

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072715\
 Data File : BF080695.D
 Acq On : 28 Jul 2015 3:28
 Operator : TP/UM
 Sample : G3084-04
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUMBO-EP-4

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-BF072715.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	2.224	9	12	25	rBV	17891	90905	8.17%	1.066%
2	4.453	205	207	213	rVB	19386	24558	2.21%	0.288%
3	5.093	261	263	266	rBV	622512	638725	57.38%	7.493%
4	5.516	297	300	302	rBV	895036	1113056	100.00%	13.057%
5	5.927	334	336	339	rVB	47992	45023	4.04%	0.528%
6	6.533	387	389	392	rBV	979119	995480	89.44%	11.678%
7	6.682	400	402	405	rBV	1049725	1075483	96.62%	12.617%
8	6.922	421	423	426	rVB	230182	191169	17.18%	2.243%
9	7.082	434	437	439	rBV	986694	829351	74.51%	9.729%
10	7.482	470	472	474	rBV	871733	674543	60.60%	7.913%
11	7.550	477	478	484	rVB2	9116	11212	1.01%	0.132%
12	8.213	534	536	538	rBV	187995	212014	19.05%	2.487%
13	9.288	627	630	632	rBV	1057445	935714	84.07%	10.977%
14	9.676	662	664	666	rBV	222262	173167	15.56%	2.031%
15	9.962	687	689	691	rVB	200943	166113	14.92%	1.949%
16	10.751	756	758	760	rBV	427271	379294	34.08%	4.450%
17	10.876	767	769	772	rVB	8177	11540	1.04%	0.135%
18	11.448	817	819	820	rBV	141550	115178	10.35%	1.351%
19	11.676	837	839	844	rBV	23395	37072	3.33%	0.435%
20	11.974	864	865	868	rBV2	9814	14878	1.34%	0.175%
