

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
 Data File : BF096513.D
 Acq On : 6 Jul 2017 5:38
 Operator : SJ/MA
 Sample : I3975-05
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B7-8-10

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	3.687	267	272	279	rVB2	20775	32397	1.21%	0.134%
2	4.904	474	479	488	rBV	311333	417765	15.57%	1.733%
3	5.328	546	551	554	rBV	2695094	2683612	100.00%	11.131%
4	6.351	720	725	735	rVB	2434117	2669357	99.47%	11.072%
5	6.487	743	748	751	rBV	2557670	2558162	95.33%	10.611%
6	6.710	783	786	790	rBV	820194	721357	26.88%	2.992%
7	6.869	809	813	817	rBV	2164432	1976899	73.67%	8.200%
8	7.275	876	882	885	rBV	1693165	1525563	56.85%	6.328%
9	7.363	894	897	903	rBV3	20609	29240	1.09%	0.121%
10	7.716	952	957	963	rBV	45640	57494	2.14%	0.238%
11	7.992	1000	1004	1007	rBV	1134773	944500	35.20%	3.918%
12	9.075	1183	1188	1191	rBV	2734320	2377517	88.59%	9.861%
13	9.169	1199	1204	1207	rVB3	37862	33638	1.25%	0.140%
14	9.469	1251	1255	1258	rBV	730905	638509	23.79%	2.648%
15	9.692	1291	1293	1298	rVB	57377	50135	1.87%	0.208%
16	9.745	1298	1302	1306	rBV	824478	776075	28.92%	3.219%
17	10.192	1375	1378	1381	rVB	68428	52287	1.95%	0.217%
18	10.533	1432	1436	1447	rVB	1186309	1047399	39.03%	4.344%
19	10.663	1455	1458	1468	rBV	69608	90127	3.36%	0.374%
20	11.116	1532	1535	1537	rVB2	41658	35853	1.34%	0.149%
21	11.227	1550	1554	1556	rBV	812869	661719	24.66%	2.745%
22	11.251	1556	1558	1562	rVB	178112	136189	5.07%	0.565%
23	11.298	1562	1566	1570	rBV	49704	50759	1.89%	0.211%
24	11.757	1642	1644	1648	rVB	28858	26968	1.00%	0.112%
25	11.839	1655	1658	1661	rBV	37845	40610	1.51%	0.168%
26	12.433	1756	1759	1763	rBV	189331	184466	6.87%	0.765%
27	12.663	1791	1798	1801	rBV	202998	288756	10.76%	1.198%
28	12.727	1807	1809	1814	rVB5	27880	32436	1.21%	0.135%
29	12.816	1820	1824	1827	rBV	2041193	1916565	71.42%	7.949%
30	12.845	1827	1829	1832	rVB2	33430	33312	1.24%	0.138%
31	13.063	1863	1866	1869	rBV2	42687	38315	1.43%	0.159%
32	13.098	1869	1872	1874	rBV2	41530	45201	1.68%	0.187%
33	13.298	1901	1906	1913	rVB	311175	315893	11.77%	1.310%
34	13.363	1913	1917	1921	rBV3	39679	82008	3.06%	0.340%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B7-8-10

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

35	13.721	1975	1978	1986	rVB	207904	233925	8.72%	0.970%
36	13.863	1997	2002	2005	rBV	806910	830849	30.96%	3.446%
37	13.886	2005	2006	2012	rVB	99080	67815	2.53%	0.281%
38	15.274	2237	2242	2246	rBV	347020	405872	15.12%	1.683%

