

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
 Data File : BF090268.D
 Acq On : 27 Sep 2016 22:43
 Operator : UM/SJ
 Sample : H4949-07 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-4-1-LOC-4(0-5)

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-BF092016.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	1.644	4	5	49	rVB	1877195	5347411	54.94%	14.310%
2	4.536	256	258	265	rBV	137424	230772	2.37%	0.618%
3	5.027	299	301	315	rBV	824650	1168969	12.01%	3.128%
4	6.136	395	398	400	rBV	914522	1133837	11.65%	3.034%
5	6.239	405	407	410	rVV	1369191	1238237	12.72%	3.314%
6	6.479	425	428	430	rBV	519042	704858	7.24%	1.886%
7	6.627	439	441	444	rBV	1126207	996592	10.24%	2.667%
8	7.039	475	477	480	rBV	503435	671325	6.90%	1.796%
9	7.759	538	540	543	rBV	900095	951571	9.78%	2.546%
10	8.833	632	634	637	rBV	1072633	1400369	14.39%	3.747%
11	9.245	667	670	672	rBV	284482	394731	4.06%	1.056%
12	9.359	678	680	685	rVB	213769	191559	1.97%	0.513%
13	9.496	690	692	694	rBV	947831	937974	9.64%	2.510%
14	10.285	758	761	763	rBV2	529678	661572	6.80%	1.770%
15	10.433	770	774	777	rBV2	59161	103528	1.06%	0.277%
16	10.971	818	821	825	rBV2	723552	1285868	13.21%	3.441%
17	11.039	825	827	829	rVB	148313	135016	1.39%	0.361%
18	11.462	862	864	866	rBV	72314	110135	1.13%	0.295%
19	11.531	868	870	872	rVV2	161087	214269	2.20%	0.573%
20	11.576	872	874	879	rVB2	113990	222398	2.28%	0.595%
21	11.782	889	892	895	rBV2	83136	121986	1.25%	0.326%
22	12.171	923	926	928	rBV	724137	933526	9.59%	2.498%
