

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
 Data File : BF096408.D
 Acq On : 2 Jul 2017 11:34
 Operator : SJ/MA
 Sample : I3950-19
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B6-12-14

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-BF070117.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	4.940	480	485	496	rVB	607313	926408	19.91%	2.306%
2	5.357	550	556	559	rBV	4103918	4652061	100.00%	11.578%
3	6.375	723	729	732	rBV	3558313	4463625	95.95%	11.109%
4	6.504	746	751	755	rBV	3841355	4514905	97.05%	11.237%
5	6.734	786	790	793	rBV	1110571	897492	19.29%	2.234%
6	6.892	812	817	820	rBV	3286024	3079199	66.19%	7.664%
7	7.292	879	885	888	rBV	2506542	2960701	63.64%	7.369%
8	7.381	897	900	910	rVB2	31635	47818	1.03%	0.119%
9	8.016	1003	1008	1011	rBV	1406701	1268246	27.26%	3.157%
10	9.092	1185	1191	1194	rBV	4090411	4417672	94.96%	10.995%
11	9.480	1252	1257	1261	rBV	773328	729776	15.69%	1.816%
12	9.710	1293	1296	1300	rVB	59239	51749	1.11%	0.129%
13	9.769	1300	1306	1309	rBV	1370113	1389065	29.86%	3.457%
14	10.210	1378	1381	1384	rVB	102515	84958	1.83%	0.211%
15	10.557	1434	1440	1443	rBV	2376749	2655112	57.07%	6.608%
16	10.680	1458	1461	1472	rBV	114911	126382	2.72%	0.315%
17	11.127	1534	1537	1541	rBV2	56978	58740	1.26%	0.146%
18	11.245	1550	1557	1559	rBV	1372101	1185375	25.48%	2.950%
19	11.269	1559	1561	1564	rVV	169863	133490	2.87%	0.332%
20	11.316	1564	1569	1573	rVB	69039	60387	1.30%	0.150%
21	11.780	1644	1648	1652	rBV2	120445	124049	2.67%	0.309%
22	12.451	1759	1762	1766	rBV	180891	146084	3.14%	0.364%
23	12.568	1778	1782	1786	rBV	45757	47960	1.03%	0.119%
24	12.657	1793	1797	1798	rBV2	46520	56592	1.22%	0.141%
25	12.674	1798	1800	1803	rVB	143542	130893	2.81%	0.326%
26	12.833	1822	1827	1830	rBV2	3264467	3495580	75.14%	8.700%
27	13.310	1898	1908	1914	rBV	142936	174781	3.76%	0.435%
28	13.727	1976	1979	1987	rVB	263936	267239	5.74%	0.665%
