

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
 Data File : BF085186.D
 Acq On : 4 Mar 2016 5:08
 Operator : SJ/UM
 Sample : H1663-03
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-39(11-13)

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-BF030316.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	4.035	150	153	156	rVB	704988	913689	25.77%	2.612%
2	5.190	251	254	259	rBV	545247	805309	22.72%	2.302%
3	5.590	286	289	291	rBV	3356947	3544955	100.00%	10.133%
4	6.596	374	377	380	rBV	2371166	3456466	97.50%	9.880%
5	6.744	387	390	393	rBV	3456654	3287680	92.74%	9.398%
6	6.973	408	410	413	rVB	680077	903383	25.48%	2.582%
7	7.133	422	424	427	rVB	2616351	2607888	73.57%	7.455%
8	7.544	457	460	462	rVB	2083028	2428425	68.50%	6.942%
9	7.613	464	466	469	rVB	52779	68722	1.94%	0.196%
10	8.264	520	523	525	rBV	1511013	1283327	36.20%	3.668%
11	8.367	529	532	535	rBV	34872	57139	1.61%	0.163%
12	8.550	545	548	550	rBV3	25361	46682	1.32%	0.133%
13	8.802	569	570	575	rBV3	39213	77972	2.20%	0.223%
14	9.007	586	588	590	rBV3	25437	40814	1.15%	0.117%
15	9.282	611	612	614	rBV2	42280	50008	1.41%	0.143%
16	9.339	614	617	619	rVV	3863584	3343685	94.32%	9.558%
17	9.419	622	624	626	rBV2	199841	227433	6.42%	0.650%
18	9.476	626	629	631	rVV3	23076	52276	1.47%	0.149%
19	9.590	635	639	640	rBV4	20229	56367	1.59%	0.161%
20	9.727	649	651	653	rBV	672185	585441	16.51%	1.673%
21	9.842	658	661	662	rBV3	36558	57724	1.63%	0.165%
22	9.887	663	665	666	rBV	126767	134055	3.78%	0.383%
23	9.933	668	669	671	rVV2	143615	185799	5.24%	0.531%
