

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
 Data File : BF134552.D
 Acq On : 01 Aug 2023 17:15
 Operator : CG\JU
 Sample : 03784-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OS-2

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: BF134552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.410	560	565	568	rBV	3228156	3140948	84.16%	9.891%
2	6.416	731	736	739	rBV	3324666	3131117	83.90%	9.861%
3	6.792	796	800	803	rBV	1257146	1025961	27.49%	3.231%
4	7.351	890	895	898	rBV	2151568	1927995	51.66%	6.072%
5	8.069	1013	1017	1020	rBV	1754906	1381454	37.02%	4.350%
6	8.534	1094	1096	1099	rVB2	88891	82601	2.21%	0.260%
7	8.622	1105	1111	1114	rBV6	45763	93131	2.50%	0.293%
8	8.692	1119	1123	1125	rBV5	49244	77335	2.07%	0.244%
9	8.757	1131	1134	1141	rVB8	61159	88876	2.38%	0.280%
10	8.816	1141	1144	1146	rBV2	87373	81440	2.18%	0.256%
11	8.892	1154	1157	1159	rBV	128477	105122	2.82%	0.331%
12	9.034	1178	1181	1183	rBV4	92859	92285	2.47%	0.291%
13	9.063	1183	1186	1188	rBV	210842	162229	4.35%	0.511%
14	9.098	1190	1192	1195	rVB4	118368	102987	2.76%	0.324%
15	9.145	1195	1200	1204	rBV	3811929	3655352	97.94%	11.511%
16	9.186	1205	1207	1209	rBV2	80878	85605	2.29%	0.270%
