

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
 Data File : BF087871.D
 Acq On : 10 Jun 2016 13:34
 Operator : UM/SJ
 Sample : H3426-13
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-5

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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	1.655	3	6	8	rVB	3838293	6033243	100.00%	14.572%
2	1.747	12	14	23	rVB	340178	762043	12.63%	1.841%
3	1.872	23	25	39	rVB	2229220	4028301	66.77%	9.729%
4	4.993	295	298	302	rBV	123692	185876	3.08%	0.449%
5	5.404	331	334	337	rVB	2037884	2210893	36.65%	5.340%
6	6.444	422	425	428	rBV	1829770	2234368	37.03%	5.397%
7	6.582	434	437	439	rBV	2392053	2604876	43.18%	6.291%
8	6.810	455	457	459	rBV	896723	724078	12.00%	1.749%
9	6.970	468	471	473	rBV	2077148	2037342	33.77%	4.921%
10	7.382	503	507	509	rBV	1458091	1796005	29.77%	4.338%
11	7.462	512	514	516	rBV	131539	103972	1.72%	0.251%
12	8.102	567	570	572	rBV	913795	1003323	16.63%	2.423%
13	9.176	661	664	666	rBV	3007704	2769123	45.90%	6.688%
14	9.565	696	698	700	rBV	219503	175013	2.90%	0.423%
15	9.850	720	723	724	rBV	928801	990520	16.42%	2.392%
16	10.628	789	791	794	rBV2	1368142	1601916	26.55%	3.869%
17	10.753	800	802	806	rVB2	58386	68110	1.13%	0.165%
18	11.199	837	841	842	rBV2	44279	65999	1.09%	0.159%
19	11.325	850	852	853	rBV	1228141	1108310	18.37%	2.677%
20	11.393	856	858	860	rVB	171913	159150	2.64%	0.384%
21	11.553	869	872	873	rBV2	68223	76317	1.26%	0.184%
22	11.816	893	895	897	rBV	49479	79880	1.32%	0.193%
23	11.851	897	898	900	rVV	122566	104497	1.73%	0.252%
24	11.931	903	905	910	rVB	146304	200934	3.33%	0.485%
25	12.114	919	921	925	rVB3	53459	103140	1.71%	0.249%
26	12.422	945	948	949	rVV2	114388	137639	2.28%	0.332%