24	10.025	674	677	679	rVV	1041843	1304232	36.79%	3.728%
25	10.059	679	680	684	rVB4	46342	94382	2.66%	0.270%
26	10.448	710	714	715	rBV	166325	189921	5.36%	0.543%
27	10.482	715	717	718	rVV	54206	68050	1.92%	0.195%
28	10.562	722	724	728	rVV3	48264	87449	2.47%	0.250%
29	10.665	730	733	736	rBV	69954	145274	4.10%	0.415%
30	10.802	743	745	748	rBV2	1487442	1735433	48.96%	4.961%
31	10.859	748	750	751	rVV2	70129	81533	2.30%	0.233%
32	10.928	754	756	760	rVB3	158698	362187	10.22%	1.035%
33	11.510	804	807	809	rBV	782583	1063422	30.00%	3.040%
34	11.568	809	812	814	rVB4	23434	59547	1.68%	0.170%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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35	12.025	850	852	857	rBV5	212347	273633	7.72%	0.782%
36	13.088	943	945	948	rBV	2183180	1972336	55.64%	5.638%
37	13.534	982	984	986	rVB	143798	134549	3.80%	0.385%
38	13.979	1021	1023	1030	rVB2	214025	320610	9.04%	0.916%
39	14.139	1035	1037	1040	rVB	817765	786618	22.19%	2.249%
40	15.614	1164	1166	1172	rVB	553361	879056	24.80%	2.513%
41	16.345	1227	1230	1239	rVB	252874	696489	19.65%	1.991%
42	16.780	1265	1268	1276	rVB	259463	513902	14.50%	1.469%

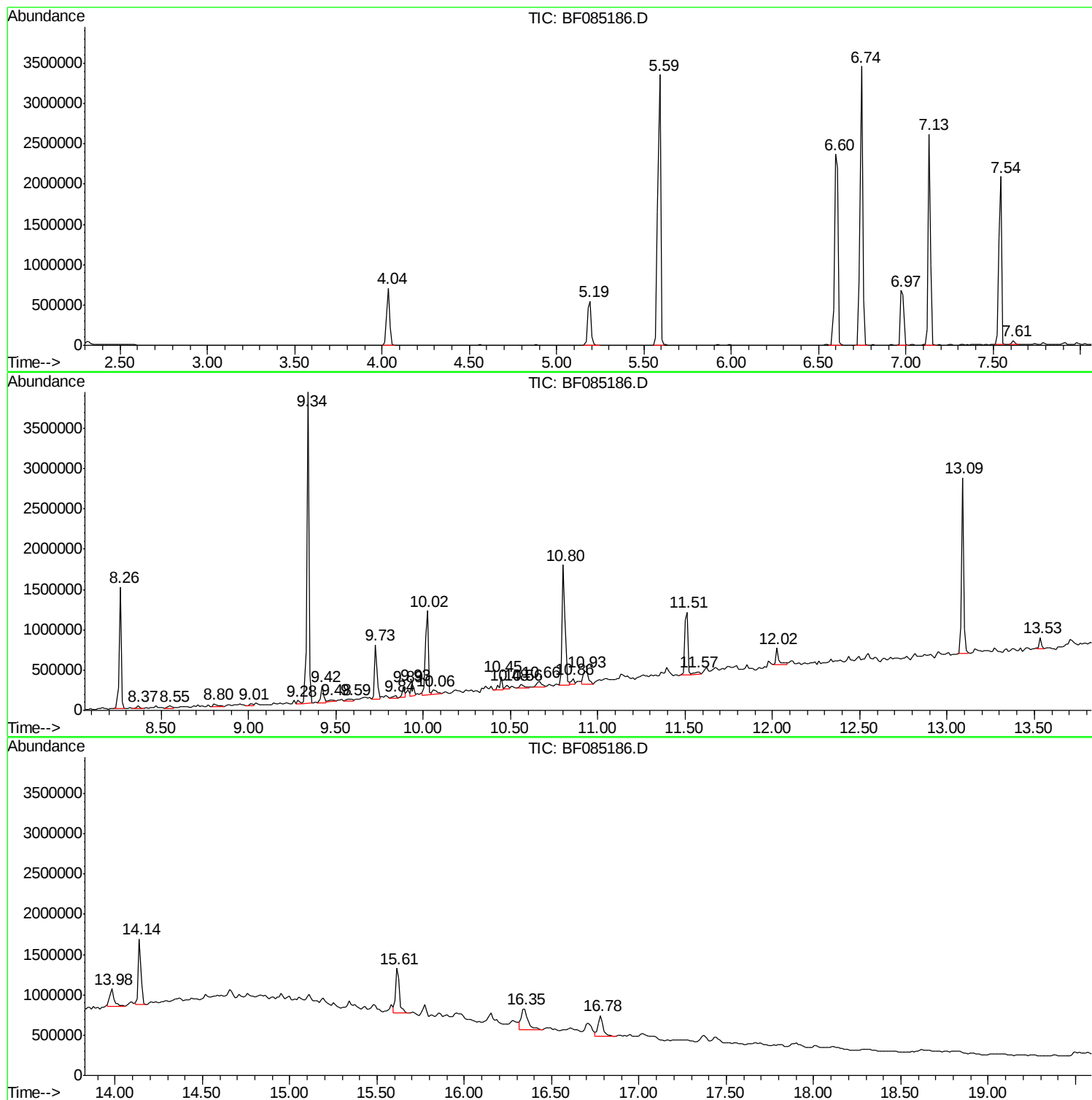
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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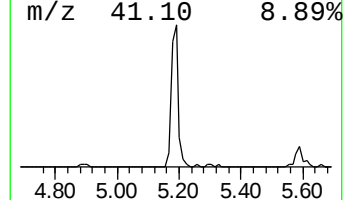
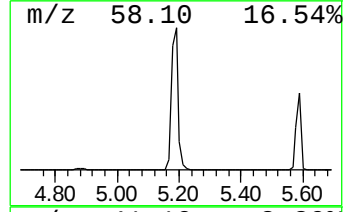
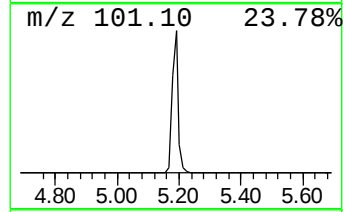
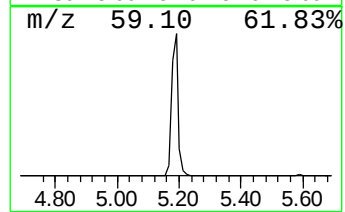
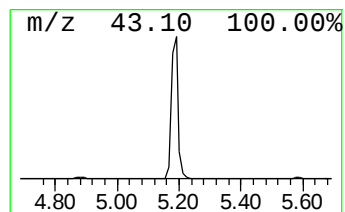
