

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
 Data File : BF095750.D
 Acq On : 7 Jun 2017 17:23
 Operator : SJ/MA
 Sample : I3506-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF060517.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	4.587	506	510	527	rBV	53007	137412	7.84%	0.794%
2	5.275	623	627	660	rBV	921355	1565287	89.30%	9.046%
3	6.945	906	911	922	rBV	1023852	1509973	86.15%	8.726%
4	7.039	922	927	943	rVB	1265729	1752823	100.00%	10.129%
5	7.381	981	985	998	rBV	343760	424326	24.21%	2.452%
6	7.622	1021	1026	1042	rBV	968371	1230182	70.18%	7.109%
7	8.298	1136	1141	1162	rBV	715663	942423	53.77%	5.446%
8	9.416	1326	1331	1345	rBV	455552	580694	33.13%	3.356%
9	11.198	1628	1634	1650	rBV	1365277	1692550	96.56%	9.781%
10	11.886	1746	1751	1764	rBV	351259	407860	23.27%	2.357%
11	12.015	1769	1773	1779	rVB	13325	19693	1.12%	0.114%
12	12.239	1806	1811	1816	rBV2	476714	574850	32.80%	3.322%
13	12.286	1816	1819	1824	rVB2	23840	31332	1.79%	0.181%
14	13.098	1953	1957	1960	rBV2	20957	26042	1.49%	0.150%
15	13.133	1960	1963	1973	rVB	17179	25803	1.47%	0.149%
16	13.533	2026	2031	2039	rBV	608754	827236	47.19%	4.781%
17	13.868	2082	2088	2095	rBV2	25418	42687	2.44%	0.247%
18	14.598	2207	2212	2213	rBV	17803	19229	1.10%	0.111%
19	14.627	2213	2217	2221	rVV2	394409	493612	28.16%	2.853%
20	14.668	2221	2224	2231	rVB	143467	180122	10.28%	1.041%
21	14.762	2236	2240	2246	rVB	33639	46942	2.68%	0.271%
22	15.168	2306	2309	2313	rVB4	15082	18404	1.05%	0.106%
23	15.433	2351	2354	2358	rBV2	39137	42346	2.42%	0.245%
