

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
 Data File : BF081688.D
 Acq On : 17 Sep 2015 20:43
 Operator : UM/IZ
 Sample : G3620-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-2

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-BF090115.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	1.258	11	15	18	rBV	1023643	1271215	63.93%	5.953%
2	1.338	20	22	26	rVB	23179	34349	1.73%	0.161%
3	1.441	29	31	37	rBV	82245	208978	10.51%	0.979%
4	1.532	37	39	70	rVB	342708	1238365	62.28%	5.799%
5	4.481	292	297	314	rBV	341975	1103687	55.50%	5.169%
6	5.339	369	372	388	rBV	875557	1873073	94.20%	8.772%
7	7.613	566	571	573	rBV	870543	1988484	100.00%	9.312%
8	7.693	574	578	581	rVB	1062396	1921208	96.62%	8.997%
9	8.173	617	620	631	rBV	201761	312871	15.73%	1.465%
10	8.505	644	649	652	rBV	833721	1405588	70.69%	6.582%
11	9.476	729	734	737	rBV	611060	1279038	64.32%	5.990%
12	11.065	870	873	877	rBV	221644	400314	20.13%	1.875%
13	13.717	1099	1105	1108	rBV	1109155	1984799	99.81%	9.295%
14	14.768	1193	1197	1200	rBV	224413	348472	17.52%	1.632%
15	15.191	1230	1234	1239	rBB	225157	417968	21.02%	1.957%
16	16.597	1354	1357	1360	rBB	15289	26183	1.32%	0.123%
17	17.100	1397	1401	1410	rBB	641169	1299892	65.37%	6.087%
18	17.740	1453	1457	1464	rBV	20950	49707	2.50%	0.233%
19	18.700	1537	1541	1544	rBV	262813	427642	21.51%	2.003%
20	18.746	1544	1545	1549	rVV	21642	33521	1.69%	0.157%