27	12.525	955	957	960	rVB	714110	762896	12.64%	1.843%
28	12.674	967	970	973	rBV3	25803	63449	1.05%	0.153%
29	12.754	973	977	980	rVV	749247	861061	14.27%	2.080%
30	12.902	988	990	993	rVB	1719975	2152700	35.68%	5.199%
31	12.982	993	997	998	rBV2	47321	84590	1.40%	0.204%
32	13.085	1000	1006	1008	rBV	117900	177113	2.94%	0.428%
33	13.154	1008	1012	1013	rBV	72534	111840	1.85%	0.270%
34	13.188	1013	1015	1016	rBV	92219	96496	1.60%	0.233%

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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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35	13.588	1047	1050	1054	rBV	46273	66785	1.11%	0.161%
36	13.691	1057	1059	1061	rBV2	79525	123690	2.05%	0.299%
37	13.805	1066	1069	1073	rVB3	171300	248621	4.12%	0.600%
38	13.942	1078	1081	1087	rVB2	764986	1556271	25.79%	3.759%
39	14.057	1087	1091	1092	rBV2	48240	86357	1.43%	0.209%
40	14.297	1108	1112	1113	rBV4	33951	64196	1.06%	0.155%
41	14.331	1113	1115	1117	rVB	69338	77540	1.29%	0.187%
42	14.708	1146	1148	1150	rBV	266948	306714	5.08%	0.741%
43	14.960	1167	1170	1174	rBV	316882	648733	10.75%	1.567%
44	15.051	1176	1178	1181	rVB2	66983	104744	1.74%	0.253%
45	15.234	1192	1194	1197	rVB	167271	245727	4.07%	0.593%
46	15.291	1197	1199	1202	rVV	223029	331049	5.49%	0.800%
47	15.360	1202	1205	1211	rVV2	626979	897899	14.88%	2.169%
48	15.851	1246	1248	1254	rVB4	33339	107363	1.78%	0.259%
49	16.022	1261	1263	1269	rVB	42118	101202	1.68%	0.244%
50	16.708	1320	1323	1328	rVB2	134075	246044	4.08%	0.594%
51	17.120	1355	1359	1364	rVB	101689	211609	3.51%	0.511%
52	17.325	1375	1377	1384	rVB2	26284	67976	1.13%	0.164%
53	19.177	1534	1539	1547	rVB4	63510	236048	3.91%	0.570%

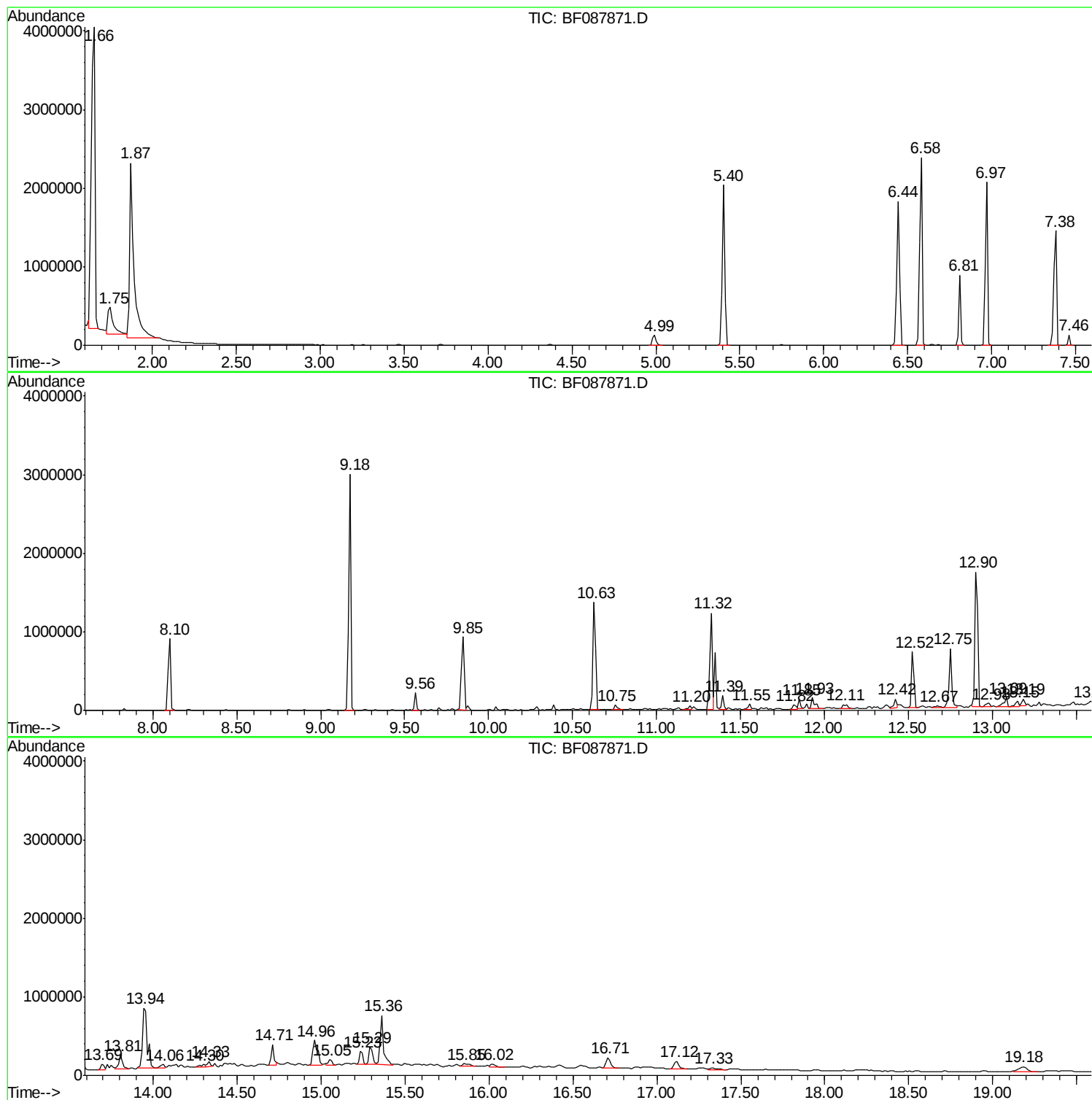
