

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122816\
 Data File : BF092006.D
 Acq On : 28 Dec 2016 20:42
 Operator : UM/SJ
 Sample : H6281-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-7

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-BF122116.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	2.167	3	7	8	rBV	22769	69841	1.18%	0.165%
2	4.853	239	242	248	rBV	656519	828743	13.98%	1.953%
3	5.310	280	282	285	rBV	2054278	2947610	49.71%	6.945%
4	6.362	372	374	377	rBV	1391506	1672667	28.21%	3.941%
5	6.476	382	384	387	rBV	4093369	4408113	74.34%	10.386%
6	6.704	401	404	406	rBV	1368467	1287949	21.72%	3.034%
7	6.864	415	418	420	rBV	3742351	4211140	71.02%	9.922%
8	7.276	451	454	456	rBV	3096778	3366326	56.77%	7.931%
9	7.985	514	516	519	rVV	1309920	1747134	29.47%	4.116%
10	8.796	583	587	589	rBV4	29940	65239	1.10%	0.154%
11	8.990	601	604	605	rVV	110555	120122	2.03%	0.283%
12	9.025	605	607	608	rVB	100686	79635	1.34%	0.188%
13	9.070	608	611	614	rBV	4804221	5929376	100.00%	13.970%
14	9.162	617	619	621	rVV3	78596	137293	2.32%	0.323%
15	9.253	624	627	629	rVV	192845	239803	4.04%	0.565%
16	9.368	635	637	638	rBV2	41562	61216	1.03%	0.144%
17	9.402	638	640	642	rVV2	108099	161718	2.73%	0.381%
18	9.470	644	646	649	rVV	235708	253108	4.27%	0.596%
19	9.539	651	652	655	rBV2	62913	122071	2.06%	0.288%
20	9.608	655	658	660	rVV2	98120	157605	2.66%	0.371%
21	9.745	667	670	672	rBV	2200386	2095540	35.34%	4.937%
22	9.813	674	676	677	rBV2	43390	76256	1.29%	0.180%
