

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
 Data File : BF087701.D
 Acq On : 5 Jun 2016 11:12
 Operator : UM/SJ
 Sample : H3312-05
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW2

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-BF060416.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	1.770	15	16	26	rVV	311810	547531	12.77%	1.757%
2	1.907	26	28	47	rVB	2303376	4288432	100.00%	13.759%
3	5.039	300	302	305	rBV	143515	165650	3.86%	0.531%
4	5.450	335	338	340	rBV	1524886	1414727	32.99%	4.539%
5	6.479	425	428	430	rBV	1095482	916112	21.36%	2.939%
6	6.627	438	441	443	rBV	2483306	2708982	63.17%	8.691%
7	6.856	459	461	464	rBV	868504	783997	18.28%	2.515%
8	7.016	472	475	477	rBV	2583430	2359994	55.03%	7.572%
9	7.382	505	507	508	rBV	60085	66340	1.55%	0.213%
10	7.427	508	511	513	rVB	1940012	2237721	52.18%	7.179%
11	7.542	519	521	523	rVB	83850	103556	2.41%	0.332%
12	8.148	571	574	576	rBV	1023257	1047104	24.42%	3.359%
13	8.479	599	603	607	rBV3	29667	70198	1.64%	0.225%
14	9.108	656	658	660	rBV	35040	44899	1.05%	0.144%
15	9.222	665	668	671	rBV	2926864	3603722	84.03%	11.562%
16	9.622	700	703	705	rVB	741094	725169	16.91%	2.327%
17	9.828	719	721	725	rBV	176331	170368	3.97%	0.547%
18	9.896	725	727	729	rVB	1135881	1109777	25.88%	3.560%
19	10.319	762	764	767	rBV3	45147	74167	1.73%	0.238%
20	10.685	793	796	799	rBV	1975203	2178333	50.80%	6.989%
21	10.811	805	807	812	rVB2	50524	54576	1.27%	0.175%
22	10.902	813	815	817	rBV	50697	49401	1.15%	0.158%
23	11.256	844	846	851	rBV2	50972	79346	1.85%	0.255%
24	11.382	854	857	859	rVB	1217064	1131161	26.38%	3.629%
