

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
 Data File : BF096359.D
 Acq On : 1 Jul 2017 1:56
 Operator : SJ/MA
 Sample : I3930-07
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B2-12.5-15

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-BF062717.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	4.957	483	488	496	rVB	471856	629121	16.02%	1.959%
2	5.375	554	559	562	rBV	3743138	3907654	99.50%	12.165%
3	6.393	726	732	735	rBV	3524753	3927365	100.00%	12.227%
4	6.528	750	755	758	rBV	3638021	3647302	92.87%	11.355%
5	6.757	790	794	798	rBV	1195820	960631	24.46%	2.991%
6	6.828	802	806	809	rBV	99593	89381	2.28%	0.278%
7	6.916	814	821	824	rBV	2823861	2557279	65.11%	7.961%
8	7.316	880	889	892	rBV	2286220	2299276	58.55%	7.158%
9	7.404	901	904	910	rVB4	61176	79007	2.01%	0.246%
10	7.687	950	952	956	rVB4	49299	45513	1.16%	0.142%
11	8.039	1008	1012	1015	rBV	1524232	1259930	32.08%	3.922%
12	8.339	1056	1063	1066	rVB6	42211	74671	1.90%	0.232%
13	8.475	1083	1086	1088	rBV	65318	65956	1.68%	0.205%
14	9.075	1185	1188	1190	rBV	87078	67808	1.73%	0.211%
15	9.116	1190	1195	1198	rVB	2926981	2653091	67.55%	8.260%
16	9.510	1258	1262	1264	rBV	496835	437550	11.14%	1.362%
17	9.528	1264	1265	1268	rVB	60998	47215	1.20%	0.147%
18	9.739	1298	1301	1304	rVB	55290	43962	1.12%	0.137%