21	18.826	1549	1552	1555	rVV2	17583	31040	1.56%	0.145%
22	20.357	1682	1686	1689	rBV	30309	69387	3.49%	0.325%
23	20.460	1692	1695	1707	rVB	83141	183437	9.22%	0.859%
24	21.386	1773	1776	1778	rVB	61877	84681	4.26%	0.397%
25	21.729	1803	1806	1814	rBV	69100	105291	5.30%	0.493%
26	21.866	1816	1818	1824	rBV3	18446	32602	1.64%	0.153%
27	22.072	1833	1836	1839	rBV	1135972	1725254	86.76%	8.079%
28	22.917	1906	1910	1912	rBV3	8632	24286	1.22%	0.114%
29	23.340	1942	1947	1949	rBV3	288416	544271	27.37%	2.549%
30	23.375	1949	1950	1953	rVV2	59176	55241	2.78%	0.259%
31	24.003	2003	2005	2011	rVB	26124	45394	2.28%	0.213%
32	24.369	2035	2037	2039	rVB	25109	22547	1.13%	0.106%
33	24.449	2041	2044	2049	rBV	63684	114962	5.78%	0.538%
34	24.609	2056	2058	2063	rBV2	23625	52088	2.62%	0.244%

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DUP-2

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	24.689	2063	2065	2067	rVV	43269	42177	2.12%	0.198%
36	24.735	2067	2069	2071	rVV	53800	51801	2.61%	0.243%
37	24.781	2071	2073	2080	rVV	222262	234432	11.79%	1.098%
38	25.215	2110	2111	2114	rVB	15926	27579	1.39%	0.129%
39	25.546	2135	2140	2144	rVV3	6675	23457	1.18%	0.110%
40	25.821	2161	2164	2168	rVB2	30902	56429	2.84%	0.264%
41	25.935	2170	2174	2176	rBV4	7194	24403	1.23%	0.114%
42	25.981	2176	2178	2182	rVB2	12986	23180	1.17%	0.109%
43	26.118	2187	2190	2193	rVV	26096	46386	2.33%	0.217%
