

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052617\
 Data File : BM010264.D
 Acq On : 26 May 2017 19:23
 Operator : SJ/MA
 Sample : I3306-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DSK-MW-LS

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

Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.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	5.522	408	414	426	rBV	1173193	1729069	15.57%	3.694%
2	7.122	679	686	698	rBV	597470	994405	8.96%	2.125%
3	7.475	739	746	757	rBV	1966239	3202234	28.84%	6.842%
4	7.939	819	825	837	rBV	420367	702714	6.33%	1.501%
5	8.257	872	879	889	rVB	2030879	3219189	29.00%	6.878%
6	9.128	1018	1027	1035	rBV	1353434	2232233	20.11%	4.769%
7	10.745	1295	1302	1308	rBV	482175	836936	7.54%	1.788%
8	12.557	1603	1610	1617	rBV2	192769	370828	3.34%	0.792%
9	13.192	1711	1718	1725	rBV	4341650	5853279	52.72%	12.506%
10	13.304	1733	1737	1749	rBV	64644	163476	1.47%	0.349%
11	13.951	1842	1847	1855	rVB	257446	379258	3.42%	0.810%
12	14.268	1895	1901	1906	rBV5	102703	190665	1.72%	0.407%
13	14.363	1912	1917	1921	rVB3	162999	242905	2.19%	0.519%
14	14.504	1934	1941	1945	rBV8	51241	129878	1.17%	0.278%
15	14.568	1947	1952	1961	rVV2	722901	1149466	10.35%	2.456%
16	16.062	2200	2206	2218	rBV	3765450	5051541	45.50%	10.793%
17	16.851	2336	2340	2353	rVB	113209	264824	2.39%	0.566%
18	17.315	2414	2419	2426	rVB2	1051568	1524339	13.73%	3.257%
19	17.956	2524	2528	2534	rVB5	99614	138124	1.24%	0.295%
20	18.051	2540	2544	2552	rVB	144285	236411	2.13%	0.505%
21	18.162	2559	2563	2568	rBV5	100341	153707	1.38%	0.328%
22	18.915	2689	2691	2699	rVB2	89486	116004	1.04%	0.248%
23	19.921	2856	2862	2871	rBV	9232797	11101608	100.00%	23.720%
24	21.480	3122	3127	3132	rBV	1794477	2312310	20.83%	4.941%
25	22.586	3310	3315	3320	rBV	1666370	2142961	19.30%	4.579%
26	23.833	3521	3527	3535	rVB2	1169308	2364135	21.30%	5.051%

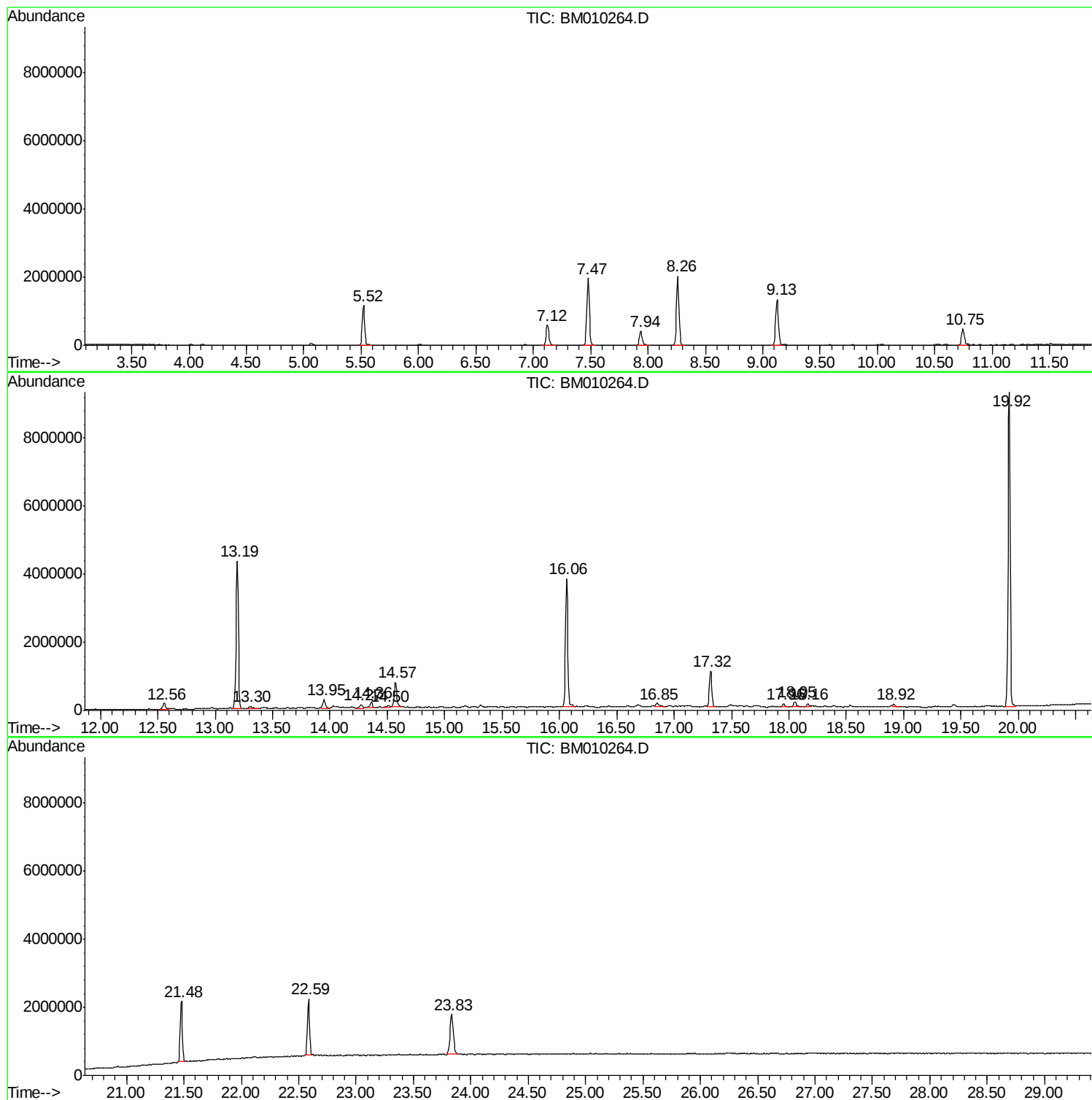
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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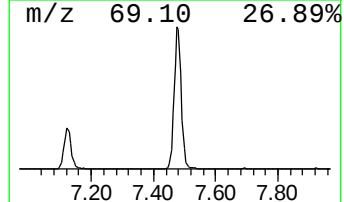
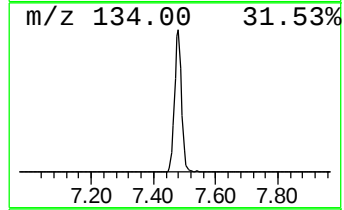
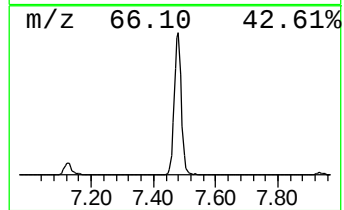
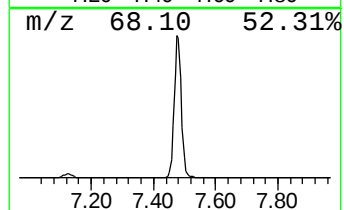
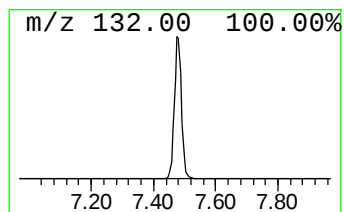
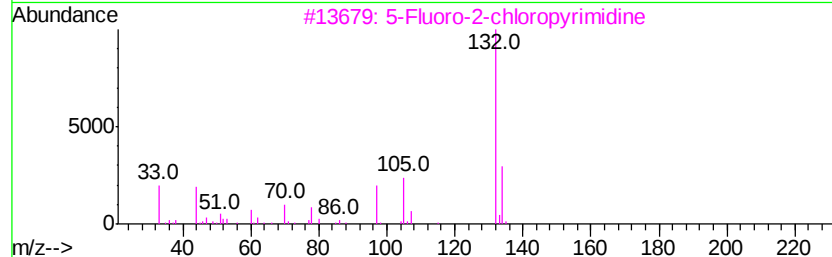
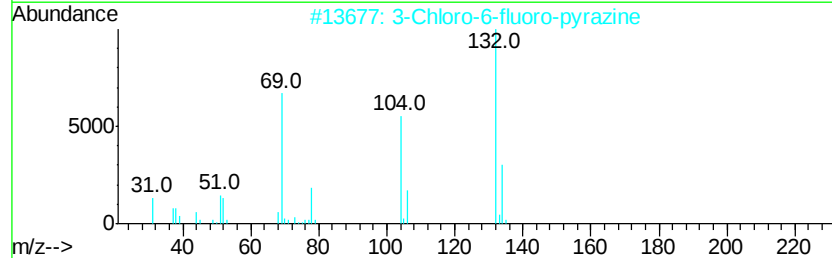
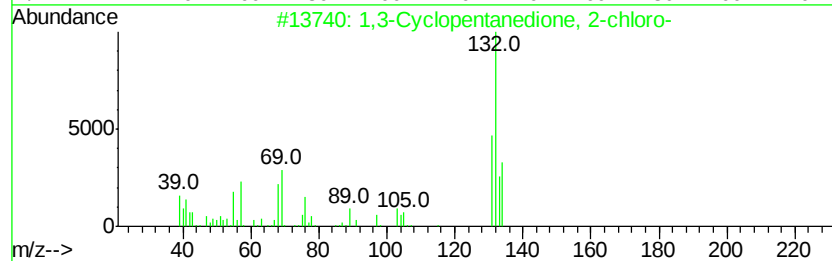
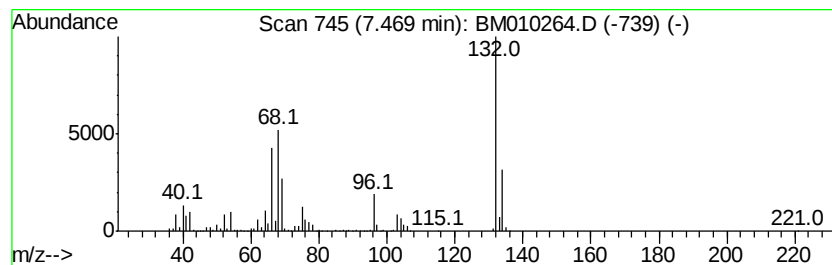
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	91.14 ng	3202230	1,4-Dichlorobenzene-d4	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10