25	11.919	902	904	908	rBV2	341553	414765	9.67%	1.331%
26	12.708	971	973	979	rBV	250192	274019	6.39%	0.879%
27	12.971	993	996	998	rBV	2835464	2841335	66.26%	9.116%
28	13.874	1073	1075	1085	rVB	196681	207120	4.83%	0.665%
29	14.011	1085	1087	1090	rVB	879749	821627	19.16%	2.636%
30	15.440	1209	1212	1215	rVB	578637	679018	15.83%	2.178%

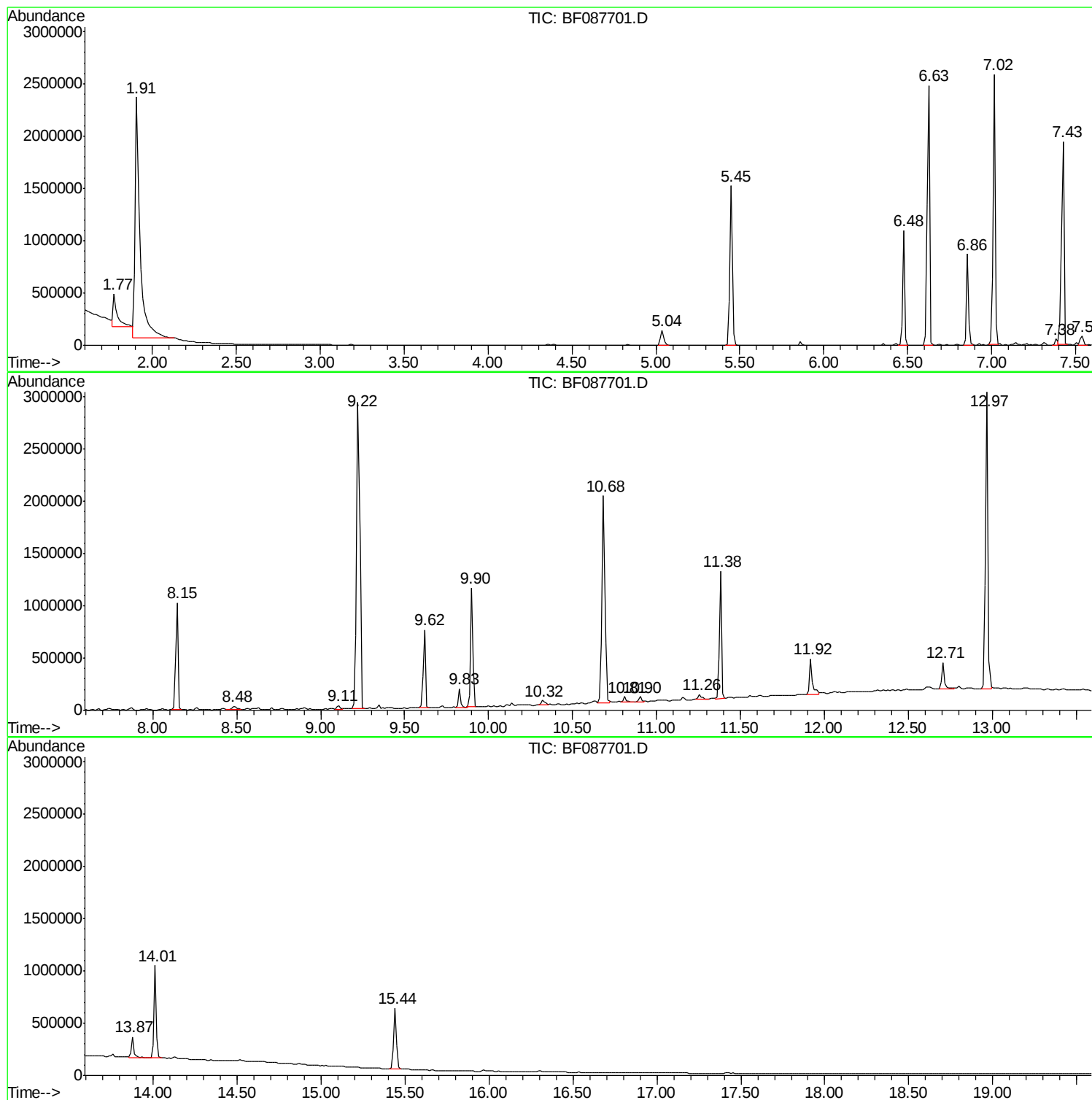
Sum of corrected areas: 31169147

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SW2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

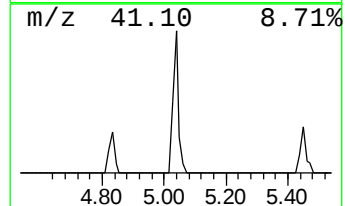
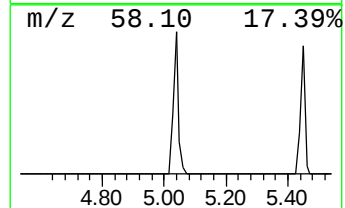
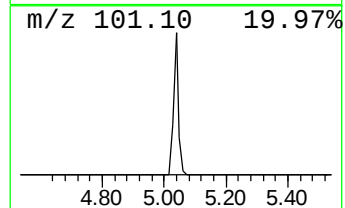
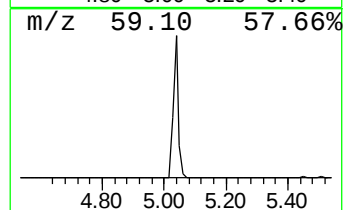
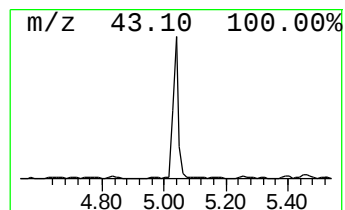
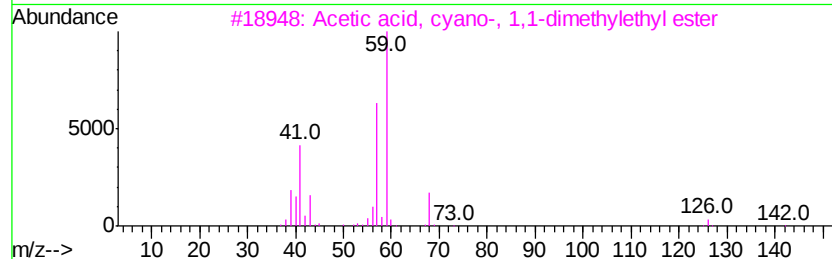
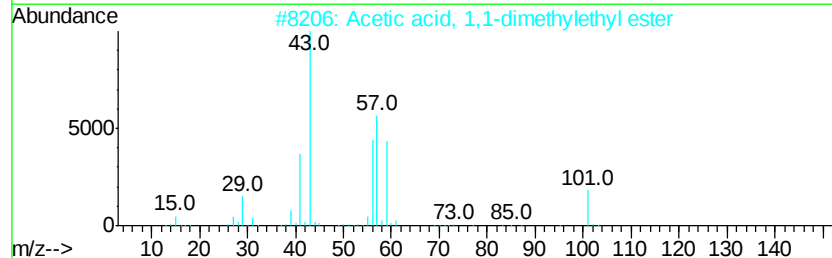
