

Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
 Data File : BF094539.D
 Acq On : 20 Apr 2017 12:42
 Operator : SJ/MA
 Sample : I2744-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-9(11-13)20170418

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-BF041717.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	3.919	333	337	344	rBV	427784	476551	14.88%	1.635%
2	4.319	401	405	419	rBV	2689648	2538758	79.30%	8.710%
3	4.701	466	470	474	rBV	30422	32337	1.01%	0.111%
4	5.389	582	587	598	rBV	2419473	2723391	85.06%	9.343%
5	5.519	604	609	612	rBV	2827780	2742940	85.67%	9.410%
6	5.766	647	651	654	rBV	773968	696912	21.77%	2.391%
7	5.942	676	681	684	rBV	2304376	2123918	66.34%	7.286%
8	5.978	684	687	692	rVB	40111	49587	1.55%	0.170%
9	6.413	755	761	764	rBV	1727709	1668692	52.12%	5.725%
10	6.583	783	790	795	rBV	47315	59565	1.86%	0.204%
11	7.254	896	904	907	rBV	986760	966313	30.18%	3.315%
12	7.283	907	909	911	rVB	63064	49566	1.55%	0.170%
13	8.125	1049	1052	1056	rVB2	51301	52041	1.63%	0.179%
14	8.201	1060	1065	1070	rVV4	37012	80829	2.52%	0.277%
15	8.583	1125	1130	1133	rVB	2964284	3101412	96.87%	10.640%
16	9.077	1205	1214	1218	rBV	906159	891697	27.85%	3.059%
17	9.389	1262	1267	1273	rVB2	1057310	1056178	32.99%	3.623%
18	9.989	1366	1369	1373	rBV2	59751	63374	1.98%	0.217%
19	10.066	1379	1382	1388	rVB	218995	211661	6.61%	0.726%
20	10.260	1409	1415	1418	rBV2	21719	35194	1.10%	0.121%
21	10.366	1428	1433	1438	rBV	1740931	1813135	56.63%	6.220%
22	10.571	1464	1468	1470	rBV	100579	95537	2.98%	0.328%
23	10.671	1481	1485	1489	rBV4	23549	35244	1.10%	0.121%
24	11.124	1558	1562	1565	rBV	62712	57717	1.80%	0.198%
25	11.213	1572	1577	1580	rBV	1071948	1100464	34.37%	3.775%
26	11.507	1622	1627	1633	rBV	76854	104736	3.27%	0.359%
27	11.560	1633	1636	1646	rVV2	136708	182234	5.69%	0.625%
28	11.754	1666	1669	1675	rBV2	167923	175753	5.49%	0.603%
29	11.924	1693	1698	1699	rBV4	41431	47421	1.48%	0.163%
30	11.948	1699	1702	1705	rVB2	79391	71922	2.25%	0.247%
31	11.989	1705	1709	1712	rBV	59090	64684	2.02%	0.222%
32	12.024	1712	1715	1717	rBV3	75042	87820	2.74%	0.301%
33	12.083	1722	1725	1730	rVB2	77311	91964	2.87%	0.315%
34	12.148	1730	1736	1738	rBV5	39858	79198	2.47%	0.272%

Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

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-BF041717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.171	1738	1740	1743	rVB2	35041	38272	1.20%	0.131%
36	12.236	1749	1751	1753	rBV	59634	56554	1.77%	0.194%
37	12.289	1758	1760	1766	rVB	50111	52747	1.65%	0.181%
38	13.189	1907	1913	1917	rBV	2712854	3201635	100.00%	10.984%
39	13.948	2039	2042	2047	rVB3	36727	39339	1.23%	0.135%
40	14.354	2106	2111	2120	rBV2	112829	183999	5.75%	0.631%
41	14.459	2124	2129	2135	rVB	949114	1079344	33.71%	3.703%
42	15.571	2314	2318	2323	rVB	41837	47573	1.49%	0.163%
43	16.083	2400	2405	2410	rBV	693698	820684	25.63%	2.815%