44	26.198	2194	2197	2202	rVV2	20306	45505	2.29%	0.213%
45	26.289	2202	2205	2209	rVV2	8381	20124	1.01%	0.094%
46	26.872	2254	2256	2265	rVB7	5708	21345	1.07%	0.100%
47	27.649	2319	2324	2329	rVB3	5902	21029	1.06%	0.098%

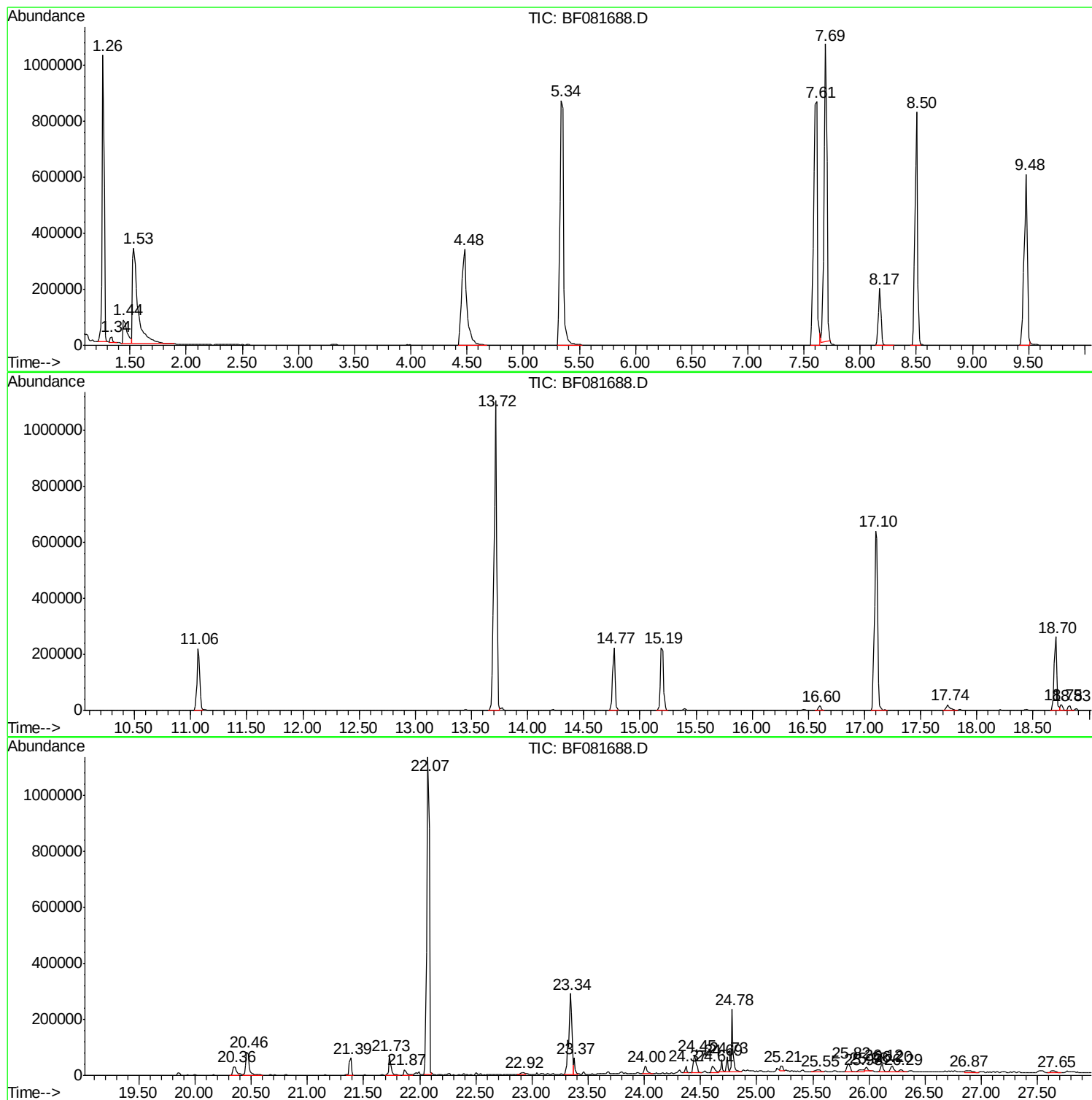
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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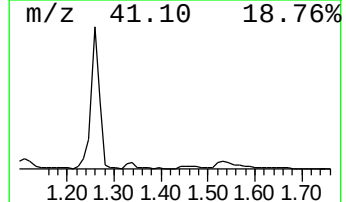
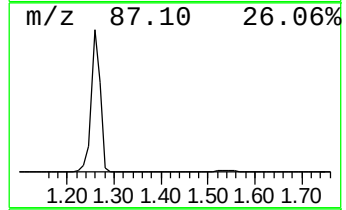
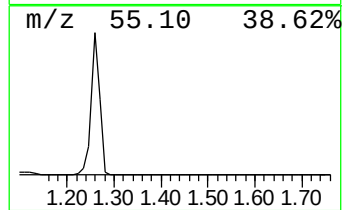
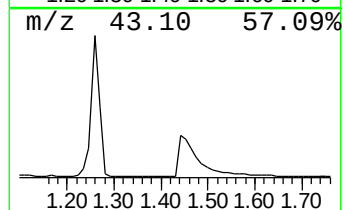
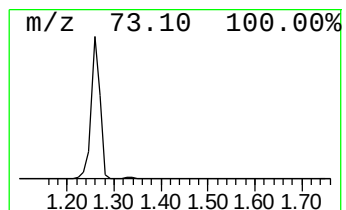
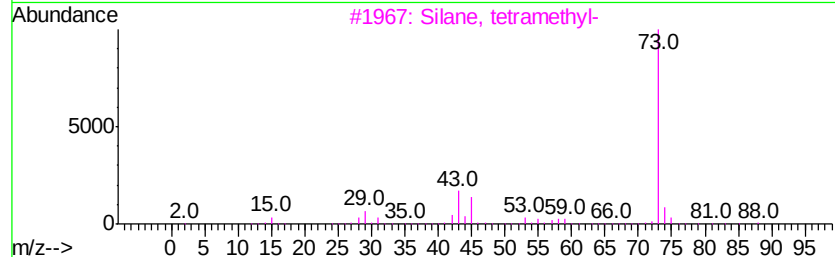
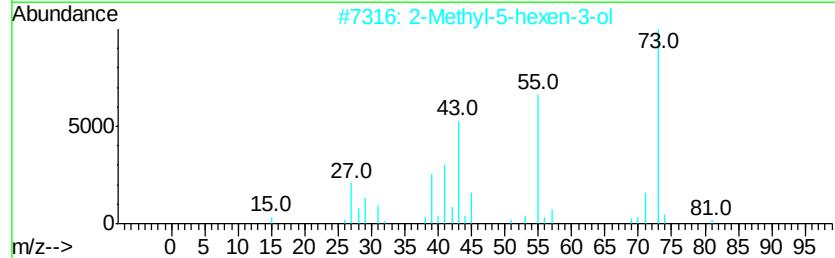
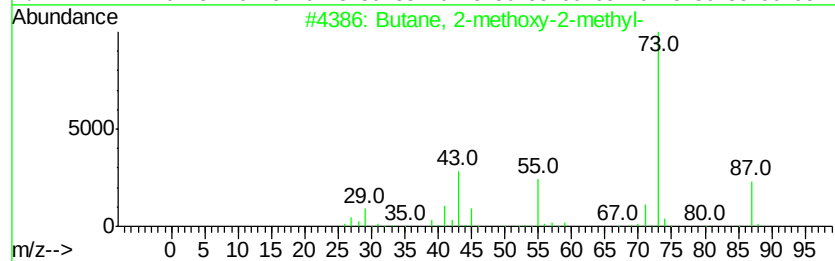
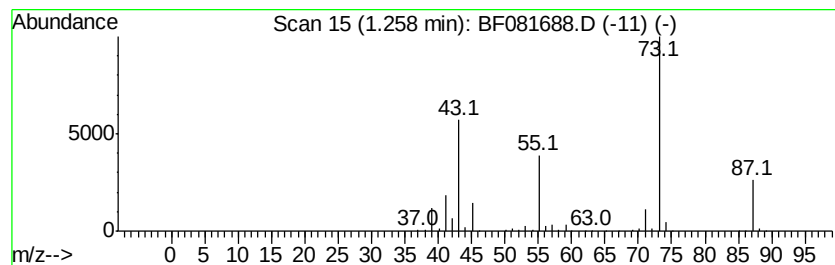
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	81.26 ng	1271220	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4		Boronic acid, ethyl-, dimethyl e...	102	C4H11B02	007318-82-3	10
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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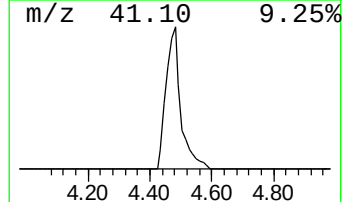
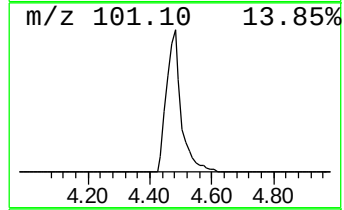
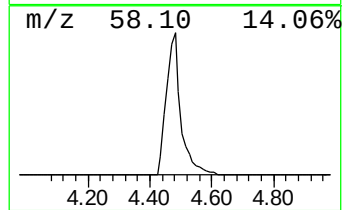
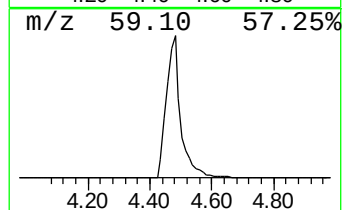
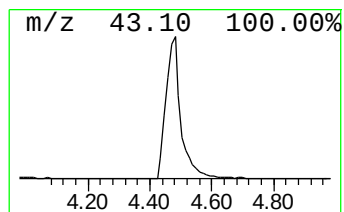
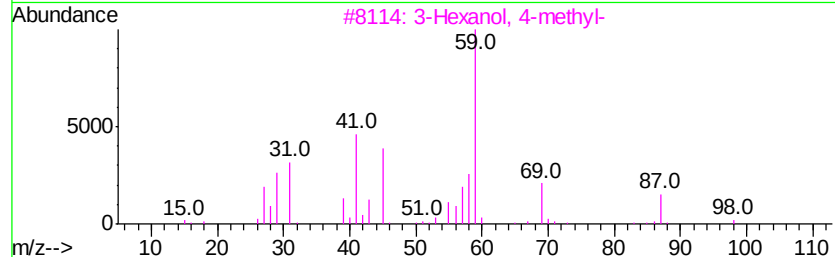
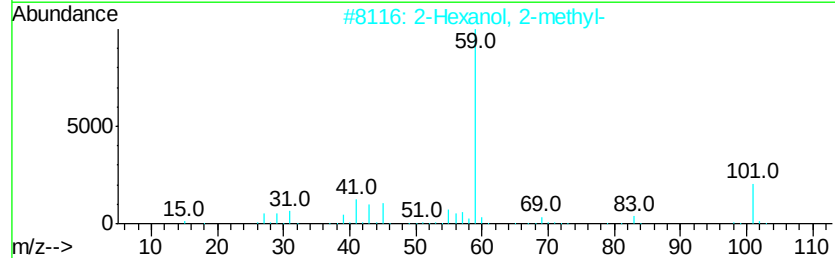
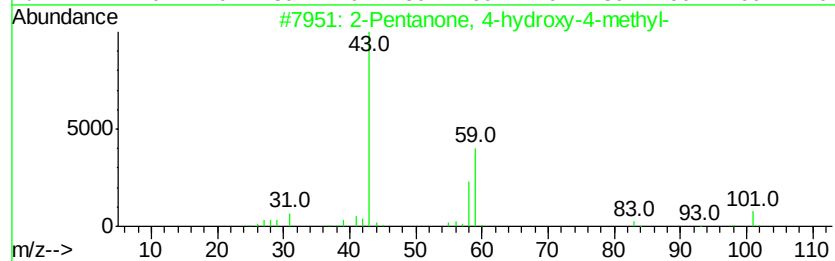