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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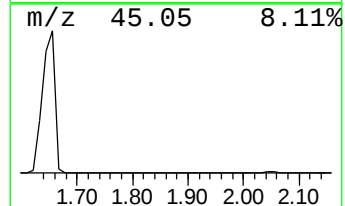
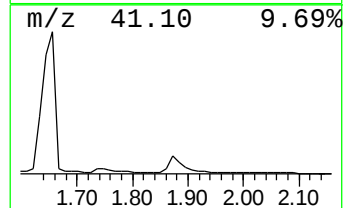
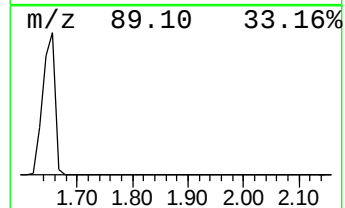
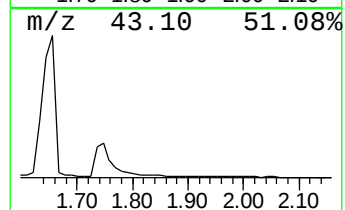
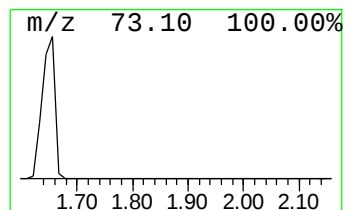
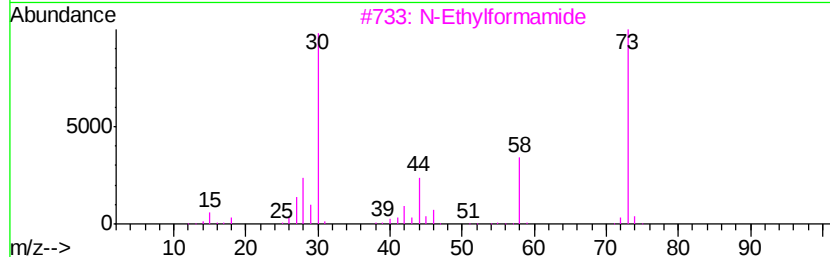
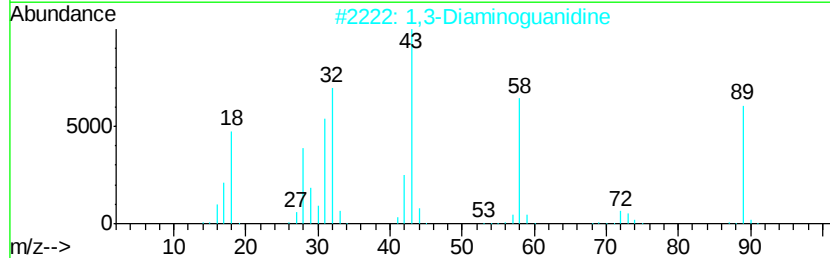
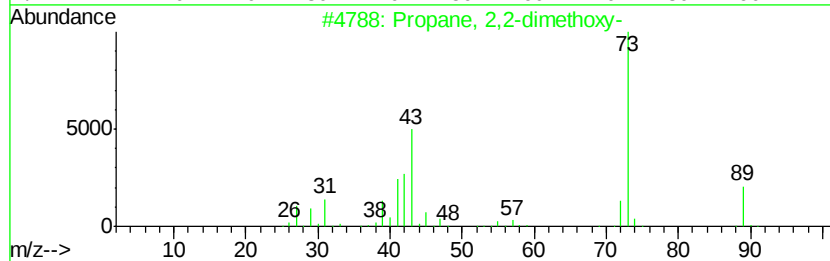
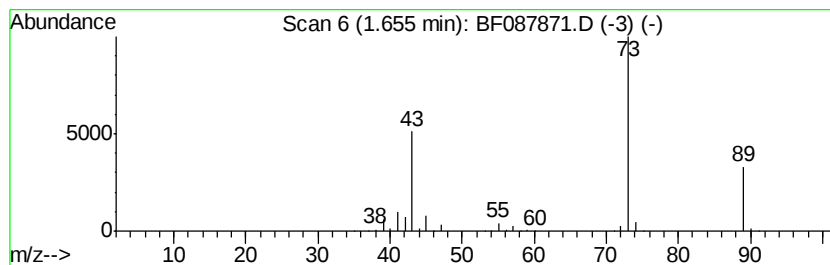
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	166.65 ng	6033240	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2		1,3-Diaminoquinidine	89	CH7N5	004364-78-7	9
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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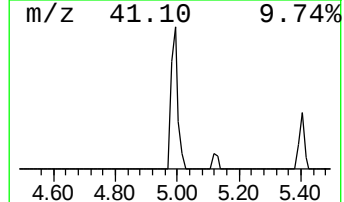
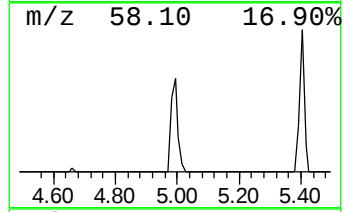
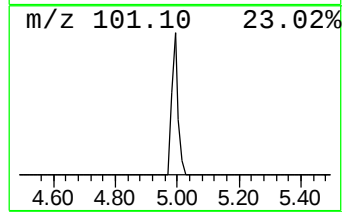
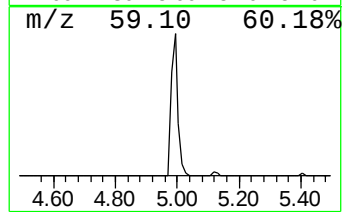
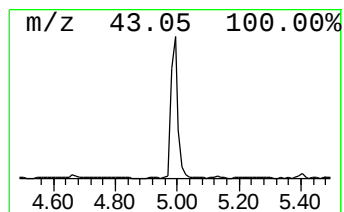
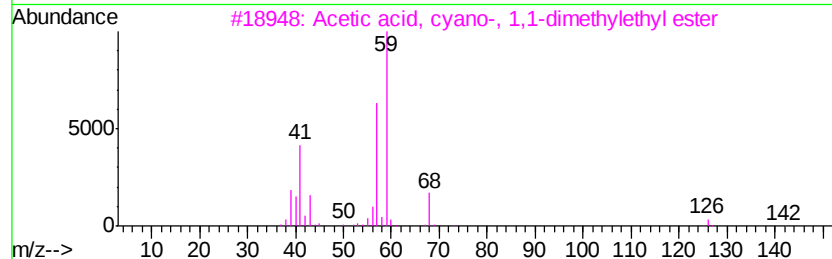
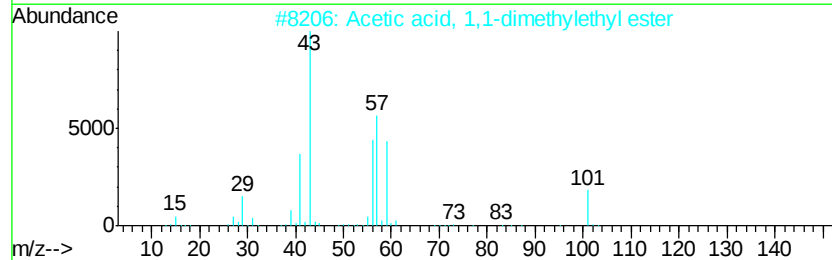
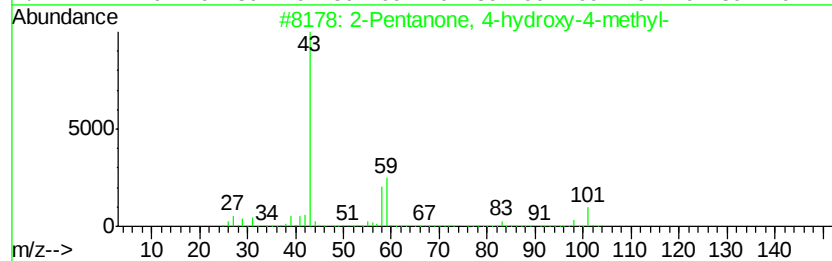
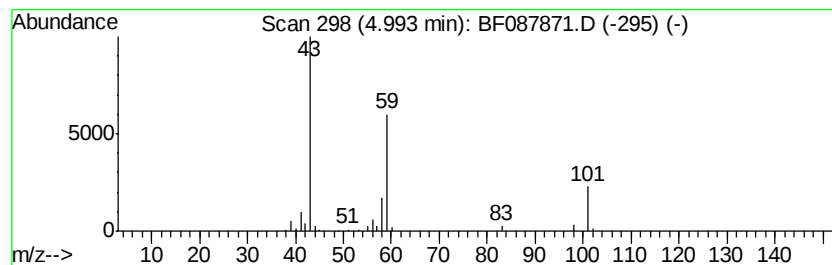
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	5.13 ng	185876	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Acetic acid, cvano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	25	
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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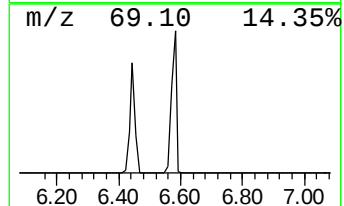
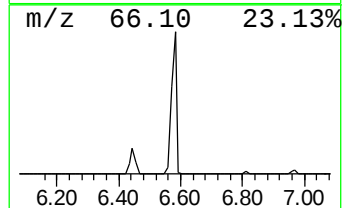
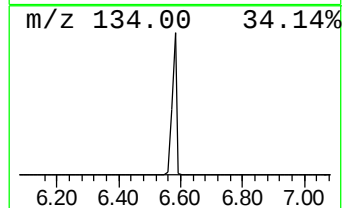
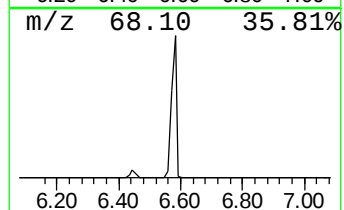
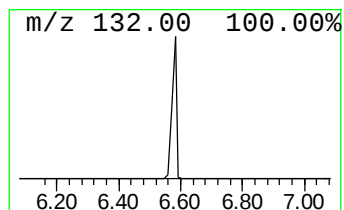
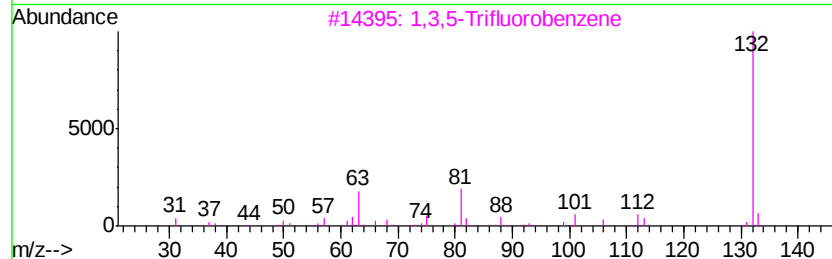
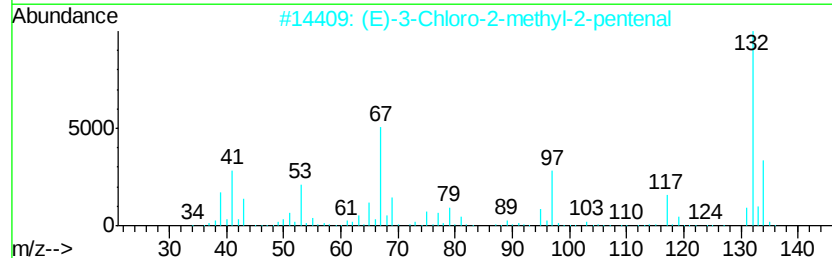