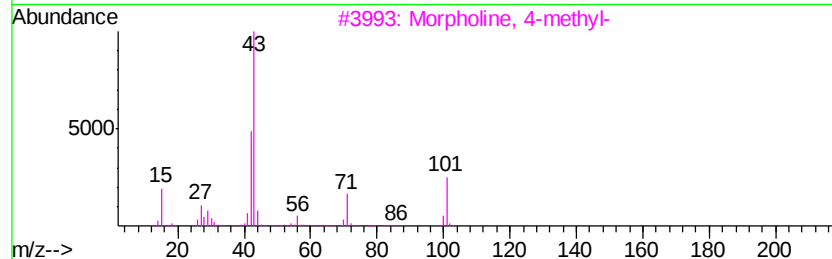
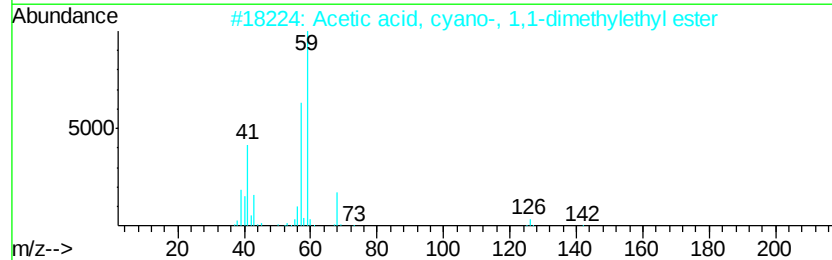
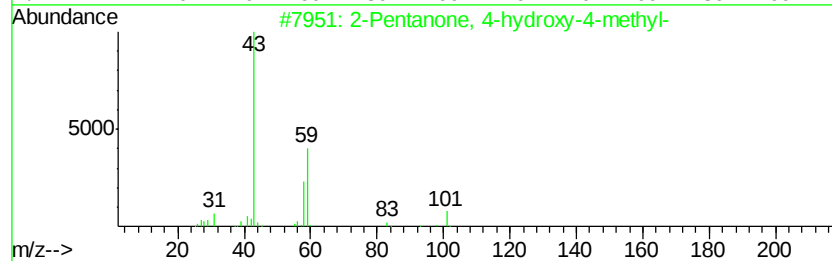
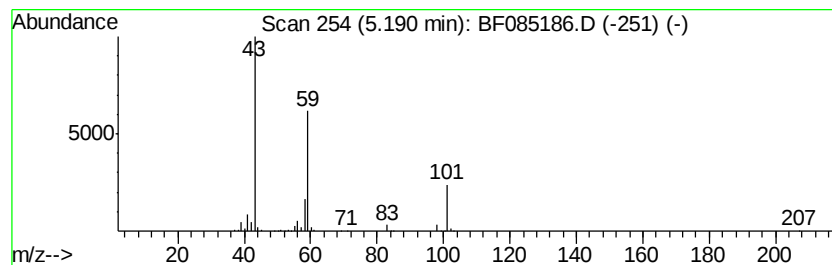
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	17.83 ng	805309	1,4-Dichlorobenzene-d4	6.98

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-dimethy...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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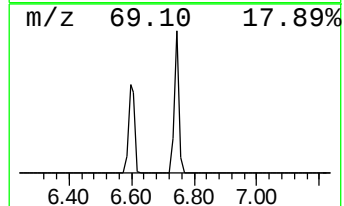
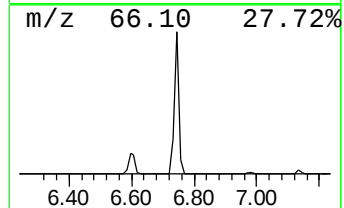
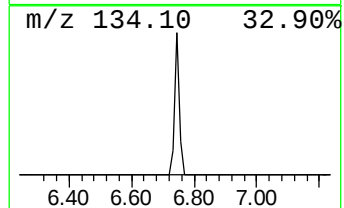
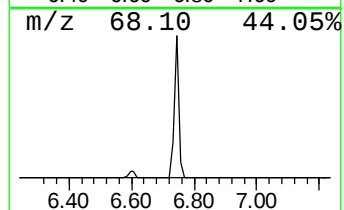
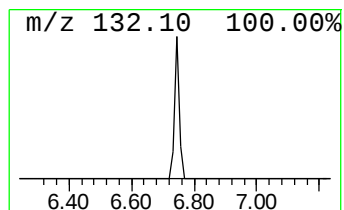
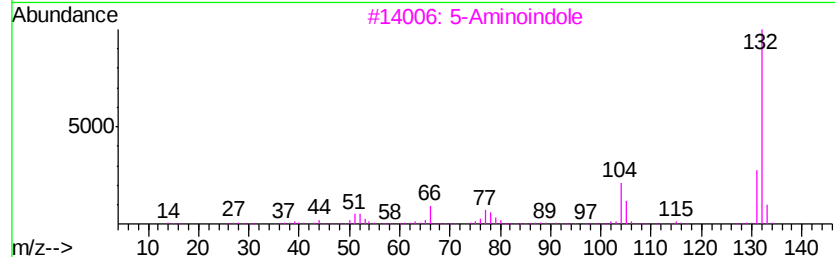
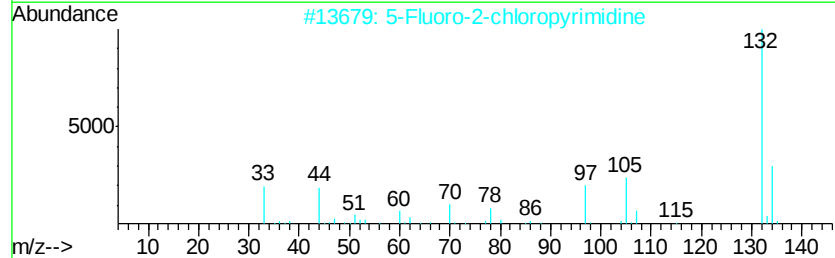
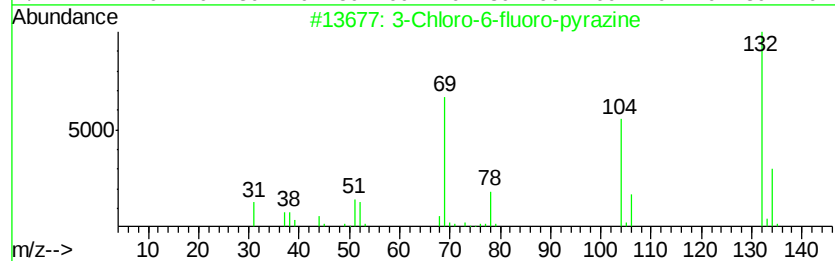
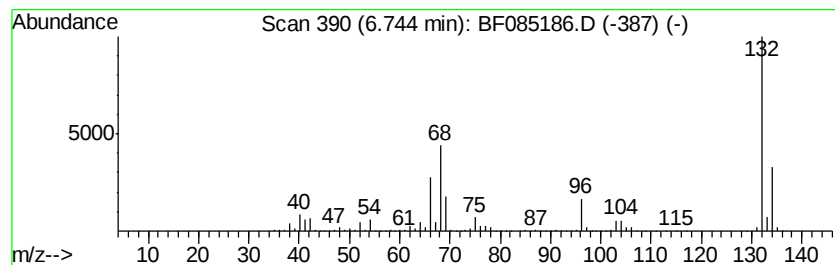
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Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	72.79 ng	3287680	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
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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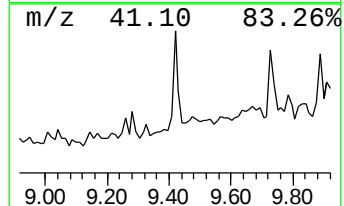
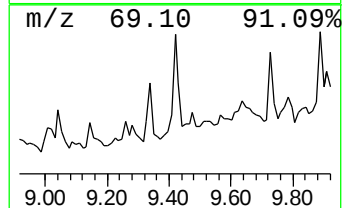
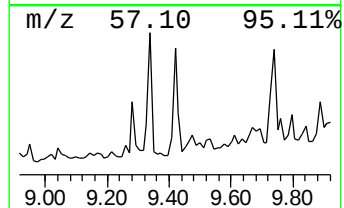
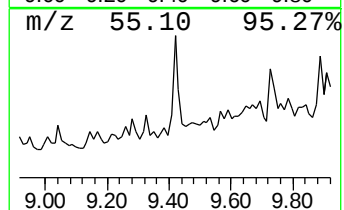
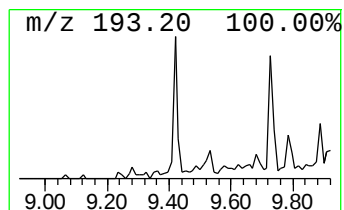
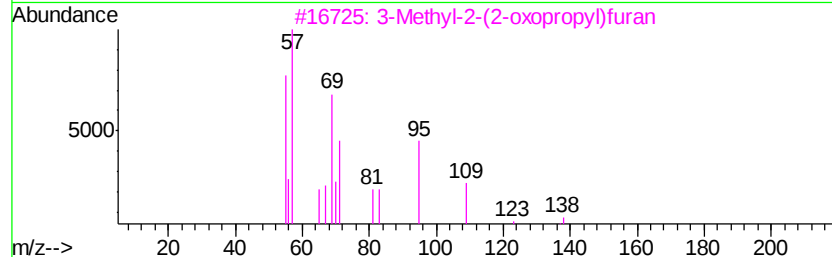
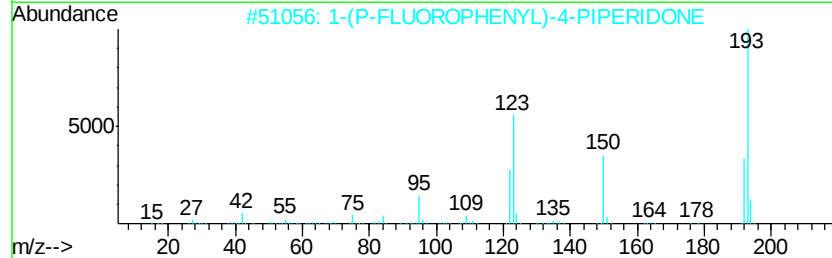
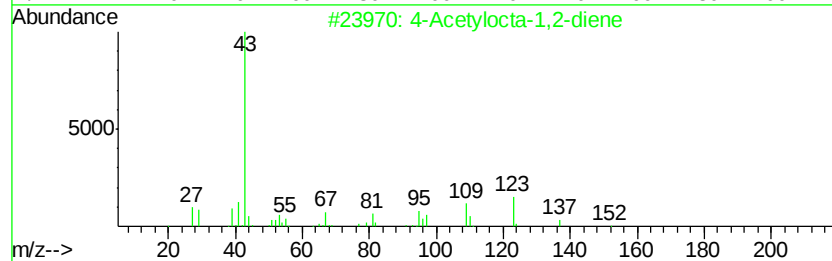
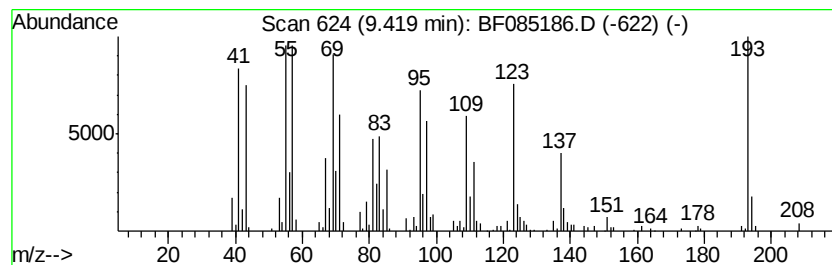