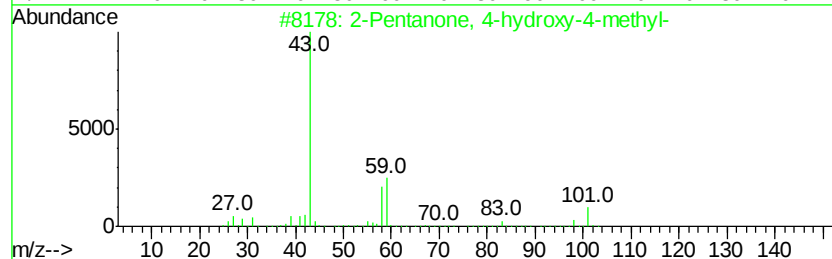
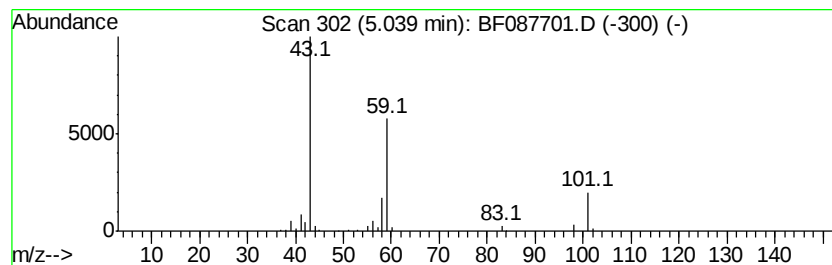
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.23 ng	165650	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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-dimethy...	141	C7H11NO2	001116-98-9	32
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

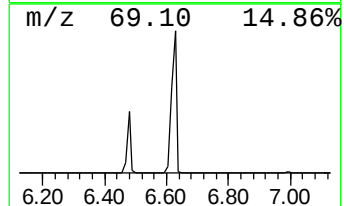
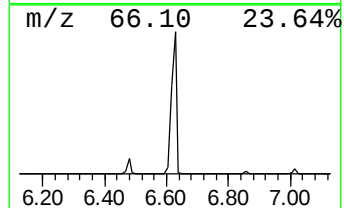
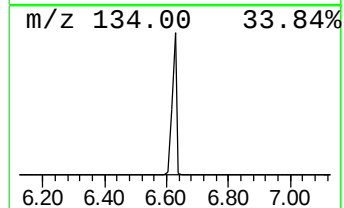
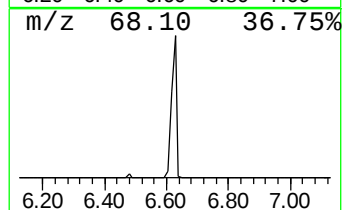
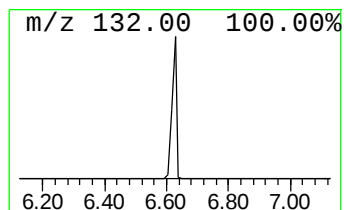
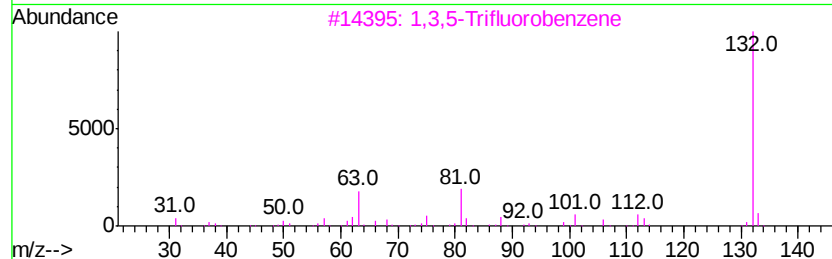
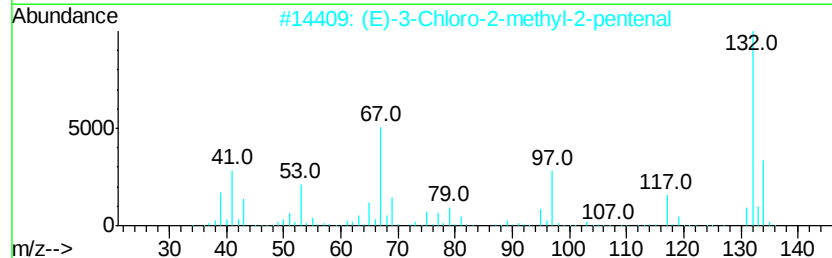
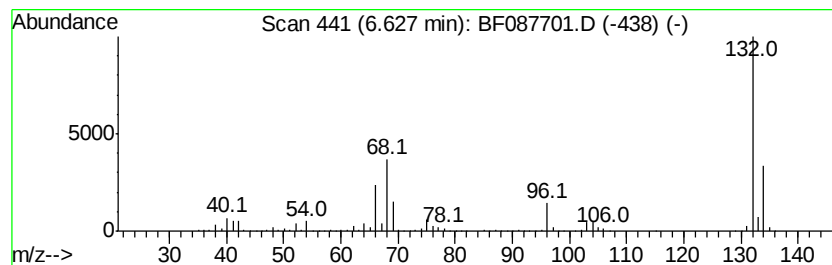
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	69.11 ng	2708980	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

