

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
 Data File : BF121339.D
 Acq On : 20 Aug 2020 11:08
 Operator : JU/CG
 Sample : L3712-05 5X
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VB-25203

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF081920.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.293	541	545	560	rBV	536529	569182	33.59%	3.021%
2	6.328	717	721	731	rBV	583864	607853	35.87%	3.227%
3	6.687	779	782	786	rBV	926623	794809	46.91%	4.219%
4	7.251	875	878	884	rBV	493033	388864	22.95%	2.064%
5	7.975	996	1001	1004	rBV	1216290	1075457	63.47%	5.709%
6	8.263	1046	1050	1053	rVB5	22834	30379	1.79%	0.161%
7	8.434	1077	1079	1082	rVB3	32490	31624	1.87%	0.168%
8	8.657	1114	1117	1121	rVB6	30615	42873	2.53%	0.228%
9	8.716	1124	1127	1129	rBV2	35887	34038	2.01%	0.181%
10	8.745	1129	1132	1135	rBV3	32666	39067	2.31%	0.207%
11	8.922	1160	1162	1166	rBV3	41042	56245	3.32%	0.299%
12	8.963	1166	1169	1171	rVV2	111059	87482	5.16%	0.464%
13	8.998	1171	1175	1178	rBV3	89335	93576	5.52%	0.497%
14	9.045	1178	1183	1186	rBV	1028311	845490	49.90%	4.488%
15	9.122	1192	1196	1200	rBV2	169023	222057	13.11%	1.179%
16	9.169	1202	1204	1206	rBV3	45692	45686	2.70%	0.243%
17	9.322	1228	1230	1232	rBV3	61655	56859	3.36%	0.302%
18	9.357	1233	1236	1238	rBV3	86138	95538	5.64%	0.507%
19	9.428	1246	1248	1251	rBV2	433623	475704	28.08%	2.525%
20	9.481	1255	1257	1263	rVB4	164255	179463	10.59%	0.953%
21	9.539	1265	1267	1269	rVB2	111195	80695	4.76%	0.428%
22	9.586	1272	1275	1278	rBV3	275658	335524	19.80%	1.781%
23	9.633	1281	1283	1286	rVB	750117	607036	35.83%	3.222%
24	9.675	1286	1290	1292	rBV3	168283	238026	14.05%	1.263%
25	9.722	1292	1298	1301	rBV	1373120	1694368	100.00%	8.994%
26	9.769	1303	1306	1308	rBV	148473	147123	8.68%	0.781%
27	9.992	1340	1344	1348	rBV2	455520	639516	37.74%	3.395%
28	10.057	1351	1355	1358	rVV4	294456	419028	24.73%	2.224%
29	10.092	1358	1361	1364	rBV4	324090	402758	23.77%	2.138%
30	10.133	1364	1368	1370	rBV2	654624	665563	39.28%	3.533%
31	10.386	1409	1411	1416	rVB	491430	506116	29.87%	2.687%
32	10.510	1428	1432	1435	rBV3	472892	760450	44.88%	4.037%
33	10.651	1452	1456	1459	rBV2	1075355	1376736	81.25%	7.308%
34	11.122	1533	1536	1539	rVB	713280	803486	47.42%	4.265%

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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

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Peak separation: 5

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35	11.210	1549	1551	1554	rBV	832346	716482	42.29%	3.803%
36	12.792	1817	1820	1828	rVB	958097	943074	55.66%	5.006%
37	13.839	1995	1998	2002	rBV	1194315	1191282	70.31%	6.324%
38	14.851	2167	2170	2178	rVB	51072	88777	5.24%	0.471%
39	15.186	2225	2227	2232	rVB	29506	44512	2.63%	0.236%
40	15.245	2232	2237	2241	rBV	1029503	1183217	69.83%	6.281%
41	15.674	2306	2310	2315	rVB	52705	75250	4.44%	0.399%
42	16.133	2383	2388	2392	rBV2	42029	65970	3.89%	0.350%
43	16.280	2410	2413	2419	rVB4	19141	29747	1.76%	0.158%
44	16.674	2474	2480	2486	rBV2	27195	51910	3.06%	0.276%

