

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120517\
 Data File : BF101122.D
 Acq On : 5 Dec 2017 14:15
 Operator : SJ/JU
 Sample : I6718-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-4651

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-BF113017.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	5.087	507	510	524	rVB	75256	118270	6.07%	0.707%
2	5.475	571	576	579	rBV	1441886	1536468	78.80%	9.180%
3	6.487	743	748	751	rBV	1367119	1568242	80.43%	9.370%
4	6.622	766	771	774	rBV	1720258	1626315	83.41%	9.717%
5	6.845	806	809	813	rBV	432900	340005	17.44%	2.031%
6	7.004	832	836	839	rBV	1443258	1278948	65.59%	7.642%
7	7.416	900	906	909	rBV	984754	994504	51.00%	5.942%
8	8.128	1024	1027	1030	rBV	532905	425816	21.84%	2.544%
9	9.204	1205	1210	1213	rBV	1953503	1949860	100.00%	11.650%
10	9.598	1273	1277	1284	rVB	217767	181594	9.31%	1.085%
11	9.804	1308	1312	1317	rBV2	35983	34451	1.77%	0.206%
12	9.886	1322	1326	1329	rVB	556436	464694	23.83%	2.777%
13	10.304	1395	1397	1400	rVB	39809	29179	1.50%	0.174%
14	10.680	1456	1461	1464	rBV	1229390	1117237	57.30%	6.675%
15	10.775	1474	1477	1487	rVB2	30633	36348	1.86%	0.217%
16	11.375	1575	1579	1581	rBV	601333	497095	25.49%	2.970%
17	11.398	1581	1583	1586	rVB	149168	111013	5.69%	0.663%
18	11.874	1661	1664	1665	rBV	48250	41289	2.12%	0.247%
19	11.892	1665	1667	1674	rVB2	77078	108772	5.58%	0.650%
20	11.986	1679	1683	1685	rVV2	53016	56059	2.88%	0.335%
21	12.010	1685	1687	1691	rVB	39949	30849	1.58%	0.184%
22	12.169	1711	1714	1717	rBV	27149	22867	1.17%	0.137%
23	12.422	1754	1757	1760	rBV	39833	35977	1.85%	0.215%
24	12.463	1760	1764	1766	rVV3	16551	24471	1.26%	0.146%
25	12.516	1769	1773	1776	rVB3	20509	22851	1.17%	0.137%