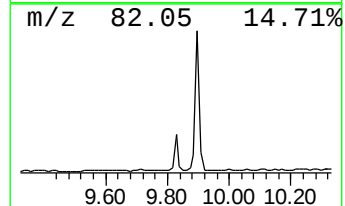
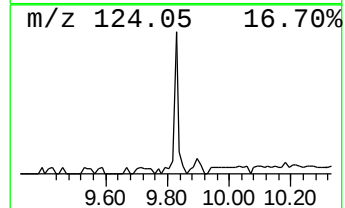
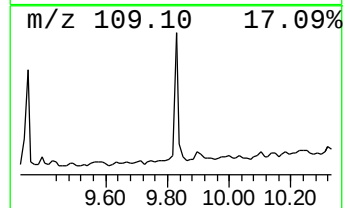
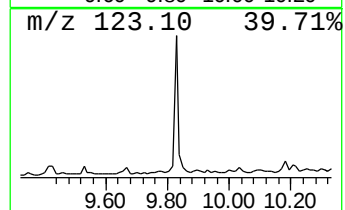
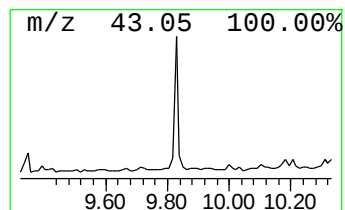
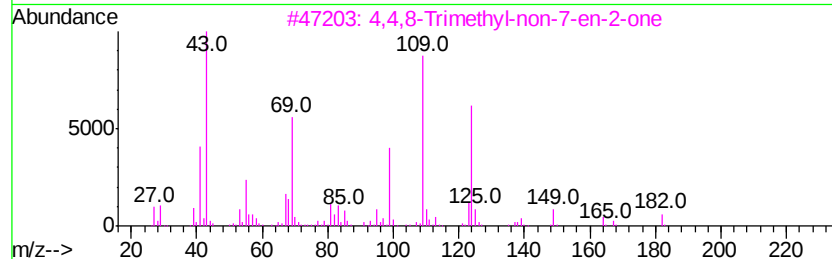
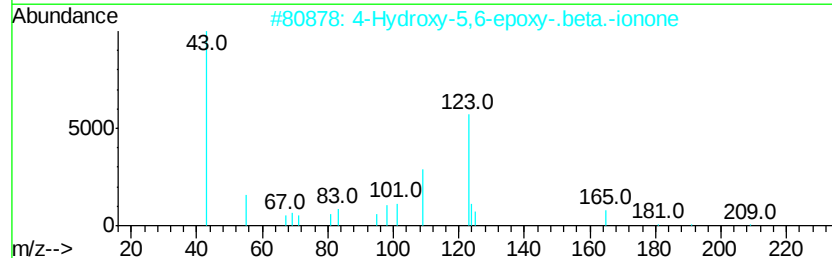
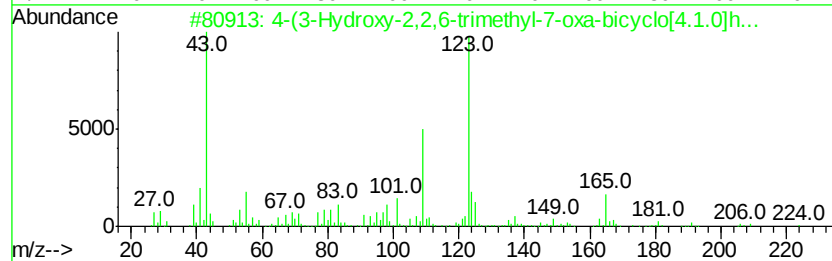
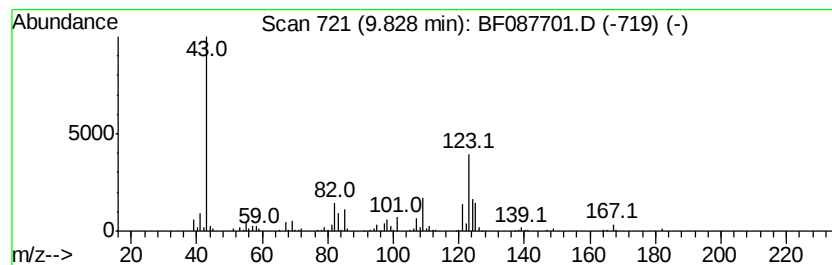
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4-(3-Hydroxy-2,2,6-trimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	3.07 ng	170368	Acenaphthene-d10	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(3-Hydroxy-2,2,6-trimethyl-7-oxa-bicyclo[4.1.0]hept-5-en-5-ylidene)-2-methyl-2-butanol	224	C13H20O3	1000190-36-6	53
2			4-Hydroxy-5,6-epoxy- β -ionone	224	C13H20O3	1000108-78-1	47