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.42 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	3.49 ng	227433	Acenaphthene-d10	10.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	4	Acetylocta-1,2-diene	152	C10H16O	1000250-44-5	27
2	1	(P-FLUOROPHENYL)-4-PIPERIDONE	193	C11H12FNO	1000238-56-7	27
3	3	Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	20
4	1,7	Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	18
5	Bicyclo[2.2.1]	heptane, 2,2,3-tri...	138	C10H18	020536-41-8	15



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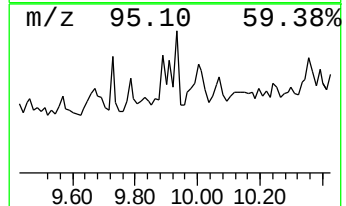
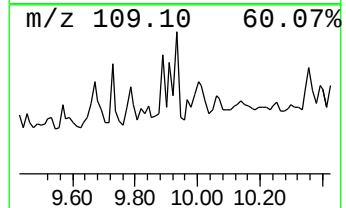
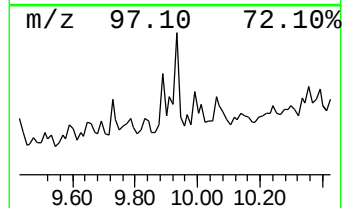
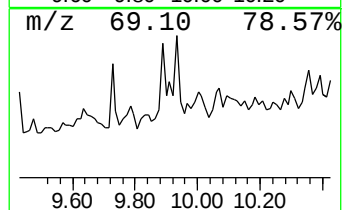
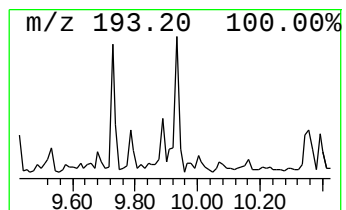
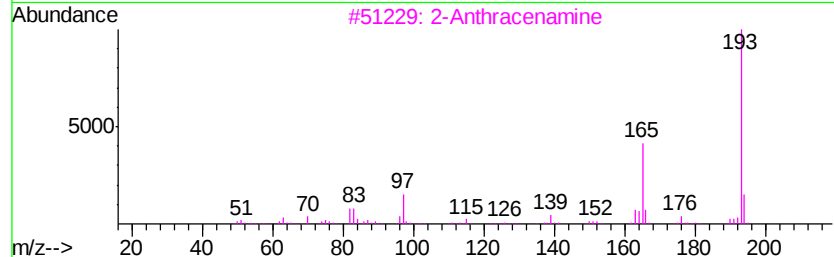
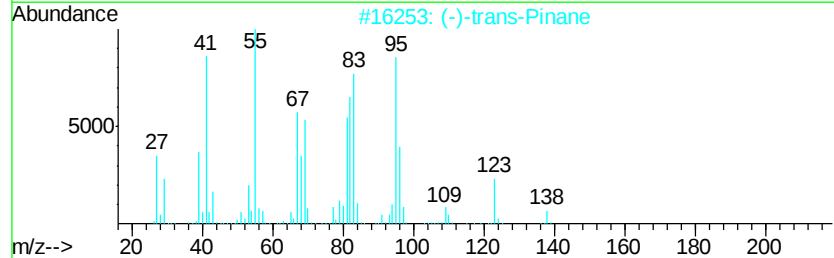
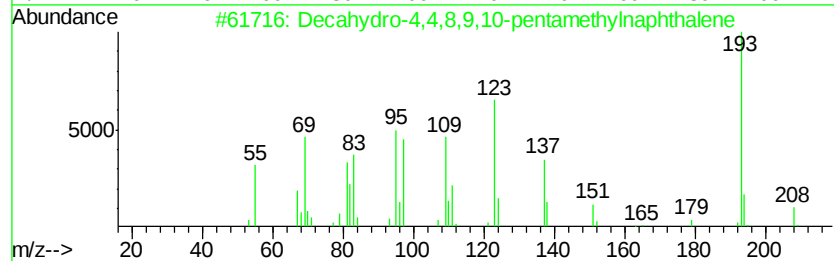
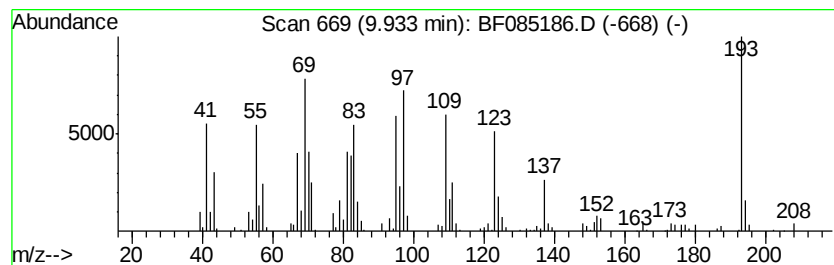
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Peak Number 7 Decahydro-4,4,8,9,10-pentam... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	2.85 ng	185799	Acenaphthene-d10	10.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	72
2		(-)-trans-Pinane	138	C10H18	033626-25-4	25
3		2-Anthracenamine	193	C14H11N	000613-13-8	25
4		1-(P-FLUOROPHENYL)-4-PIPERIDONE	193	C11H12FNO	1000238-56-7	25
5		2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	22



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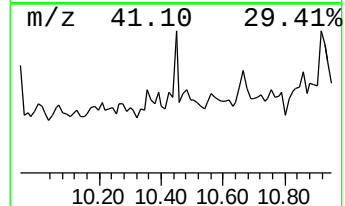
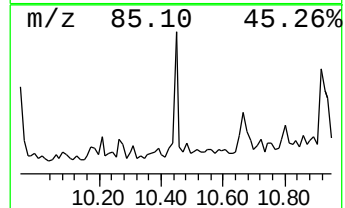
