

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
 Data File : BF094260.D
 Acq On : 7 Apr 2017 8:17
 Operator : SJ/MA
 Sample : I2542-17
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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	3.993	353	358	368	rBV	592986	712800	20.45%	2.127%
2	4.393	421	426	429	rBV	3141985	3152657	90.46%	9.407%
3	4.775	488	491	497	rVB	44408	41842	1.20%	0.125%
4	5.063	536	540	543	rVB	48263	42139	1.21%	0.126%
5	5.463	602	608	613	rBV	2923343	3485231	100.00%	10.400%
6	5.598	626	631	635	rBV	3196380	3380234	96.99%	10.087%
7	5.851	670	674	678	rBV	1031063	910172	26.12%	2.716%
8	6.034	700	705	708	rBV	2520291	2479579	71.15%	7.399%
9	6.504	778	785	788	rBV	1977341	2104334	60.38%	6.279%
10	7.357	925	930	933	rBV	1237720	1207021	34.63%	3.602%
11	8.681	1149	1155	1158	rBV	3015896	2965822	85.10%	8.850%
12	9.175	1235	1239	1244	rBV	325623	293185	8.41%	0.875%
13	9.492	1285	1293	1302	rBV	1163511	1288477	36.97%	3.845%
14	10.086	1389	1394	1398	rVB	64259	63585	1.82%	0.190%
15	10.363	1435	1441	1444	rBV2	23377	36182	1.04%	0.108%
16	10.469	1454	1459	1470	rBV	1732639	1777175	50.99%	5.303%
17	10.675	1490	1494	1502	rVB	83229	110852	3.18%	0.331%
18	11.227	1584	1588	1592	rBV	61493	66582	1.91%	0.199%
19	11.316	1599	1603	1607	rBV	1106937	1105233	31.71%	3.298%
20	12.180	1746	1750	1753	rBV2	38472	43733	1.25%	0.130%
21	12.692	1834	1837	1843	rVB	89615	92044	2.64%	0.275%
22	12.810	1854	1857	1860	rVB	60771	60345	1.73%	0.180%
23	13.086	1900	1904	1907	rBV	48341	54920	1.58%	0.164%
24	13.133	1907	1912	1915	rVV3	45194	54824	1.57%	0.164%
25	13.298	1935	1940	1944	rBV	1994299	2073394	59.49%	6.187%
26	13.510	1957	1976	1978	rBV	73642	288298	8.27%	0.860%
27	13.610	1990	1993	1997	rBV6	27541	59034	1.69%	0.176%
28	13.645	1997	1999	2002	rVB	53264	51387	1.47%	0.153%
29	13.774	2018	2021	2024	rVB3	33328	35913	1.03%	0.107%
30	13.910	2038	2044	2046	rBV6	23964	39053	1.12%	0.117%
31	14.468	2134	2139	2147	rBV3	160167	260996	7.49%	0.779%
32	14.568	2151	2156	2160	rBV	853406	882582	25.32%	2.634%
33	14.868	2203	2207	2210	rBV	81465	92427	2.65%	0.276%
34	15.251	2268	2272	2280	rVB2	181229	240214	6.89%	0.717%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

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_F\METHODS\8270-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.357	2287	2290	2294	rBV3	41571	54596	1.57%	0.163%
36	15.398	2294	2297	2300	rVB	53310	58188	1.67%	0.174%
37	15.568	2323	2326	2329	rBV2	34623	37688	1.08%	0.112%
38	15.609	2330	2333	2337	rVV	62246	69355	1.99%	0.207%
39	15.762	2356	2359	2361	rBV2	39674	37406	1.07%	0.112%
40	15.962	2389	2393	2404	rVB	228471	328802	9.43%	0.981%
41	16.198	2428	2433	2440	rVB	649177	762552	21.88%	2.275%
42	16.321	2451	2454	2458	rVB	47684	57196	1.64%	0.171%
43	16.498	2481	2484	2489	rVB3	63986	77257	2.22%	0.231%
44	16.715	2518	2521	2525	rBV	87127	122862	3.53%	0.367%
45	16.762	2525	2529	2535	rVV	410917	621926	17.84%	1.856%
46	16.892	2548	2551	2558	rBV	56809	97693	2.80%	0.292%
47	17.421	2637	2641	2649	rVB3	80194	148845	4.27%	0.444%
48	18.086	2749	2754	2766	rBV5	108503	258125	7.41%	0.770%
49	18.556	2829	2834	2844	rVB8	117506	287920	8.26%	0.859%
50	18.780	2864	2872	2887	rVB7	226101	729286	20.93%	2.176%
51	18.980	2902	2906	2915	rVB4	98255	210391	6.04%	0.628%

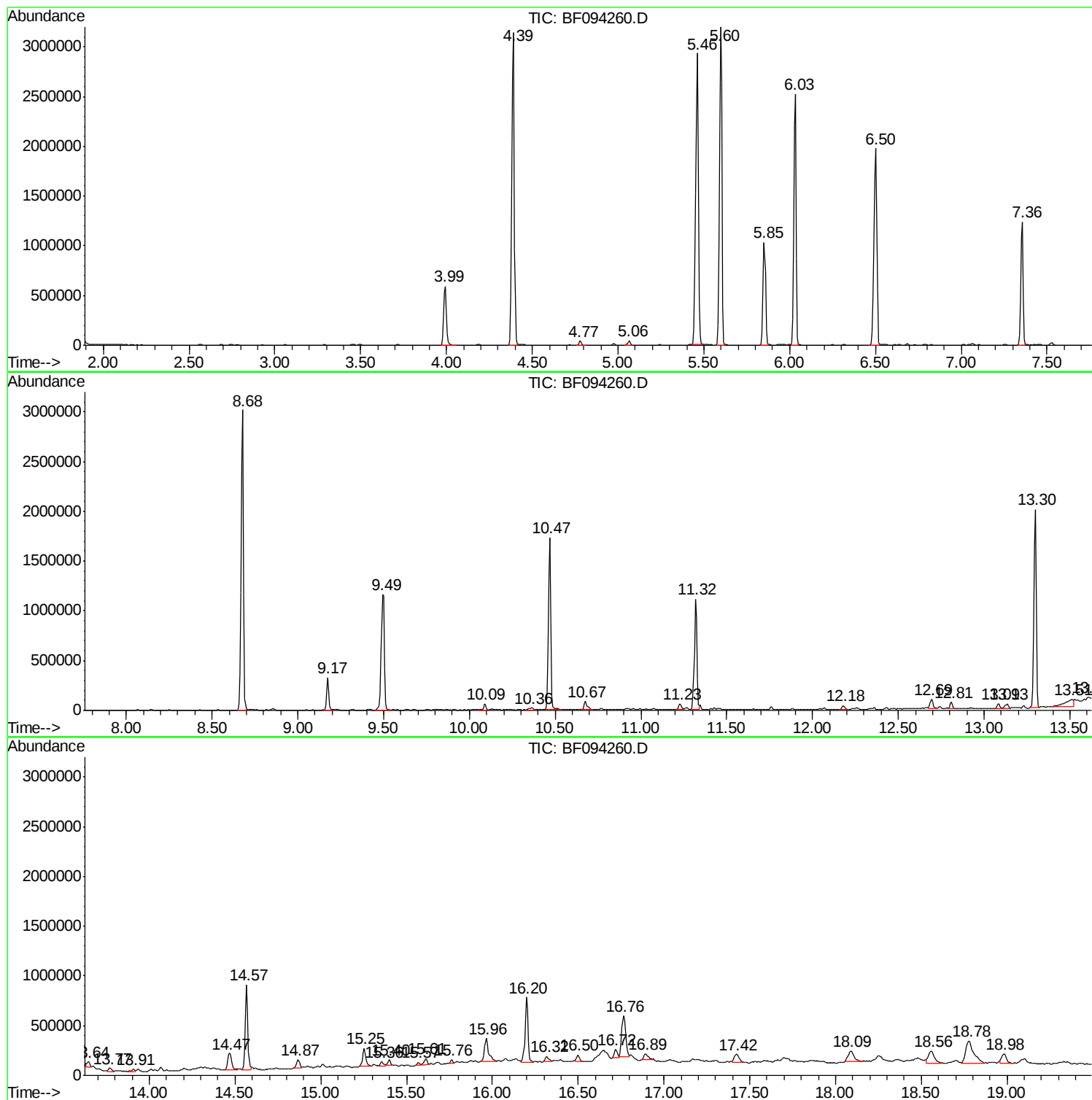
Sum of corrected areas: 33512354

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

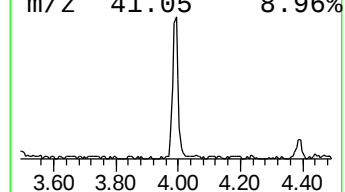
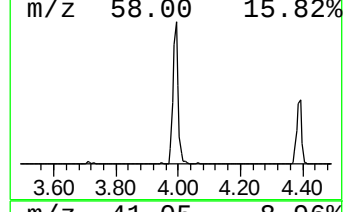
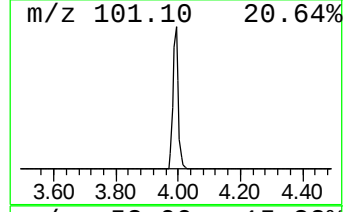
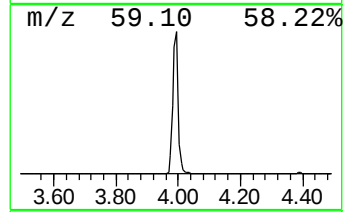
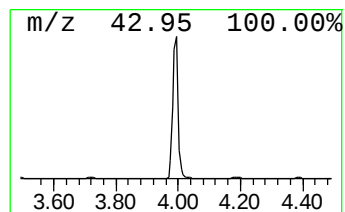
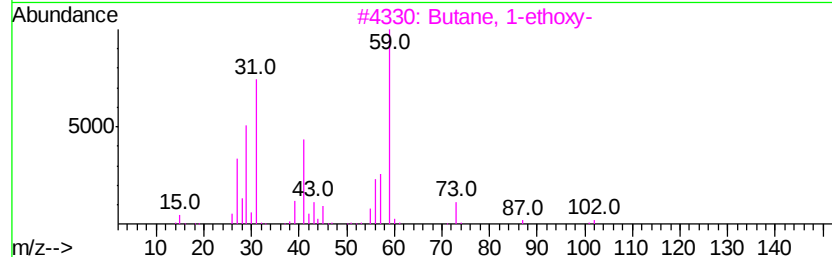
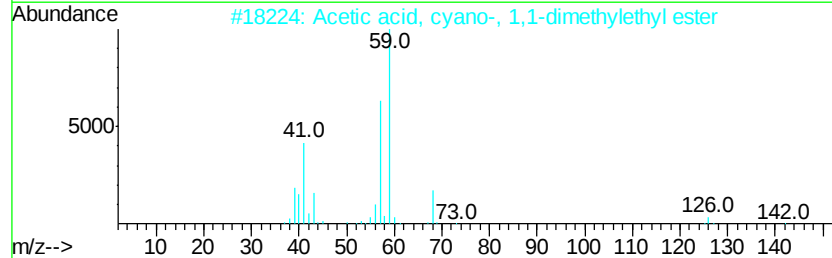
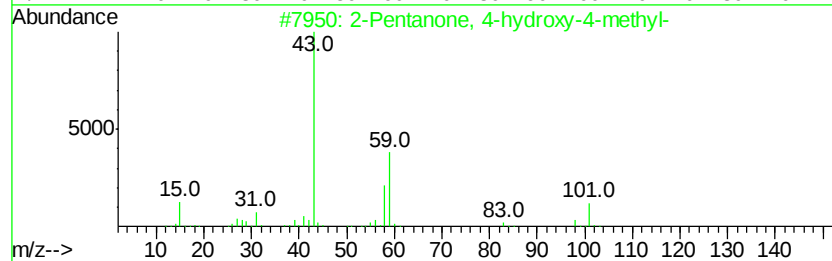
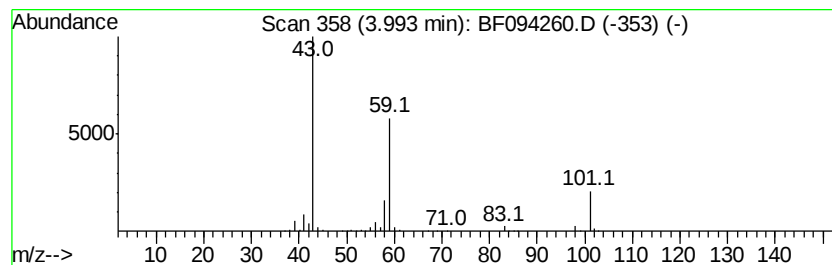
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	15.66 ng	712800	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

