

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
 Data File : BF095795.D
 Acq On : 8 Jun 2017 21:34
 Operator : SJ/MA
 Sample : I3457-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-17

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	4.581	505	509	518	rBV	47657	121796	6.83%	0.648%
2	5.257	620	624	654	rBV	901292	1589604	89.08%	8.453%
3	6.928	903	908	920	rBV	1033364	1562851	87.58%	8.311%
4	7.022	920	924	937	rVB	1254225	1784512	100.00%	9.490%
5	7.369	979	983	997	rBV	305513	420018	23.54%	2.234%
6	7.604	1018	1023	1041	rBV	941052	1233875	69.14%	6.561%
7	8.286	1133	1139	1160	rBV	666847	974705	54.62%	5.183%
8	9.398	1324	1328	1342	rBV	438191	565684	31.70%	3.008%
9	11.180	1625	1631	1642	rBV	1350667	1642450	92.04%	8.734%
10	11.874	1745	1749	1754	rBV	153973	190850	10.69%	1.015%
11	12.004	1767	1771	1776	rVB	14650	19903	1.12%	0.106%
12	12.221	1803	1808	1813	rBV2	480414	581661	32.59%	3.093%
13	12.268	1813	1816	1822	rVB3	17984	27808	1.56%	0.148%
14	13.080	1947	1954	1958	rBV	16456	22833	1.28%	0.121%
15	13.121	1958	1961	1965	rBV	17852	23053	1.29%	0.123%
16	13.515	2022	2028	2042	rBV	714788	977718	54.79%	5.199%
17	14.615	2210	2215	2218	rBV	430906	543817	30.47%	2.892%
18	14.651	2218	2221	2229	rVB	235880	306859	17.20%	1.632%
19	14.745	2233	2237	2243	rBV	34348	46292	2.59%	0.246%
20	15.051	2286	2289	2294	rBV2	15591	21082	1.18%	0.112%
21	15.421	2347	2352	2356	rBV	37917	42647	2.39%	0.227%
22	15.462	2356	2359	2364	rVB	42753	51893	2.91%	0.276%
23	15.574	2374	2378	2382	rBV3	45638	60832	3.41%	0.323%
24	15.633	2382	2388	2394	rVB5	65815	101437	5.68%	0.539%