17	9.228	1210	1214	1217	rBV2	447843	578429	15.50%	1.822%
18	9.269	1219	1221	1223	rBV3	155997	156736	4.20%	0.494%
19	9.457	1251	1253	1255	rBV3	216252	237908	6.37%	0.749%
20	9.481	1255	1257	1259	rVV2	237361	230619	6.18%	0.726%
21	9.533	1264	1266	1269	rBV2	1258793	1181148	31.65%	3.720%
22	9.563	1269	1271	1273	rVB2	375153	258091	6.92%	0.813%
23	9.592	1273	1276	1280	rBV3	569215	654605	17.54%	2.061%
24	9.645	1283	1285	1287	rBV2	317877	253136	6.78%	0.797%
25	9.698	1290	1294	1297	rBV3	1102374	1672474	44.81%	5.267%
26	9.739	1298	1301	1304	rVB	2184248	2090536	56.02%	6.584%
27	9.781	1305	1308	1310	rBV3	635633	849620	22.77%	2.676%
28	9.828	1310	1316	1321	rBV2	2073547	3732085	100.00%	11.753%
29	10.104	1360	1363	1367	rBV3	858179	1104345	29.59%	3.478%
30	10.245	1384	1387	1390	rBV2	1721075	1630071	43.68%	5.133%
31	13.968	2017	2020	2023	rVB	868787	778359	20.86%	2.451%
32	15.415	2262	2266	2271	rVB	892783	1031387	27.64%	3.248%
33	16.139	2386	2389	2397	rVB6	44997	80133	2.15%	0.252%

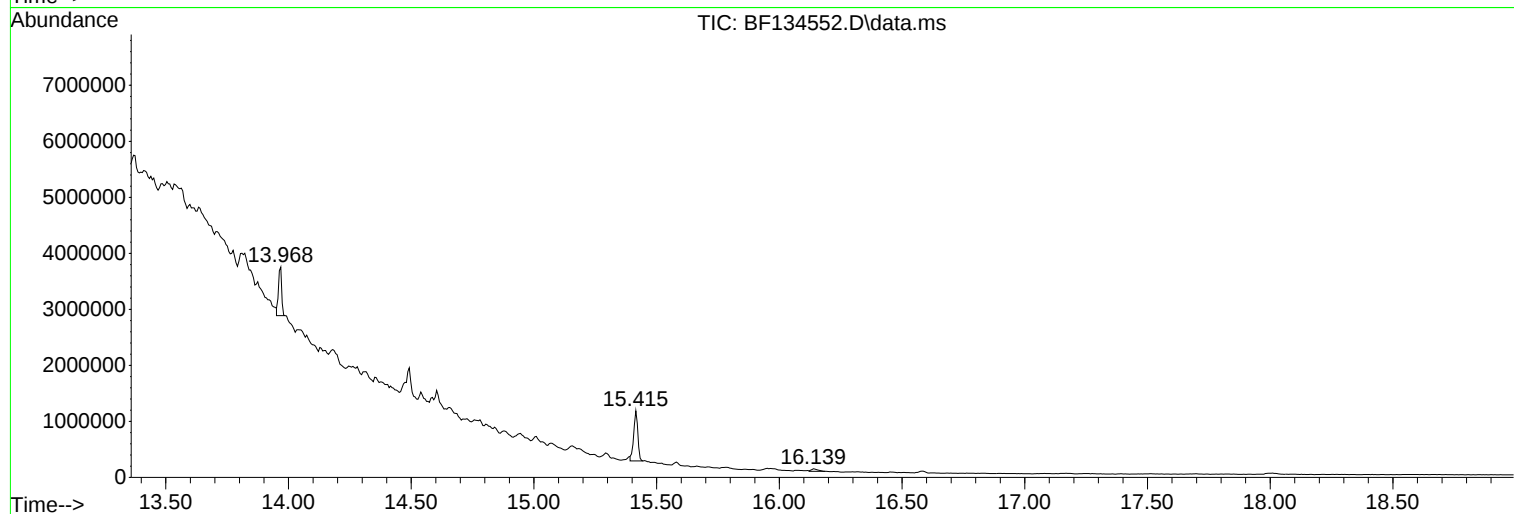
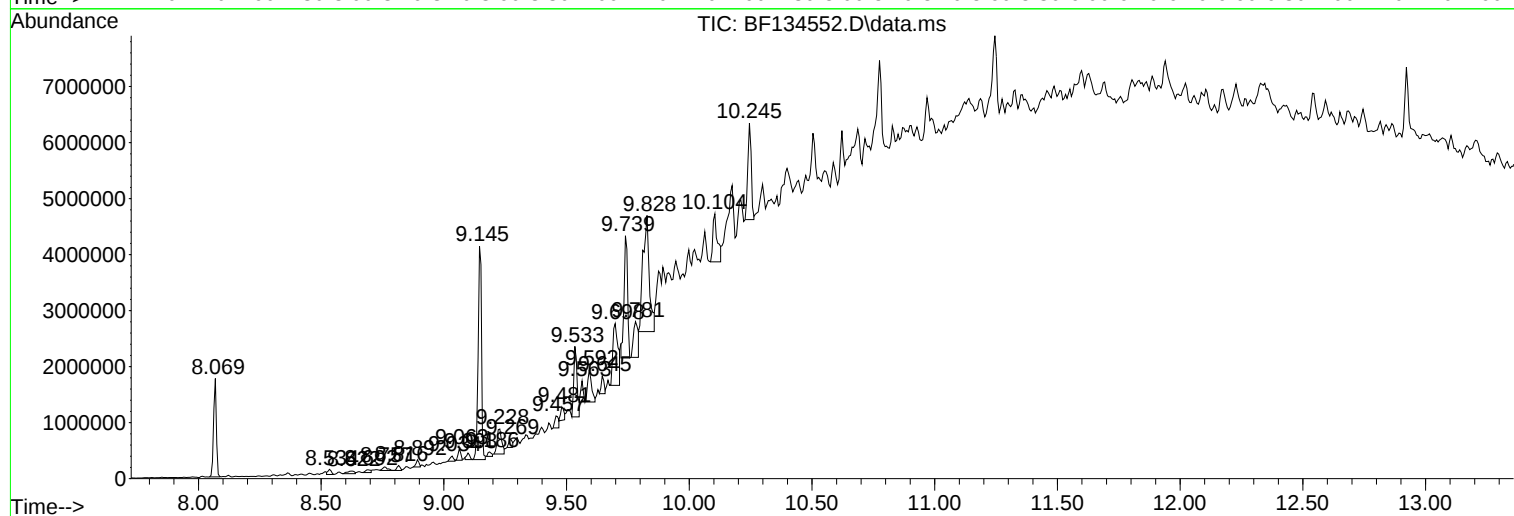
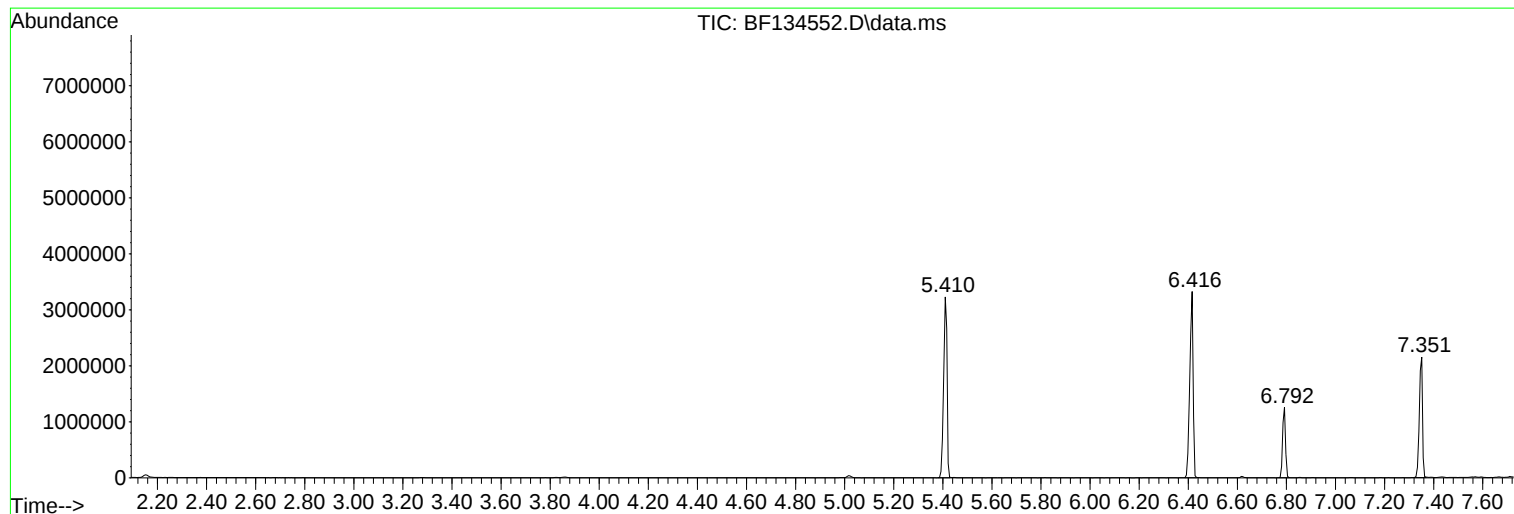