23	10.042	695	696	698	rBV2	71672	109742	1.85%	0.259%
24	10.362	722	724	729	rBV4	100771	260983	4.40%	0.615%
25	10.499	734	736	737	rBV2	79525	97099	1.64%	0.229%
26	10.533	737	739	742	rVV2	2973288	4104143	69.22%	9.670%
27	10.933	772	774	778	rBV3	117694	224585	3.79%	0.529%
28	11.025	780	782	785	rVB4	138272	185459	3.13%	0.437%
29	11.231	798	800	802	rVB	1093950	1265682	21.35%	2.982%
30	11.265	802	803	807	rVB2	209207	263541	4.44%	0.621%
31	11.425	815	817	821	rVB3	211978	413937	6.98%	0.975%
32	11.494	821	823	825	rBV2	261617	469980	7.93%	1.107%
33	11.779	847	848	853	rVB3	249809	365332	6.16%	0.861%
34	12.568	915	917	922	rVB	139813	233456	3.94%	0.550%

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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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.819	936	939	941	rBV	3467531	3464839	58.44%	8.163%
36	13.859	1027	1030	1032	rBV	557962	539120	9.09%	1.270%
37	15.242	1149	1151	1154	rBV	344729	407366	6.87%	0.960%

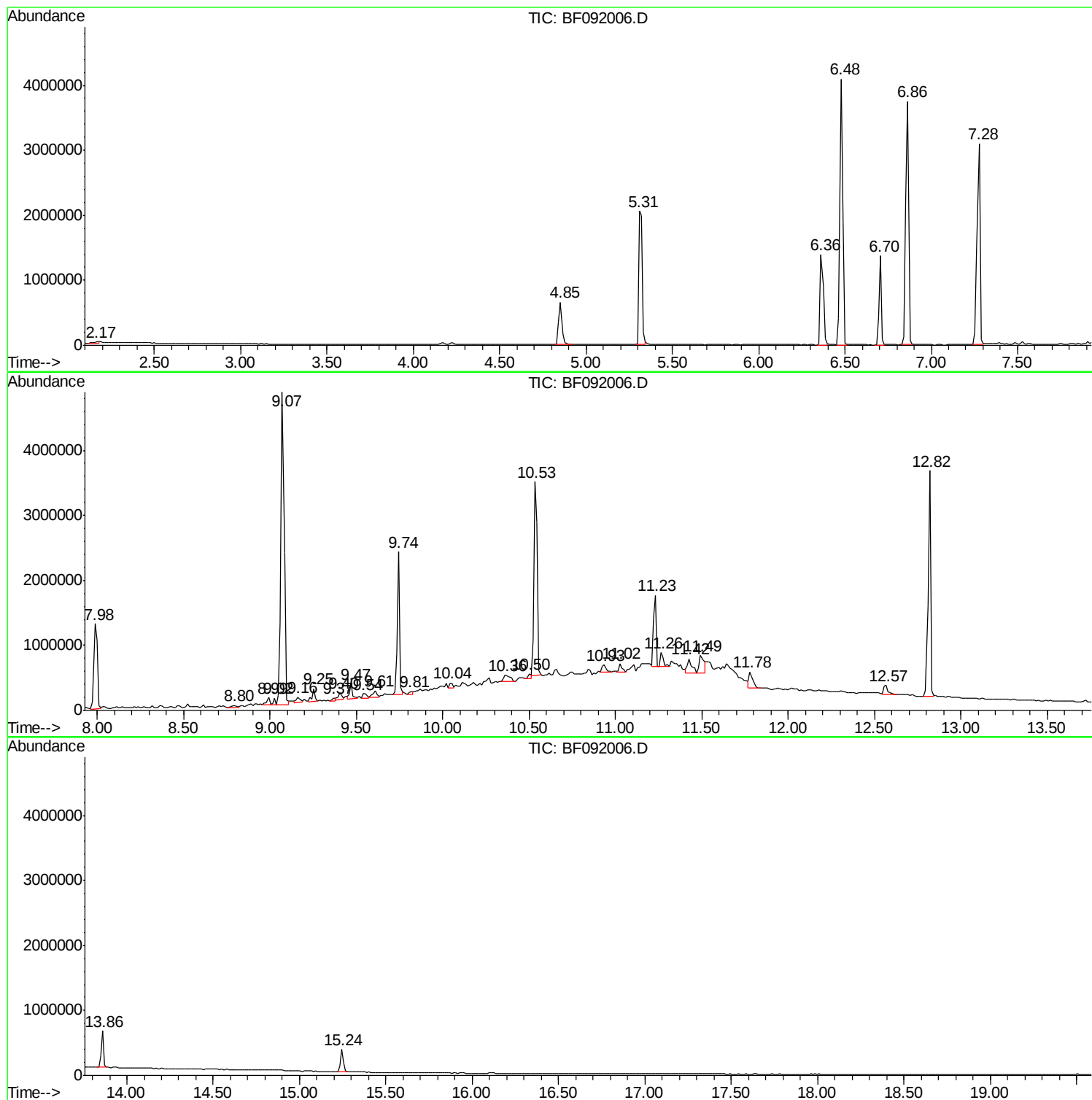
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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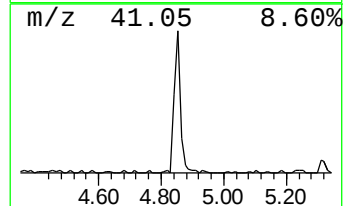
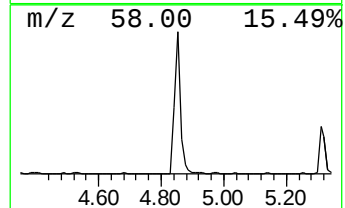
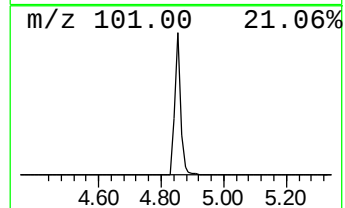
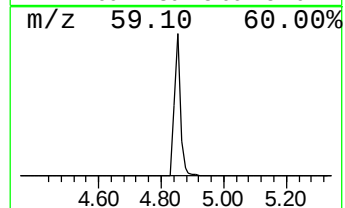
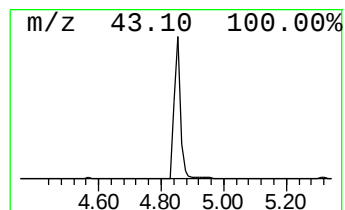
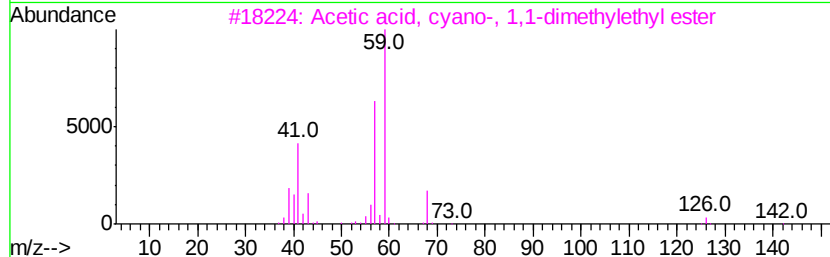
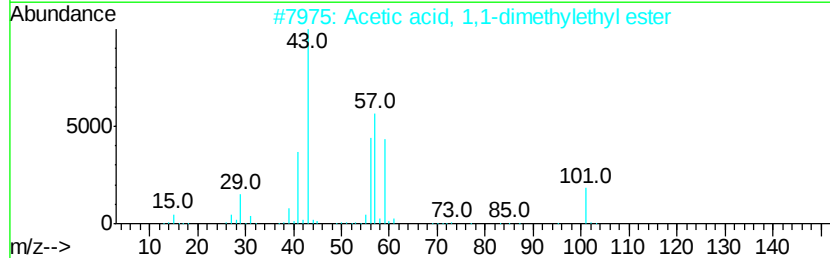
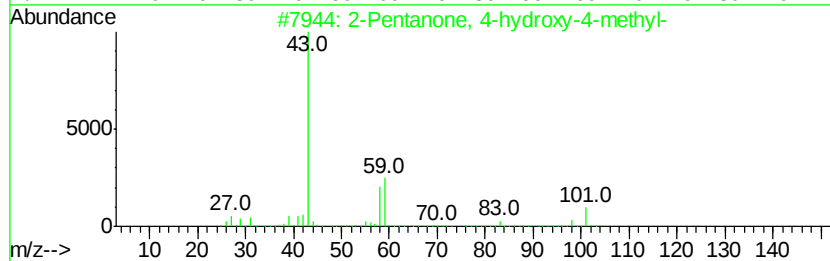
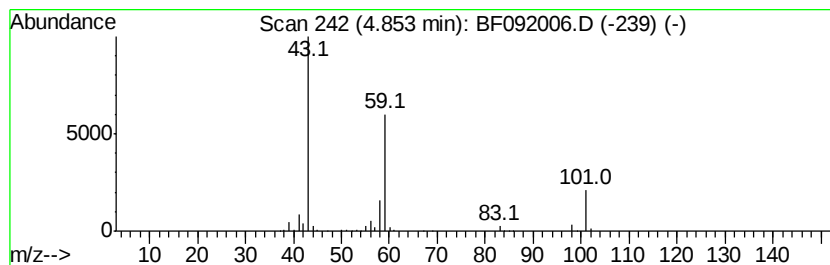
