

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
 Data File : BF085488.D
 Acq On : 17 Mar 2016 3:52
 Operator : UM/SJ
 Sample : H1788-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5(9-10)

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-BF031516.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	4.527	194	196	198	rVB	86759	110553	3.90%	0.425%
2	5.098	244	246	253	rVB	46056	61623	2.17%	0.237%
3	5.498	278	281	284	rBV	2357936	2619952	92.36%	10.083%
4	6.527	368	371	374	rBV	2405294	2525573	89.03%	9.720%
5	6.664	381	383	386	rBV	2796446	2711076	95.57%	10.434%
6	6.904	401	404	406	rBV	609131	709953	25.03%	2.732%
7	7.053	415	417	420	rBV	2110990	2230396	78.63%	8.584%
8	7.464	450	453	455	rBV	2027380	1926740	67.92%	7.415%
9	7.544	458	460	465	rVB	33430	39019	1.38%	0.150%
10	8.184	514	516	518	rBV	1129211	937019	33.03%	3.606%
11	9.076	592	594	595	rVB	68682	48335	1.70%	0.186%
12	9.259	608	610	613	rBV	2636340	2836674	100.00%	10.917%
13	9.659	643	645	647	rBV	464511	531925	18.75%	2.047%
14	9.876	660	664	666	rBV	90104	109193	3.85%	0.420%
15	9.945	668	670	672	rVB	854827	929226	32.76%	3.576%
16	10.105	681	684	685	rBV	29882	46407	1.64%	0.179%
17	10.196	690	692	694	rVB2	29956	32163	1.13%	0.124%
18	10.368	706	707	709	rVB	154919	135736	4.79%	0.522%
19	10.585	723	726	730	rBV	50335	103692	3.66%	0.399%
20	10.722	736	738	741	rBV2	1122623	1597256	56.31%	6.147%
21	10.848	747	749	753	rBV	127518	204783	7.22%	0.788%
22	11.042	763	766	768	rBV2	18762	41662	1.47%	0.160%
23	11.293	785	788	789	rBV	65659	68707	2.42%	0.264%
24	11.316	789	790	793	rVB	36247	47367	1.67%	0.182%
25	11.373	793	795	797	rBV3	15720	34234	1.21%	0.132%
26	11.419	797	799	802	rVV2	725478	806104	28.42%	3.102%
27	11.488	802	805	808	rVB4	27888	53040	1.87%	0.204%
28	11.899	837	841	842	rBV3	10447	28490	1.00%	0.110%
29	11.945	843	845	851	rVV3	70476	127099	4.48%	0.489%
30	12.036	851	853	857	rVB4	14989	43909	1.55%	0.169%
31	12.676	908	909	911	rVB2	37780	29685	1.05%	0.114%
32	12.733	912	914	916	rBV3	37366	45752	1.61%	0.176%
33	12.882	923	927	930	rBV4	20723	66611	2.35%	0.256%
34	13.008	935	938	940	rBV	2168185	1941740	68.45%	7.473%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

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-BF031516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.454	975	977	979	rVB	31779	37956	1.34%	0.146%
36	13.899	1014	1016	1020	rBV	76296	128622	4.53%	0.495%
37	14.059	1026	1030	1032	rBV2	690185	778158	27.43%	2.995%
38	15.511	1154	1157	1162	rVB	487338	748116	26.37%	2.879%
39	16.197	1215	1217	1224	rVB2	110633	257565	9.08%	0.991%
40	16.620	1252	1254	1257	rVB	72489	104724	3.69%	0.403%
41	17.260	1308	1310	1314	rVB3	83725	146469	5.16%	0.564%