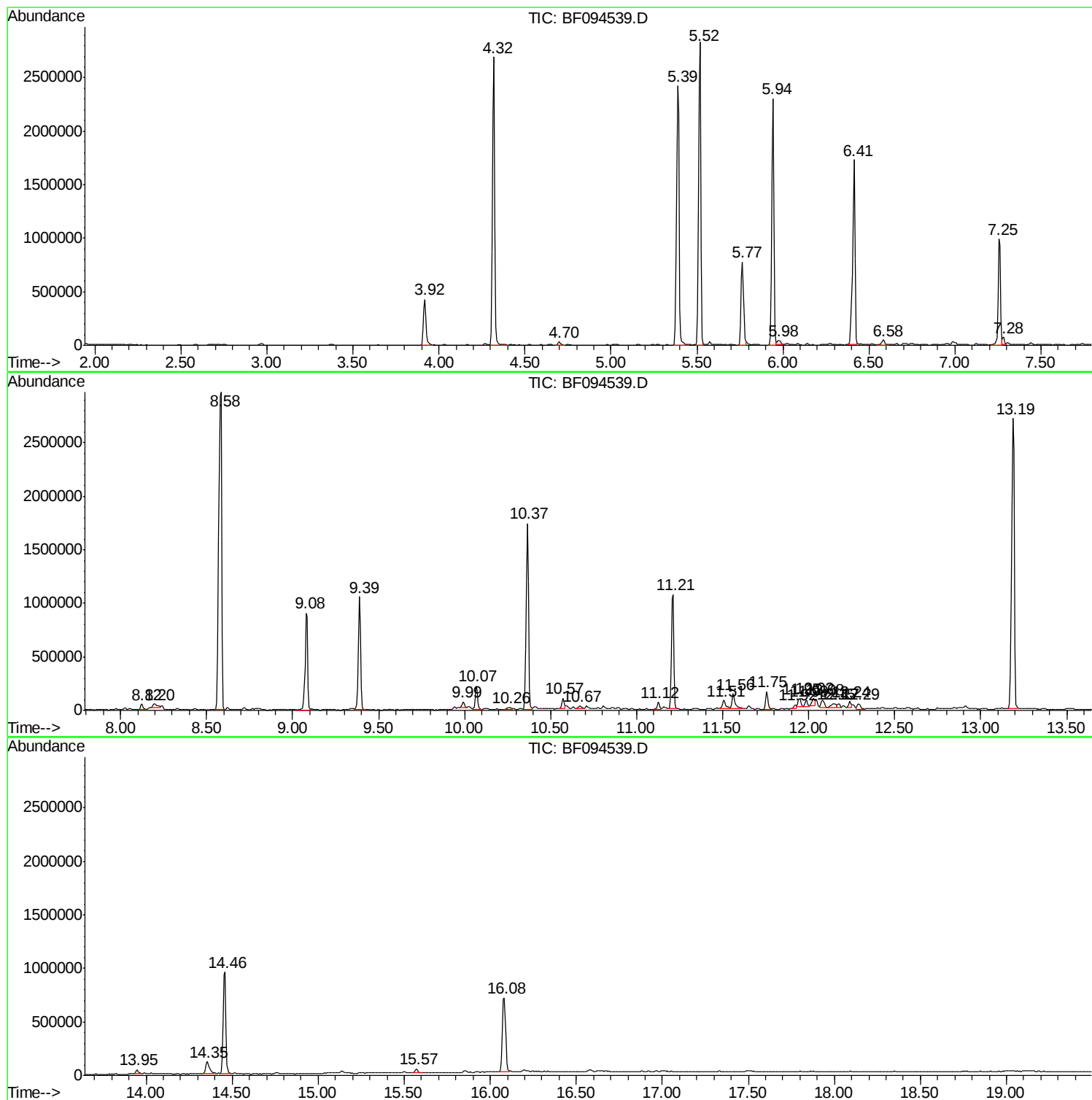
Sum of corrected areas: 29148892

Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.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\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

