

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
 Data File : BF090029.D
 Acq On : 8 Sep 2016 17:26
 Operator : UM/SJ
 Sample : H4704-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2-7.0-8.0

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-BF083116.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	1.724	10	12	59	rVB	4481752	11982696	100.00%	19.157%
2	4.730	272	275	289	rBV	785252	1409362	11.76%	2.253%
3	5.176	311	314	317	rBV	3403659	5246246	43.78%	8.387%
4	6.250	405	408	415	rBV	3895888	5326884	44.45%	8.516%
5	6.364	415	418	421	rVV	4249909	5045266	42.10%	8.066%
6	6.593	436	438	441	rBV	783839	1101917	9.20%	1.762%
7	6.753	450	452	455	rBV	3734664	3883762	32.41%	6.209%
8	7.164	485	488	491	rBV	2176368	3393964	28.32%	5.426%
9	7.290	496	499	507	rVB	85806	187363	1.56%	0.300%
10	7.884	549	551	561	rBV	1581452	1564410	13.06%	2.501%
11	8.970	643	646	648	rBV	5577823	6334870	52.87%	10.128%
12	9.370	678	681	683	rBV	1699346	2118078	17.68%	3.386%
13	9.633	701	704	706	rBV	1706217	1768296	14.76%	2.827%
14	10.410	769	772	775	rBV2	2474155	3496253	29.18%	5.590%
15	10.559	783	785	789	rVB	94065	169107	1.41%	0.270%
16	11.096	830	832	835	rBV	1377423	1578018	13.17%	2.523%
17	11.656	879	881	888	rBV2	85526	125251	1.05%	0.200%
18	12.685	968	971	974	rBV	4326550	4905867	40.94%	7.843%
19	13.588	1048	1050	1056	rBV	231738	297733	2.48%	0.476%
20	13.714	1059	1061	1069	rVV	1298883	1404994	11.73%	2.246%
21	15.051	1176	1178	1183	rBV	908320	1208951	10.09%	1.933%

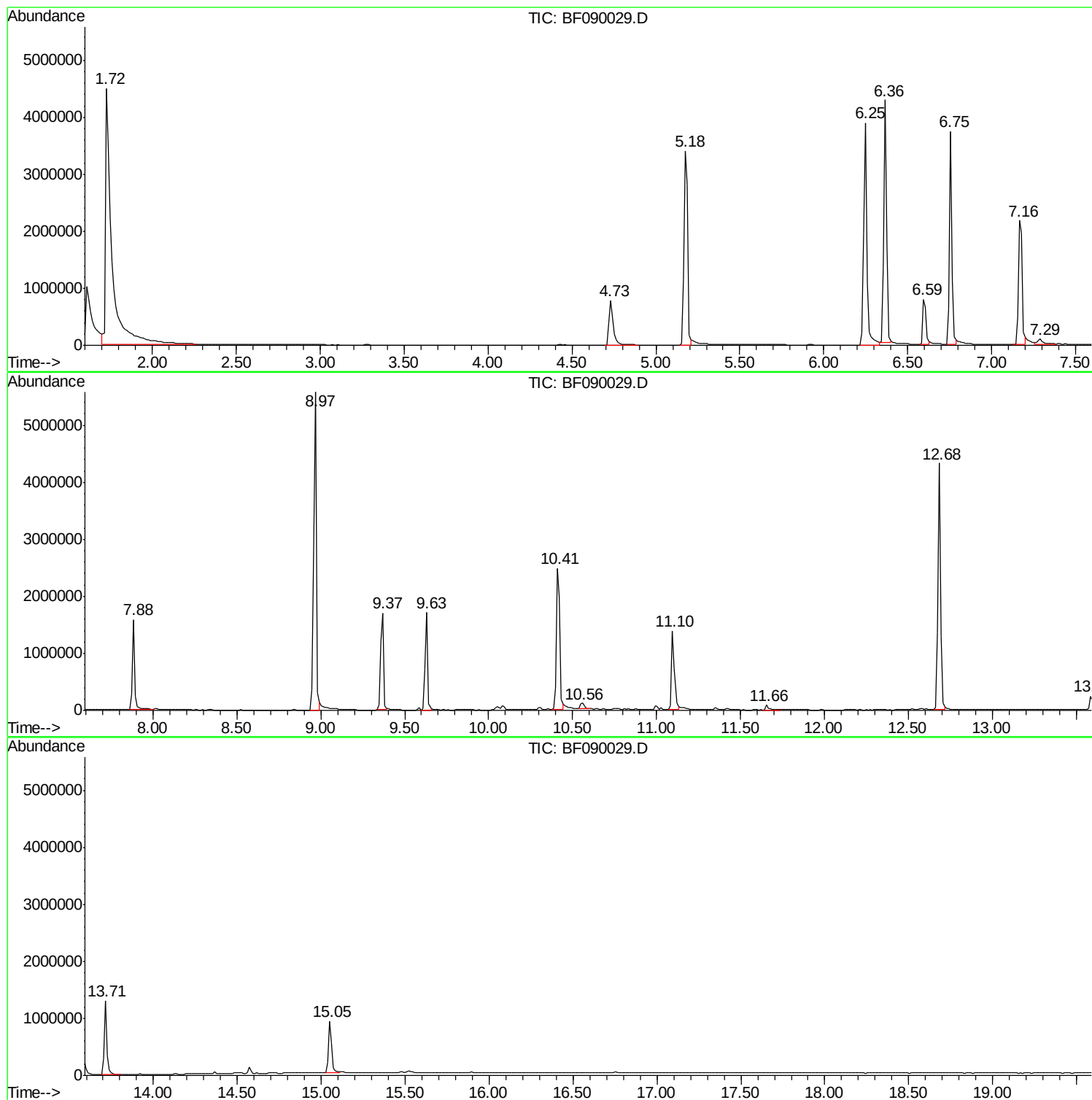
Sum of corrected areas: 62549288

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
Data File : BF090029.D
Acq On : 8 Sep 2016 17:26
Operator : UM/SJ
Sample : H4704-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-7.0-8.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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\BF090816\