25	15.868	2425	2428	2434	rVV	20867	28246	1.58%	0.150%
26	15.939	2436	2440	2450	rVB9	28889	48030	2.69%	0.255%
27	16.233	2486	2490	2493	rBV	34309	43724	2.45%	0.233%
28	16.268	2493	2496	2500	rVV3	25750	37088	2.08%	0.197%
29	16.350	2506	2510	2517	rVB3	24736	35777	2.00%	0.190%
30	16.433	2519	2524	2530	rBV	403776	505481	28.33%	2.688%
31	16.533	2537	2541	2544	rBV5	15071	21618	1.21%	0.115%
32	16.633	2554	2558	2562	rBV2	16039	20464	1.15%	0.109%
33	16.733	2571	2575	2582	rBV	464972	523648	29.34%	2.785%
34	16.933	2606	2609	2613	rBV2	18770	19038	1.07%	0.101%

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Integrator: RTE
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 Sampling : 1
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 Stop Thrs : 0

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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35	16.986	2613	2618	2625	rVB	1017757	1184095	66.35%	6.297%
36	17.068	2628	2632	2637	rVB2	26692	41069	2.30%	0.218%
37	17.180	2646	2651	2653	rBV4	24259	39586	2.22%	0.211%
38	17.209	2653	2656	2661	rVB	57669	71308	4.00%	0.379%
39	17.292	2666	2670	2675	rVB	44869	57201	3.21%	0.304%
40	17.339	2675	2678	2685	rBV4	42430	75339	4.22%	0.401%
41	17.456	2694	2698	2701	rVB	26816	29745	1.67%	0.158%
42	17.492	2702	2704	2711	rVB3	15172	24303	1.36%	0.129%
43	17.897	2771	2773	2777	rVB4	19035	25343	1.42%	0.135%
44	18.009	2789	2792	2795	rBV	41891	46684	2.62%	0.248%
45	18.039	2795	2797	2800	rVV2	27417	29157	1.63%	0.155%
46	18.115	2805	2810	2814	rVB5	25561	44620	2.50%	0.237%
47	18.244	2829	2832	2835	rBV4	41530	59167	3.32%	0.315%
