

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
 Data File : BF100936.D
 Acq On : 28 Nov 2017 16:19
 Operator : SJ/JU
 Sample : I6579-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HAR-4-E(7-8)

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-BF110817.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	5.081	505	509	521	rBB	141842	174575	13.24%	1.225%
2	5.481	572	577	580	rBV	1229520	1153494	87.49%	8.096%
3	6.487	743	748	751	rBV	1170954	1200210	91.03%	8.424%
4	6.628	768	772	775	rBV	1413960	1226949	93.06%	8.611%
5	6.857	808	811	815	rBV	436664	338126	25.65%	2.373%
6	7.016	834	838	841	rBV	1132767	942539	71.49%	6.615%
7	7.422	902	907	910	rBV	836729	729492	55.33%	5.120%
8	8.139	1025	1029	1031	rBV	542262	425791	32.29%	2.988%
9	8.157	1031	1032	1036	rVB	39630	29903	2.27%	0.210%
10	8.692	1120	1123	1126	rBV	69301	53731	4.08%	0.377%
11	9.216	1207	1212	1215	rBV	1527119	1318463	100.00%	9.254%
12	9.604	1275	1278	1285	rVB2	54632	60015	4.55%	0.421%
13	9.757	1300	1304	1307	rBV	177326	145384	11.03%	1.020%
14	9.892	1319	1327	1331	rBV2	493555	444407	33.71%	3.119%
15	10.098	1355	1362	1366	rVB2	15158	16263	1.23%	0.114%
16	10.345	1402	1404	1408	rBV	19090	16194	1.23%	0.114%
17	10.439	1418	1420	1425	rBV2	10592	15815	1.20%	0.111%
18	10.604	1445	1448	1455	rVB	261426	215997	16.38%	1.516%
19	10.680	1457	1461	1472	rVB	697615	669102	50.75%	4.696%
20	10.786	1476	1479	1481	rBV3	13664	15707	1.19%	0.110%
21	11.380	1577	1580	1582	rBV	439451	364004	27.61%	2.555%
22	11.404	1582	1584	1590	rVB	146787	112227	8.51%	0.788%
23	11.457	1590	1593	1596	rVB	60935	49403	3.75%	0.347%
