

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
 Data File : BF123453.D
 Acq On : 24 Mar 2021 22:38
 Operator : JU/CG
 Sample : M1775-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 11979

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-BF032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123453.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	15	20	27	rVB	857419	1053886	29.14%	2.665%
2	2.310	35	38	44	rVB3	54822	72815	2.01%	0.184%
3	5.134	515	518	524	rVB	51531	58129	1.61%	0.147%
4	5.534	581	586	589	rBV	3750675	3580207	98.98%	9.052%
5	6.533	751	756	762	rBV	3491675	3616977	100.00%	9.145%
6	6.739	787	791	796	rBV2	53942	54359	1.50%	0.137%
7	6.916	817	821	824	rBV	1680163	1291651	35.71%	3.266%
8	6.975	827	831	834	rBV	149366	124750	3.45%	0.315%
9	7.475	905	916	919	rBV	2573560	2241231	61.96%	5.667%
10	8.069	1012	1017	1020	rBV2	53554	52315	1.45%	0.132%
11	8.198	1034	1039	1042	rBV	1888636	1538901	42.55%	3.891%
12	8.804	1138	1142	1145	rBV3	30959	47606	1.32%	0.120%
13	9.098	1187	1192	1193	rBV5	32867	52114	1.44%	0.132%
14	9.157	1199	1202	1206	rBV5	38359	70079	1.94%	0.177%
15	9.198	1206	1209	1211	rBV2	93561	73086	2.02%	0.185%
16	9.227	1211	1214	1218	rBV4	58501	64470	1.78%	0.163%
17	9.274	1218	1222	1225	rBV	2411072	1868068	51.65%	4.723%
18	9.357	1233	1236	1240	rBV	248106	276534	7.65%	0.699%
19	9.592	1274	1276	1277	rBV2	75061	63183	1.75%	0.160%
20	9.616	1277	1280	1282	rVV2	297849	243637	6.74%	0.616%
21	9.639	1282	1284	1287	rVB2	170001	154550	4.27%	0.391%
22	9.669	1287	1289	1293	rBV2	1153194	1156948	31.99%	2.925%
23	9.727	1297	1299	1303	rVB3	342892	333050	9.21%	0.842%
24	9.833	1313	1317	1319	rBV4	682080	713264	19.72%	1.803%
25	9.857	1319	1321	1322	rVV2	202007	168079	4.65%	0.425%
26	9.874	1322	1324	1327	rVB	1351046	1135580	31.40%	2.871%
27	9.916	1328	1331	1333	rBV2	333132	285224	7.89%	0.721%
28	9.963	1333	1339	1342	rBV2	1810133	2334692	64.55%	5.903%
29	10.004	1343	1346	1349	rBV3	370766	521397	14.42%	1.318%
30	10.074	1355	1358	1361	rBV5	241635	293602	8.12%	0.742%
31	10.104	1361	1363	1365	rBV2	250950	211559	5.85%	0.535%
32	10.163	1370	1373	1375	rVB2	351433	298169	8.24%	0.754%
33	10.192	1375	1378	1381	rBV4	272232	367210	10.15%	0.928%
34	10.221	1381	1383	1386	rBV2	359599	397591	10.99%	1.005%
35	10.286	1391	1394	1395	rBV2	512630	531885	14.71%	1.345%
36	10.304	1395	1397	1400	rVB3	583625	505912	13.99%	1.279%

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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	10.339	1400	1403	1405	rBV4	545627	550977	15.23%	1.393%
38	10.374	1405	1409	1414	rBV3	1430933	1672515	46.24%	4.229%
39	10.433	1416	1419	1420	rBV2	496046	496248	13.72%	1.255%
40	10.504	1429	1431	1433	rBV2	393578	448347	12.40%	1.134%
41	10.751	1470	1473	1476	rBV2	1735023	1593110	44.05%	4.028%
42	10.886	1492	1496	1502	rBV2	1343894	2249569	62.19%	5.688%
43	11.457	1591	1593	1595	rBV	1098318	928547	25.67%	2.348%
44	11.986	1681	1683	1686	rBV2	580523	493543	13.65%	1.248%
45	13.045	1860	1863	1870	rVB	1311956	1235414	34.16%	3.124%
46	13.945	2013	2016	2023	rVB3	289669	406217	11.23%	1.027%
47	14.104	2037	2043	2046	rBV	1241542	1354714	37.45%	3.425%
48	14.739	2149	2151	2155	rVB2	148455	138200	3.82%	0.349%
49	15.251	2236	2238	2242	rVB	155966	149864	4.14%	0.379%
50	15.609	2295	2299	2303	rVB	732561	873675	24.15%	2.209%
51	15.868	2339	2343	2348	rVB2	152745	206416	5.71%	0.522%
52	16.168	2389	2394	2402	rVB	525599	900056	24.88%	2.276%