48	18.327	2841	2846	2850	rBV2	455528	656812	36.81%	3.493%
49	18.362	2850	2852	2857	rVV2	152809	204148	11.44%	1.086%
50	18.409	2857	2860	2865	rVB	172024	180276	10.10%	0.959%
51	18.462	2865	2869	2874	rBV2	32746	42103	2.36%	0.224%
52	18.621	2892	2896	2899	rBV5	19329	28351	1.59%	0.151%
53	18.662	2900	2903	2910	rVB4	26957	38134	2.14%	0.203%
54	18.739	2913	2916	2920	rVB2	16995	22093	1.24%	0.117%
55	18.839	2931	2933	2937	rBV	29239	28001	1.57%	0.149%
56	19.597	3058	3062	3065	rBV	190977	247117	13.85%	1.314%
57	19.709	3078	3081	3085	rVB	26665	28725	1.61%	0.153%
58	19.768	3088	3091	3095	rVV	74659	81117	4.55%	0.431%
59	19.886	3107	3111	3115	rBV	117806	131596	7.37%	0.700%
60	19.944	3118	3121	3125	rVB	153444	167771	9.40%	0.892%
61	19.997	3126	3130	3140	rVB	330253	429997	24.10%	2.287%
62	20.268	3173	3176	3182	rVB7	34417	56281	3.15%	0.299%
63	20.450	3204	3207	3209	rBV	26861	26841	1.50%	0.143%
64	20.527	3217	3220	3228	rVB7	45053	78145	4.38%	0.416%
65	20.850	3272	3275	3280	rVB4	40701	55417	3.11%	0.295%
66	21.027	3301	3305	3309	rBV5	26482	37975	2.13%	0.202%
67	21.174	3326	3330	3337	rVB	69718	118963	6.67%	0.633%
68	21.321	3350	3355	3359	rBV6	13407	31727	1.78%	0.169%
69	21.509	3383	3387	3394	rBV2	53214	95836	5.37%	0.510%
70	21.662	3406	3413	3415	rBV8	14420	32061	1.80%	0.170%
71	21.944	3455	3461	3467	rBV10	12376	30216	1.69%	0.161%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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72	23.003	3637	3641	3648	rVB8	13758	30171	1.69%	0.160%
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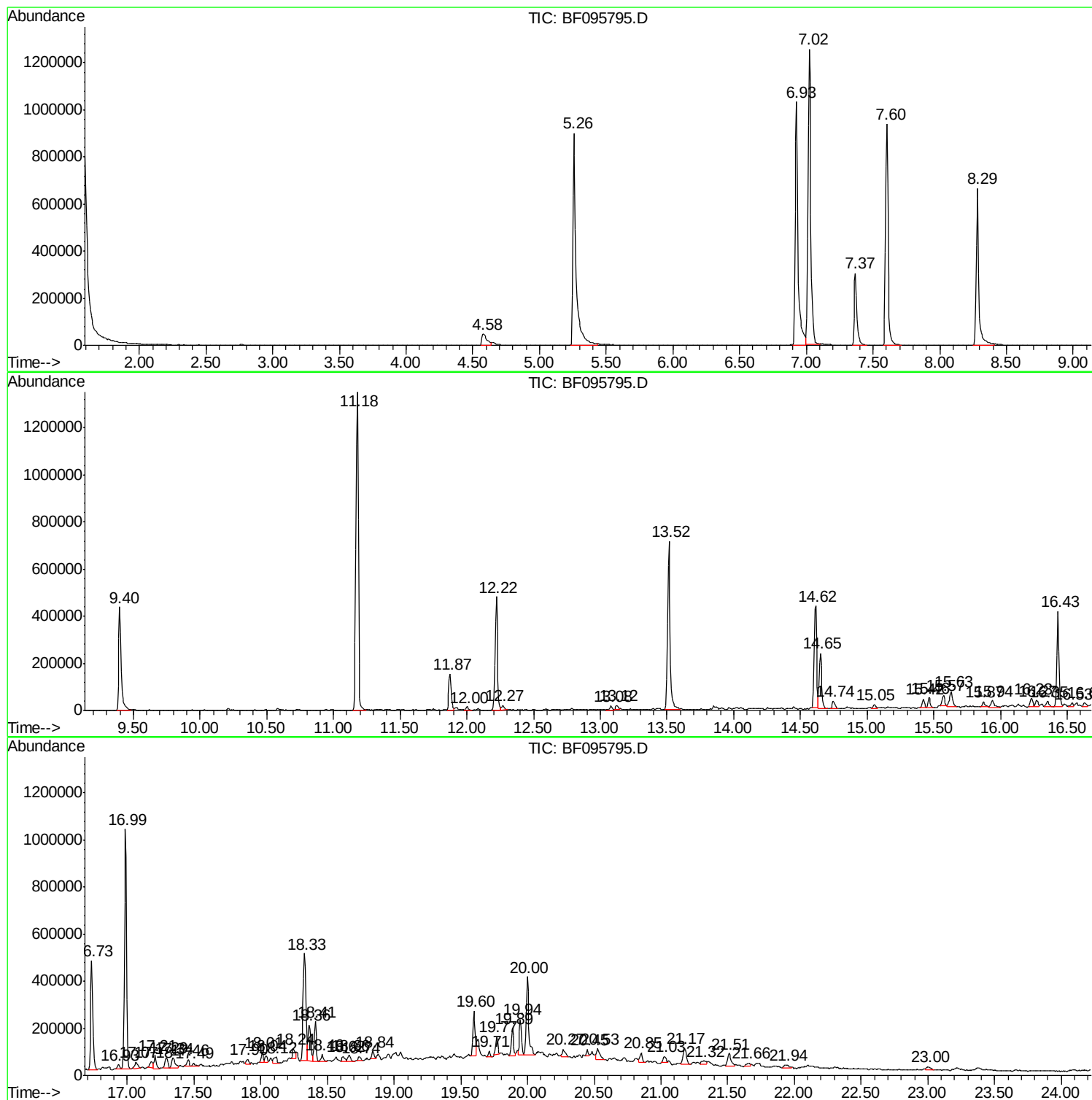
