

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
 Data File : BF100795.D
 Acq On : 21 Nov 2017 21:54
 Operator : SJ/JU
 Sample : I6499-07 2X
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PG1-4-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	5.087	507	510	522	rVB	61895	63818	5.24%	0.415%
2	5.486	573	578	581	rBV	963737	877543	72.07%	5.712%
3	6.498	745	750	759	rVB	989496	988086	81.15%	6.431%
4	6.639	770	774	777	rBV	1173523	948836	77.93%	6.176%
5	6.869	810	813	817	rBV	531603	479090	39.35%	3.118%
6	7.028	836	840	843	rBV	900112	715018	58.73%	4.654%
7	7.433	905	909	912	rBV	635484	548567	45.06%	3.571%
8	7.504	918	921	925	rBV	22190	20689	1.70%	0.135%
9	7.869	979	983	993	rVB	13899	17159	1.41%	0.112%
10	8.151	1027	1031	1034	rBV	732986	608213	49.95%	3.959%
11	8.480	1083	1087	1095	rBV	15516	20064	1.65%	0.131%
12	9.227	1210	1214	1217	rBV	1498390	1217543	100.00%	7.925%
13	9.616	1277	1280	1283	rBV	76170	60495	4.97%	0.394%
14	9.769	1303	1306	1308	rBV	30699	23513	1.93%	0.153%
15	9.833	1312	1317	1321	rVB	32793	31390	2.58%	0.204%
16	9.910	1326	1330	1333	rVV	700830	613327	50.37%	3.992%
17	9.939	1333	1335	1338	rVB	24699	17591	1.44%	0.114%
18	10.110	1359	1364	1368	rBV2	23459	37300	3.06%	0.243%
19	10.304	1394	1397	1399	rBV3	15249	15699	1.29%	0.102%
20	10.327	1399	1401	1404	rVB	36473	29747	2.44%	0.194%
21	10.451	1419	1422	1426	rVB	21236	21034	1.73%	0.137%
22	10.692	1460	1463	1470	rVB	622854	579310	47.58%	3.771%
23	10.804	1479	1482	1491	rVB	36445	43615	3.58%	0.284%
24	11.045	1521	1523	1527	rVB2	18974	17087	1.40%	0.111%
25	11.198	1546	1549	1552	rVV	27147	21221	1.74%	0.138%
26	11.251	1554	1558	1560	rVV2	32546	31231	2.57%	0.203%
27	11.292	1560	1565	1568	rVB2	20406	27593	2.27%	0.180%