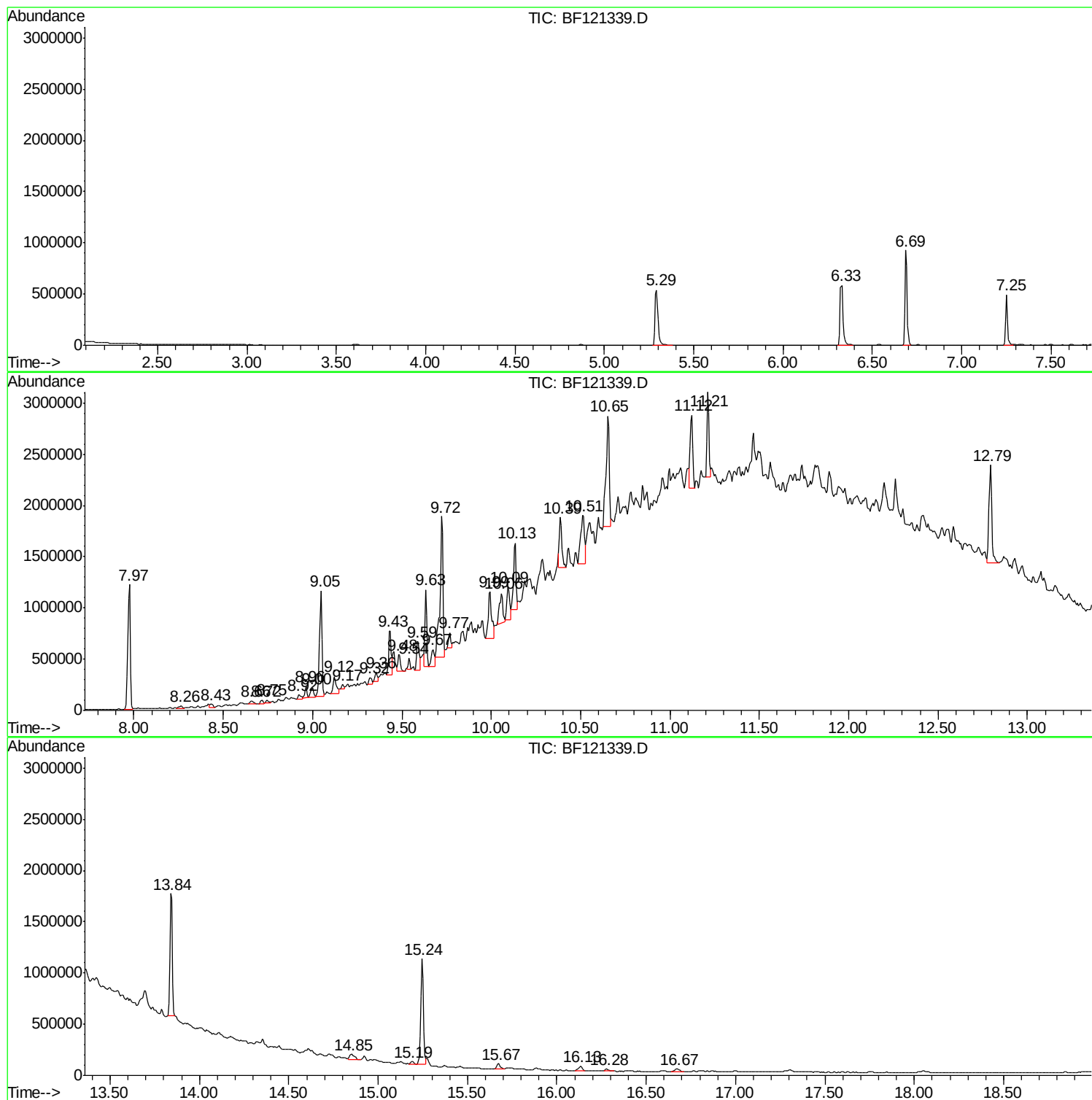
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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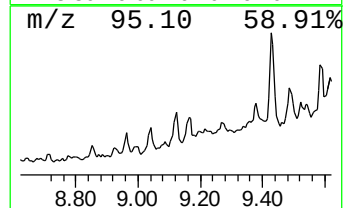
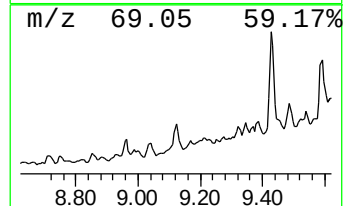
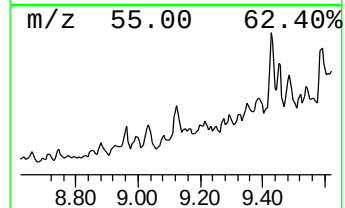
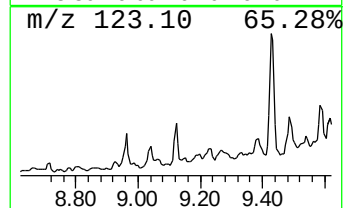
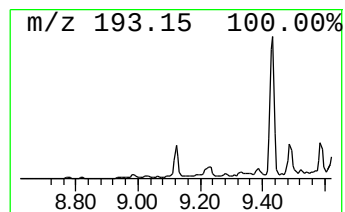
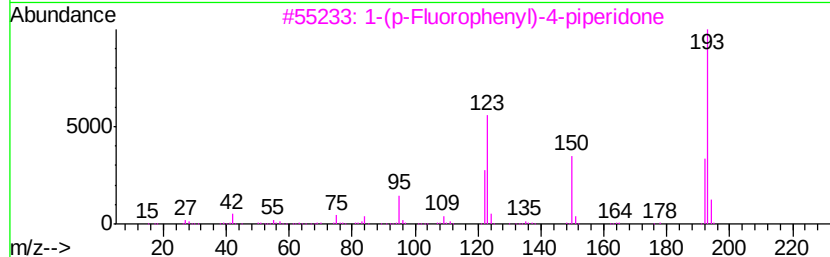
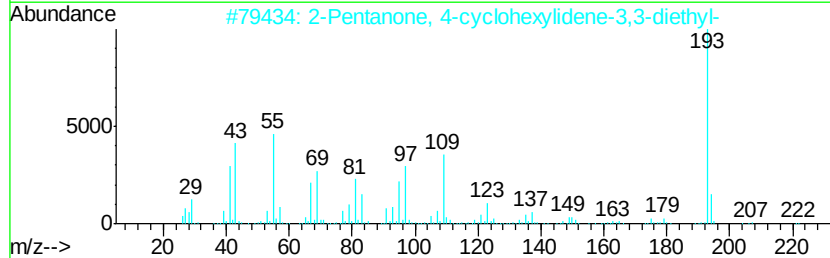
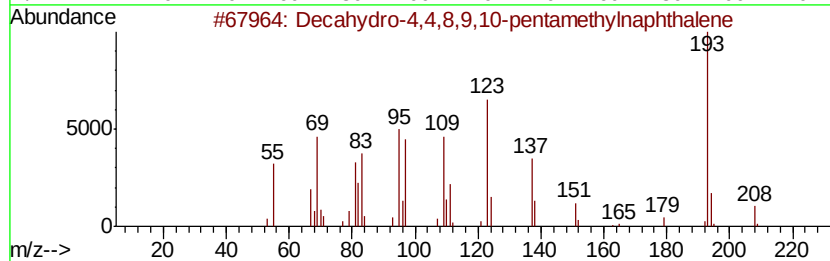
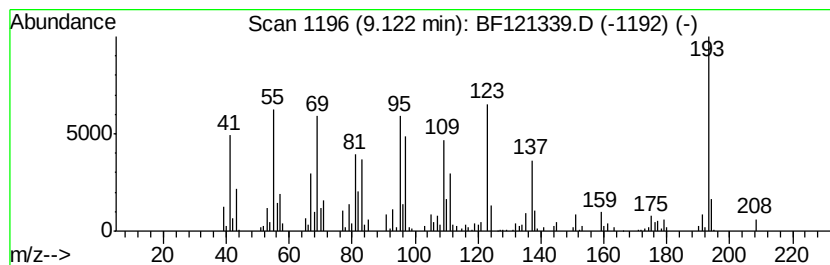
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown9.12 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.12	2.62 ng	222057	Acenaphthene-d10	9.72		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	49
2		2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	47
3		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FN0	1000238-56-7	35
4		Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25B0	057387-76-5	22
5		2-Aminobenzothiazol-6-carboxamide	193	C8H7N3OS	111962-90-4	14



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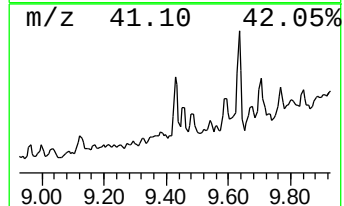
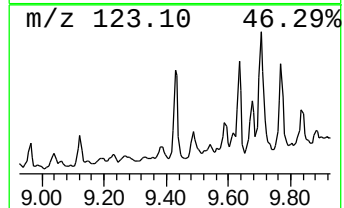
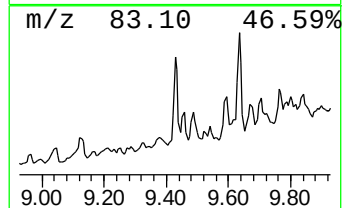
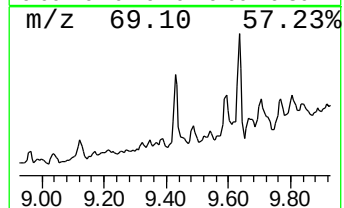
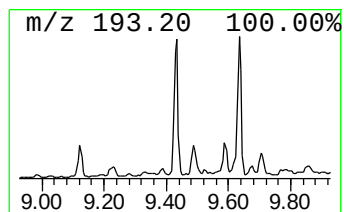
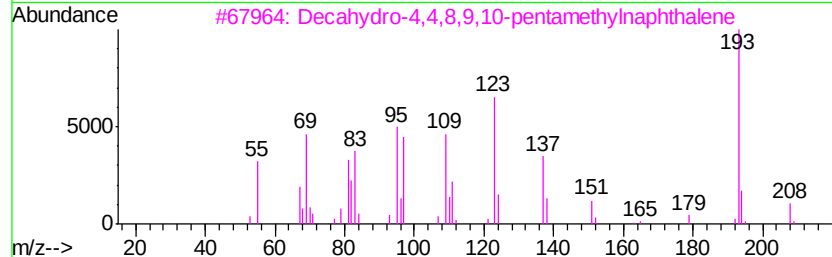
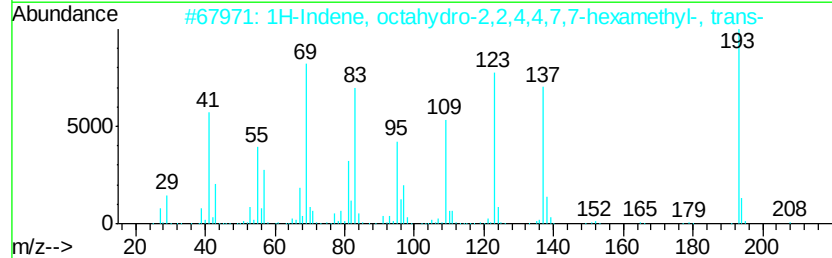
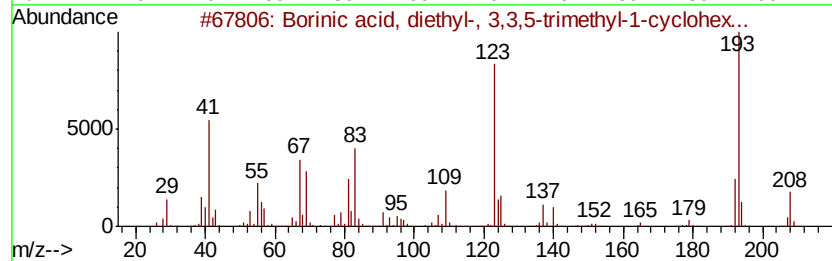
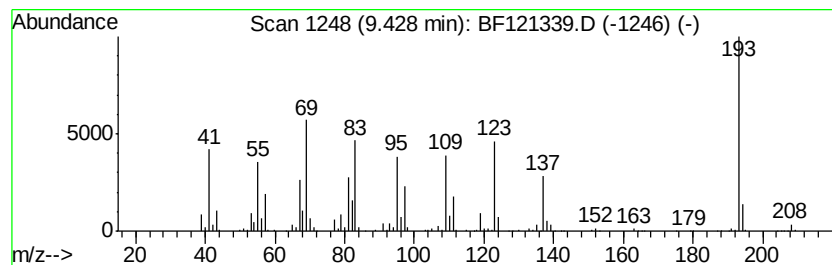
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown9.43 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.43	5.62 ng	475704	Acenaphthene-d10	9.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25B0	057387-76-5	25
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	25
3	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	23
4	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21B02	074630-04-9	17
5	diallyl(2,2,4a,7,7-pentamethyl-1...	384	C19H33N2O4P	1000187-42-4	16



