

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052815\
 Data File : BF079544.D
 Acq On : 28 May 2015 15:07
 Operator : TP/IZ
 Sample : G2359-05 2X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-29AS

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-BF052615.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	1.370	14	16	23	rVB	135952	211904	2.85%	0.891%
2	1.564	32	33	40	rVV	229412	358298	4.82%	1.507%
3	1.667	40	42	88	rVB	3507685	7431638	100.00%	31.255%
4	5.233	352	354	365	rVB	538193	708402	9.53%	2.979%
5	6.559	468	470	478	rBV	692473	772048	10.39%	3.247%
6	6.673	478	480	483	rVV	651502	794654	10.69%	3.342%
7	6.959	503	505	508	rBV	510033	471580	6.35%	1.983%
8	7.142	519	521	524	rBV	616383	608129	8.18%	2.558%
9	7.656	564	566	569	rBV	433859	451088	6.07%	1.897%
10	8.536	641	643	648	rBV	755461	696104	9.37%	2.928%
11	9.885	759	761	764	rBV	1102431	966525	13.01%	4.065%
12	10.708	830	833	835	rVB	562924	717695	9.66%	3.018%
13	11.679	916	918	921	rBV	568549	595796	8.02%	2.506%
14	12.536	990	993	994	rBV	772749	742160	9.99%	3.121%
15	12.559	994	995	998	rVV	167280	226672	3.05%	0.953%
16	13.291	1053	1059	1067	rBV4	78868	216174	2.91%	0.909%
17	14.034	1121	1124	1126	rBV	407810	392037	5.28%	1.649%
18	14.308	1146	1148	1151	rBV	358006	409567	5.51%	1.723%
19	14.525	1164	1167	1170	rVB	938479	1041205	14.01%	4.379%
20	14.857	1194	1196	1201	rVB4	47807	128035	1.72%	0.538%
21	15.245	1227	1230	1234	rBV2	71670	111129	1.50%	0.467%