3			4,4,8-Trimethyl-non-7-en-2-one	182	C12H22O	1000187-18-6	10
4			3-Cyclohexen-1-carboxaldehyde, 3-methyl-	124	C8H12O	056980-32-6	9
5			Bicyclo[2.2.2]octane-1,4-diol, methyl-	184	C10H16O3	054774-94-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

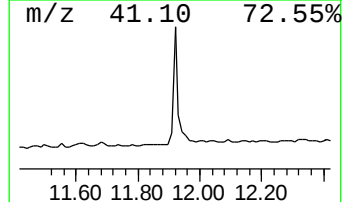
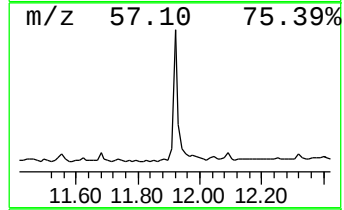
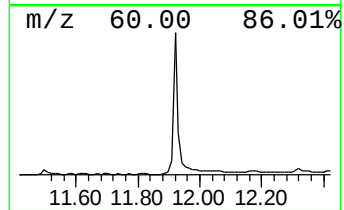
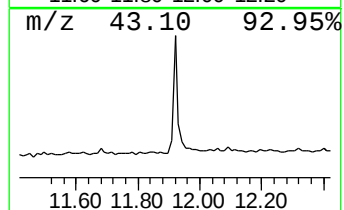
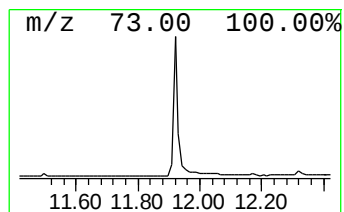
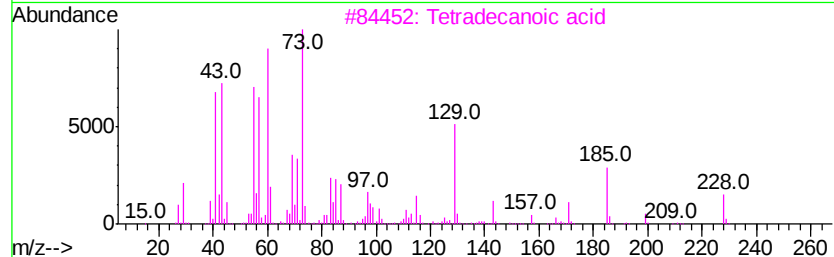
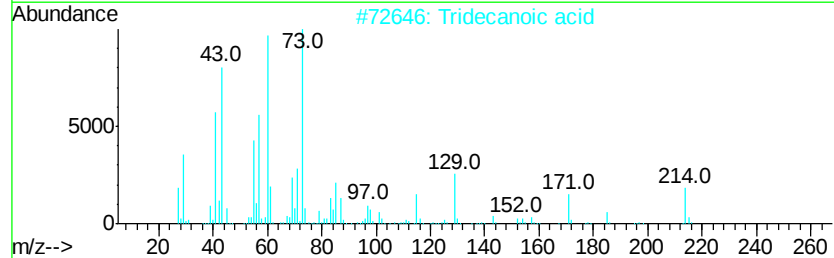
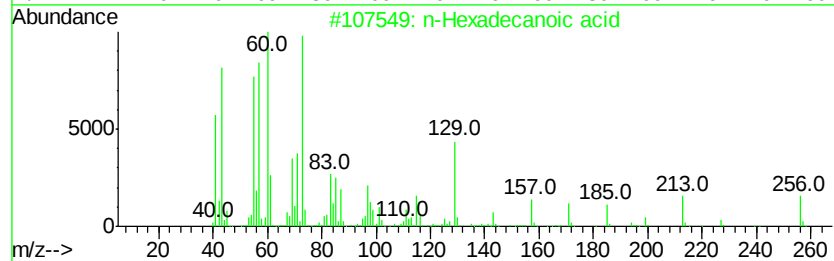
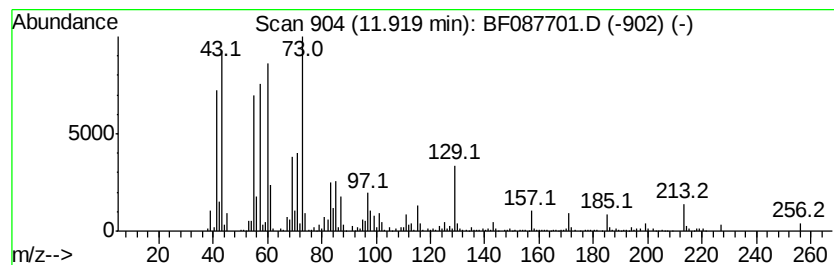
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.33 ng	414765	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	70



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

