

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091118\
 Data File : BF108937.D
 Acq On : 11 Sep 2018 16:08
 Operator : JU/SJ
 Sample : PB112707BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB112707BL

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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	4.943	438	443	451	rBV	434473	601260	12.99%	1.631%
2	5.354	508	513	517	rBV	3478242	3858184	83.38%	10.463%
3	6.372	680	686	689	rBV	3599214	4049204	87.51%	10.981%
4	6.507	704	709	712	rBV	4197381	4013448	86.74%	10.884%
5	6.737	744	748	751	rBV	1308702	1020192	22.05%	2.767%
6	6.895	770	775	778	rBV	3597752	3160882	68.31%	8.572%
7	7.295	838	843	846	rBV	2680539	2603013	56.26%	7.059%
8	8.019	961	966	969	rBV	1399801	1299782	28.09%	3.525%
9	9.095	1144	1149	1152	rBV	4950208	4627136	100.00%	12.549%
10	9.766	1259	1263	1267	rBV2	1655346	1445026	31.23%	3.919%
11	10.554	1392	1397	1400	rBV	2355564	2348175	50.75%	6.368%
12	11.242	1510	1514	1518	rBV	1537793	1378328	29.79%	3.738%
13	12.830	1779	1784	1787	rBV	3922881	3760704	81.27%	10.199%
14	13.866	1957	1960	1964	rBV	1018480	951895	20.57%	2.582%
15	14.654	2091	2094	2099	rVB	54563	55776	1.21%	0.151%
16	14.977	2144	2149	2153	rBV	92938	110522	2.39%	0.300%
17	15.277	2195	2200	2205	rBV	941380	1086879	23.49%	2.948%
18	15.330	2205	2209	2215	rVB	125119	162347	3.51%	0.440%
19	15.742	2274	2279	2284	rBV	108918	159853	3.45%	0.434%
20	16.212	2353	2359	2364	rBV	75851	124935	2.70%	0.339%