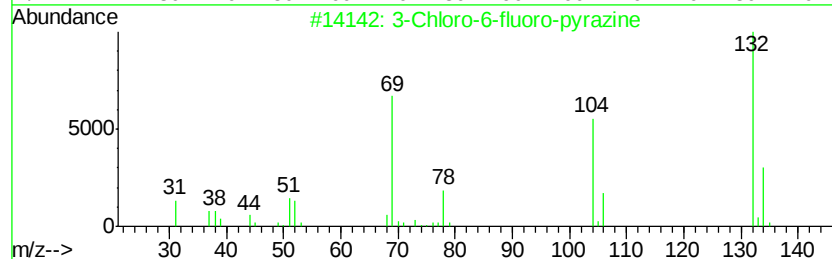
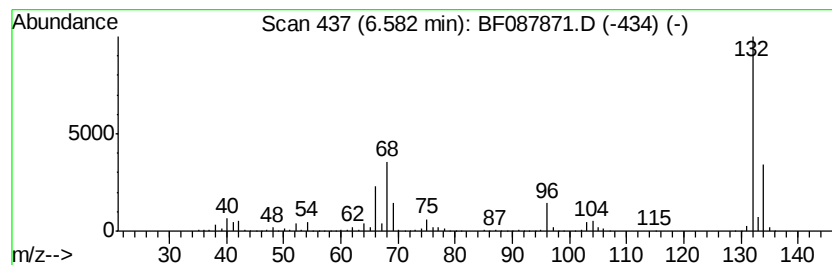
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	71.95 ng	2604880	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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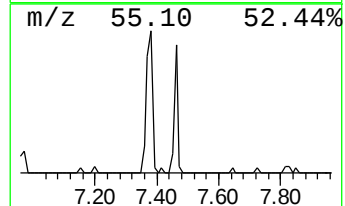
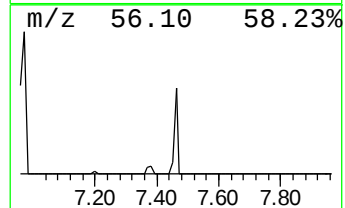
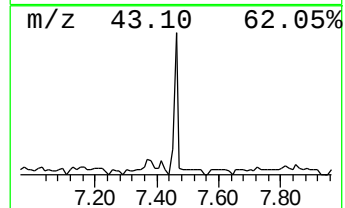
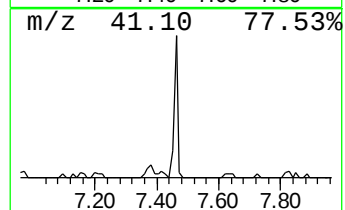
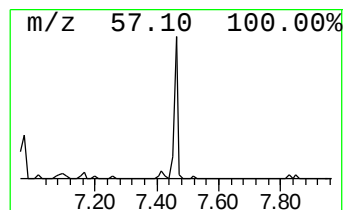
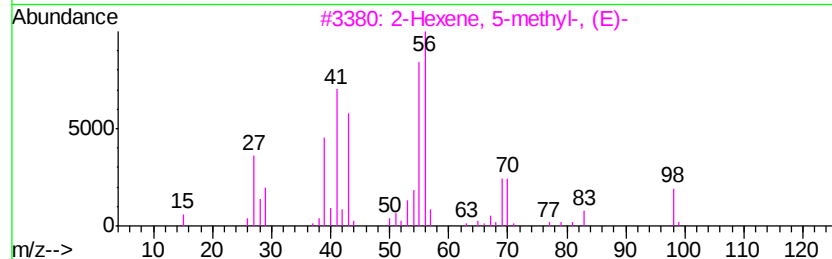
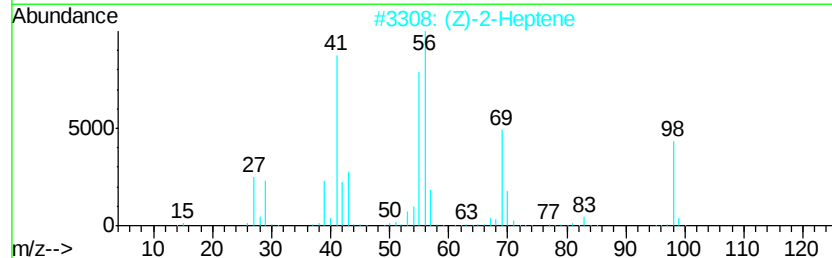
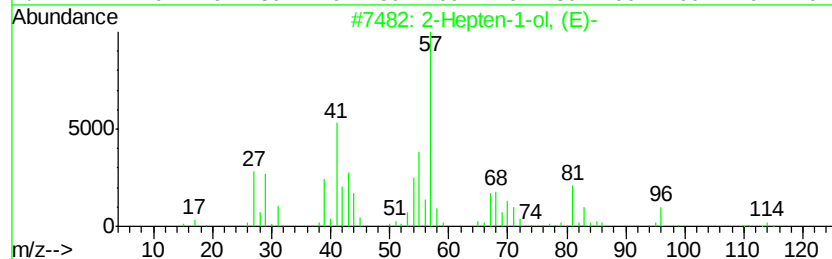
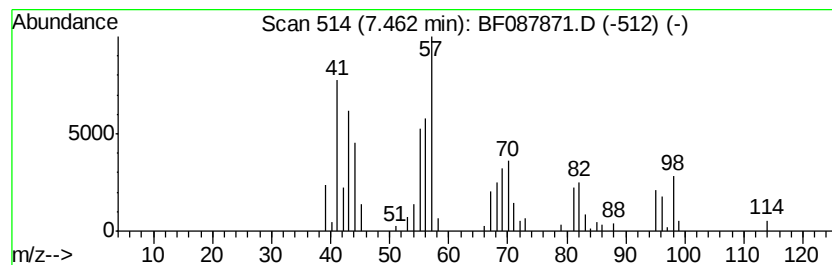
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 unknown7.46 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	2.07 ng	103972	Naphthalene-d8	8.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-1-ol, (E)-			114	C7H14O	033467-76-4	27
2	(Z)-2-Heptene			98	C7H14	006443-92-1	25
3	2-Hexene, 5-methyl-, (E)-			98	C7H14	007385-82-2	22
4	Heptane, 2-chloro-			134	C7H15Cl	001001-89-4	22
5	2-Heptene			98	C7H14	000592-77-8	22



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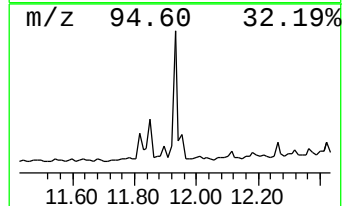
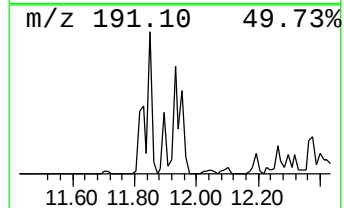
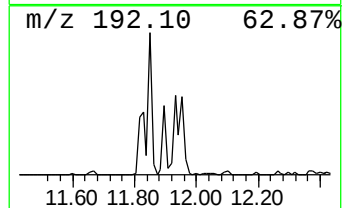
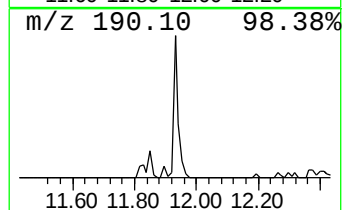
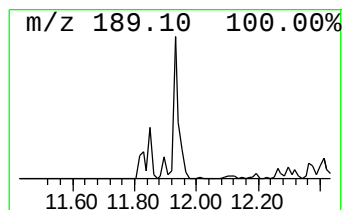
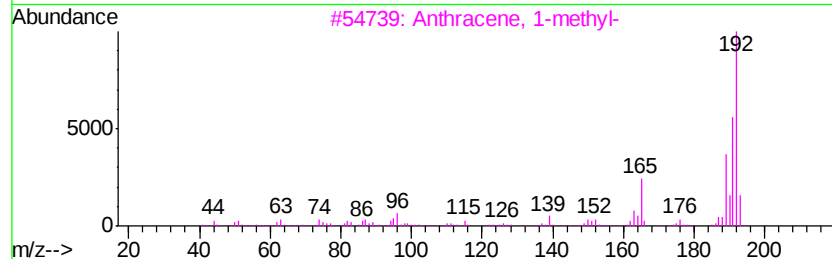
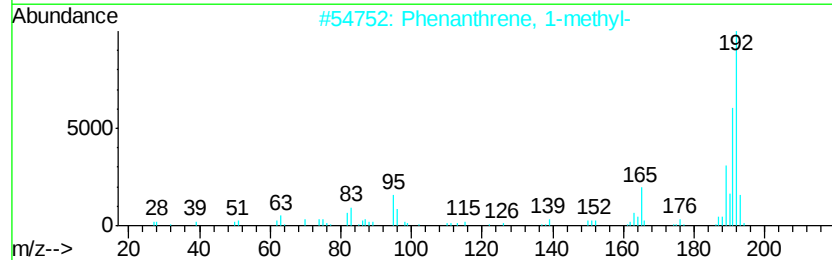
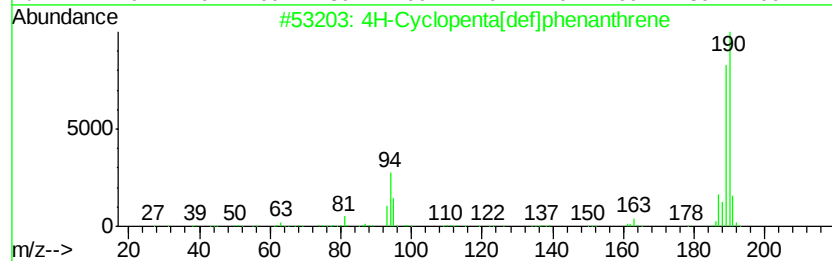
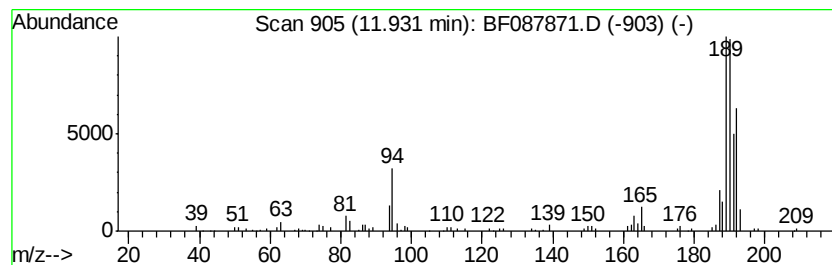
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	3.63 ng	200934	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35
3		Anthracene, 1-methyl-	192	C15H12	000610-48-0	25
4		Benzene, 1,1'-(2-cyclopropen-1-yl)-	192	C15H12	022825-21-4	22