24	11.492	1596	1599	1601	rBV	16614	15425	1.17%	0.108%
25	11.880	1661	1665	1666	rBV2	21681	18684	1.42%	0.131%
26	11.898	1666	1668	1675	rVB2	35438	46267	3.51%	0.325%
27	11.957	1675	1678	1681	rBV	17244	15278	1.16%	0.107%
28	11.992	1681	1684	1687	rBV2	32137	37010	2.81%	0.260%
29	12.427	1754	1758	1760	rBV4	21570	23919	1.81%	0.168%
30	12.516	1770	1773	1777	rVB2	14192	17549	1.33%	0.123%
31	12.592	1783	1786	1789	rBV	232540	192544	14.60%	1.351%
32	12.686	1799	1802	1806	rBV	66564	65378	4.96%	0.459%
33	12.763	1813	1815	1820	rVB	31783	27544	2.09%	0.193%
34	12.821	1820	1825	1829	rBV	210608	211591	16.05%	1.485%

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HAR-4-E(7-8)

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35	12.963	1845	1849	1852	rBV	1044821	909576	68.99%	6.384%
36	13.039	1858	1862	1866	rBV4	16472	27761	2.11%	0.195%
37	13.145	1874	1880	1884	rVB2	41164	66770	5.06%	0.469%
38	13.186	1884	1887	1889	rBV2	11849	15186	1.15%	0.107%
39	13.216	1890	1892	1894	rVB	25435	19485	1.48%	0.137%
40	13.257	1894	1899	1901	rBV2	27578	31129	2.36%	0.218%
41	13.321	1907	1910	1912	rBV2	23268	27673	2.10%	0.194%
42	13.657	1965	1967	1971	rBV	19569	22044	1.67%	0.155%
43	13.768	1984	1986	1989	rBV2	19062	15030	1.14%	0.105%
44	13.821	1993	1995	1998	rVV2	20218	26019	1.97%	0.183%
45	13.857	1998	2001	2009	rVB3	53753	83471	6.33%	0.586%
46	14.021	2024	2029	2032	rBV3	484908	591681	44.88%	4.153%
47	14.045	2032	2033	2036	rVB	127498	84583	6.42%	0.594%
48	14.127	2044	2047	2049	rBV2	29160	25940	1.97%	0.182%
49	14.168	2051	2054	2056	rVV	39859	35882	2.72%	0.252%
50	14.651	2134	2136	2143	rVB2	39737	47223	3.58%	0.331%
