

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
 Data File : BF088140.D
 Acq On : 18 Jun 2016 18:08
 Operator : UM/SJ
 Sample : H3501-22
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB14(1-3)

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-BF060716.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	1.667	5	7	11	rBV	95857	136347	6.99%	0.730%
2	1.735	11	13	15	rVV	21390	31493	1.62%	0.169%
3	1.781	15	17	24	rVV	855805	1233241	63.26%	6.600%
4	1.884	24	26	57	rVB2	74985	348836	17.89%	1.867%
5	2.913	115	116	128	rVB2	12971	36816	1.89%	0.197%
6	4.844	283	285	292	rBV	89671	119436	6.13%	0.639%
7	5.290	322	324	326	rBV	1727822	1757891	90.17%	9.408%
8	6.342	413	416	419	rBV2	1439139	1810585	92.88%	9.690%
9	6.456	424	426	429	rBV	1694737	1645024	84.38%	8.804%
10	6.685	444	446	449	rBV	677526	563701	28.92%	3.017%
11	6.845	457	460	462	rBV	1642458	1594911	81.81%	8.536%
12	7.256	493	496	498	rBV	993252	989177	50.74%	5.294%
13	7.370	501	506	512	rVB3	10531	28557	1.46%	0.153%
14	7.976	556	559	561	rBV	625046	710185	36.43%	3.801%
15	9.050	650	653	655	rBV	2163743	1949456	100.00%	10.433%
16	9.451	685	688	690	rBV	738148	627190	32.17%	3.357%
17	9.553	692	697	703	rBV	11167	22163	1.14%	0.119%
18	9.725	709	712	714	rBV	696982	693433	35.57%	3.711%
19	10.159	749	750	752	rVB	24289	21331	1.09%	0.114%
20	10.513	778	781	783	rBV2	531942	719746	36.92%	3.852%
21	10.628	789	791	798	rVB	28104	47489	2.44%	0.254%
22	11.074	829	830	832	rBV	30978	42424	2.18%	0.227%
23	11.199	839	841	843	rBV	706368	599034	30.73%	3.206%
24	11.451	861	863	866	rBV	15113	23275	1.19%	0.125%
25	11.508	866	868	870	rVB	51541	50296	2.58%	0.269%
26	11.908	901	903	907	rVB	38700	32976	1.69%	0.176%
27	12.788	977	980	982	rBV	1362312	1617608	82.98%	8.657%
28	13.634	1051	1054	1058	rBV	11380	22099	1.13%	0.118%
29	13.702	1058	1060	1063	rBV	45064	66050	3.39%	0.353%
30	13.828	1068	1071	1074	rBV	650611	597772	30.66%	3.199%
31	13.931	1074	1080	1082	rBV	32963	39065	2.00%	0.209%
32	14.308	1111	1113	1115	rBV2	14182	22340	1.15%	0.120%