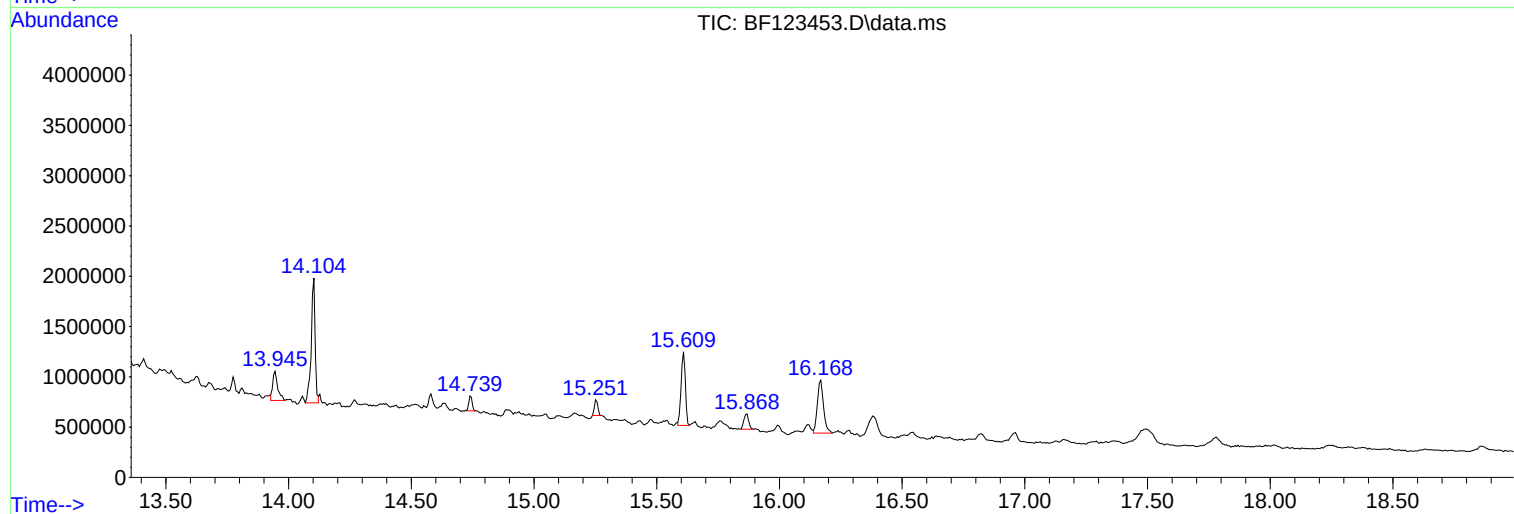
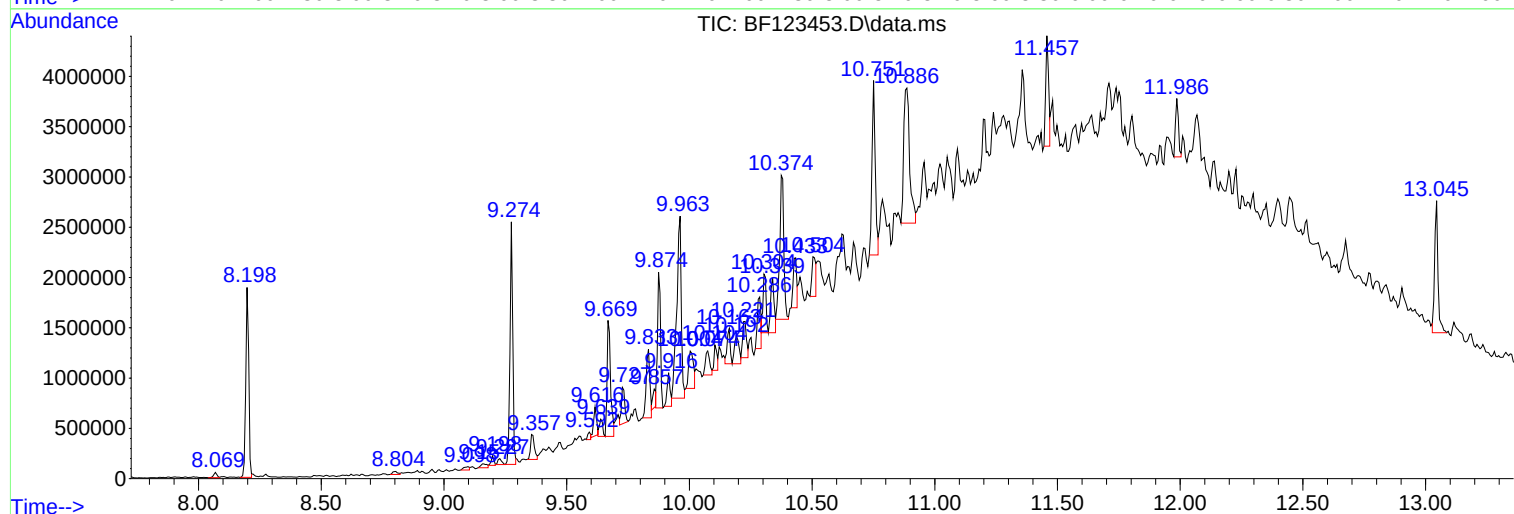
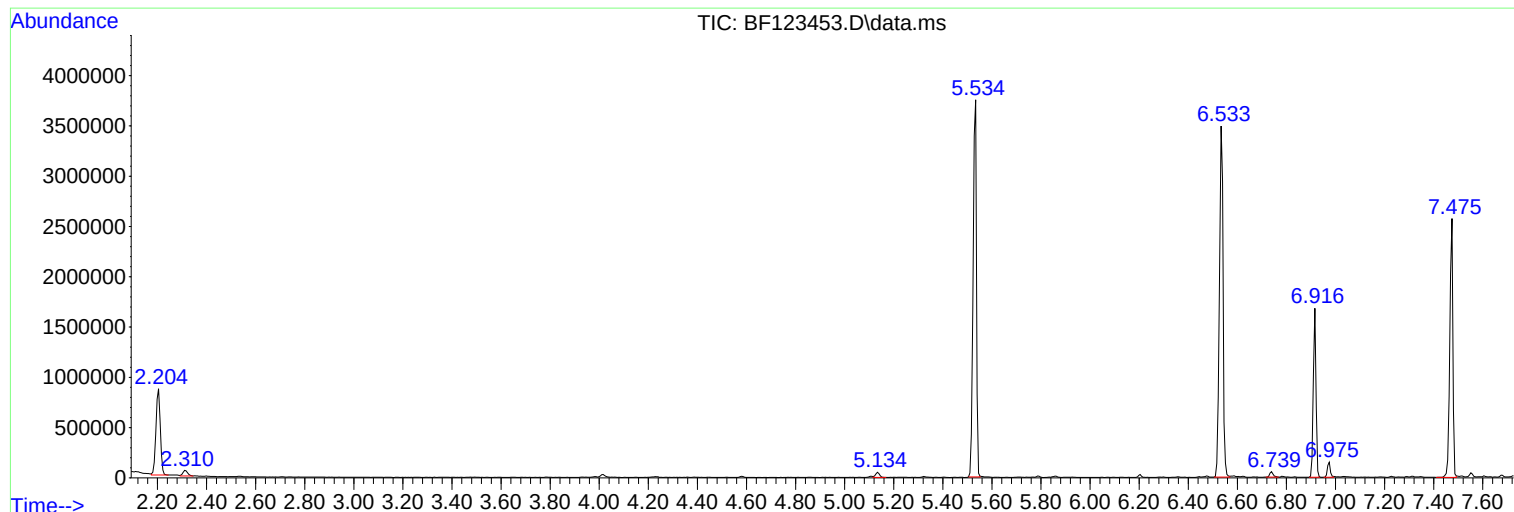
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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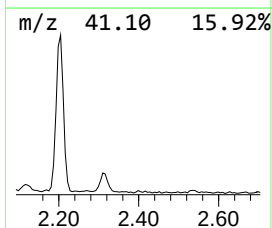
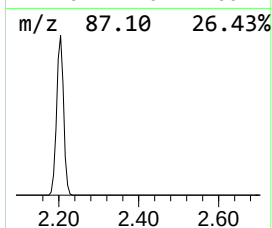
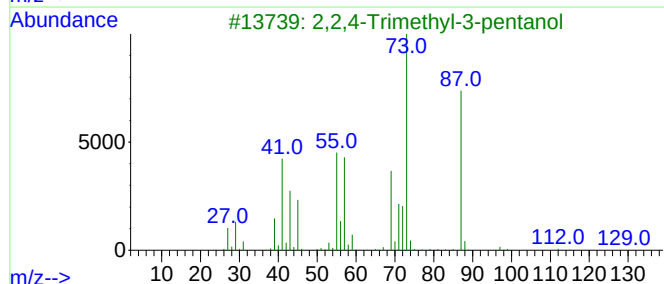
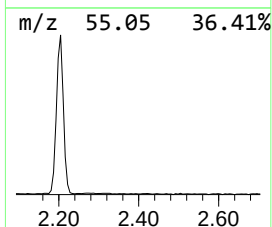
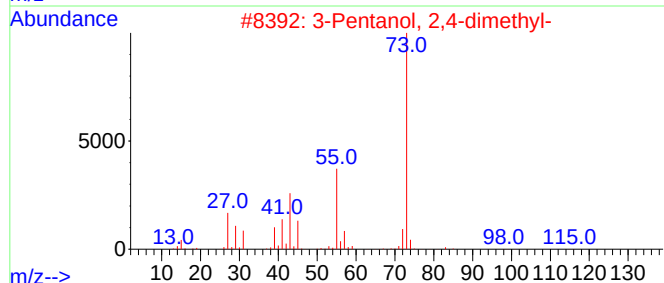
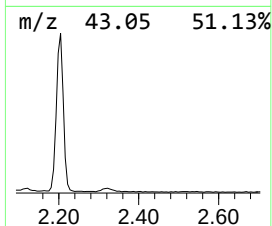
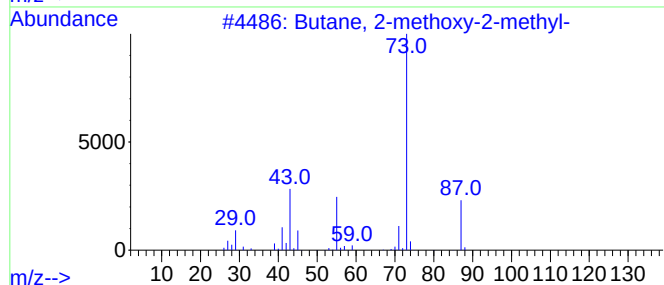
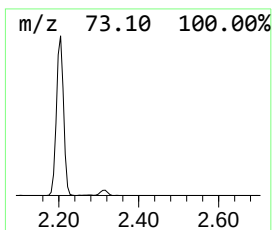
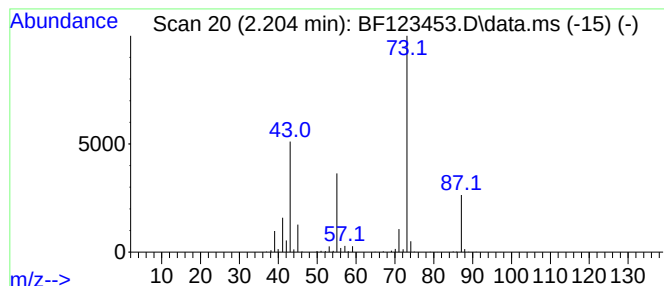
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	16.32 ng	1053890	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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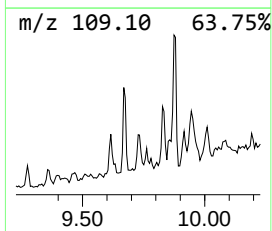
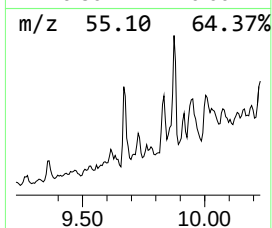
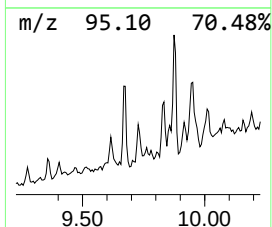
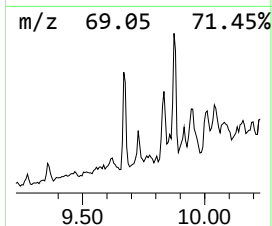
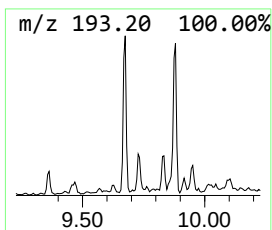
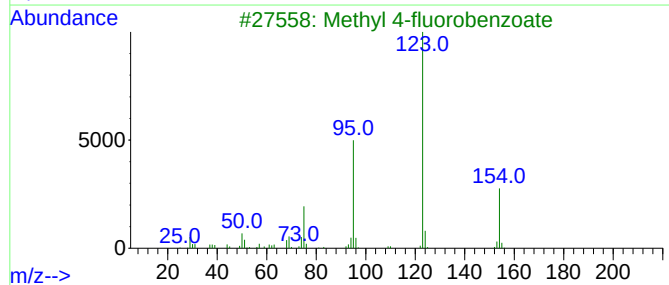
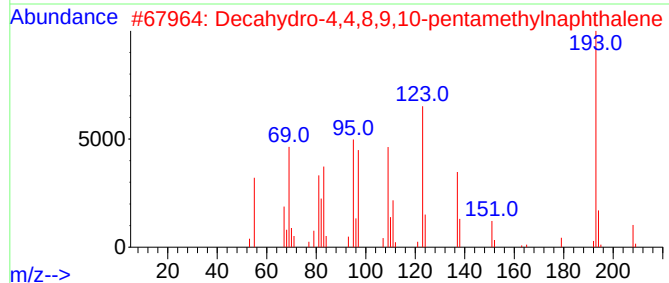
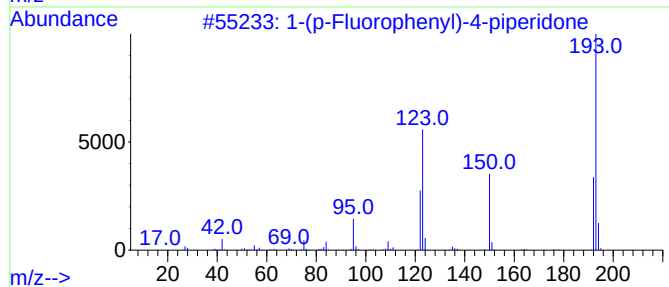
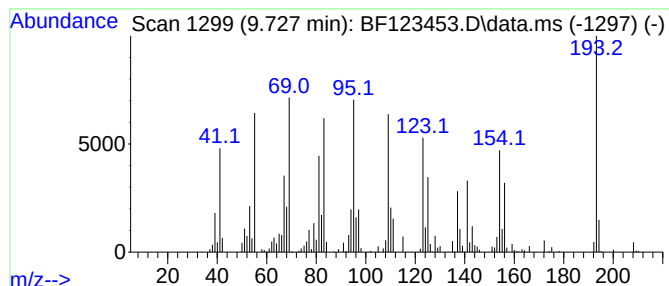
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown9.727 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.727	2.85 ng	333050	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27		
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	22		
3	Methyl 4-fluorobenzoate	154	C8H7FO2	000403-33-8	22		
4	3,5-Diamino-6-[2-thienyl]-1,2,4-...	193	C7H7N5S	058848-66-1	16		
5	2-(Phenylthio)ethanol	154	C8H10OS	000699-12-7	15		



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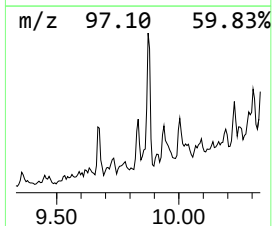
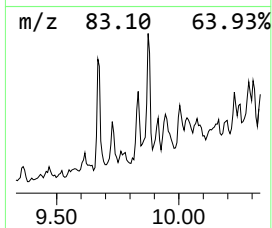
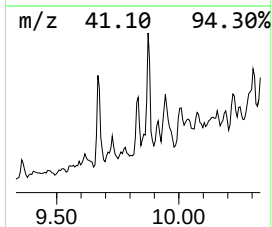
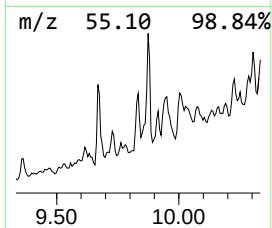
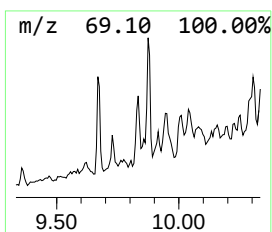
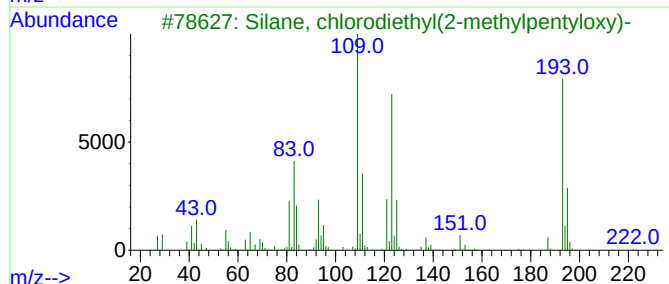
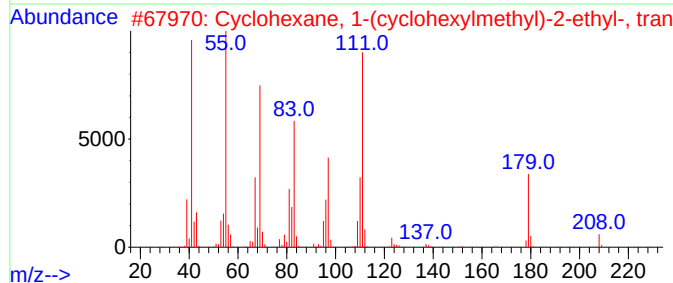
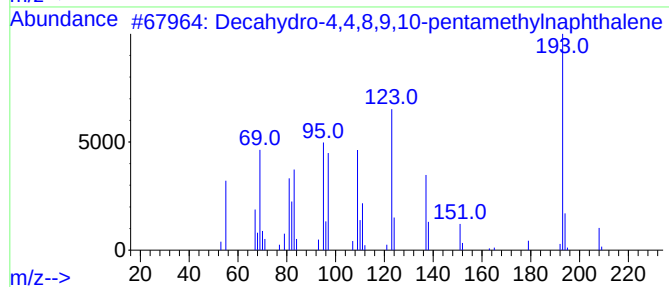
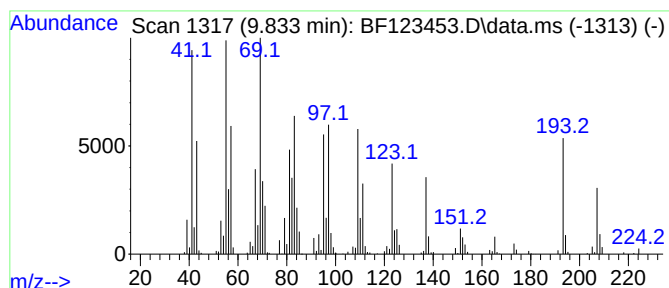
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Decahydro-4,4,8,9,10-pentam... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.833	6.11 ng	713264	Acenaphthene-d10	9.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	78
2	Cyclohexane, 1-(cyclohexylmethyl)...	208	C15H28	054934-92-8	38
3	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	38
4	1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5	30
5	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	30