23	12.308	936	938	942	rBV2	95946	144347	1.48%	0.386%
24	12.388	942	945	948	rBV	906813	914857	9.40%	2.448%
25	12.548	957	959	962	rBV	1100743	1002249	10.30%	2.682%
26	12.616	962	965	966	rVV2	120833	162710	1.67%	0.435%
27	12.719	970	974	976	rVB2	106621	198959	2.04%	0.532%
28	12.822	981	983	985	rBV	134004	148306	1.52%	0.397%
29	13.039	999	1002	1004	rBV	543040	698736	7.18%	1.870%
30	13.222	1016	1018	1020	rVB	116648	113588	1.17%	0.304%
31	13.325	1025	1027	1028	rBV	119291	126157	1.30%	0.338%
32	13.577	1046	1049	1050	rBV2	936235	1410318	14.49%	3.774%
33	13.622	1050	1053	1056	rVB	5535813	9733938	100.00%	26.048%
34	13.965	1081	1083	1085	rBV	72397	104953	1.08%	0.281%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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35	14.102	1092	1095	1099	rBV5	65447	142947	1.47%	0.383%
36	14.571	1133	1136	1140	rBV	486687	989200	10.16%	2.647%
37	14.800	1154	1156	1159	rVB	289837	342758	3.52%	0.917%
38	14.857	1159	1161	1163	rBV	316034	416317	4.28%	1.114%
39	14.902	1163	1165	1170	rVV2	523644	706264	7.26%	1.890%
40	15.314	1199	1201	1203	rBV2	78336	117497	1.21%	0.314%
41	15.794	1241	1243	1250	rVB4	86903	162925	1.67%	0.436%
42	16.045	1262	1265	1269	rVB2	180836	318433	3.27%	0.852%
43	16.377	1291	1294	1298	rVB	145464	256752	2.64%	0.687%

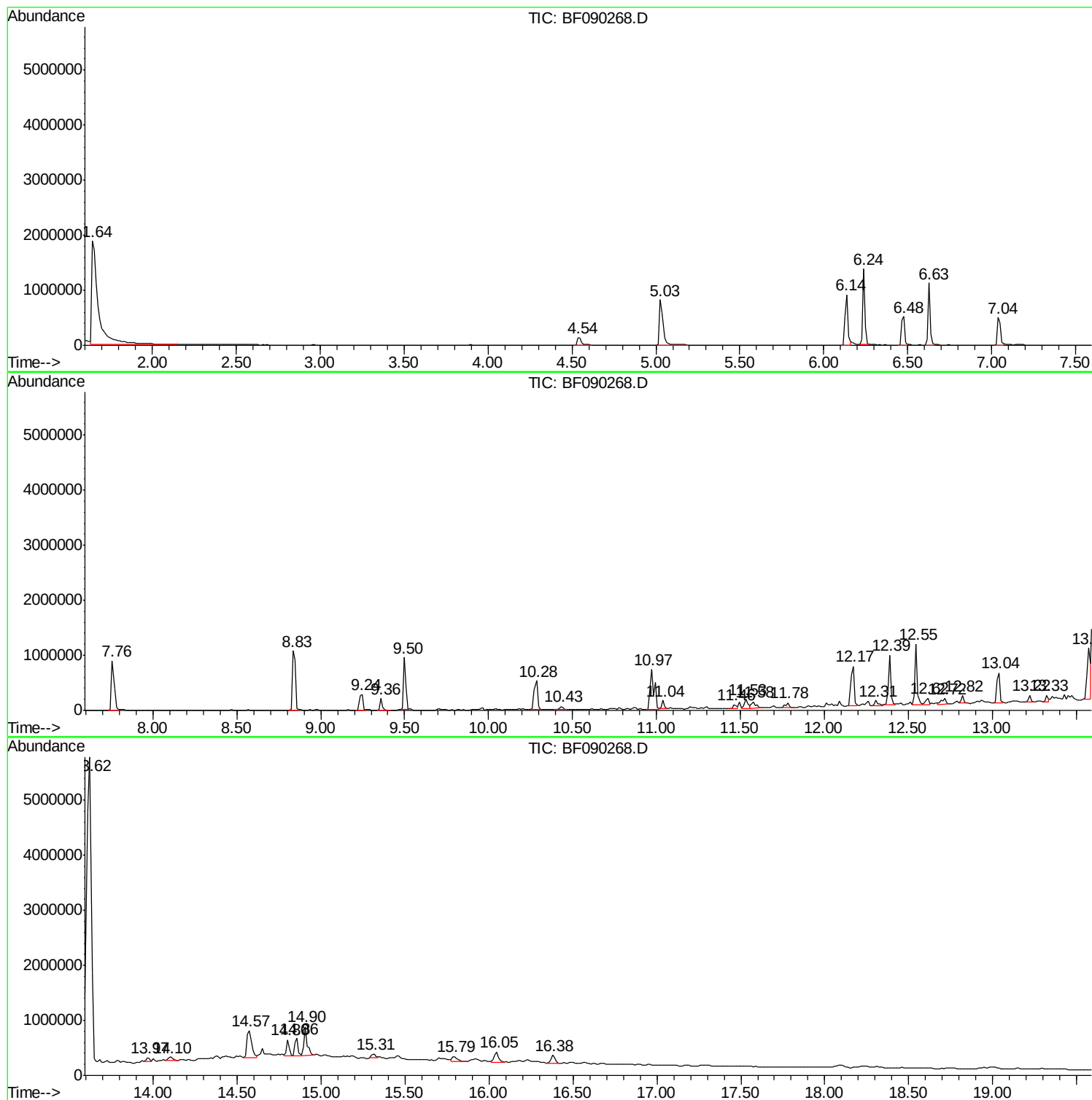
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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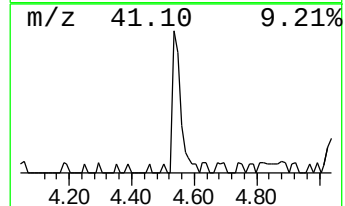
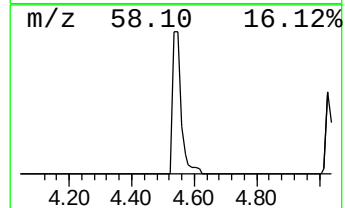