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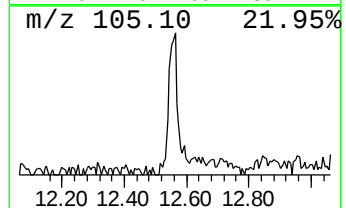
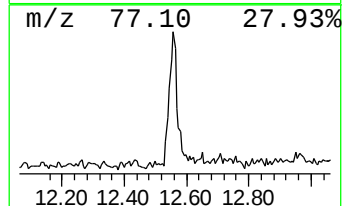
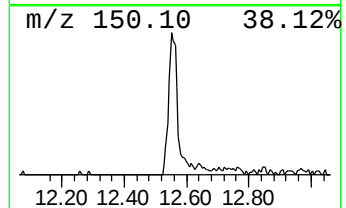
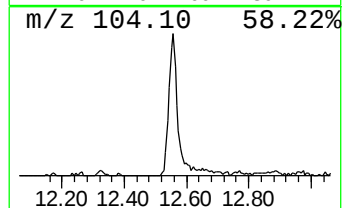
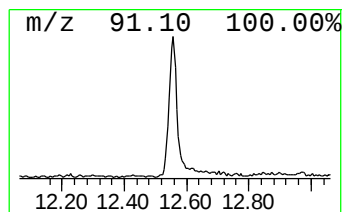
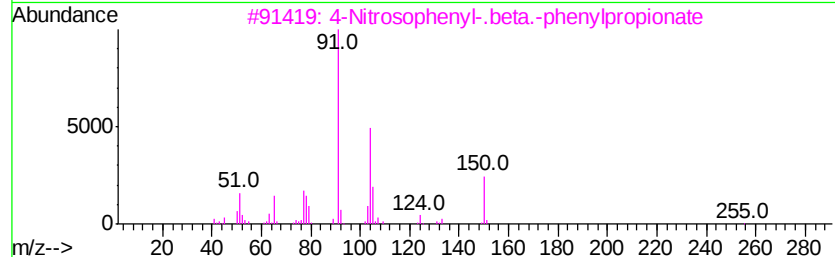
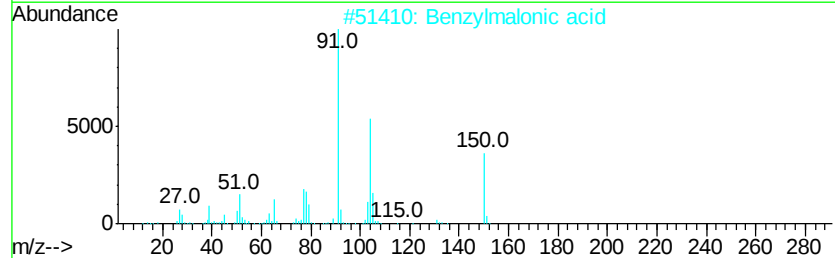
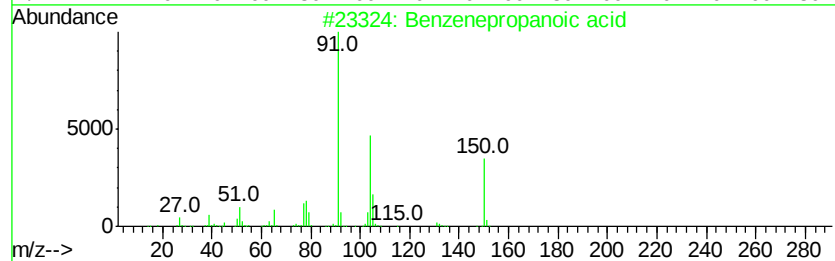
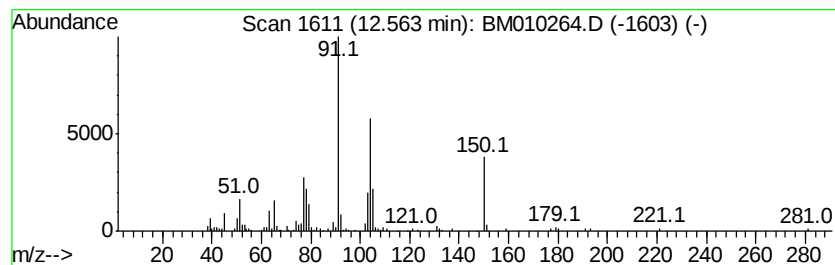
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Peak Number 3 Benzenepropanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.56	8.86 ng	370828	Napthalene-d8	10.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid	150	C9H10O2	000501-52-0	74
2	Benzylmalonic acid	194	C10H10O4	000616-75-1	72
3	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	64
4	3-Phenyl-propionic acid, isoprop...	192	C12H16O2	022767-95-9	64
5	2-Phenethyl-.beta.-phenylpropionate	254	C17H18O2	028049-10-7	50



