

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
 Data File : BF090180.D
 Acq On : 22 Sep 2016 1:03
 Operator : UM/SJ
 Sample : H4856-06 2X
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BH-7-0.5-2FT

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-BF092016.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.667	6	7	39	rVB	1942714	4872547	100.00%	21.909%
2	4.581	260	262	271	rVB	186834	248648	5.10%	1.118%
3	5.061	302	304	307	rBV	1087497	1183923	24.30%	5.323%
4	6.159	398	400	408	rBV	1297379	1268065	26.02%	5.702%
5	6.273	408	410	412	rBV	1478170	1370292	28.12%	6.161%
6	6.502	428	430	433	rBV	607448	670541	13.76%	3.015%
7	6.662	441	444	446	rBV	1215689	1063395	21.82%	4.781%
8	7.073	478	480	488	rBV	788785	773540	15.88%	3.478%
9	7.793	541	543	547	rBV	1033852	904026	18.55%	4.065%
10	8.879	635	638	640	rBV	1122146	1323132	27.15%	5.949%
11	9.279	671	673	675	rBV	344140	392430	8.05%	1.765%
12	9.542	694	696	698	rBV	807425	1007043	20.67%	4.528%
13	10.319	761	764	766	rBV	823647	804705	16.52%	3.618%
14	10.468	775	777	781	rVB2	54609	78078	1.60%	0.351%
15	11.005	821	824	825	rBV	1032726	898763	18.45%	4.041%
16	11.565	872	873	876	rVV3	48010	85325	1.75%	0.384%
17	11.611	876	877	881	rVB	45471	63503	1.30%	0.286%
18	12.205	926	929	931	rBV	325554	333839	6.85%	1.501%
19	12.422	945	948	950	rVV	327666	360709	7.40%	1.622%
20	12.491	950	954	958	rVB3	18887	51429	1.06%	0.231%
21	12.582	960	962	965	rVV	1010837	1100595	22.59%	4.949%
22	12.857	984	986	990	rVB3	37079	51878	1.06%	0.233%
23	13.417	1031	1035	1036	rBV2	27532	56642	1.16%	0.255%
24	13.508	1040	1043	1046	rVB2	212709	297497	6.11%	1.338%
25	13.611	1049	1052	1057	rBV	709067	1275583	26.18%	5.736%
26	14.137	1095	1098	1100	rBV3	67177	117536	2.41%	0.528%
27	14.400	1119	1121	1124	rBV2	122732	209565	4.30%	0.942%
28	14.594	1136	1138	1143	rBV	142043	326553	6.70%	1.468%
29	14.845	1158	1160	1162	rVB	95272	121620	2.50%	0.547%
30	14.891	1162	1164	1166	rBV	124469	155932	3.20%	0.701%
31	14.948	1166	1169	1171	rBV	505165	772596	15.86%	3.474%

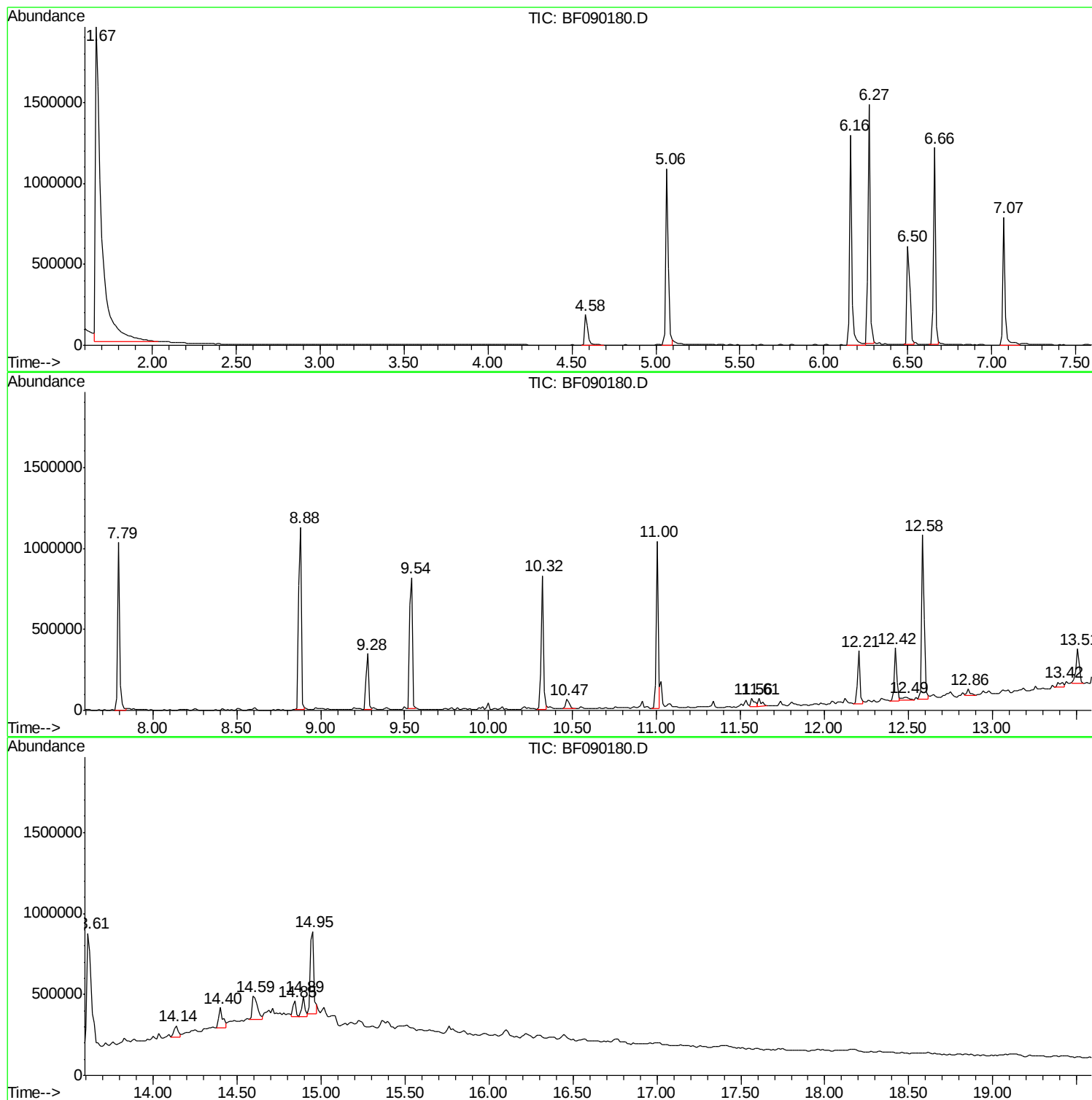
Sum of corrected areas: 22239930