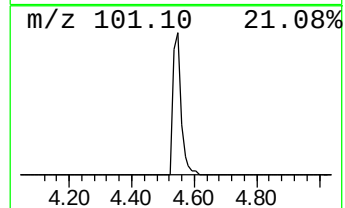
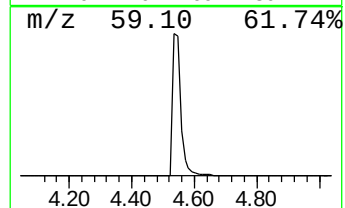
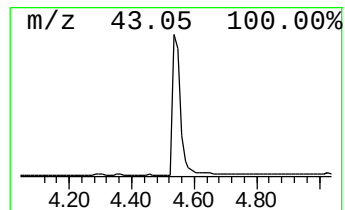
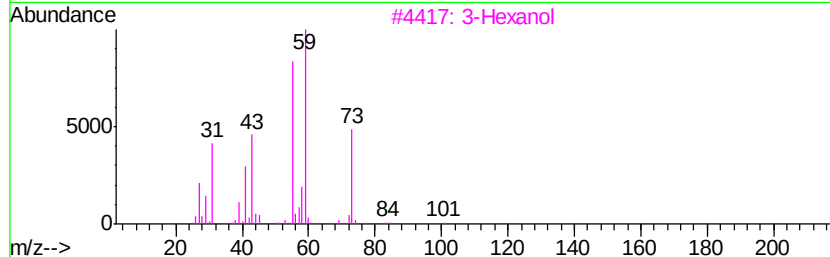
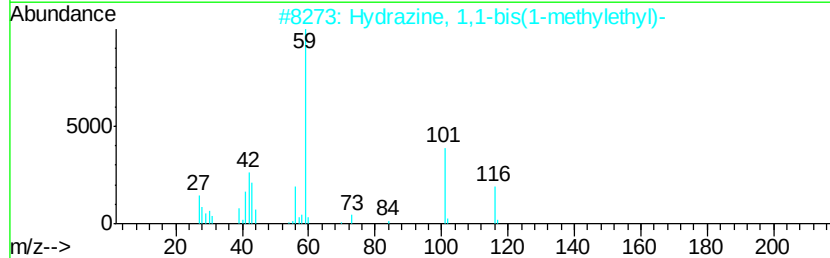
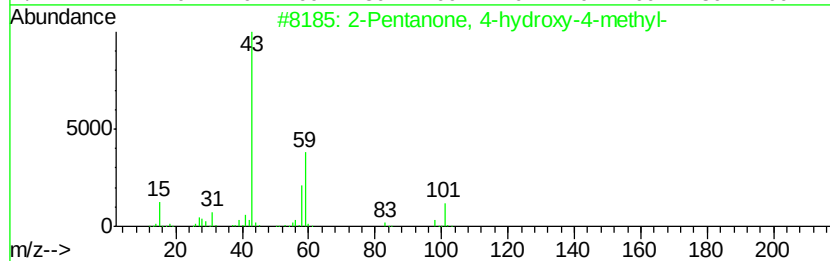
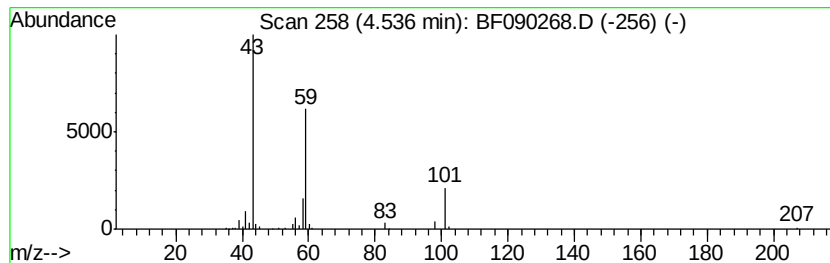
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	6.55 ng	230772	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3		3-Hexanol	102	C6H14O	000623-37-0	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		Butane	58	C4H10	000106-97-8	9



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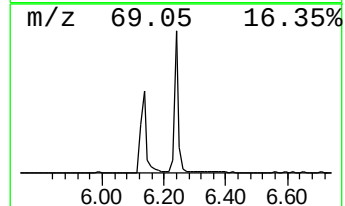
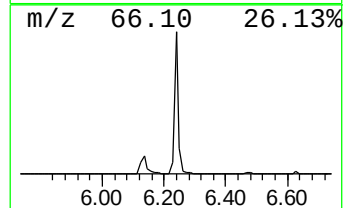
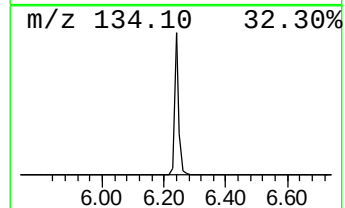
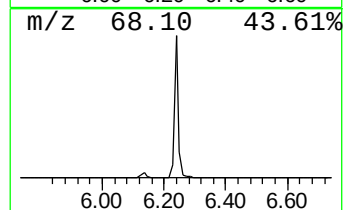
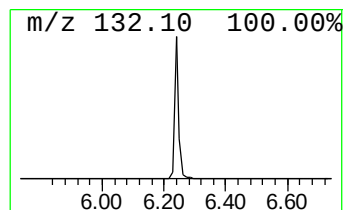
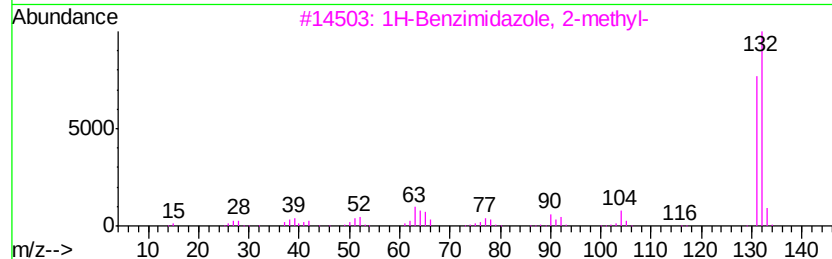
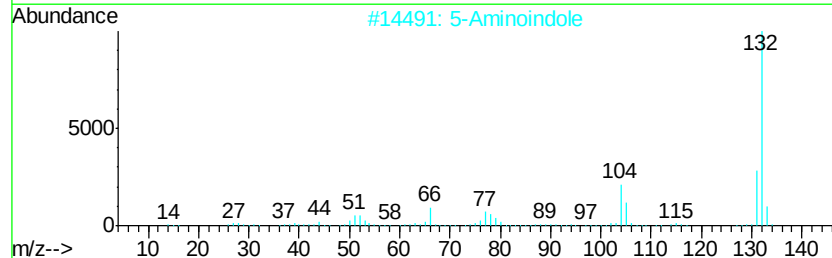
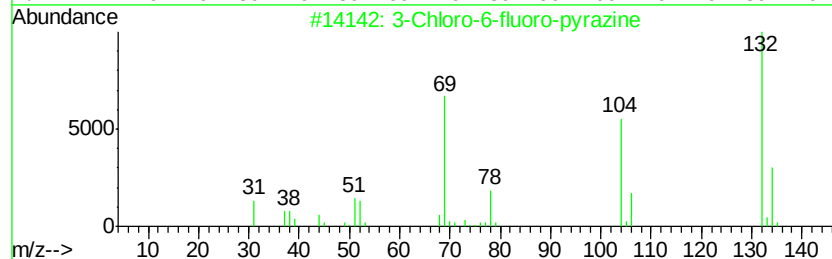
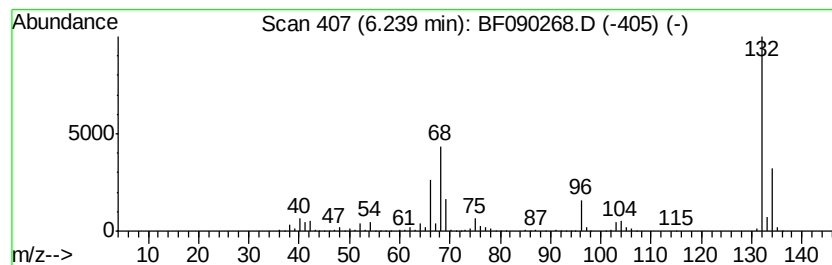
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Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	35.13 ng	1238240	1,4-Dichlorobenzene-d4	6.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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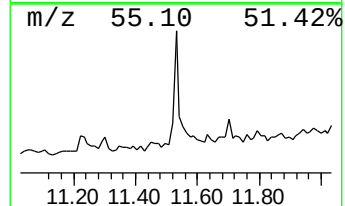
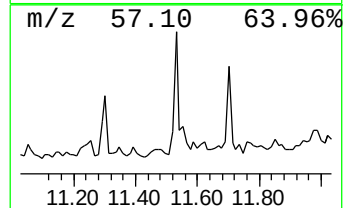
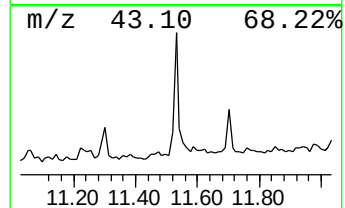
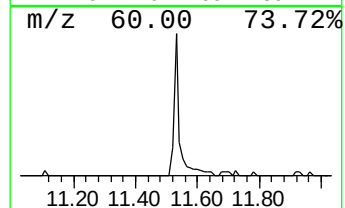
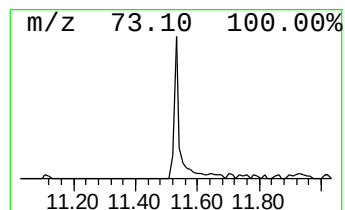
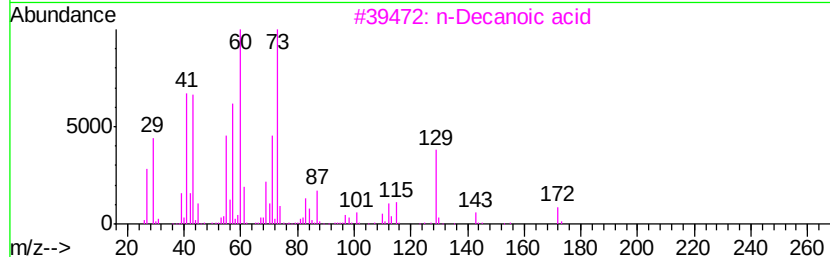
