

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080318\
 Data File : BF107949.D
 Acq On : 3 Aug 2018 20:27
 Operator : JU/SJ
 Sample : J4318-03 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BEEBEE-SITE-DEMO-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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	5.178	479	483	493	rBV	20951	40241	3.67%	0.368%
2	5.660	558	565	566	rBV3	10953	17609	1.60%	0.161%
3	6.660	724	735	745	rBV3	35701	181079	16.50%	1.654%
4	6.748	745	750	765	rVV	83786	299453	27.29%	2.736%
5	6.954	782	785	808	rBV	209594	577613	52.64%	5.277%
6	7.107	808	811	830	rVB	147326	314868	28.70%	2.877%
7	7.572	881	890	901	rBV5	27141	133402	12.16%	1.219%
8	8.236	999	1003	1030	rBV	386321	889624	81.08%	8.127%
9	9.307	1182	1185	1206	rBV	207558	451805	41.18%	4.128%
10	9.989	1297	1301	1324	rBV	693812	914137	83.31%	8.351%
11	10.795	1434	1438	1449	rBV2	78765	167882	15.30%	1.534%
12	10.901	1454	1456	1460	rVB2	10668	13564	1.24%	0.124%
13	11.489	1552	1556	1572	rBV	468105	884402	80.60%	8.080%
14	12.007	1638	1644	1645	rBV6	16477	27567	2.51%	0.252%
15	12.030	1645	1648	1650	rVB	17039	19518	1.78%	0.178%
16	12.107	1656	1661	1665	rBV7	16814	30465	2.78%	0.278%
17	12.266	1685	1688	1690	rBV3	12153	15495	1.41%	0.142%
18	12.542	1732	1735	1738	rBV4	14541	14608	1.33%	0.133%
19	12.642	1748	1752	1753	rBV3	20621	22513	2.05%	0.206%
20	12.707	1759	1763	1770	rBV	169902	250012	22.78%	2.284%
21	12.836	1783	1785	1787	rBV3	10996	12065	1.10%	0.110%