28	11.392	1579	1582	1585	rBV	553513	550133	45.18%	3.581%
29	11.416	1585	1586	1590	rVV	382798	286503	23.53%	1.865%
30	11.468	1592	1595	1598	rVB	71505	55192	4.53%	0.359%
31	11.621	1615	1621	1628	rBV2	28154	49761	4.09%	0.324%
32	11.680	1628	1631	1636	rVB2	20175	26946	2.21%	0.175%
33	11.780	1643	1648	1651	rBV6	18313	21276	1.75%	0.138%
34	11.851	1655	1660	1662	rVV5	13070	16063	1.32%	0.105%

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Integration Parameters: rteint.p
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 Sampling : 1
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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.892	1664	1667	1668	rVV	54957	48301	3.97%	0.314%
36	11.915	1668	1671	1677	rVV2	154569	217590	17.87%	1.416%
37	11.968	1677	1680	1683	rVV	26426	33345	2.74%	0.217%
38	12.004	1683	1686	1689	rVV2	58937	72818	5.98%	0.474%
39	12.027	1689	1690	1694	rVB	39379	27718	2.28%	0.180%
40	12.086	1694	1700	1705	rBV2	26665	43138	3.54%	0.281%
41	12.186	1715	1717	1720	rBV	39073	33807	2.78%	0.220%
42	12.215	1720	1722	1724	rBV	33738	26175	2.15%	0.170%
43	12.445	1757	1761	1764	rBV	41071	58298	4.79%	0.379%
44	12.480	1764	1767	1769	rVV3	34199	46767	3.84%	0.304%
45	12.527	1773	1775	1779	rVB	39310	37927	3.12%	0.247%
46	12.610	1785	1789	1794	rBV	491463	438720	36.03%	2.856%
47	12.698	1801	1804	1807	rBV2	69117	61491	5.05%	0.400%
48	12.839	1822	1828	1833	rBV	443298	470019	38.60%	3.059%
49	12.880	1833	1835	1840	rVB2	25214	30542	2.51%	0.199%
50	12.974	1845	1851	1860	rVB	1031291	985396	80.93%	6.414%
51	13.057	1860	1865	1868	rBV4	39074	66948	5.50%	0.436%
52	13.139	1876	1879	1880	rBV2	25844	26094	2.14%	0.170%
53	13.157	1880	1882	1887	rVB	38638	41519	3.41%	0.270%
54	13.268	1896	1901	1903	rBV3	46823	62078	5.10%	0.404%