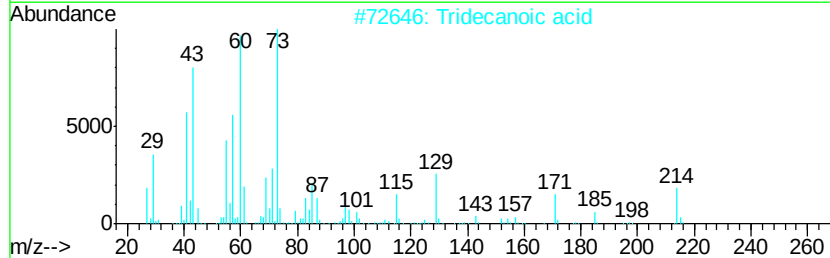
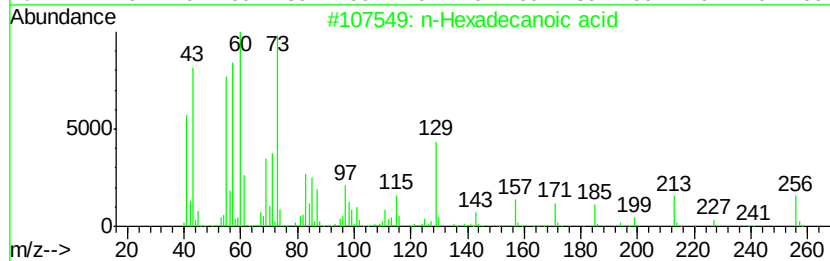
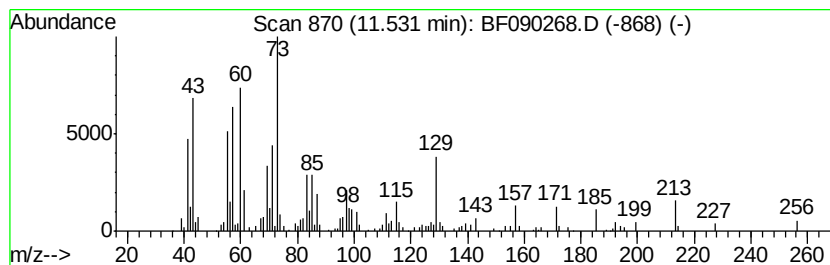
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	3.33 ng	214269	Phenanthrene-d10	10.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	81
3		n-Decanoic acid	172	C10H20O2	000334-48-5	76
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		2,5-Cyclohexadiene-1,4-dione, 2,...	176	C6H2Cl2O2	000615-93-0	18



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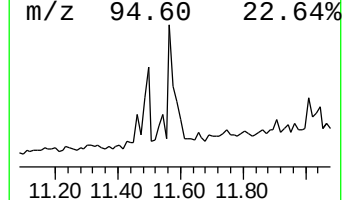
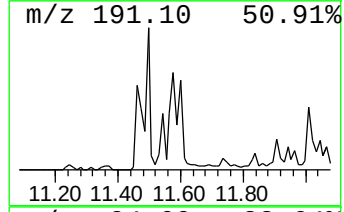
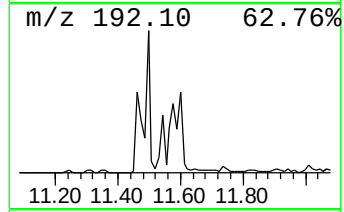
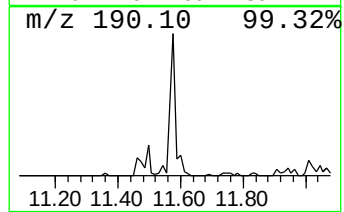
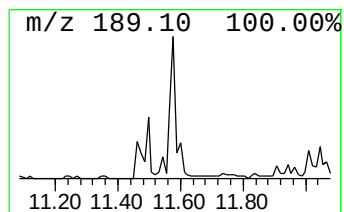
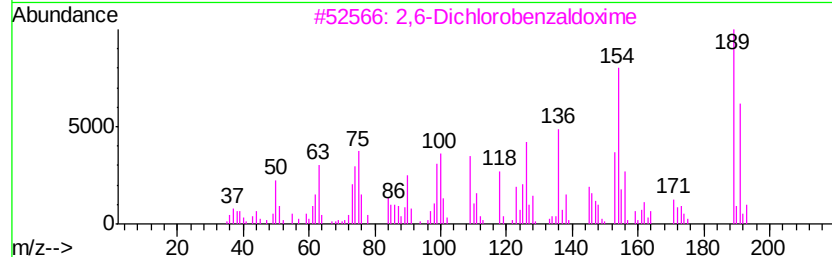
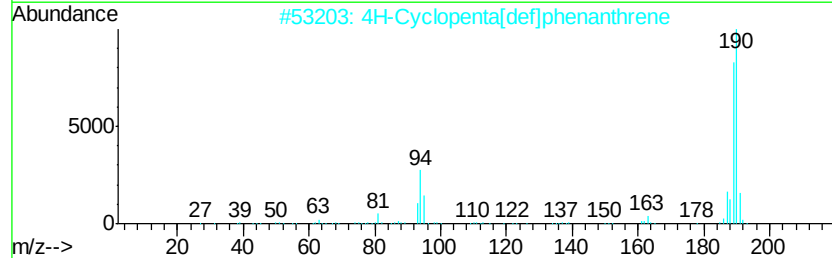
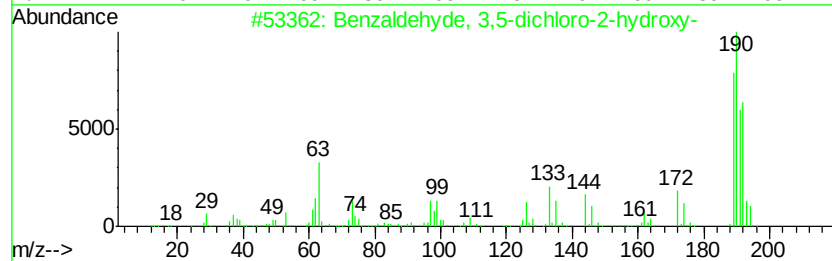
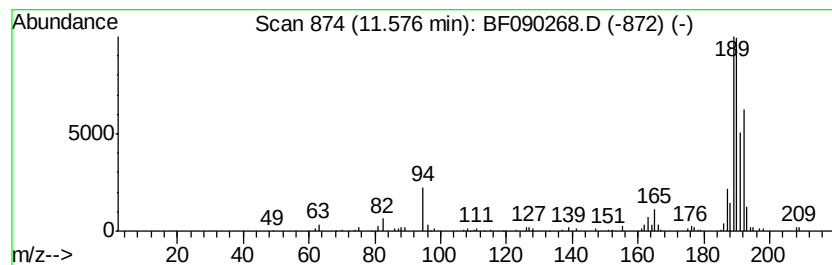
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.58	3.46 ng	222398	Phenanthrene-d10	10.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
3	2,6-Dichlorobenzaloxime	189	C7H5Cl2NO	025185-95-9	42
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	38
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30



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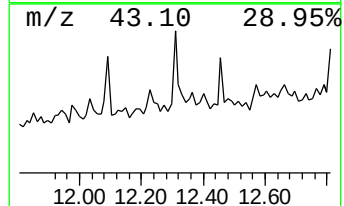
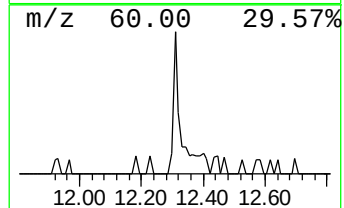
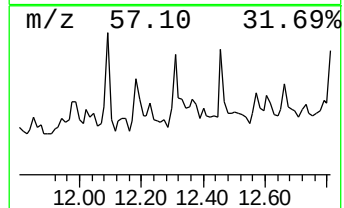
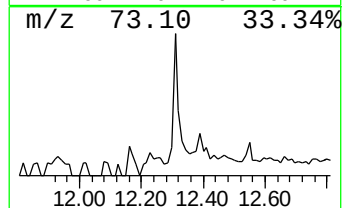
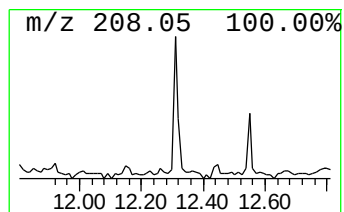
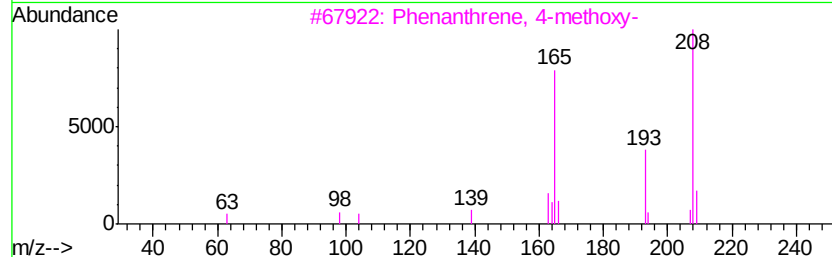
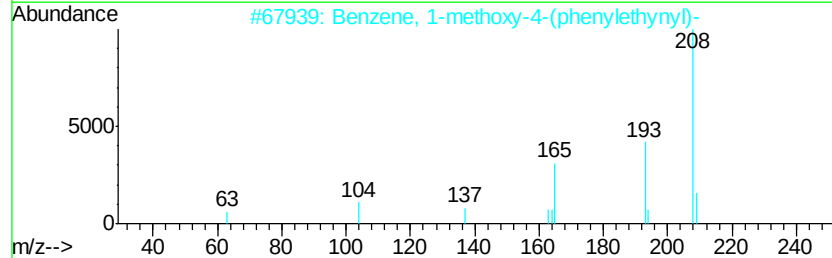
