

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
 Data File : BF095323.D
 Acq On : 22 May 2017 20:02
 Operator : SJ/MA
 Sample : I3236-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01 003

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-BF050217.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	5.119	537	541	558	rBV	143684	358277	12.56%	1.617%
2	5.719	639	643	680	rBV	1133999	2465635	86.45%	11.125%
3	7.301	908	912	928	rBV	1398934	2221825	77.90%	10.025%
4	7.419	928	932	949	rVB	1642773	2651258	92.96%	11.963%
5	7.760	986	990	1004	rVB	365740	470706	16.50%	2.124%
6	7.995	1025	1030	1046	rBV	1541784	1926227	67.54%	8.691%
7	8.660	1138	1143	1168	rBV	912274	1504274	52.74%	6.788%
8	9.777	1329	1333	1353	rBV	363265	656178	23.01%	2.961%
9	11.548	1628	1634	1655	rBV	1988107	2852143	100.00%	12.869%
10	12.248	1749	1753	1770	rBV	226854	381357	13.37%	1.721%
11	12.613	1810	1815	1830	rBV2	450790	737721	25.87%	3.329%
12	13.442	1950	1956	1961	rBV	26823	32139	1.13%	0.145%
13	13.907	2030	2035	2055	rBV	800894	1341521	47.04%	6.053%
14	14.212	2083	2087	2098	rBV	25685	42614	1.49%	0.192%
15	15.012	2219	2223	2244	rVB	312712	524621	18.39%	2.367%
16	15.977	2382	2387	2395	rBV4	13908	34046	1.19%	0.154%
17	17.330	2612	2617	2631	rBV	1362037	1693717	59.38%	7.642%
18	18.683	2843	2847	2860	rBV	328893	490424	17.19%	2.213%
19	20.083	3081	3085	3089	rBV	48635	54022	1.89%	0.244%