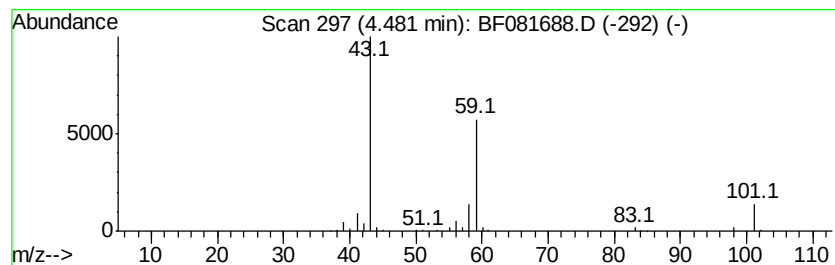
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	70.55 ng	1103690	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9



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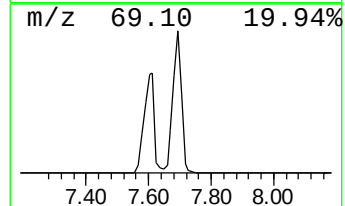
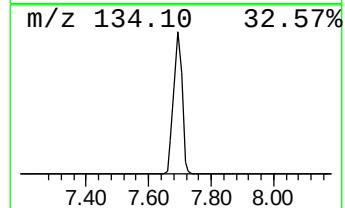
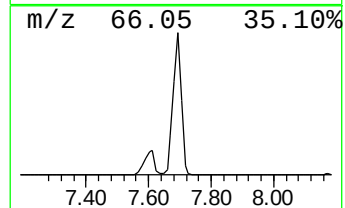
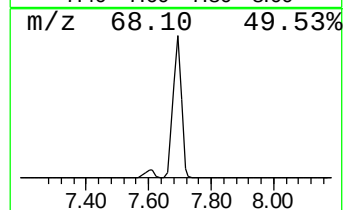
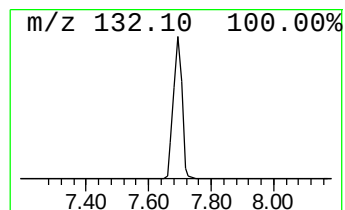
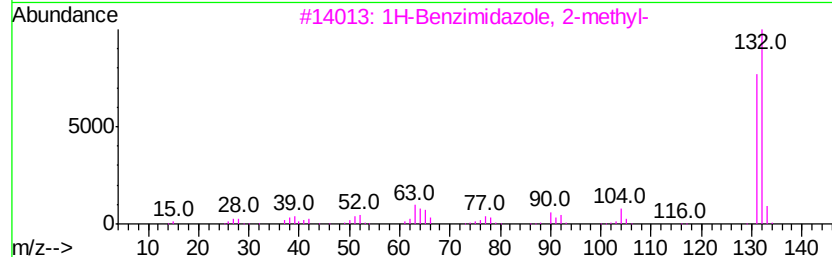
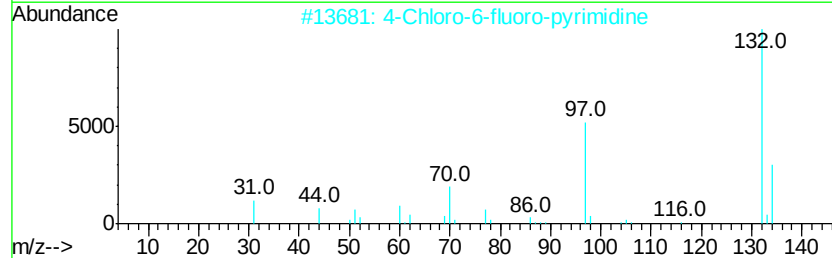
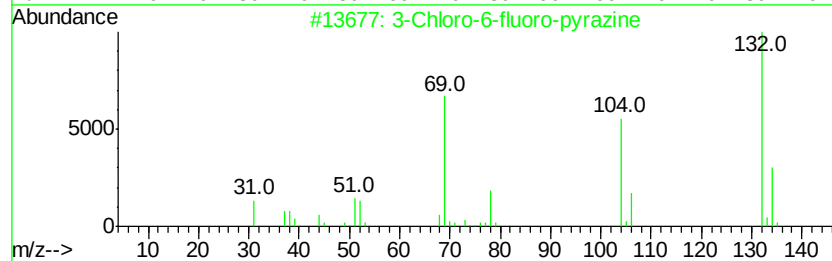
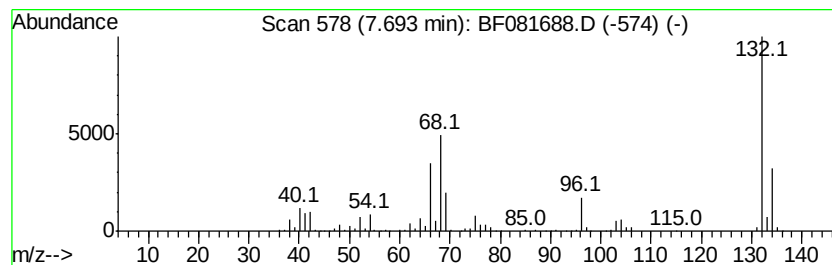
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	122.81 ng	1921210	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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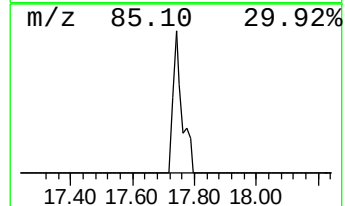
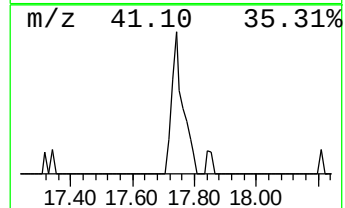
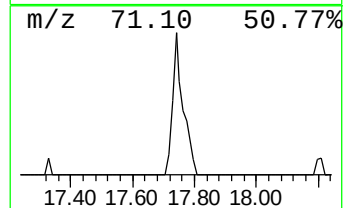
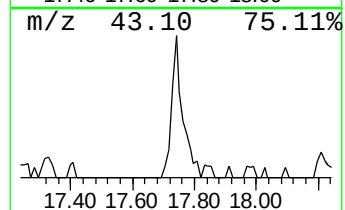
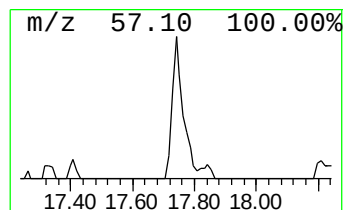
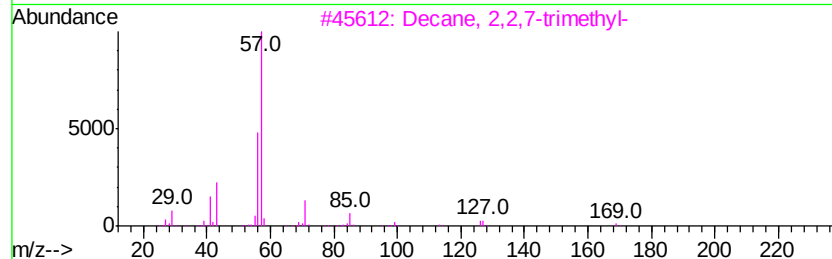
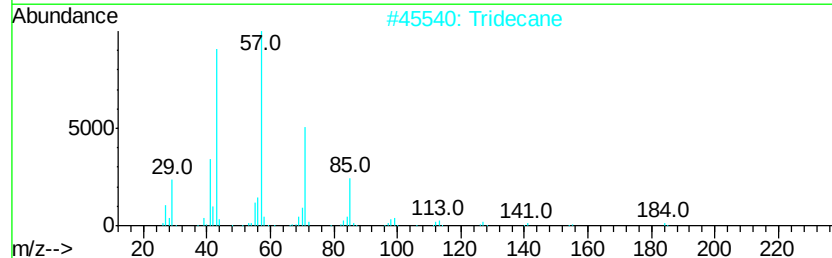
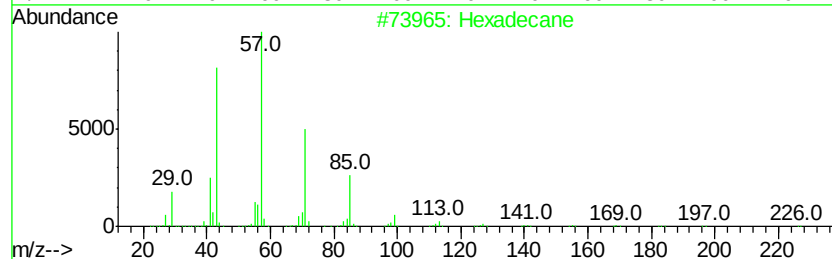
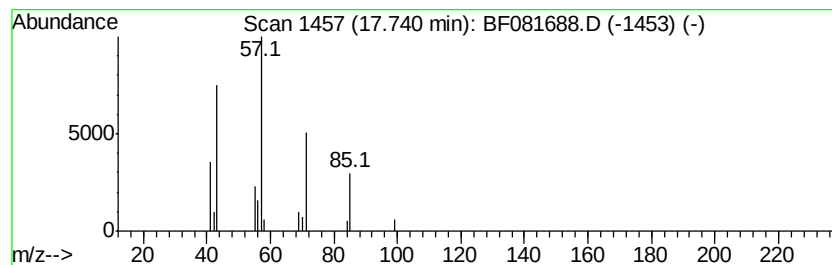
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.74	2.32 ng	49707	Phenanthrene-d10	18.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	83
2	Tridecane		184	C13H28	000629-50-5	78