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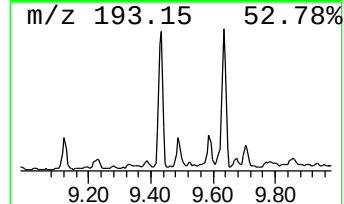
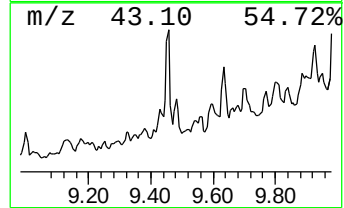
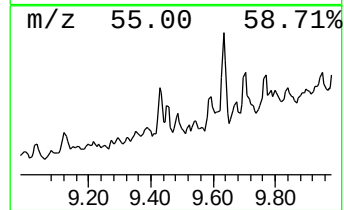
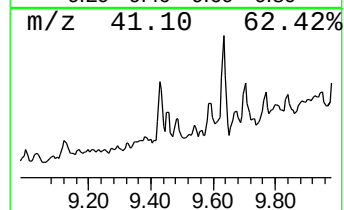
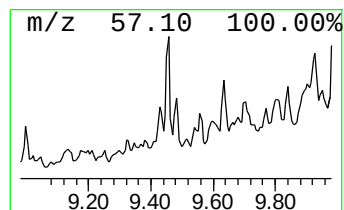
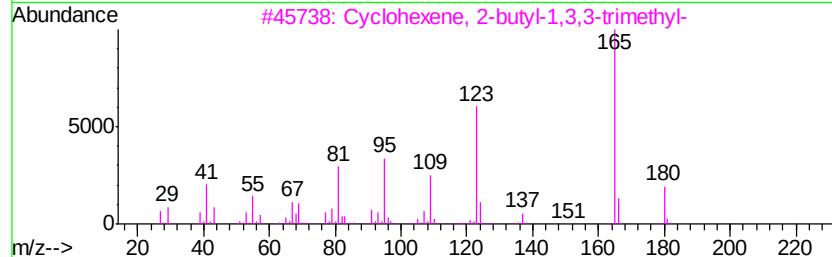
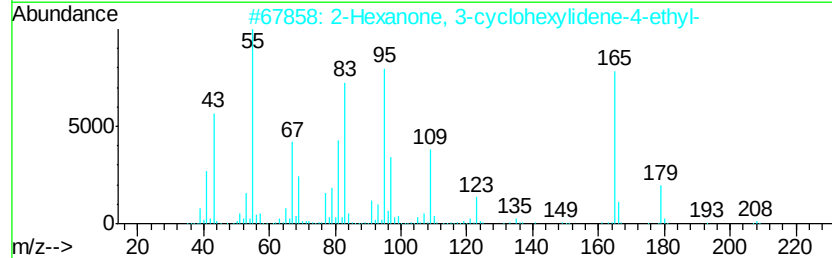
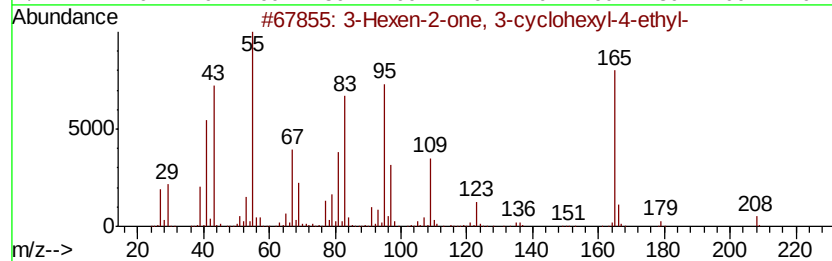
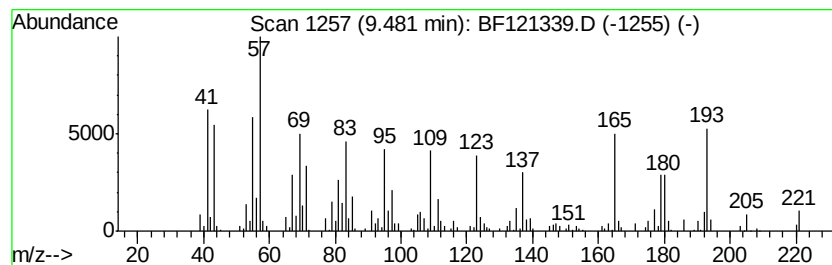
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.48 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	2.12 ng	179463	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one, 3-cyclohexyl-4-ethyl-	208	C14H24O	1000150-19-1	42
2		2-Hexanone, 3-cyclohexylidene-4-ethyl-	208	C14H24O	1000150-19-2	38
3		Cyclohexene, 2-butyl-1,3,3-trimethyl-	180	C13H24	003293-50-3	38
4		[1,2,4]Triazolo[1,5-a]pyrimidin-5-yl-	193	C8H11N5O	1000351-50-1	38
5		3-Hydroxymethylene-1,7,7-trimethyl-	180	C11H16O2	015051-75-9	35



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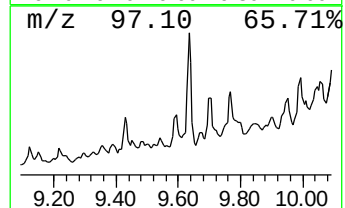
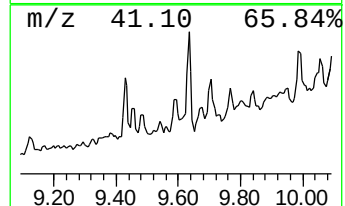
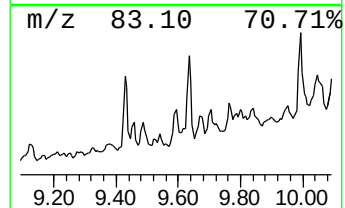
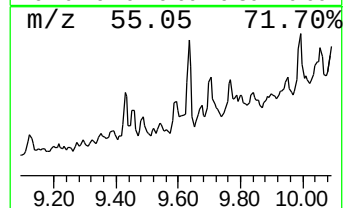
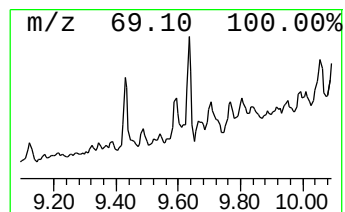
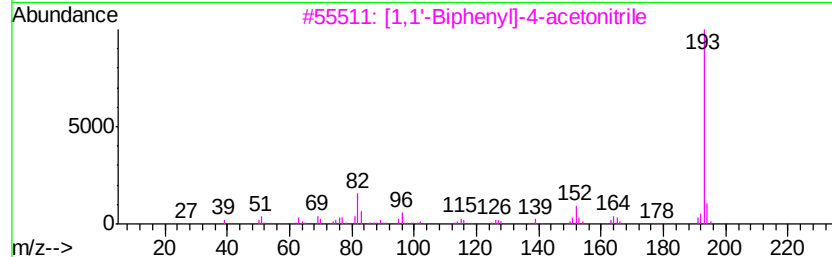
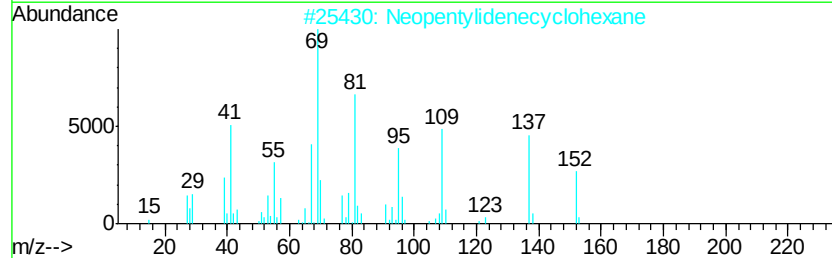
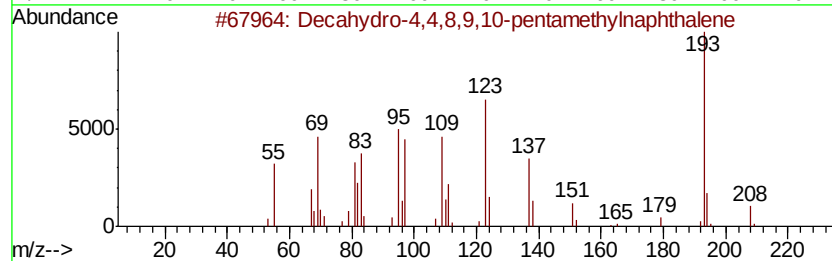
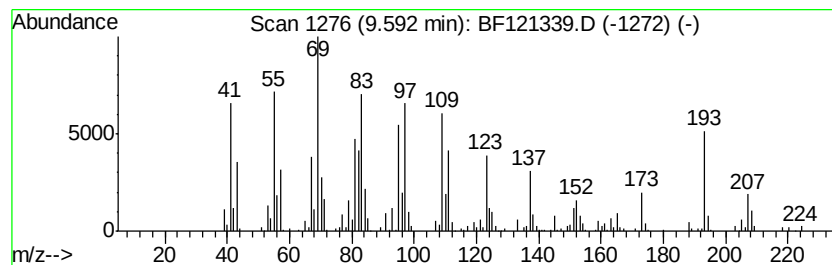
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Decahydro-4,4,8,9,10-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	3.96 ng	335524	Acenaphthene-d10	9.72
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Decahydro-4,4,8,9,10-pentamethyl...	208 C15H28	080655-44-3 89
2		Neopentylidenecyclohexane	152 C11H20	039546-80-0 30
3		[1,1'-Biphenyl]-4-acetonitrile	193 C14H11N	031603-77-7 25
4		Benzo[flquinoline, 3-methyl-	193 C14H11N	000085-06-3 25
5		2,6-Heptadienal, 2,4-dimethyl-	138 C9H14O	085136-08-9 20