26	12.586	1781	1785	1789	rBV	200447	167768	8.60%	1.002%
27	12.816	1818	1824	1827	rBV	193603	206776	10.60%	1.235%
28	12.869	1831	1833	1837	rVB2	18348	20309	1.04%	0.121%
29	12.963	1844	1849	1852	rBV	1895445	1780211	91.30%	10.637%
30	13.033	1858	1861	1868	rBV5	21664	35440	1.82%	0.212%
31	13.121	1873	1876	1878	rVV4	20298	22645	1.16%	0.135%
32	13.145	1878	1880	1883	rVB2	28401	28127	1.44%	0.168%
33	13.251	1894	1898	1900	rBV2	32106	28929	1.48%	0.173%
34	13.345	1911	1914	1916	rVB	25277	21201	1.09%	0.127%

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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

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35	13.374	1916	1919	1922	rBV	25590	22718	1.17%	0.136%
36	13.769	1981	1986	1988	rBV3	19785	27334	1.40%	0.163%
37	13.839	1995	1998	2001	rBV	175681	157890	8.10%	0.943%
38	14.016	2024	2028	2031	rBV2	413746	446796	22.91%	2.670%
39	14.045	2031	2033	2036	rVB	71365	58144	2.98%	0.347%
40	14.163	2049	2053	2056	rBV4	15779	20641	1.06%	0.123%
41	14.404	2089	2094	2097	rBV	28569	31092	1.59%	0.186%
42	14.474	2102	2106	2109	rBV3	33915	46210	2.37%	0.276%
43	14.527	2113	2115	2118	rBV2	18235	19946	1.02%	0.119%
44	14.598	2125	2127	2141	rVB2	21468	42765	2.19%	0.256%
45	14.845	2166	2169	2175	rVB	46617	53243	2.73%	0.318%
46	14.910	2175	2180	2185	rVB7	11236	23022	1.18%	0.138%
47	15.063	2201	2206	2208	rBV	48854	65253	3.35%	0.390%
48	15.368	2253	2258	2261	rVB	31859	38733	1.99%	0.231%
49	15.427	2264	2268	2274	rBV	47178	60521	3.10%	0.362%
50	15.492	2274	2279	2291	rVB	261592	352161	18.06%	2.104%
51	15.745	2318	2322	2326	rVB5	13577	19973	1.02%	0.119%
52	15.915	2347	2351	2356	rBV4	18794	30003	1.54%	0.179%
53	15.974	2356	2361	2368	rVV6	27520	49382	2.53%	0.295%