20	20.359	3128	3132	3142	rBV	307903	458826	16.09%	2.070%
21	20.600	3170	3173	3176	rBV4	33795	39460	1.38%	0.178%
22	20.706	3187	3191	3198	rVB7	18137	40441	1.42%	0.182%
23	20.806	3205	3208	3212	rVB2	32234	38994	1.37%	0.176%
24	21.483	3318	3323	3328	rBV7	24885	47552	1.67%	0.215%
25	22.153	3429	3437	3446	rBV7	52501	167046	5.86%	0.754%
26	22.571	3504	3508	3519	rVB10	49290	139792	4.90%	0.631%
27	22.994	3574	3580	3589	rVB7	52077	118817	4.17%	0.536%
28	23.218	3613	3618	3623	rBV9	20436	47153	1.65%	0.213%
29	23.700	3691	3700	3713	rBV9	44712	193513	6.78%	0.873%
30	23.841	3716	3724	3737	rVB3	145828	431980	15.15%	1.949%

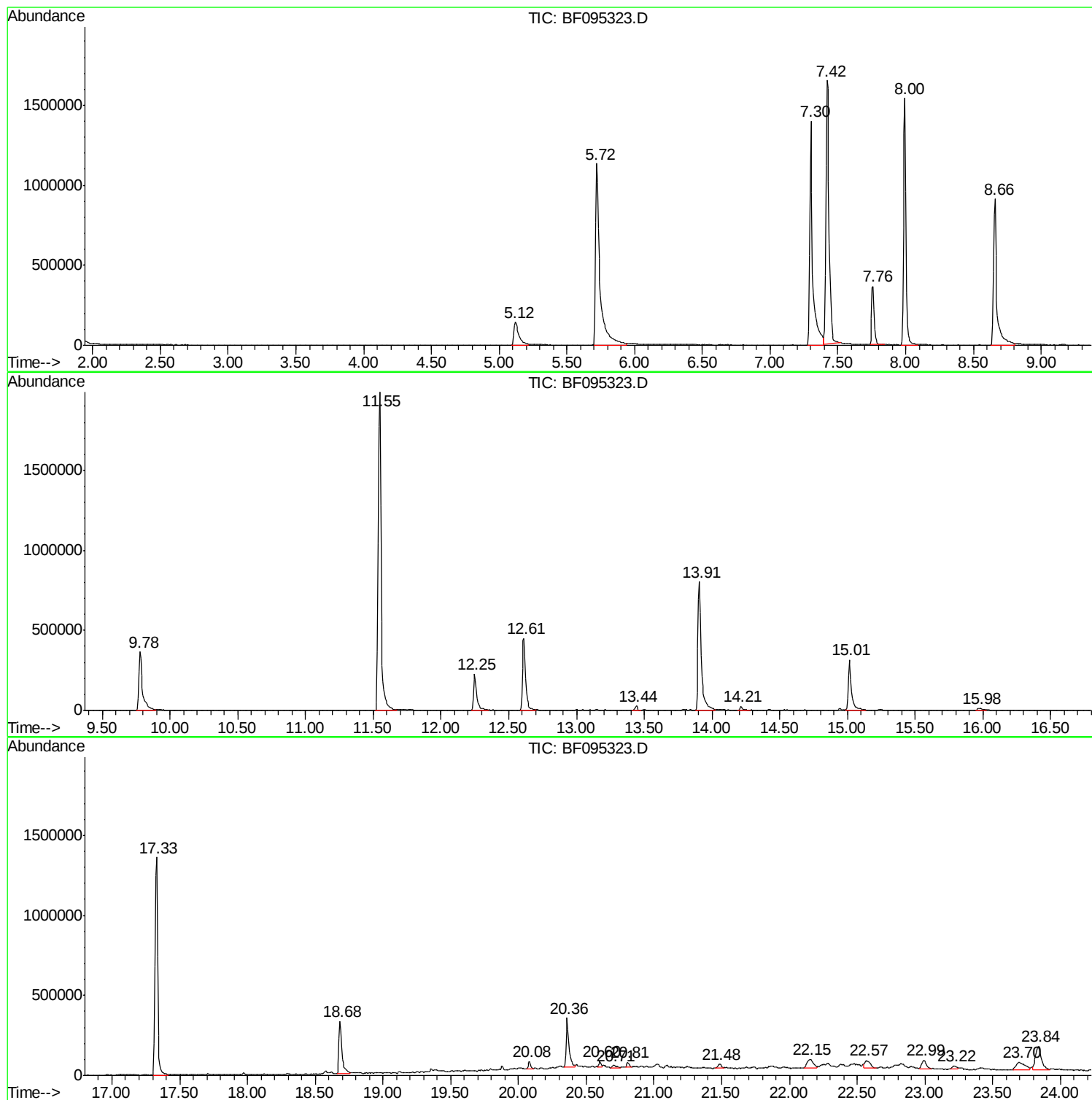
Sum of corrected areas: 22162279

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

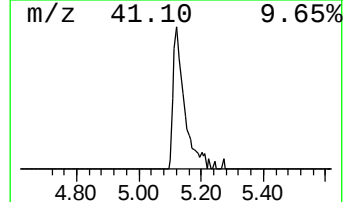
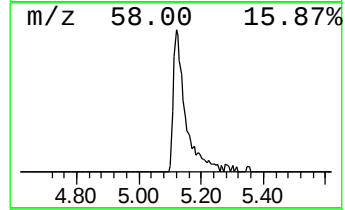
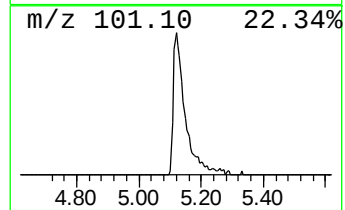
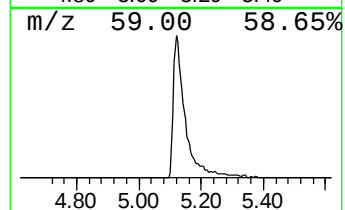
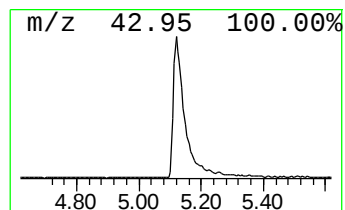
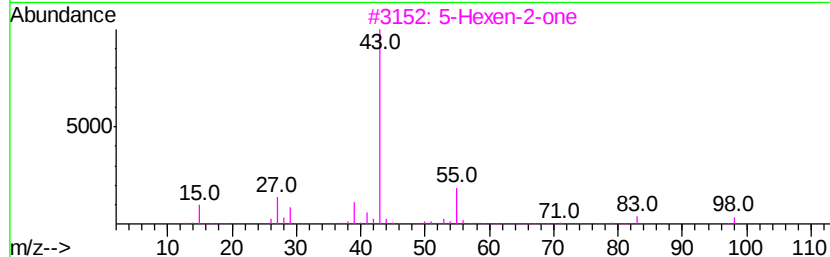
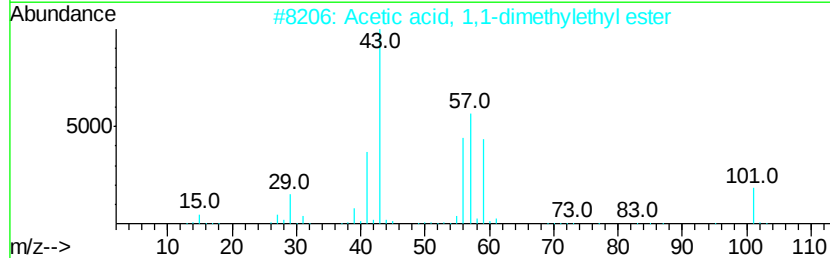
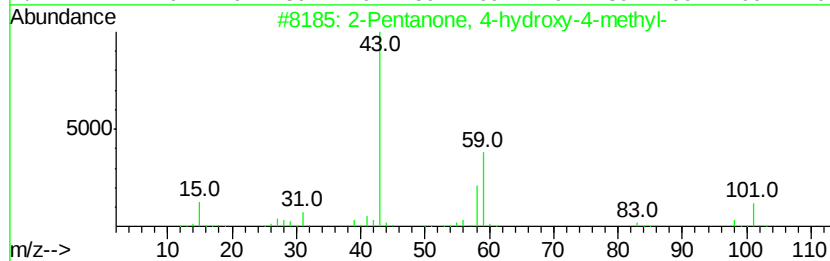
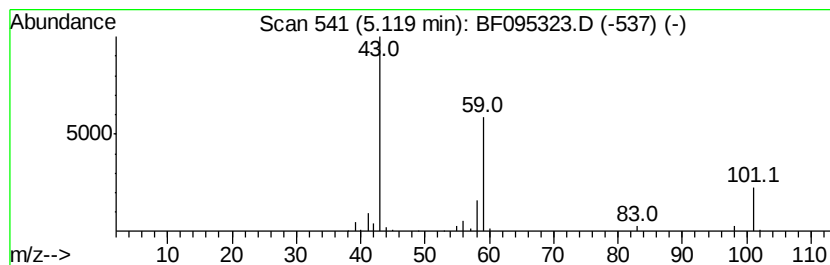
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	15.22 ng	358277	1,4-Dichlorobenzene-d4	7.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

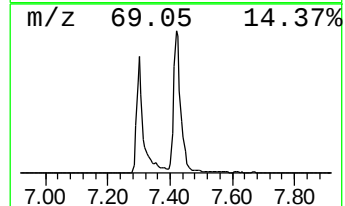
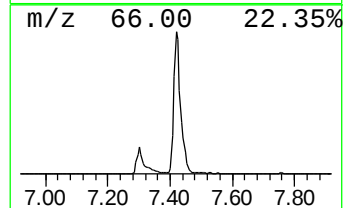
