

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
 Data File : BF093797.D
 Acq On : 21 Mar 2017 14:47
 Operator : SJ/MA
 Sample : I2263-21
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-103D

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-BF032017.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	2.070	14	16	20	rVB2	55040	78234	1.39%	0.200%
2	4.984	269	271	274	rBV	295092	352672	6.28%	0.903%
3	5.419	306	309	311	rBV	2152214	2006462	35.74%	5.137%
4	5.830	343	345	347	rBV	101075	88914	1.58%	0.228%
5	6.447	397	399	402	rBV	1507803	1317563	23.47%	3.374%
6	6.596	409	412	414	rVB	3188686	4088731	72.84%	10.469%
7	6.825	430	432	434	rBV	1301568	1090180	19.42%	2.791%
8	6.985	443	446	448	rBV	4102889	3788664	67.49%	9.701%
9	7.385	478	481	483	rBV	2791738	3043466	54.22%	7.793%
10	7.933	523	529	533	rVB2	63359	131074	2.34%	0.336%
11	8.105	542	544	546	rBV	1220969	1414256	25.19%	3.621%
12	8.219	552	554	560	rVB3	30545	68743	1.22%	0.176%
13	8.413	569	571	573	rVB	75291	58094	1.03%	0.149%
14	8.630	588	590	592	rVB	128117	122840	2.19%	0.315%
15	9.190	636	639	641	rVB	5575816	5613312	100.00%	14.373%
16	9.362	651	654	658	rVB	73174	73221	1.30%	0.187%
17	9.625	675	677	681	rVB	309511	301086	5.36%	0.771%
18	9.762	686	689	691	rVB	99407	115136	2.05%	0.295%
19	9.865	695	698	700	rVB	1614029	1688918	30.09%	4.324%
20	9.968	703	707	708	rBV	46804	58665	1.05%	0.150%
21	10.196	724	727	729	rVB2	81455	105166	1.87%	0.269%
22	10.242	729	731	733	rBV	124473	130007	2.32%	0.333%
23	10.288	733	735	736	rVV	369327	438959	7.82%	1.124%
24	10.642	763	766	769	rBV2	2394239	3128108	55.73%	8.009%
25	10.779	776	778	782	rVB	51460	69973	1.25%	0.179%
26	10.871	784	786	790	rBV3	35262	60530	1.08%	0.155%