54	16.968	2525	2530	2541	rVB4	21617	59134	3.03%	0.353%
55	17.104	2549	2553	2558	rBV8	9720	19555	1.00%	0.117%
56	17.421	2601	2607	2613	rBV3	16889	34269	1.76%	0.205%
57	17.521	2617	2624	2631	rBV9	15809	39004	2.00%	0.233%
58	19.021	2873	2879	2892	rVB9	20088	54303	2.78%	0.324%

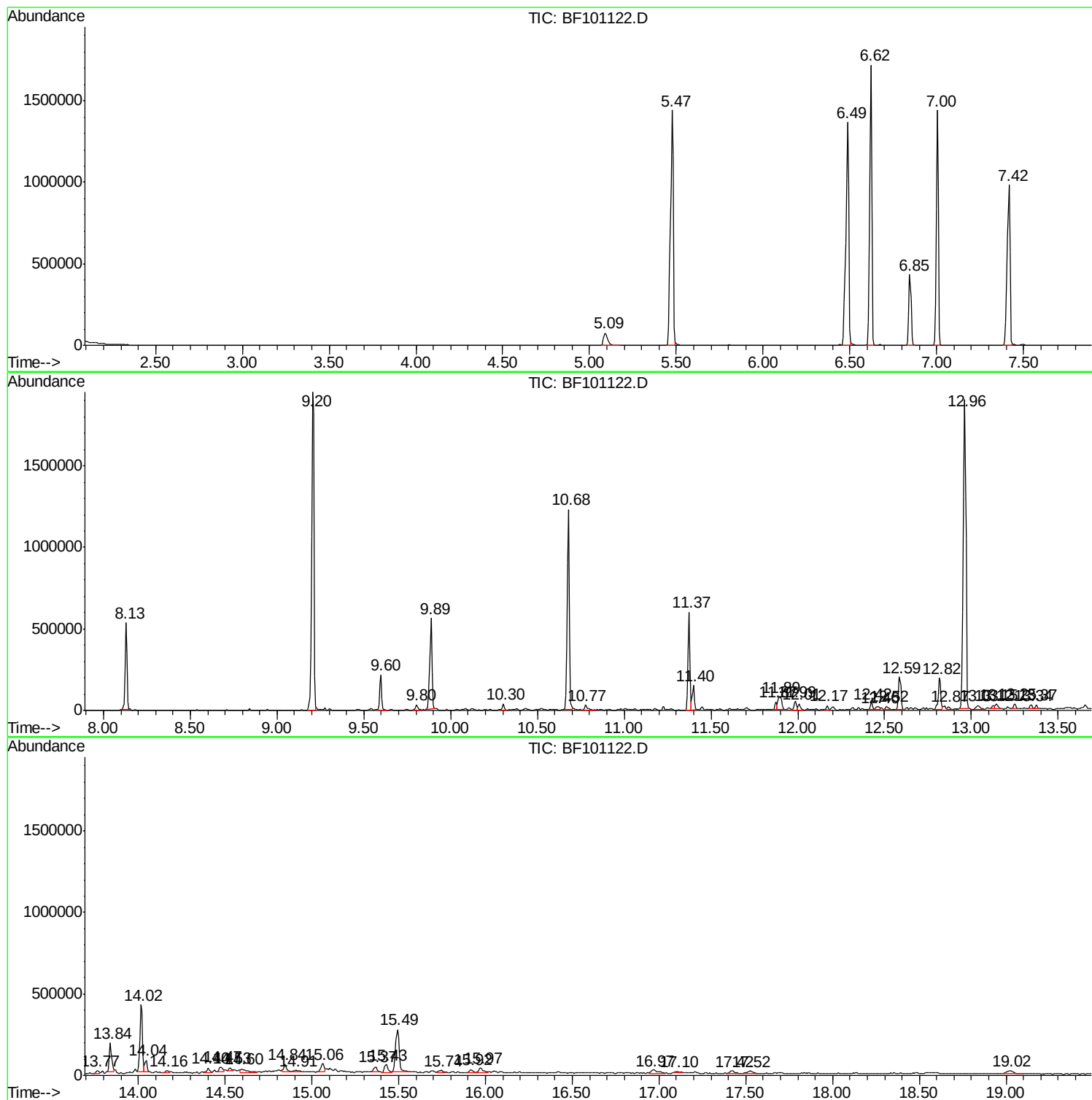
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ClientSampled :
RT-4651

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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ClientSampleId :
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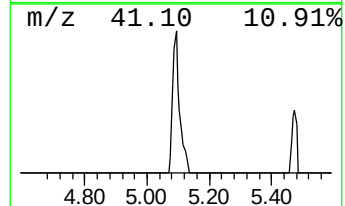
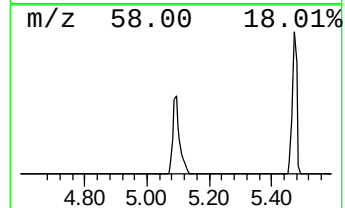
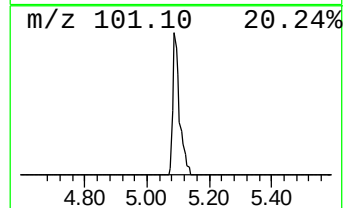
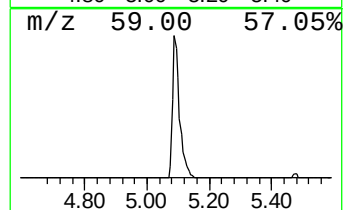
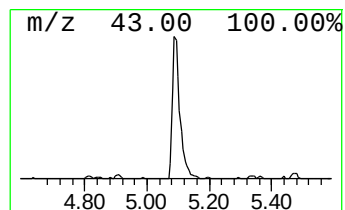
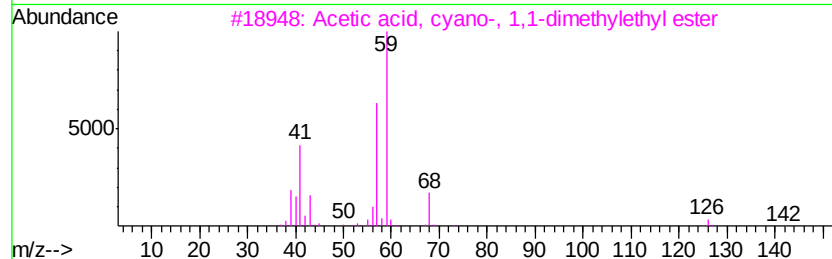
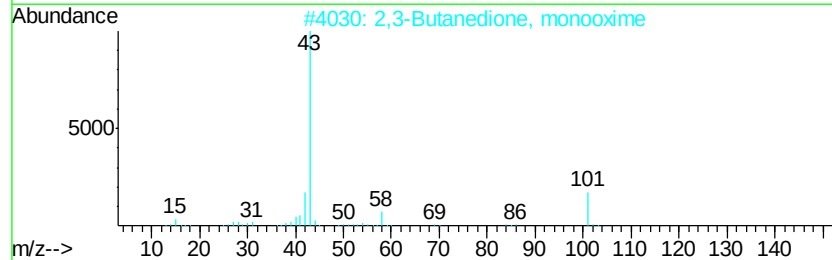
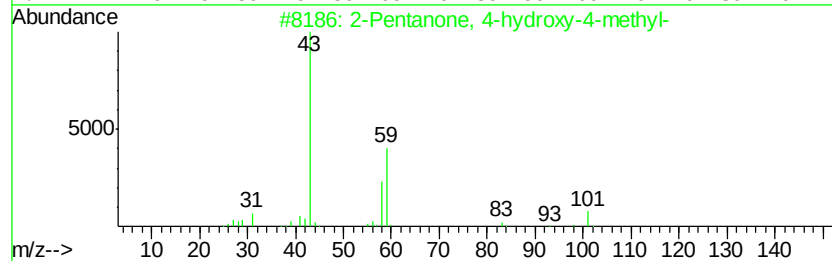
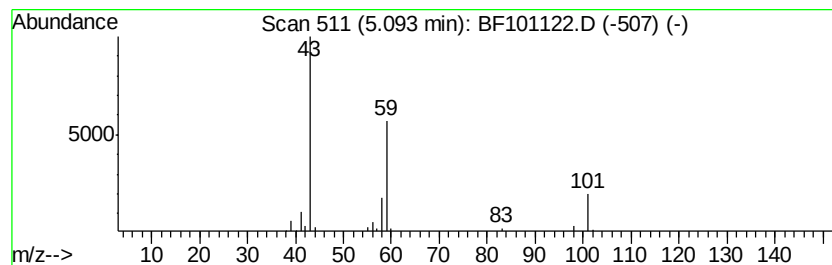
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.09	6.96 ng	118270	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10	
5	Acetone	58	C3H6O	000067-64-1	10	



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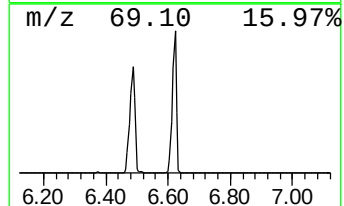
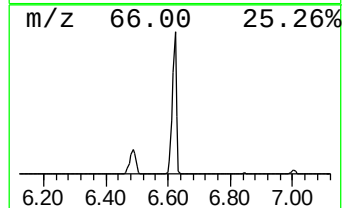
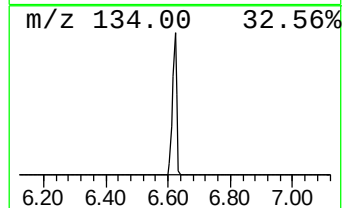
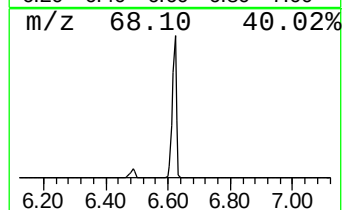
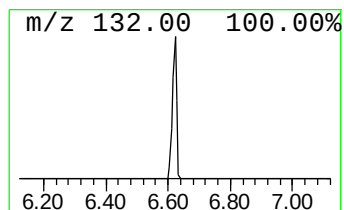
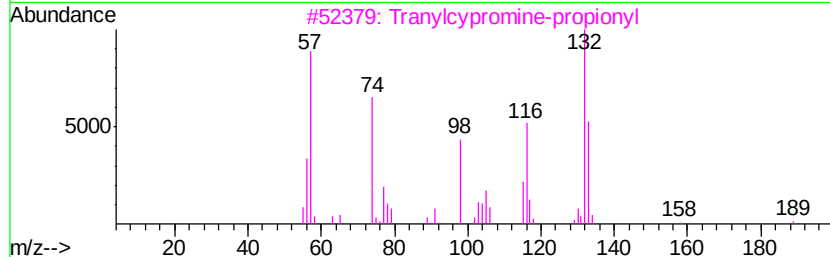
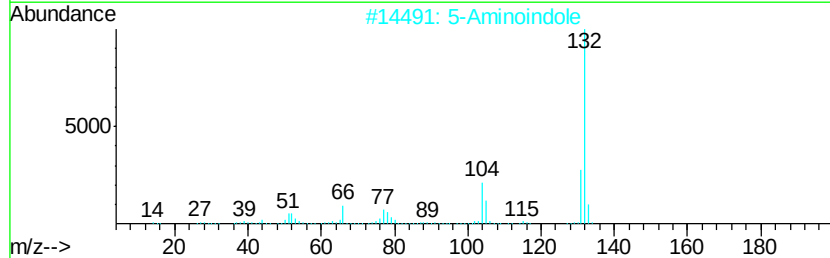
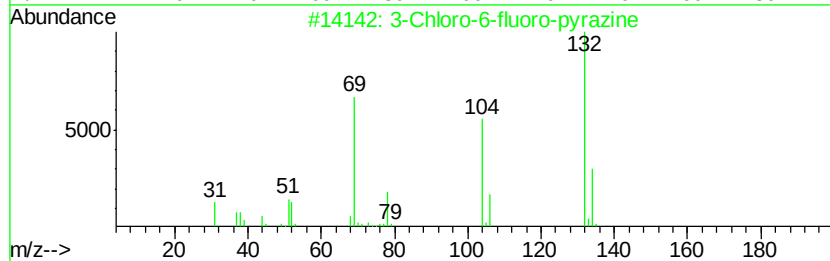
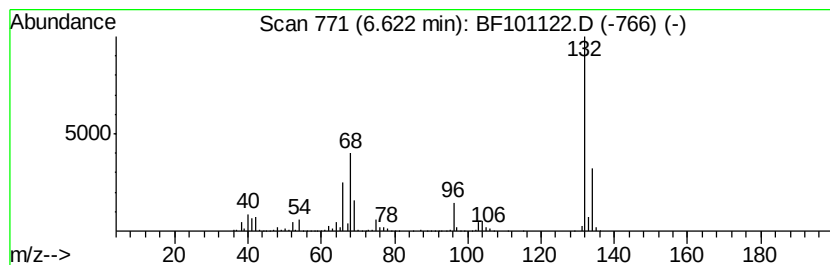
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	95.66 ng	1626320	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	Tranvlcyproline-propionyl			189	C12H15NO	1000123-86-3	10