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092116\
Data File : BF090180.D
Acq On : 22 Sep 2016 1:03
Operator : UM/SJ
Sample : H4856-06 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
BH-7-0.5-2FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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\BF092116\
Data File : BF090180.D
Acq On : 22 Sep 2016 1:03
Operator : UM/SJ
Sample : H4856-06 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BH-7-0.5-2FT

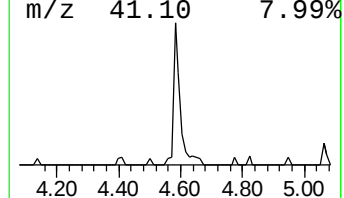
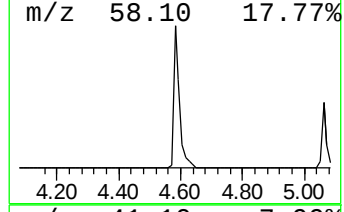
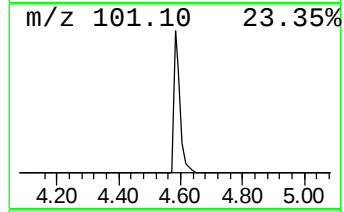
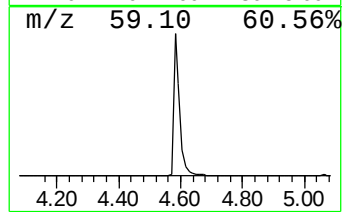
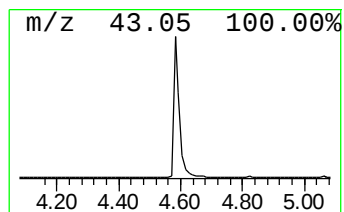
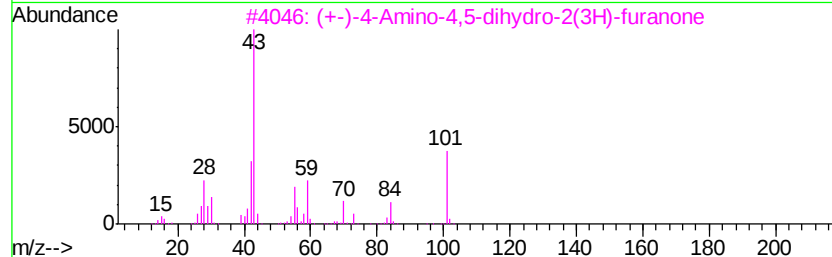
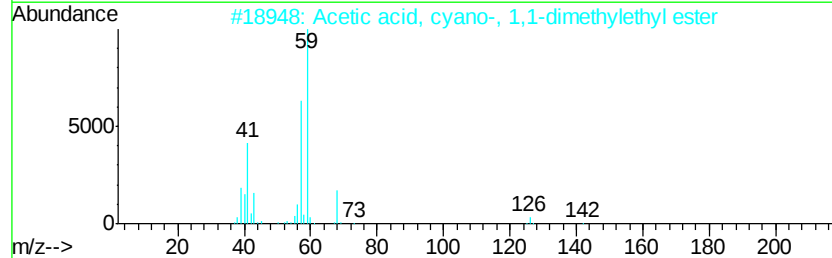
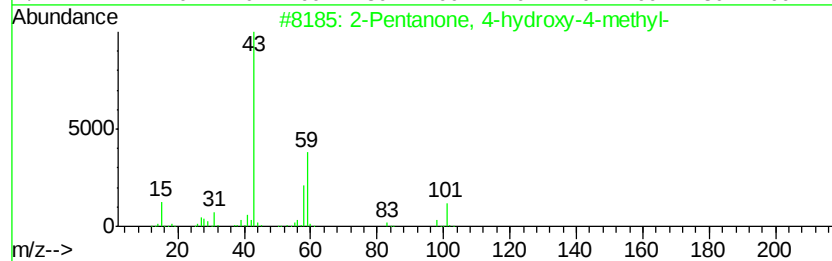
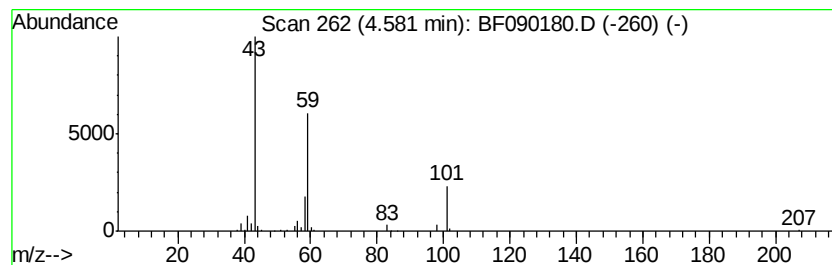
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	7.42 ng	248648	1,4-Dichlorobenzene-d4	6.50

