

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
 Data File : BF089518.D
 Acq On : 1 Aug 2016 18:56
 Operator : UM/SJ
 Sample : H4256-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-6

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-BF072716.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	1.655	4	6	36	rVB	802447	1856473	100.00%	19.839%
2	4.547	257	259	268	rVB	47943	63356	3.41%	0.677%
3	5.039	300	302	317	rBV4	157130	265907	14.32%	2.842%
4	6.136	396	398	405	rBV3	105119	174378	9.39%	1.863%
5	6.239	405	407	423	rVB	507130	627584	33.81%	6.707%
6	6.479	426	428	434	rBV	192846	213977	11.53%	2.287%
7	6.559	434	435	439	rVB	58949	62043	3.34%	0.663%
8	6.627	439	441	444	rBV	680334	742007	39.97%	7.929%
9	7.050	476	478	489	rBV	534786	628560	33.86%	6.717%
10	7.759	538	540	544	rBV	233244	302026	16.27%	3.228%
11	7.816	544	545	551	rVB	16821	24222	1.30%	0.259%
12	8.010	560	562	563	rBV	21253	20040	1.08%	0.214%
13	8.033	563	564	566	rVV	19880	21441	1.15%	0.229%
14	8.113	569	571	574	rVB	26193	28354	1.53%	0.303%
15	8.422	596	598	606	rVB	53920	72211	3.89%	0.772%
16	8.845	632	635	637	rBV	1419956	1285311	69.23%	13.736%
17	9.245	668	670	672	rBV	153680	130199	7.01%	1.391%
18	9.508	691	693	695	rBV	371609	348938	18.80%	3.729%
19	10.285	759	761	764	rBV2	317189	454921	24.50%	4.862%
20	10.982	819	822	824	rBV	213050	288716	15.55%	3.085%
21	11.176	832	839	842	rBV2	53460	73715	3.97%	0.788%
22	11.233	842	844	847	rVV2	18732	25822	1.39%	0.276%
23	11.531	868	870	873	rBV	31379	44484	2.40%	0.475%
24	11.576	873	874	876	rVV	14420	22185	1.20%	0.237%
25	11.611	876	877	880	rVV2	25340	40632	2.19%	0.434%
26	11.725	883	887	891	rVV3	13050	35991	1.94%	0.385%
27	12.319	936	939	948	rVB2	14744	26917	1.45%	0.288%
28	12.559	958	960	963	rBV	753246	691670	37.26%	7.392%
29	13.142	1009	1011	1014	rBV	24271	21627	1.16%	0.231%
30	13.474	1037	1040	1044	rBV	22126	32115	1.73%	0.343%
31	13.599	1048	1051	1054	rBV2	187387	246968	13.30%	2.639%
32	14.445	1123	1125	1127	rVB	19568	23966	1.29%	0.256%
33	14.925	1165	1167	1174	rBV	180312	215689	11.62%	2.305%
34	15.462	1211	1214	1221	rVB3	25506	54566	2.94%	0.583%

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ALS Vial : 13 Sample Multiplier: 1

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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	15.611	1224	1227	1233	rVB	78157	141988	7.65%	1.517%
36	16.194	1275	1278	1284	rVB6	9079	19382	1.04%	0.207%
37	16.503	1302	1305	1309	rVB3	11949	29182	1.57%	0.312%