27	11.225	815	817	819	rBV	93851	91430	1.63%	0.234%
28	11.339	824	827	829	rVB	1875930	1614997	28.77%	4.135%
29	11.876	872	874	876	rBV	143725	153606	2.74%	0.393%
30	12.665	940	943	949	rBV	108191	147701	2.63%	0.378%
31	12.928	963	966	968	rBV	4691392	4959566	88.35%	12.699%
32	13.831	1042	1045	1051	rBV2	56863	88757	1.58%	0.227%
33	13.968	1054	1057	1059	rBV	1108263	1279524	22.79%	3.276%
34	14.162	1071	1074	1077	rBV	82637	96102	1.71%	0.246%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103D

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-BF032017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.562	1107	1109	1111	rBV	94600	94343	1.68%	0.242%
36	15.374	1177	1180	1182	rBV	637888	875120	15.59%	2.241%
37	15.843	1218	1221	1231	rVB	34911	63640	1.13%	0.163%
38	16.311	1258	1262	1267	rBV	32986	60548	1.08%	0.155%
39	16.494	1275	1278	1282	rBV	54581	97129	1.73%	0.249%

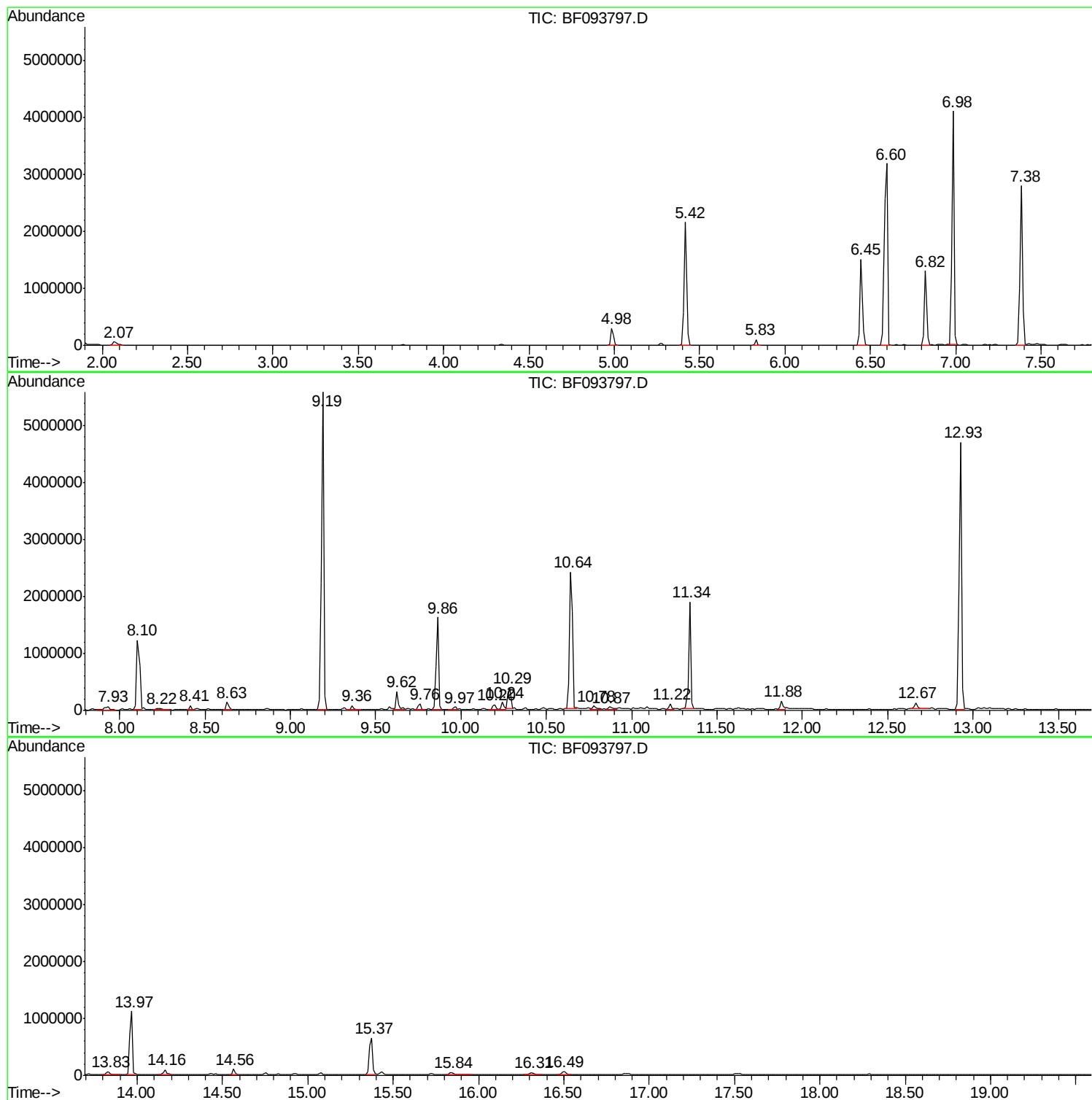
Sum of corrected areas: 39055437

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103D

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.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\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103D

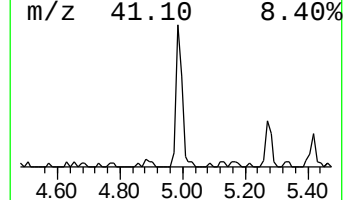
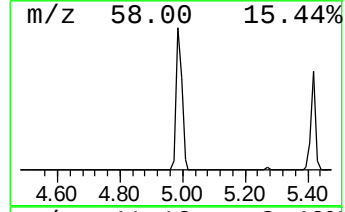
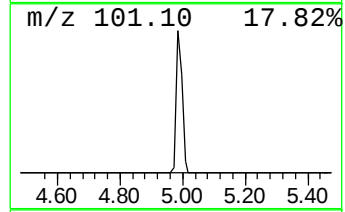
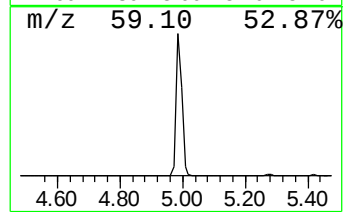
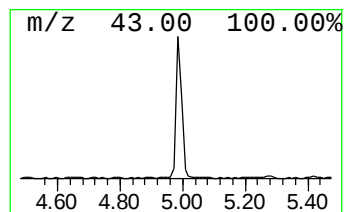
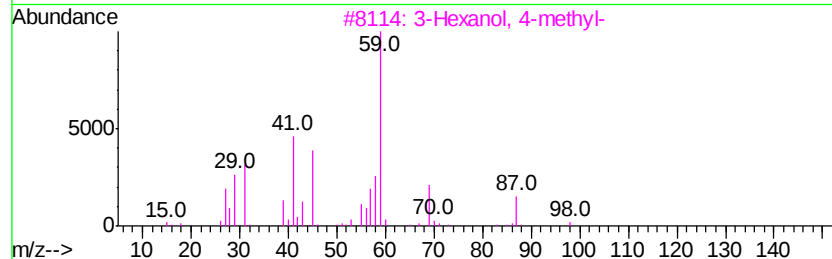
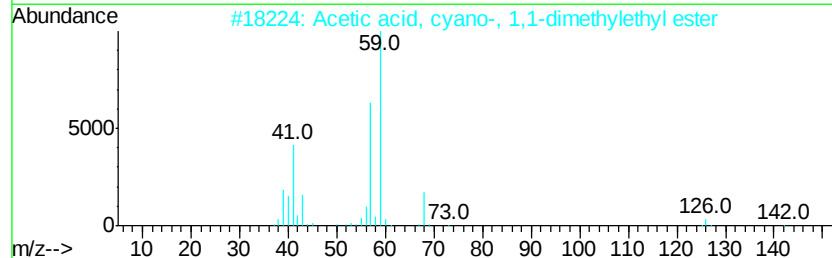
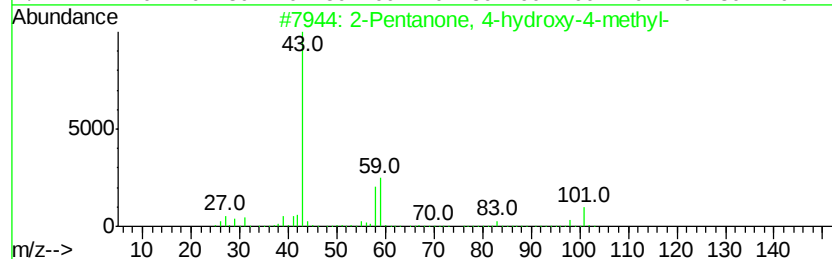
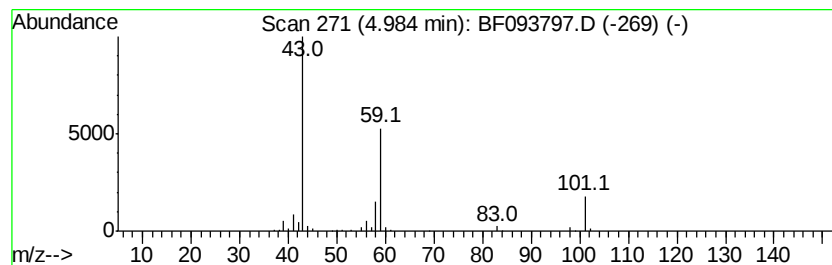
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.98	6.47 ng	352672	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	37
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103D