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	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Guanidine	59	CH5N3	000113-00-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092116\
Data File : BF090180.D
Acq On : 22 Sep 2016 1:03
Operator : UM/SJ
Sample : H4856-06 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BH-7-0.5-2FT

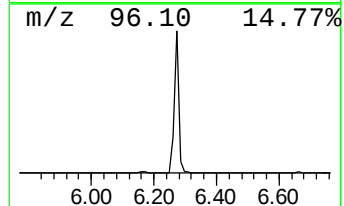
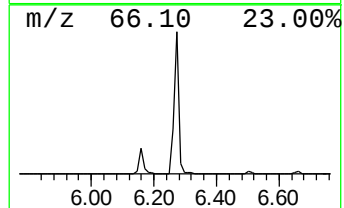
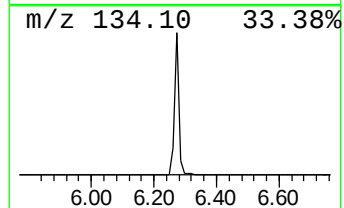
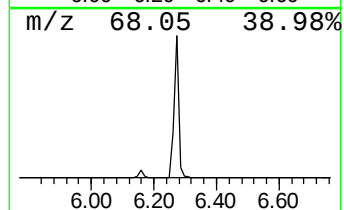
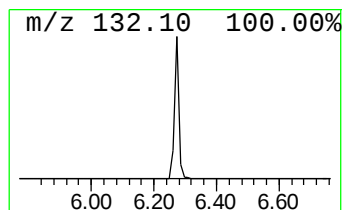
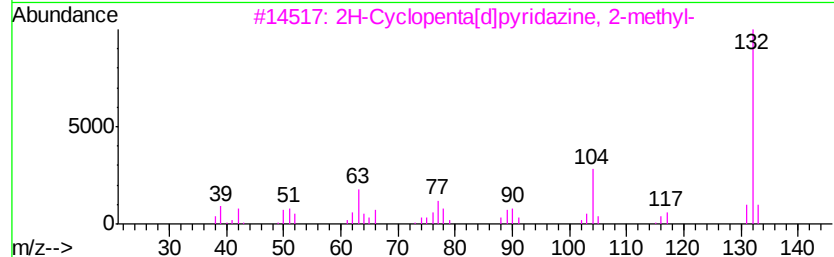
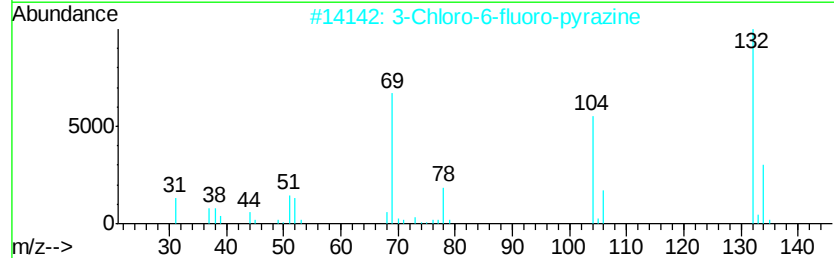
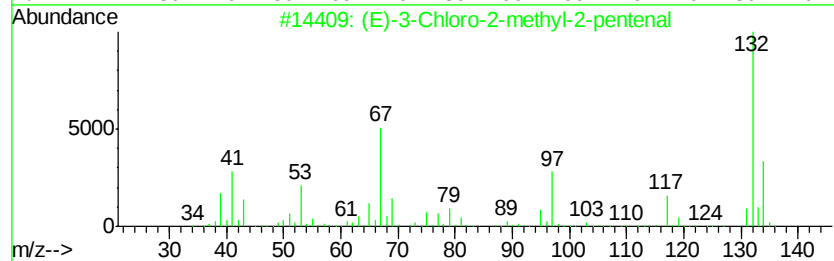
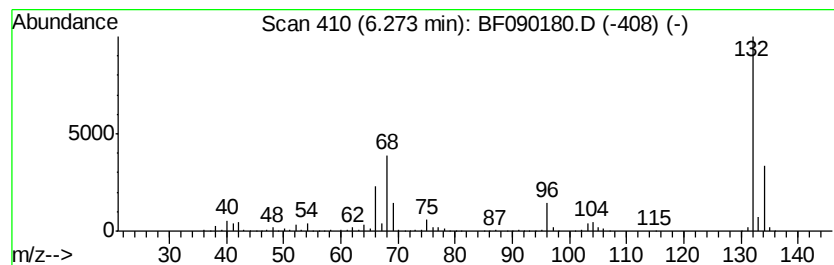
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	40.87 ng	1370290	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090180.D
Acq On : 22 Sep 2016 1:03
Operator : UM/SJ
Sample : H4856-06 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BH-7-0.5-2FT

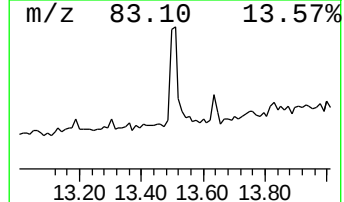
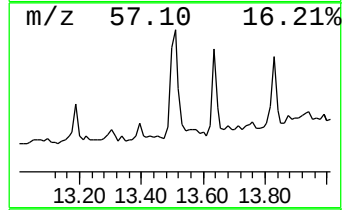
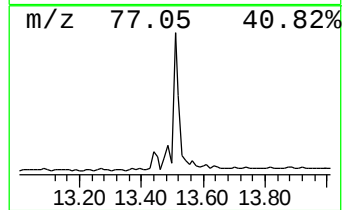
