

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
 Data File : BF091033.D
 Acq On : 4 Nov 2016 21:07
 Operator : UM/SJ
 Sample : H5526-05
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-100-1.0-1.5

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-BF110316.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	1.778	7	8	31	rVB	3311483	7758952	100.00%	12.406%
2	2.121	31	38	78	rVB	1896644	4083004	52.62%	6.528%
3	4.853	274	277	285	rBV	633523	1111903	14.33%	1.778%
4	5.299	314	316	319	rBV	3836334	4355004	56.13%	6.963%
5	6.362	406	409	411	rBV	3856660	4970007	64.06%	7.947%
6	6.476	416	419	421	rBV	4623564	4811722	62.02%	7.693%
7	6.705	437	439	441	rBV	1039336	1086541	14.00%	1.737%
8	6.853	450	452	455	rBV	2770288	3612658	46.56%	5.776%
9	7.276	486	489	491	rBV	2640092	3190554	41.12%	5.101%
10	7.402	497	500	506	rVB	68182	119073	1.53%	0.190%
11	7.985	549	551	554	rBV	1343074	1443695	18.61%	2.308%
12	8.750	609	618	630	rBV	61320	222698	2.87%	0.356%
13	9.070	643	646	648	rBV	5200368	4724374	60.89%	7.554%
14	9.470	678	681	683	rBV	1288243	1203925	15.52%	1.925%
15	9.745	702	705	707	rBV	1376089	1565851	20.18%	2.504%
16	10.533	771	774	776	rBV	2698242	2898151	37.35%	4.634%
17	10.659	783	785	791	rVB	116843	186052	2.40%	0.297%
18	11.105	819	824	825	rBV	93540	114946	1.48%	0.184%
19	11.219	832	834	838	rBV2	1452963	1540854	19.86%	2.464%
20	11.299	838	841	843	rVB2	68968	96075	1.24%	0.154%
21	11.459	852	855	859	rBV5	44869	81609	1.05%	0.130%
22	11.722	872	878	879	rBV3	59484	79429	1.02%	0.127%