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.85	12.87 ng	828743	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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-dimethyl...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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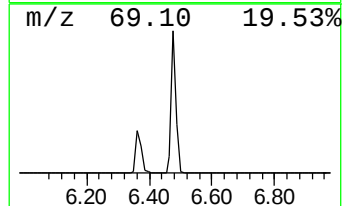
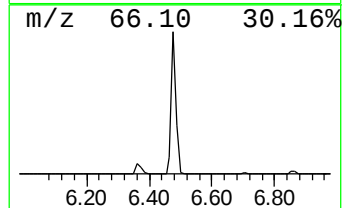
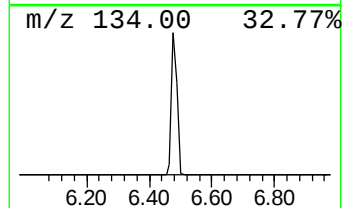
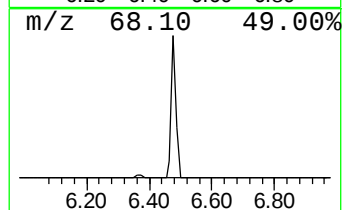
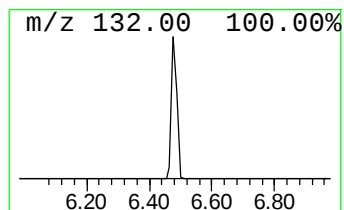
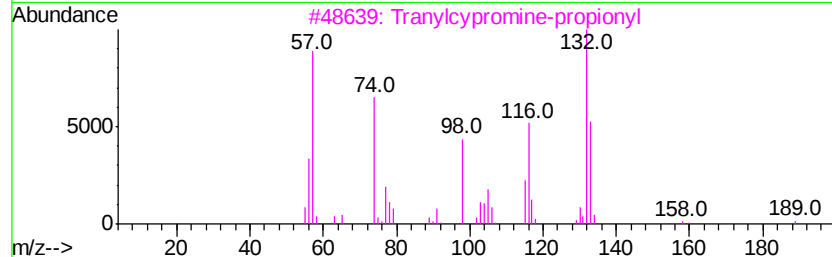
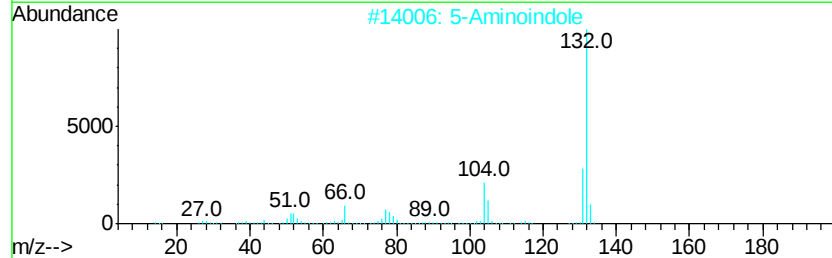
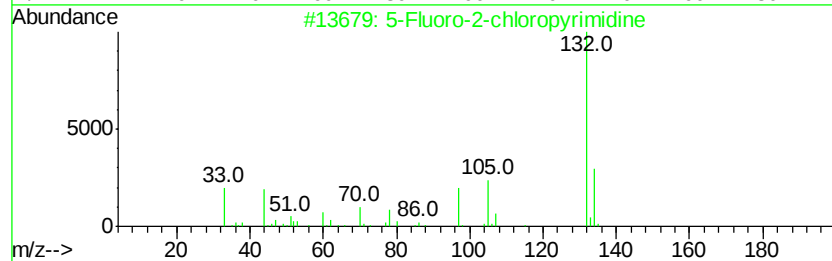
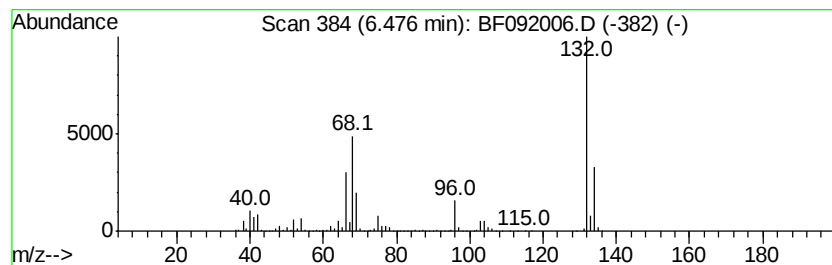
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	68.45 ng	4408110	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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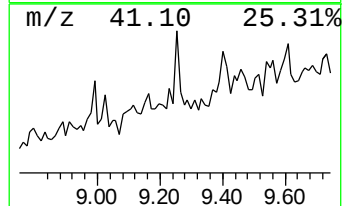
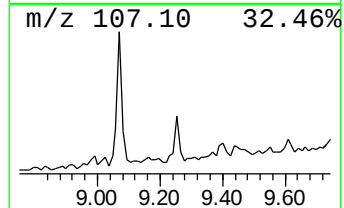
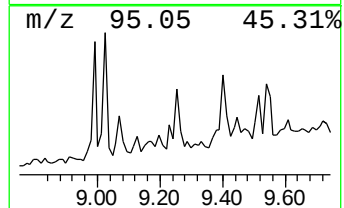
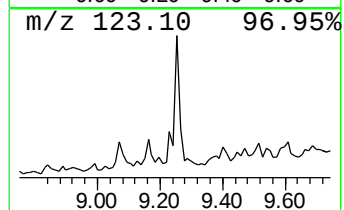
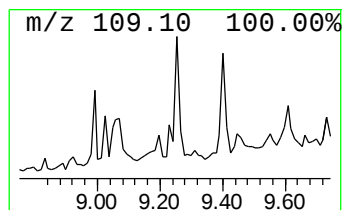
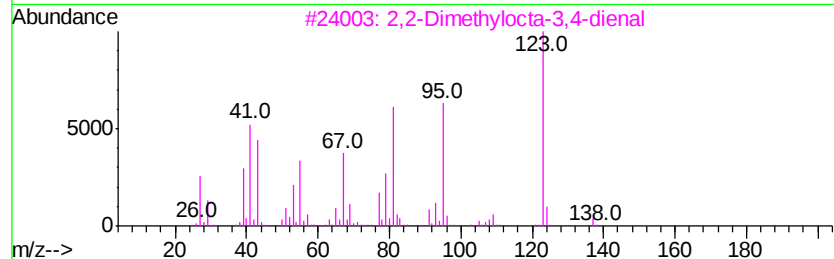
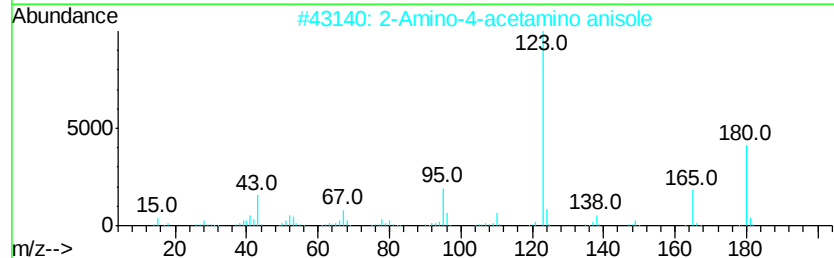
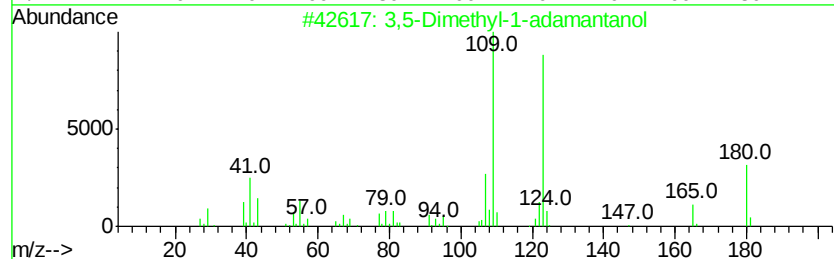
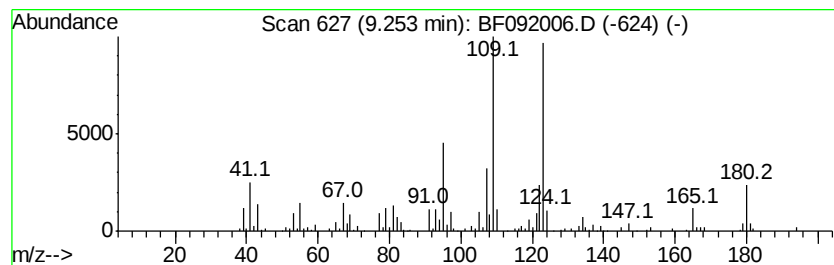
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3,5-Dimethyl-1-adamantanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.25	2.29 ng	239803	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Dimethyl-1-adamantanol	180	C12H20O	000707-37-9	87
2		2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	49