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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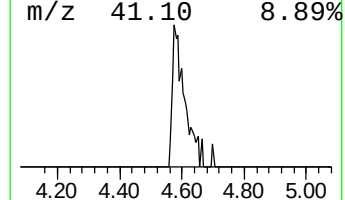
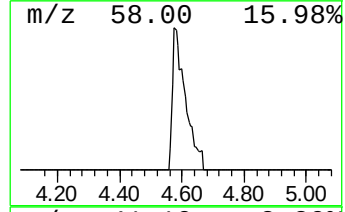
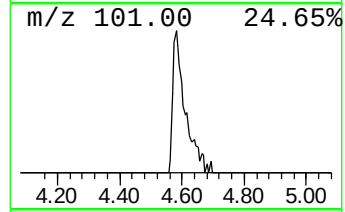
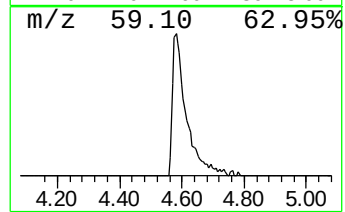
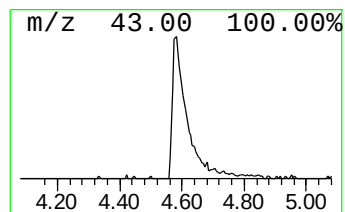
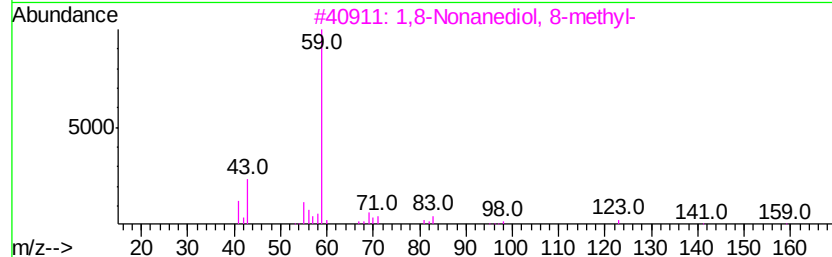
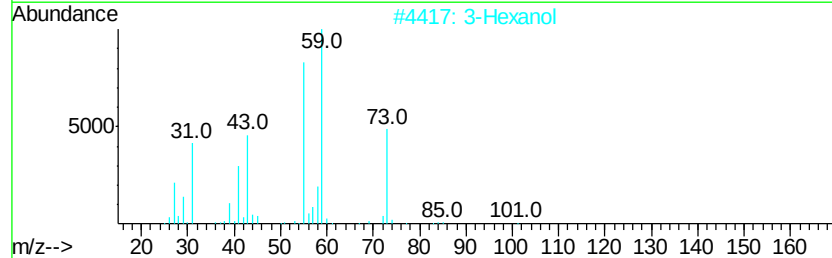
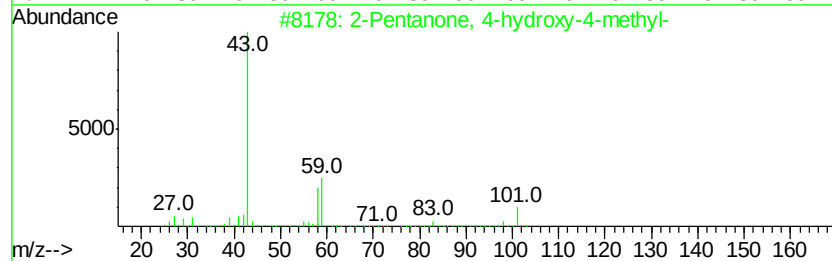
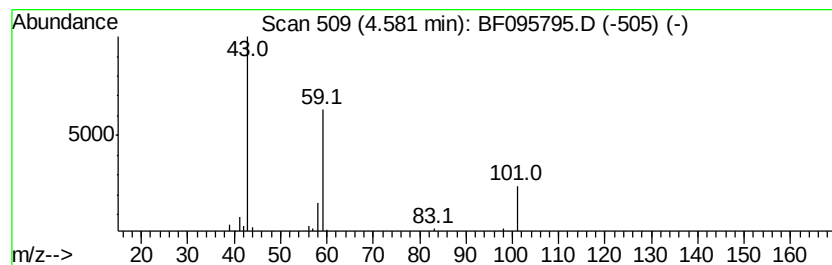
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	5.80 ng	121796	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	3-Octanol	130	C8H18O	000589-98-0	9



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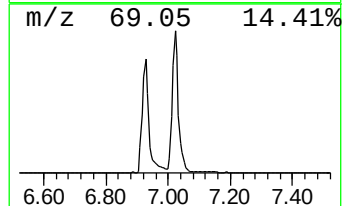
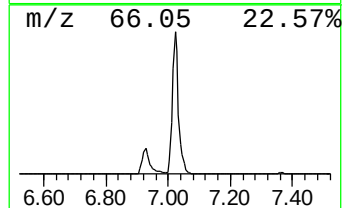
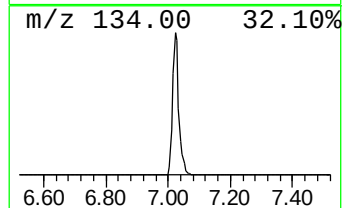
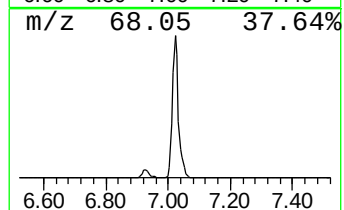
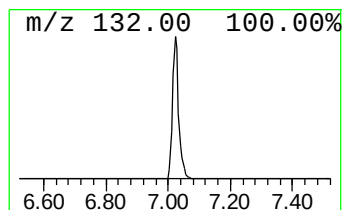
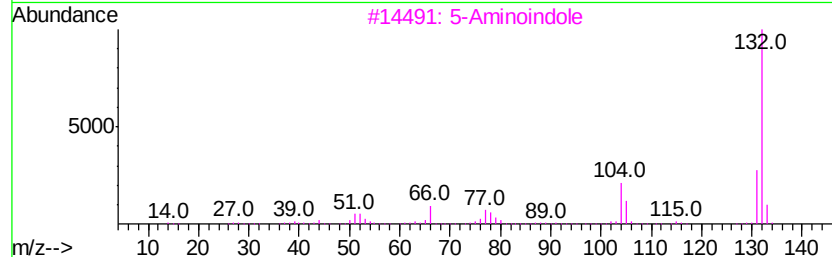
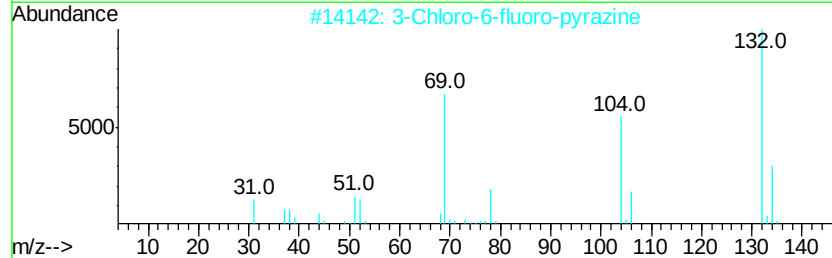
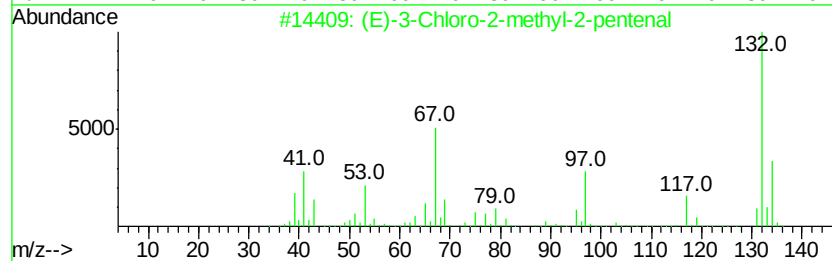
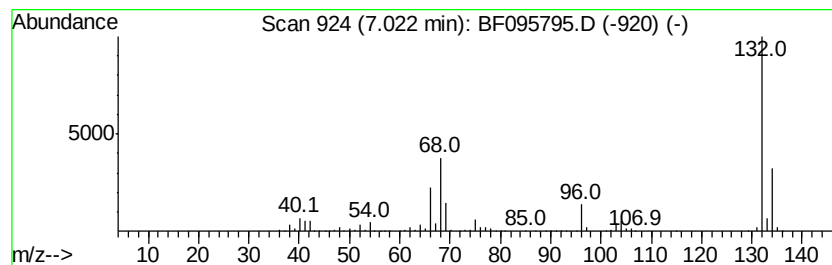
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	84.97 ng	1784510	1,4-Dichlorobenzene-d4	7.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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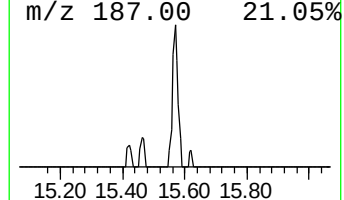
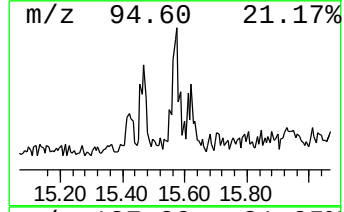
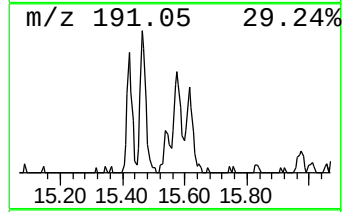
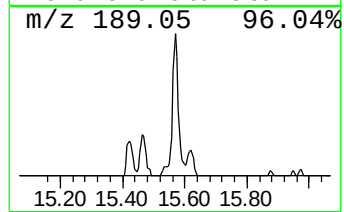
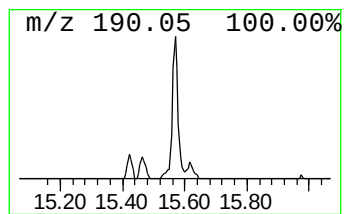
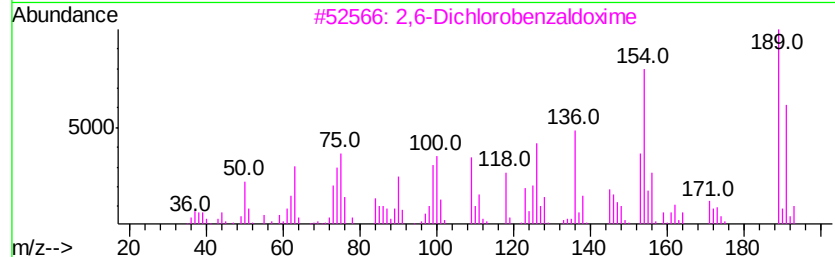
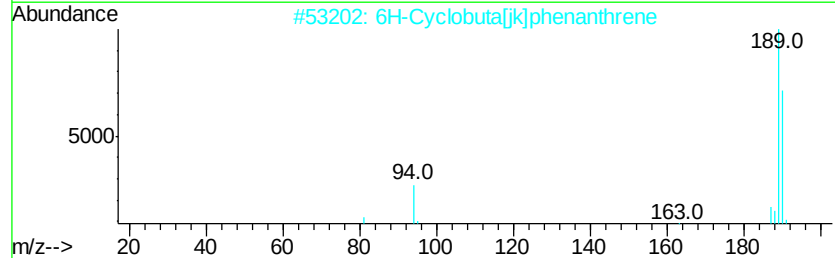