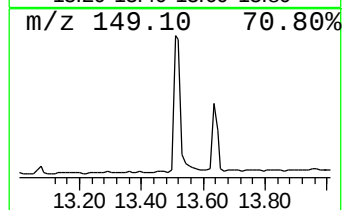
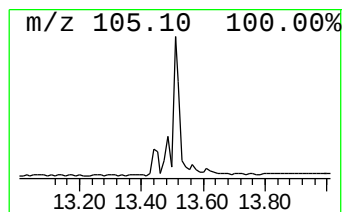
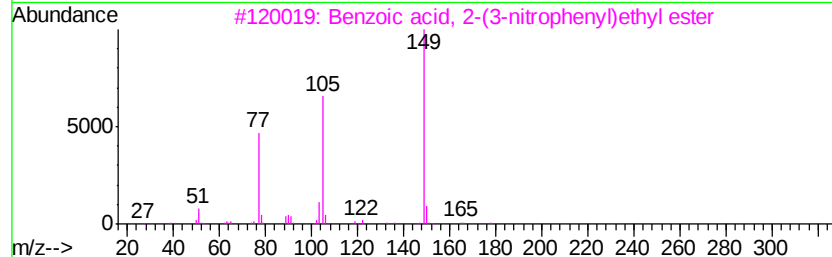
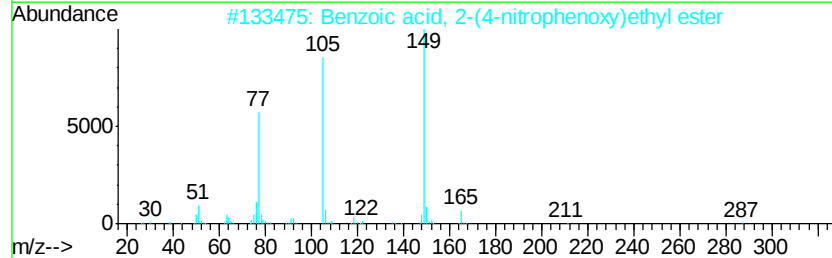
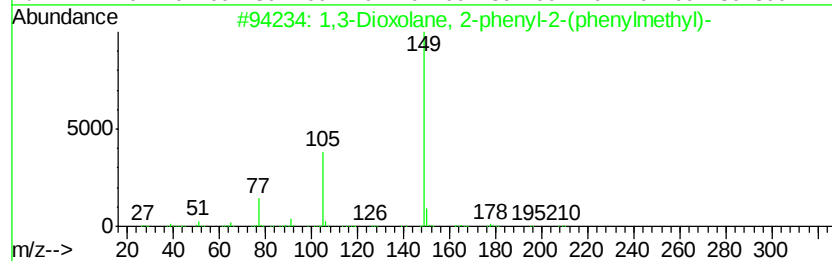
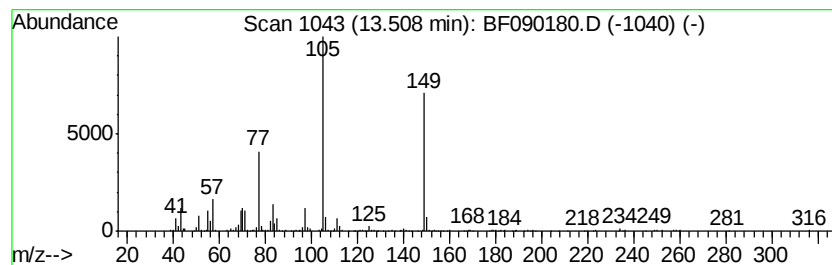
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,3-Dioxolane, 2-phenyl-2-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	4.66 ng	297497	Chrysene-d12	13.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-phenyl-2-(phenyl...	240	C16H16O2	004362-19-0	64
2		Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
3		Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	64
4		2,2'-(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	50
5		Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092116\
Data File : BF090180.D
Acq On : 22 Sep 2016 1:03
Operator : UM/SJ
Sample : H4856-06 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BH-7-0.5-2FT

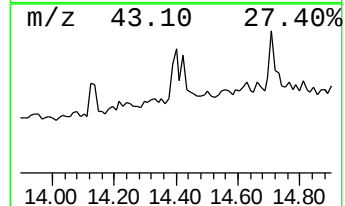
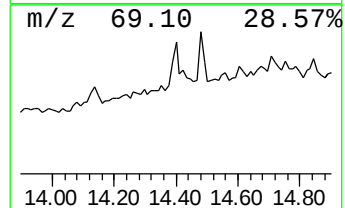
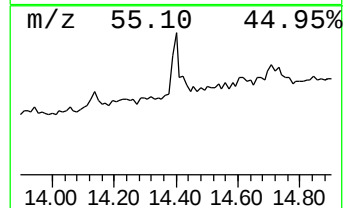