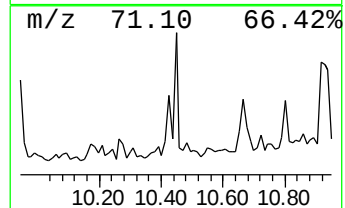
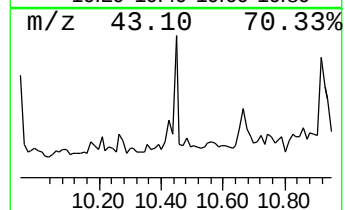
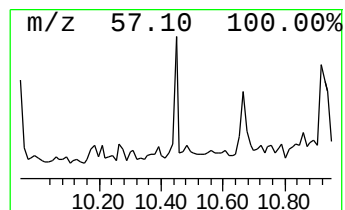
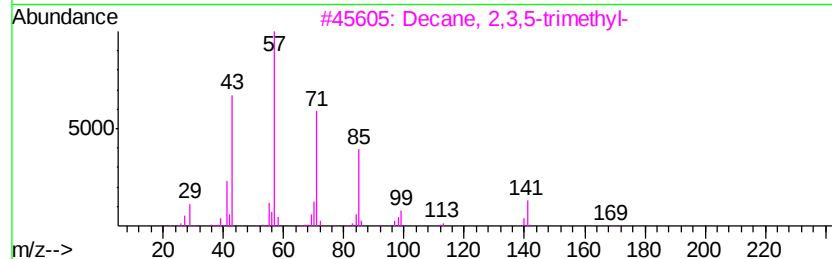
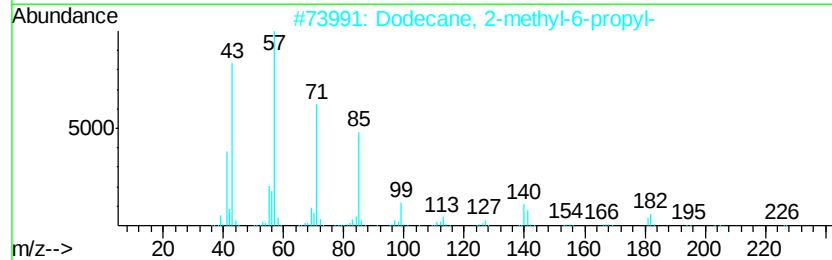
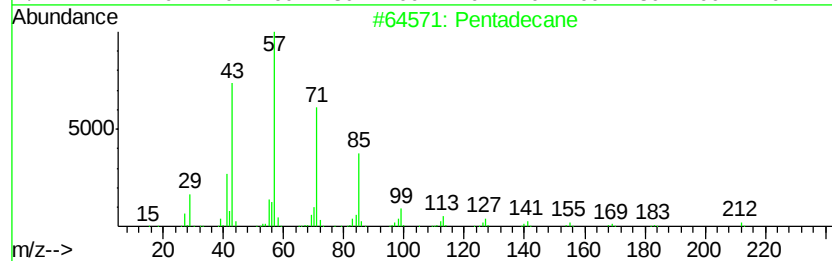
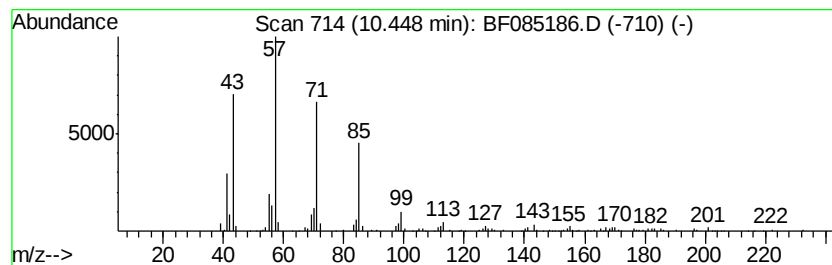
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.91 ng	189921	Acenaphthene-d10	10.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	86
2	Dodecane, 2-methyl-6-propyl-	226 C16H34	055045-08-4	80
3	Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3	80
4	Nonane, 3,7-dimethyl-	156 C11H24	017302-32-8	72
5	Decane, 3,6-dimethyl-	170 C12H26	017312-53-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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Acq On : 4 Mar 2016 5:08
Operator : SJ/UM
Sample : H1663-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

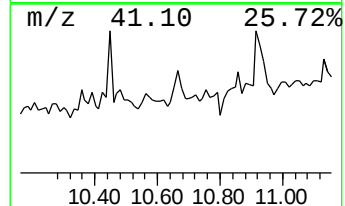
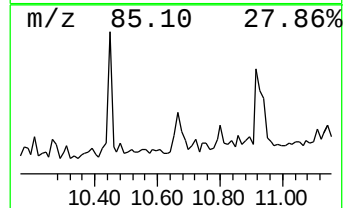
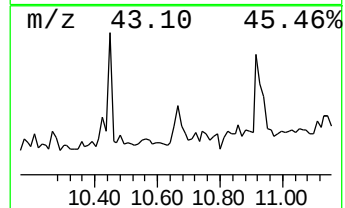
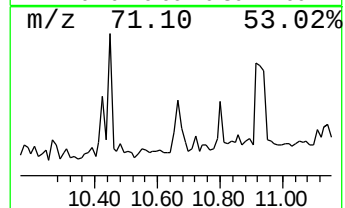
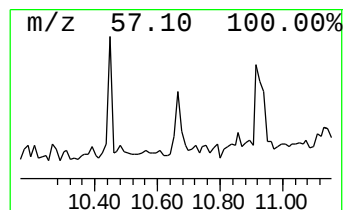
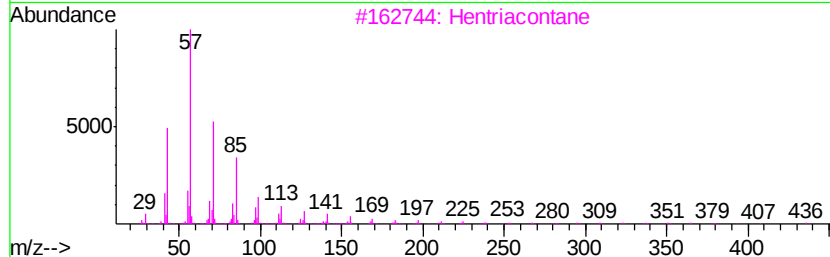
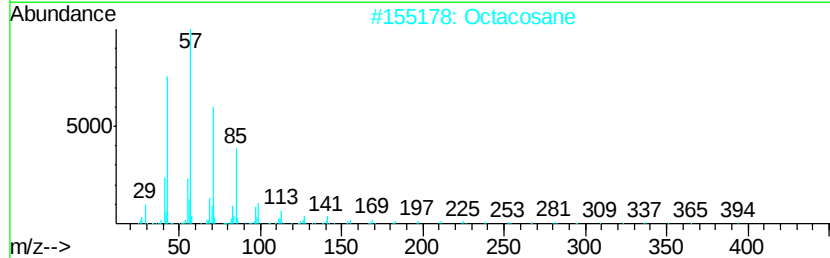
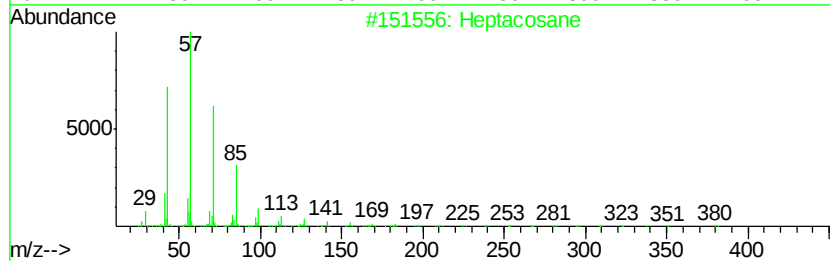
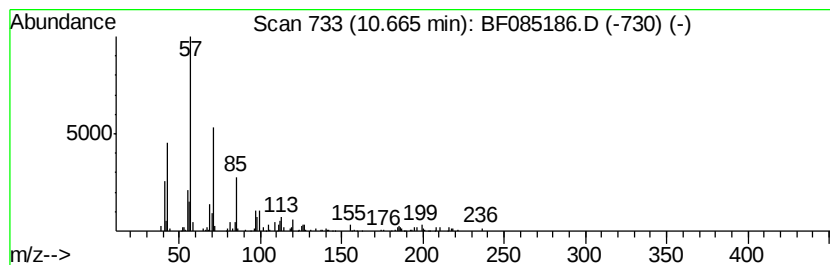
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ClientSampleId :
SB-39(11-13)

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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 9 Heptacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.23 ng	145274	Acenaphthene-d10	10.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	80