55	13.345	1912	1914	1915	rBV	22651	18772	1.54%	0.122%
56	13.392	1919	1922	1925	rBV2	35095	39857	3.27%	0.259%
57	13.668	1965	1969	1974	rVB	81872	88219	7.25%	0.574%
58	13.780	1985	1988	1991	rBV2	40308	48901	4.02%	0.318%
59	13.809	1991	1993	1995	rVV	42566	33163	2.72%	0.216%
60	13.833	1995	1997	1999	rVV	31657	32552	2.67%	0.212%
61	13.874	2000	2004	2007	rVB2	70400	105287	8.65%	0.685%
62	14.033	2026	2031	2034	rBV2	660900	793487	65.17%	5.165%
63	14.057	2034	2035	2043	rVB	205555	187545	15.40%	1.221%
64	14.415	2094	2096	2099	rVB	42884	41131	3.38%	0.268%
65	15.074	2204	2208	2212	rBV	182012	292205	24.00%	1.902%
66	15.380	2258	2260	2267	rVB	90950	117035	9.61%	0.762%
67	15.445	2268	2271	2277	rVV	145228	203440	16.71%	1.324%
68	15.509	2278	2282	2293	rVB	370714	543879	44.67%	3.540%
69	15.651	2302	2306	2314	rVB4	87535	127810	10.50%	0.832%
70	16.215	2398	2402	2410	rVB2	161195	307796	25.28%	2.003%
71	16.656	2472	2477	2486	rVB2	157095	326562	26.82%	2.126%

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Integrator: RTE
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72	17.239	2571	2576	2582	rvB4	75781	146347	12.02%	0.953%
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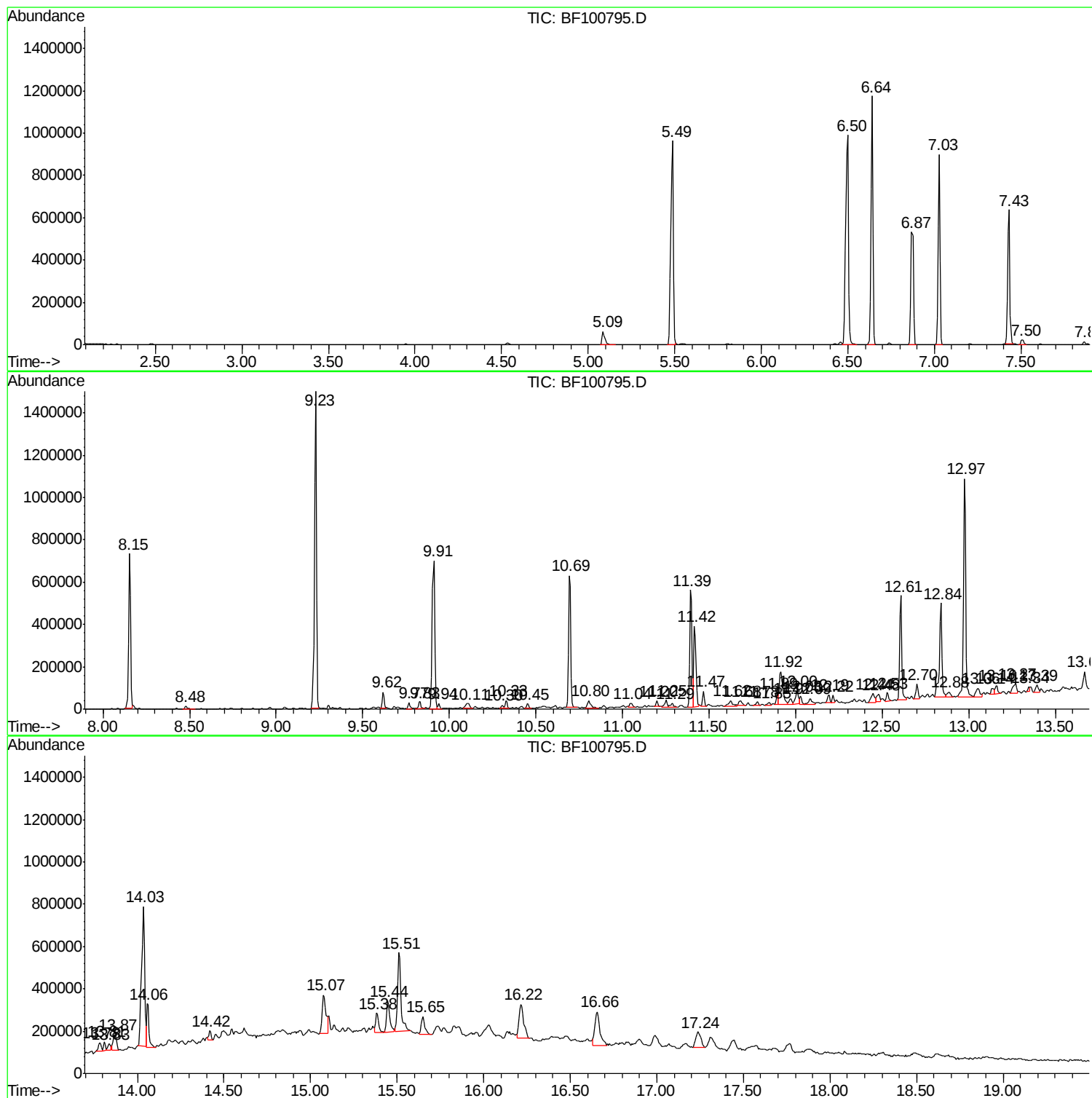
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Instrument :
BNA_F
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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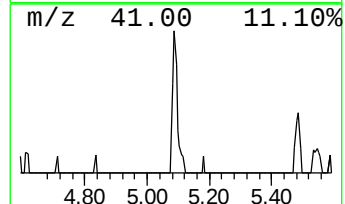
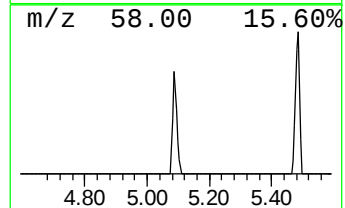
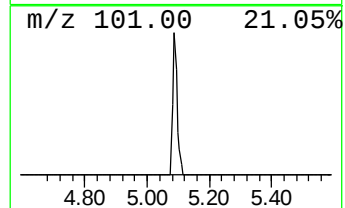
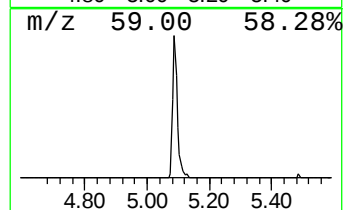
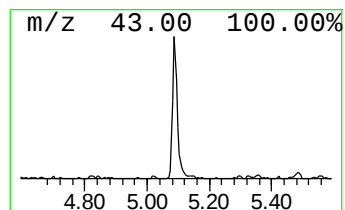
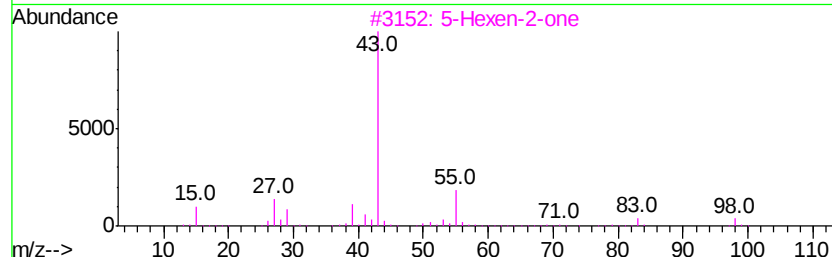
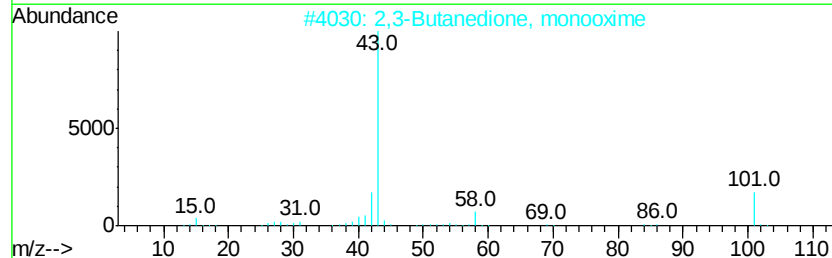
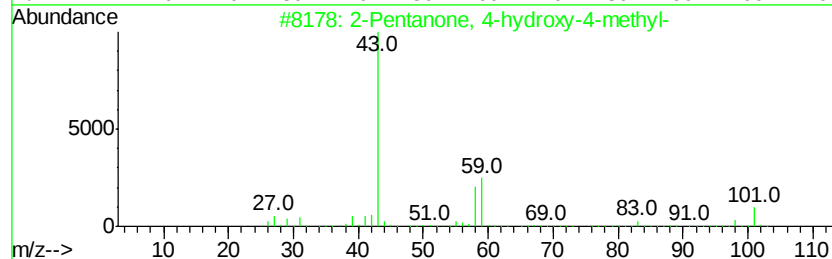