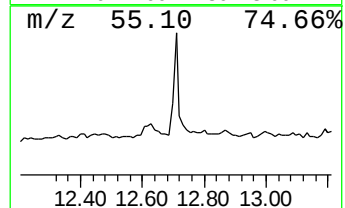
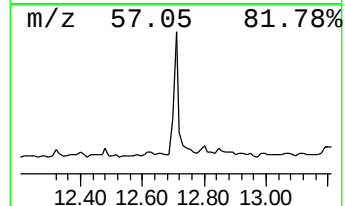
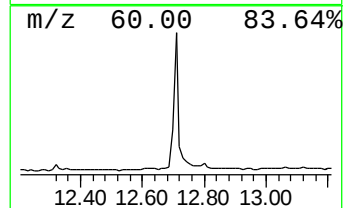
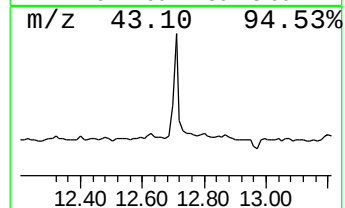
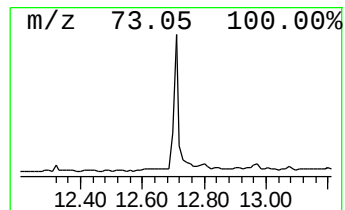
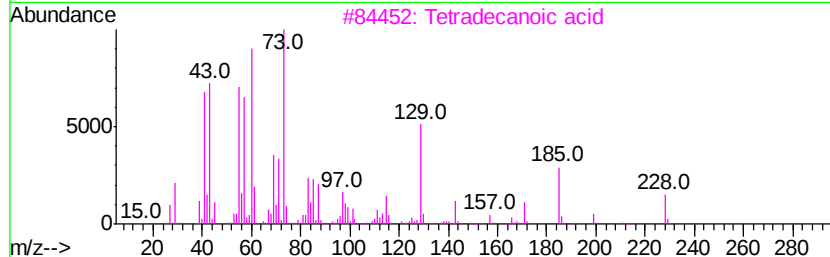
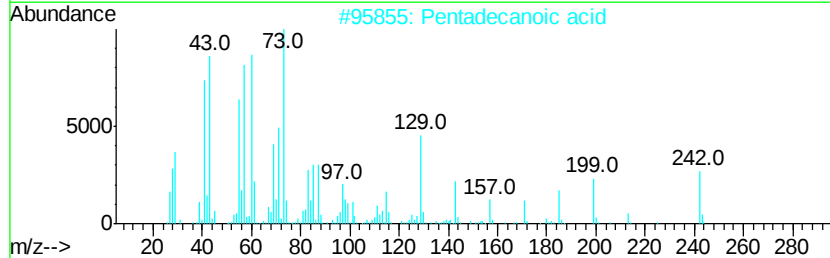
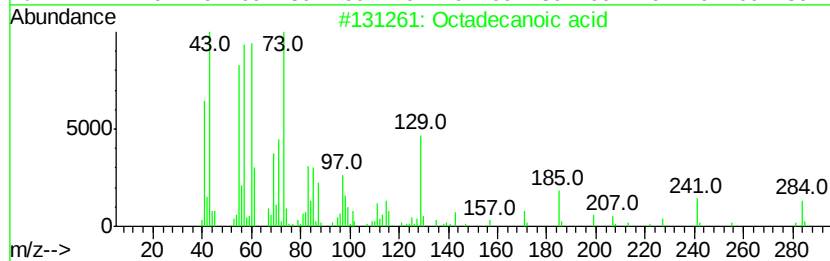
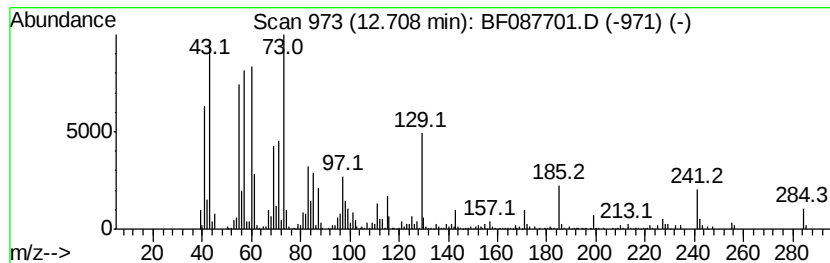
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	6.67 ng	274019	Chrysene-d12	14.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

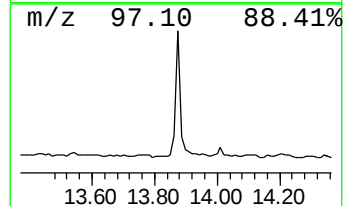
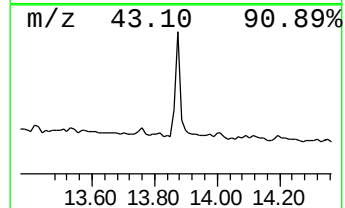
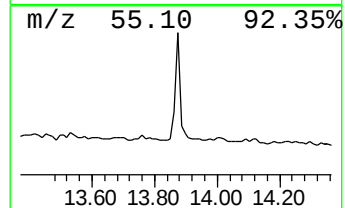
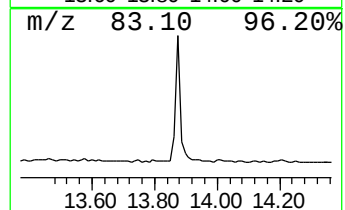
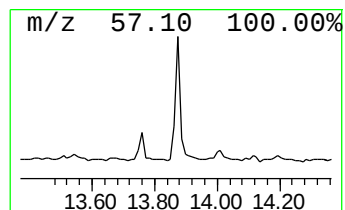
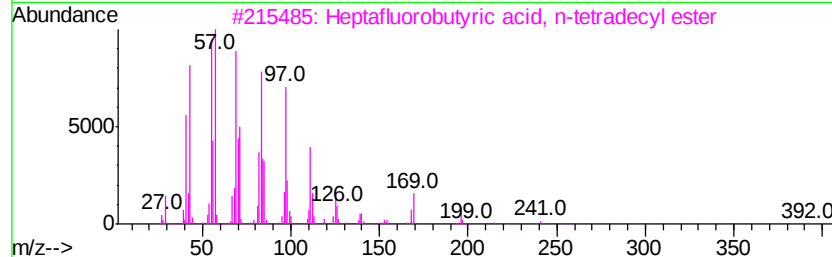