22	12.942	1796	1803	1806	rBV	145477	218900	19.95%	2.000%
23	13.071	1821	1825	1836	rBV	289963	532691	48.55%	4.866%
24	13.160	1836	1840	1843	rVV2	251941	383382	34.94%	3.502%
25	13.201	1843	1847	1849	rVV2	209485	333157	30.36%	3.044%
26	13.224	1849	1851	1855	rVV	184887	247612	22.57%	2.262%
27	13.283	1855	1861	1867	rVV5	231707	604892	55.13%	5.526%
28	13.336	1867	1870	1875	rVV	293126	396407	36.13%	3.621%
29	13.377	1875	1877	1889	rVB	203262	316753	28.87%	2.894%
30	13.613	1915	1917	1920	rBV3	20280	21269	1.94%	0.194%
31	13.948	1971	1974	1979	rBV3	37838	43308	3.95%	0.396%
32	14.048	1989	1991	1994	rBV2	45937	55624	5.07%	0.508%
33	14.083	1994	1997	2000	rVB	172867	146424	13.34%	1.338%
34	14.142	2003	2007	2017	rVV2	625613	1097267	100.00%	10.024%

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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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.248	2022	2025	2031	rVB3	101930	167804	15.29%	1.533%
36	15.230	2187	2192	2200	rVB3	93730	223008	20.32%	2.037%
37	15.542	2241	2245	2250	rBV	53073	104057	9.48%	0.951%
38	15.671	2263	2267	2279	rVB	405213	775632	70.69%	7.086%

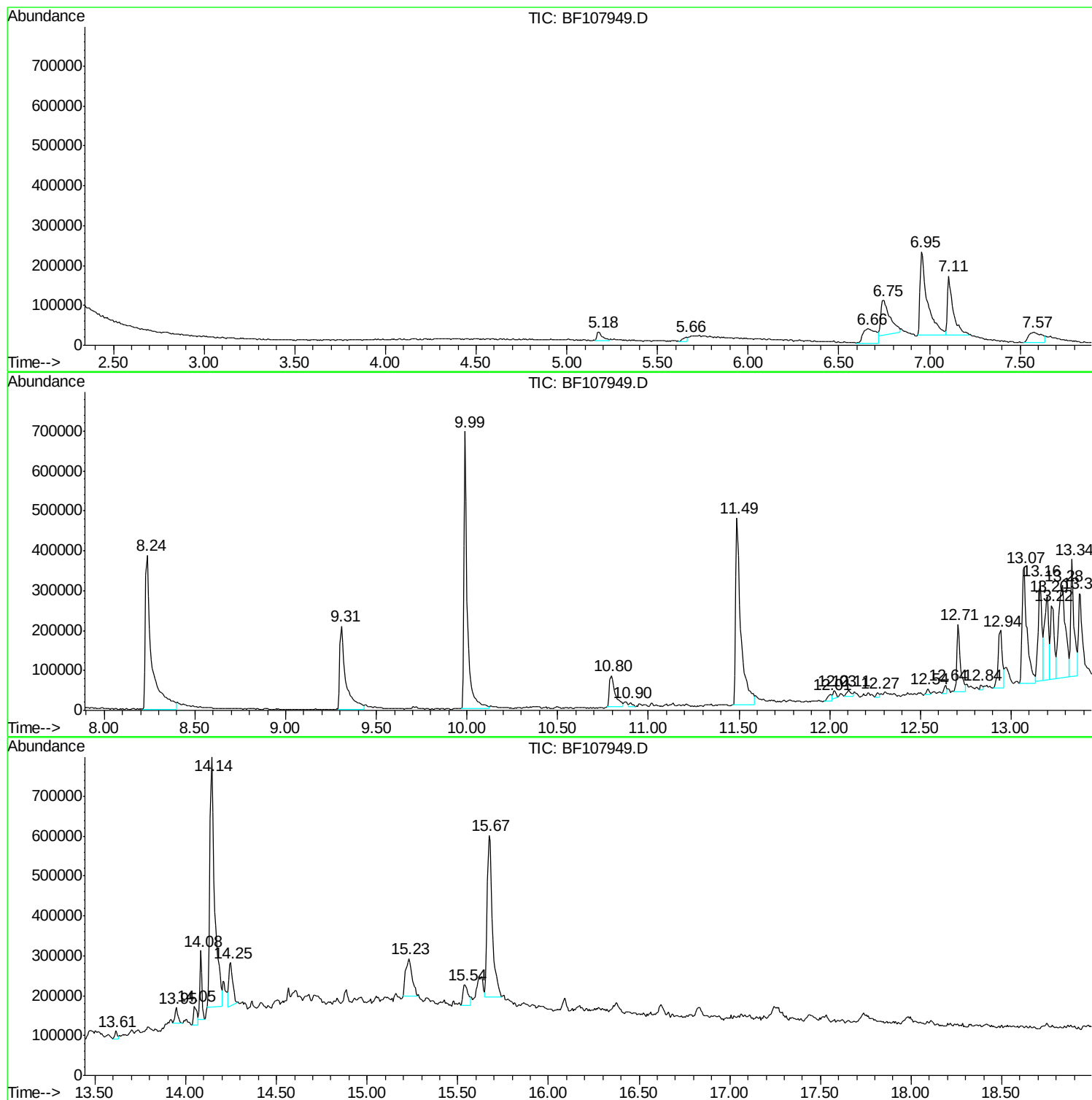
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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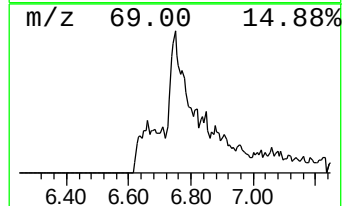
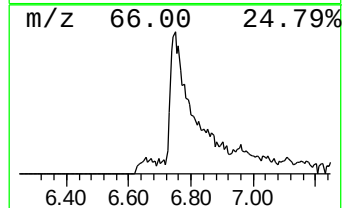
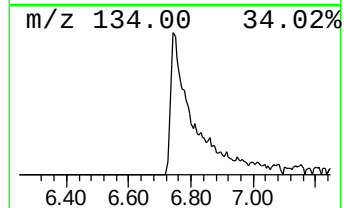
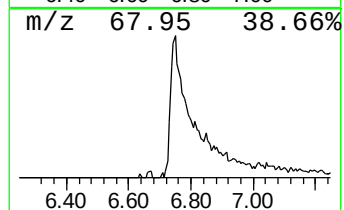