19	9.792	1306	1310	1314	rBV	1234597	1050411	26.75%	3.270%
20	10.233	1383	1385	1388	rVB	73850	64726	1.65%	0.202%
21	10.457	1417	1423	1426	rBV	28271	43721	1.11%	0.136%
22	10.575	1439	1443	1447	rBV	1731739	1553510	39.56%	4.836%
23	10.710	1463	1466	1473	rVB	80741	94505	2.41%	0.294%
24	11.269	1557	1561	1564	rBV	931517	848663	21.61%	2.642%
25	11.810	1649	1653	1662	rBV	173802	194865	4.96%	0.607%
26	12.592	1783	1786	1788	rBV2	68357	63290	1.61%	0.197%
27	12.674	1797	1800	1804	rBV3	42181	48046	1.22%	0.150%
28	12.857	1827	1831	1834	rBV	2090745	1887486	48.06%	5.876%
29	13.339	1910	1913	1917	rVB	85032	79825	2.03%	0.249%
30	13.404	1920	1924	1927	rBV3	68961	85558	2.18%	0.266%
31	13.557	1947	1950	1956	rVB3	55984	55722	1.42%	0.173%
32	13.757	1980	1984	1991	rBV	270870	303271	7.72%	0.944%
33	13.898	2005	2008	2012	rBV	908286	904846	23.04%	2.817%
34	14.392	2089	2092	2096	rBV5	53357	98306	2.50%	0.306%

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ALS Vial : 36 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B2-12.5-15

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.321	2244	2250	2254	rVB	485390	668464	17.02%	2.081%
36	15.474	2273	2276	2281	rVB4	121300	177108	4.51%	0.551%
37	16.010	2363	2367	2382	rVB2	230269	555088	14.13%	1.728%
38	16.427	2433	2438	2445	rVB	306409	550765	14.02%	1.715%

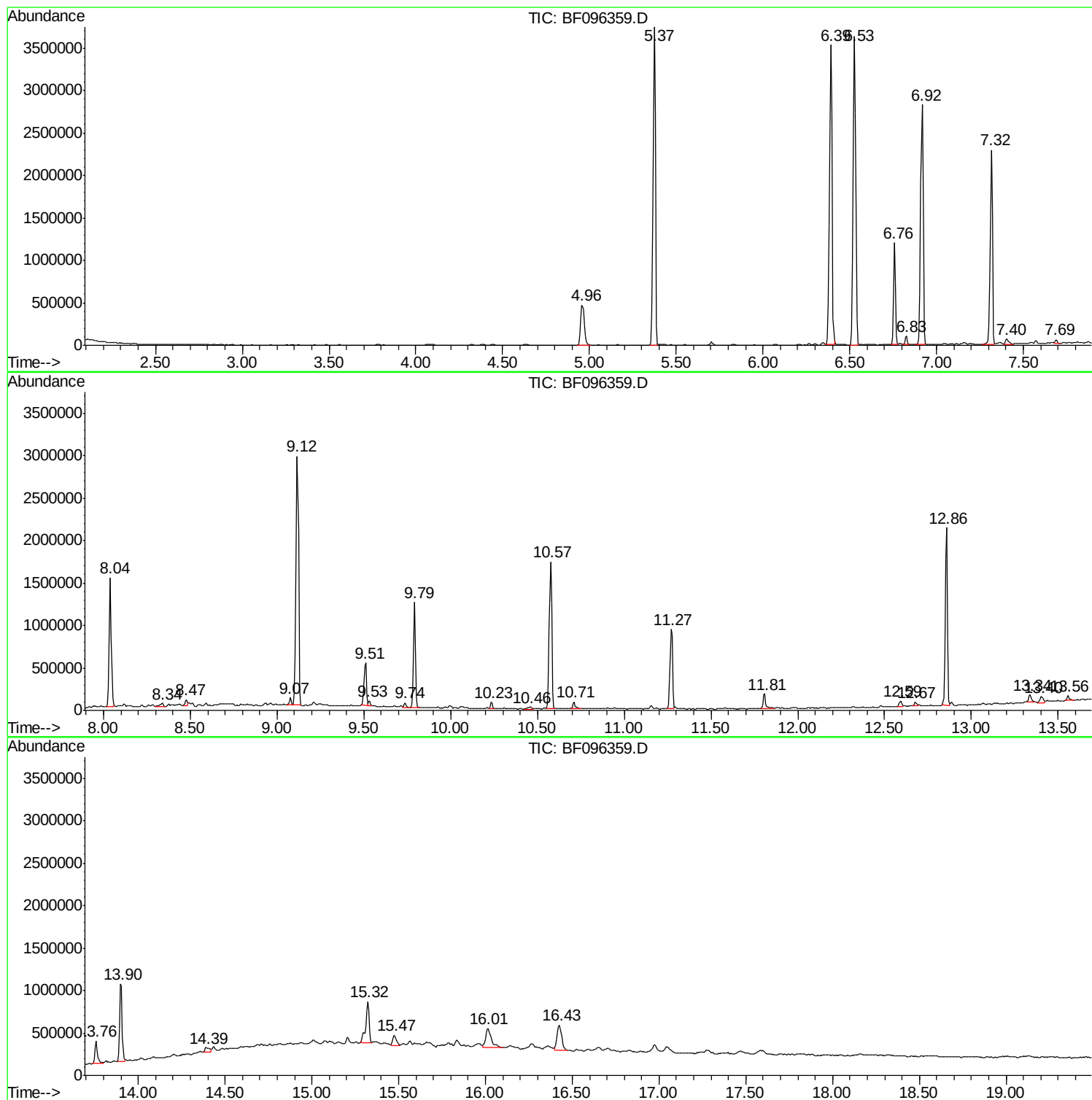