4	2H-Cyclopenta[dl]pyridazine, 2-me...			132	C8H8N2	022291-85-6	9
5	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9



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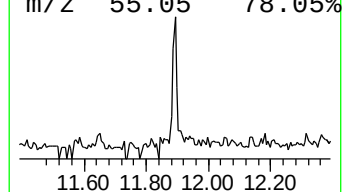
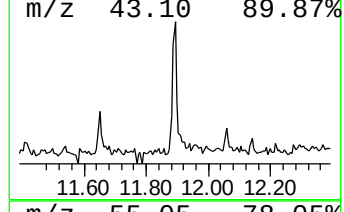
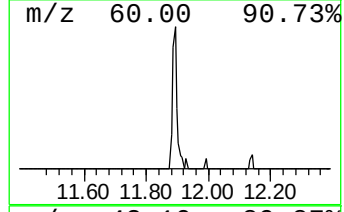
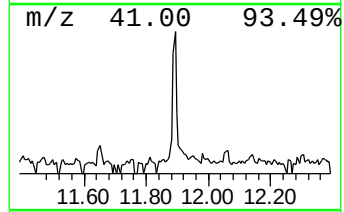
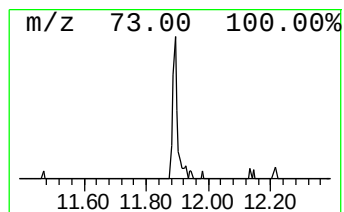
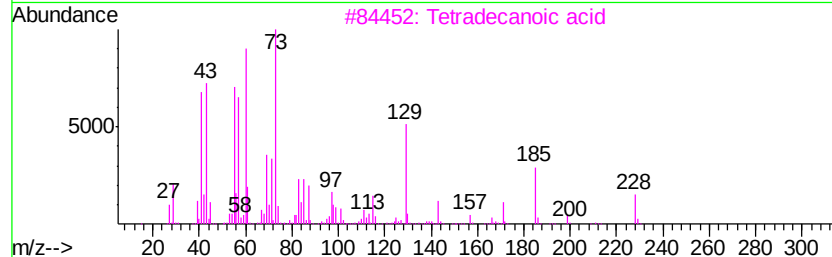
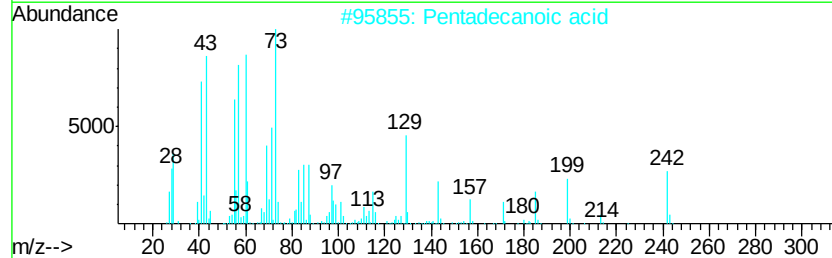
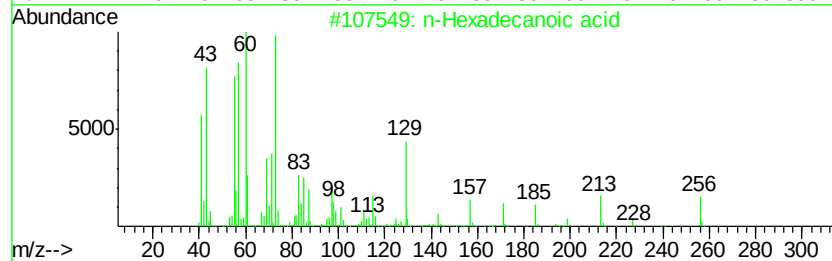
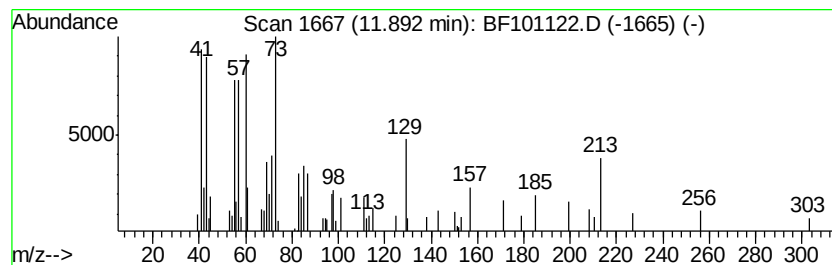
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	4.38 ng	108772	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4		Dodecanoic acid	200	C12H24O2	000143-07-7	50
5		Octadecanoic acid	284	C18H36O2	000057-11-4	46



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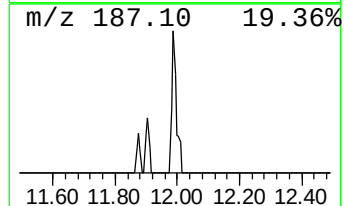
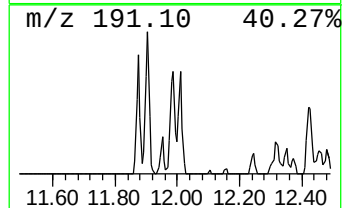
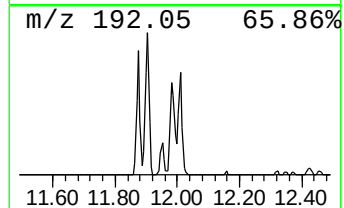
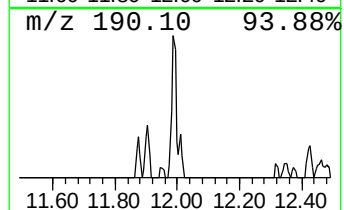
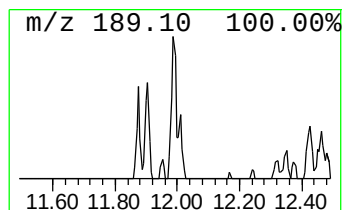
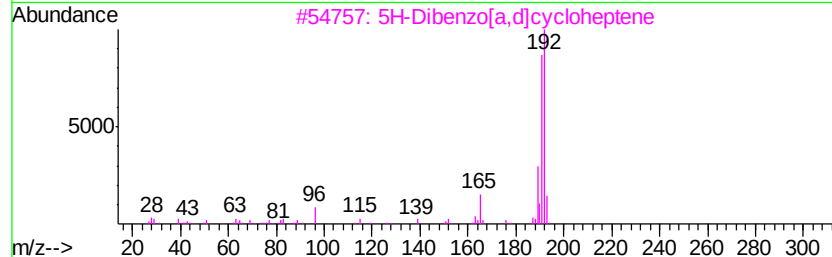
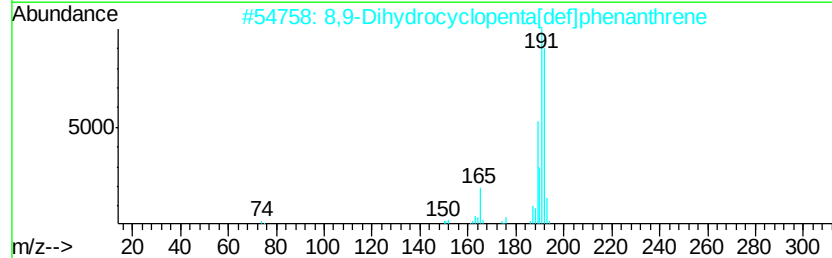
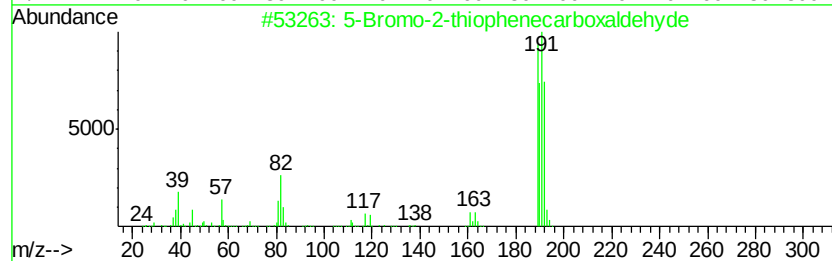
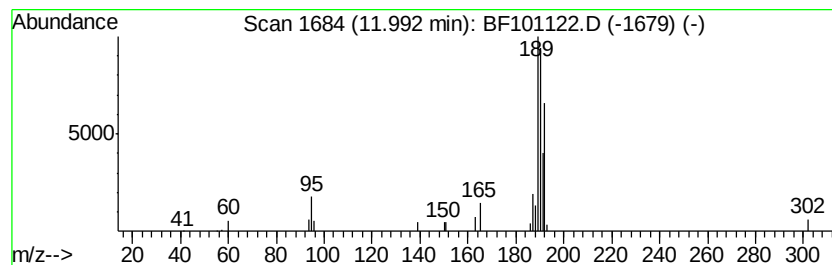
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Bromo-2-thiophenecarboxal... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.26 ng	56059	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	58
2		8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	50
3		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	43
4		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43
5		Benzene, 1,1'-(1,2-propadienyli...	192	C15H12	014251-57-1	43