21	16.765	2449	2453	2460	rVB3	28194	55977	1.21%	0.152%

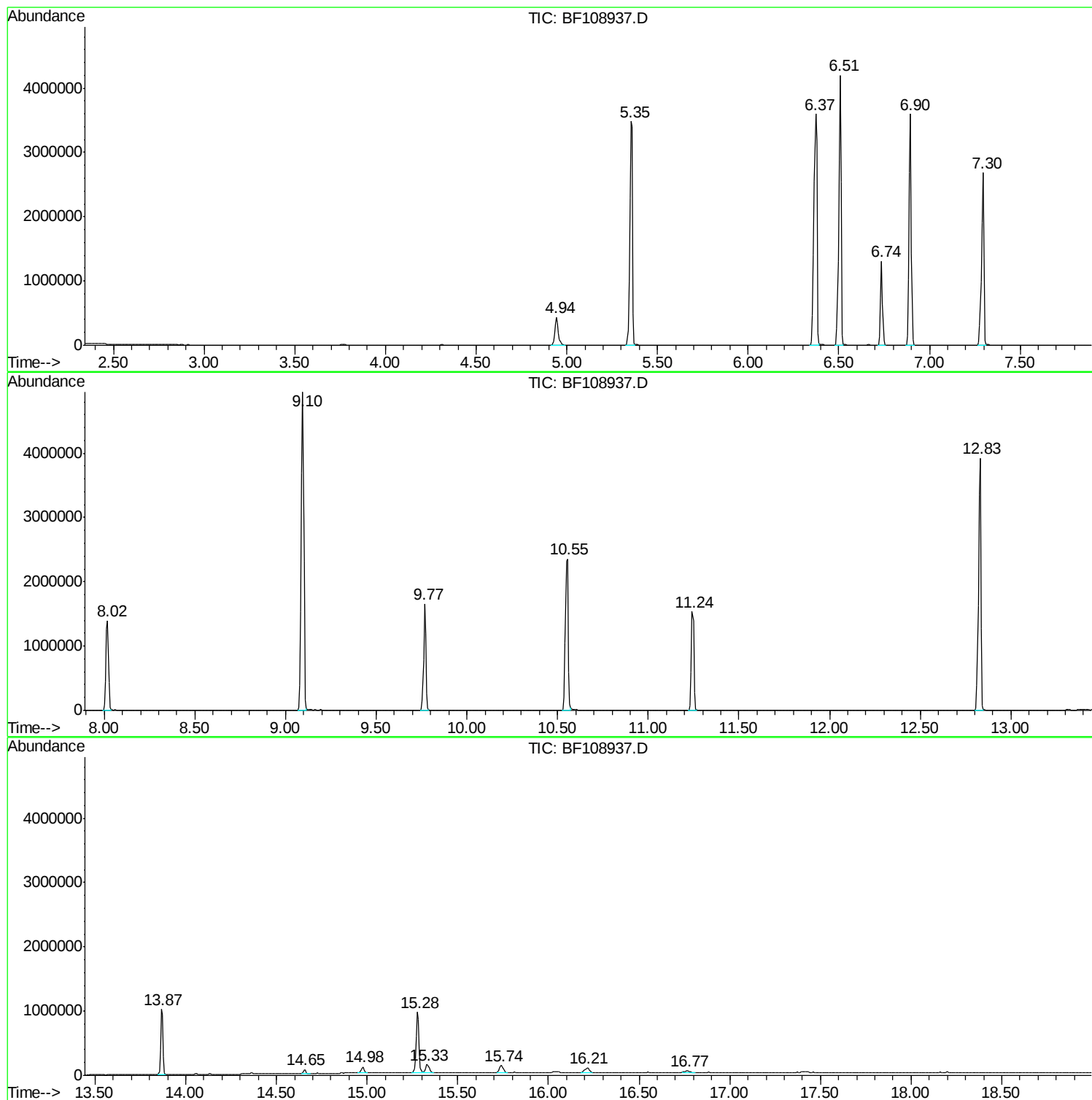
Sum of corrected areas: 36873518

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

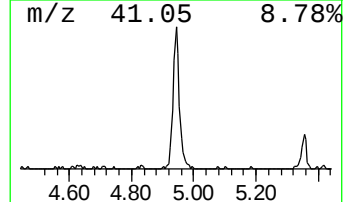
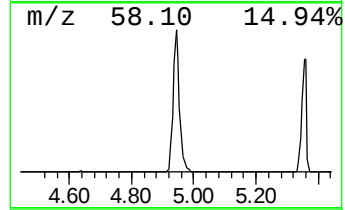
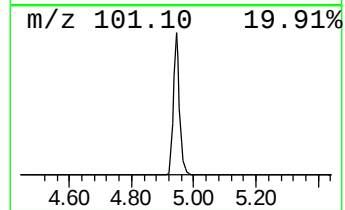
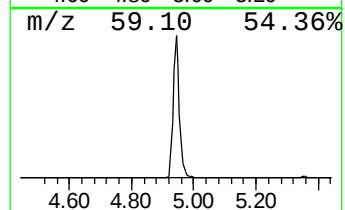
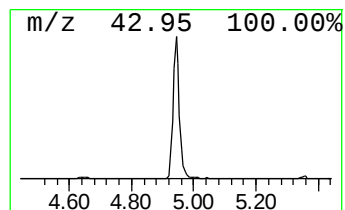
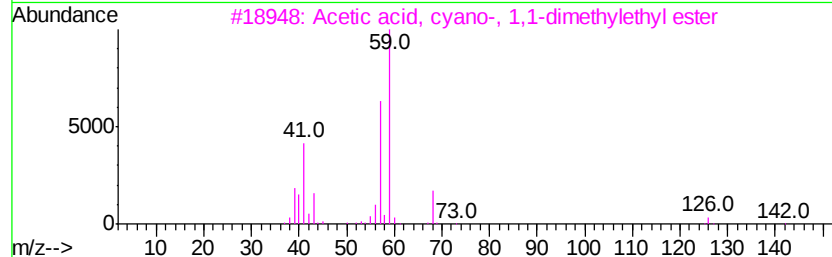
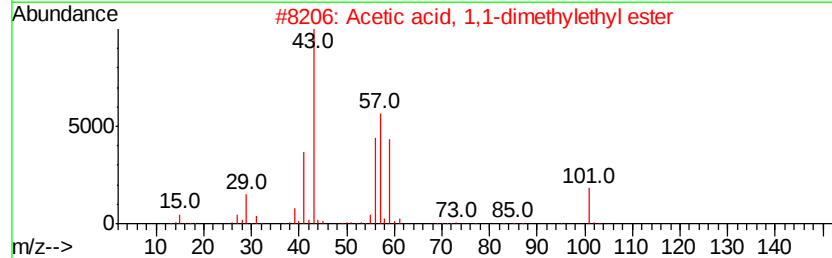
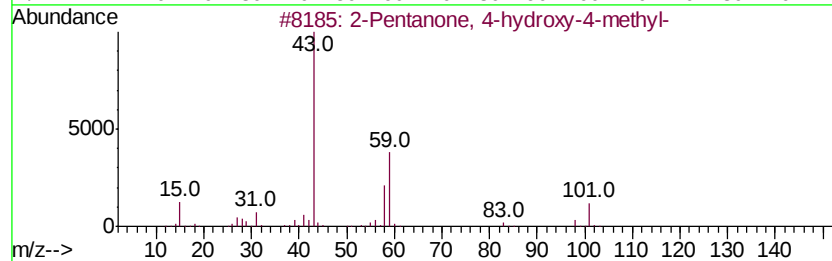
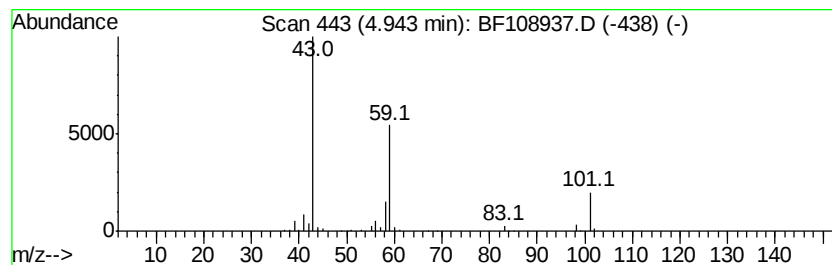
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	11.79 ng	601260	1,4-Dichlorobenzene-d4	6.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