51	15.062	2201	2206	2214	rBV	215493	387514	29.39%	2.720%
52	15.174	2221	2225	2227	rBV	81377	84751	6.43%	0.595%
53	15.368	2254	2258	2264	rVB	128610	157713	11.96%	1.107%
54	15.433	2265	2269	2274	rVB	190334	229368	17.40%	1.610%
55	15.498	2275	2280	2283	rBV	290936	396281	30.06%	2.781%
56	16.621	2468	2471	2476	rVB8	22558	34635	2.63%	0.243%
57	16.968	2524	2530	2538	rVB2	93386	177106	13.43%	1.243%
58	17.145	2556	2560	2565	rBV3	14493	25141	1.91%	0.176%
59	17.209	2567	2571	2575	rVB5	23921	39993	3.03%	0.281%
60	17.421	2599	2607	2618	rBV	116768	256690	19.47%	1.802%
61	17.656	2642	2647	2652	rBV2	19696	40612	3.08%	0.285%

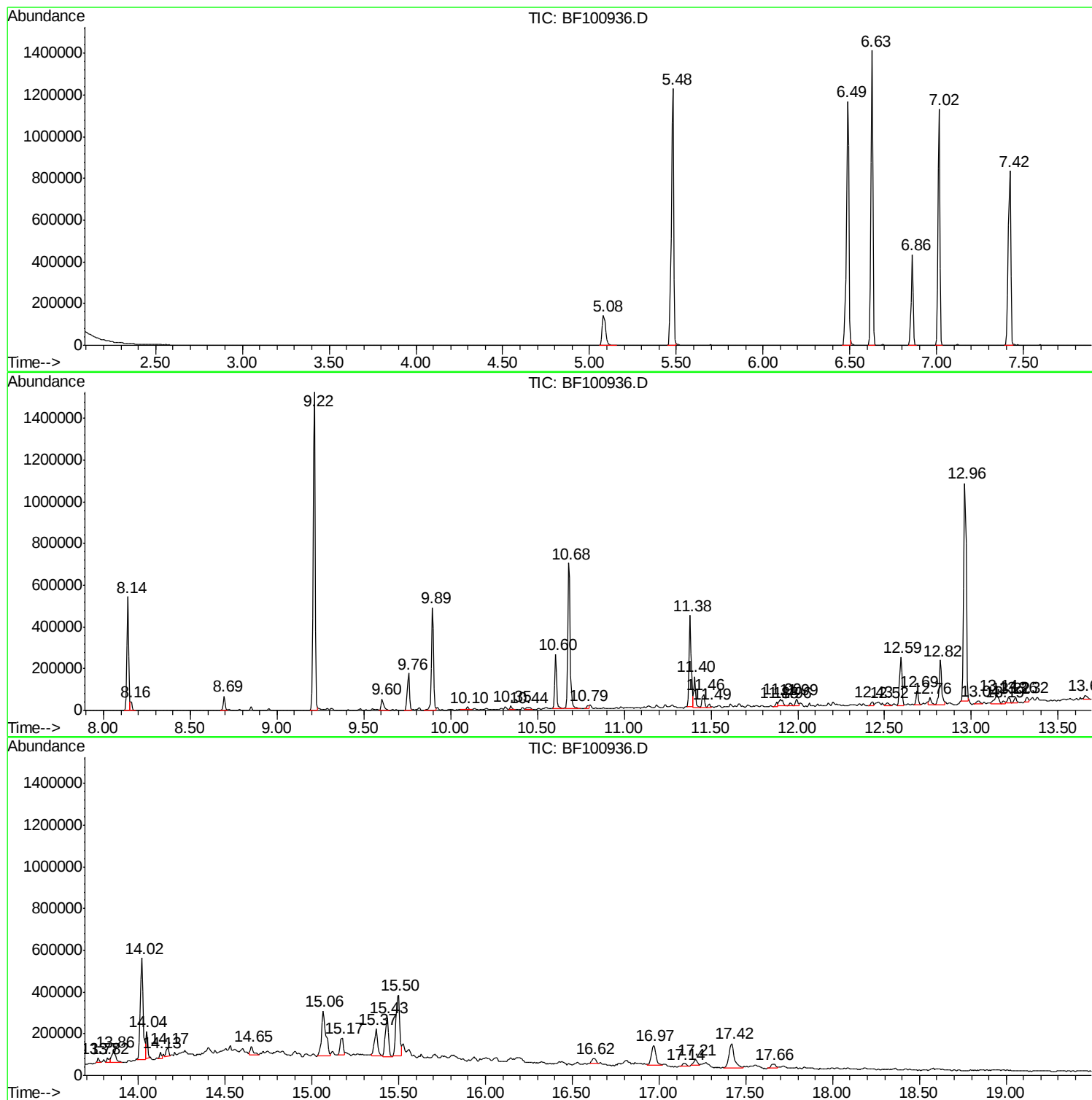
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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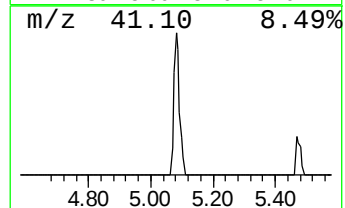
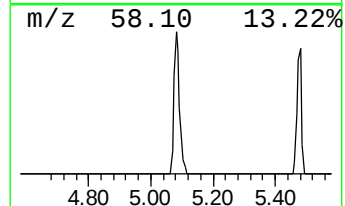
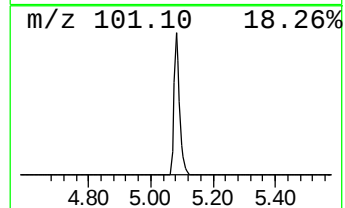
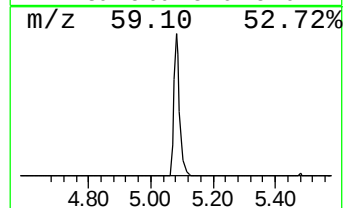
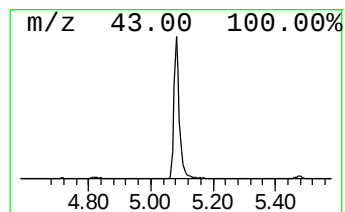
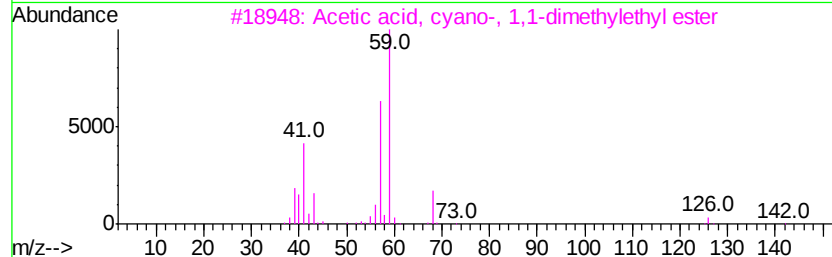
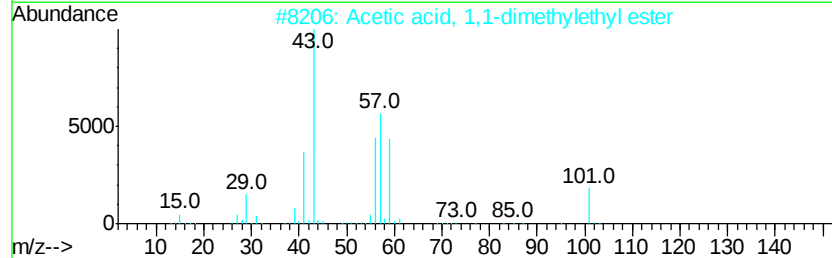
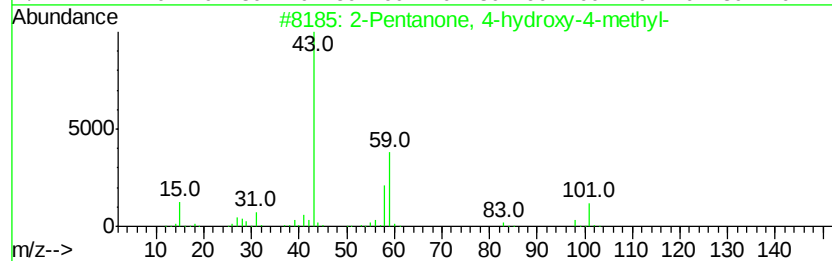
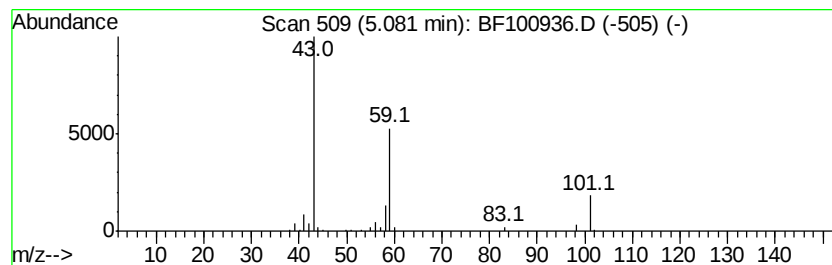
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.08	10.33 ng	174575	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
4			3-Pentanol	88	C5H12O	000584-02-1	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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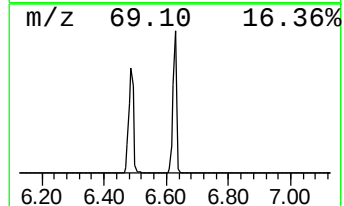
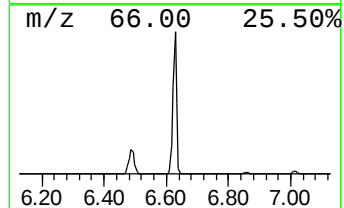
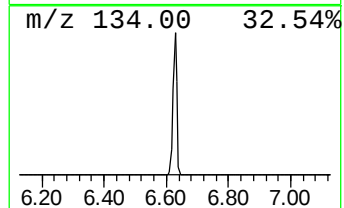
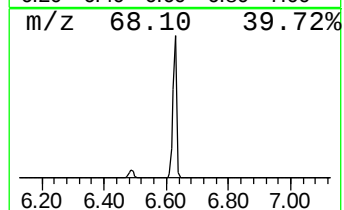