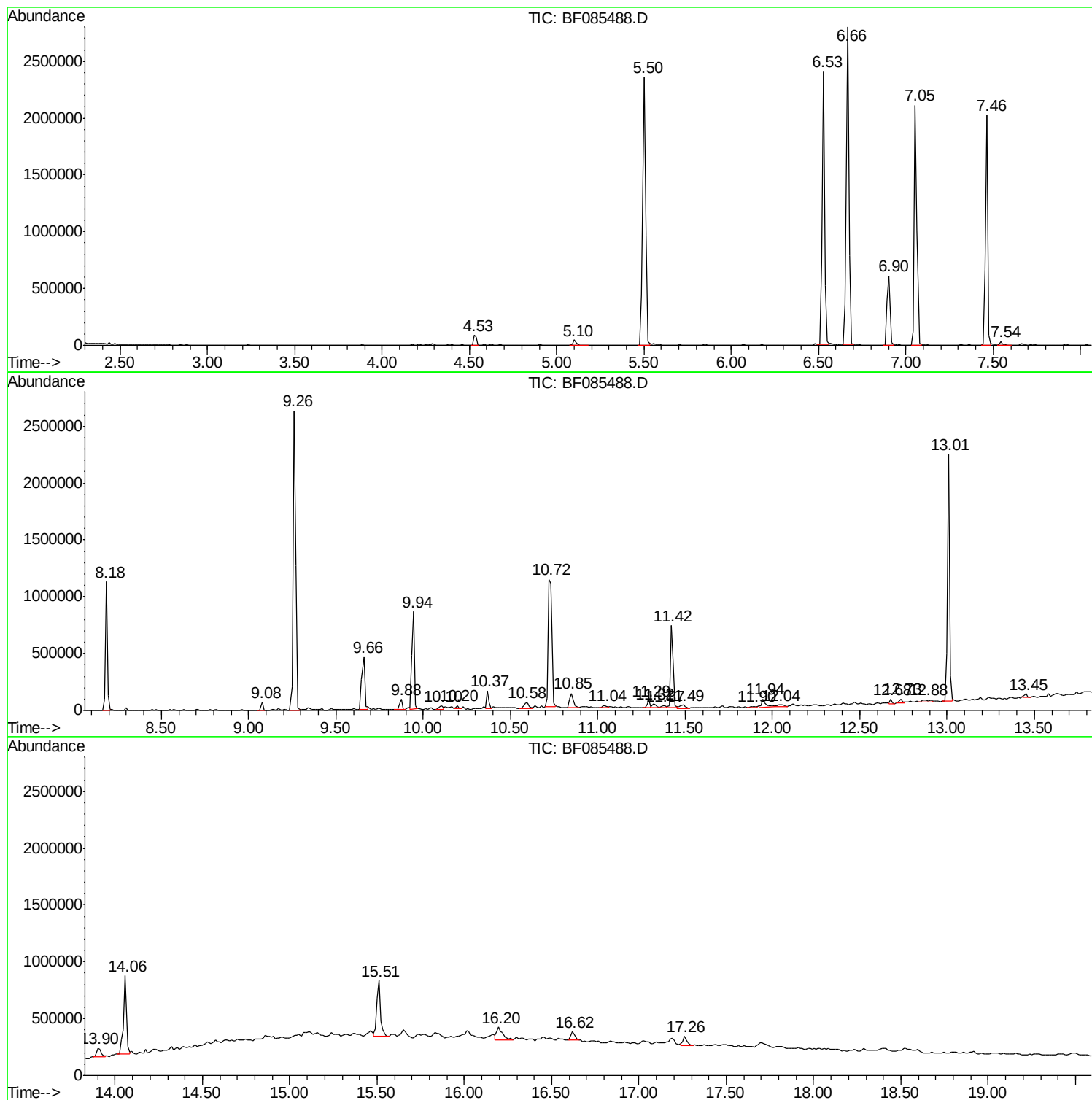
Sum of corrected areas: 25983304

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

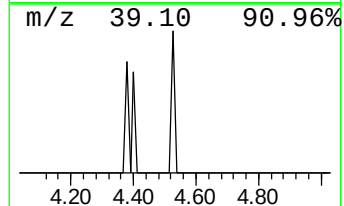
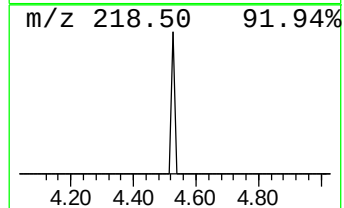
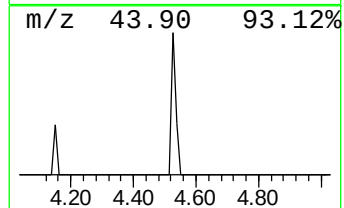
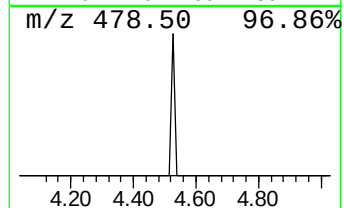
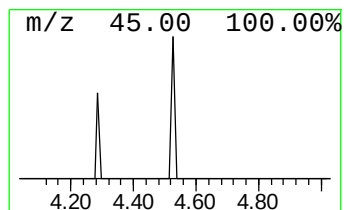
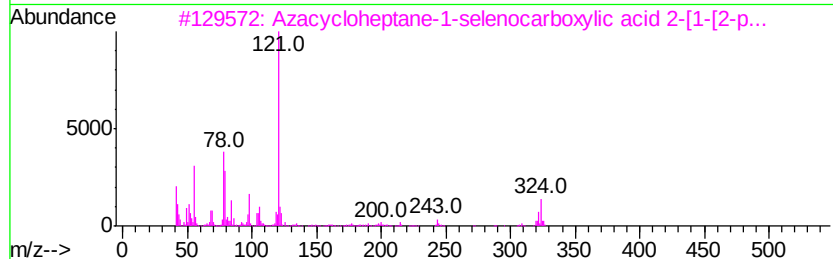
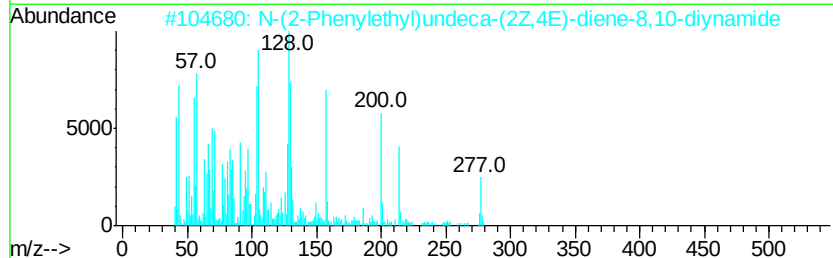
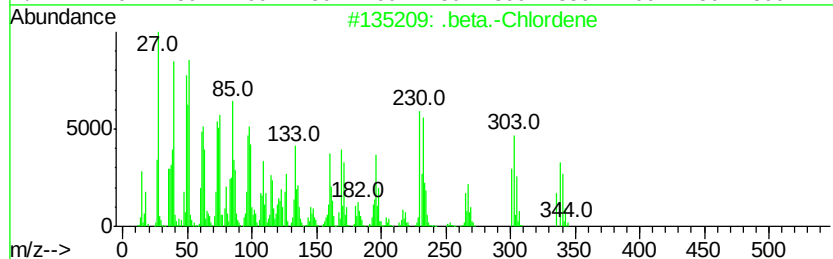
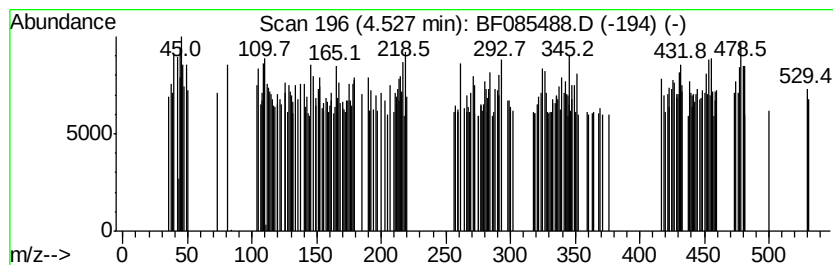
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.53 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.11 ng	110553	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-Chlordene	336	C10H6Cl6	056534-03-3	30	
2	N-(2-Phenylethyl)undeca-(2Z,4E)-...	277	C19H19NO	099615-80-2	22		
3	Azacycloheptane-1-selenocarboxyl...	324	C14H20N4Se	079514-45-7	22		
4	Epi-epoxy-buphanamine	317	C17H19NO5	006835-78-5	22		
5	Dibenzo[a,d]bicyclo[3,2,1]-8-aza...	339	C21H25NO3	1000128-43-4	22		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