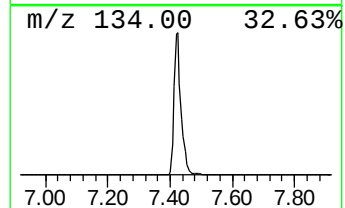
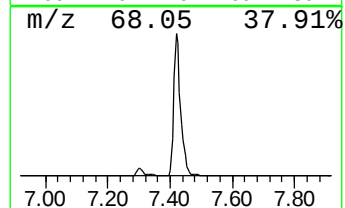
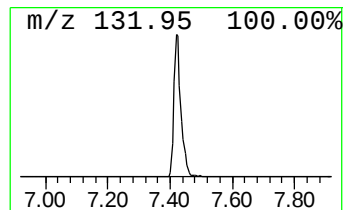
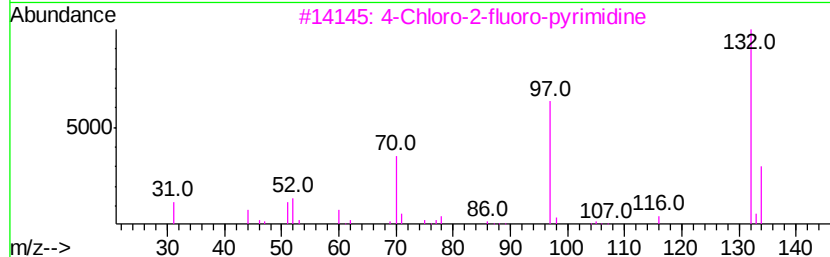
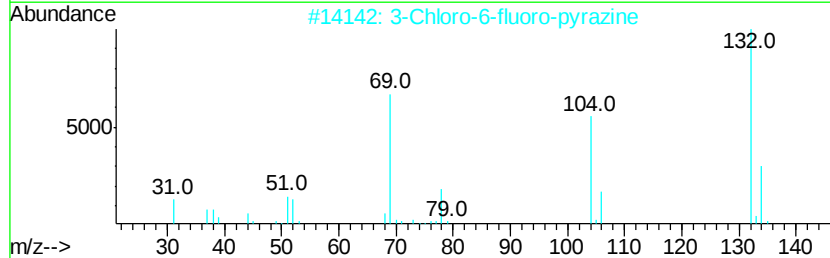
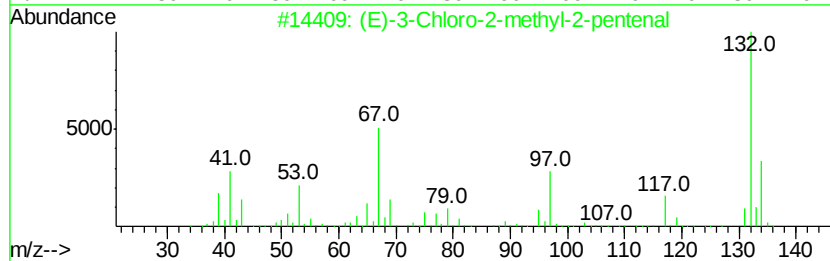
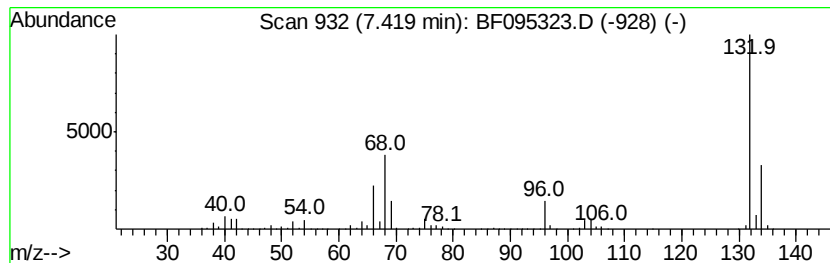
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	112.65 ng	2651260	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

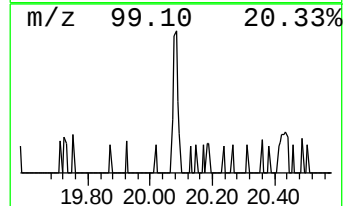
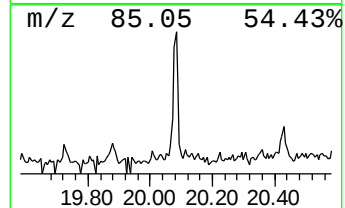
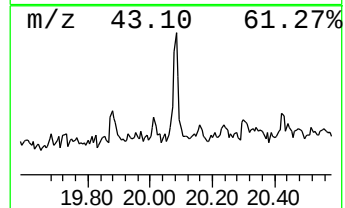
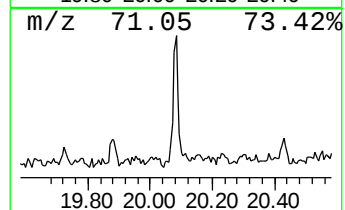
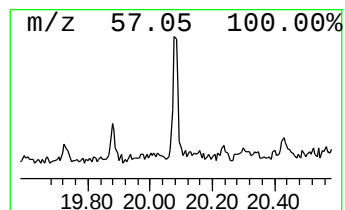
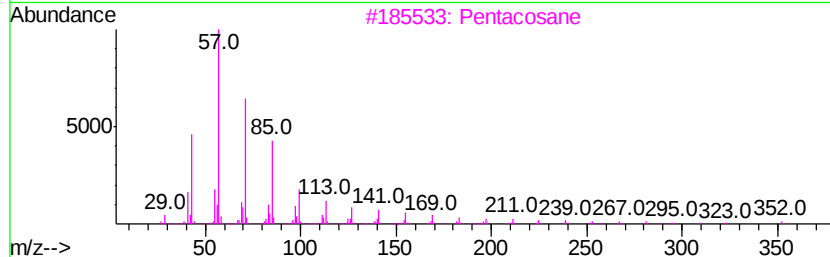
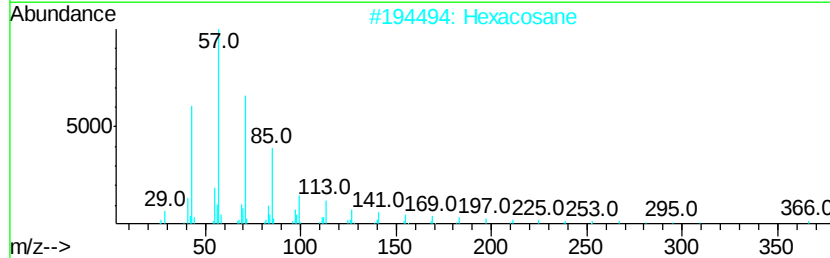
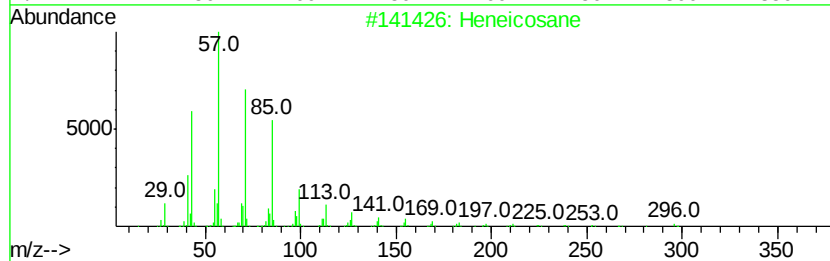
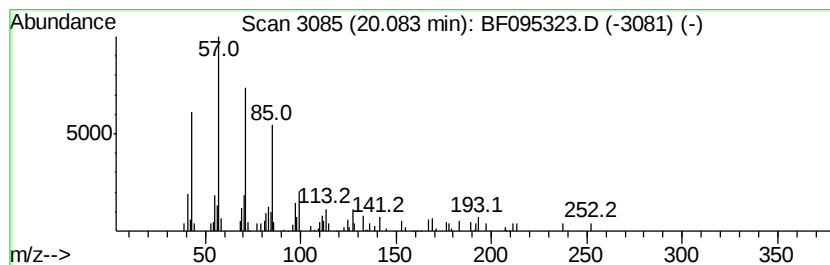
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.08	2.35 ng	54022	Perylene-d12	20.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Pentacosane		352	C25H52	000629-99-2	90
4	Hentriacontane		437	C31H64	000630-04-6	87
5	Heptadecane		240	C17H36	000629-78-7	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

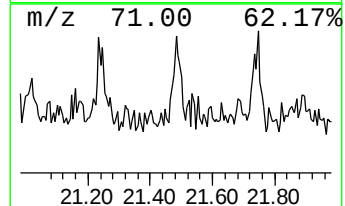
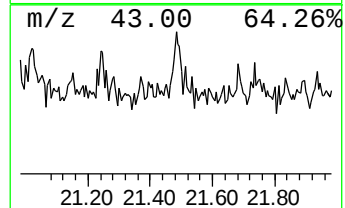
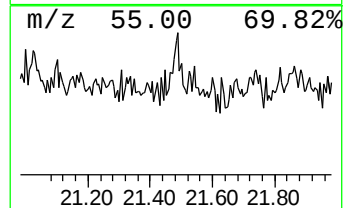
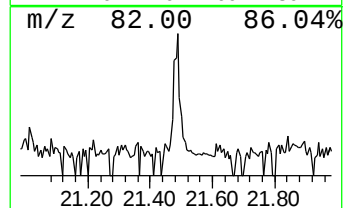
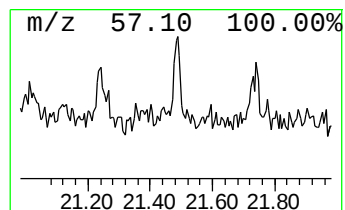
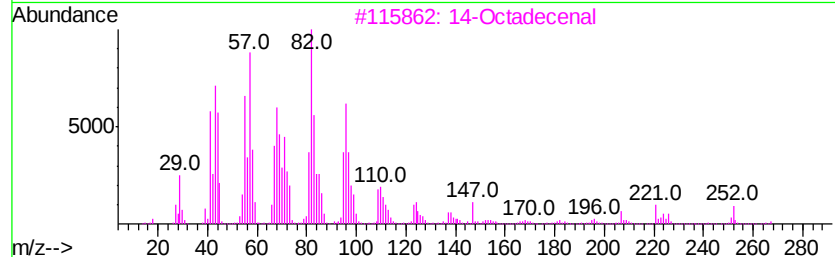
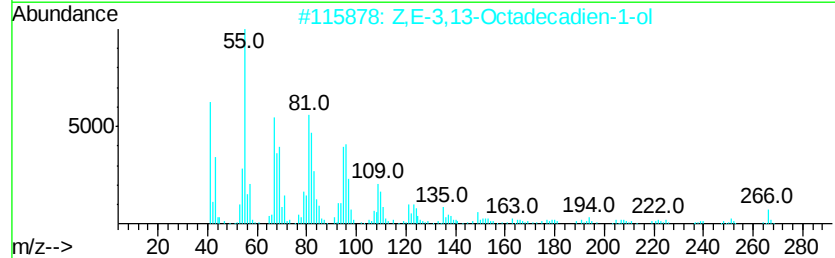