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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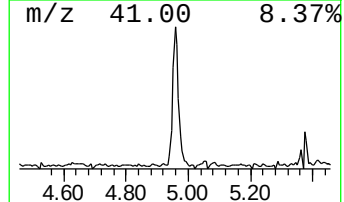
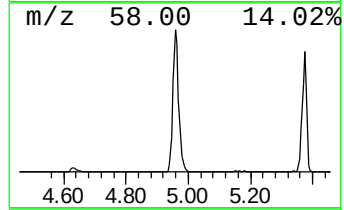
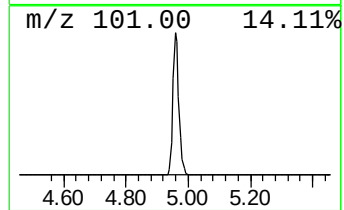
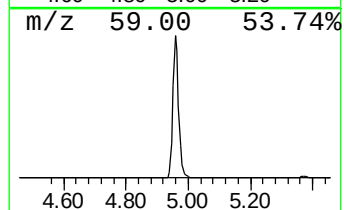
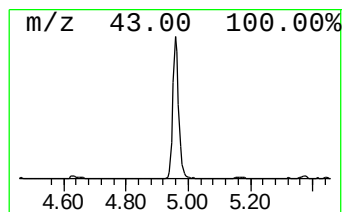
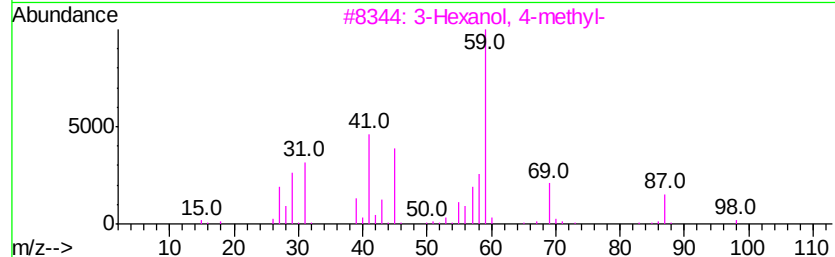
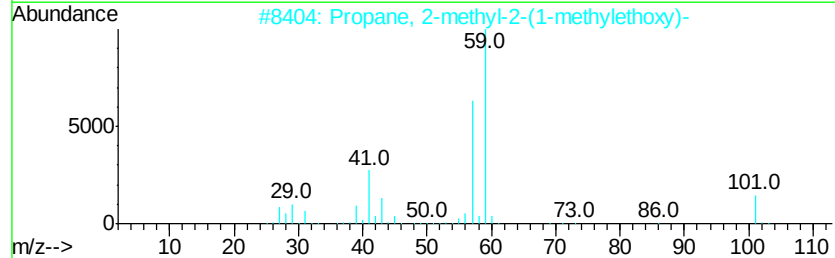
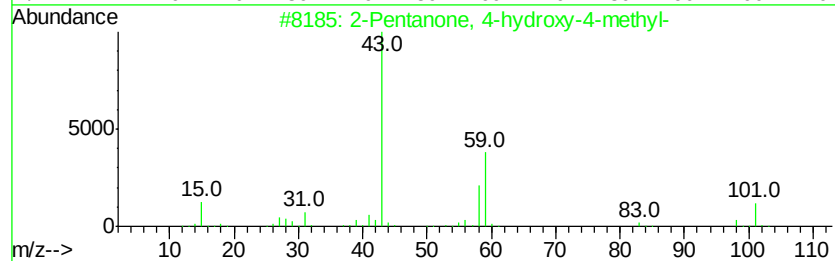
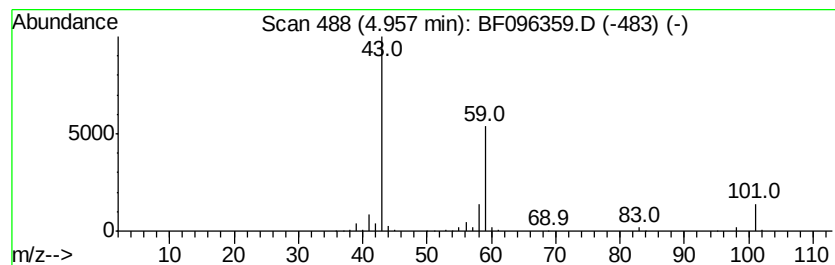
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	13.10 ng	629121	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		3-Hexanol	102	C6H14O	000623-37-0	33



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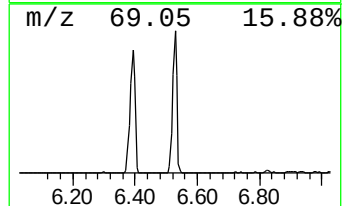
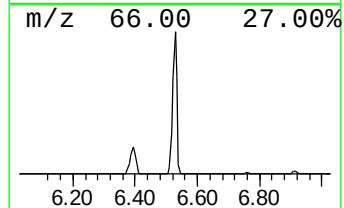
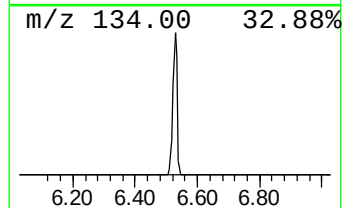
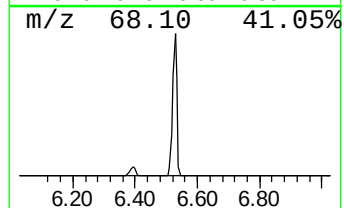
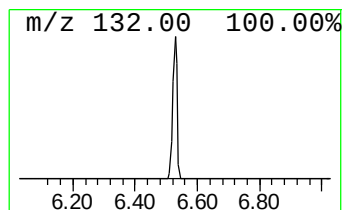
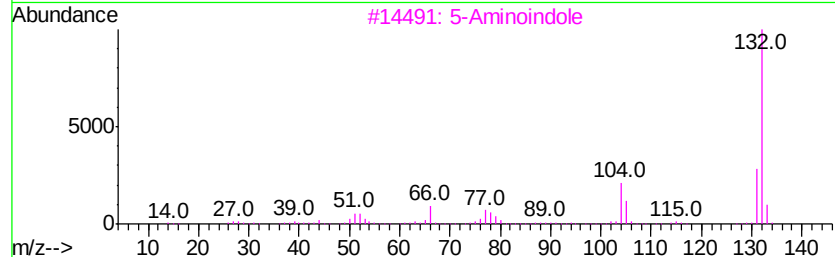
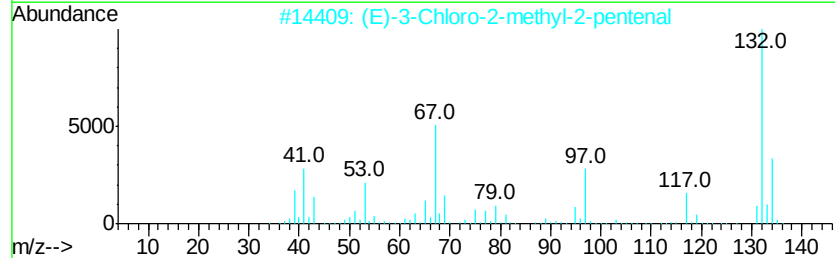
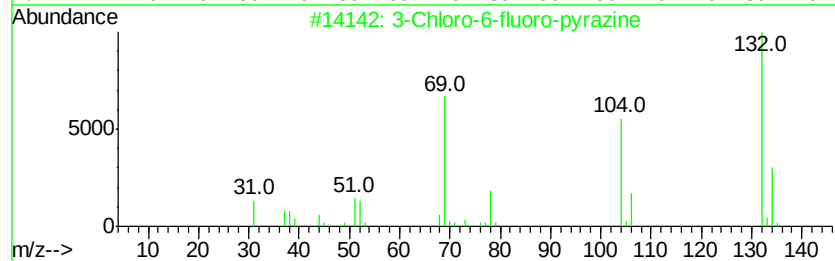
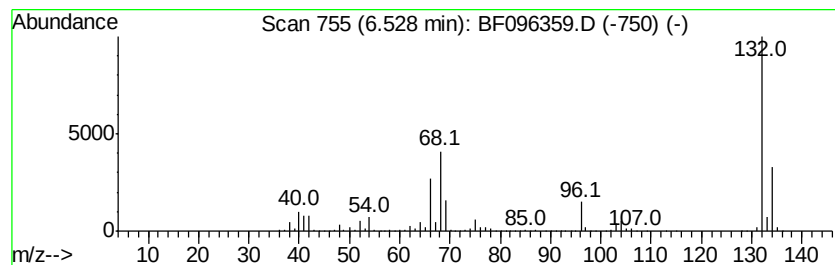
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	75.94 ng	3647300	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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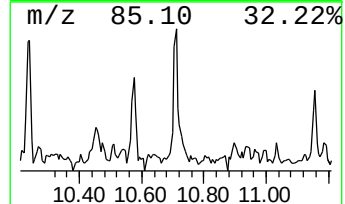
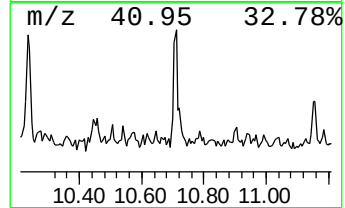