33	14.662	1142	1144	1147	rBV	16109	27086	1.39%	0.145%
34	15.211	1190	1192	1198	rVB	401389	457936	23.49%	2.451%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088140.D
Acq On : 18 Jun 2016 18:08
Operator : UM/SJ
Sample : H3501-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB14(1-3)

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

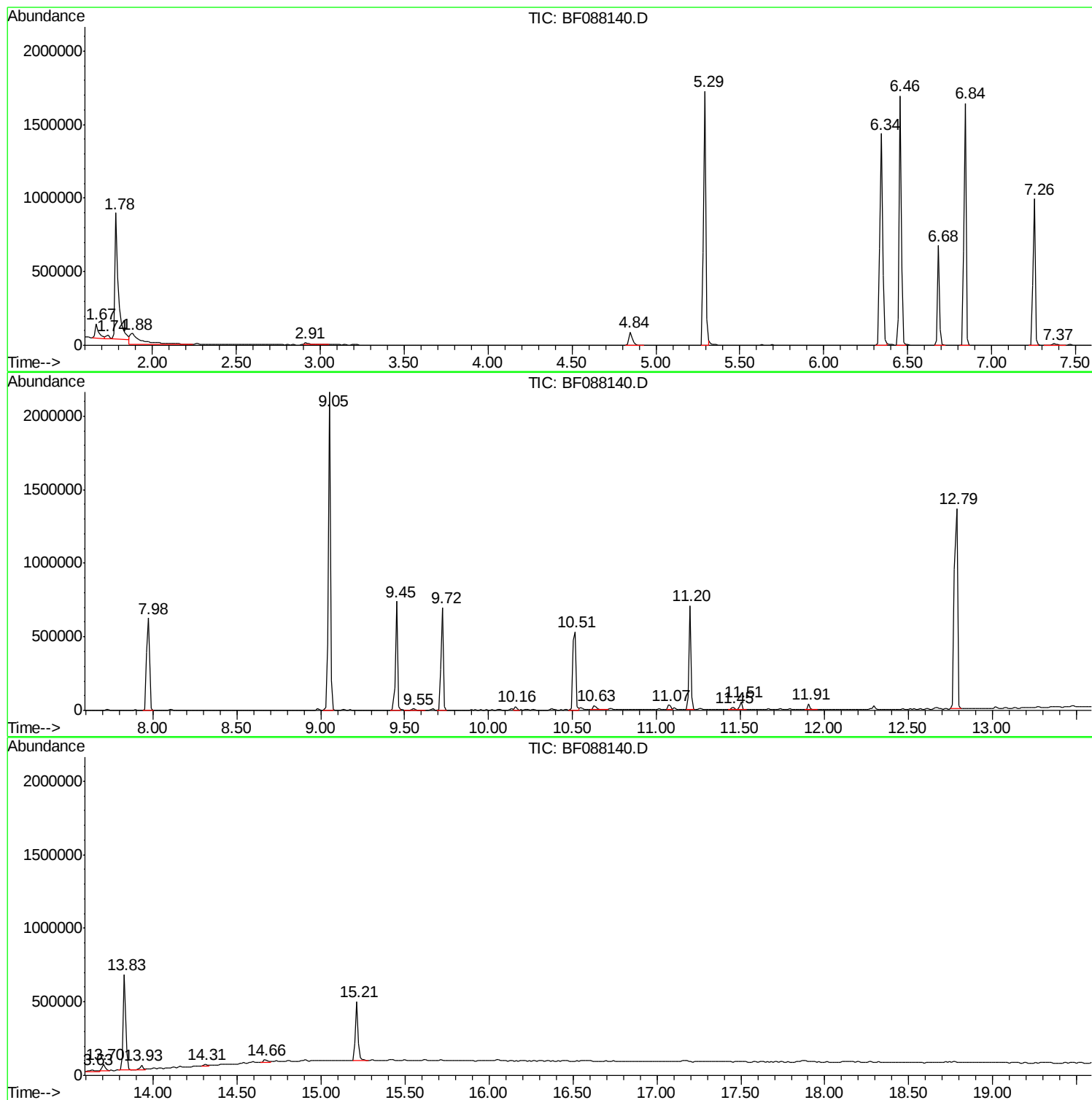
Sum of corrected areas: 18684969

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088140.D
Acq On : 18 Jun 2016 18:08
Operator : UM/SJ
Sample : H3501-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB14(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061816\
Data File : BF088140.D
Acq On : 18 Jun 2016 18:08
Operator : UM/SJ
Sample : H3501-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB14(1-3)

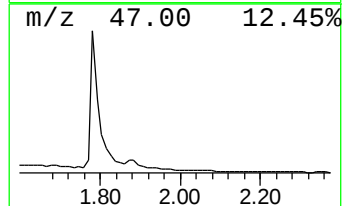
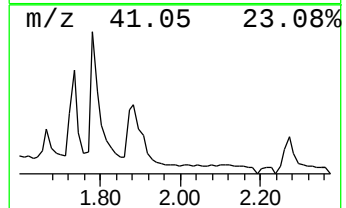
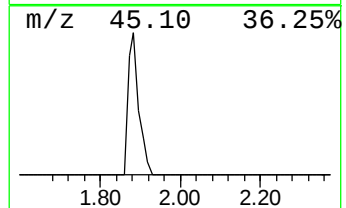
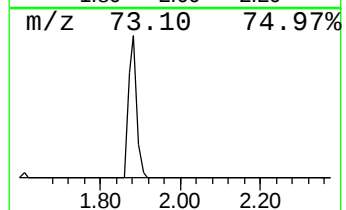