22	15.702	1267	1270	1275	rBV	273426	395895	5.33%	1.665%
23	15.805	1275	1279	1283	rBV2	796480	1348139	18.14%	5.670%
24	15.874	1283	1285	1287	rVB	246127	275172	3.70%	1.157%
25	16.114	1304	1306	1310	rBV2	48237	110495	1.49%	0.465%
26	16.514	1339	1341	1349	rVB3	212521	337904	4.55%	1.421%
27	17.085	1387	1391	1396	rBV	209883	497543	6.69%	2.093%
28	17.280	1406	1408	1413	rBV2	150535	355492	4.78%	1.495%
29	17.394	1416	1418	1421	rVV	141260	172084	2.32%	0.724%
30	17.451	1421	1423	1427	rVB	152851	223633	3.01%	0.941%
31	17.520	1427	1429	1435	rBV	766099	975056	13.12%	4.101%
32	18.057	1473	1476	1477	rBV	98771	143065	1.93%	0.602%
33	18.811	1540	1542	1548	rVB2	106979	218787	2.94%	0.920%
34	19.189	1572	1575	1579	rVB	95461	188113	2.53%	0.791%

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Instrument :
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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

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35	19.326	1584	1587	1591	rBV2	137751	310658	4.18%	1.307%
36	20.183	1659	1662	1666	rBV2	63258	174333	2.35%	0.733%

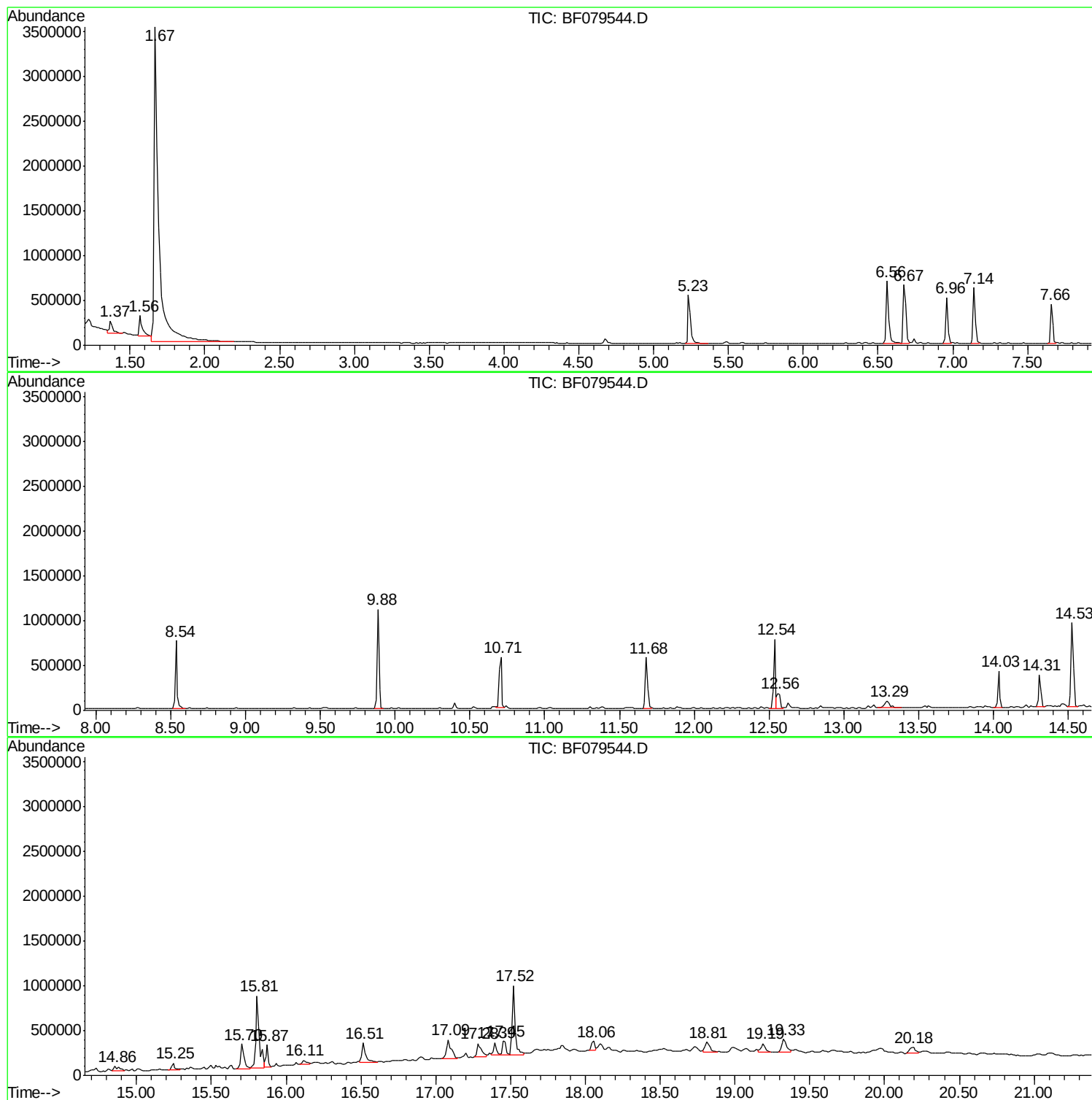
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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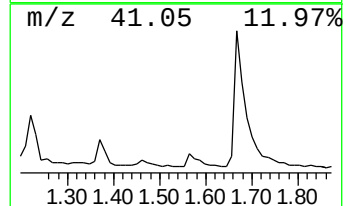
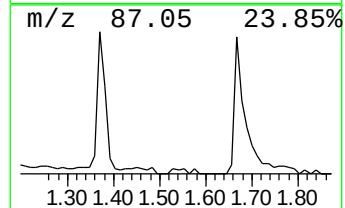
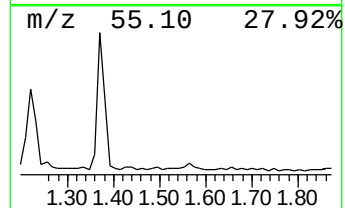
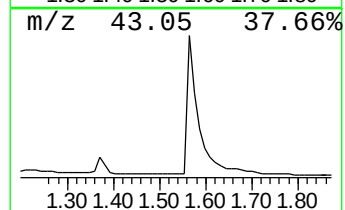
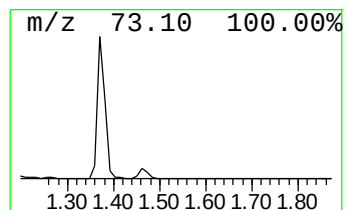