24	15.480	2358	2362	2368	rVB	34732	42791	2.44%	0.247%
25	15.586	2376	2380	2384	rVV2	44942	62854	3.59%	0.363%
26	15.645	2384	2390	2399	rVB3	93655	144760	8.26%	0.837%
27	15.886	2427	2431	2435	rBV3	24026	32470	1.85%	0.188%
28	16.245	2486	2492	2495	rBV	39556	46498	2.65%	0.269%
29	16.286	2495	2499	2503	rVV2	19608	27389	1.56%	0.158%
30	16.362	2508	2512	2517	rVV2	41007	51791	2.95%	0.299%
31	16.445	2520	2526	2532	rVV	259458	311529	17.77%	1.800%
32	16.551	2539	2544	2547	rBV5	12394	19639	1.12%	0.113%
33	16.745	2573	2577	2583	rBV	330804	383560	21.88%	2.217%
34	16.945	2608	2611	2614	rBV3	17935	21496	1.23%	0.124%

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35	17.003	2616	2621	2625	rVV	1045093	1130627	64.50%	6.534%
36	17.080	2627	2634	2637	rBV2	22347	35927	2.05%	0.208%
37	17.192	2649	2653	2655	rBV4	19081	34566	1.97%	0.200%
38	17.221	2655	2658	2664	rVB	32143	41339	2.36%	0.239%
39	17.309	2670	2673	2677	rVB2	21374	20844	1.19%	0.120%
40	17.350	2677	2680	2686	rBV3	36247	63206	3.61%	0.365%
41	17.462	2697	2699	2703	rBV	31863	31679	1.81%	0.183%
42	17.509	2703	2707	2712	rVB	23306	30671	1.75%	0.177%
43	17.909	2772	2775	2782	rVB	23048	36208	2.07%	0.209%
44	18.021	2790	2794	2797	rBV2	30228	40169	2.29%	0.232%
45	18.050	2797	2799	2802	rVB2	34381	32653	1.86%	0.189%
46	18.086	2802	2805	2807	rBV	18453	18859	1.08%	0.109%
47	18.203	2823	2825	2829	rVB2	18311	19564	1.12%	0.113%
48	18.256	2829	2834	2843	rBV3	65779	122903	7.01%	0.710%
49	18.345	2843	2849	2852	rBV2	427039	602275	34.36%	3.481%