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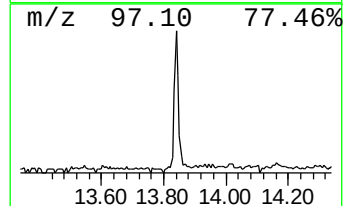
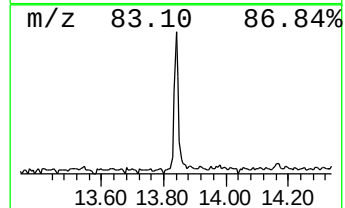
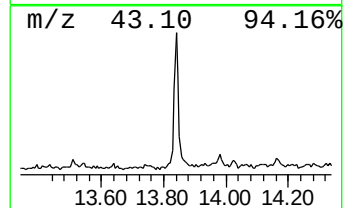
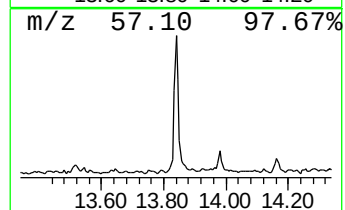
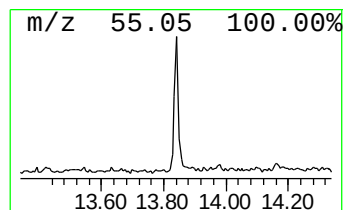
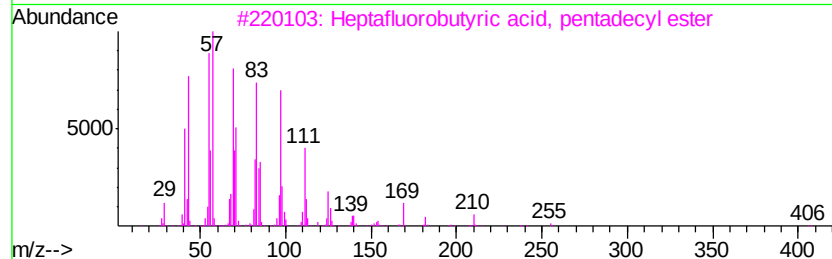
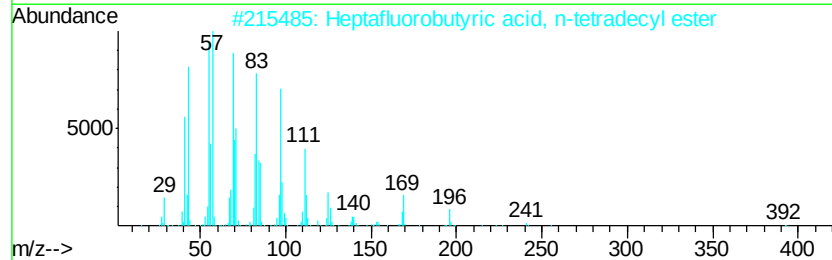
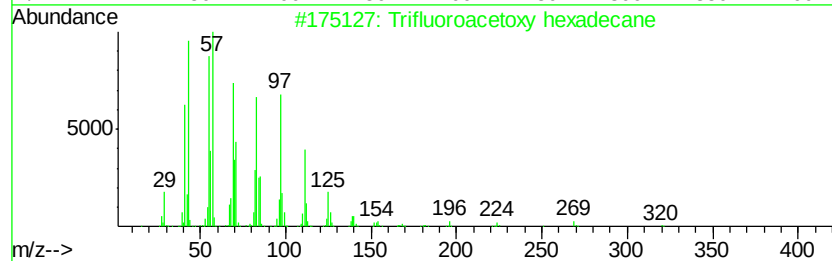
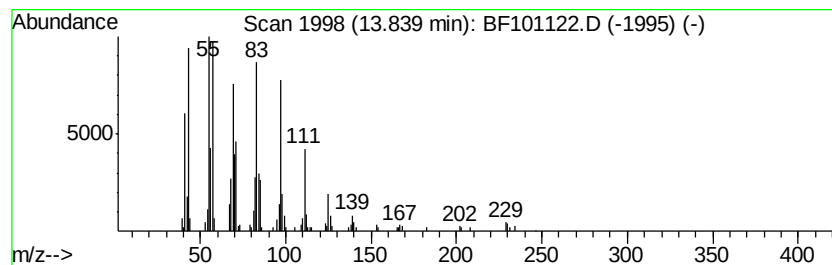
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.84	7.07 ng	157890	Chrysene-d12		14.02	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120517\
Data File : BF101122.D
Acq On : 5 Dec 2017 14:15
Operator : SJ/JU
Sample : I6718-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

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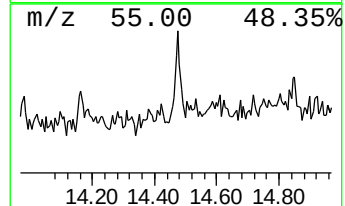
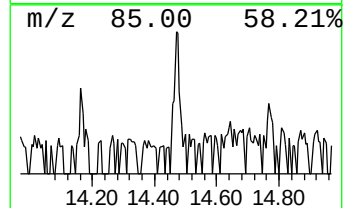
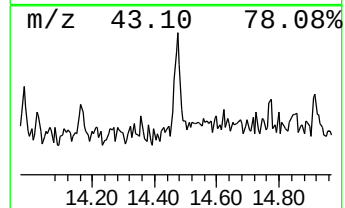
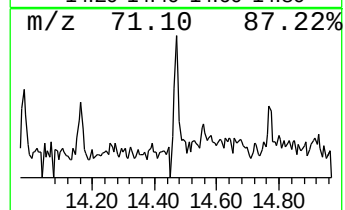
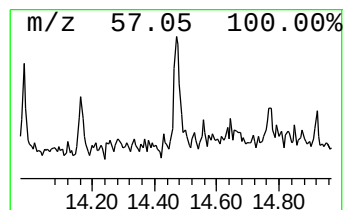
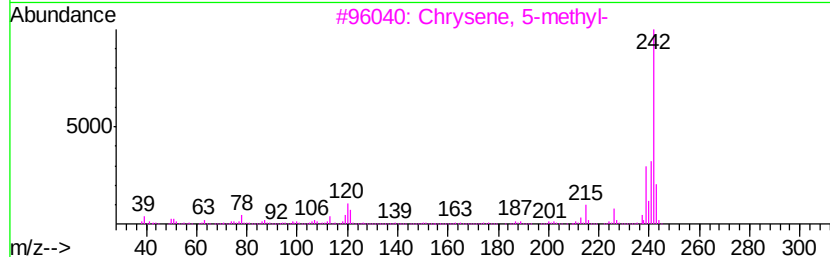
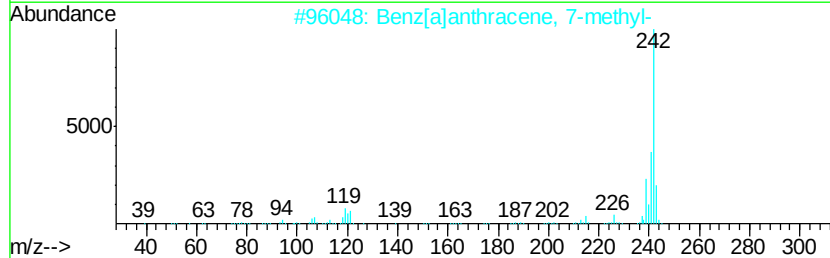
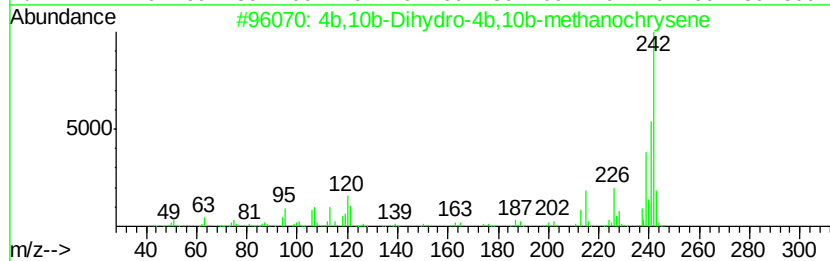
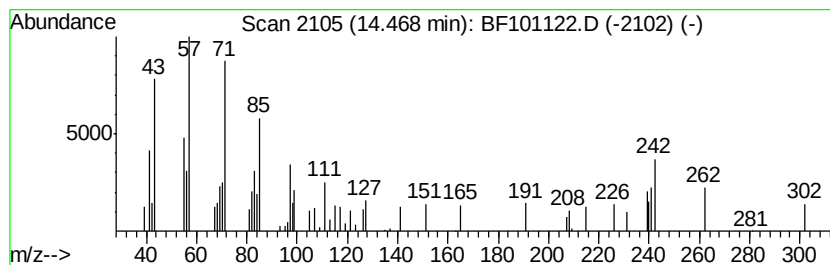
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4b,10b-Dihydro-4b,10b-metha... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.07 ng	46210	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4b,10b-Dihydro-4b,10b-methanochr...	242	C19H14	071949-03-6	86
2		Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	50
3		Chrysene, 5-methyl-	242	C19H14	003697-24-3	41
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	25
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120517\
Data File : BF101122.D
Acq On : 5 Dec 2017 14:15