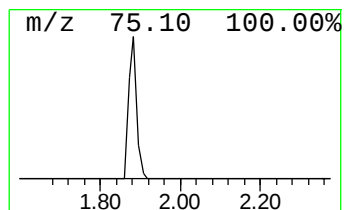
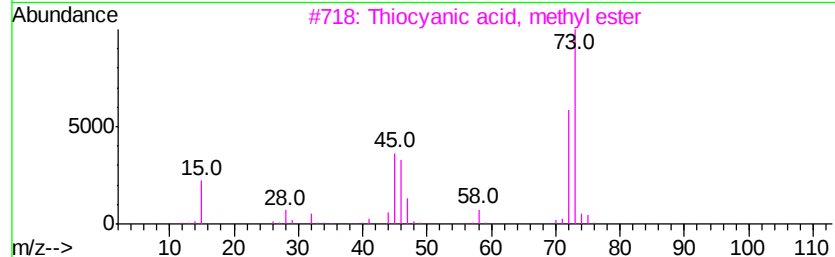
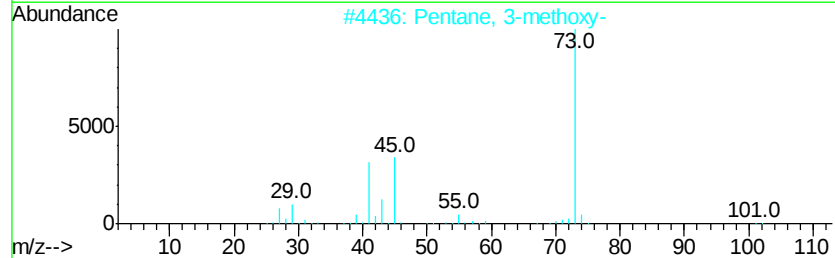
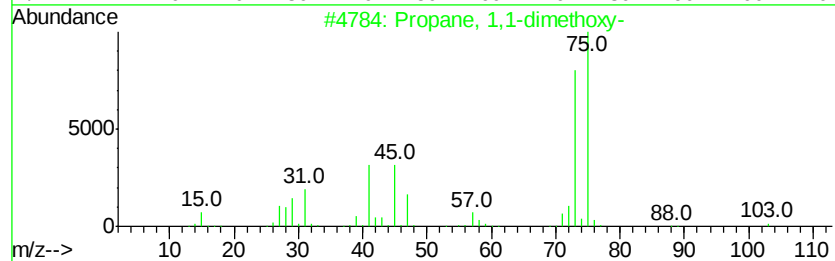
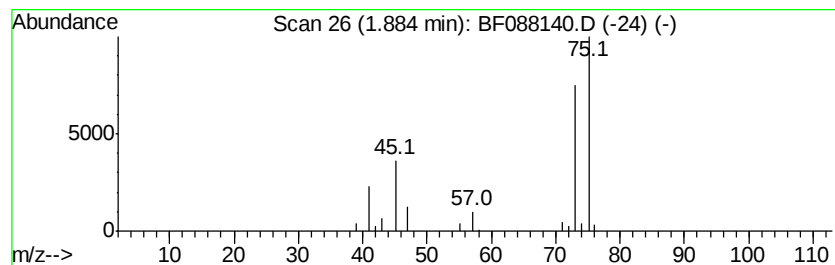
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	12.38 ng	348836	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	12
4		Glycine	75	C2H5NO2	000056-40-6	9
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088140.D
Acq On : 18 Jun 2016 18:08
Operator : UM/SJ
Sample : H3501-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB14(1-3)

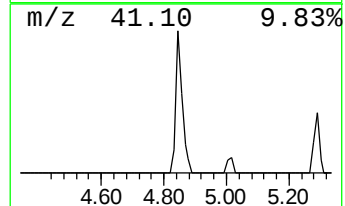
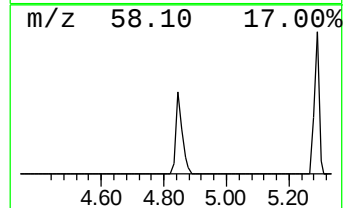
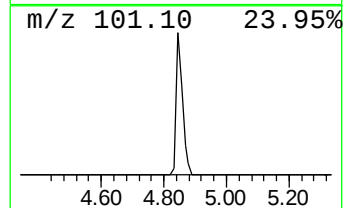
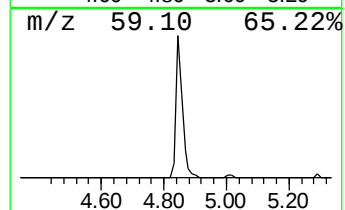
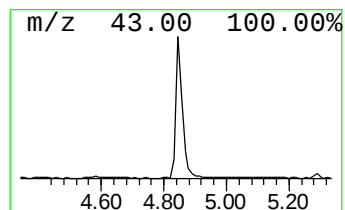
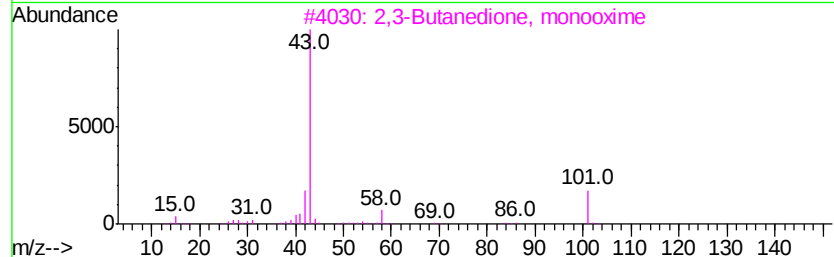
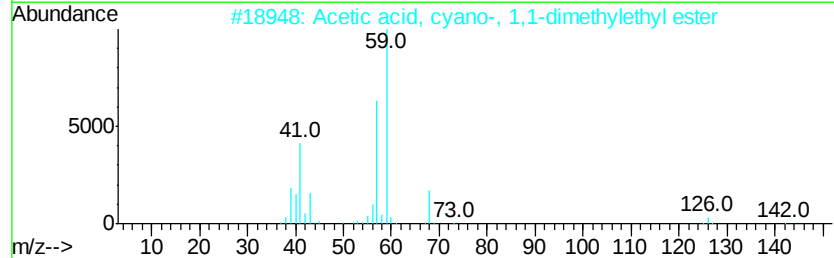
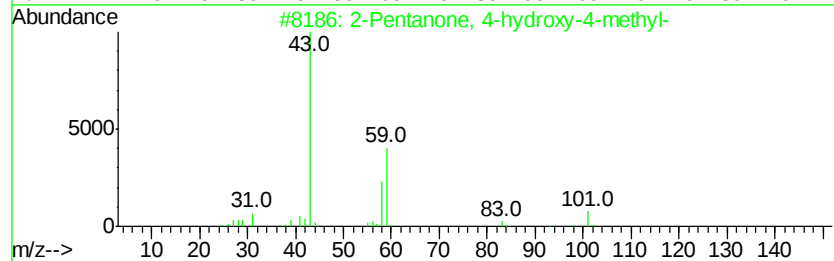
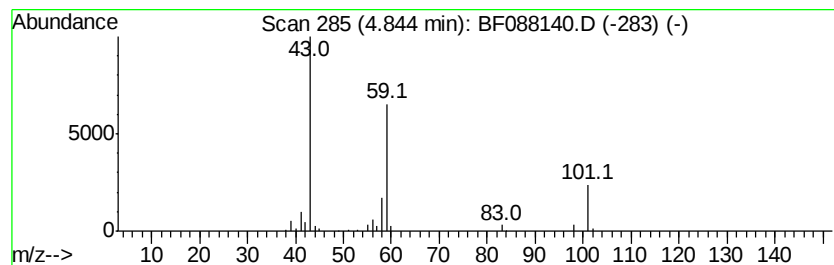
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	4.24 ng	119436	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088140.D