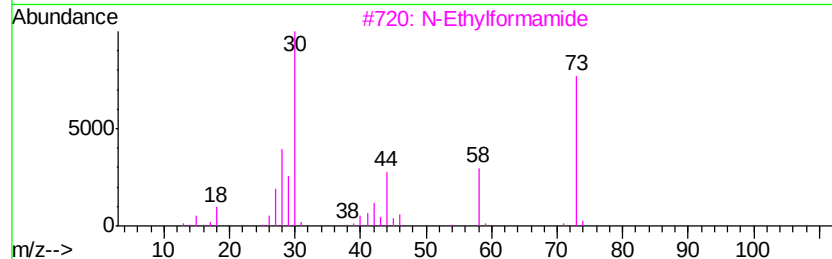
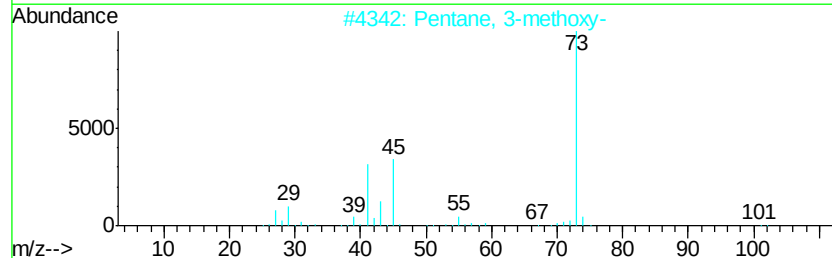
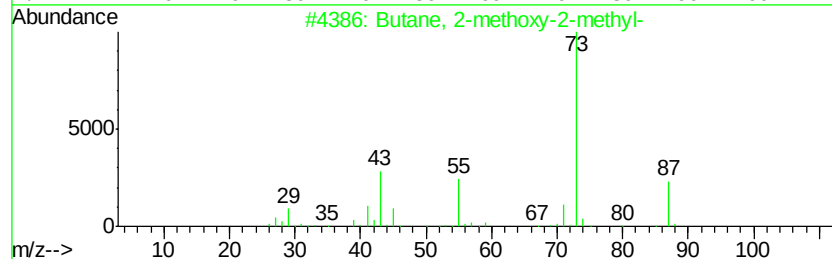
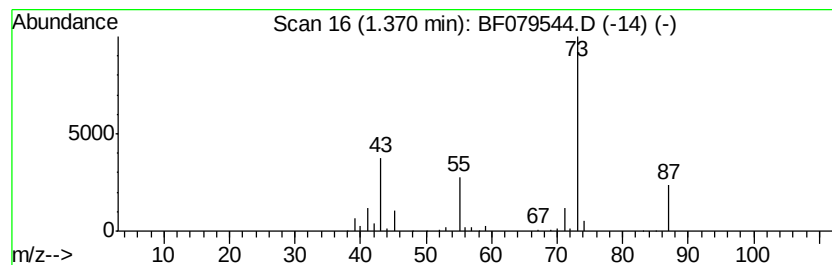
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	8.99 ng	211904	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9



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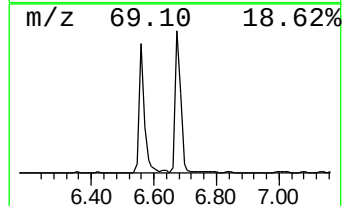
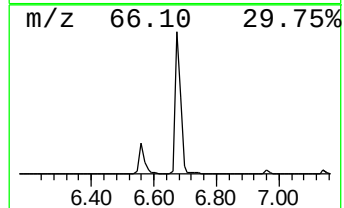
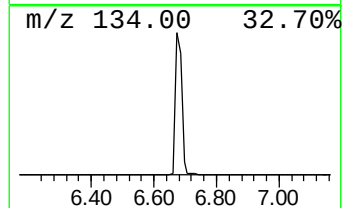
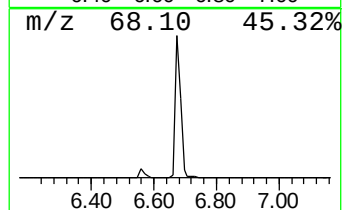
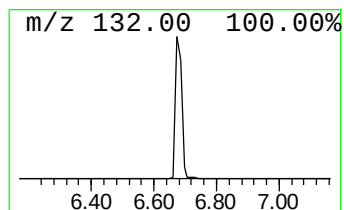
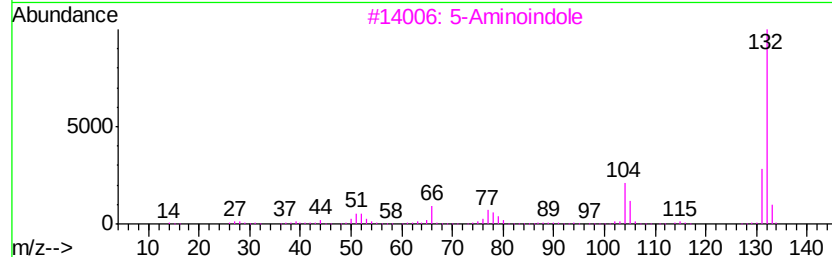
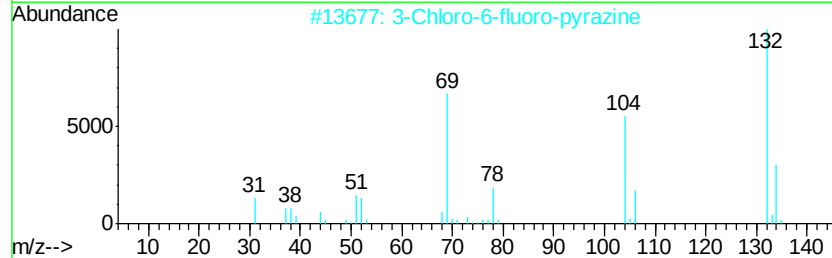
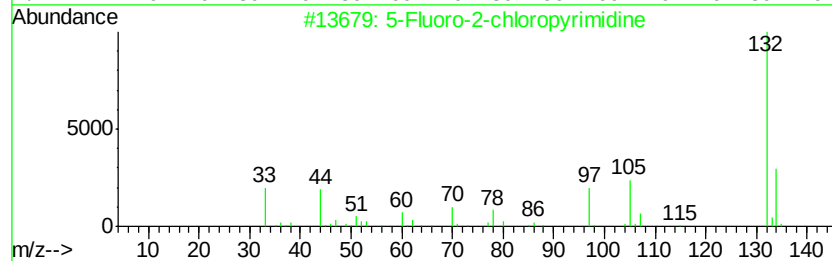
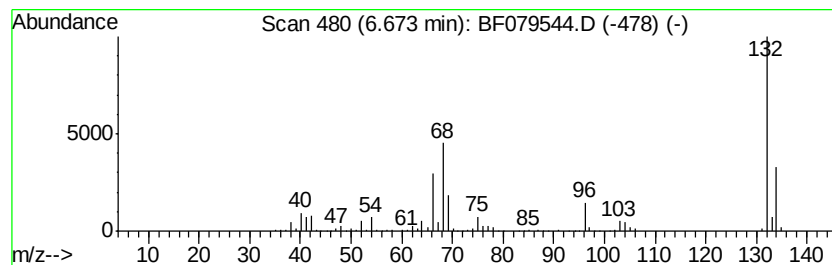
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	33.70 ng	794654	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16	
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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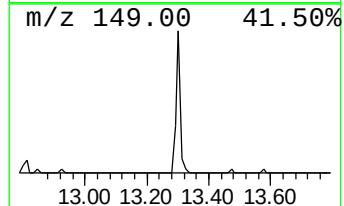
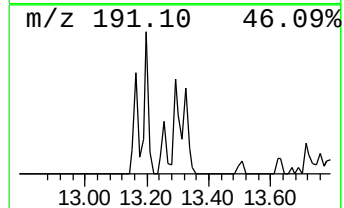
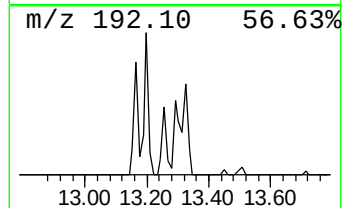
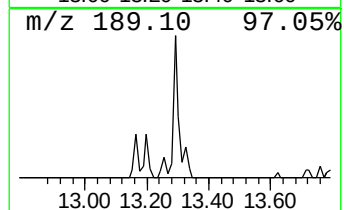
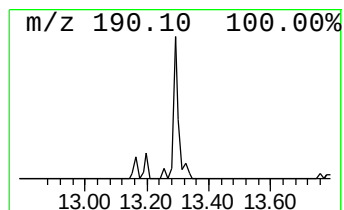
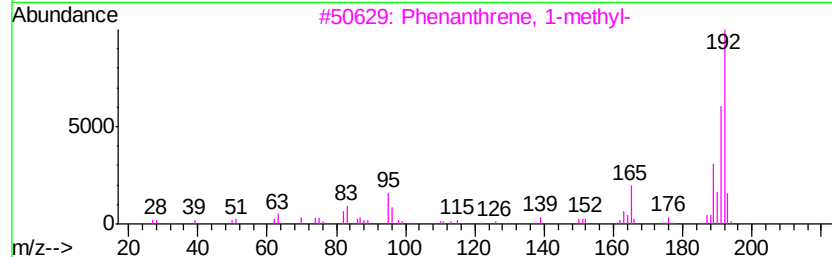
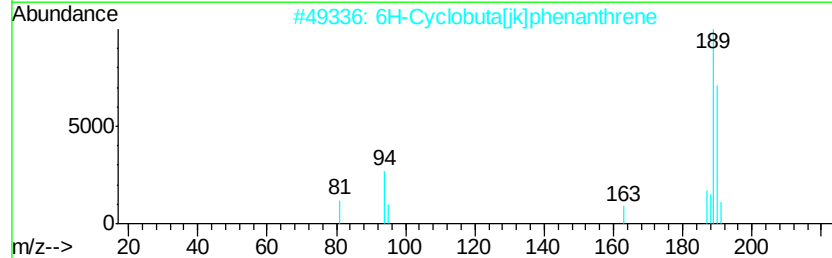
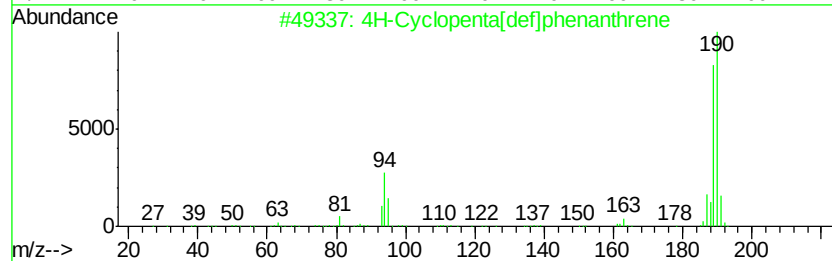
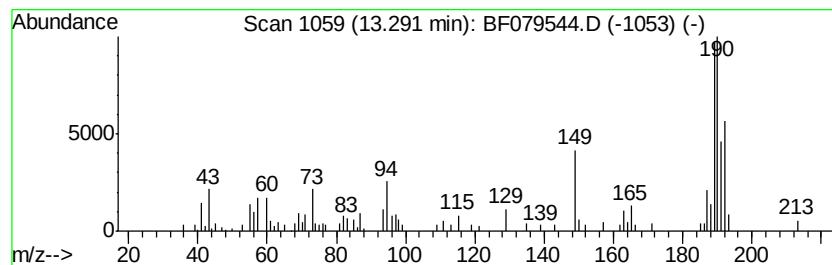
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown13.29 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.29	5.83 ng	216174	Phenanthrene-d10	12.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