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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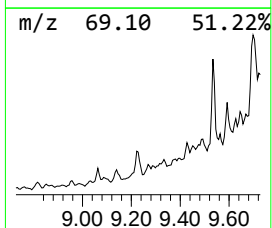
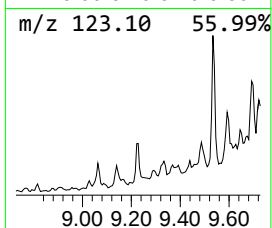
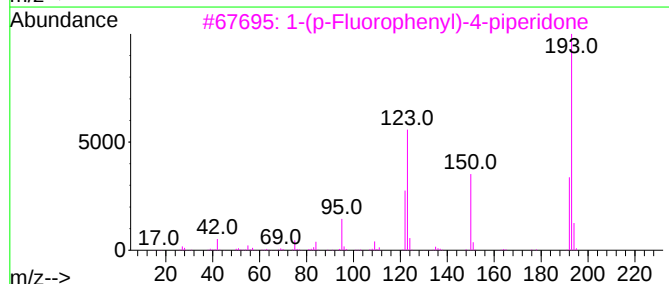
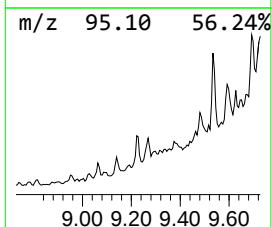
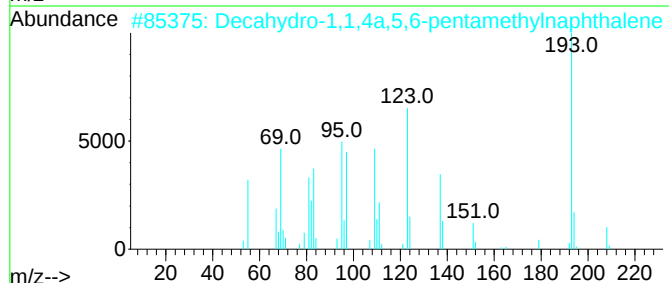
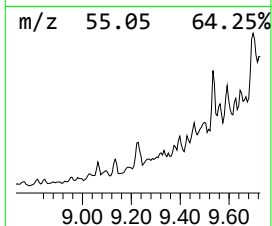
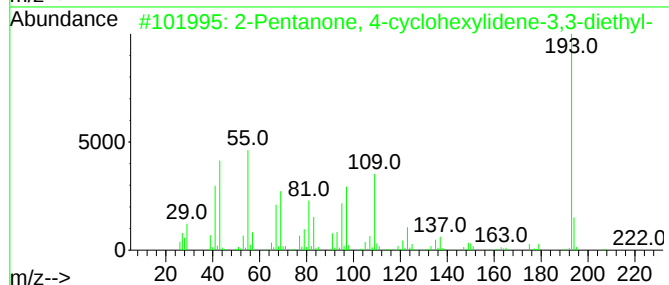
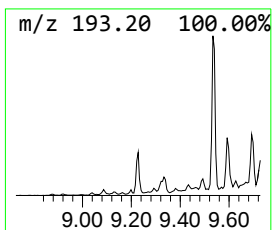
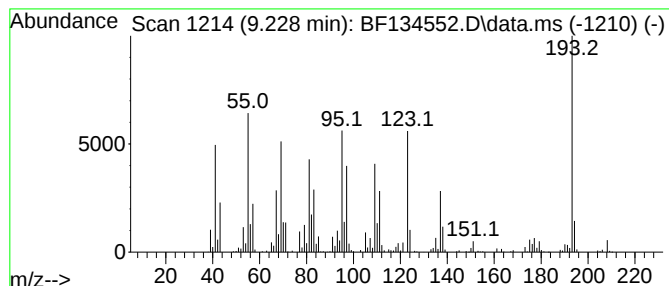
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown9.228 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.228	3.10 ng	578429	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	43		
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38		
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
4	Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	27		
5	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	25		



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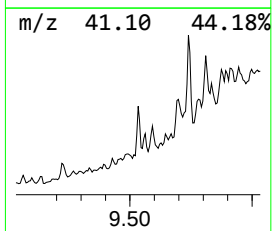
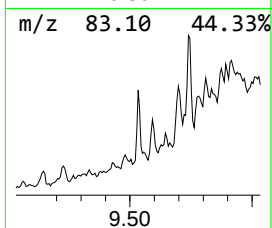
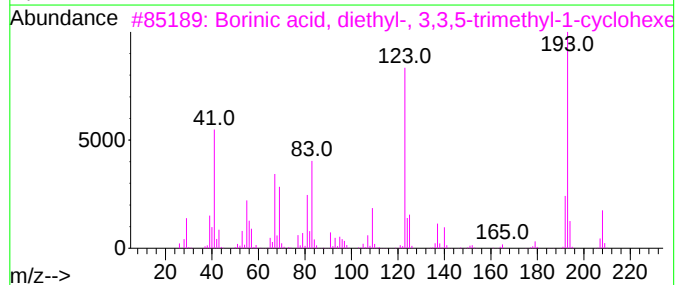
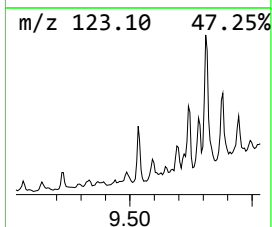
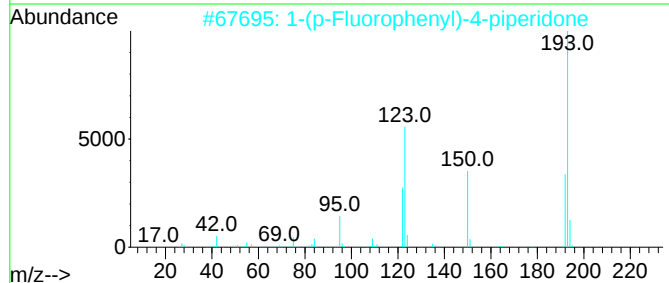
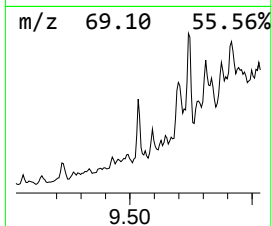