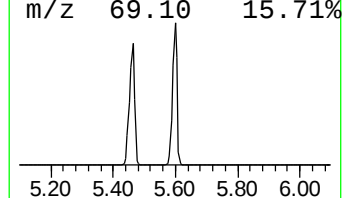
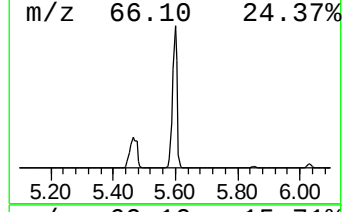
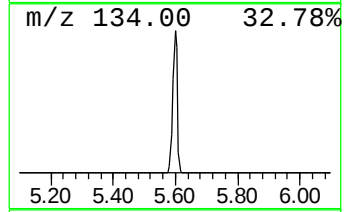
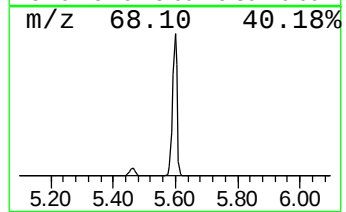
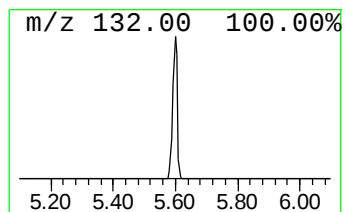
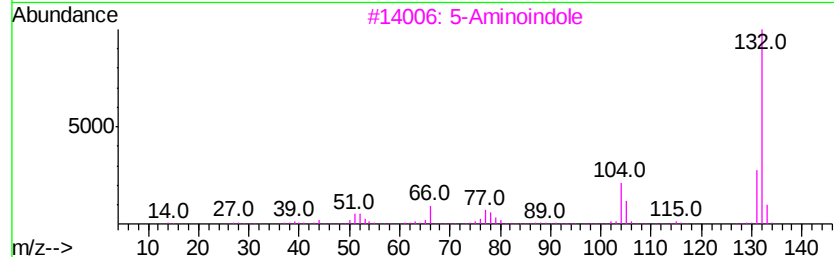
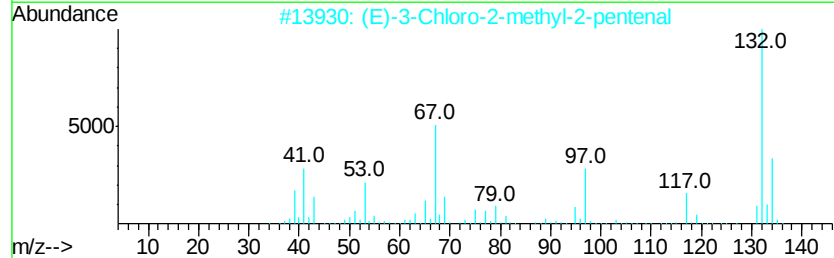
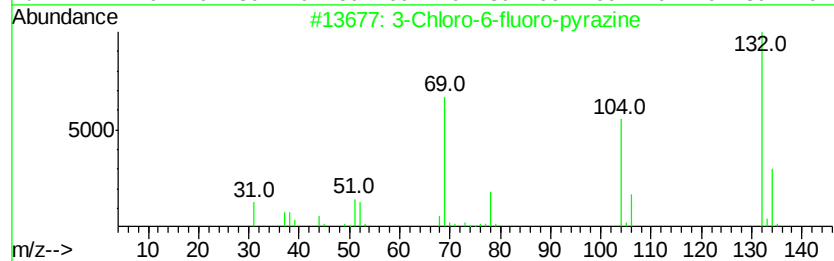
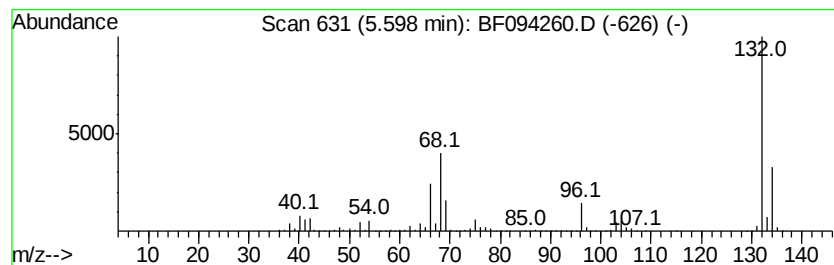
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	74.28 ng	3380230	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

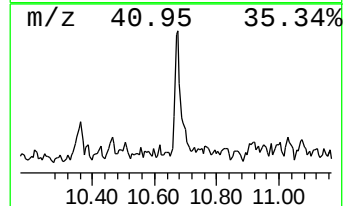
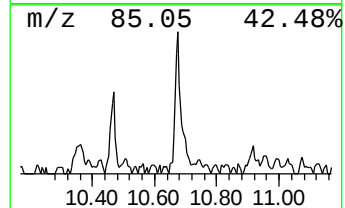
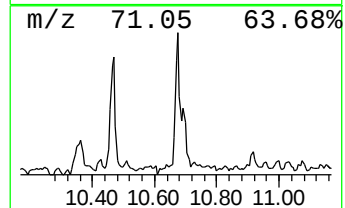
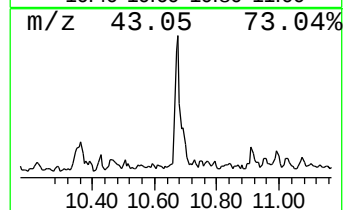
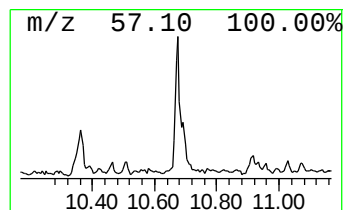
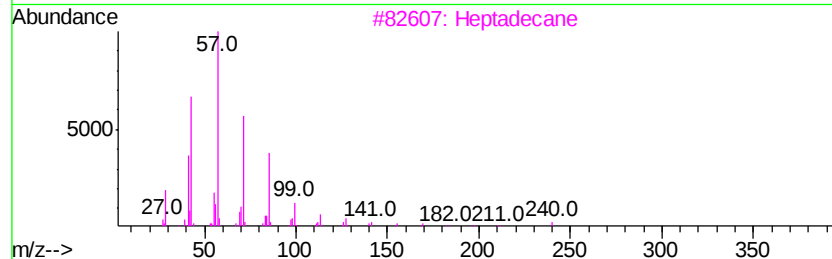
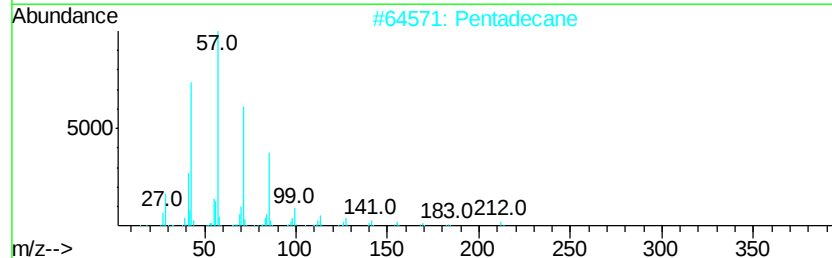
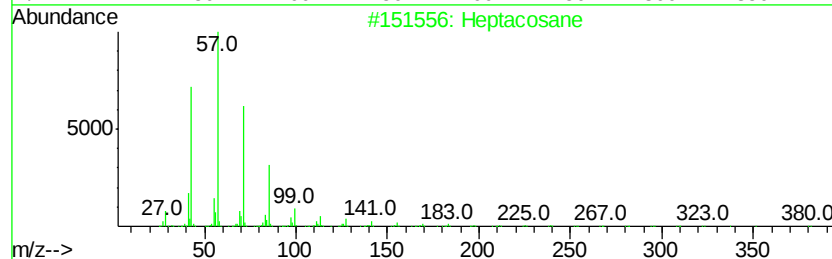
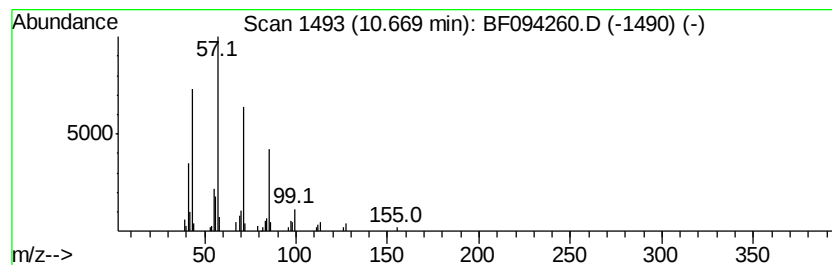
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptacosane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.01 ng	110852	Phenanthrene-d10	11.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Pentadecane	212	C15H32	000629-62-9	90
3			Heptadecane	240	C17H36	000629-78-7	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Tetradecane	198	C14H30	000629-59-4	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