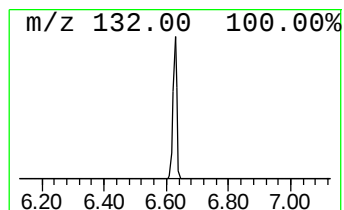
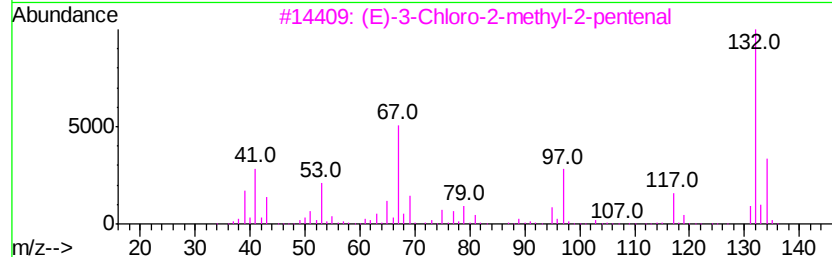
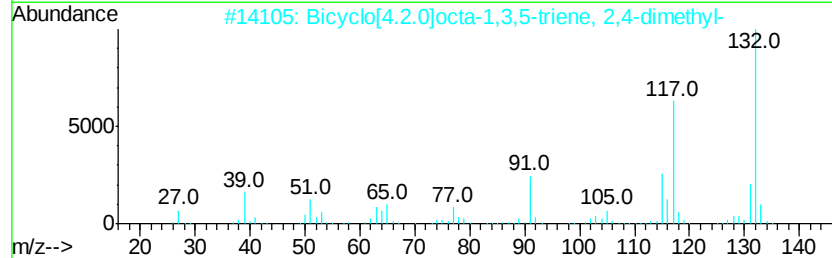
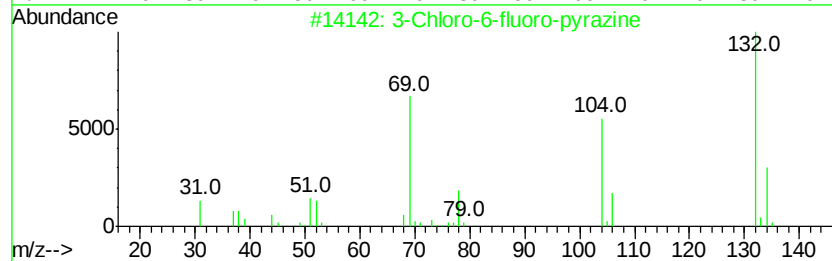
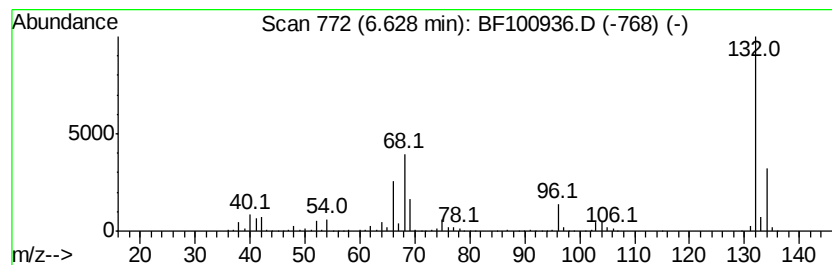
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	72.57 ng	1226950	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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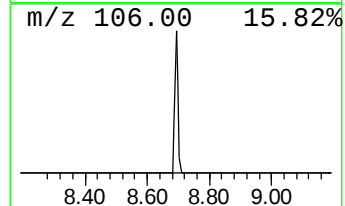
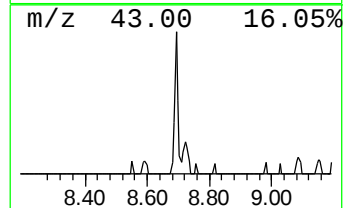
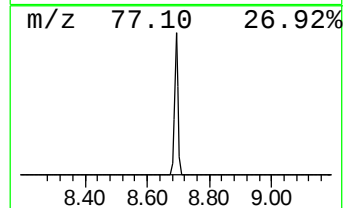
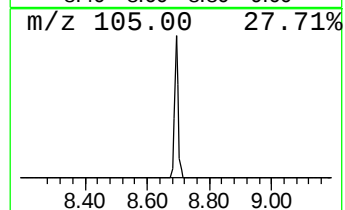
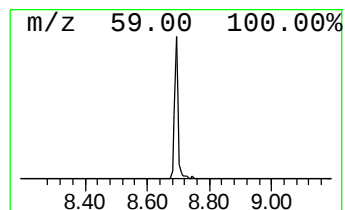
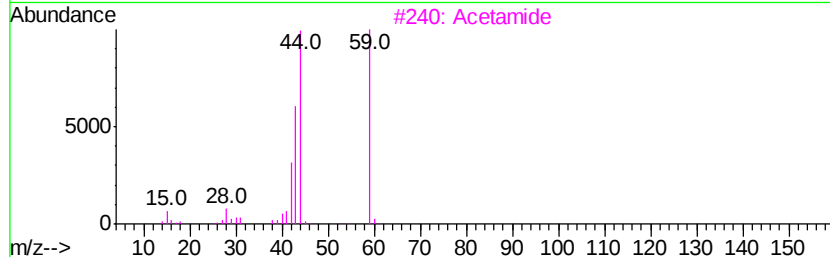
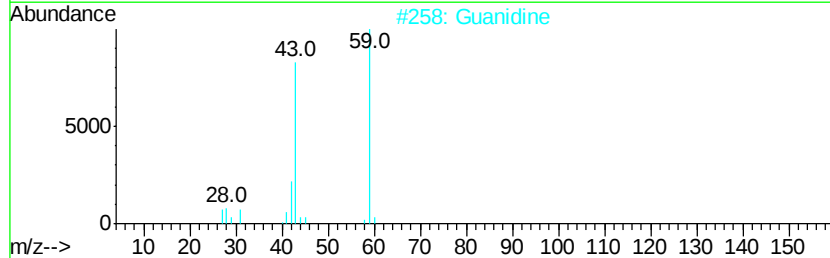
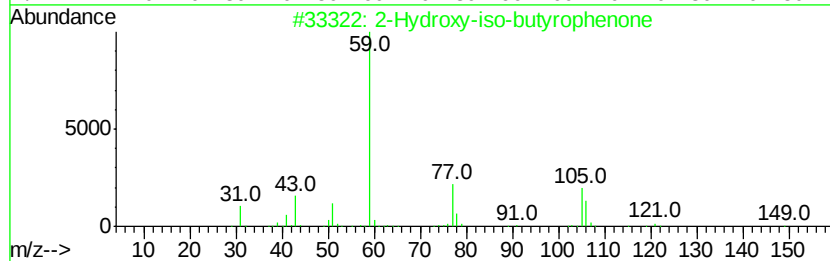
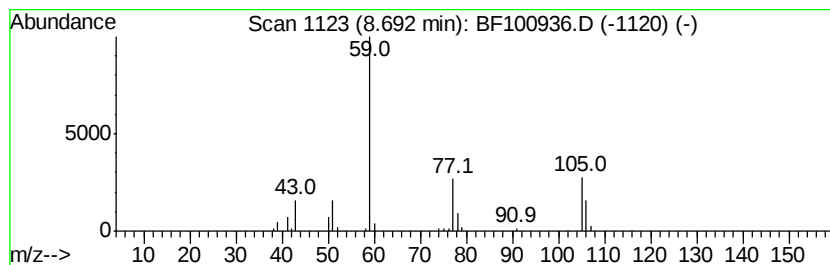
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	2.52 ng	53731	Naphthalene-d8	8.14

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2			Guanidine	59	CH5N3	000113-00-8	7
3			Acetamide	59	C2H5NO	000060-35-5	5
4			Formamide, N-methyl-	59	C2H5NO	000123-39-7	4
5			Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	4



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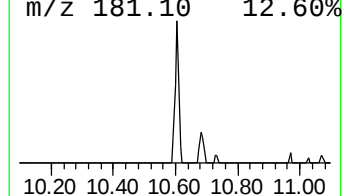
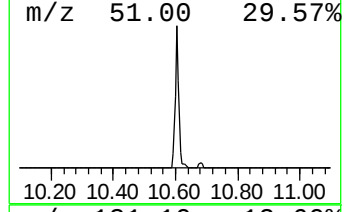
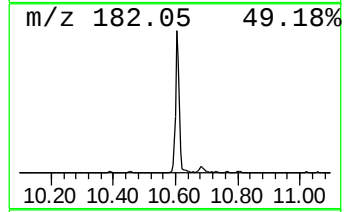
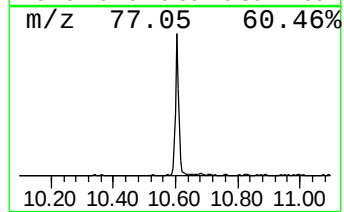
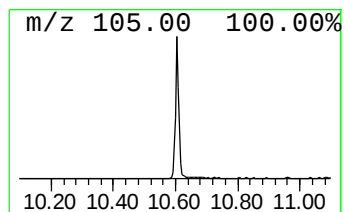
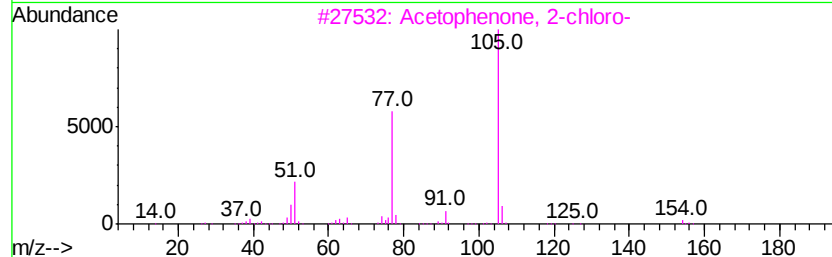
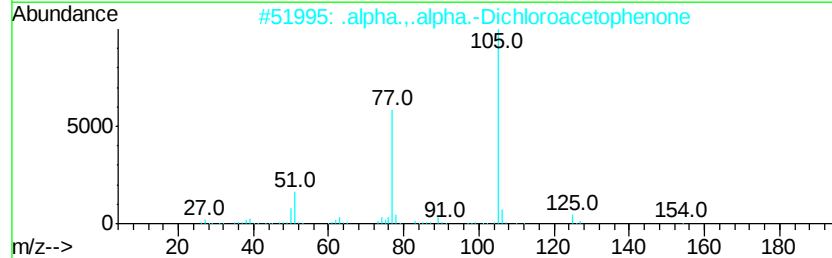
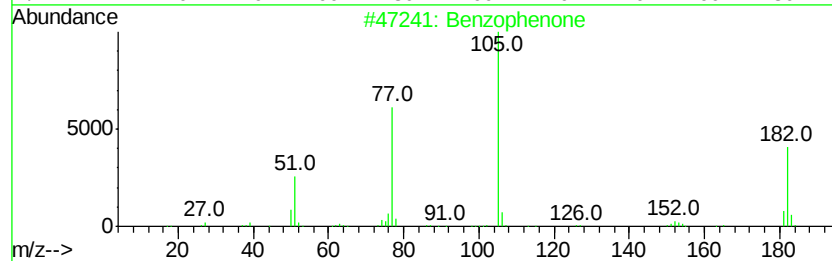
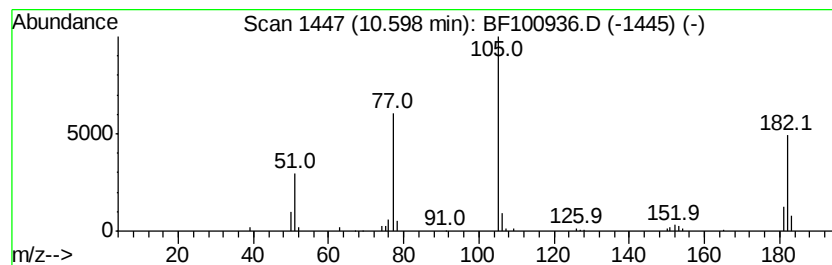
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	9.72 ng	215997	Acenaphthene-d10	9.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		.alpha.,.alpha.-Dichloroacetophe...	188 C8H6Cl2O	002648-61-5 47