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Instrument :
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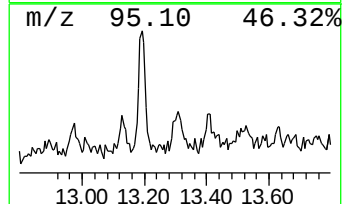
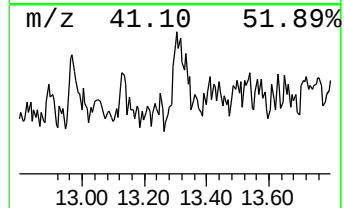
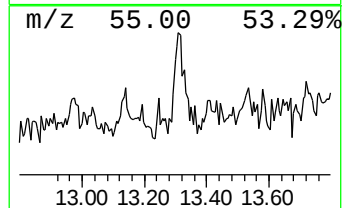
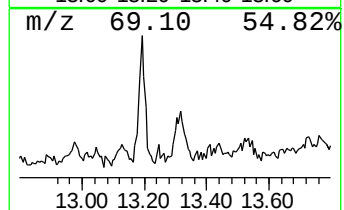
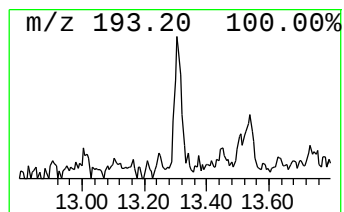
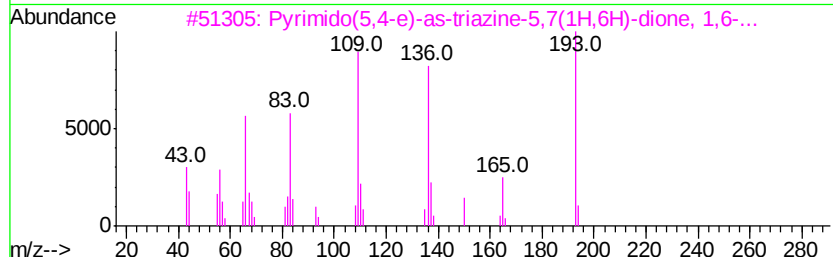
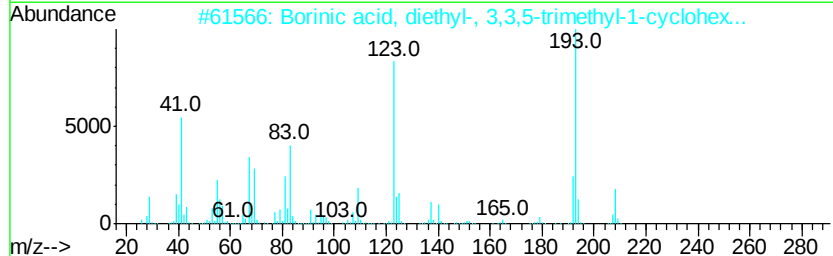
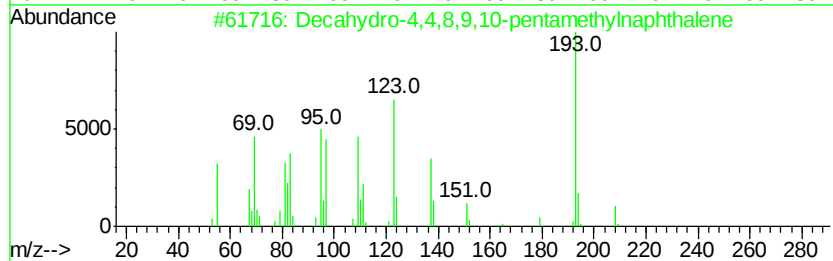
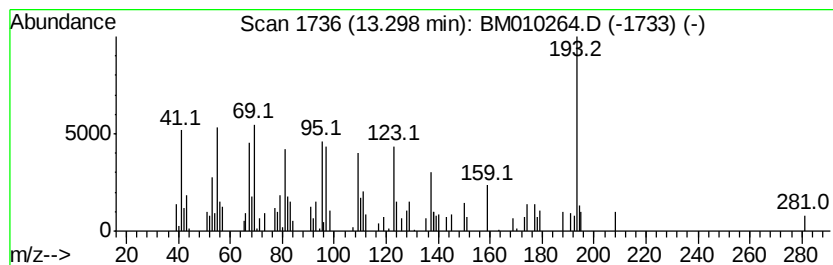
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Peak Number 4 Decahydro-4,4,8,9,10-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	2.84 ng	163476	Acenaphthene-d10	14.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	86
2		Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
3		Pvrimido(5,4-e)-as-triazine-5,7(...	193	C7H7N5O2	000084-82-2	38
4		6-Methylphenanthridine	193	C14H11N	003955-65-5	27
5		2-Anthracenamine	193	C14H11N	000613-13-8	27



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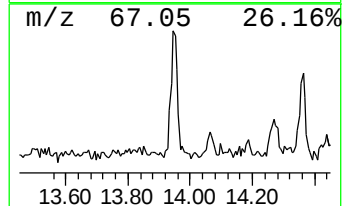
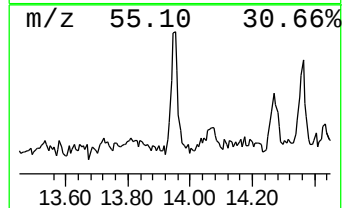
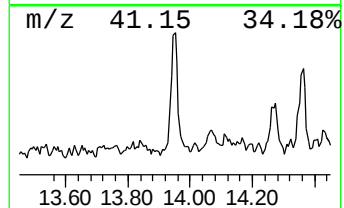
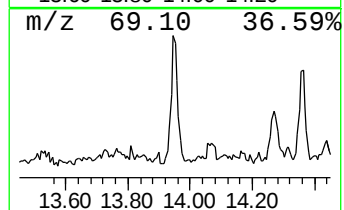
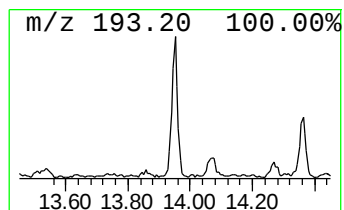
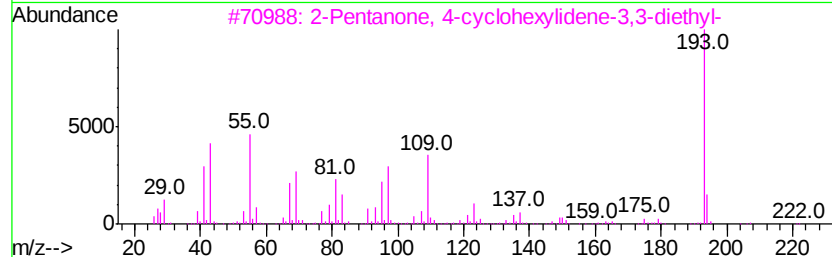
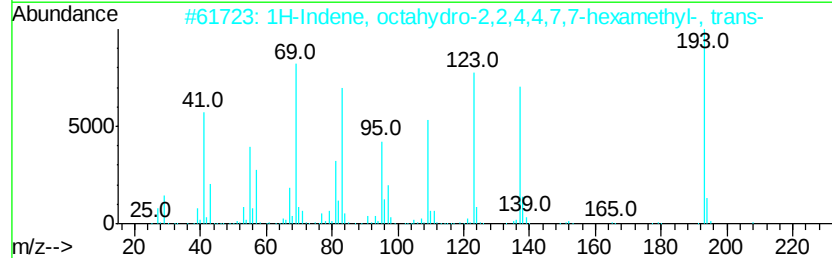
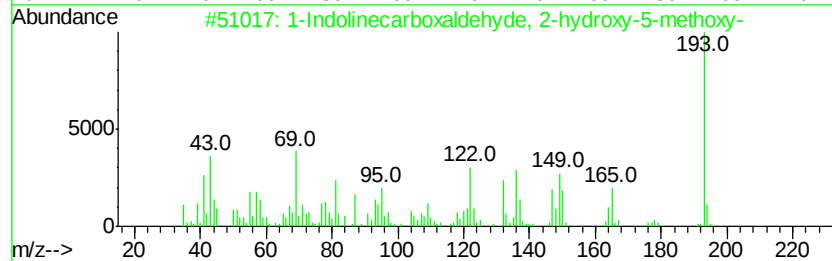
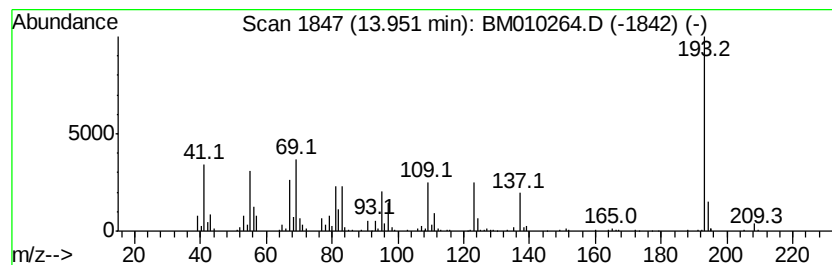
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Peak Number 5 1-Indolinecarboxaldehyde, 2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.95	6.60 ng	379258	Acenaphthene-d10	14.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11N03	013303-70-3	50
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	42
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	42
5	1-(P-FLUOROPHENYL)-4-PIPERIDONE	193	C11H12FNO	1000238-56-7	38



