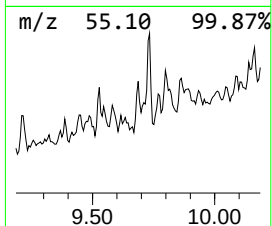
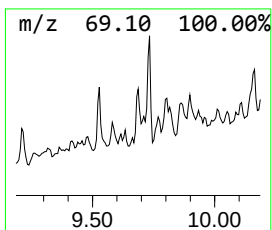
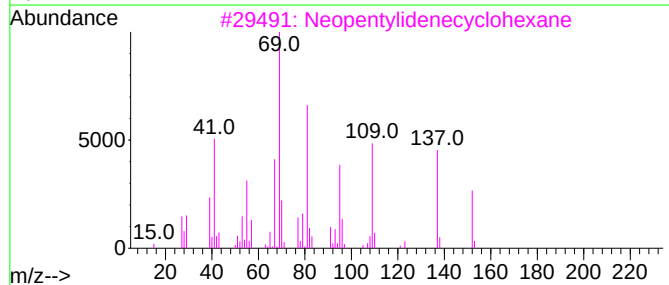
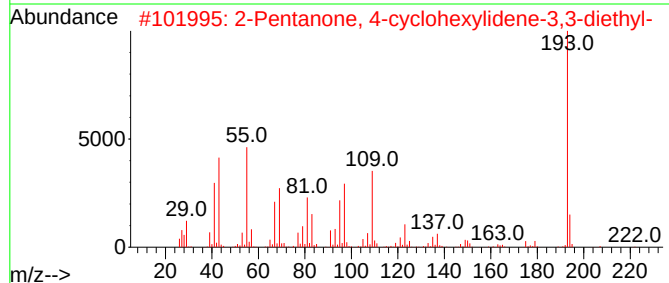
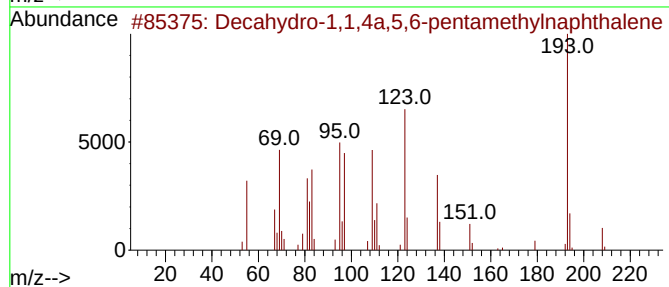
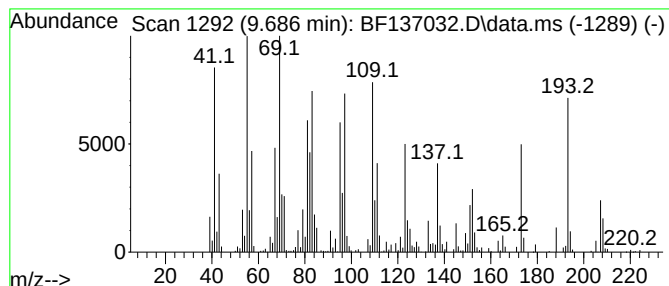
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown9.686 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.686	15.23 ng	520270	Acenaphthene-d10	9.828	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	45
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
3	Neopentylidenecyclohexane	152	C11H20	039546-80-0	35
4	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	30
5	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
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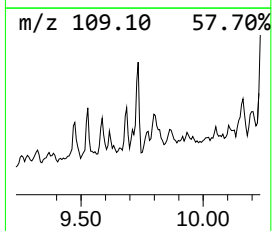
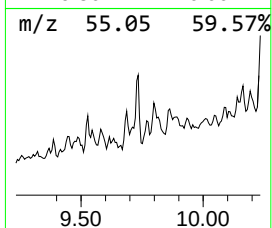
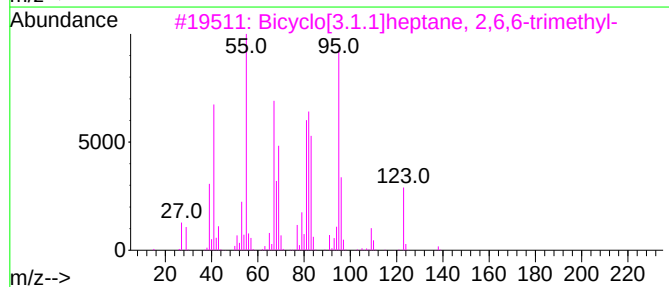
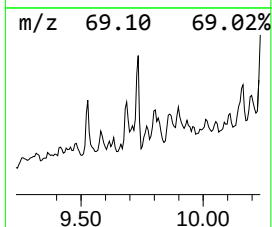
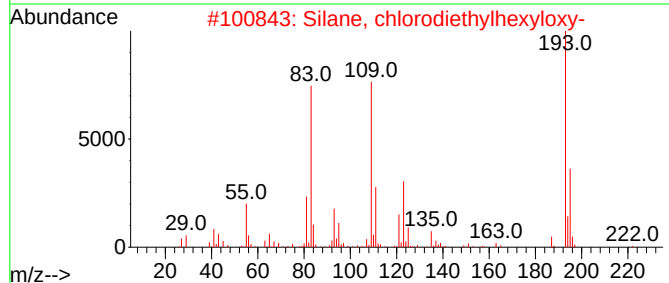
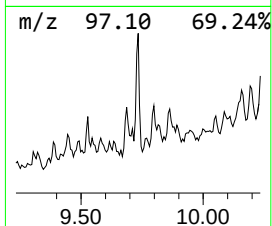