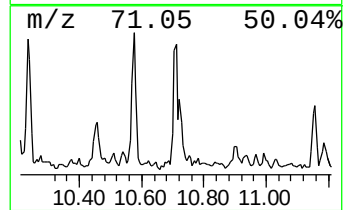
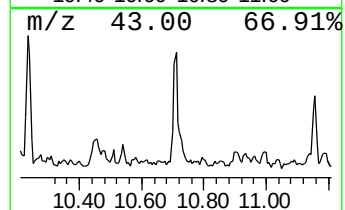
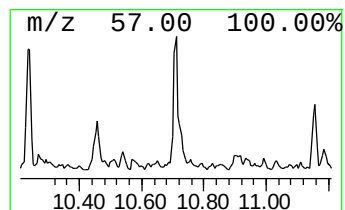
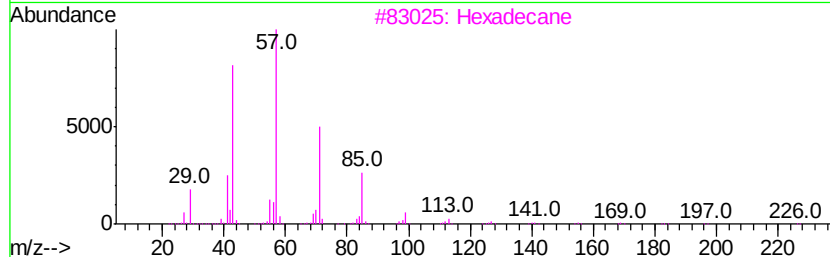
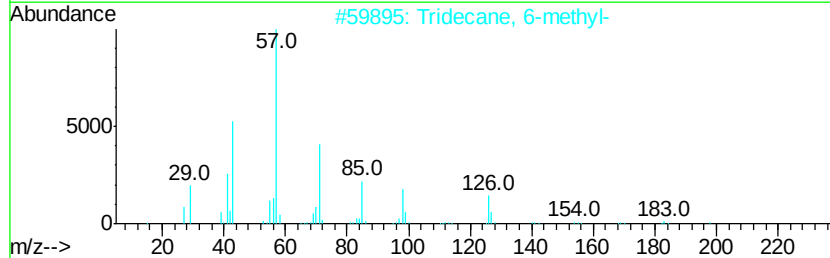
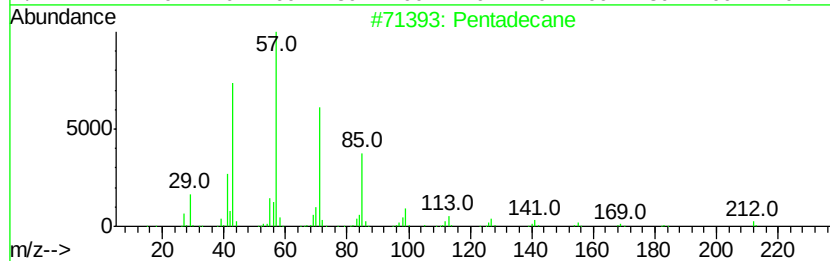
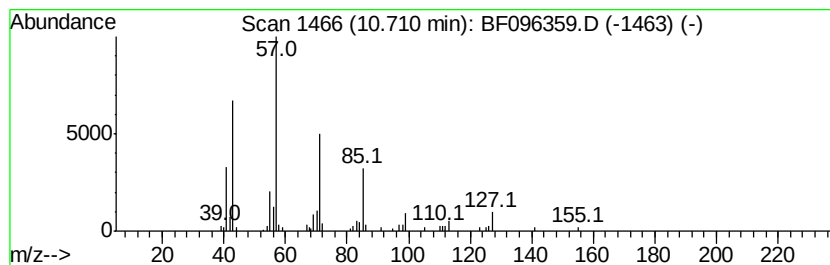
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	2.23 ng	94505	Phenanthrene-d10	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	90
2	Tridecane, 6-methyl-		198	C14H30	013287-21-3	83
3	Hexadecane		226	C16H34	000544-76-3	83
4	Heptadecane, 8-methyl-		254	C18H38	013287-23-5	80
5	Nonadecane		268	C19H40	000629-92-5	80



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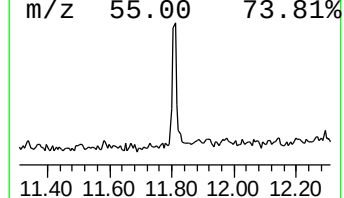
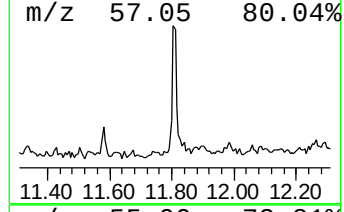
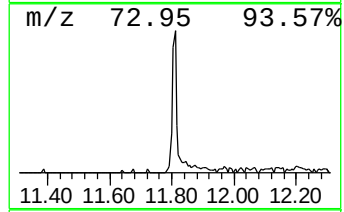
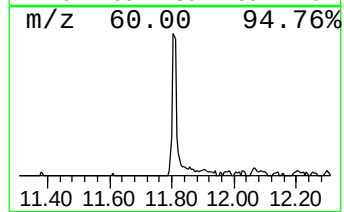
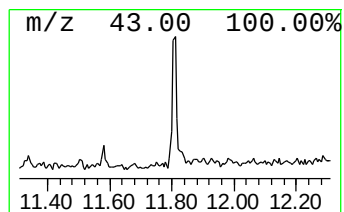
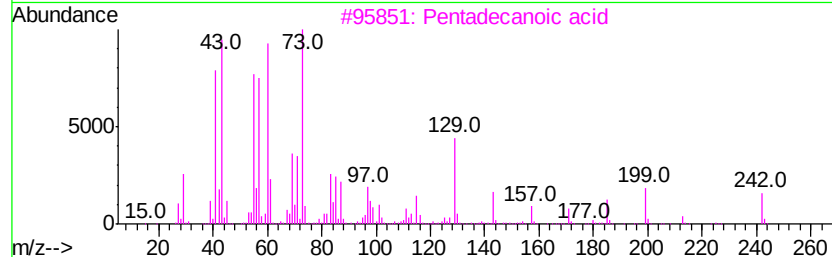
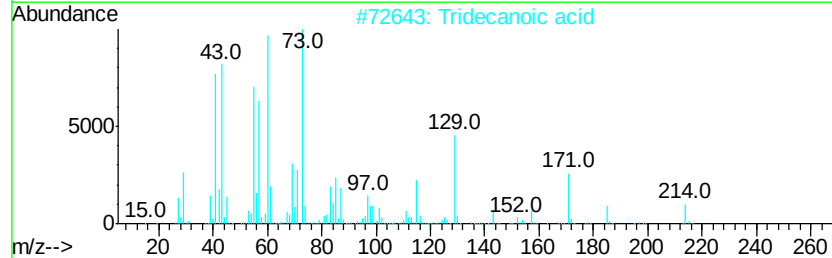
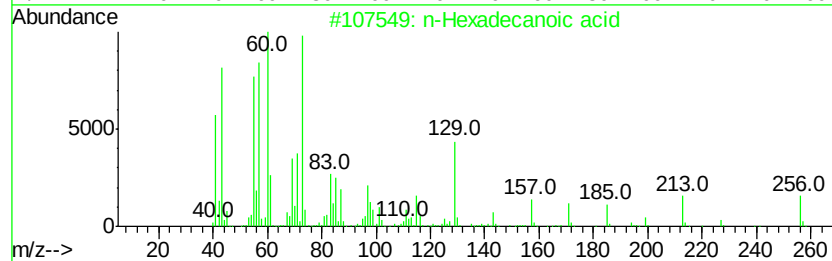
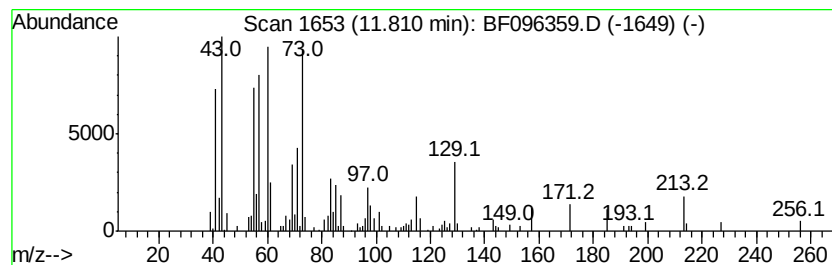
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	4.59 ng	194865	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	30



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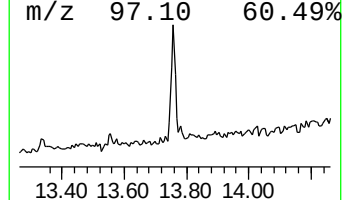
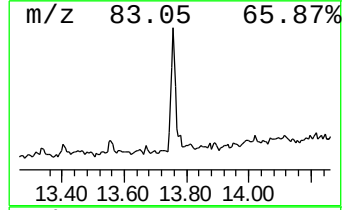