23	11.768	879	882	883	rVV2	167959	231180	2.98%	0.370%
24	11.791	883	884	886	rVV2	59526	80884	1.04%	0.129%
25	11.836	886	888	893	rVB2	60742	140654	1.81%	0.225%
26	12.431	938	940	942	rBV	667578	637695	8.22%	1.020%
27	12.659	957	960	961	rBV	461827	651840	8.40%	1.042%
28	12.694	961	963	968	rVB3	74227	153271	1.98%	0.245%
29	12.808	970	973	975	rVV	4114213	3655940	47.12%	5.845%
30	12.877	975	979	983	rVB4	49973	95692	1.23%	0.153%
31	12.979	985	988	990	rVB2	53362	119980	1.55%	0.192%
32	13.082	996	997	1001	rVV2	54564	103011	1.33%	0.165%
33	13.357	1019	1021	1023	rBV	97390	119351	1.54%	0.191%
34	13.494	1031	1033	1037	rBV	72194	89214	1.15%	0.143%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.597	1040	1042	1044	rBV	74481	141273	1.82%	0.226%
36	13.711	1050	1052	1056	rBV2	465750	544926	7.02%	0.871%
37	13.848	1061	1064	1069	rBV2	1142844	2031323	26.18%	3.248%
38	14.237	1096	1098	1100	rBV	61784	89876	1.16%	0.144%
39	14.340	1105	1107	1110	rBV4	95076	198269	2.56%	0.317%
40	14.522	1121	1123	1130	rBV	136033	305439	3.94%	0.488%
41	14.854	1150	1152	1157	rBV	493414	863333	11.13%	1.380%
42	14.957	1159	1161	1164	rVB	109469	142873	1.84%	0.228%
43	15.128	1174	1176	1179	rVV	257281	298841	3.85%	0.478%
44	15.185	1179	1181	1183	rVB	337536	377123	4.86%	0.603%
45	15.242	1183	1186	1193	rBV	809419	1093761	14.10%	1.749%
46	15.711	1225	1227	1239	rVB3	101688	317718	4.09%	0.508%
47	16.557	1297	1301	1305	rBV2	130201	273500	3.52%	0.437%
48	16.694	1310	1313	1317	rBV2	89666	245877	3.17%	0.393%