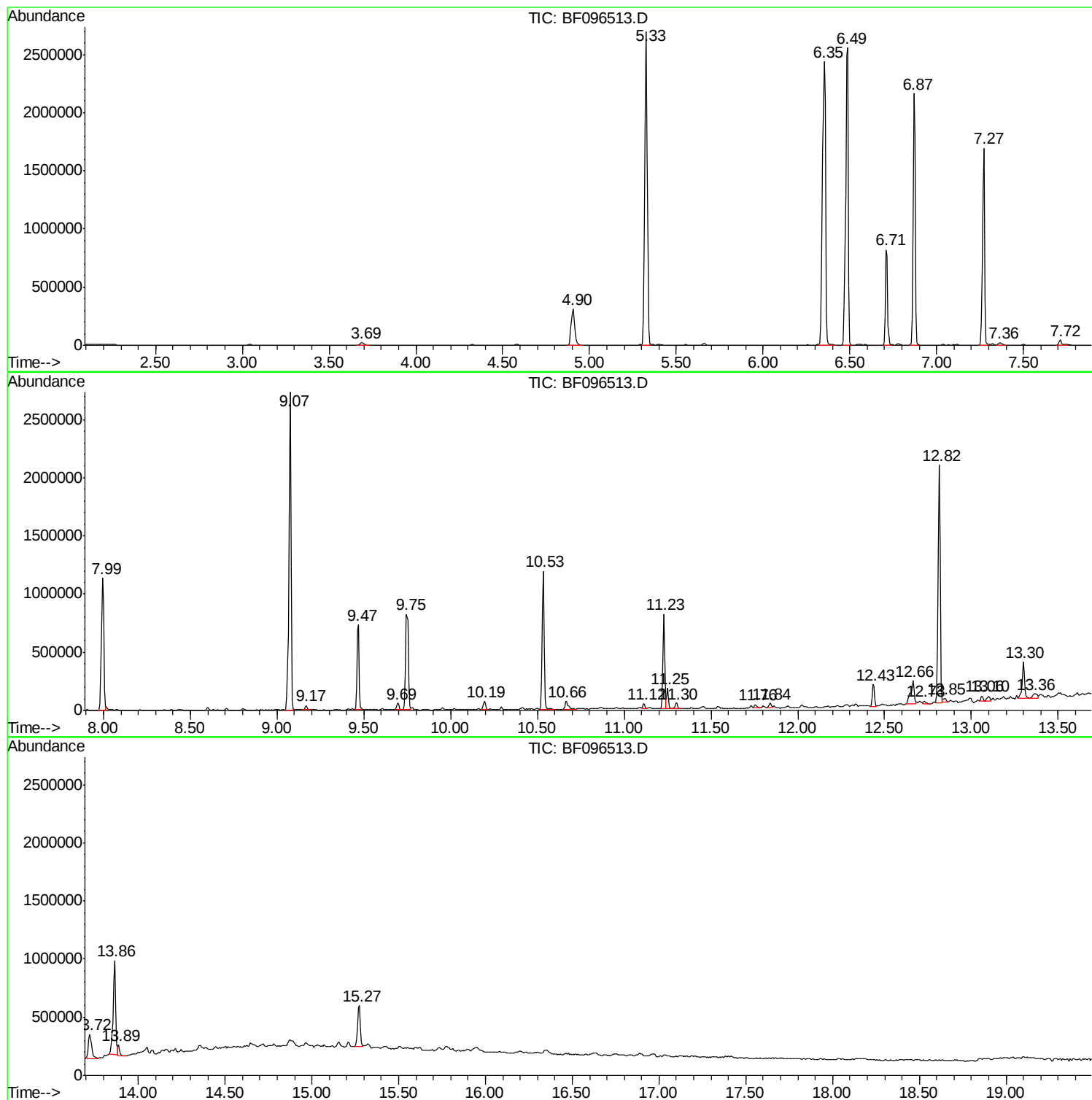
Sum of corrected areas: 24109544

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
B7-8-10

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\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B7-8-10