Acq On : 18 Jun 2016 18:08
Operator : UM/SJ
Sample : H3501-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB14(1-3)

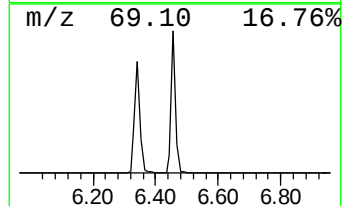
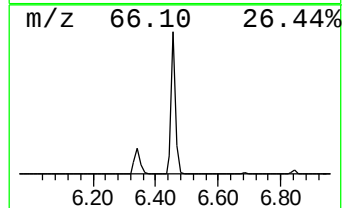
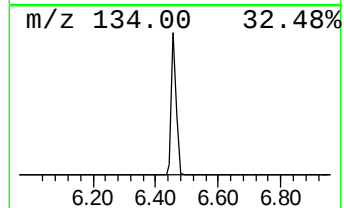
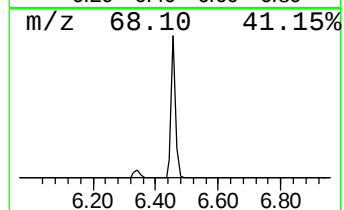
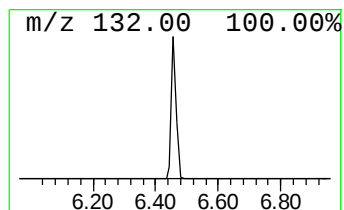
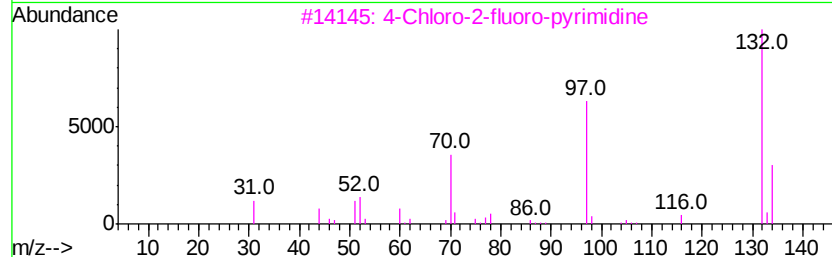
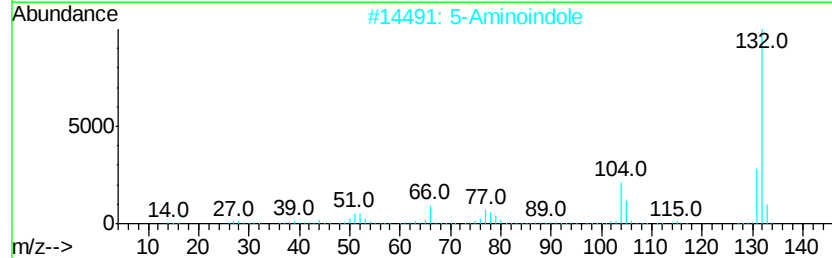
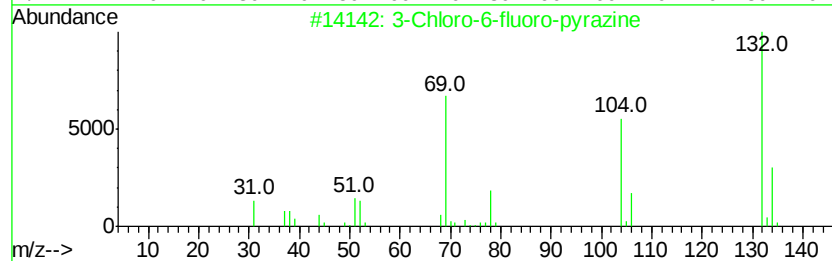
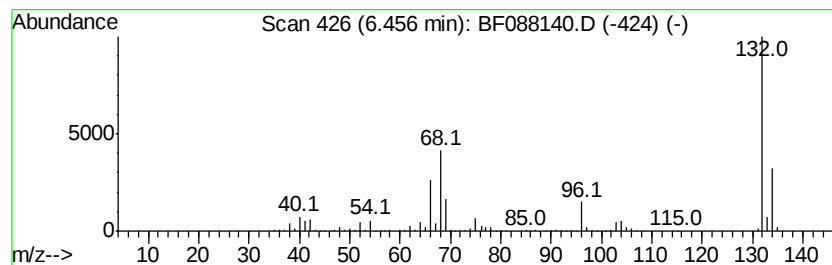
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	58.37 ng	1645020	1,4-Dichlorobenzene-d4	6.68

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-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088140.D
Acq On : 18 Jun 2016 18:08
Operator : UM/SJ
Sample : H3501-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB14(1-3)

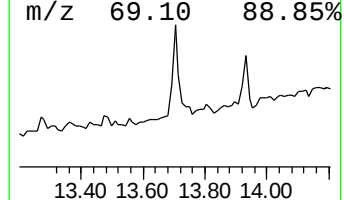
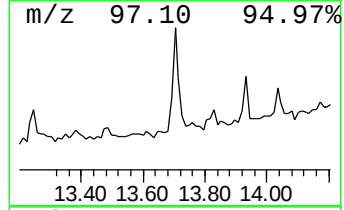
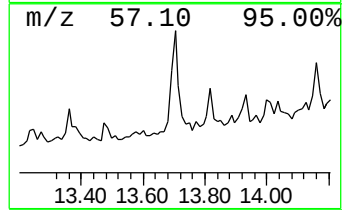