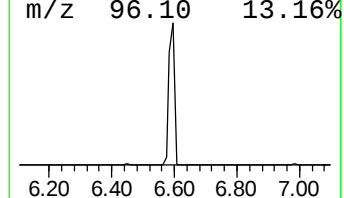
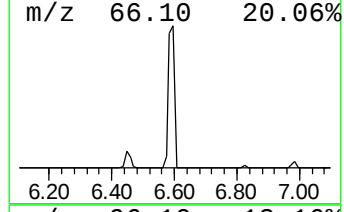
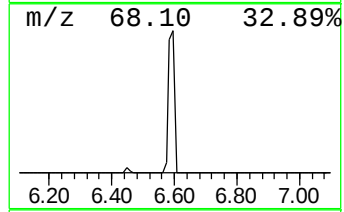
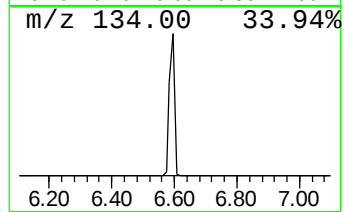
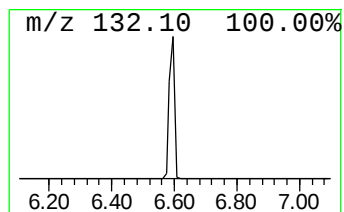
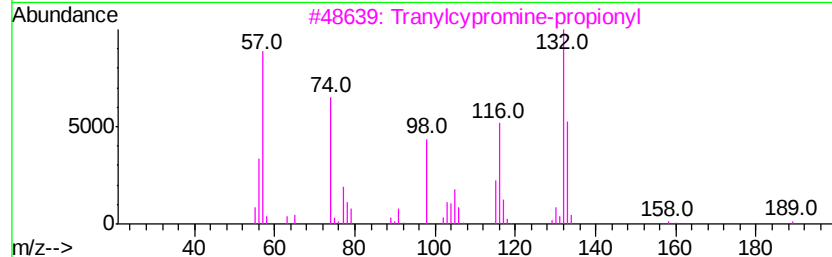
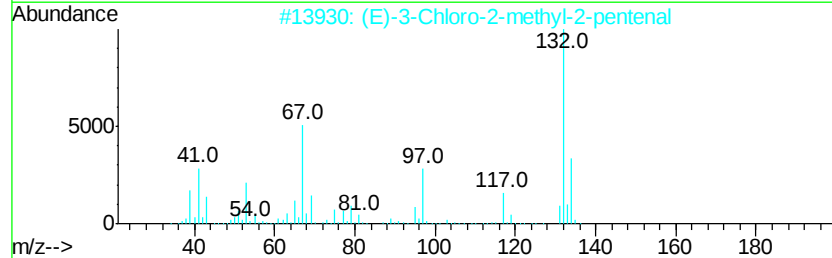
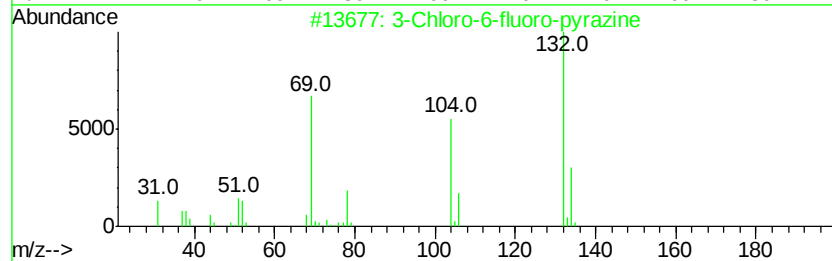
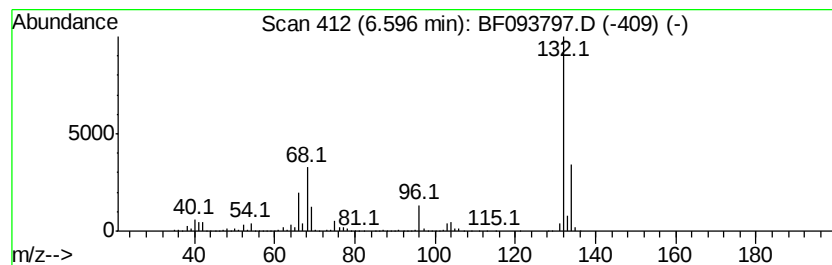
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	75.01 ng	4088730	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103D

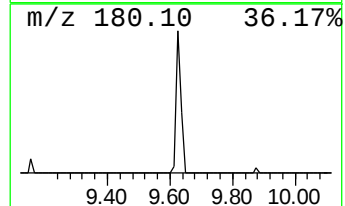
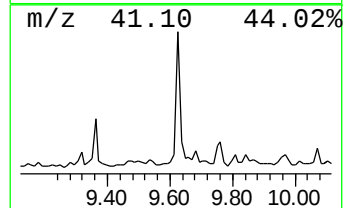
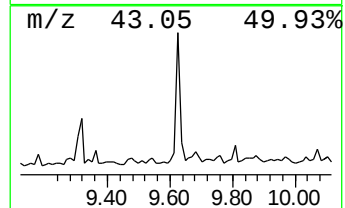
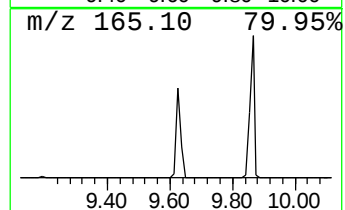
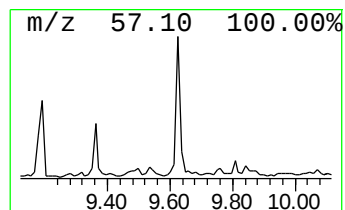
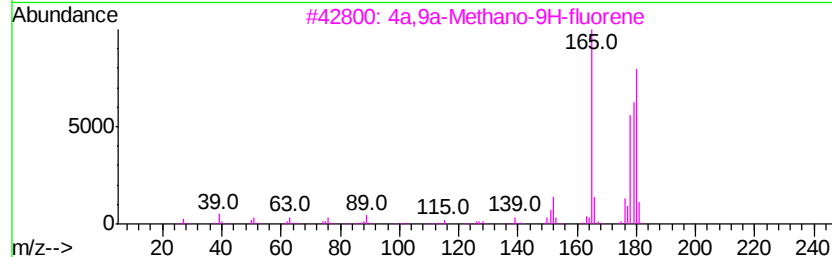
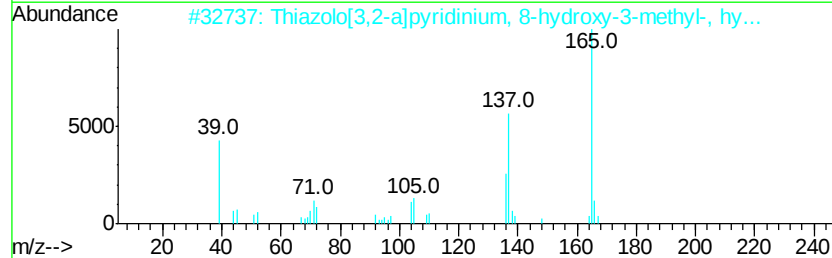
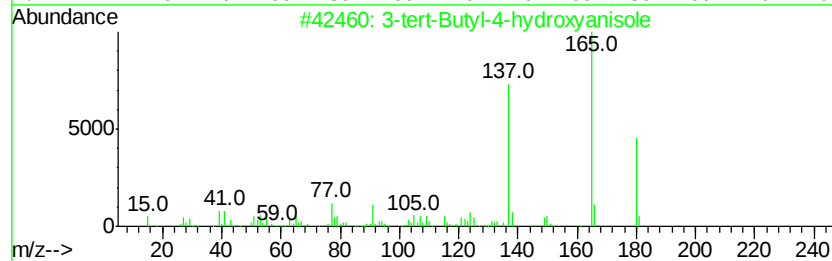