21	12.236	886	888	890	rBV	59804	54033	4.85%	0.634%
22	12.671	924	926	928	rBV	45818	39332	3.53%	0.461%
23	12.911	943	947	949	rBV	41197	43116	3.87%	0.506%
24	13.059	958	960	963	rVB	520019	455053	40.88%	5.338%
25	14.054	1045	1047	1051	rVB4	7007	12497	1.12%	0.147%
26	14.202	1058	1060	1062	rBV	60698	75212	6.76%	0.882%
27	15.162	1141	1144	1146	rBV3	4886	12530	1.13%	0.147%
28	15.242	1148	1151	1153	rVV	23573	29383	2.64%	0.345%
29	15.391	1162	1164	1169	rBV4	6729	18197	1.63%	0.213%
30	15.825	1200	1202	1206	rVB	19163	31755	2.85%	0.373%
31	17.757	1368	1371	1374	rVB2	9132	18712	1.68%	0.220%

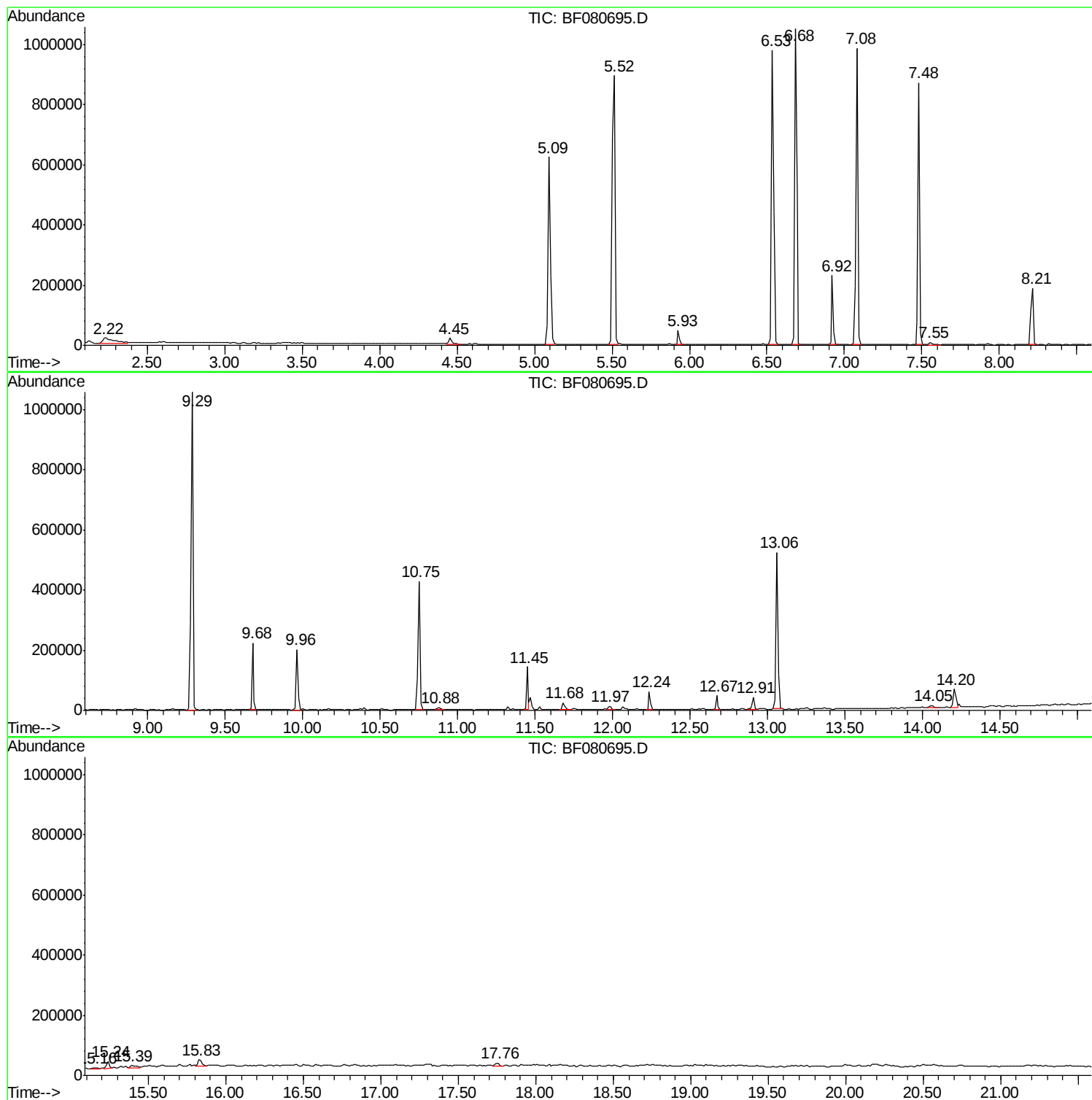
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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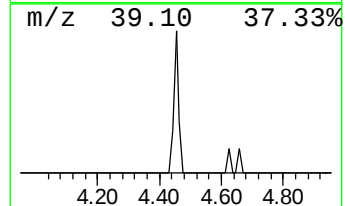
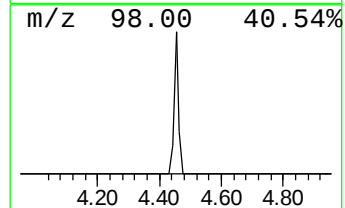
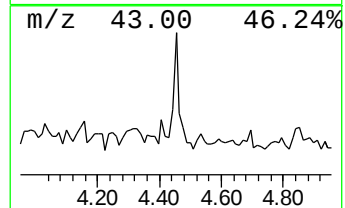
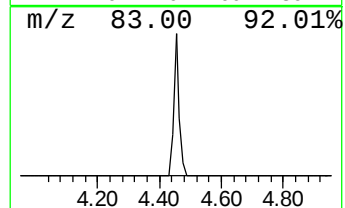
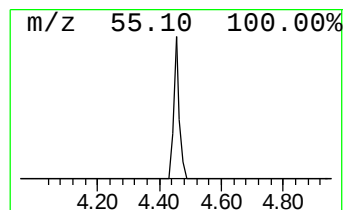
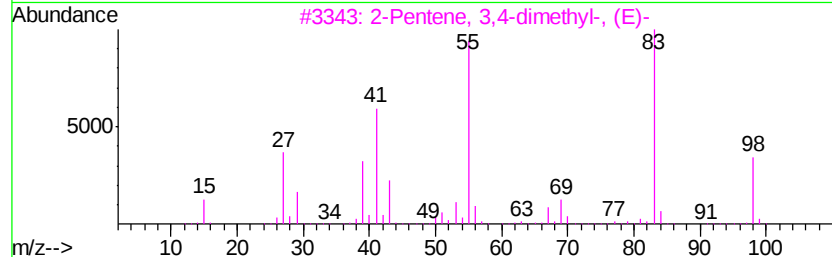
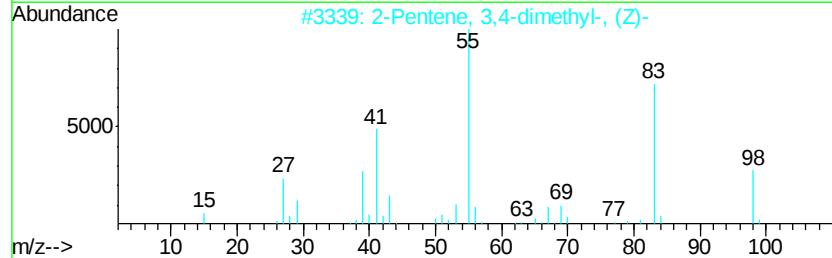
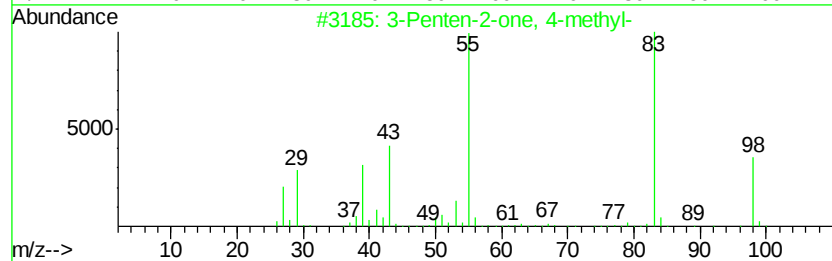
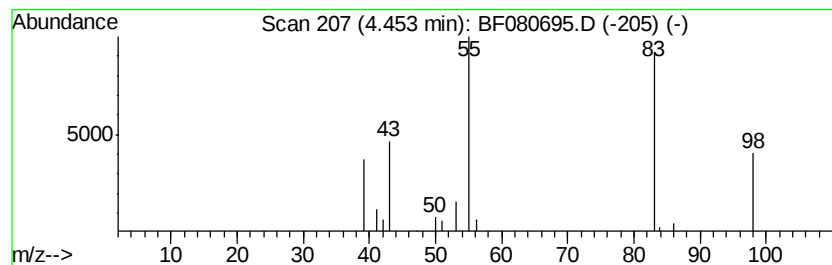
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	2.57 ng	24558	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4			3-Hexen-2-one	98	C6H10O	000763-93-9	78
5			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	56