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	23	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

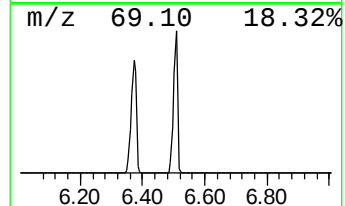
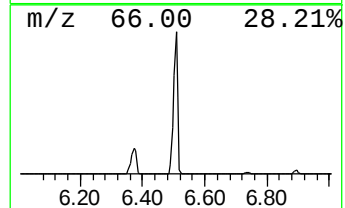
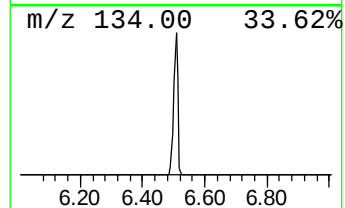
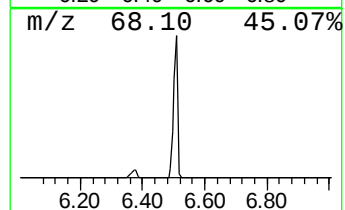
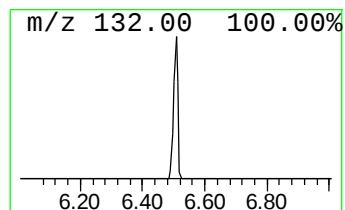
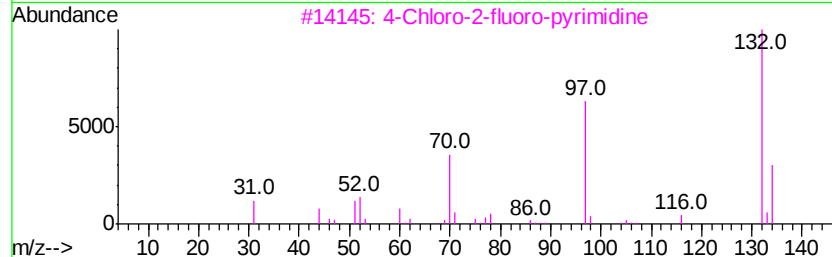
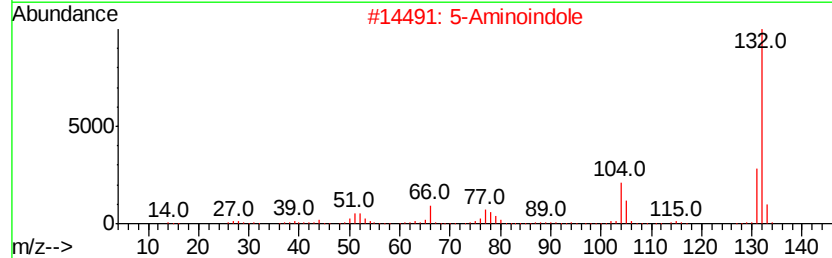
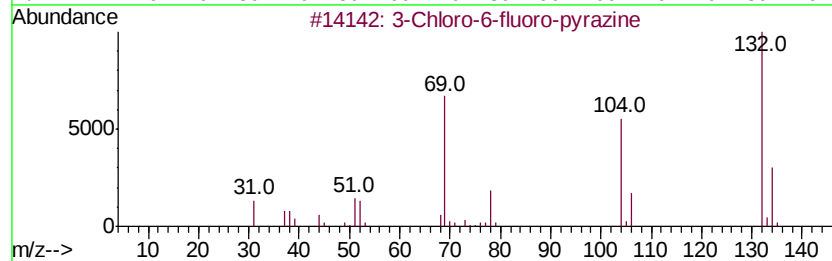
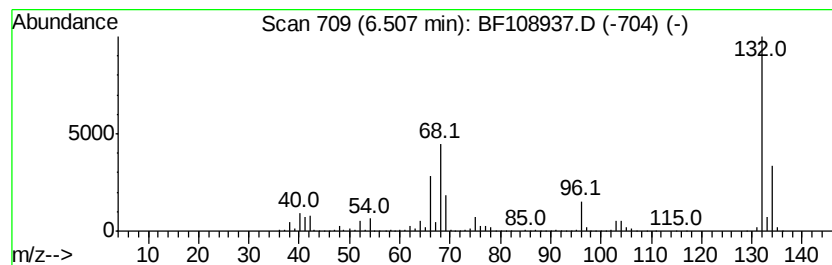
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	78.68 ng	4013450	1,4-Dichlorobenzene-d4	6.74

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			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