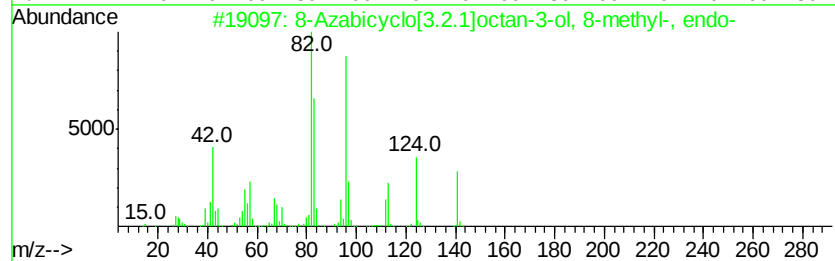
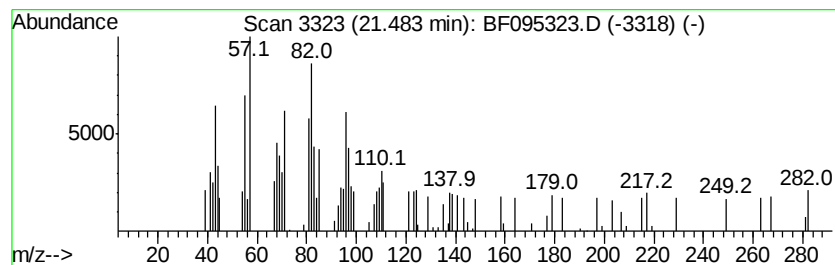
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown21.48 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.48	2.07 ng	47552	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	8-Azabicyclo[3.2.1]octan-3-ol, 8...	141	C8H15NO	000120-29-6	43
2		Z,E-3,13-Octadecadien-1-ol	266	C18H34O	1000131-10-4	43
3		14-Octadecenal	266	C18H34O	056554-89-3	35
4		16-Octadecenal	266	C18H34O	056554-87-1	35
5		12-Methyl-E,E-2,13-octadecadien-...	280	C19H36O	1000130-90-4	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

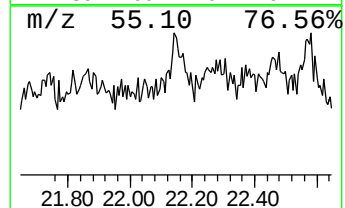
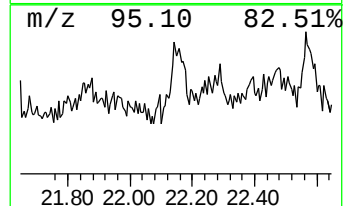
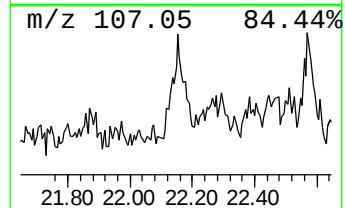
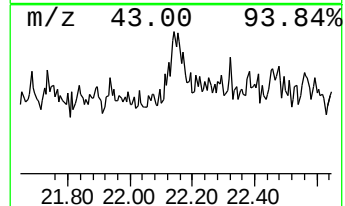
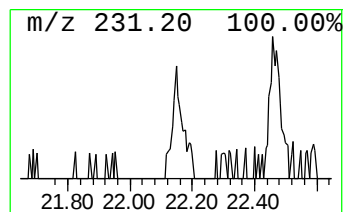
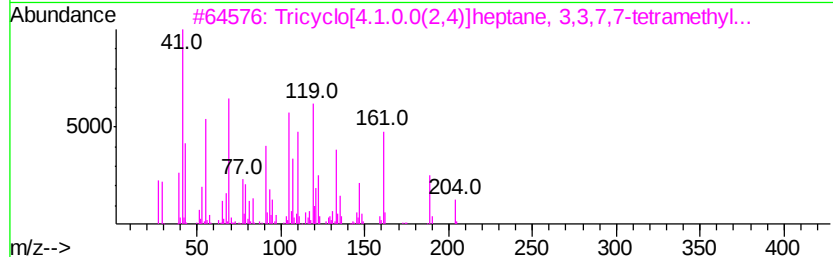
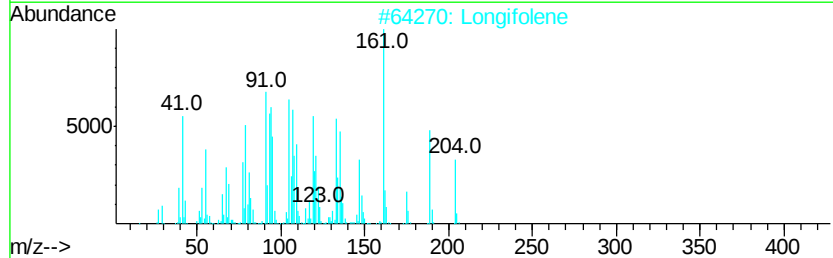
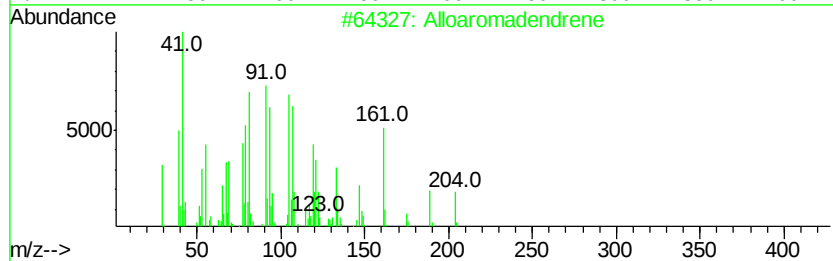
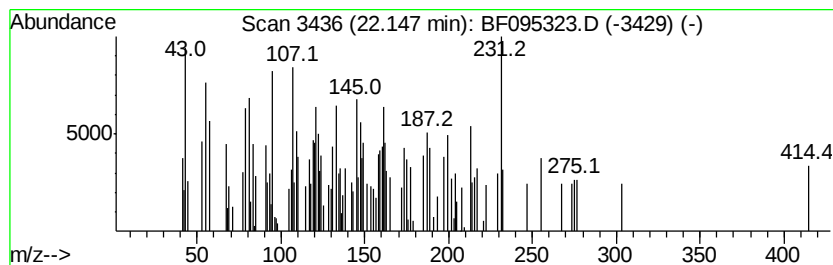
Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown22.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.15	7.28 ng	167046	Perylene-d12	20.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Alloaromadendrene	204 C15H24	025246-27-9 38
2		Longifolene	204 C15H24	000475-20-7 25
3		Tricyclo[4.1.0.0(2,4)]heptane, 3...	204 C15H24	067843-59-8 22
4		1,3-Oxazine, tetrahydro-2-(4-dim...	206 C12H18N2O	109086-78-4 20