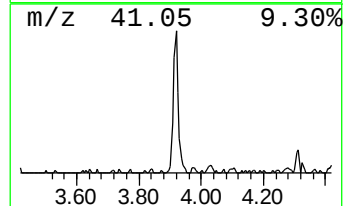
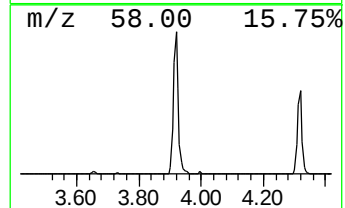
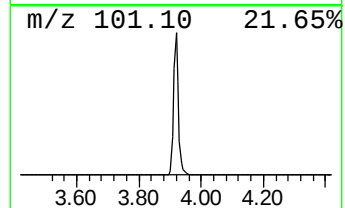
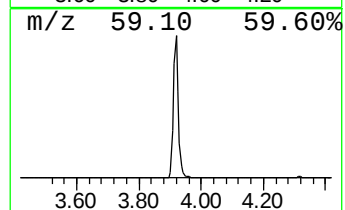
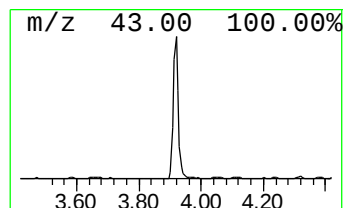
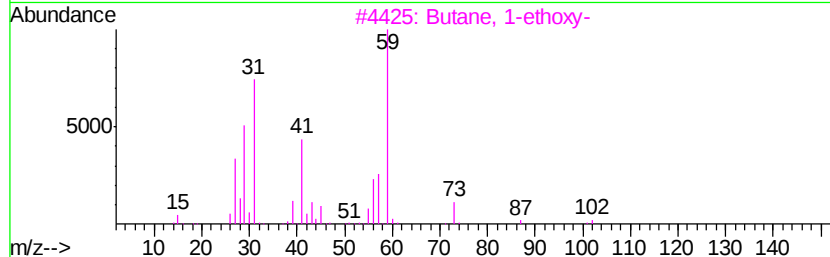
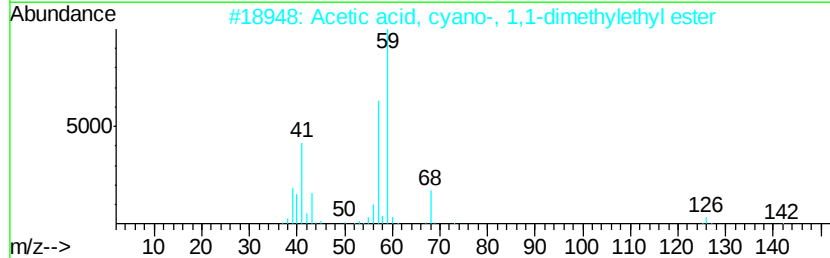
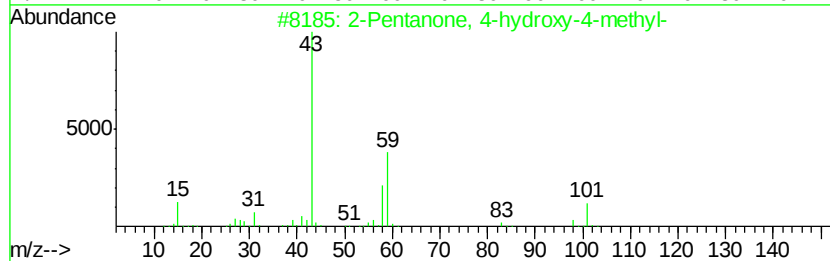
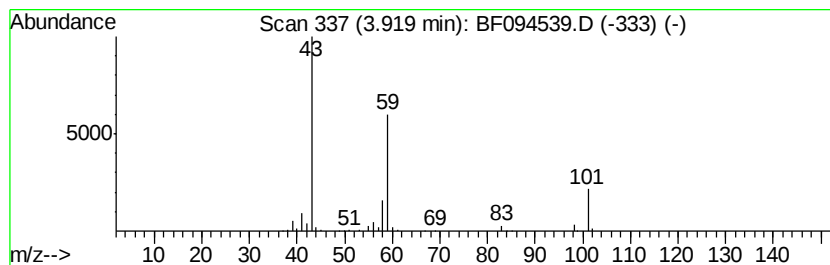
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	13.68 ng	476551	1,4-Dichlorobenzene-d4	5.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA_F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