3		2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	38
4		Benzoic acid, 4-fluoro-, anhydride	262	C14H8F2O3	025569-77-1	35
5		Tricyclo[4.3.1.1(3,8)]undecane, ...	180	C12H20O	021898-95-3	35



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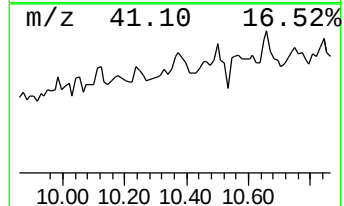
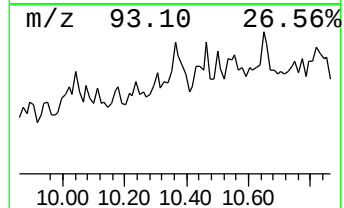
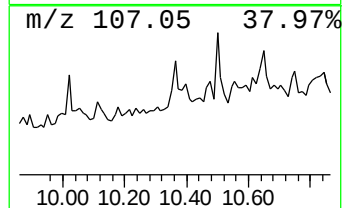
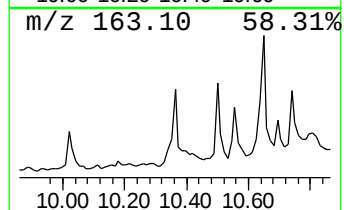
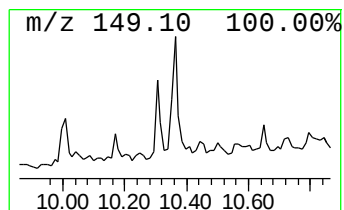
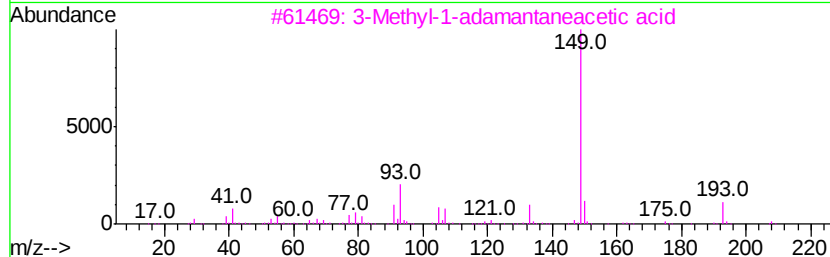
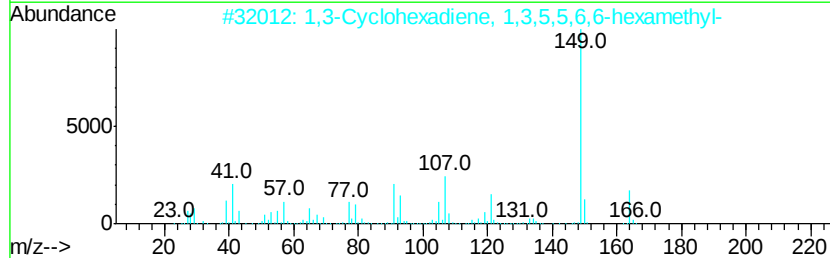
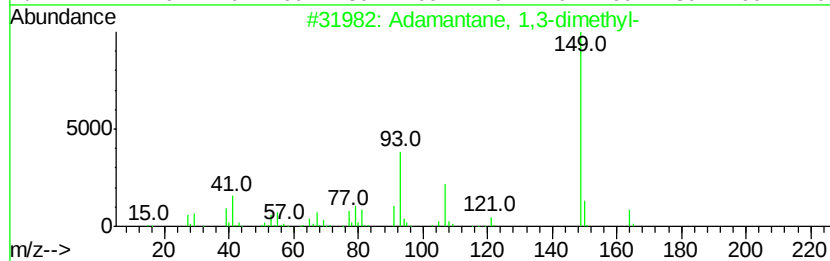
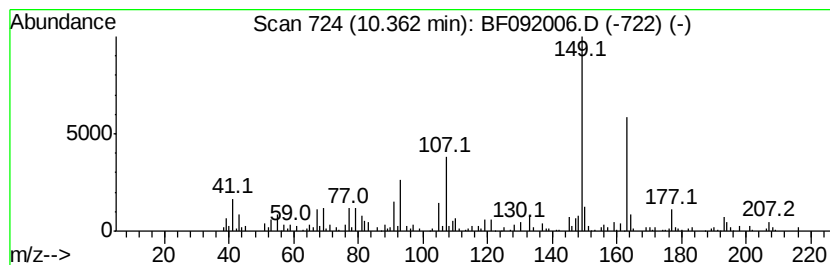
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Adamantane, 1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	2.49 ng	260983	Acenaphthene-d10	9.74
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Adamantane, 1,3-dimethyl-	164 C12H20	000702-79-4	60
2	1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164 C12H20	1000150-39-4	47
3	3-Methyl-1-adamantaneacetic acid	208 C13H20O2	014202-13-2	43
4	Diethyl Phthalate	222 C12H14O4	000084-66-2	43
5	Pyridinium, 1-(acetylamino)-2,6-...	164 C9H12N2O	031020-35-6	43



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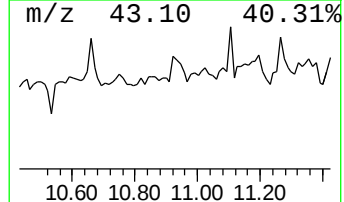
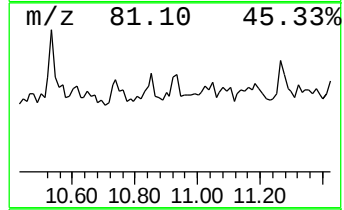
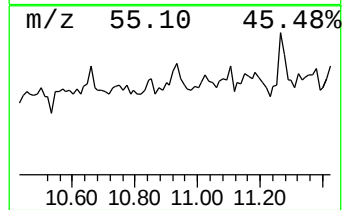
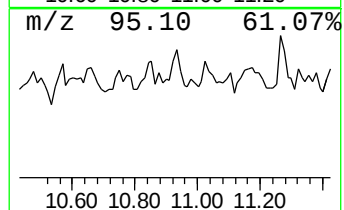
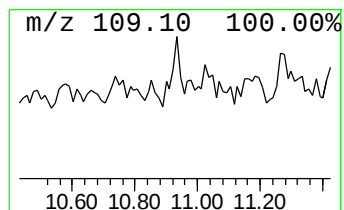
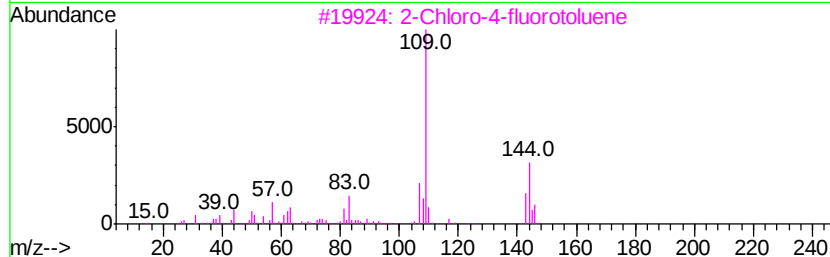