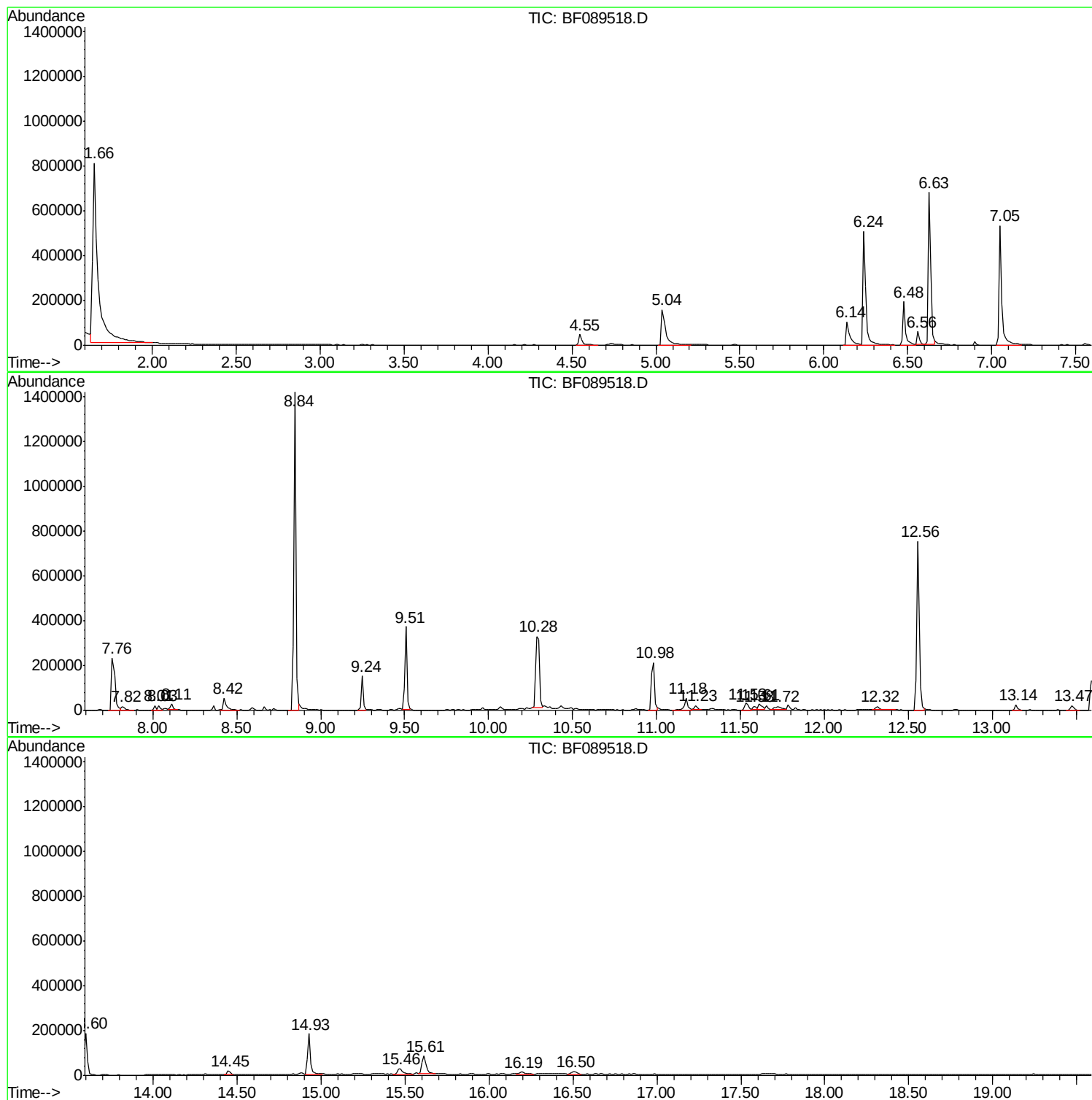
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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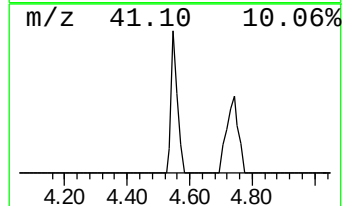
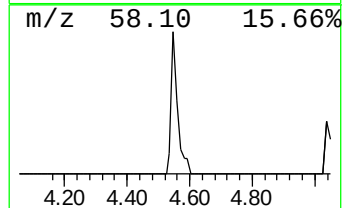
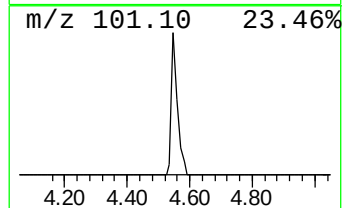
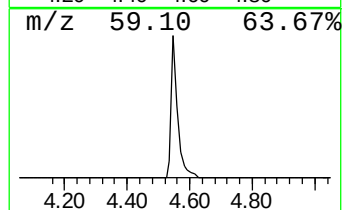
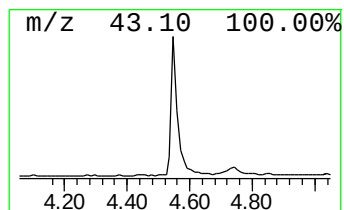
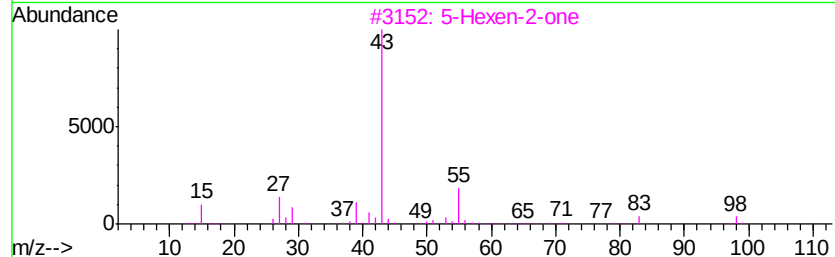
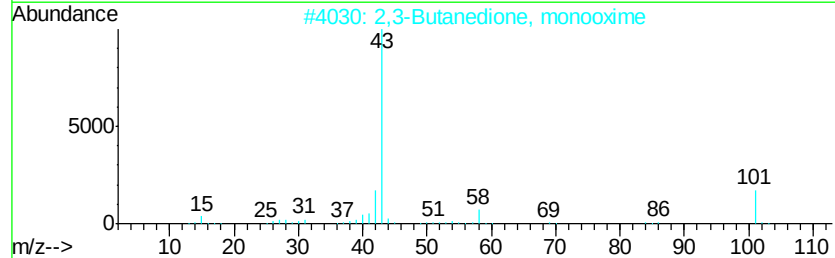
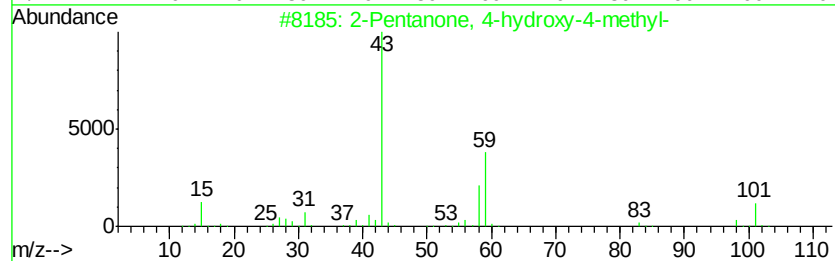
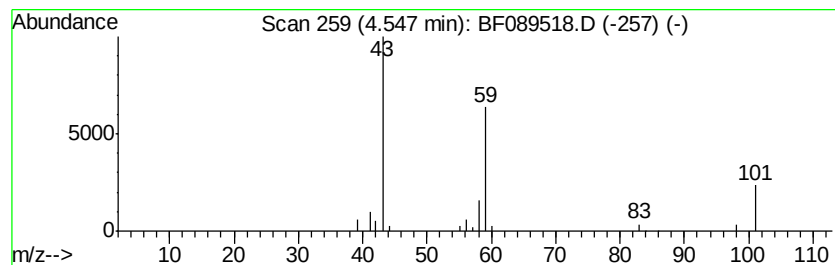
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	5.92 ng	63356	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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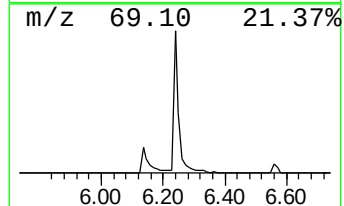
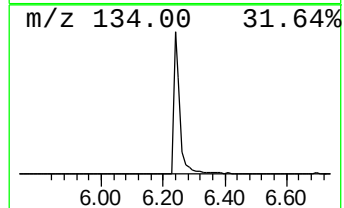
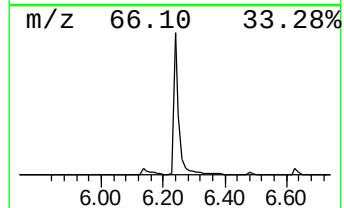
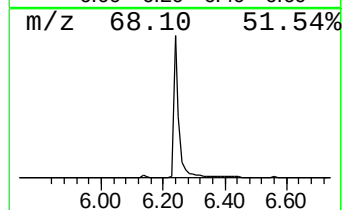
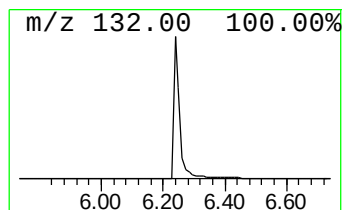
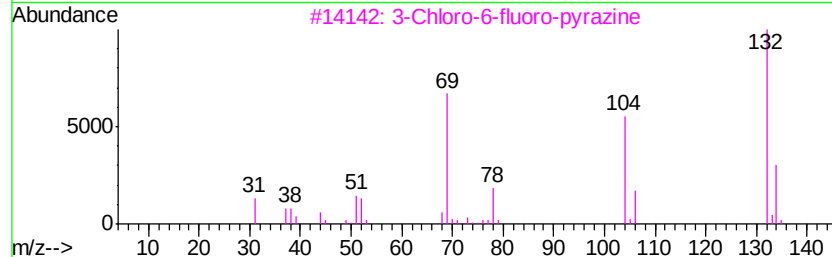
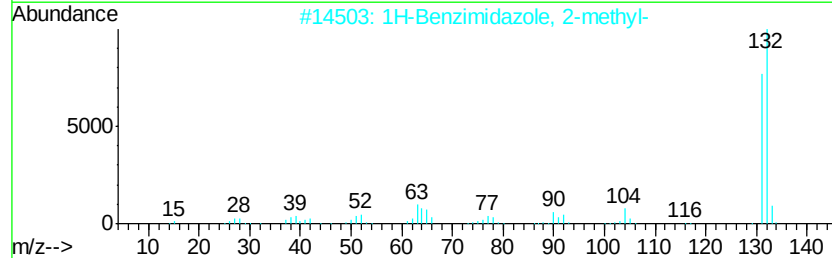
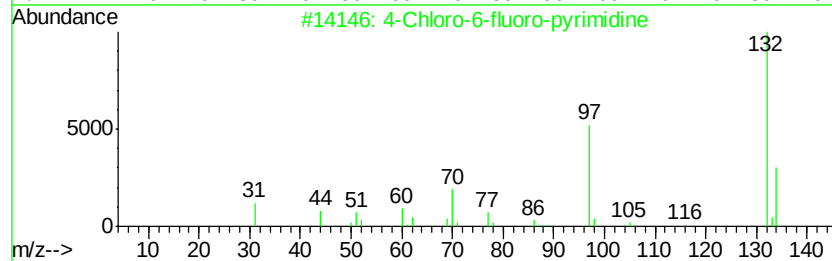
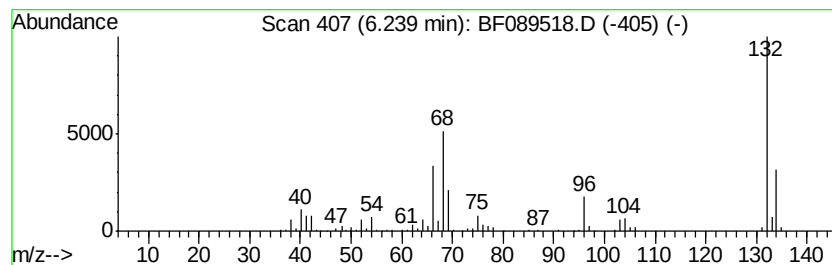
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown6.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	58.66 ng	627584	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10



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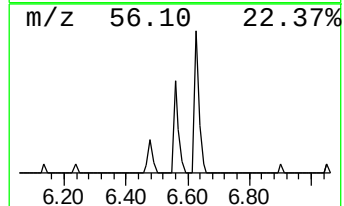
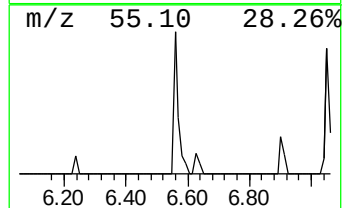
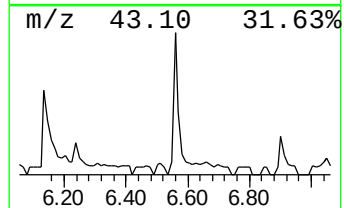
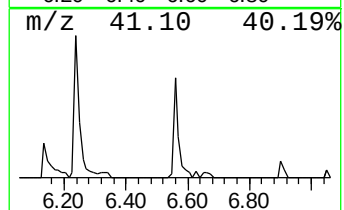
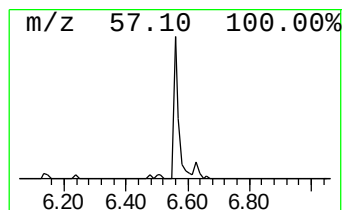
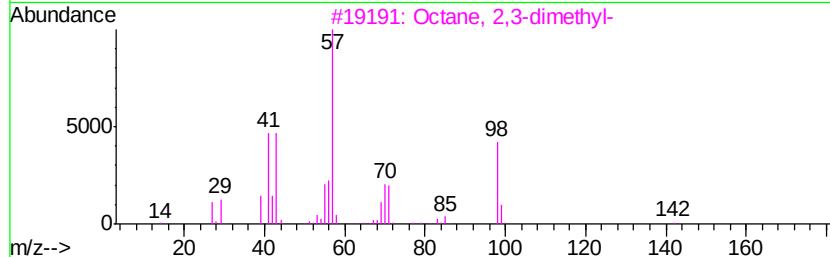
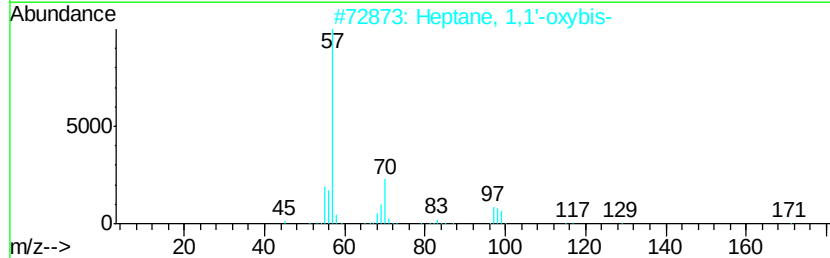
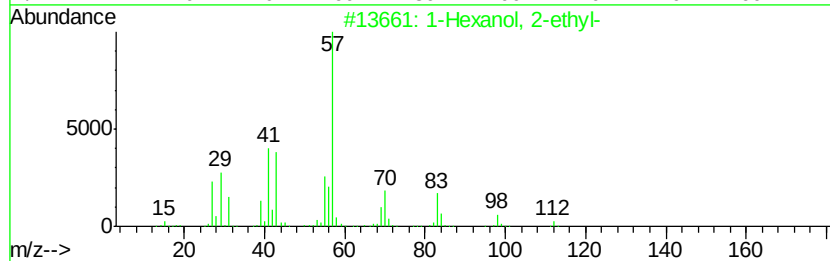
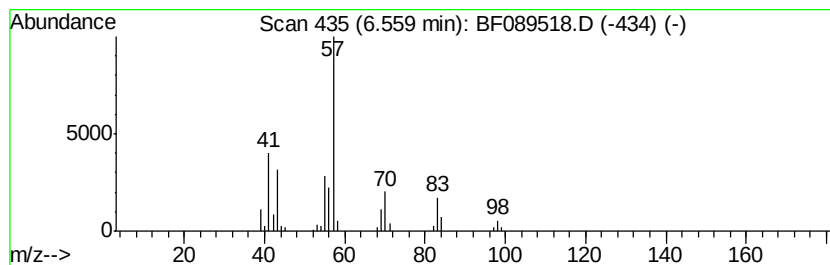
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	5.80 ng	62043	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	59
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53