Data File : BF090029.D
Acq On : 8 Sep 2016 17:26
Operator : UM/SJ
Sample : H4704-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-7.0-8.0

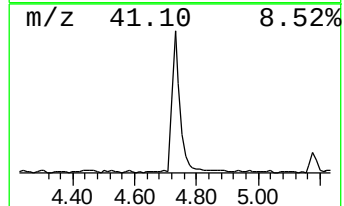
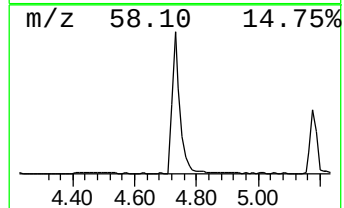
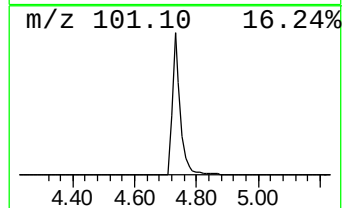
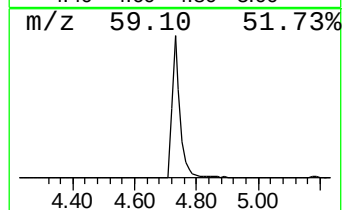
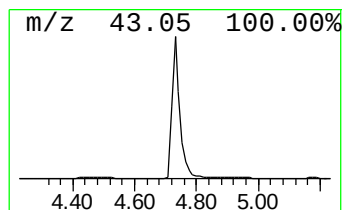
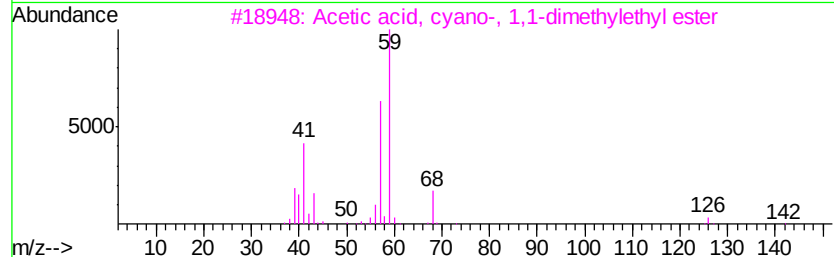
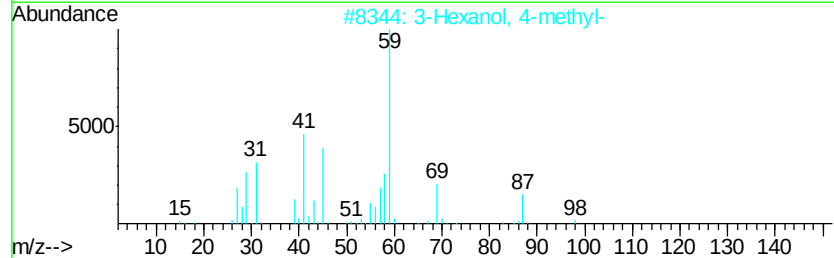
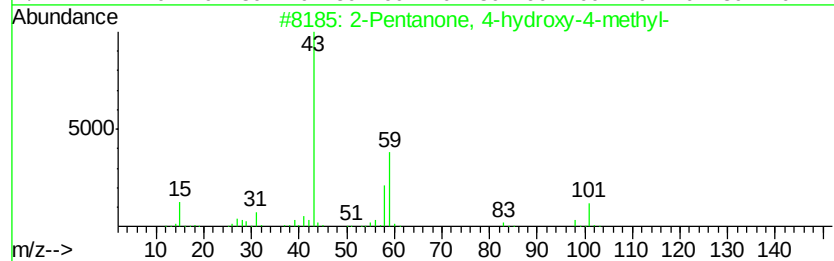
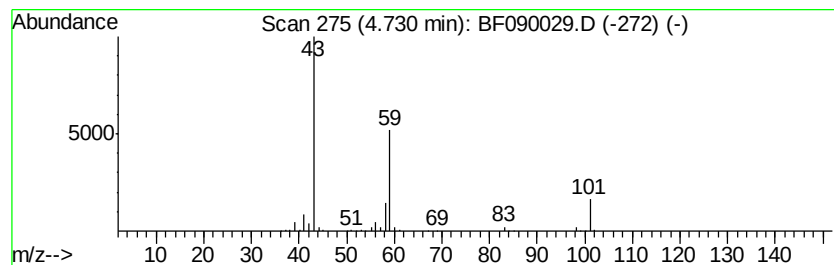
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.73	25.58 ng	1409360	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
Data File : BF090029.D
Acq On : 8 Sep 2016 17:26
Operator : UM/SJ
Sample : H4704-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-7.0-8.0