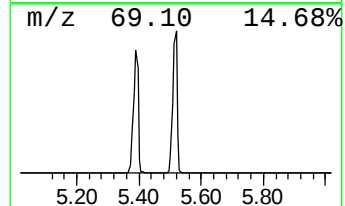
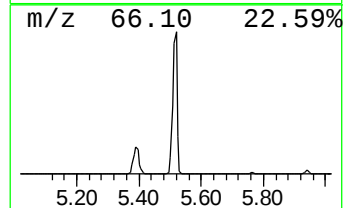
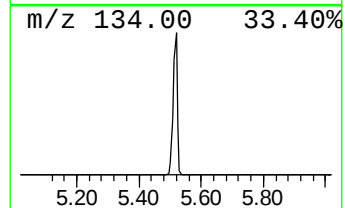
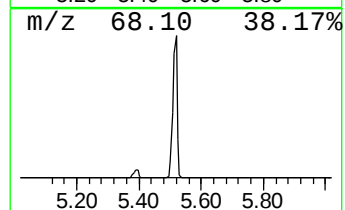
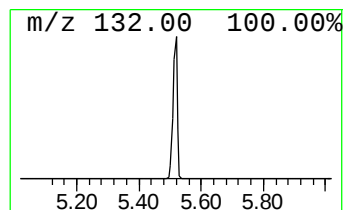
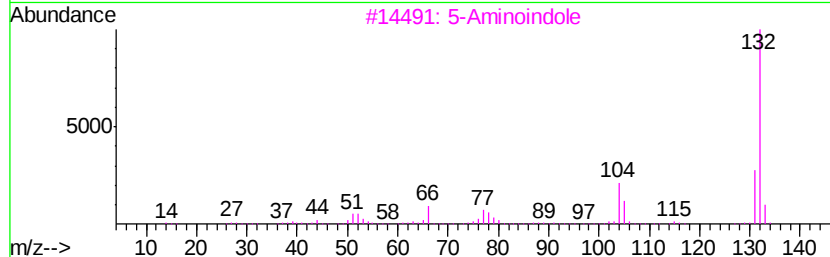
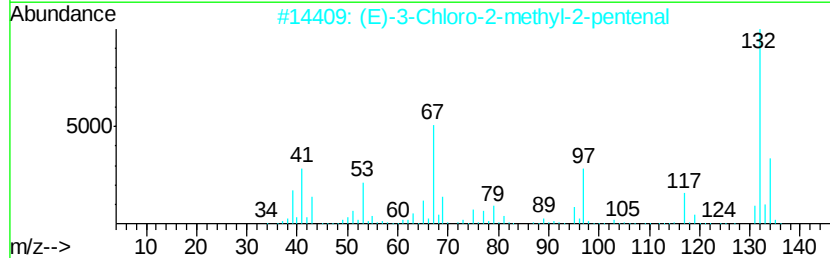
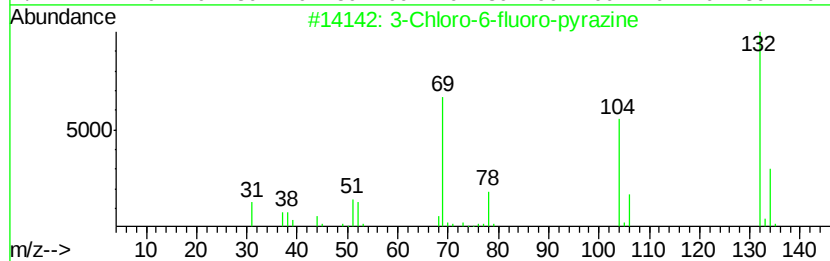
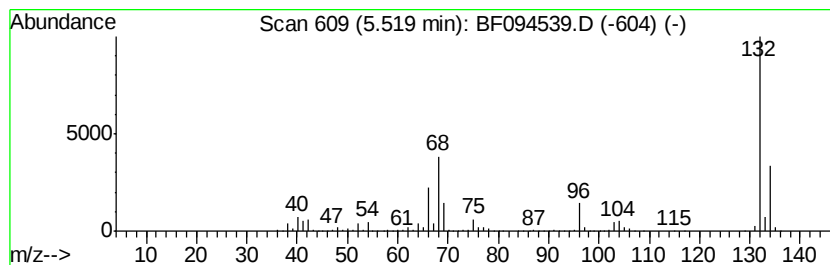
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	78.72 ng	2742940	1,4-Dichlorobenzene-d4	5.77

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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