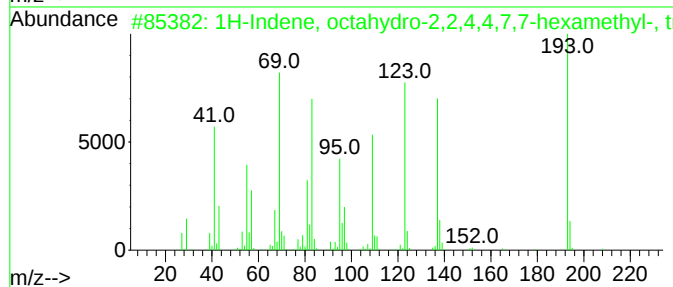
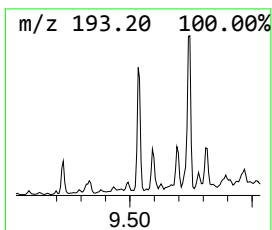
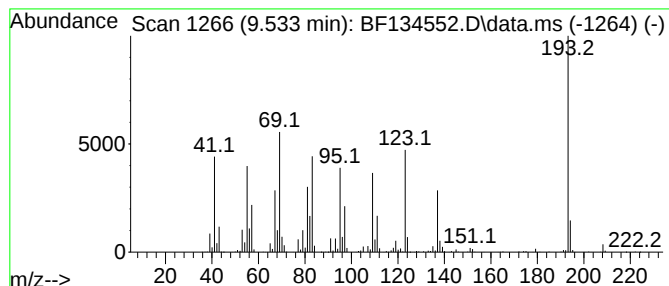
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown9.533 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.533	6.33 ng	1181150	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
3			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	37
4			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37
5			4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	32



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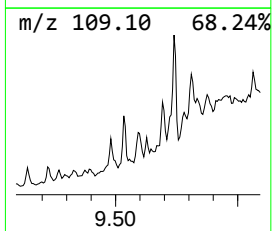
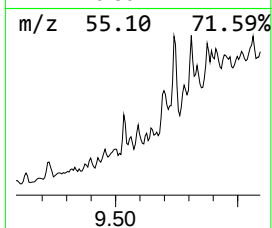
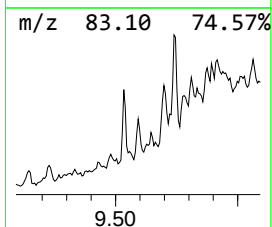
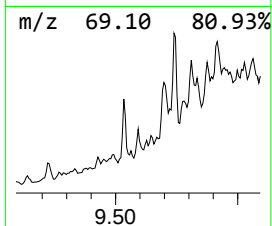
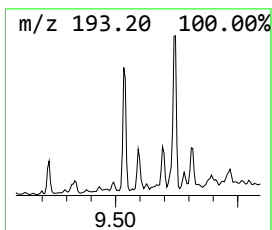
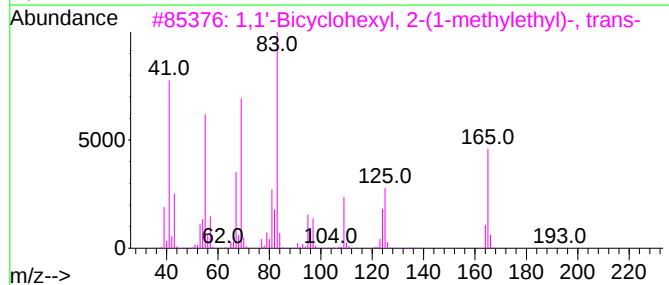
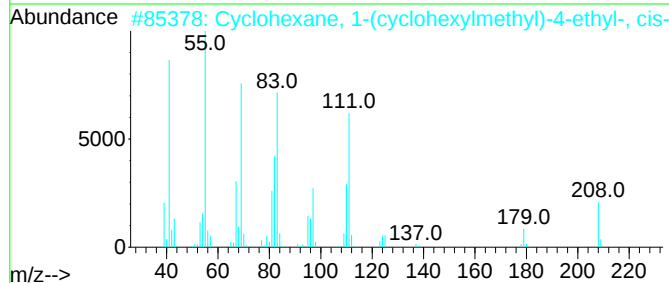
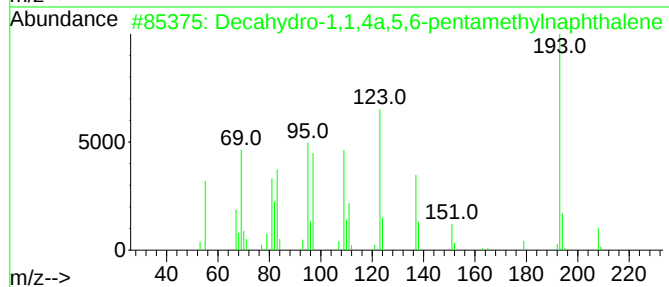
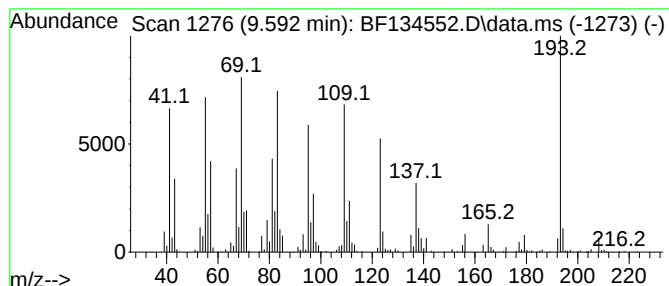
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown9.592 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	3.51 ng	654605	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			Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-95-1	38