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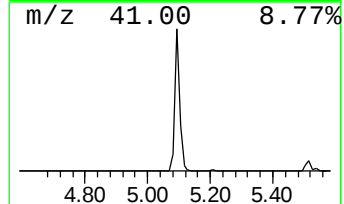
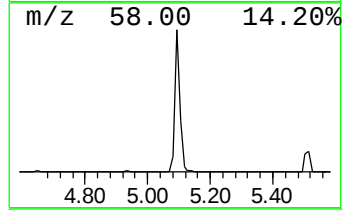
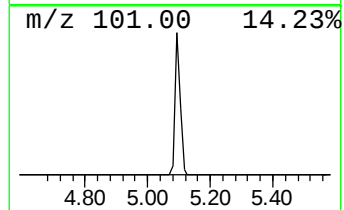
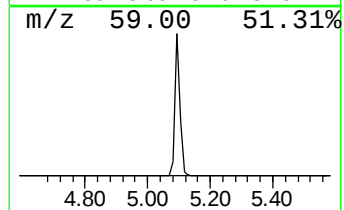
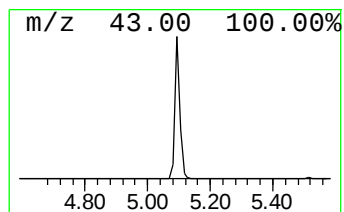
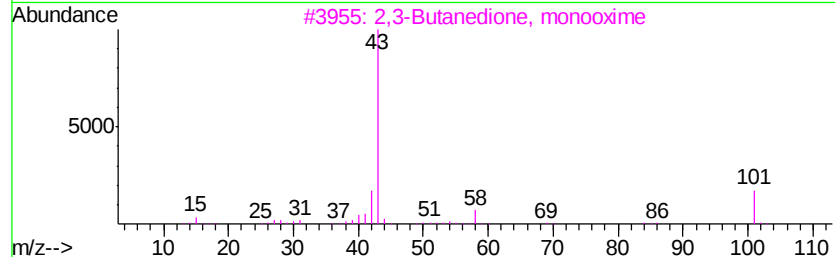
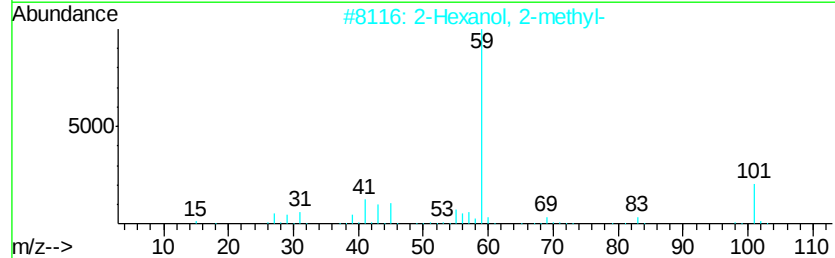
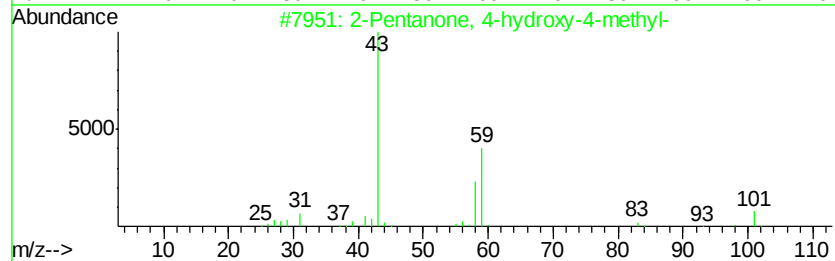
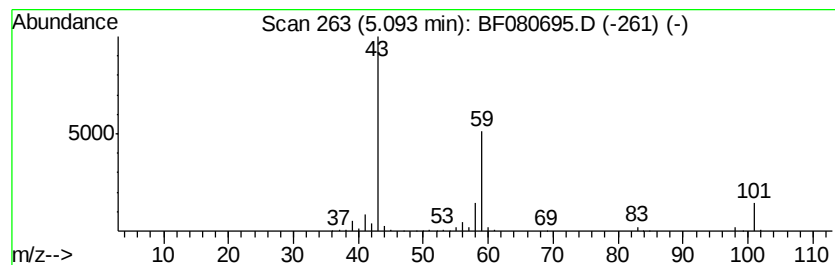
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	66.82 ng	638725	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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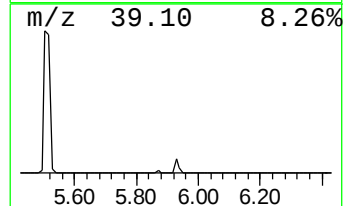
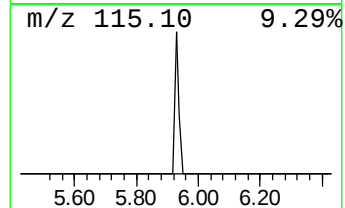
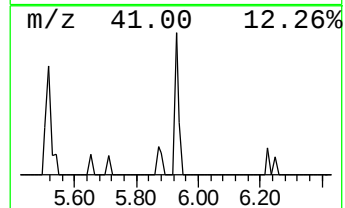
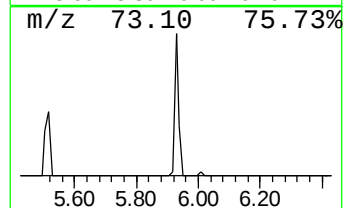
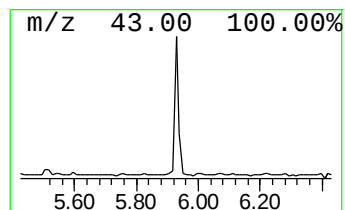
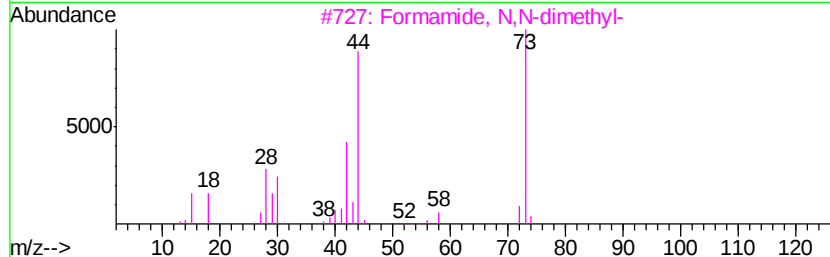
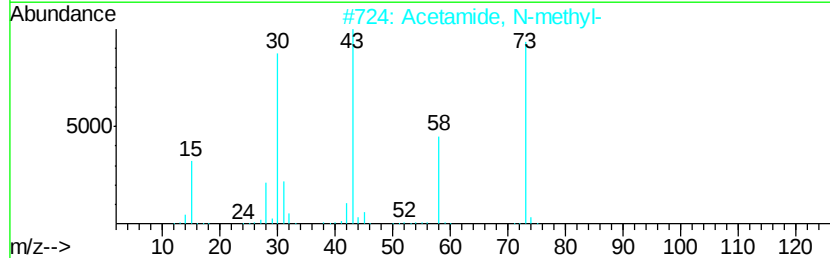
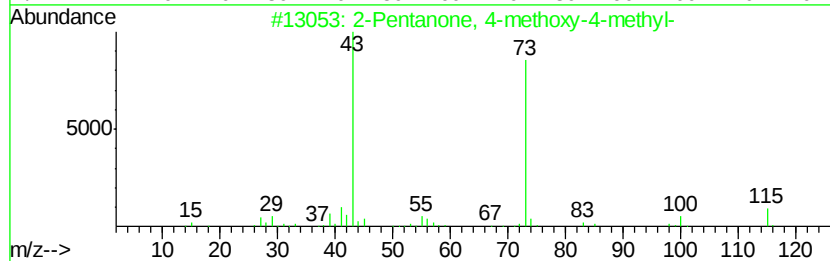
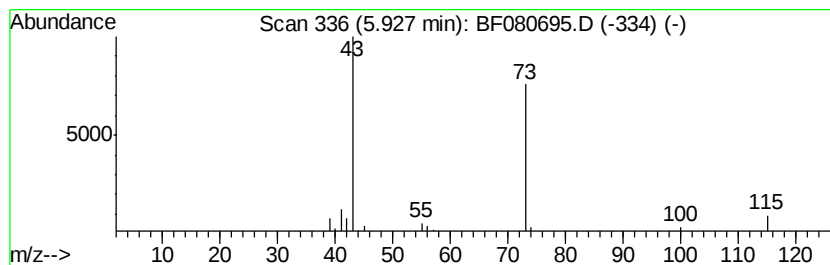
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	4.71 ng	45023	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3		Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		Heptane	100	C7H16	000142-82-5	7



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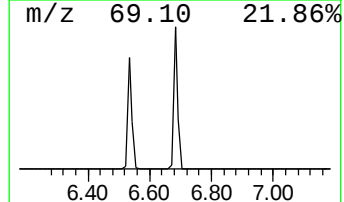
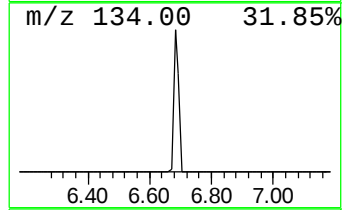
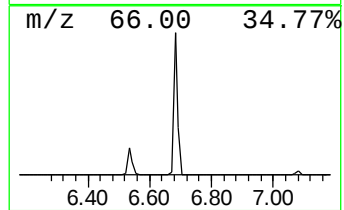