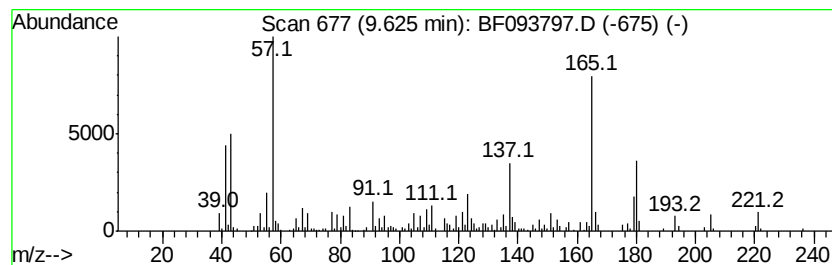
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-tert-Butyl-4-hydroxyanisole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	3.57 ng	301086	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	64
2		Thiazolo[3,2-a]pyridinium, 8-hyd...	165	C8H7NOS	030276-99-4	55
3		4a,9a-Methano-9H-fluorene	180	C14H12	019540-84-2	53
4		9H-Fluorene, 4-methyl-	180	C14H12	001556-99-6	53
5		3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103D

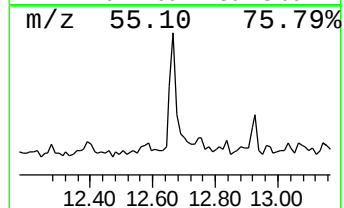
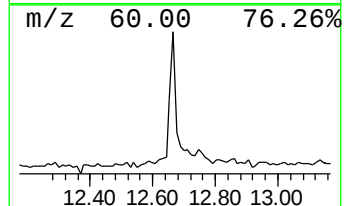
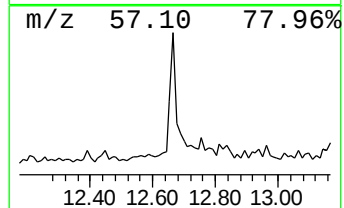
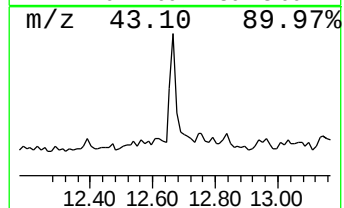
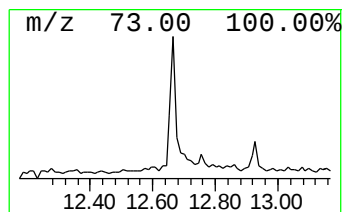
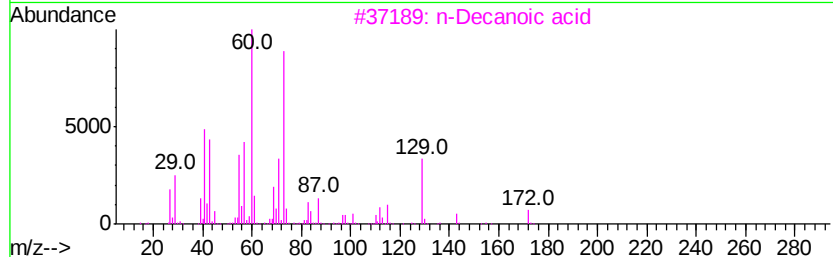
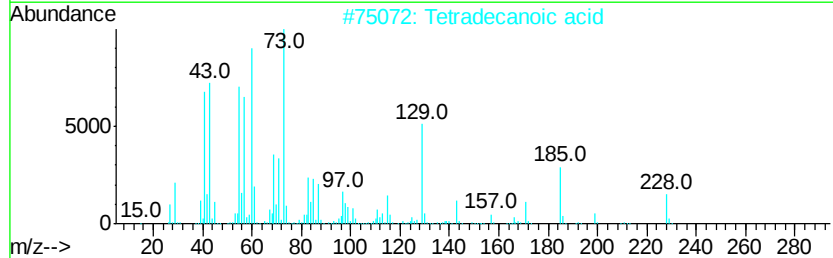
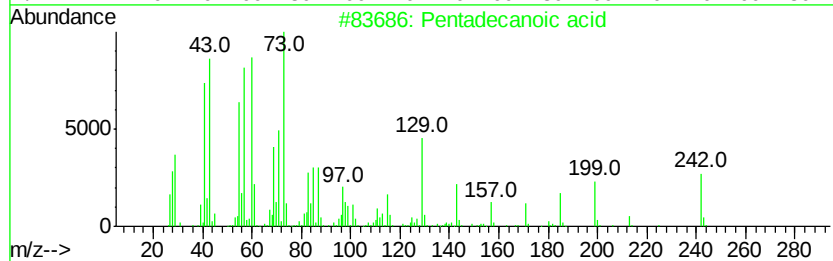
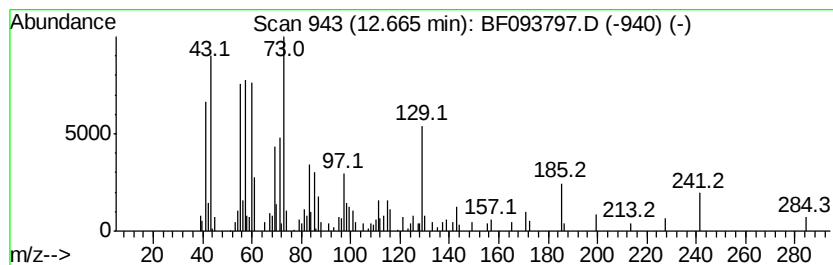
