

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
 Data File : BF097337.D
 Acq On : 4 Aug 2017 00:48
 Operator : SJ/JU
 Sample : I4560-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-STOCKPILE-COMP

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-BF072517.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	4.575	454	457	470	rBV	124218	198672	7.42%	0.906%
2	5.045	533	537	556	rBV	1941096	2264500	84.55%	10.332%
3	6.122	713	720	733	rBV	2243693	2678265	100.00%	12.220%
4	6.222	733	737	745	rVB	2498873	2379642	88.85%	10.857%
5	6.445	772	775	784	rVB	711984	623062	23.26%	2.843%
6	6.604	798	802	811	rVB	1794055	1699129	63.44%	7.753%
7	7.016	868	872	880	rBV	1555125	1436404	53.63%	6.554%
8	7.728	990	993	1001	rBV	999734	879400	32.83%	4.012%
9	8.439	1110	1114	1117	rBV2	38435	38774	1.45%	0.177%
10	8.804	1172	1176	1179	rBV	2493125	2068801	77.24%	9.439%
11	8.904	1190	1193	1198	rVB3	31642	30697	1.15%	0.140%
12	9.204	1241	1244	1249	rBV	258277	227972	8.51%	1.040%
13	9.333	1262	1266	1269	rBV	41225	38564	1.44%	0.176%
14	9.427	1278	1282	1285	rBV	54456	42569	1.59%	0.194%
15	9.469	1285	1289	1292	rVV	888621	760846	28.41%	3.471%
16	9.498	1292	1294	1302	rVB2	34165	37096	1.39%	0.169%
17	9.674	1318	1324	1328	rBV3	32827	46866	1.75%	0.214%
18	9.921	1363	1366	1369	rVB	74271	56990	2.13%	0.260%
19	10.145	1398	1404	1406	rBV2	36040	49083	1.83%	0.224%
20	10.257	1419	1423	1430	rBV	882810	872476	32.58%	3.981%