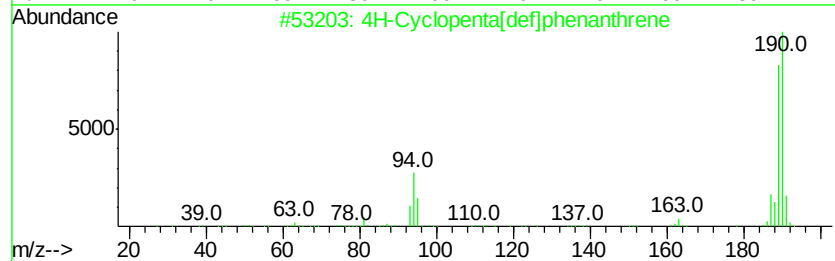
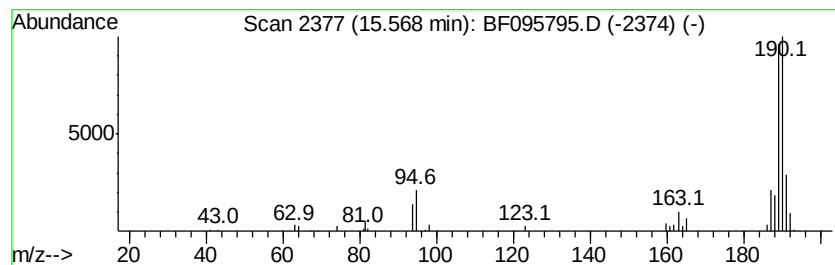
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.57	2.24 ng	60832	Phenanthrene-d10	14.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
2	6H-Cyclobuta[i]kphenanthrene	190	C15H10	083469-43-6	40
3	2,6-Dichlorobenzaloxime	189	C7H5Cl2NO	025185-95-9	38
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	14
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	14



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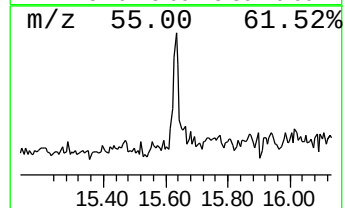
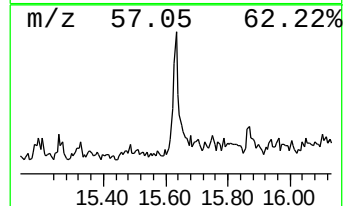
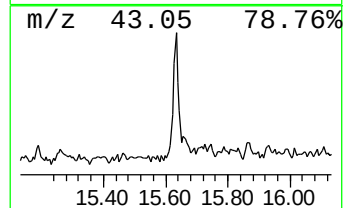
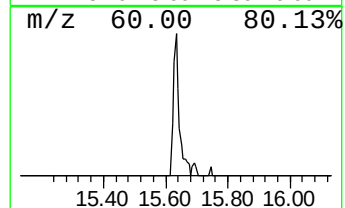
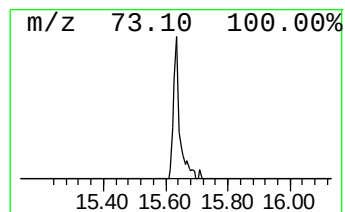
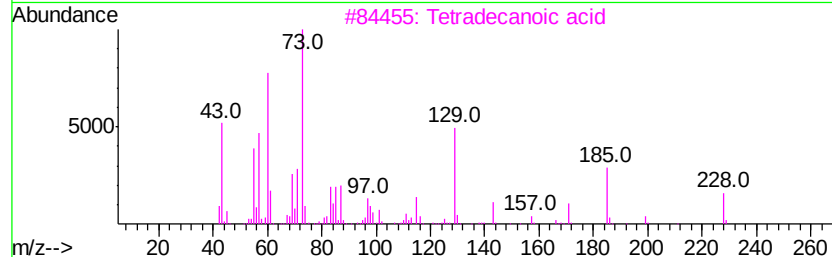
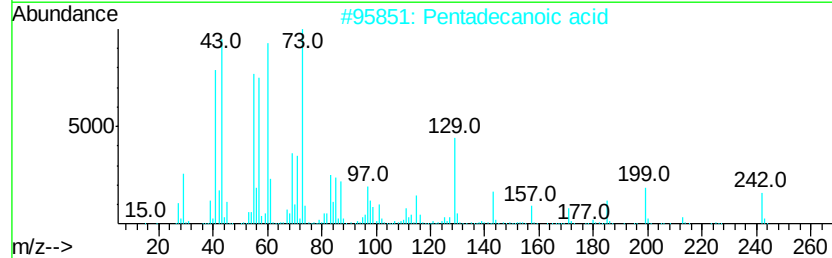
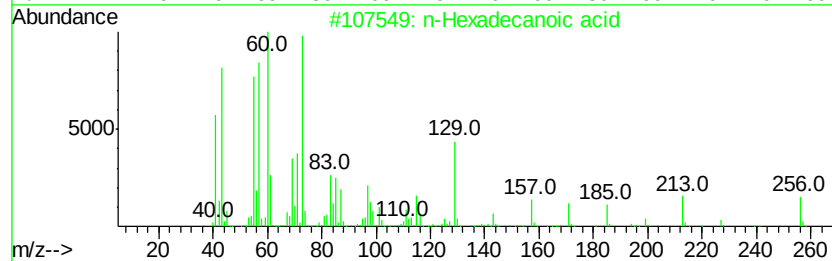
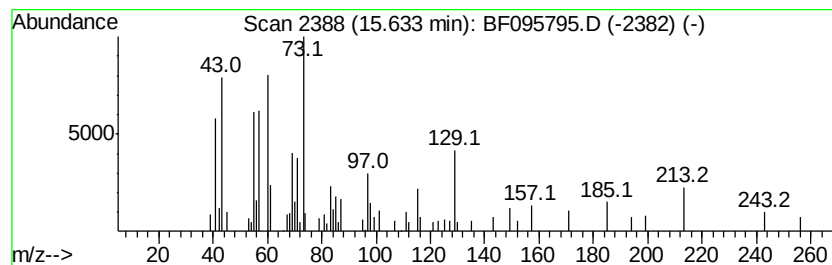
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.63	3.73 ng	101437	Phenanthrene-d10		14.62
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095795.D
Acq On : 8 Jun 2017 21:34
Operator : SJ/MA
Sample : I3457-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

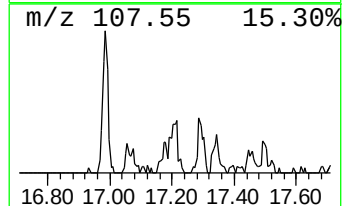
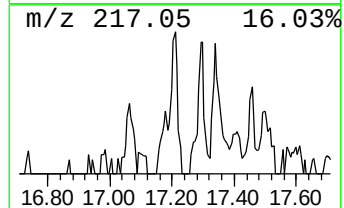
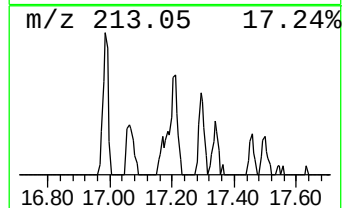
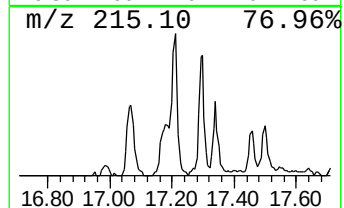
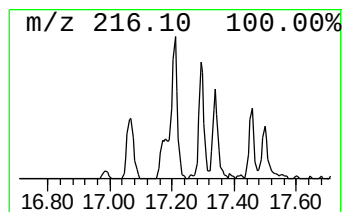
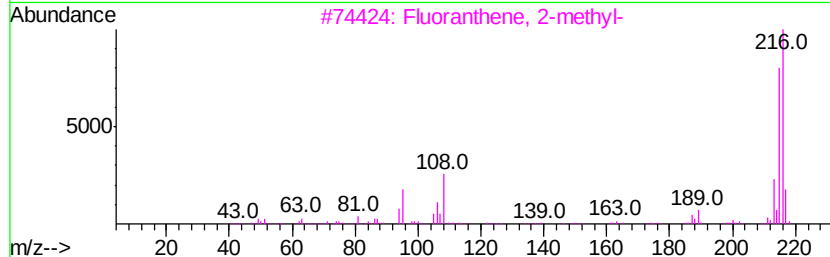
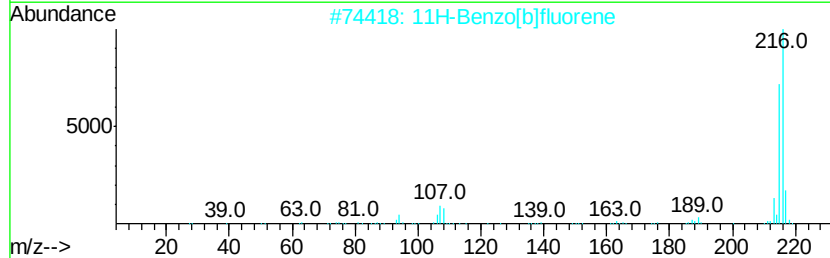
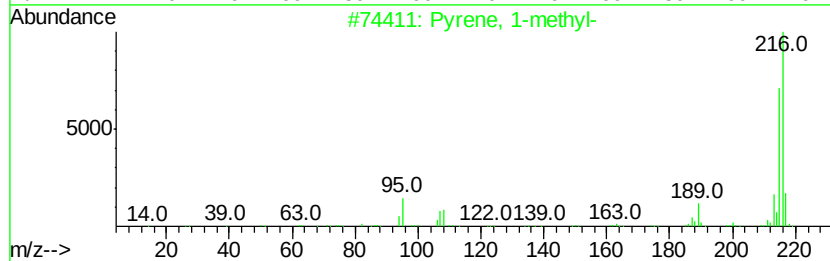
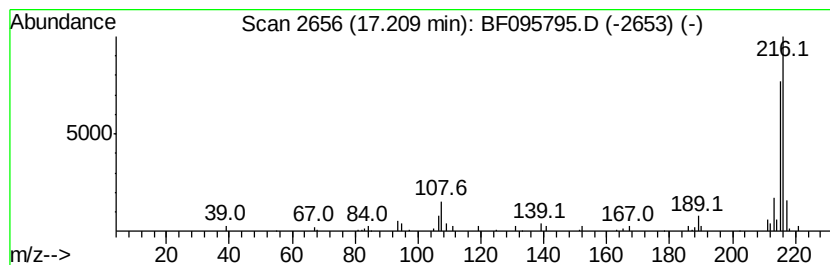
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.		