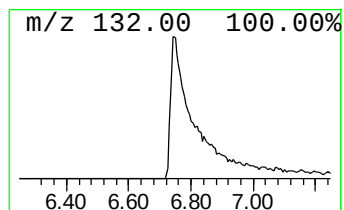
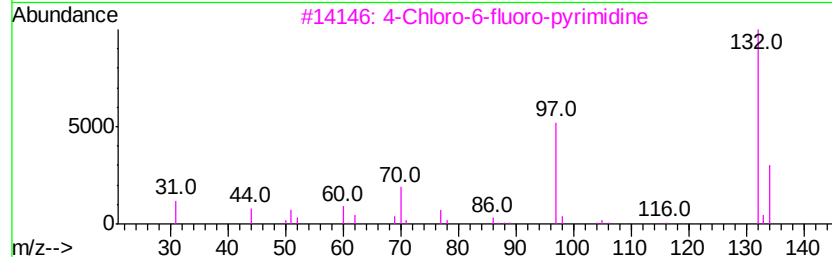
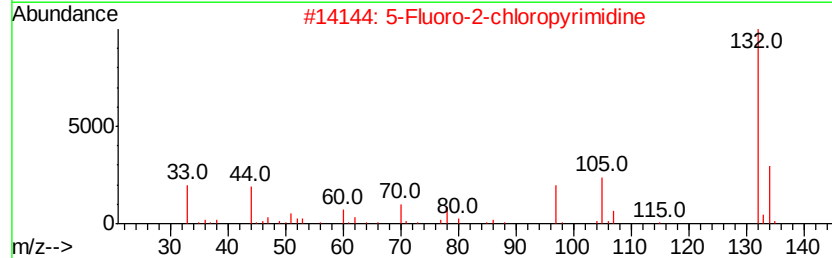
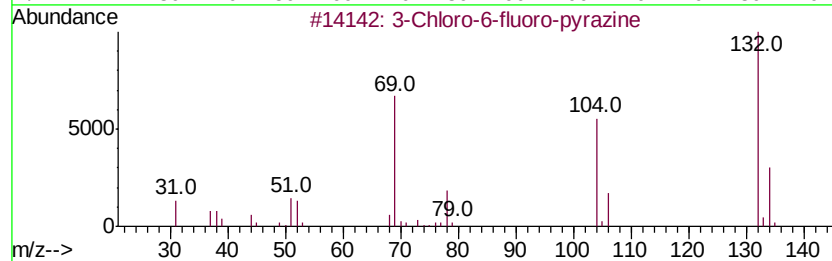
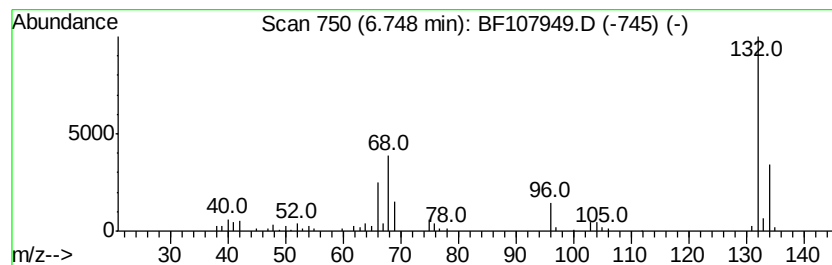
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.75 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	10.37 ng	299453	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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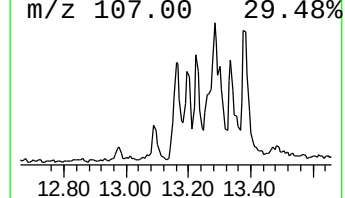
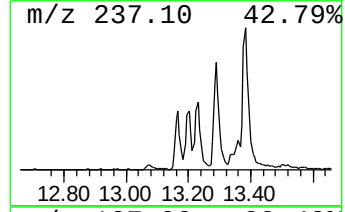
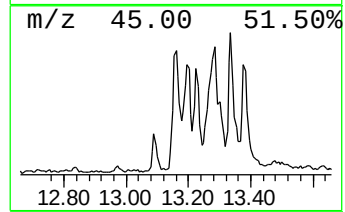
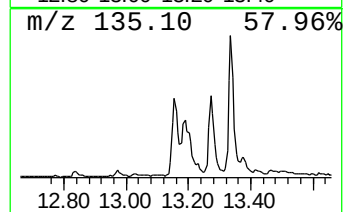
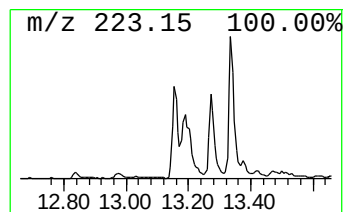
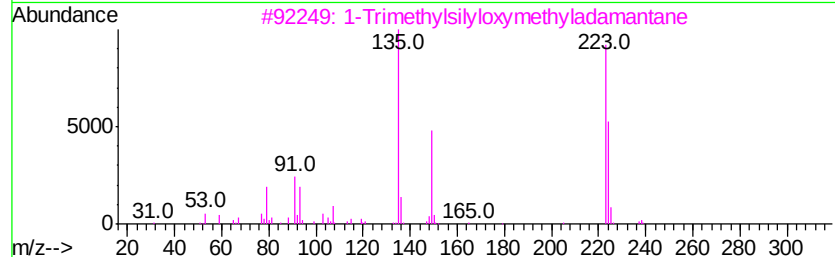
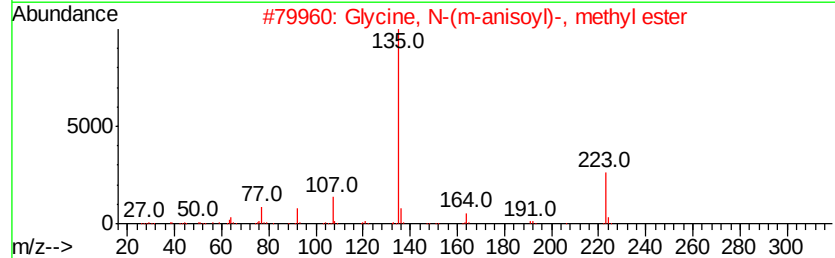
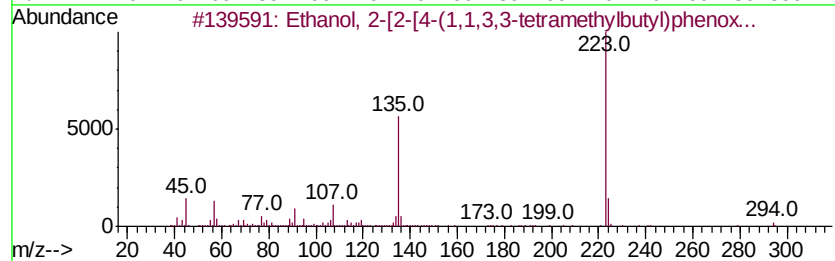
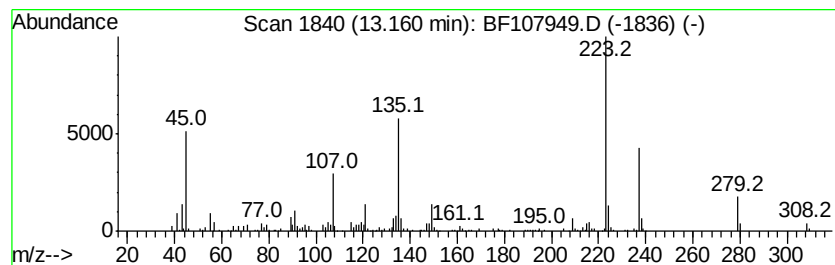
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.16	6.99 ng	383382	Chrysene-d12	14.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	46
2	Glycine, N-(m-anisoyl)-, methyl ...	223	C11H13NO4	1000299-70-7	38
3	1-Trimethylsilyloxymethyladamantane	238	C14H26OSi	079671-68-4	32
4	5-Acetonvl-5-(2-bromo-2-propenyl...	302	C10H11BrN2O4	021248-31-7	27
5	9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	22



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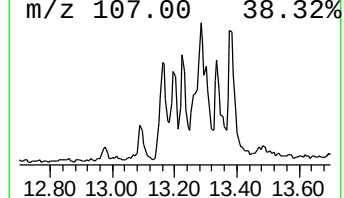
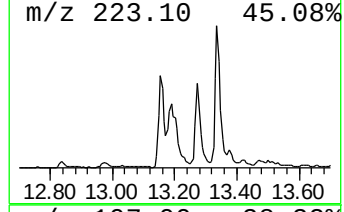
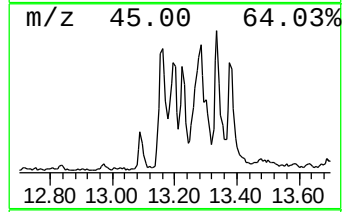
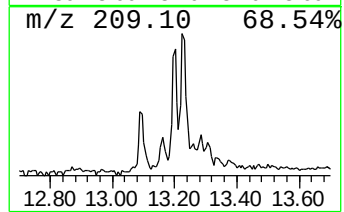