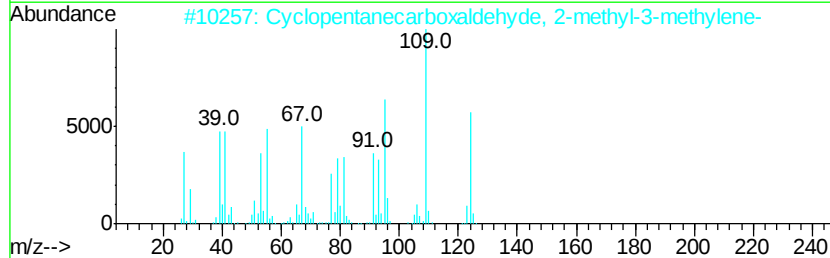
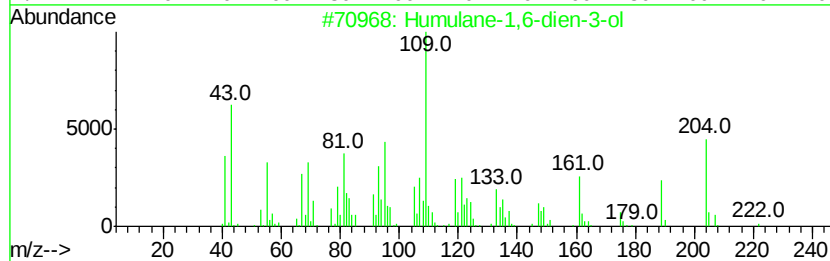
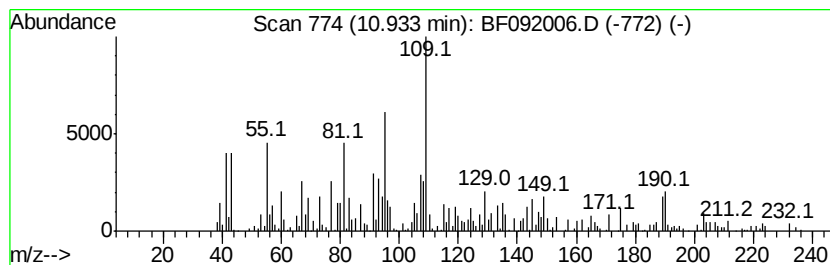
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ClientSampled :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown10.93 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.93	3.55 ng	224585	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Humulane-1,6-dien-3-ol	222	C15H26O	1000140-23-1	43
2	Cyclopentanecarboxaldehyde, 2-me...	124	C8H12O	1000154-24-0	35
3	2-Chloro-4-fluorotoluene	144	C7H6ClF	000452-73-3	35
4	Bicyclo[3.3.1]nonan-9-one, 1,2,4...	225	C12H19NO3	129967-65-3	27
5	Cyclohexanol, 3,3,5-trimethyl-, ...	184	C11H20O2	024691-16-5	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122816\
Data File : BF092006.D
Acq On : 28 Dec 2016 20:42
Operator : UM/SJ
Sample : H6281-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

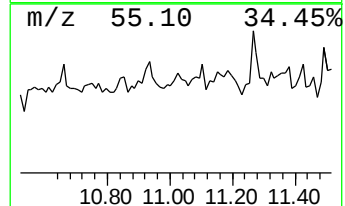
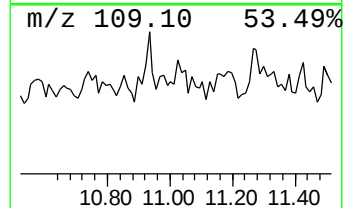
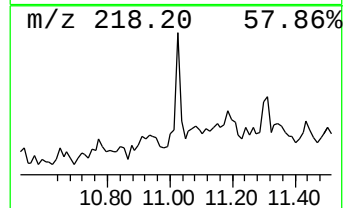
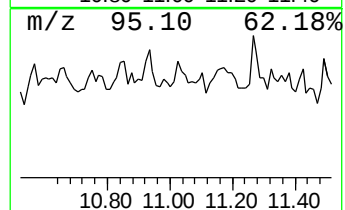
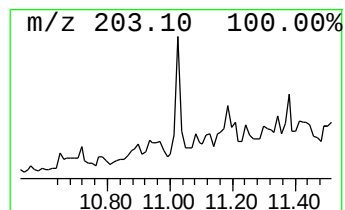
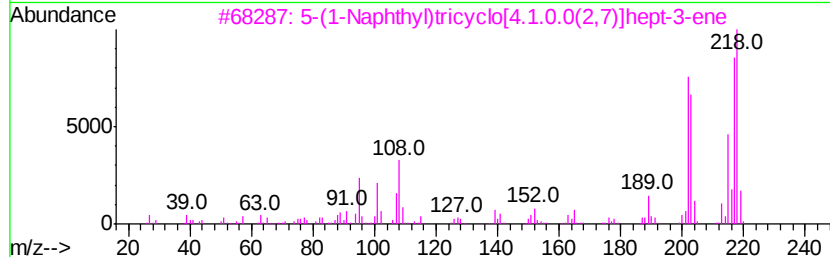
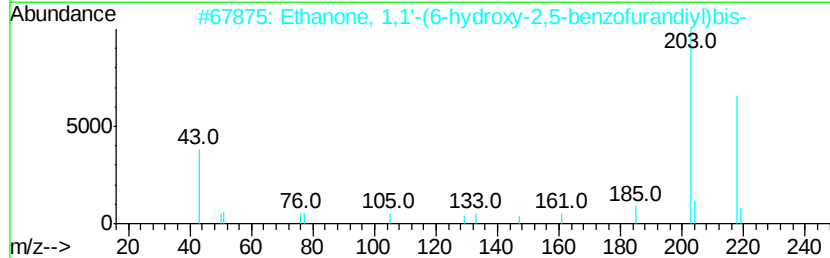
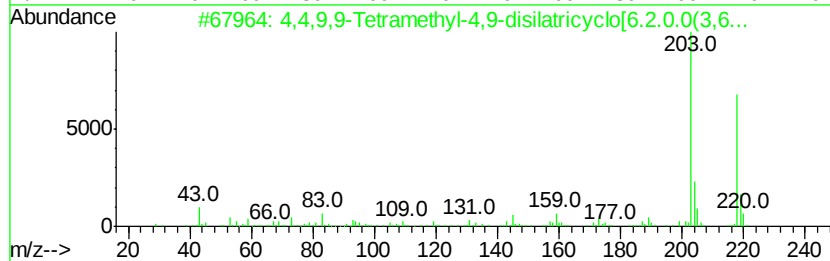
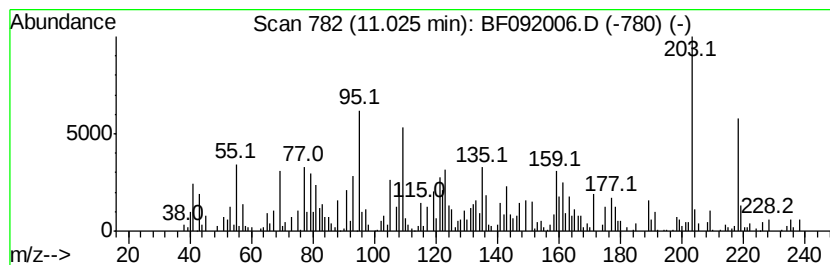
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown11.02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	2.93 ng	185459	Phenanthrene-d10	11.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4,9,9-Tetramethyl-4,9-disilatr...	218	C12H18Si2	1000280-67-7	27		