49	16.934	1332	1334	1342	rVB	117495	282919	3.65%	0.452%

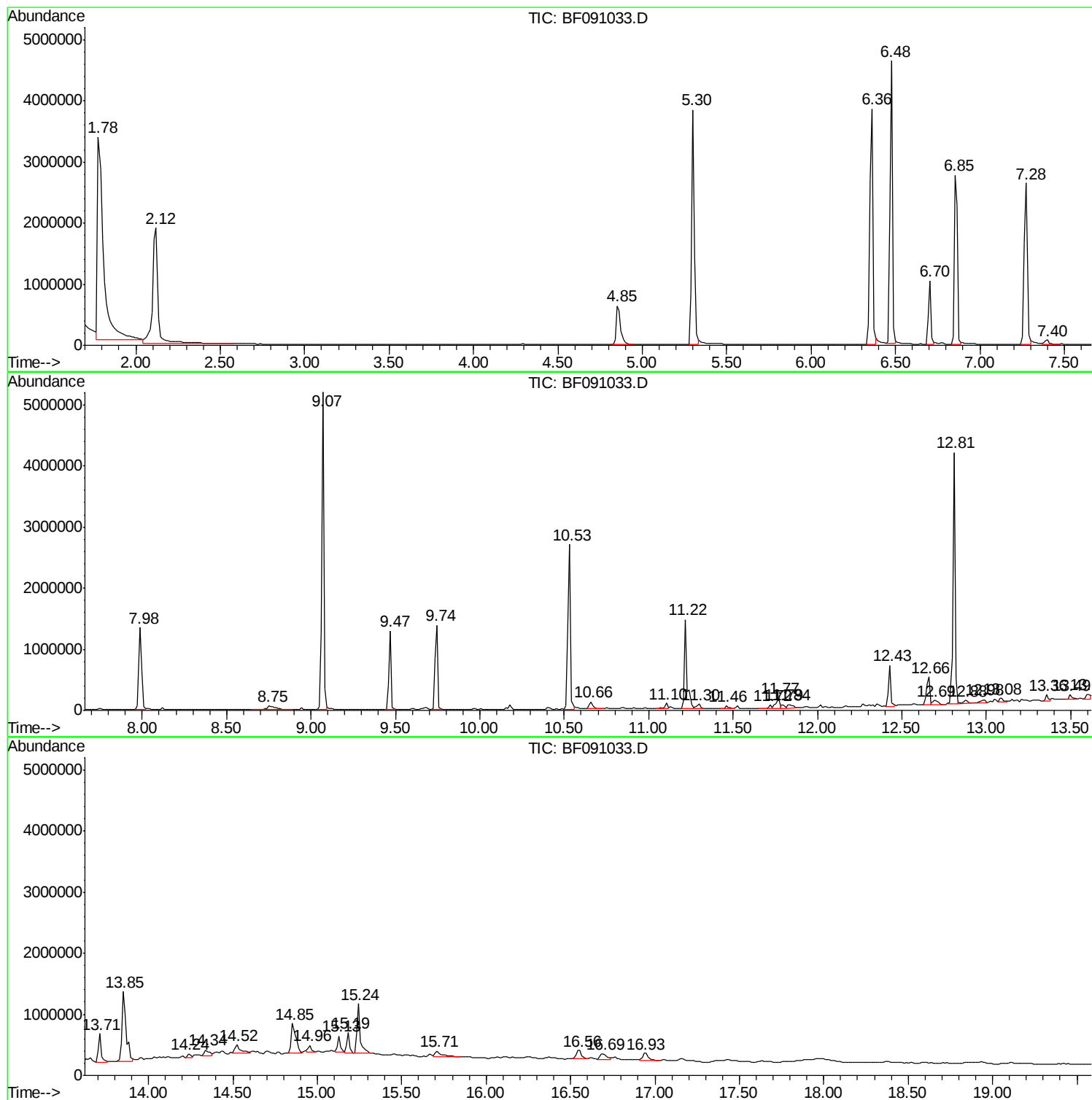
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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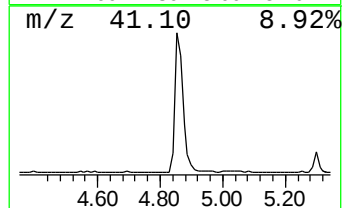
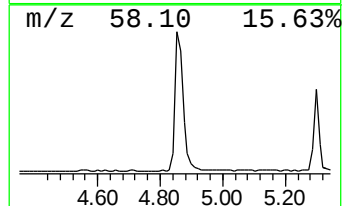
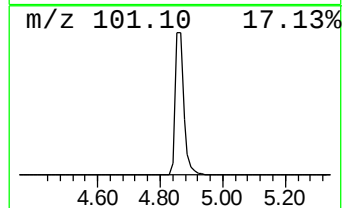
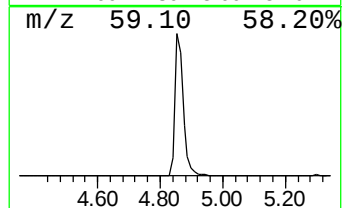
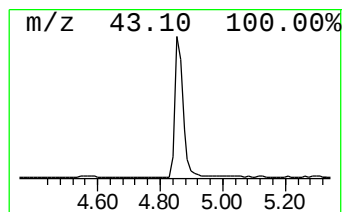
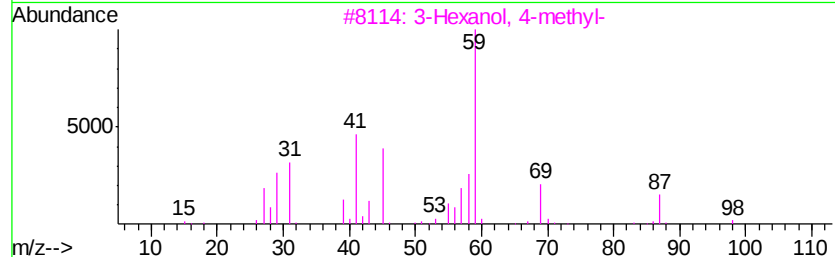
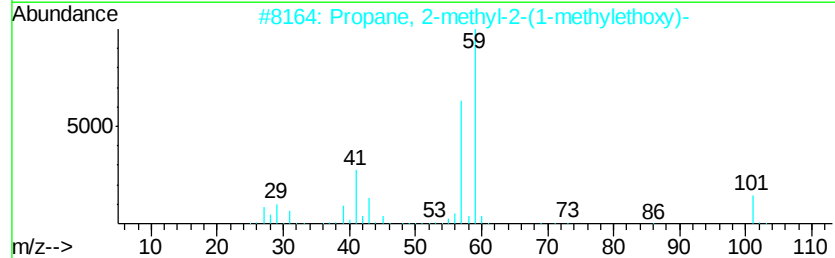
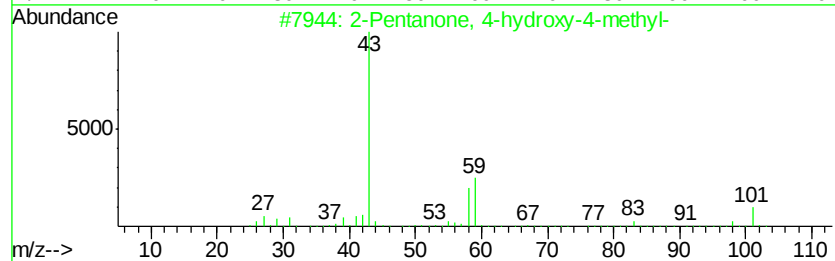
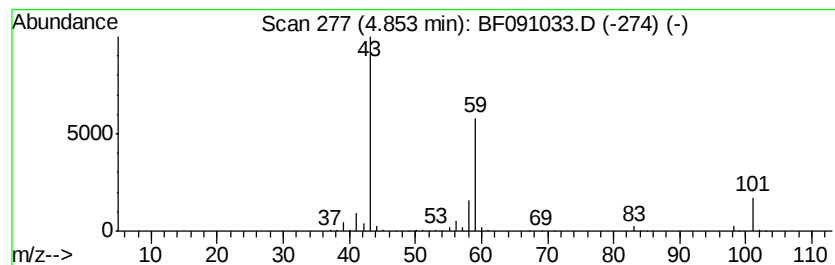
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	20.47 ng	1111900	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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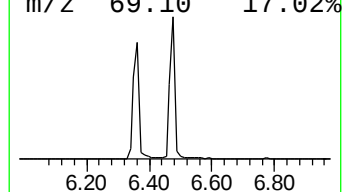
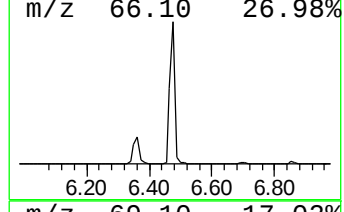
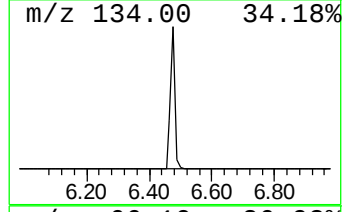
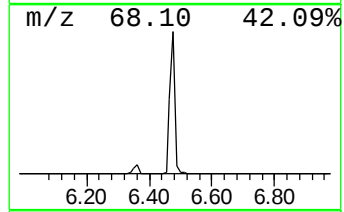
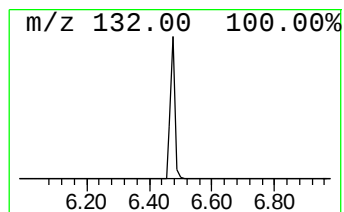
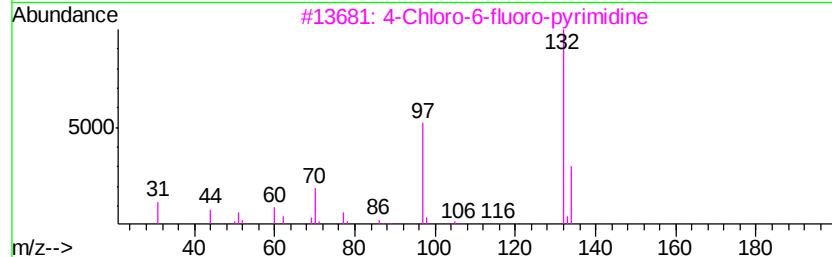
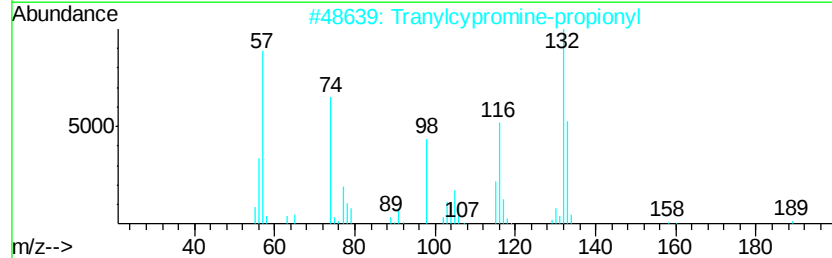
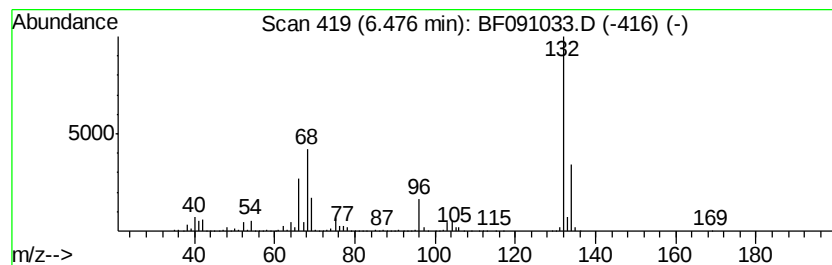
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	88.57 ng	4811720	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9



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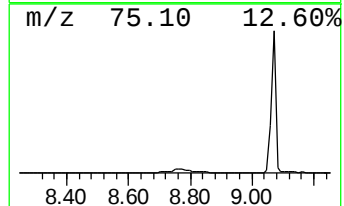
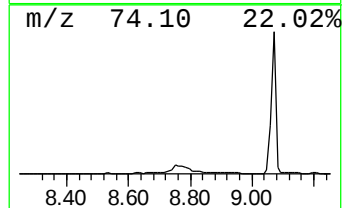
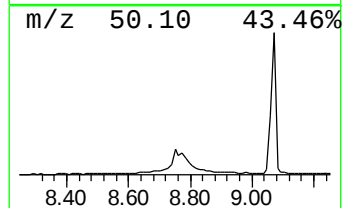
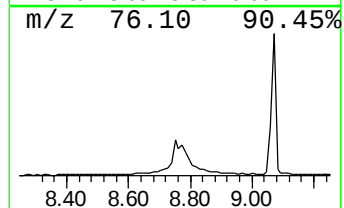
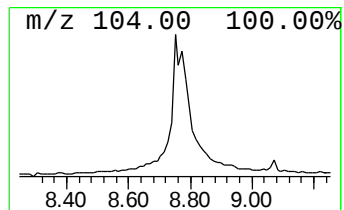
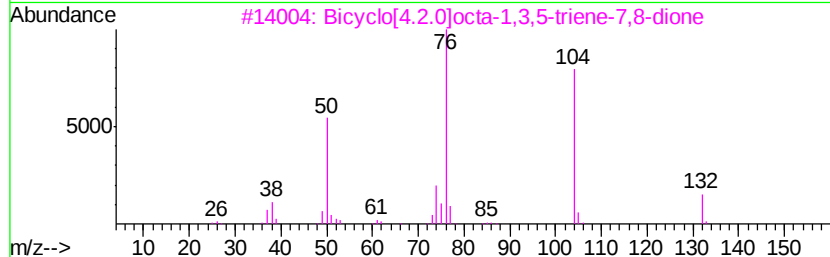