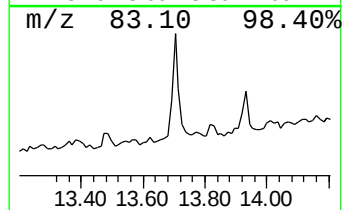
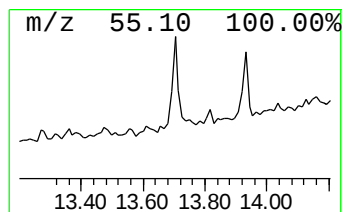
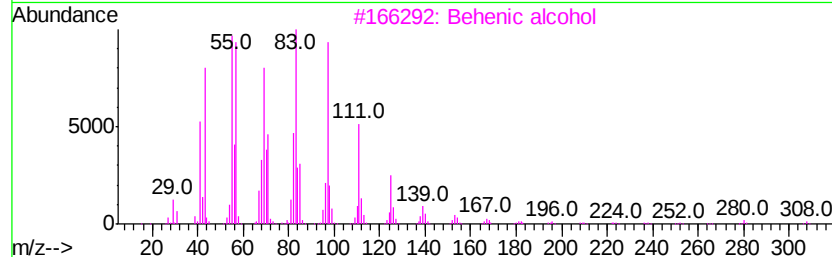
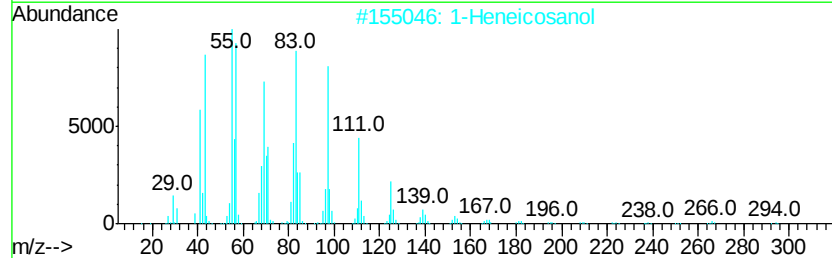
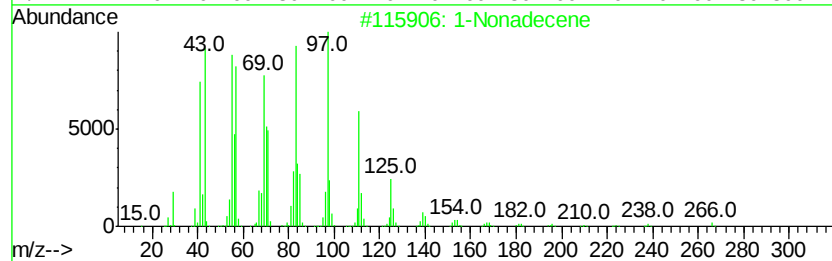
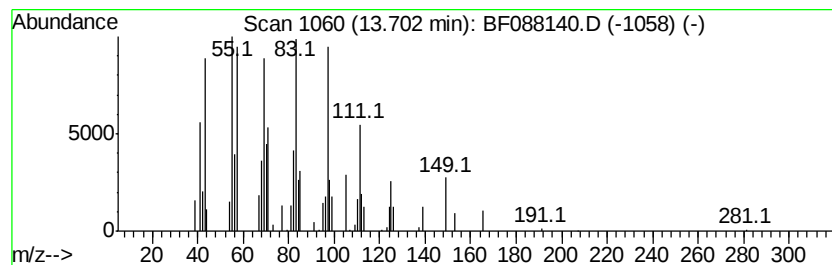
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.21 ng	66050	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	93
2	1-Heneicosanol		312	C21H44O	015594-90-8	93
3	Behenic alcohol		326	C22H46O	000661-19-8	93
4	Pentafluoropropionic acid, hexad...		388	C19H33F5O2	006222-07-7	93
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088140.D
Acq On : 18 Jun 2016 18:08
Operator : UM/SJ
Sample : H3501-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB14(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
Propane, 1,1-dime...	1.88	12.4	ng	348836	1	6.68	563701	20.0
2-Pentanone, 4-hy...	4.84	4.2	ng	119436	1	6.68	563701	20.0
unknown6.46	6.46	58.4	ng	1645020	1	6.68	563701	20.0
1-Nonadecene	13.70	2.2	ng	66050	5	13.83	597772	20.0