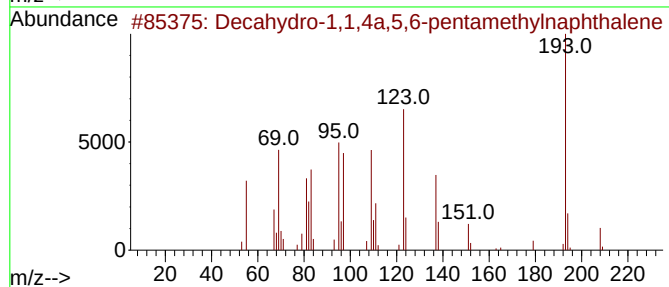
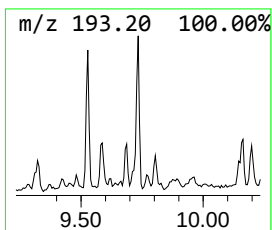
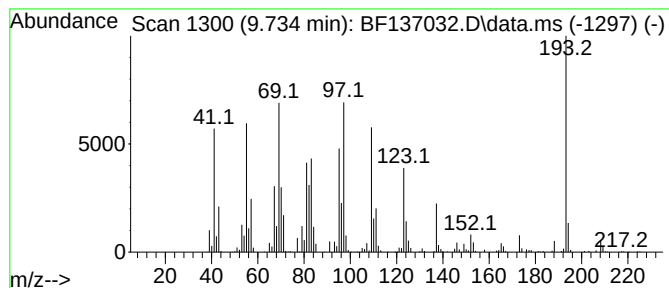
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown9.734 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.734	23.56 ng	804875	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2			Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	35
3			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	30
4			Hexadecanedinitrile	248	C16H28N2	006812-44-8	22
5			(-)-trans-Pinane	138	C10H18	033626-25-4	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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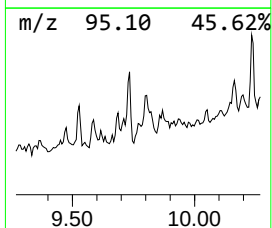
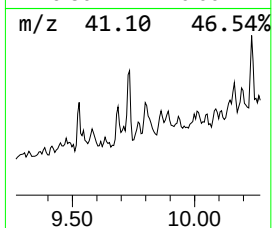
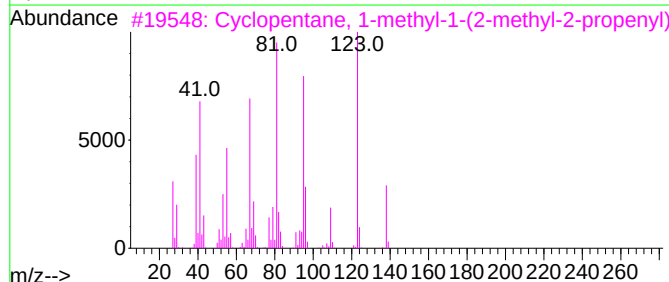
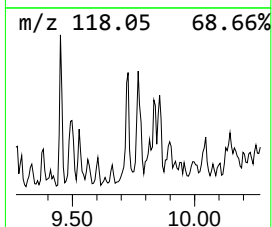
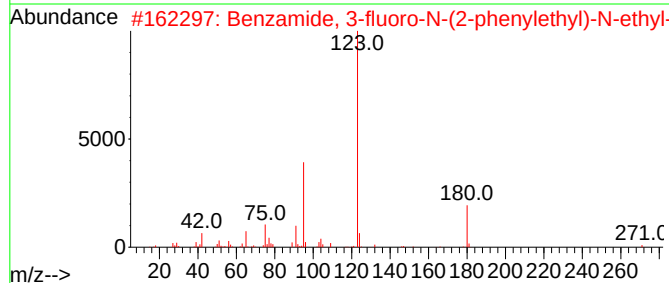
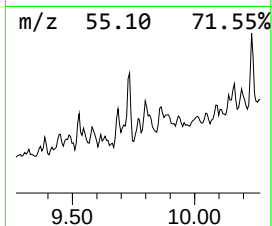
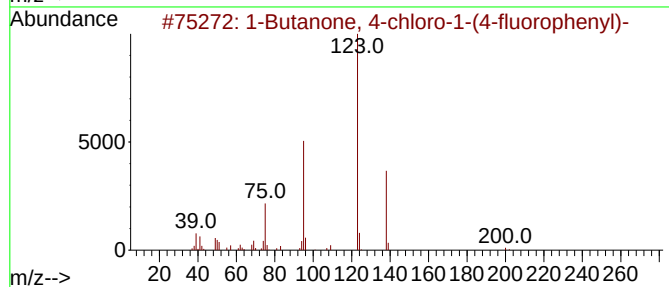
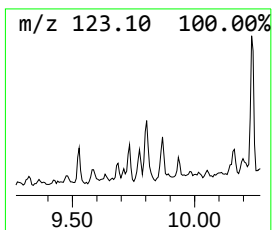