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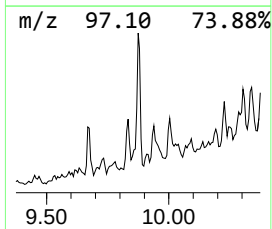
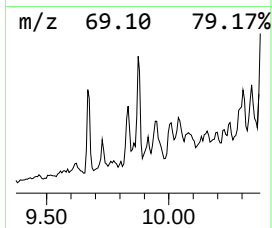
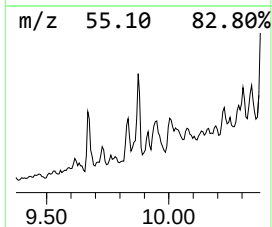
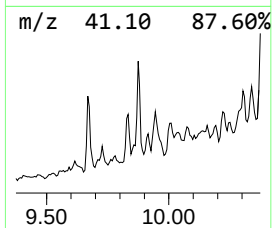
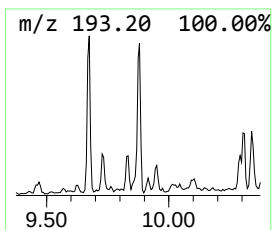
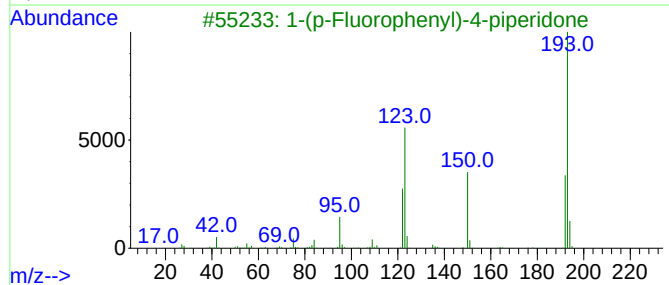
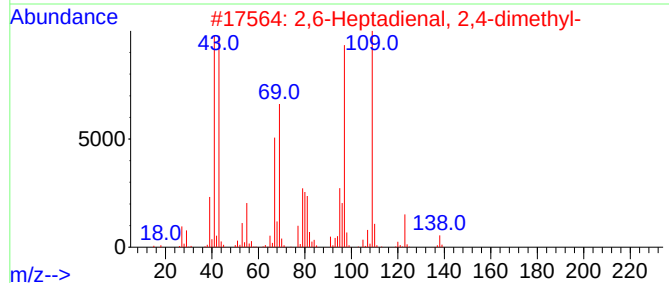
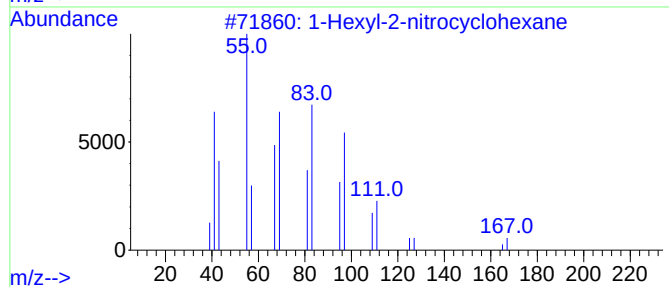
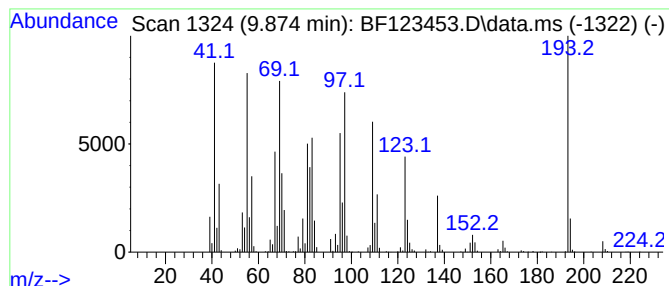
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown9.874 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.874	9.73 ng	1135580	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	43
2			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
4			Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-96-0	18
5			Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	14



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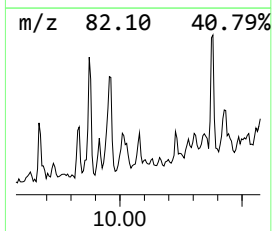
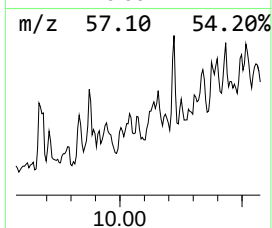
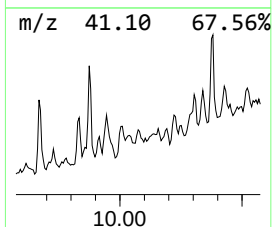
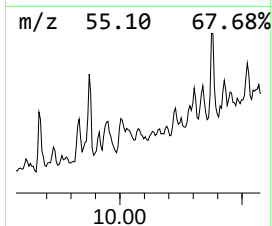
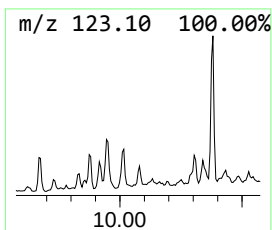
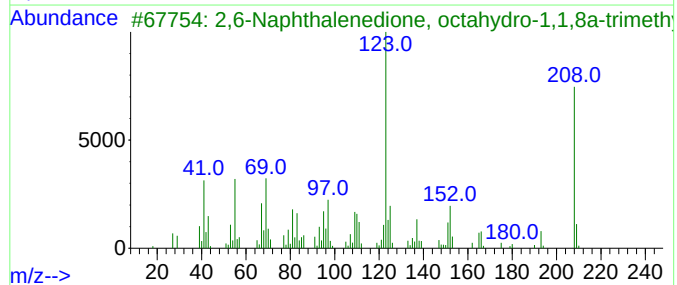
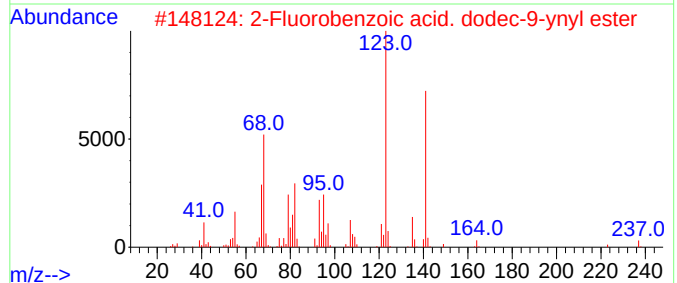
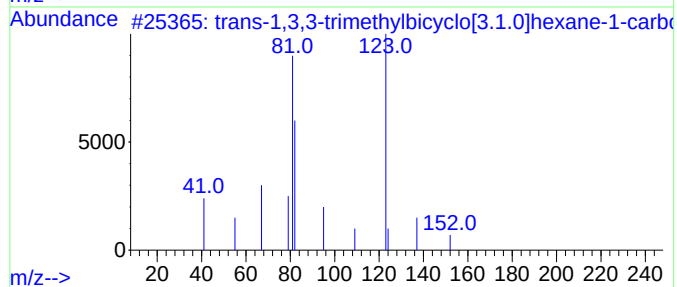
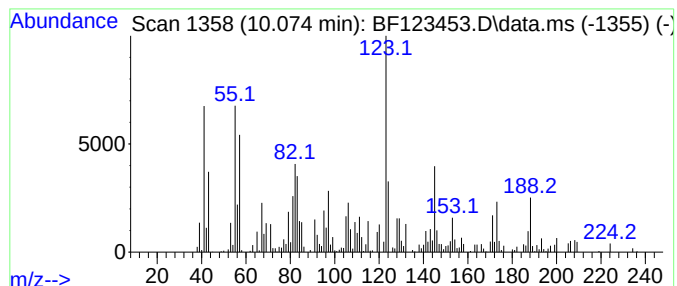
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.074 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.074	2.52 ng	293602	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-1,3,3-trimethylbicyclo[3.1...	152	C10H16O	1000365-94-1	43
2			2-Fluorobenzoic acid. dodec-9-yn...	304	C19H25FO2	1000282-96-4	35
3			2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-17-5	35
4			2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	35
5			Phenol, 2-amino-4-methyl-	123	C7H9NO	000095-84-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123453.D
Acq On : 24 Mar 2021 22:38
Operator : JU/CG
Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

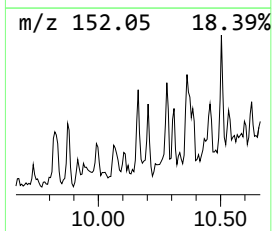
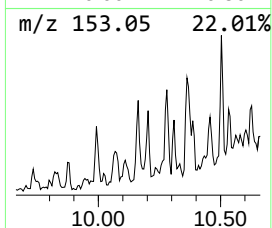
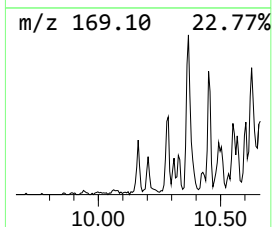
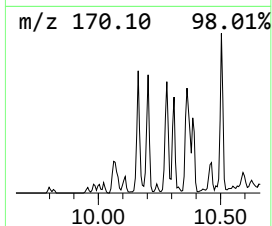
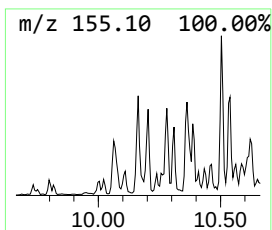
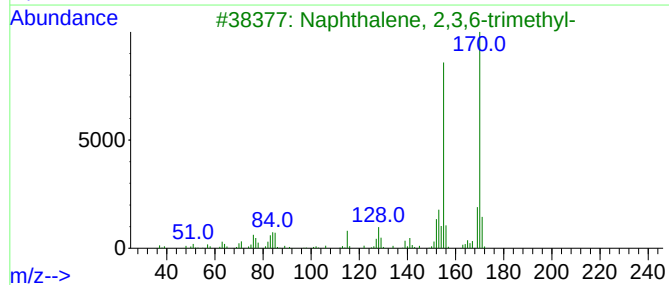
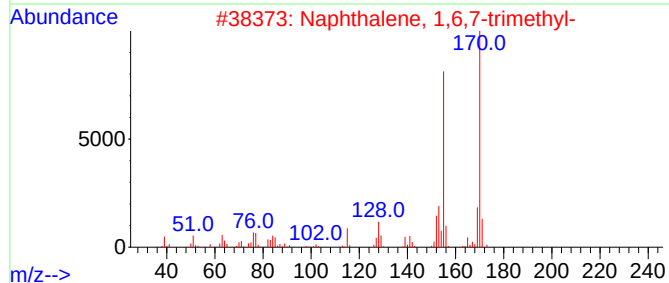
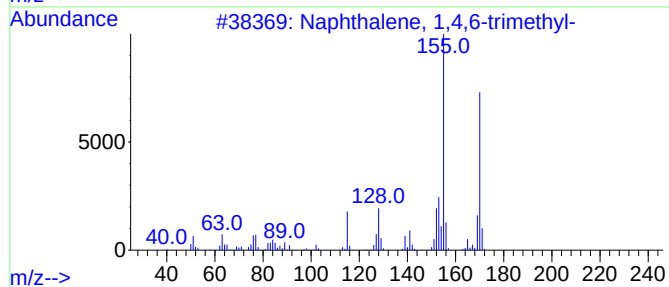
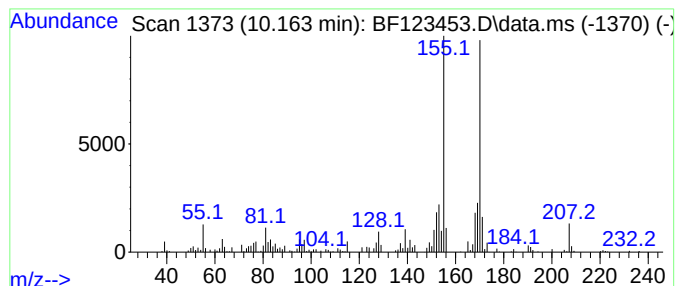
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ClientSampled :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 1,4,6-trimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.163	2.55 ng	298169	Acenaphthene-d10	9.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	94
2	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	93
3	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	93
4	1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	87
5	3-(2-Methyl-propenyl)-1H-indene	170	C13H14	1000187-78-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