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.31 ng	147701	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3		n-Decanoic acid	172	C10H20O2	000334-48-5	60
4		Undecanoic acid	186	C11H22O2	000112-37-8	41
5		2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

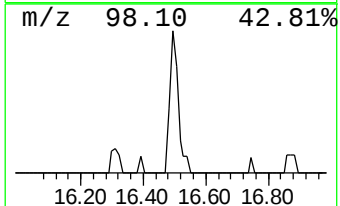
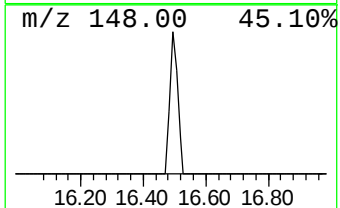
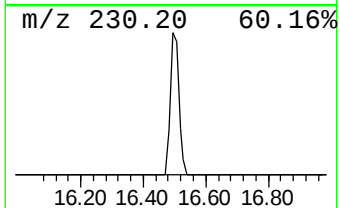
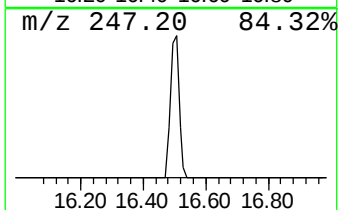
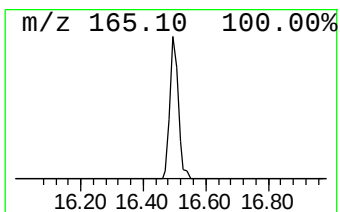
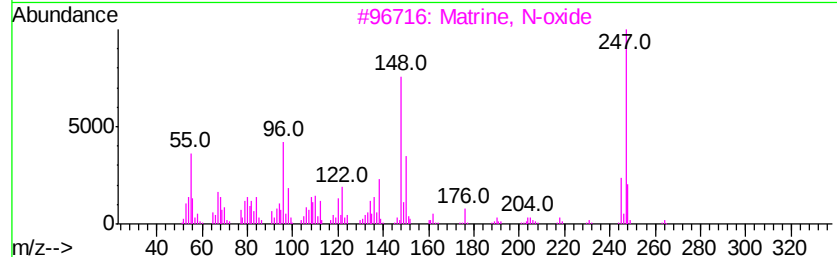
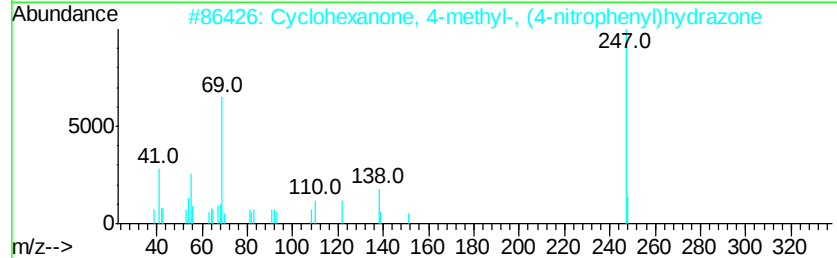
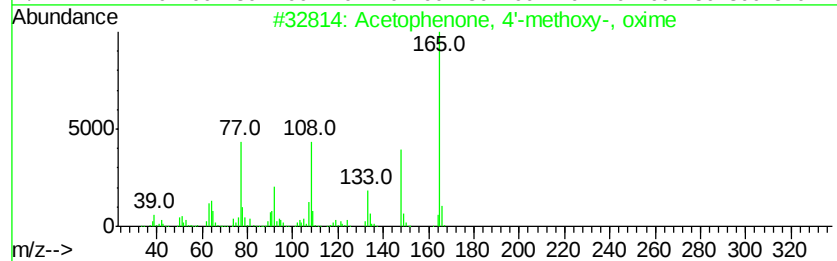
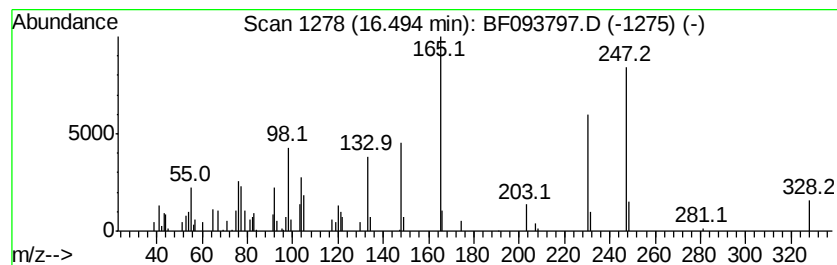
Instrument :
BNA_F
ClientSampleId :
MW-103D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.49 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.22 ng	97129	Perylene-d12	15.37
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Acetophenone, 4'-methoxy-, oxime	165 C9H11NO2	002475-92-5	27
2	Cyclohexanone, 4-methyl-, (4-nit...	247 C13H17N3O2	025117-42-4	15
3	Matrine, N-oxide	264 C15H24N2O2	059091-53-1	12
4	4-O-Nitrophenylhydrazono-3-methy...	247 C10H9N5O3	065855-04-1	11
5	4-Iodo-2,6-dimethylaniline	247 C8H10IN	004102-53-8	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093797.D
Acq On : 21 Mar 2017 14:47
Operator : SJ/MA
Sample : I2263-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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
2-Pentanone, 4-hy...	4.98	6.5	ng	352672	1	6.82	1090180	20.0
unknown6.60	6.60	75.0	ng	4088730	1	6.82	1090180	20.0
3-tert-Butyl-4-hy...	9.62	3.6	ng	301086	3	9.86	1688920	20.0
Pentadecanoic acid	12.67	2.3	ng	147701	5	13.97	1279520	20.0
unknown16.49	16.49	2.2	ng	97129	6	15.37	875120	20.0