17.21	2.17 ng	71308	Chrysene-d12		18.33		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	86
4			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	86
5			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
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Sample : I3457-01
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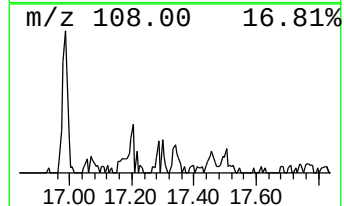
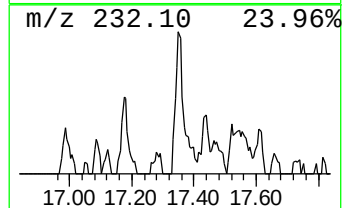
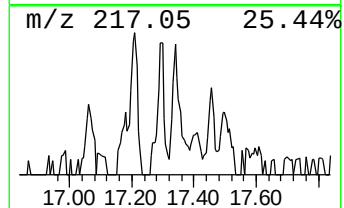
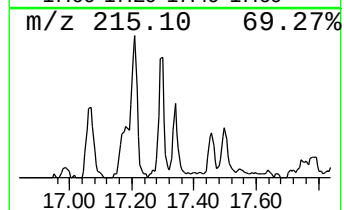
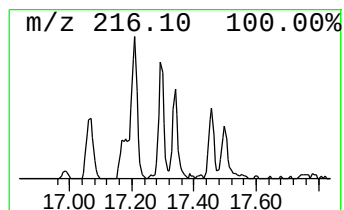
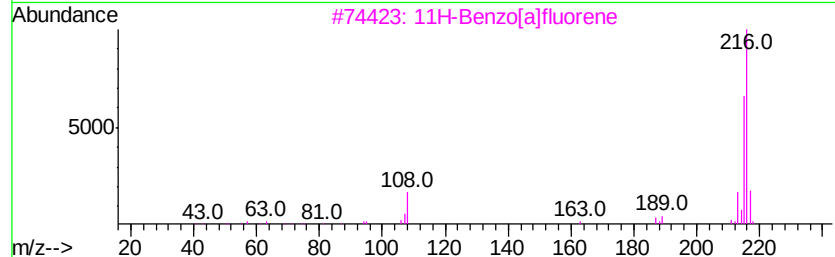
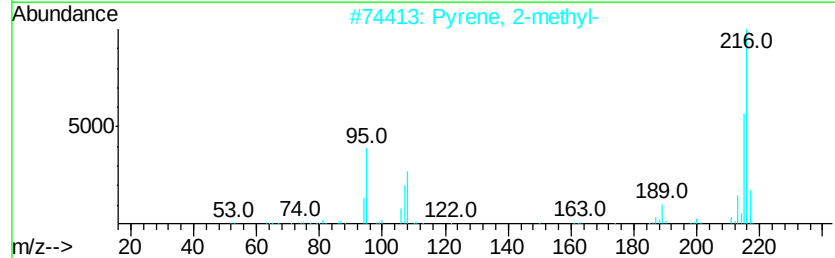
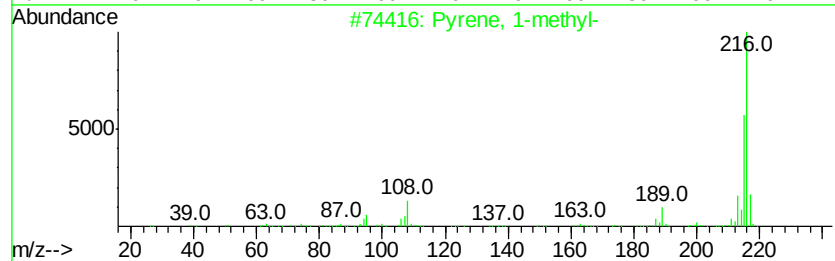
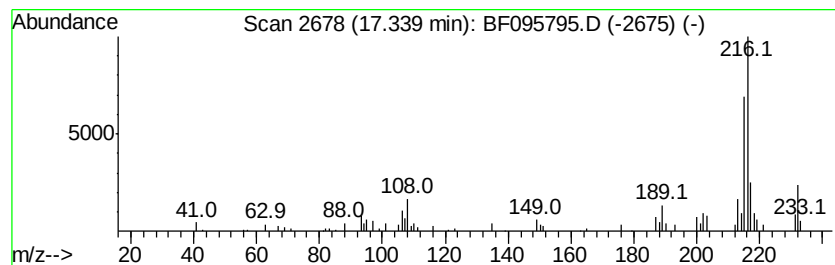
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	2.29 ng	75339	Chrysene-d12	18.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyrene, 1-methyl-	216 C17H12	002381-21-7 94
2		Pyrene, 2-methyl-	216 C17H12	003442-78-2 81
3		11H-Benzo[a]fluorene	216 C17H12	000238-84-6 76
4		11H-Benzo[b]fluorene	216 C17H12	000243-17-4 70
5		Fluoranthene, 2-methyl-	216 C17H12	033543-31-6 70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095795.D
Acq On : 8 Jun 2017 21:34
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Sample : I3457-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-17

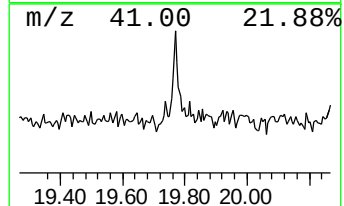
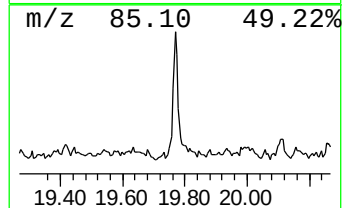
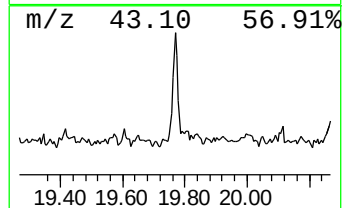
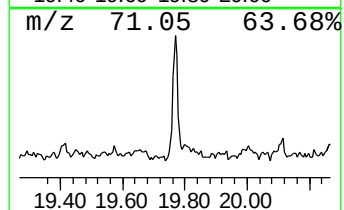
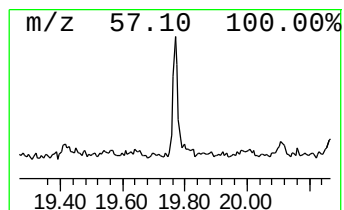
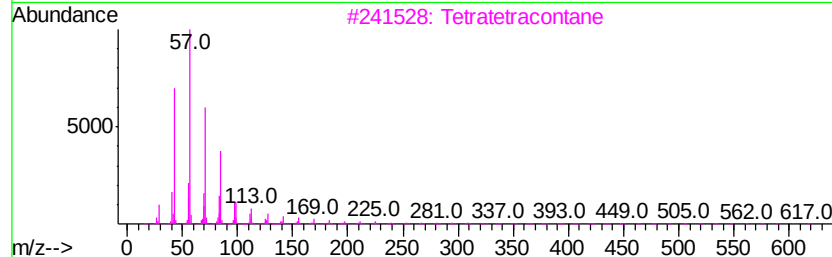
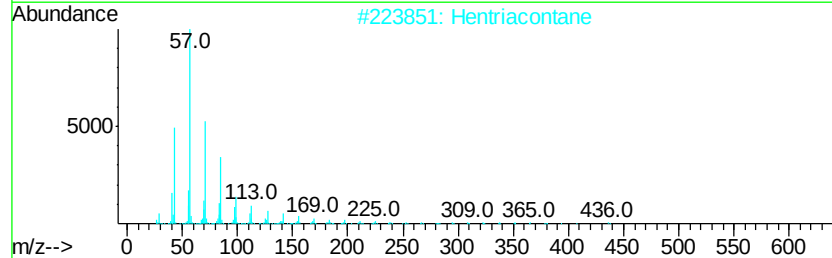
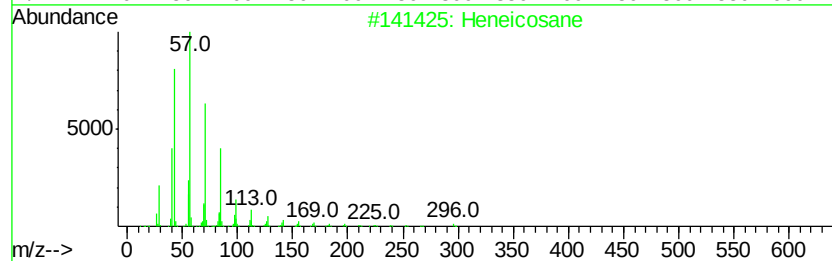