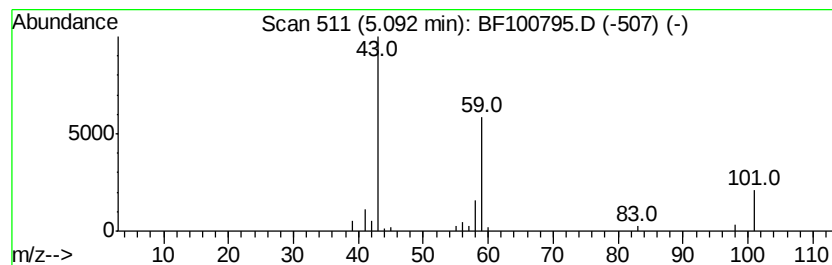
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.66 ng	63818	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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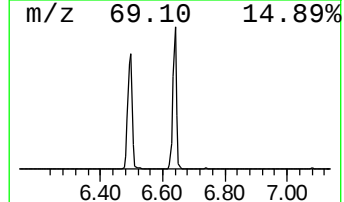
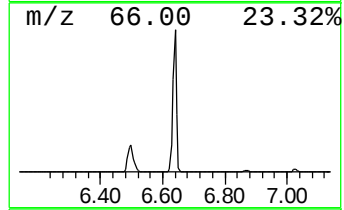
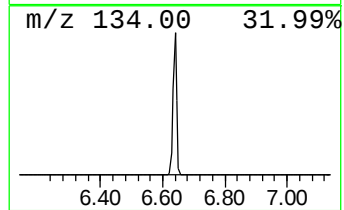
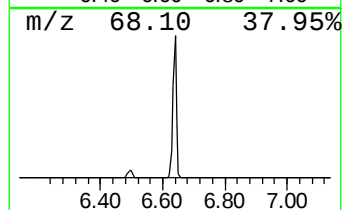
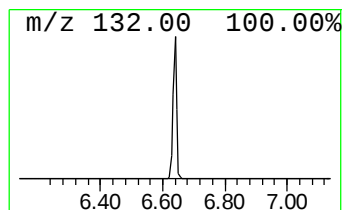
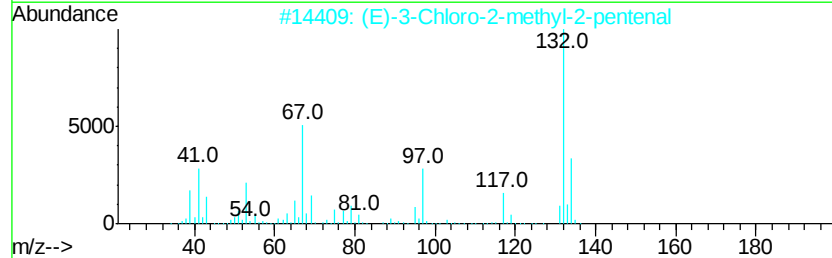
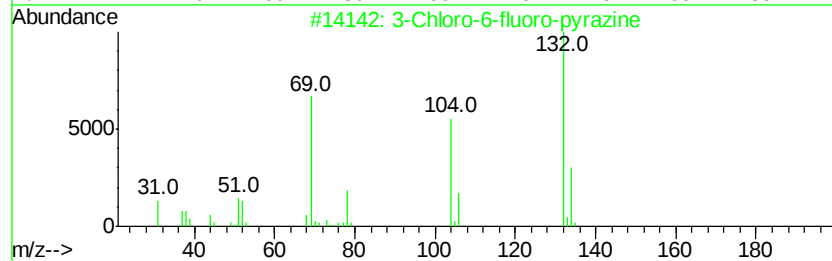
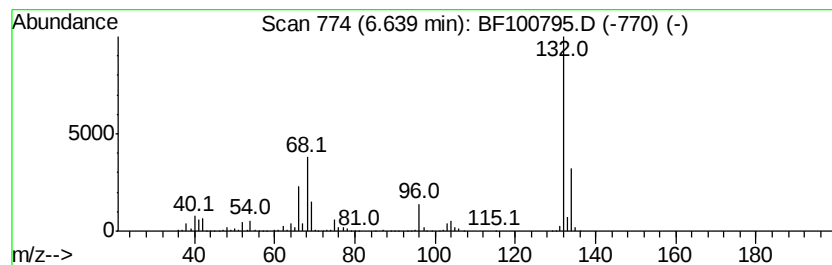
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	39.61 ng	948836	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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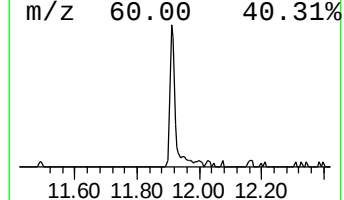
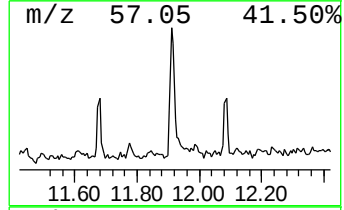
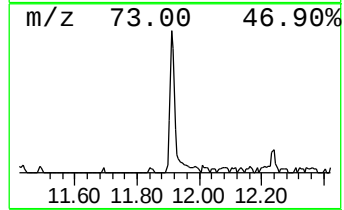
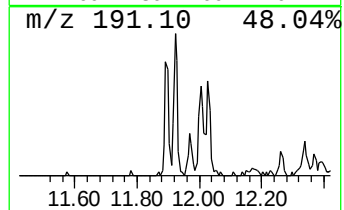
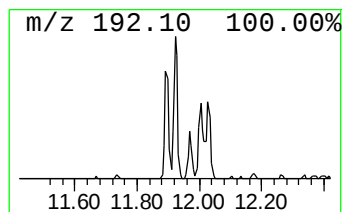
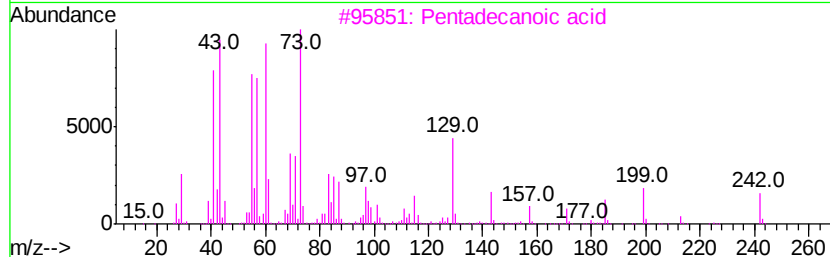
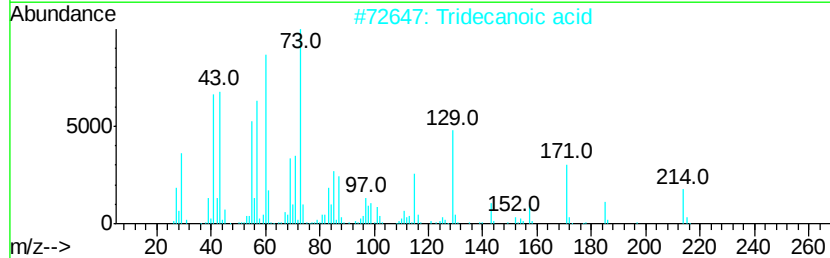
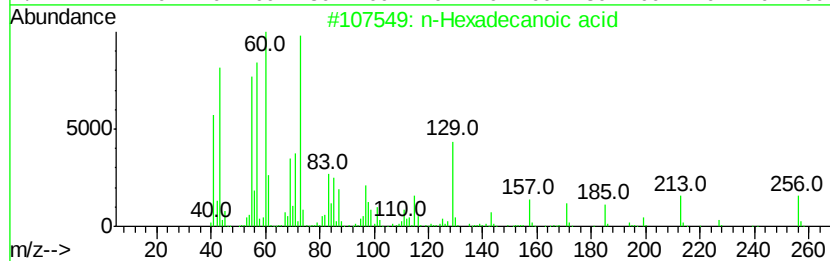
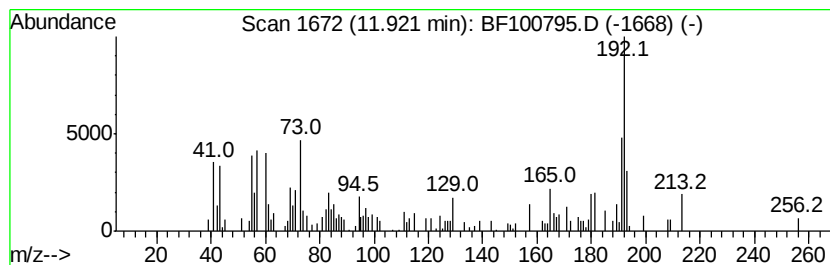
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.91 ng	217590	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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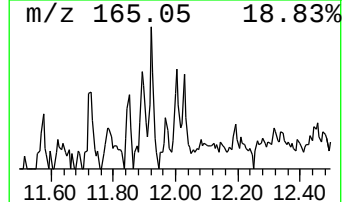
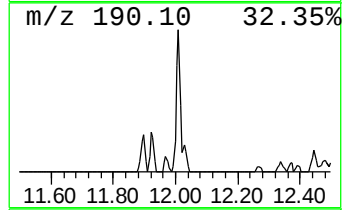
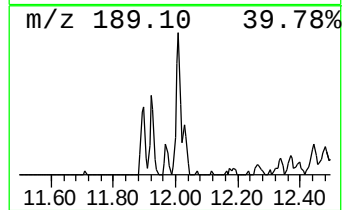
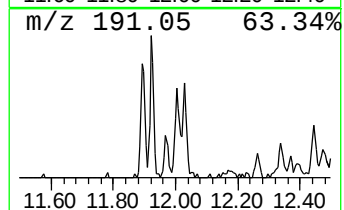
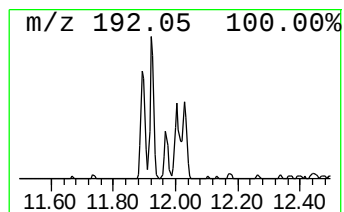
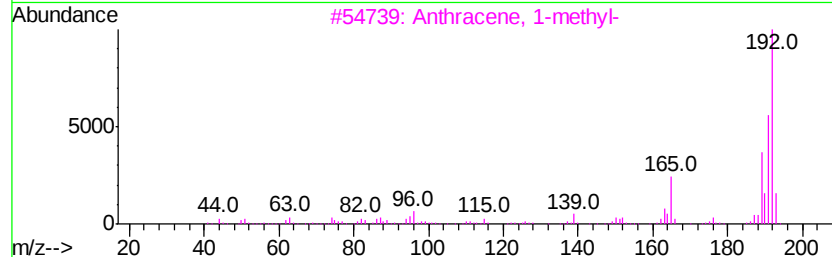
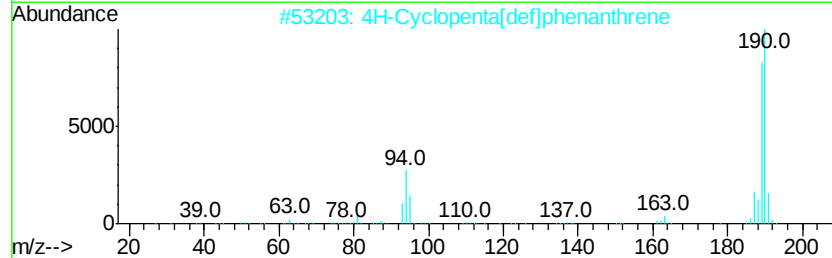
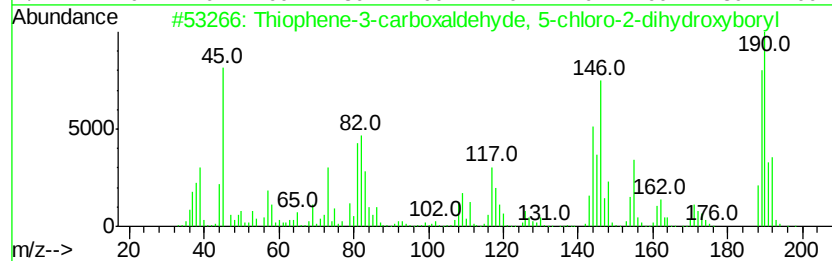
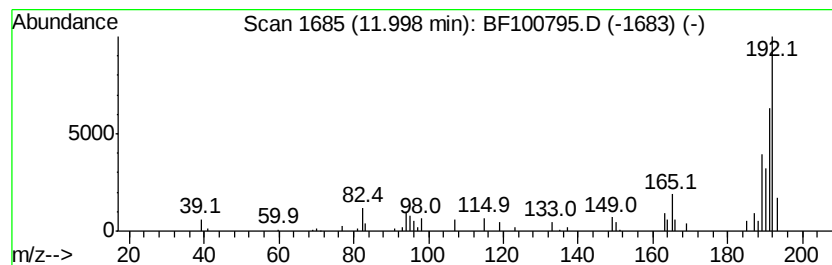