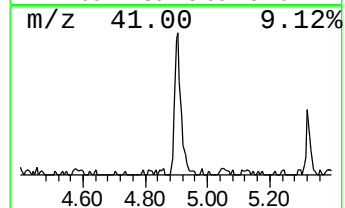
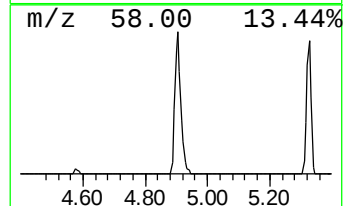
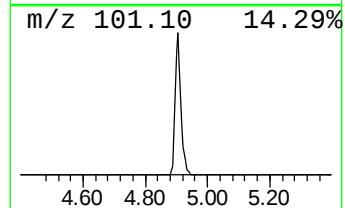
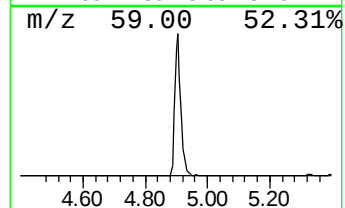
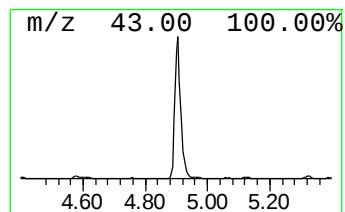
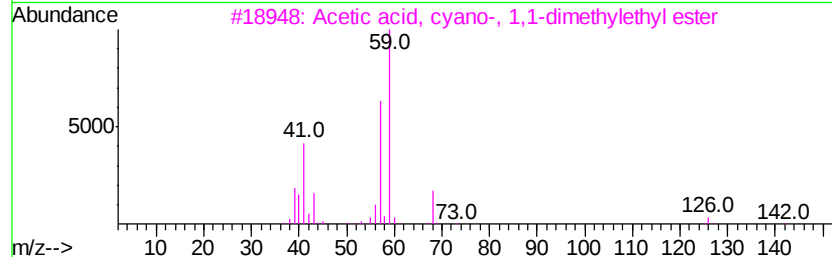
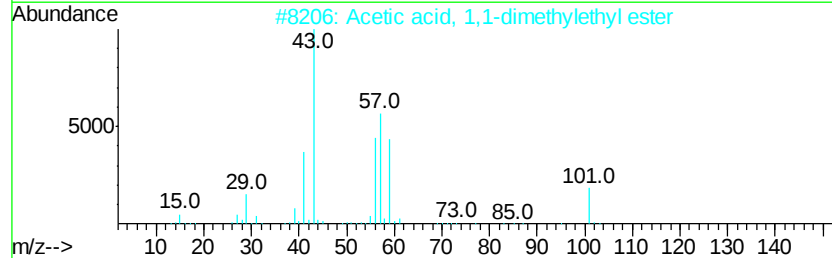
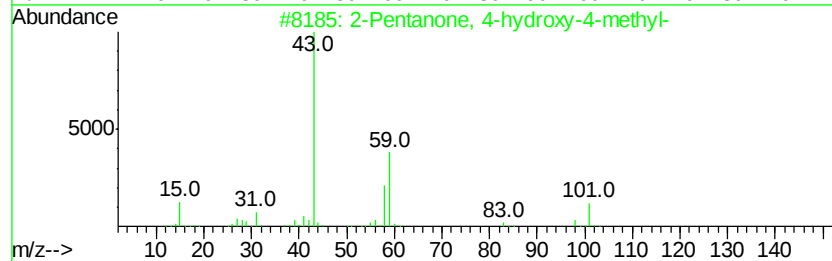
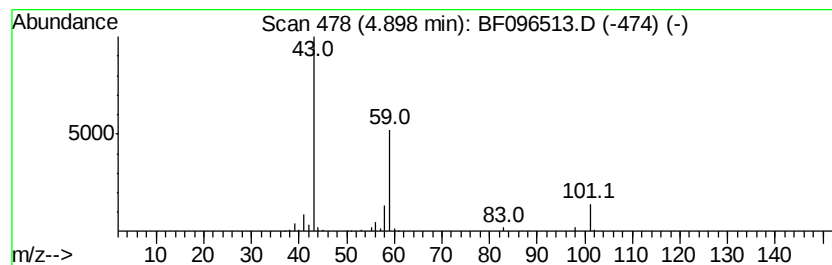
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	11.58 ng	417765	1,4-Dichlorobenzene-d4	6.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B7-8-10