2	Octacosane	394 C28H58	000630-02-4	72
3	Hentriacontane	437 C31H64	000630-04-6	72
4	Pentadecane	212 C15H32	000629-62-9	72
5	Tetratetracontane	619 C44H90	007098-22-8	72



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ClientSampleId :
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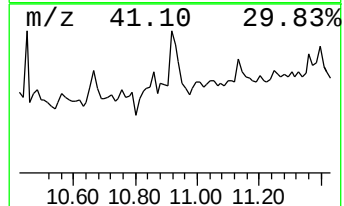
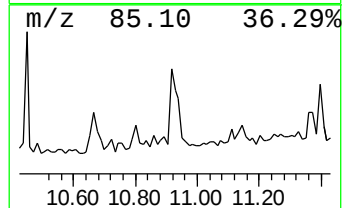
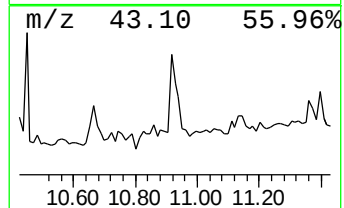
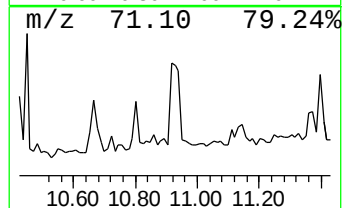
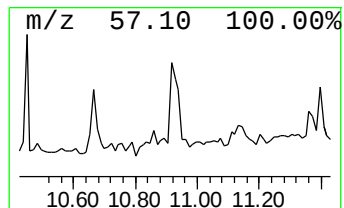
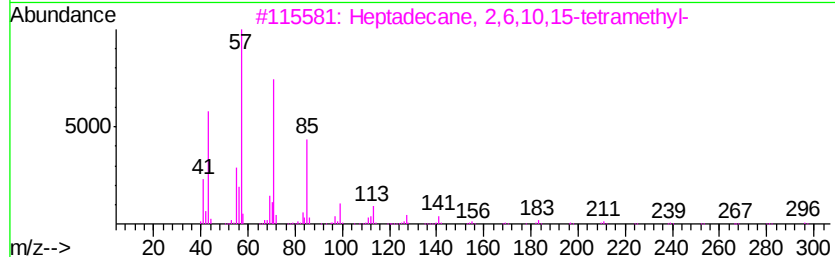
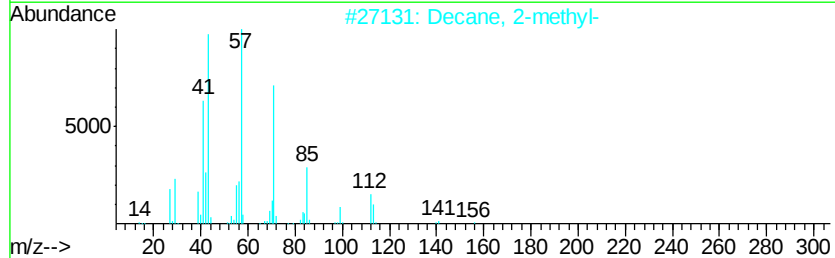
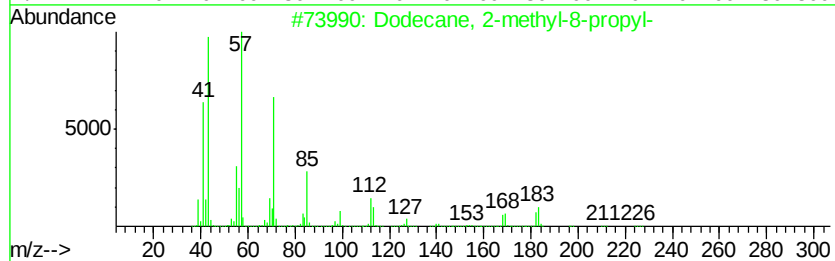
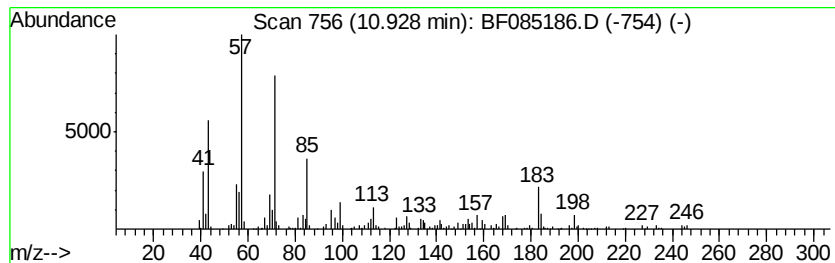
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dodecane, 2-methyl-8-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	6.81 ng	362187	Phenanthrene-d10	11.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	80
2			Decane, 2-methyl-	156	C11H24	006975-98-0	74
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74
4			Tridecane	184	C13H28	000629-50-5	74
5			Tetradecane	198	C14H30	000629-59-4	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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Acq On : 4 Mar 2016 5:08
Operator : SJ/UM
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ClientSampleId :
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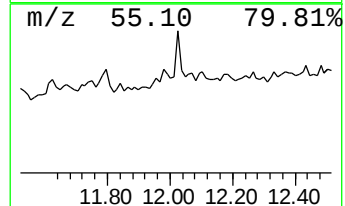
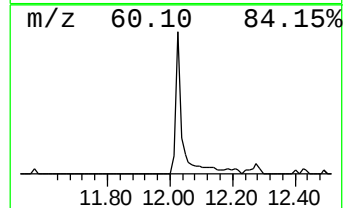
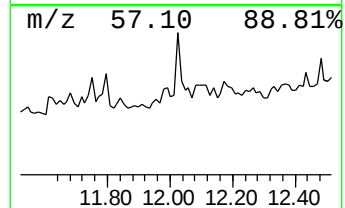