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown12.00 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	2.65 ng	72818	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	47
2		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
3		Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	41
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100795.D
Acq On : 21 Nov 2017 21:54
Operator : SJ/JU
Sample : I6499-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

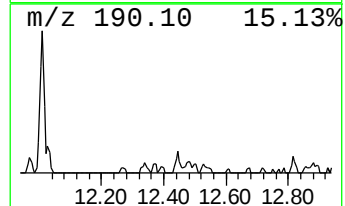
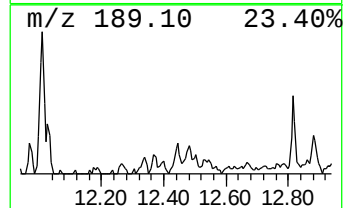
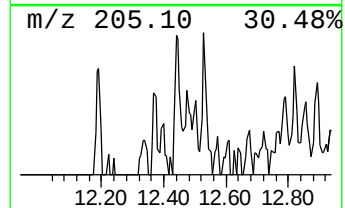
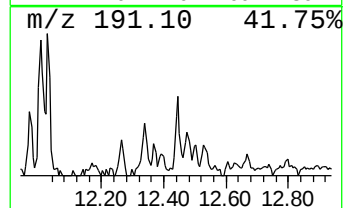
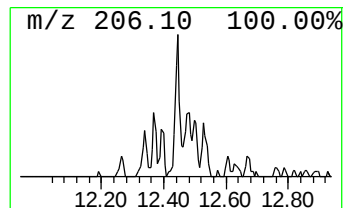
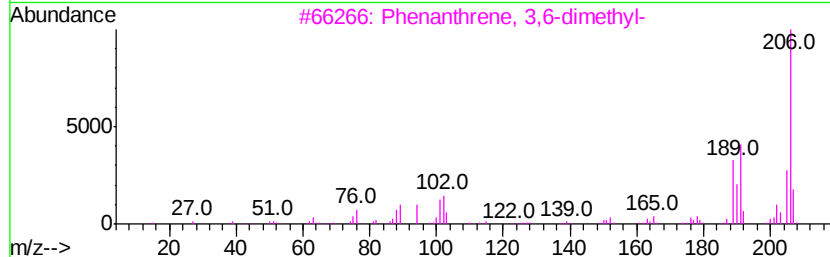
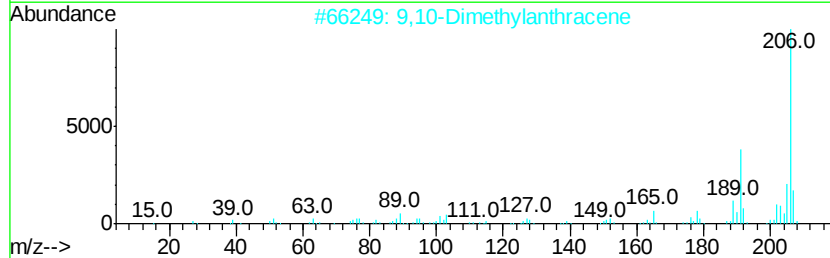
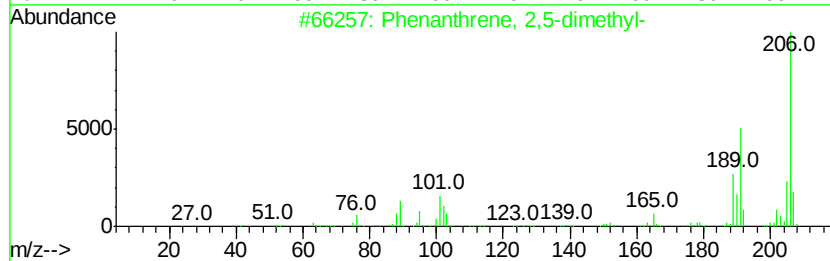
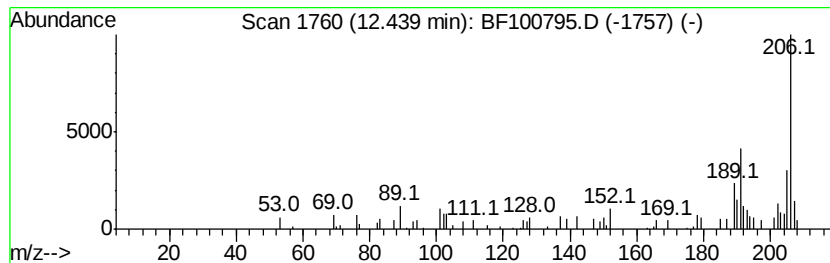
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ClientSampleId :
PG1-4-E(7-8)

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 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.44	2.12 ng	58298	Phenanthrene-d10	11.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91	
2	9,10-Dimethylantracene	206	C16H14	000781-43-1	91	
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	83	
4	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	81	
5	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	81	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100795.D
Acq On : 21 Nov 2017 21:54
Operator : SJ/JU
Sample : I6499-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PG1-4-E(7-8)

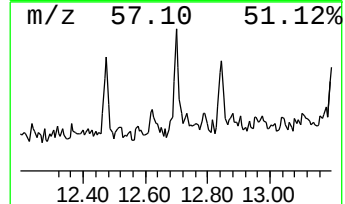
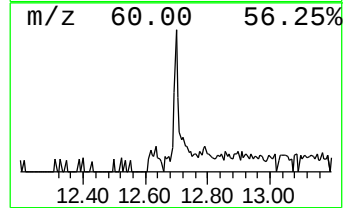
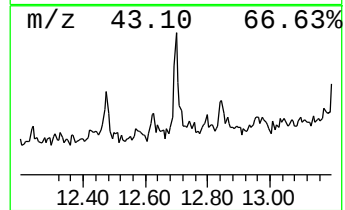
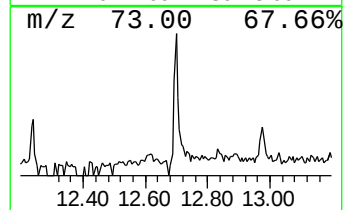
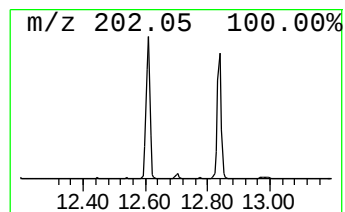
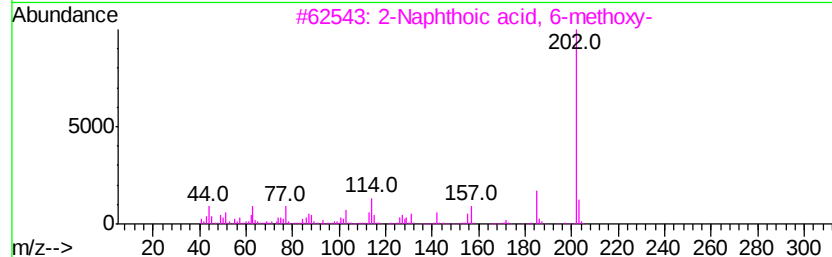