21	10.392	1442	1446	1451	rVB	90233	109633	4.09%	0.500%
22	10.839	1517	1522	1524	rBV2	62920	63371	2.37%	0.289%
23	10.939	1535	1539	1541	rBV	672636	577503	21.56%	2.635%
24	10.963	1541	1543	1548	rVB	249285	196845	7.35%	0.898%
25	11.016	1550	1552	1556	rVB	93422	80040	2.99%	0.365%
26	11.180	1576	1580	1582	rBV	33412	30521	1.14%	0.139%
27	11.263	1592	1594	1602	rVB3	36349	40408	1.51%	0.184%
28	11.439	1622	1624	1627	rBV	47598	45826	1.71%	0.209%
29	11.468	1627	1629	1632	rVV	62203	58014	2.17%	0.265%
30	11.498	1632	1634	1636	rVV2	42227	43430	1.62%	0.198%
31	11.515	1636	1637	1640	rVV2	40435	35216	1.31%	0.161%
32	11.551	1640	1643	1645	rVV	83132	84965	3.17%	0.388%
33	11.574	1645	1647	1653	rVB2	43954	44163	1.65%	0.202%
34	11.668	1660	1663	1667	rBV5	28410	37273	1.39%	0.170%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.733	1672	1674	1678	rVV	28746	39236	1.46%	0.179%
36	11.768	1678	1680	1685	rVB4	27492	34779	1.30%	0.159%
37	11.986	1714	1717	1720	rBV	48440	53394	1.99%	0.244%
38	12.080	1730	1733	1737	rVB2	46797	48071	1.79%	0.219%
39	12.145	1740	1744	1749	rBV	425228	385014	14.38%	1.757%
40	12.292	1767	1769	1774	rVB5	31029	27838	1.04%	0.127%
41	12.368	1778	1782	1786	rBV	424626	419944	15.68%	1.916%
42	12.521	1805	1808	1814	rVB	1477748	1448458	54.08%	6.609%
43	12.804	1853	1856	1864	rBV2	57309	88940	3.32%	0.406%
44	13.445	1962	1965	1970	rVB2	154093	187092	6.99%	0.854%
45	13.562	1981	1985	1988	rBV2	597360	709819	26.50%	3.239%