50	18.380	2852	2855	2861	rVB2	109441	141427	8.07%	0.817%
51	18.468	2867	2870	2875	rVB3	29992	40328	2.30%	0.233%
52	18.680	2902	2906	2911	rVB4	21666	31357	1.79%	0.181%
53	18.850	2933	2935	2939	rVB	37773	34564	1.97%	0.200%
54	18.892	2940	2942	2946	rVB	23880	21487	1.23%	0.124%
55	18.968	2952	2955	2957	rVB4	17210	19080	1.09%	0.110%
56	19.003	2958	2961	2965	rBV4	22676	36744	2.10%	0.212%
57	19.386	3020	3026	3030	rBV	110966	154514	8.82%	0.893%
58	19.491	3042	3044	3051	rVB4	30428	40559	2.31%	0.234%
59	19.609	3061	3064	3067	rBV	128652	166580	9.50%	0.963%
60	19.721	3081	3083	3087	rVB	29972	30535	1.74%	0.176%
61	19.897	3110	3113	3118	rBV	90189	105569	6.02%	0.610%
62	19.956	3120	3123	3128	rBV	116226	124358	7.09%	0.719%
63	20.015	3128	3133	3137	rBV	277216	358982	20.48%	2.075%

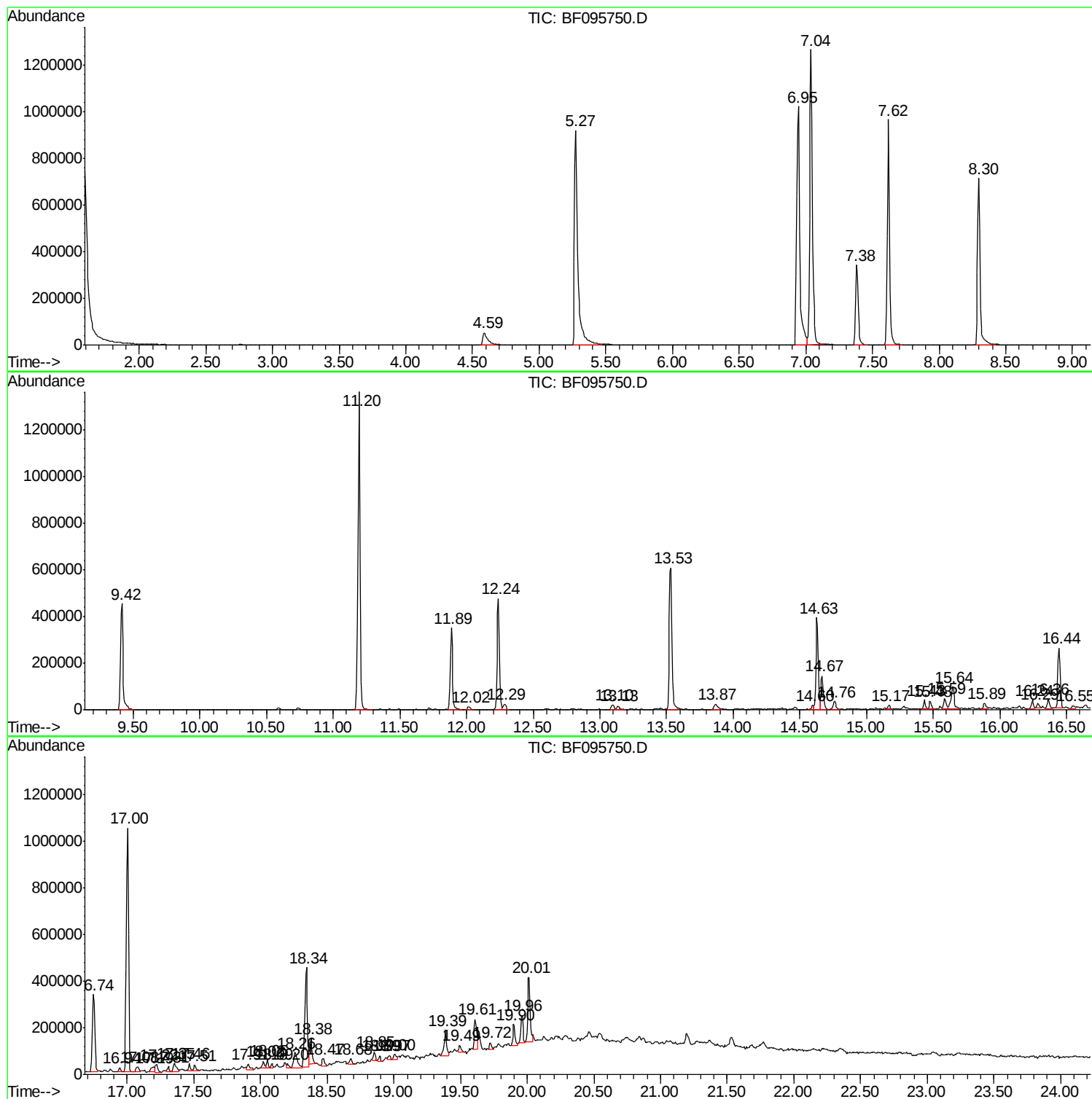
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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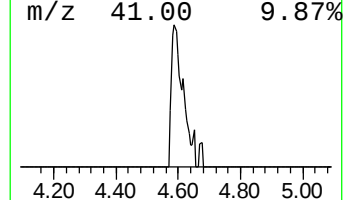
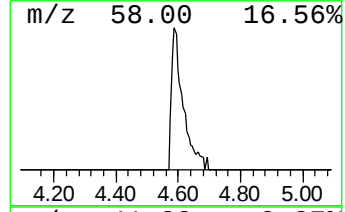
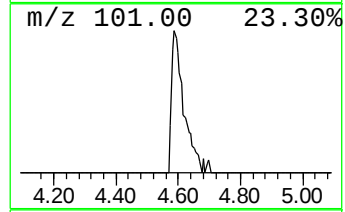
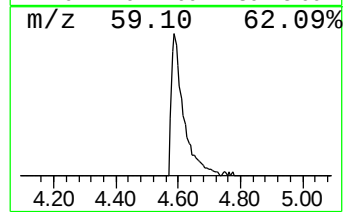
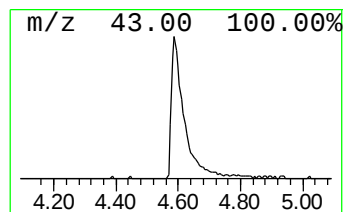
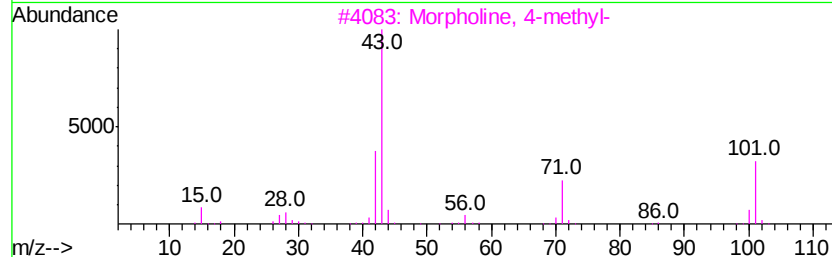
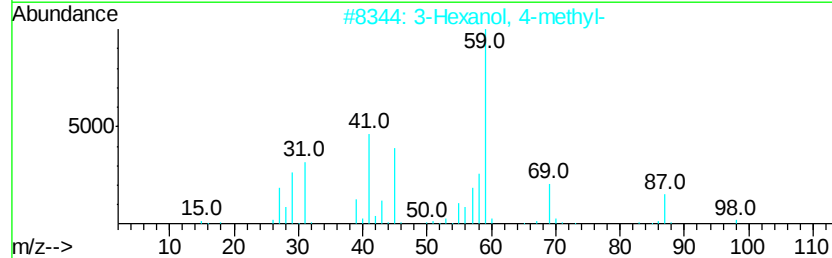
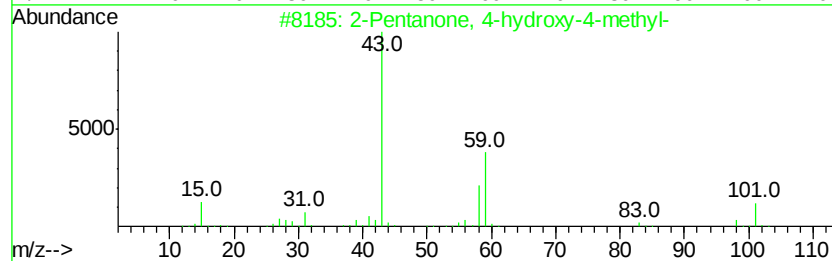
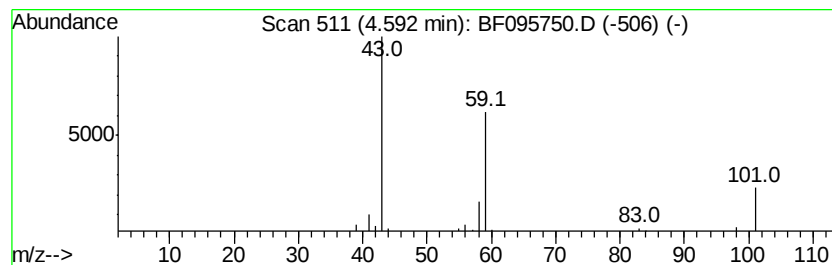
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	6.48 ng	137412	1,4-Dichlorobenzene-d4	7.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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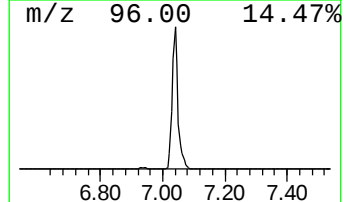