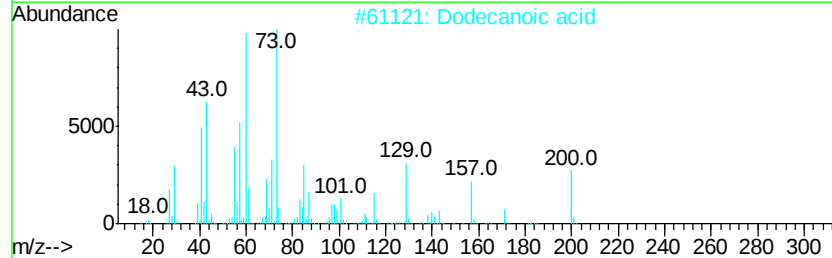
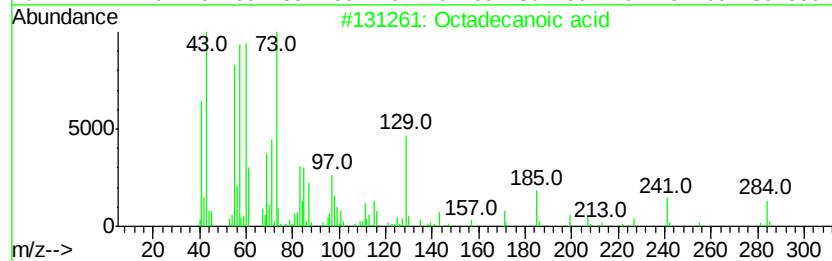
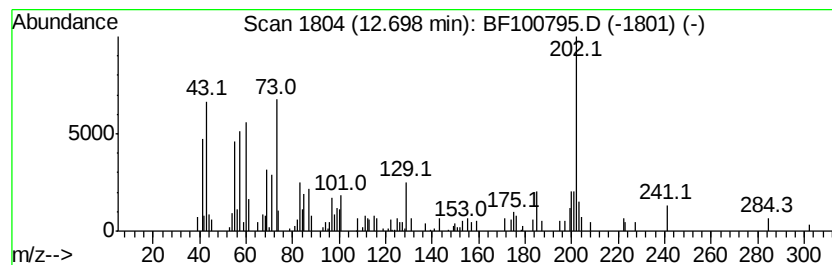
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.24 ng	61491	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Dodecanoic acid	200	C12H24O2	000143-07-7	46
3		2-Naphthoic acid, 6-methoxy-	202	C12H10O3	002471-70-7	38
4		Pyrene	202	C16H10	000129-00-0	30
5		Fluoranthene	202	C16H10	000206-44-0	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100795.D
Acq On : 21 Nov 2017 21:54
Operator : SJ/JU
Sample : I6499-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

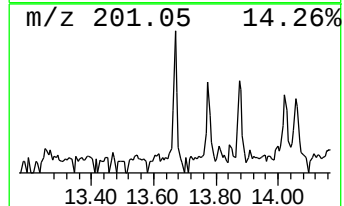
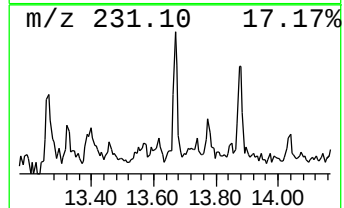
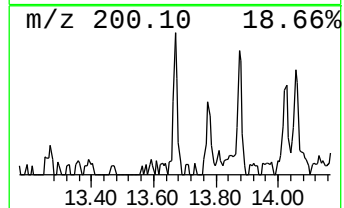
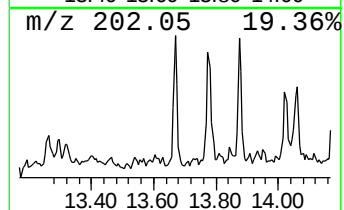
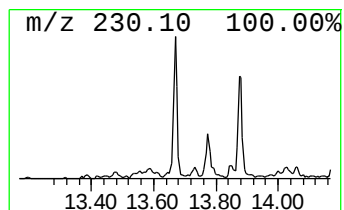
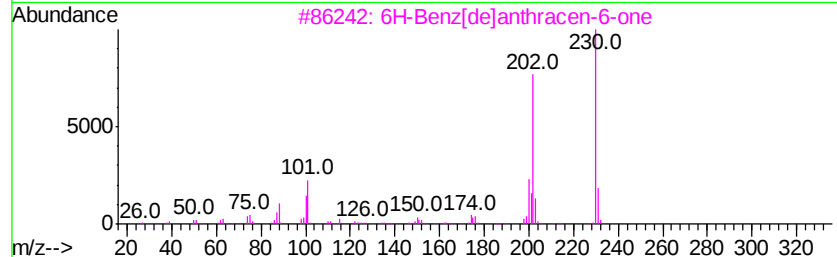
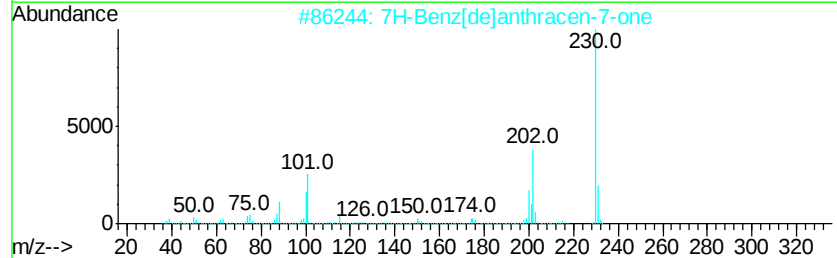
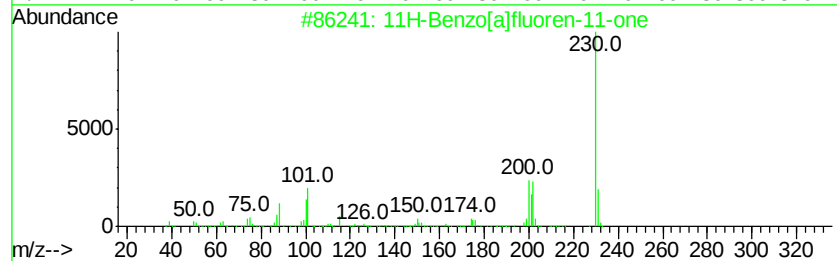
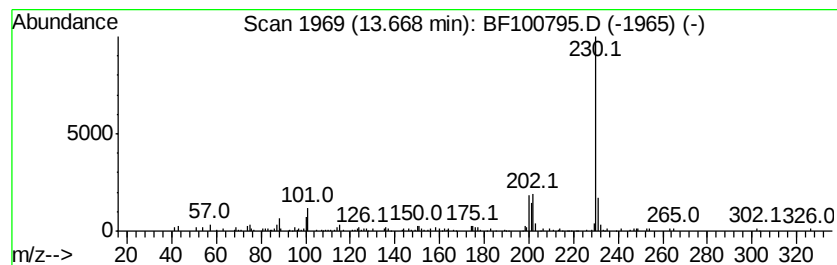
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ClientSampleId :
PG1-4-E(7-8)

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 8 11H-Benzo[a]fluoren-11-one Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.67	2.22 ng	88219	Chrysene-d12		14.03		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	83
3			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	72
4			o-Terphenyl	230	C18H14	000084-15-1	72
5			9-Chloro-1-phenazinol	230	C12H7ClN2O	091268-03-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100795.D
Acq On : 21 Nov 2017 21:54
Operator : SJ/JU
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PG1-4-E(7-8)

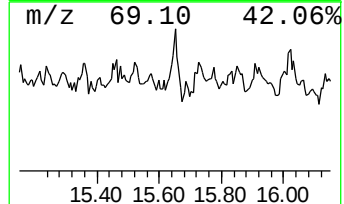
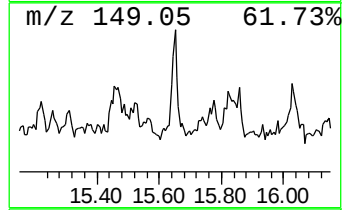
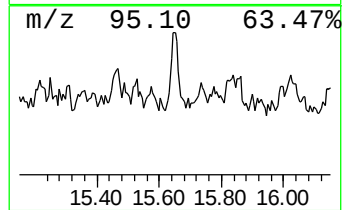