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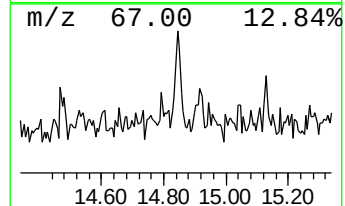
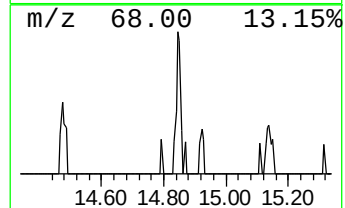
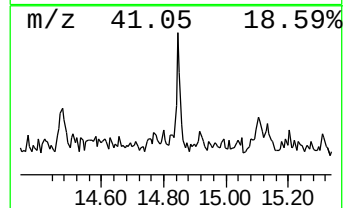
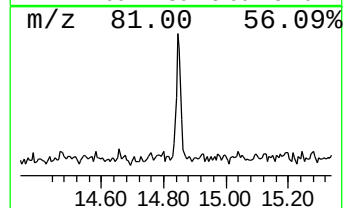
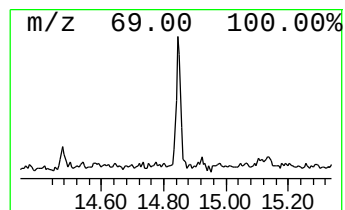
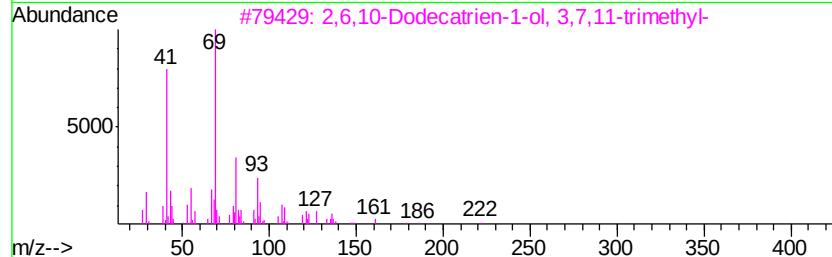
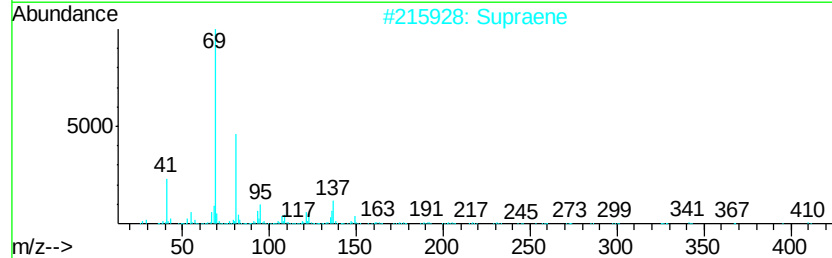
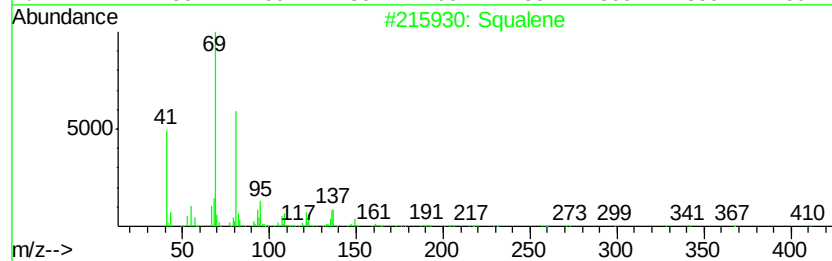
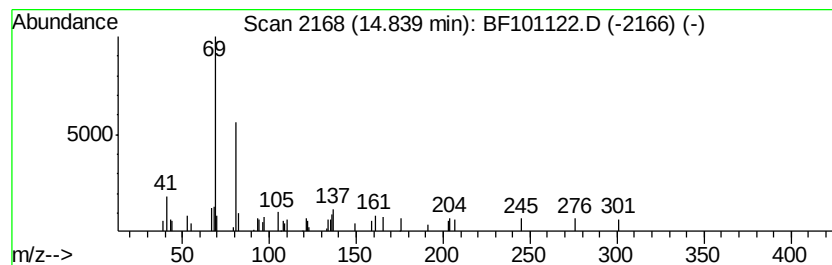
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.02 ng	53243	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	68
2		Supraene	410	C30H50	007683-64-9	64
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	50
4		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	49
5		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120517\
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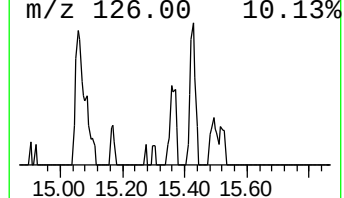
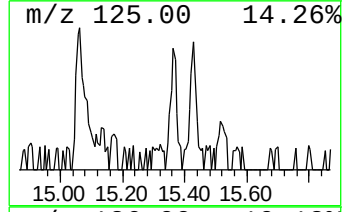
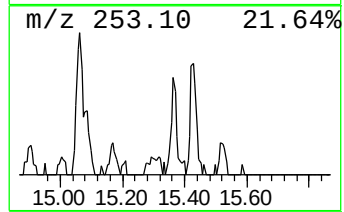
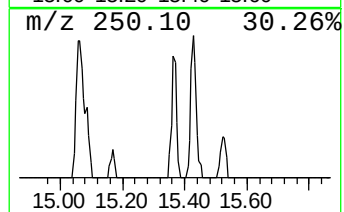
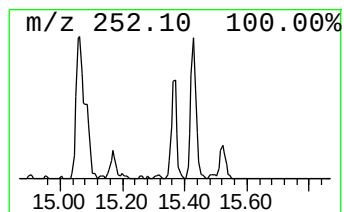
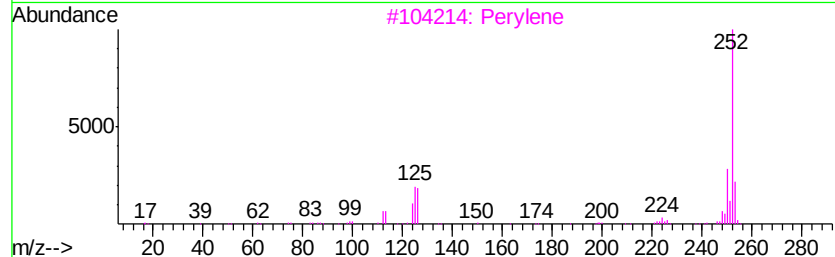
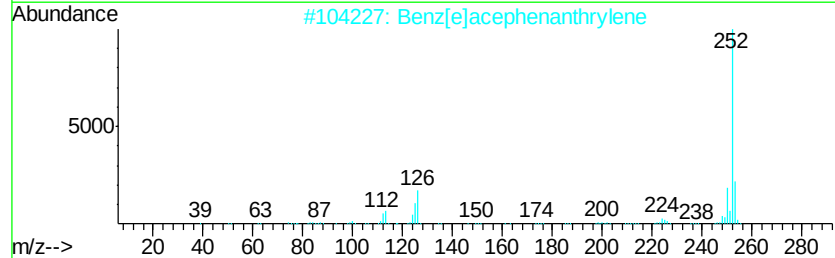
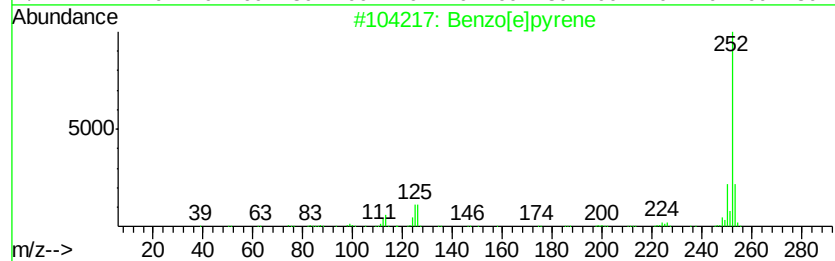
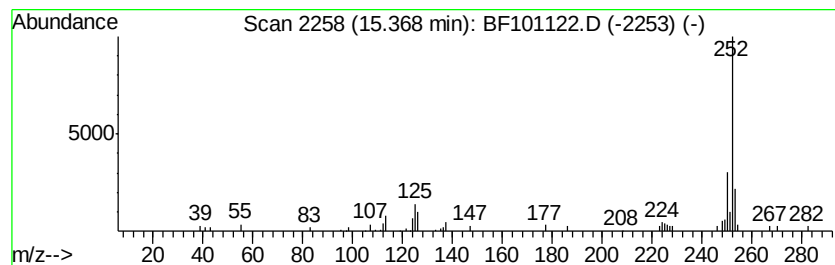
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.37	2.20 ng	38733	Perylene-d12		15.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	90
3	Perylene	252	C20H12	000198-55-0	87
4	Benzo[a]pyrene	252	C20H12	000050-32-8	87
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120517\
Data File : BF101122.D
Acq On : 5 Dec 2017 14:15
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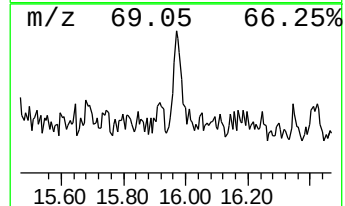
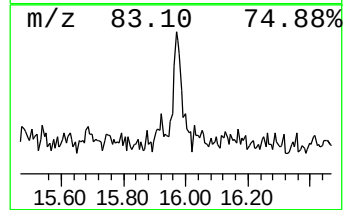
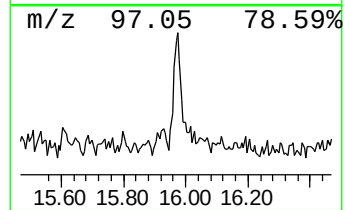