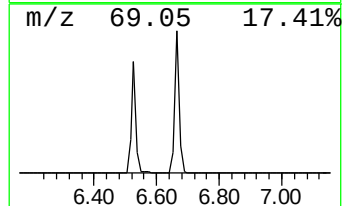
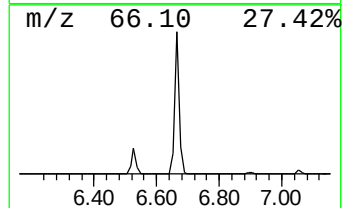
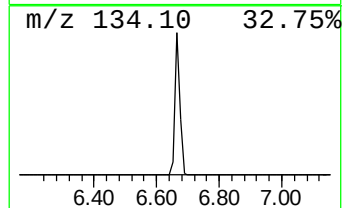
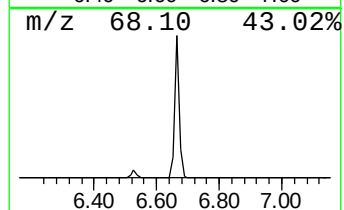
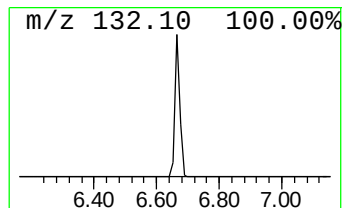
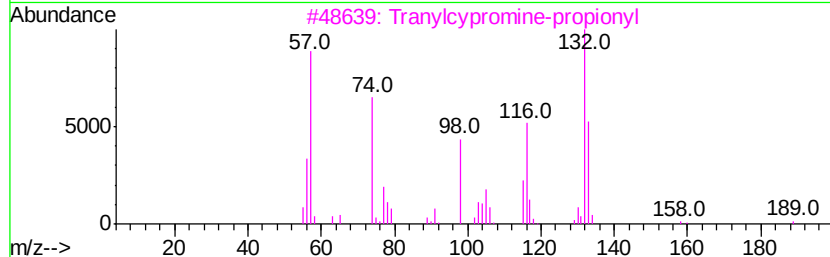
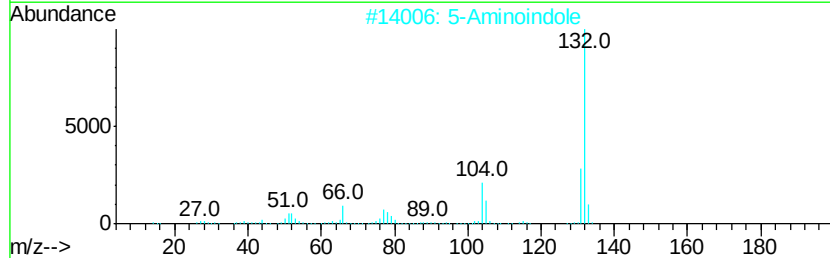
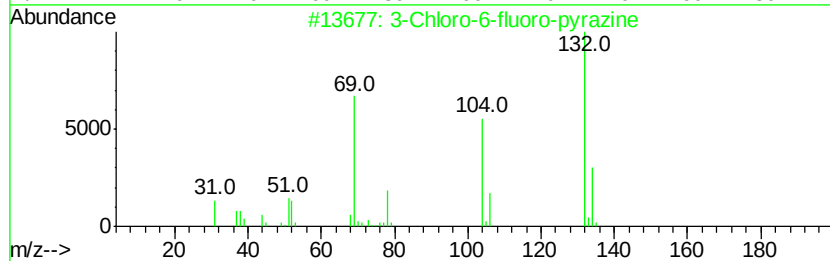
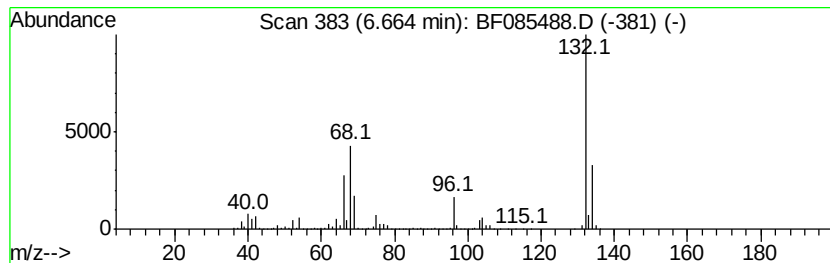
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	76.37 ng	2711080	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-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\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

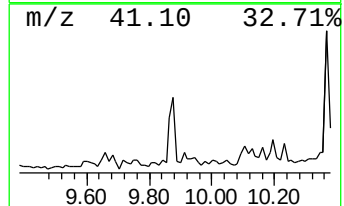
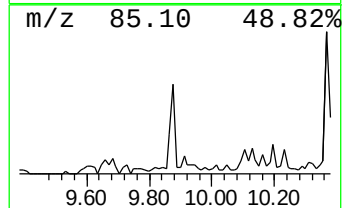
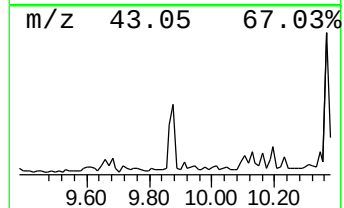
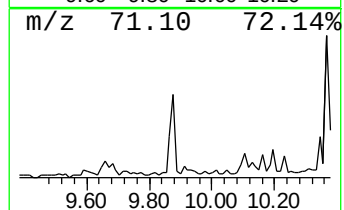
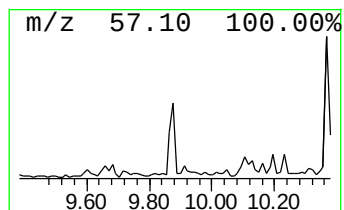
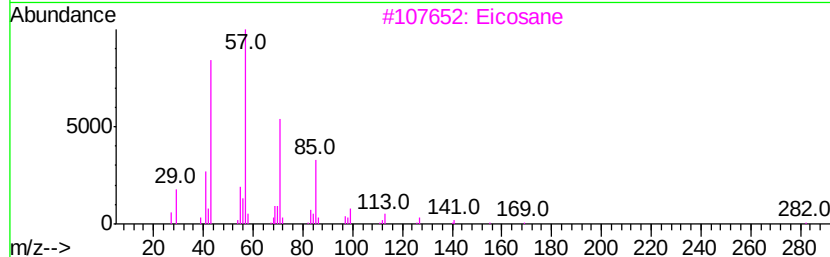
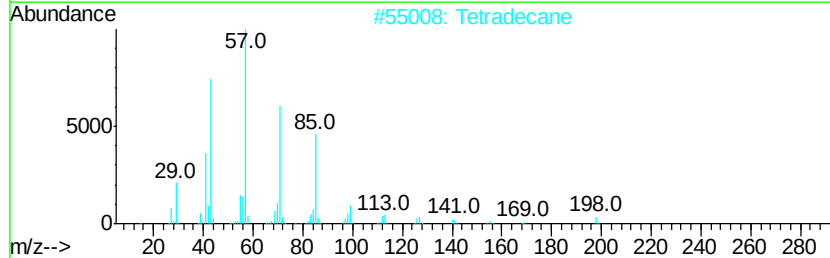
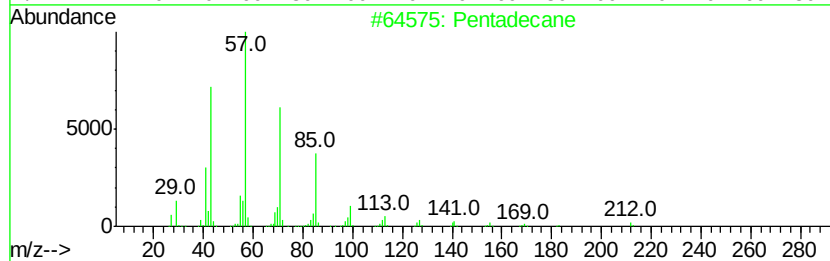
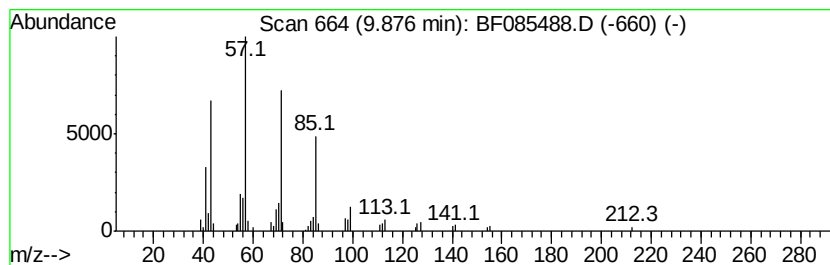
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.88	2.35 ng	109193	Acenaphthene-d10	9.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	96
2		Tetradecane	198	C14H30	000629-59-4	91
3		Eicosane	282	C20H42	000112-95-8	91
4		Hexadecane	226	C16H34	000544-76-3	90
5		Tritetracontane	605	C43H88	007098-21-7	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