2	6H-Cyclobuta[i]kphenanthrene	190	C15H10	083469-43-6	38
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	15
4	Benzene, 1,1'-(2-cyclopropen-1-yl)-	192	C15H12	022825-21-4	15
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	11



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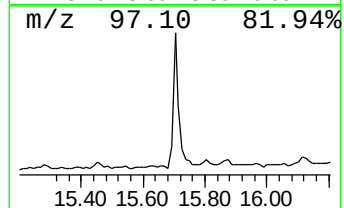
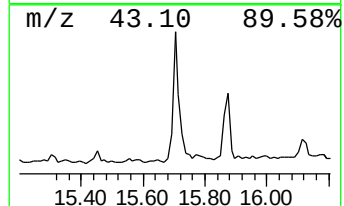
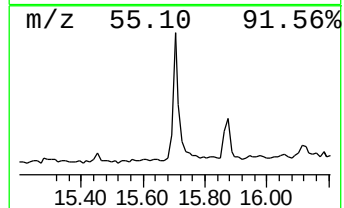
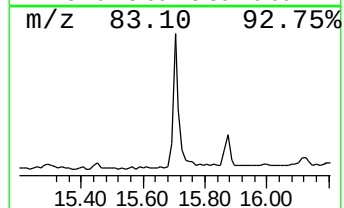
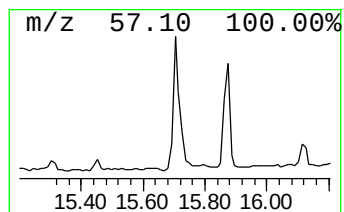
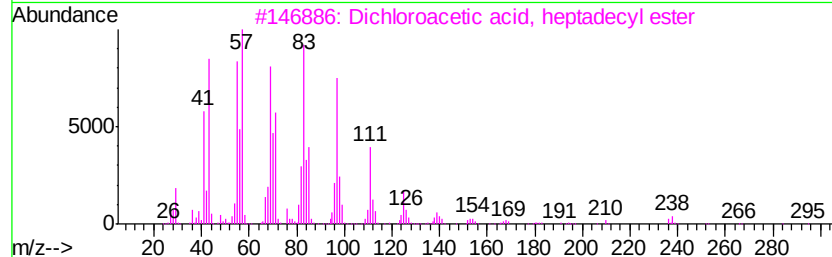
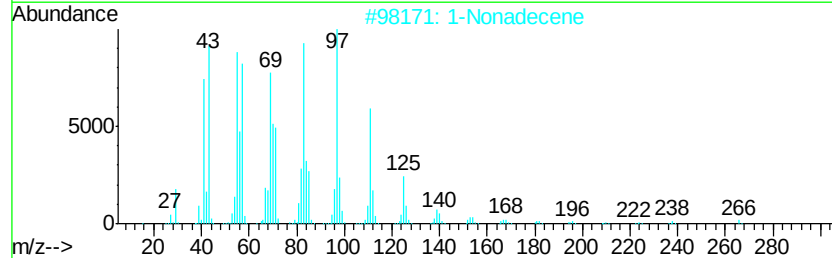
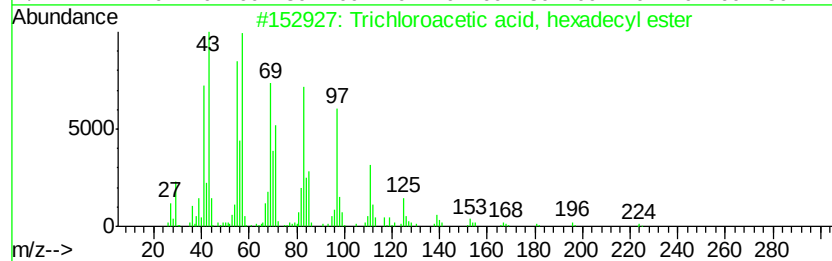
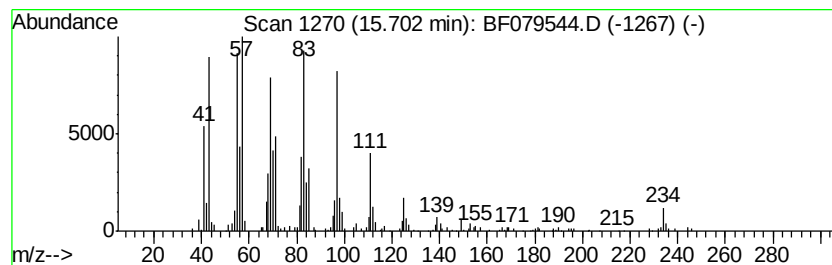
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	5.87 ng	395895	Chrysene-d12	15.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	83



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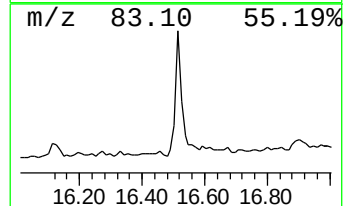
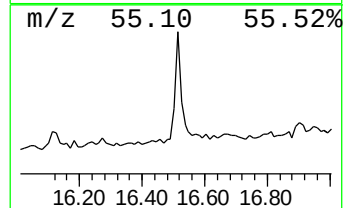
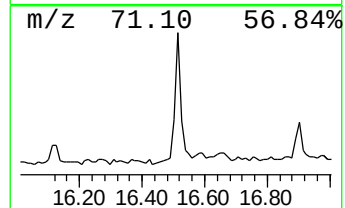
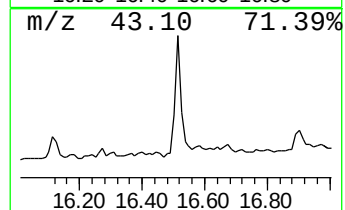
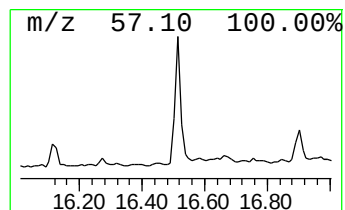
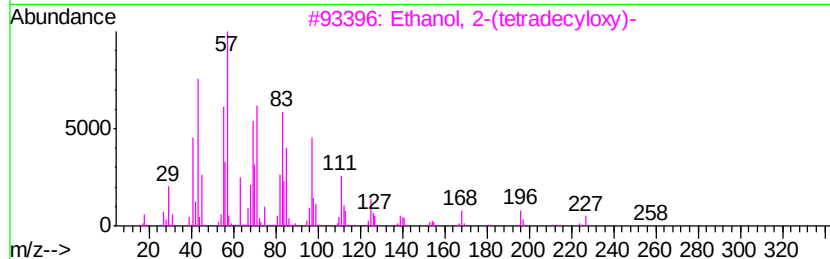
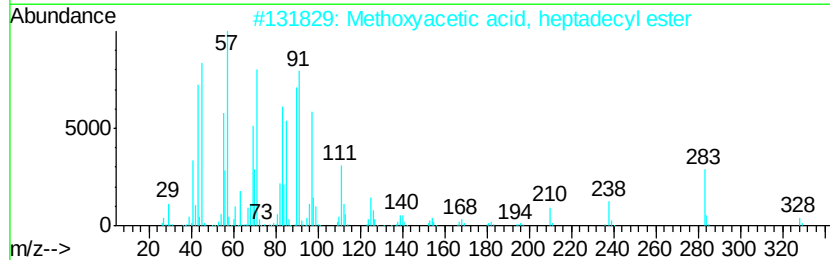
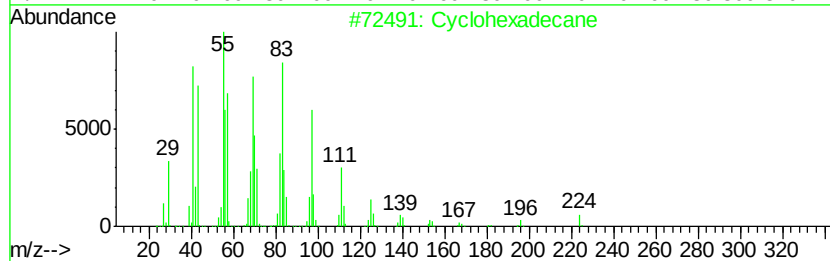
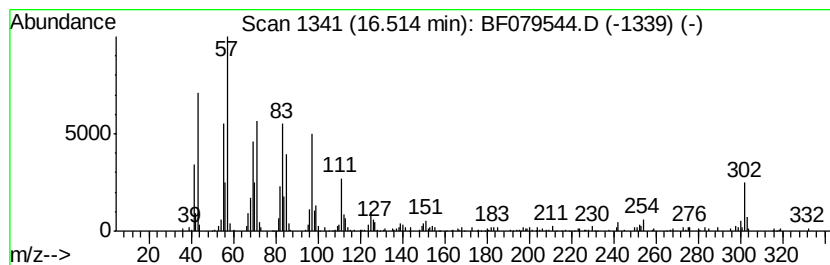
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Cyclohexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.51	5.01 ng	337904	Chrysene-d12	15.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	95