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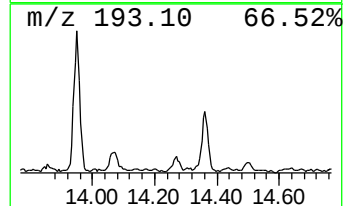
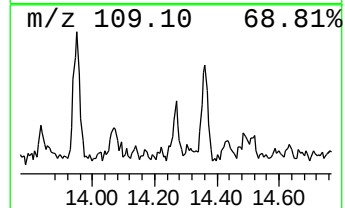
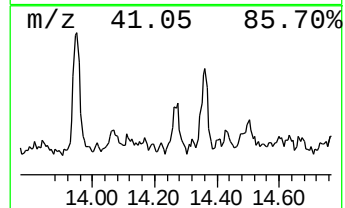
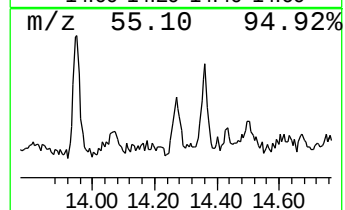
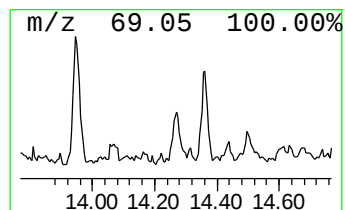
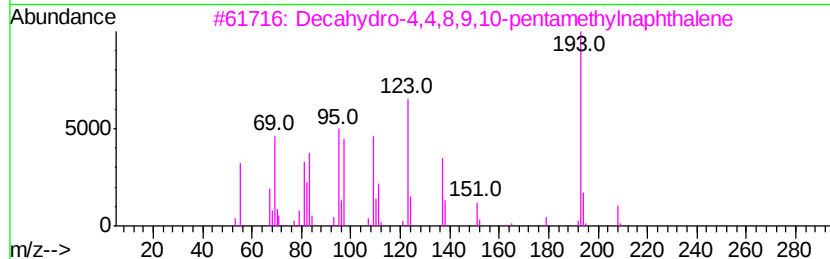
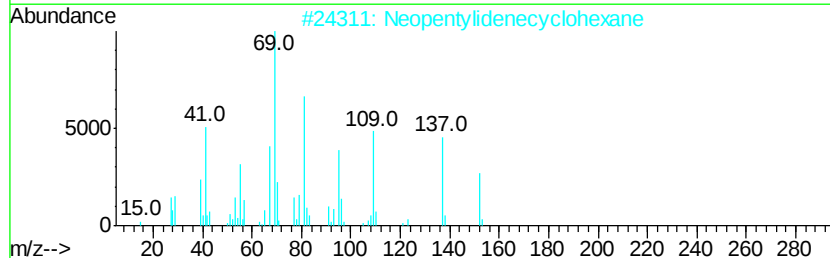
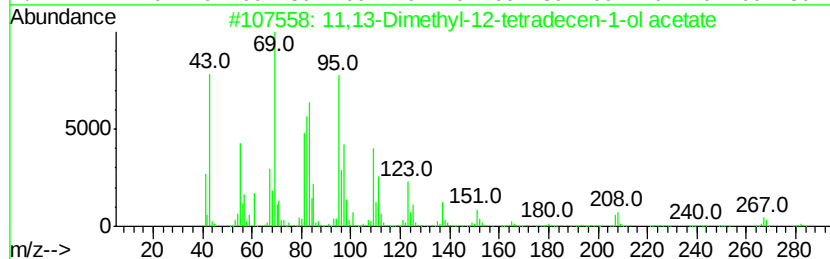
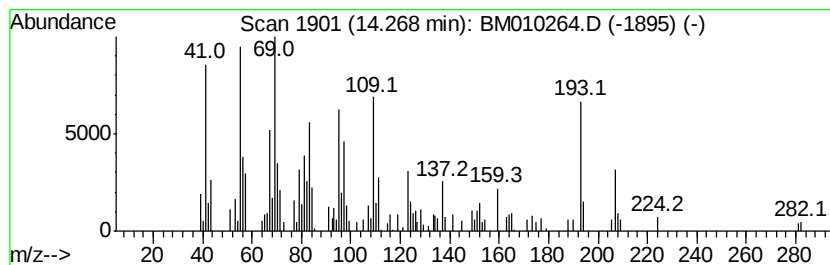
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Peak Number 6 11,13-Dimethyl-12-tetradec... Concentration Rank 8

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14.27	3.32 ng	190665	Acenaphthene-d10	14.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11,13-Dimethyl-12-tetradecen-1-o...	282	C18H34O2	1000130-81-0	53
2			Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
3			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	42
4			1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	35
5			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	27