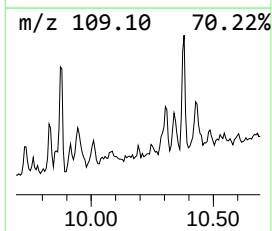
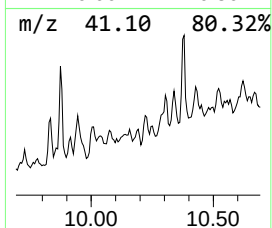
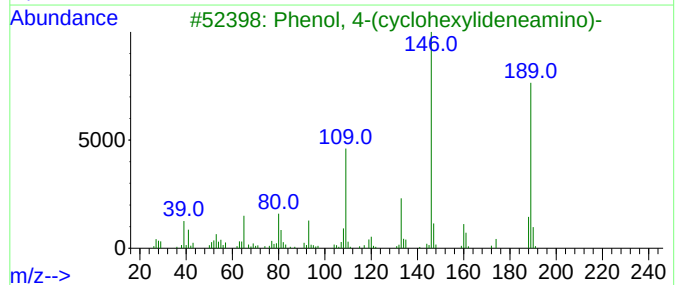
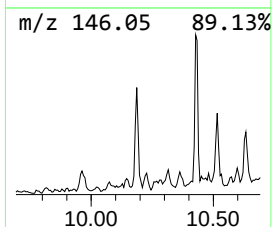
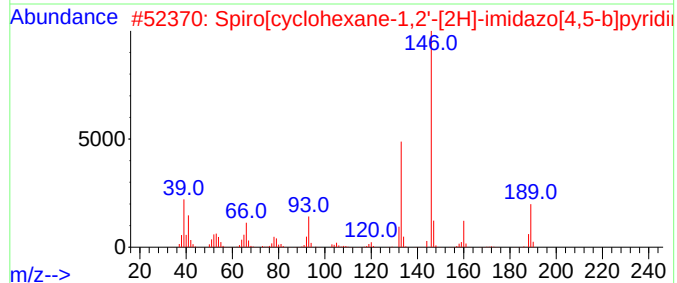
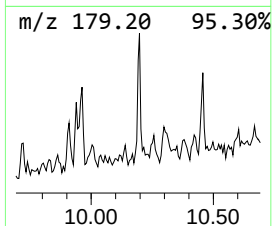
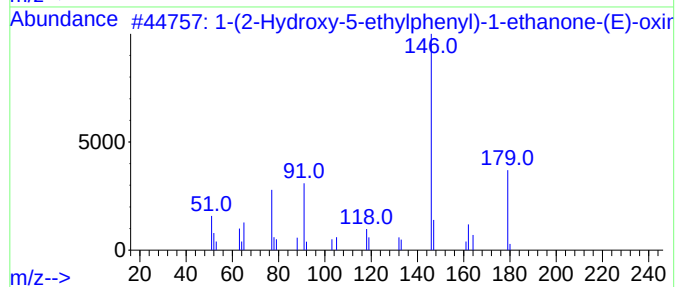
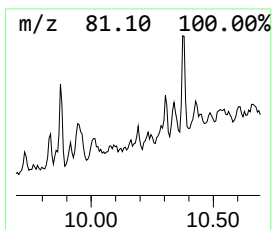
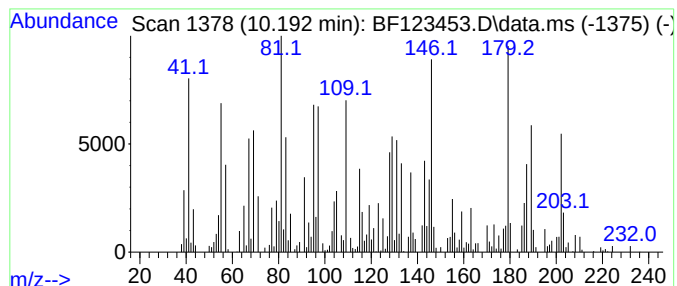
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown10.192 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.192	3.15 ng	367210	Acenaphthene-d10	9.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Hydroxy-5-ethylphenyl)-1-et...	179	C10H13NO2	1000146-46-9	22
2	Spiro[cyclohexane-1,2'-[2H]-imid...	189	C11H15N3	076902-24-4	22
3	Phenol, 4-(cyclohexylideneamino)-	189	C12H15NO	059651-96-6	15
4	4-Acetyl-1,2,3,4-tetrahydro-2-ox...	189	C11H11NO2	092287-78-0	15
5	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123453.D
Acq On : 24 Mar 2021 22:38
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Sample : M1775-02
Misc :
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Instrument :
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ClientSampleId :
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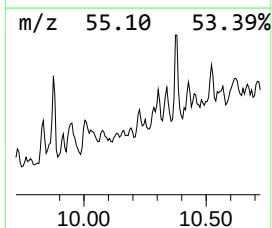
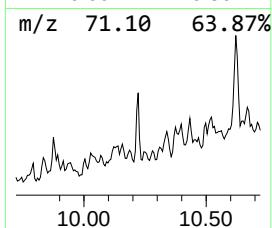
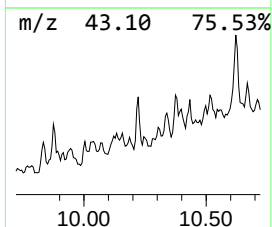
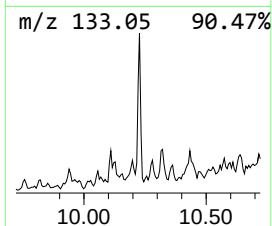
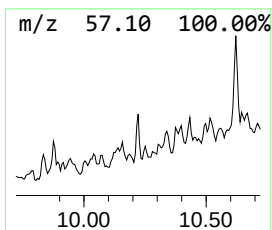
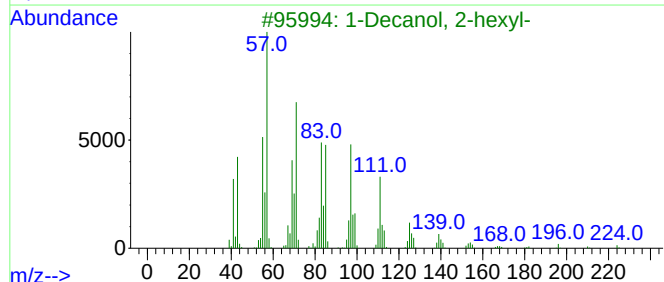
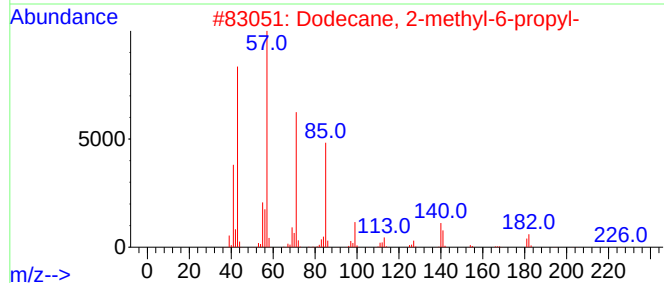
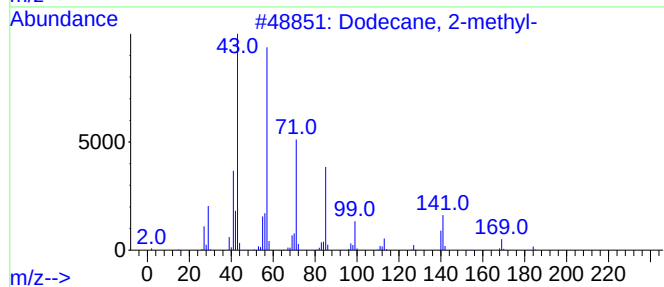
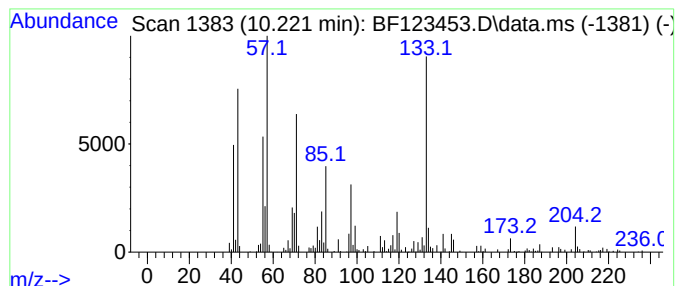
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown10.222 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.222	3.41 ng	397591	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-	184	C13H28	001560-97-0	45
2			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	43
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
4			Heptacosane	380	C27H56	000593-49-7	38
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

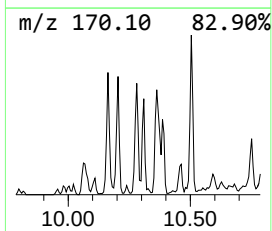
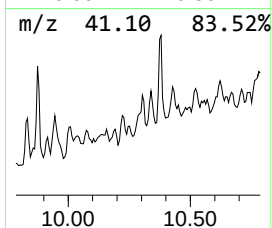
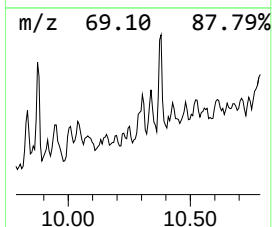
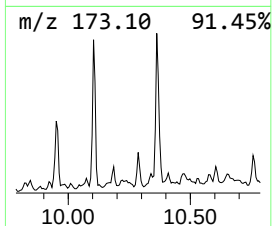
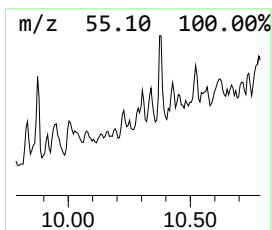
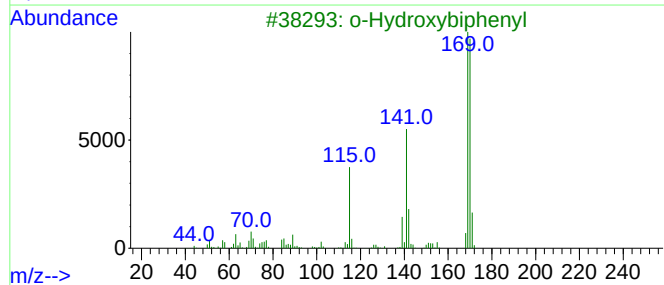
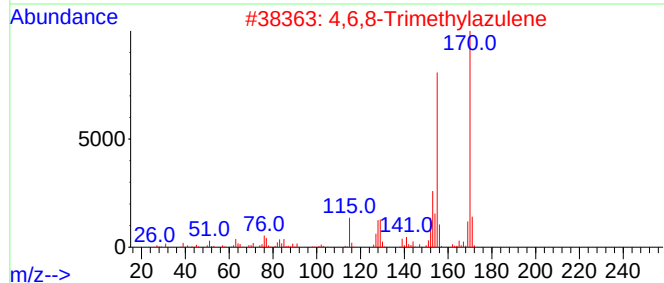
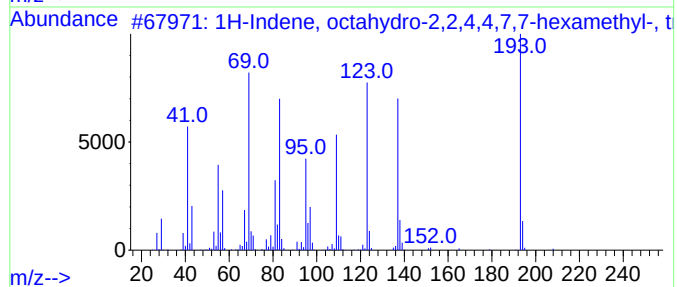
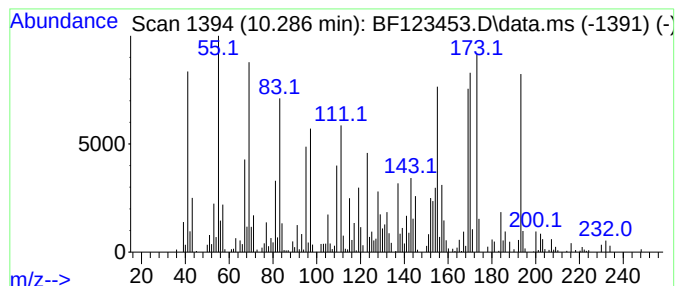
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown10.286 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.286	4.56 ng	531885	Acenaphthene-d10	9.963	
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	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	15
3	o-Hydroxybiphenyl	170	C12H10O	000090-43-7	15
4	6-Fluorovanillin	170	C8H7FO3	079418-77-2	15
5	1H,3H-Thieno[3,4-c]thiophene, 4,...	170	C8H10S2	015441-54-0	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123453.D
Acq On : 24 Mar 2021 22:38
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Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