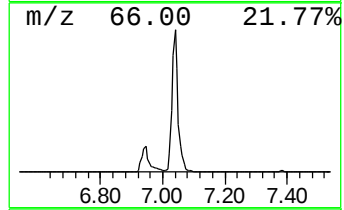
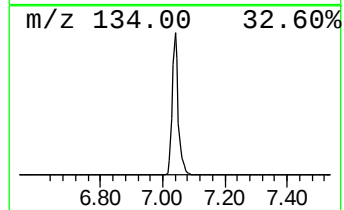
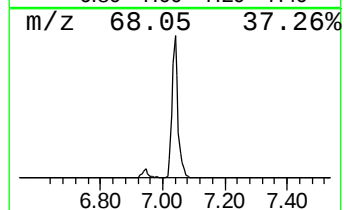
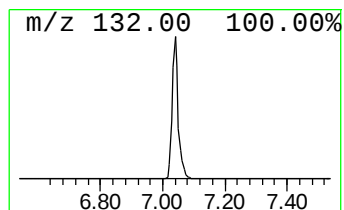
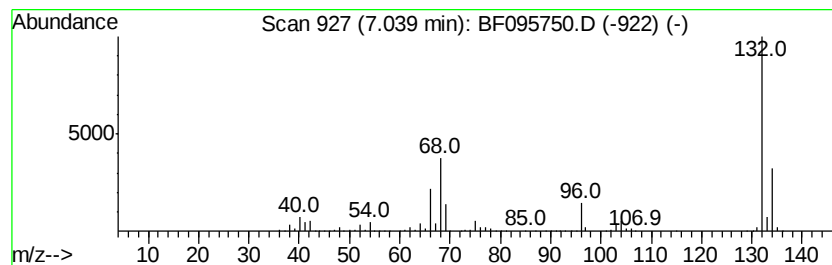
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	82.62 ng	1752820	1,4-Dichlorobenzene-d4	7.38

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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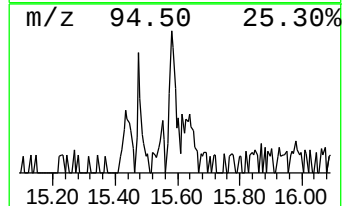
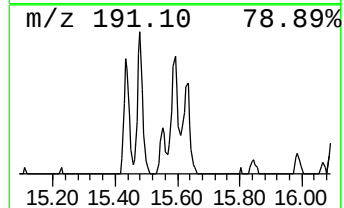
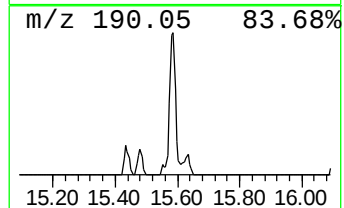
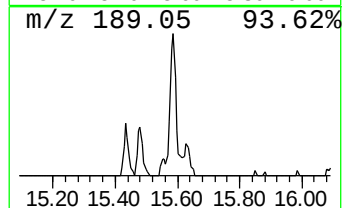
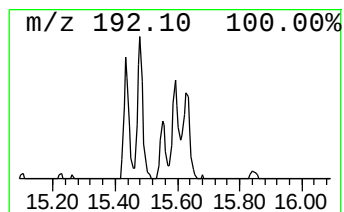
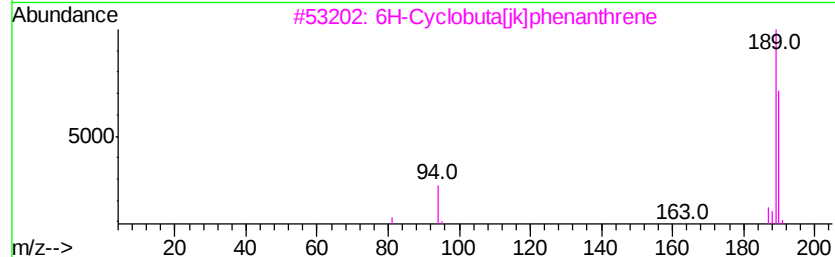
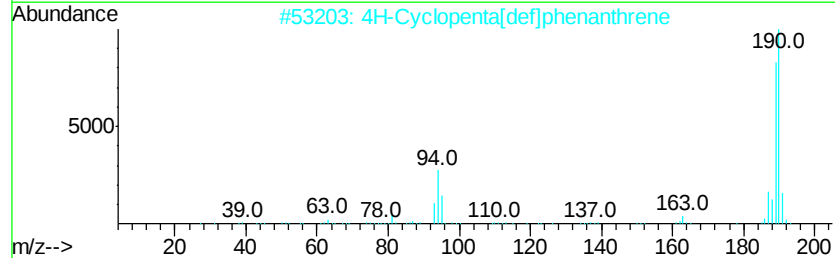
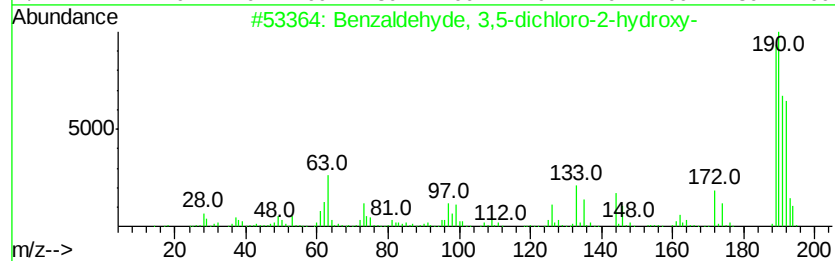
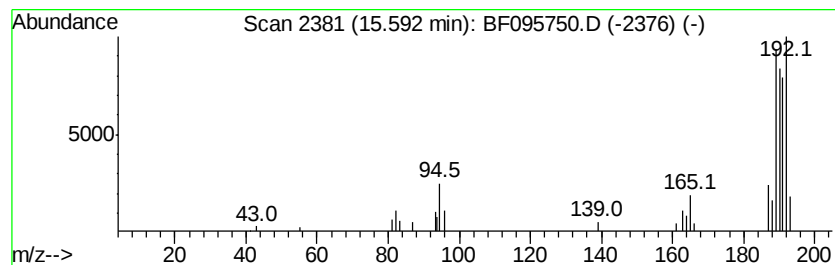
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.59	2.55 ng	62854	Phenanthrene-d10		14.63
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
3	6H-Cyclobuta[f]kphenanthrene	190	C15H10	083469-43-6	58
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	Methyl diselenide	190	C2H6Se2	007101-31-7	22



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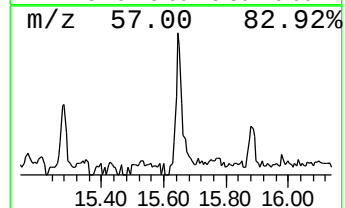
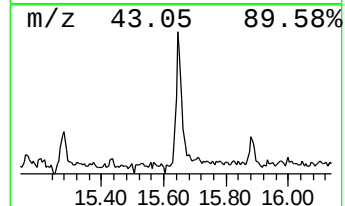
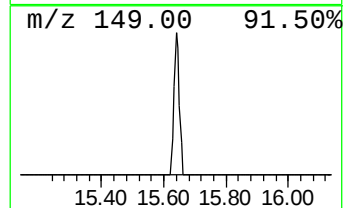
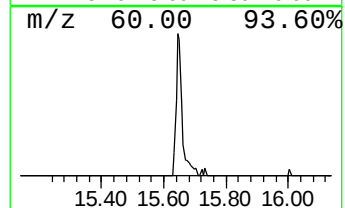
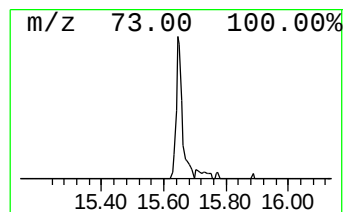
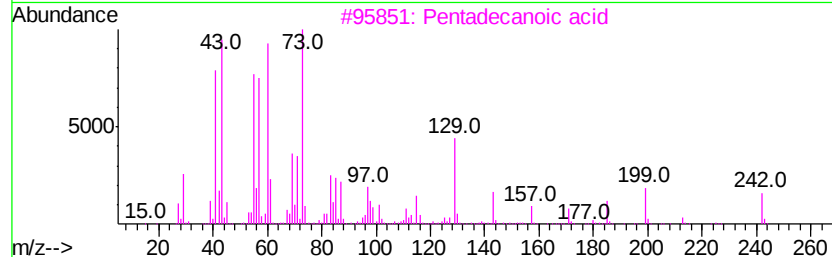
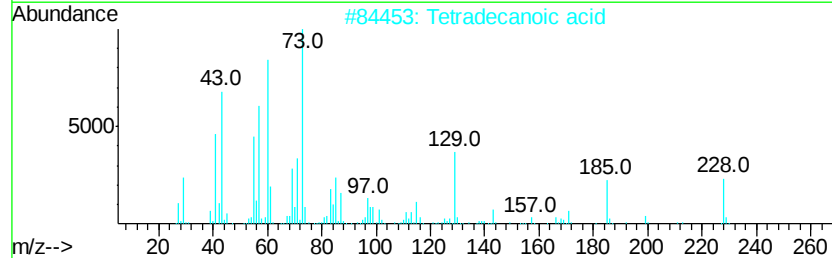
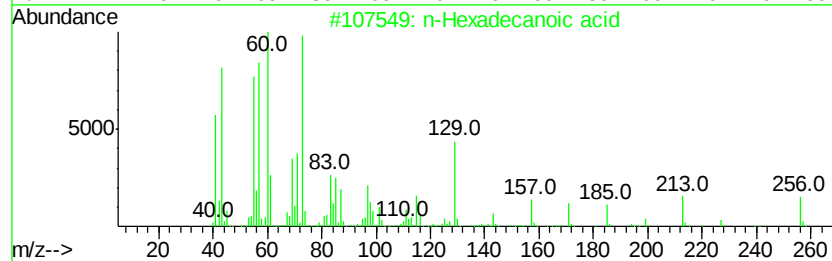
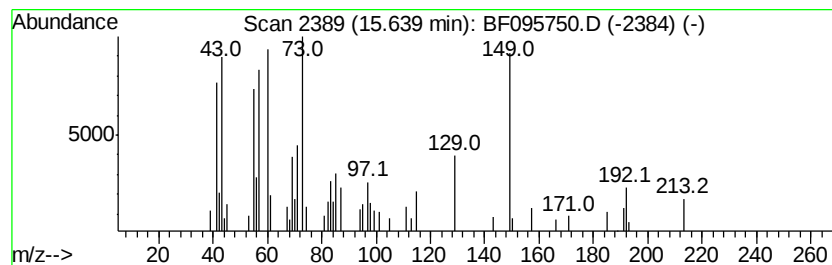