5		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
Data File : BF087871.D
Acq On : 10 Jun 2016 13:34
Operator : UM/SJ
Sample : H3426-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

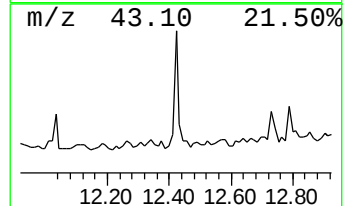
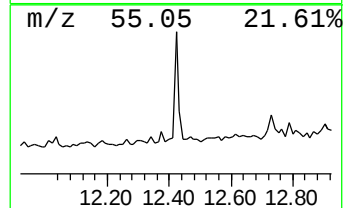
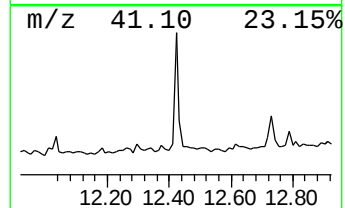
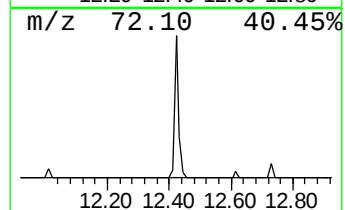
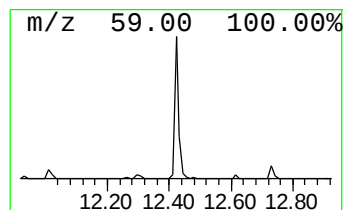
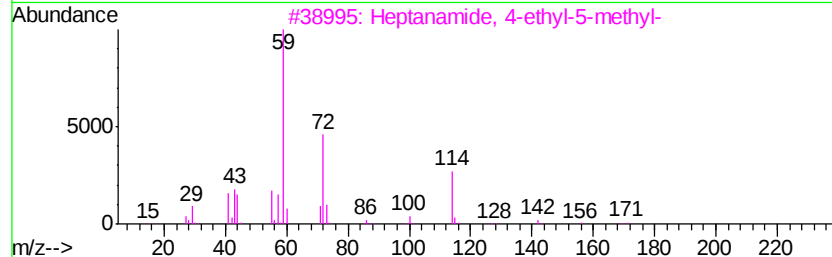
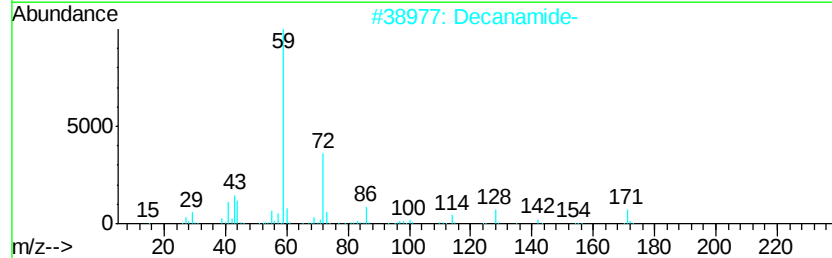
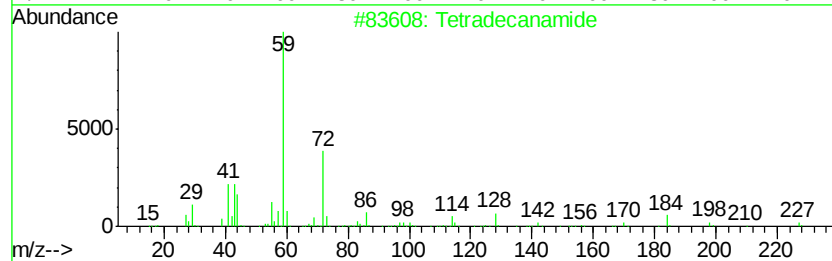
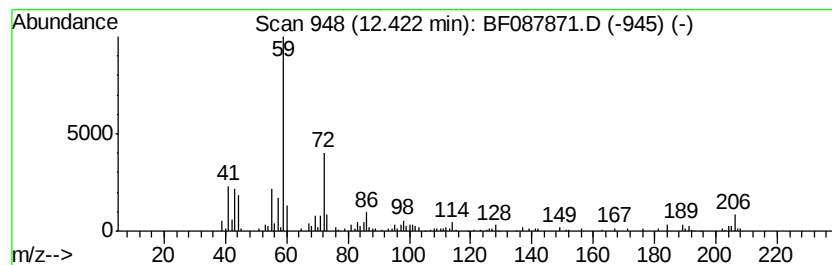
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetradecanamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.42	2.48 ng	137639	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	78
2	Decanamide-	171	C10H21NO	002319-29-1	78
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	72
5	Pentanamide	101	C5H11NO	000626-97-1	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
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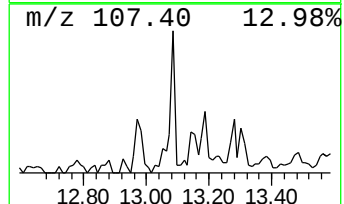
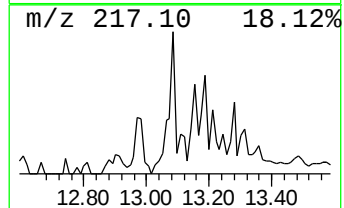
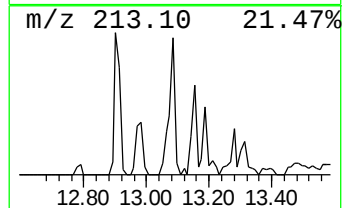
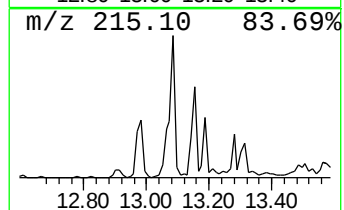
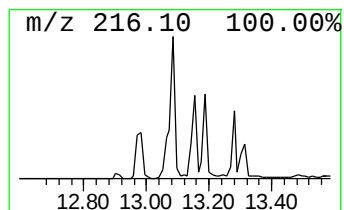
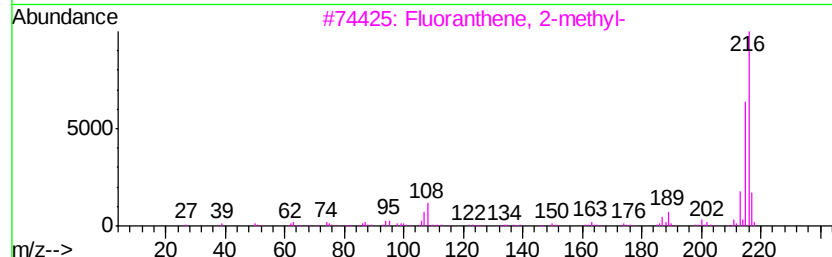
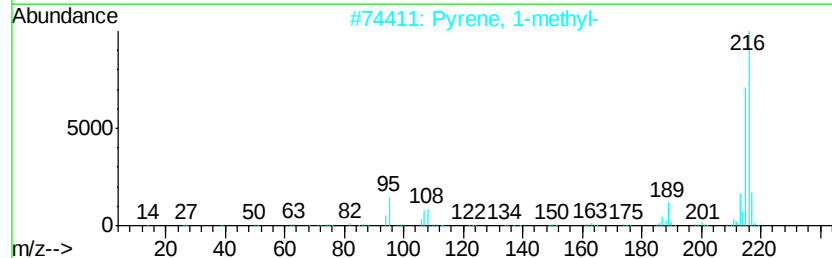
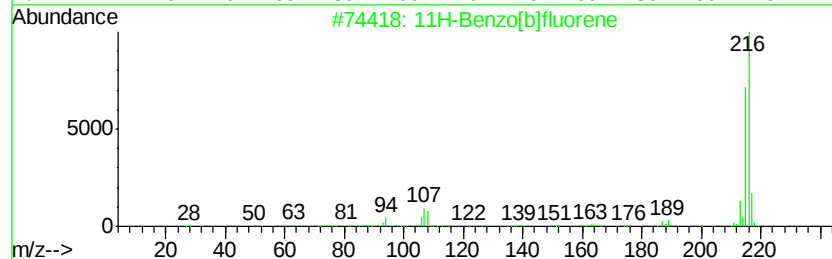
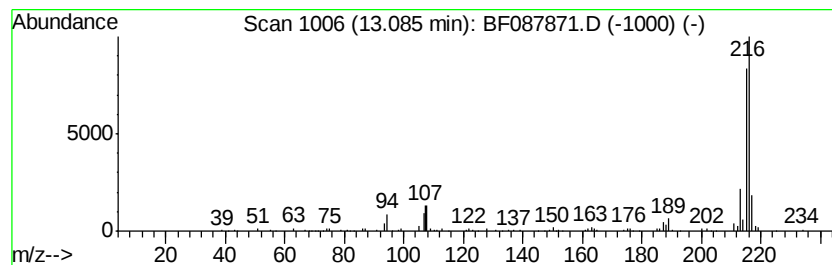
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 11H-Benzo[b]fluorene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	2.28 ng	177113	Chrysene-d12	13.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
4			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
5			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87