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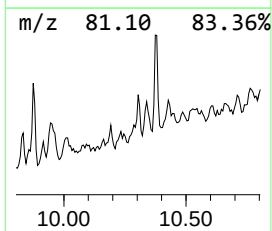
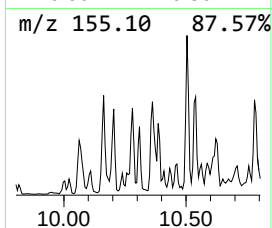
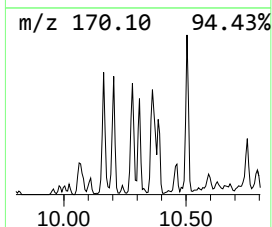
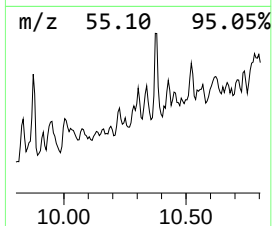
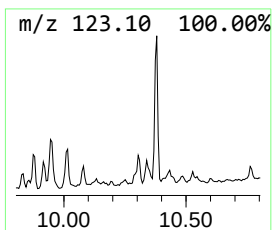
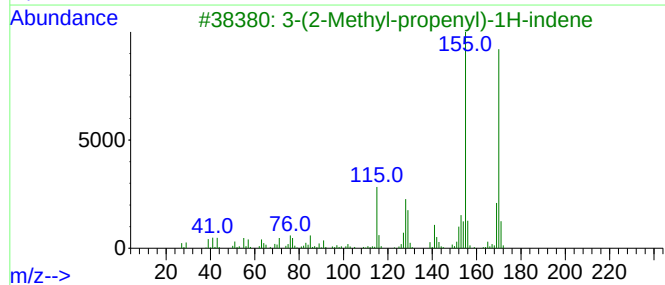
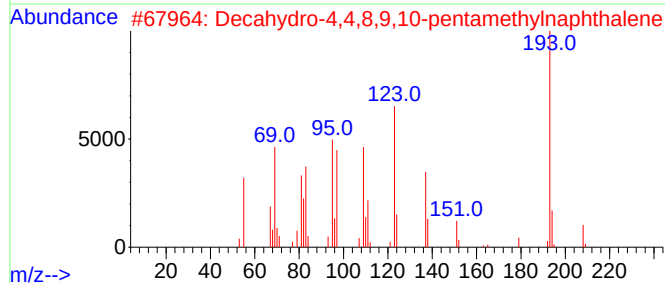
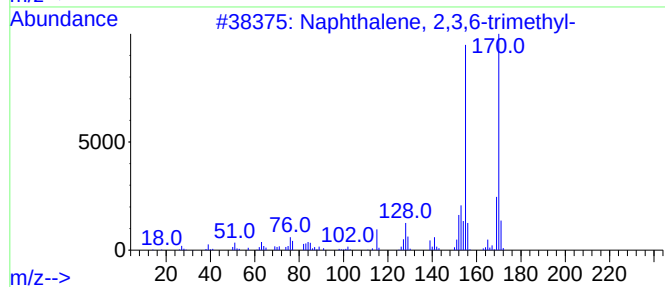
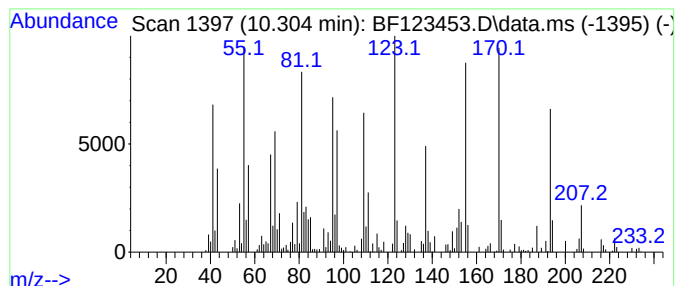
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown10.304 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.304	4.33 ng	505912	Acenaphthene-d10	9.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	48
2		Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
3		3-(2-Methyl-propenyl)-1H-indene	170	C13H14	1000187-78-5	35
4		Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	35
5		2-Naphthyl methyl ketone	170	C12H10O	000093-08-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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Misc :
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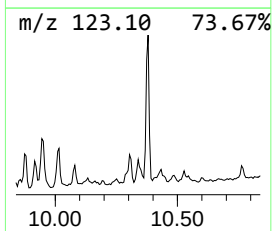
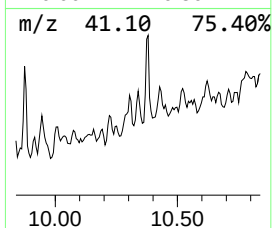
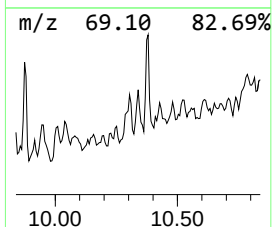
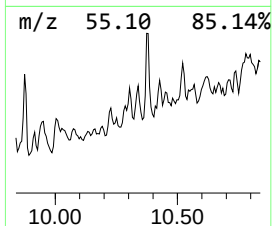
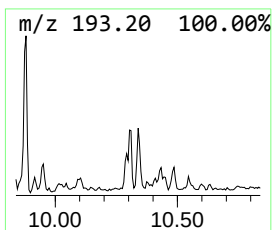
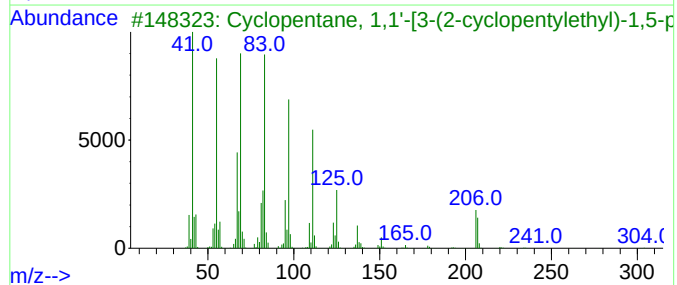
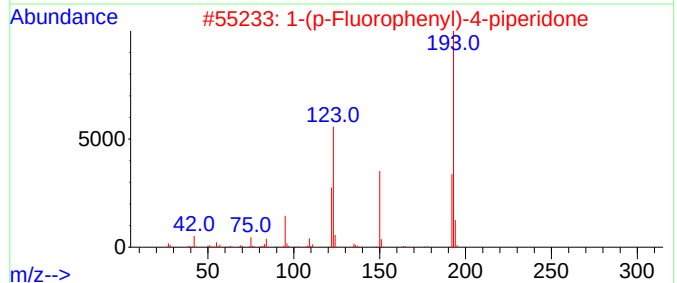
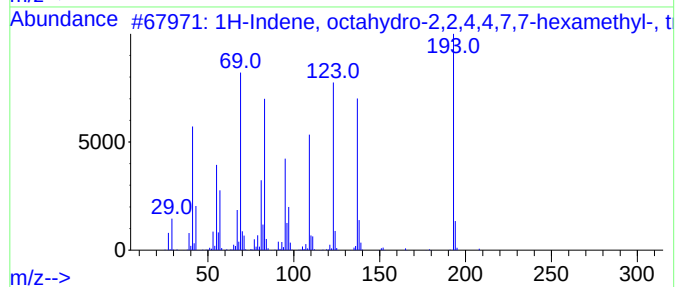
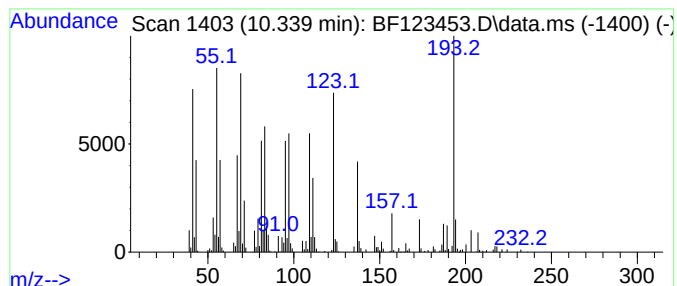
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1H-Indene, octahydro-2,2,4,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.339	4.72 ng	550977	Acenaphthene-d10	9.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	70
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	30
3	Cyclopentane, 1,1'-[3-(2-cyclope...	304	C22H40	055255-85-1	27
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
5	Neopentylidenecyclohexane	152	C11H20	039546-80-0	22