46	13.592	1988	1990	1994	rVB	163957	140135	5.23%	0.639%
47	14.556	2152	2154	2157	rBV	138908	133629	4.99%	0.610%
48	14.909	2211	2214	2217	rVB	286714	259323	9.68%	1.183%
49	15.803	2364	2366	2369	rBV3	81290	64398	2.40%	0.294%

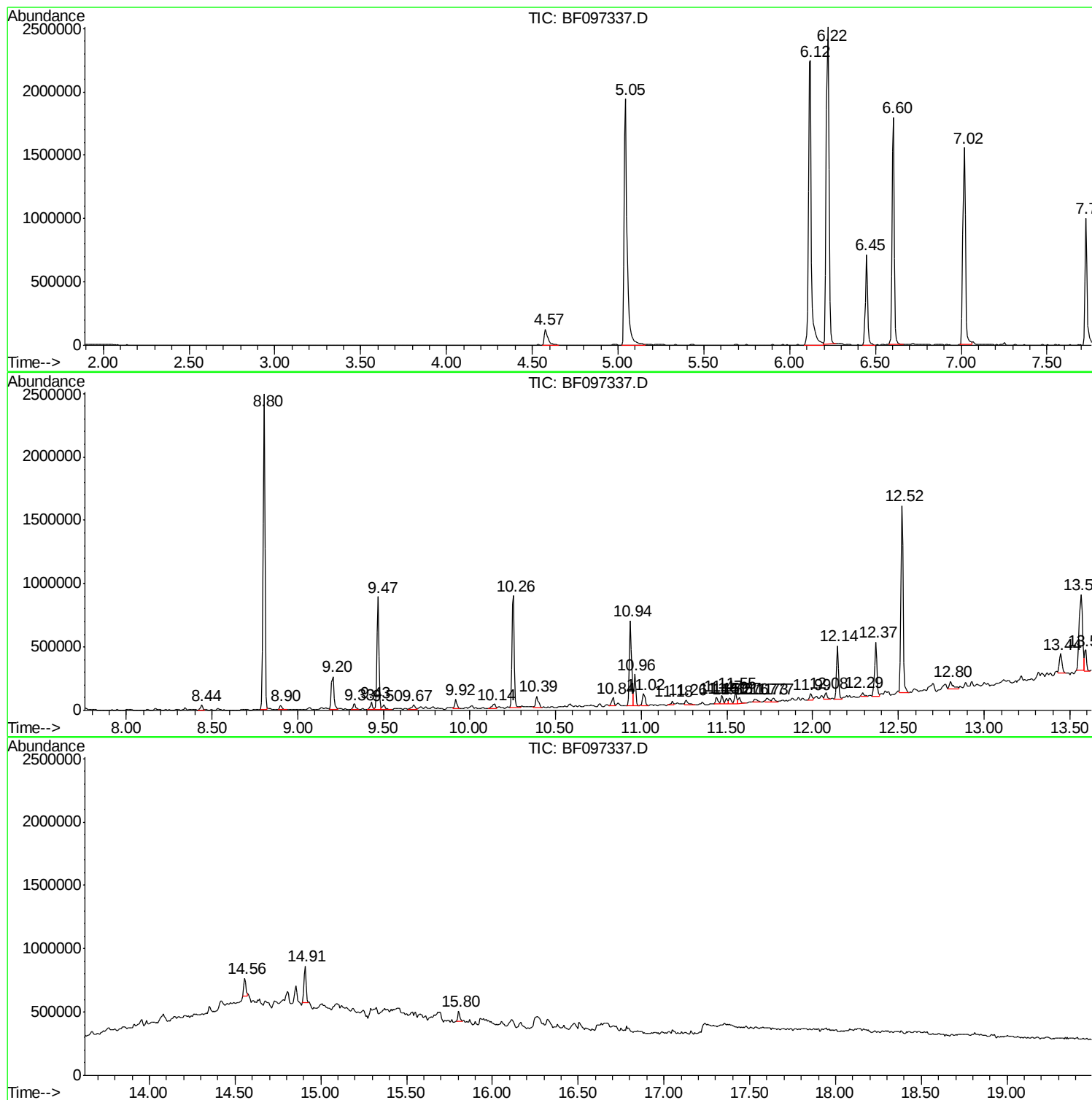
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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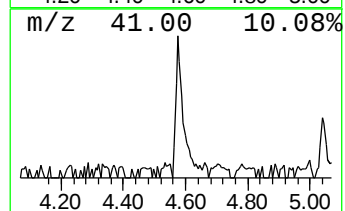
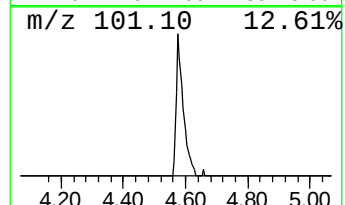
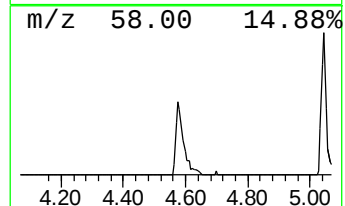
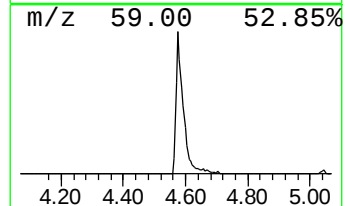
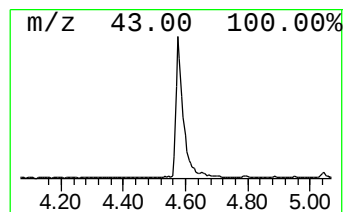
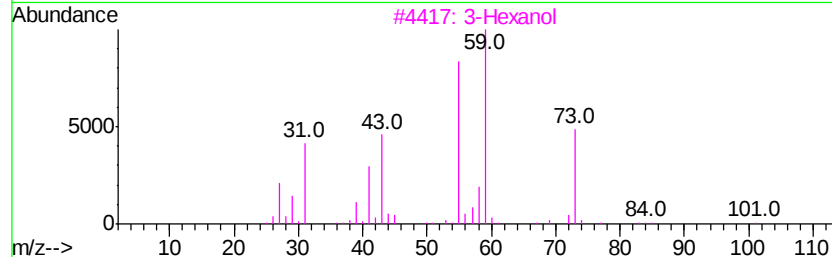
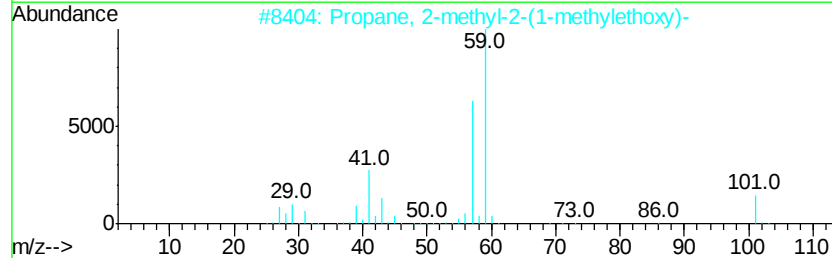
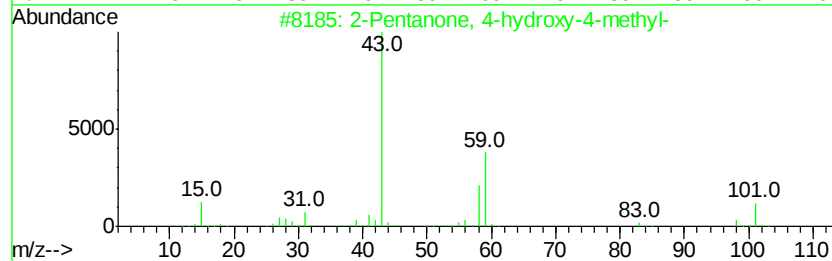
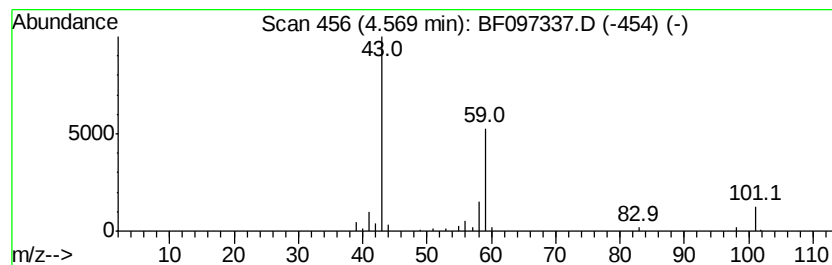
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	6.38 ng	198672	1,4-Dichlorobenzene-d4	6.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol	102	C6H14O	000623-37-0	9
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9
5			1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9



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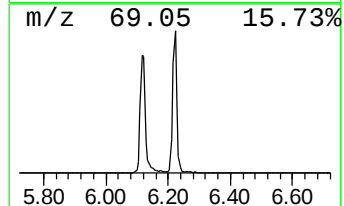
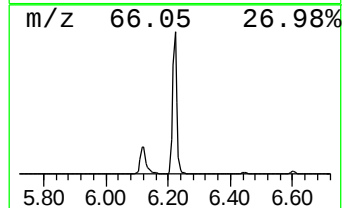
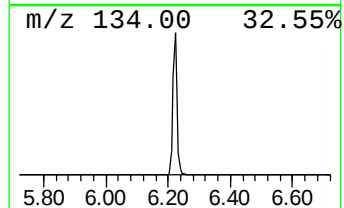
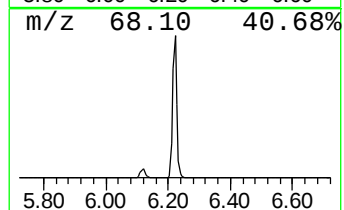
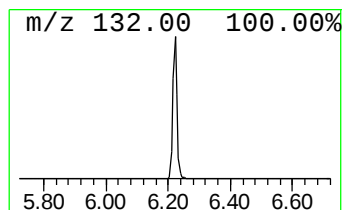
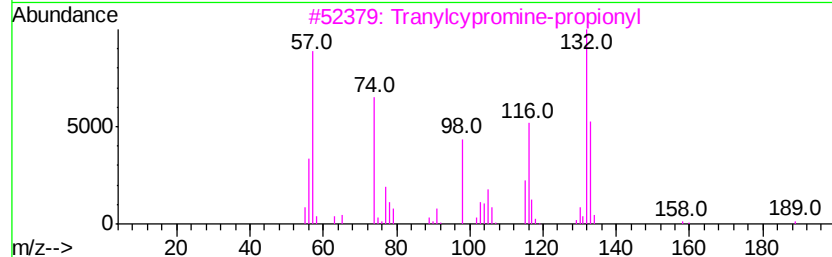
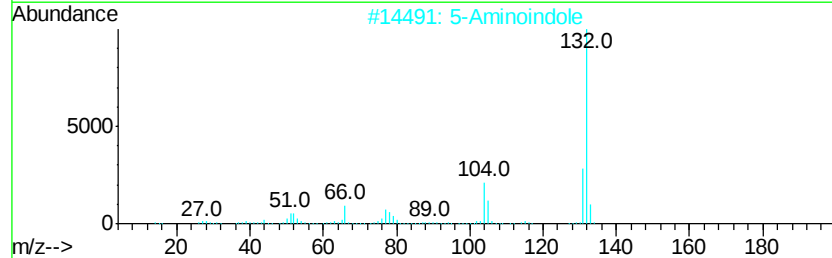
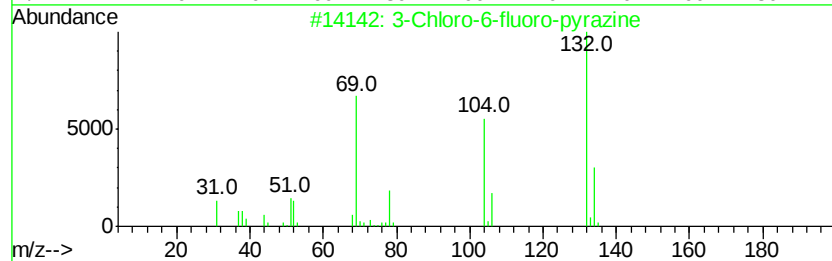
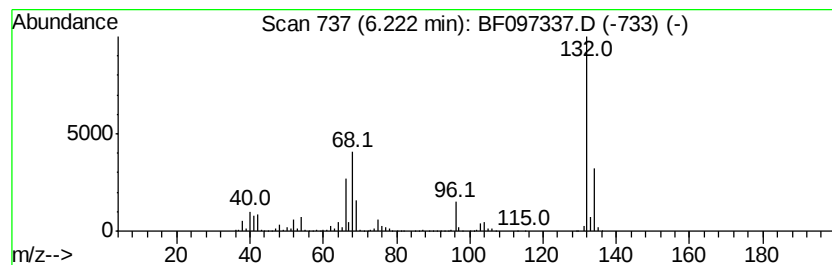