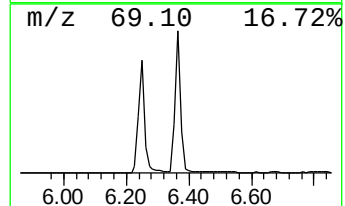
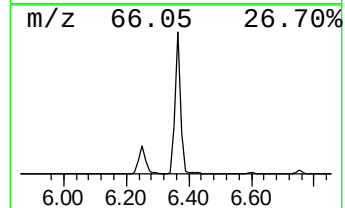
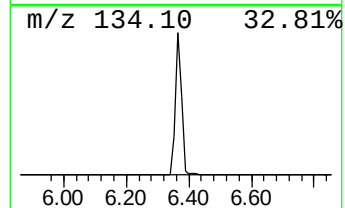
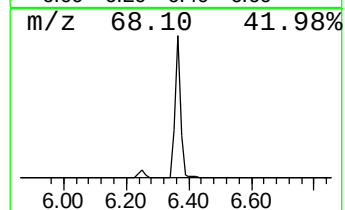
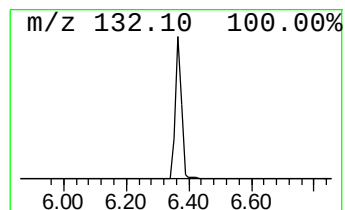
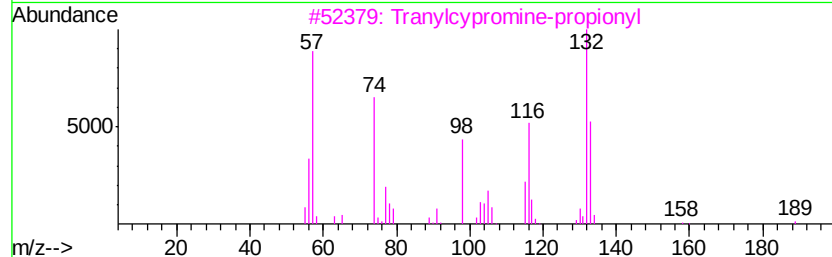
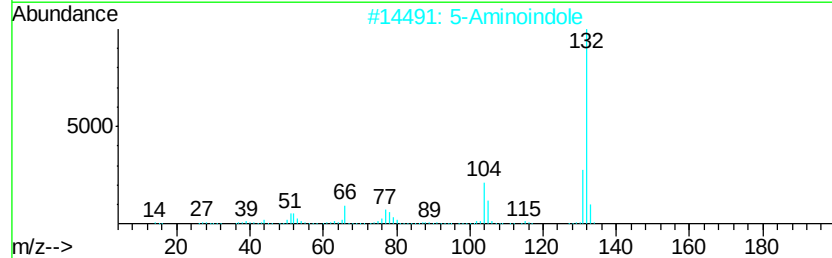
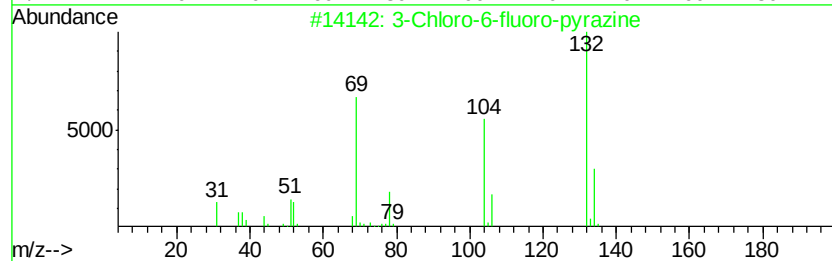
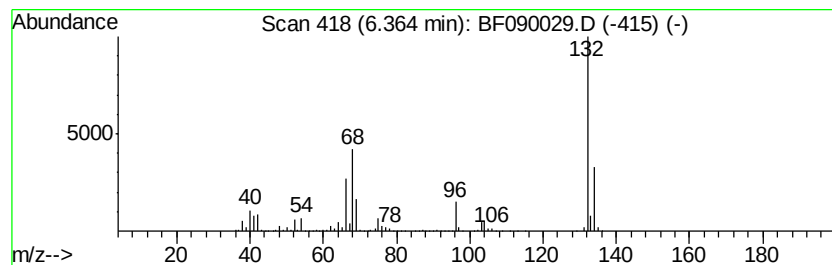
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	91.57 ng	5045270	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
Data File : BF090029.D
Acq On : 8 Sep 2016 17:26
Operator : UM/SJ
Sample : H4704-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

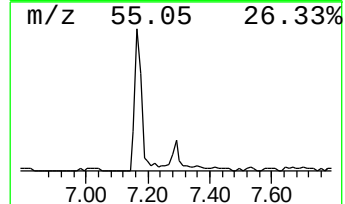
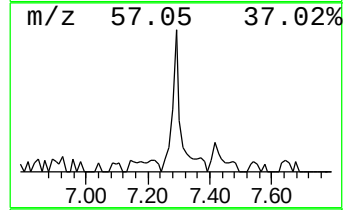
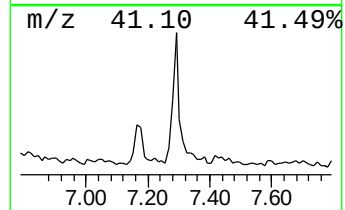
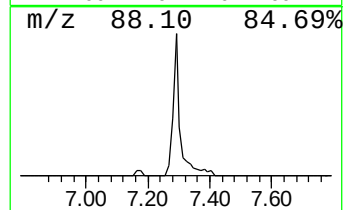
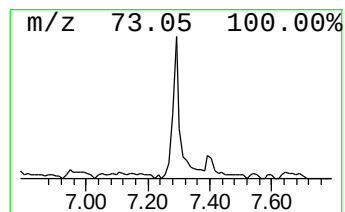
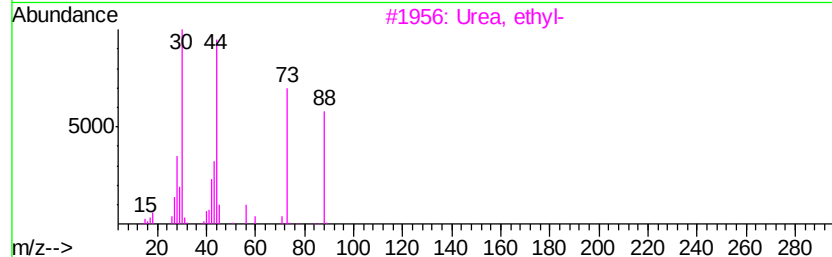