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Operator : JU/CG
Sample : M1775-02
Misc :
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ClientSampleId :
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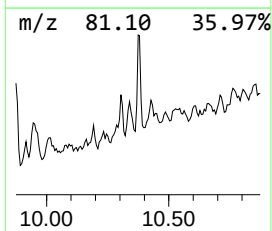
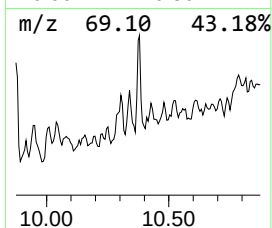
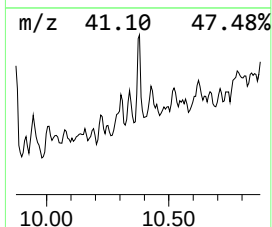
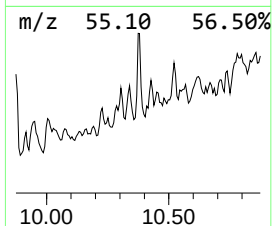
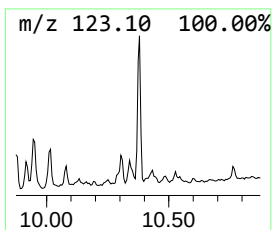
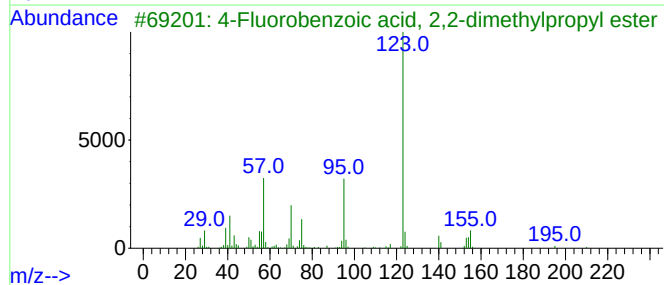
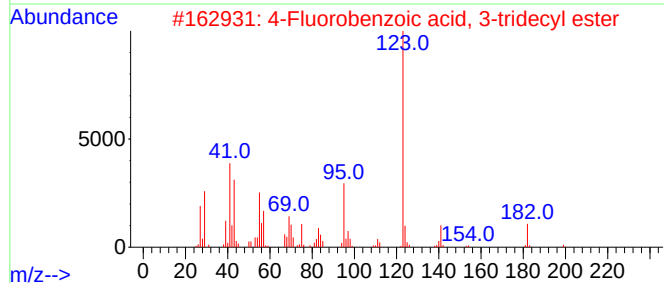
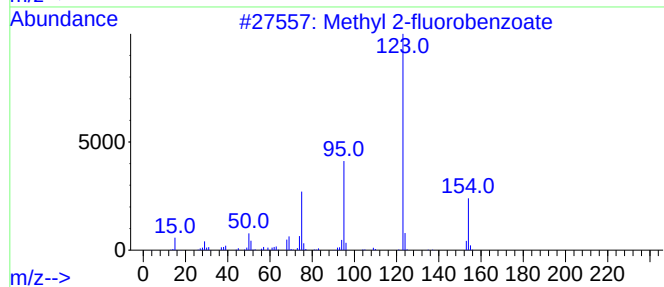
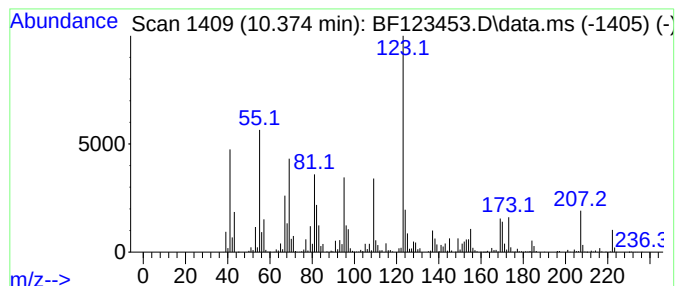
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown10.374 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.374	14.33 ng	1672520	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 2-fluorobenzoate	154	C8H7FO2	000394-35-4	43
2			4-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-67-9	38
3			4-Fluorobenzoic acid, 2,2-dimeth...	210	C12H15FO2	069912-03-4	38
4			4-Fluorobenzoic acid, pentafluor...	306	C13H4F6O2	1000355-67-4	38
5			3-Fluorobenzoic acid, undec-2-en...	292	C18H25FO2	1000292-60-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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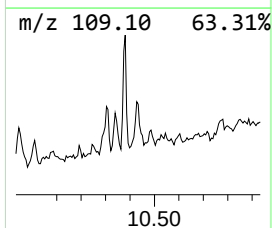
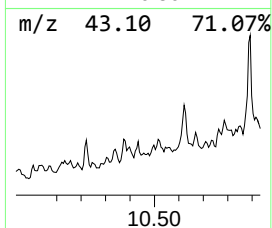
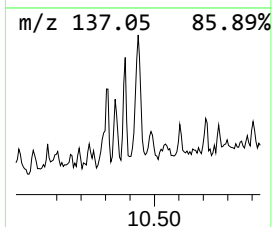
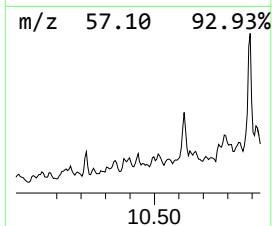
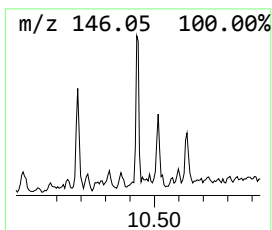
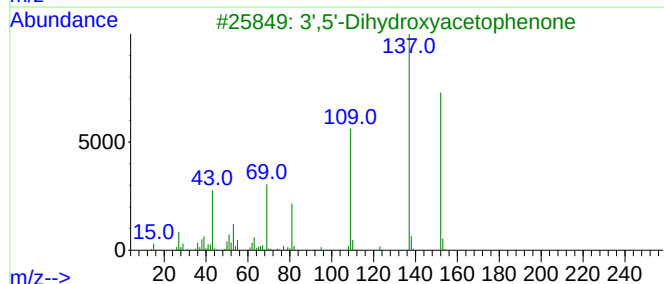
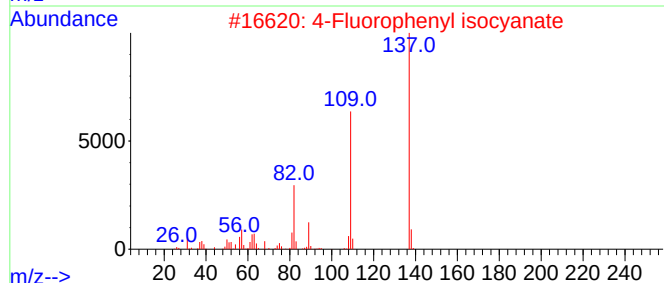
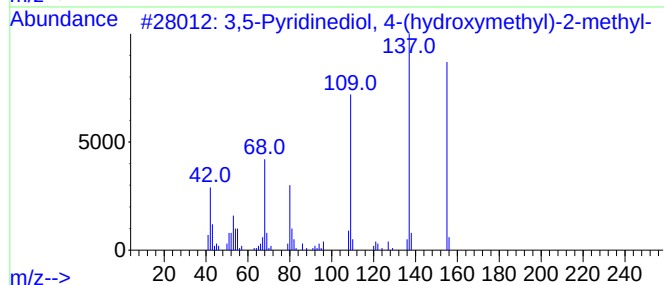
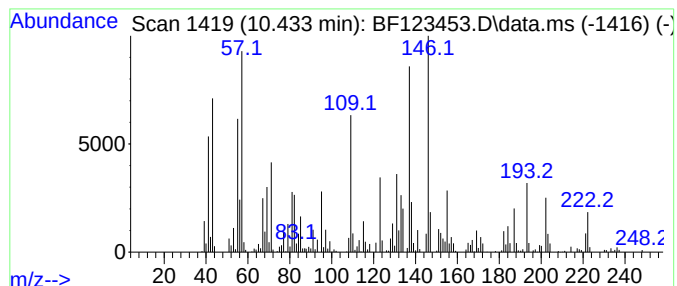
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown10.433 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.433	4.25 ng	496248	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Pyridinediol, 4-(hydroxymeth...	155	C7H9NO3	002029-60-9	35
2			4-Fluorophenyl isocyanate	137	C7H4FNO	001195-45-5	30
3			3',5'-Dihydroxyacetophenone	152	C8H8O3	051863-60-6	27
4			Mandelic acid, o-methoxy-, methy...	196	C10H12O4	021165-11-7	27
5			Ethyl Vanillin	166	C9H10O3	000121-32-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123453.D
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Sample : M1775-02
Misc :
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Instrument :
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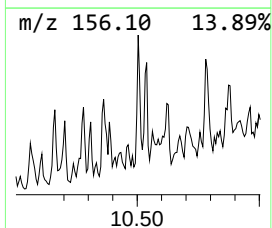
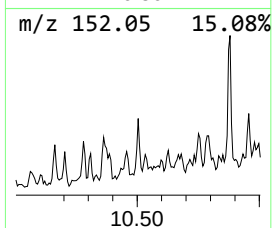
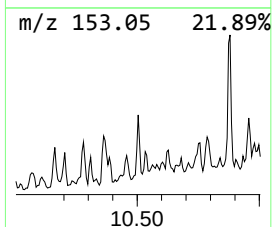
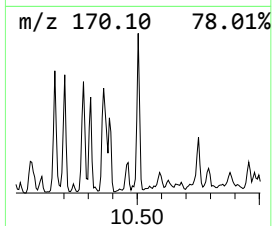
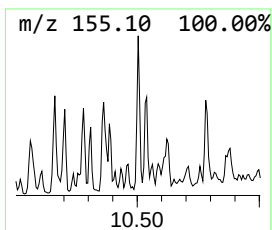
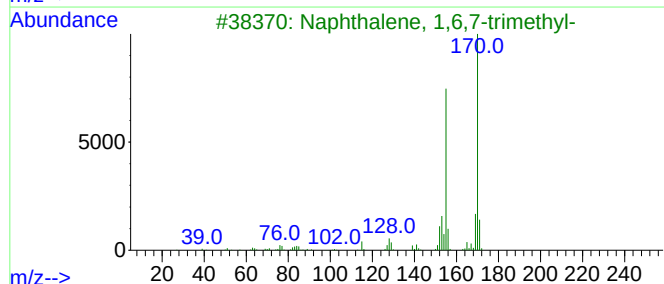
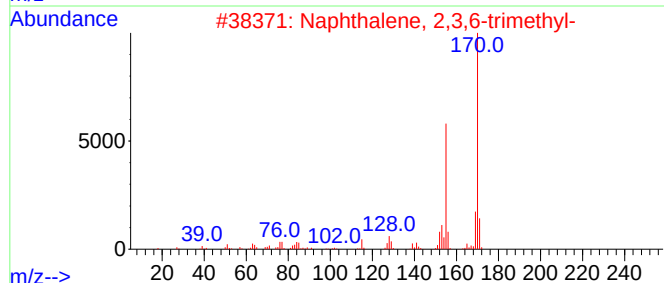
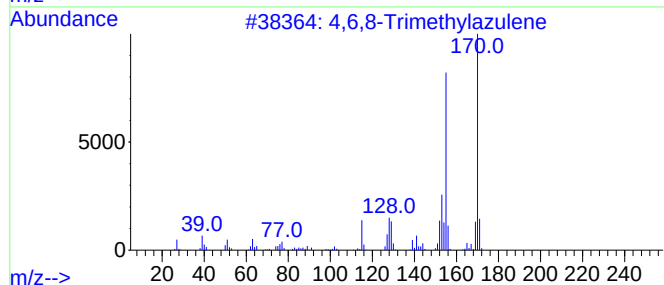
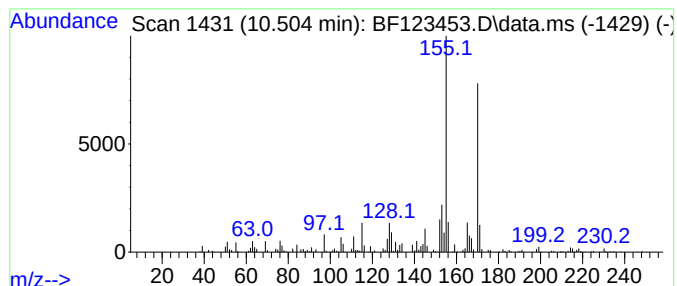
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 4,6,8-Trimethylazulene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.504	3.84 ng	448347	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,6,8-Trimethylazulene	170	C13H14	000941-81-1	93
2			Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	93
3			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	93
4			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	87
5			3-(2-Methyl-propenyl)-1H-indene	170	C13H14	1000187-78-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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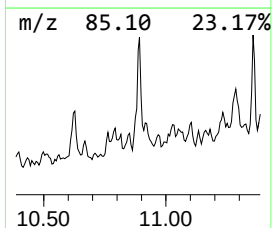
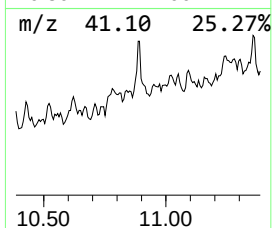
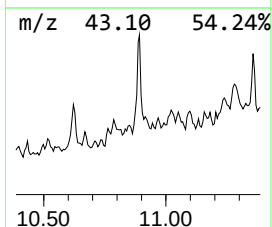
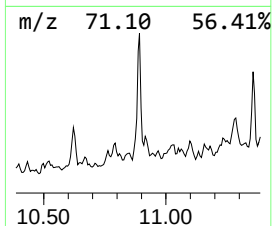
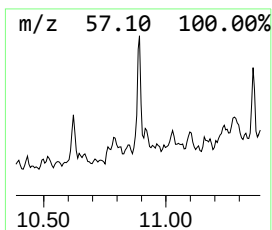
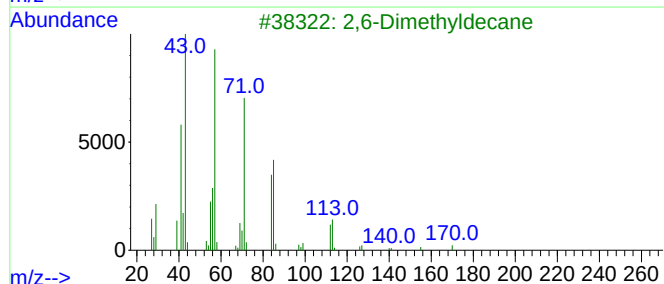
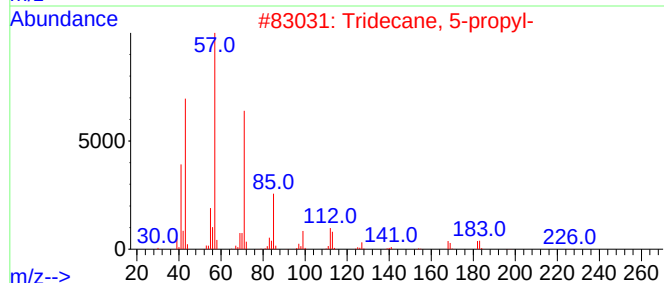
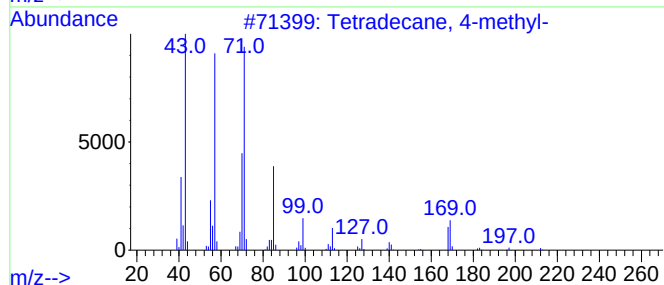
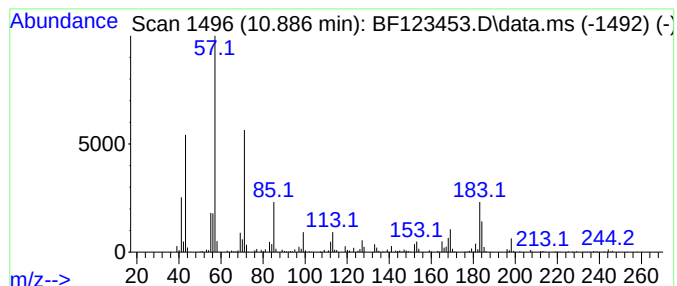
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Tetradecane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.886	48.45 ng	2249570	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	64
2			Tridecane, 5-propyl-	226	C16H34	055045-11-9	58
3			2,6-Dimethyldecane	170	C12H26	013150-81-7	55
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	55
5			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123453.D
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Misc :
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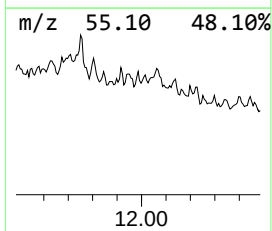
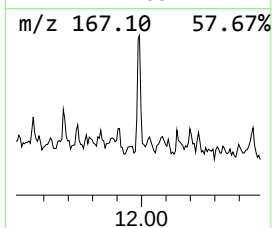
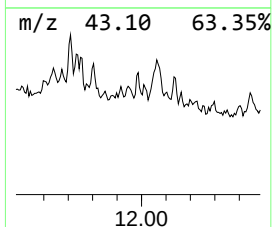
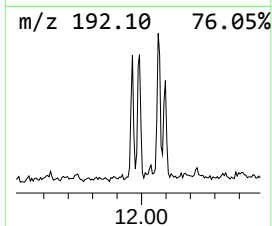
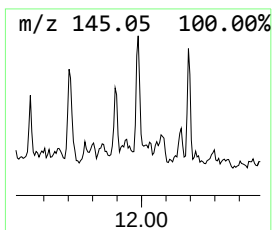
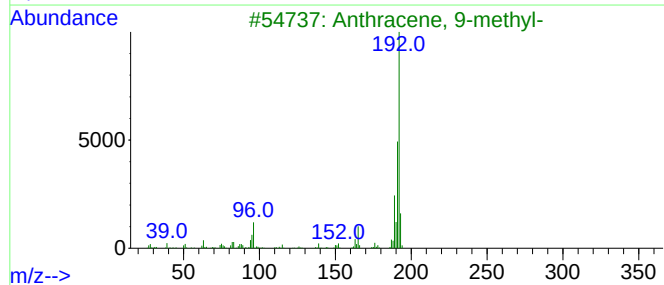
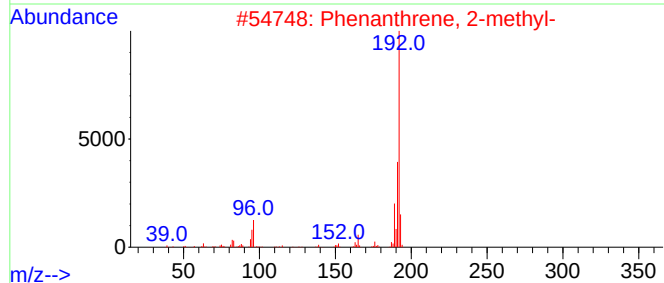
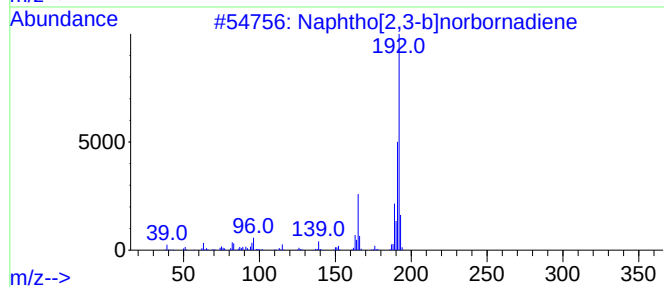
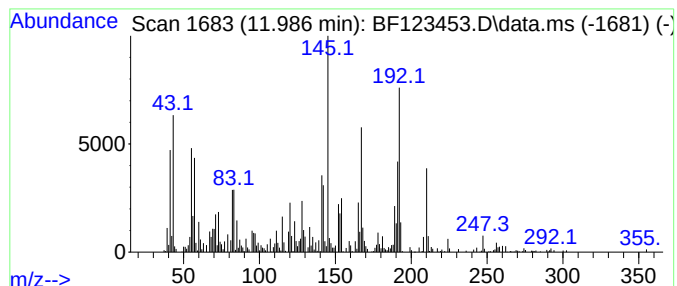
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Naphtho[2,3-b]norbornadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	10.63 ng	493543	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	52
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38
3			Anthracene, 9-methyl-	192	C15H12	000779-02-2	35
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	35
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