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	76.39 ng	2379640	1,4-Dichlorobenzene-d4	6.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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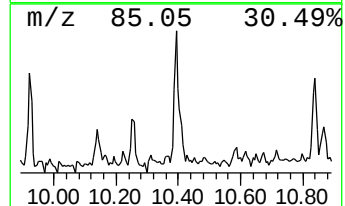
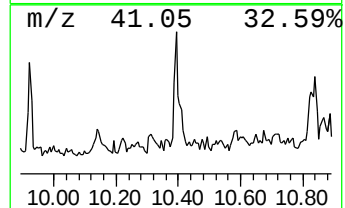
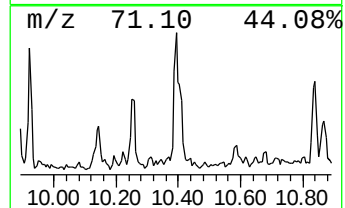
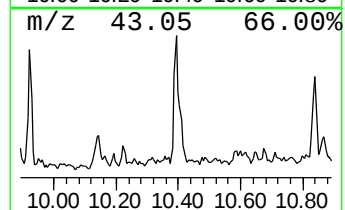
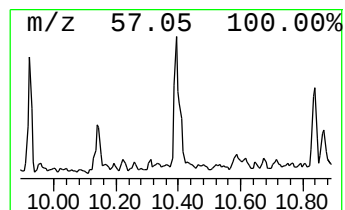
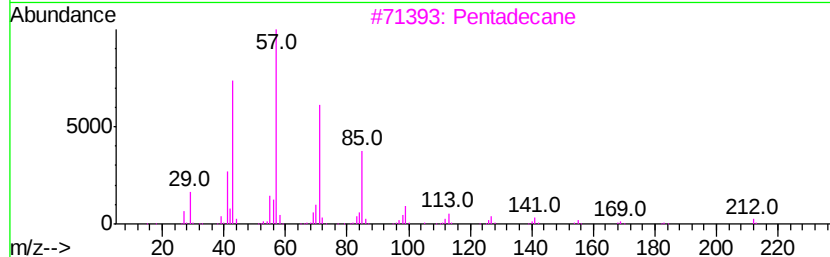
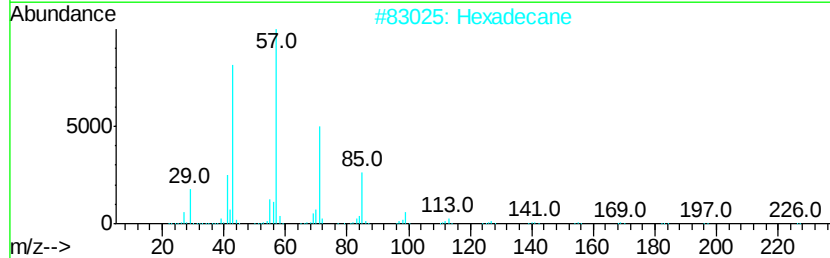
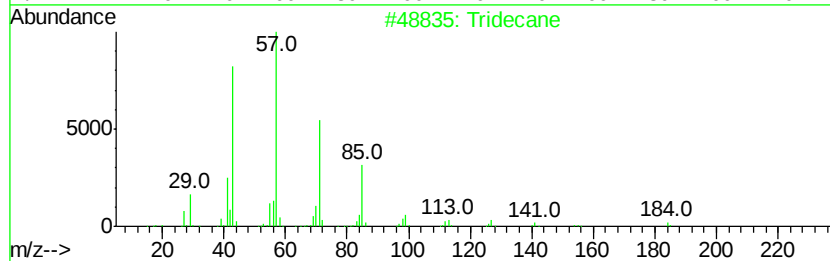
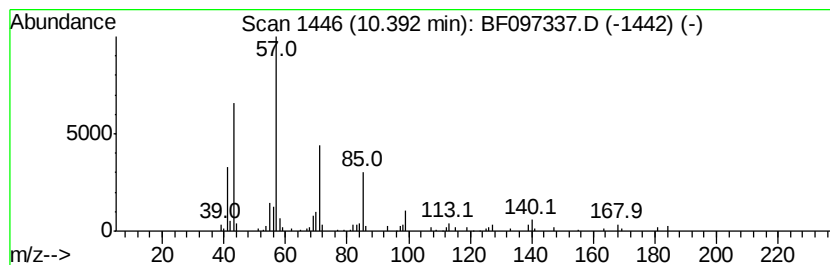
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.39	3.80 ng	109633	Phenanthrene-d10	10.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Hexadecane	226	C16H34	000544-76-3	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	78
5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	78



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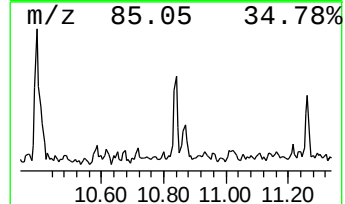
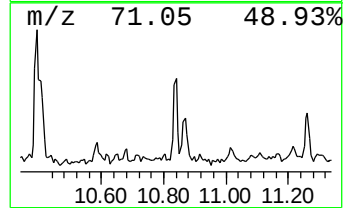
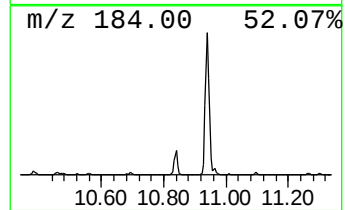
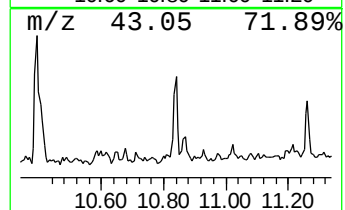
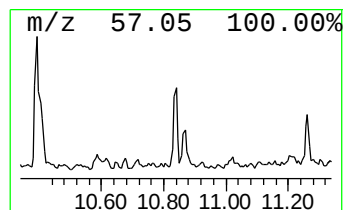
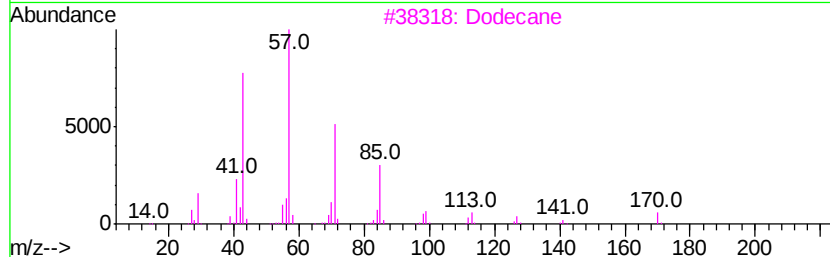
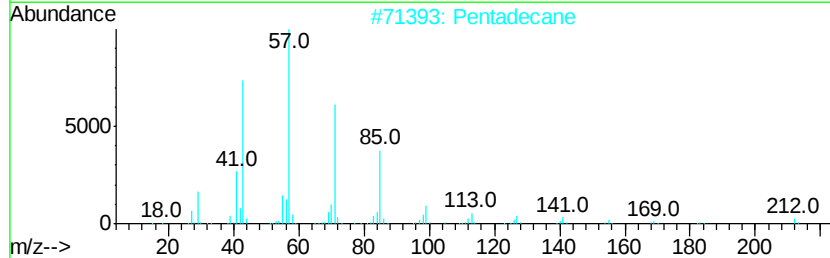
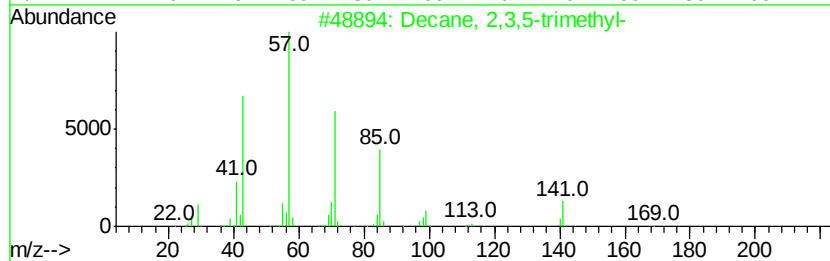
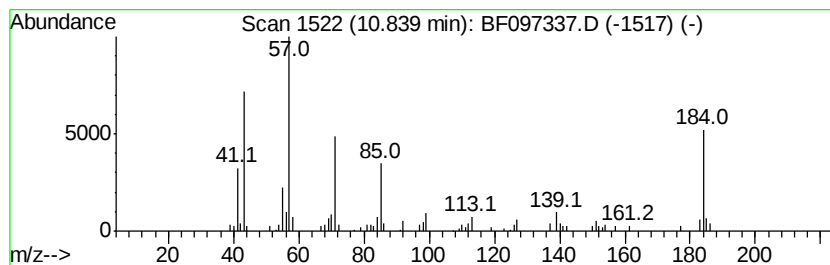
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.84 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.19 ng	63371	Phenanthrene-d10	10.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	46