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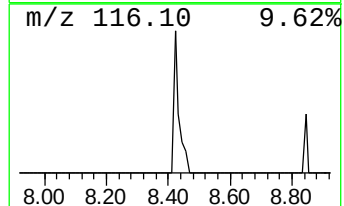
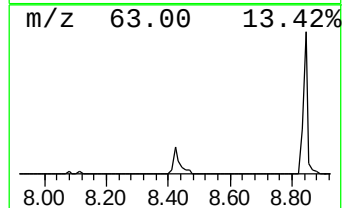
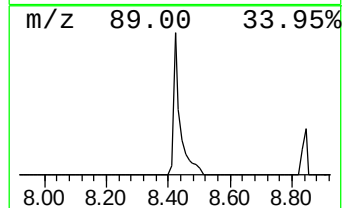
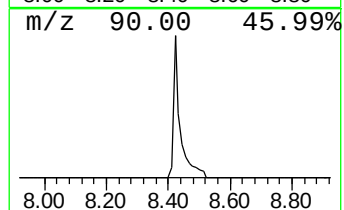
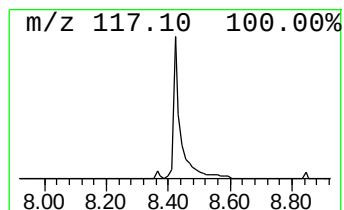
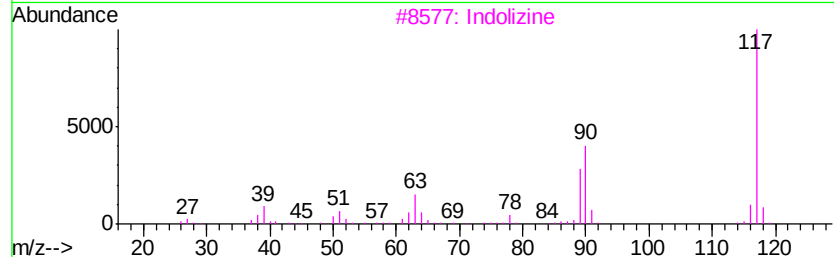
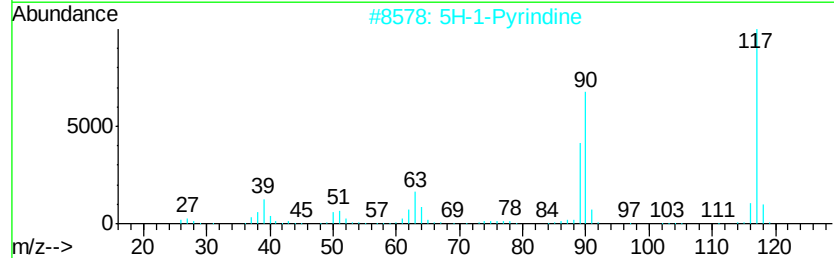
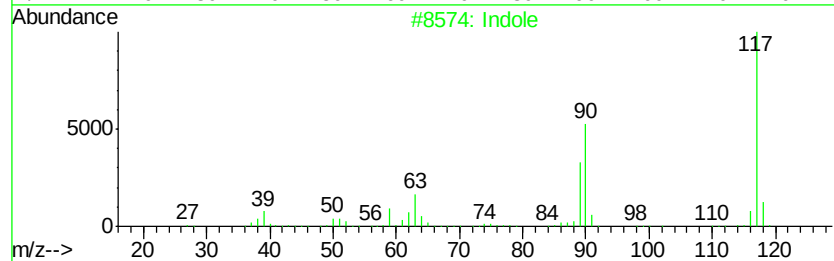
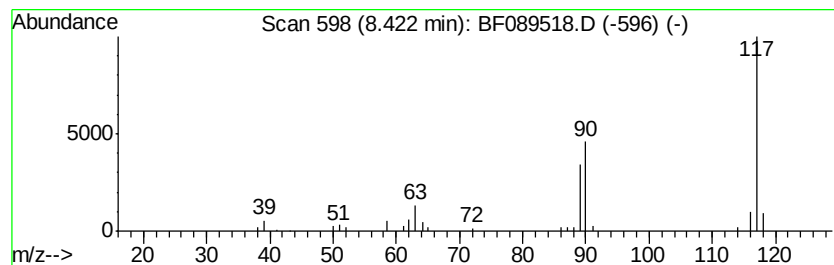
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Indole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	4.78 ng	72211	Naphthalene-d8	7.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole		117	C8H7N	000120-72-9	95
2	5H-1-Pyridine		117	C8H7N	000270-91-7	91
3	Indolizine		117	C8H7N	000274-40-8	91
4	Benzene, 1-isocvano-2-methyl-		117	C8H7N	010468-64-1	90
5	Benzonitrile, 2-methyl-		117	C8H7N	000529-19-1	87



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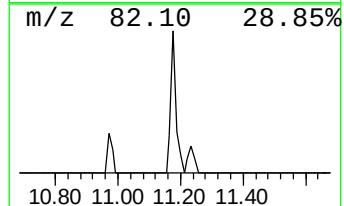
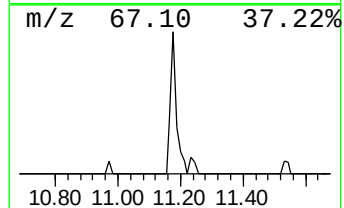
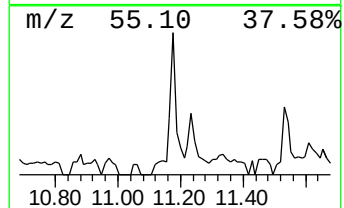
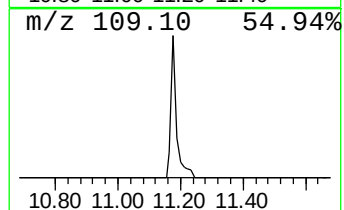
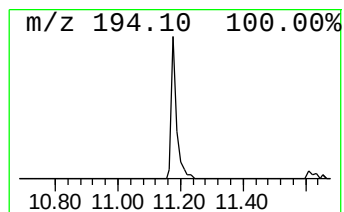
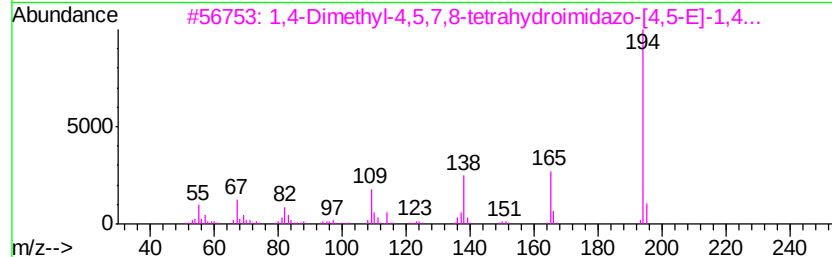
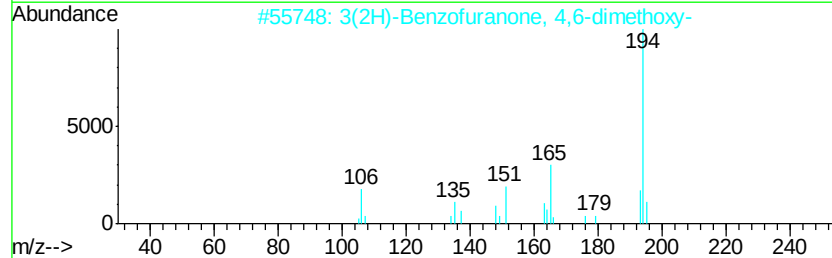
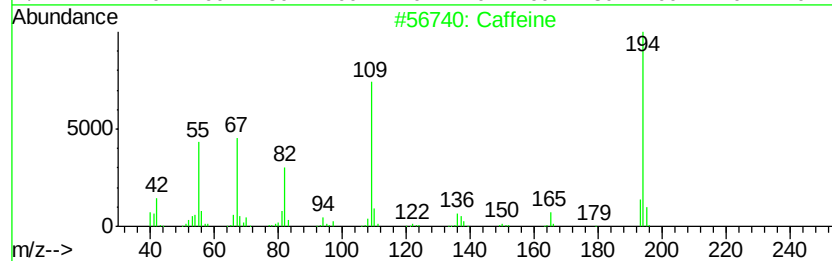
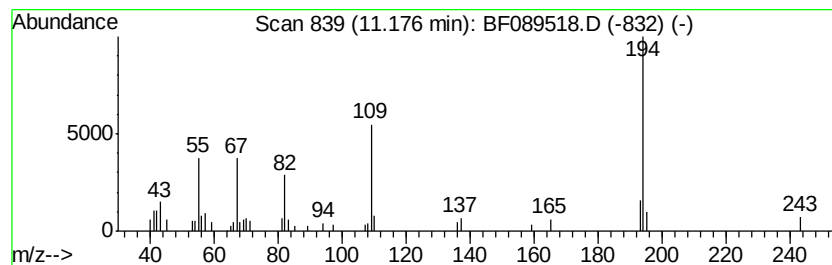
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Caffeine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.18	5.11 ng	73715	Phenanthrene-d10	10.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	96
2	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	50
3	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	47
4	2-(2,5-dimethoxy-4-propylphenyl)...	223	C13H21NO2	207740-22-5	37
5	Benzaldehyde, 4,6-dimethoxy-2,3-...	194	C11H14O3	034883-13-1	32