2	Ethanone, 1,1'-(6-hydroxy-2,5-be...	218	C12H10O4	053947-86-7	27		
3	5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	25		
4	2H-Cyclopropafalnaphthalen-2-one...	218	C15H22O	006831-17-0	25		
5	Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	22		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122816\
Data File : BF092006.D
Acq On : 28 Dec 2016 20:42
Operator : UM/SJ
Sample : H6281-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

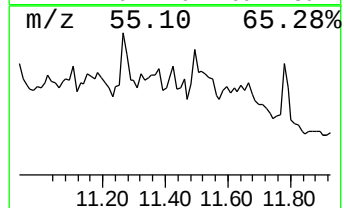
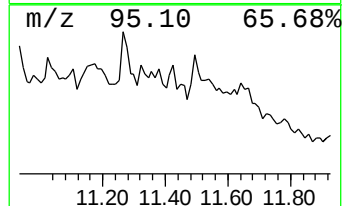
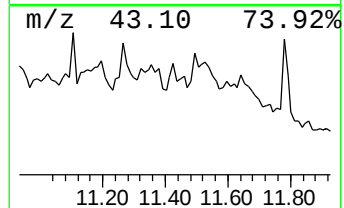
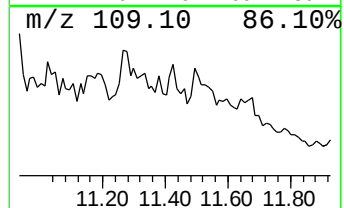
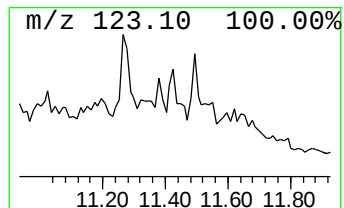
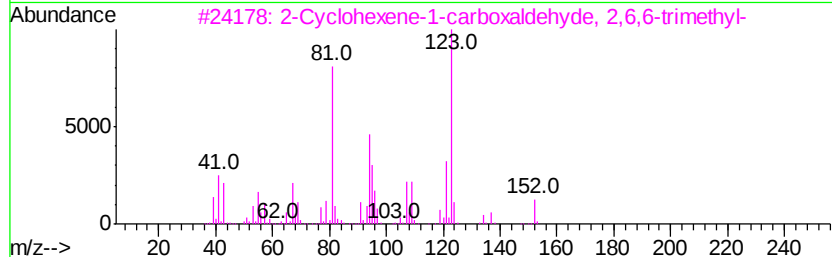
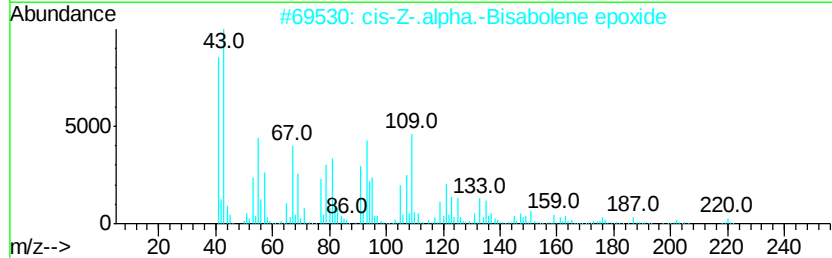
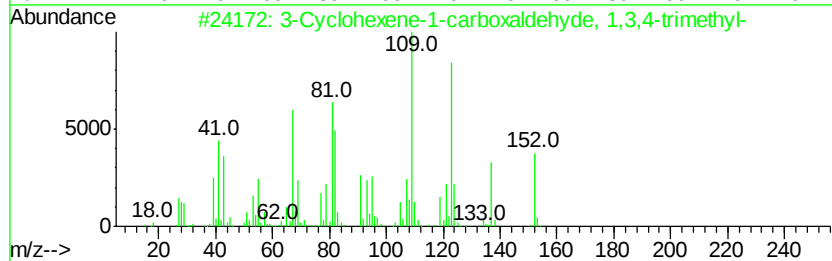
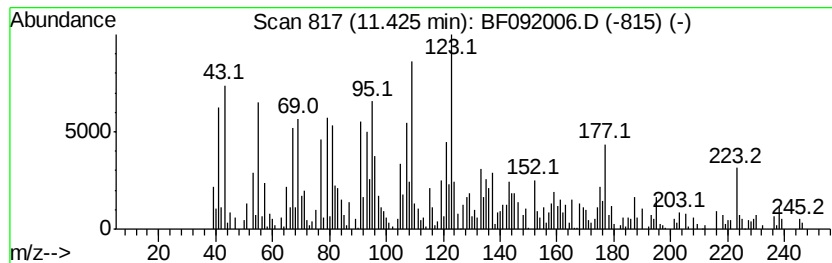
Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown11.43 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.43	6.54 ng	413937	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cvclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	46
2	cis-Z-.alpha.-Bisabolene epoxide	220	C15H24O	1000131-71-2	41
3	2-Cvclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	30
4	2,6-Dimethyl-3,5,7-octatriene-2-...	152	C10H16O	1000141-11-9	30
5	Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122816\
Data File : BF092006.D
Acq On : 28 Dec 2016 20:42
Operator : UM/SJ
Sample : H6281-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