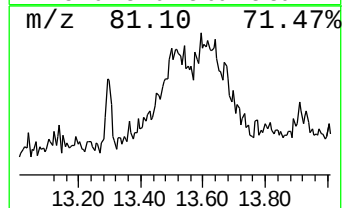
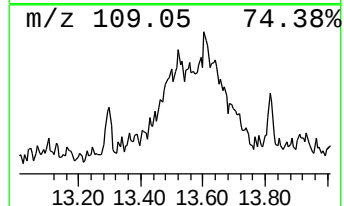
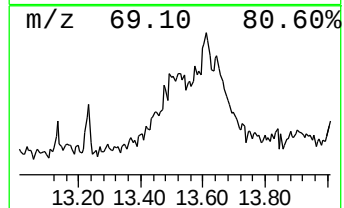
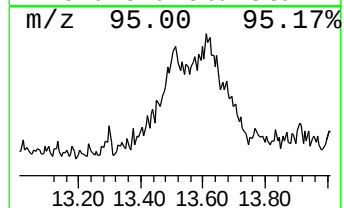
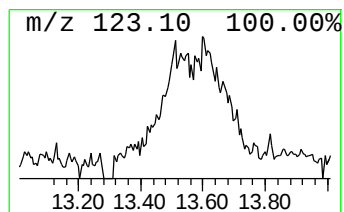
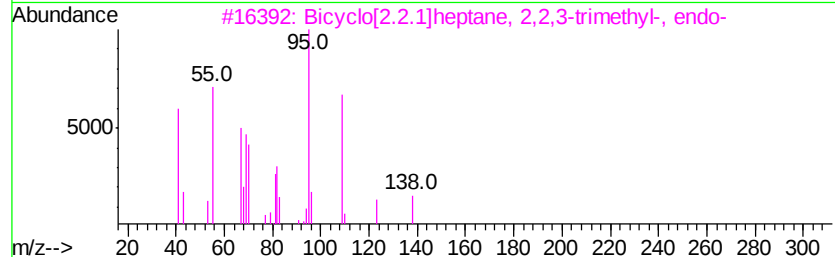
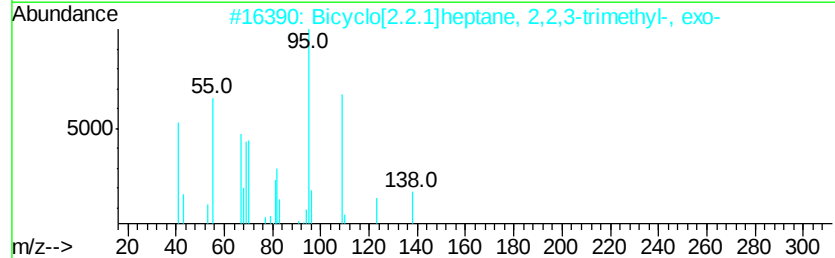
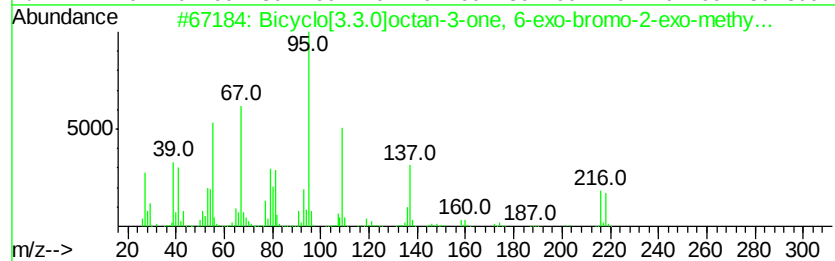
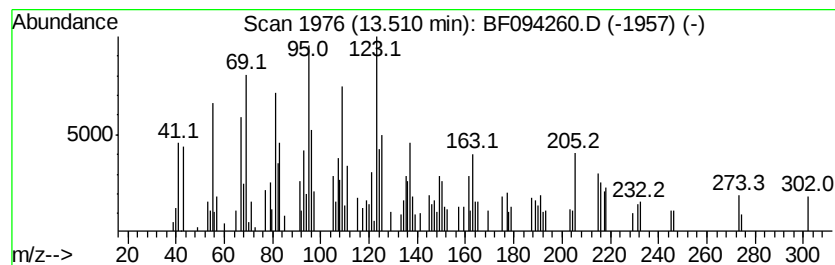
Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.51 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.51	6.53 ng	288298	Chrysene-d12	14.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicvclo[3.3.0]octan-3-one, 6-exo...	216	C9H13BrO	1000149-28-6	41
2	Bicvclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	38
3	Bicvclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38
4	Cyclopentanecarboxaldehyd, 2-me...	124	C8H12O	1000154-24-0	25
5	4,4-Diallyl-cyclohexanone	178	C12H18O	1000186-50-2	20



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

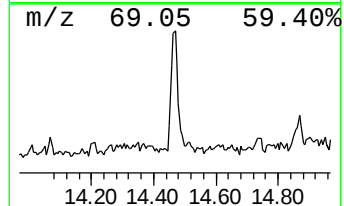
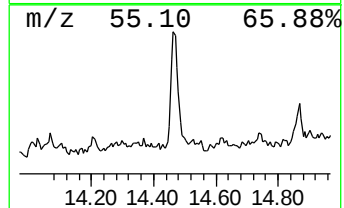
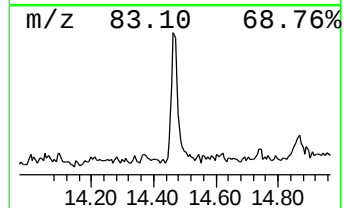
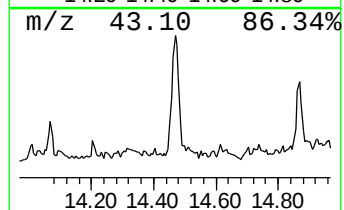
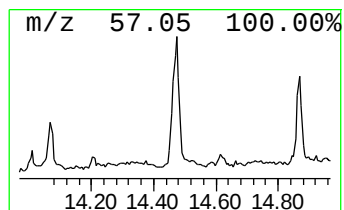
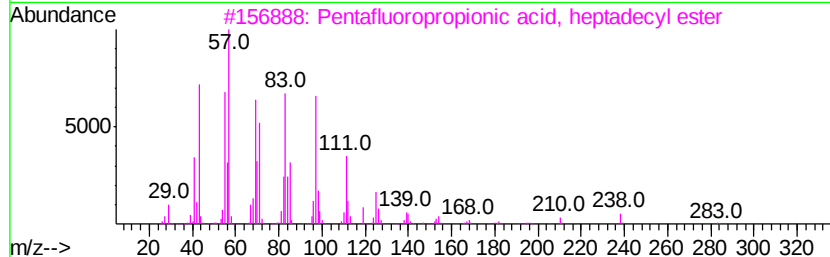
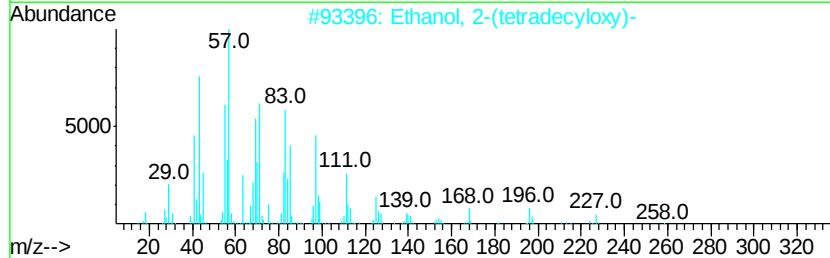
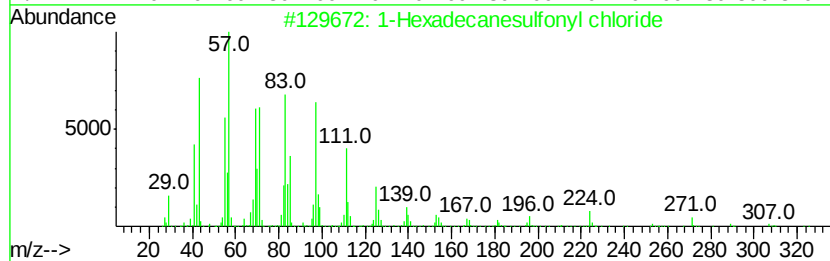
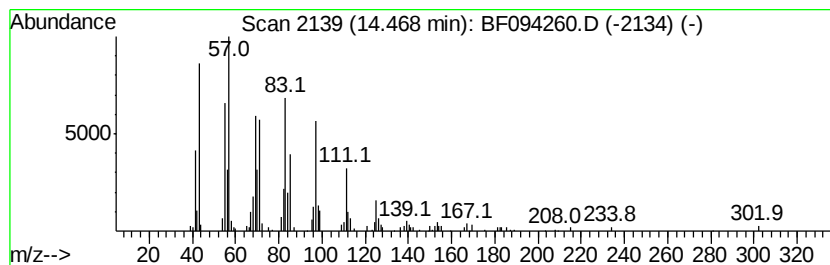
Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexadecanesulfonyl chloride Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.47	5.91 ng	260996	Chrysene-d12	14.57		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
4		Tridecane, 7-cyclohexyl-	266	C19H38	013151-92-3	83
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

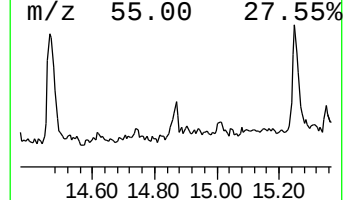
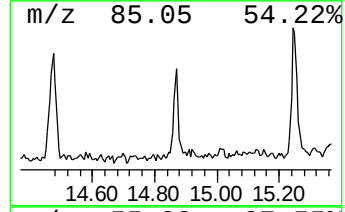
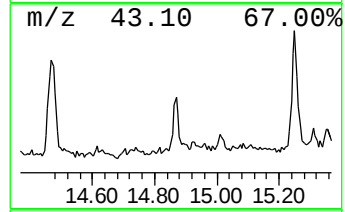
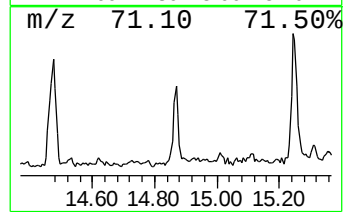
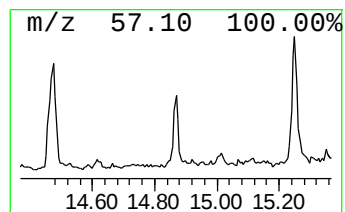
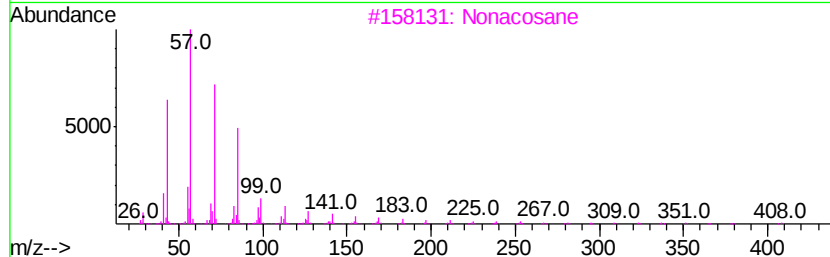
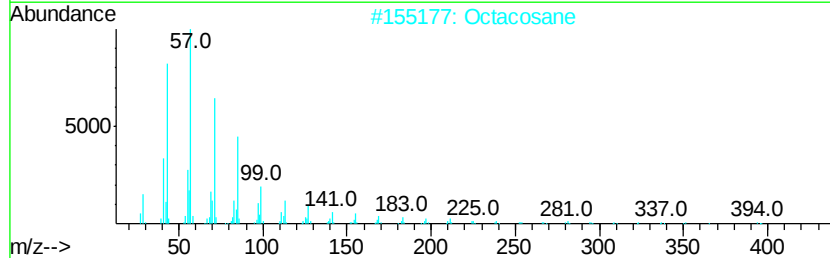
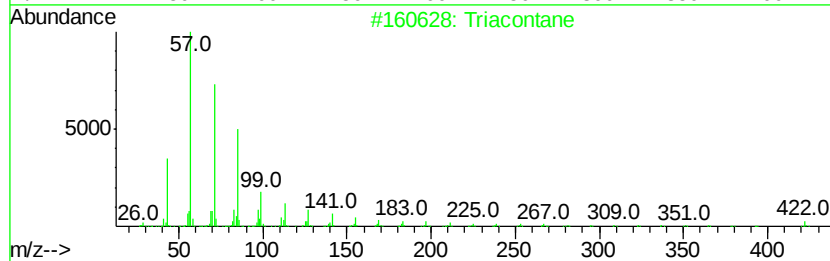
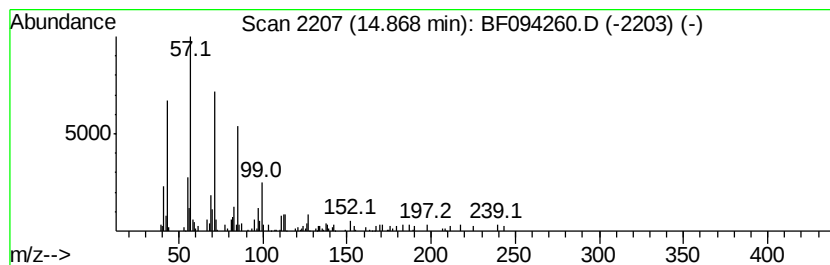
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.09 ng	92427	Chrysene-d12	14.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	86
2		Octacosane	394	C28H58	000630-02-4	80
3		Nonacosane	408	C29H60	000630-03-5	80
4		Heneicosane	296	C21H44	000629-94-7	72
5		Tetracosane	338	C24H50	000646-31-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