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	5.87 ng	144760	Phenanthrene-d10	14.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4		Tridecanoic acid	214	C13H26O2	000638-53-9	47
5		Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	18



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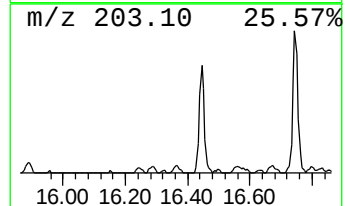
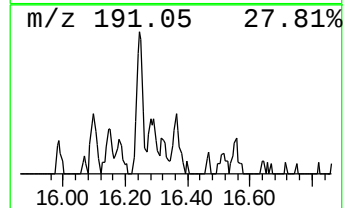
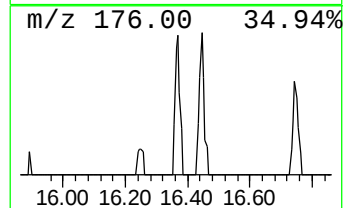
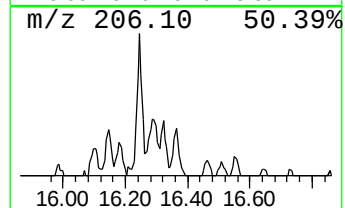
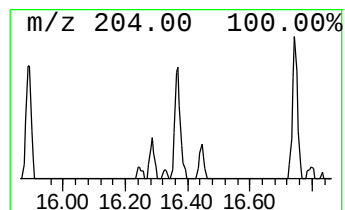
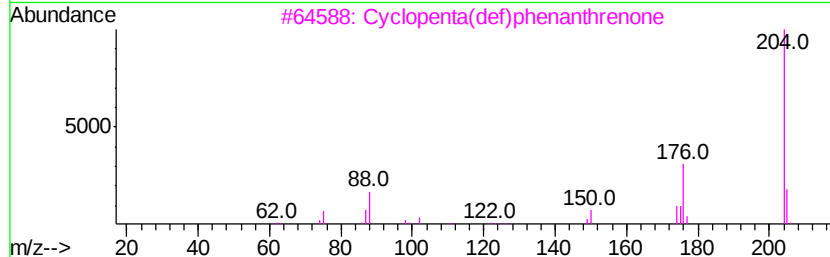
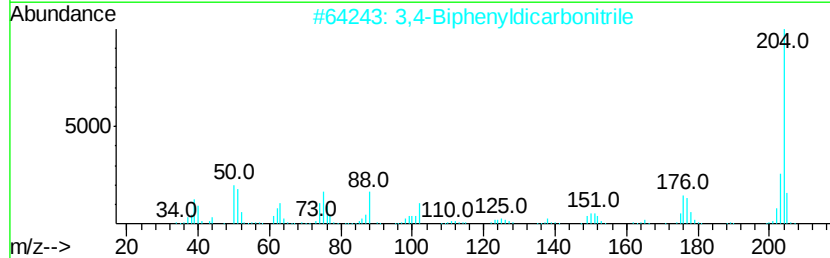
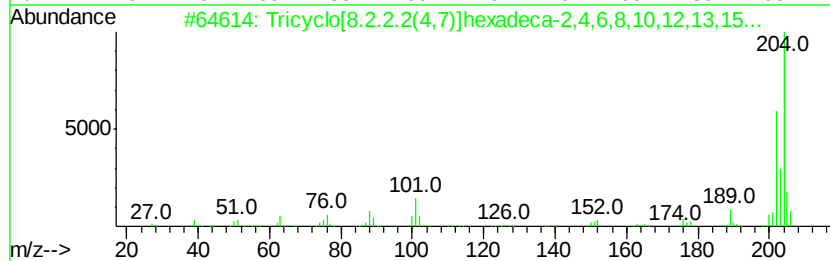
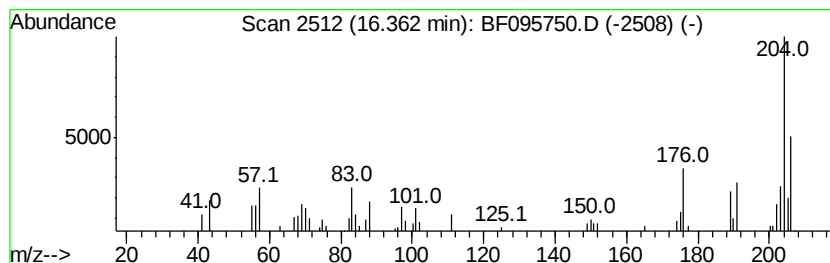
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tricyclo[8.2.2.2(4,7)]hexad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	2.10 ng	51791	Phenanthrene-d10	14.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	55
2		3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	55
3		Cyclopenta(def)phenanthrene	204	C15H8O	005737-13-3	50
4		[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	46
5		[1,1'-Biphenyl]-2-ol, 3-chloro-	204	C12H9ClO	000085-97-2	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095750.D
Acq On : 7 Jun 2017 17:23
Operator : SJ/MA
Sample : I3506-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

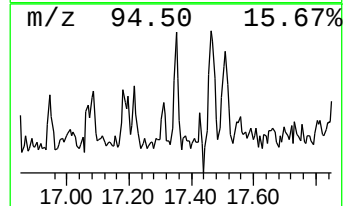
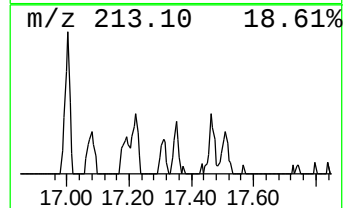
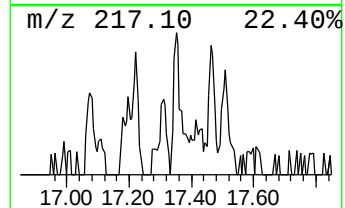
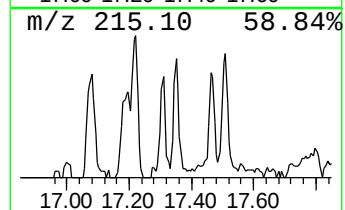
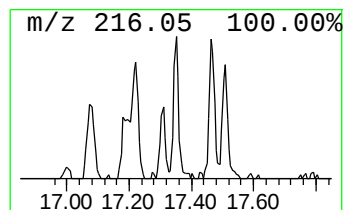