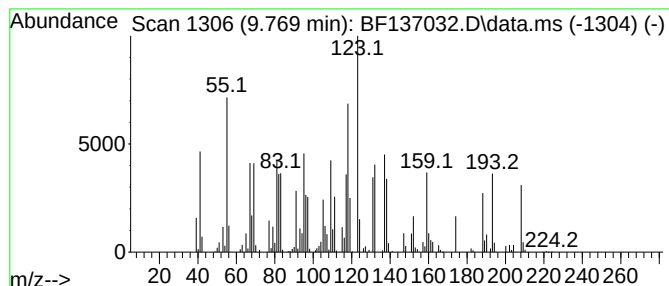
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown9.769 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	4.96 ng	169376	Acenaphthene-d10	9.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanone, 4-chloro-1-(4-fluoro...	200	C10H10ClFO	003874-54-2	22
2		Benzamide, 3-fluoro-N-(2-phenyle...	271	C17H18FNO	1000451-30-0	22
3		Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	22
4		Benzamide, 3-fluoro-N-(2-phenyle...	257	C16H16FNO	1000451-29-9	22
5		2-Cyclopenten-1-one, 2,3,4,5-tet...	138	C9H14O	054458-61-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
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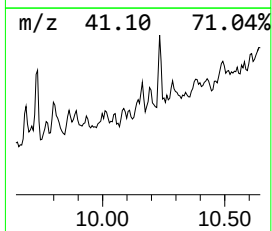
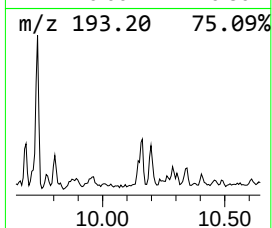
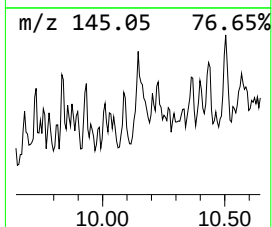
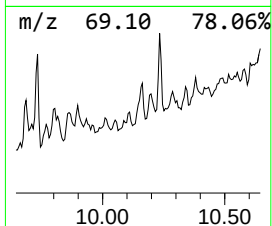
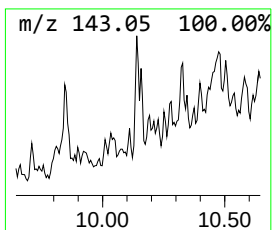
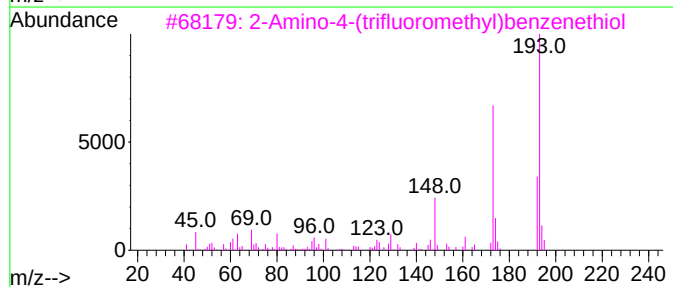
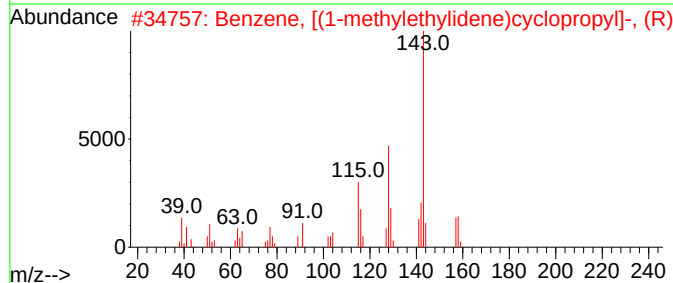