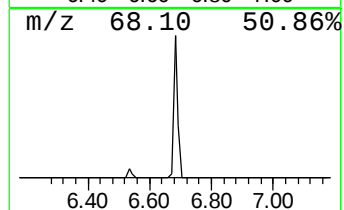
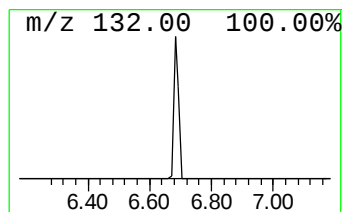
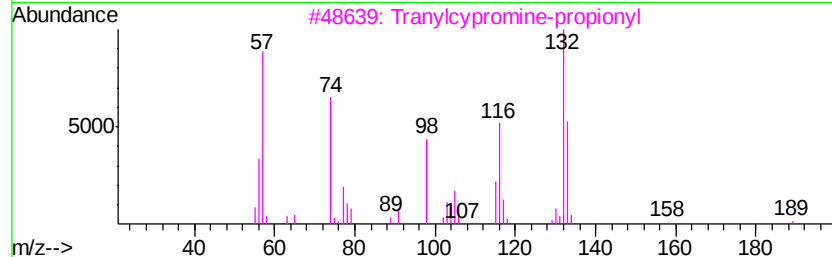
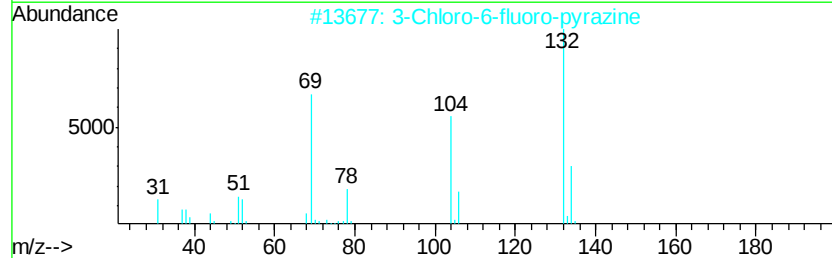
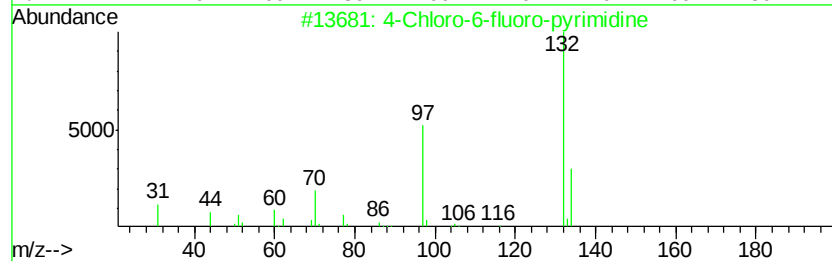
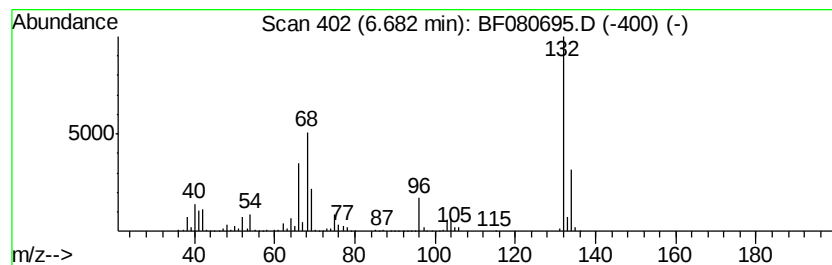
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown6.88 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	112.52 ng	1075480	1,4-Dichlorobenzene-d4	6.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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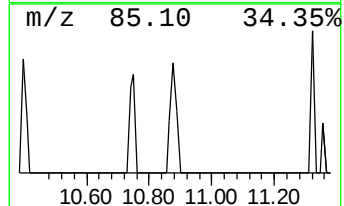
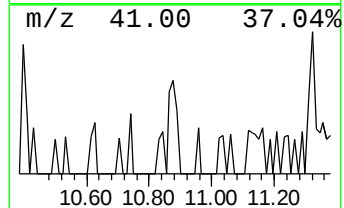
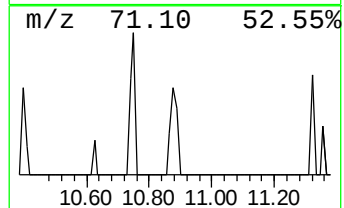
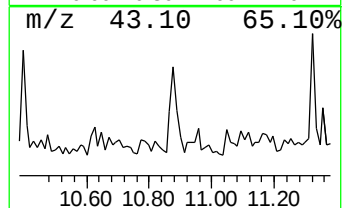
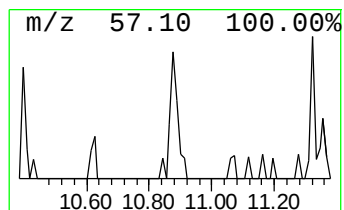
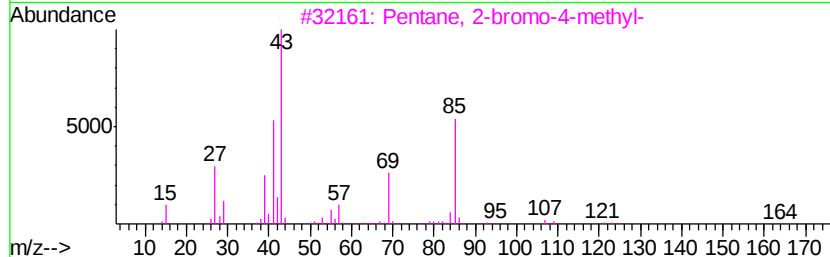
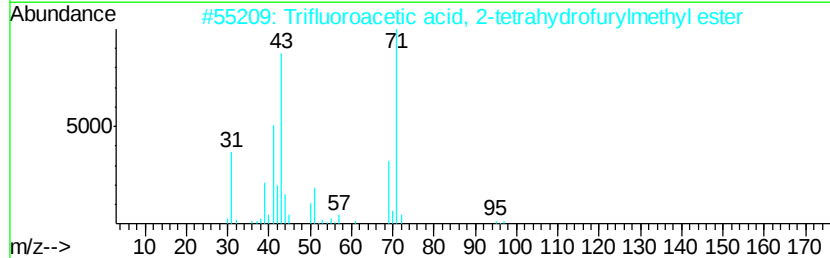
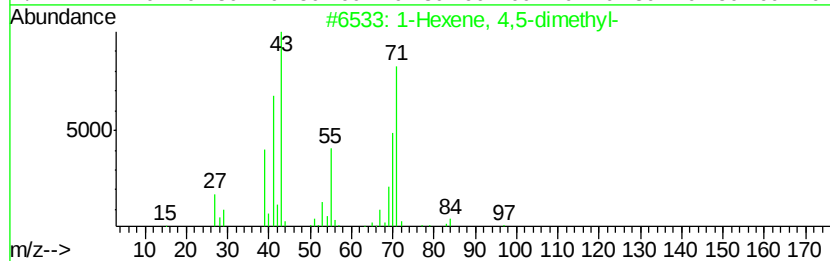
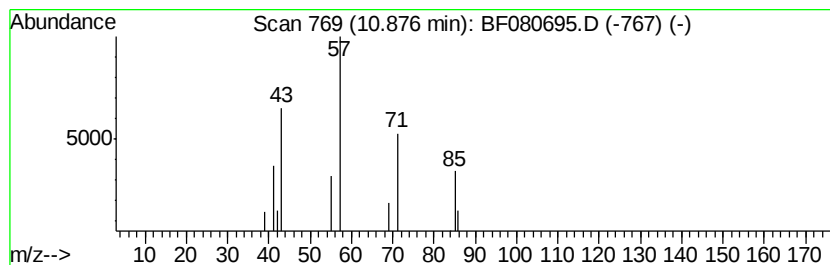
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown10.88 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.00 ng	11540	Phenanthrene-d10	11.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	25
2		Trifluoroacetic acid, 2-tetrahyd...	198	C7H9F3O3	071239-15-1	25
3		Pentane, 2-bromo-4-methyl-	164	C6H13Br	030310-22-6	25
4		Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5		Pentane, 2-bromo-2-methyl-	164	C6H13Br	004283-80-1	9