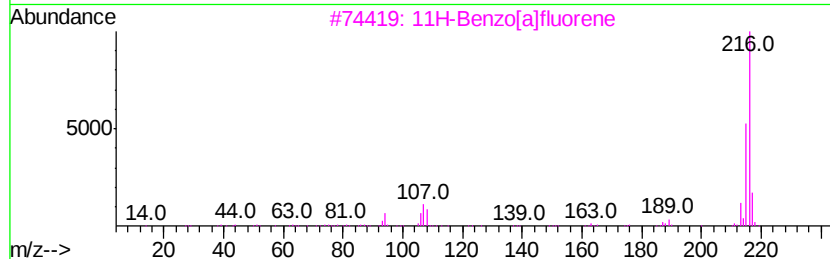
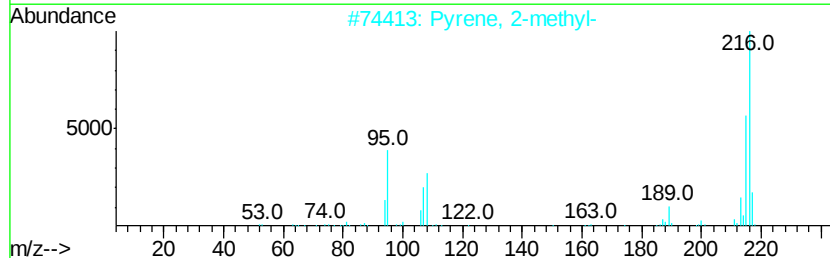
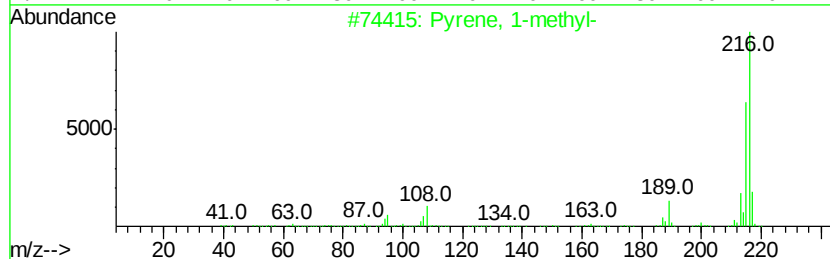
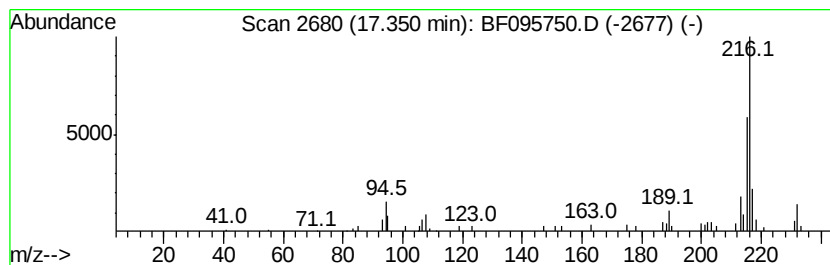
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.35	2.10 ng	63206	Chrysene-d12	18.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2		Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5		Pyrene, 4-methyl-	216	C17H12	003353-12-6	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095750.D
Acq On : 7 Jun 2017 17:23
Operator : SJ/MA
Sample : I3506-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

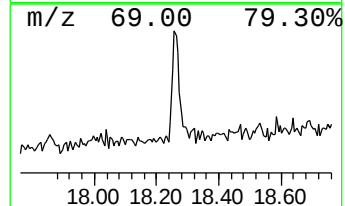
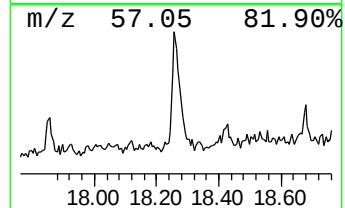
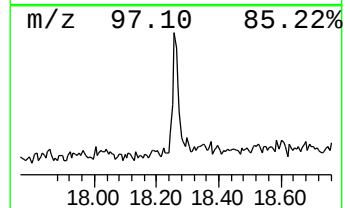
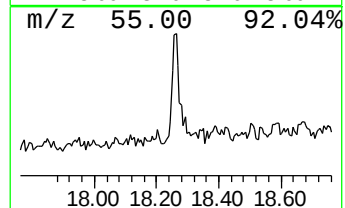
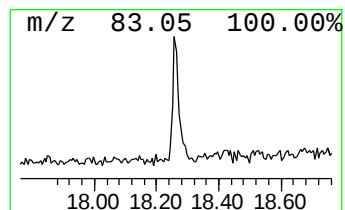
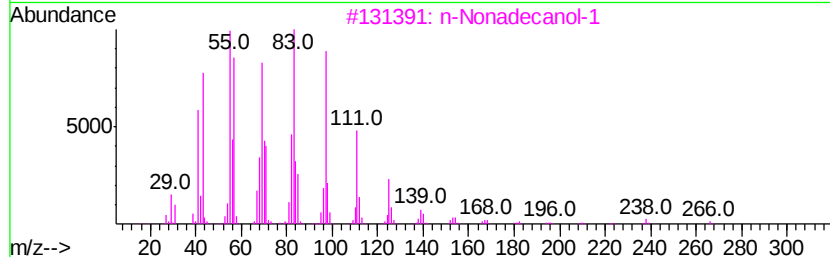
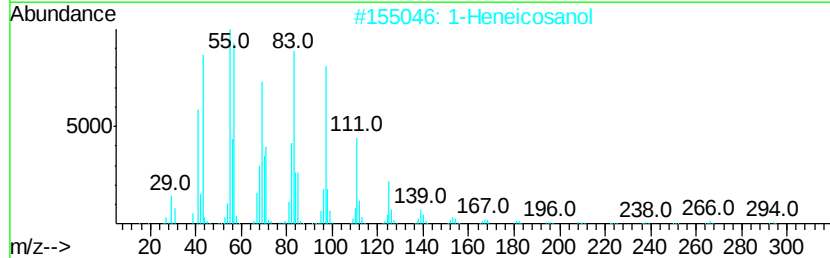
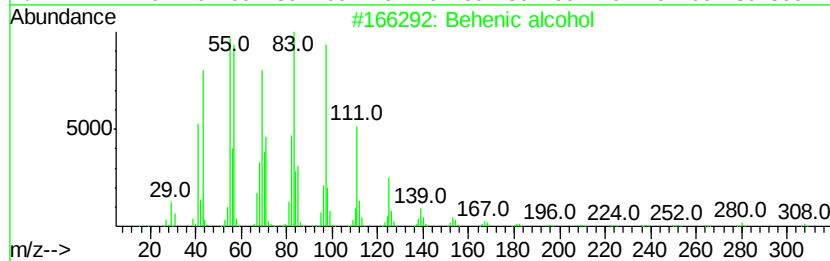
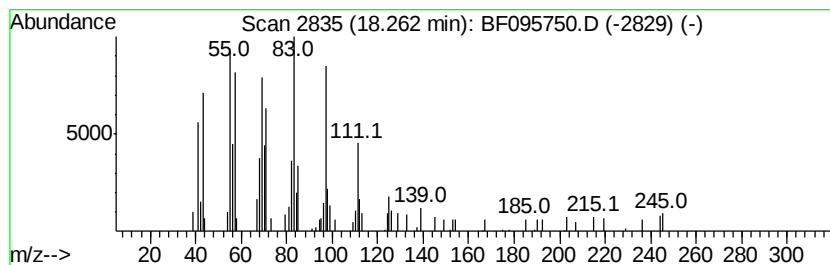
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.26	4.08 ng	122903	Chrysene-d12	18.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095750.D
Acq On : 7 Jun 2017 17:23
Operator : SJ/MA
Sample : I3506-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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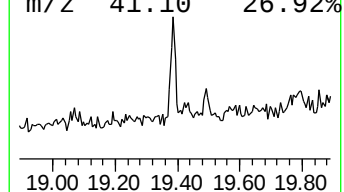
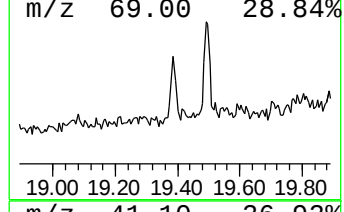
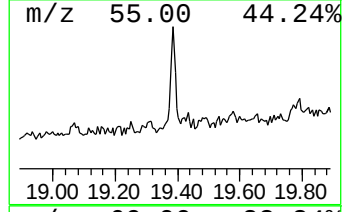
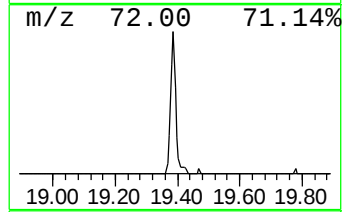
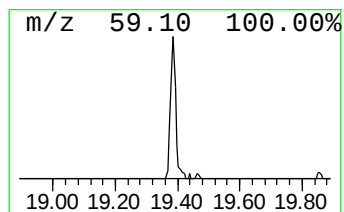
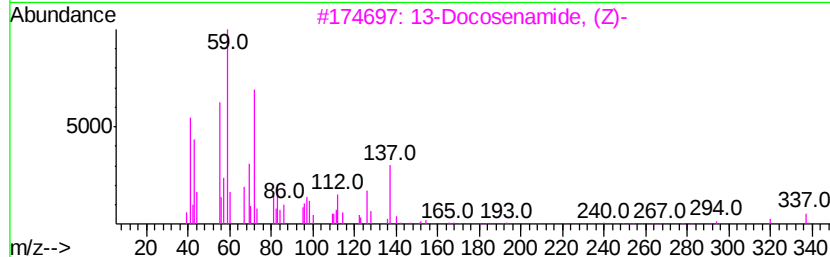