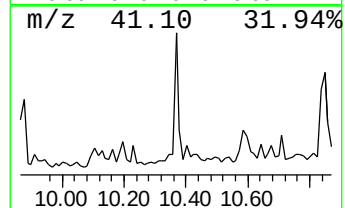
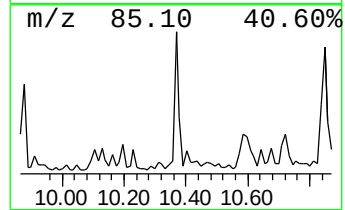
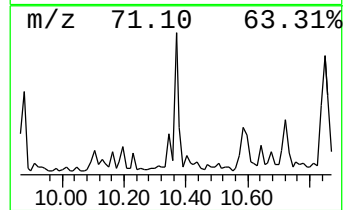
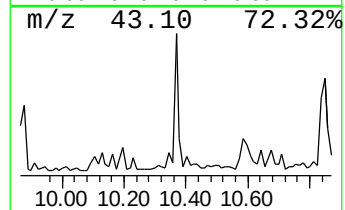
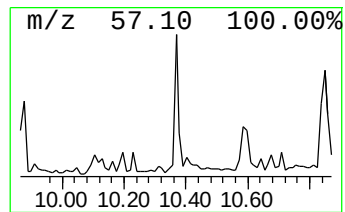
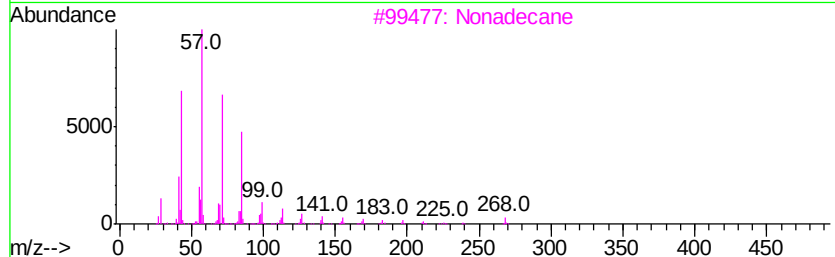
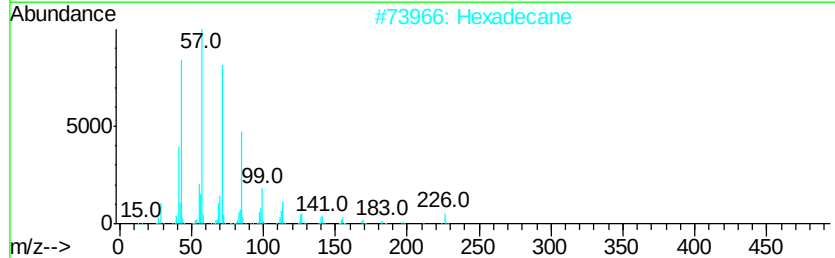
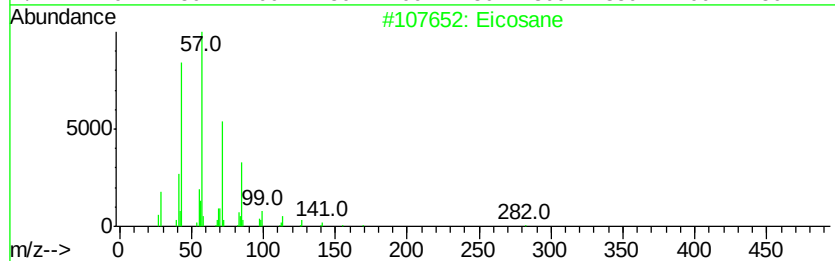
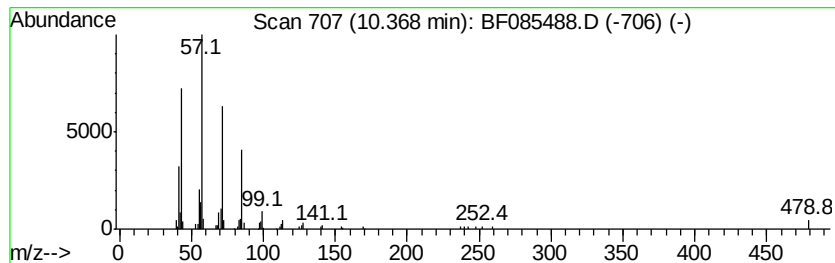
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	2.92 ng	135736	Acenaphthene-d10	9.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	87
2	Hexadecane		226	C16H34	000544-76-3	86
3	Nonadecane		268	C19H40	000629-92-5	86
4	Tridecane		184	C13H28	000629-50-5	86
5	Heptadecane		240	C17H36	000629-78-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