3		Acetophenone, 2-chloro-	154 C8H7ClO	000532-27-4 47
4		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
5		N-Methoxy-N-methylbenzamide	165 C9H11NO2	006919-61-5 47



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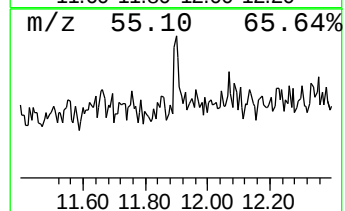
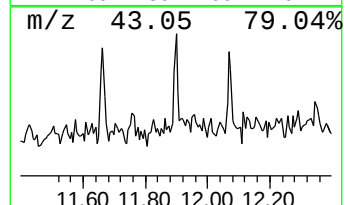
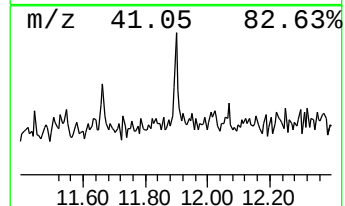
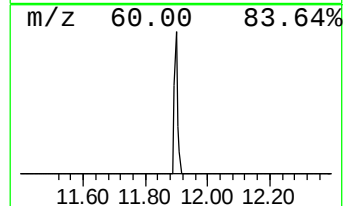
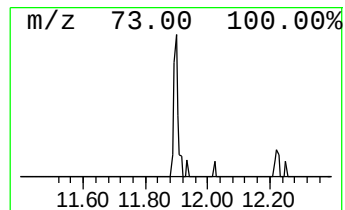
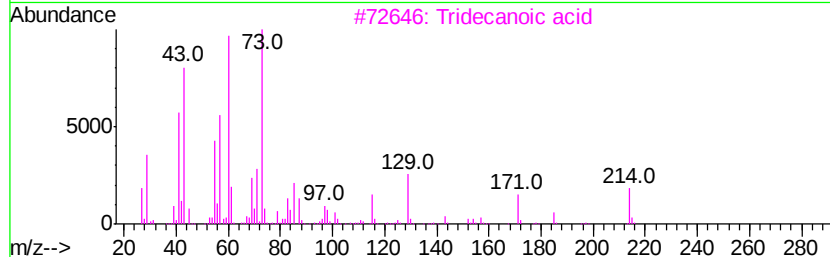
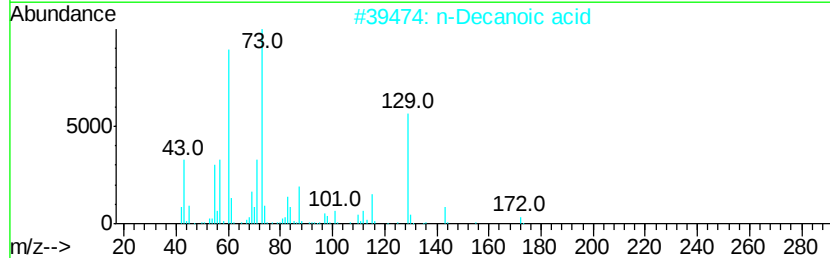
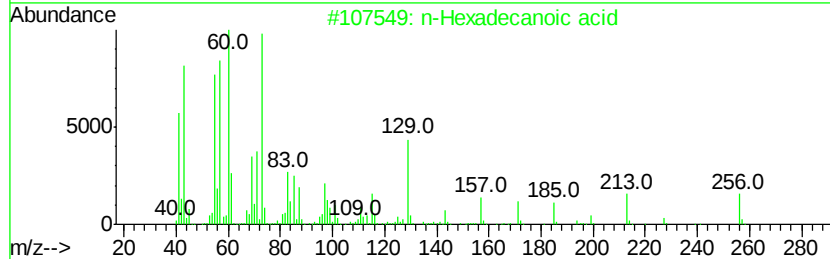
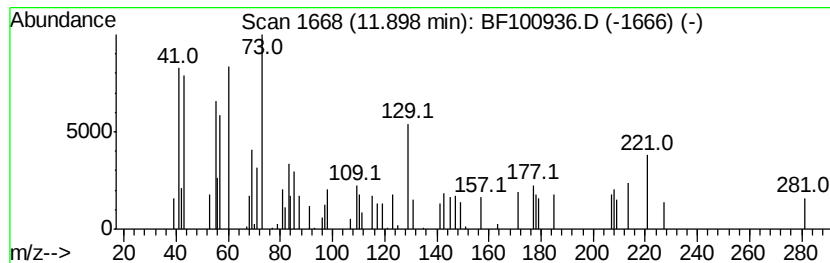
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.90 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.54 ng	46267	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	37
2		n-Decanoic acid	172	C10H20O2	000334-48-5	35
3		Tridecanoic acid	214	C13H26O2	000638-53-9	35
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	35
5		Dodecanoic acid	200	C12H24O2	000143-07-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100936.D
Acq On : 28 Nov 2017 16:19
Operator : SJ/JU
Sample : I6579-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-4-E(7-8)

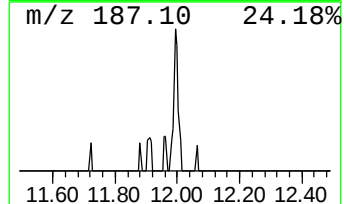
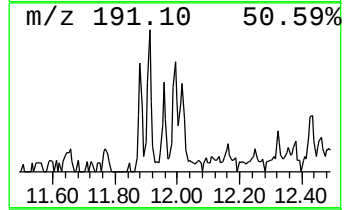
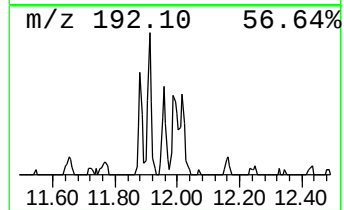
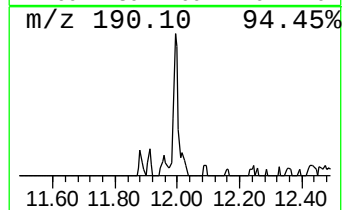
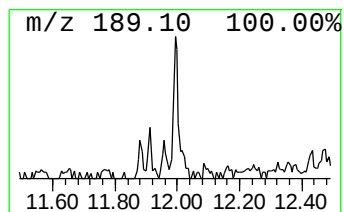
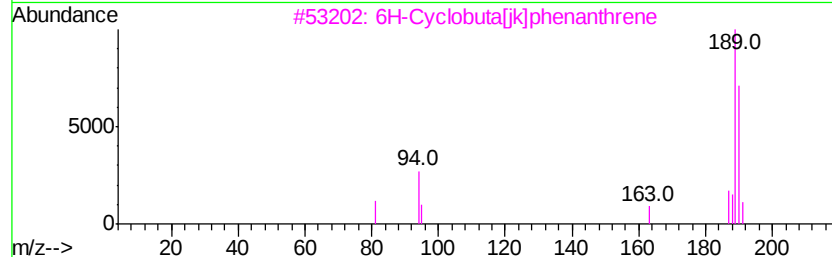
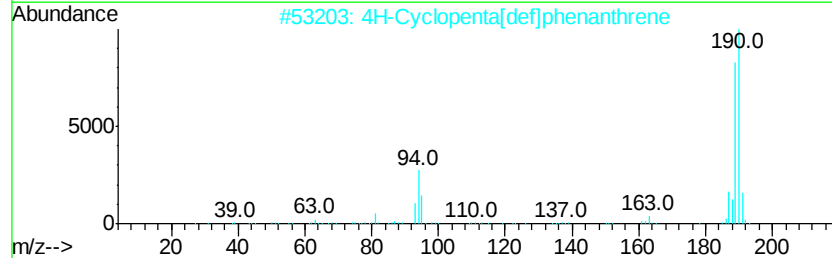
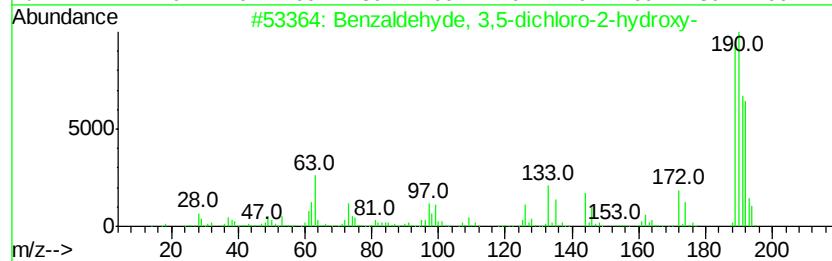