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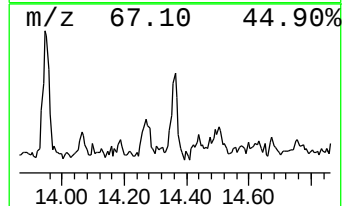
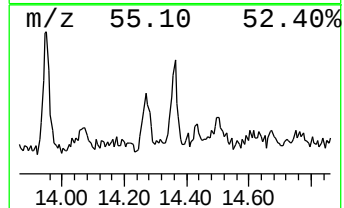
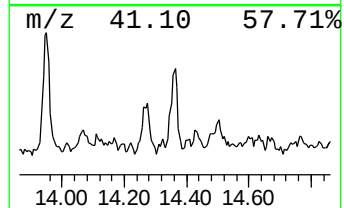
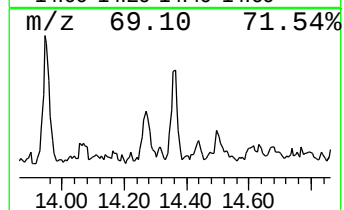
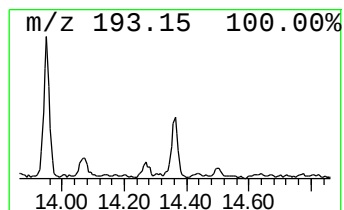
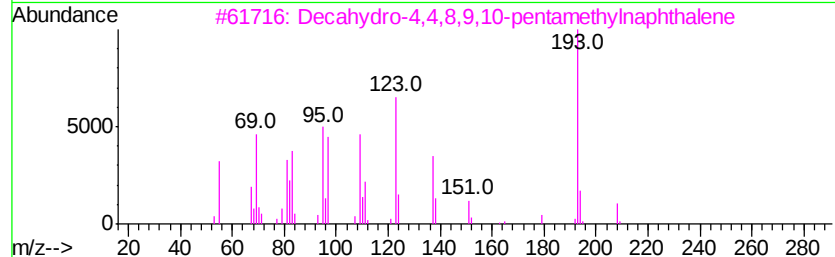
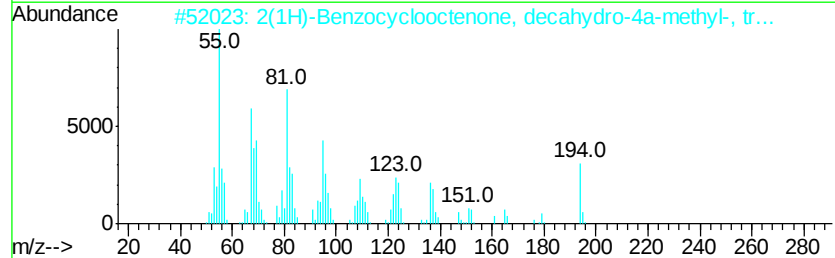
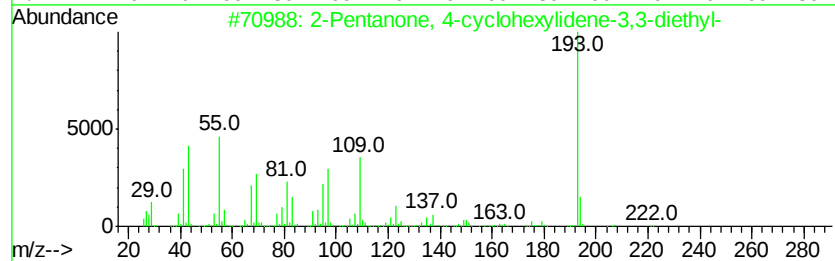
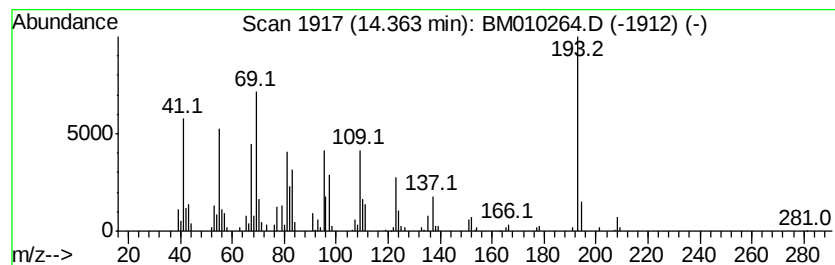
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ClientSampleId :
DSK-MW-LS

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Pentanone, 4-cyclohexylidene-3,3-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	4.23 ng	242905	Acenaphthene-d10	14.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Pentanone, 4-cvclohexvlidene-3...	222 C15H26O	313253-65-5	53
2	2(1H)-Benzocyclooctenone, decahy...	194 C13H22O	055103-66-7	49
3	Decahydro-4,4,8,9,10-pentamethyl...	208 C15H28	080655-44-3	43
4	Borinic acid, diethyl-, 3,3,5-tr...	208 C13H25BO	057387-76-5	37
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138 C10H18	004863-59-6	35



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052617\
Data File : BM010264.D
Acq On : 26 May 2017 19:23
Operator : SJ/MA
Sample : I3306-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DSK-MW-LS

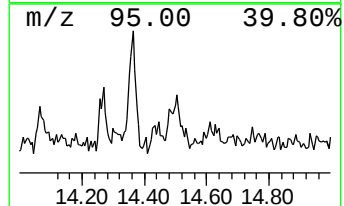
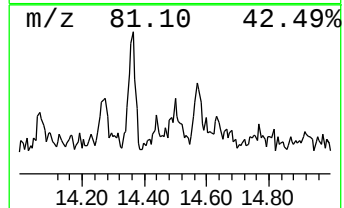
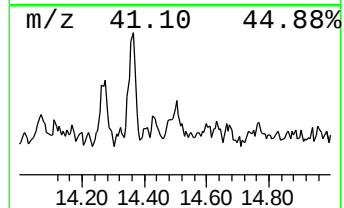
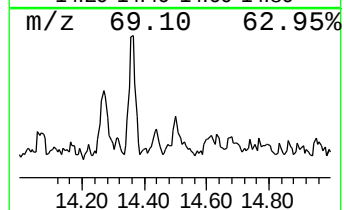
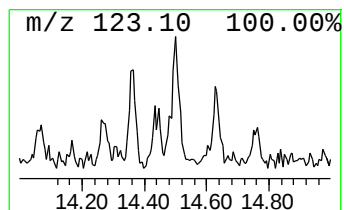
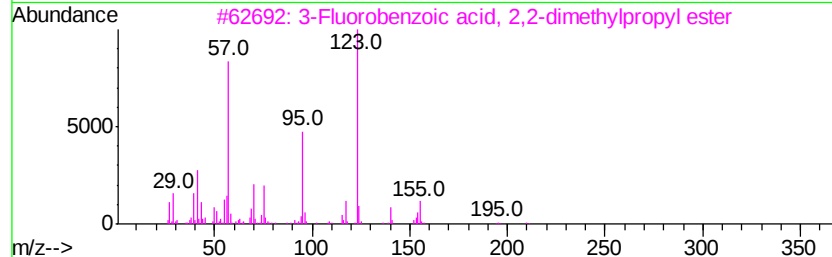
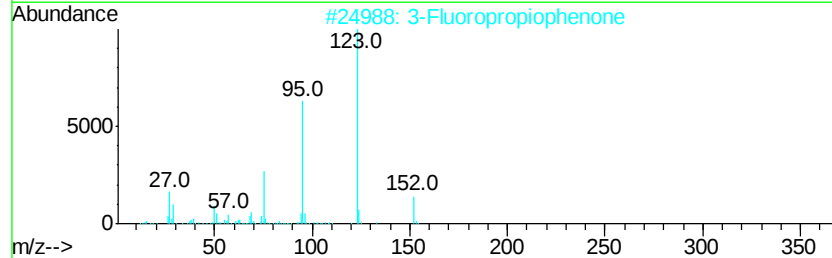
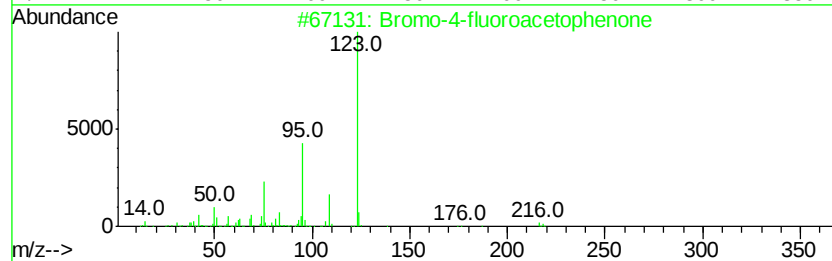
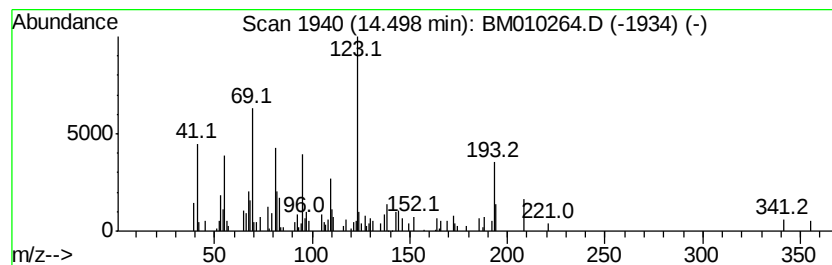
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.50 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.26 ng	129878	Acenaphthene-d10	14.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromo-4-fluoroacetophenone	216	C8H6BrFO	000403-29-2	35
2		3-Fluoropropiophenone	152	C9H9FO	000455-67-4	30
3		3-Fluorobenzoic acid, 2,2-dimeth...	210	C12H15FO2	204779-85-1	27
4		4-Fluorobenzoic acid, isopropyl ...	182	C10H11FO2	002928-09-8	27
5		Benzoyl chloride, 3-fluoro-	158	C7H4ClFO	001711-07-5	27