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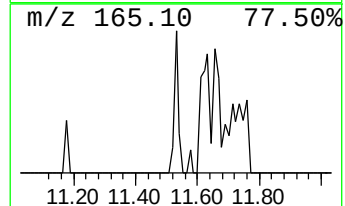
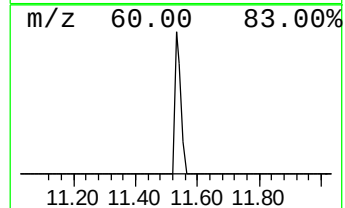
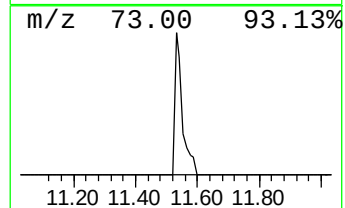
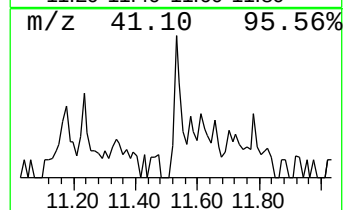
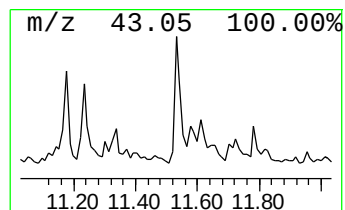
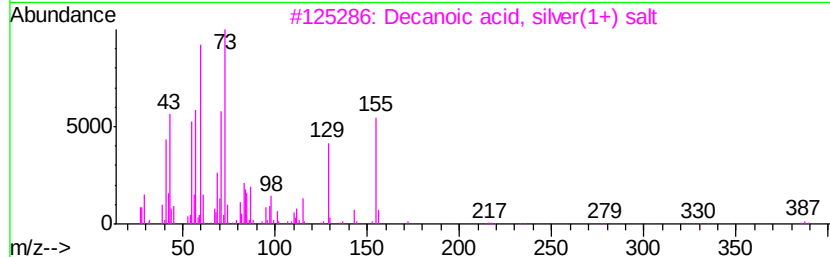
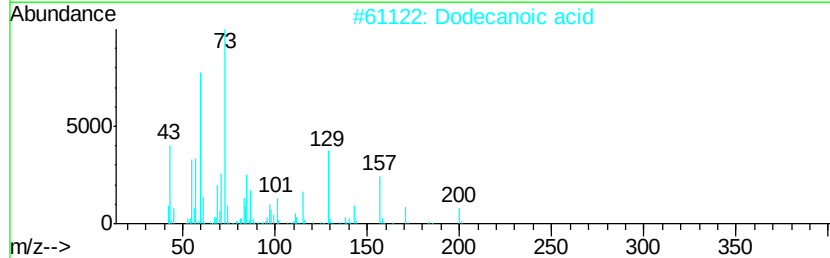
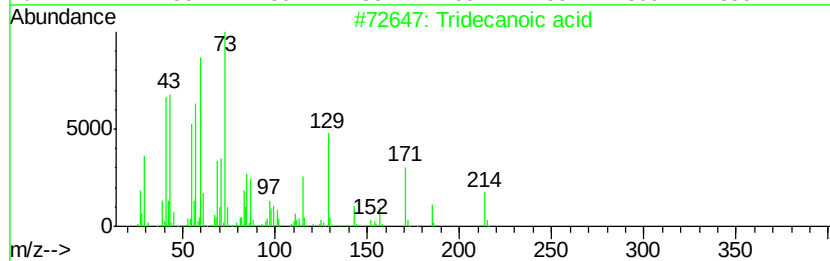
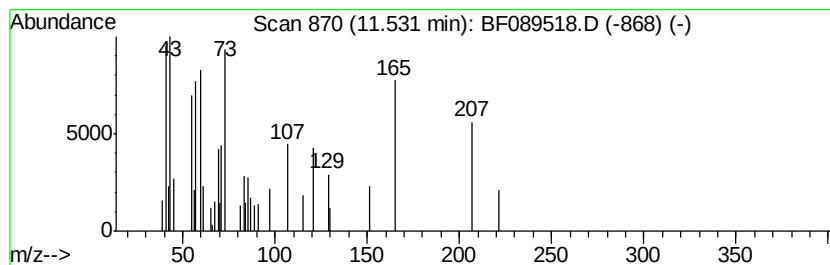
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown11.53 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	3.08 ng	44484	Phenanthrene-d10	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanoic acid	214	C13H26O2	000638-53-9	27
2		Dodecanoic acid	200	C12H24O2	000143-07-7	27
3		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	22
4		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	22
5		Undecanoic acid	186	C11H22O2	000112-37-8	16



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089518.D
Acq On : 1 Aug 2016 18:56
Operator : UM/SJ
Sample : H4256-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