2		Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	83
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	76
4		E-15-Heptadecenal	252	C17H32O	1000130-97-9	70
5		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	68



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ALS Vial : 5 Sample Multiplier: 1

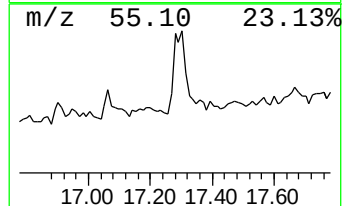
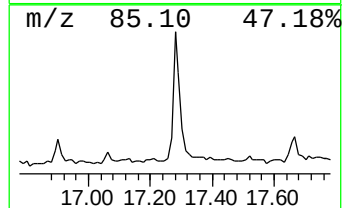
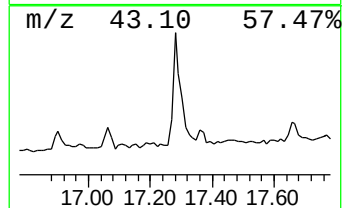
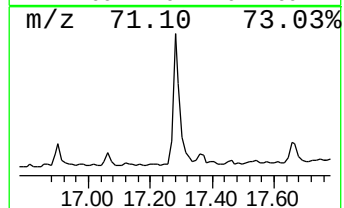
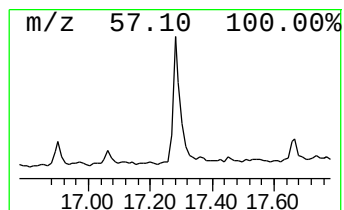
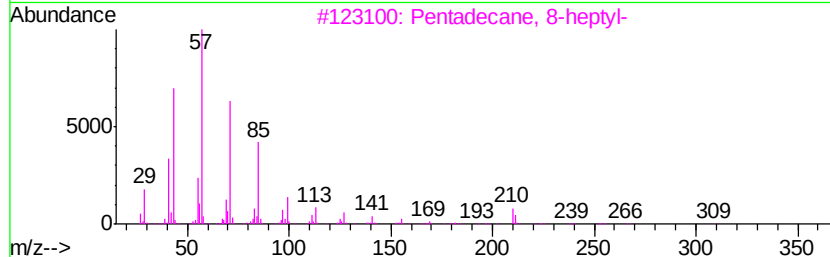
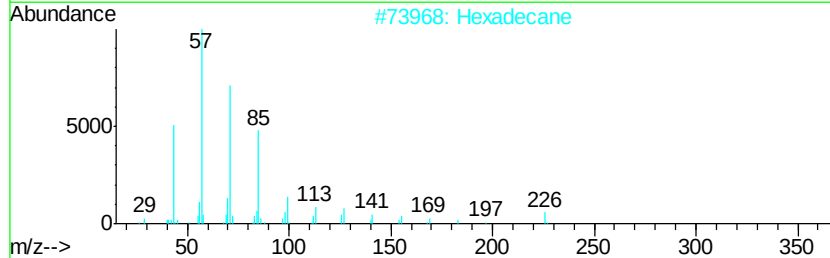
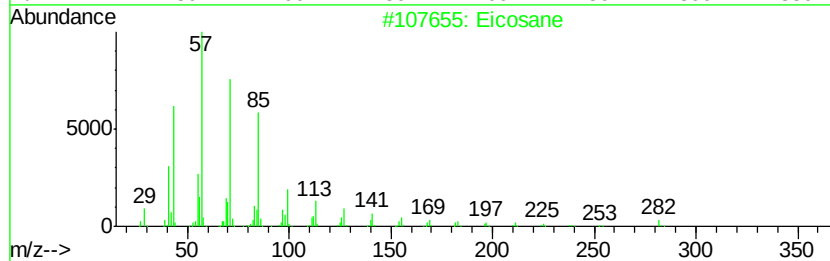
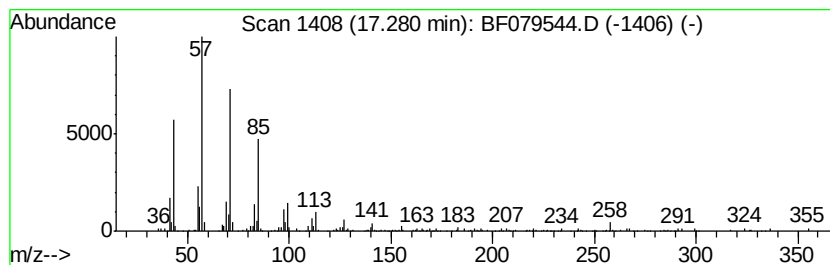
Instrument :
BNA_F
ClientSampleId :
SB-29AS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	7.29 ng	355492	Perylene-d12	17.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	93
2	Hexadecane	226 C16H34	000544-76-3	91
3	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	87
4	Tetracosane	338 C24H50	000646-31-1	87
5	Heneicosane	296 C21H44	000629-94-7	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052815\
Data File : BF079544.D
Acq On : 28 May 2015 15:07
Operator : TP/IZ
Sample : G2359-05 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29AS

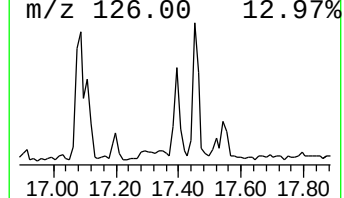
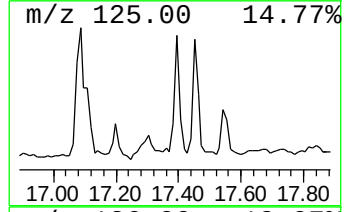
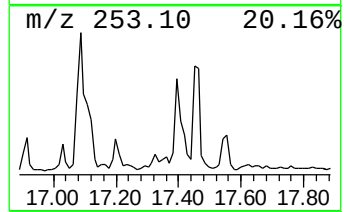