3	Decane, 2,2,7-trimethyl-		184	C13H28	062237-99-4	59
4	Octane, 2-methyl-		128	C9H20	003221-61-2	59
5	Decane, 2,2,6-trimethyl-		184	C13H28	062237-97-2	59



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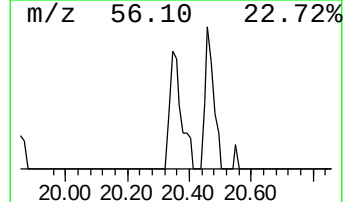
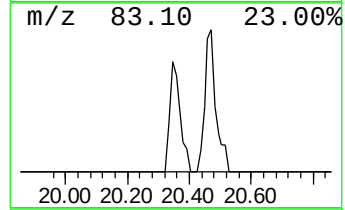
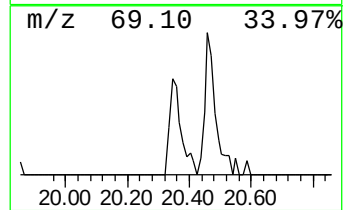
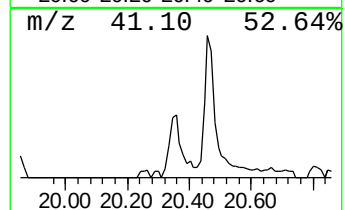
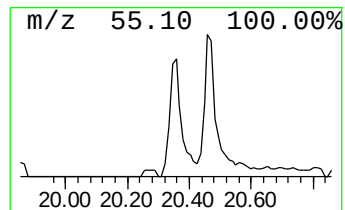
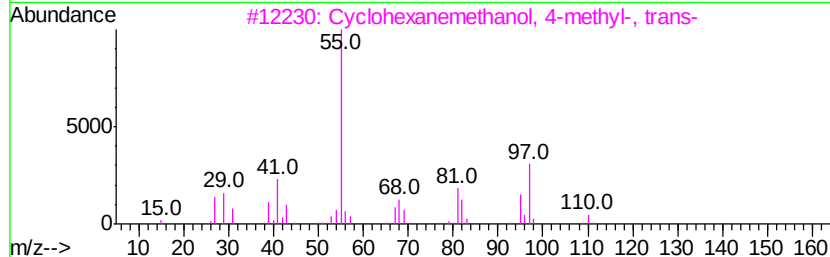
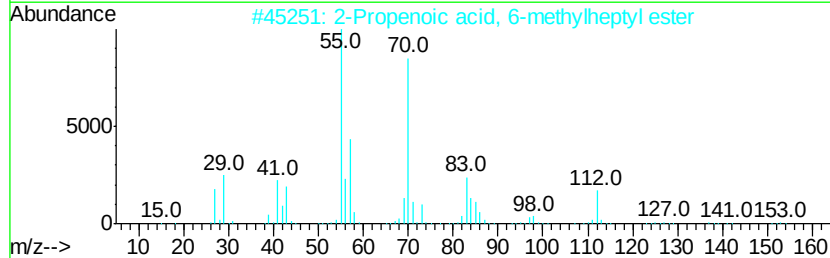
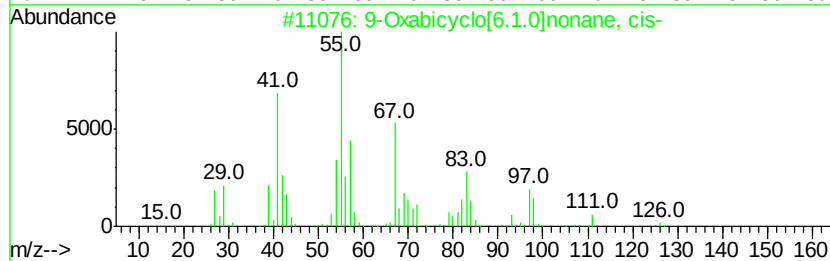
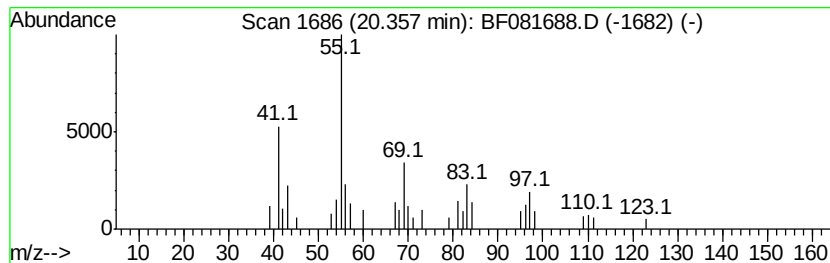
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown20.36 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.36	3.25 ng	69387	Phenanthrene-d10	18.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Oxabicyclo[6.1.0]nonane, cis-	126	C8H14O	004925-71-7	40
2	2-Propenoic acid, 6-methylheptyl...	184	C11H20O2	054774-91-3	38
3	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	27
4	2-Decenal, (E)-	154	C10H18O	003913-81-3	27
5	Dichloroacetic acid, 1-cyclopent...	224	C9H14Cl2O2	1000282-56-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081688.D
Acq On : 17 Sep 2015 20:43
Operator : UM/IZ
Sample : G3620-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-2

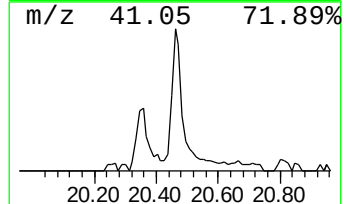
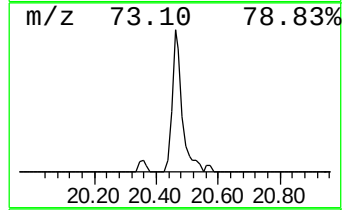
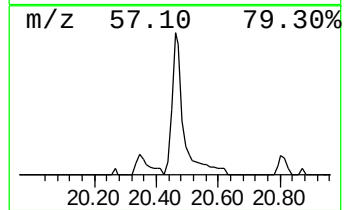