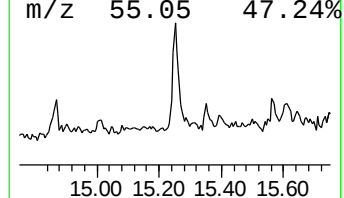
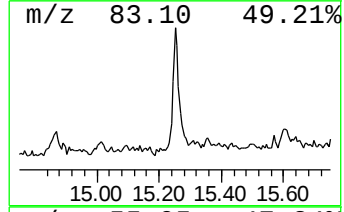
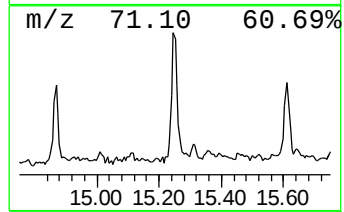
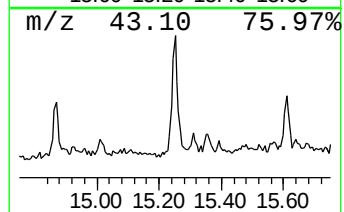
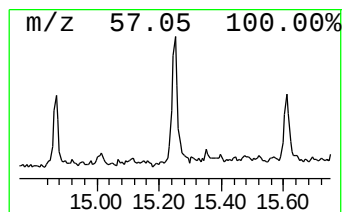
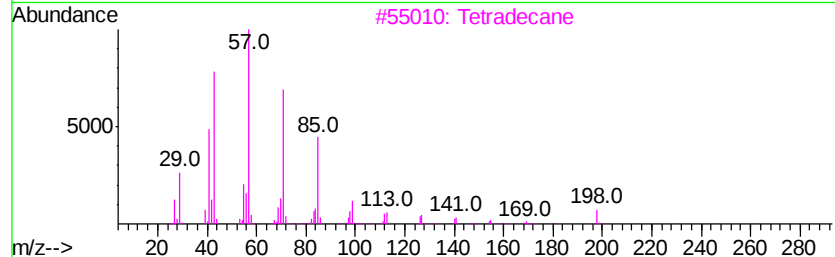
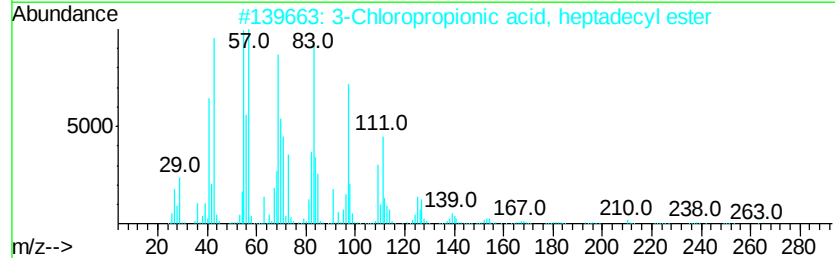
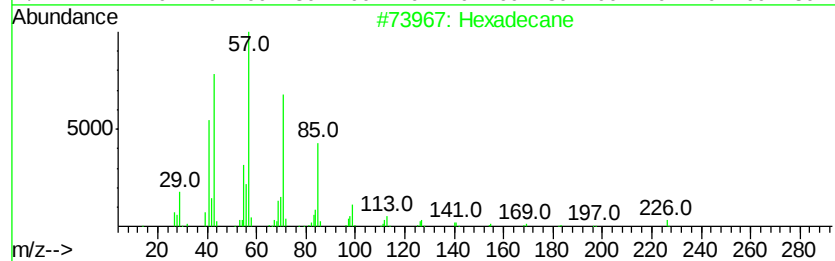
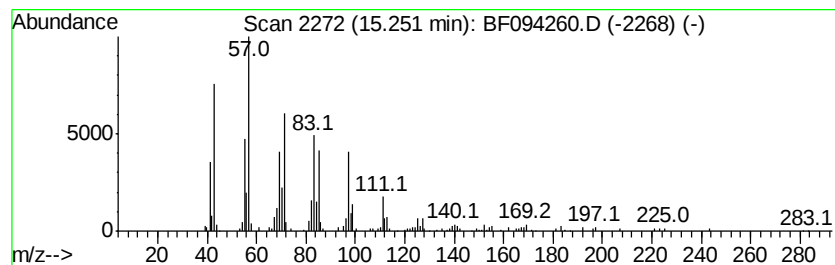
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.25 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	5.44 ng	240214	Chrysene-d12	14.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	49
2		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	49
3		Tetradecane	198	C14H30	000629-59-4	46
4		Heptadecane	240	C17H36	000629-78-7	46
5		Pentadecane	212	C15H32	000629-62-9	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

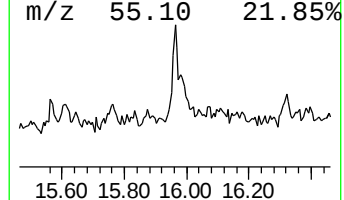
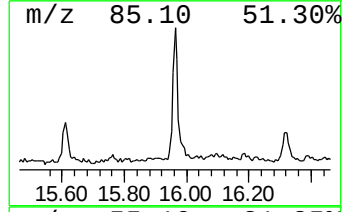
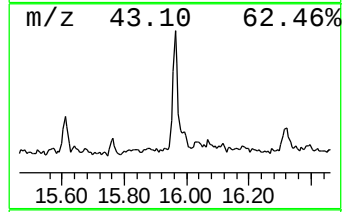
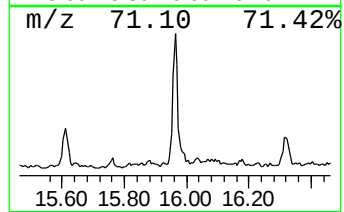
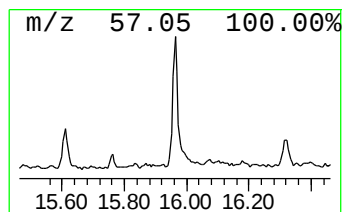
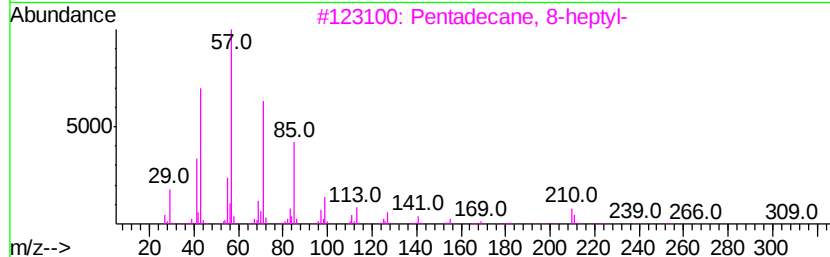
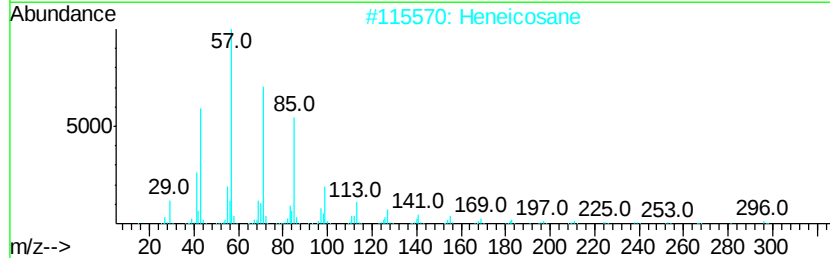
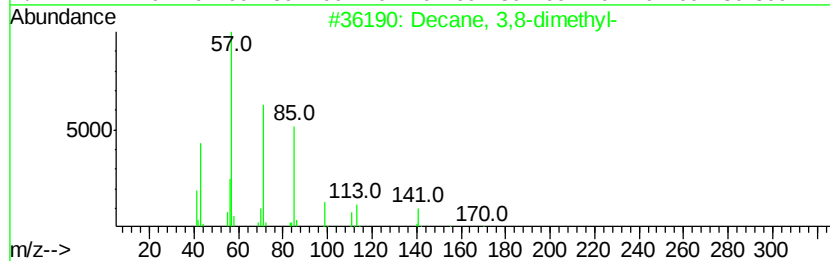
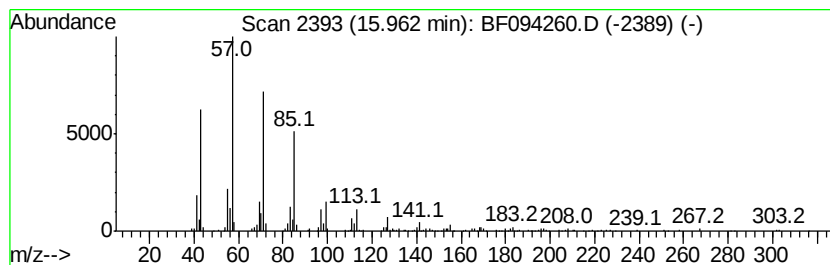
Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Decane, 3,8-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.96	8.62 ng	328802	Perylene-d12	16.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Nonacosane	408	C29H60	000630-03-5	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