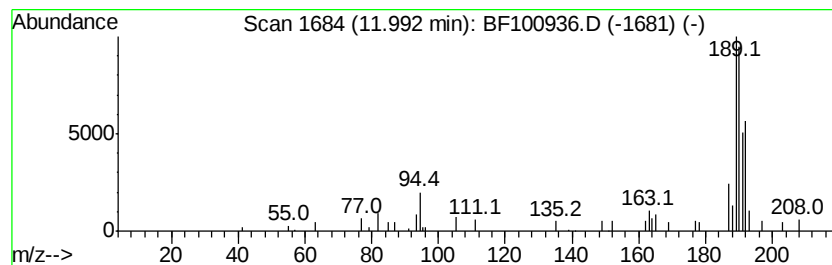
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzaldehyde, 3,5-dichloro-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.03 ng	37010	Phenanthrene-d10	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehydve, 3,5-dichloro-2-hvd...	190	C7H4Cl2O2	000090-60-8	72
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
3			6H-Cyclobuta[f]kphenanthrene	190	C15H10	083469-43-6	50
4			Methyl diselenide	190	C2H6Se2	007101-31-7	41
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100936.D
Acq On : 28 Nov 2017 16:19
Operator : SJ/JU
Sample : I6579-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

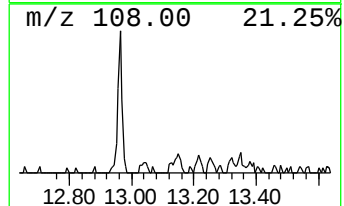
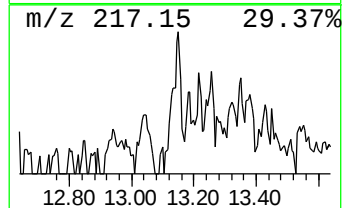
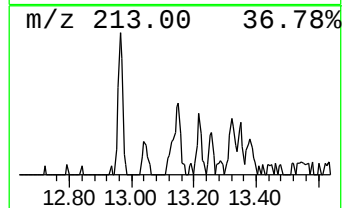
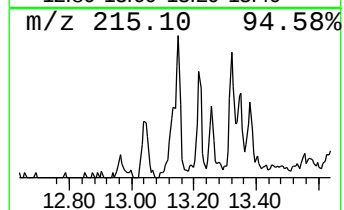
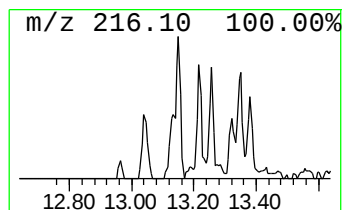
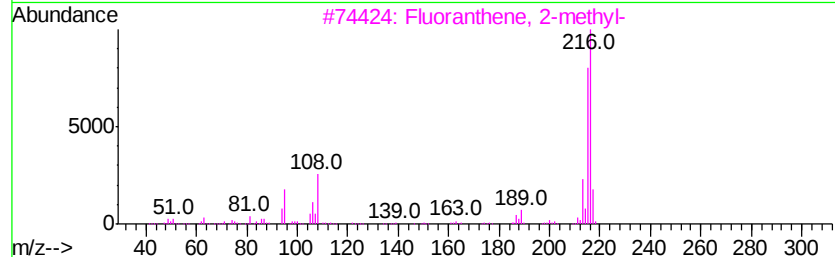
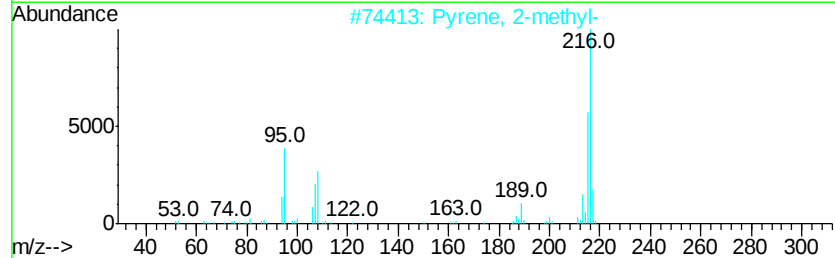
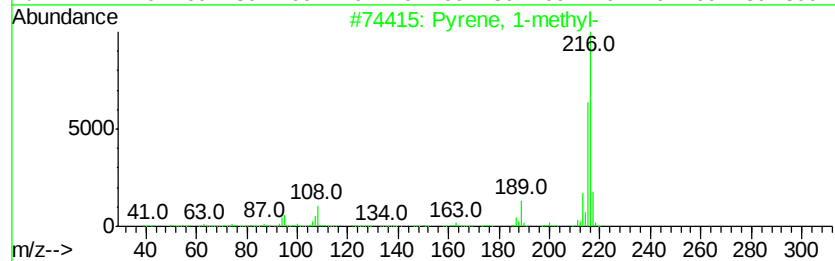
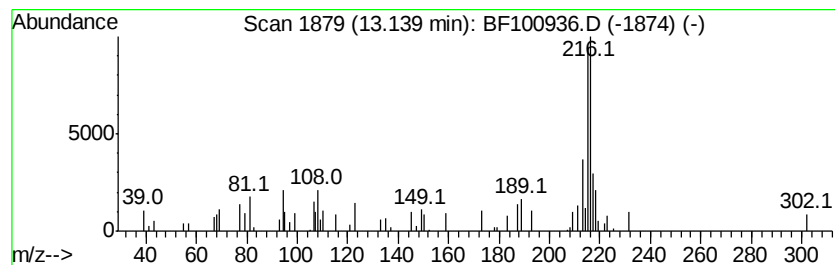
Instrument :
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ClientSampleId :
HAR-4-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	2.26 ng	66770	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyrene, 1-methyl-	216 C17H12	002381-21-7 93
2		Pyrene, 2-methyl-	216 C17H12	003442-78-2 83
3		Fluoranthene, 2-methyl-	216 C17H12	033543-31-6 76
4		11H-Benzo[b]fluorene	216 C17H12	000243-17-4 72
5		11H-Benzo[a]fluorene	216 C17H12	000238-84-6 72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100936.D
Acq On : 28 Nov 2017 16:19
Operator : SJ/JU