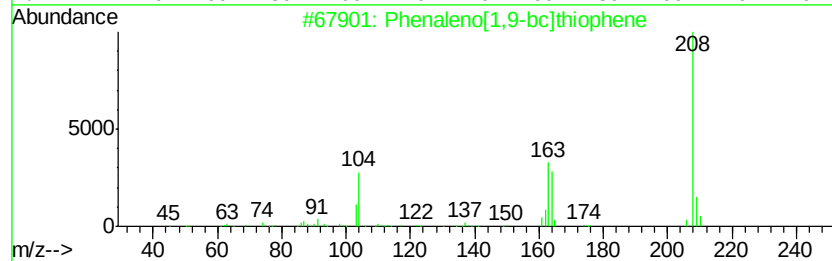
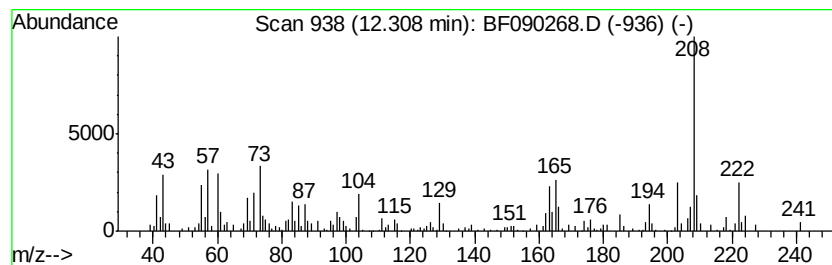
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.31 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	2.05 ng	144347	Chrysene-d12	13.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenaleno[1,9-bc]thiophene	208	C14H8S	079965-99-4	46
2		Benzene, 1-methoxy-4-(phenylethy...	208	C15H12O	007380-78-1	38
3		Phenanthrene, 4-methoxy-	208	C15H12O	015638-06-9	35
4		Asarone	208	C12H16O3	002883-98-9	35
5		Anthracene, 1-methoxy-	208	C15H12O	054458-84-3	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090268.D
Acq On : 27 Sep 2016 22:43
Operator : UM/SJ
Sample : H4949-07 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-1-LOC-4(0-5)

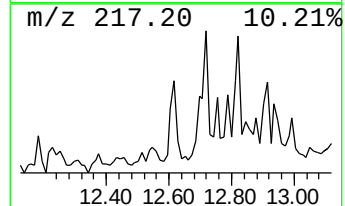
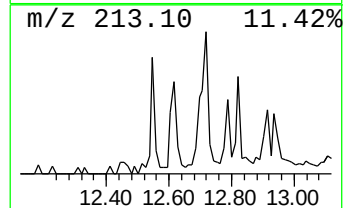
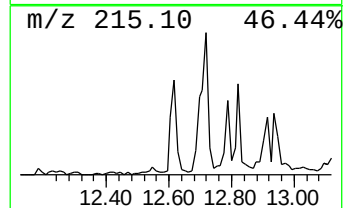
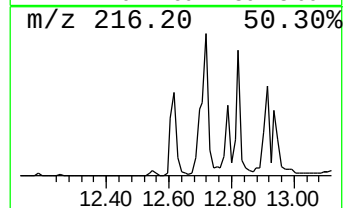
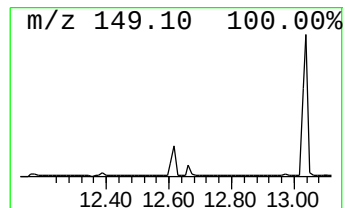
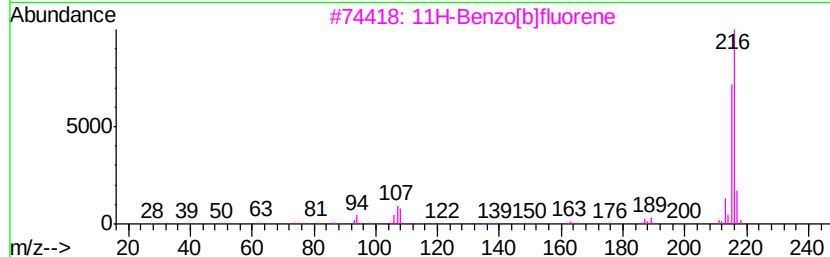
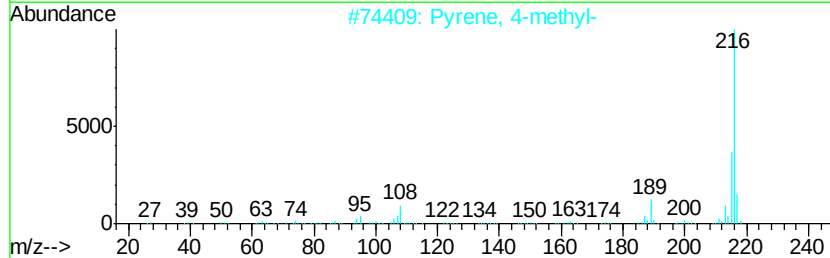
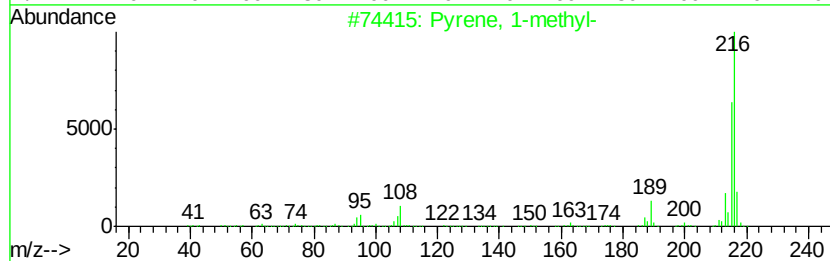
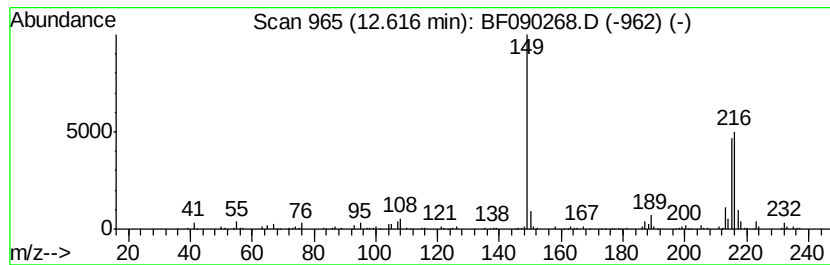
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	2.31 ng	162710	Chrysene-d12	13.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	66
2		Pyrene, 4-methyl-	216	C17H12	003353-12-6	60
3		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	50
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	38
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