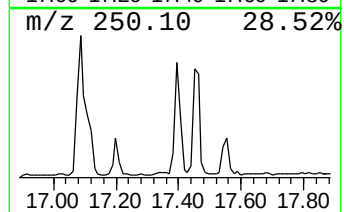
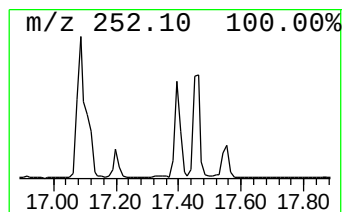
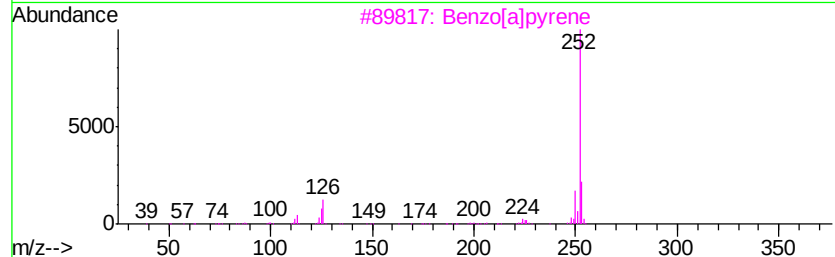
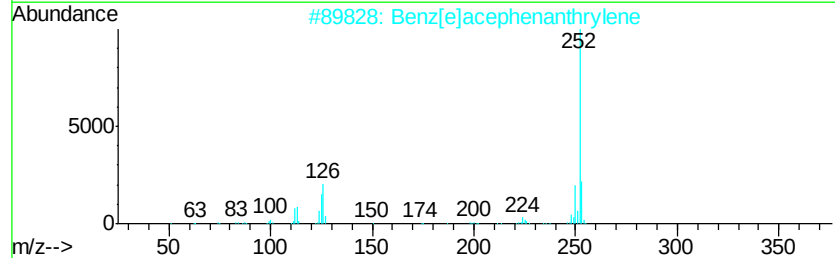
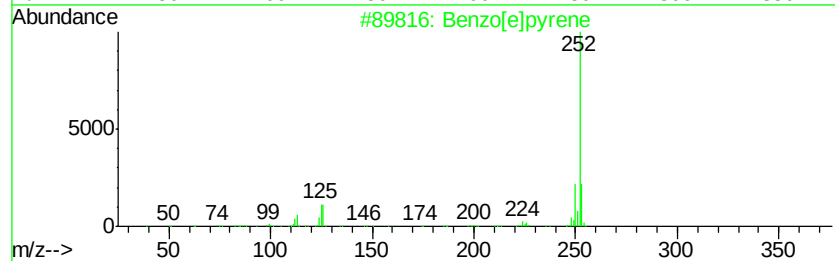
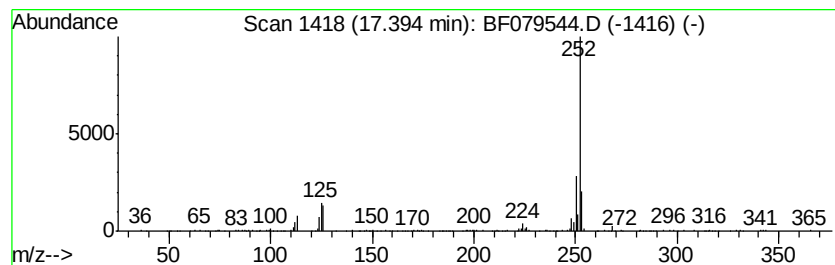
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	3.53 ng	172084	Perylene-d12	17.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]bpvrene	252	C20H12	000192-97-2	94
2			Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	94
3			Benzo[a]bpvrene	252	C20H12	000050-32-8	93
4			Perylene	252	C20H12	000198-55-0	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052815\
Data File : BF079544.D
Acq On : 28 May 2015 15:07
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Sample : G2359-05 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-29AS

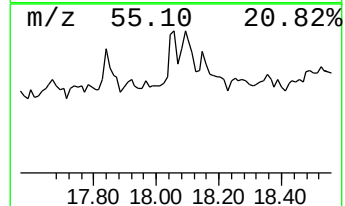
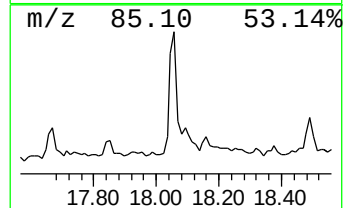
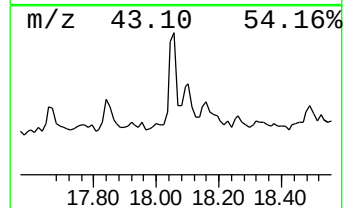
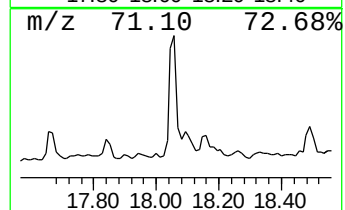
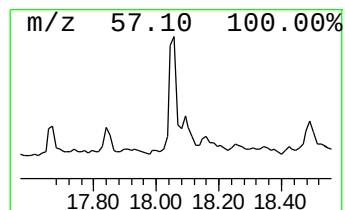
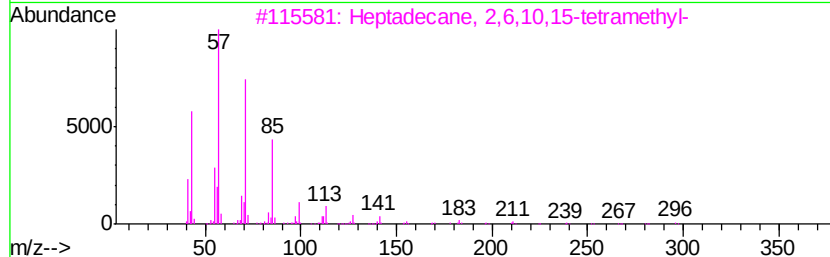
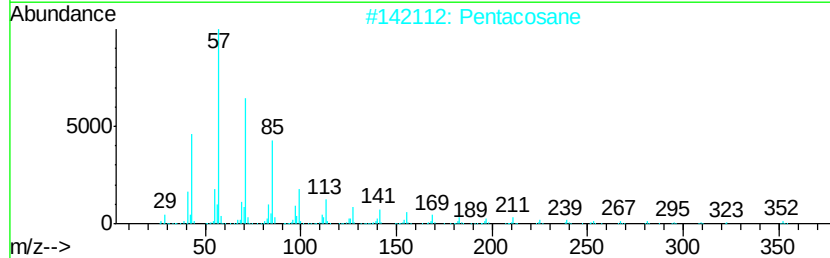
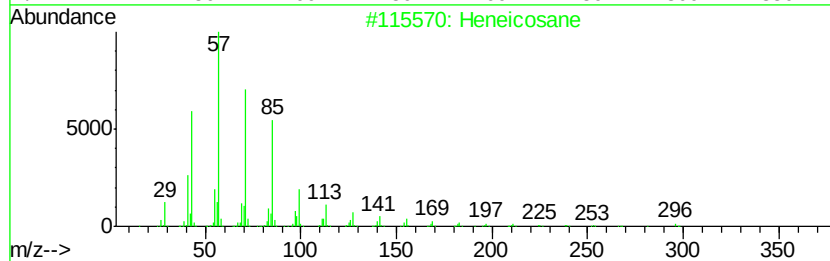
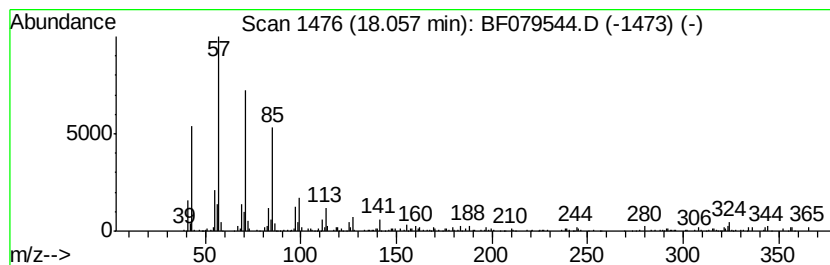
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	2.93 ng	143065	Perylene-d12	17.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	93
2		Pentacosane	352	C25H52	000629-99-2	93
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
4		Octacosane	394	C28H58	000630-02-4	90