2		Pentadecane	212	C15H32	000629-62-9	43
3		Dodecane	170	C12H26	000112-40-3	43
4		Eicosane	282	C20H42	000112-95-8	43
5		Heptadecane	240	C17H36	000629-78-7	43



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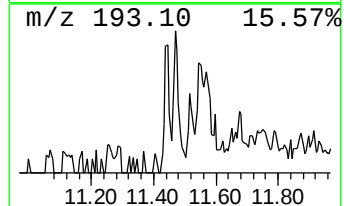
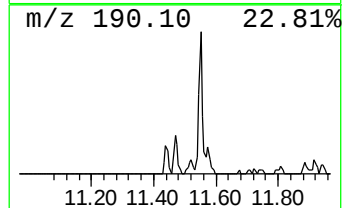
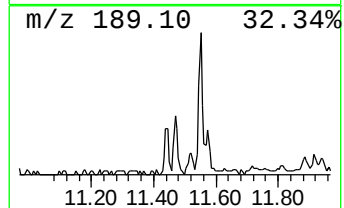
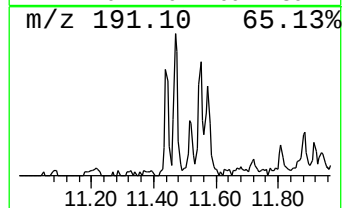
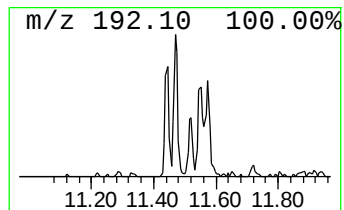
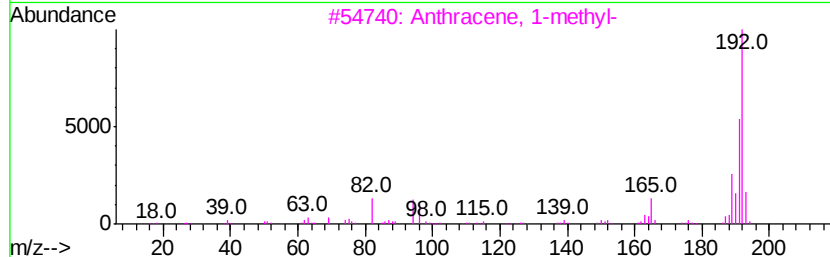
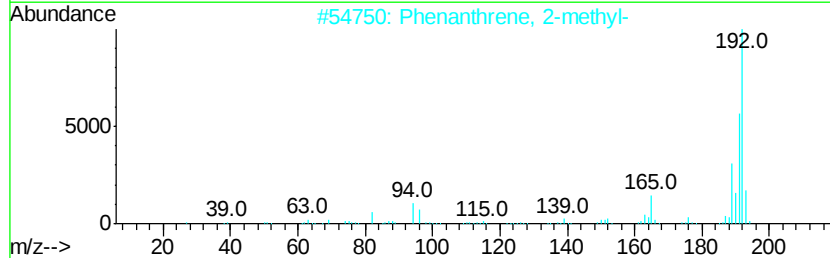
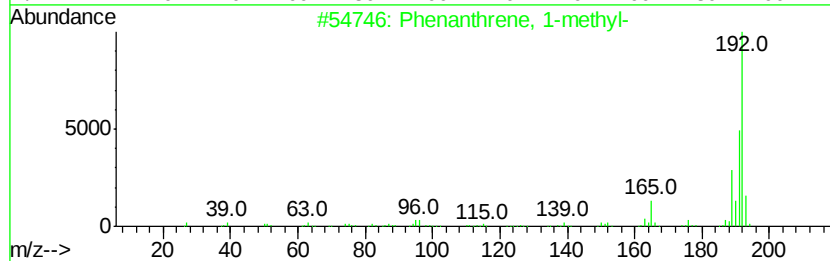
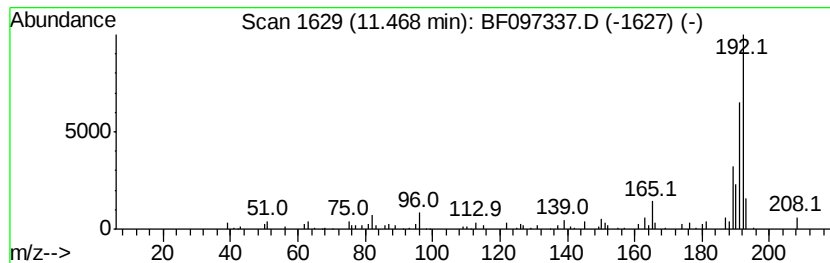
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	2.01 ng	58014	Phenanthrene-d10	10.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	81
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	81
3		Anthracene, 1-methyl-	192	C15H12	000610-48-0	76
4		1H-Cyclopropa[1,1]phenanthrene, 1a,...	192	C15H12	000949-41-7	76
5		Anthracene, 2-methyl-	192	C15H12	000613-12-7	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
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Acq On : 4 Aug 2017 00:48
Operator : SJ/JU
Sample : I4560-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

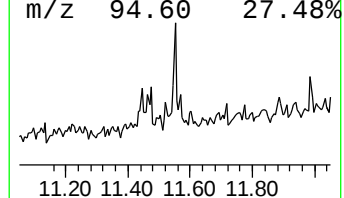
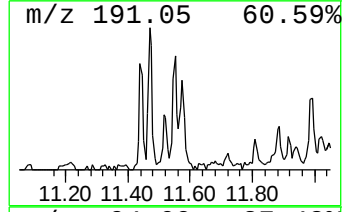
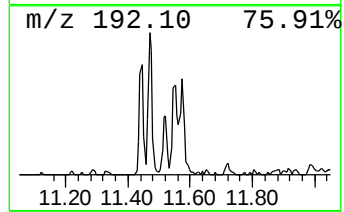
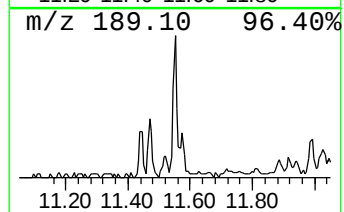
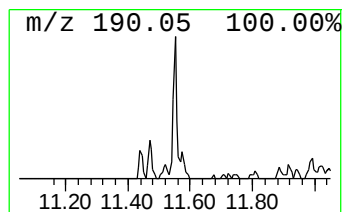