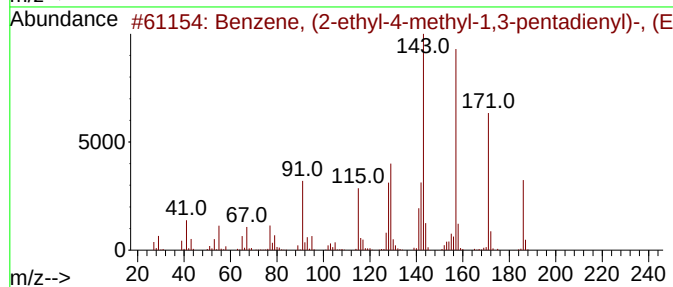
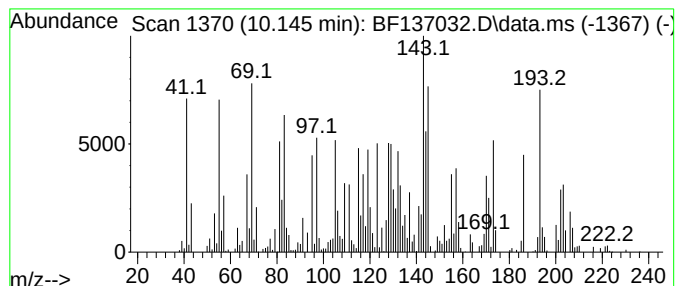
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown10.145 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.145	10.63 ng	363337	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-ethyl-4-methyl-1,3-p...	186	C14H18	074663-67-5	30
2			Benzene, [(1-methylethylidene)cy...	158	C12H14	024524-55-8	25
3			2-Amino-4-(trifluoromethyl)benze...	193	C7H6F3NS	004274-38-8	25
4			1H-Indene, 3-butyl-1-methyl-	186	C14H18	111400-84-1	25
5			1H-Indene, 3-ethyl-1-(1-methylet...	186	C14H18	111400-85-2	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
Operator : CG\JU
Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

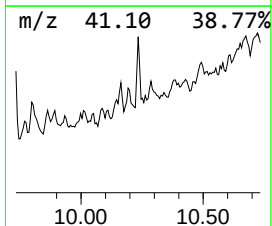
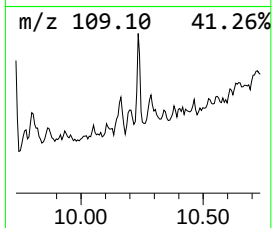
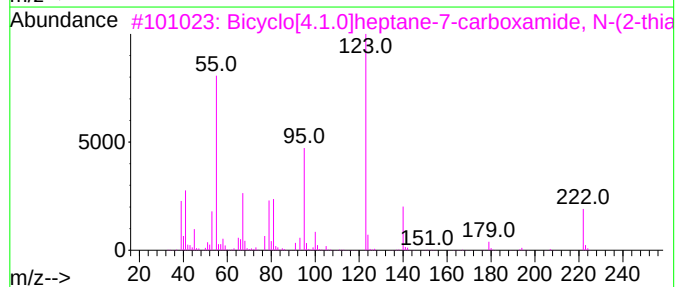
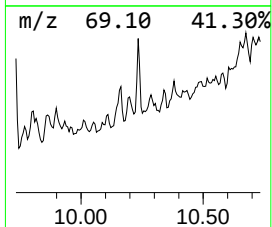
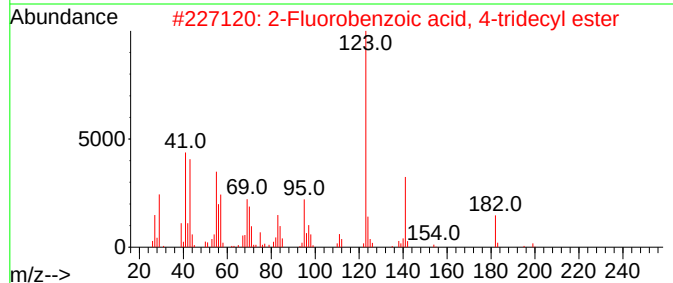
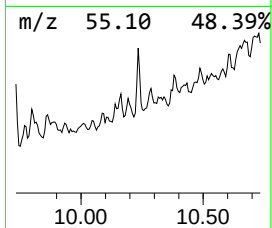
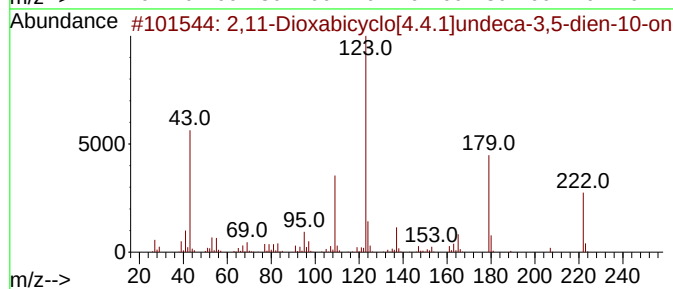