3			1,1'-Bicyclohexyl, 2-(1-methylet...	208	C15H28	050991-16-7	35
4			Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	30
5			Bicyclo[3.1.1]heptan-3-one, 2-(b...	192	C13H20O	1010163-96-1	30



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ALS Vial : 7 Sample Multiplier: 1

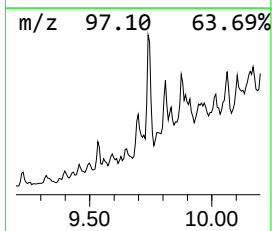
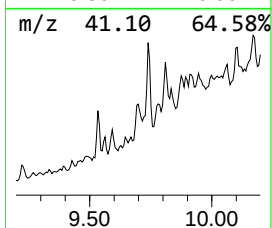
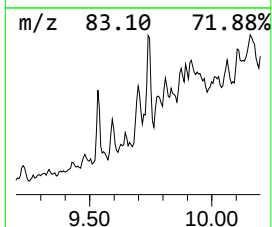
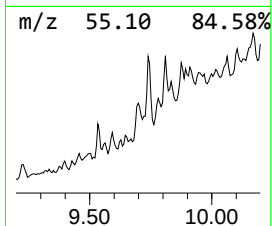
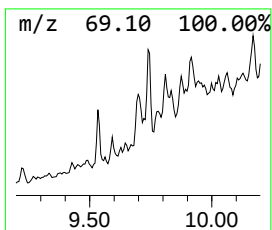
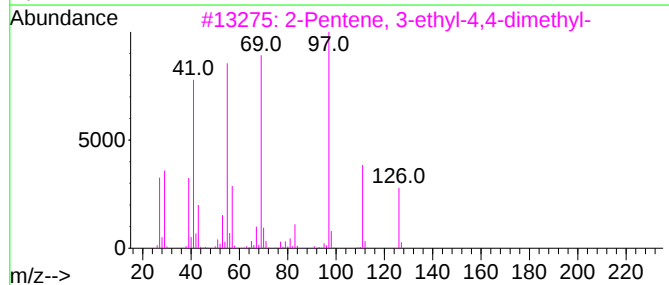
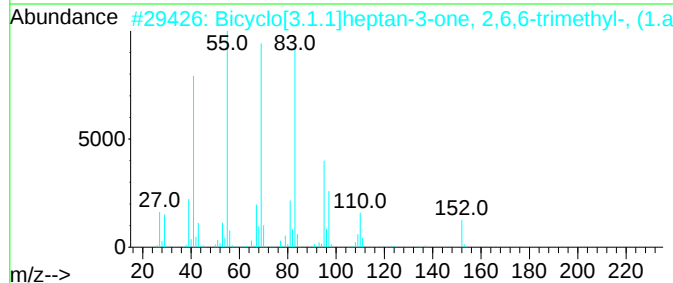
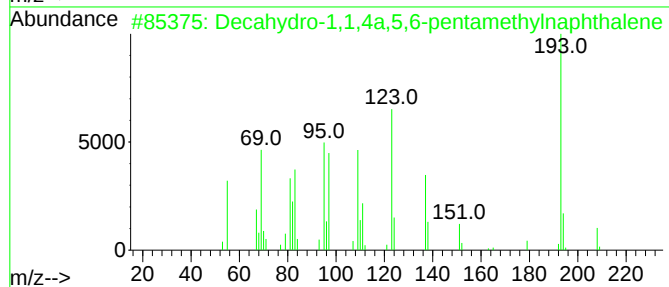
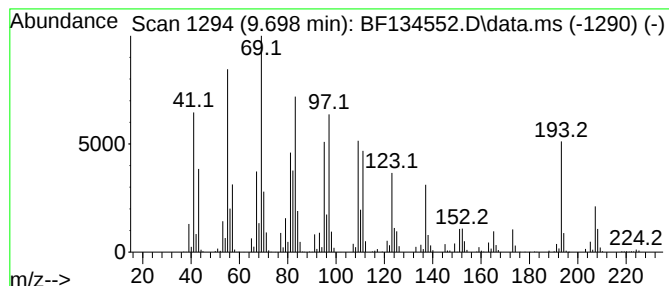
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Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.698	8.96 ng	1672470	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	95
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...		152	C10H16O	000547-60-4	25
3	2-Pentene, 3-ethyl-4,4-dimethyl-		126	C9H18	053907-59-8	22
4	2-propenamide, N-(2,6-dihydroxyp...		193	C10H11NO3	1000395-98-7	22
5	Cyclohexane, 1,1,2-trimethyl-		126	C9H18	007094-26-0	22