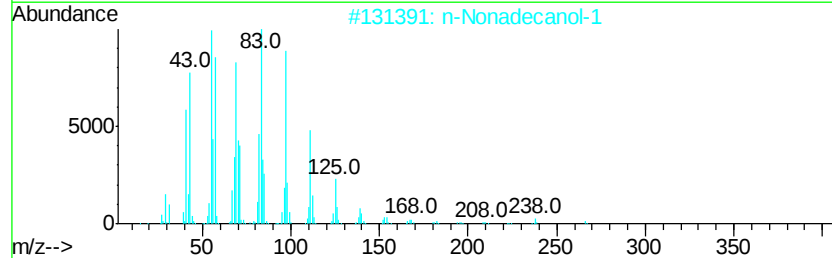
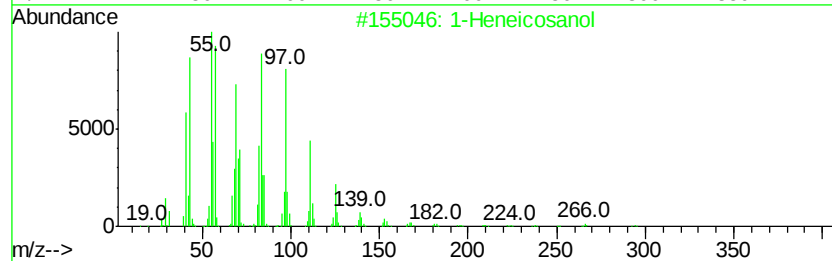
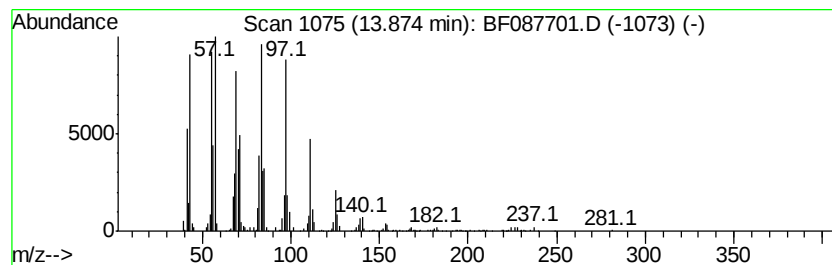
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	5.04 ng	207120	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5		Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087701.D
Acq On : 5 Jun 2016 11:12
Operator : UM/SJ
Sample : H3312-05
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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...	5.04	4.2	ng	165650	1	6.86	783997	20.0
unknown6.63	6.63	69.1	ng	2708980	1	6.86	783997	20.0
4-(3-Hydroxy-2,2,...	9.83	3.1	ng	170368	3	9.90	1109780	20.0
n-Hexadecanoic acid	11.92	7.3	ng	414765	4	11.38	1131160	20.0
Octadecanoic acid	12.71	6.7	ng	274019	5	14.01	821627	20.0
1-Heneicosanol	13.87	5.0	ng	207120	5	14.01	821627	20.0