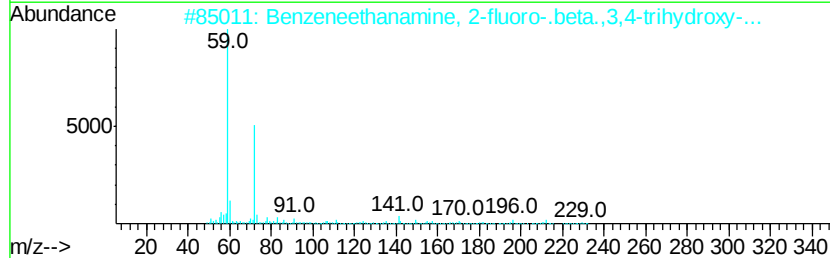
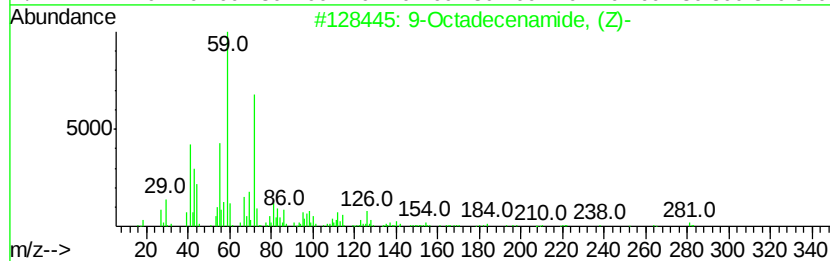
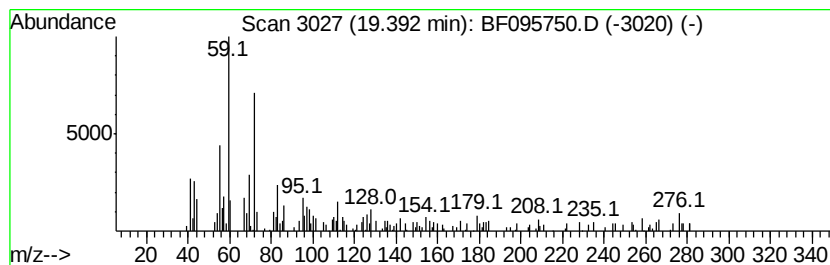
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	8.61 ng	154514	Perylene-d12	20.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	68
3		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
4		d-Glucosamine	179	C6H13NO5	000090-77-7	59
5		Dodecanamide	199	C12H25NO	001120-16-7	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095750.D
Acq On : 7 Jun 2017 17:23
Operator : SJ/MA
Sample : I3506-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

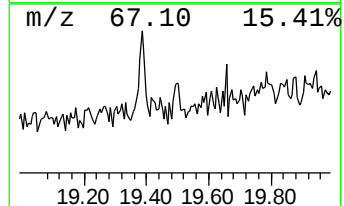
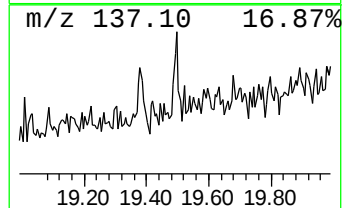
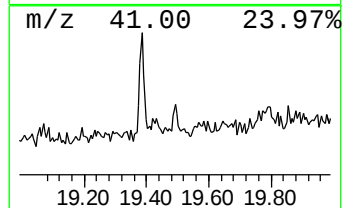
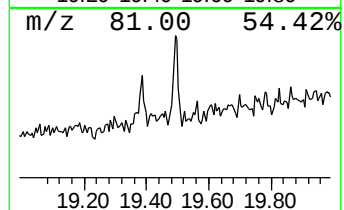
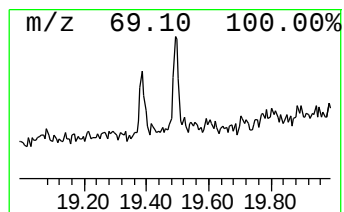
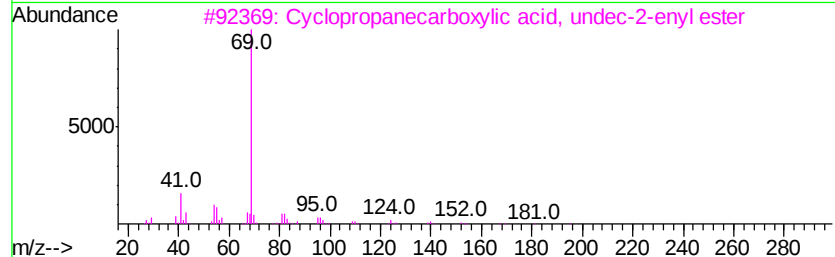
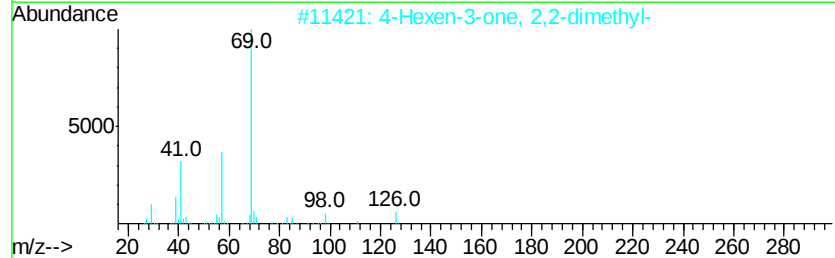
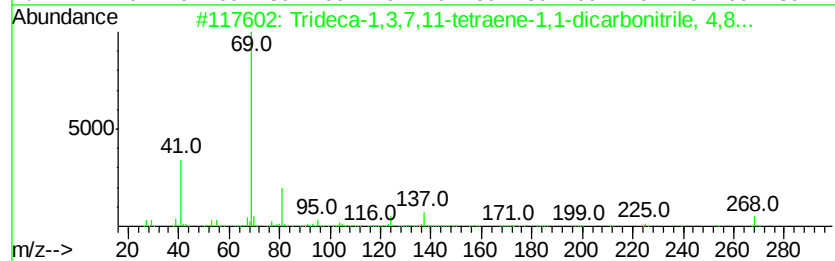
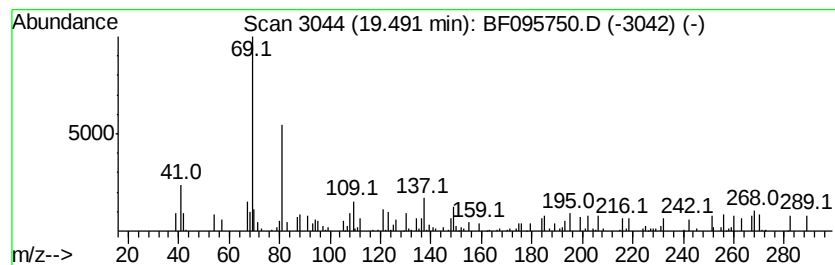
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trideca-1,3,7,11-tetraene-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.49	2.26 ng	40559	Perylene-d12	20.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53
2	4-Hexen-3-one, 2,2-dimethyl-	126	C8H14O	020971-19-1	49
3	Cvclopropanecarboxvlic acid, und...	238	C15H26O2	1000299-38-1	47
4	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47
5	(E)-all-trans-3,7,11-Trimethyl-2...	235	C15H25NO	1000161-30-7	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