29	13.874	1998	2004	2007	rBV	1147294	1135796	24.41%	2.827%
30	15.221	2230	2233	2237	rVB	34325	47551	1.02%	0.118%
31	15.280	2238	2243	2250	rBV	591242	770860	16.57%	1.919%
32	15.798	2326	2331	2339	rBV	33815	78054	1.68%	0.194%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-12-14

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

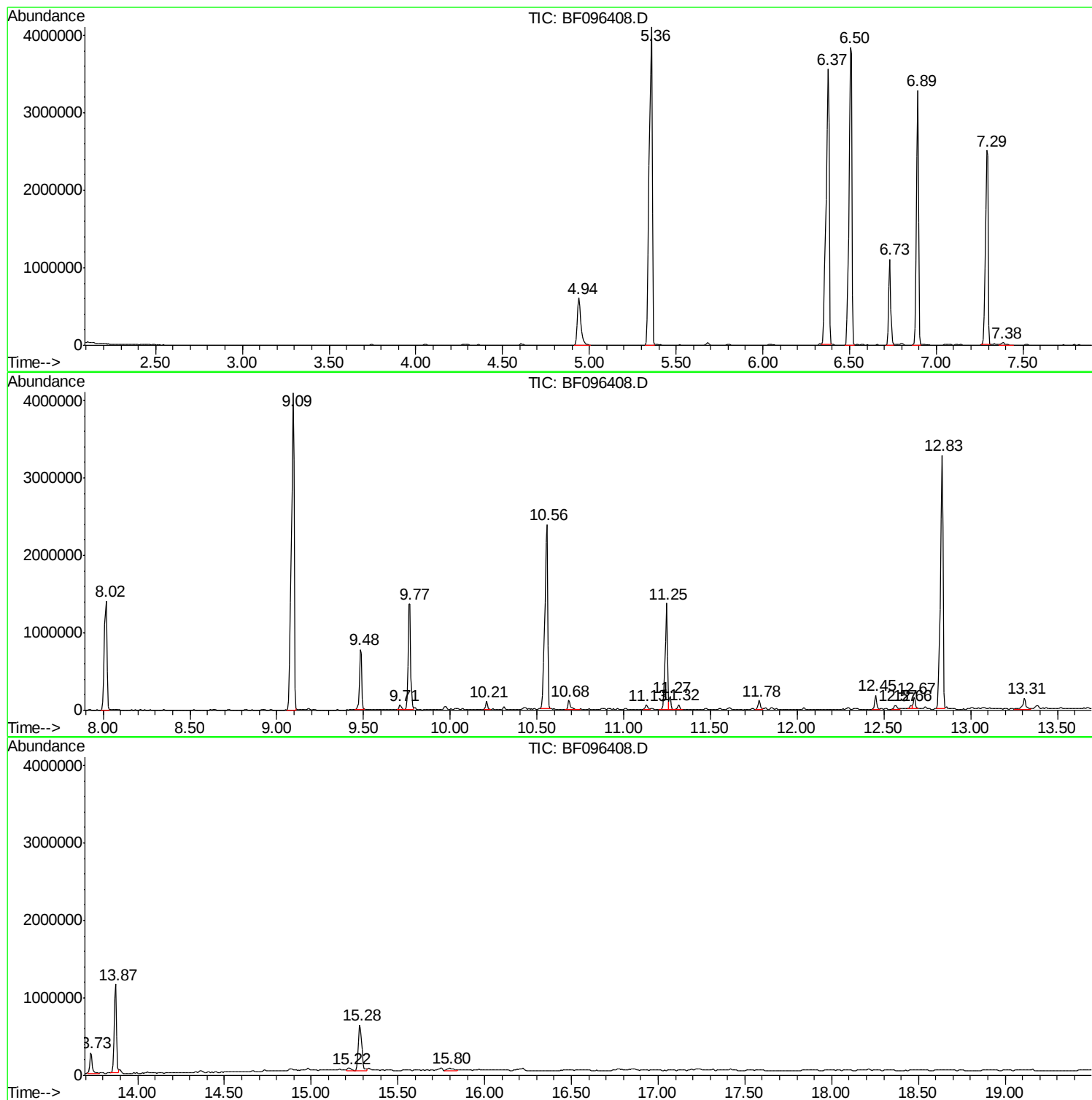
Sum of corrected areas: 40178600

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
B6-12-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-12-14

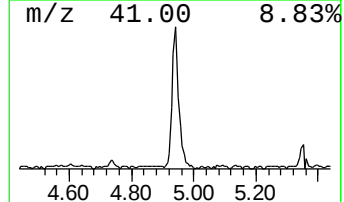
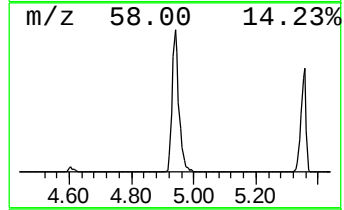
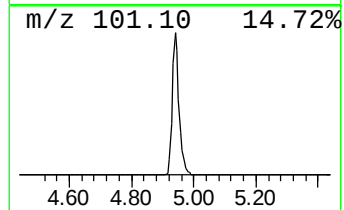
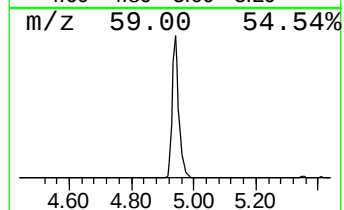
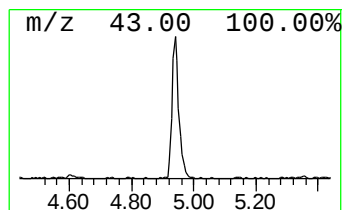
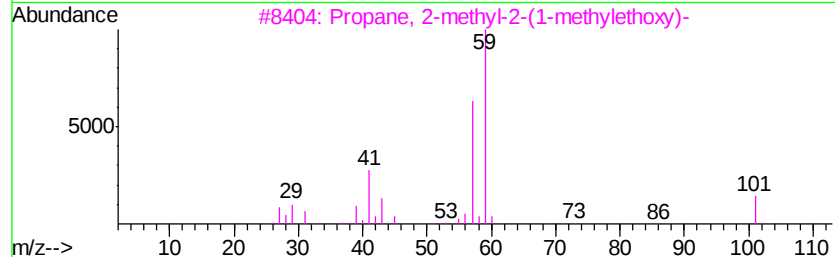
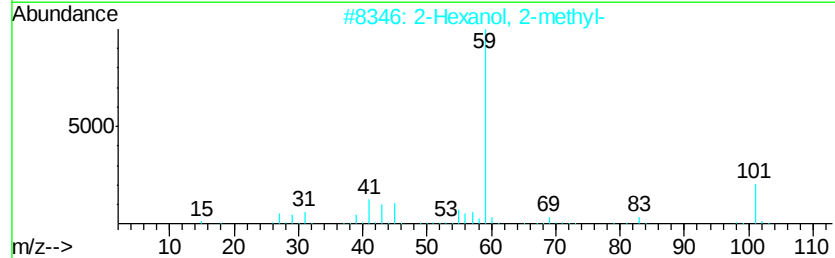
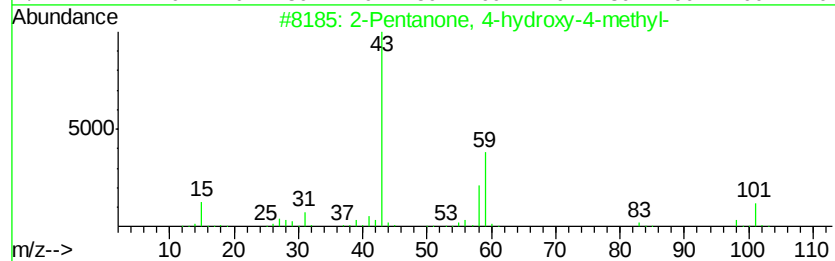
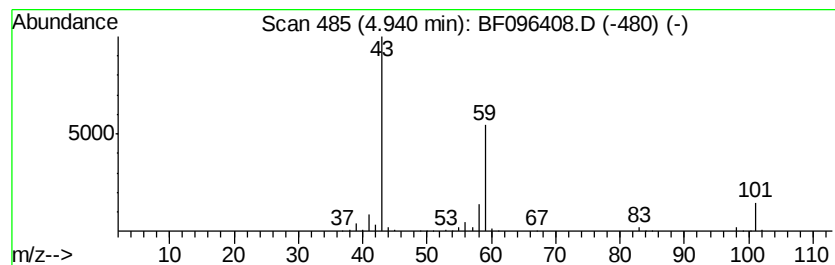