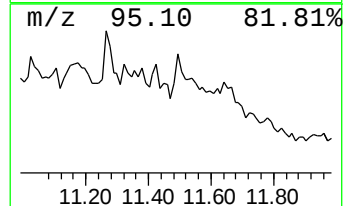
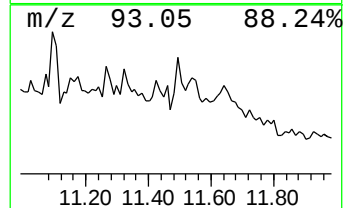
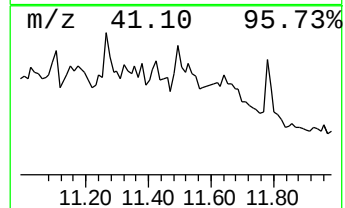
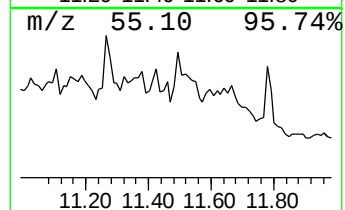
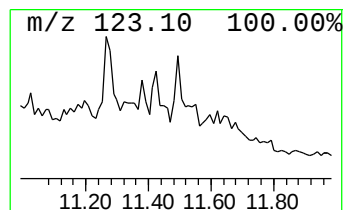
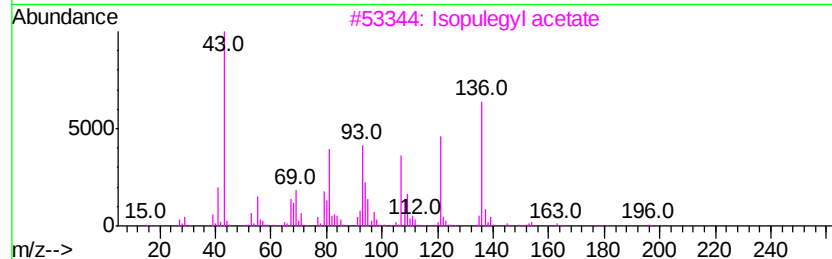
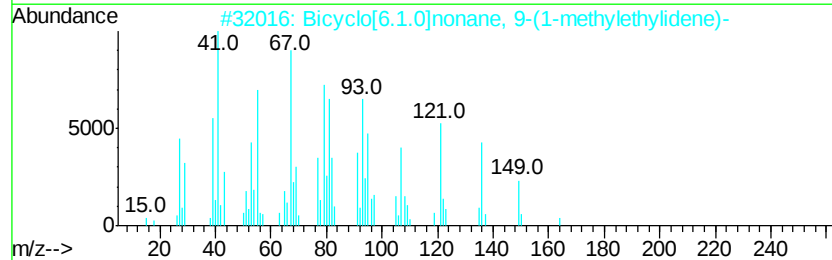
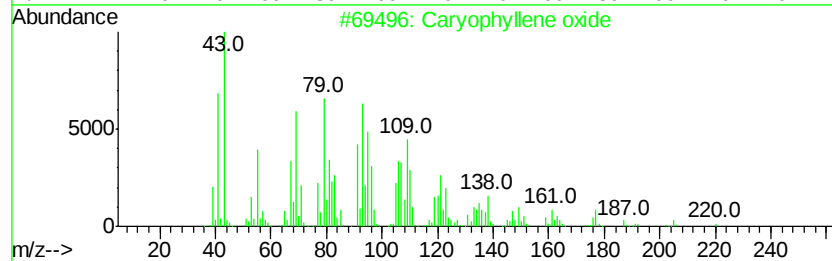
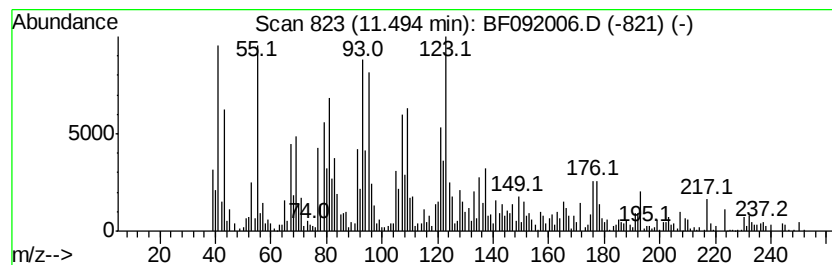
Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Caryophyllene oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.49	7.43 ng	469980	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carvophyllene oxide	220	C15H24O	001139-30-6	62
2	Bicyclo[6.1.0]nonane, 9-(1-methy...	164	C12H20	056666-90-1	46
3	Isopuleavl acetate	196	C12H20O2	000089-49-6	38
4	o-Mentha-1(7),8-dien-3-ol	152	C10H16O	015358-81-3	38
5	Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122816\
Data File : BF092006.D
Acq On : 28 Dec 2016 20:42
Operator : UM/SJ
Sample : H6281-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

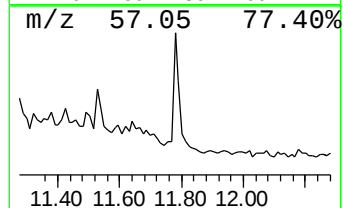
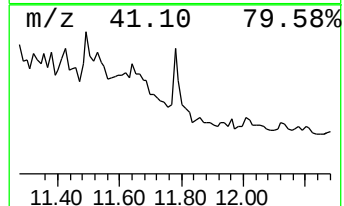
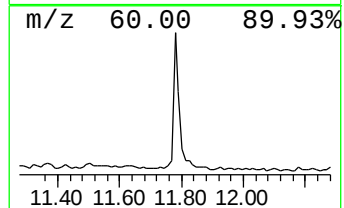
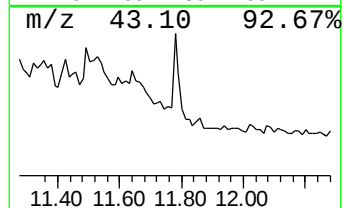
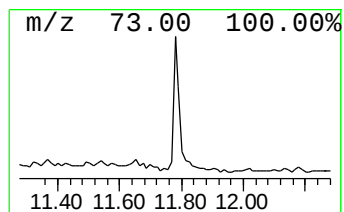
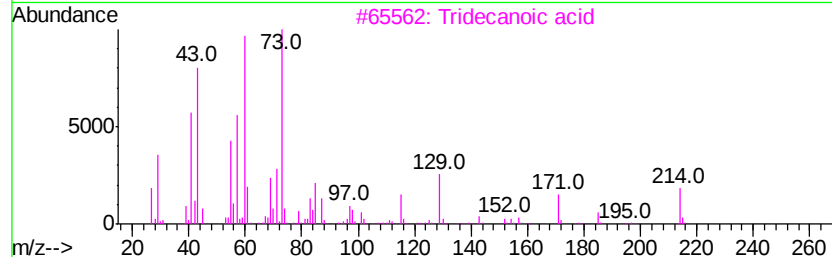
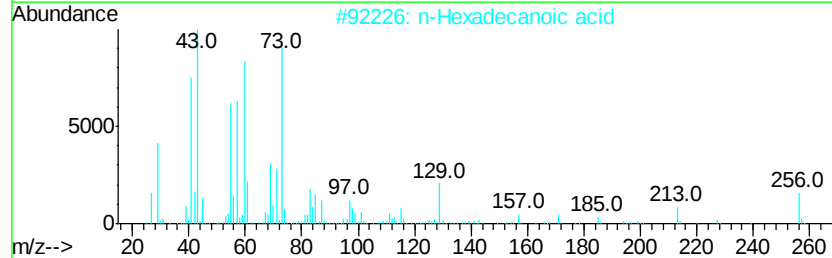
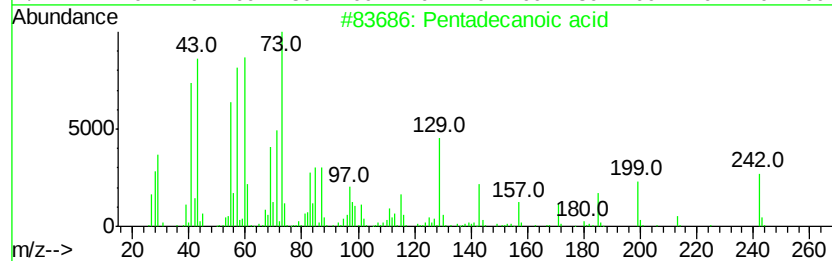
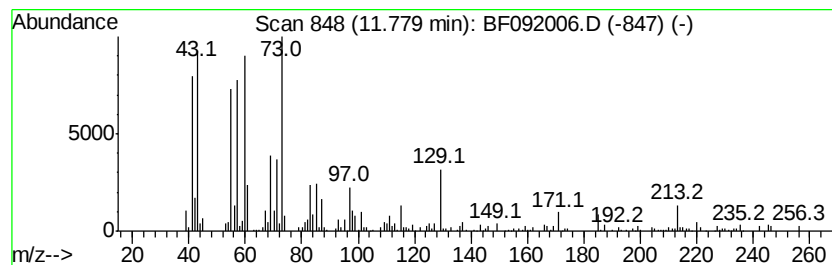
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	5.77 ng	365332	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122816\
Data File : BF092006.D