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Operator : SJ/MA
Sample : I3506-01
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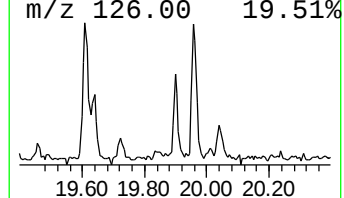
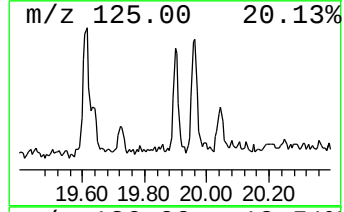
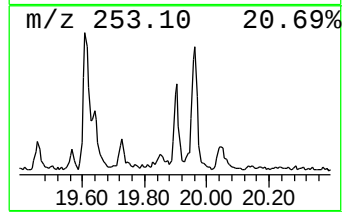
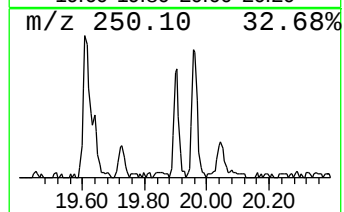
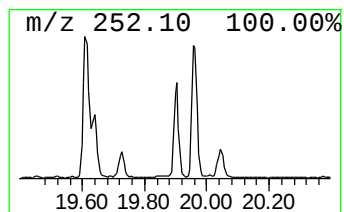
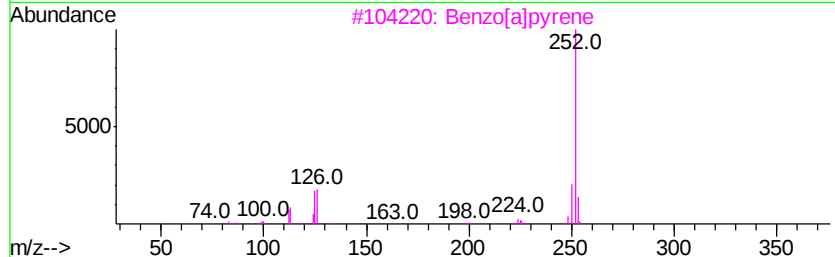
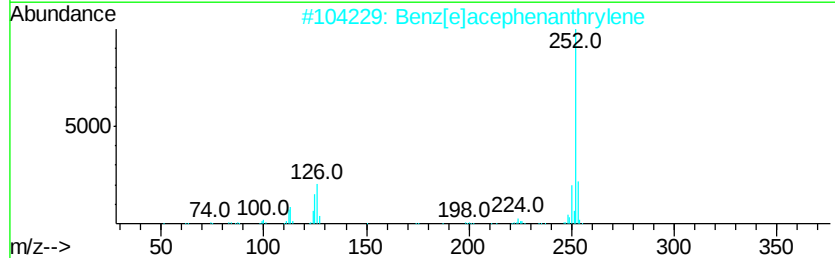
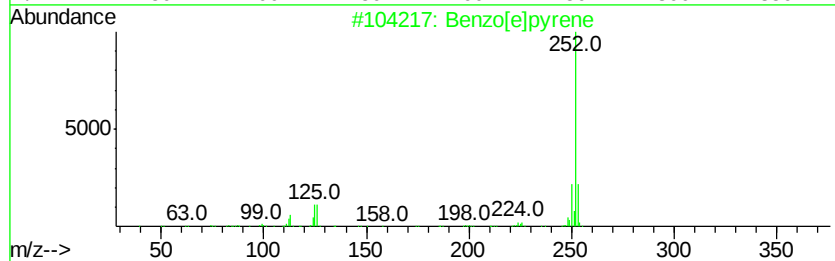
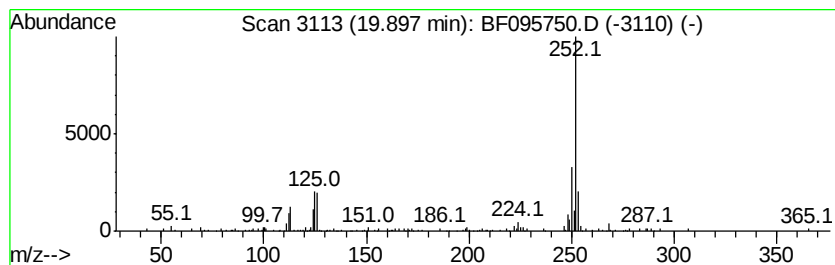
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.90	5.88 ng	105569	Perylene-d12	20.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	94
4	Benzo[i]fluoranthene	252	C20H12	000205-82-3	94
5	Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060717\
Data File : BF095750.D
Acq On : 7 Jun 2017 17:23
Operator : SJ/MA
Sample : I3506-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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
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unknown7.04	7.04	82.6	ng	1752820	1	7.38	424326	20.0
Benzaldehyde, 3,5...	15.59	2.5	ng	62854	4	14.63	493612	20.0
n-Hexadecanoic acid	15.64	5.9	ng	144760	4	14.63	493612	20.0
Tricyclo[8.2.2.2(...	16.36	2.1	ng	51791	4	14.63	493612	20.0
Pyrene, 1-methyl-	17.35	2.1	ng	63206	5	18.34	602275	20.0
Behenic alcohol	18.26	4.1	ng	122903	5	18.34	602275	20.0
9-Octadecenamide, ...	19.39	8.6	ng	154514	6	20.02	358982	20.0
Trideca-1,3,7,11-...	19.49	2.3	ng	40559	6	20.02	358982	20.0
Benzo[e]pyrene	19.90	5.9	ng	105569	6	20.02	358982	20.0