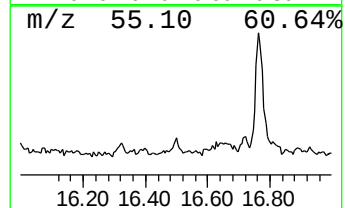
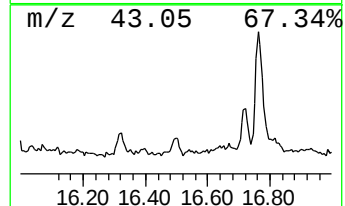
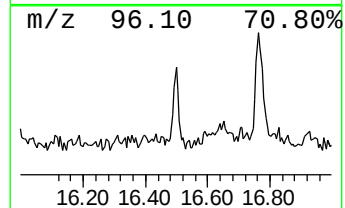
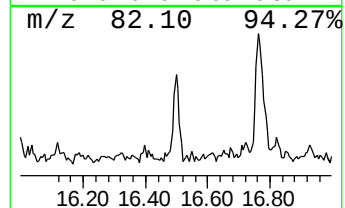
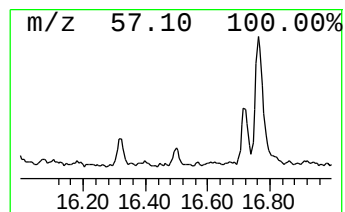
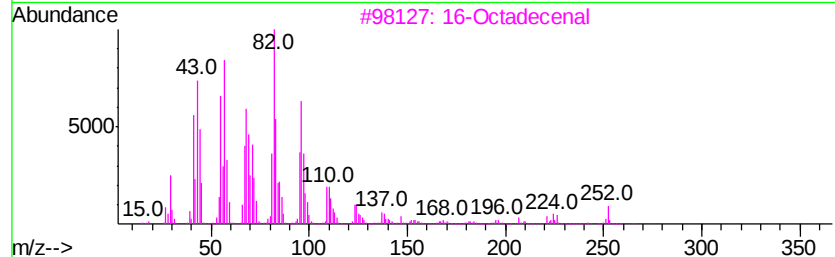
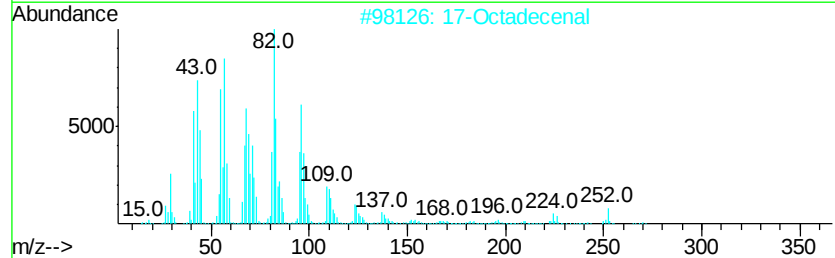
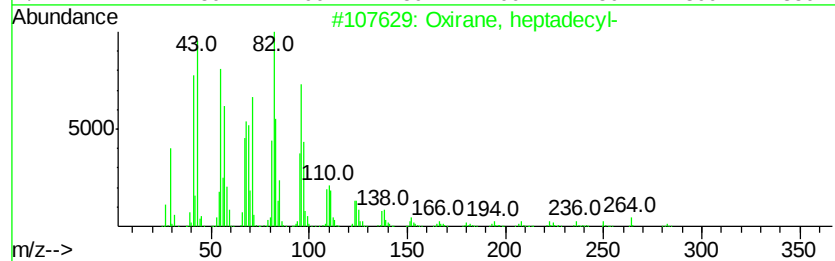
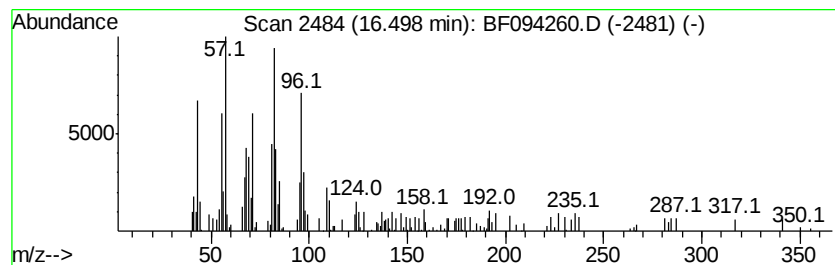
Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxirane, heptadecyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	2.03 ng	77257	Perylene-d12	16.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Oxirane, heptadecyl-	282 C19H38O	067860-04-2	80
2	17-Octadecenal	266 C18H34O	056554-86-0	72
3	16-Octadecenal	266 C18H34O	056554-87-1	72
4	15-Octadecenal	266 C18H34O	056554-93-9	72
5	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

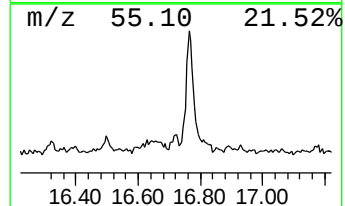
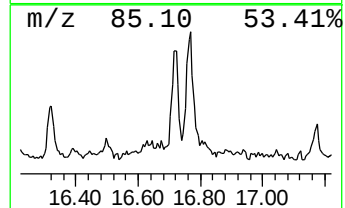
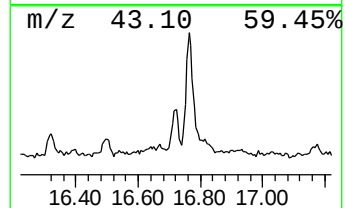
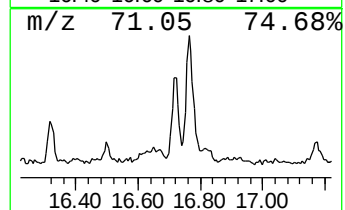
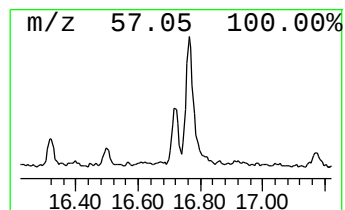
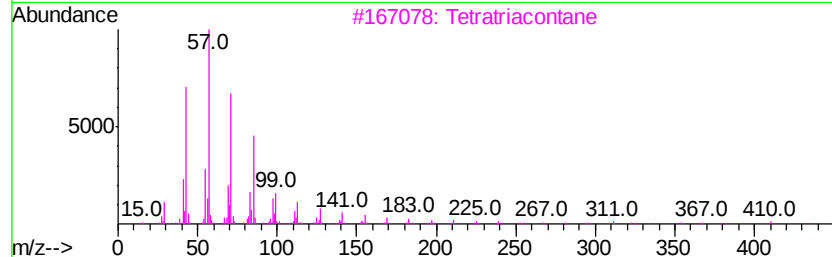
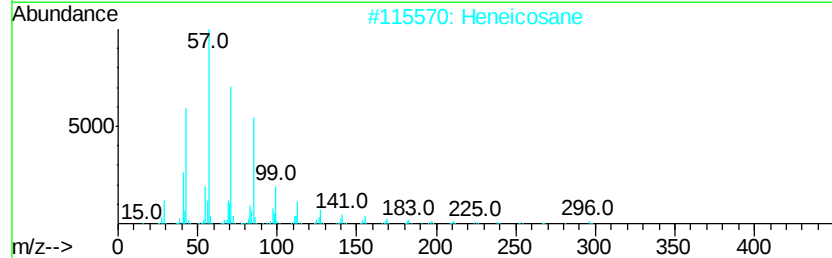
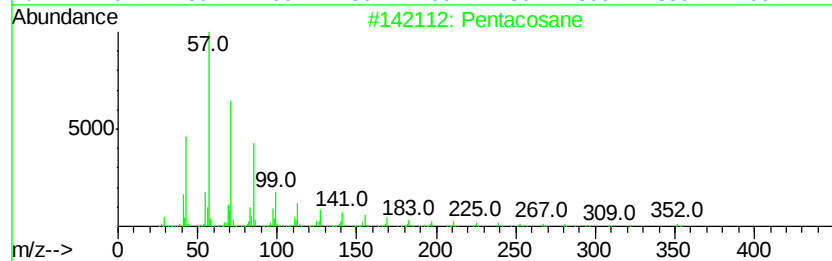
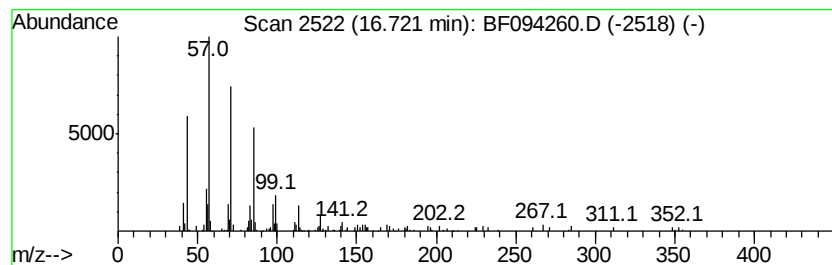
Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	3.22 ng	122862	Perylene-d12	16.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	93
2	Heneicosane	296 C21H44	000629-94-7	91
3	Tetratriacontane	479 C34H70	014167-59-0	91
4	Octacosane	394 C28H58	000630-02-4	91
5	Tetracosane, 11-decyl-	479 C34H70	055429-84-0	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