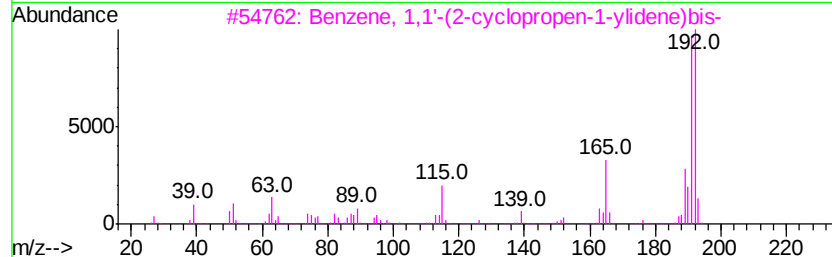
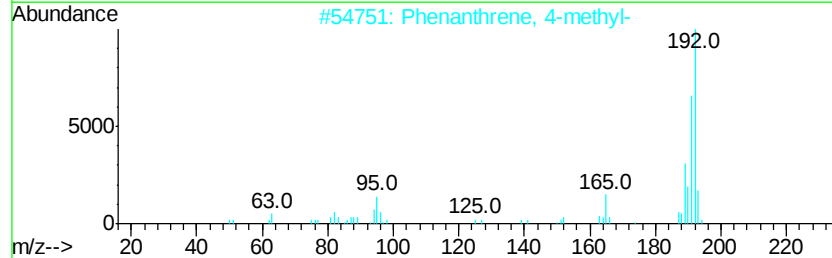
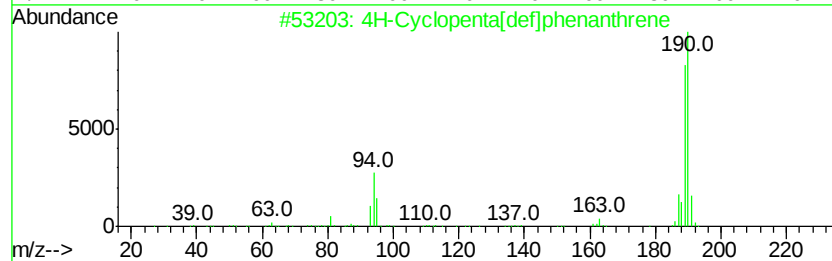
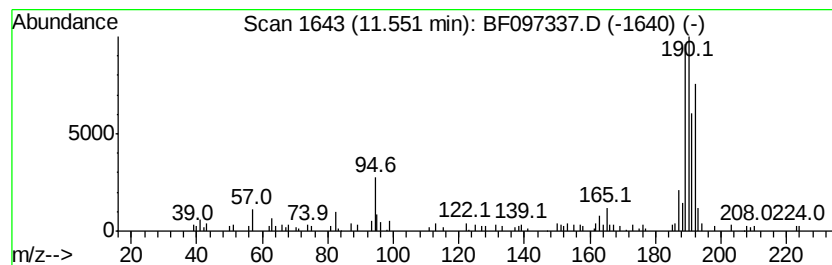
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ClientSampleId :
S-STOCKPILE-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.55	2.94 ng	84965	Phenanthrene-d10	10.94		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
2		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
3		Benzene, 1,1'-(2-cyclopropen-1-ylidene)bis-	192	C15H12	022825-21-4	38
4		Benzene, 1,1'-(1,2-propadienyldiylidene)bis-	192	C15H12	014251-57-1	38
5		8,9-Dihydrocyclopenta[def]phenanthrene	192	C15H12	027410-55-5	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097337.D
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Misc :
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Instrument :
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ClientSampleId :
S-STOCKPILE-COMP

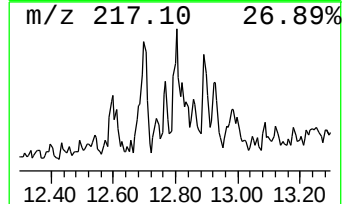
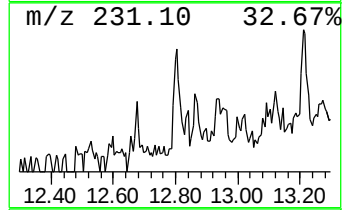
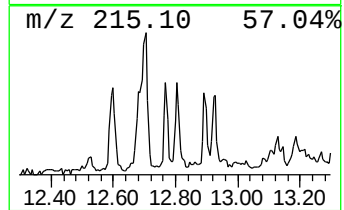
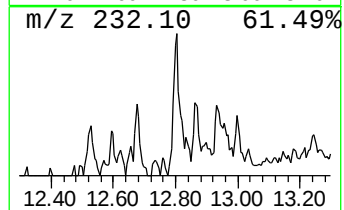
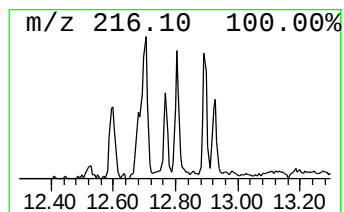
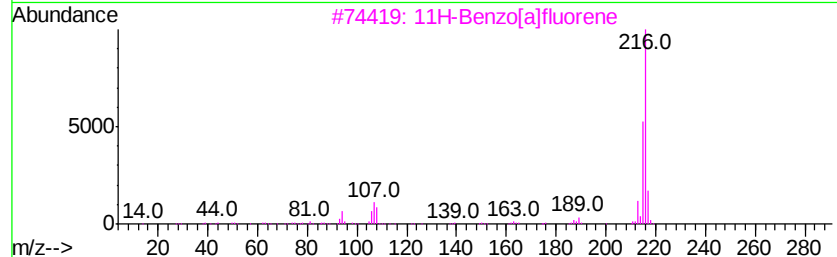
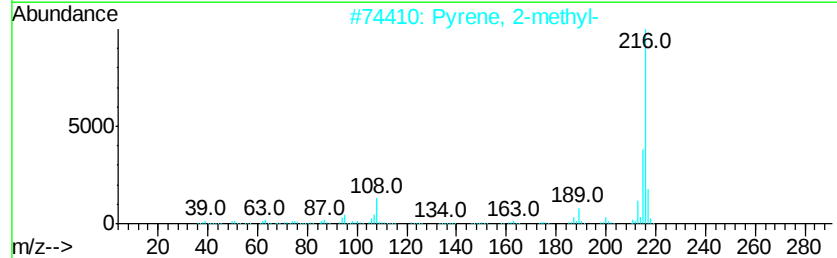
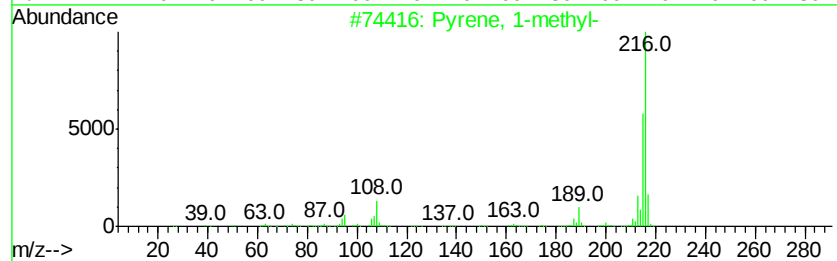
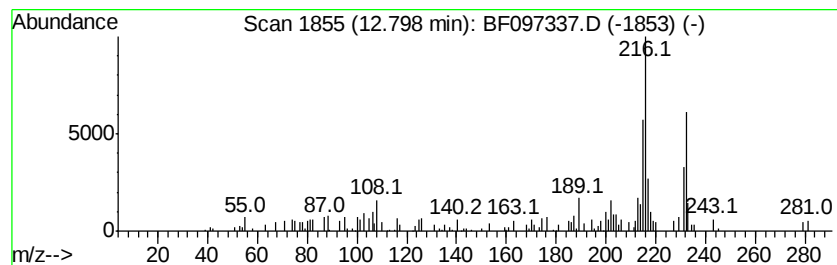
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.51 ng	88940	Chrysene-d12	13.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2		Pyrene, 2-methyl-	216	C17H12	003442-78-2	81