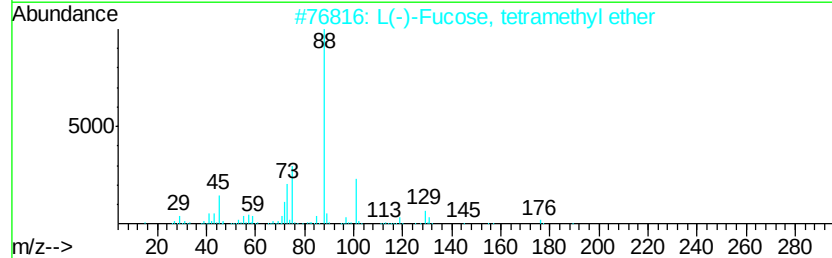
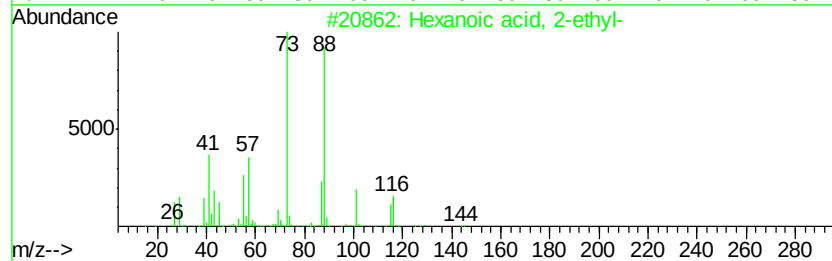
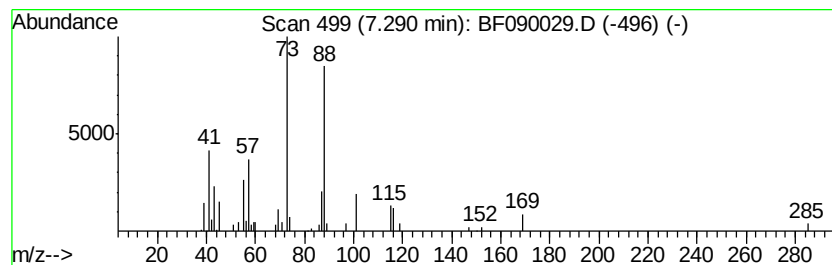
Instrument :
BNA_F
ClientSampleId :
SB-2-7.0-8.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	2.40 ng	187363	Naphthalene-d8	7.88
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Hexanoic acid, 2-ethyl-	144 C8H16O2	000149-57-5 86
2		L(-)-Fucose, tetramethyl ether	220 C10H20O5	1000332-75-0 50
3		Urea, ethyl-	88 C3H8N2O	000625-52-5 43
4		Undecanoic acid, 2-methyl-, meth...	214 C13H26O2	055955-69-6 42
5		Heptanoic acid, 2,6-dimethyl-, m...	172 C10H20O2	033315-72-9 38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
Data File : BF090029.D
Acq On : 8 Sep 2016 17:26
Operator : UM/SJ
Sample : H4704-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-7.0-8.0

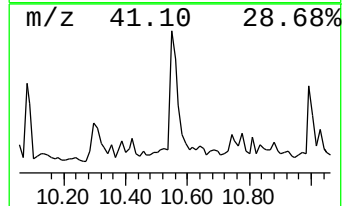
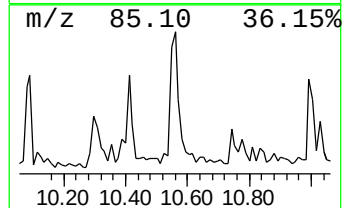
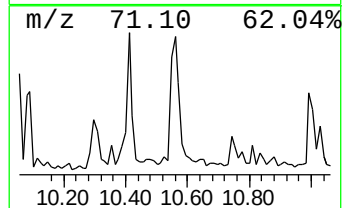