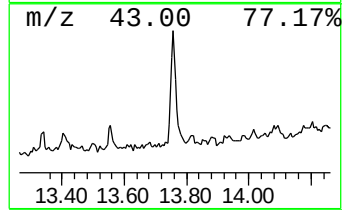
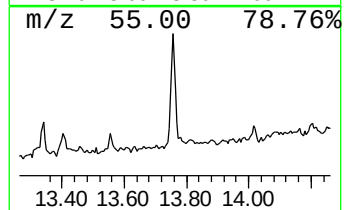
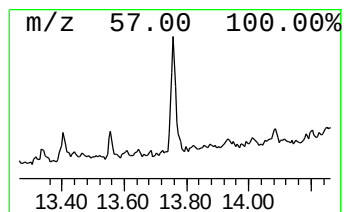
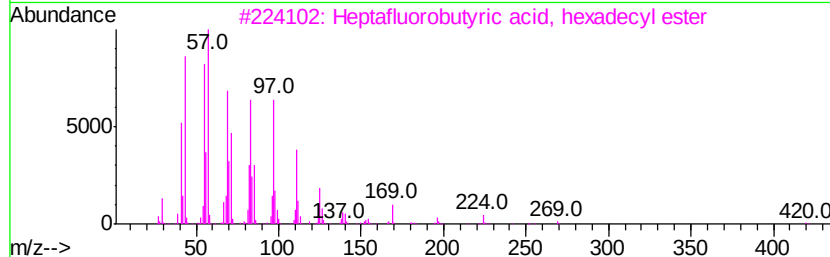
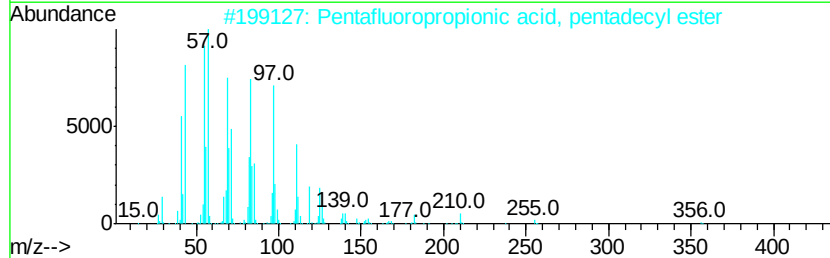
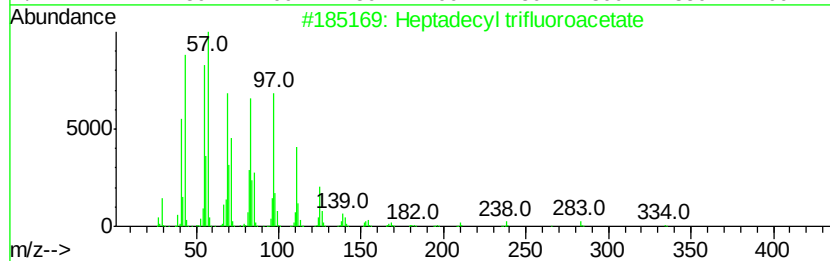
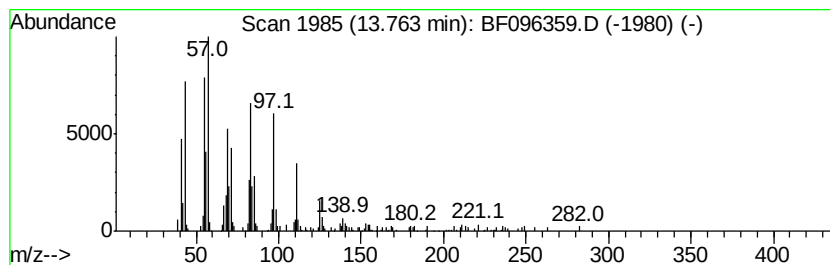
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.76	6.70 ng	303271	Chrysene-d12	13.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptafluorobutvric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



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ALS Vial : 36 Sample Multiplier: 1

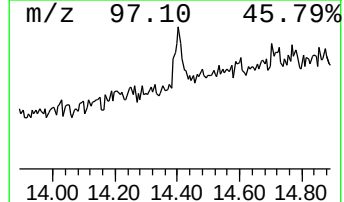
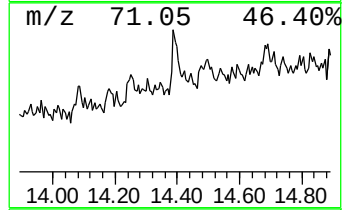
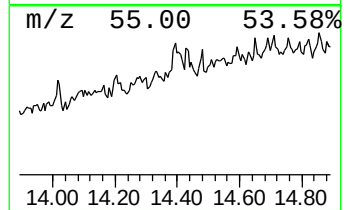
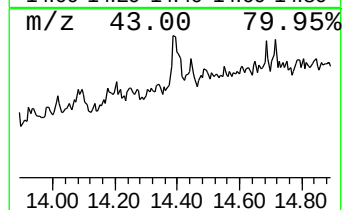
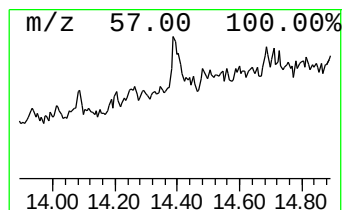
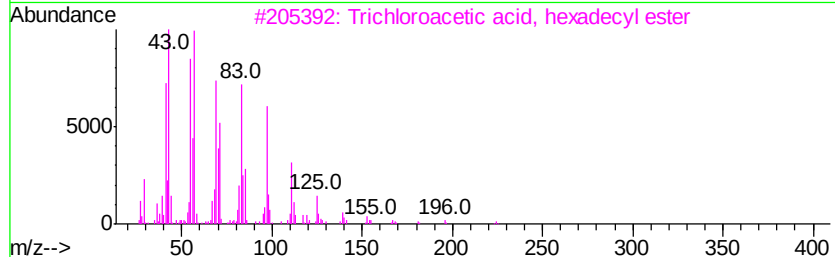
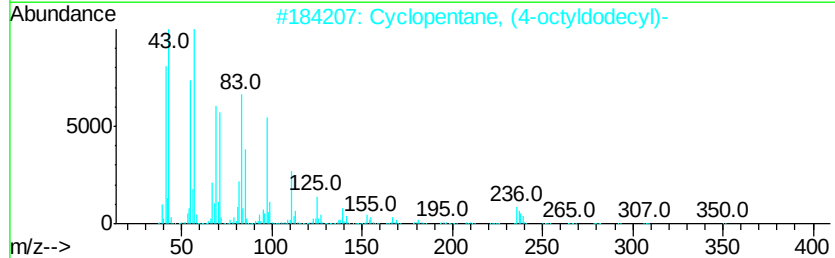
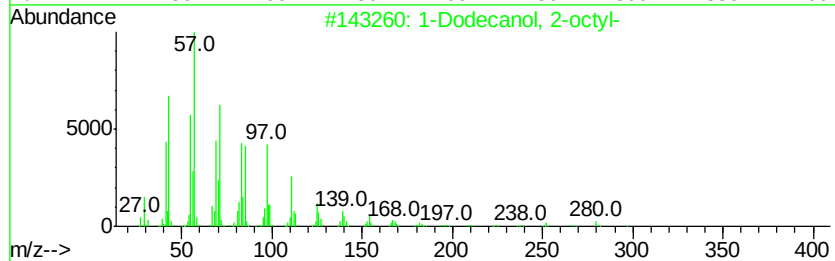
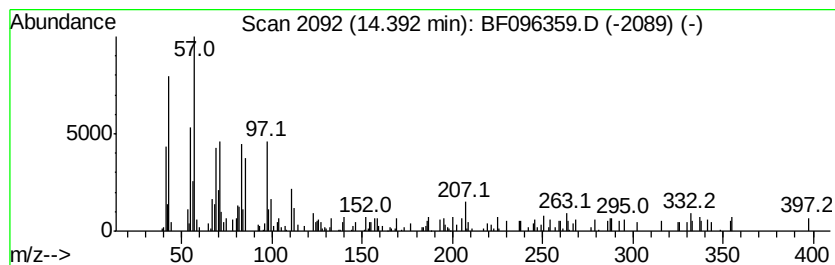
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BNA_F
ClientSampleId :
B2-12.5-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	2.17 ng	98306	Chrysene-d12	13.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Dodecanol, 2-octyl-	298 C20H42O	005333-42-6	81
2	Cyclopentane, (4-octyldodecyl)-	350 C25H50	005638-09-5	72
3	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	52