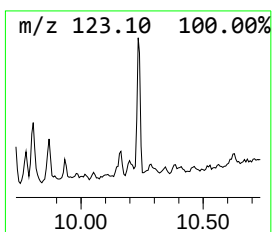
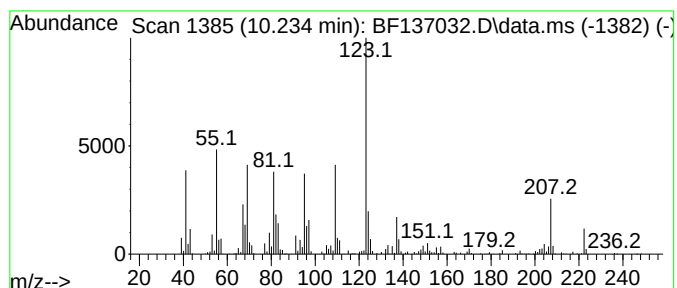
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.233	26.03 ng	889213	Acenaphthene-d10			9.828
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...		222	C13H18O3	070412-52-1	59
2	2-Fluorobenzoic acid, 4-tridecyl...		322	C20H31FO2	1000280-61-2	43
3	Bicyclo[4.1.0]heptane-7-carboxam...		222	C11H14N2O5	329912-72-3	43
4	Pentanamide, N-(4-methoxyphenyl)-		207	C12H17NO2	1000306-89-3	43
5	1-Trimethylsilylpent-1-en-4-yne		138	C8H14Si	079516-25-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
Operator : CG\JU
Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
332

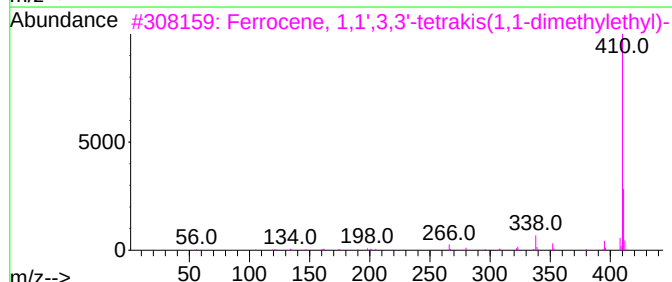
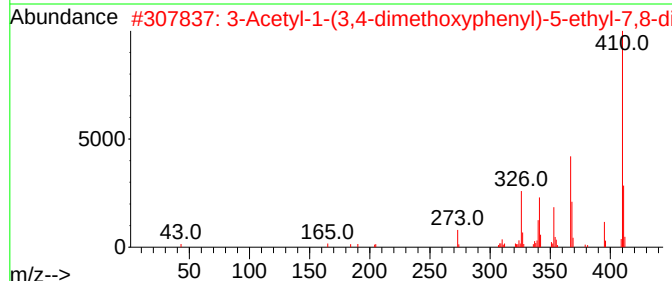
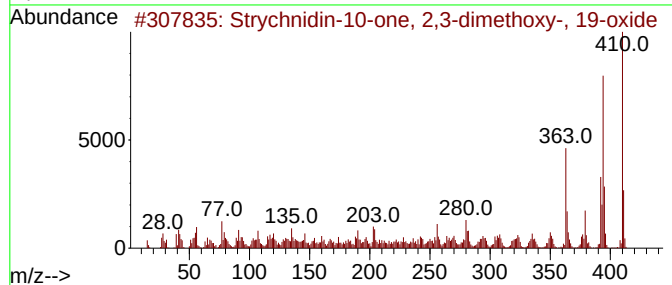
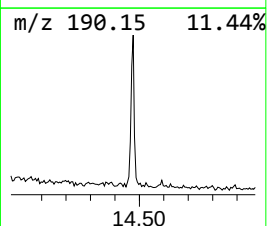
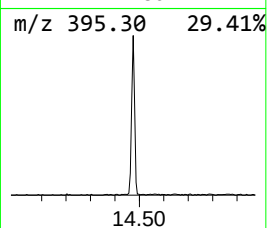
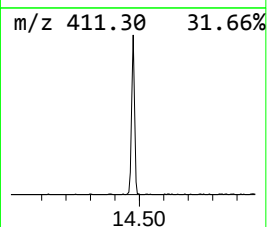
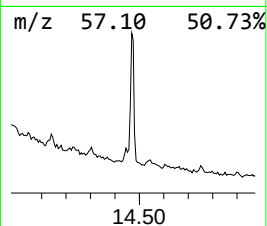