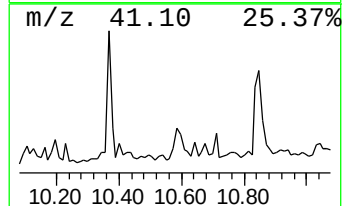
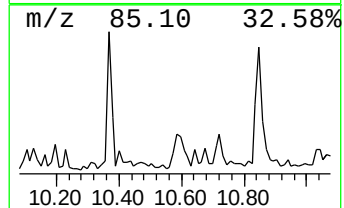
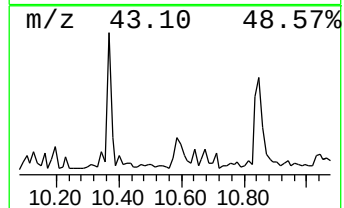
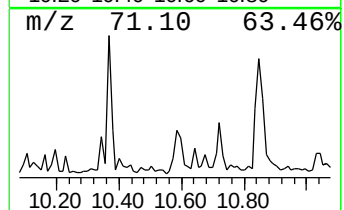
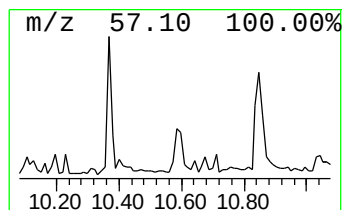
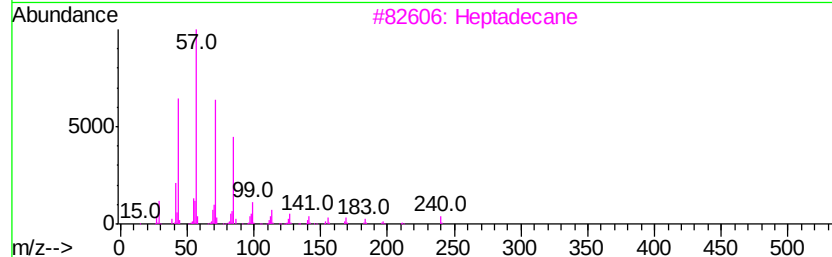
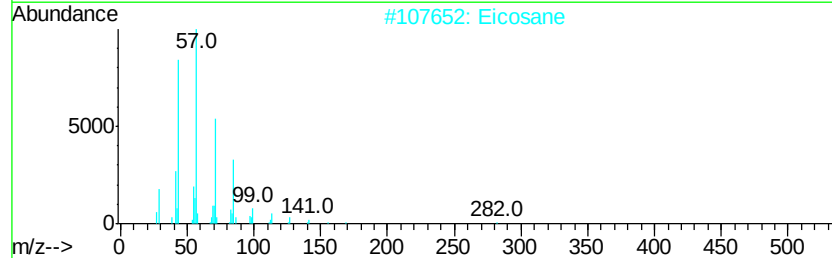
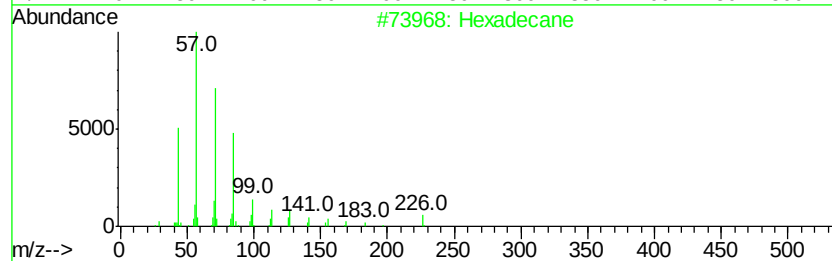
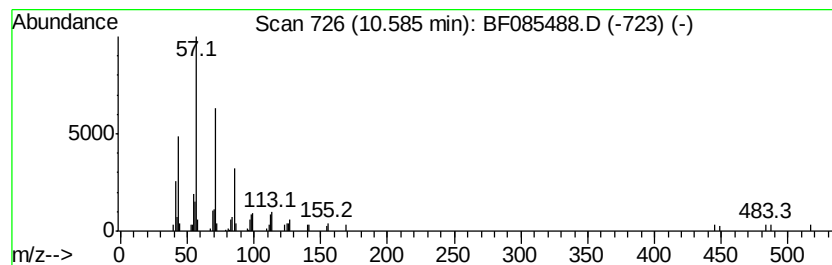
Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.58	2.23 ng	103692	Acenaphthene-d10		9.94
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Eicosane	282	C20H42	000112-95-8	83
3	Heptadecane	240	C17H36	000629-78-7	80
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
5	Heptacosane	380	C27H56	000593-49-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

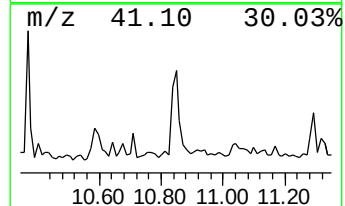
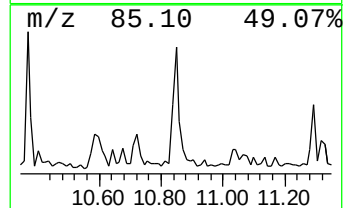
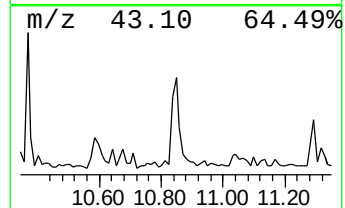
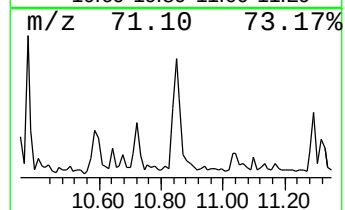
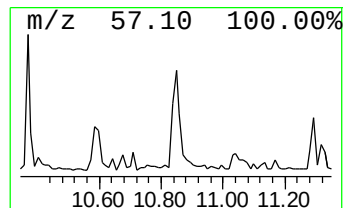
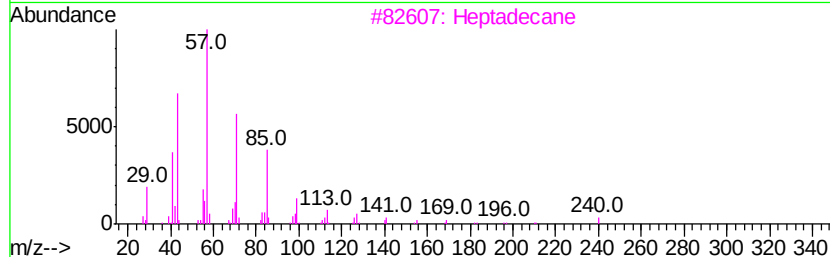
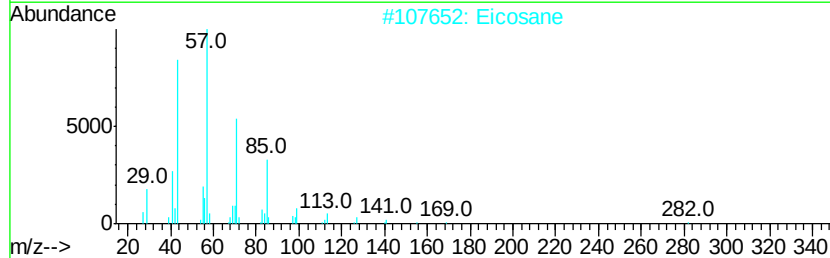
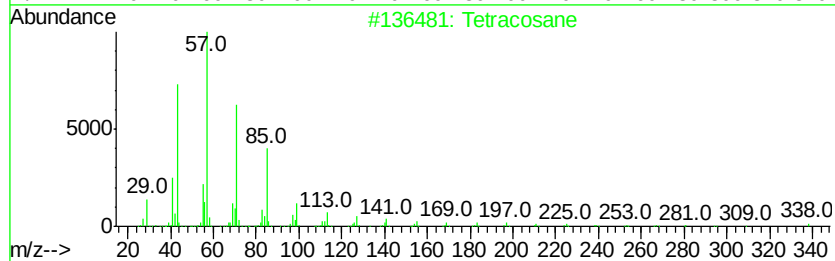
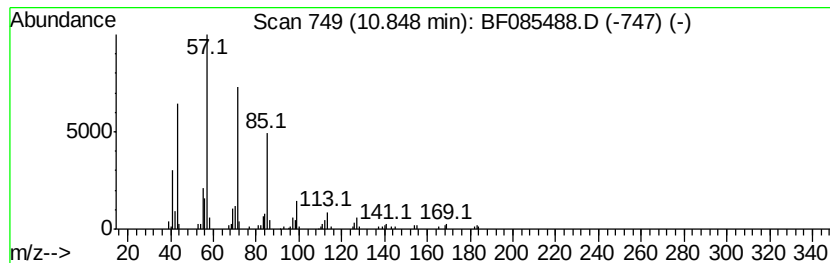
Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.85	5.08 ng	204783	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Pentadecane	212	C15H32	000629-62-9	91
5	Hexadecane	226	C16H34	000544-76-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