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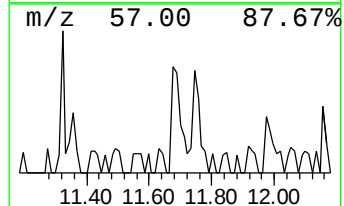
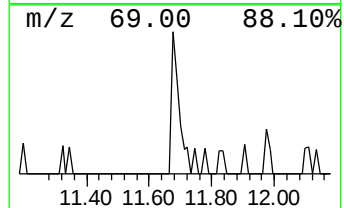
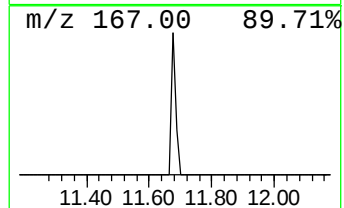
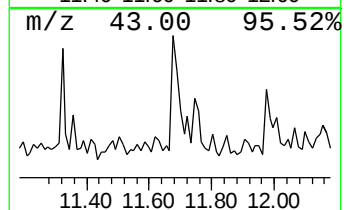
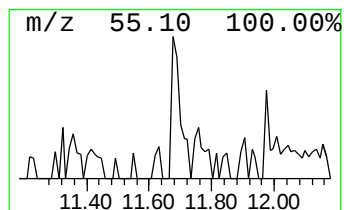
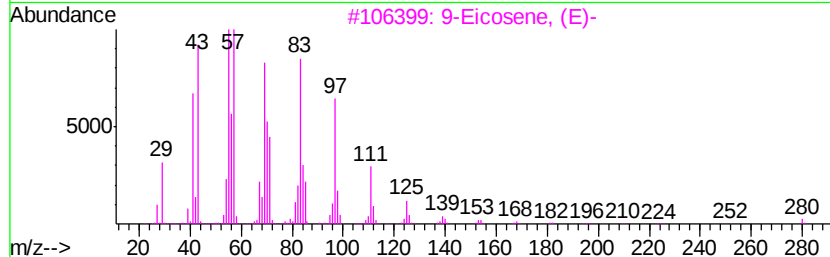
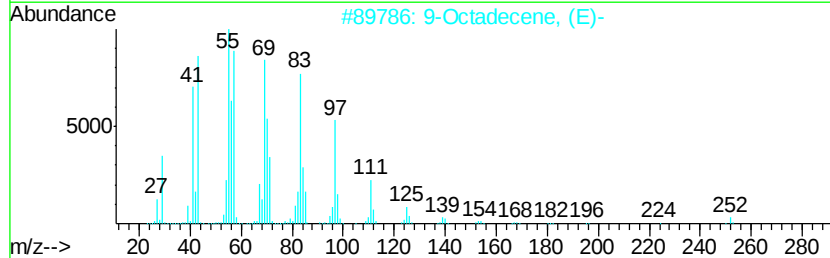
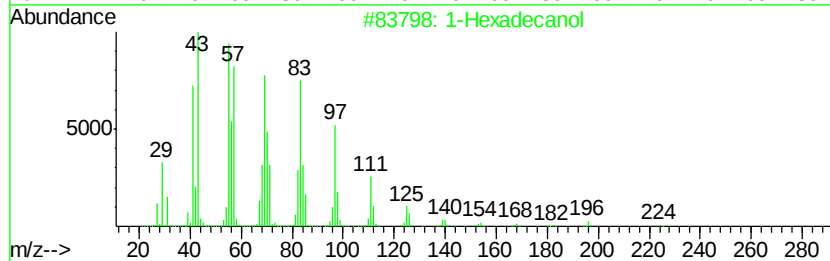
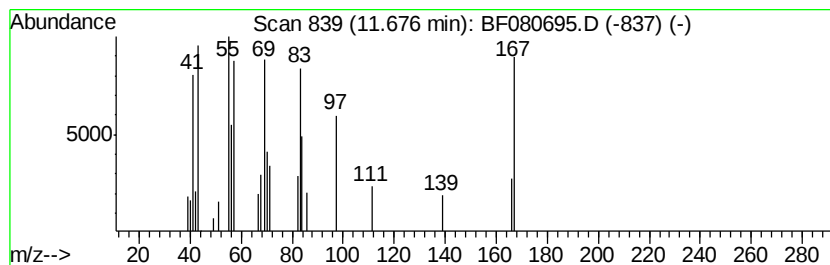
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	6.44 ng	37072	Phenanthrene-d10	11.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanol	242	C16H34O	036653-82-4	62
2		9-Octadecene, (E)-	252	C18H36	007206-25-9	58
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	58
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	50
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072715\
Data File : BF080695.D
Acq On : 28 Jul 2015 3:28
Operator : TP/UM
Sample : G3084-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUMBO-EP-4

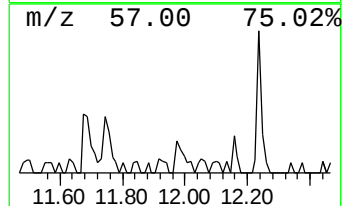
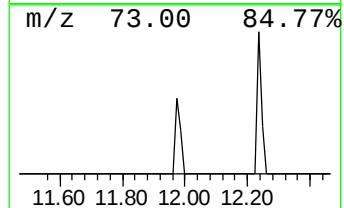
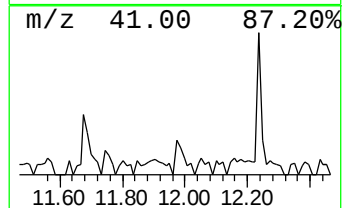
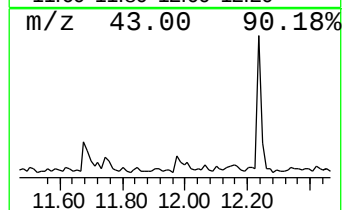
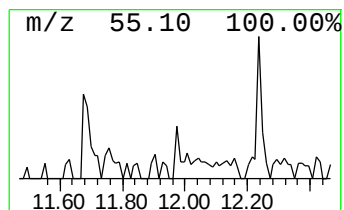
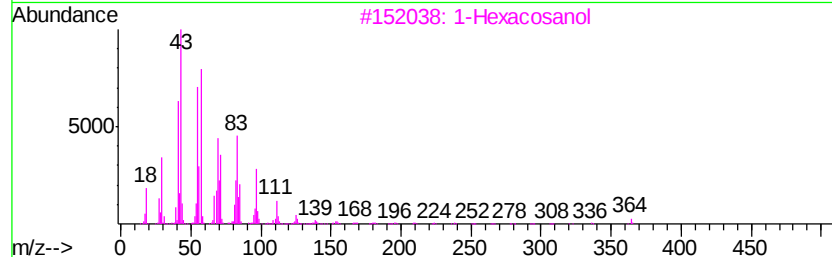
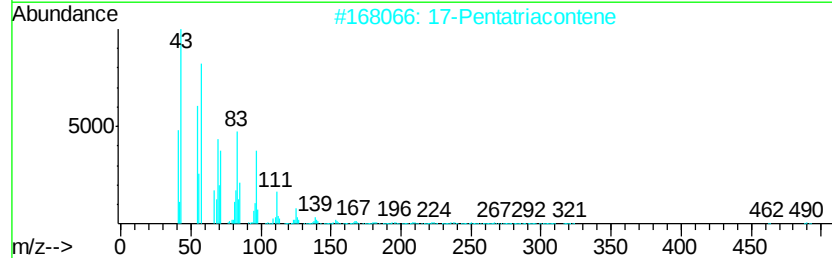
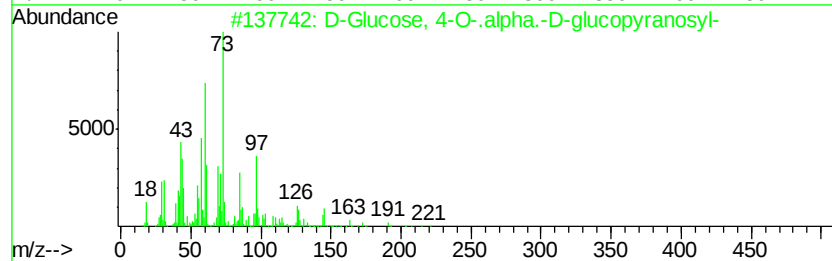
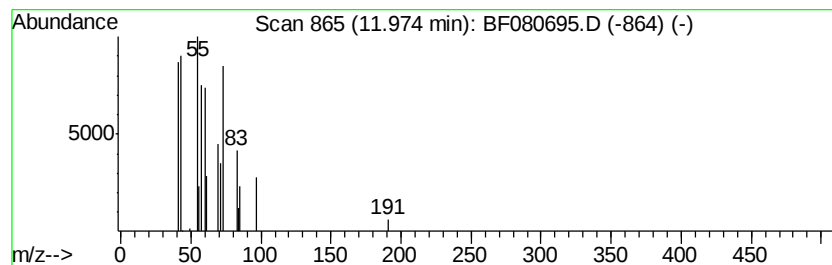