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Sample : H4949-07 2X
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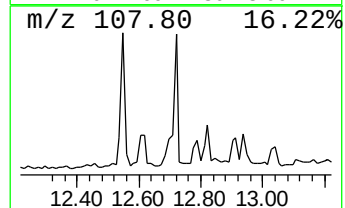
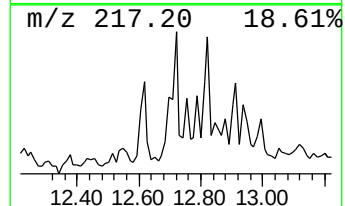
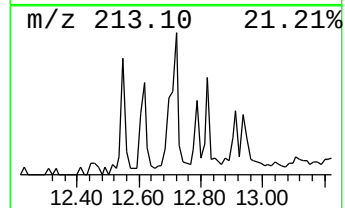
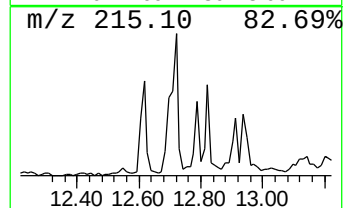
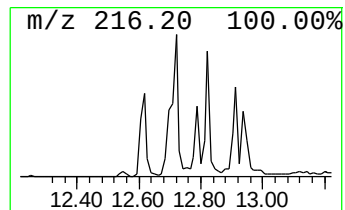
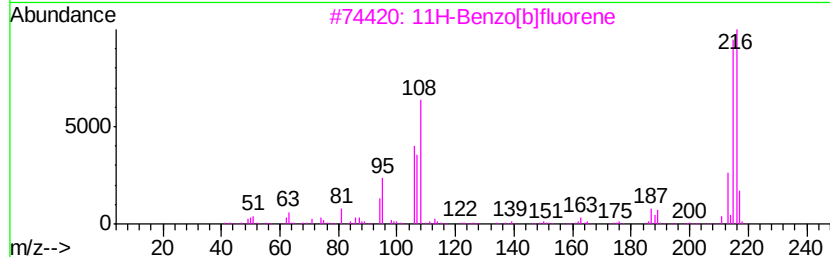
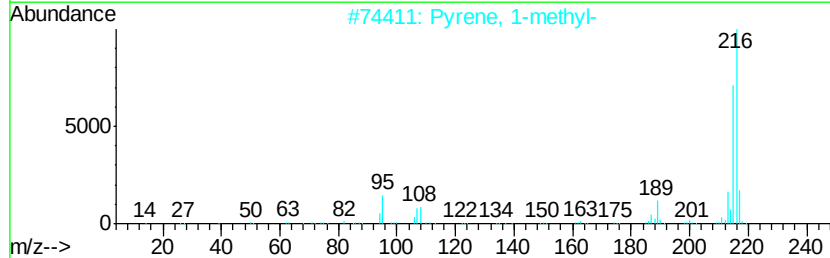
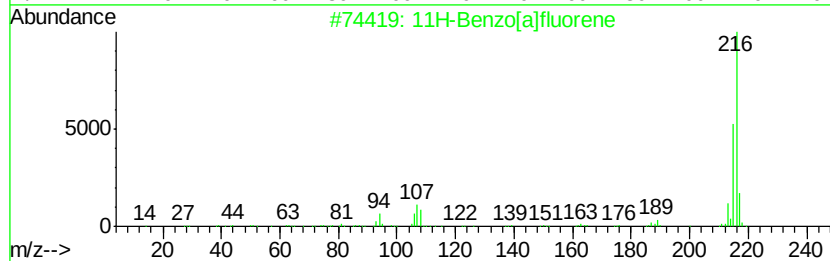
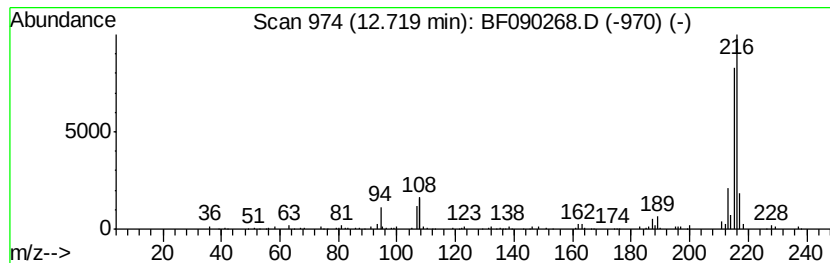
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 11H-Benzo[a]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.72	2.82 ng	198959	Chrysene-d12	13.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[alfluorene	216	C17H12	000238-84-6	91
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090268.D
Acq On : 27 Sep 2016 22:43
Operator : UM/SJ
Sample : H4949-07 2X
Misc :
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Instrument :
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ClientSampleId :
S-4-1-LOC-4(0-5)

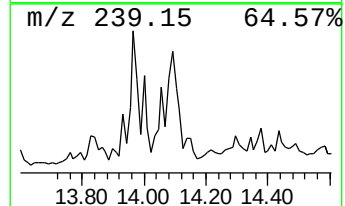
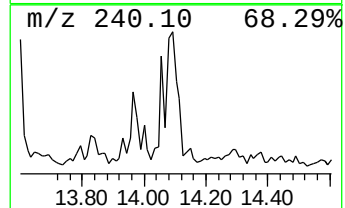
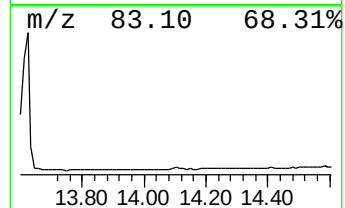
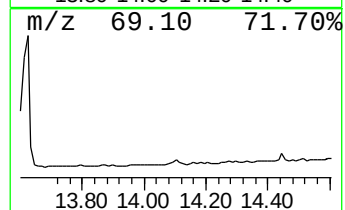
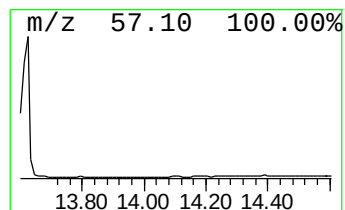
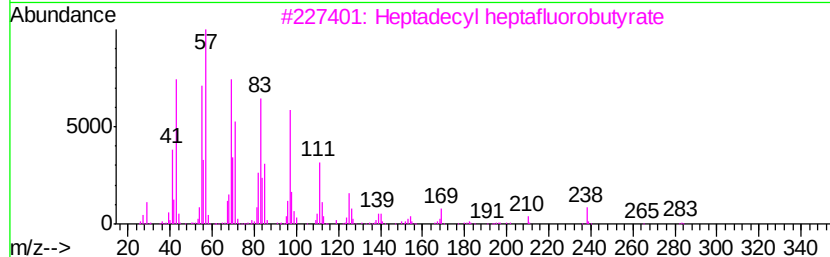
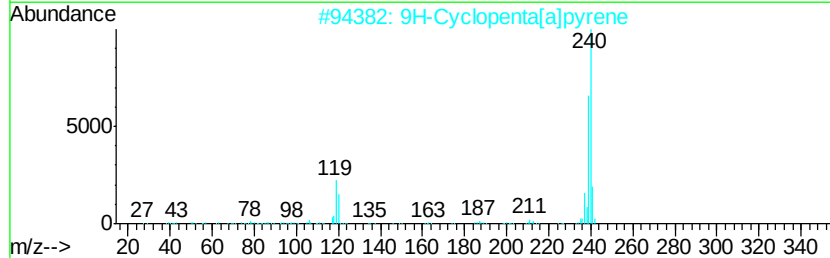
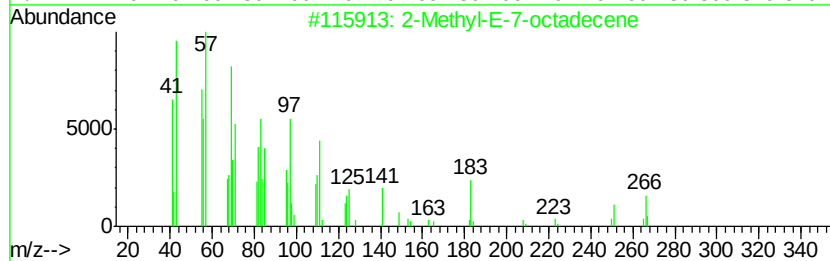
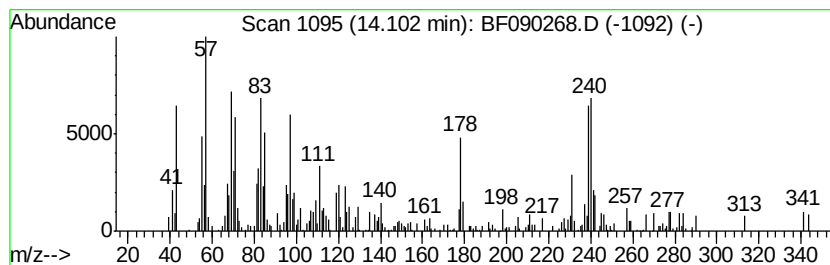