Acq On : 28 Dec 2016 20:42
Operator : UM/SJ
Sample : H6281-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

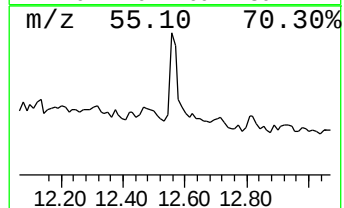
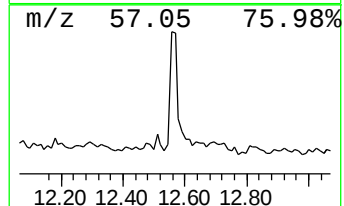
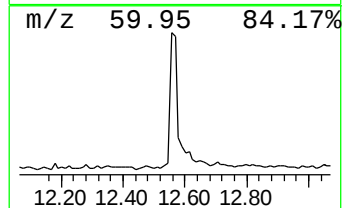
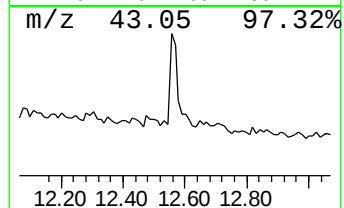
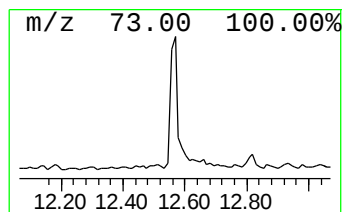
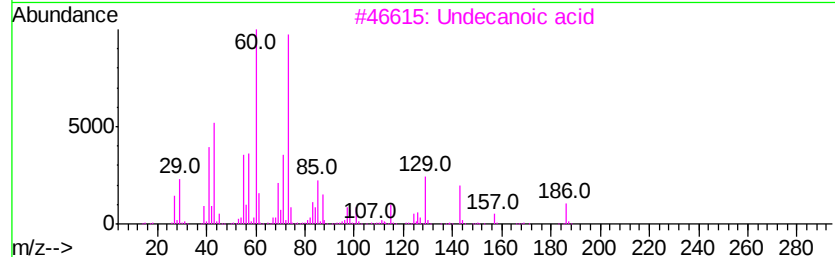
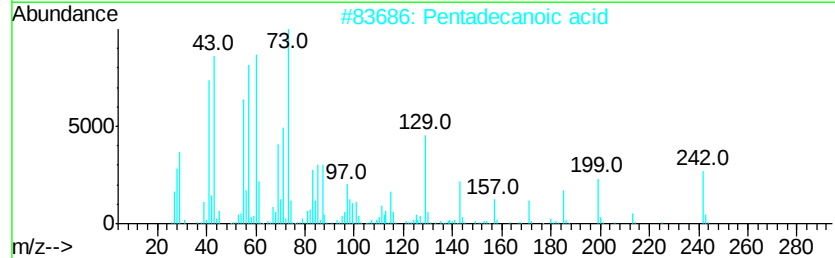
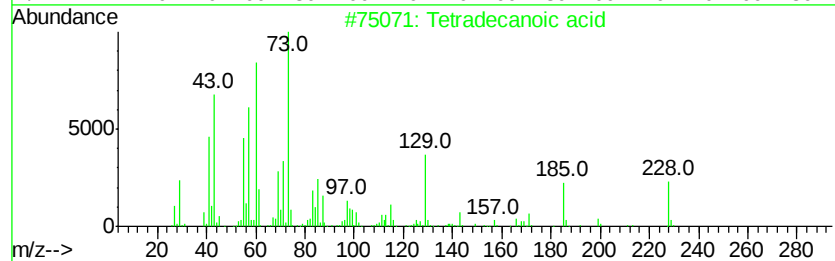
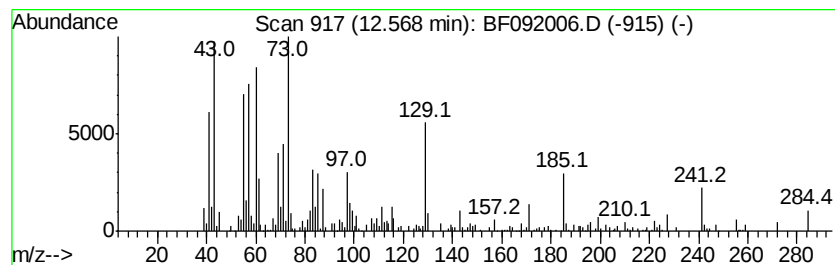
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	8.66 ng	233456	Chrysene-d12	13.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3			Undecanoic acid	186	C11H22O2	000112-37-8	62
4			2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18
5			Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122816\
Data File : BF092006.D
Acq On : 28 Dec 2016 20:42
Operator : UM/SJ
Sample : H6281-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.85	12.9	ng	828743	1	6.70	1287950	20.0
unknown6.48	6.48	68.5	ng	4408110	1	6.70	1287950	20.0
3,5-Dimethyl-1-ad...	9.25	2.3	ng	239803	3	9.74	2095540	20.0
Adamantane, 1,3-d...	10.36	2.5	ng	260983	3	9.74	2095540	20.0
unknown10.93	10.93	3.5	ng	224585	4	11.23	1265680	20.0
unknown11.02	11.02	2.9	ng	185459	4	11.23	1265680	20.0
unknown11.43	11.43	6.5	ng	413937	4	11.23	1265680	20.0
Caryophyllene oxide	11.49	7.4	ng	469980	4	11.23	1265680	20.0
Pentadecanoic acid	11.78	5.8	ng	365332	4	11.23	1265680	20.0
Tetradecanoic acid	12.57	8.7	ng	233456	5	13.86	539120	20.0