4	1-Octadecanethiol	286 C18H38S	002885-00-9	50
5	1-Docosene	308 C22H44	001599-67-3	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096359.D
Acq On : 1 Jul 2017 1:56
Operator : SJ/MA
Sample : I3930-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B2-12.5-15

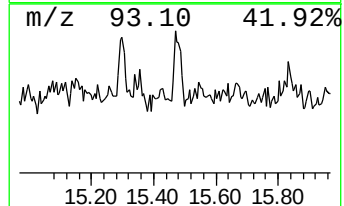
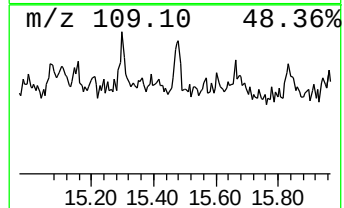
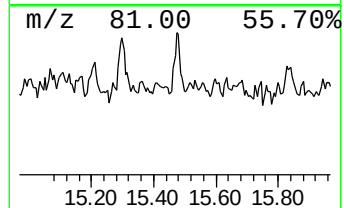
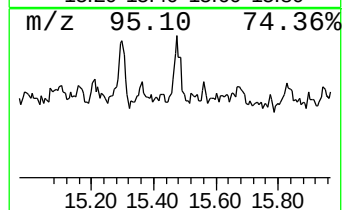
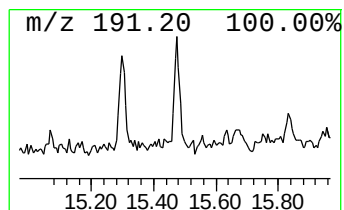
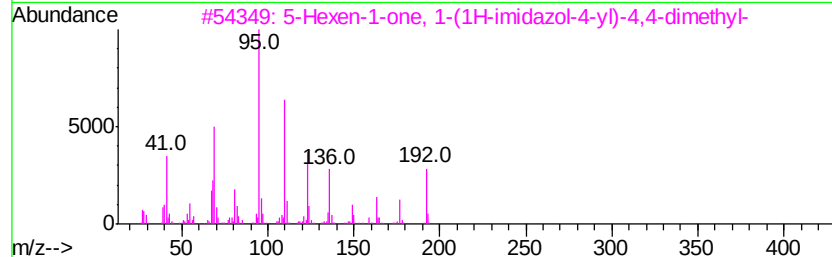
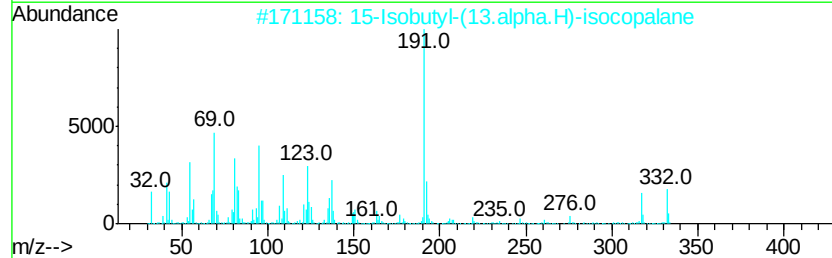
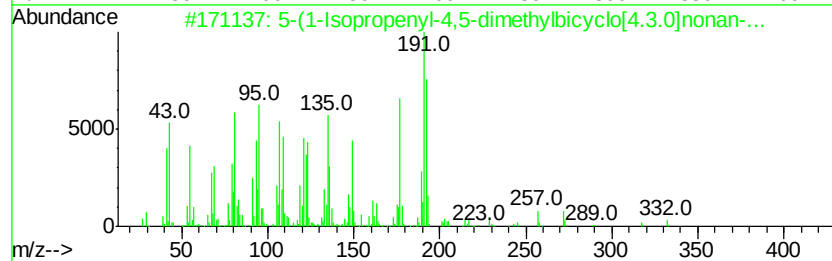
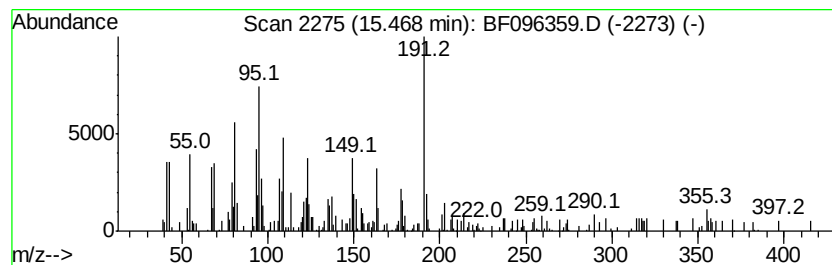
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-(1-Isopropenyl-4,5-dimeth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	5.30 ng	177108	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-(1-Isopropenyl-4,5-dimethylbic...	332	C22H36O2	1000195-69-8	50
2		15-Isobutyl-(13.alpha.H)-isocopa...	332	C24H44	087953-47-7	49
3		5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	30
4		Benzene, 1,1'-[1,2-cyclohexanedi...	300	C18H20S2	1000362-19-6	30
5		Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096359.D
Acq On : 1 Jul 2017 1:56
Operator : SJ/MA
Sample : I3930-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B2-12.5-15