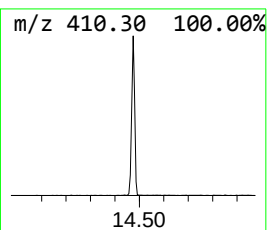
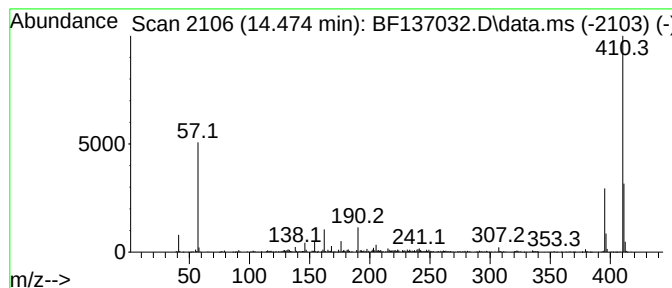
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Strychnidin-10-one, 2,3-dim... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	28.95 ng	528819	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Strychnidin-10-one, 2,3-dimethox...	410	C23H26N2O5	017301-81-4	72
2			3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	59
3			Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	58
4			6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	40
5			2'-Hydroxy-3,3',4'-trimethoxycha...	410	C20H17F3O6	1010453-84-8	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137032.D
Acq On : 10 Jan 2024 21:37
Operator : CG\JU
Sample : P1086-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
332

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
Furan, tetrahyd...	2.128	12.6	ng	163665	1	6.787	259317	20.0
unknown7.422	7.422	5.3	ng	69360	1	6.787	259317	20.0
1,4-Dimethylada...	8.292	6.1	ng	111754	2	8.063	363987	20.0