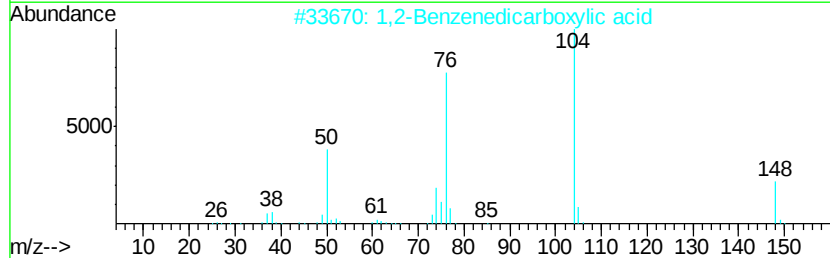
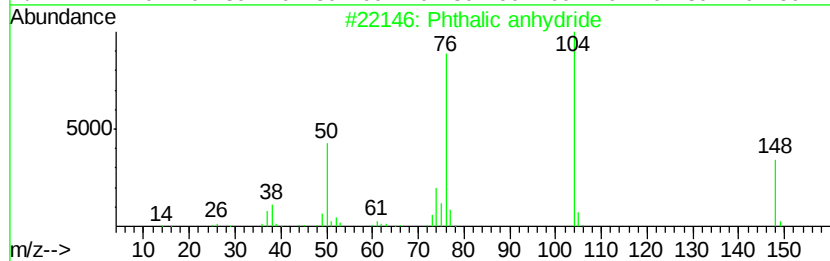
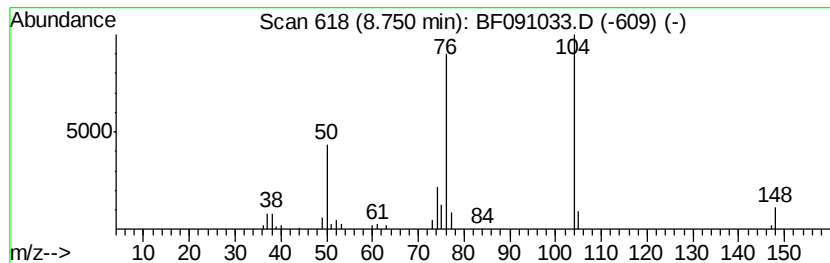
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phthalic anhydride Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.75	3.09 ng	222698	Naphthalene-d8	7.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic anhydride	148	C8H4O3	000085-44-9	94
2		1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
3		Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	78
4		Phthalamic acid	165	C8H7NO3	000088-97-1	74
5		N-[2-Acetamidoethylthio]phthalimide	264	C12H12N2O3S	025158-14-9	64



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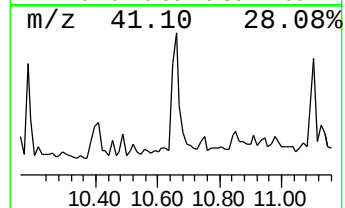
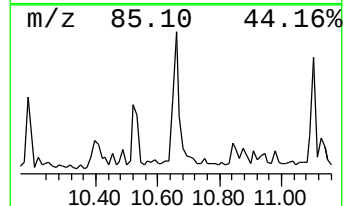
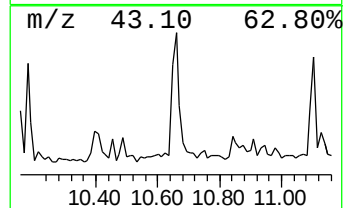
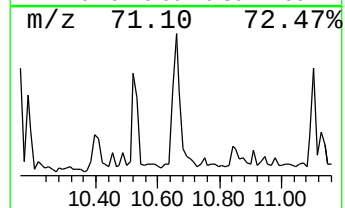
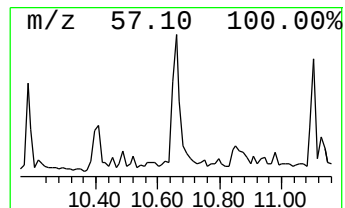
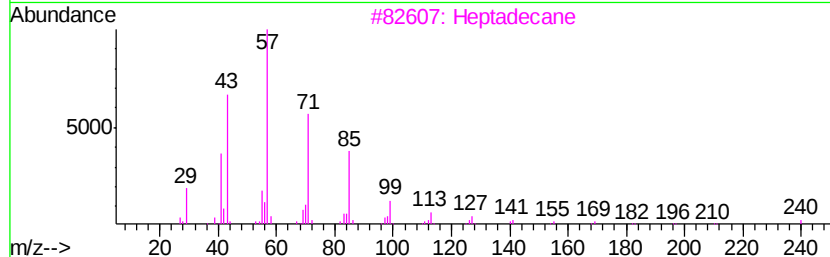
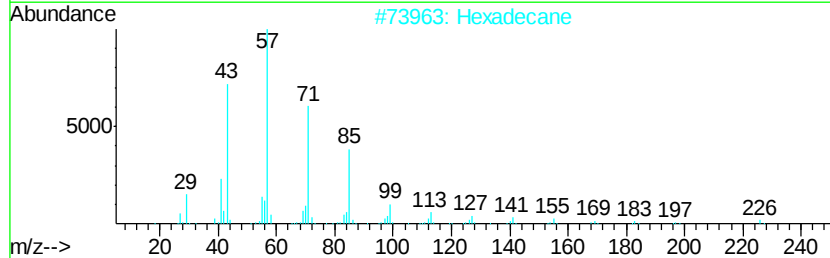
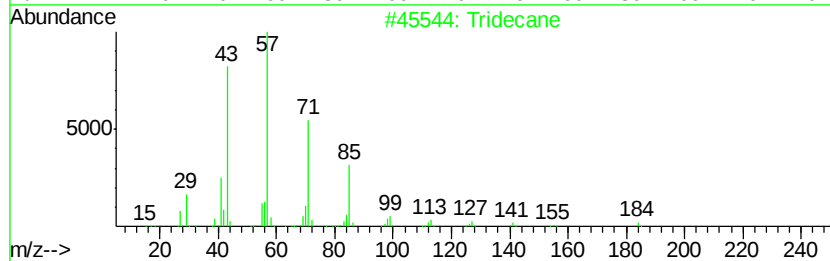
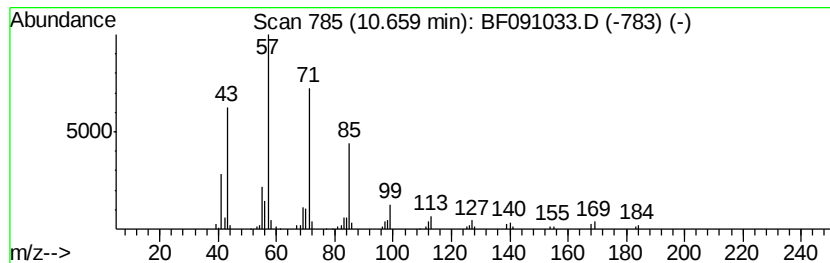
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tridecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.66	2.41 ng	186052	Phenanthrene-d10	11.22		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Heptadecane		240	C17H36	000629-78-7	90
4	Heptacosane		380	C27H56	000593-49-7	87
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	87



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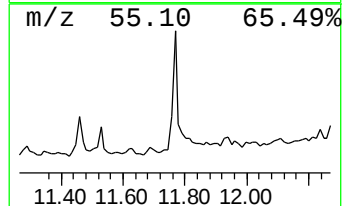