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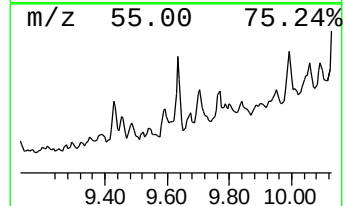
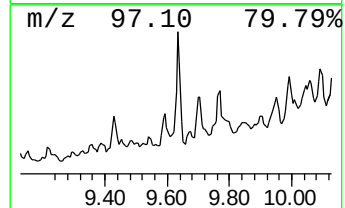
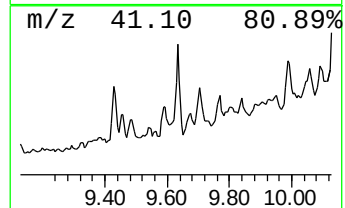
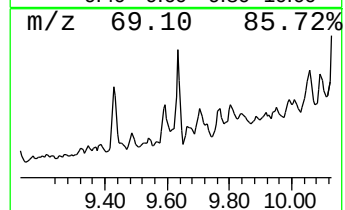
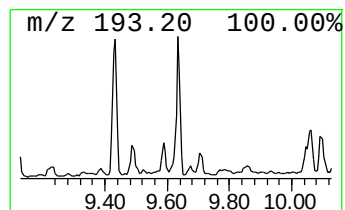
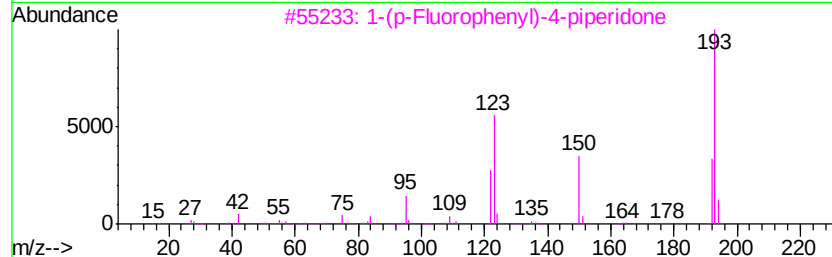
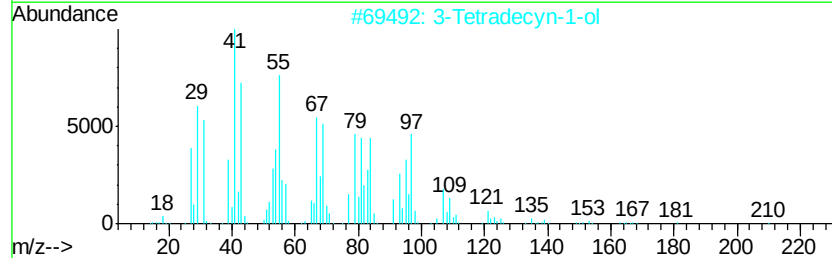
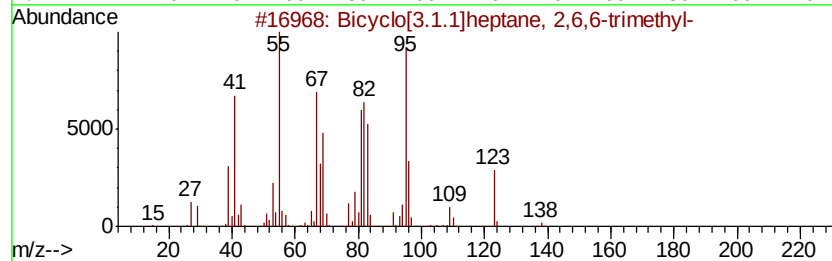
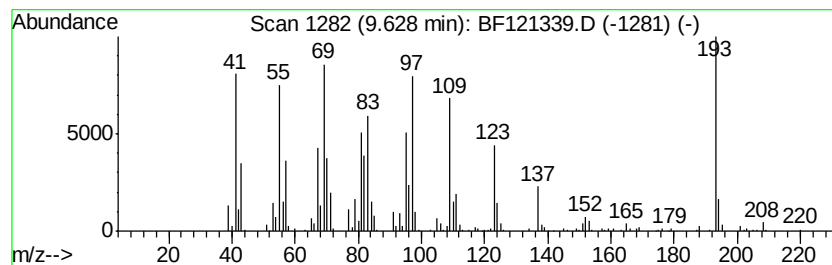
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.63 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	7.17 ng	607036	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	30
2		3-Tetradecyn-1-ol	210	C14H26O	055182-74-6	27
3		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
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\BF082020\
Data File : BF121339.D
Acq On : 20 Aug 2020 11:08
Operator : JU/CG
Sample : L3712-05 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