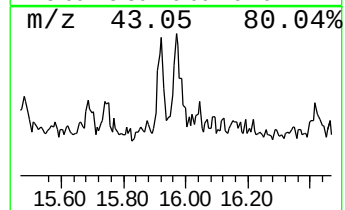
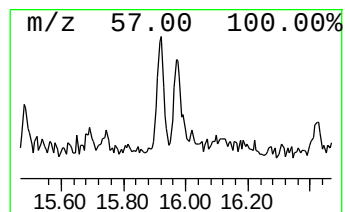
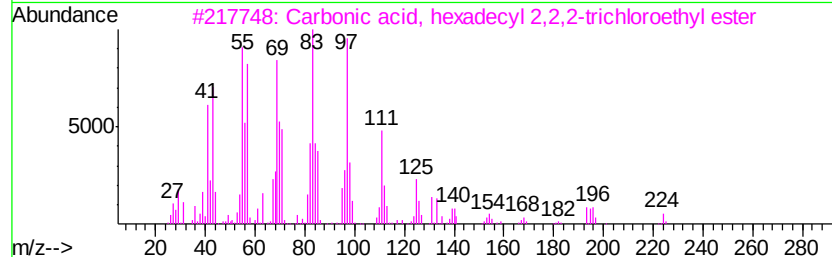
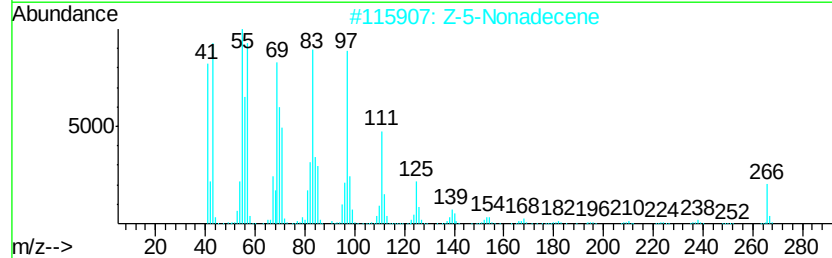
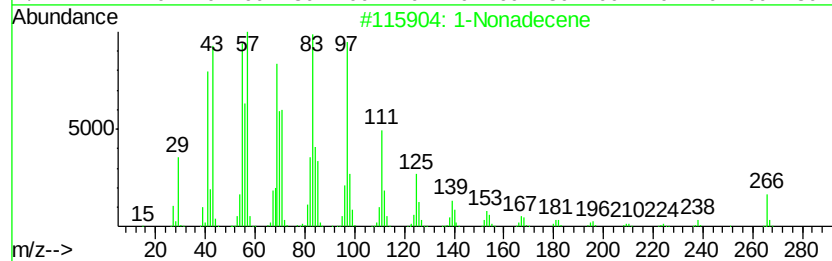
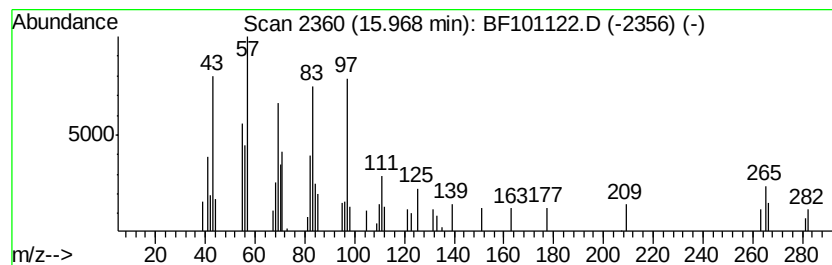
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.80 ng	49382	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	96
2			Z-5-Nonadecene	266	C19H38	1000131-11-8	92
3			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	76
4			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	76
5			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	70



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120517\
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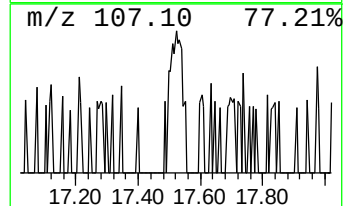
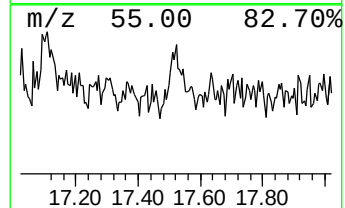
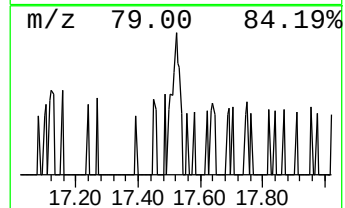
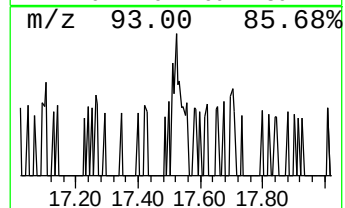
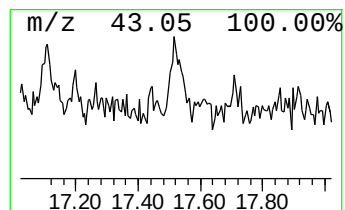
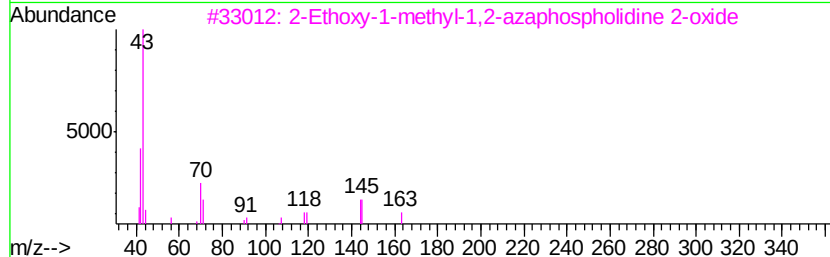
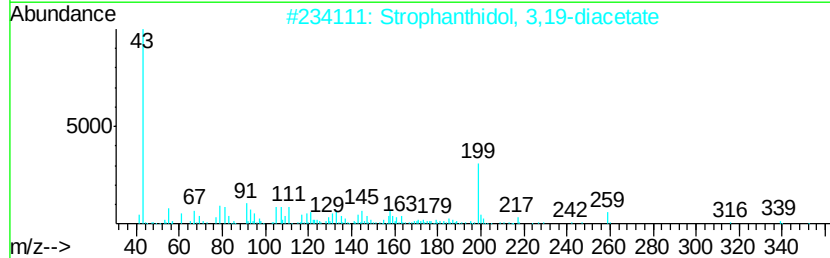
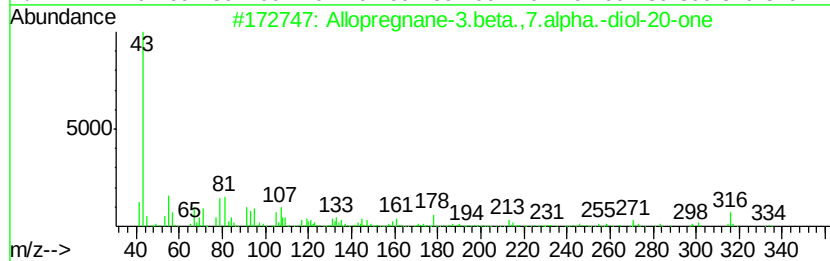
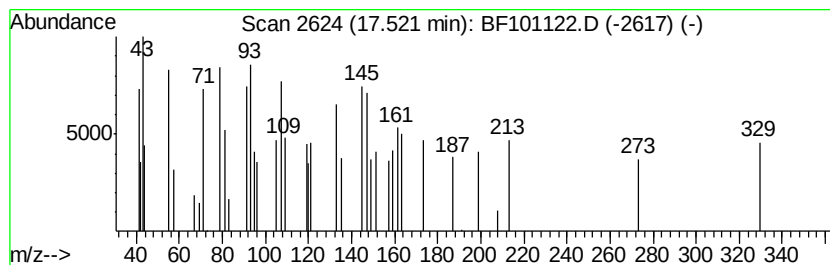
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.52 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.52	2.22 ng	39004	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Allopregnane-3.beta.,7.alpha.-di...	334	C21H34O3	000566-20-1	35
2		Strophanthidol, 3,19-diacetate	490	C27H38O8	083349-11-5	27
3		2-Ethoxy-1-methyl-1,2-azaphospho...	163	C6H14N02P	054008-32-1	14
4		2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	10
5		4aH-Cycloprop[e]azulen-4a-ol, de...	222	C15H26O	005986-49-2	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120517\
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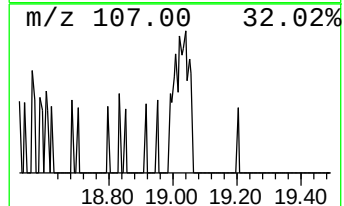