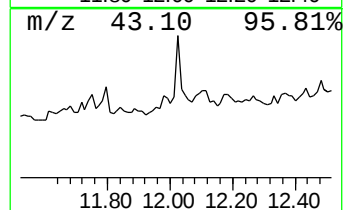
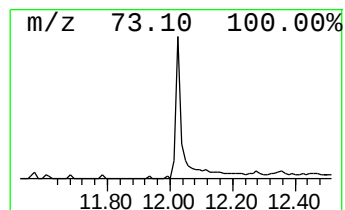
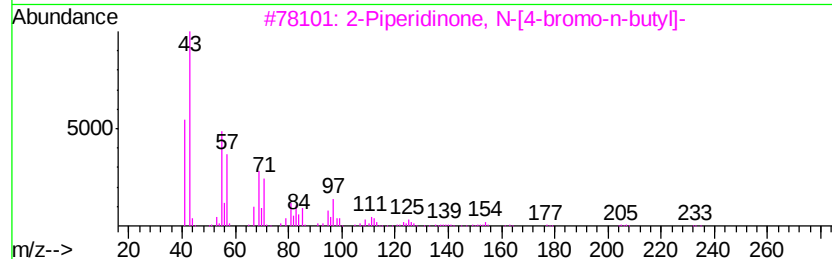
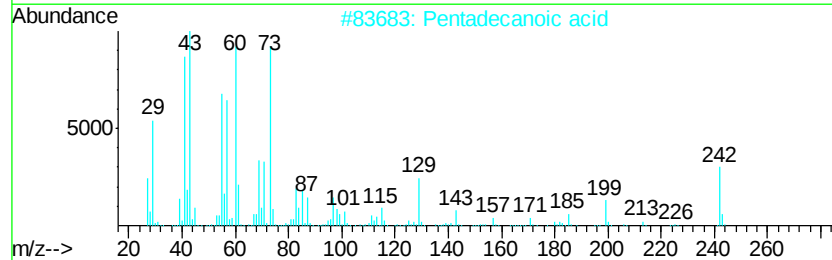
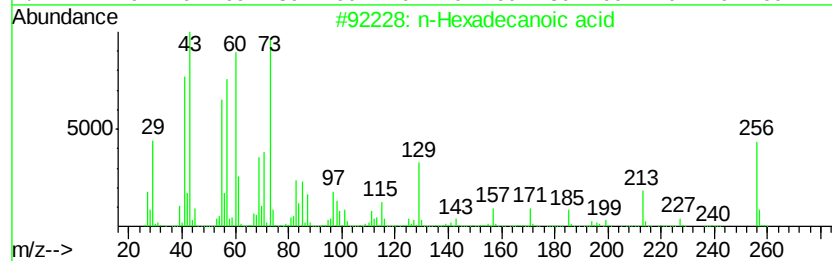
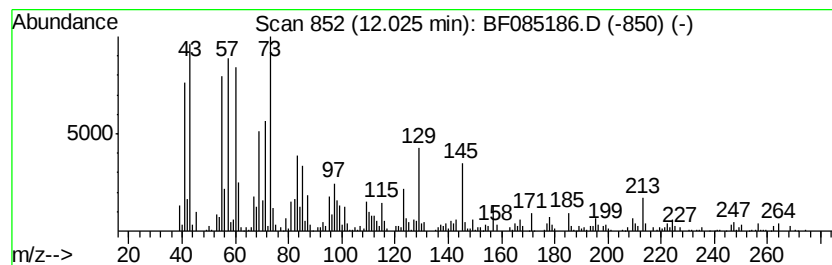
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	5.15 ng	273633	Phenanthrene-d10	11.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	44
4			n-Decanoic acid	172	C10H20O2	000334-48-5	43
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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Acq On : 4 Mar 2016 5:08
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Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-39(11-13)

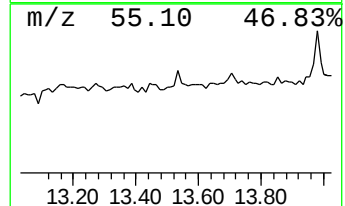
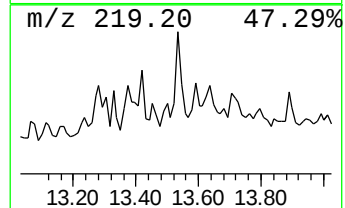
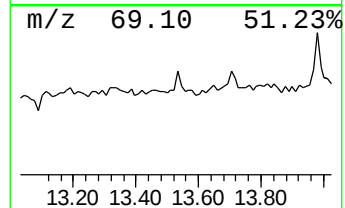
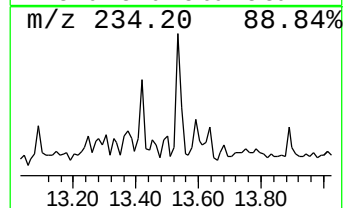
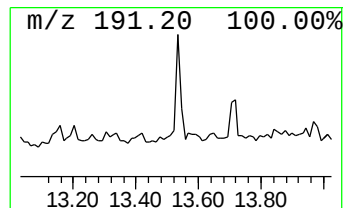
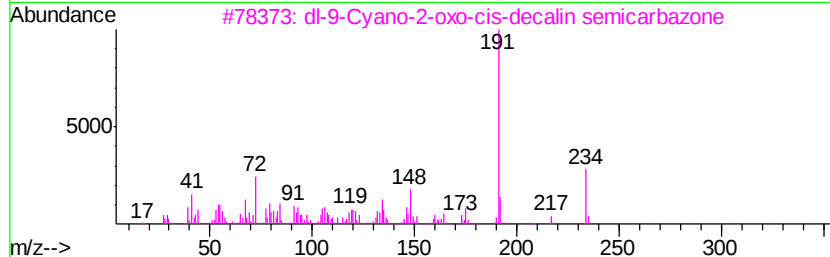
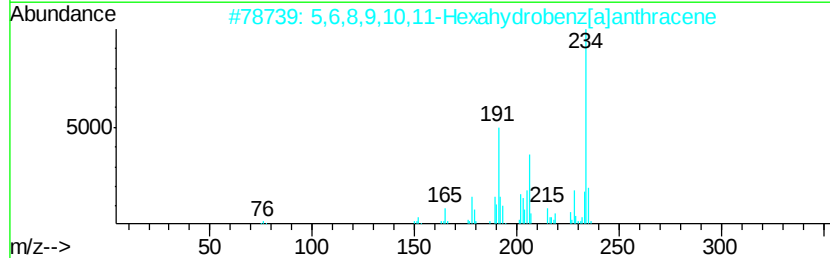
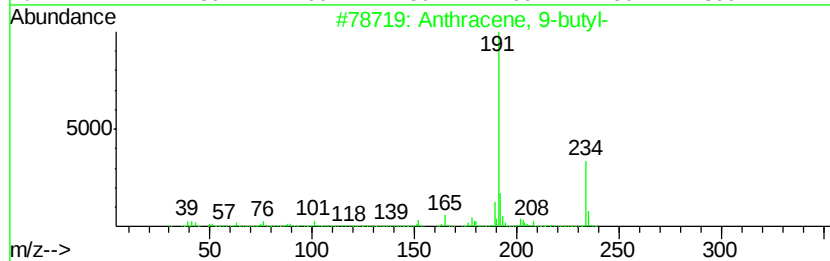
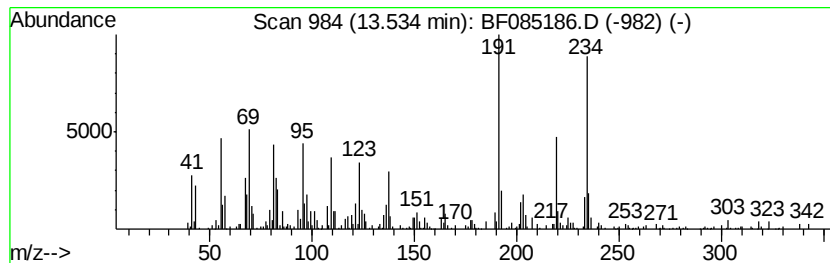
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown13.53 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	3.42 ng	134549	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-butyl-	234	C18H18	001498-69-7	49
2		5,6,8,9,10,11-Hexahydrobenz[a]an...	234	C18H18	067064-61-3	47
3		dl-9-Cyano-2-oxo-cis-decalin sem...	234	C12H18N4O	002740-39-8	43
4		Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	42