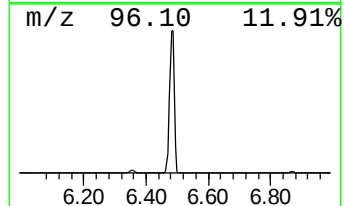
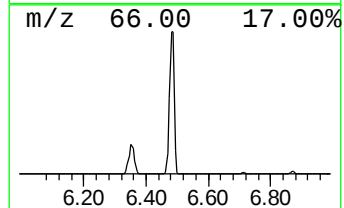
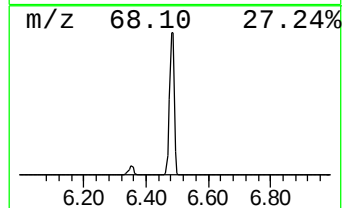
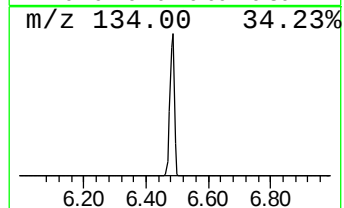
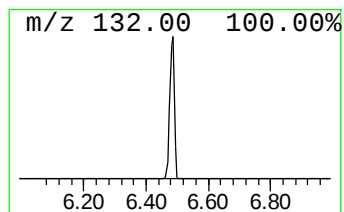
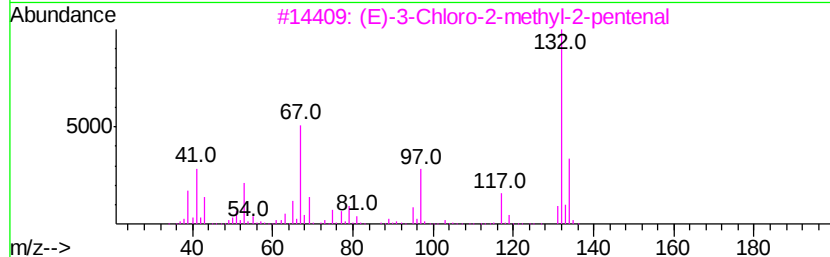
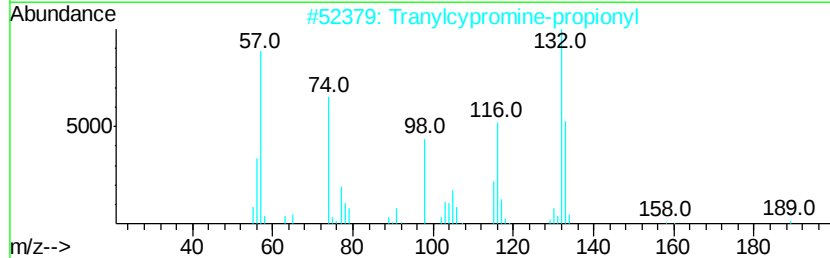
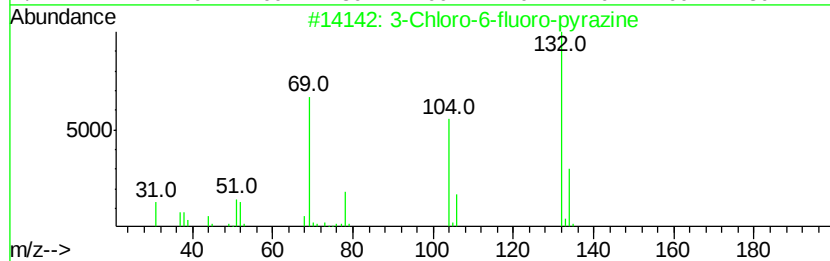
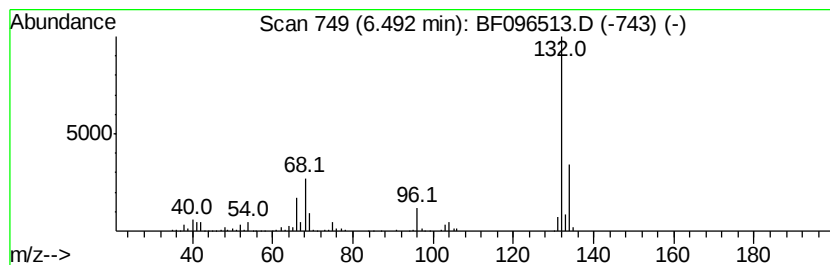
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	70.93 ng	2558160	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B7-8-10