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052617\
Data File : BM010264.D
Acq On : 26 May 2017 19:23
Operator : SJ/MA
Sample : I3306-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

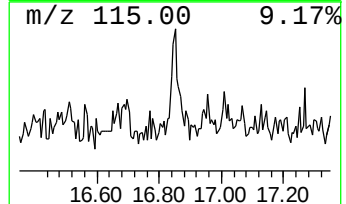
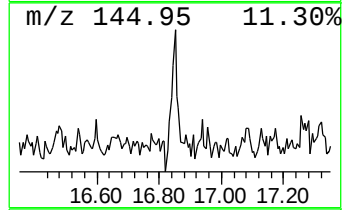
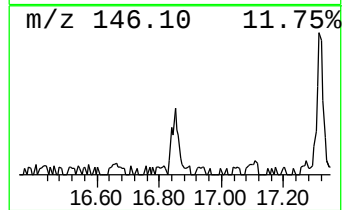
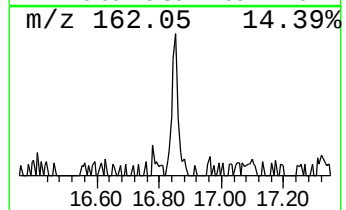
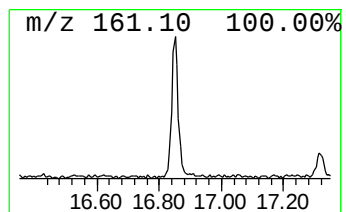
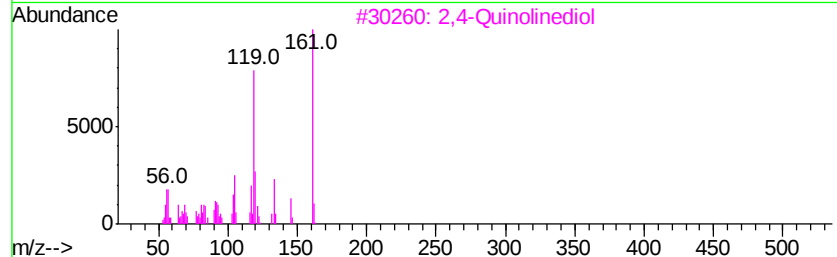
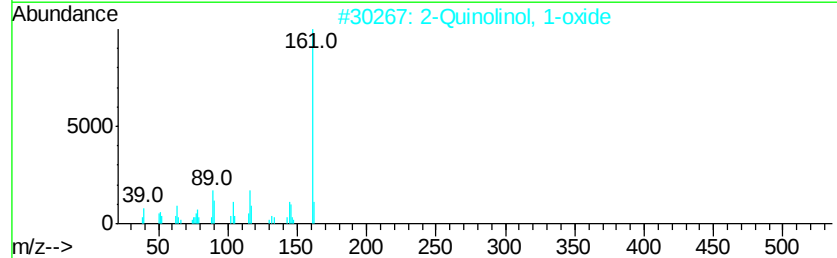
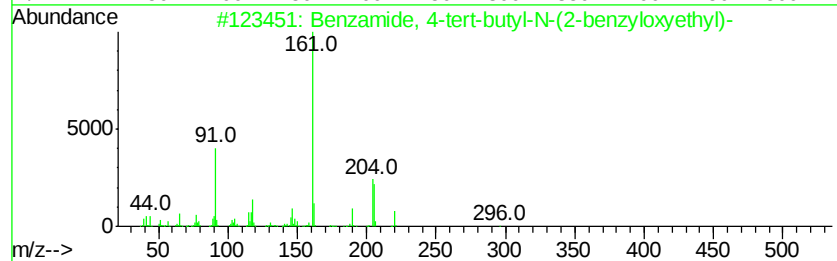
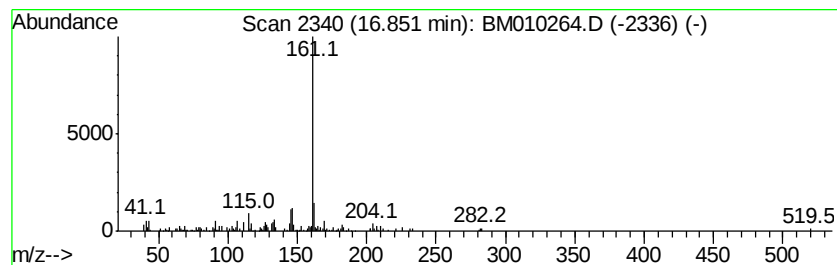
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ClientSampled :
DSK-MW-LS

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzamide, 4-tert-butyl-N-(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.85	3.47 ng	264824	Phenanthrene-d10	17.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, 4-tert-butyl-N-(2-ben...	311	C20H25N02	349491-49-2	72
2	2-Quinolinol, 1-oxide	161	C9H7N02	010285-97-9	64
3	2,4-Quinolinediol	161	C9H7N02	000086-95-3	64
4	Benzoic acid, 4-(1,1-dimethyleth...	204	C13H16O2	015484-80-7	64
5	Benzoyl chloride, 4-(1,1-dimethy...	196	C11H13ClO	001710-98-1	64



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052617\
Data File : BM010264.D
Acq On : 26 May 2017 19:23
Operator : SJ/MA
Sample : I3306-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DSK-MW-LS