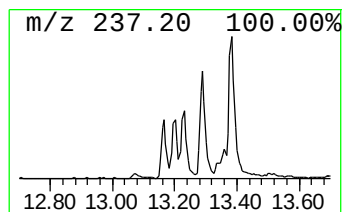
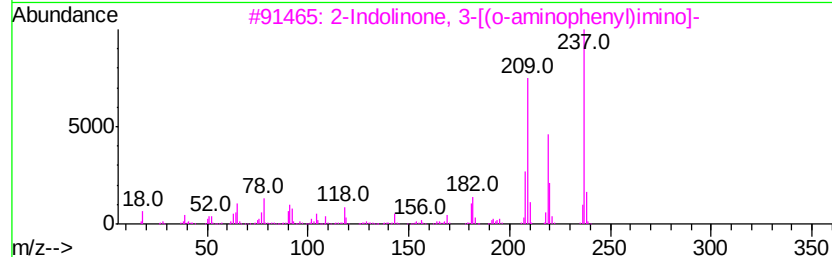
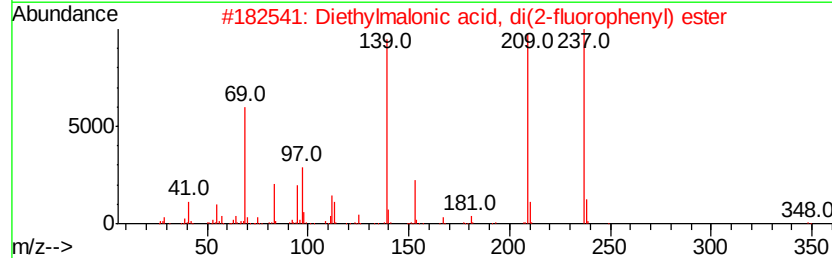
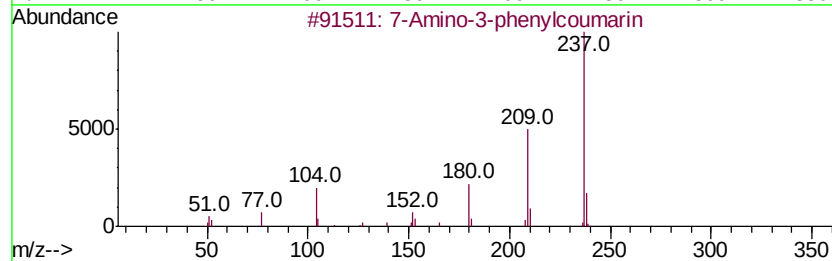
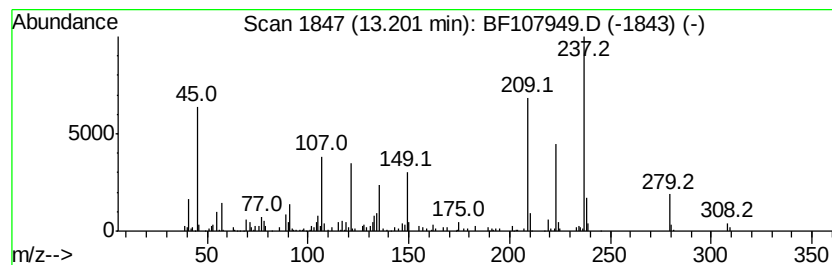
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown13.20 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	6.07 ng	333157	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Amino-3-phenylcoumarin	237	C15H11NO2	004108-61-6	43
2		Diethylmalonic acid, di(2-fluoro...	348	C19H18F2O4	1000370-14-3	35
3		2-Indolinone, 3-[(o-aminophenyl)...]	237	C14H11N3O	033829-08-2	35
4		Thieno[2,3-d]pyrimidine-6-carbon...	237	C8H7N5S2	1000311-13-6	35
5		2H-Indol-2-one, 3-[(4-aminopheny...	237	C14H11N3O	033829-07-1	35



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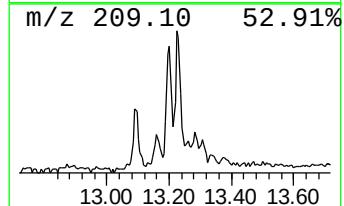
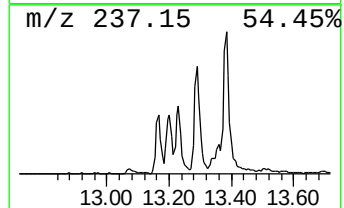
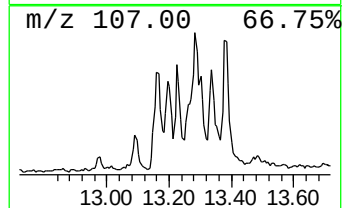
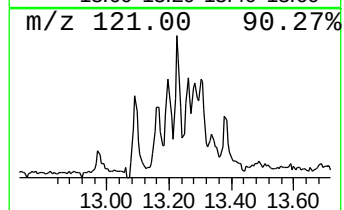
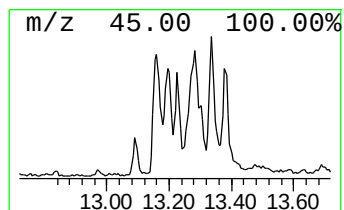
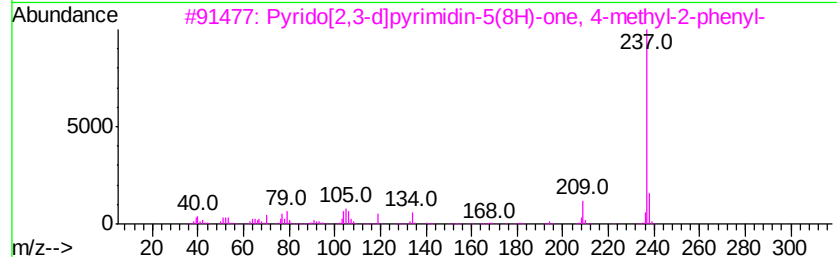
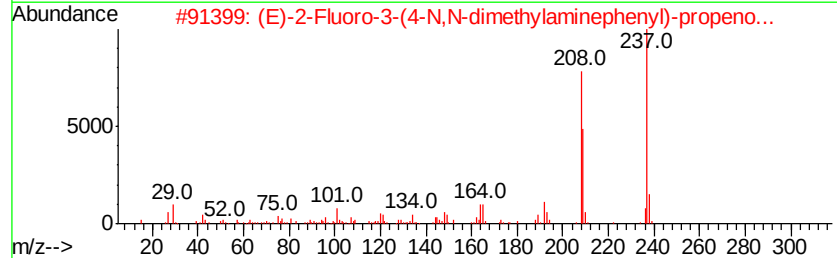
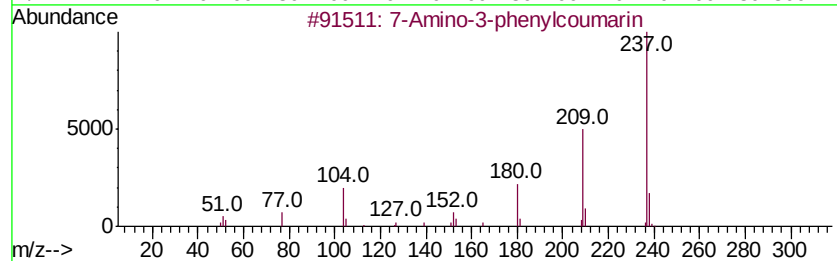
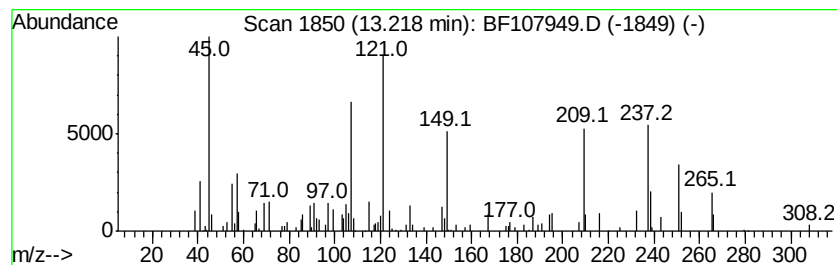
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Peak Number 5 unknown13.22 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.22	4.51 ng	247612	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Amino-3-phenylcoumarin	237	C15H11N02	004108-61-6	27
2		(E)-2-Fluoro-3-(4-N,N-dimethylam...	237	C13H16FN02	110915-65-6	25