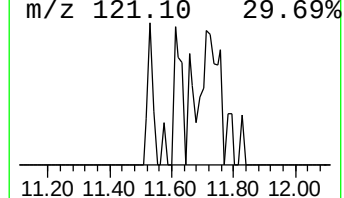
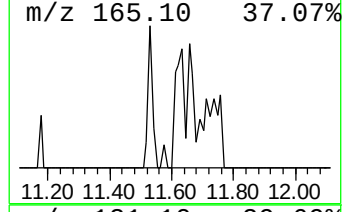
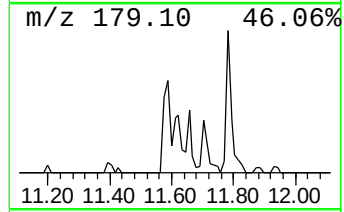
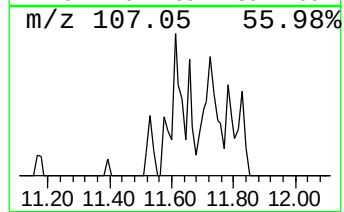
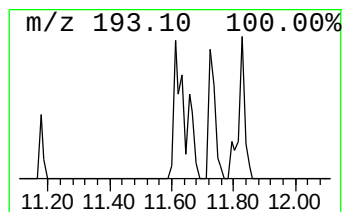
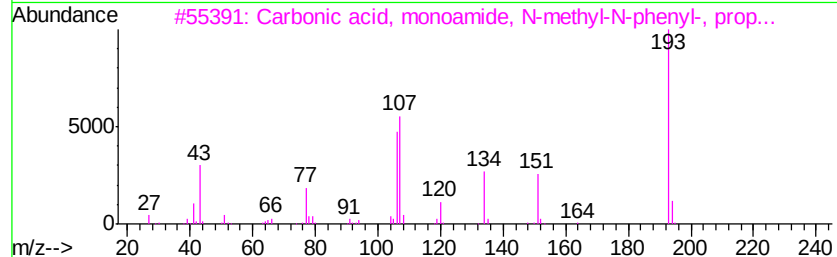
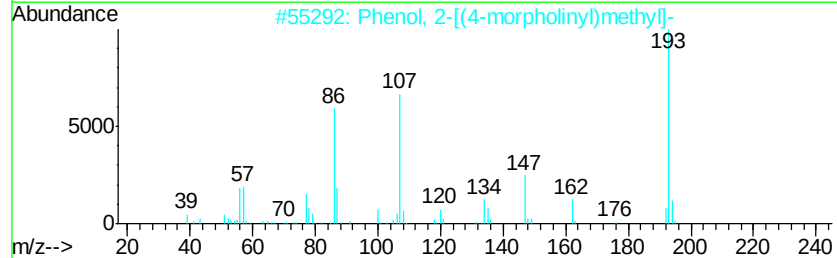
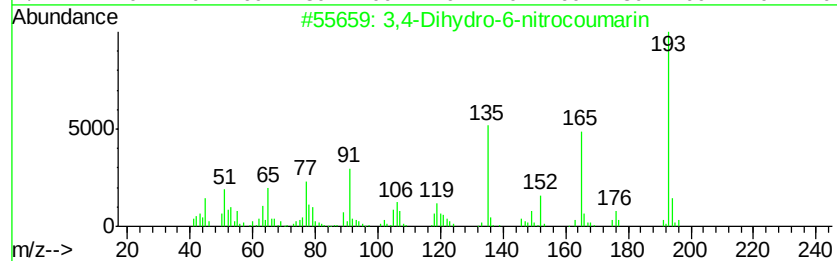
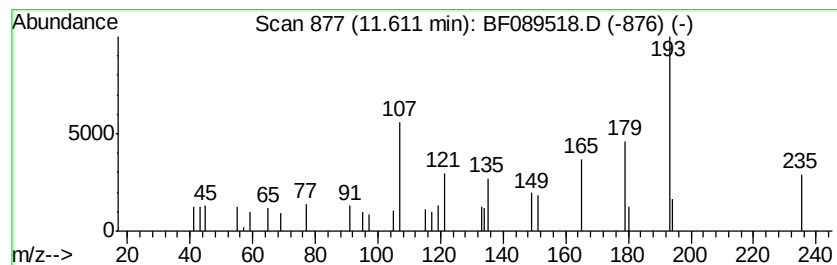
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown11.61 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.61	2.81 ng	40632	Phenanthrene-d10		10.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dihydro-6-nitrocoumarin	193	C9H7NO4	020920-99-4	38
2	Phenol, 2-[(4-morpholinyl)methyl]-	193	C11H15NO2	004438-01-1	38
3	Carbonic acid, monoamide, N-meth...	193	C11H15NO2	1000340-19-0	35
4	Benzonitrile, 2,3,4-trimethoxy-	193	C10H11NO3	043020-38-8	32
5	Carbamic acid, 3-methylphenyl-, ...	193	C11H15NO2	1000314-76-5	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
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Sample : H4256-01
Misc :
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Instrument :
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ClientSampleId :
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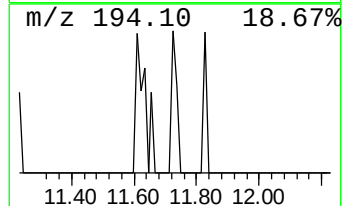
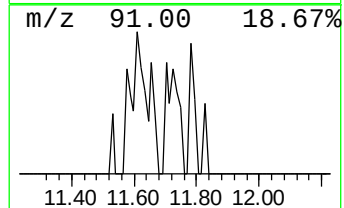
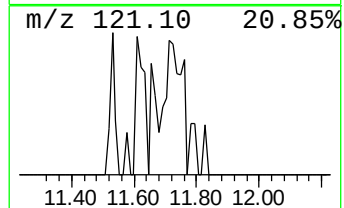
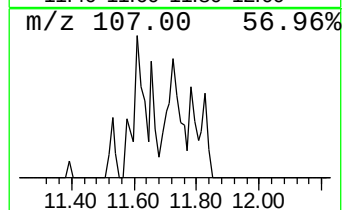
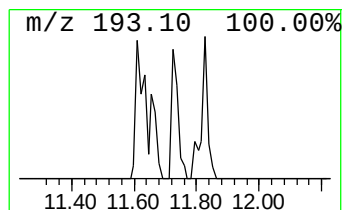
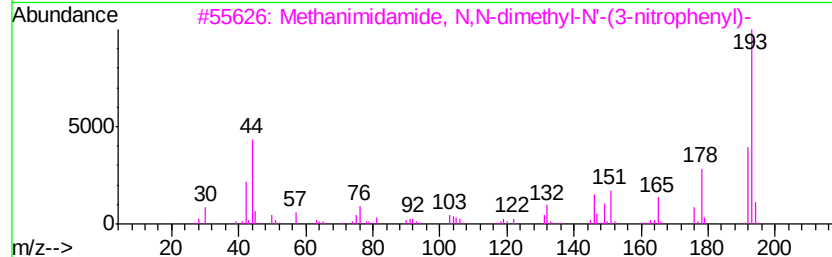
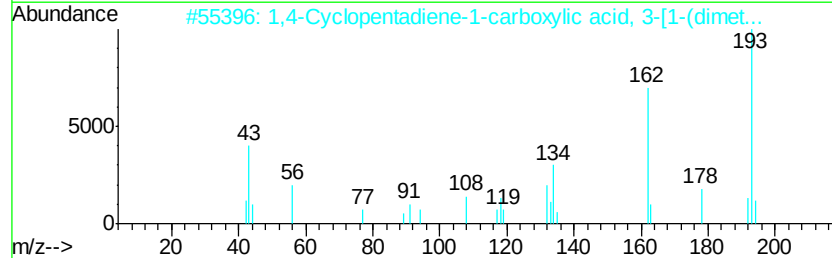
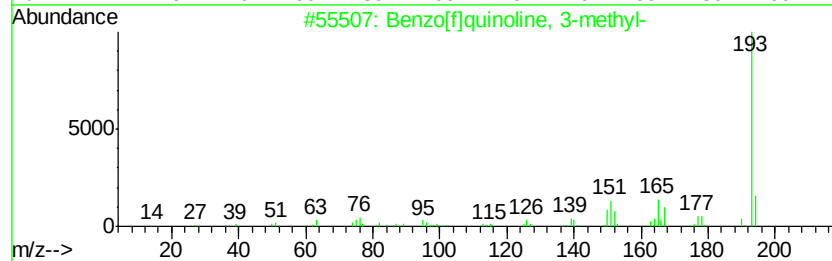
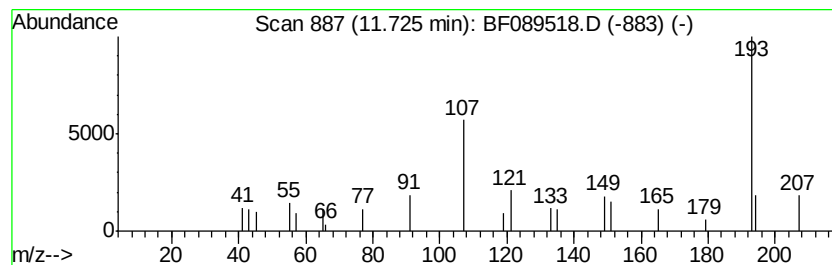
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown11.73 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.49 ng	35991	Phenanthrene-d10	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[f]quinoline, 3-methyl-	193	C14H11N	000085-06-3	43
2		1,4-Cyclopentadiene-1-carboxylic...	193	C11H15N02	014485-75-7	38
3		Methanimidamide, N,N-dimethyl-N'...	193	C9H11N3O2	002103-47-1	38
4		3-Oxabicyclo[5.3.0]decan-2-one, ...	194	C12H18O2	1000155-87-7	38
5		Methanimidamide, N,N-dimethyl-N'...	193	C9H11N3O2	001205-59-0	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089518.D
Acq On : 1 Aug 2016 18:56
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Sample : H4256-01
Misc :
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Instrument :
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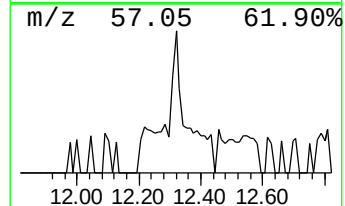
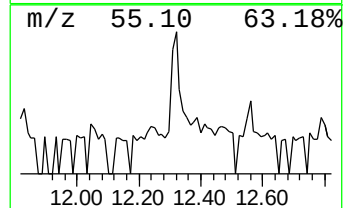
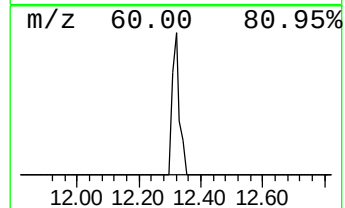
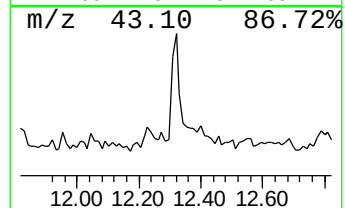
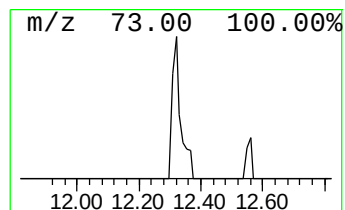
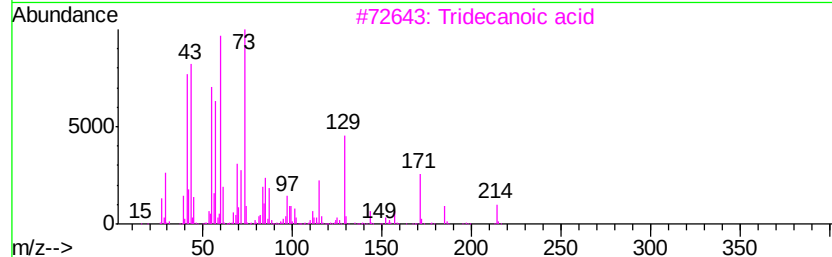
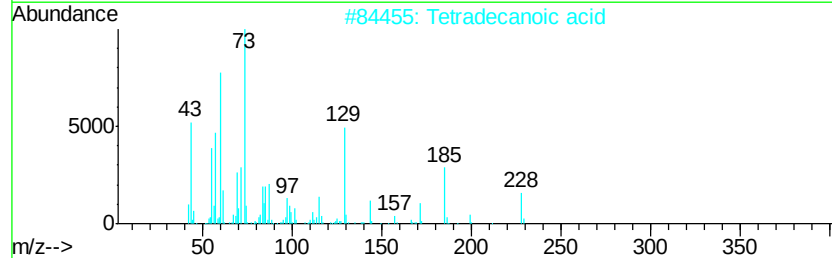
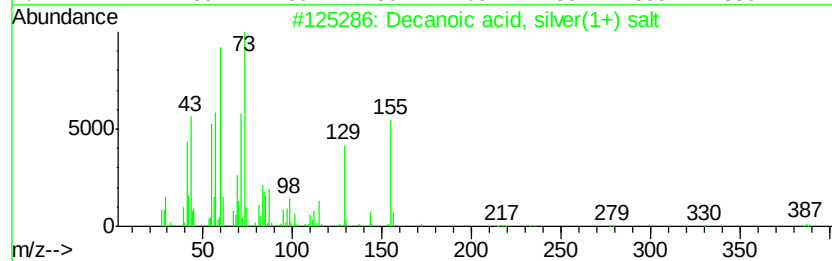
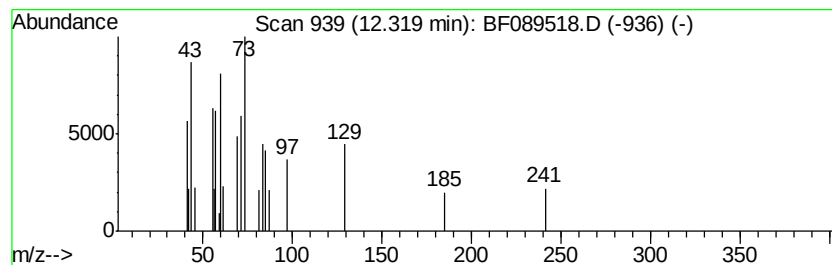
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Decanoic acid, silver(1+) salt Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	2.18 ng	26917	Chrysene-d12	13.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3		Tridecanoic acid	214	C13H26O2	000638-53-9	50