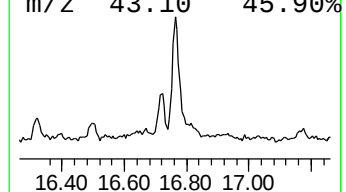
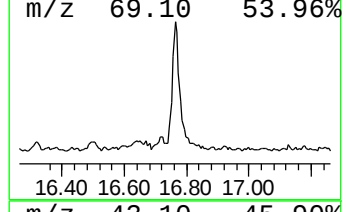
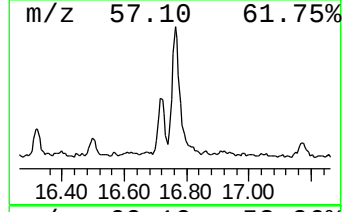
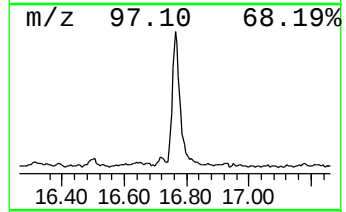
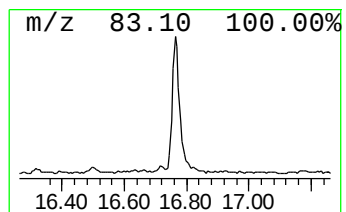
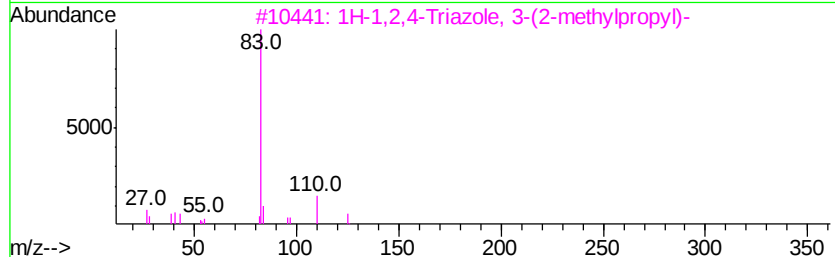
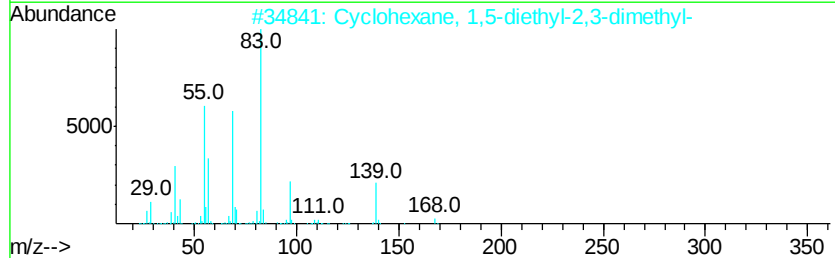
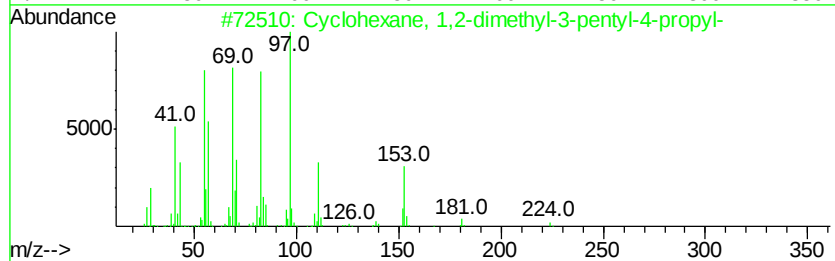
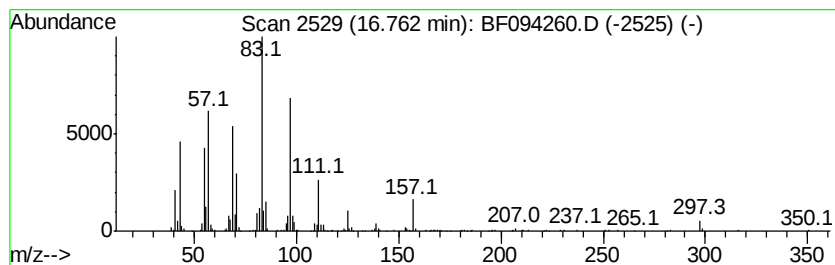
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.76 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	16.31 ng	621926	Perylene-d12	16.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	43
2		Cyclohexane, 1,5-diethyl-2,3-dim...	168	C12H24	074663-66-4	38
3		1H-1,2,4-Triazole, 3-(2-methylpr...	125	C6H11N3	040515-29-5	38
4		dl-Noformicin sulfate	197	C8H15N5O	1000131-37-1	35
5		Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

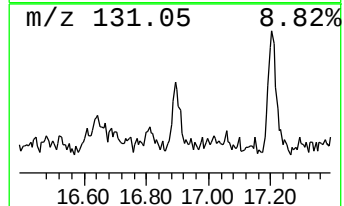
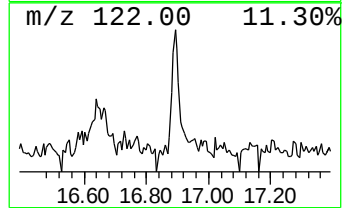
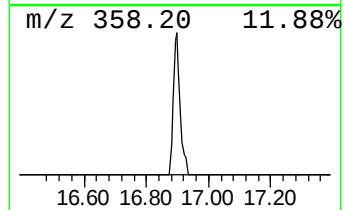
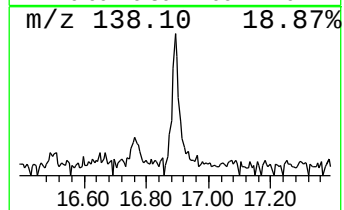
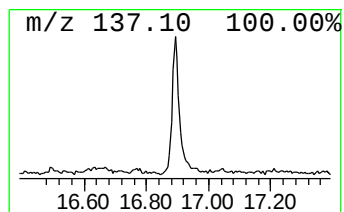
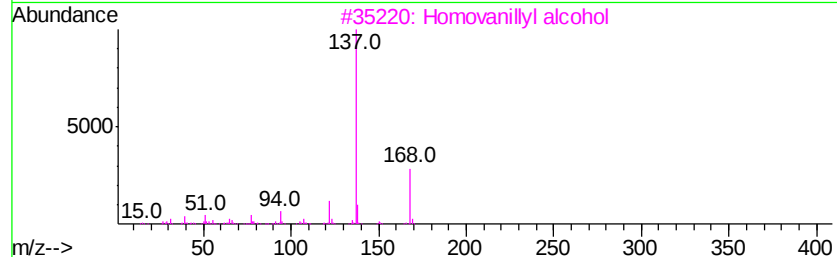
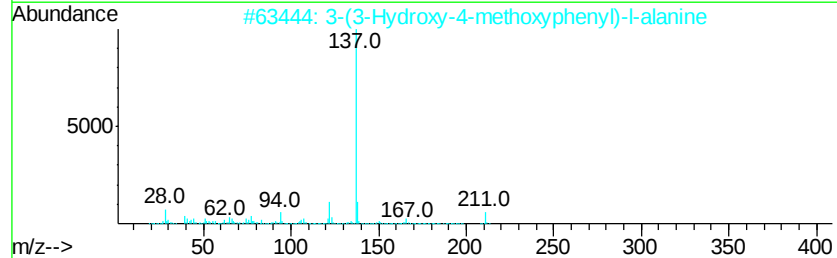
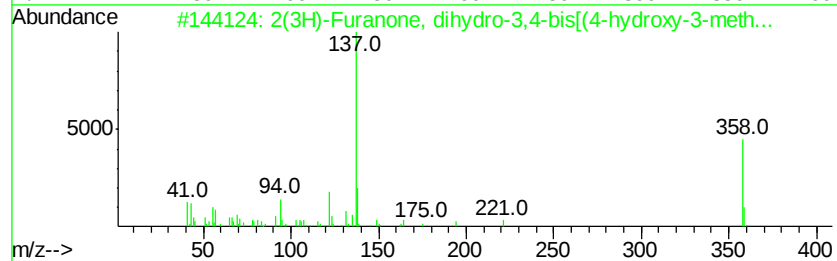
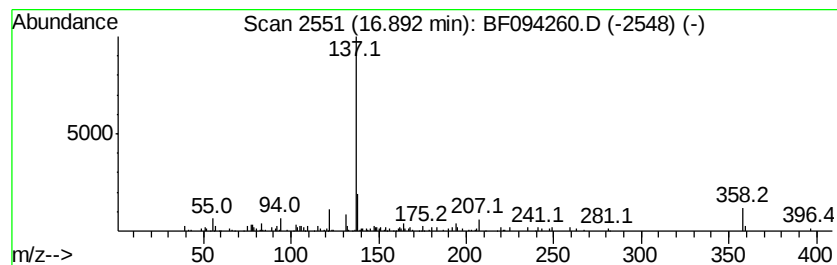
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Furanone, dihydro-3,4... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	2.56 ng	97693	Perylene-d12	16.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, dihydro-3,4-bis[...	358	C20H22O6	000580-72-3	60
2		3-(3-Hydroxy-4-methoxyphenyl)-l-...	211	C10H13NO4	1000103-80-4	59
3		Homovanillyl alcohol	168	C9H12O3	002380-78-1	59
4		Ketone, 1-cyclohexen-1-yl methyl...	181	C9H15N3O	007499-13-0	49
5		(-)-Nortrachelogenin	374	C20H22O7	034444-37-6	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

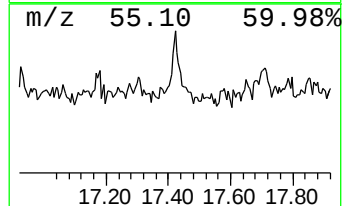
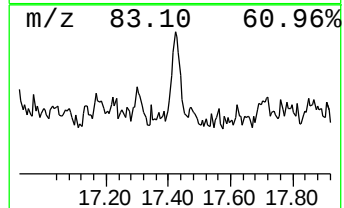
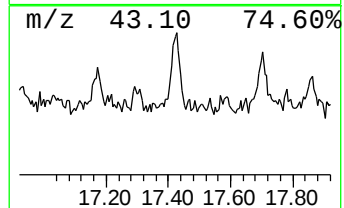
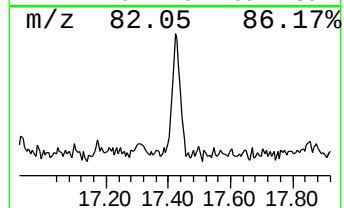
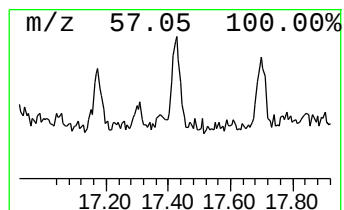
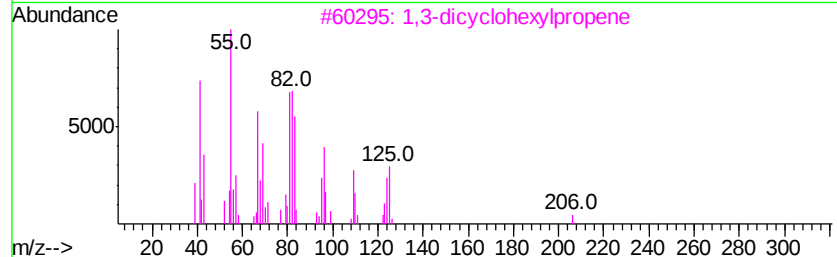
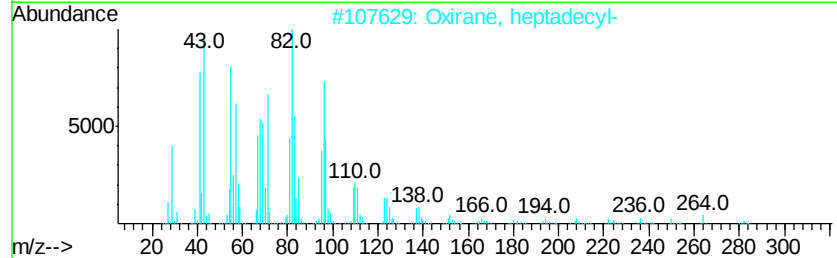
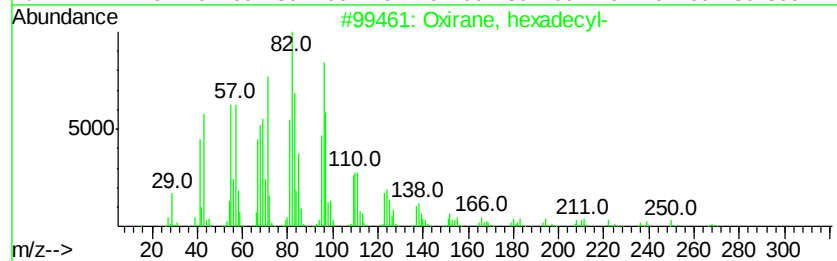
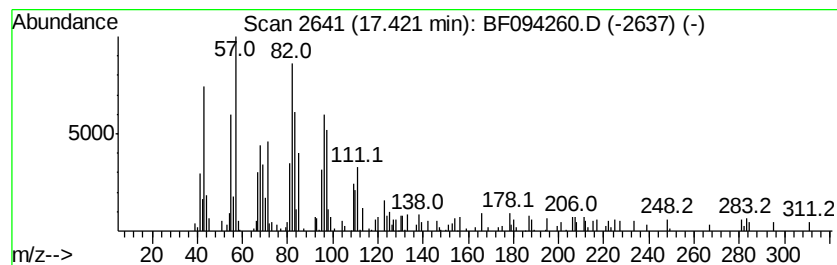
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Oxirane, hexadecyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	3.90 ng	148845	Perylene-d12	16.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	83
3		1,3-dicyclohexylpropene	206	C15H26	1000214-96-8	60
4		1,19-Eicosadiene	278	C20H38	014811-95-1	58
5		Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