Sample : I6579-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-4-E(7-8)

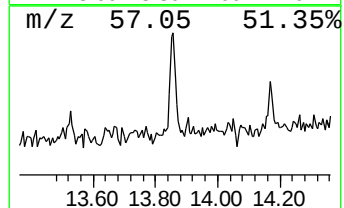
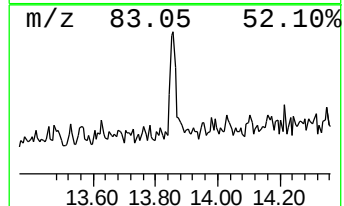
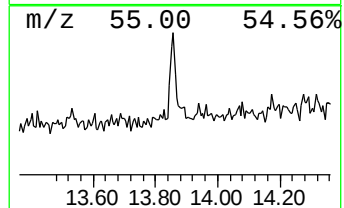
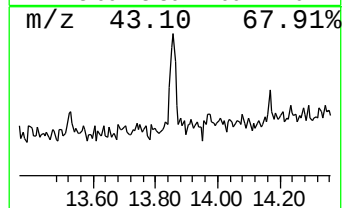
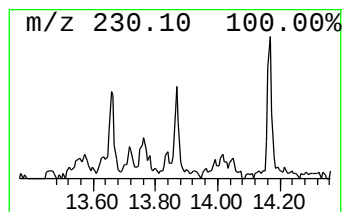
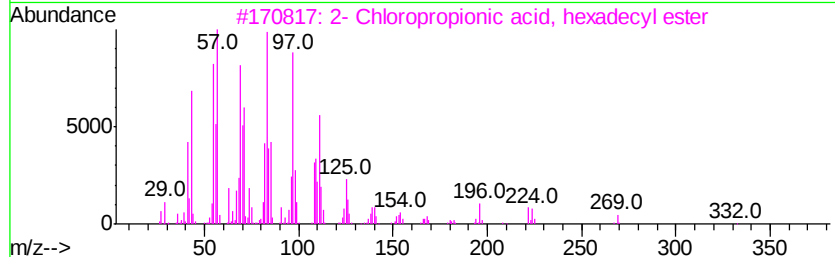
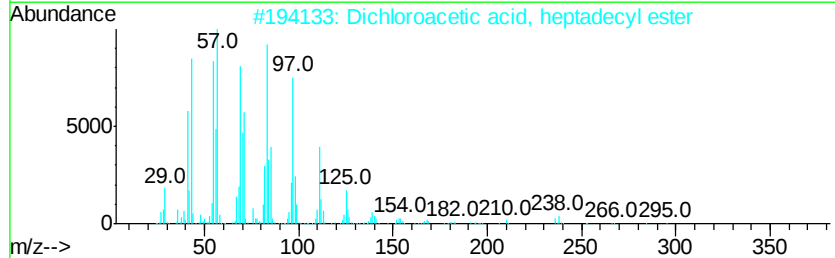
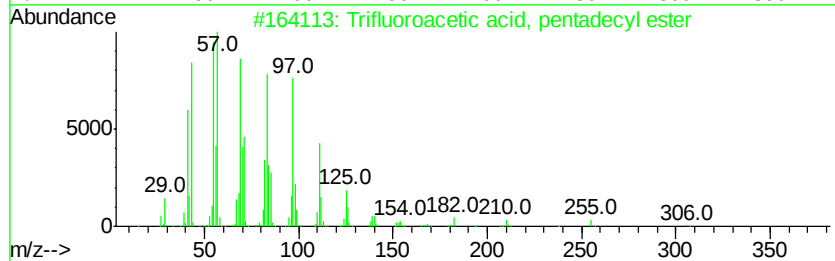
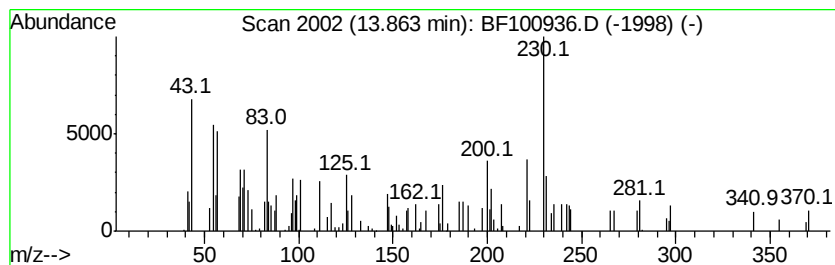
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown13.86 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.82 ng	83471	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	42
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	38
3		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	38
4		Octadecane, 1-(ethenvloxy)-	296	C20H40O	000930-02-9	38
5		Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100936.D
Acq On : 28 Nov 2017 16:19
Operator : SJ/JU
Sample : I6579-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-4-E(7-8)

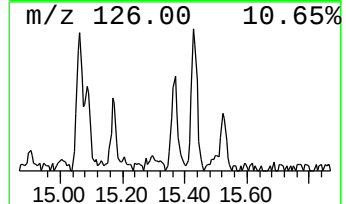
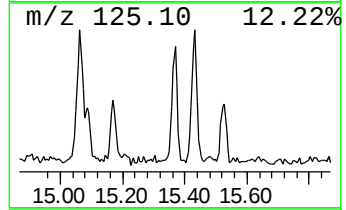
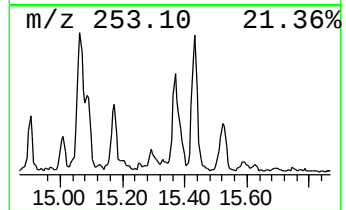
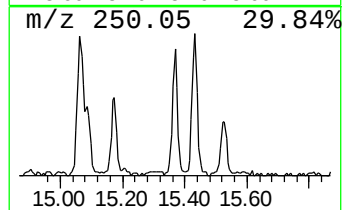
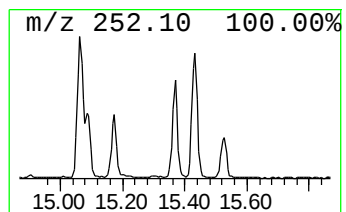
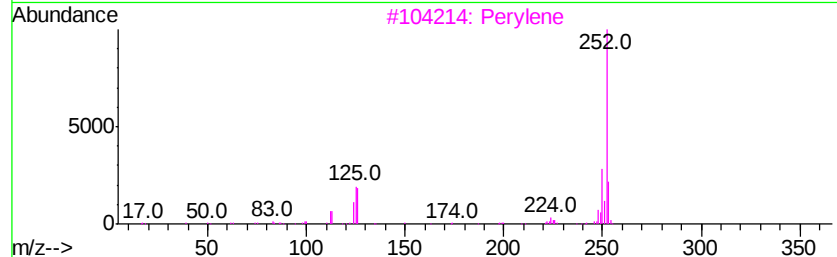
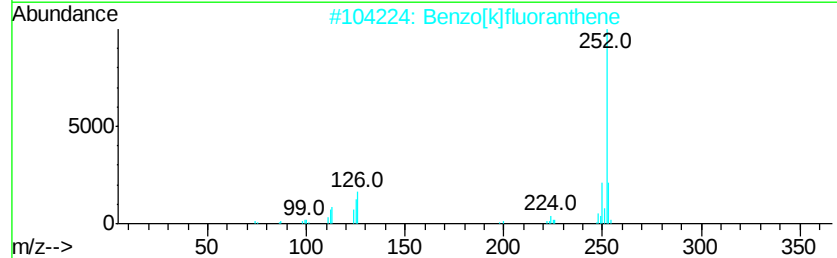
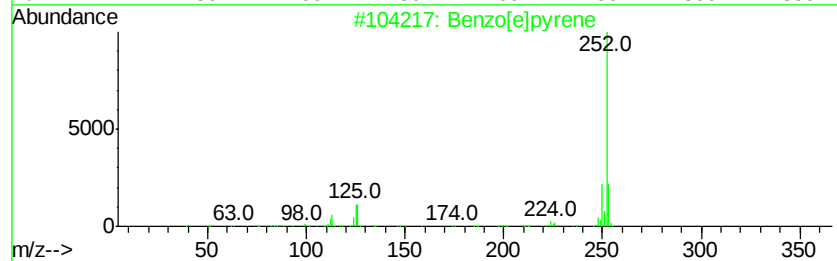
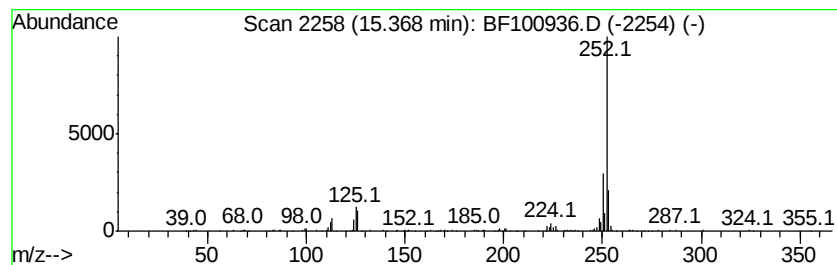
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	7.96 ng	157713	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Perylene	252	C20H12	000198-55-0	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	95
5			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