5		Benzene, 1-ethoxy-4-(4-propylcyc...	246 C17H26O	080944-44-1 14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

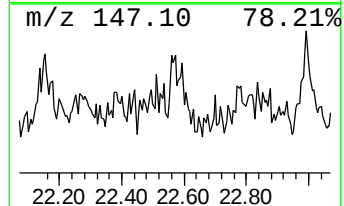
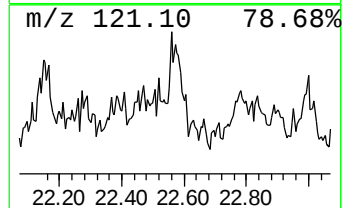
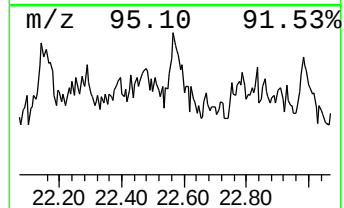
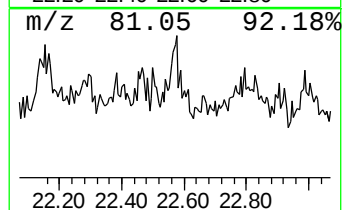
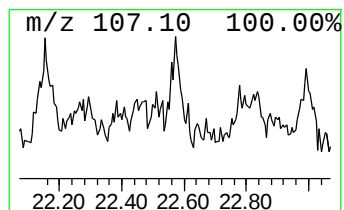
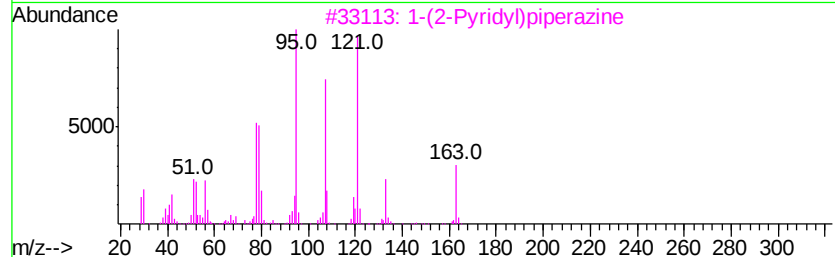
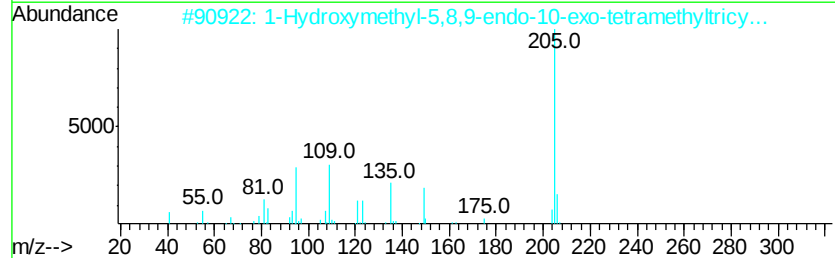
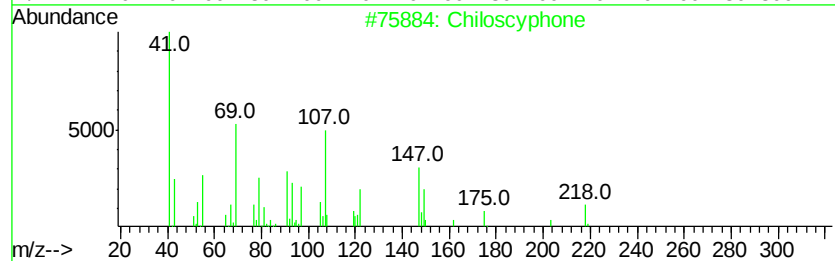
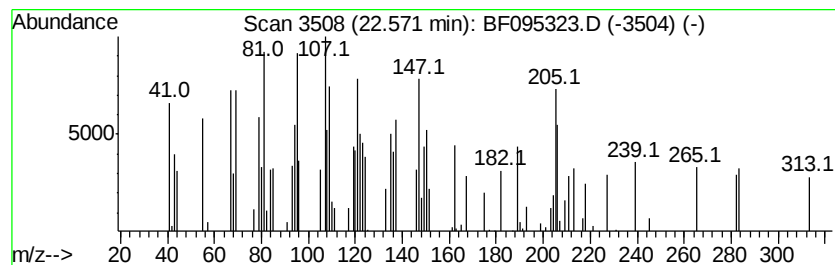
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown22.57 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.57	6.09 ng	139792	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chiloscyphone	218	C15H22O	023538-45-6	35
2		1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	27
3		1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	25
4		Acetoacetanilide, 2',4'-dimethyl-	205	C12H15NO2	000097-36-9	22
5		Isocyclocitral	152	C10H16O	001335-66-6	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

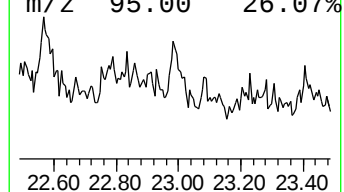
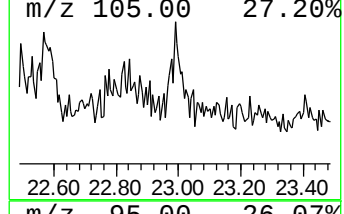
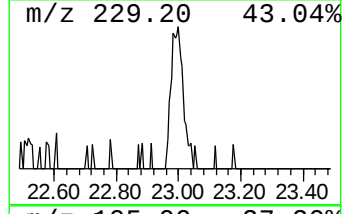
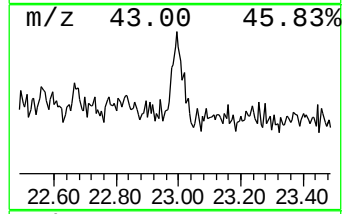
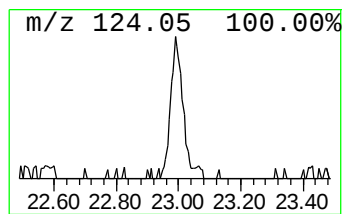
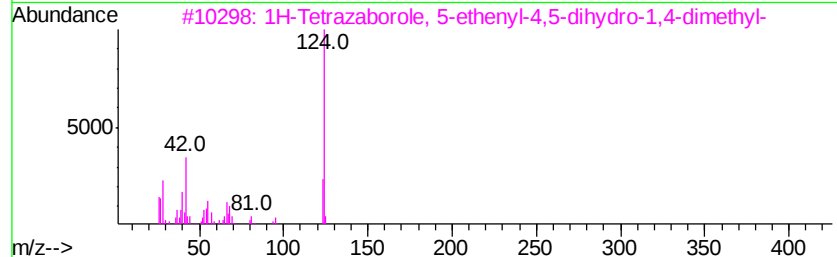
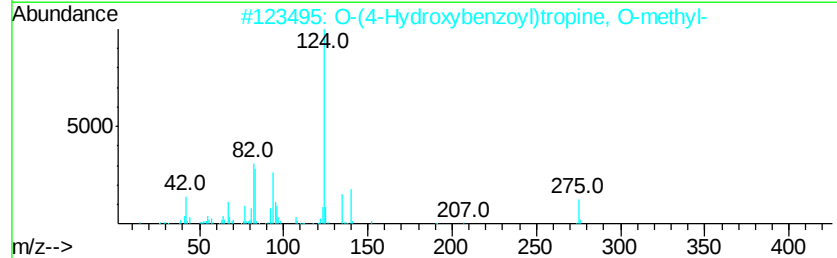
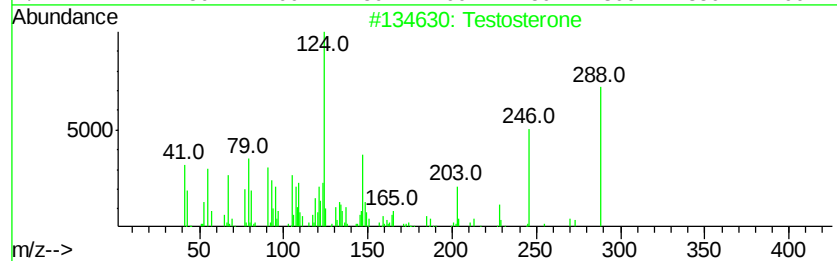