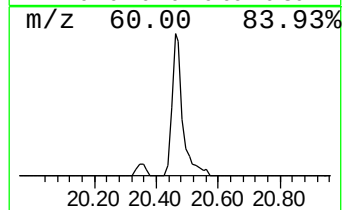
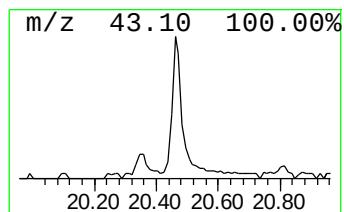
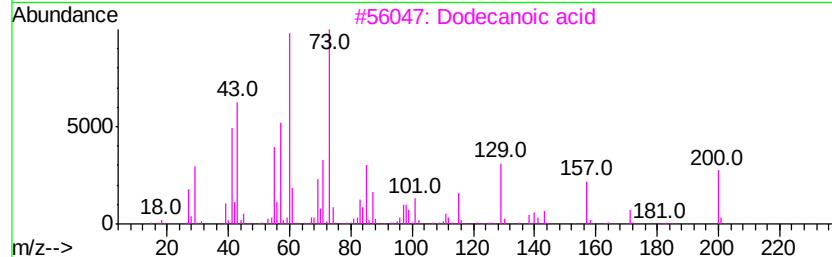
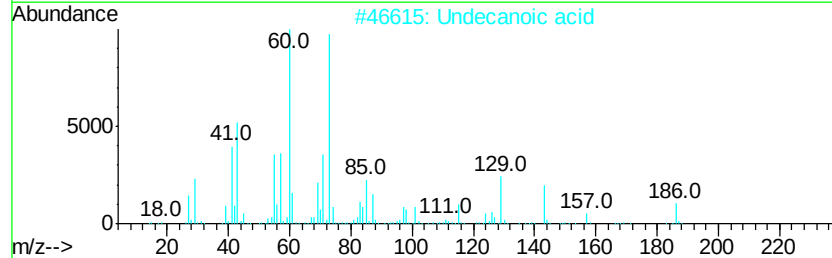
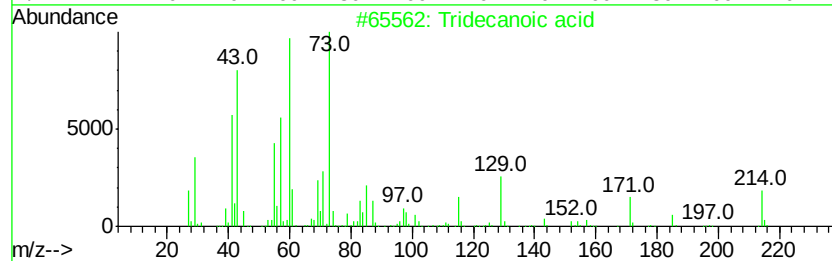
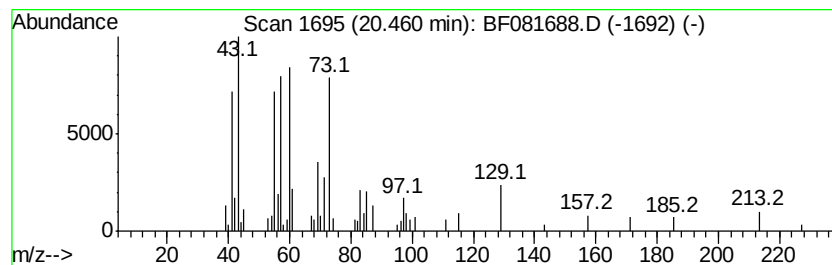
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	8.58 ng	183437	Phenanthrene-d10	18.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	86
2			Undecanoic acid	186	C11H22O2	000112-37-8	80
3			Dodecanoic acid	200	C12H24O2	000143-07-7	59
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081688.D
Acq On : 17 Sep 2015 20:43
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Sample : G3620-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

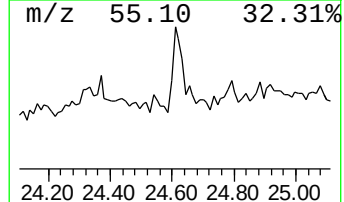
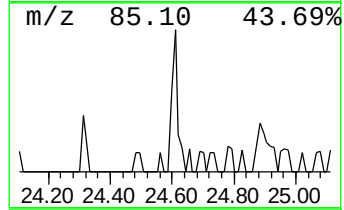
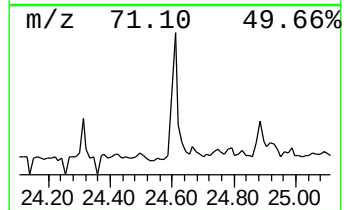
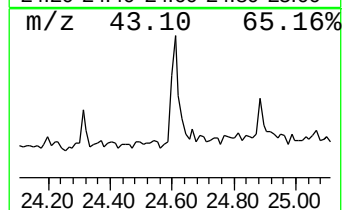
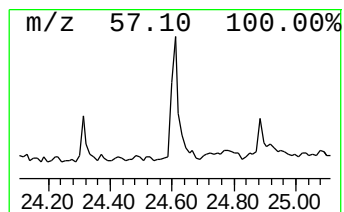
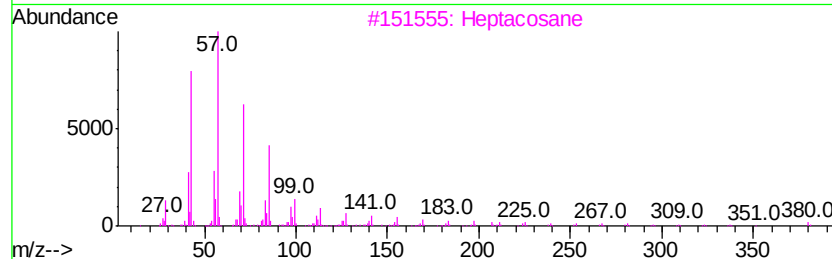
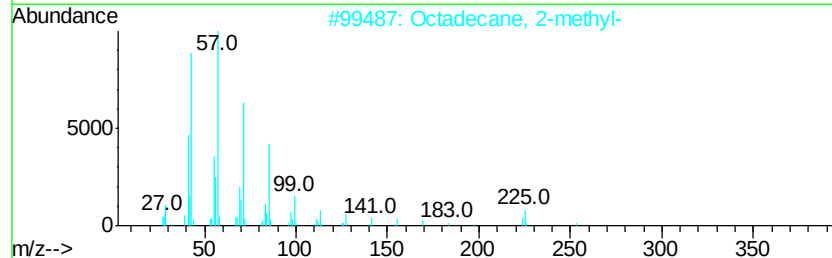
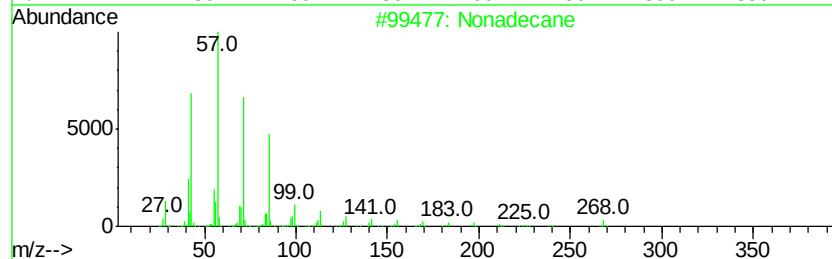
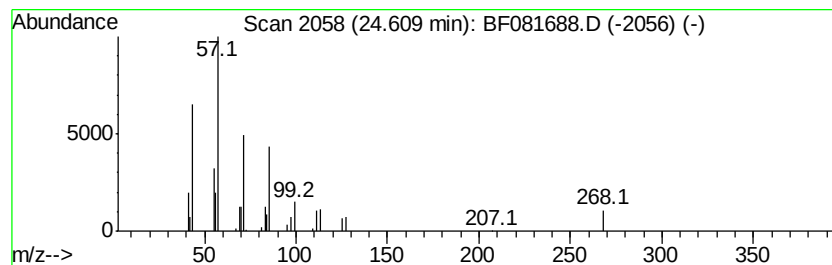
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
24.61	4.44 ng	52088	Perylene-d12		24.78
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	83
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
3	Heptacosane	380	C27H56	000593-49-7	72
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