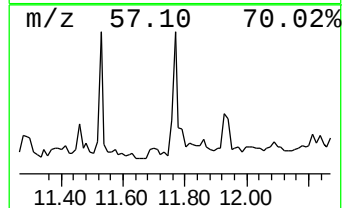
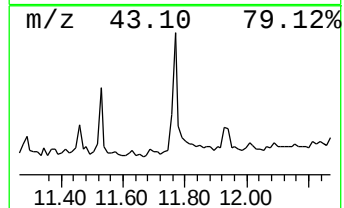
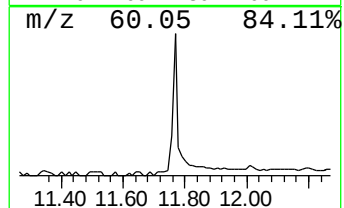
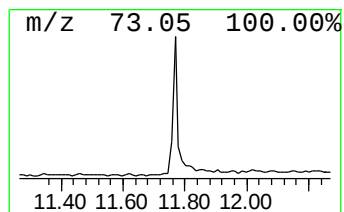
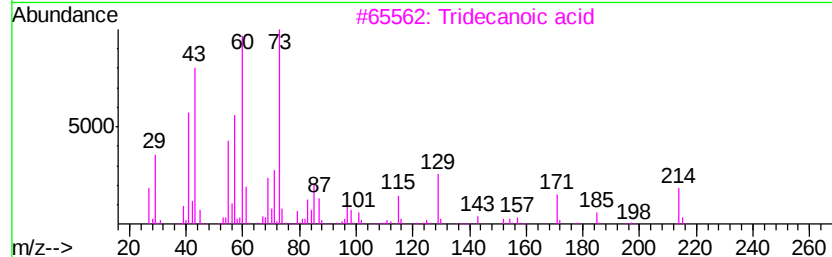
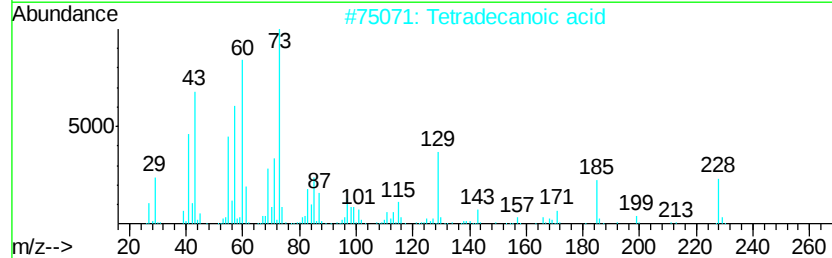
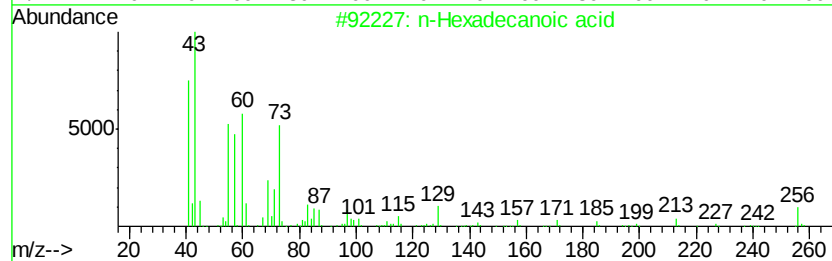
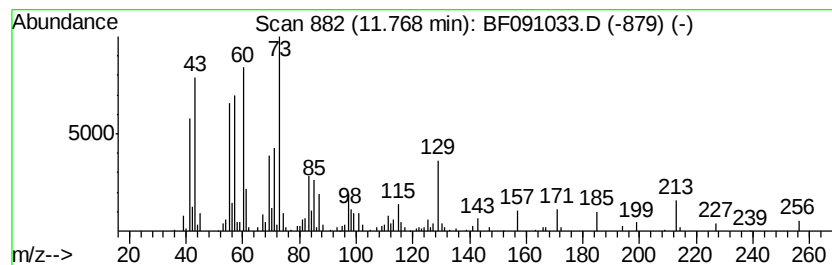
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.00 ng	231180	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	76
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5		n-Decanoic acid	172	C10H20O2	000334-48-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
Data File : BF091033.D
Acq On : 4 Nov 2016 21:07
Operator : UM/SJ
Sample : H5526-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-100-1.0-1.5

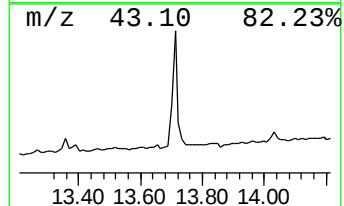
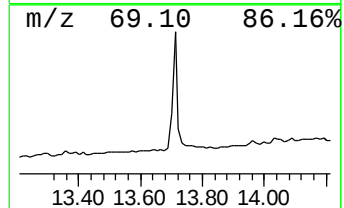
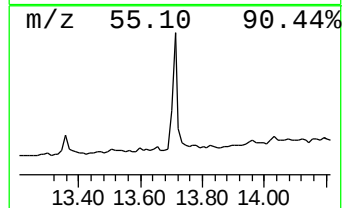
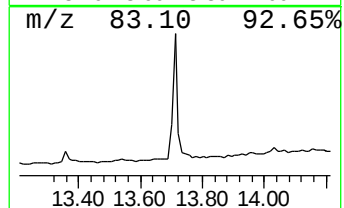
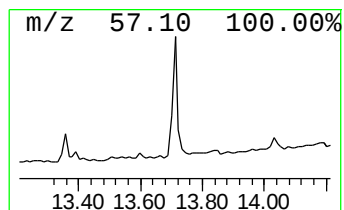
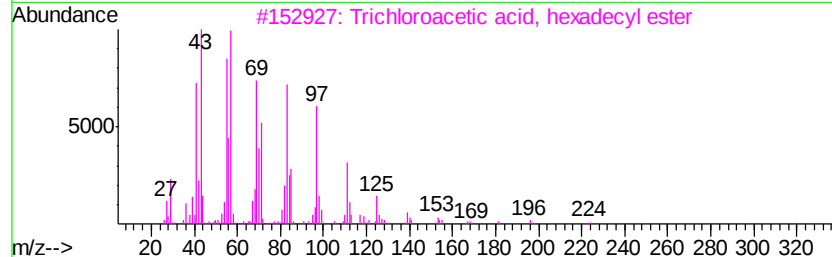
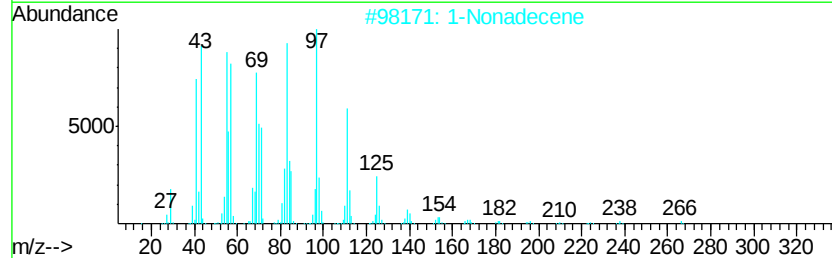
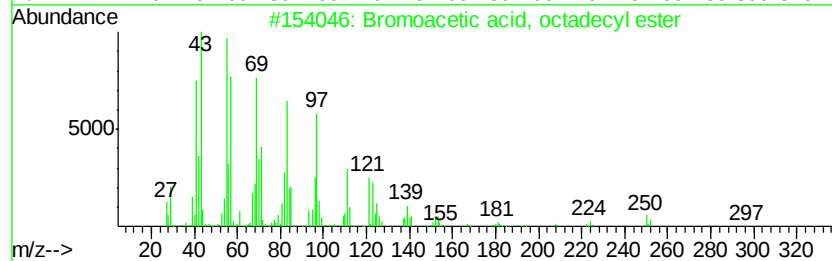
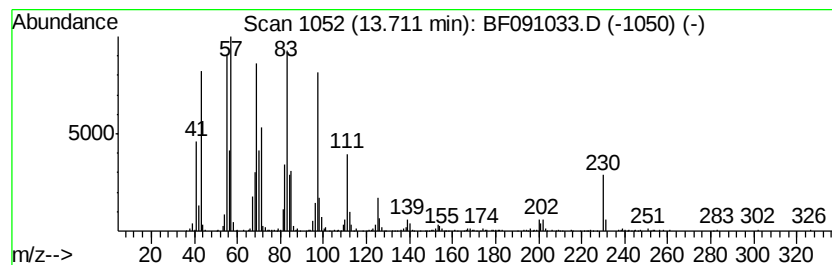
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Bromoacetic acid, octadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	5.37 ng	544926	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
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Operator : UM/SJ
Sample : H5526-05
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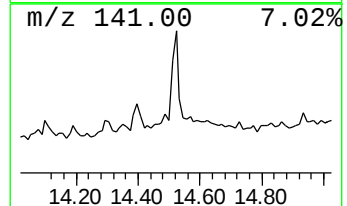