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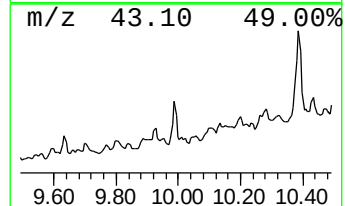
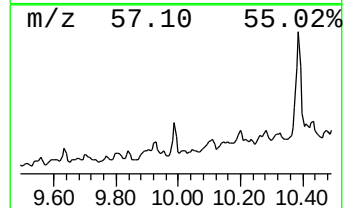
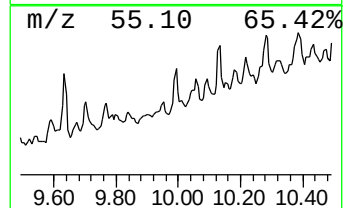
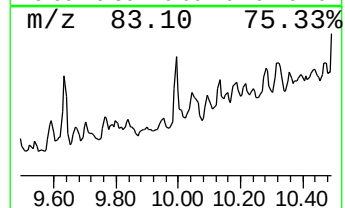
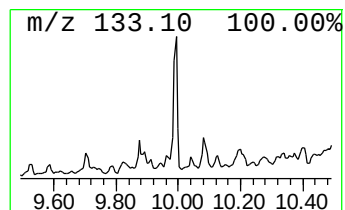
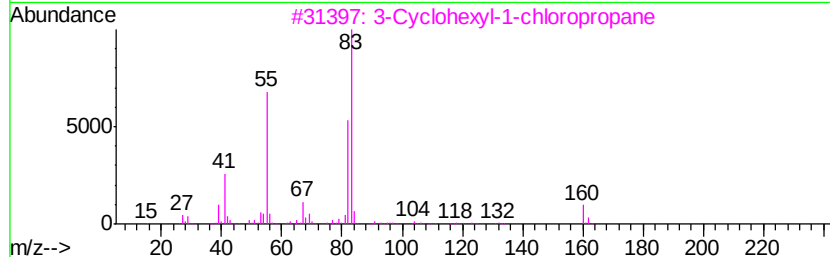
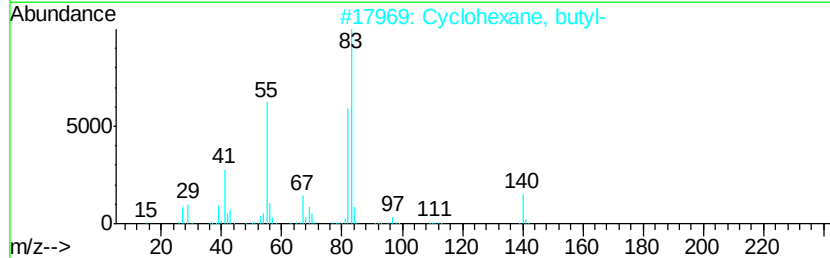
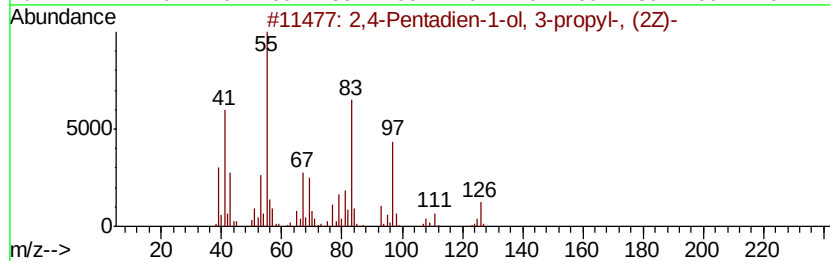
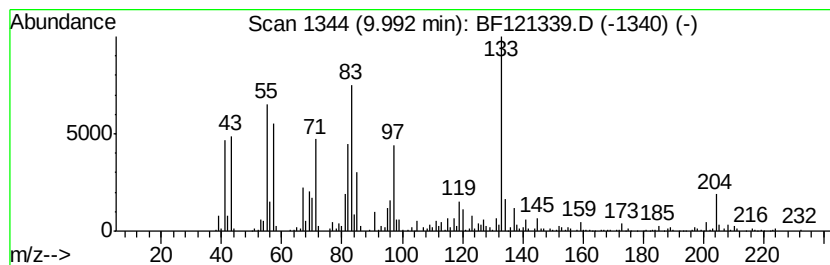
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.99 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.99	7.55 ng	639516	Acenaphthene-d10		9.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Pentadien-1-ol, 3-propyl-, (...)	126	C8H14O	1000142-17-9	30		
2	Cyclohexane, butyl-	140	C10H20	001678-93-9	25		
3	3-Cyclohexyl-1-chloropropane	160	C9H17Cl	001124-62-5	25		
4	Cyclohexane, propyl-	126	C9H18	001678-92-8	25		
5	Cyclohexane, pentyl-	154	C11H22	004292-92-6	25		



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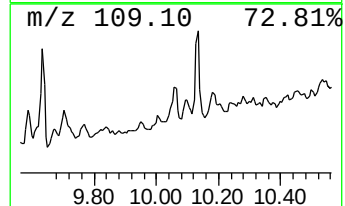
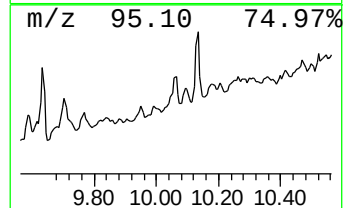
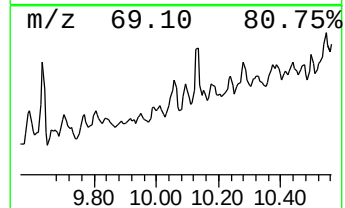
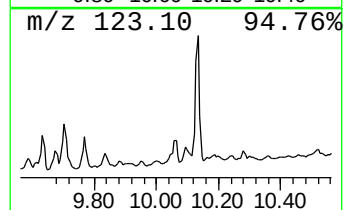
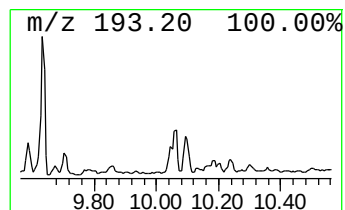
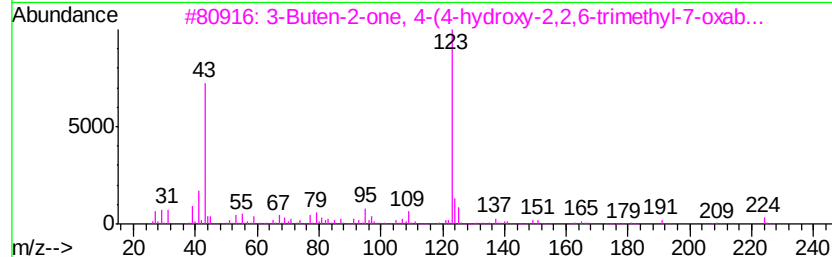
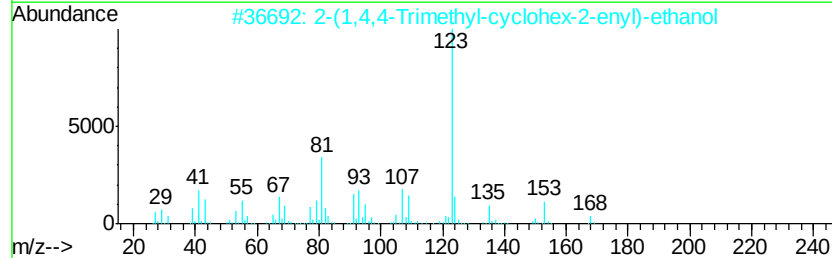
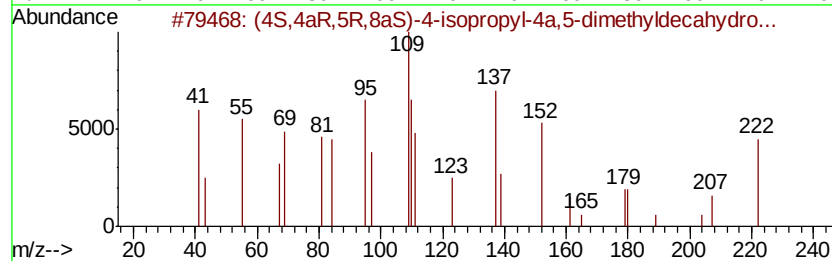
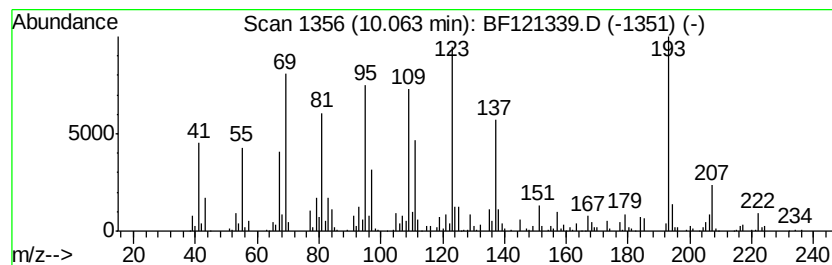
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.06 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.06	4.95 ng	419028	Acenaphthene-d10	9.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4S,4aR,5R,8aS)-4-isopropyl-4a,5...	222	C15H26O	055897-99-9	18
2	2-(1,4,4-Trimethyl-cyclohex-2-en...	168	C11H20O	1000190-92-3	11
3	3-Buten-2-one, 4-(4-hydroxy-2,2,...	224	C13H20O3	038274-01-0	11
4	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	11
5	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	11