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.94	20.64 ng	926408	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			1,2-Butanediol	90	C4H10O2	000584-03-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-12-14

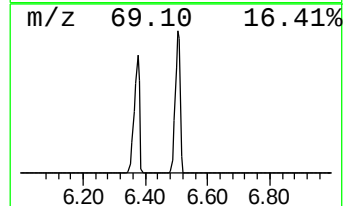
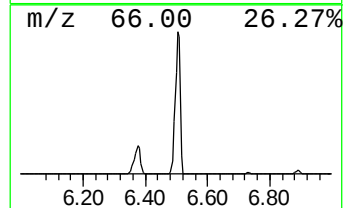
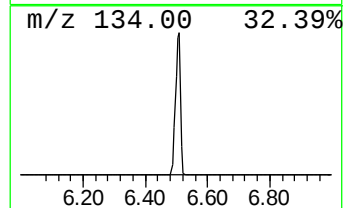
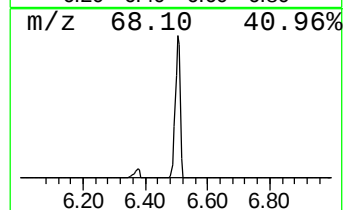
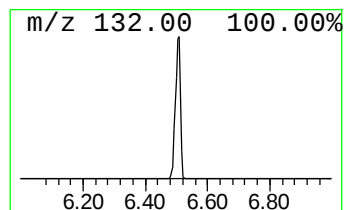
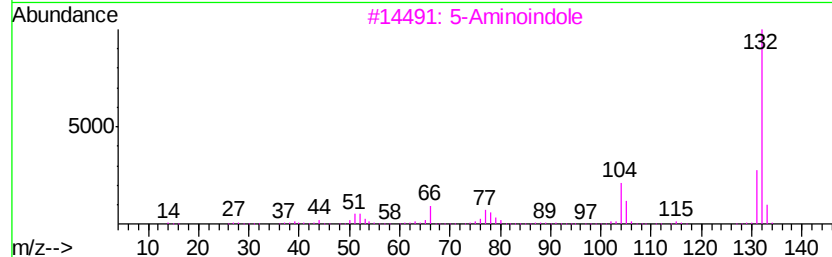
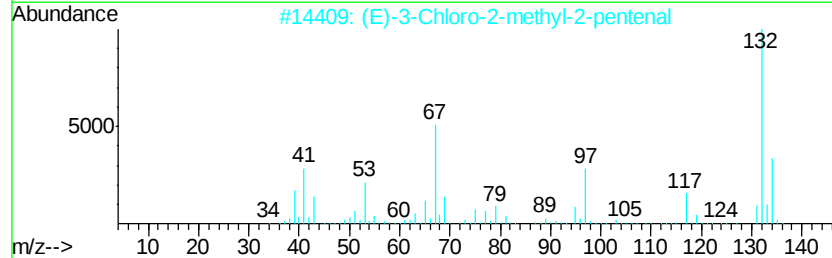
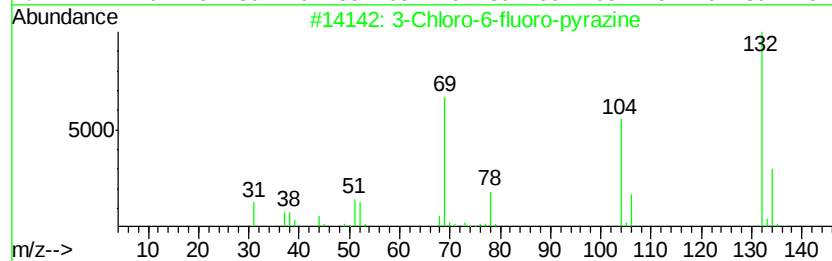
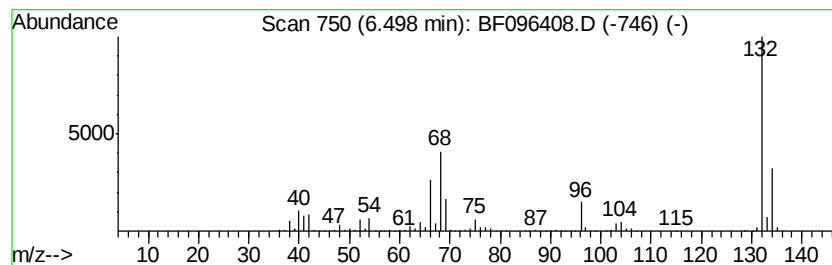
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	100.61 ng	4514910	1,4-Dichlorobenzene-d4	6.73

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

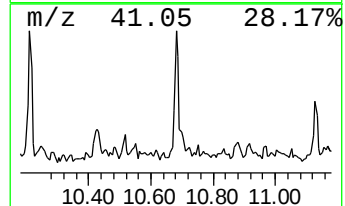
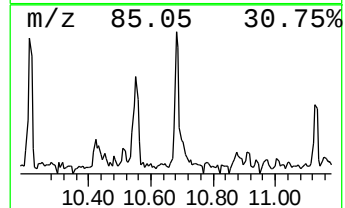
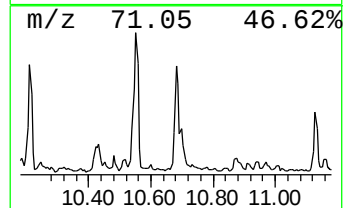
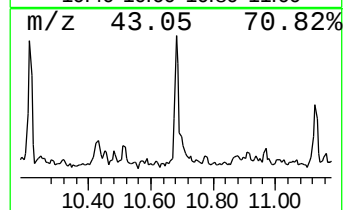
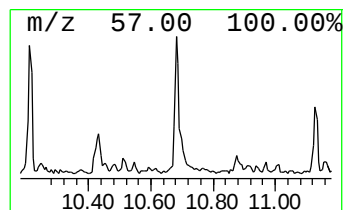