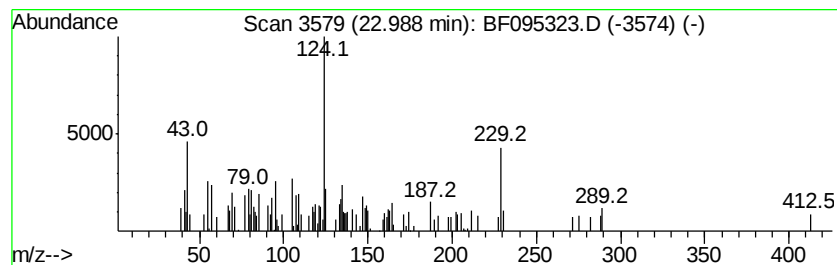
Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown22.99 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.99	5.18 ng	118817	Perylene-d12	20.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Testosterone	288 C19H28O2	000058-22-0 38
2		O-(4-Hydroxybenzoyl)tropine, O-m...	275 C16H21NO3	1000374-67-0 27
3		1H-Tetrazaborole, 5-ethenyl-4,5-...	124 C4H9BN4	020534-02-5 25
4		2-Piperidinobicyclo[3.3.1]nonan-...	221 C14H23NO	302589-52-2 22
5		2-Methylphenyl-1-thio-.alpha.-D-...	286 C13H18O5S	1000126-63-0 22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

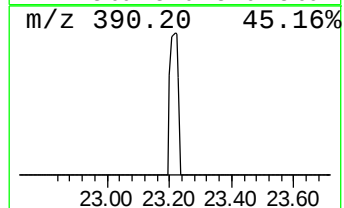
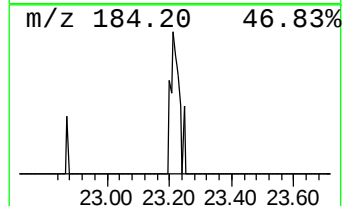
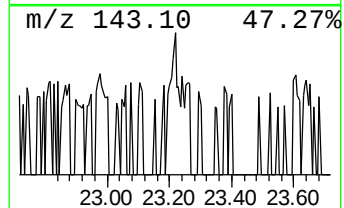
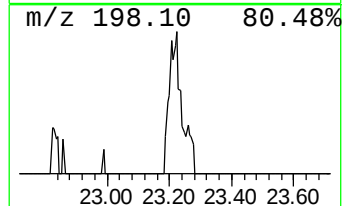
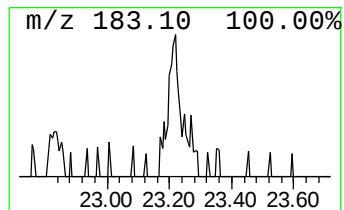
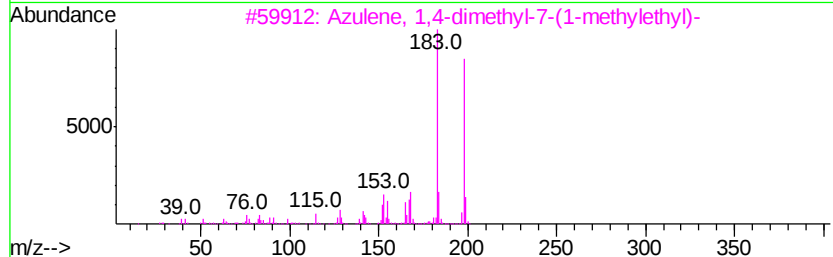
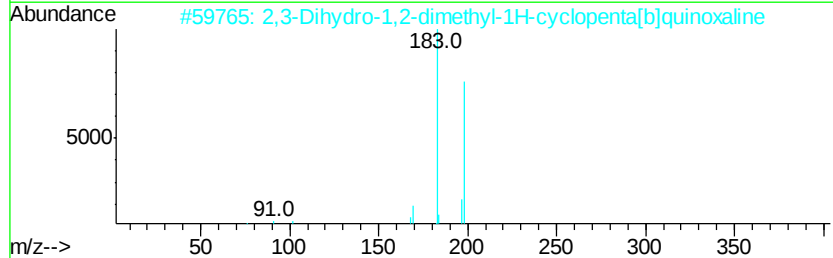
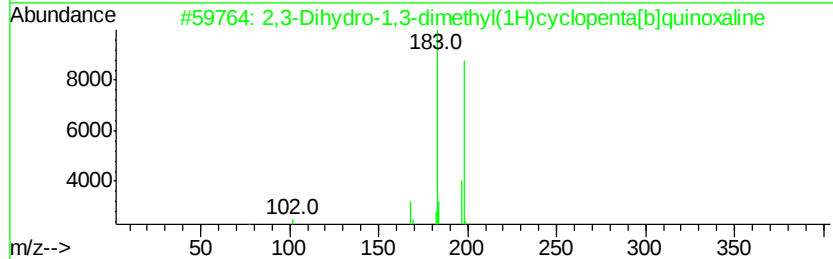
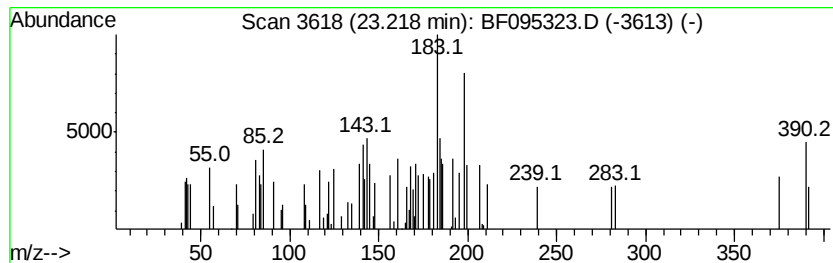
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown23.22 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.22	2.06 ng	47153	Perylene-d12	20.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dihydro-1,3-dimethyl(1H)cycl...	198	C13H14N2	1000112-95-8	38		
2	2,3-Dihydro-1,2-dimethyl-1H-cycl...	198	C13H14N2	109682-78-2	25		
3	Azulene, 1,4-dimethyl-7-(1-methv...	198	C15H18	000489-84-9	25		