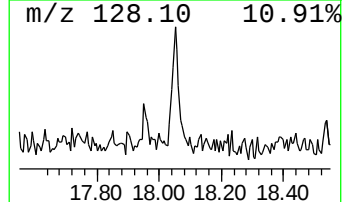
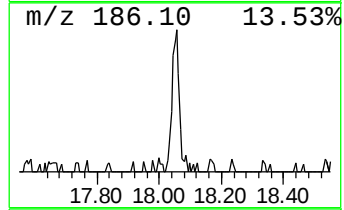
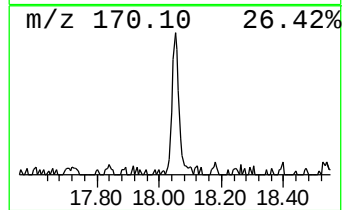
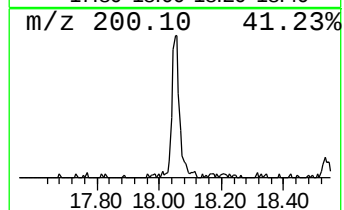
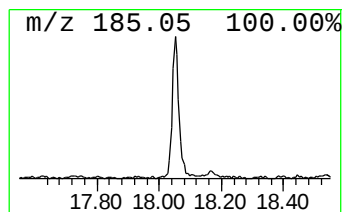
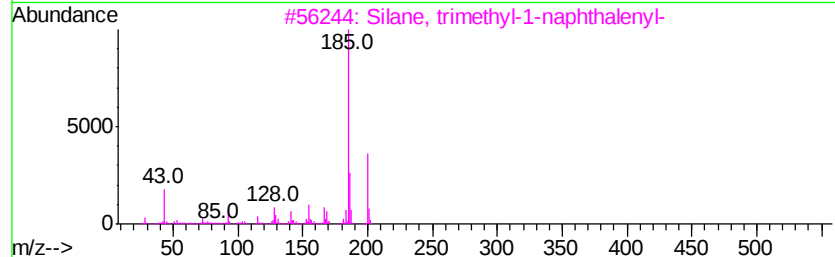
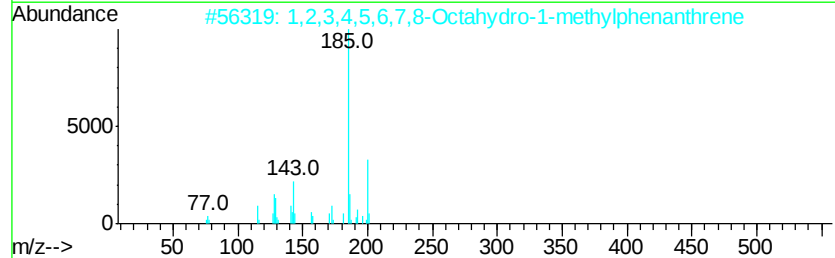
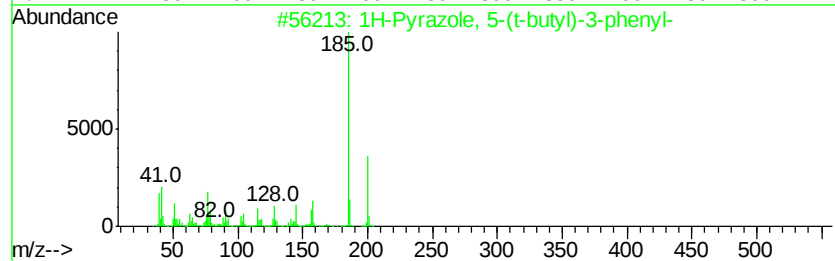
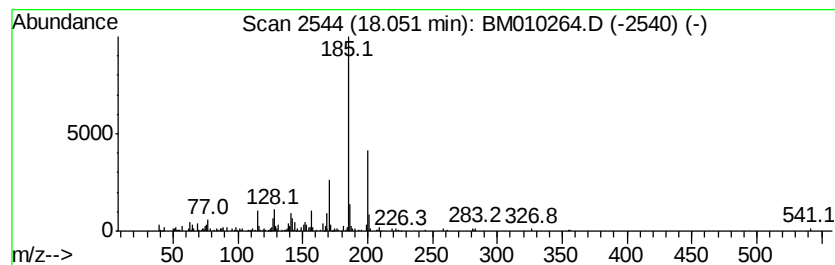
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1H-Pyrazole, 5-(t-butyl)-3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	3.10 ng	236411	Phenanthrene-d10	17.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrazole, 5-(t-butyl)-3-phenyl-	200	C13H16N2	1000261-34-8	81
2			1,2,3,4,5,6,7,8-Octahydro-1-meth...	200	C15H20	1000080-19-4	64
3			Silane, trimethyl-1-naphthalenyl-	200	C13H16Si	018052-80-7	59
4			Ethanone, 1-(6-methoxy-1-naphtha...	200	C13H12O2	058149-89-6	58
5			2-Acetyl-6-methoxynaphthalene	200	C13H12O2	003900-45-6	53



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052617\
Data File : BM010264.D
Acq On : 26 May 2017 19:23
Operator : SJ/MA
Sample : I3306-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
DSK-MW-LS

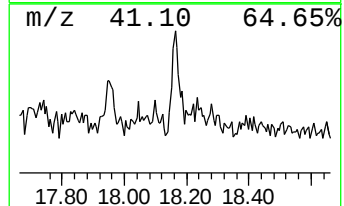
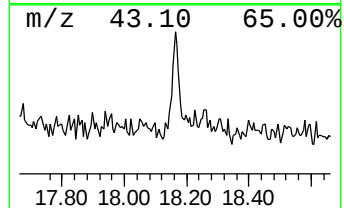
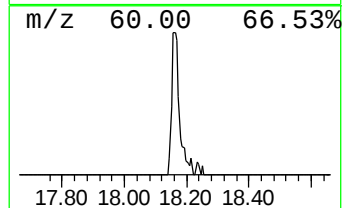
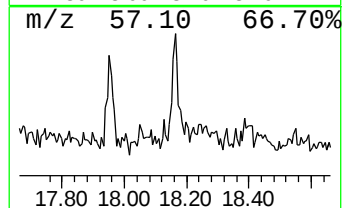
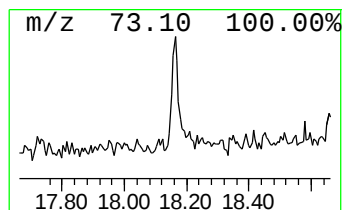
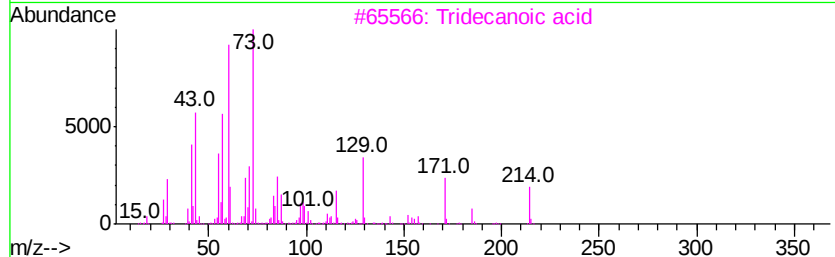
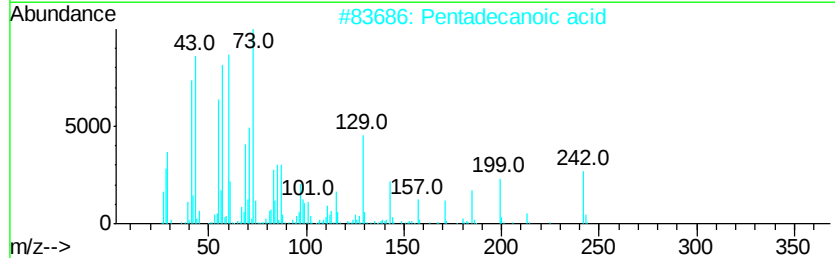
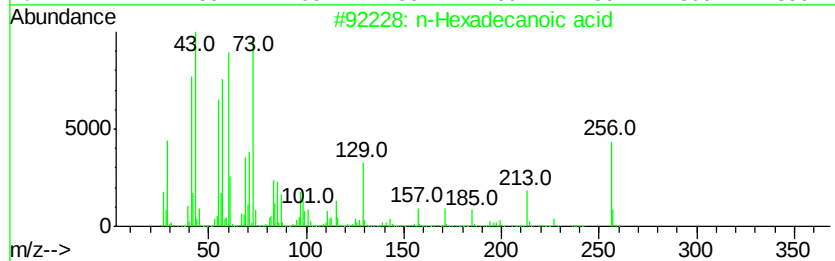
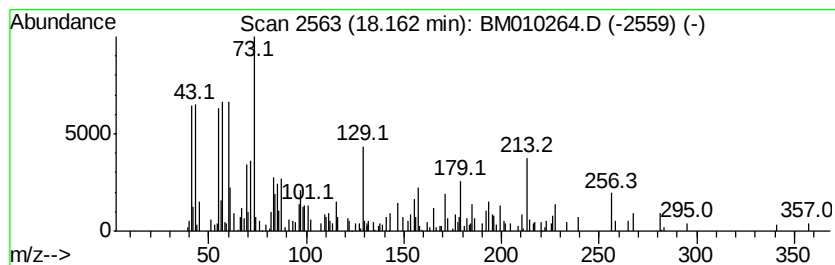
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	2.02 ng	153707	Phenanthrene-d10	17.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3		Tridecanoic acid	214	C13H26O2	000638-53-9	49
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5		n-Decanoic acid	172	C10H20O2	000334-48-5	38