4		Oxalic acid, allvl octadecyl ester	382	C23H42O4	1000309-24-5	27
5		Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
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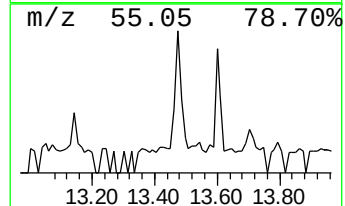
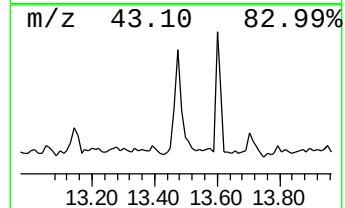
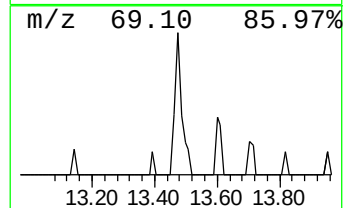
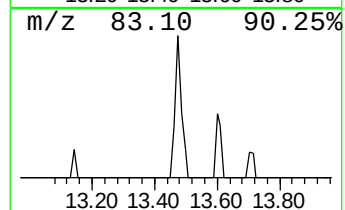
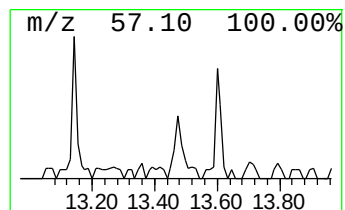
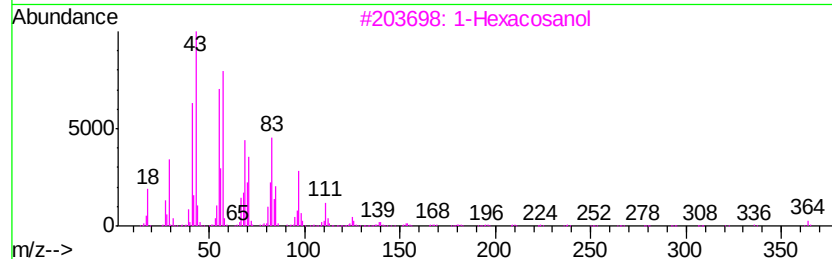
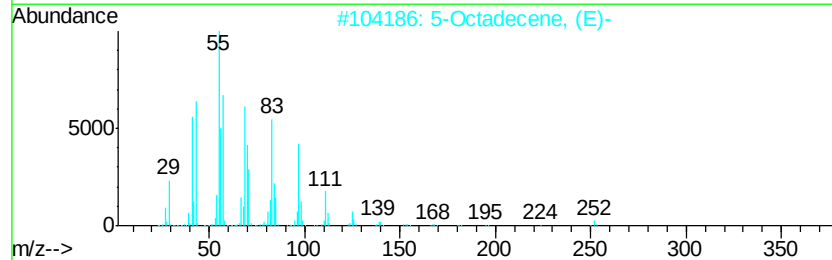
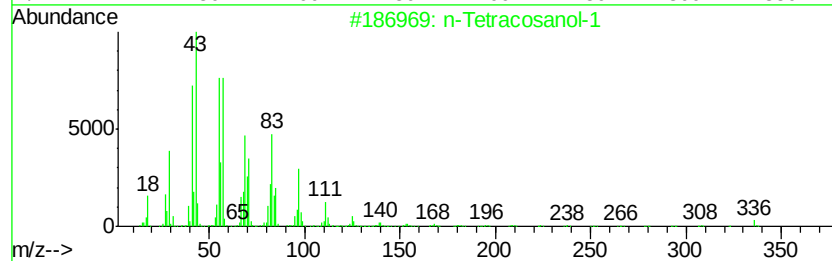
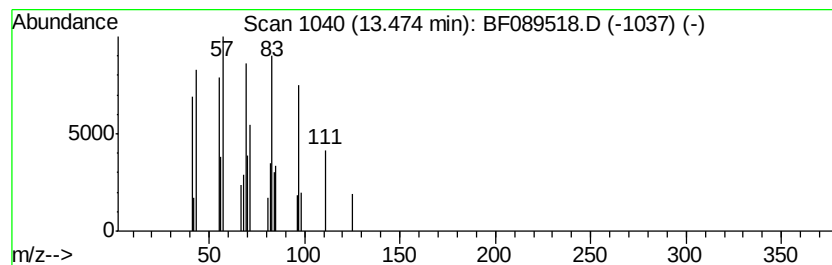
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Tetracosanol-1 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2.60 ng	32115	Chrysene-d12	13.60
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Tetracosanol-1	354 C24H50O	000506-51-4 90
2		5-Octadecene, (E)-	252 C18H36	007206-21-5 72
3		1-Hexacosanol	382 C26H54O	000506-52-5 68
4		Carbonic acid, isobutyl octadecyl ester	370 C23H46O3	1000314-61-5 53
5		Oxalic acid, allyl dodecyl ester	298 C17H30O4	1000309-24-0 50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
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Sample : H4256-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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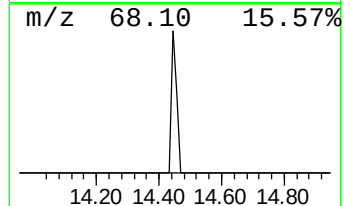
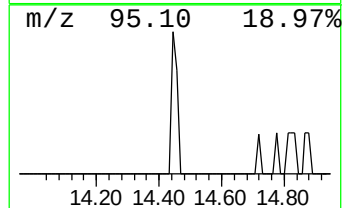
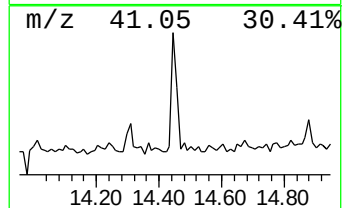
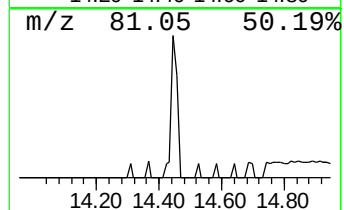
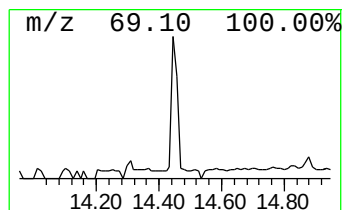
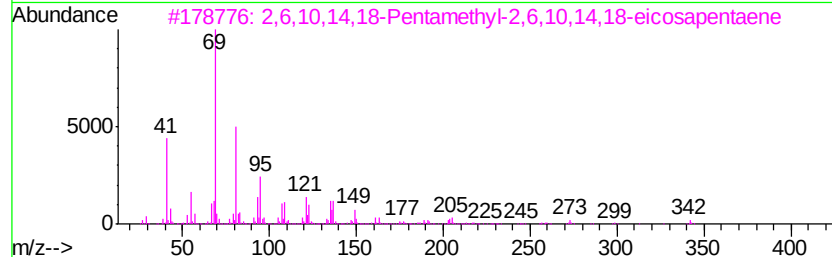
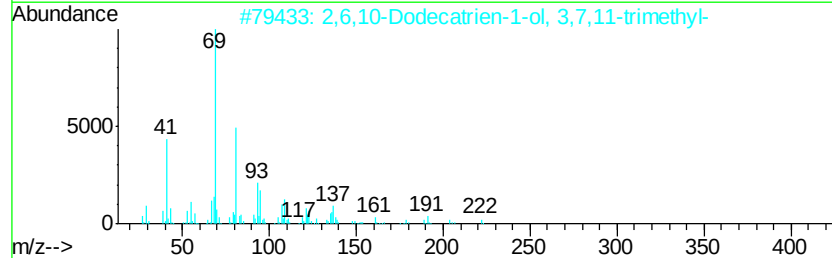
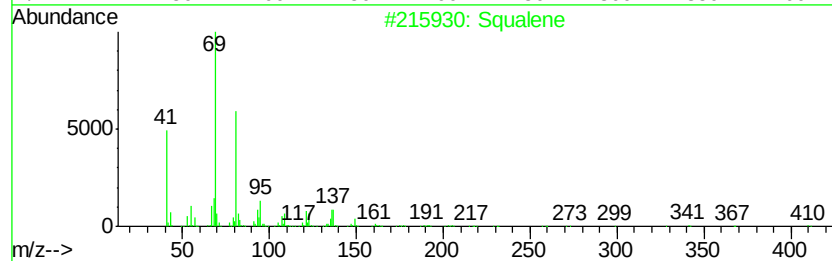
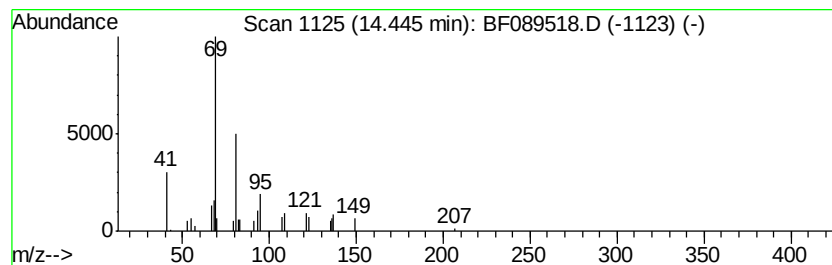
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Squalene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.22 ng	23966	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	83
3		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
4		trans-Farnesol	222	C15H26O	000106-28-5	78
5		Supraene	410	C30H50	007683-64-9	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
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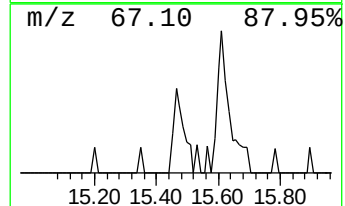
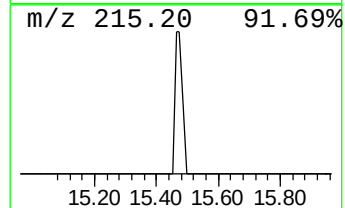
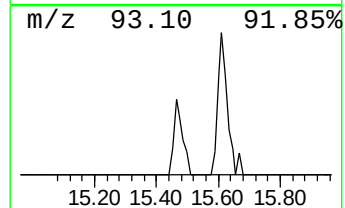
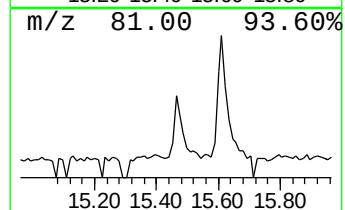
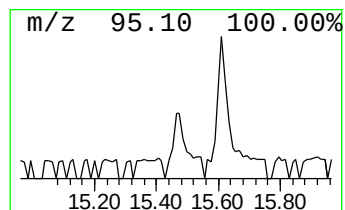
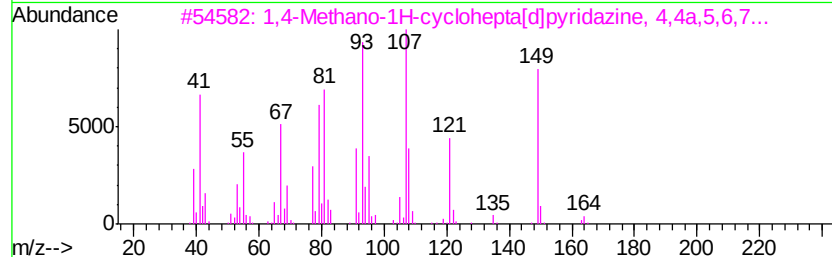
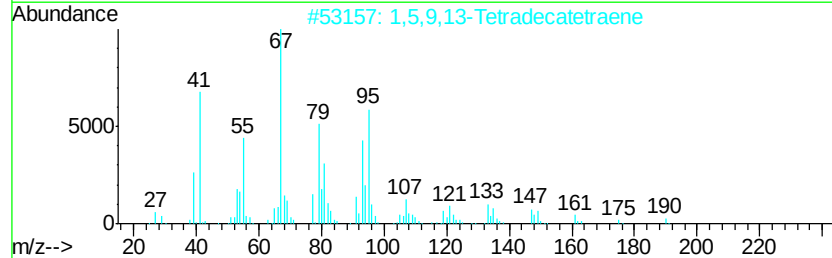
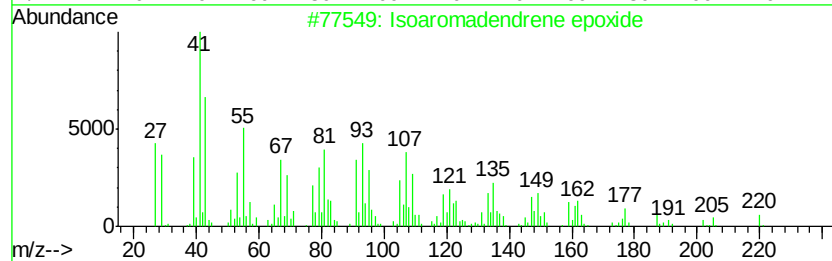
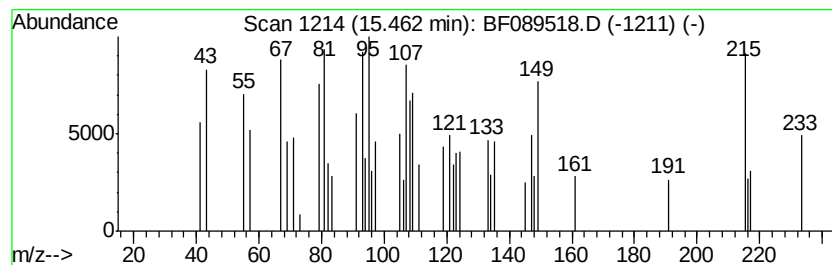
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown15.46 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	5.06 ng	54566	Perylene-d12	14.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoaromadendrene epoxide	220	C15H24O	1000159-36-6	35
2			1,5,9,13-Tetradecatetraene	190	C14H22	051487-38-8	35
3			1,4-Methano-1H-cyclohepta[d]pyri...	192	C12H20N2	1000221-85-4	22
4			1,8-Nonadiene, 2,7-dimethyl-5-(1...	192	C14H24	068702-20-5	22
5			Longipinane, (E)-	206	C15H26	1000156-14-5	22