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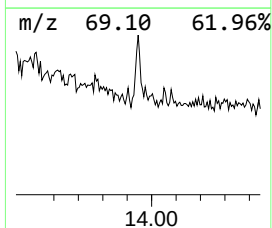
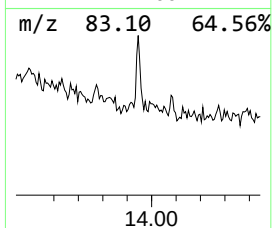
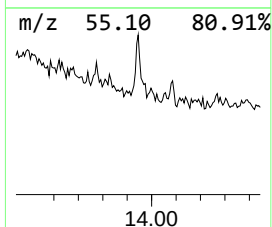
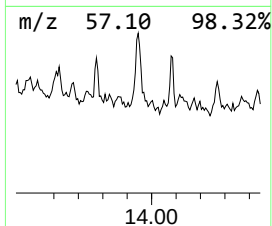
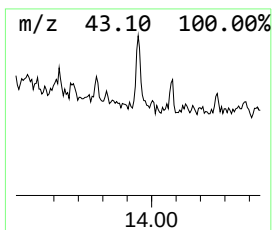
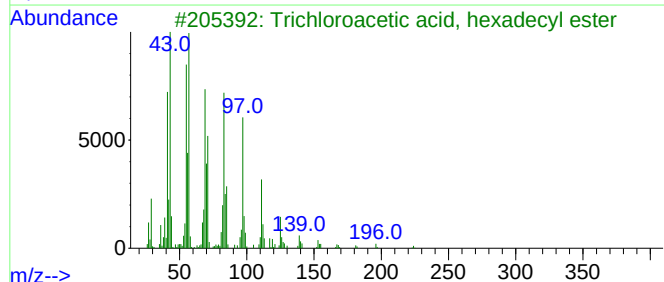
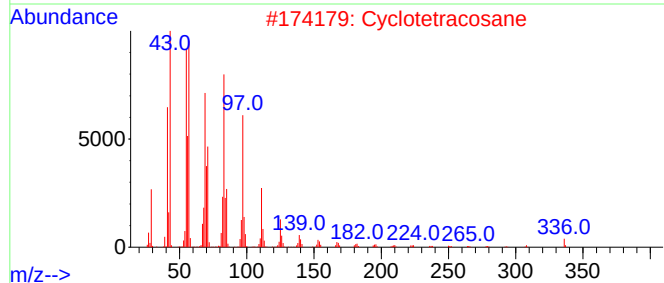
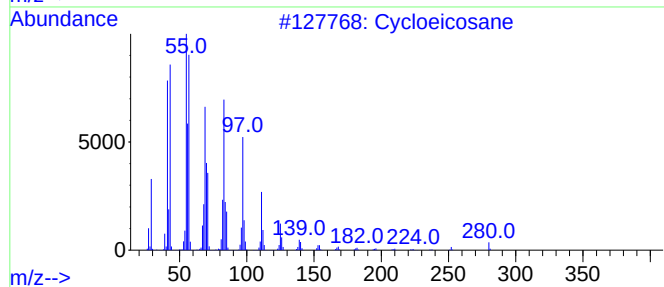
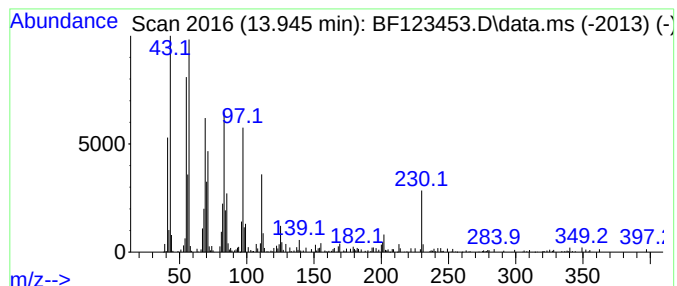
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Cycloeicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	6.00 ng	406217	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	96
2			Cyclotetracosane	336	C24H48	000297-03-0	93
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
5			Cyclooctacosane	392	C28H56	000297-24-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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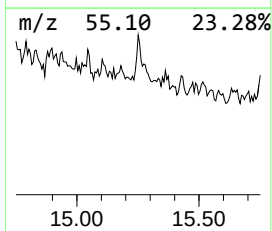
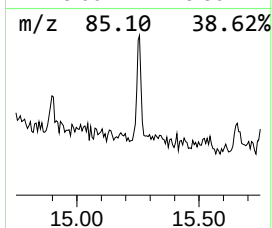
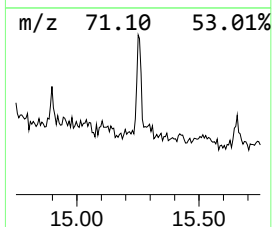
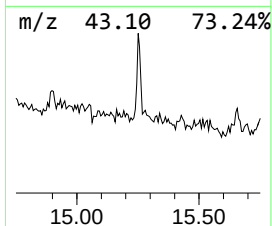
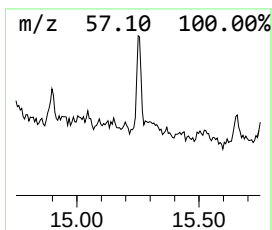
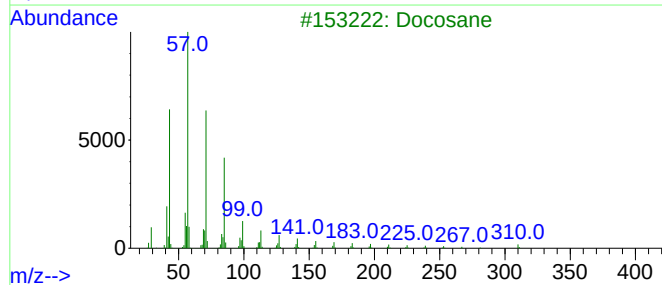
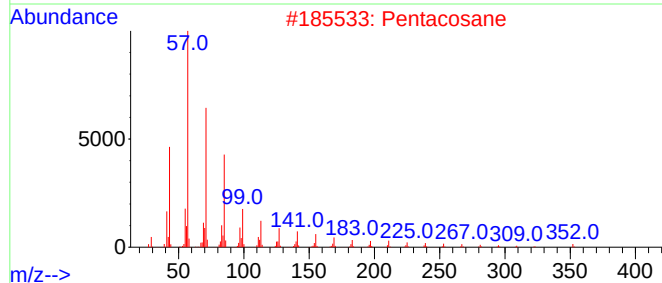
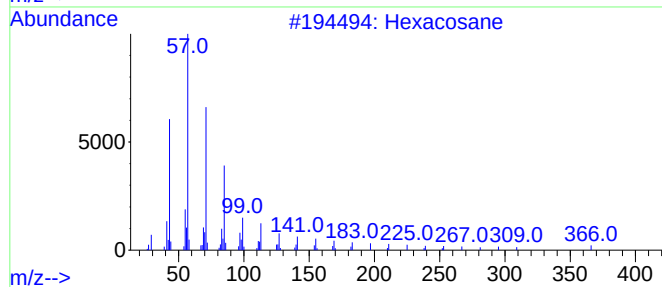
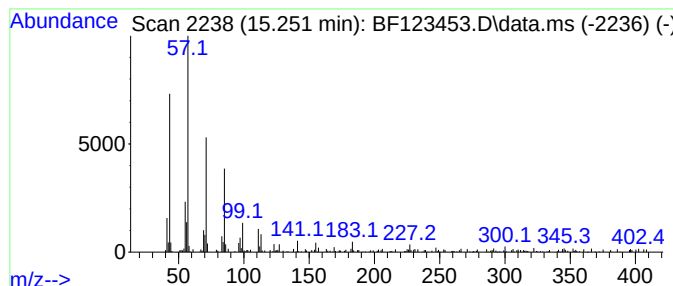
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BNA_F
ClientSampleId :
11979