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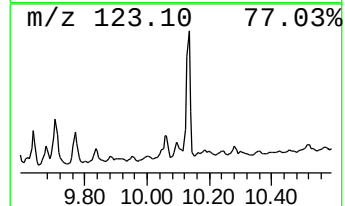
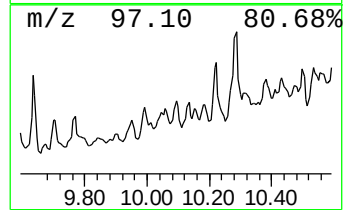
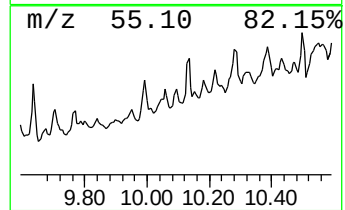
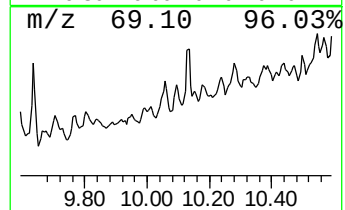
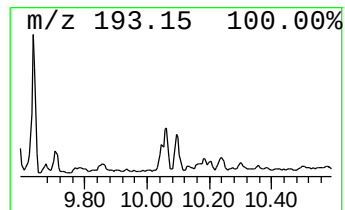
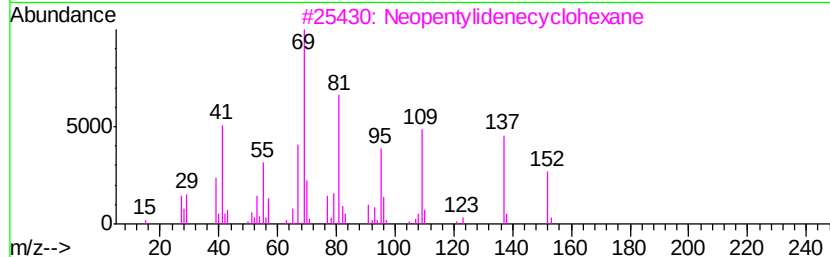
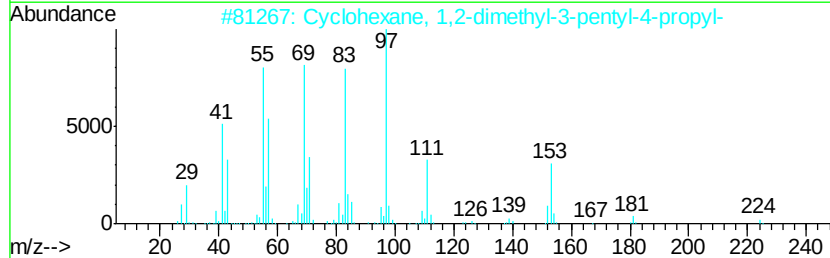
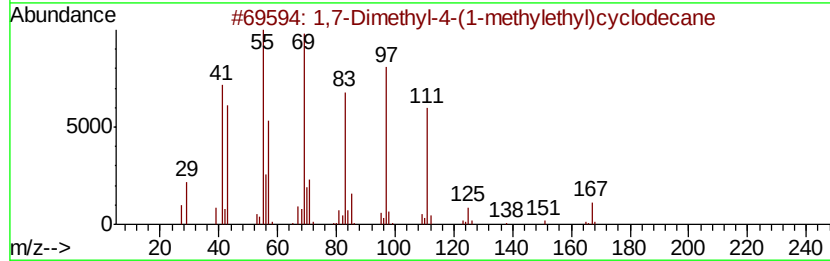
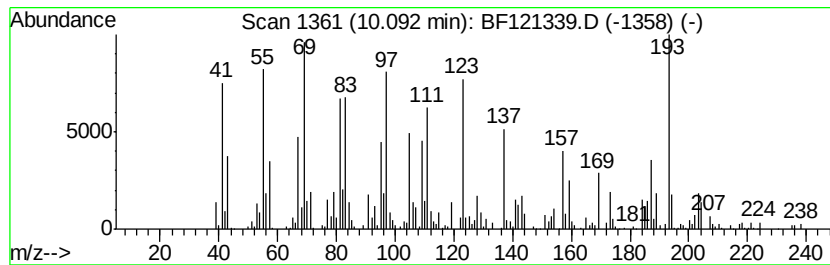
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.09 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.09	4.75 ng	402758	Acenaphthene-d10	9.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cyclohexane	210	C15H30	000645-10-3	27
2	Cyclohexane, 1,2-dimethyl-3-pentyl-4-propyl-	224	C16H32	062376-17-4	25
3	Neopentylidenecyclohexane	152	C11H20	039546-80-0	25
4	2-(3-Chloro-propyl)-1,1-dimethylcyclohexane	200	C12H21Cl	1000191-45-6	18
5	Cyclohexane, 1,2,4,5-tetraethyl-	196	C14H28	061142-24-3	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
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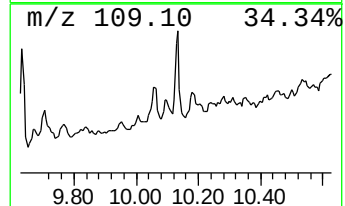
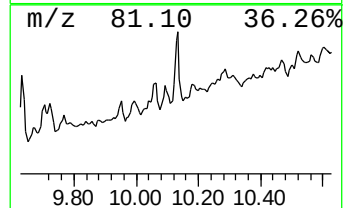
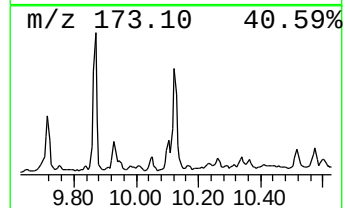
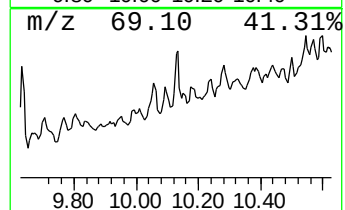
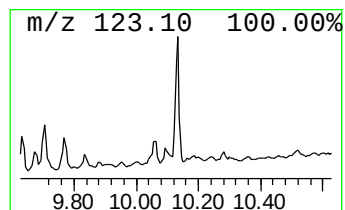
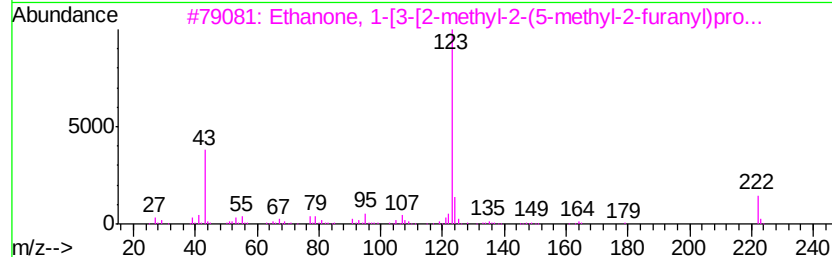
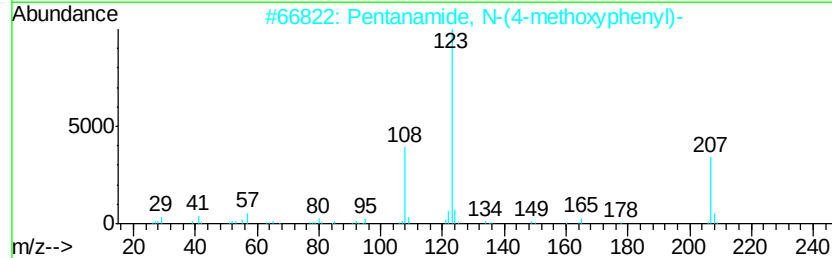
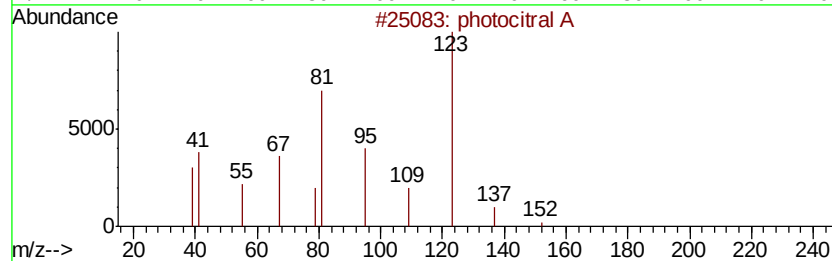
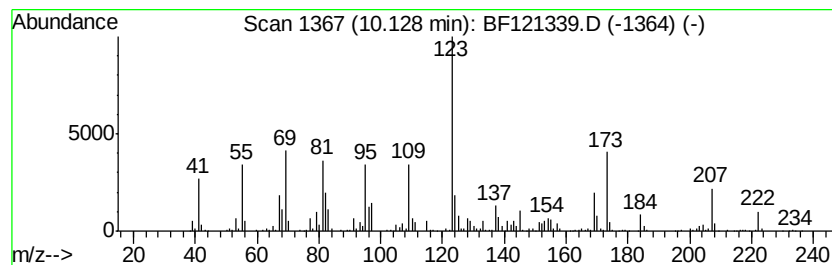
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 photocitral A Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.13	7.86 ng	665563	Acenaphthene-d10	9.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	photocitral A	152	C10H16O	055253-28-6	50
2	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	49
3	Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	43
4	4-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-68-3	43
5	4-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-67-9	43