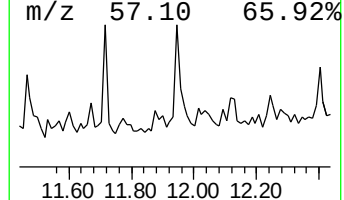
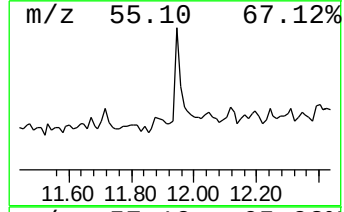
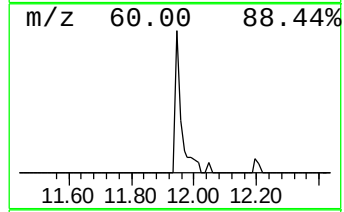
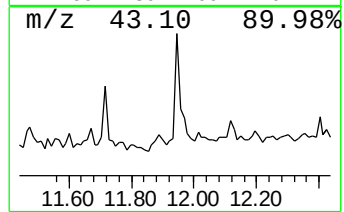
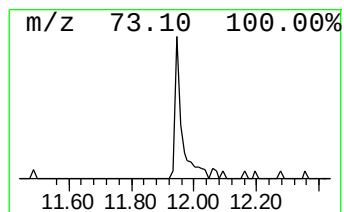
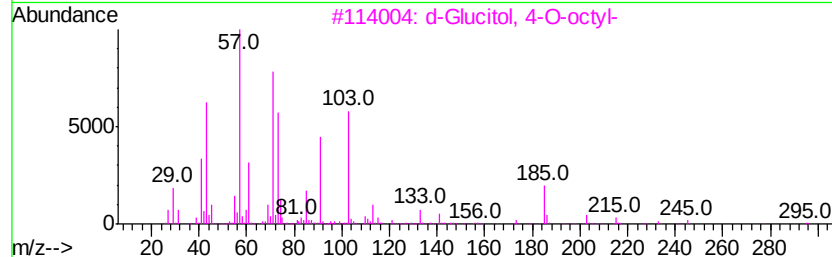
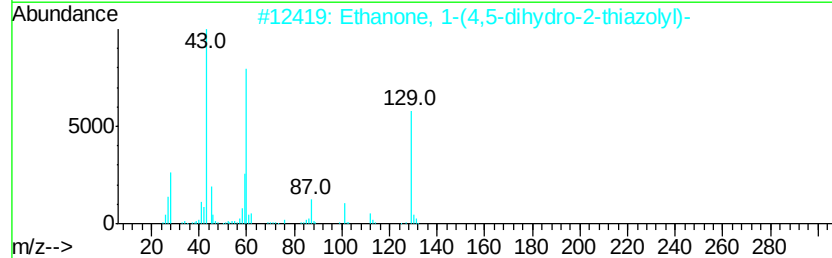
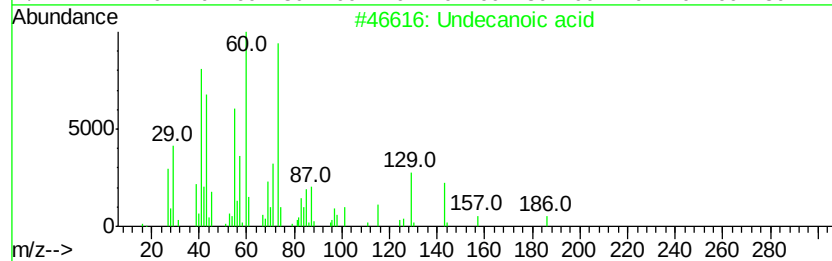
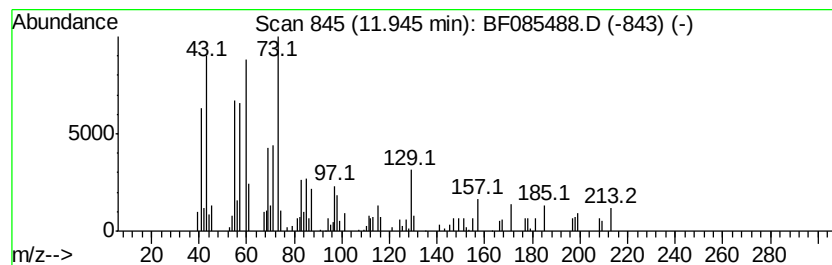
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.15 ng	127099	Phenanthrene-d10	11.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	53	
2	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35	
3	d-Glucitol, 4-O-octyl-	294	C14H30O6	132696-01-6	22	
4	Dodecane	170	C12H26	000112-40-3	11	
5	Tridecane	184	C13H28	000629-50-5	10	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