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70
5		Pyrene, 4-methyl-	216	C17H12	003353-12-6	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097337.D
Acq On : 4 Aug 2017 00:48
Operator : SJ/JU
Sample : I4560-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

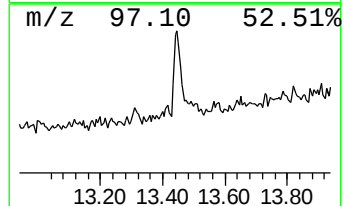
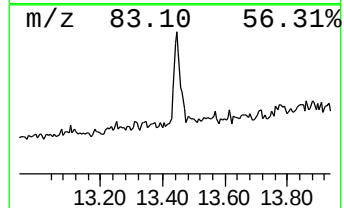
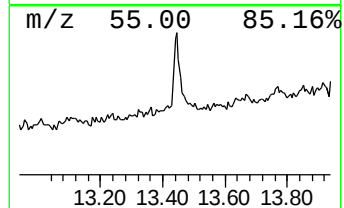
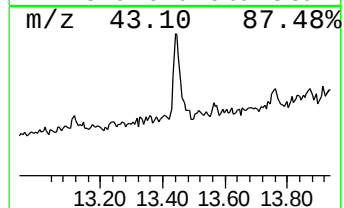
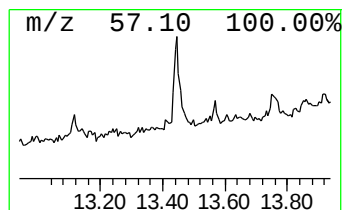
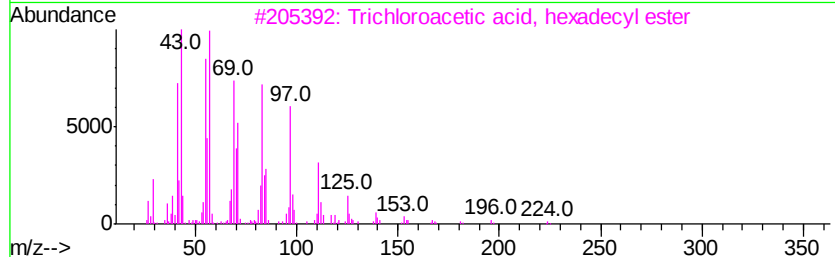
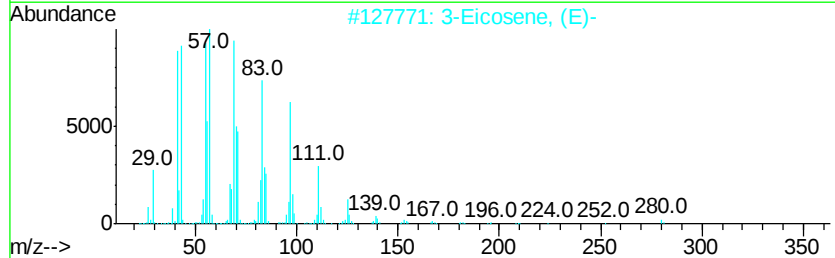
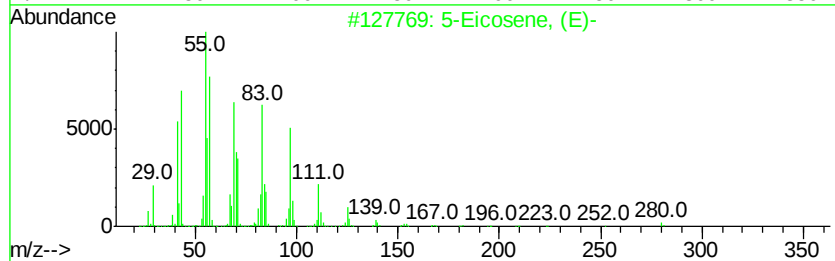
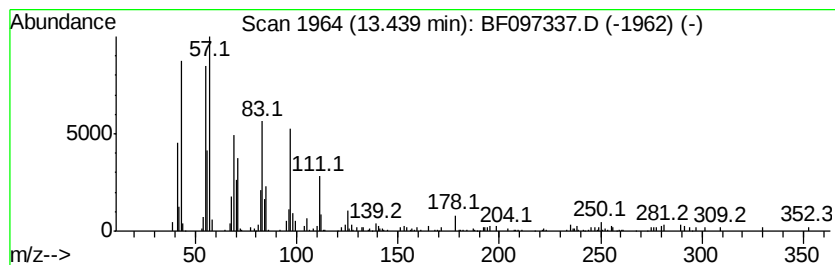
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	5.27 ng	187092	Chrysene-d12	13.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	5-Eicosene, (E)-	280 C20H40	074685-30-6	96
2	3-Eicosene, (E)-	280 C20H40	074685-33-9	91
3	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	91
4	9-Eicosene, (E)-	280 C20H40	074685-29-3	91
5	Heptafluorobutyric acid, hexadec...	438 C20H33F7O2	006385-15-5	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097337.D
Acq On : 4 Aug 2017 00:48
Operator : SJ/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-STOCKPILE-COMP

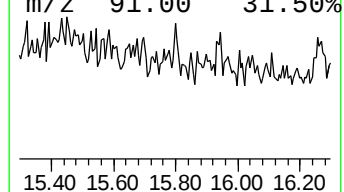
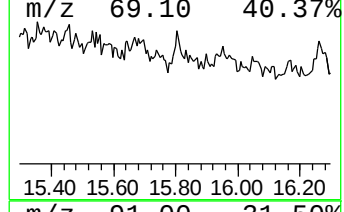
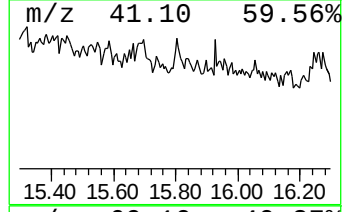