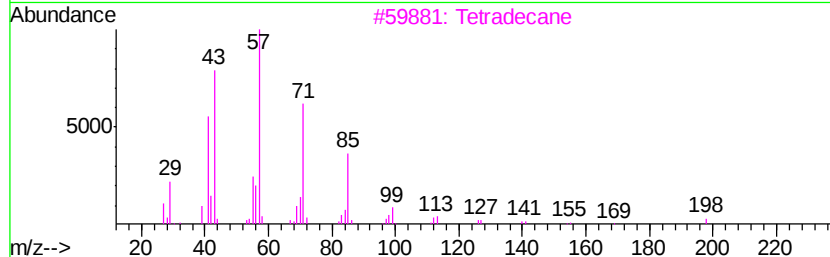
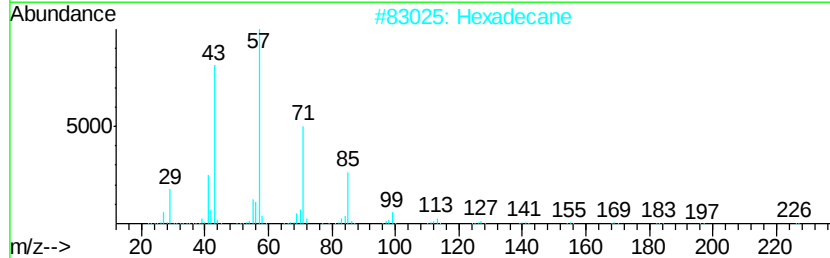
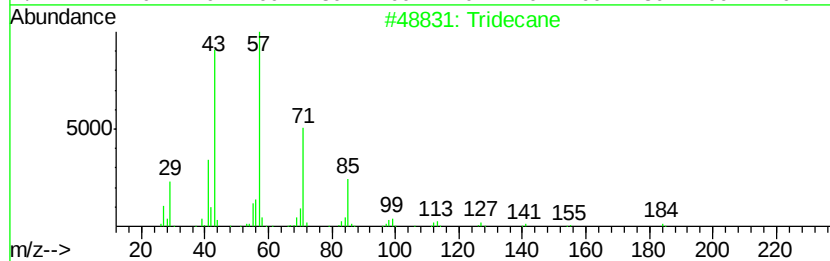
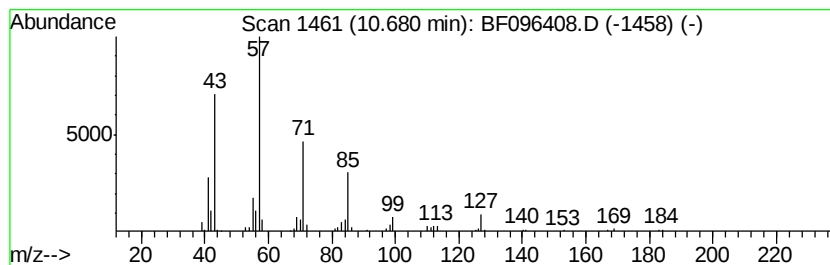
Instrument :
BNA_F
ClientSampleId :
B6-12-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.68	2.13 ng	126382	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Hexadecane	226	C16H34	000544-76-3	80
3	Tetradecane	198	C14H30	000629-59-4	78
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	64
5	Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

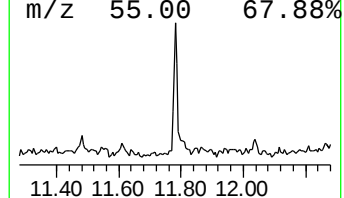
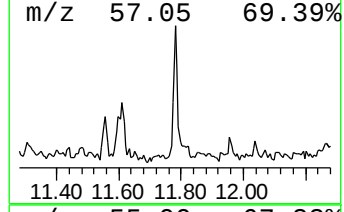
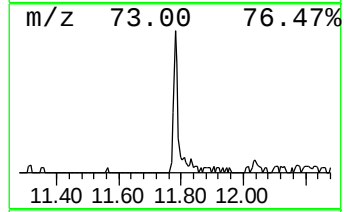
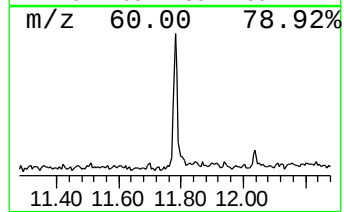
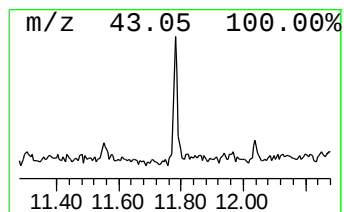
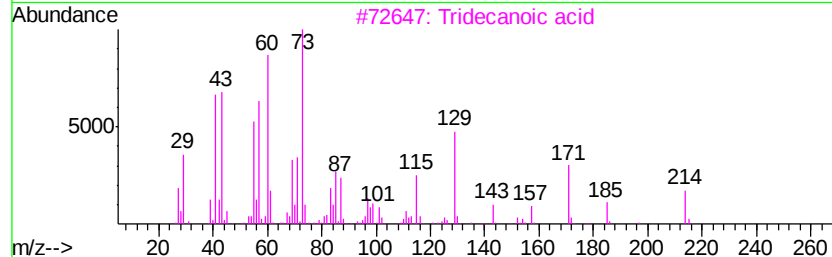
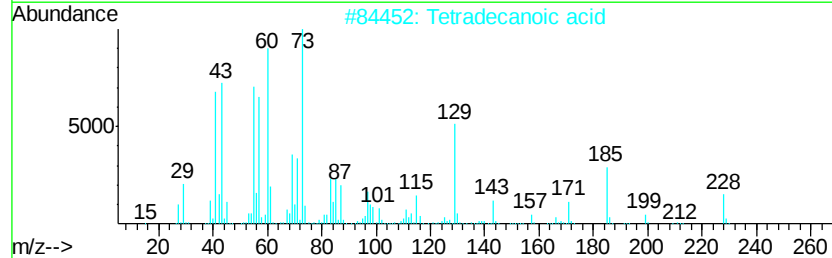
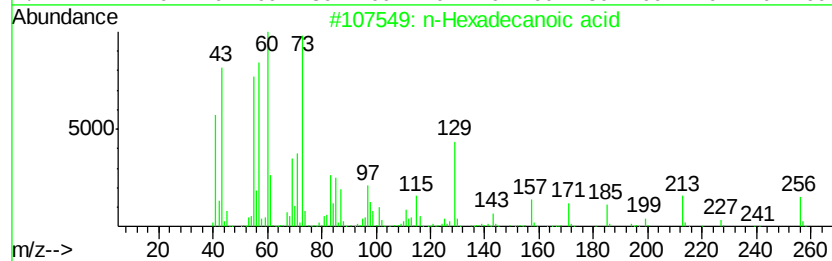
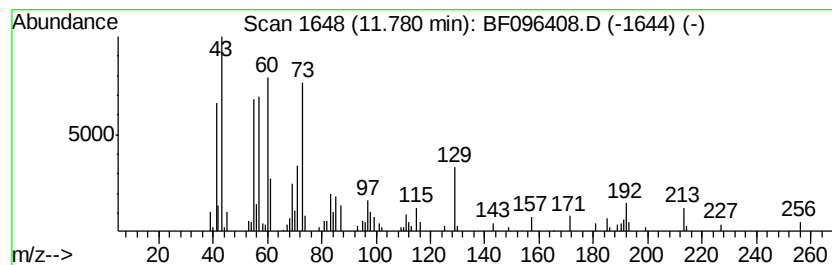
Instrument :
BNA_F
ClientSampleId :