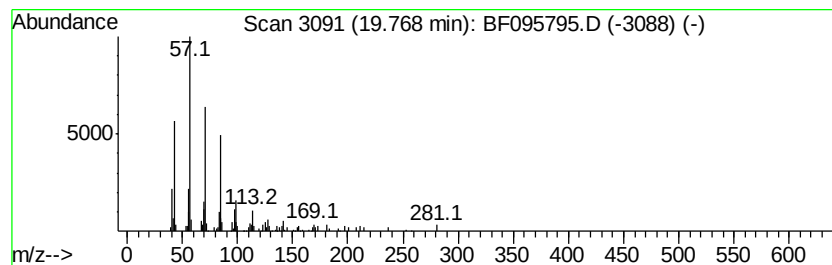
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	3.77 ng	81117	Perylene-d12	20.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hentriacontane		437	C31H64	000630-04-6	91
3	Tetratetracontane		619	C44H90	007098-22-8	90
4	Triacontane		422	C30H62	000638-68-6	90
5	Heptadecane		240	C17H36	000629-78-7	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095795.D
Acq On : 8 Jun 2017 21:34
Operator : SJ/MA
Sample : I3457-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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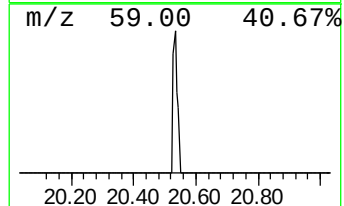
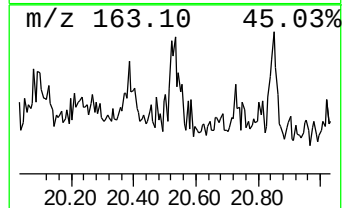
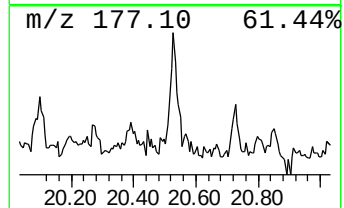
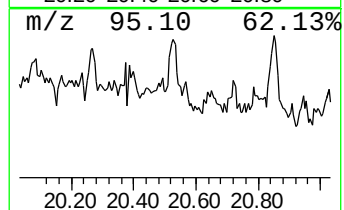
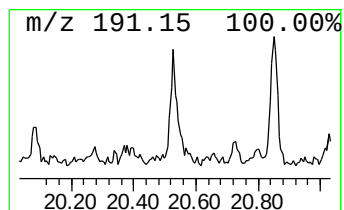
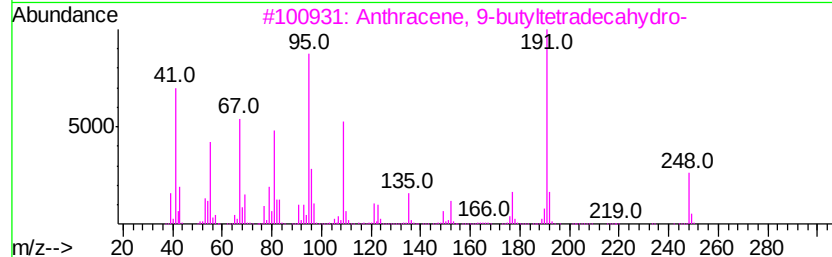
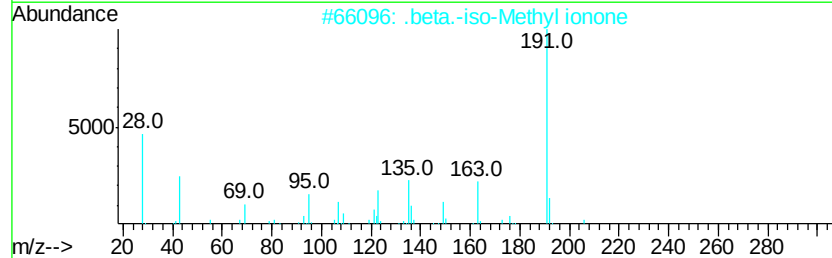
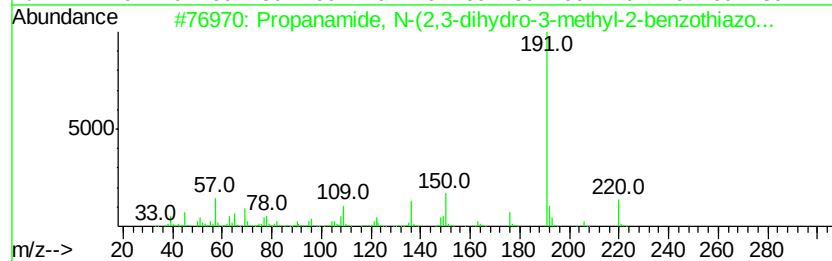
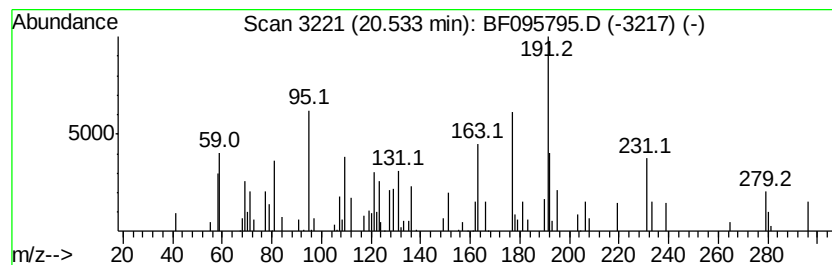
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown20.53 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.53	3.63 ng	78145	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	35
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	32
3		Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	28
4		1,3,4-Thiadiazol-2-amino, 5-(p-t...	191	C9H9N3S	026907-54-0	27
5		Silane, 1,3-decadiynyltrimethyl-	206	C13H22Si	084751-17-7	17



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
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Acq On : 8 Jun 2017 21:34
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Sample : I3457-01
Misc :
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Instrument :