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 D-Glucose, 4-O-.alpha.-D-gl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.58 ng	14878	Phenanthrene-d10	11.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	50
2			17-Pentatriacontene	491	C35H70	006971-40-0	43
3			1-Hexacosanol	382	C26H54O	000506-52-5	43
4			1-Tetracosanol	354	C24H50O	000506-51-4	38
5			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072715\
Data File : BF080695.D
Acq On : 28 Jul 2015 3:28
Operator : TP/UM
Sample : G3084-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUMBO-EP-4

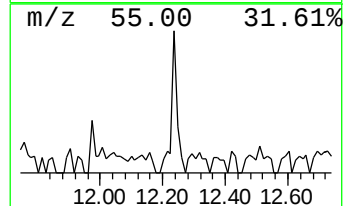
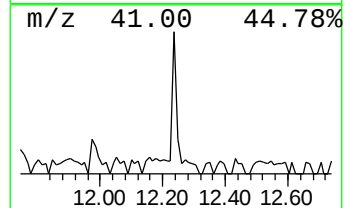
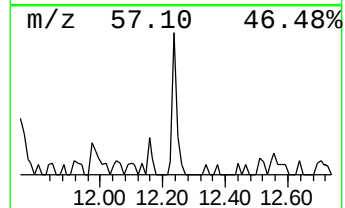
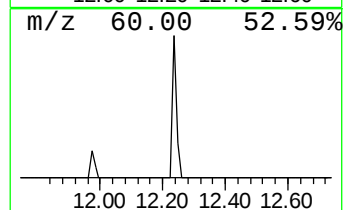
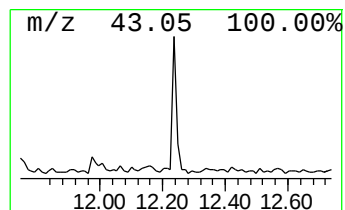
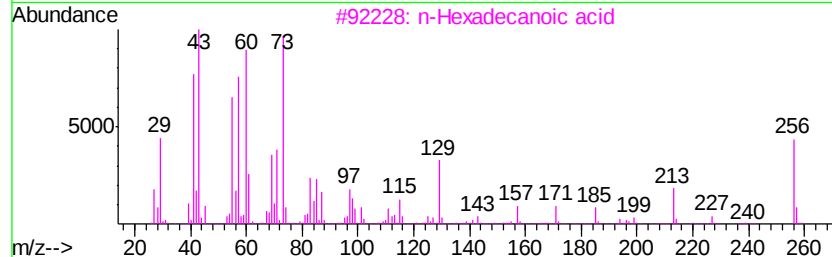
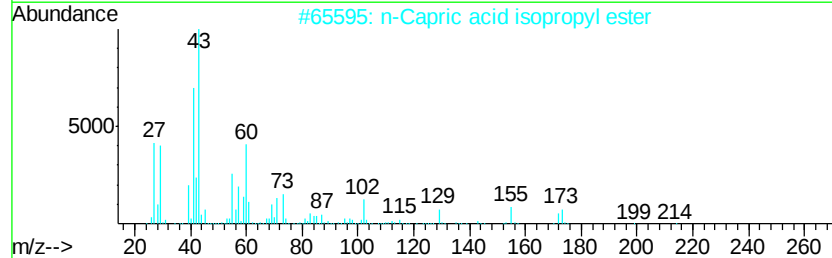
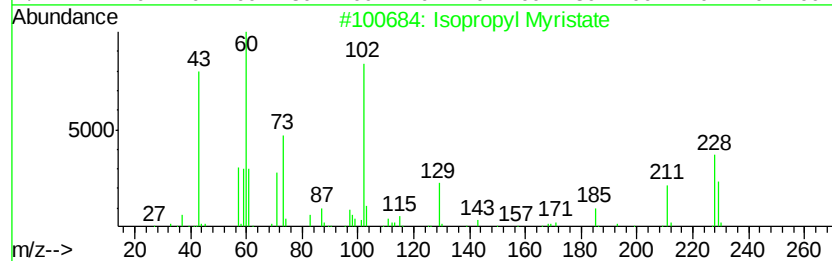
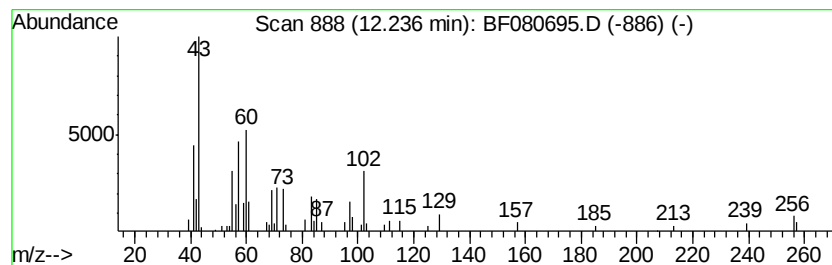
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Isopropyl Myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.24	9.38 ng	54033	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Myristate	270	C17H34O2	000110-27-0	59
2	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	59
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
4	Heptanoic acid, propyl ester	172	C10H20O2	007778-87-2	43