B6-12-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.78	2.09 ng	124049	Phenanthrene-d10	11.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Tridecanoic acid	214	C13H26O2	000638-53-9	70
4		Undecanoic acid	186	C11H22O2	000112-37-8	59
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-12-14

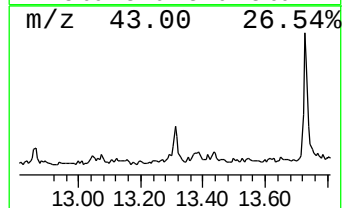
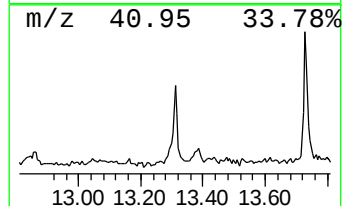
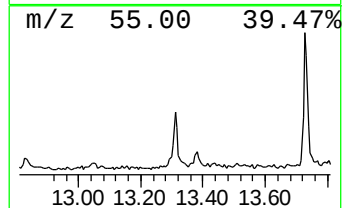
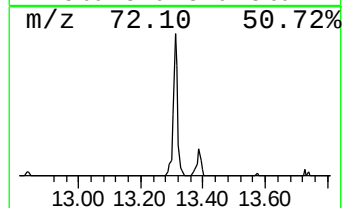
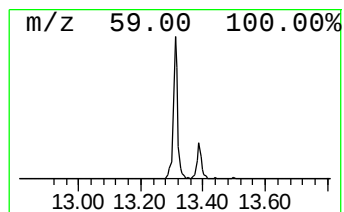
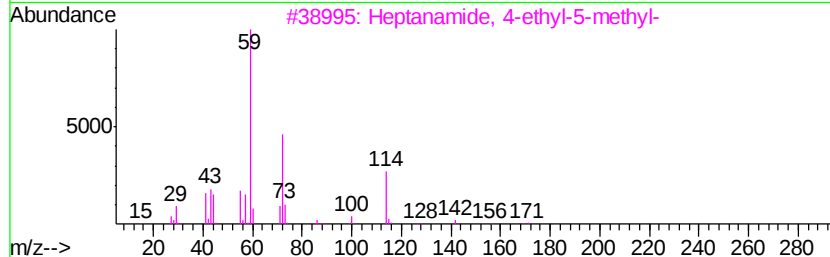
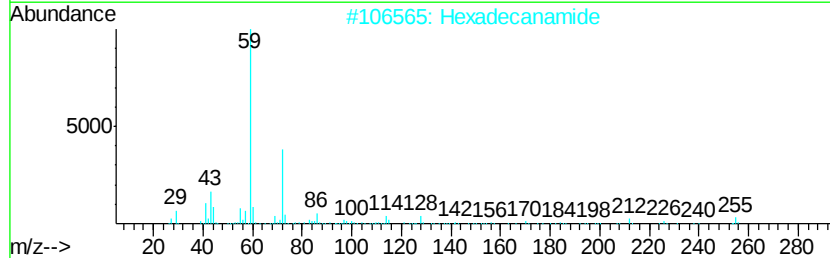
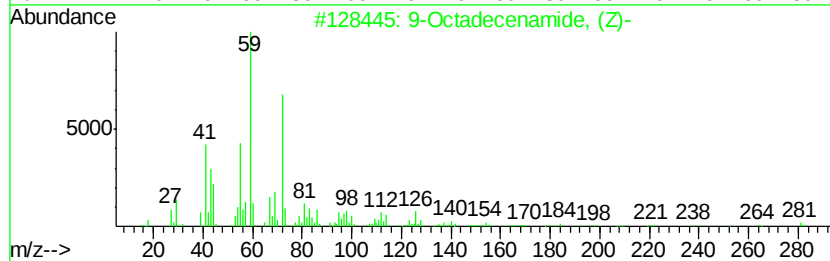
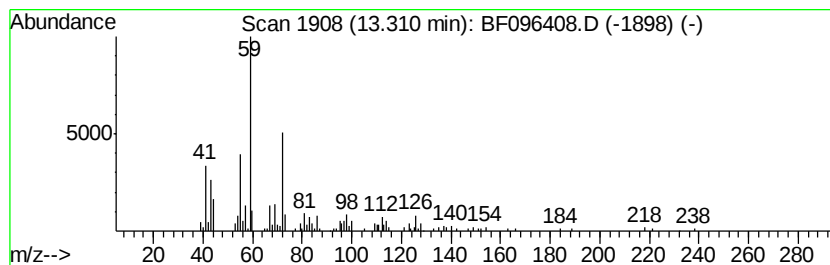
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.31	3.08 ng	174781	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Hexadecanamide	255	C16H33NO	000629-54-9	72
3		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