5	Octacosane	394	C28H58	000630-02-4	72



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Acq On : 17 Sep 2015 20:43
Operator : UM/IZ
Sample : G3620-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

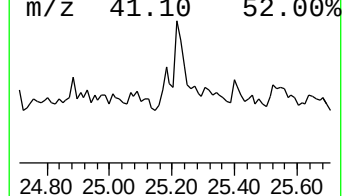
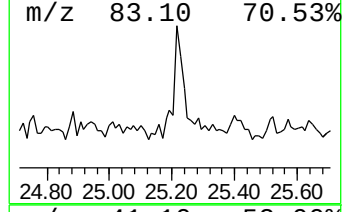
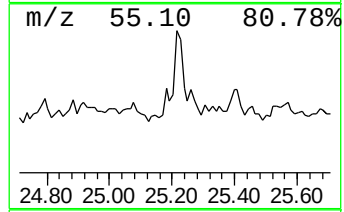
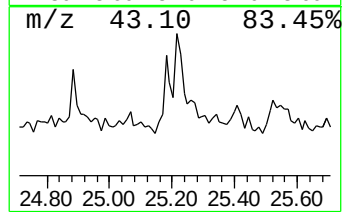
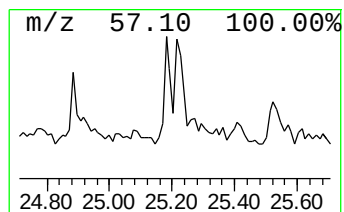
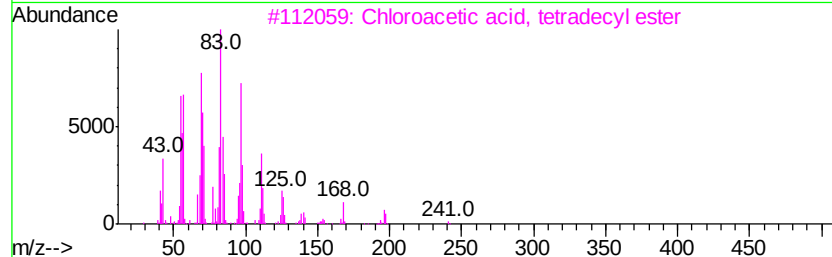
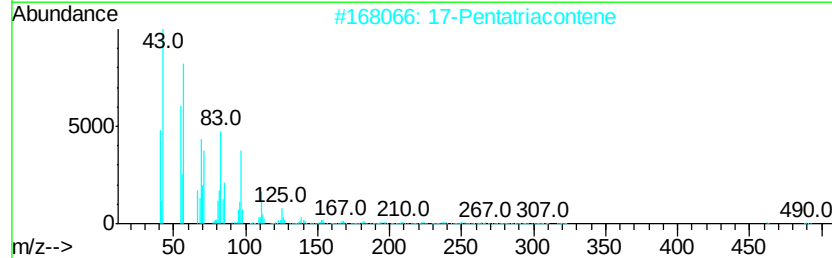
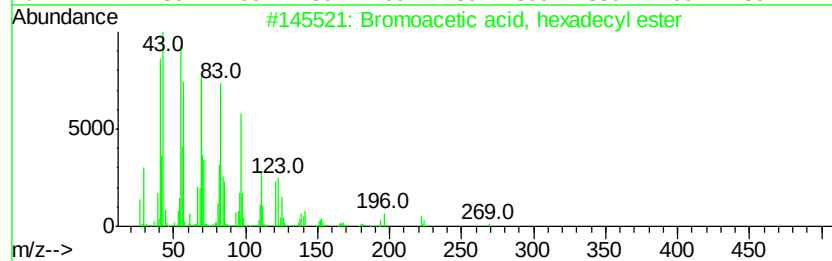
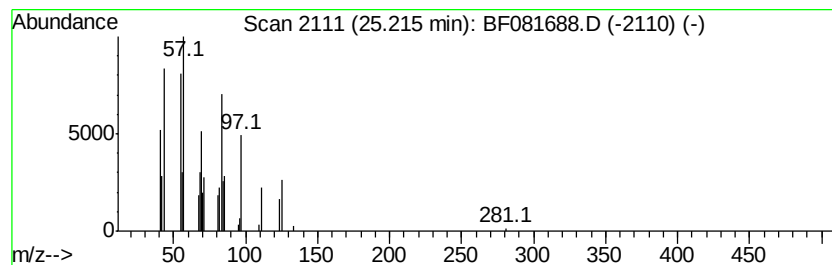
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Bromoacetic acid, hexadecyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
25.21	2.35 ng	27579	Perylene-d12	24.78		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	64
2		17-Pentatriacontene	491	C35H70	006971-40-0	64
3		Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	59
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	59
5		1-Hexadecanol	242	C16H34O	036653-82-4	59



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Operator : UM/IZ
Sample : G3620-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

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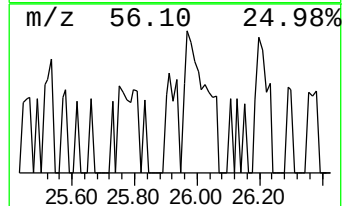
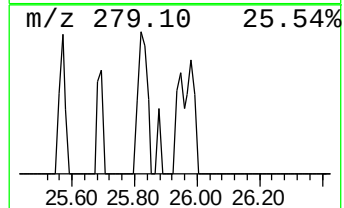
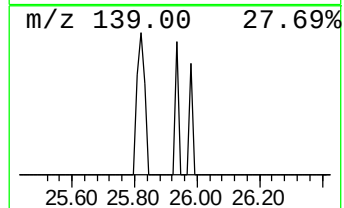
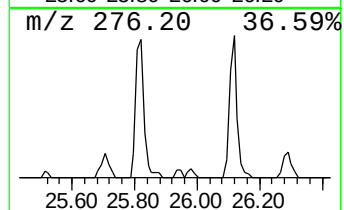