3		Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	11
4		1-(2-Phenoxyethyl)-1H-indole	237	C16H15NO	1000322-52-5	10
5		2-Amino-10-oxo-10H-9-oxa-1-aza-a...	237	C13H7N3O2	061424-81-5	10



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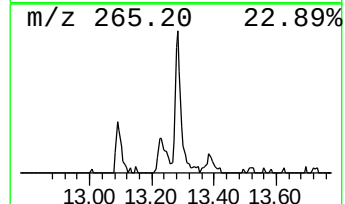
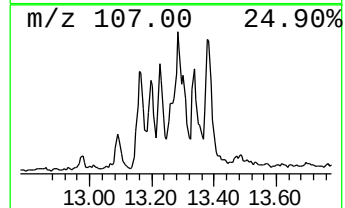
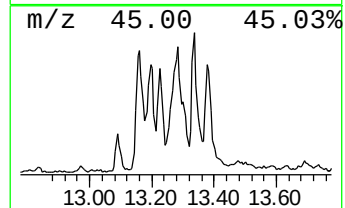
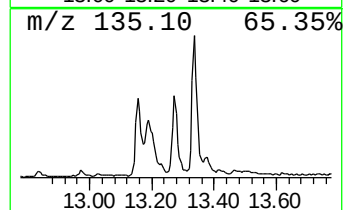
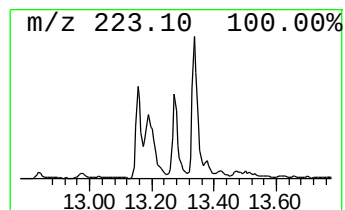
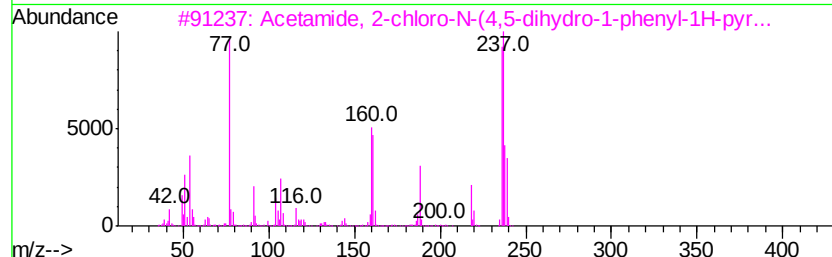
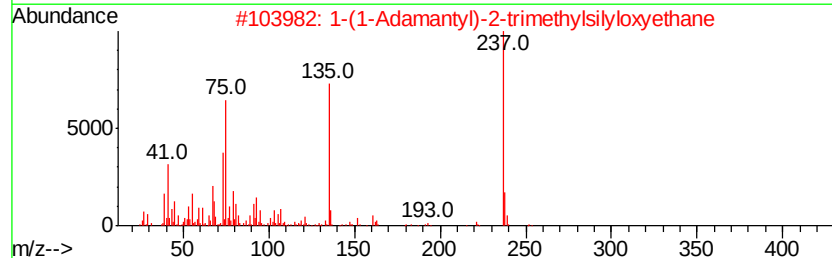
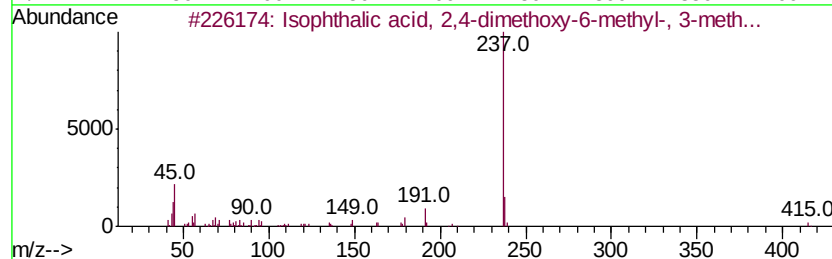
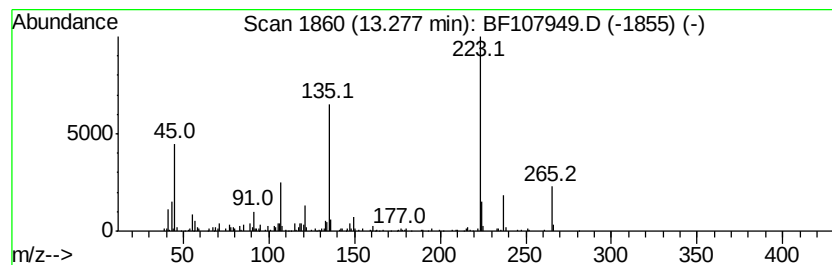
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Peak Number 6 unknown13.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	11.03 ng	604892	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isophthalic acid, 2,4-dimethoxyv-...	446	C23H26O9	019314-77-3	25
2		1-(1-Adamantyl)-2-trimethylsilyl...	252	C15H28OSi	1000283-09-0	25
3		Acetamide, 2-chloro-N-(4,5-dihyd...	237	C11H12ClN3O	1000337-23-3	22
4		2,4-Diphenylthiazole	237	C15H11NS	001826-14-8	18
5		2-Benzo[1,3]dioxol-5-yl-indolizine	237	C15H11NO2	1000301-42-4	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107949.D
Acq On : 3 Aug 2018 20:27
Operator : JU/SJ
Sample : J4318-03 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

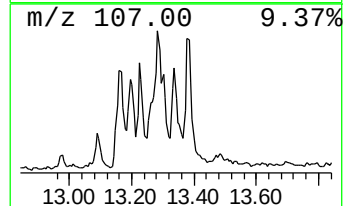
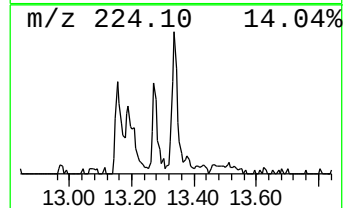
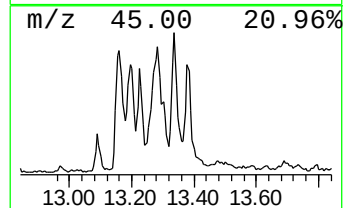