5	Vitamin d3	384	C27H44O	001406-16-2	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072715\
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Acq On : 28 Jul 2015 3:28
Operator : TP/UM
Sample : G3084-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUMBO-EP-4

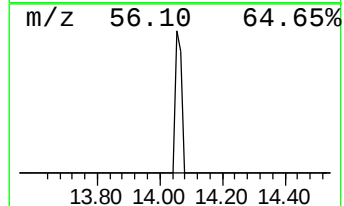
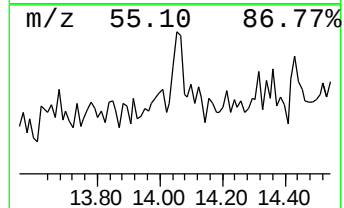
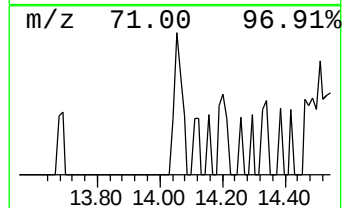
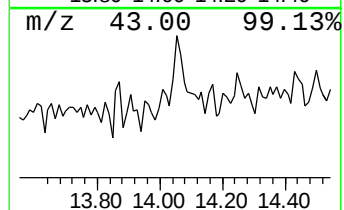
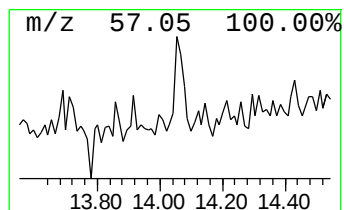
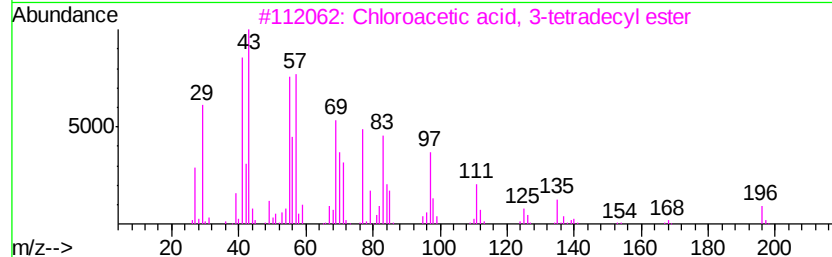
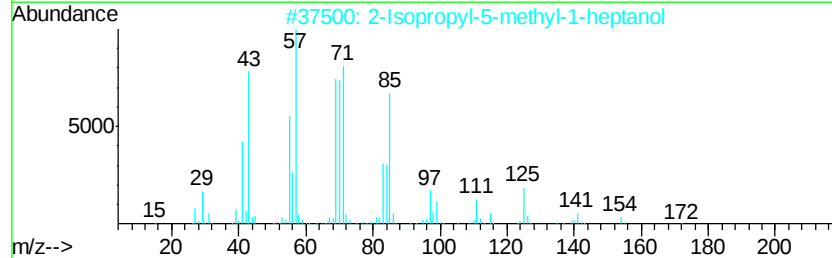
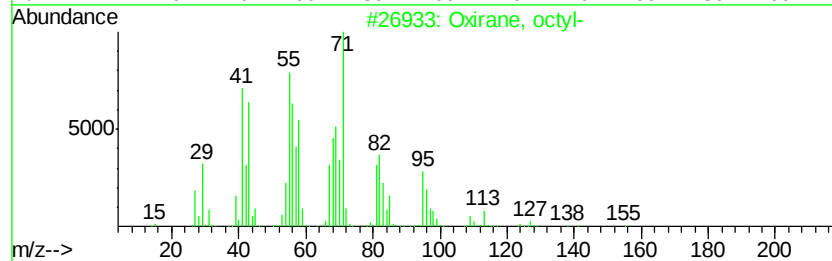
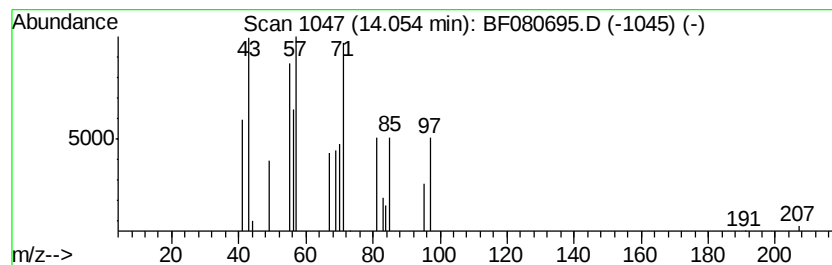
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.05 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	3.32 ng	12497	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, octyl-	156	C10H20O	002404-44-6	38
2		2-Isopropyl-5-methyl-1-heptanol	172	C11H24O	091337-07-4	22
3		Chloroacetic acid, 3-tetradecyl ...	290	C16H31ClO2	1000280-08-5	14
4		17-Pentatriacontene	491	C35H70	006971-40-0	14
5		1-(Cyclopropyl-nitro-methyl)-cyc...	185	C9H15NO3	1000186-67-0	14



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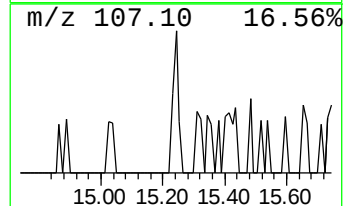
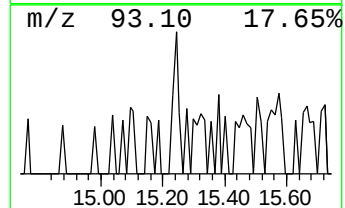
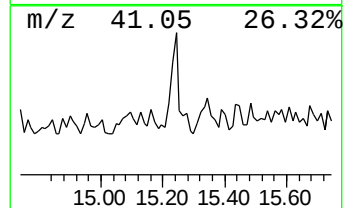
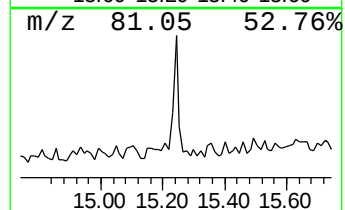
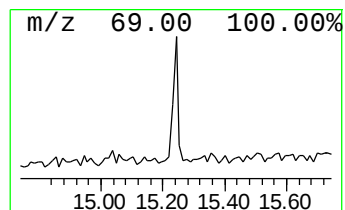
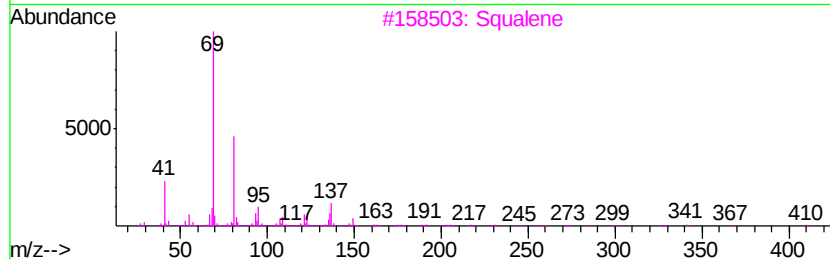