5		Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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SB-39(11-13)

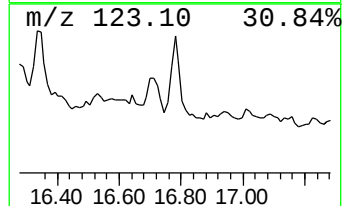
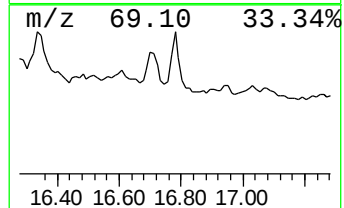
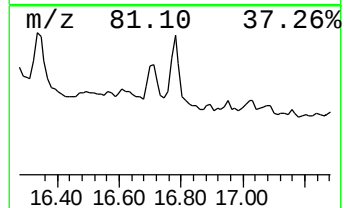
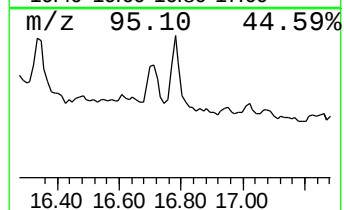
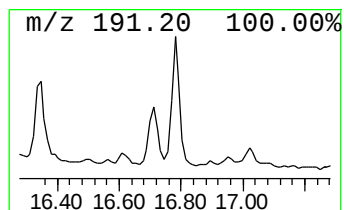
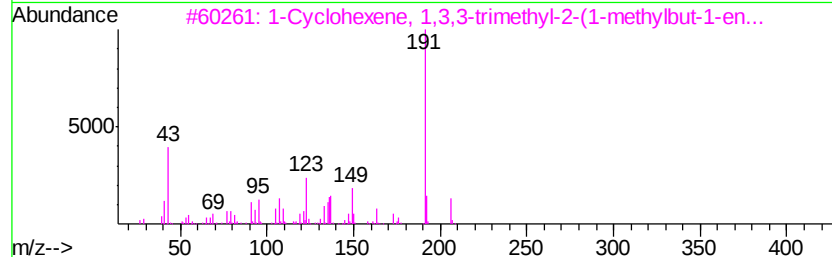
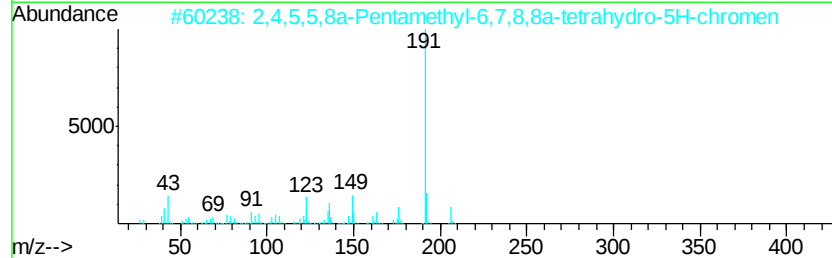
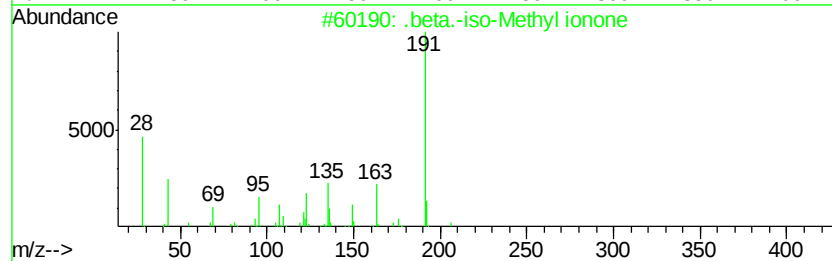
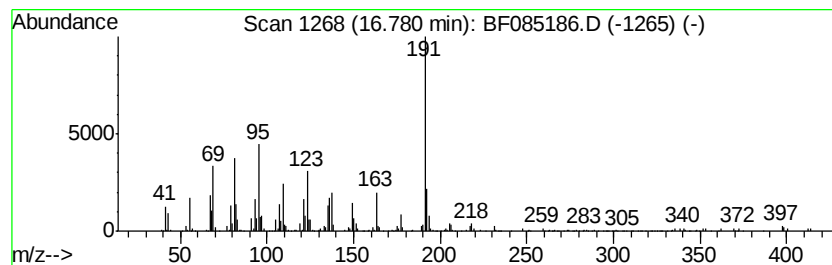
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .beta.-iso-Methyl ionone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	11.69 ng	513902	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	60
2		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	47
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	40
4		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
5		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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...	5.19	17.8	ng	805309	1	6.98	903383	20.0
unknown6.74	6.74	72.8	ng	3287680	1	6.98	903383	20.0
unknown9.42	9.42	3.5	ng	227433	3	10.02	1304230	20.0
Decahydro-4,4,8,9...	9.93	2.9	ng	185799	3	10.02	1304230	20.0
Pentadecane	10.45	2.9	ng	189921	3	10.02	1304230	20.0
Heptacosane	10.66	2.2	ng	145274	3	10.02	1304230	20.0
Dodecane, 2-methy...	10.93	6.8	ng	362187	4	11.51	1063420	20.0
n-Hexadecanoic acid	12.02	5.2	ng	273633	4	11.51	1063420	20.0
unknown13.53	13.53	3.4	ng	134549	5	14.14	786618	20.0
.beta.-iso-Methyl...	16.78	11.7	ng	513902	6	15.61	879056	20.0