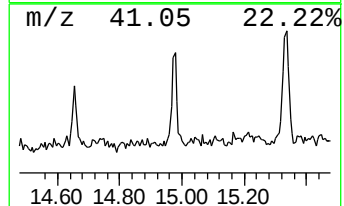
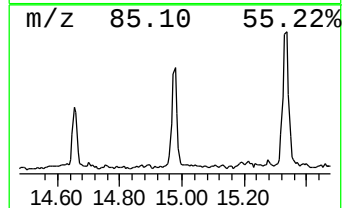
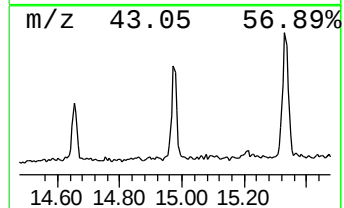
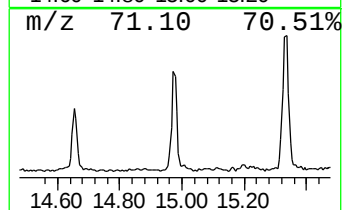
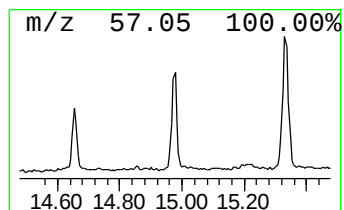
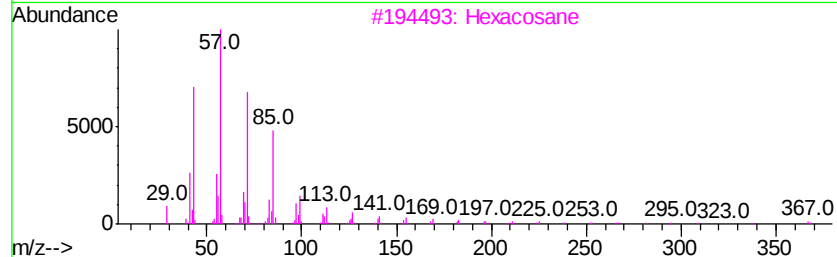
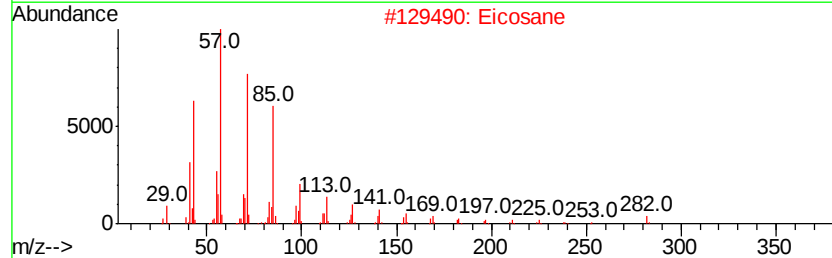
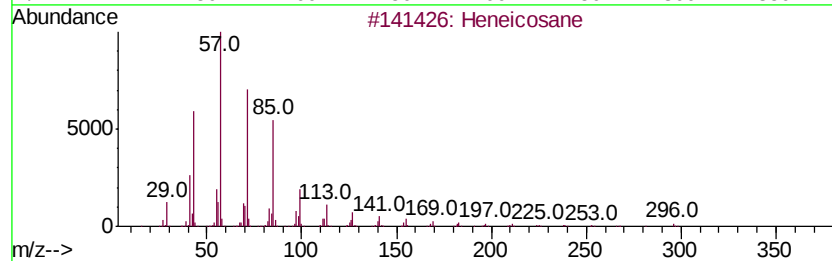
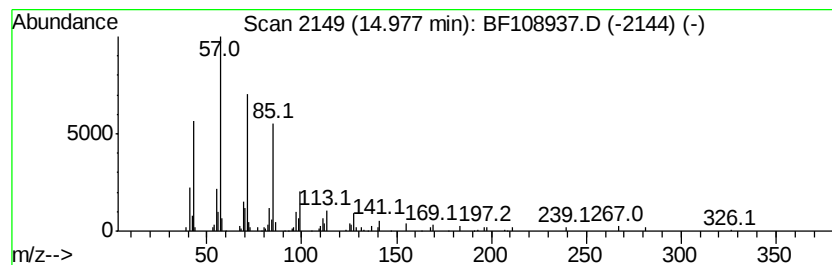
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.03 ng	110522	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Hexacosane		366	C26H54	000630-01-3	90
4	Docosane		310	C22H46	000629-97-0	87
5	Heptadecane		240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

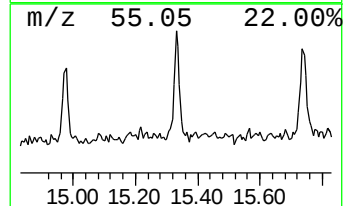
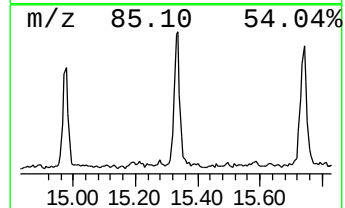