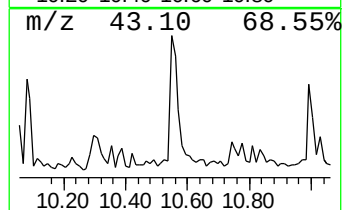
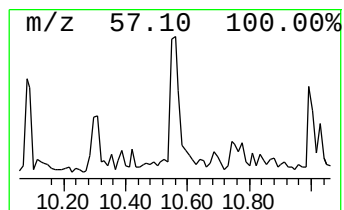
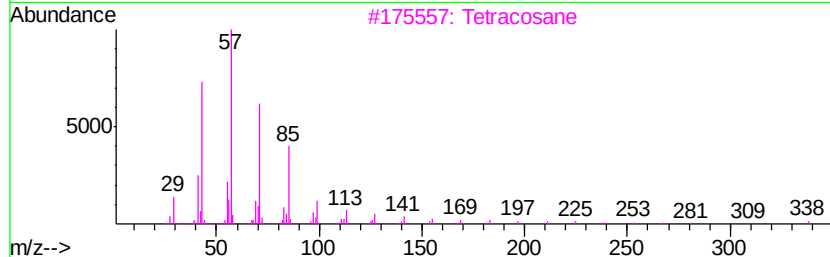
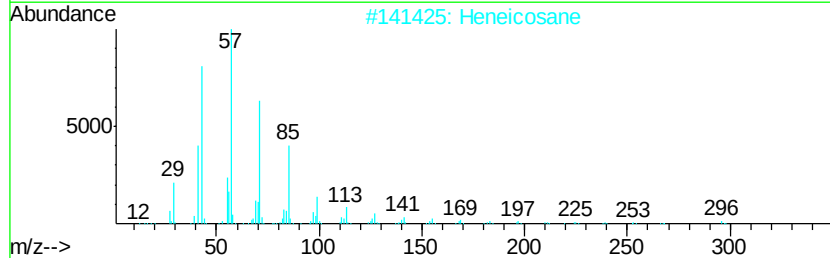
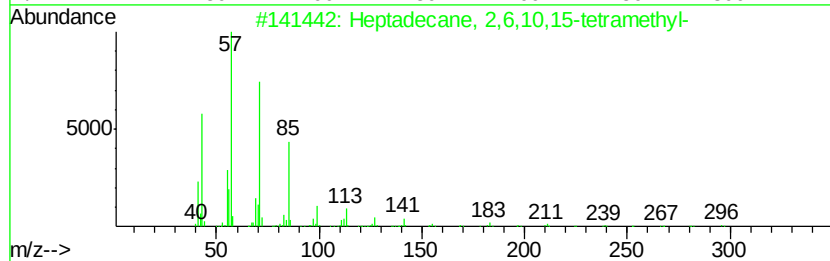
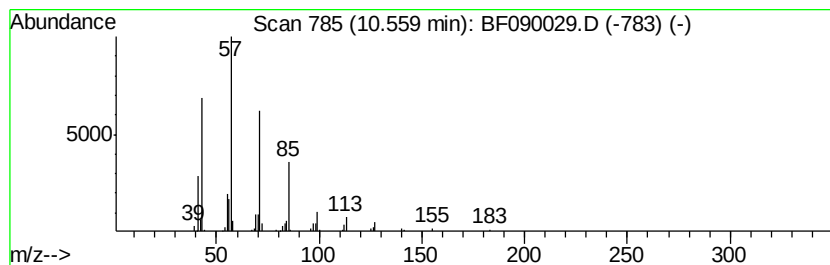
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.14 ng	169107	Phenanthrene-d10	11.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Heptadecane	240	C17H36	000629-78-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
Data File : BF090029.D
Acq On : 8 Sep 2016 17:26
Operator : UM/SJ
Sample : H4704-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

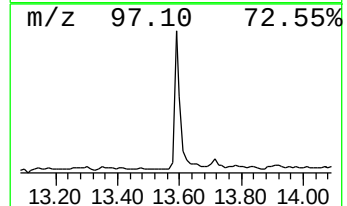
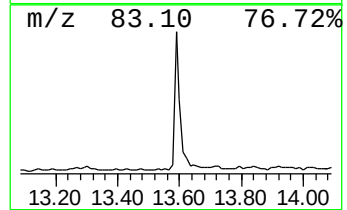
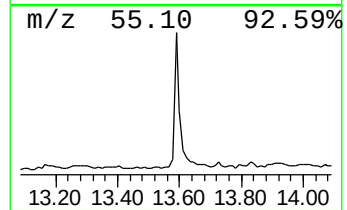
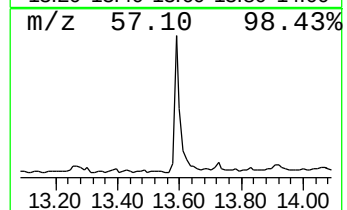
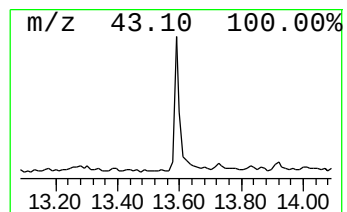
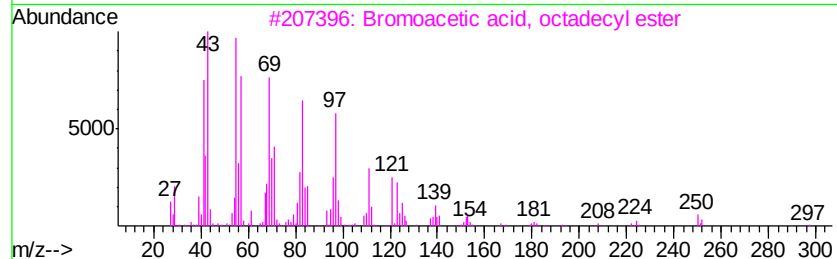