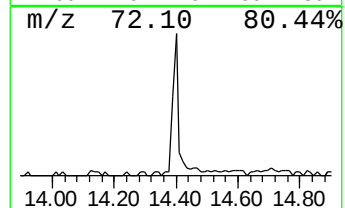
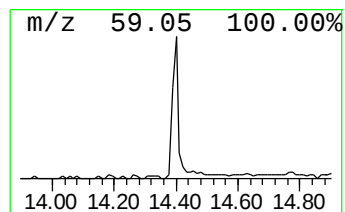
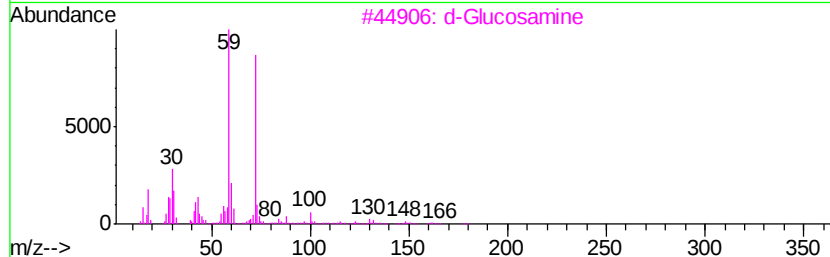
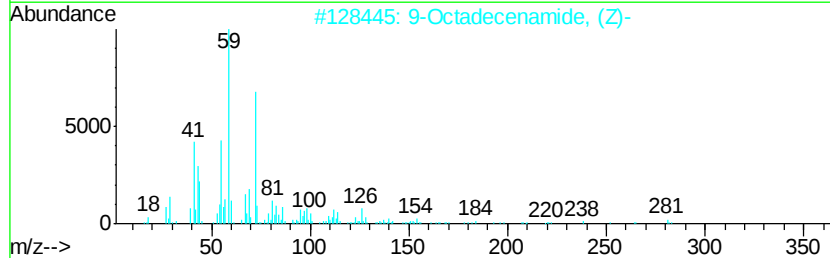
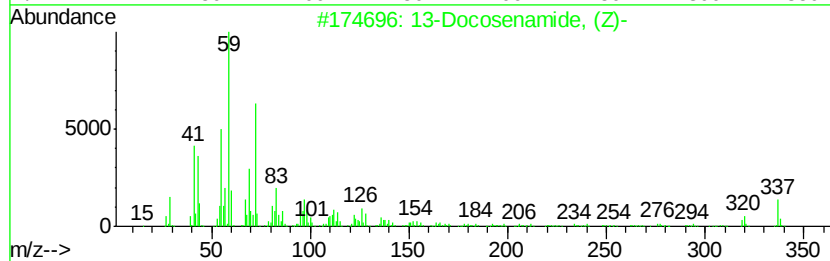
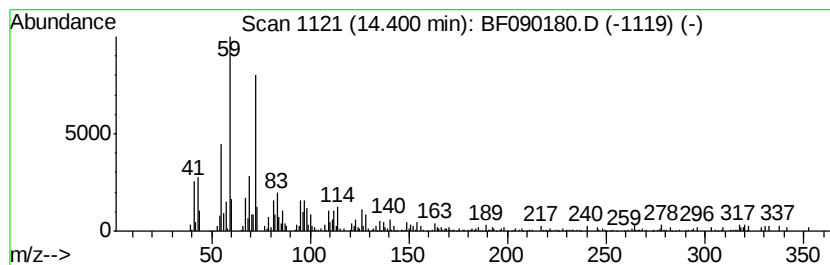
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	5.42 ng	209565	Perylene-d12	14.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	89
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3		d-Glucosamine	179	C6H13NO5	000090-77-7	50
4		Octadecanamide	283	C18H37NO	000124-26-5	43
5		trans-13-Docosenamide	337	C22H43NO	010436-09-6	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092116\
Data File : BF090180.D
Acq On : 22 Sep 2016 1:03
Operator : UM/SJ
Sample : H4856-06 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BH-7-0.5-2FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.58	7.4	ng	248648	1	6.50	670541	20.0
unknown6.27	6.27	40.9	ng	1370290	1	6.50	670541	20.0
1,3-Dioxolane, 2-...	13.51	4.7	ng	297497	5	13.62	1275580	20.0
13-Docosenamide, ...	14.40	5.4	ng	209565	6	14.95	772596	20.0