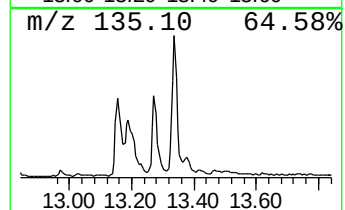
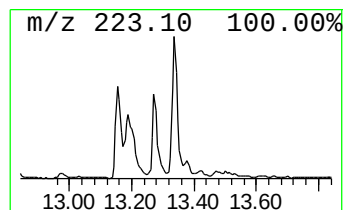
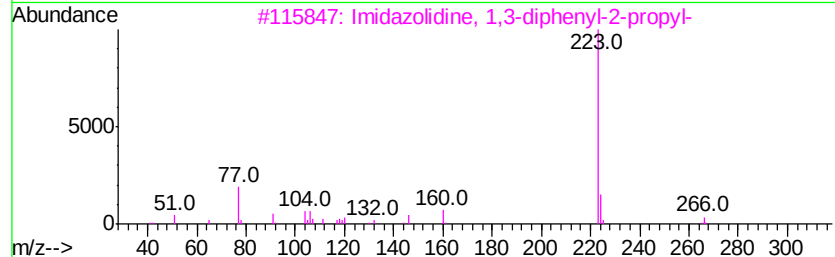
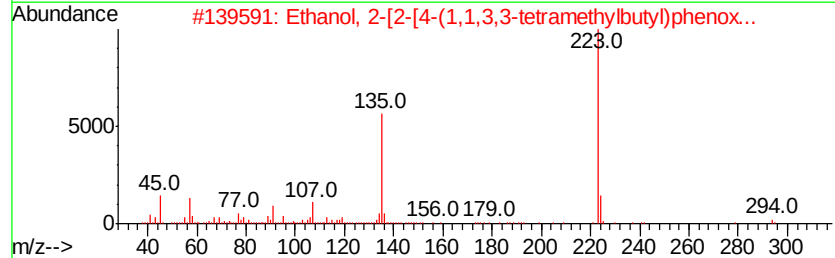
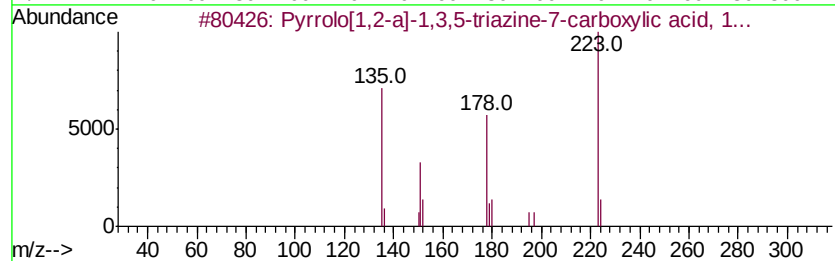
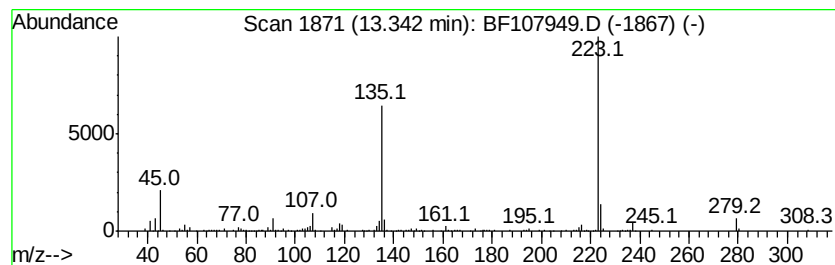
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.34	7.23 ng	396407	Chrysene-d12		14.14		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	86
2			Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	38
3			Imidazolidine, 1,3-diphenyl-2-pr...	266	C18H22N2	055320-82-6	32
4			Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6N02	296242-69-8	14
5			Sarcosine, N-(4-methoxybenzoyl)-...	279	C15H21N04	1000321-42-1	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107949.D
Acq On : 3 Aug 2018 20:27
Operator : JU/SJ
Sample : J4318-03 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

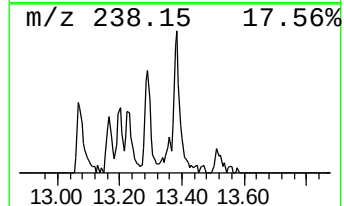
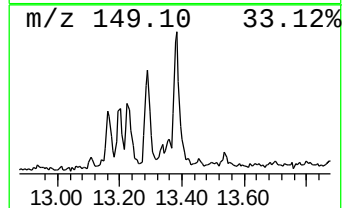
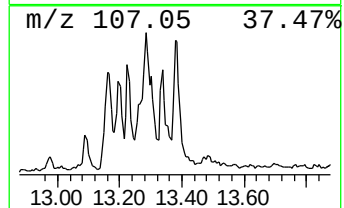
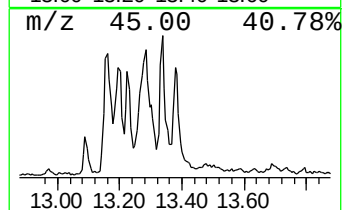
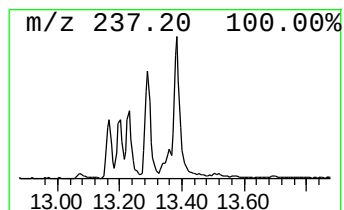
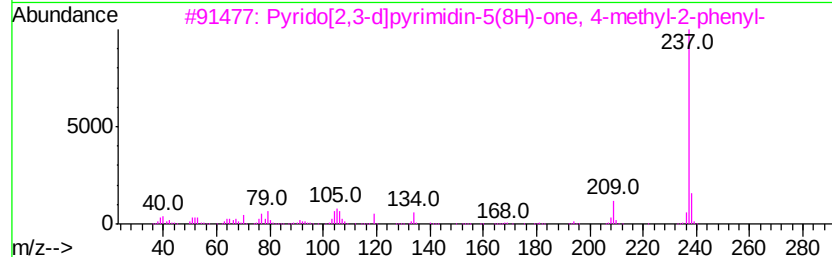
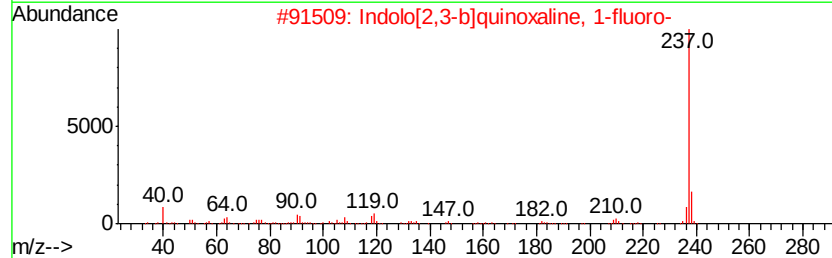
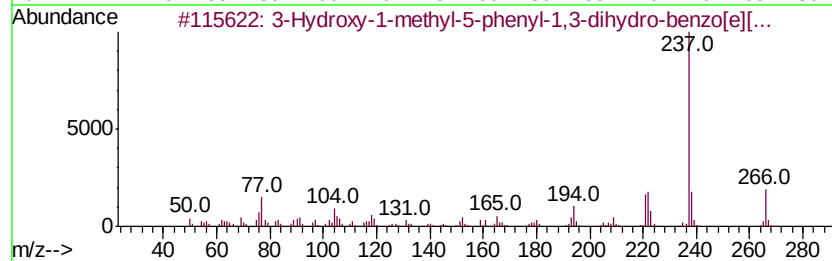
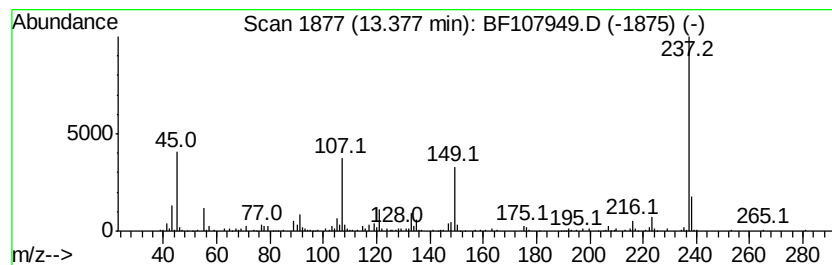
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.38 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.38	5.77 ng	316753	Chrysene-d12	14.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hydroxy-1-methyl-5-phenyl-1,3-...	266	C16H14N2O2	025177-93-9	40