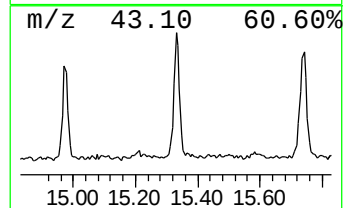
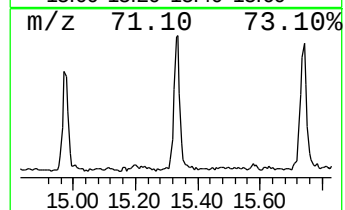
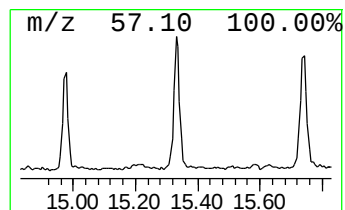
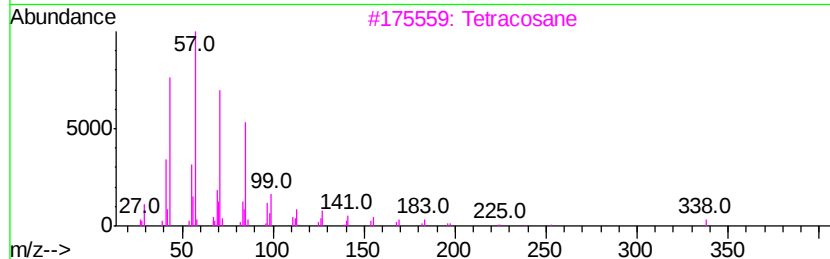
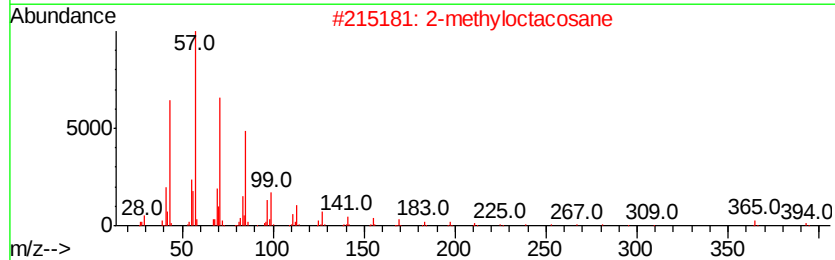
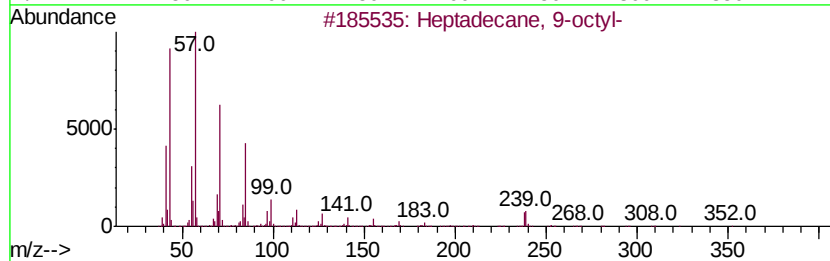
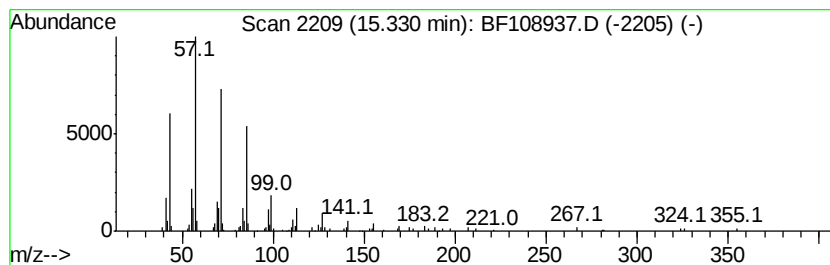
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	2.99 ng	162347	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

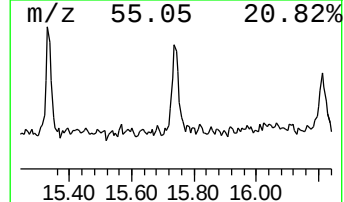
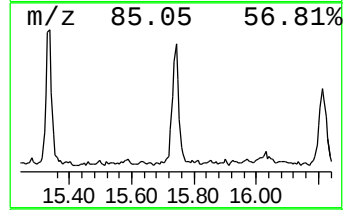
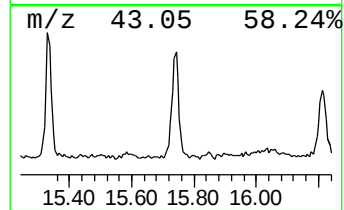
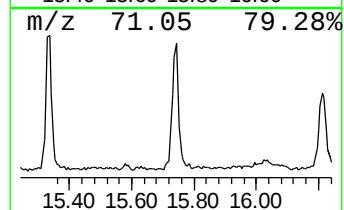
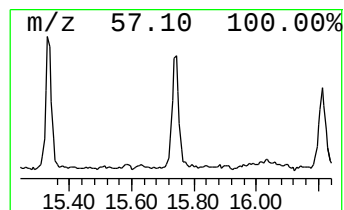
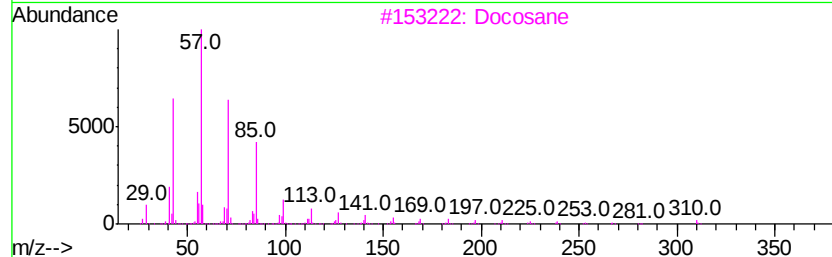
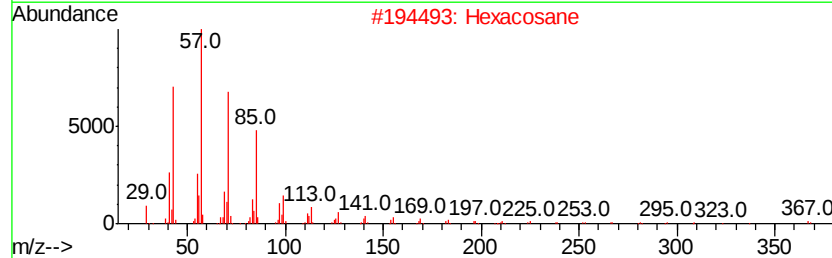