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.10 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	2.03 ng	142947	Chrysene-d12	13.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-E-7-octadecene	266	C19H38	1000130-92-3	44
2			9H-Cyclopenta[a]pyrene	240	C19H12	050861-05-7	35
3			Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	25
4			4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	25
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090268.D
Acq On : 27 Sep 2016 22:43
Operator : UM/SJ
Sample : H4949-07 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-4-1-LOC-4(0-5)

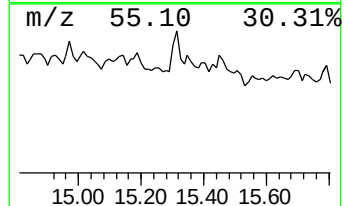
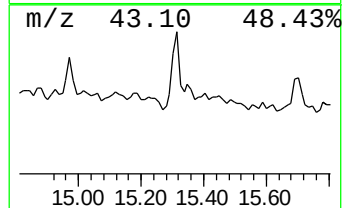
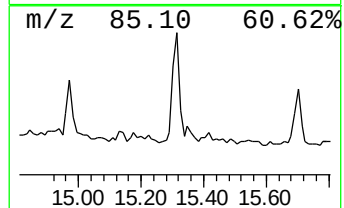
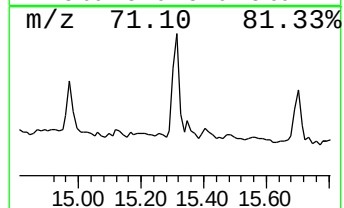
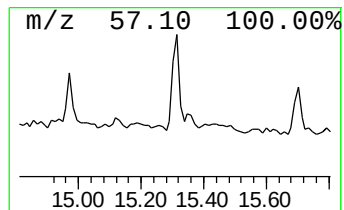
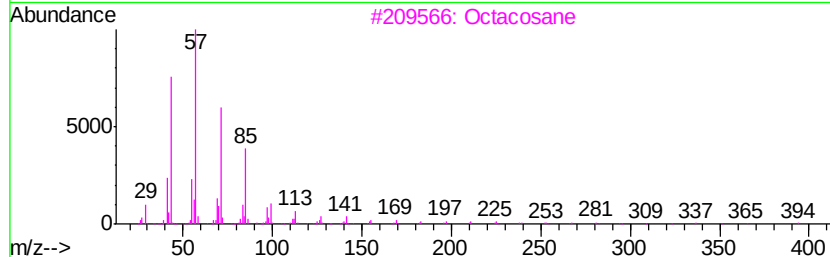
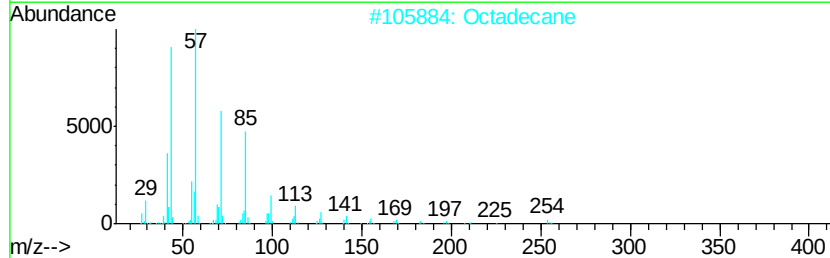
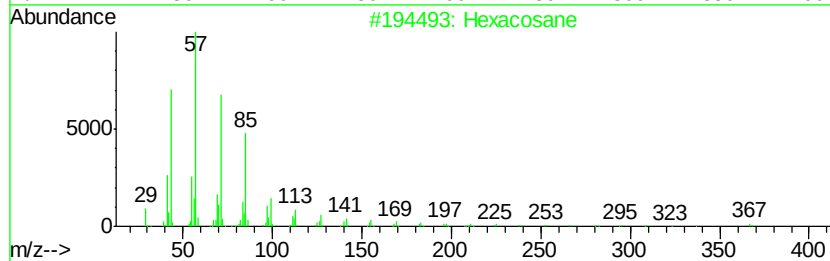
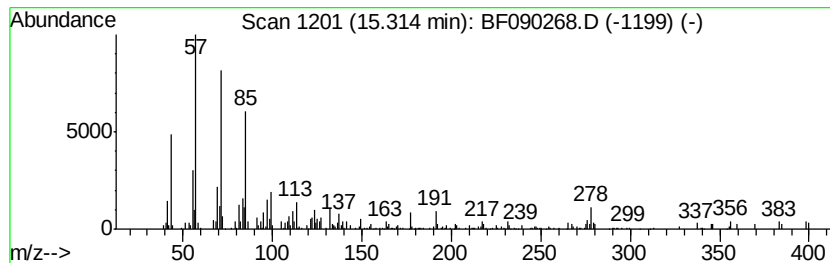
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	3.33 ng	117497	Perylene-d12	14.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	68
2		Octadecane	254	C18H38	000593-45-3	64
3		Octacosane	394	C28H58	000630-02-4	64
4		Hexadecane	226	C16H34	000544-76-3	64
5		Heptadecane	240	C17H36	000629-78-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090268.D
Acq On : 27 Sep 2016 22:43
Operator : UM/SJ
Sample : H4949-07 2X
Misc :
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S-4-1-LOC-4(0-5)

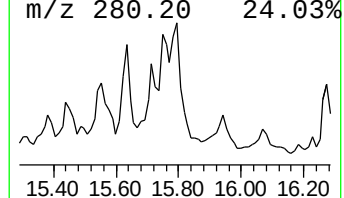
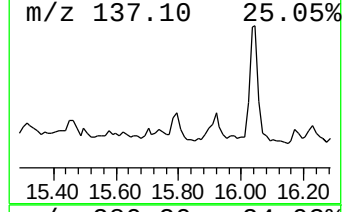
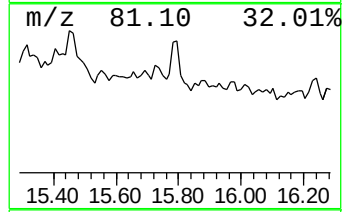