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Data File : BF089518.D
Acq On : 1 Aug 2016 18:56
Operator : UM/SJ
Sample : H4256-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-6

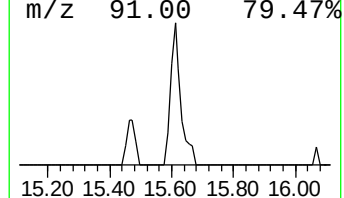
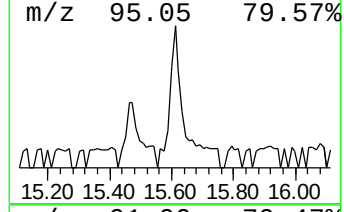
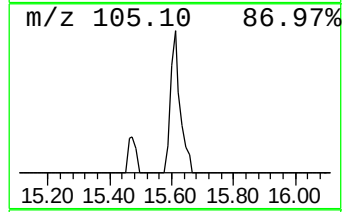
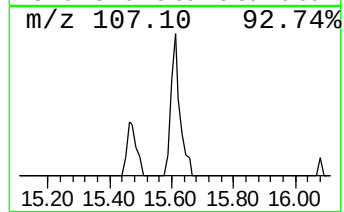
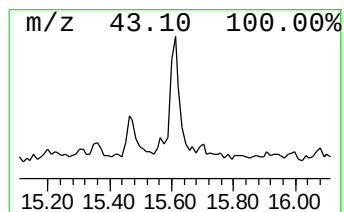
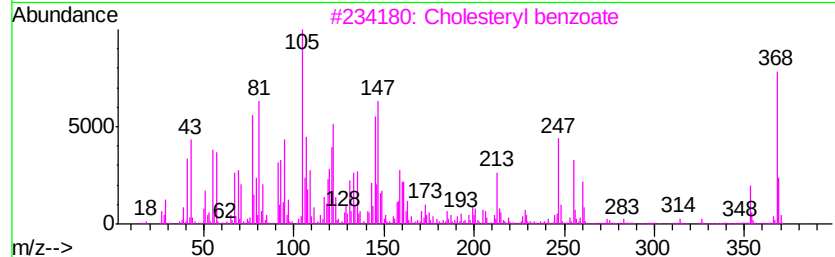
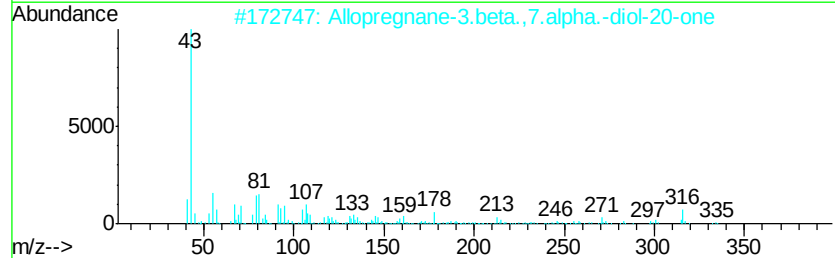
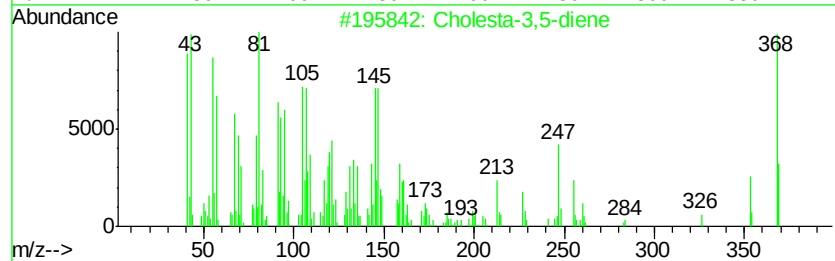
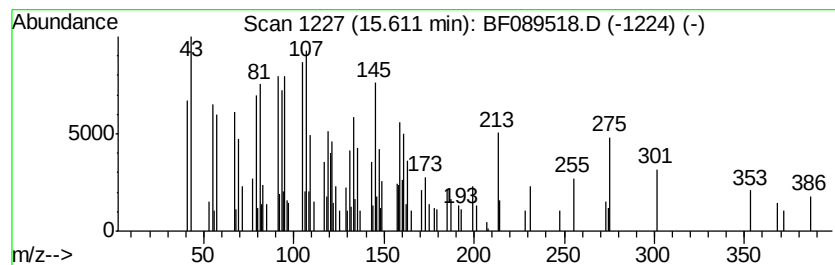
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Cholesta-3,5-diene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	13.17 ng	141988	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholesta-3,5-diene	368	C27H44	000747-90-0	53
2		Allopregnane-3.beta.,7.alpha.-di...	334	C21H34O3	000566-20-1	43
3		Cholesteryl benzoate	490	C34H50O2	000604-32-0	37
4		Cholest-5-en-3-ol (3.beta.)-, pr...	442	C30H50O2	000633-31-8	32
5		1,4-Methanocycloocta[d]pyridazin...	204	C13H20N2	1000221-85-9	14