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Data File : BF121339.D
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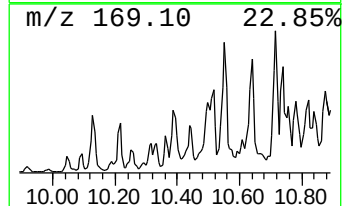
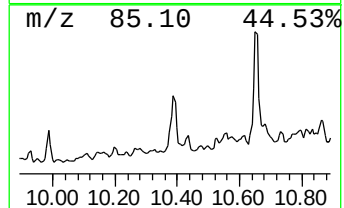
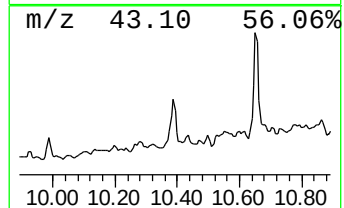
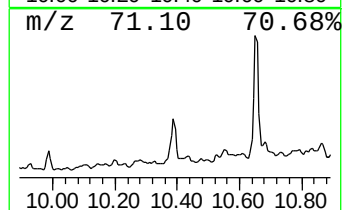
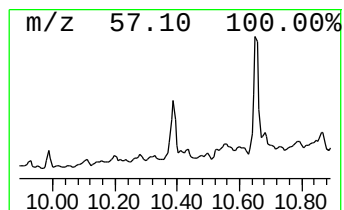
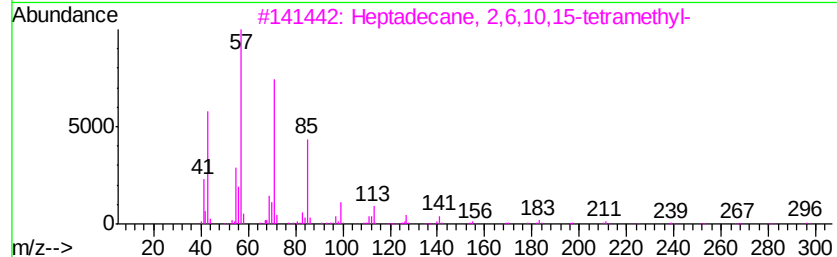
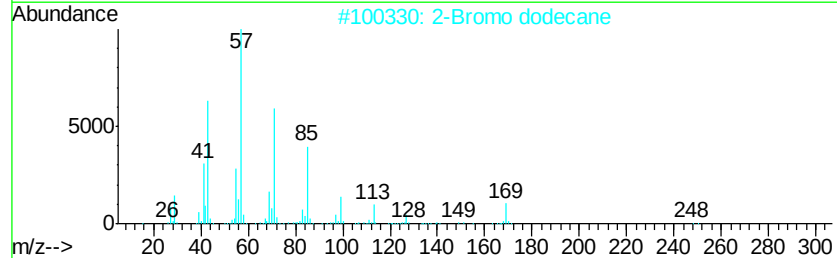
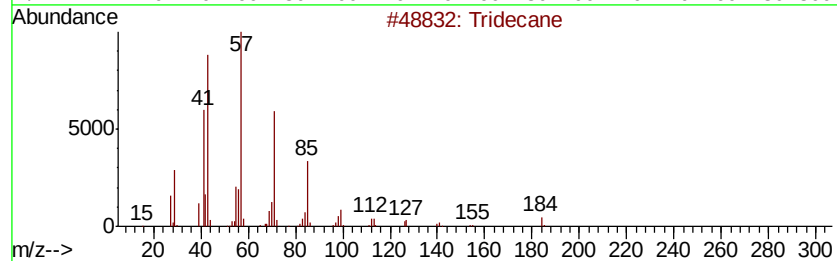
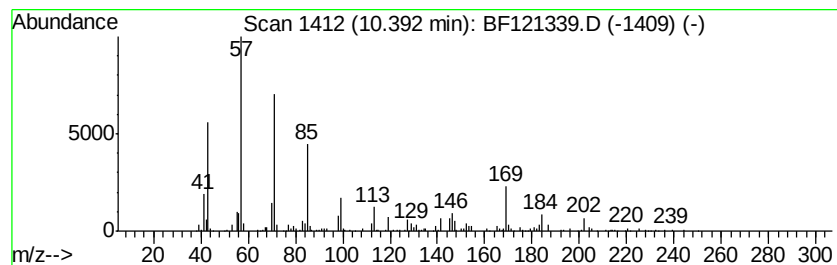
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.39	5.97 ng	506116	Acenaphthene-d10		9.72
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	72
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	60
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58
4	Hexadecane	226	C16H34	000544-76-3	58
5	Tetradecane	198	C14H30	000629-59-4	53