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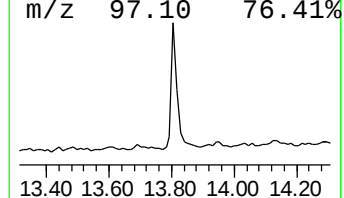
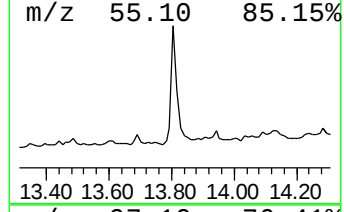
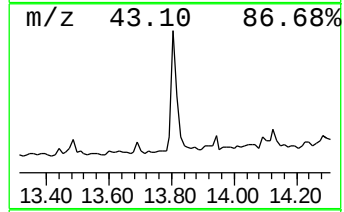
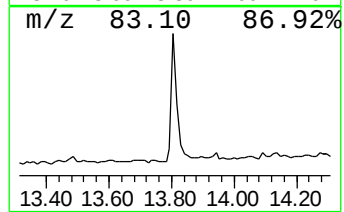
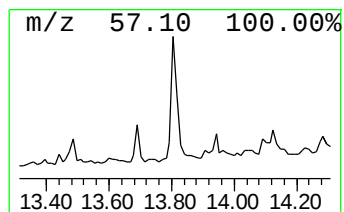
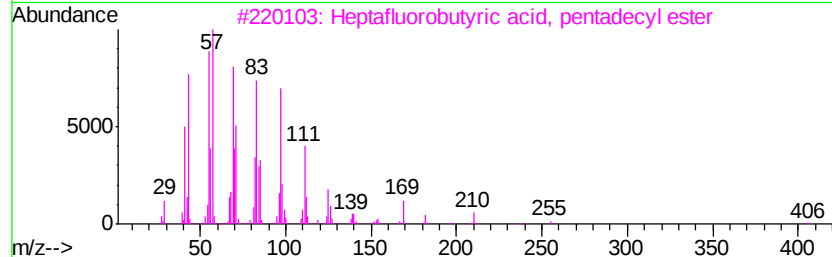
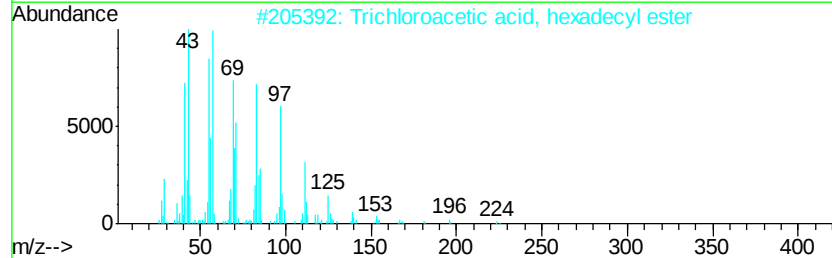
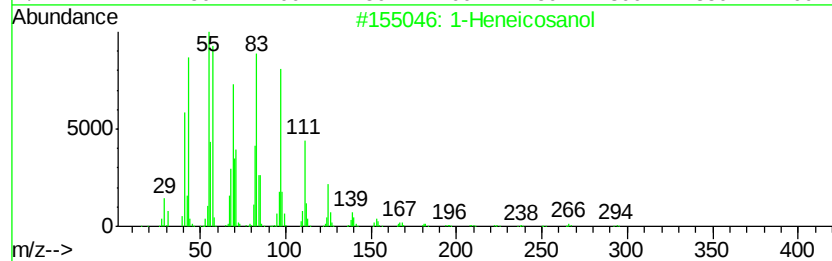
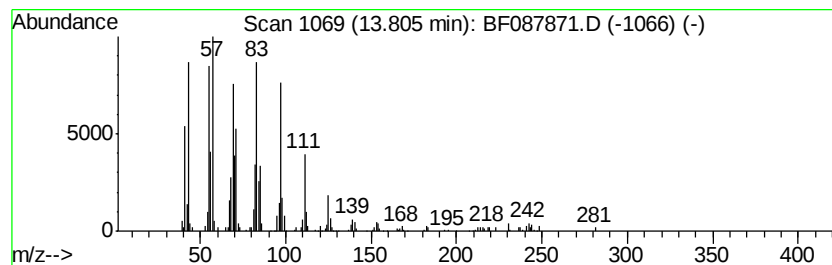
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heneicosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	3.20 ng	248621	Chrysene-d12	13.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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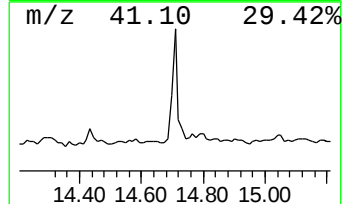
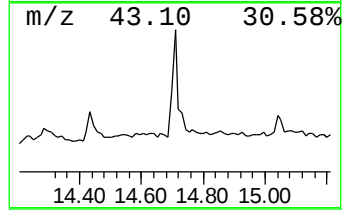
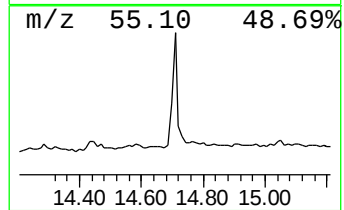
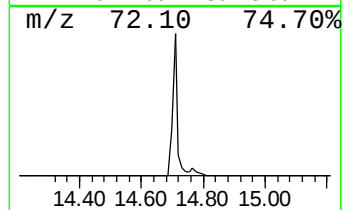
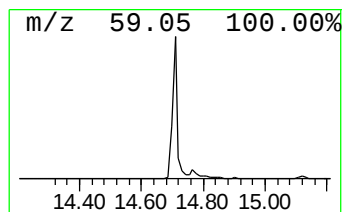
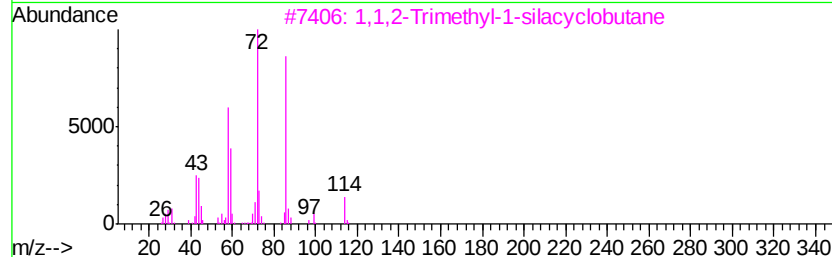
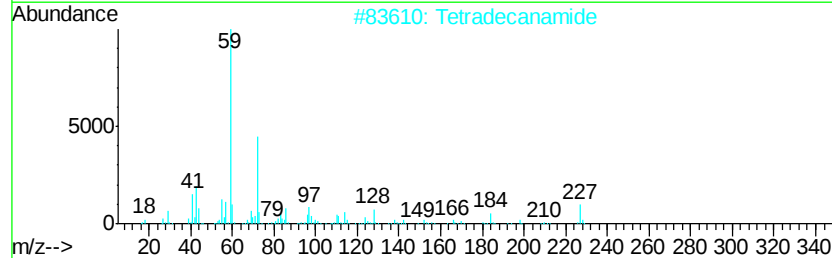
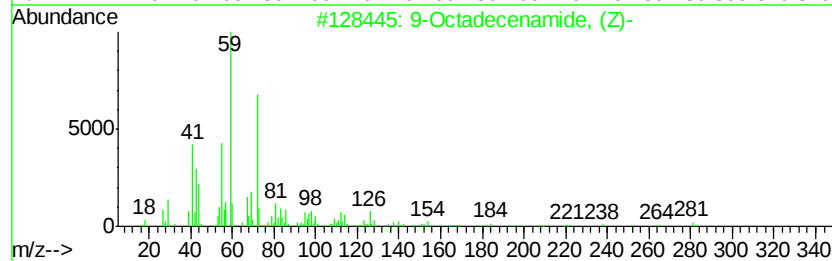
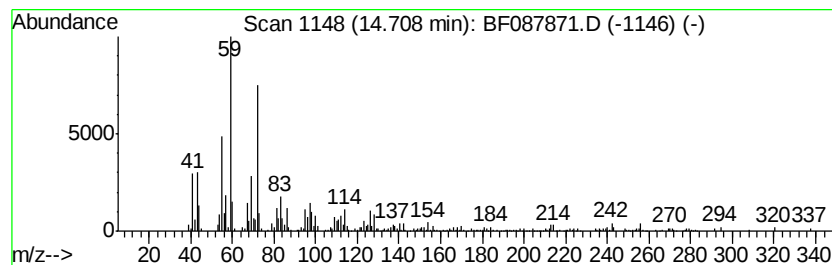
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	6.83 ng	306714	Perylene-d12	15.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2			Tetradecanamide	227	C14H29NO	000638-58-4	53
3			1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	43
4			Cyclopentylsilane	100	C5H12Si	080249-74-7	30
5			Urea, N-tert-butyl-N',N'-dipropyl-	200	C11H24N2O	1000360-40-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
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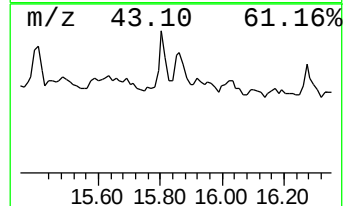
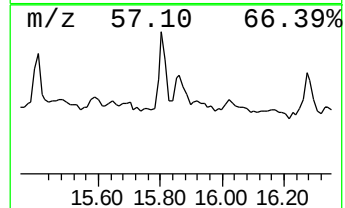
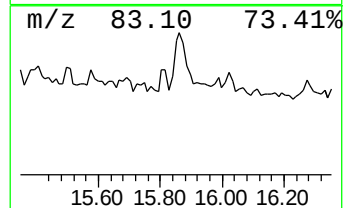
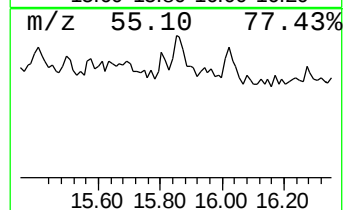