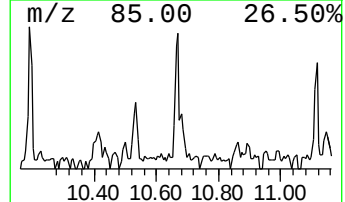
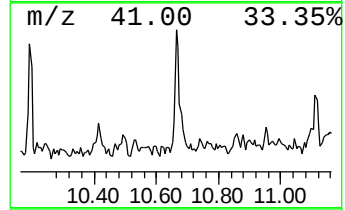
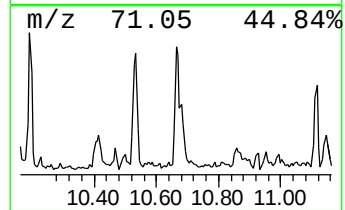
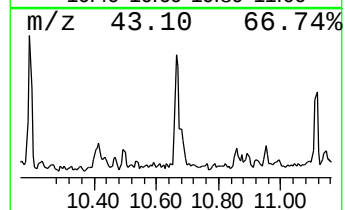
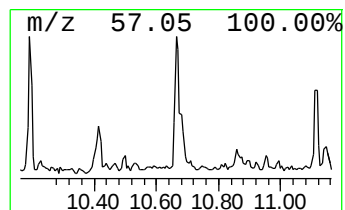
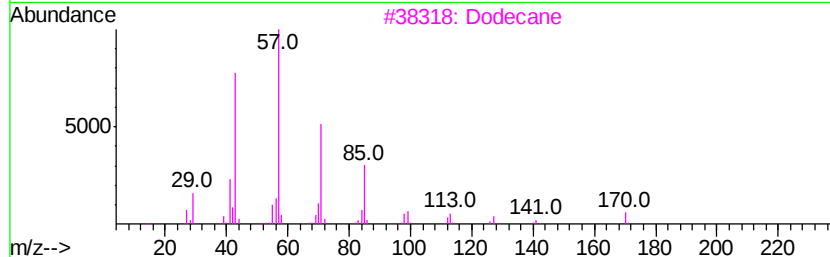
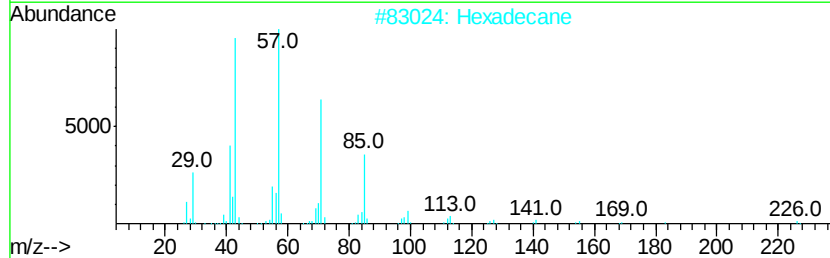
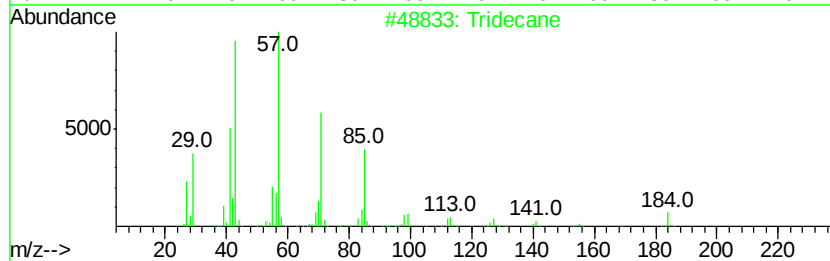
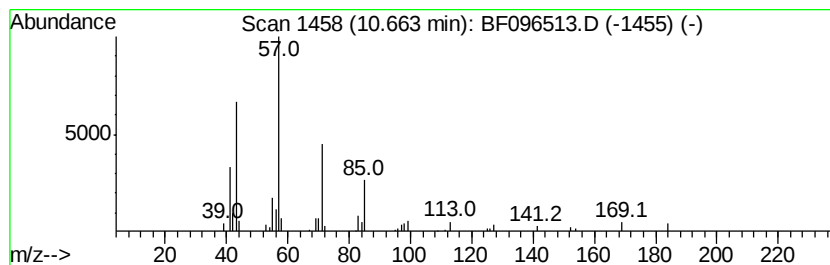
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.72 ng	90127	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	93
2	Hexadecane		226	C16H34	000544-76-3	80
3	Dodecane		170	C12H26	000112-40-3	80
4	Eicosane		282	C20H42	000112-95-8	72
5	Tetracosane		338	C24H50	000646-31-1	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