2	Indolo[2,3-b]quinoxaline, 1-fluoro-	237	C14H8FN3	296244-71-8	35
3	Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	35
4	1-(1-Adamantyl)-2-dichloromethyl...	320	C15H26Cl2OSi	1000283-10-6	17
5	2-p-Tolylisoindole-1,3-dione	237	C15H11N02	002142-03-2	17



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107949.D
Acq On : 3 Aug 2018 20:27
Operator : JU/SJ
Sample : J4318-03 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BEEBEE-SITE-DEMO-2

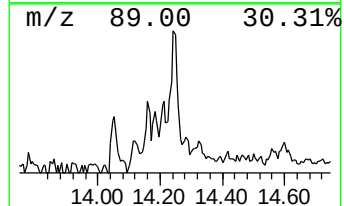
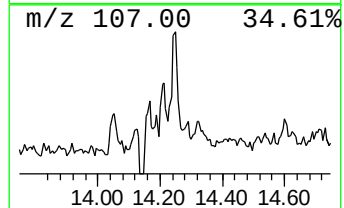
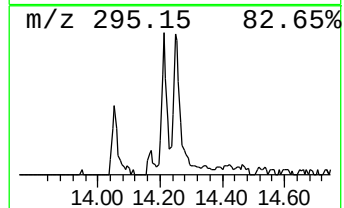
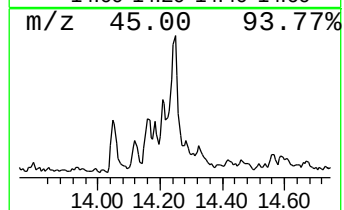
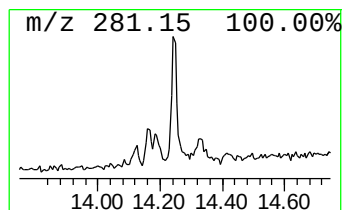
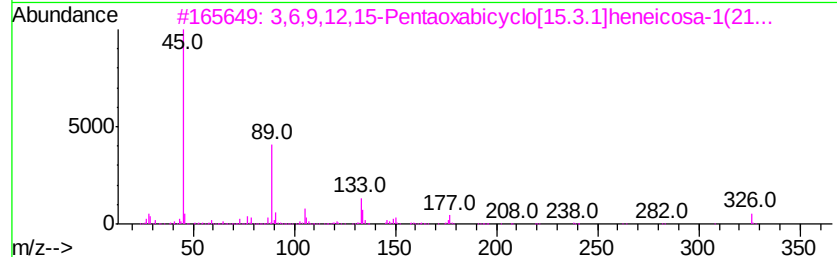
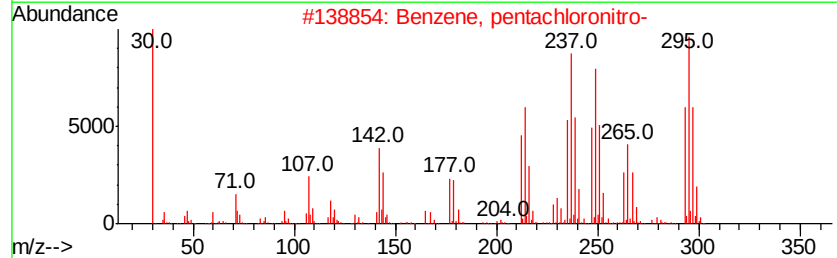
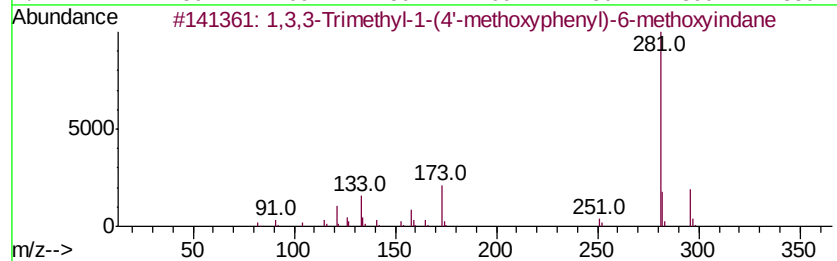
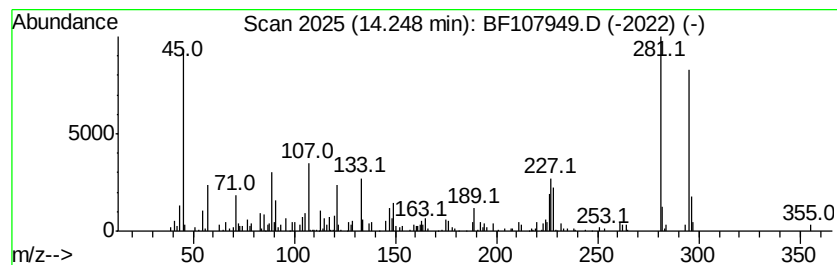
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.25 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	3.06 ng	167804	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,3-Trimethyl-1-(4'-methoxyvphe...	296	C20H24O2	108122-20-9	22
2		Benzene, pentachloronitro-	293	C6Cl5NO2	000082-68-8	15
3		3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	14
4		4-Morpholinobenzaldehyde m-tolyl...	295	C18H21N3O	300865-04-7	11
5		2,6-Di[p-cyanophenyl]-4-picoline	295	C20H13N3	1000212-46-7	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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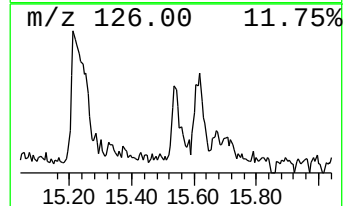