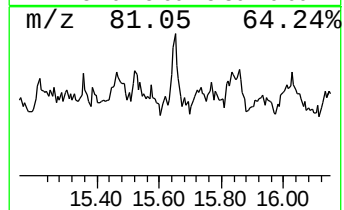
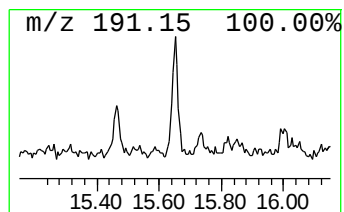
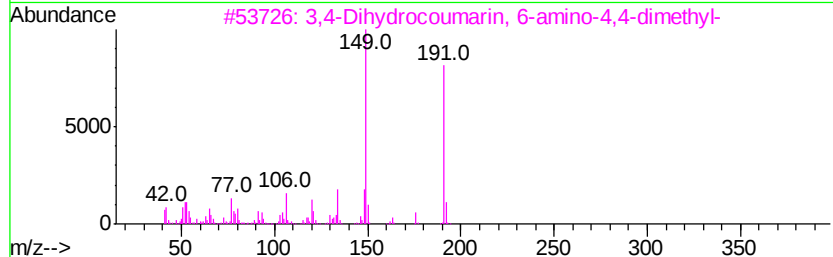
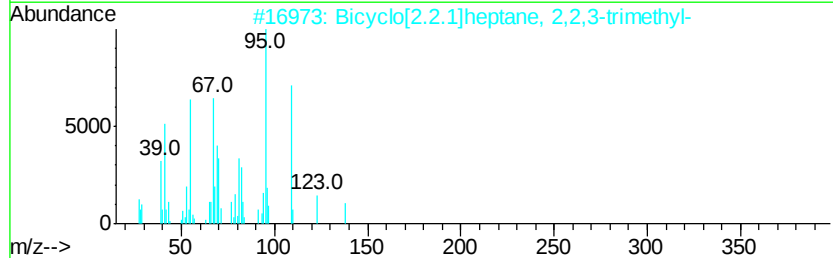
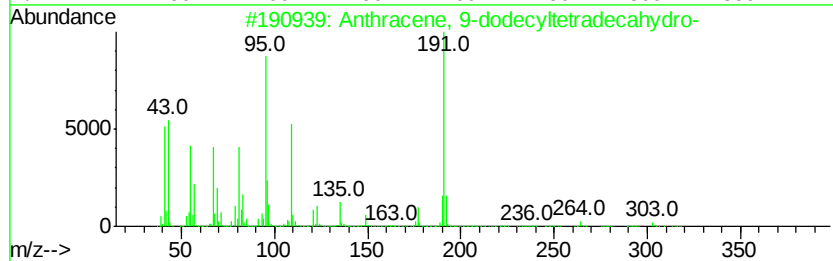
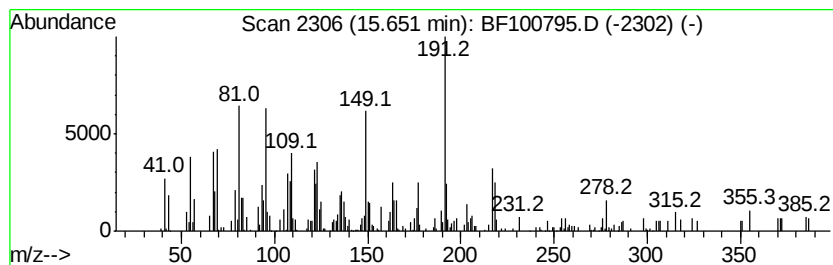
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.65 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	4.70 ng	127810	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	47
2		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	44
3		3,4-Dihydrocoumarin, 6-amino-4,4...	191	C11H13N02	1000128-49-9	35
4		Furan-2-carboxylic acid, [4-(4-m...	315	C18H21N04	1000305-72-3	35
5		Butanoic acid, 4-(4-hydroxypheny...	209	C10H11N04	062558-67-2	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100795.D
Acq On : 21 Nov 2017 21:54
Operator : SJ/JU
Sample : I6499-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PG1-4-E(7-8)

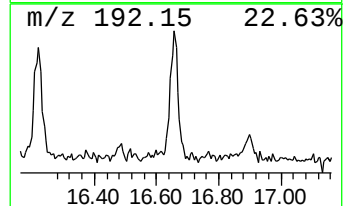
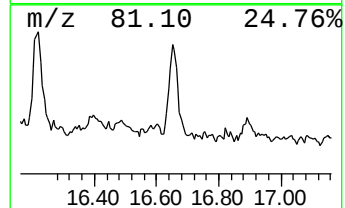
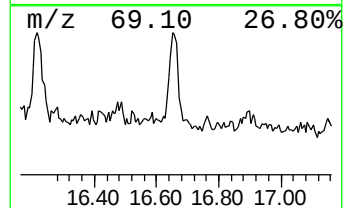
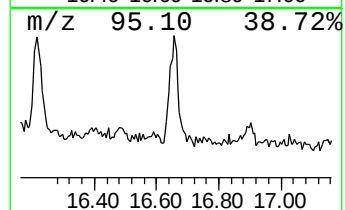
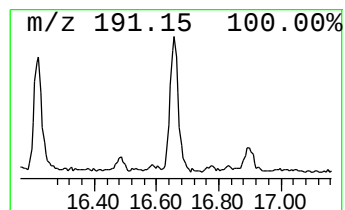
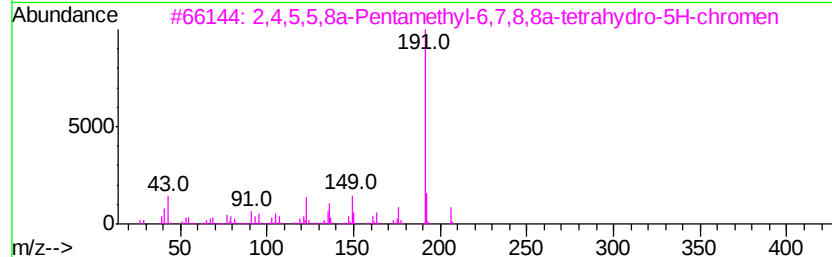
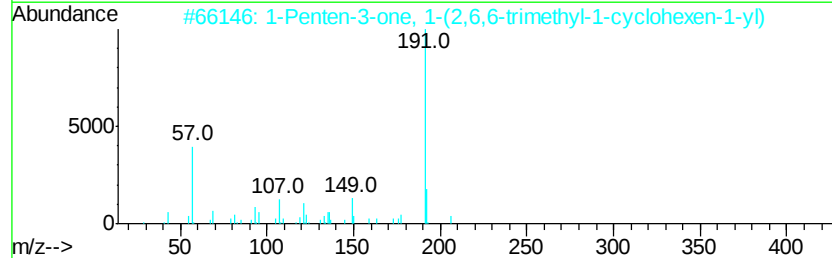
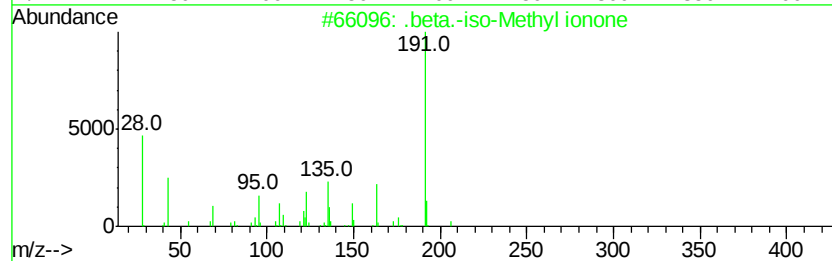
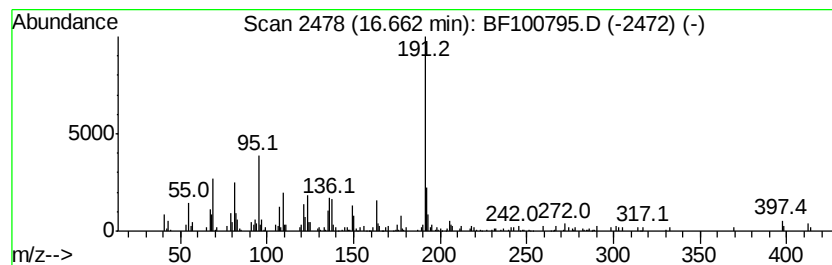
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .beta.-iso-Methyl ionone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	12.01 ng	326562	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	60
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
3		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	37
4		Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	37
5		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100795.D
Acq On : 21 Nov 2017 21:54