1H-1,4-Diazepin...	8.351	6.0	ng	108208	2	8.063	363987	20.0
unknown8.498	8.498	5.9	ng	107247	2	8.063	363987	20.0
unknown8.522	8.522	6.6	ng	119422	2	8.063	363987	20.0
Naphthalene, 1,...	8.563	7.3	ng	132159	2	8.063	363987	20.0
unknown8.687	8.687	6.8	ng	124532	2	8.063	363987	20.0
unknown8.745	8.745	5.8	ng	104928	2	8.063	363987	20.0
1,1'-Bicyclohexyl	8.834	5.3	ng	97385	2	8.063	363987	20.0
Naphthalene, 1,...	8.887	11.0	ng	200322	2	8.063	363987	20.0
unknown9.210	9.210	15.4	ng	526390	3	9.828	683331	20.0
Benzene, 1-cycl...	9.451	7.7	ng	261501	3	9.828	683331	20.0
unknown9.528	9.528	12.1	ng	414361	3	9.828	683331	20.0
unknown9.686	9.686	15.2	ng	520270	3	9.828	683331	20.0
unknown9.734	9.734	23.6	ng	804875	3	9.828	683331	20.0
unknown9.769	9.769	5.0	ng	169376	3	9.828	683331	20.0
unknown10.145	10.145	10.6	ng	363337	3	9.828	683331	20.0
2,11-Dioxabicyc...	10.233	26.0	ng	889213	3	9.828	683331	20.0
Strychnidin-10-...	14.474	28.9	ng	528819	5	13.998	365384	20.0