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Acq On : 28 Nov 2017 16:19
Operator : SJ/JU
Sample : I6579-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HAR-4-E(7-8)

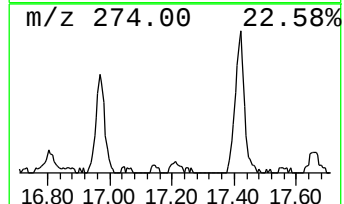
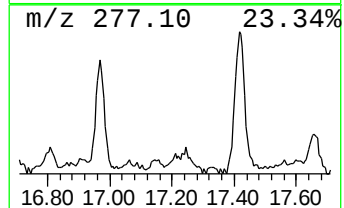
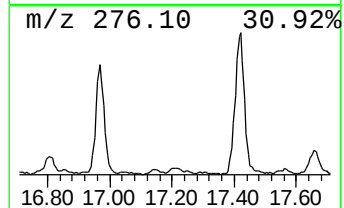
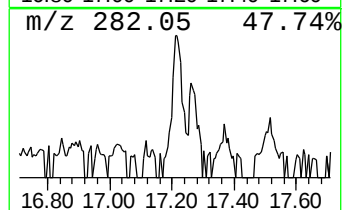
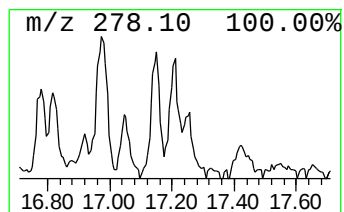
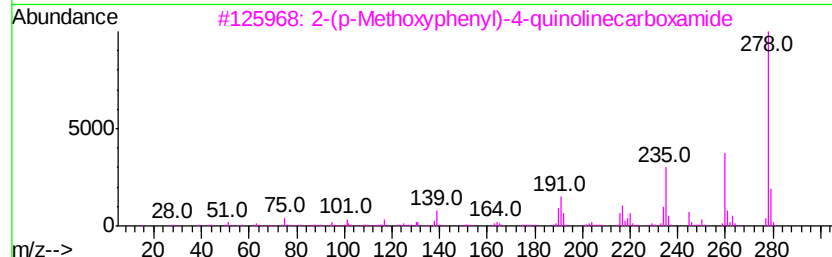
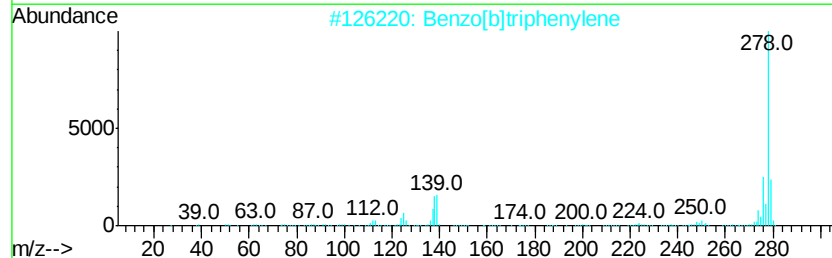
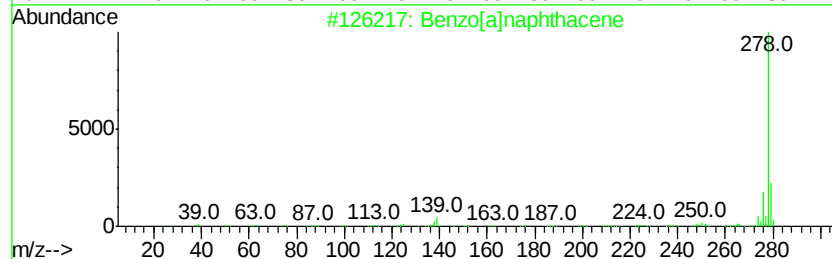
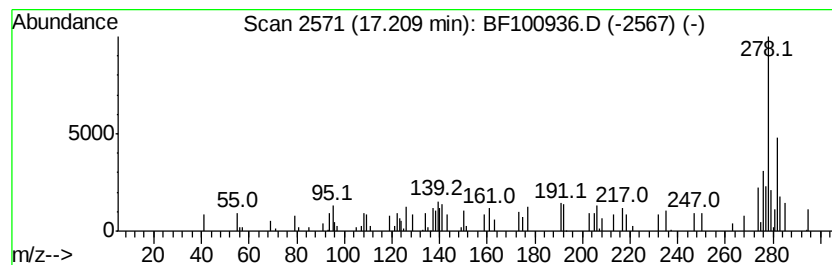
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.21 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	2.02 ng	39993	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[a]naphthacene	278	C22H14	000226-88-0	43
2		Benzo[b]triphenylene	278	C22H14	000215-58-7	41
3		2-(p-Methoxyphenyl)-4-quinolinec...	278	C17H14N2O2	051842-82-1	38
4		Dibenz[a,i]anthracene	278	C22H14	000224-41-9	38
5		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HAR-4-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.08	10.3	ng	174575	1	6.86	338126	20.0
unknown6.63	6.63	72.6	ng	1226950	1	6.86	338126	20.0
2-Hydroxy-iso-but...	8.69	2.5	ng	53731	2	8.14	425791	20.0
Benzophenone	10.60	9.7	ng	215997	3	9.89	444407	20.0
unknown11.90	11.90	2.5	ng	46267	4	11.38	364004	20.0
Benzaldehyde, 3,5...	11.99	2.0	ng	37010	4	11.38	364004	20.0
Pyrene, 1-methyl-	13.14	2.3	ng	66770	5	14.02	591681	20.0
unknown13.86	13.86	2.8	ng	83471	5	14.02	591681	20.0
Benzo[e]pyrene	15.37	8.0	ng	157713	6	15.50	396281	20.0
unknown17.21	17.21	2.0	ng	39993	6	15.50	396281	20.0