Operator : SJ/JU
Sample : I6499-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

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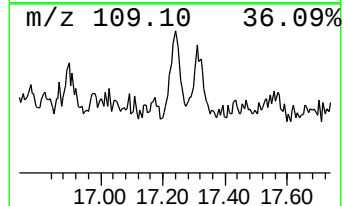
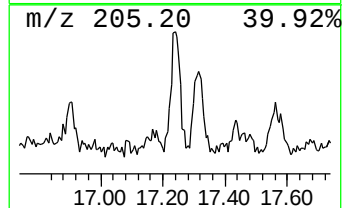
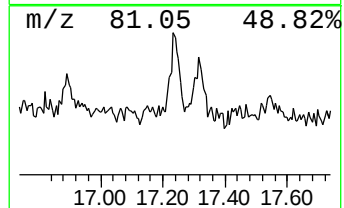
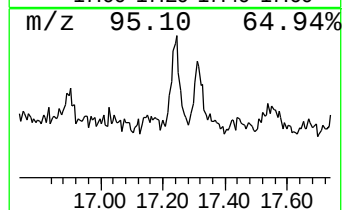
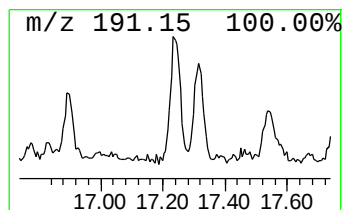
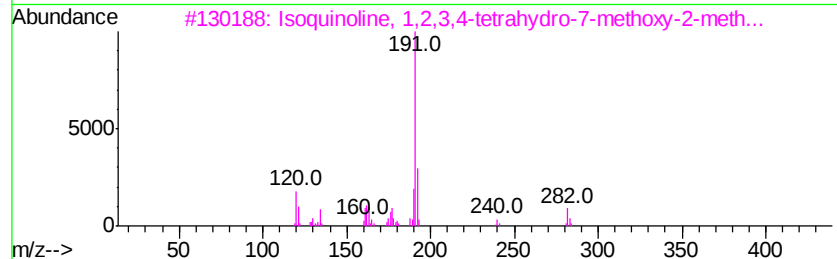
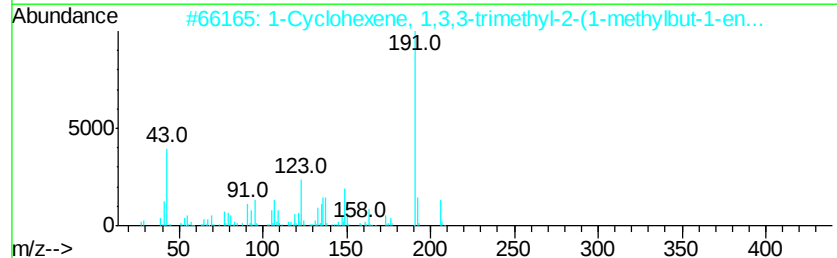
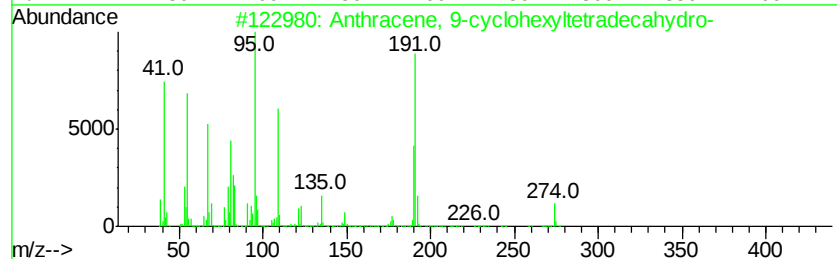
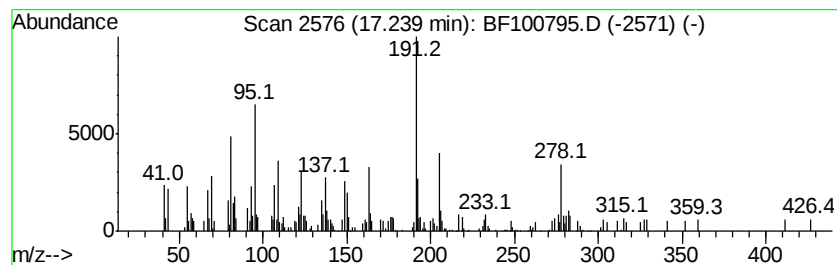
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Anthracene, 9-cyclohexyltet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.24	5.38 ng	146347	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	50
2		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	41
3		Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	35
4		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	30
5		Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
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Acq On : 21 Nov 2017 21:54
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Sample : I6499-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	2.7 ng		63818	1	6.87	479090	20.0
unknown6.64	6.64	39.6 ng		948836	1	6.87	479090	20.0
n-Hexadecanoic acid	11.92	7.9 ng		217590	4	11.39	550133	20.0
unknown12.00	12.00	2.6 ng		72818	4	11.39	550133	20.0
Phenanthrene, 2,5...	12.44	2.1 ng		58298	4	11.39	550133	20.0
Octadecanoic acid	12.70	2.2 ng		61491	4	11.39	550133	20.0
11H-Benzo[a]fluor...	13.67	2.2 ng		88219	5	14.03	793487	20.0
unknown15.65	15.65	4.7 ng		127810	6	15.51	543879	20.0
.beta.-iso-Methyl...	16.66	12.0 ng		326562	6	15.51	543879	20.0
Anthracene, 9-cyc...	17.24	5.4 ng		146347	6	15.51	543879	20.0