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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-6

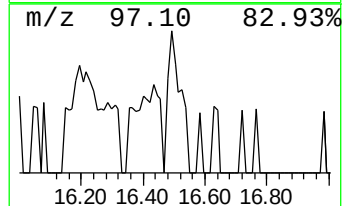
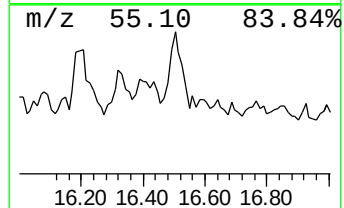
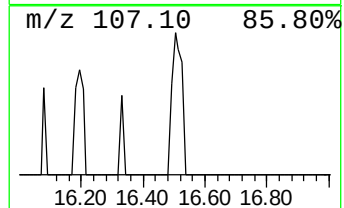
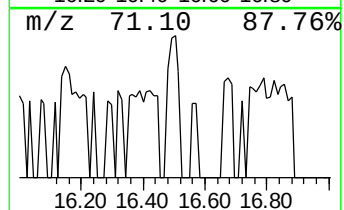
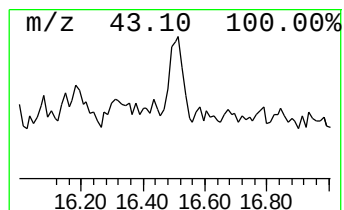
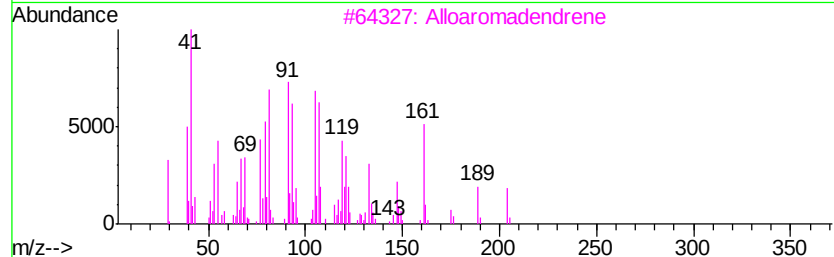
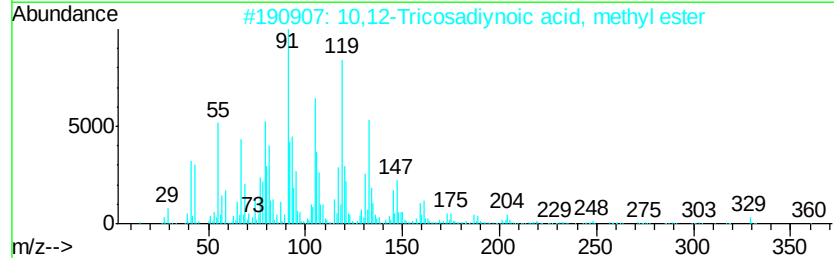
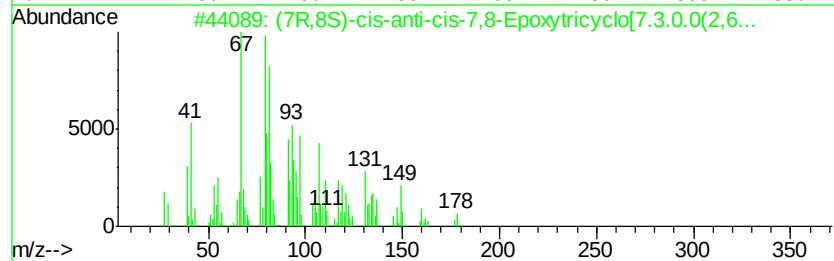
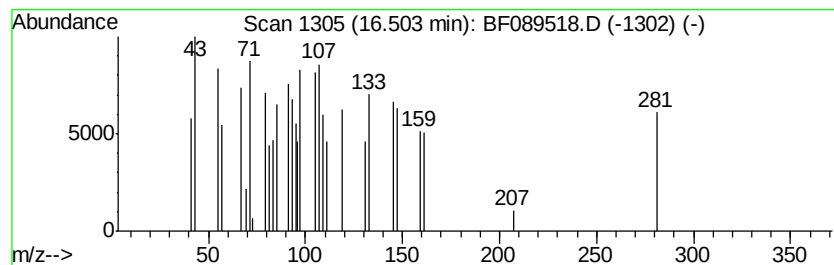
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown16.50 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	2.71 ng	29182	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(7R,8S)-cis-anti-cis-7,8-Epoxytr...	178	C12H18O	073285-35-5	35
2		10,12-Tricosadiynoic acid, methy...	360	C24H40O2	1000333-59-4	27
3		Alloaromadendrene	204	C15H24	025246-27-9	27
4		1,4-Methanocycloocta[d]pyridazin...	204	C13H20N2	1000221-85-9	16
5		Caryophyllene	204	C15H24	000087-44-5	16



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 Sample : H4256-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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...	4.55	5.9	ng	63356	1	6.48	213977	20.0
unknown6.24	6.24	58.7	ng	627584	1	6.48	213977	20.0
1-Hexanol, 2-ethyl-	6.56	5.8	ng	62043	1	6.48	213977	20.0
Indole	8.42	4.8	ng	72211	2	7.76	302026	20.0
Caffeine	11.18	5.1	ng	73715	4	10.98	288716	20.0
unknown11.53	11.53	3.1	ng	44484	4	10.98	288716	20.0
unknown11.61	11.61	2.8	ng	40632	4	10.98	288716	20.0
unknown11.73	11.73	2.5	ng	35991	4	10.98	288716	20.0
Decanoic acid, si...	12.32	2.2	ng	26917	5	13.60	246968	20.0
n-Tetracosanol-1	13.47	2.6	ng	32115	5	13.60	246968	20.0
Squalene	14.45	2.2	ng	23966	6	14.93	215689	20.0
unknown15.46	15.46	5.1	ng	54566	6	14.93	215689	20.0
Cholesta-3,5-diene	15.61	13.2	ng	141988	6	14.93	215689	20.0
unknown16.50	16.50	2.7	ng	29182	6	14.93	215689	20.0