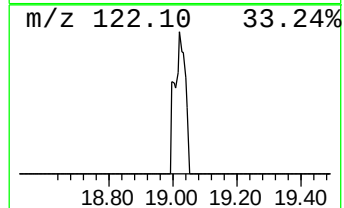
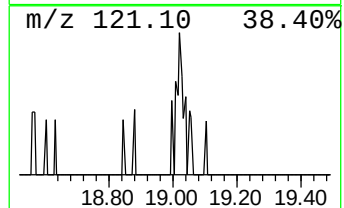
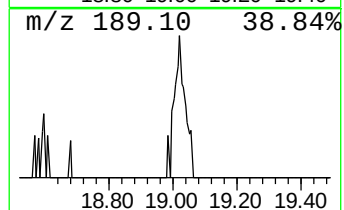
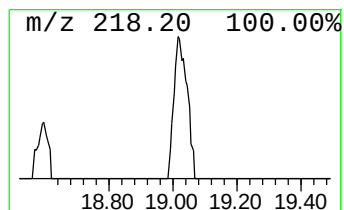
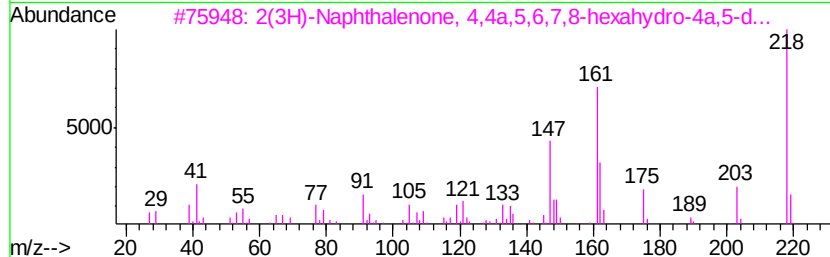
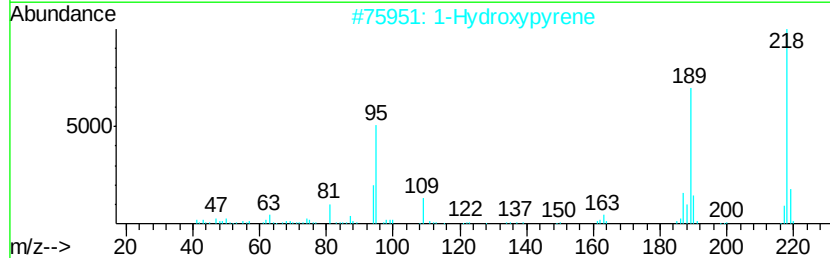
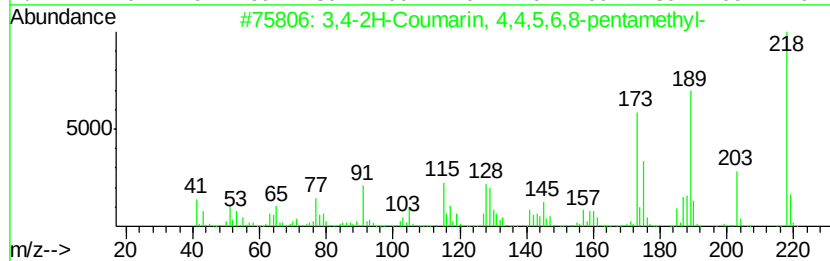
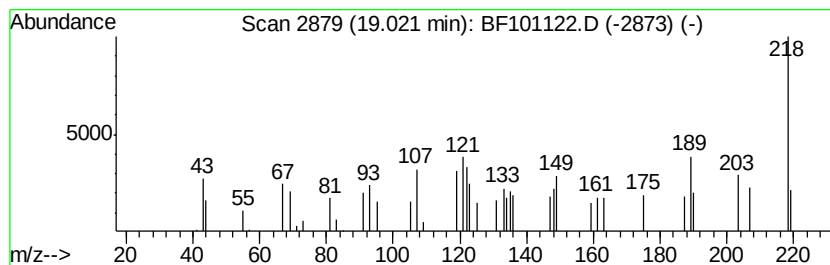
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown19.02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	3.08 ng	54303	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,4-2H-Coumarin, 4,4,5,6,8-penta...	218	C14H18O2	1000129-70-7	46
2		1-Hydroxypyrene	218	C16H10O	005315-79-7	38
3		2(3H)-Naphthalenone, 4,4a,5,6,7,...	218	C15H22O	019598-45-9	37
4		4-(p-N,N-dimethylaminophenyl)imin...	218	C13H18N2O	1000100-07-8	35
5		Benzo(b)naphtho(1,2-d)furan	218	C16H10O	000205-39-0	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120517\
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ALS Vial : 11 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\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	7.0 ng		118270	1	6.85	340005	20.0
unknown6.62	6.62	95.7 ng		1626320	1	6.85	340005	20.0
n-Hexadecanoic acid	11.89	4.4 ng		108772	4	11.37	497095	20.0
5-Bromo-2-thiophe...	11.99	2.3 ng		56059	4	11.37	497095	20.0
Trifluoroacetoxy ...	13.84	7.1 ng		157890	5	14.02	446796	20.0
4b,10b-Dihydro-4b...	14.47	2.1 ng		46210	5	14.02	446796	20.0
Squalene	14.84	3.0 ng		53243	6	15.49	352161	20.0
Benzo[e]pyrene	15.37	2.2 ng		38733	6	15.49	352161	20.0
1-Nonadecene	15.97	2.8 ng		49382	6	15.49	352161	20.0
unknown17.52	17.52	2.2 ng		39004	6	15.49	352161	20.0
unknown19.02	19.02	3.1 ng		54303	6	15.49	352161	20.0