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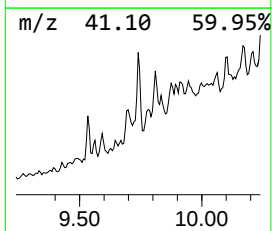
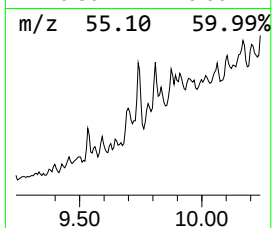
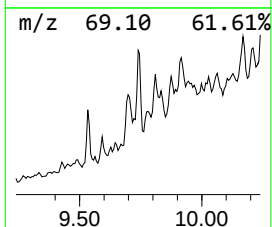
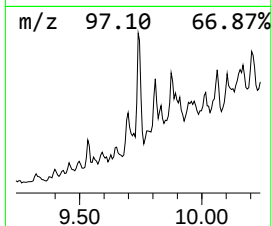
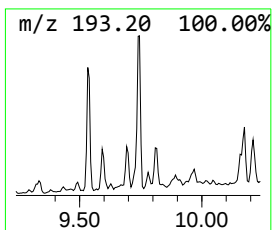
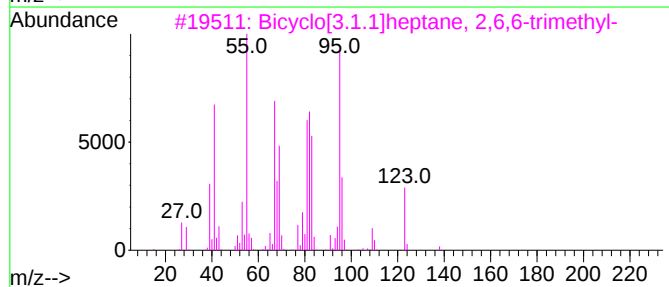
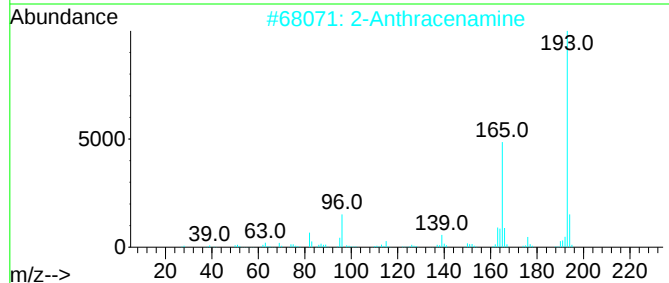
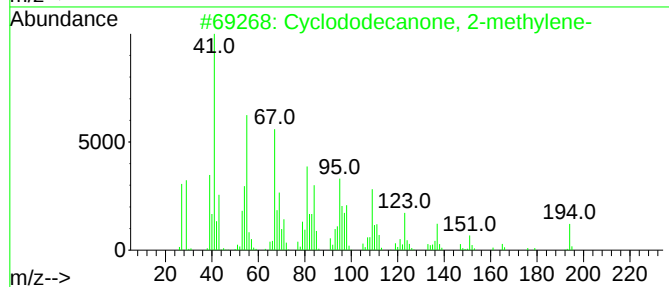
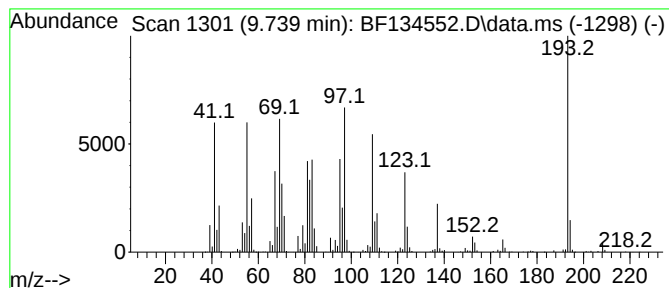
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Peak Number 5 unknown9.739 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.739	11.20 ng	2090540	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	22
2			2-Anthracenamine	193	C14H11N	000613-13-8	22
3			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	18
4			Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	14
5			Hexadecanedinitrile	248	C16H28N2	006812-44-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134552.D
Acq On : 01 Aug 2023 17:15
Operator : CG\JU
Sample : 03784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-2

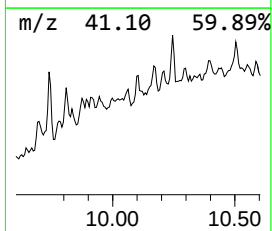
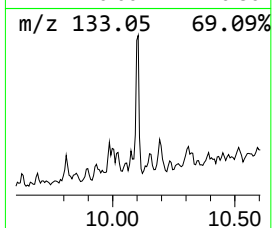
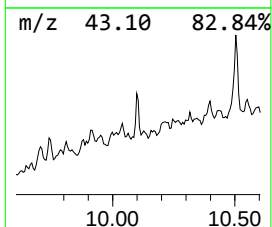
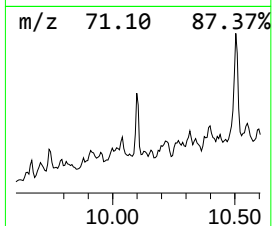