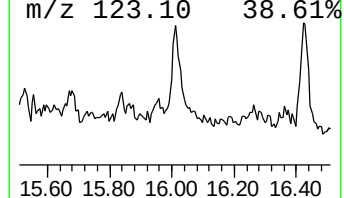
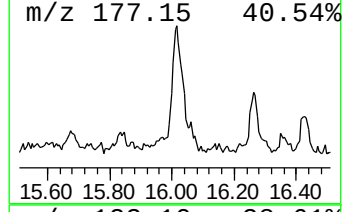
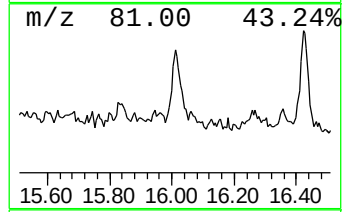
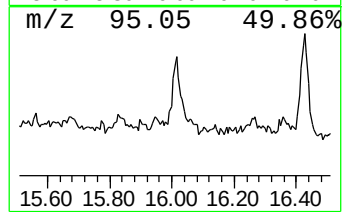
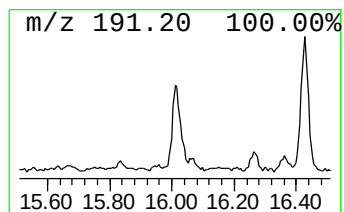
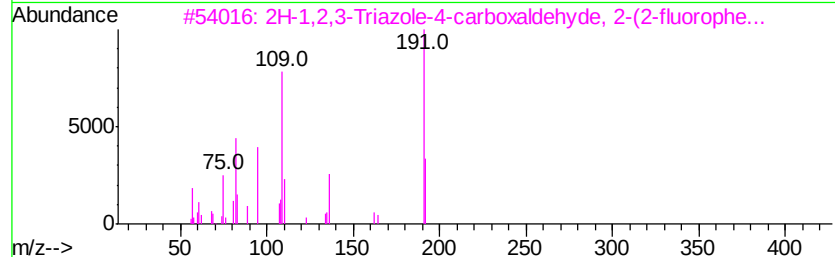
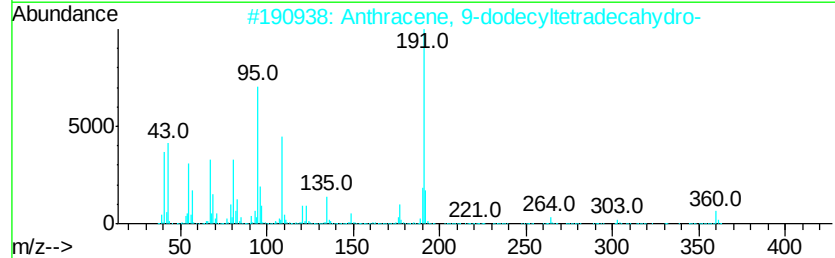
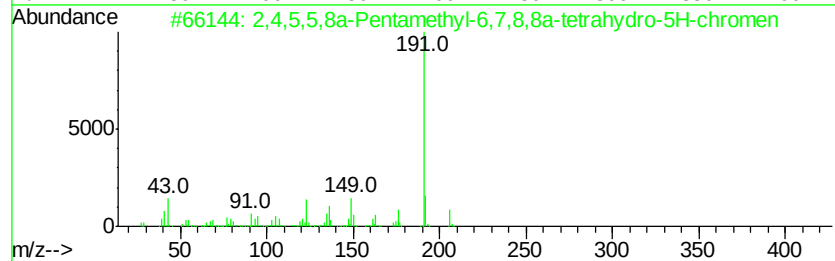
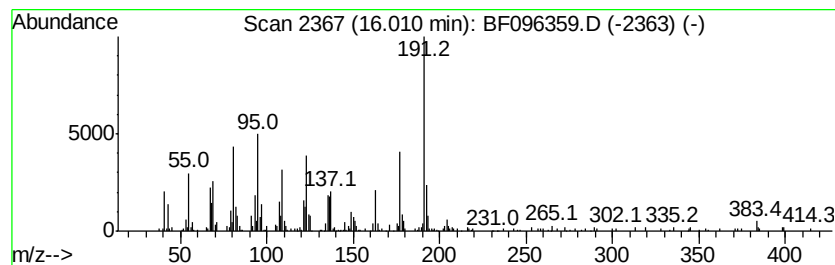
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	16.61 ng	555088	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	37
2		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	37
3		2H-1,2,3-Triazole-4-carboxaldehv...	191	C9H6FN3O	051306-43-5	35
4		1,4-Benzenediol, 2-[(1,4,4a,5,6,...	314	C21H30O2	039707-55-6	25
5		Pentanoic acid, 4-methyl-2-(2,5-...	278	C13H18N4O3	1000294-63-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096359.D
Acq On : 1 Jul 2017 1:56
Operator : SJ/MA
Sample : I3930-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

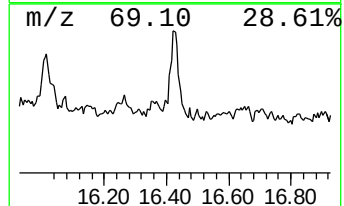
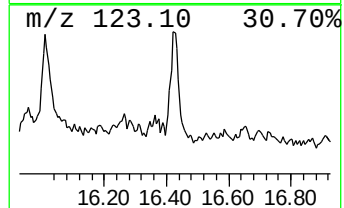
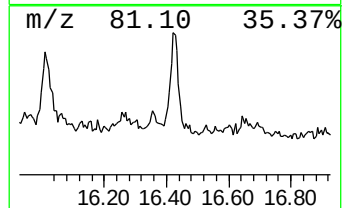
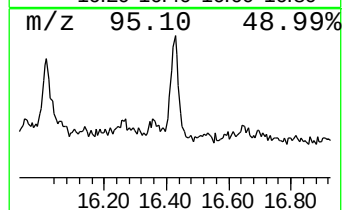
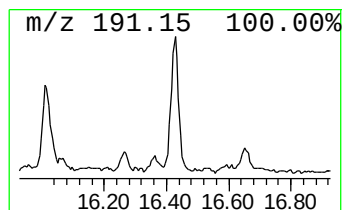
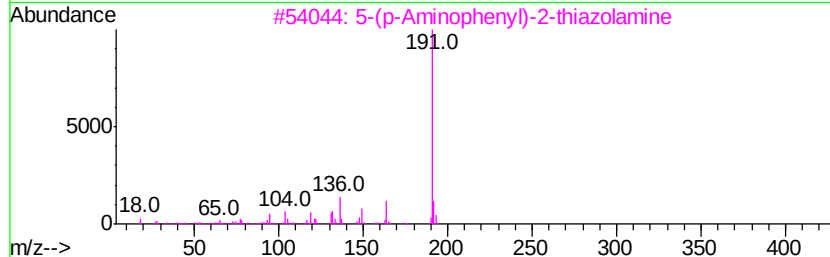
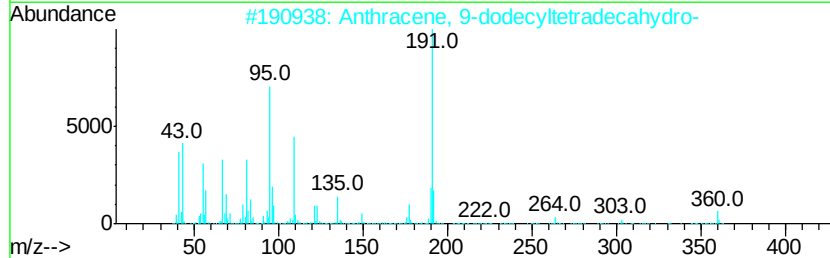
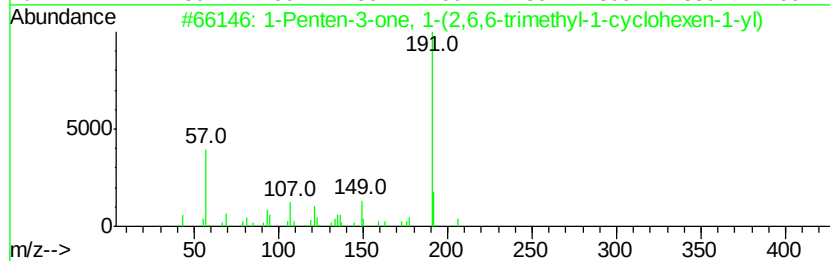
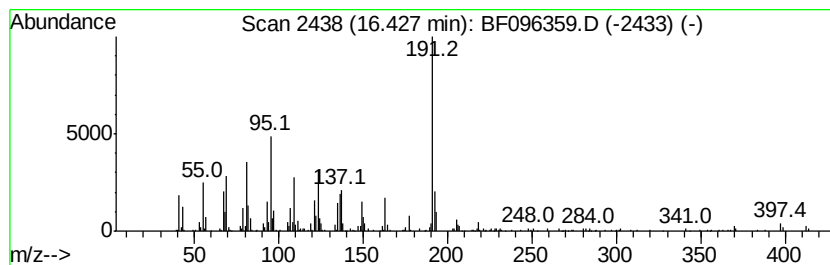