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ClientSampleId :
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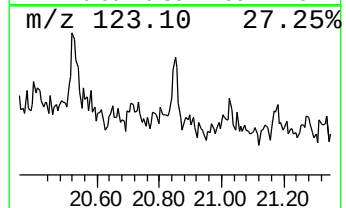
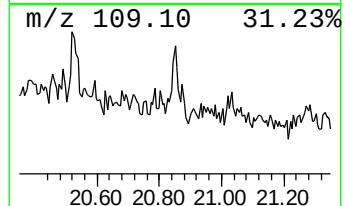
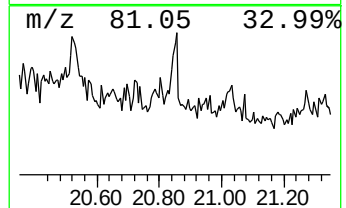
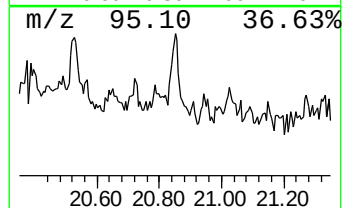
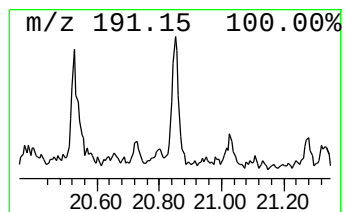
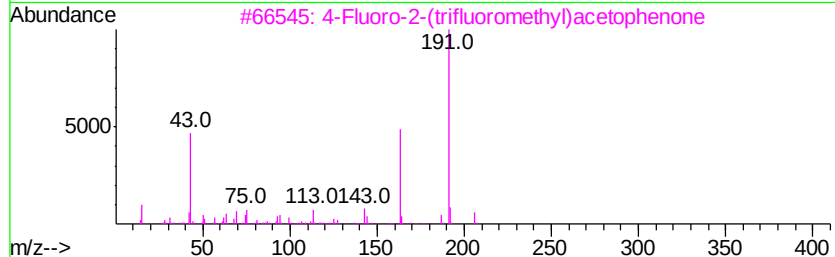
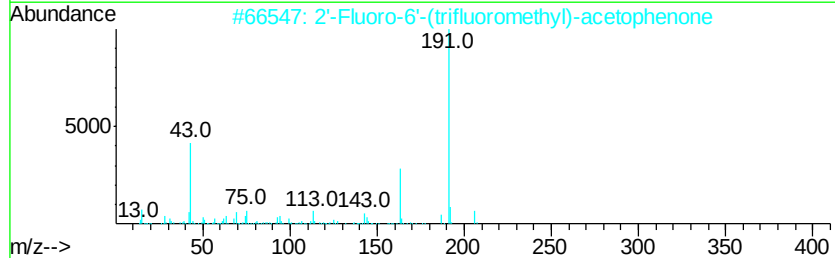
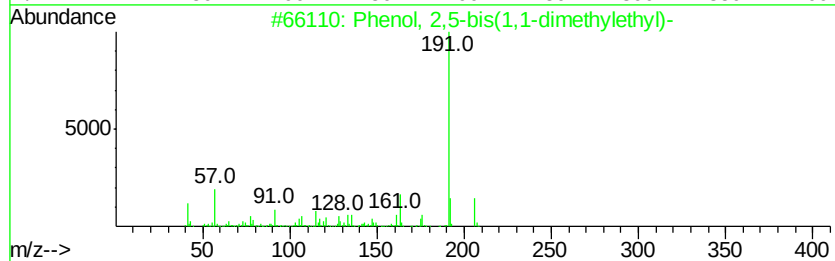
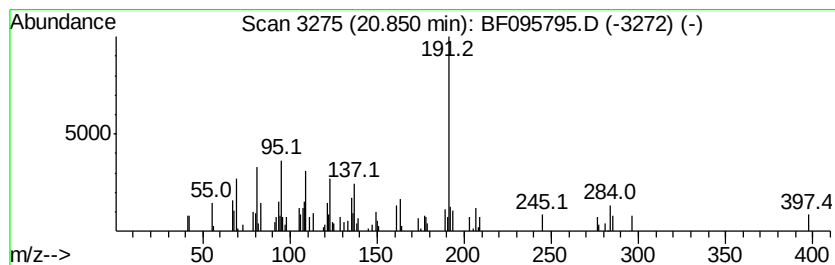
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown20.85 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	2.58 ng	55417	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	43
2		2'-Fluoro-6'-(trifluoromethyl)-a...	206	C9H6F4O	174013-29-7	43
3		4-Fluoro-2-(trifluoromethyl)acet...	206	C9H6F4O	208173-21-1	43
4		Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	43
5		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	41



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Instrument :
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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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unknown7.02	7.02	85.0	ng	1784510	1	7.37	420018	20.0
4H-Cyclopenta[def...	15.57	2.2	ng	60832	4	14.62	543817	20.0
n-Hexadecanoic acid	15.63	3.7	ng	101437	4	14.62	543817	20.0
Pyrene, 1-methyl-	17.21	2.2	ng	71308	5	18.33	656812	20.0
11H-Benzo[b]fluorene	17.34	2.3	ng	75339	5	18.33	656812	20.0
Heneicosane	19.77	3.8	ng	81117	6	20.00	429997	20.0
6-Isopropenyl-4,8...	20.27	2.6	ng	56281	6	20.00	429997	20.0
unknown20.53	20.53	3.6	ng	78145	6	20.00	429997	20.0
unknown20.85	20.85	2.6	ng	55417	6	20.00	429997	20.0