4	1-Phenanthrenol, 1,2,3,4,4a,9,10...	216	C15H20O	098304-41-7	25		
5	1,3-Dioxolane, 2-(4-chlorophenyl)-	184	C9H9ClO2	002403-54-5	22		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

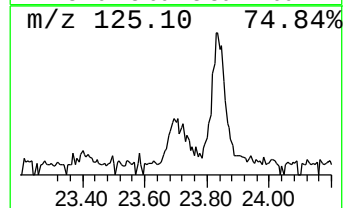
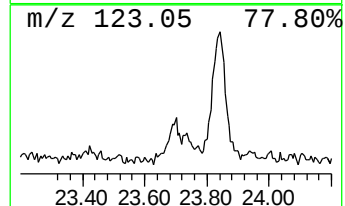
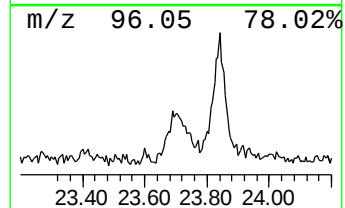
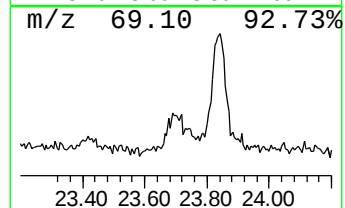
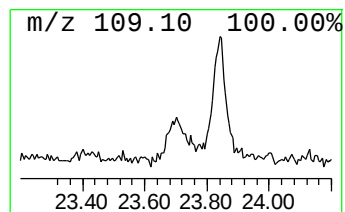
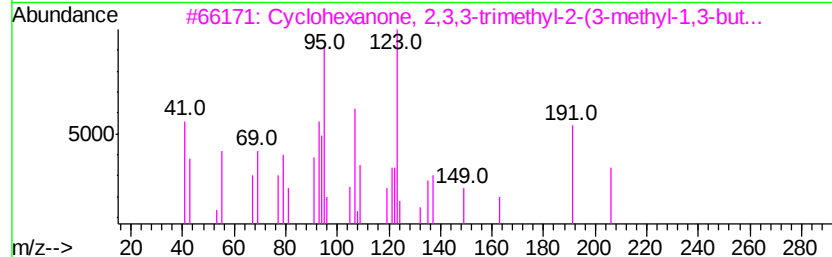
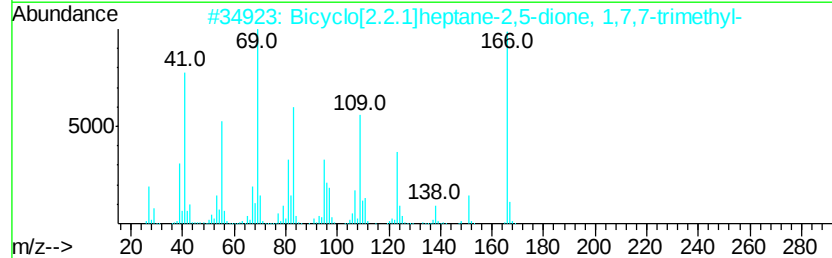
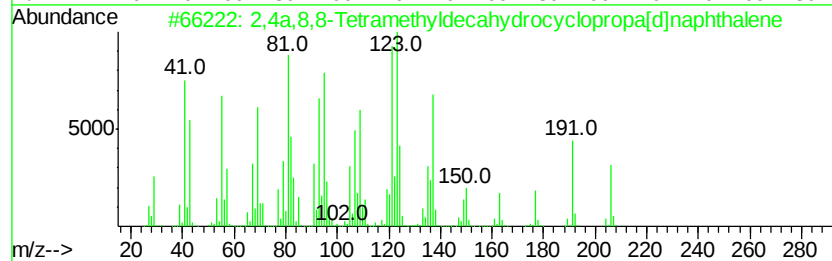
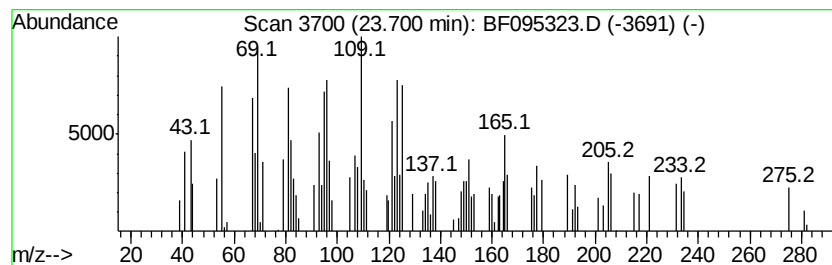
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown23.70 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.70	8.44 ng	193513	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	43
2		Bicyclo[2.2.1]heptane-2,5-dione,...	166	C10H14O2	004230-32-4	42
3		Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	41
4		1,E-11,Z-13-Heptadecatriene	234	C17H30	080625-35-0	35
5		2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_003

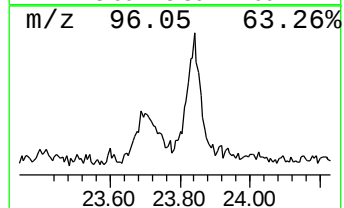
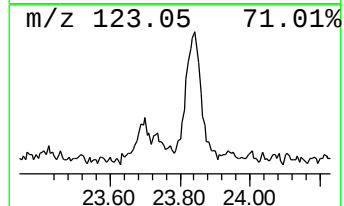
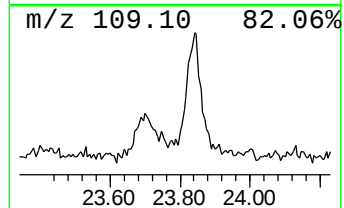
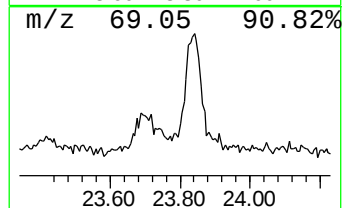
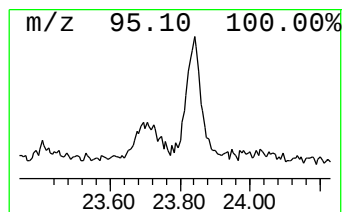
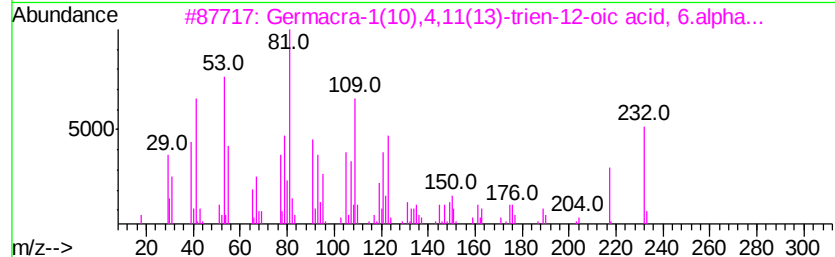
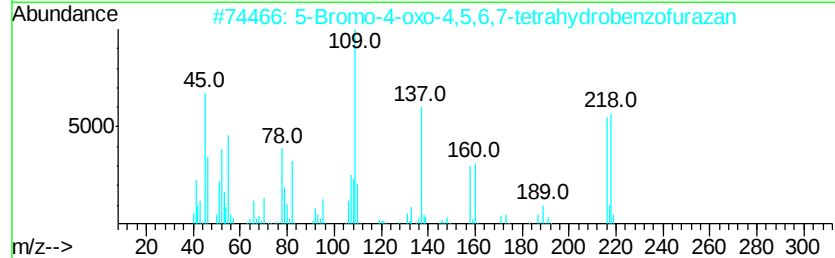
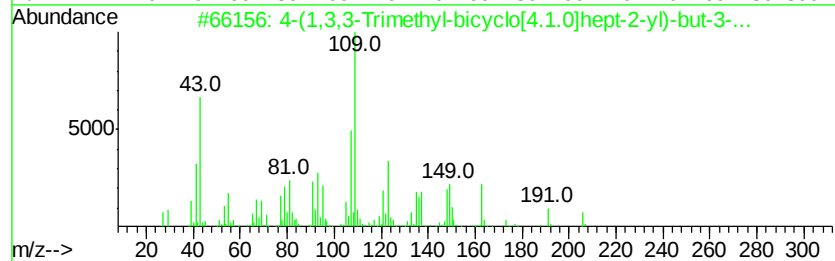
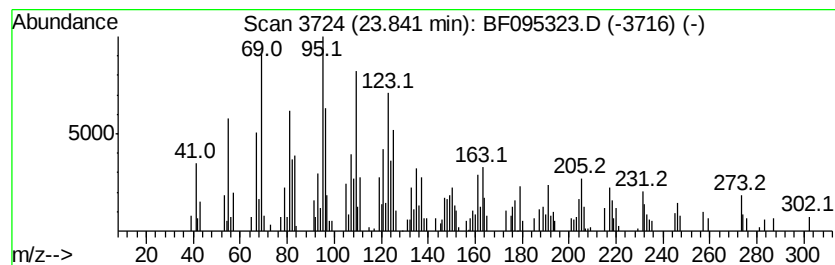