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Penten-3-one, 1-(2,6,6-tr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	16.48 ng	550765	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Penten-3-one, 1-(2,6,6-trimeth...	206 C14H22O	000127-43-5 50
2		Anthracene, 9-dodecyltetradecahy...	360 C26H48	055401-75-7 40
3		5-(p-Aminophenyl)-2-thiazolamine	191 C9H9N3S	090349-87-4 38
4		Pyrido[3,4-d]pyridazin-1(2H)-one...	191 C8H9N5O	1000263-69-7 30
5		Silane, dimethyl(dimethyl(2,6-di...	356 C18H36O3Si2	1000347-91-3 30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096359.D
Acq On : 1 Jul 2017 1:56
Operator : SJ/MA
Sample : I3930-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B2-12.5-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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
2-Pentanone, 4-hy...	4.96	13.1	ng	629121	1	6.76	960631	20.0
unknown6.53	6.53	75.9	ng	3647300	1	6.76	960631	20.0
Pentadecane	10.71	2.2	ng	94505	4	11.27	848663	20.0
n-Hexadecanoic acid	11.81	4.6	ng	194865	4	11.27	848663	20.0
Heptadecyl triflu...	13.76	6.7	ng	303271	5	13.90	904846	20.0
1-Dodecanol, 2-oc...	14.39	2.2	ng	98306	5	13.90	904846	20.0
5-(1-Isopropenyl-...	15.47	5.3	ng	177108	6	15.32	668464	20.0
unknown16.01	16.01	16.6	ng	555088	6	15.32	668464	20.0
1-Penten-3-one, 1...	16.43	16.5	ng	550765	6	15.32	668464	20.0