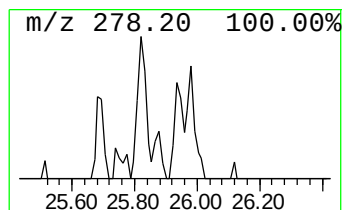
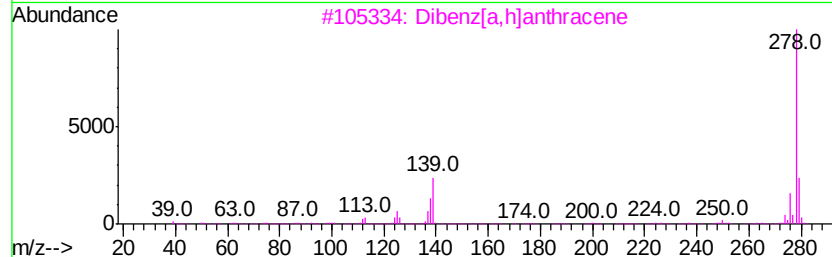
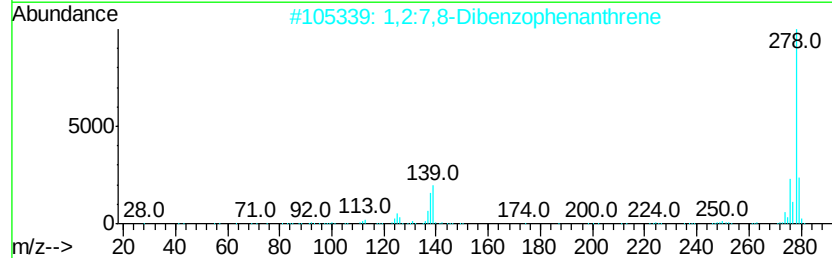
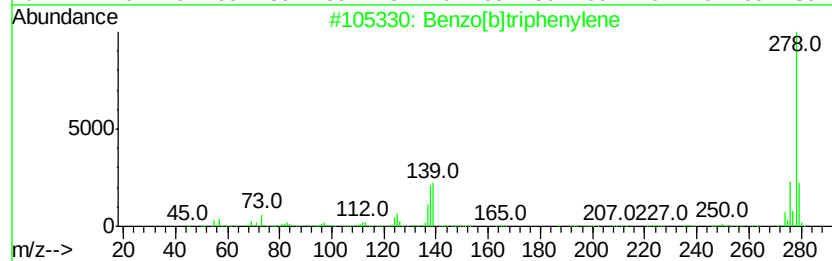
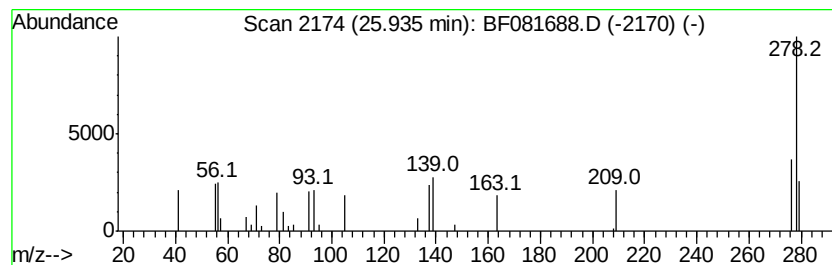
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown25.93 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.93	2.08 ng	24403	Perylene-d12	24.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]triphenylene	278	C22H14	000215-58-7	38
2		1,2:7,8-Dibenzophenanthrene	278	C22H14	000213-46-7	38
3		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	32
4		6-(Adamantyl-1)naphthol-2	278	C20H22O	037436-35-4	27
5		1H-1,4-Benzodiazepine-2,5-dione,...	278	C17H14N2O2	031965-37-4	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
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Acq On : 17 Sep 2015 20:43
Operator : UM/IZ
Sample : G3620-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.26	81.3	ng	1271220	1	8.17	312871	20.0
2-Pentanone, 4-hy...	4.48	70.5	ng	1103690	1	8.17	312871	20.0
unknown7.69	7.69	122.8	ng	1921210	1	8.17	312871	20.0
Hexadecane	17.74	2.3	ng	49707	4	18.70	427642	20.0
unknown20.36	20.36	3.3	ng	69387	4	18.70	427642	20.0
Tridecanoic acid	20.46	8.6	ng	183437	4	18.70	427642	20.0
Nonadecane	24.61	4.4	ng	52088	6	24.78	234432	20.0
Bromoacetic acid,...	25.21	2.4	ng	27579	6	24.78	234432	20.0
unknown25.93	25.93	2.1	ng	24403	6	24.78	234432	20.0