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4-(1,3,3-Trimethyl-bicyclo[... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.84	18.83 ng	431980	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-(1,3,3-Trimethyl-bicyclo[4.1.0]hept-2-yl)-but-3-en-2-ol	206	C14H22O	077143-31-8	70
2		5-Bromo-4-oxo-4,5,6,7-tetrahydro-2H-pyran	216	C6H5BrN2O2	300574-36-1	68
3		Germacra-1(10),4,11(13)-trien-12-ol	232	C15H20O2	000553-21-9	50
4		1-Formyl-2,2-dimethyl-3-trans-(3-methylbut-3-en-1-yl)cyclobutane	220	C15H24O	1000144-09-7	38
5		3(4H)-Phenanthrenone, 4a,4b,5,6,10,10a-hexahydro-1,2-benz[a]phenanthrene	246	C17H26O	057684-12-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095323.D
Acq On : 22 May 2017 20:02
Operator : SJ/MA
Sample : I3236-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01 003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.12	15.2	ng	358277	1	7.76	470706	20.0
unknown7.42	7.42	112.7	ng	2651260	1	7.76	470706	20.0
Heneicosane	20.08	2.4	ng	54022	6	20.36	458826	20.0
unknown21.48	21.48	2.1	ng	47552	6	20.36	458826	20.0
unknown22.15	22.15	7.3	ng	167046	6	20.36	458826	20.0
unknown22.57	22.57	6.1	ng	139792	6	20.36	458826	20.0
unknown22.99	22.99	5.2	ng	118817	6	20.36	458826	20.0
unknown23.22	23.22	2.1	ng	47153	6	20.36	458826	20.0
unknown23.70	23.70	8.4	ng	193513	6	20.36	458826	20.0
4-(1,3,3-Trimethy...	23.84	18.8	ng	431980	6	20.36	458826	20.0