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052617\
Data File : BM010264.D
Acq On : 26 May 2017 19:23
Operator : SJ/MA
Sample : I3306-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DSK-MW-LS

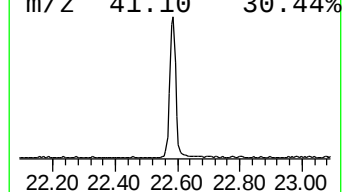
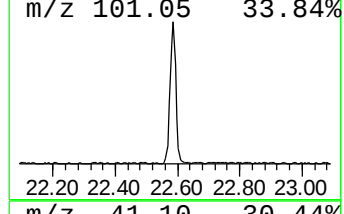
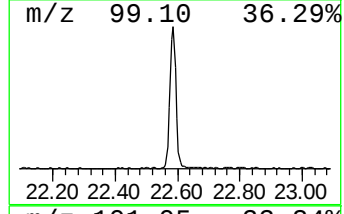
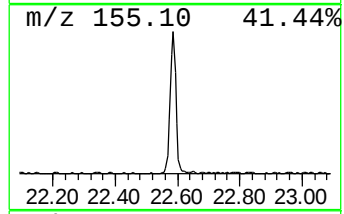
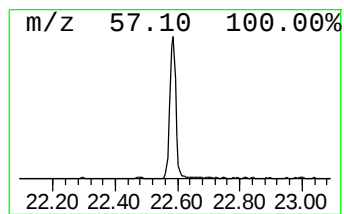
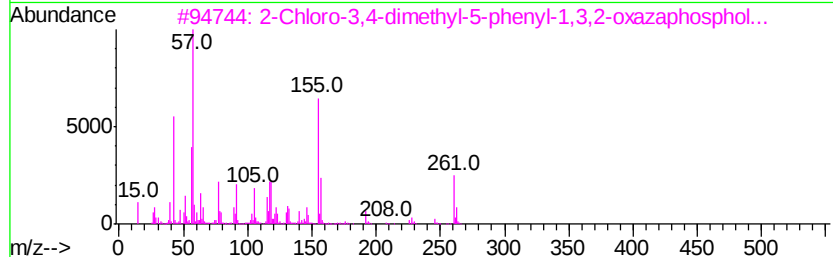
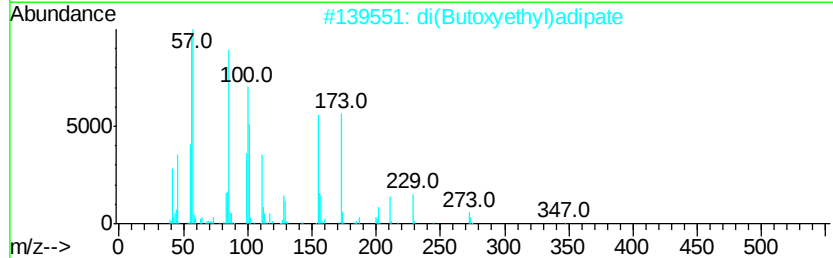
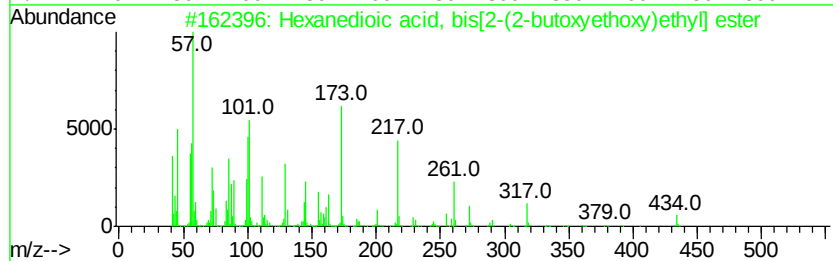
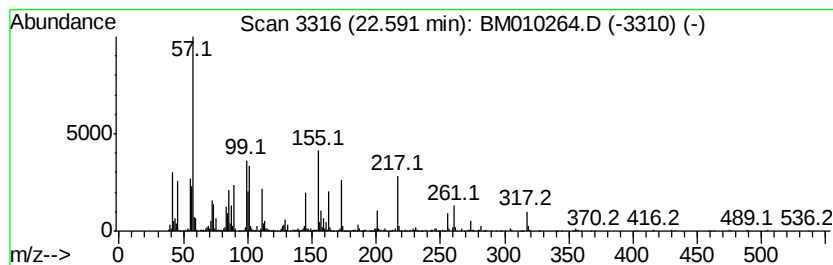
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown22.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.59	18.54 ng	2142960	Chrysene-d12	21.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	38
2		di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	16
3		2-Chloro-3,4-dimethyl-5-phenyl-1...	261	C10H13ClNOPS	1000298-05-5	9
4		N-Carbethoxy-2,2-difluoro-3-trif...	277	C8H8F5N04	059223-03-9	9
5		1,2-Propanediol, 3-(tetradecyloxy)-	288	C17H36O3	001561-06-4	9



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052617\
Data File : BM010264.D
Acq On : 26 May 2017 19:23
Operator : SJ/MA
Sample : I3306-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DSK-MW-LS

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.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
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Benzenepropanoic ...	12.56	8.9	ng	370828	2	10.75	836936	20.0
Decahydro-4,4,8,9...	13.30	2.8	ng	163476	3	14.57	1149470	20.0
1-Indolinecarboxa...	13.95	6.6	ng	379258	3	14.57	1149470	20.0
11,13-Dimethyl-12...	14.27	3.3	ng	190665	3	14.57	1149470	20.0
2-Pentanone, 4-cy...	14.36	4.2	ng	242905	3	14.57	1149470	20.0
unknown14.50	14.50	2.3	ng	129878	3	14.57	1149470	20.0
Benzamide, 4-tert...	16.85	3.5	ng	264824	4	17.32	1524340	20.0
1H-Pyrazole, 5-(t...	18.05	3.1	ng	236411	4	17.32	1524340	20.0
n-Hexadecanoic acid	18.16	2.0	ng	153707	4	17.32	1524340	20.0
unknown22.59	22.59	18.5	ng	2142960	5	21.48	2312310	20.0