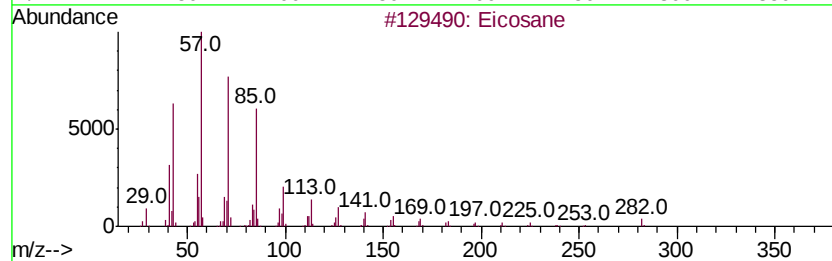
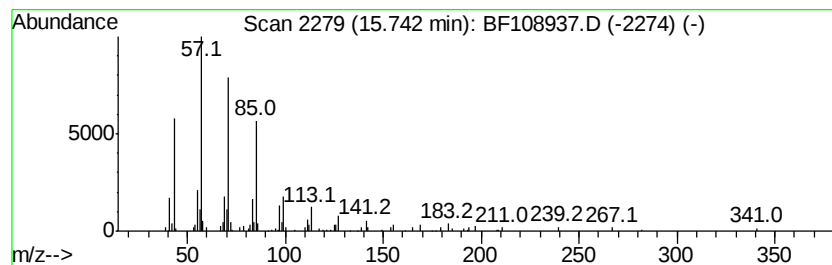
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.94 ng	159853	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Docosane	310	C22H46	000629-97-0	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

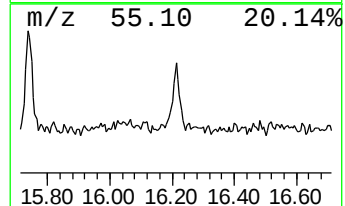
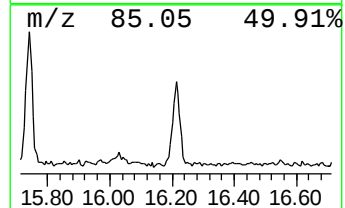
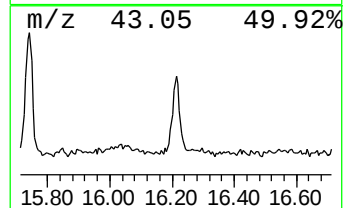
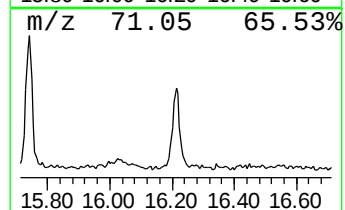
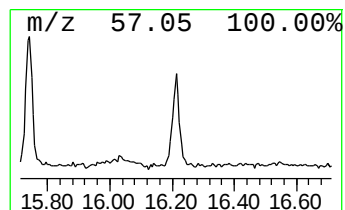
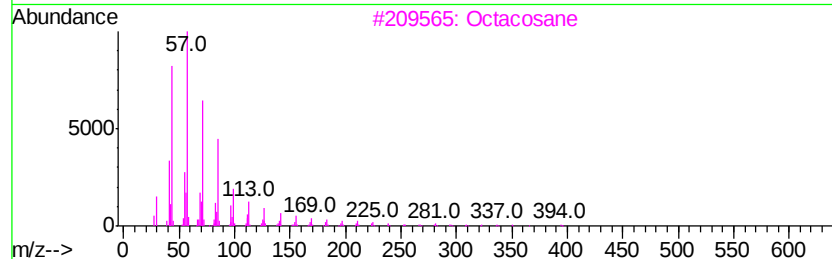
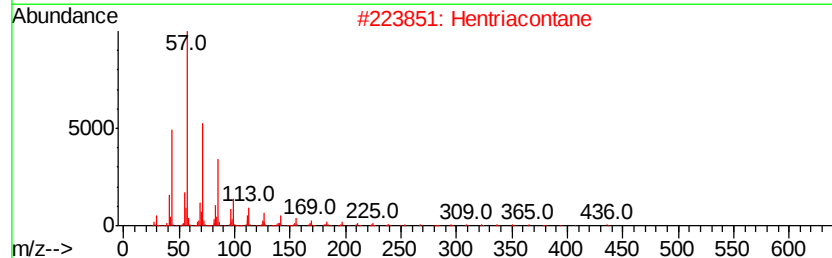
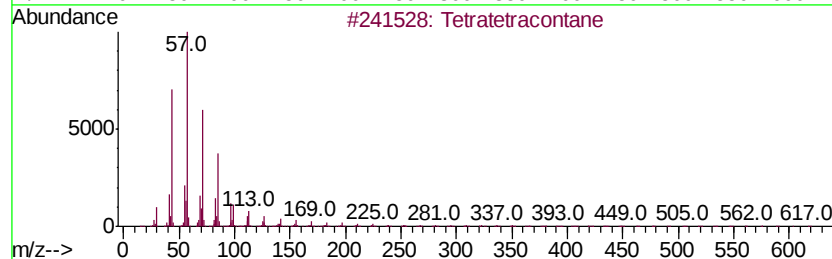
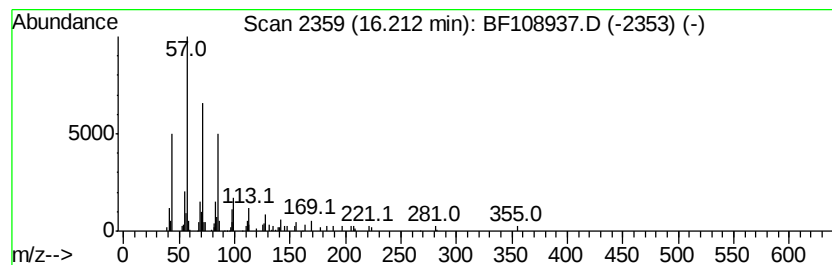
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.30 ng	124935	Perylene-d12	15.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Octacosane	394	C28H58	000630-02-4	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091118\
Data File : BF108937.D
Acq On : 11 Sep 2018 16:08
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112707BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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	11.8	ng	601260	1	6.74	1020190	20.0
unknown6.51	6.51	78.7	ng	4013450	1	6.74	1020190	20.0
Heneicosane	14.98	2.0	ng	110522	6	15.28	1086880	20.0
Heptadecane, 9-oc...	15.33	3.0	ng	162347	6	15.28	1086880	20.0
Eicosane	15.74	2.9	ng	159853	6	15.28	1086880	20.0
Tetratetracontane	16.21	2.3	ng	124935	6	15.28	1086880	20.0