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052815\
Data File : BF079544.D
Acq On : 28 May 2015 15:07
Operator : TP/IZ
Sample : G2359-05 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

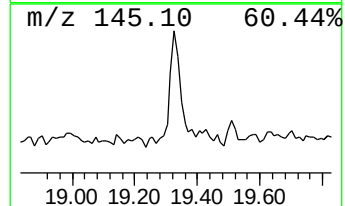
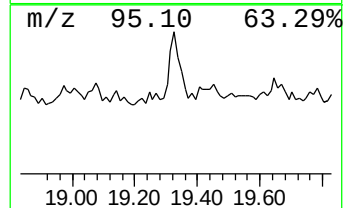
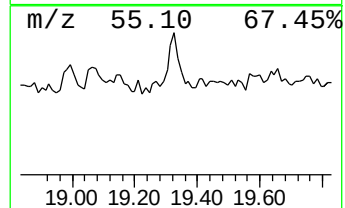
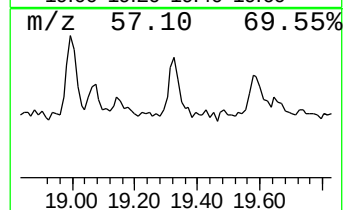
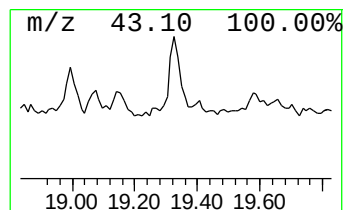
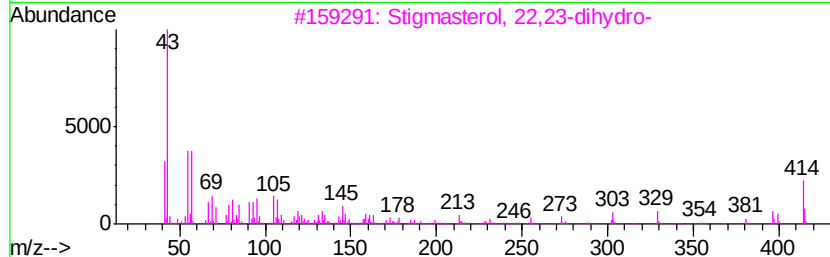
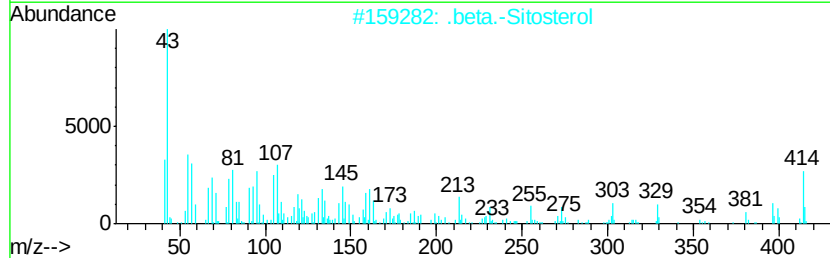
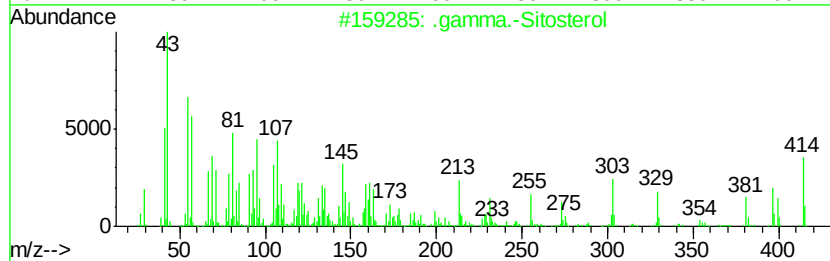
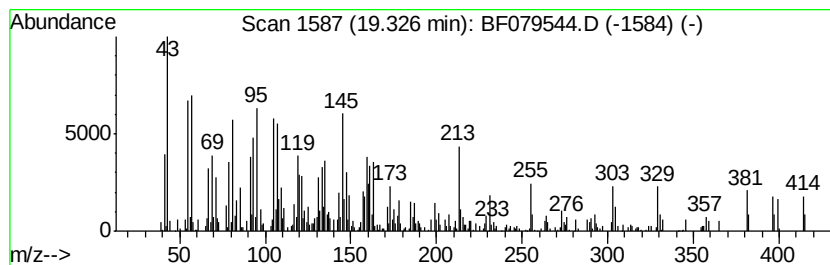
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .gamma.-Sitosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	6.37 ng	310658	Perylene-d12	17.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.gamma.-Sitosterol	414 C29H50O	000083-47-6 90
2		.beta.-Sitosterol	414 C29H50O	000083-46-5 78
3		Stigmasterol, 22,23-dihydro-	414 C29H50O	1000214-20-7 55
4		Kauren-18-ol, acetate, (4.beta.)-	330 C22H34O2	072150-74-4 49
5		Cholest-5-ene, 3-methoxy-, (3.be...	400 C28H48O	001174-92-1 43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052815\
Data File : BF079544.D
Acq On : 28 May 2015 15:07
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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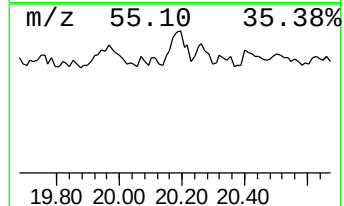
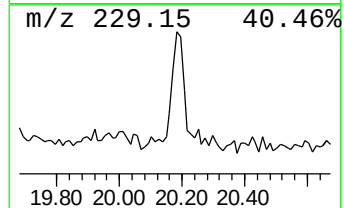
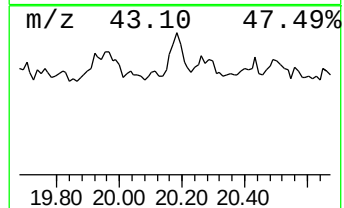
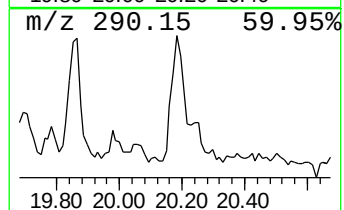