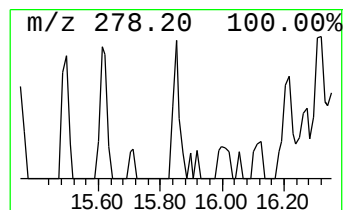
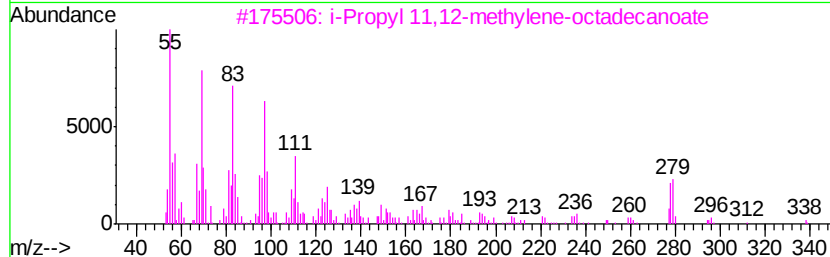
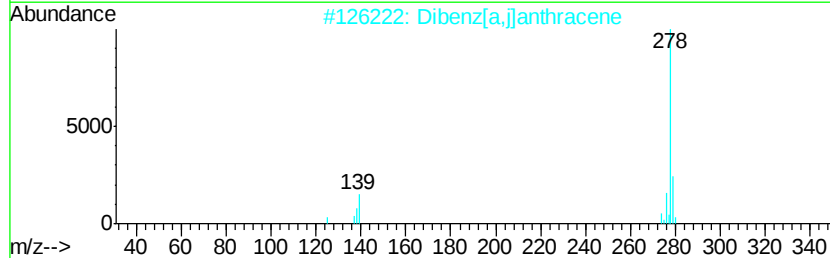
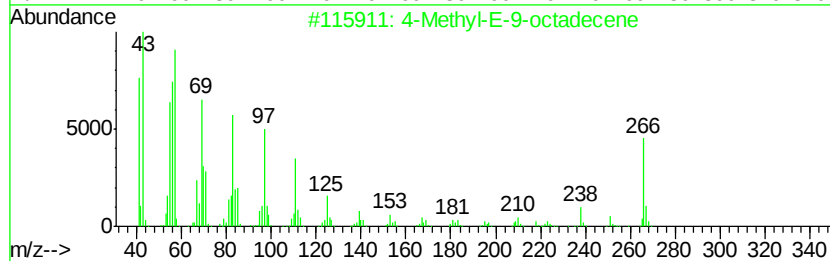
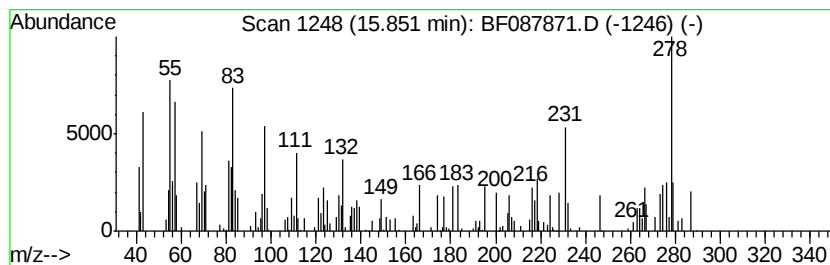
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown15.85 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	2.39 ng	107363	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	35	
2	Dibenz[a,i]anthracene	278	C22H14	000224-41-9	27	
3	i-Propyl 11,12-methylene-octadec...	338	C22H42O2	1000336-77-0	25	
4	Z-5-Nonadecene	266	C19H38	1000131-11-8	20	
5	Benzo[b]triphenylene	278	C22H14	000215-58-7	18	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
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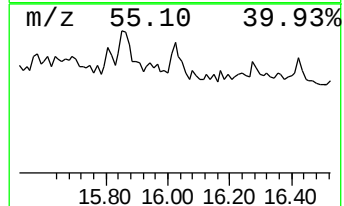
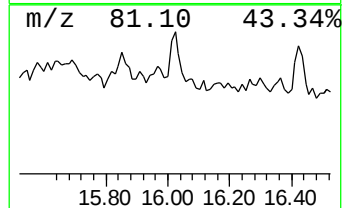
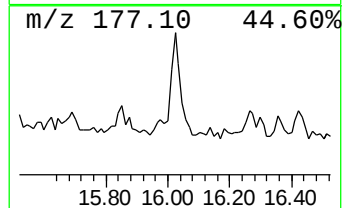
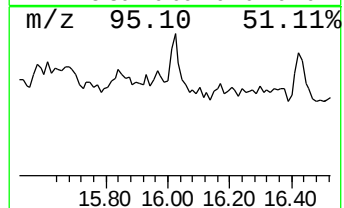
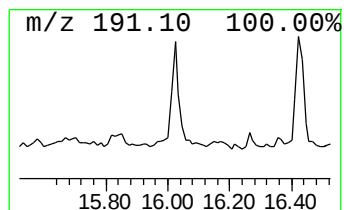
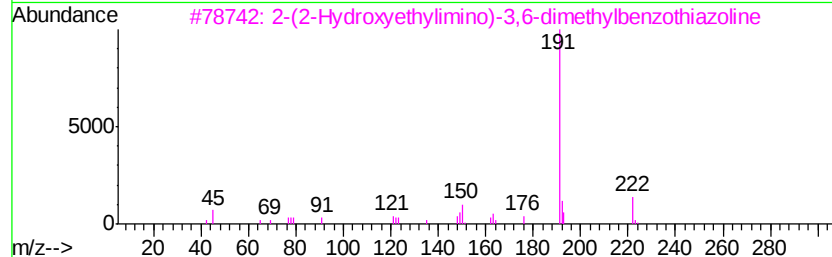
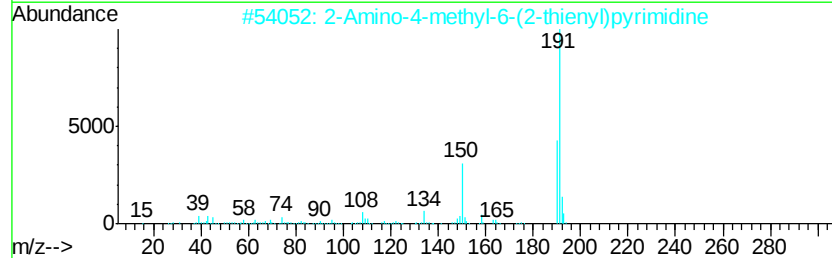
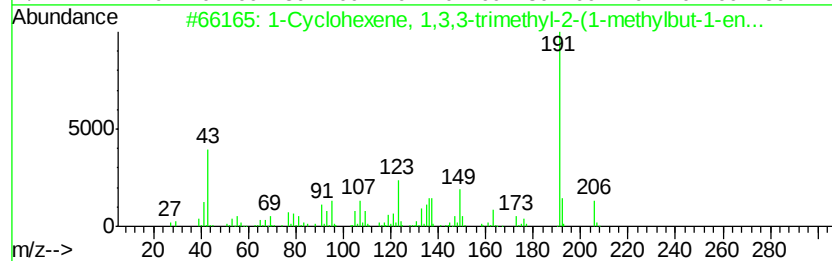
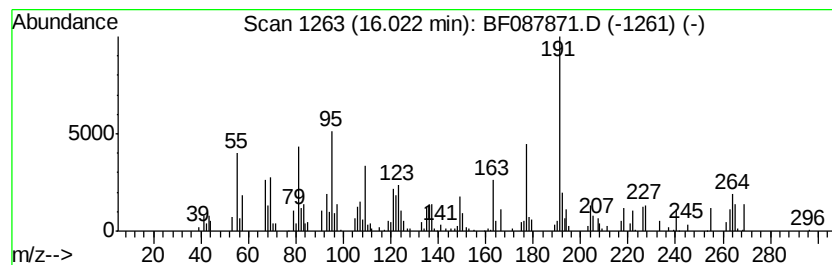
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown16.02 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.25 ng	101202	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Cyclohexene, 1,3,3-trimethyl-2...	206 C14H22O	1000197-08-4	38
2	2-Amino-4-methyl-6-(2-thienyl)py...	191 C9H9N3S	026963-43-9	30
3	2-(2-Hydroxyethylimino)-3,6-dime...	222 C11H14N2OS	068720-70-7	27
4	4H-Benzo[def]carbazole	191 C14H9N	000203-65-6	27
5	1H-Pyrazole-4-acetic acid, 1-(4-...	264 C11H16N6O2	1000337-51-2	27



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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP-5