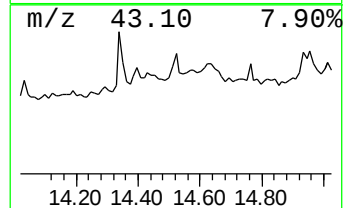
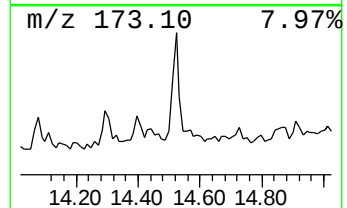
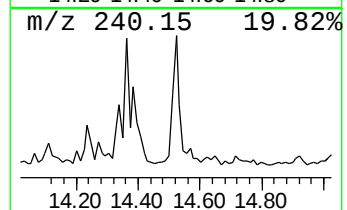
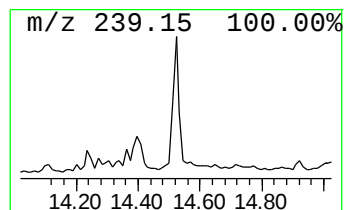
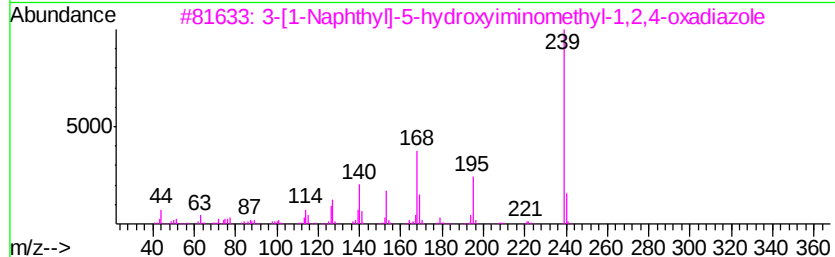
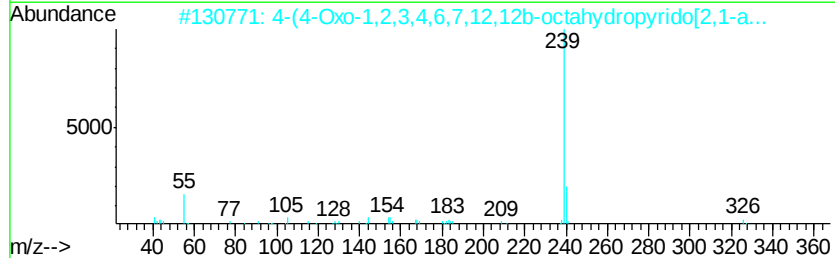
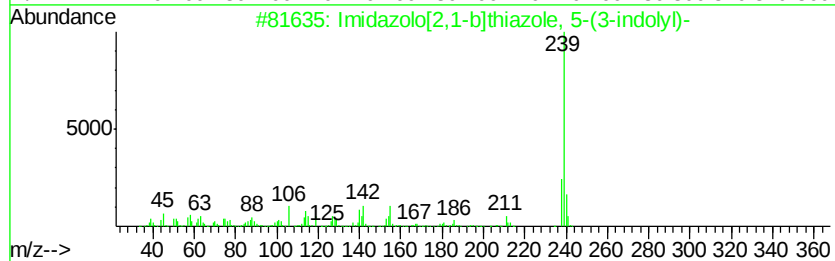
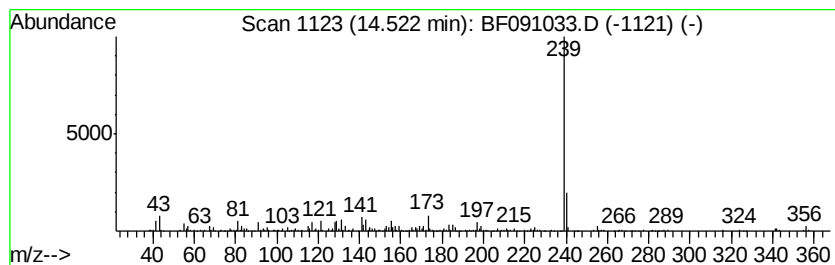
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Imidazolo[2,1-b]thiazole, 5... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.52	3.01 ng	305439	Chrysene-d12	13.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Imidazolo[2,1-b]thiazole, 5-(3-i...	239	C13H9N3S	327097-37-0	50
2		4-(4-Oxo-1,2,3,4,6,7,12,12b-octa...	326	C19H22N2O3	1000137-91-1	50
3		3-[1-Naphthyl]-5-hydroxyiminomet...	239	C13H9N3O2	103499-04-3	45
4		2-Methoxy-4-methyl-10H-acridin-9...	239	C15H13N02	1000210-25-6	39
5		2,5-Dimethoxymandelic acid, di-TMS	356	C16H28O5Si2	1000072-02-8	39



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
Data File : BF091033.D
Acq On : 4 Nov 2016 21:07
Operator : UM/SJ
Sample : H5526-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

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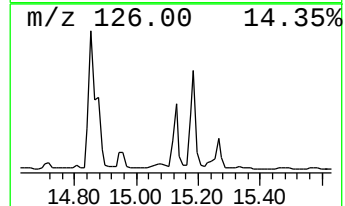
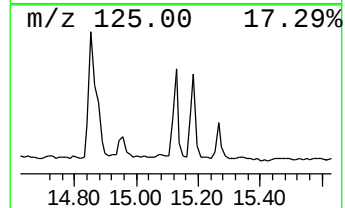
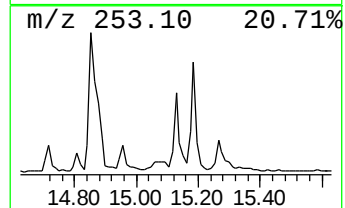
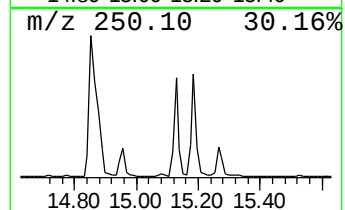
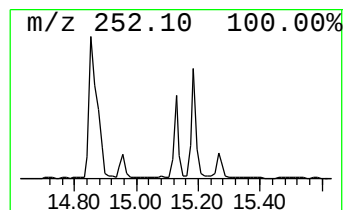
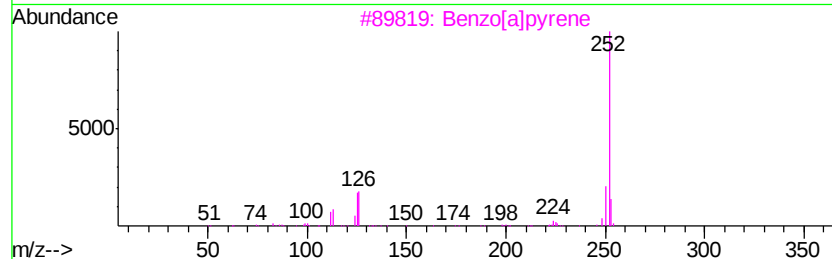
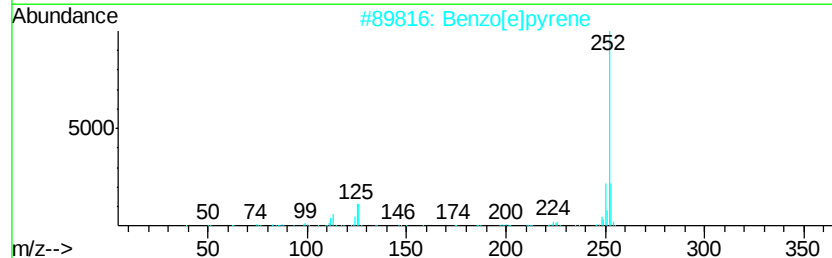
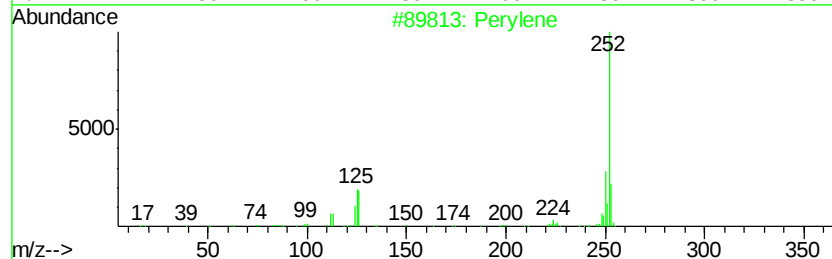