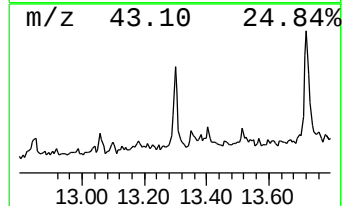
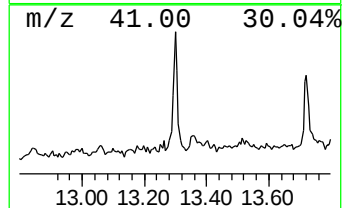
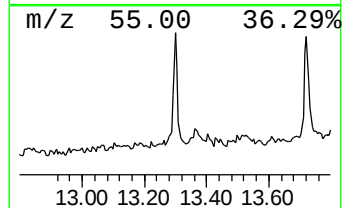
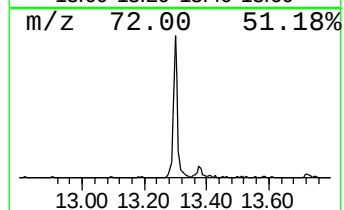
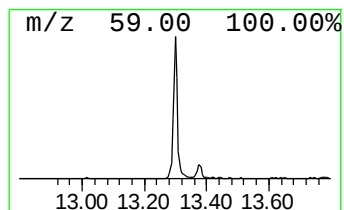
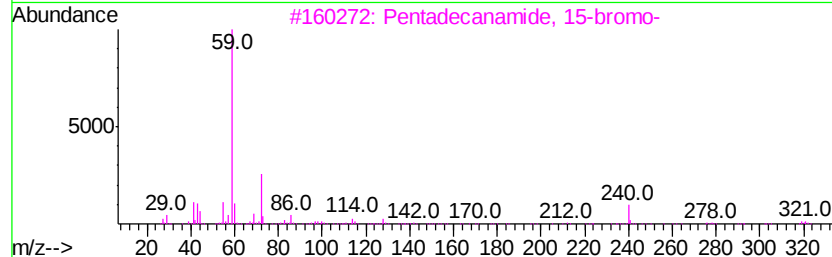
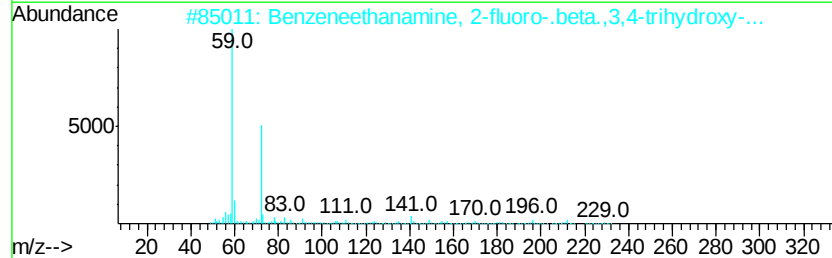
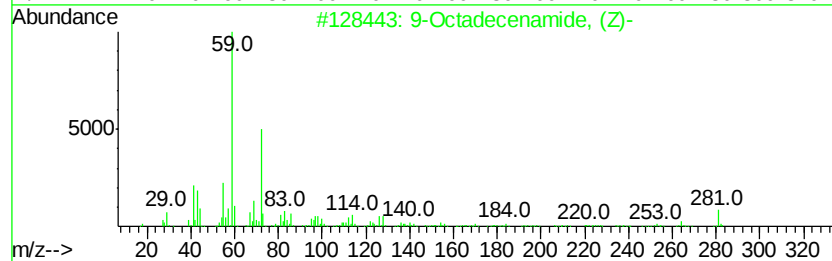
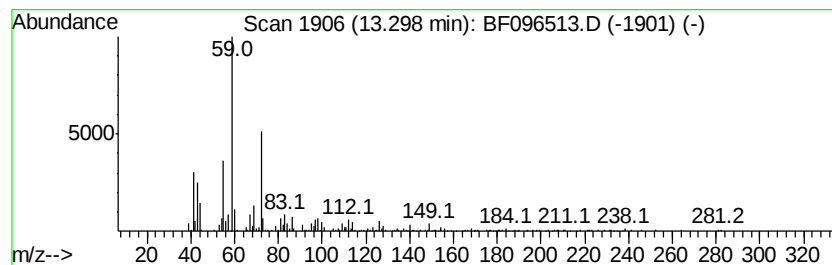
Instrument :
BNA_F
ClientSampleId :
B7-8-10