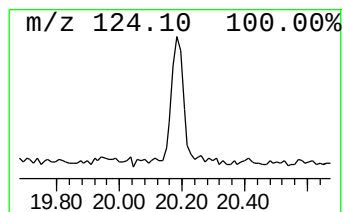
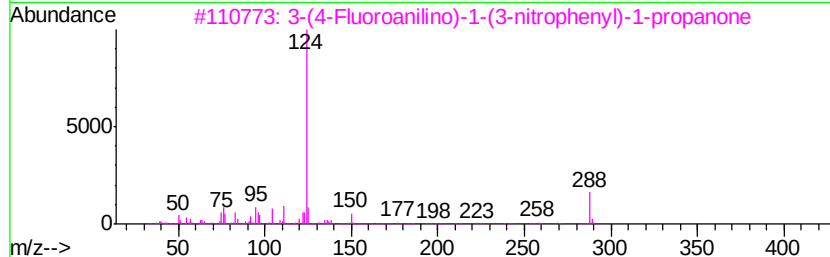
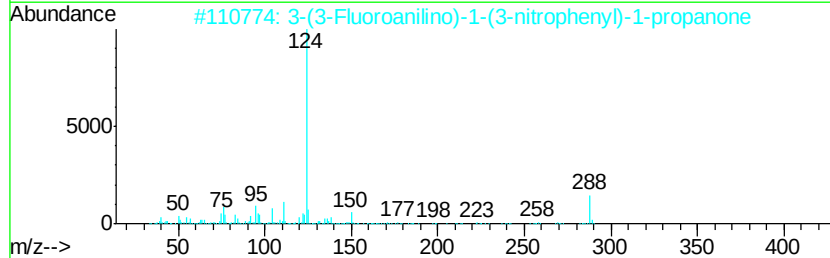
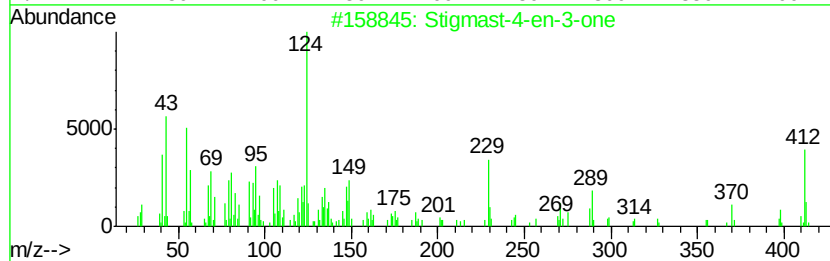
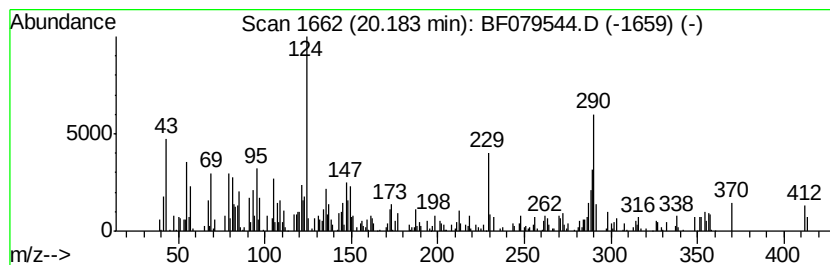
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Stigmast-4-en-3-one Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.18	3.58 ng	174333	Perylene-d12	17.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmast-4-en-3-one	412	C29H48O	001058-61-3	90
2		3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	27
3		3-(4-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	350039-84-8	27
4		4,5-Dimethyl-2-pyrimidone	124	C6H8N2O	034939-17-8	18
5		2,3-Diaminophenol	124	C6H8N2O	059649-56-8	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052815\
Data File : BF079544.D
Acq On : 28 May 2015 15:07
Operator : TP/IZ
Sample : G2359-05 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.37	9.0	ng	211904	1	6.96	471580	20.0
unknown6.67	6.67	33.7	ng	794654	1	6.96	471580	20.0
unknown13.29	13.29	5.8	ng	216174	4	12.54	742160	20.0
Trichloroacetic a...	15.70	5.9	ng	395895	5	15.81	1348140	20.0
Cyclohexadecane	16.51	5.0	ng	337904	5	15.81	1348140	20.0
Eicosane	17.28	7.3	ng	355492	6	17.52	975056	20.0
Benzo[e]pyrene	17.39	3.5	ng	172084	6	17.52	975056	20.0
Heneicosane	18.06	2.9	ng	143065	6	17.52	975056	20.0
.gamma.-Sitosterol	19.33	6.4	ng	310658	6	17.52	975056	20.0
Stigmast-4-en-3-one	20.18	3.6	ng	174333	6	17.52	975056	20.0