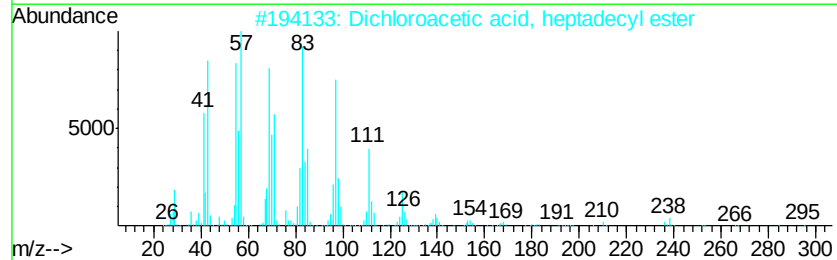
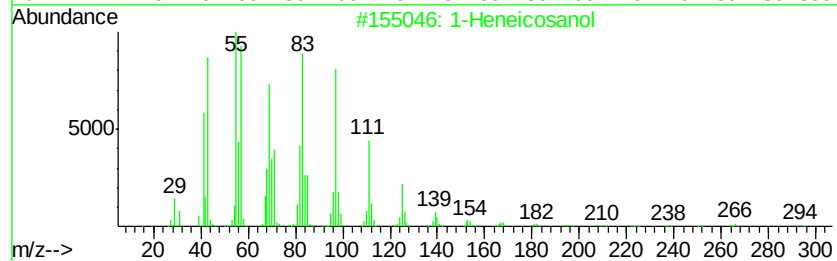
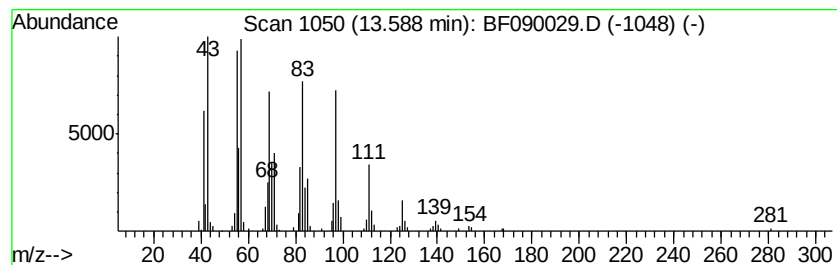
Instrument :
BNA_F
ClientSampleId :
SB-2-7.0-8.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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.	
13.59	4.24 ng	297733	Chrysene-d12	13.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
Data File : BF090029.D
Acq On : 8 Sep 2016 17:26
Operator : UM/SJ
Sample : H4704-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-7.0-8.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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...	4.73	25.6	ng	1409360	1	6.60	1101920	20.0
unknown6.36	6.36	91.6	ng	5045270	1	6.60	1101920	20.0
Hexanoic acid, 2-...	7.29	2.4	ng	187363	2	7.88	1564410	20.0
Heptadecane, 2,6,...	10.56	2.1	ng	169107	4	11.10	1578020	20.0
1-Heneicosanol	13.59	4.2	ng	297733	5	13.71	1404990	20.0