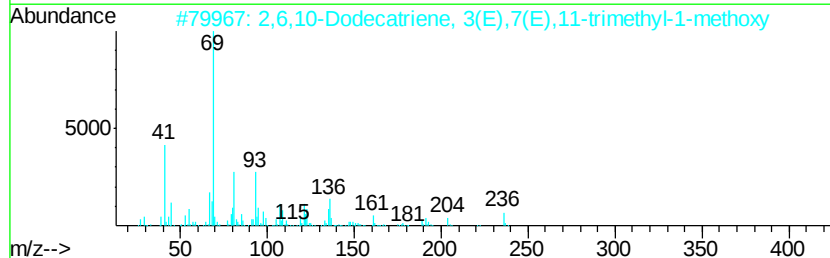
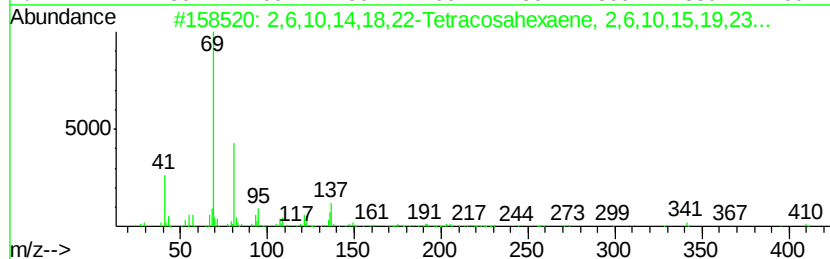
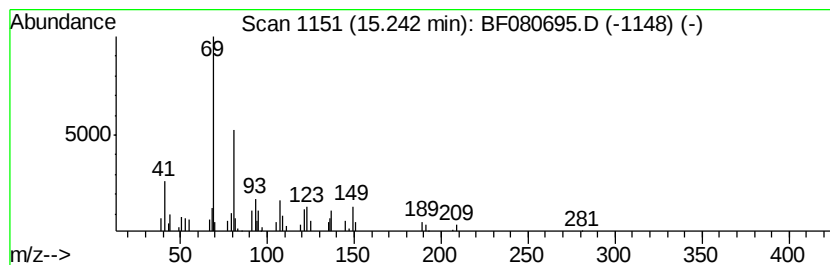
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	18.51 ng	29383	Perylene-d12	15.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64		
2	2,6,10-Dodecatriene, 3(E),7(E),1...	236	C16H28O	1000159-57-9	59		
3	Squalene	410	C30H50	007683-64-9	59		
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59		
5	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	56		



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 ALS Vial : 23 Sample Multiplier: 1

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 ClientSampleId :
 DUMBO-EP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072715.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
3-Penten-2-one, 4...	4.45	2.6	ng	24558	1	6.92	191169	20.0
2-Pentanone, 4-hy...	5.09	66.8	ng	638725	1	6.92	191169	20.0
2-Pentanone, 4-me...	5.93	4.7	ng	45023	1	6.92	191169	20.0
unknown6.88	6.68	112.5	ng	1075480	1	6.92	191169	20.0
unknown10.88	10.88	2.0	ng	11540	4	11.45	115178	20.0
1-Hexadecanol	11.68	6.4	ng	37072	4	11.45	115178	20.0
D-Glucose, 4-O-.a...	11.97	2.6	ng	14878	4	11.45	115178	20.0
Isopropyl Myristate	12.24	9.4	ng	54033	4	11.45	115178	20.0
unknown14.05	14.05	3.3	ng	12497	5	14.20	75212	20.0
2,6,10,14,18,22-T...	15.24	18.5	ng	29383	6	15.84	31755	20.0