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Hexacosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.251	3.43 ng	149864	Perylene-d12		15.609	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Pentacosane		352	C25H52	000629-99-2	91
3	Docosane		310	C22H46	000629-97-0	89
4	Heneicosane		296	C21H44	000629-94-7	83
5	Octacosane		394	C28H58	000630-02-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123453.D
Acq On : 24 Mar 2021 22:38
Operator : JU/CG
Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
11979

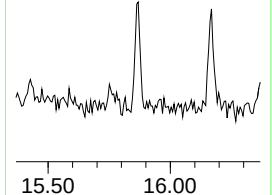
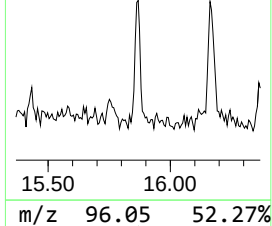
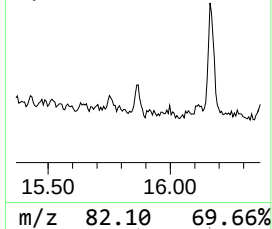
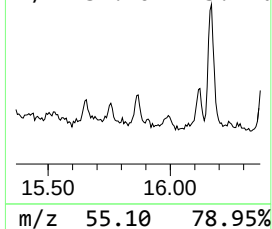
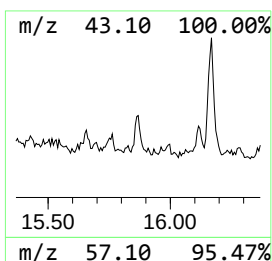
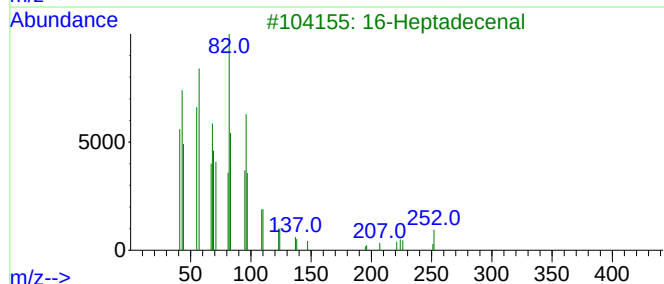
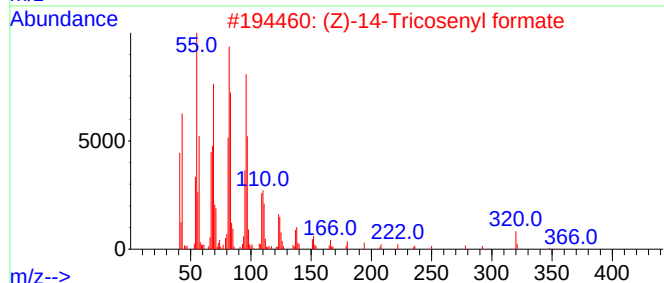
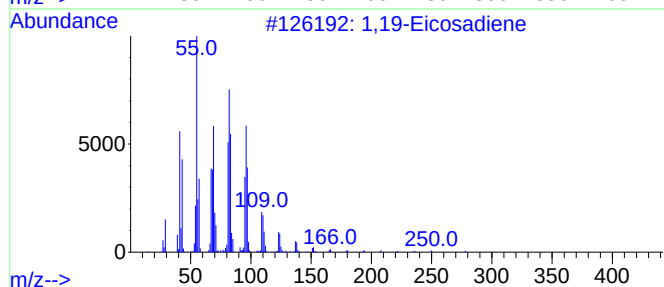
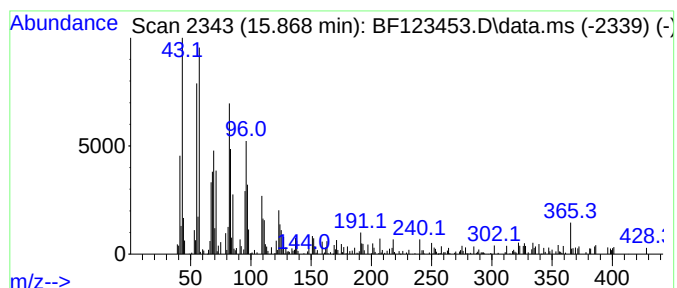
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 1,19-Eicosadiene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.868	4.73 ng	206416	Perylene-d12	15.609

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene		278	C20H38	014811-95-1	91
2	(Z)-14-Tricosenyl formate		366	C24H46O2	077899-10-6	83
3	16-Heptadecenal		252	C17H32O	1000144-57-9	81
4	Heptadecanal		254	C17H34O	1000376-70-0	81
5	Octadecanal		268	C18H36O	000638-66-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123453.D
Acq On : 24 Mar 2021 22:38
Operator : JU/CG
Sample : M1775-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11979

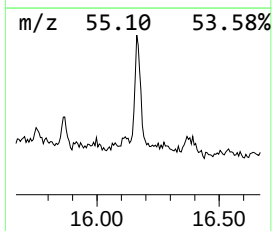
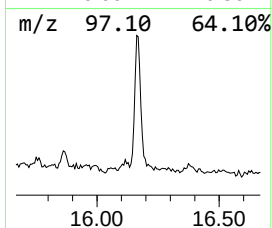
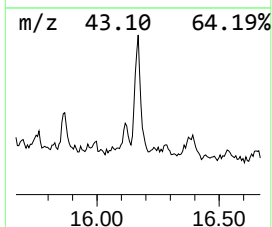
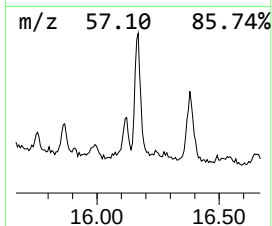
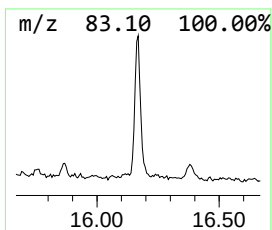
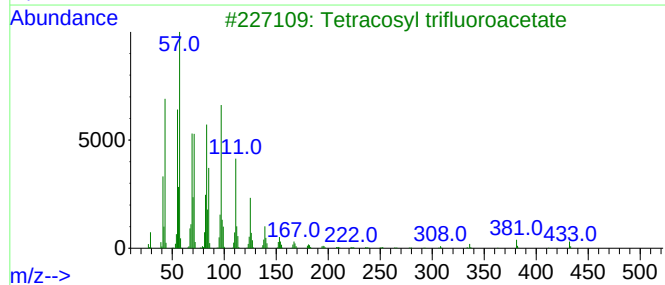
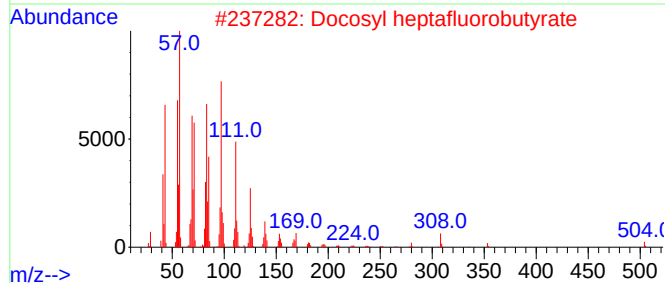
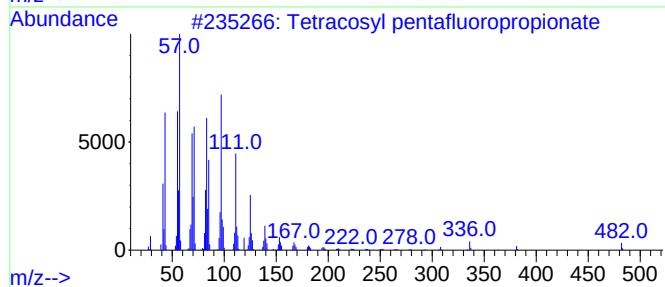
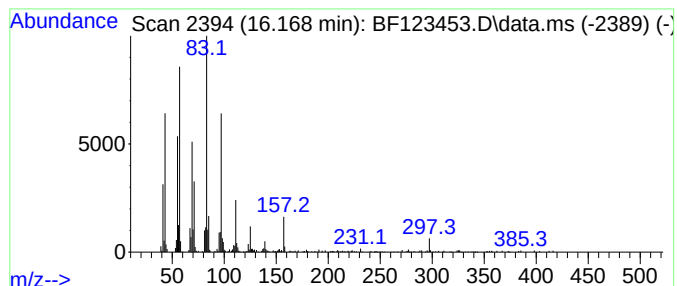
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown16.168 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.168	20.60 ng	900056	Perylene-d12	15.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	49
2			Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	46
3			Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	46
4			Octacosyl pentafluoropropionate	556	C31H57F5O2	1000351-88-9	46
5			Cyclobutanecarboxylic acid, unde...	252	C16H28O2	1000299-13-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
 Data File : BF123453.D
 Acq On : 24 Mar 2021 22:38
 Operator : JU/CG
 Sample : M1775-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 11979

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.204	16.3	ng	1053890	1	6.916	1291650	20.0
unknown9.727	9.727	2.9	ng	333050	3	9.963	2334690	20.0
Decahydro-4,4,8...	9.833	6.1	ng	713264	3	9.963	2334690	20.0
unknown9.874	9.874	9.7	ng	1135580	3	9.963	2334690	20.0
unknown10.074	10.074	2.5	ng	293602	3	9.963	2334690	20.0
Naphthalene, 1,...	10.163	2.5	ng	298169	3	9.963	2334690	20.0
unknown10.192	10.192	3.1	ng	367210	3	9.963	2334690	20.0
unknown10.222	10.222	3.4	ng	397591	3	9.963	2334690	20.0
unknown10.286	10.286	4.6	ng	531885	3	9.963	2334690	20.0
unknown10.304	10.304	4.3	ng	505912	3	9.963	2334690	20.0
1H-Indene, octa...	10.339	4.7	ng	550977	3	9.963	2334690	20.0
unknown10.374	10.374	14.3	ng	1672520	3	9.963	2334690	20.0
unknown10.433	10.433	4.3	ng	496248	3	9.963	2334690	20.0
4,6,8-Trimethyl...	10.504	3.8	ng	448347	3	9.963	2334690	20.0
Tetradecane, 4-...	10.886	48.5	ng	2249570	4	11.457	928547	20.0
Naphtho[2,3-b]n...	11.986	10.6	ng	493543	4	11.457	928547	20.0
Cycloeicosane	13.945	6.0	ng	406217	5	14.104	1354710	20.0
Hexacosane	15.251	3.4	ng	149864	6	15.609	873675	20.0
1,19-Eicosadiene	15.868	4.7	ng	206416	6	15.609	873675	20.0
unknown16.168	16.168	20.6	ng	900056	6	15.609	873675	20.0