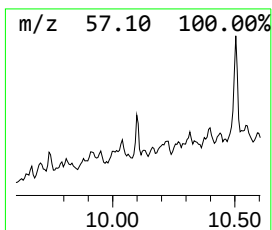
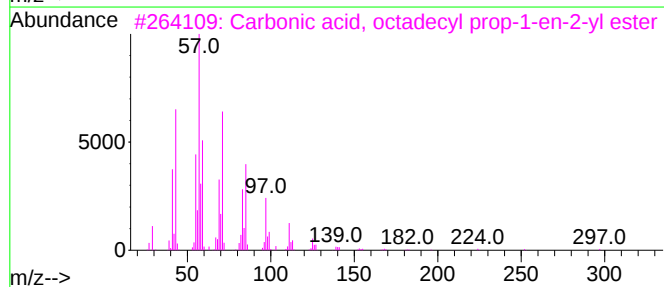
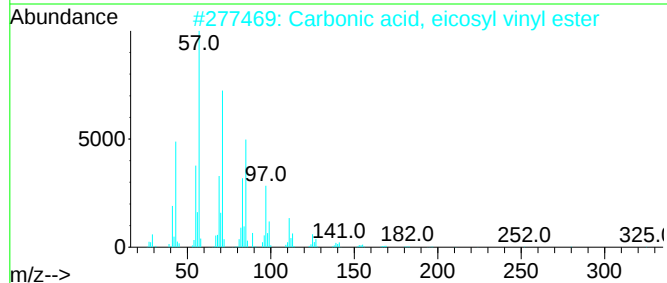
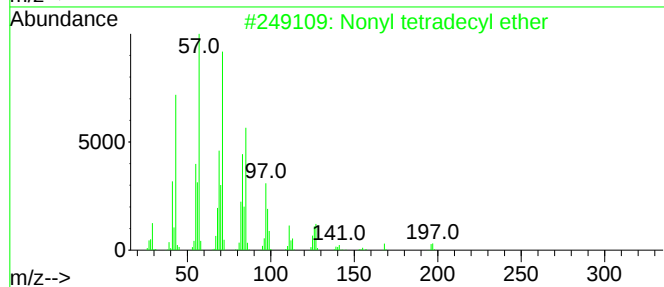
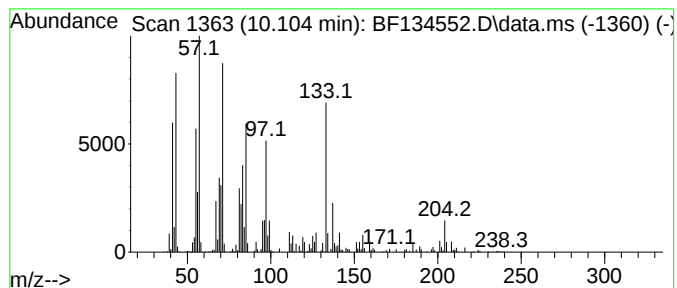
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonyl tetradecyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.104	5.92 ng	1104350	Acenaphthene-d10	9.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	58
2		Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	53
3		Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	53
4		Tritetracontane	605	C43H88	007098-21-7	46
5		2-Methyltetracosane	352	C25H52	001560-78-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134552.D
Acq On : 01 Aug 2023 17:15
Operator : CG\JU
Sample : 03784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-2

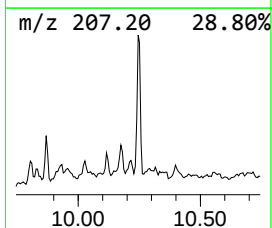
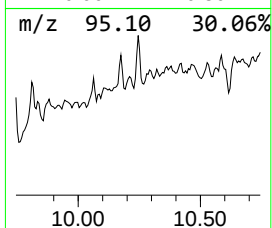
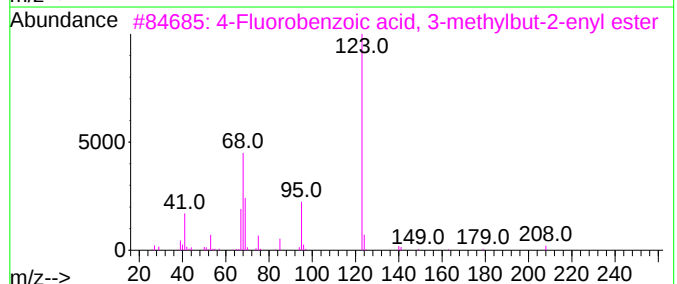
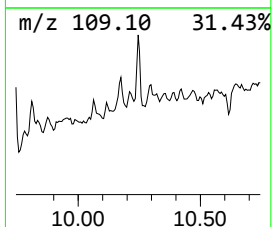
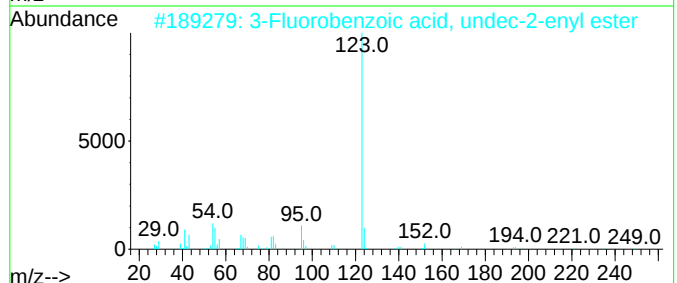
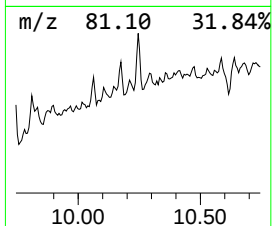
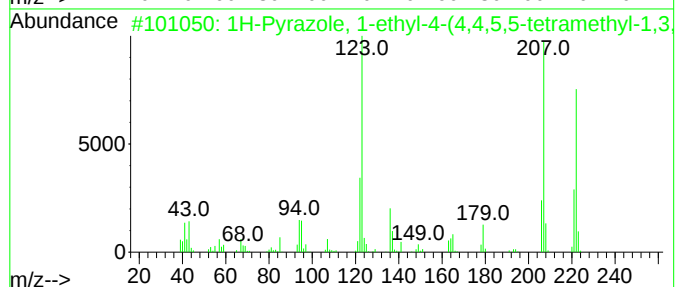
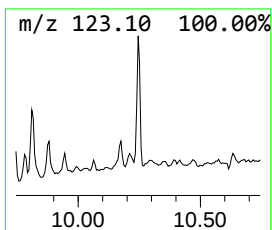
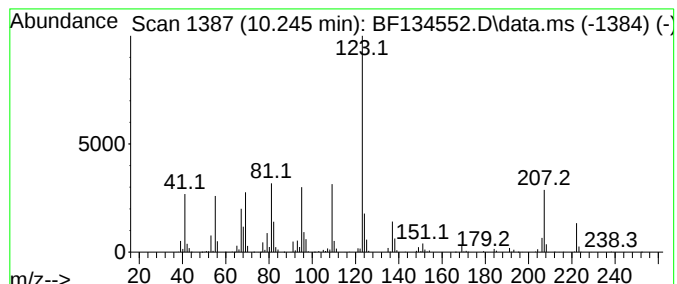
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1H-Pyrazole, 1-ethyl-4-(4,4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	8.74 ng	1630070	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 1-ethyl-4-(4,4,5,5-...	222	C11H19BN2O2	1010319-69-6	53		
2	3-Fluorobenzoic acid, undec-2-en...	292	C18H25FO2	1000292-60-8	50		
3	4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	49		
4	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	49		
5	3-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-60-7	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
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Sample : 03784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-2

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
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unknown9.533	9.533	6.3	ng	1181150	3	9.828	3732090	20.0
unknown9.592	9.592	3.5	ng	654605	3	9.828	3732090	20.0
Decahydro-1,1,4...	9.698	9.0	ng	1672470	3	9.828	3732090	20.0
unknown9.739	9.739	11.2	ng	2090540	3	9.828	3732090	20.0
Nonyl tetradecy...	10.104	5.9	ng	1104350	3	9.828	3732090	20.0
1H-Pyrazole, 1-...	10.245	8.7	ng	1630070	3	9.828	3732090	20.0