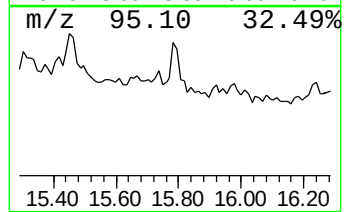
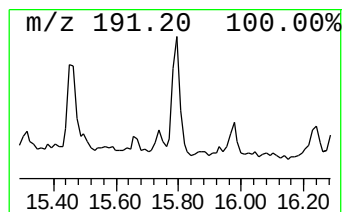
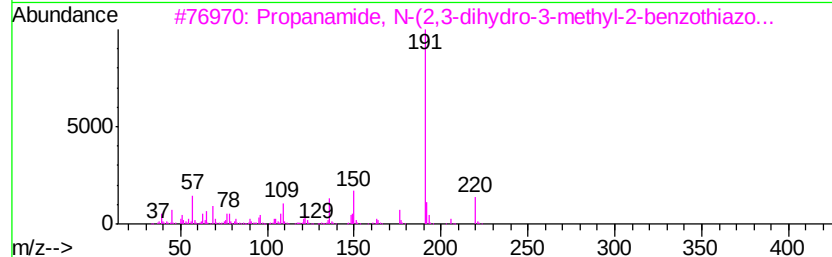
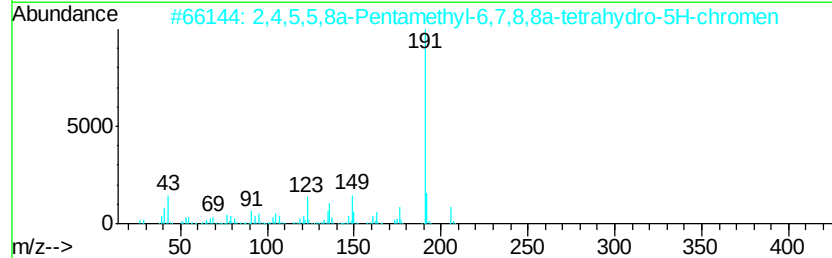
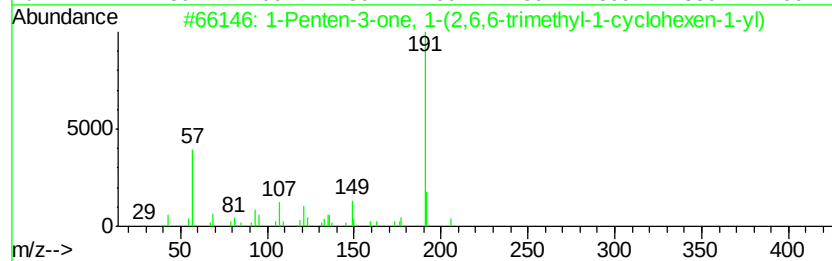
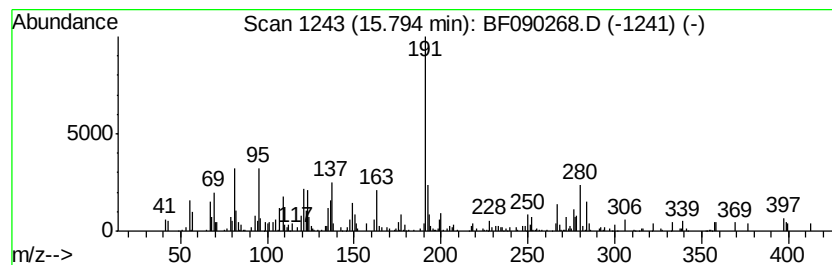
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown15.79 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	4.61 ng	162925	Perylene-d12	14.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
2			2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	43
3			Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	35
4			Benzoic acid, 4-[3-(3,4-dimethox...	397	C23H27NO5	1000317-25-8	35
5			Amiphenazole	191	C9H9N3S	000490-55-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
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 Operator : UM/SJ
 Sample : H4949-07 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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
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unknown6.24	6.24	35.1	ng	1238240	1	6.48	704858	20.0
n-Hexadecanoic acid	11.53	3.3	ng	214269	4	10.97	1285870	20.0
Benzaldehyde, 3,5...	11.58	3.5	ng	222398	4	10.97	1285870	20.0
unknown12.31	12.31	2.0	ng	144347	5	13.58	1410320	20.0
Pyrene, 1-methyl-	12.62	2.3	ng	162710	5	13.58	1410320	20.0
11H-Benzo[a]fluorene	12.72	2.8	ng	198959	5	13.58	1410320	20.0
unknown14.10	14.10	2.0	ng	142947	5	13.58	1410320	20.0
Hexacosane	15.31	3.3	ng	117497	6	14.90	706264	20.0
unknown15.79	15.79	4.6	ng	162925	6	14.90	706264	20.0