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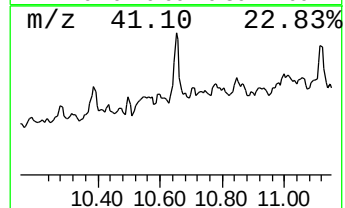
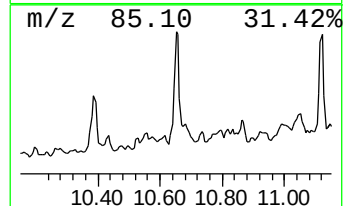
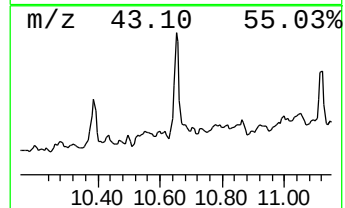
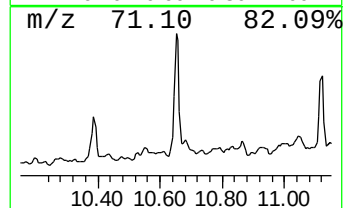
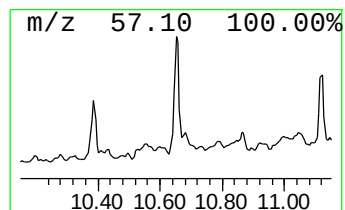
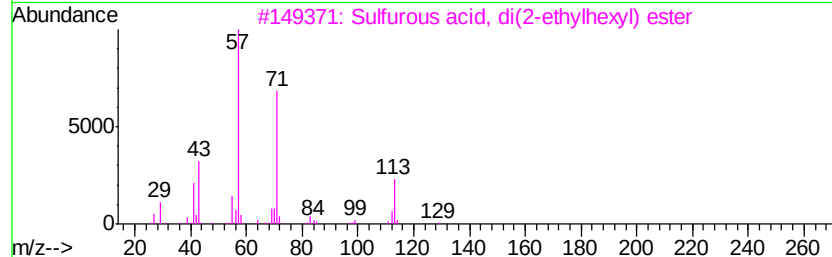
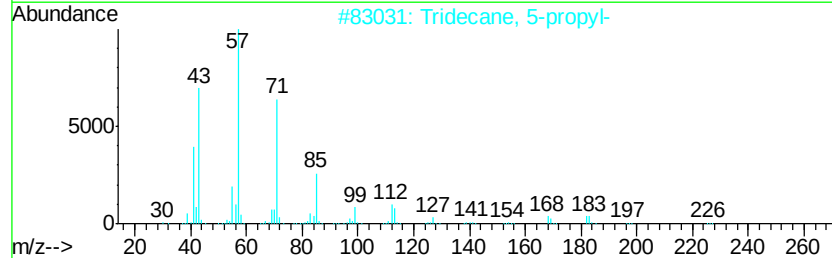
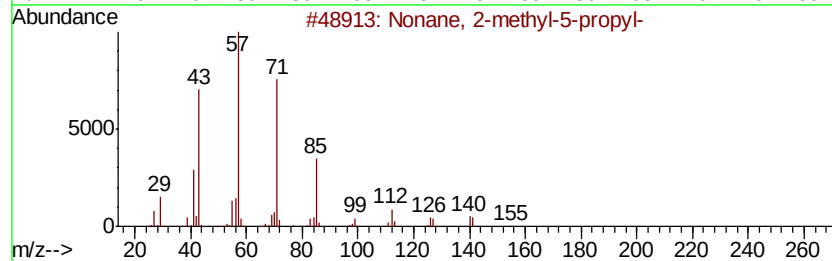
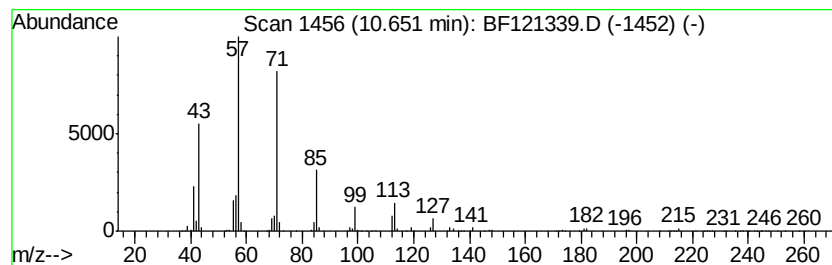
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonane, 2-methyl-5-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.65	38.43 ng	1376740	Phenanthrene-d10	11.21		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	78	
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	74	
3	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	64	
4	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64	
5	Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	59	



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Misc :
ALS Vial : 6 Sample Multiplier: 1

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ClientSampleId :
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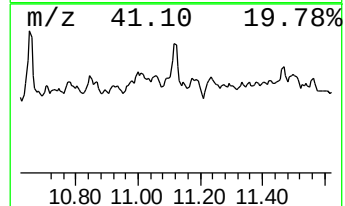
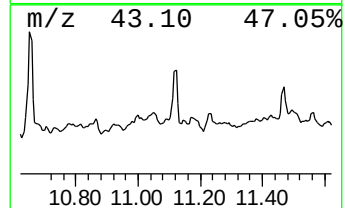
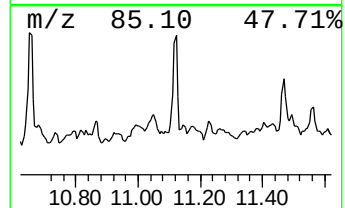
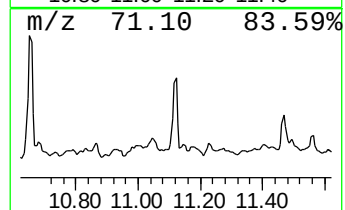
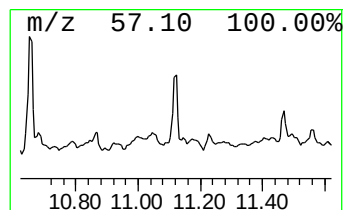
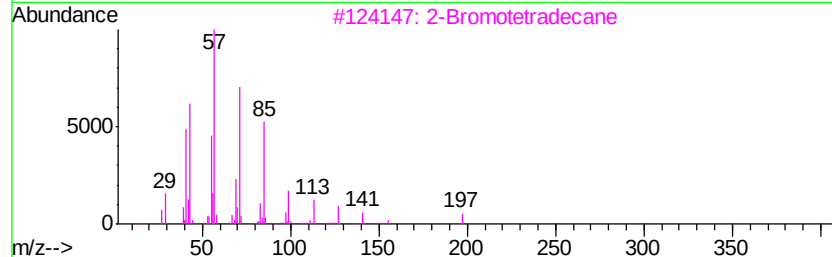
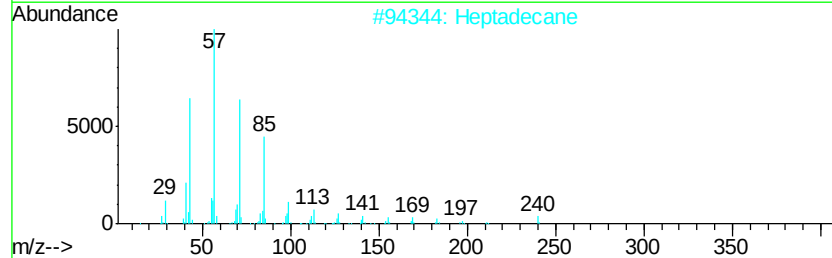
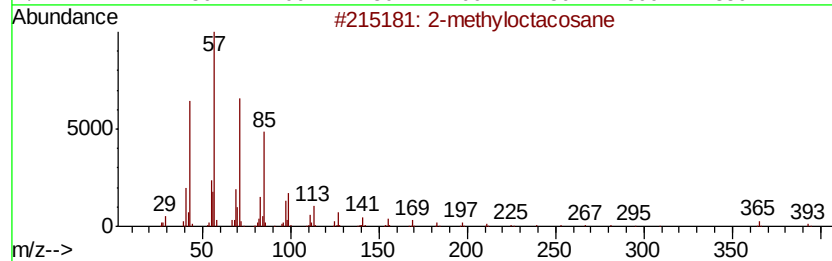
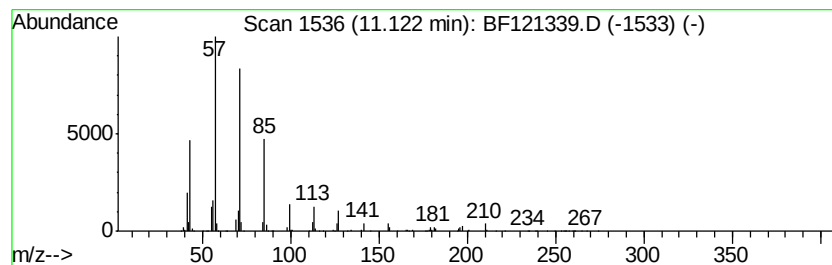
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	22.43 ng	803486	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Heptadecane	240	C17H36	000629-78-7	90
3		2-Bromotetradecane	276	C14H29Br	074036-95-6	90
4		Hexacosane	366	C26H54	000630-01-3	86
5		Tetratetracontane	619	C44H90	007098-22-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082020\
 Data File : BF121339.D
 Acq On : 20 Aug 2020 11:08
 Operator : JU/CG
 Sample : L3712-05 5X
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VB-25203

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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
unknown9.12	9.12	2.6	ng	222057	3	9.72	1694370	20.0
unknown9.43	9.43	5.6	ng	475704	3	9.72	1694370	20.0
unknown9.48	9.48	2.1	ng	179463	3	9.72	1694370	20.0
Decahydro-4,4,8,9...	9.59	4.0	ng	335524	3	9.72	1694370	20.0
unknown9.63	9.63	7.2	ng	607036	3	9.72	1694370	20.0
unknown9.99	9.99	7.5	ng	639516	3	9.72	1694370	20.0
unknown10.06	10.06	5.0	ng	419028	3	9.72	1694370	20.0
unknown10.09	10.09	4.8	ng	402758	3	9.72	1694370	20.0
photocitral A	10.13	7.9	ng	665563	3	9.72	1694370	20.0
Tridecane	10.39	6.0	ng	506116	3	9.72	1694370	20.0
Nonane, 2-methyl-...	10.65	38.4	ng	1376740	4	11.21	716482	20.0
2-methyloctacosane	11.12	22.4	ng	803486	4	11.21	716482	20.0