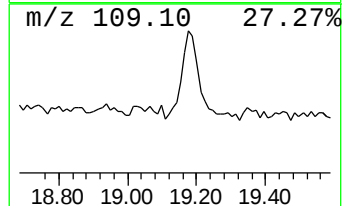
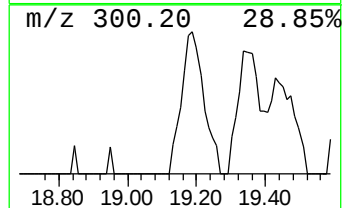
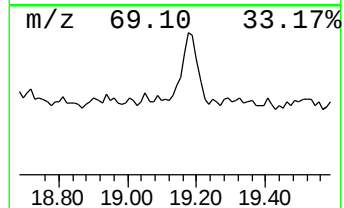
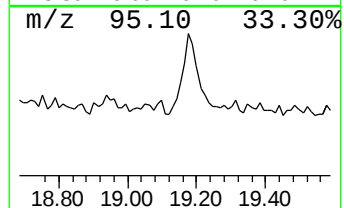
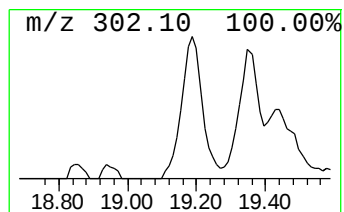
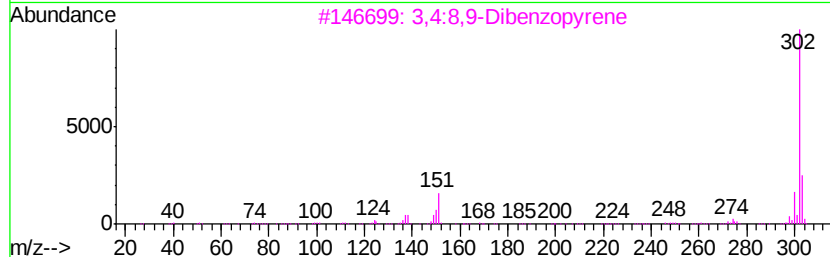
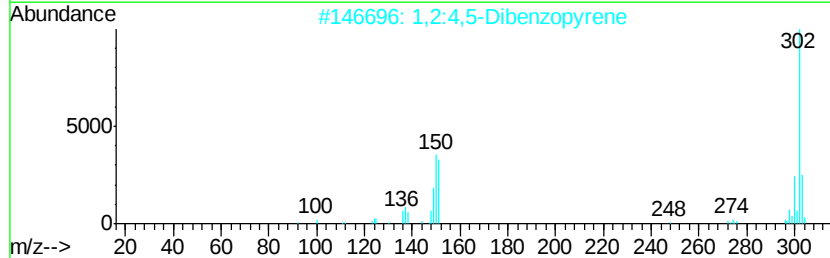
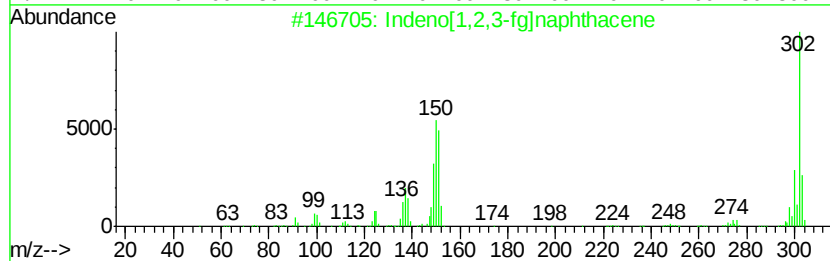
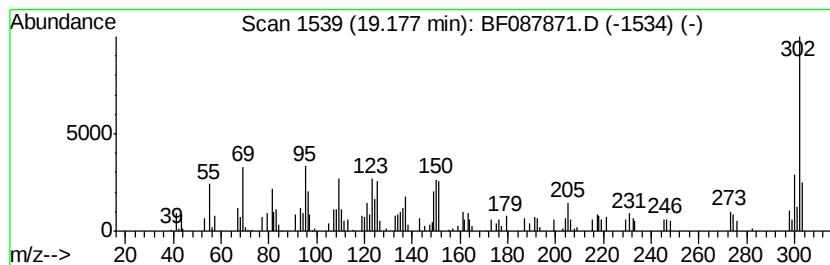
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Indeno[1,2,3-fg]naphthacene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.18	5.26 ng	236048	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	70
2		1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	58
3		3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	47
4		10,11-Dihydro-10-hydroxy-2,3,6-t...	302	C17H18O5	019172-35-1	43
5		2H-1-Benzopyran-2-one, 7-(3-meth...	302	C19H14N2O2	006025-18-9	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
 Data File : BF087871.D
 Acq On : 10 Jun 2016 13:34
 Operator : UM/SJ
 Sample : H3426-13
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
unknown1.66	1.66	166.7	ng	6033240	1	6.81	724078	20.0
2-Pentanone, 4-hy...	4.99	5.1	ng	185876	1	6.81	724078	20.0
unknown6.58	6.58	72.0	ng	2604880	1	6.81	724078	20.0
unknown7.46	7.46	2.1	ng	103972	2	8.10	1003320	20.0
4H-Cyclopenta[def...	11.93	3.6	ng	200934	4	11.32	1108310	20.0
Tetradecanamide	12.42	2.5	ng	137639	4	11.32	1108310	20.0
11H-Benzo[b]fluorene	13.09	2.3	ng	177113	5	13.95	1556270	20.0
1-Heneicosanol	13.81	3.2	ng	248621	5	13.95	1556270	20.0
9-Octadecenamide, ...	14.71	6.8	ng	306714	6	15.36	897899	20.0
unknown15.85	15.85	2.4	ng	107363	6	15.36	897899	20.0
unknown16.02	16.02	2.3	ng	101202	6	15.36	897899	20.0
Indeno[1,2,3-fg]n...	19.18	5.3	ng	236048	6	15.36	897899	20.0