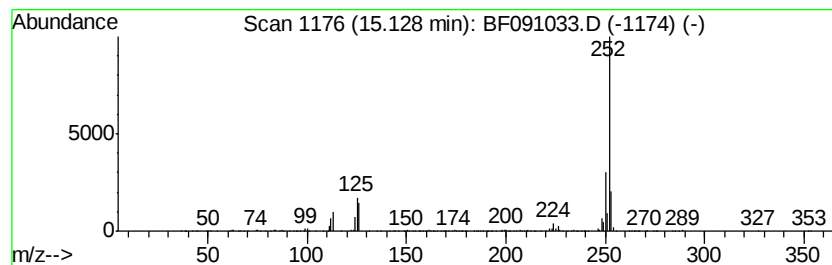
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	5.46 ng	298841	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	99
2		Benzo[e]pyrene	252	C20H12	000192-97-2	98
3		Benzo[a]pyrene	252	C20H12	000050-32-8	95
4		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
Data File : BF091033.D
Acq On : 4 Nov 2016 21:07
Operator : UM/SJ
Sample : H5526-05
Misc :
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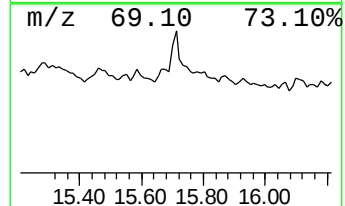
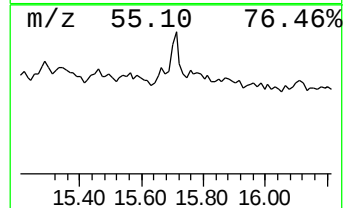
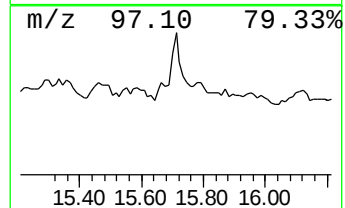
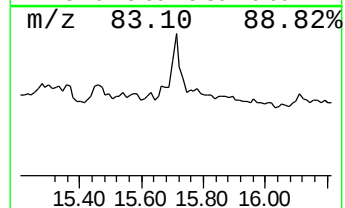
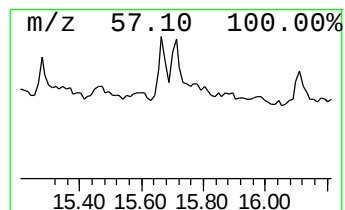
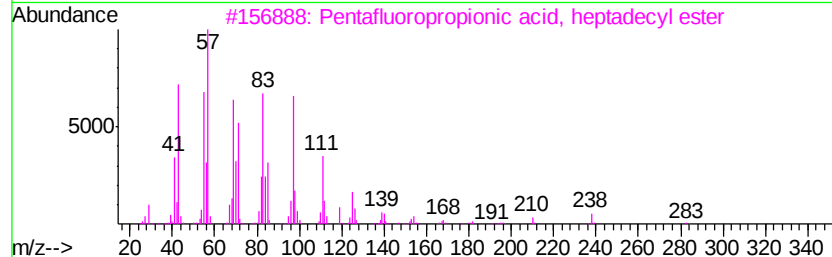
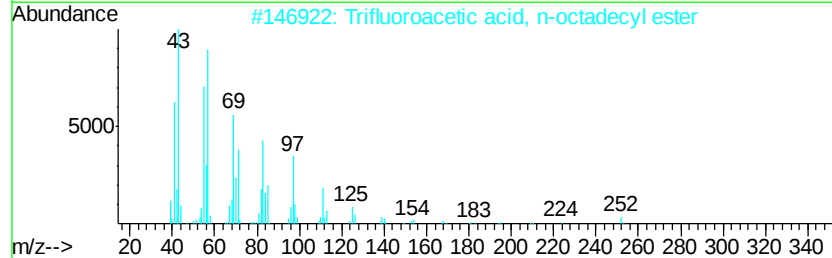
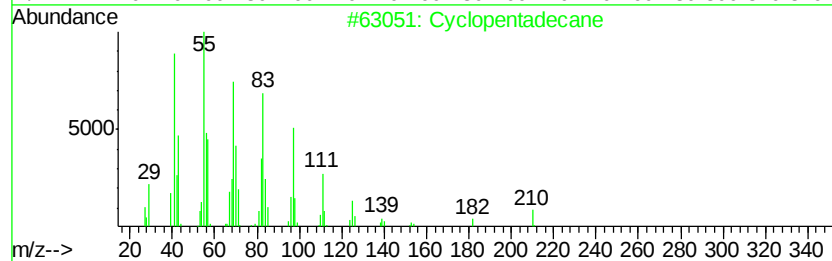
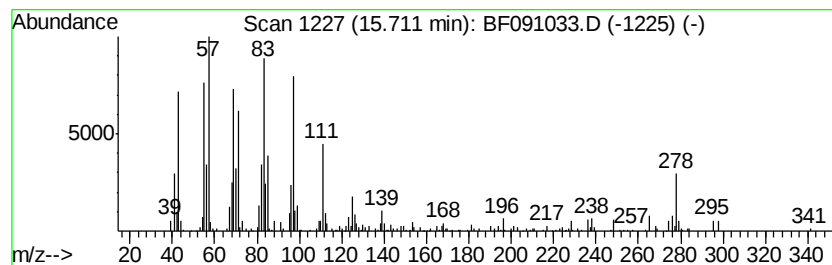
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.71	5.81 ng	317718	Perylene-d12	15.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	89
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	83
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	83
4	17-Pentatriacontene	491	C35H70	006971-40-0	80
5	Cyclotetracosane	336	C24H48	000297-03-0	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
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Acq On : 4 Nov 2016 21:07
Operator : UM/SJ
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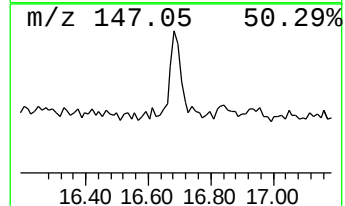
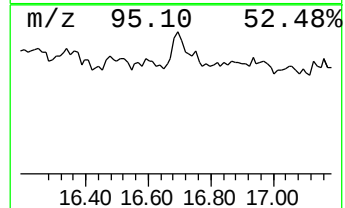
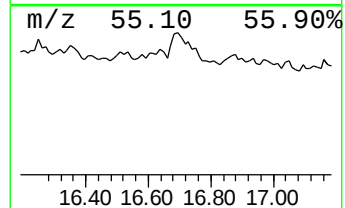