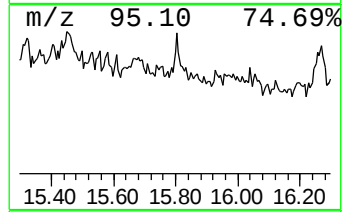
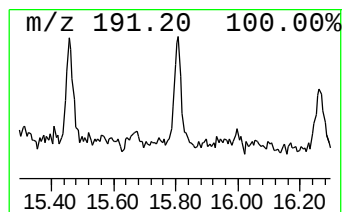
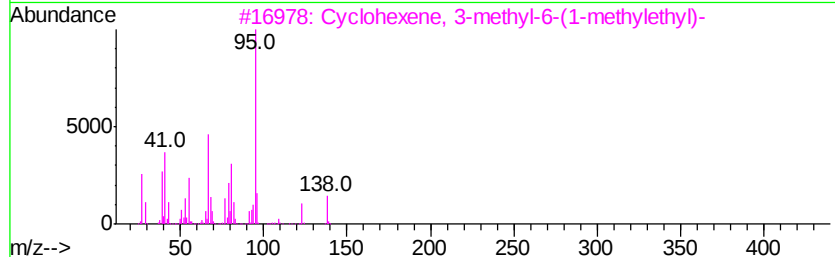
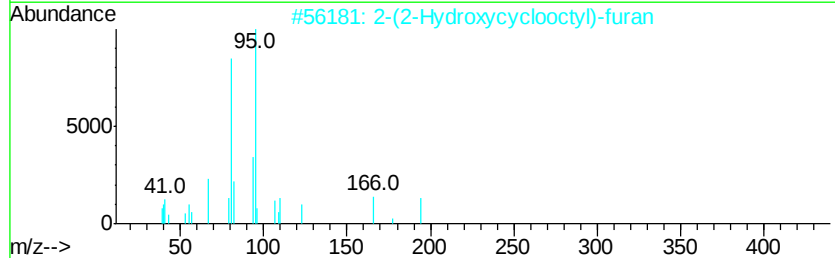
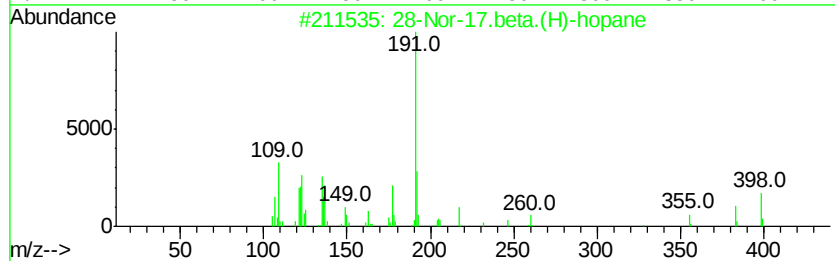
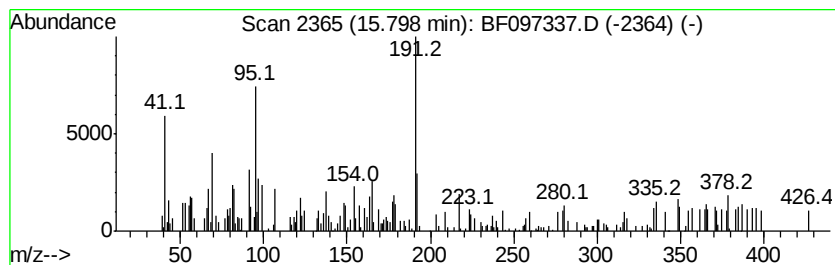
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 28-Nor-17.beta.(H)-hopane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	4.97 ng	64398	Perylene-d12	14.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	55
2		2-(2-Hydroxycyclooctyl)-furan	194	C12H18O2	115754-90-0	30
3		Cyclohexene, 3-methyl-6-(1-methyl...	138	C10H18	005256-65-5	25
4		N-(4-Morpholin-4-yl-phenyl)-2-ni...	377	C17H19N3O5S	1000374-81-7	25
5		Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097337.D
Acq On : 4 Aug 2017 00:48
Operator : SJ/JU
Sample : I4560-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-STOCKPILE-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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...	4.57	6.4	ng	198672	1	6.45	623062	20.0
unknown6.22	6.22	76.4	ng	2379640	1	6.45	623062	20.0
Tridecane	10.39	3.8	ng	109633	4	10.94	577503	20.0
unknown10.84	10.84	2.2	ng	63371	4	10.94	577503	20.0
Phenanthrene, 1-m...	11.47	2.0	ng	58014	4	10.94	577503	20.0
4H-Cyclopenta[def...	11.55	2.9	ng	84965	4	10.94	577503	20.0
Pyrene, 1-methyl-	12.80	2.5	ng	88940	5	13.56	709819	20.0
5-Eicosene, (E)-	13.44	5.3	ng	187092	5	13.56	709819	20.0
28-Nor-17.beta.(H...	15.80	5.0	ng	64398	6	14.91	259323	20.0