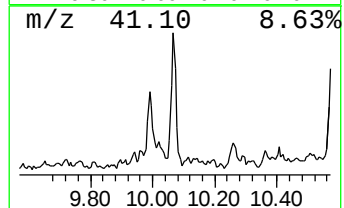
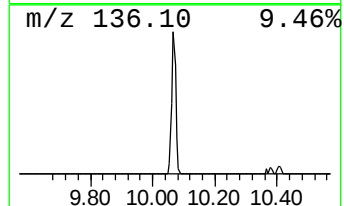
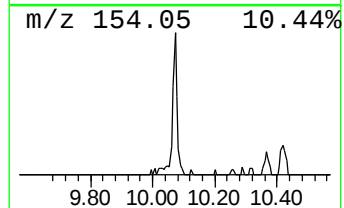
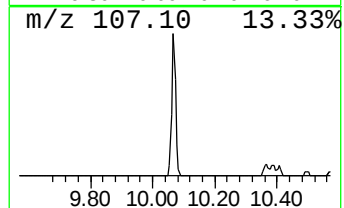
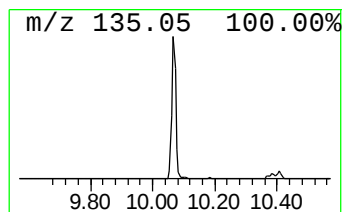
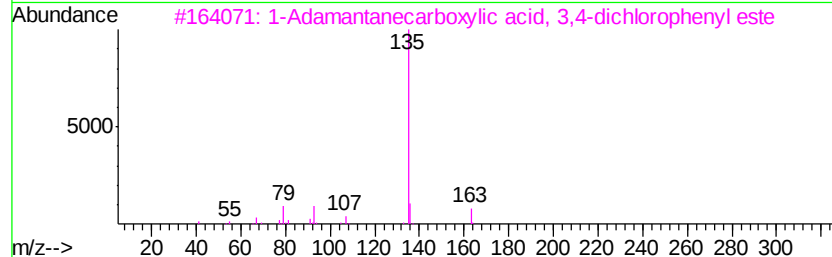
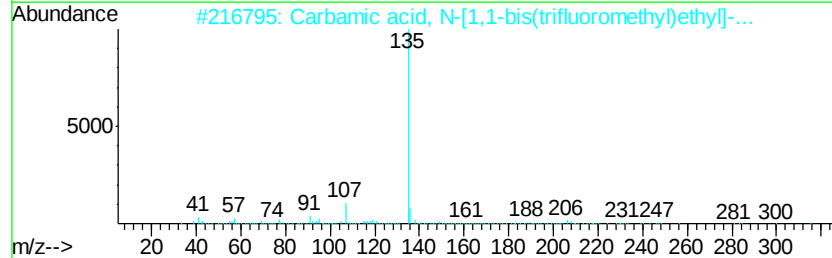
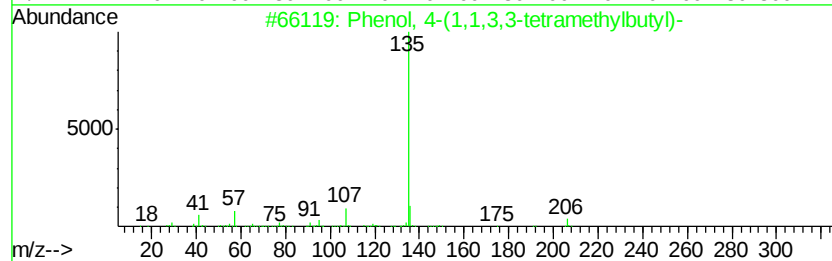
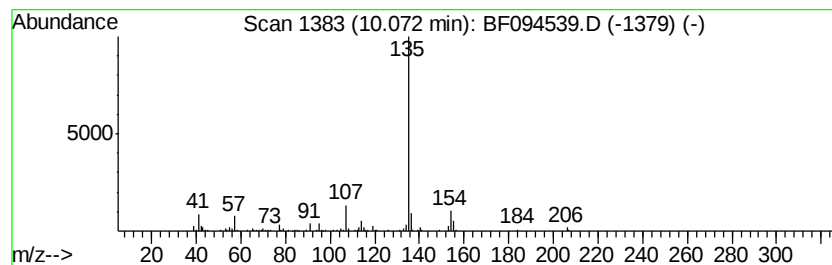
Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.07	4.01 ng	211661	Acenaphthene-d10	9.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206 C14H22O	000140-66-9	72
2	Carbamic acid, N-[1,1-bis(triflu...	413 C19H25F6N02	296242-69-8	64
3	1-Adamantanecarboxylic acid, 3,4...	324 C17H18Cl2O2	1000307-66-4	59
4	1-Adamantanecarboxylic acid, 3,5...	284 C19H24O2	1000307-66-1	59
5	Pentanoic acid, 5-hydroxy-, p-t...	250 C15H22O3	166273-37-6	50



Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

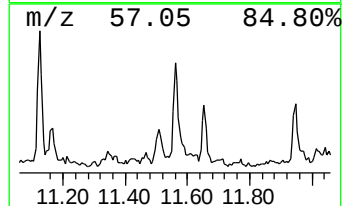
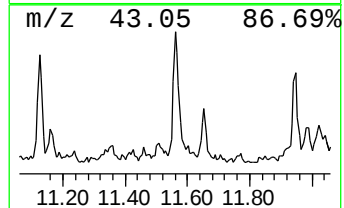
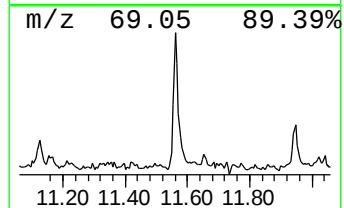
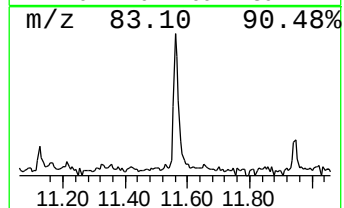
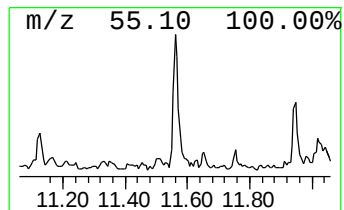
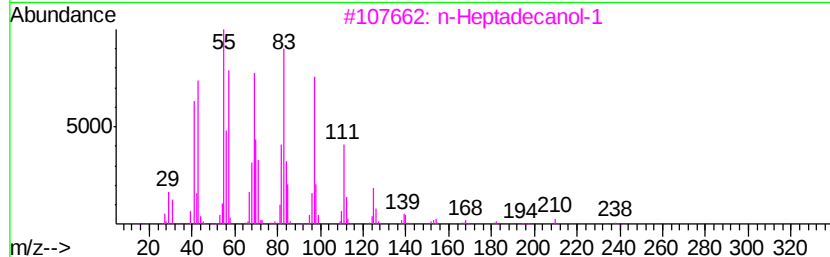
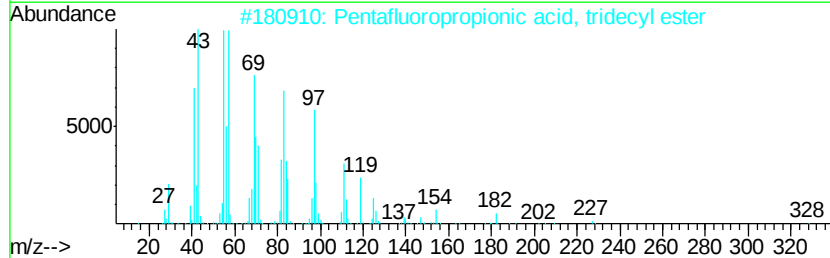
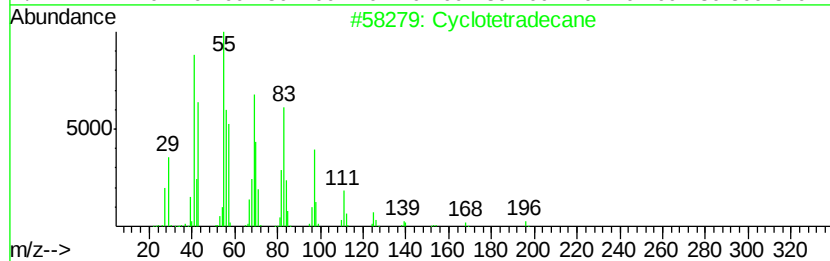
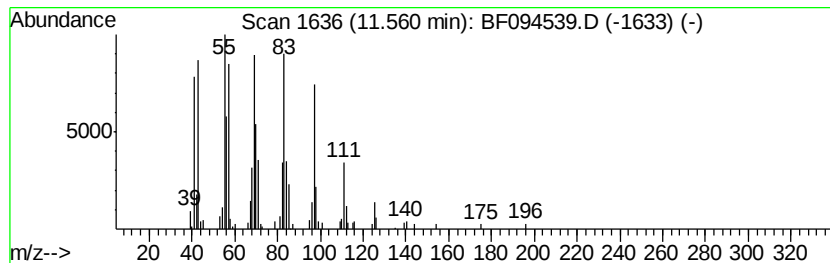
Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.56	3.31 ng	182234	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	98
2	Pentafluoropropionic acid, tridecyl ester	346	C16H27F5O2	959261-22-4	93
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91



Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

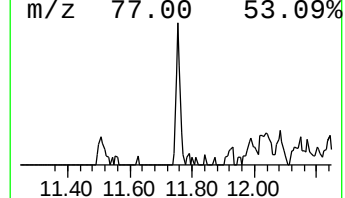
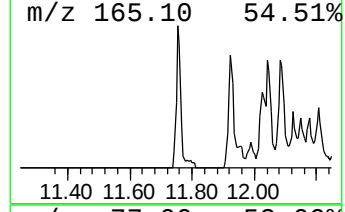
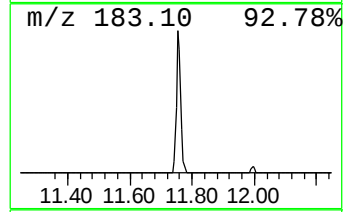
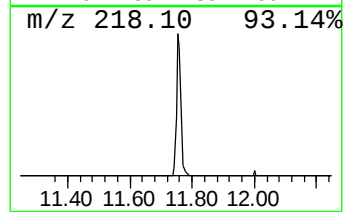
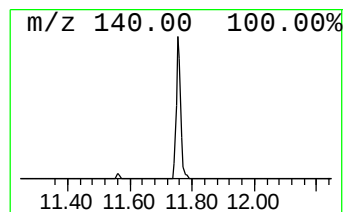
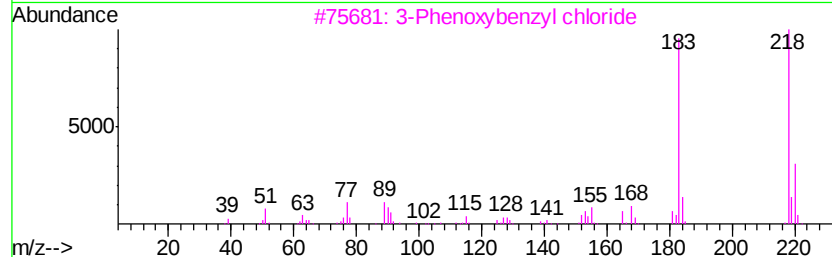
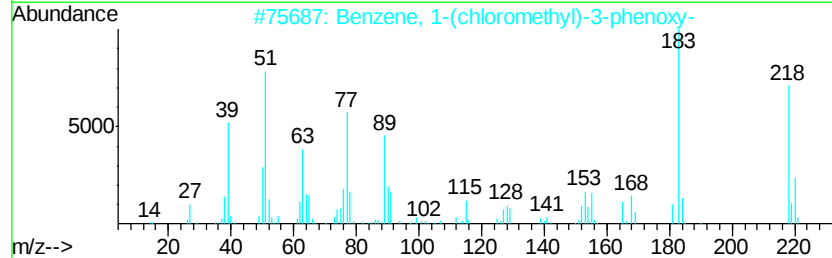
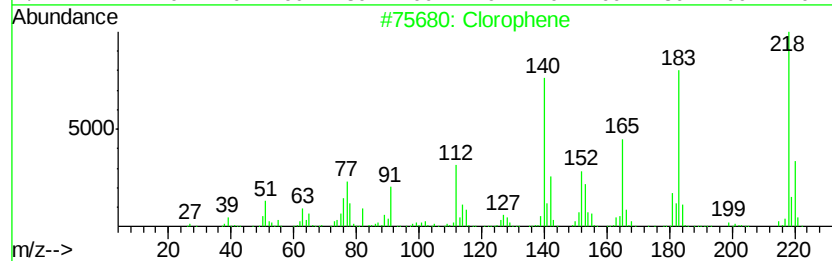
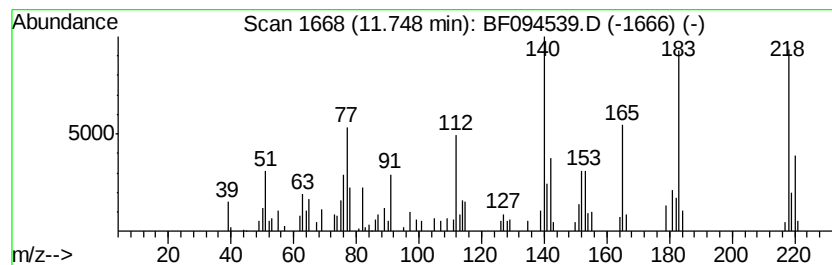
Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Clorophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.75	3.19 ng	175753	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Clorophene	218	C13H11ClO	000120-32-1	99
2	Benzene, 1-(chloromethyl)-3-phen...	218	C13H11ClO	053874-66-1	50
3	3-Phenoxybenzyl chloride	218	C13H11ClO	1000353-82-2	50
4	Benzofuro[3,2-d]pyrimidine, 4-ch...	218	C11H7ClN2O	039786-40-8	46
5	6-Methoxy-2-naphthonitrile	183	C12H9NO	067886-70-8	46



Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

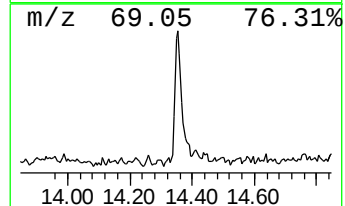
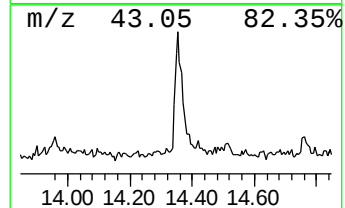
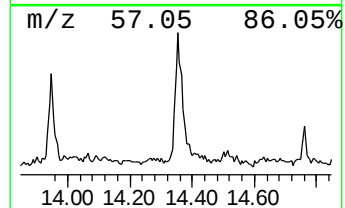
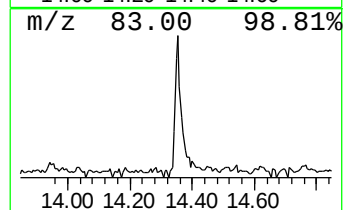
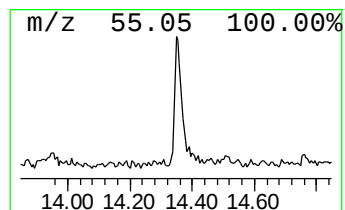
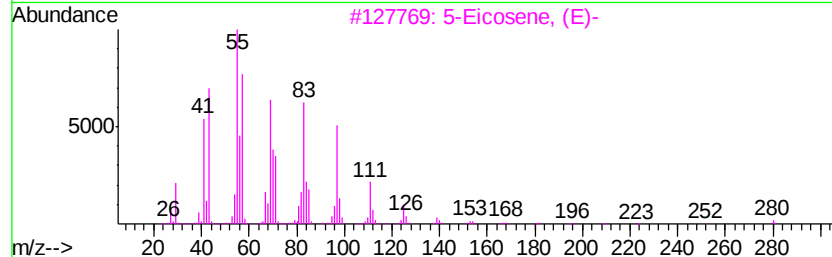
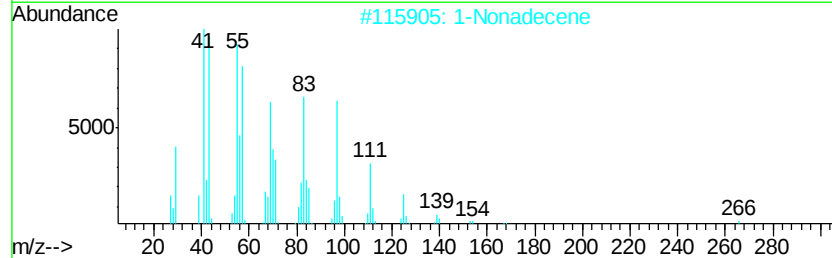
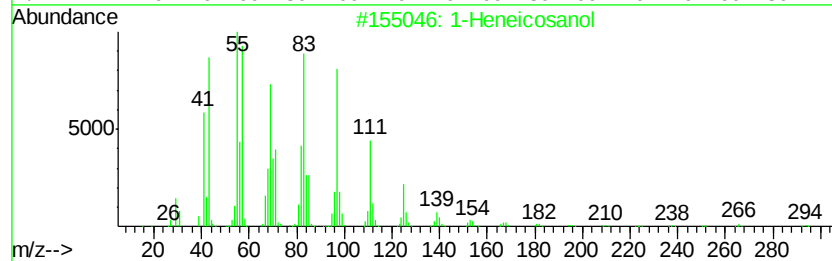
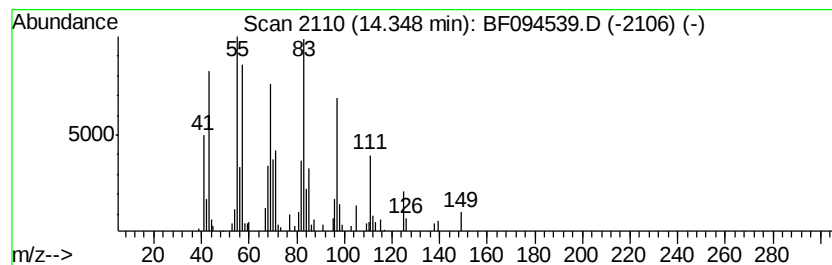
Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.41 ng	183999	Chrysene-d12	14.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	1-Nonadecene	266 C19H38	018435-45-5	91
3	5-Eicosene, (E)-	280 C20H40	074685-30-6	91
4	Behenic alcohol	326 C22H46O	000661-19-8	91
5	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	90



Data Path : Z:\HPCHEM1\BNA_F\Data\BF042017\
Data File : BF094539.D
Acq On : 20 Apr 2017 12:42
Operator : SJ/MA
Sample : I2744-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9(11-13)20170418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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...	3.92	13.7	ng	476551	1	5.77	696912	20.0
unknown5.52	5.52	78.7	ng	2742940	1	5.77	696912	20.0
Phenol, 4-(1,1,3,...	10.07	4.0	ng	211661	3	9.39	1056180	20.0
Cyclotetradecane	11.56	3.3	ng	182234	4	11.21	1100460	20.0
Clorophene	11.75	3.2	ng	175753	4	11.21	1100460	20.0
1-Heneicosanol	14.35	3.4	ng	183999	5	14.46	1079340	20.0