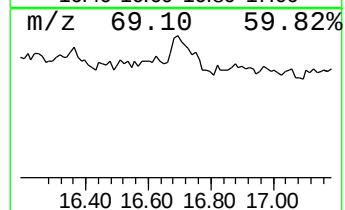
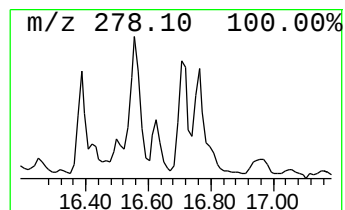
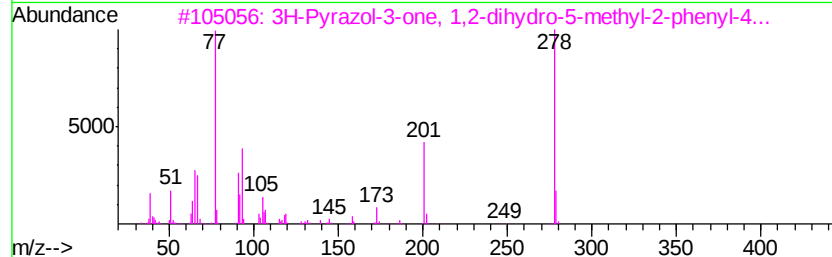
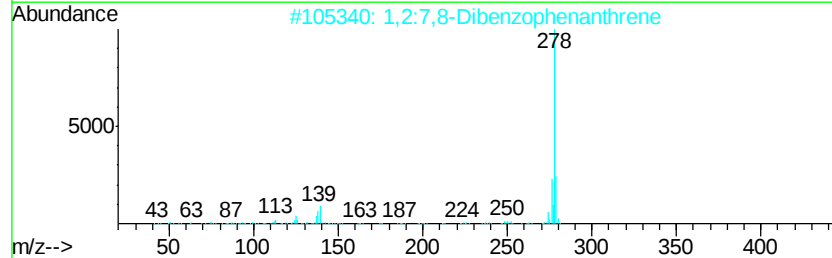
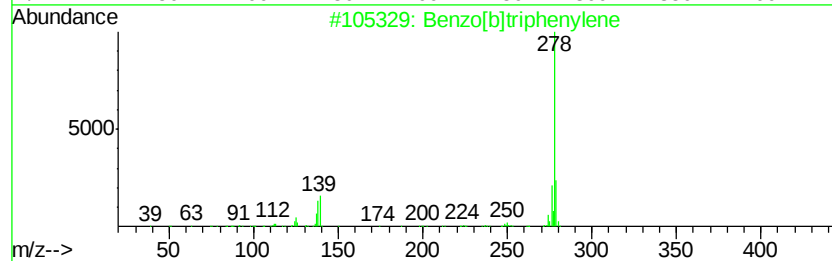
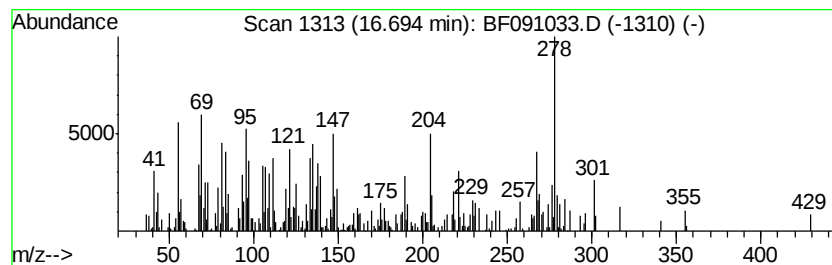
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown16.69 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	4.50 ng	245877	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]triphenylene	278	C22H14	000215-58-7	25
2		1,2:7,8-Dibenzophenanthrene	278	C22H14	000213-46-7	25
3		3H-Pyrazol-3-one, 1,2-dihydro-5-...	278	C16H14N4O	053847-70-4	25
4		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	25
5		2,3,4,5-Tetrahydro-2,4-dimethyl-...	278	C11H10N4O5	020113-63-7	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
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Acq On : 4 Nov 2016 21:07
Operator : UM/SJ
Sample : H5526-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	20.5	ng	1111900	1	6.70	1086540	20.0
unknown6.48	6.48	88.6	ng	4811720	1	6.70	1086540	20.0
Phthalic anhydride	8.75	3.1	ng	222698	2	7.98	1443700	20.0
Tridecane	10.66	2.4	ng	186052	4	11.22	1540850	20.0
n-Hexadecanoic acid	11.77	3.0	ng	231180	4	11.22	1540850	20.0
Bromoacetic acid,...	13.71	5.4	ng	544926	5	13.85	2031320	20.0
Imidazolo[2,1-b]t...	14.52	3.0	ng	305439	5	13.85	2031320	20.0
Perylene	15.13	5.5	ng	298841	6	15.24	1093760	20.0
Cyclopentadecane	15.71	5.8	ng	317718	6	15.24	1093760	20.0
unknown16.69	16.69	4.5	ng	245877	6	15.24	1093760	20.0