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 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	7.60 ng	315893	Chrysene-d12	13.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	95
2	Benzeneethanamine, 2-fluoro-.bet...	229 C11H16FN03	061338-98-5	80
3	Pentadecanamide, 15-bromo-	319 C15H30BrNO	1000163-86-1	59
4	Dodecanamide	199 C12H25NO	001120-16-7	58
5	Tetradecanamide	227 C14H29NO	000638-58-4	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

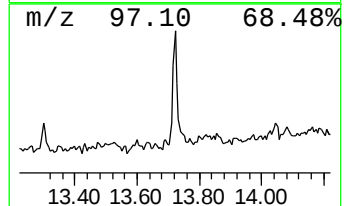
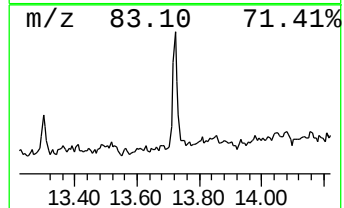
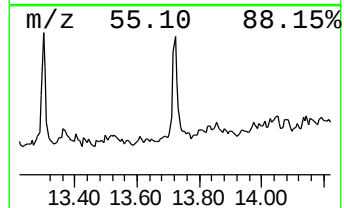
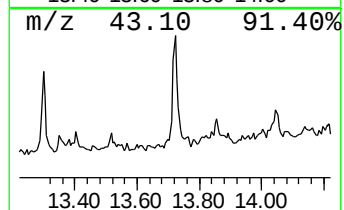
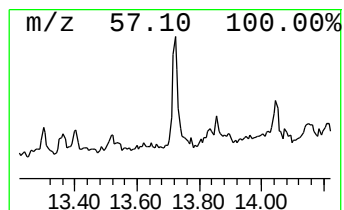
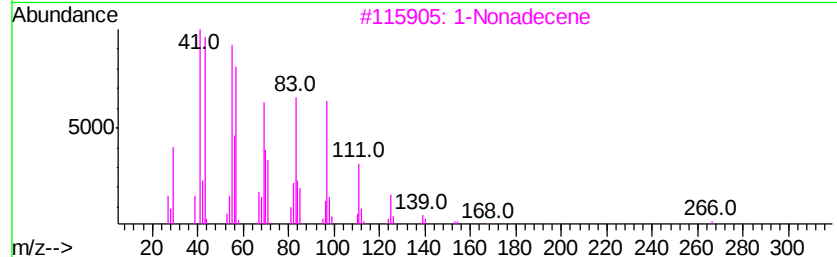
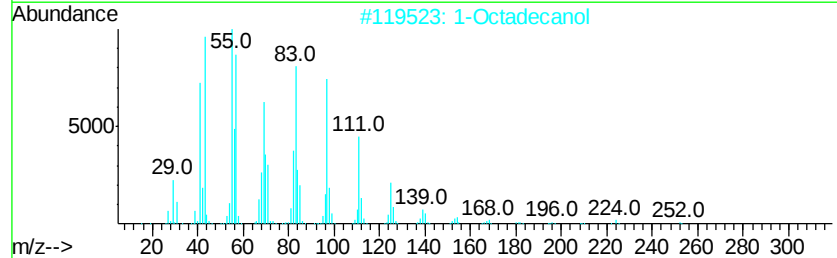
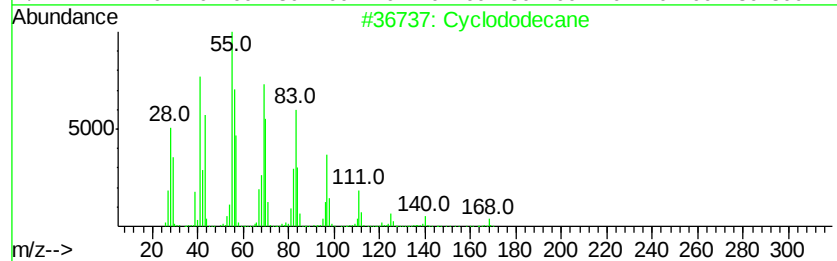
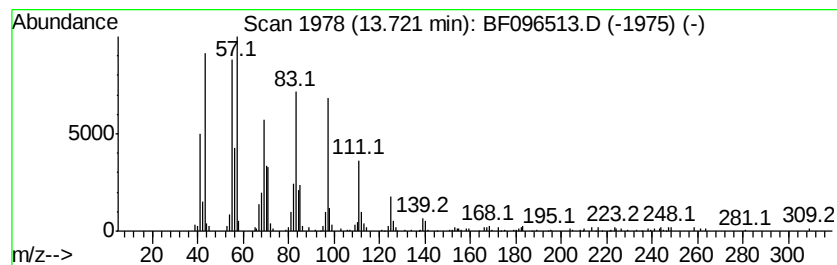
Instrument :
BNA_F
ClientSampleId :
B7-8-10

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 6 Cyclododecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	5.63 ng	233925	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecane	168	C12H24	000294-62-2	92
2	1-Octadecanol	270	C18H38O	000112-92-5	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	Cyclohexadecane	224	C16H32	000295-65-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096513.D
Acq On : 6 Jul 2017 5:38
Operator : SJ/MA
Sample : I3975-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B7-8-10

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...	4.90	11.6	ng	417765	1	6.72	721357	20.0
unknown6.49	6.49	70.9	ng	2558160	1	6.72	721357	20.0
Tridecane	10.66	2.7	ng	90127	4	11.23	661719	20.0
9-Octadecenamide, ...	13.30	7.6	ng	315893	5	13.86	830849	20.0
Cyclododecane	13.72	5.6	ng	233925	5	13.86	830849	20.0