5		Nonanamide	157	C9H19NO	001120-07-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-12-14

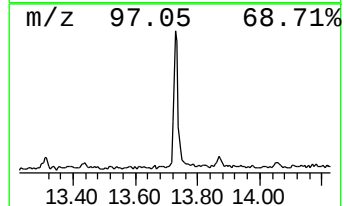
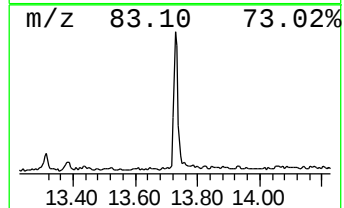
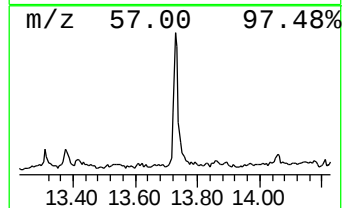
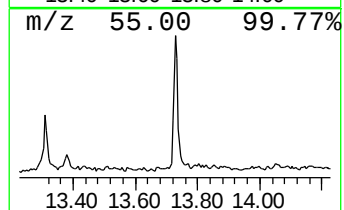
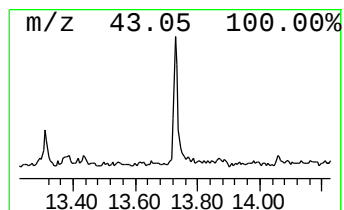
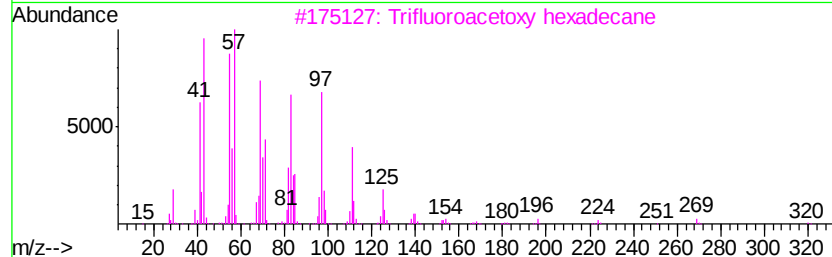
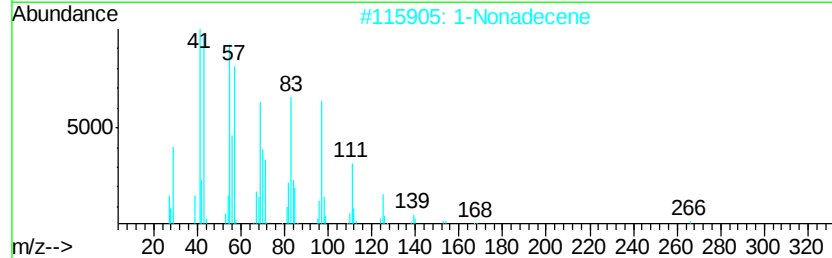
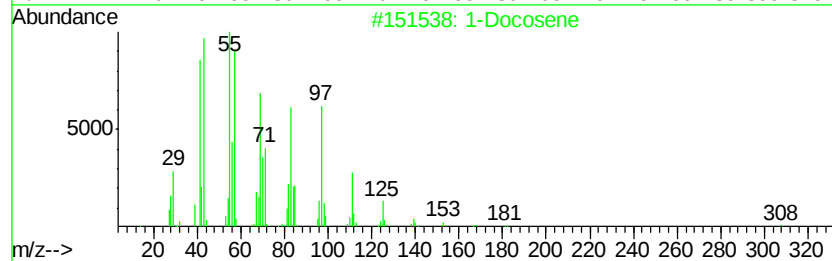
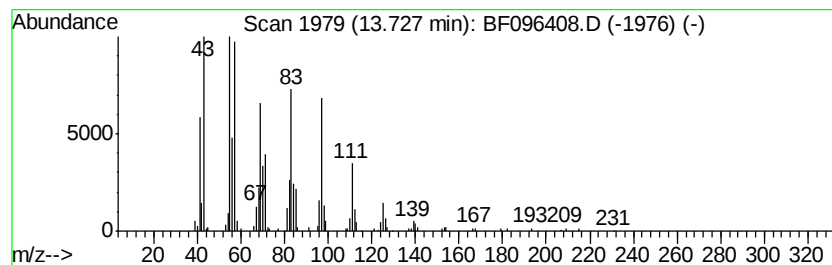
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.71 ng	267239	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
B6-12-14

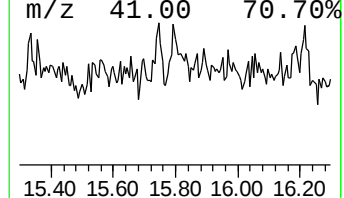
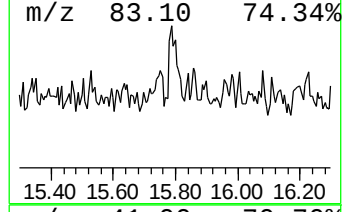
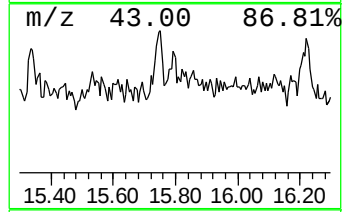
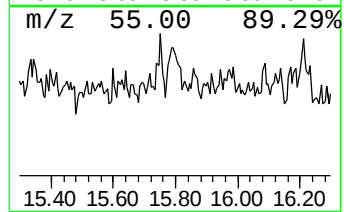
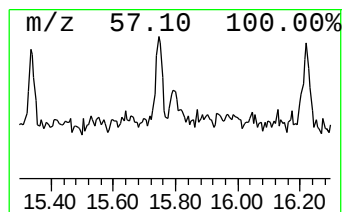
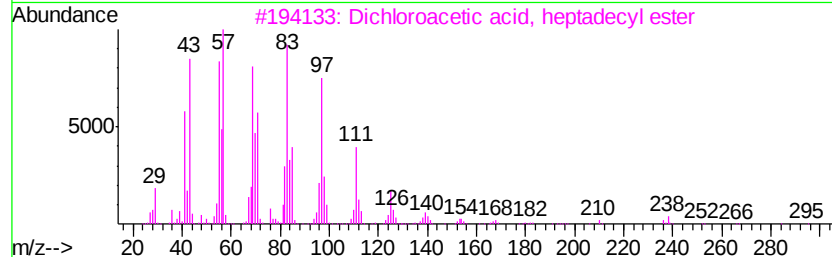
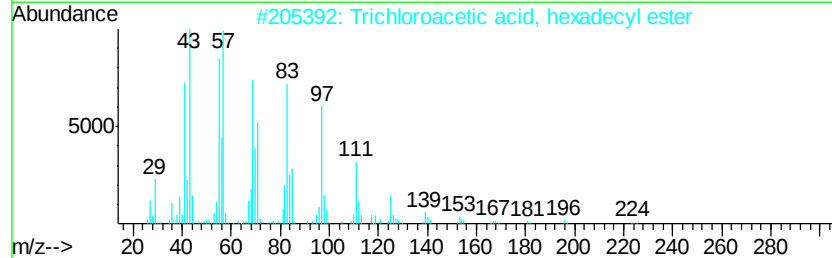
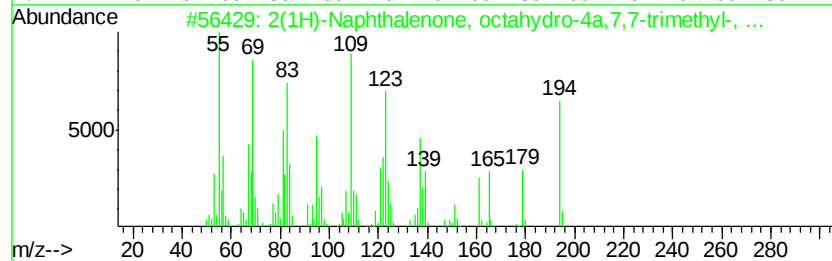
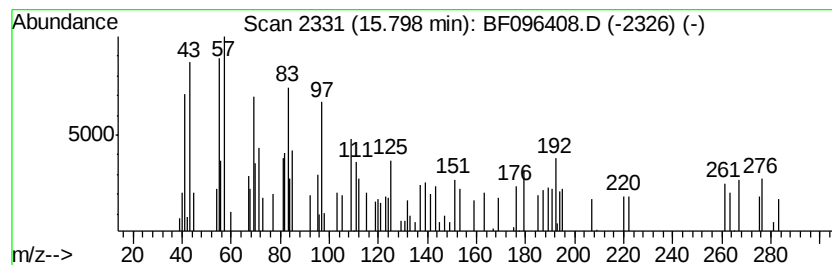
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.80 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	2.03 ng	78054	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	054699-31-9	41
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	38
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	38
4		Behenic alcohol	326	C22H46O	000661-19-8	30
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096408.D
Acq On : 2 Jul 2017 11:34
Operator : SJ/MA
Sample : I3950-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-12-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.94	20.6	ng	926408	1	6.73	897492	20.0
unknown6.50	6.50	100.6	ng	4514910	1	6.73	897492	20.0
Tridecane	10.68	2.1	ng	126382	4	11.24	1185380	20.0
n-Hexadecanoic acid	11.78	2.1	ng	124049	4	11.24	1185380	20.0
9-Octadecenamide,...	13.31	3.1	ng	174781	5	13.87	1135800	20.0
1-Docosene	13.73	4.7	ng	267239	5	13.87	1135800	20.0
unknown15.80	15.80	2.0	ng	78054	6	15.28	770860	20.0