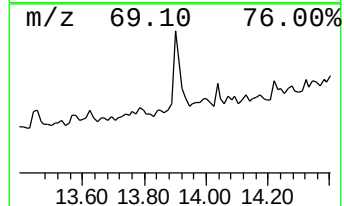
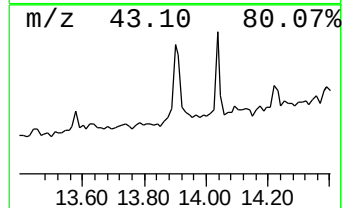
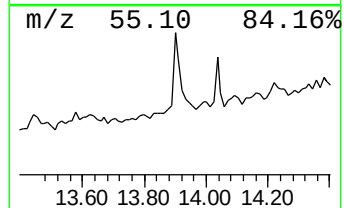
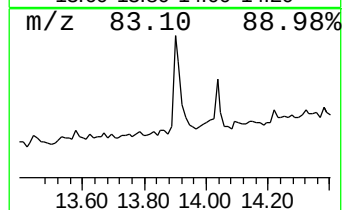
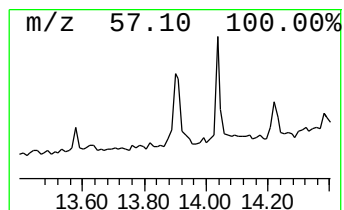
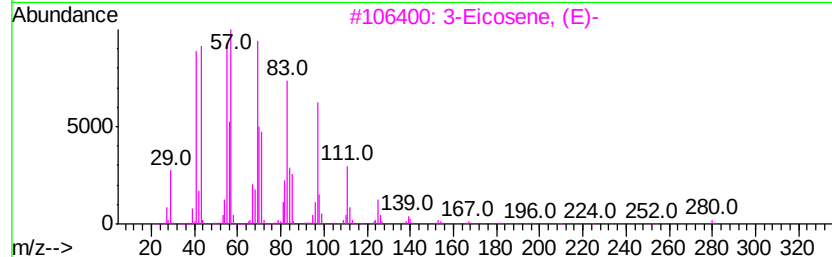
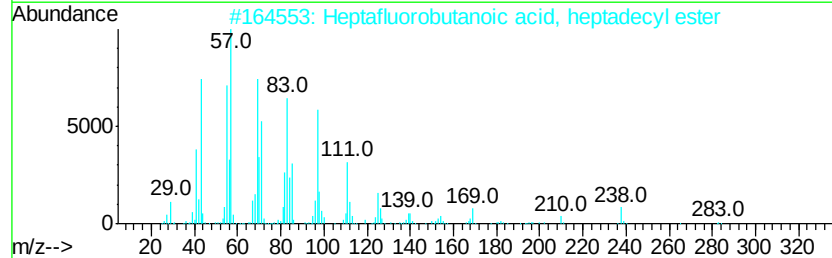
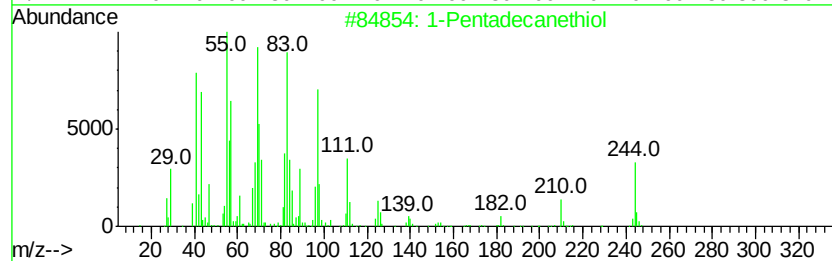
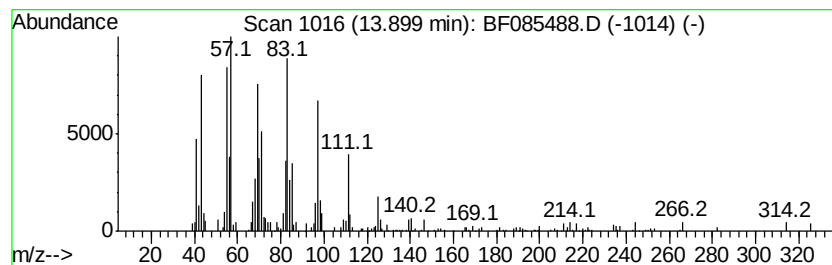
Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Pentadecanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.31 ng	128622	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Pentadecanethiol	244 C15H32S	025276-70-4	94
2	Heptafluorobutanoic acid, heptad...	452 C21H35F7O2	1000282-97-3	91
3	3-Eicosene, (E)-	280 C20H40	074685-33-9	91
4	2-Chloropropionic acid, octadec...	360 C21H41ClO2	088104-31-8	91
5	17-Pentatriacontene	491 C35H70	006971-40-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

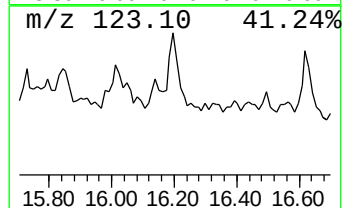
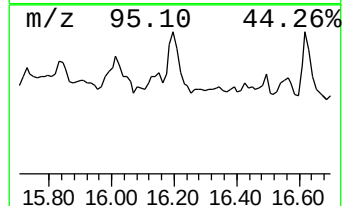
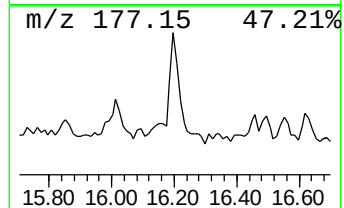
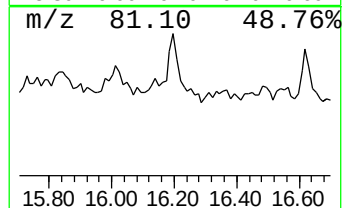
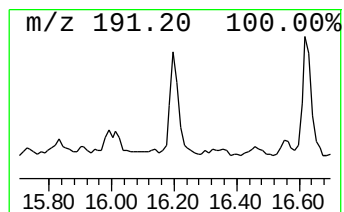
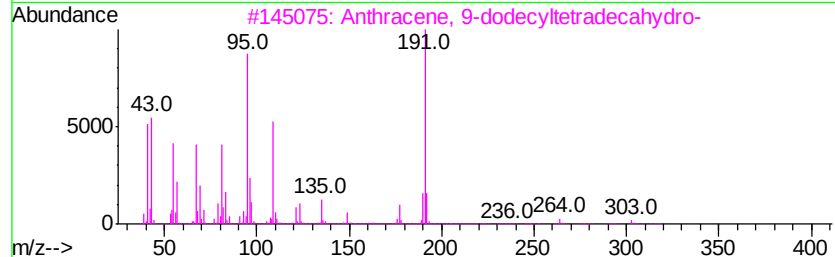
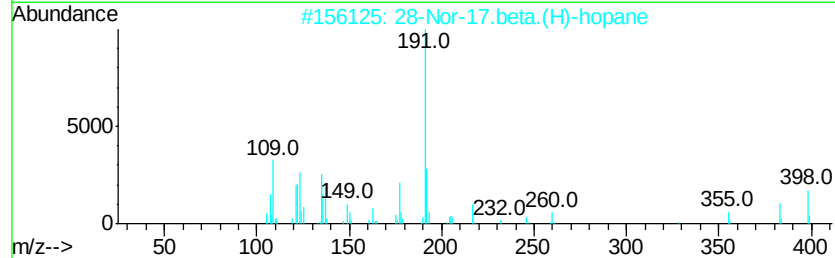
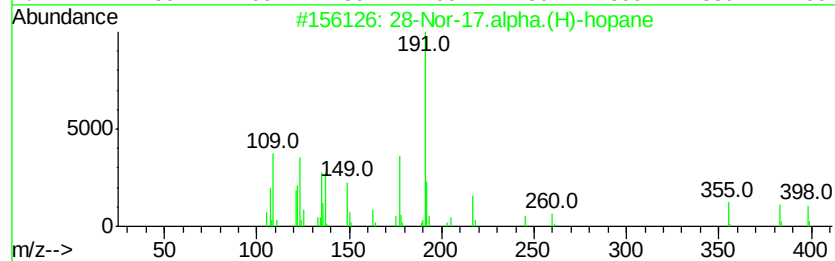
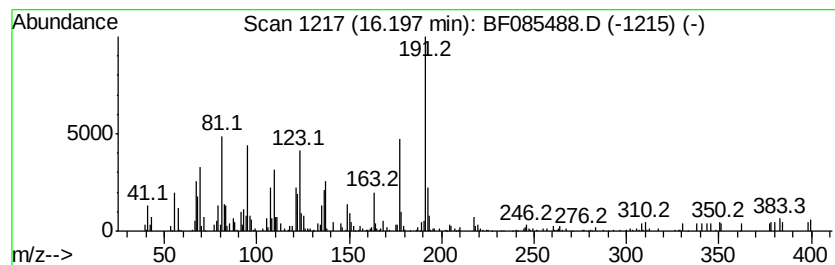
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	6.89 ng	257565	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	90
2		28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	49
3		Anthracene, 9-dodecyltetradecahydro-	360	C26H48	055401-75-7	32
4		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	27
5		Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