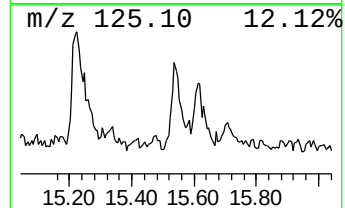
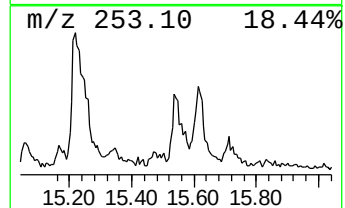
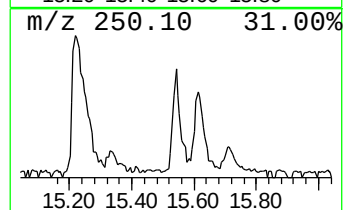
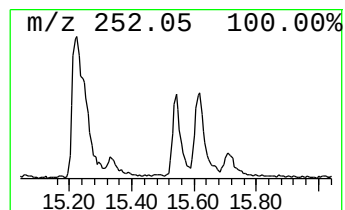
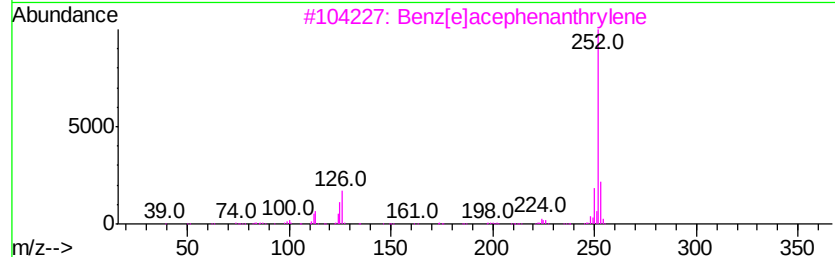
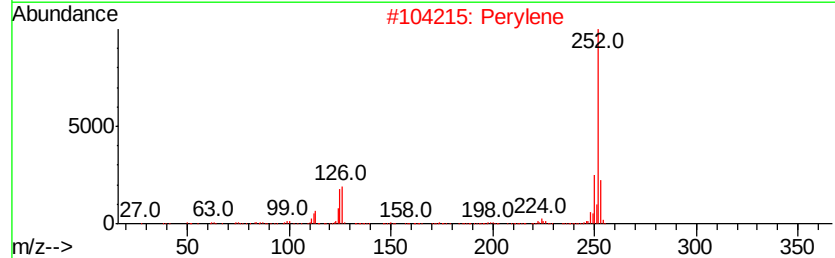
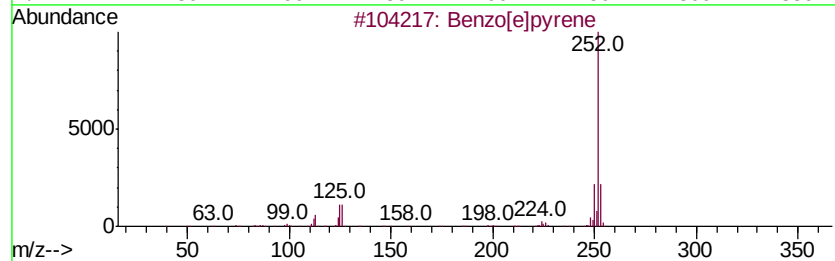
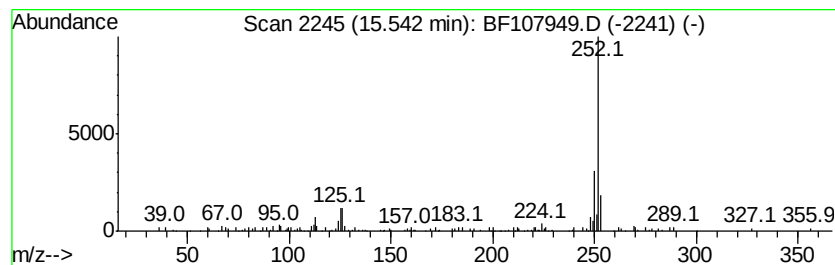
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	2.68 ng	104057	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2		Perylene	252	C20H12	000198-55-0	94
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	91
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5		Benzo[a]pyrene	252	C20H12	000050-32-8	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080318\
Data File : BF107949.D
Acq On : 3 Aug 2018 20:27
Operator : JU/SJ
Sample : J4318-03 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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
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unknown13.16	13.16	7.0	ng	383382	5	14.14	1097270	20.0
unknown13.20	13.20	6.1	ng	333157	5	14.14	1097270	20.0
unknown13.22	13.22	4.5	ng	247612	5	14.14	1097270	20.0
unknown13.28	13.28	11.0	ng	604892	5	14.14	1097270	20.0
Pyrrolo[1,2-a]-1,...	13.34	7.2	ng	396407	5	14.14	1097270	20.0
unknown13.38	13.38	5.8	ng	316753	5	14.14	1097270	20.0
unknown14.25	14.25	3.1	ng	167804	5	14.14	1097270	20.0
Benzo[e]pyrene	15.54	2.7	ng	104057	6	15.67	775632	20.0