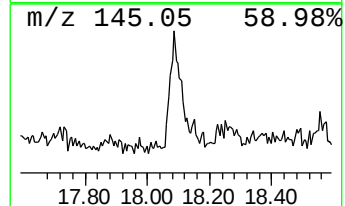
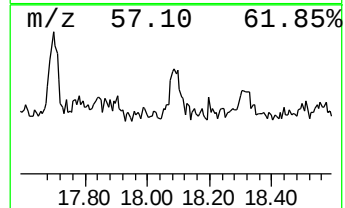
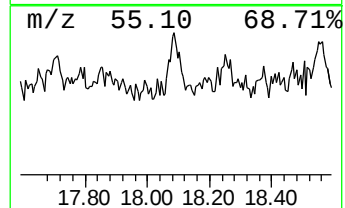
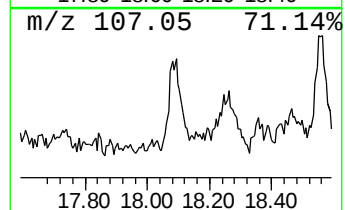
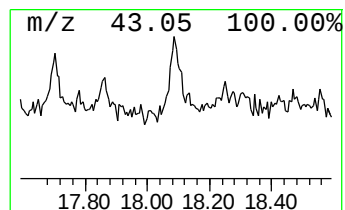
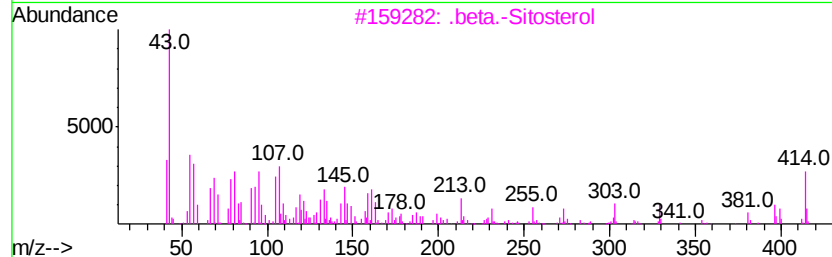
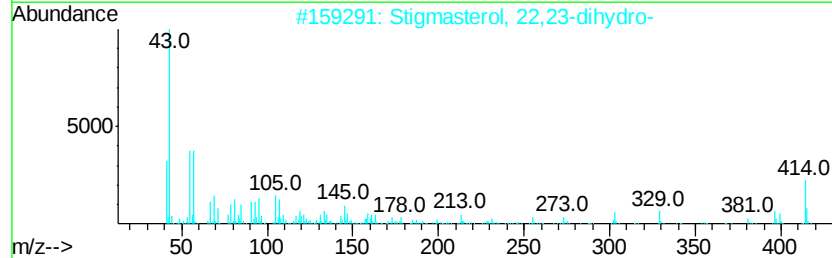
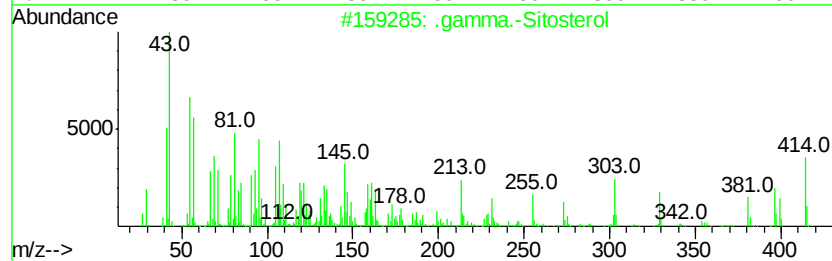
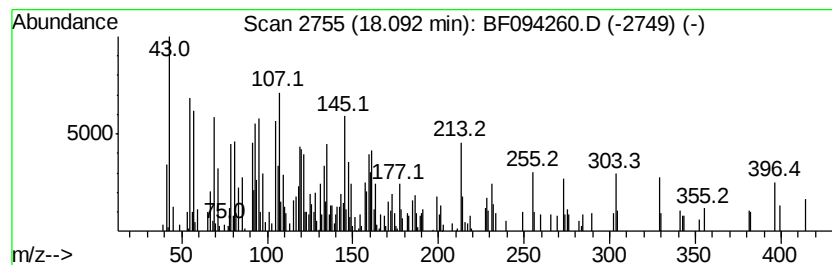
Instrument :
BNA_F
ClientSampleId :
COMP-4

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .gamma.-Sitosterol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.09	6.77 ng	258125	Perylene-d12	16.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	93
2	Stigmasterol, 22,23-dihydro-	414	C29H50O	1000214-20-7	78
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	70
4	Kauren-18-ol, acetate, (4.beta.)-	330	C22H34O2	072150-74-4	43
5	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

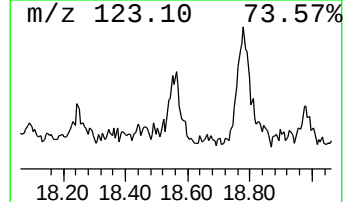
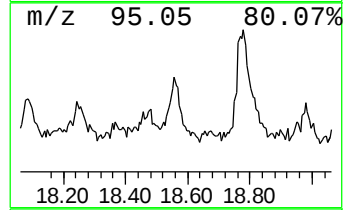
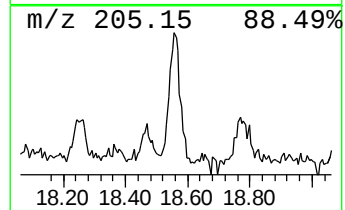
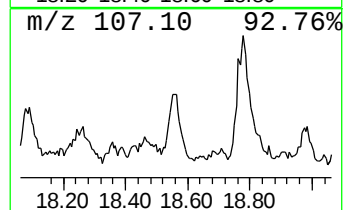
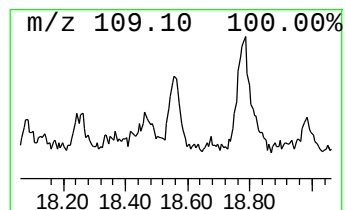
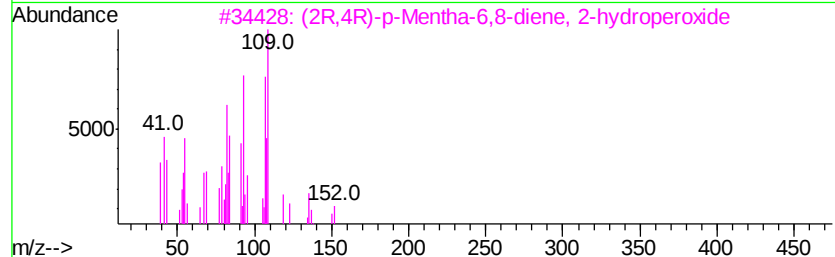
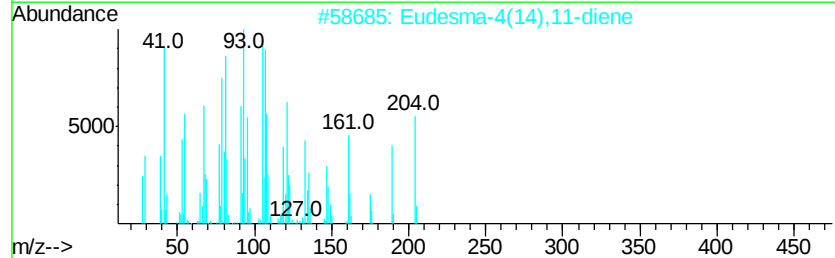
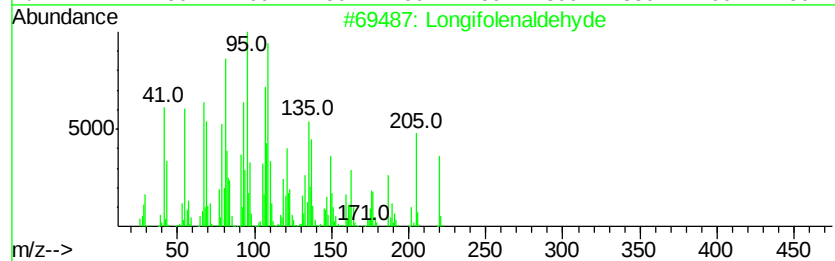
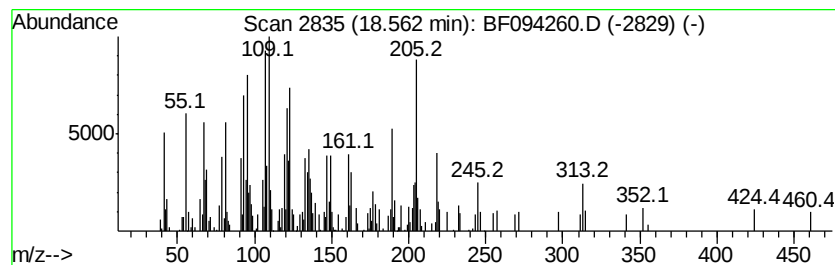
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown18.56 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	7.55 ng	287920	Perylene-d12	16.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Longifolenaldehyd	220	C15H24O	019890-84-7	47
2		Eudesma-4(14),11-diene	204	C15H24	1000152-04-3	35
3		(2R,4R)-p-Mentha-6,8-diene, 2-hv...	168	C10H16O2	1000292-74-2	27
4		Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	25
5		Propanoic acid, 2-bromo-, ethyl ...	180	C5H9BrO2	000535-11-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-4