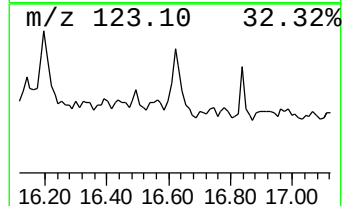
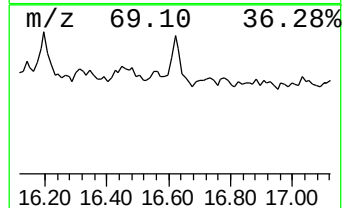
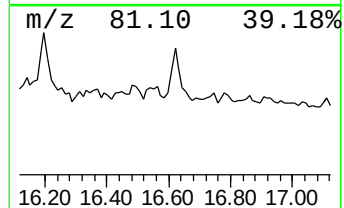
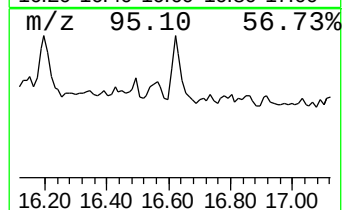
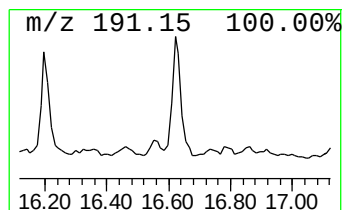
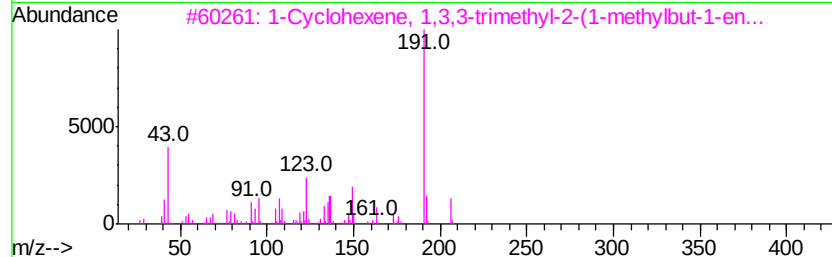
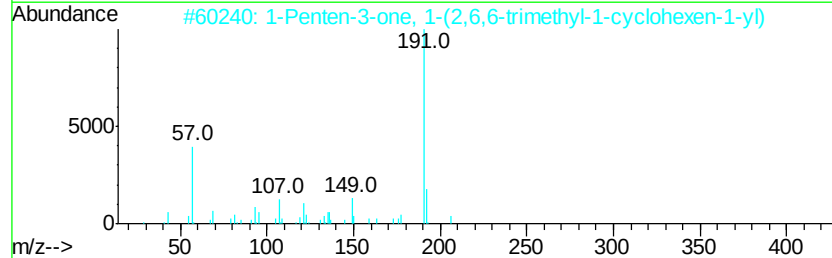
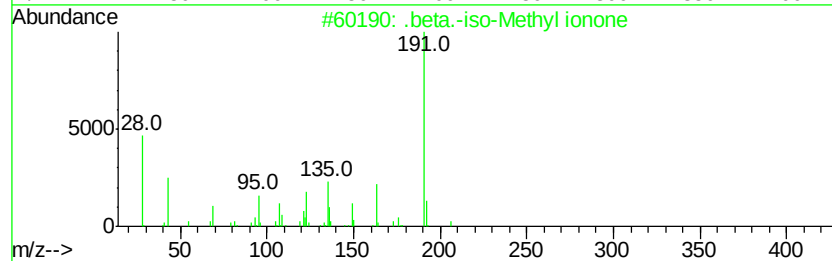
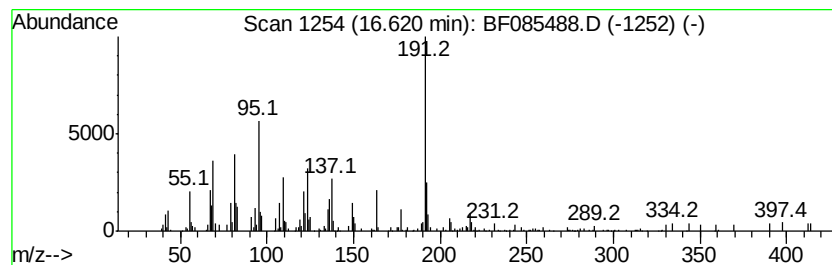
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 .beta.-iso-Methyl ionone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	2.80 ng	104724	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	76
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	41
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	37
4		4,5-Dihydrothiazol-4-one, 2-(2-m...	222	C10H10N2O2S	022476-61-5	35
5		2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085488.D
Acq On : 17 Mar 2016 3:52
Operator : UM/SJ
Sample : H1788-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(9-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.53	4.53	3.1 ng		110553	1	6.90	709953	20.0
unknown6.66	6.66	76.4 ng		2711080	1	6.90	709953	20.0
Pentadecane	9.88	2.4 ng		109193	3	9.94	929226	20.0
Eicosane	10.37	2.9 ng		135736	3	9.94	929226	20.0
Hexadecane	10.58	2.2 ng		103692	3	9.94	929226	20.0
Tetracosane	10.85	5.1 ng		204783	4	11.42	806104	20.0
Undecanoic acid	11.94	3.1 ng		127099	4	11.42	806104	20.0
1-Pentadecanethiol	13.90	3.3 ng		128622	5	14.06	778158	20.0
28-Nor-17.alpha.(...	16.20	6.9 ng		257565	6	15.51	748116	20.0
.beta.-iso-Methyl...	16.62	2.8 ng		104724	6	15.51	748116	20.0