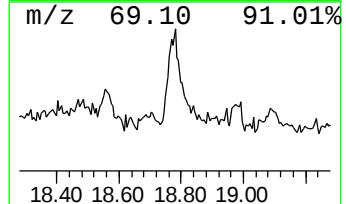
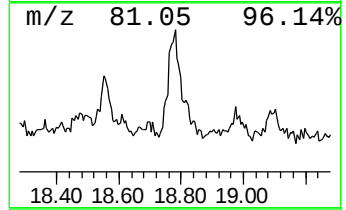
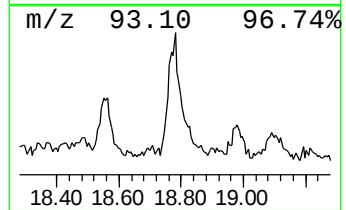
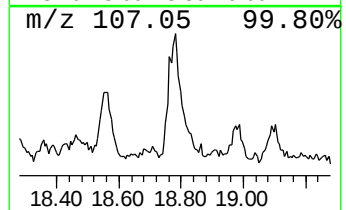
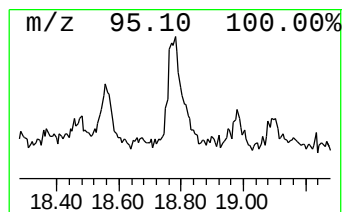
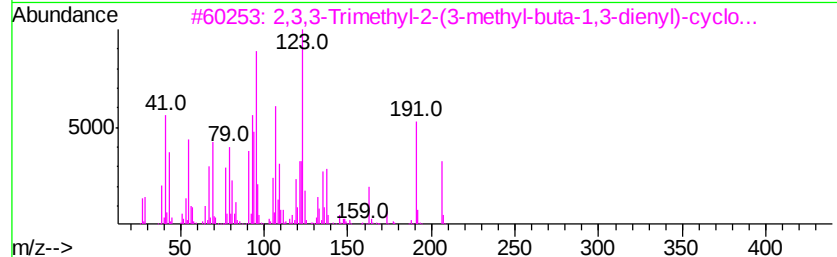
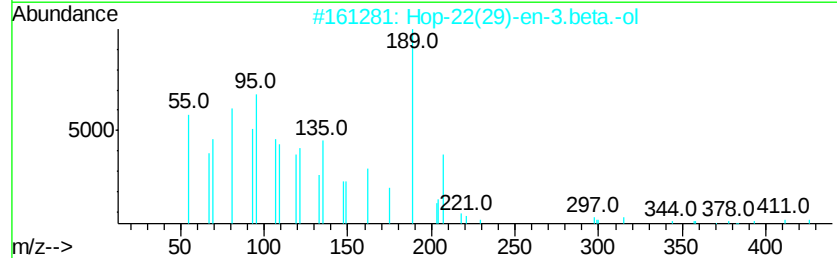
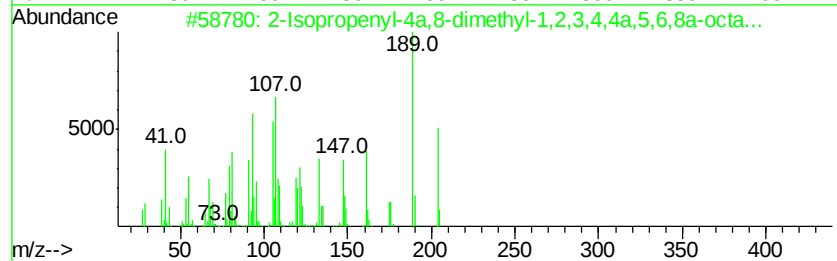
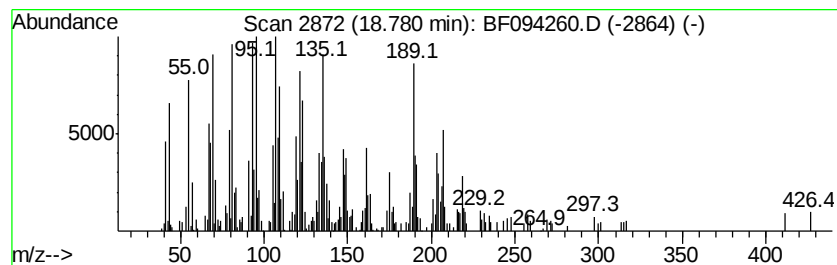
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2-Isopropenyl-4a,8-dimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.78	19.13 ng	729286	Perylene-d12	16.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	92
2			Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	64
3			2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	53
4			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	44
5			1R,3Z,9S-2,6,10,10-Tetramethylbi...	204	C15H24	1000140-07-4	41



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094260.D
Acq On : 7 Apr 2017 8:17
Operator : SJ/MA
Sample : I2542-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
COMP-4

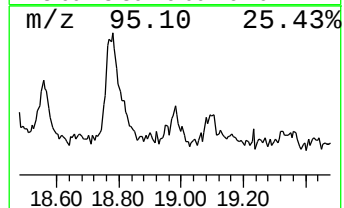
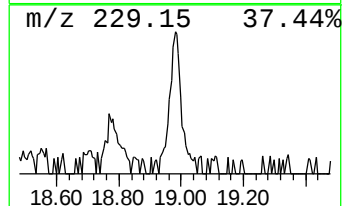
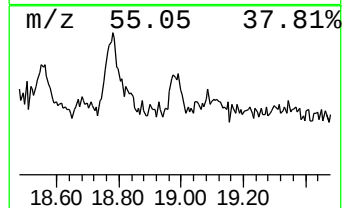
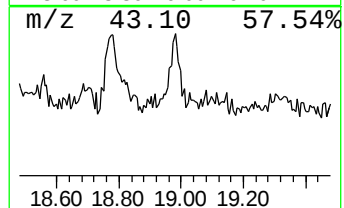
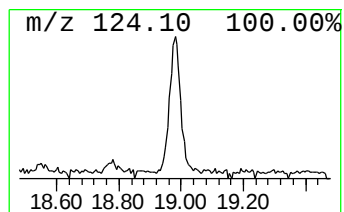
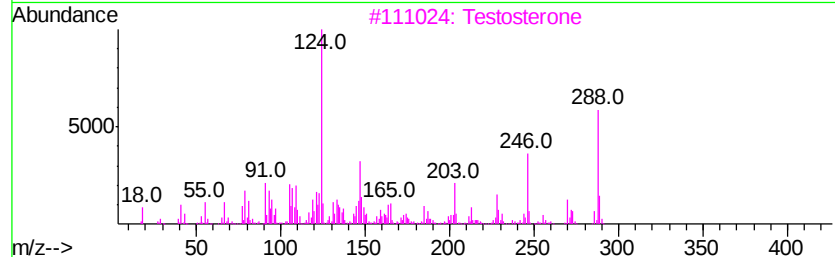
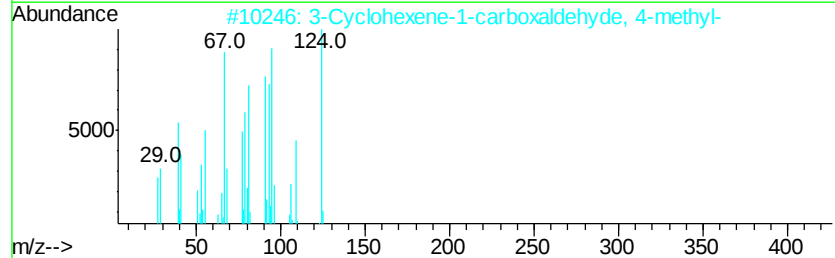
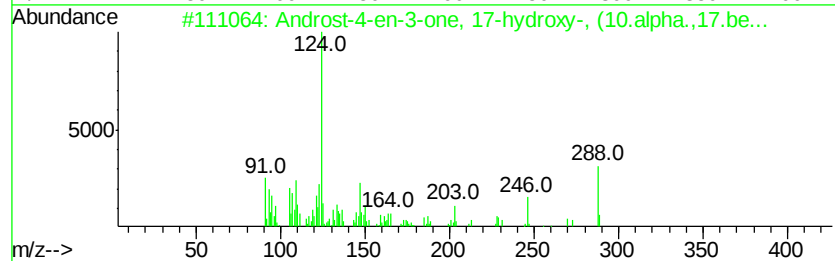
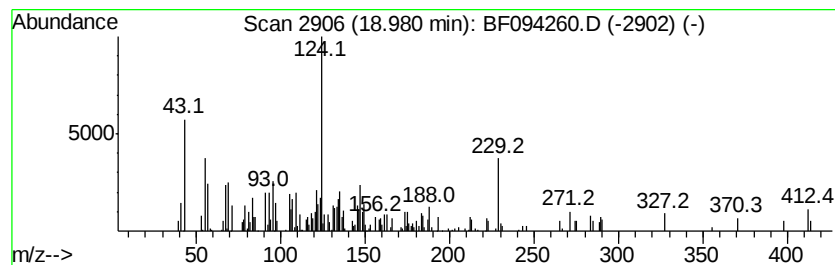
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Androst-4-en-3-one, 17-hydr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.98	5.52 ng	210391	Perylene-d12	16.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Androst-4-en-3-one, 17-hydroxy-, ...	288	C19H28O2	000604-39-7	64
2			3-Cyclohexene-1-carboxaldehyde, ...	124	C8H12O	007560-64-7	55
3			Testosterone	288	C19H28O2	000058-22-0	43
4			2,3a-Dimethylhexahydrobenzofuran...	170	C10H18O2	1000186-53-6	43
5			Pregn-4-ene-3,20-dione, (9.beta....	314	C21H30O2	002755-10-4	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
 Data File : BF094260.D
 Acq On : 7 Apr 2017 8:17
 Operator : SJ/MA
 Sample : I2542-17
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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
2-Pentanone, 4-hy...	3.99	15.7	ng	712800	1	5.85	910172	20.0
unknown5.60	5.60	74.3	ng	3380230	1	5.85	910172	20.0
Heptacosane	10.67	2.0	ng	110852	4	11.32	1105230	20.0
unknown13.51	13.51	6.5	ng	288298	5	14.57	882582	20.0
1-Hexadecanesulfo...	14.47	5.9	ng	260996	5	14.57	882582	20.0
triacontane	14.87	2.1	ng	92427	5	14.57	882582	20.0
unknown15.25	15.25	5.4	ng	240214	5	14.57	882582	20.0
Decane, 3,8-dimet...	15.96	8.6	ng	328802	6	16.20	762552	20.0
Oxirane, heptadecyl-	16.50	2.0	ng	77257	6	16.20	762552	20.0
Pentacosane	16.72	3.2	ng	122862	6	16.20	762552	20.0
unknown16.76	16.76	16.3	ng	621926	6	16.20	762552	20.0
2(3H)-Furanone, d...	16.89	2.6	ng	97693	6	16.20	762552	20.0
Oxirane, hexadecyl-	17.42	3.9	ng	148845	6	16.20	762552	20.0
.gamma.-Sitosterol	18.09	6.8	ng	258125	6	16.20	762552	20.0
unknown18.56	18.56	7.5	ng	287920	6	16.20	762552	20.0
2-Isopropenyl-4a,...	18.78	19.1	ng	729286	6	16.20	762552	20.0
Androst-4-en-3-on...	18.98	5.5	ng	210391	6	16.20	762552	20.0