

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091417\
 Data File : BF098545.D
 Acq On : 14 Sep 2017 23:18
 Operator : SJ/JU
 Sample : I5161-13
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RL-12-0-13

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-BF091117.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	3.551	240	249	257	rBV	269883	445592	12.75%	1.257%
2	4.163	350	353	365	rBV	35740	60154	1.72%	0.170%
3	4.828	462	466	479	rBV	860120	1160094	33.19%	3.273%
4	5.257	535	539	560	rBV	3082222	3320260	94.98%	9.367%
5	6.310	713	718	733	rBV	2792730	3495746	100.00%	9.862%
6	6.422	733	737	743	rVV	3555918	3396646	97.17%	9.582%
7	6.481	743	747	753	rVB3	23472	37364	1.07%	0.105%
8	6.645	772	775	782	rVB	1025907	846487	24.21%	2.388%
9	6.804	798	802	805	rBV	2596919	2264765	64.79%	6.389%
10	7.098	849	852	860	rBV	51732	78428	2.24%	0.221%
11	7.216	868	872	875	rBV	2080354	2037272	58.28%	5.747%
12	7.928	989	993	996	rBV	1215233	1141917	32.67%	3.221%
13	7.951	996	997	1003	rVB2	83684	69915	2.00%	0.197%
14	8.357	1062	1066	1070	rBV2	39055	43392	1.24%	0.122%
15	8.739	1126	1131	1137	rVB	31007	38200	1.09%	0.108%
16	8.957	1165	1168	1171	rVB	43748	39924	1.14%	0.113%
17	9.004	1172	1176	1180	rBV	2705737	2393577	68.47%	6.752%
18	9.086	1186	1190	1192	rBV3	34685	39625	1.13%	0.112%
19	9.404	1241	1244	1248	rVB	584798	447272	12.79%	1.262%
20	9.545	1265	1268	1273	rVB	46623	49271	1.41%	0.139%
21	9.616	1278	1280	1284	rBV	44799	44719	1.28%	0.126%
22	9.680	1287	1291	1294	rVV	1388311	1162743	33.26%	3.280%
23	9.710	1294	1296	1301	rVB	61121	65405	1.87%	0.185%
24	10.080	1355	1359	1362	rBV5	28293	35369	1.01%	0.100%
25	10.116	1362	1365	1367	rVV	63208	47863	1.37%	0.135%
26	10.227	1381	1384	1389	rVB	64671	63668	1.82%	0.180%
27	10.333	1399	1402	1408	rVB3	56364	81857	2.34%	0.231%
28	10.469	1419	1425	1429	rBV	1576548	1404585	40.18%	3.962%
29	10.586	1442	1445	1453	rVB2	110850	178276	5.10%	0.503%
30	11.033	1519	1521	1523	rBV	49219	43130	1.23%	0.122%
31	11.063	1523	1526	1531	rVB2	79511	86320	2.47%	0.244%
32	11.163	1539	1543	1545	rBV	1095893	973279	27.84%	2.746%
33	11.186	1545	1547	1550	rVV	546546	427387	12.23%	1.206%
34	11.233	1550	1555	1558	rVB	93465	110940	3.17%	0.313%

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 Start Thrs: 0.2
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	11.398	1581	1583	1590	rVB2	51979	63075	1.80%	0.178%
36	11.663	1625	1628	1630	rBV	68681	57899	1.66%	0.163%
37	11.692	1630	1633	1637	rVB	97221	90924	2.60%	0.257%
38	11.774	1644	1647	1649	rBV	127669	116816	3.34%	0.330%
39	11.957	1676	1678	1680	rBV	51141	42037	1.20%	0.119%
40	11.992	1681	1684	1689	rVB	68785	70946	2.03%	0.200%
41	12.139	1706	1709	1711	rBV3	52163	56589	1.62%	0.160%
42	12.210	1718	1721	1723	rBV2	58774	62150	1.78%	0.175%
43	12.369	1745	1748	1752	rBV	767835	723775	20.70%	2.042%
44	12.598	1781	1787	1790	rBV	707730	705374	20.18%	1.990%
45	12.745	1808	1812	1815	rBV	1819871	1594953	45.63%	4.499%
46	12.927	1841	1843	1846	rVB	137349	118666	3.39%	0.335%
47	12.992	1852	1854	1857	rVB	105902	86916	2.49%	0.245%
48	13.027	1857	1860	1868	rVB4	82517	124524	3.56%	0.351%
49	13.363	1914	1917	1922	rVB6	83429	106910	3.06%	0.302%
50	13.439	1928	1930	1934	rVB	53244	47154	1.35%	0.133%
51	13.545	1946	1948	1950	rBV	54644	47744	1.37%	0.135%
52	13.616	1958	1960	1962	rBV2	56357	51396	1.47%	0.145%
53	13.645	1962	1965	1969	rVB2	172280	188611	5.40%	0.532%
54	13.792	1985	1990	1993	rBV2	894204	1197296	34.25%	3.378%
55	13.821	1993	1995	2000	rVB	363331	301130	8.61%	0.850%
56	13.898	2006	2008	2010	rVB	74315	50559	1.45%	0.143%
57	14.180	2054	2056	2059	rVB	77178	63639	1.82%	0.180%
58	14.274	2069	2072	2074	rBV2	96645	107321	3.07%	0.303%
59	14.804	2158	2162	2169	rBV	399583	674218	19.29%	1.902%
60	14.868	2170	2173	2175	rVV2	108942	111819	3.20%	0.315%
61	14.898	2176	2178	2184	rVB2	102880	123764	3.54%	0.349%
62	15.080	2206	2209	2215	rVB	247899	289159	8.27%	0.816%
63	15.133	2215	2218	2224	rBV	353184	432410	12.37%	1.220%
64	15.192	2224	2228	2232	rBV	663609	832036	23.80%	2.347%
65	15.604	2295	2298	2301	rVB	97462	115982	3.32%	0.327%
66	16.192	2395	2398	2411	rVB6	93879	205234	5.87%	0.579%
67	16.527	2450	2455	2460	rBV	167721	286982	8.21%	0.810%
68	16.927	2519	2523	2530	rBV	88038	168380	4.82%	0.475%

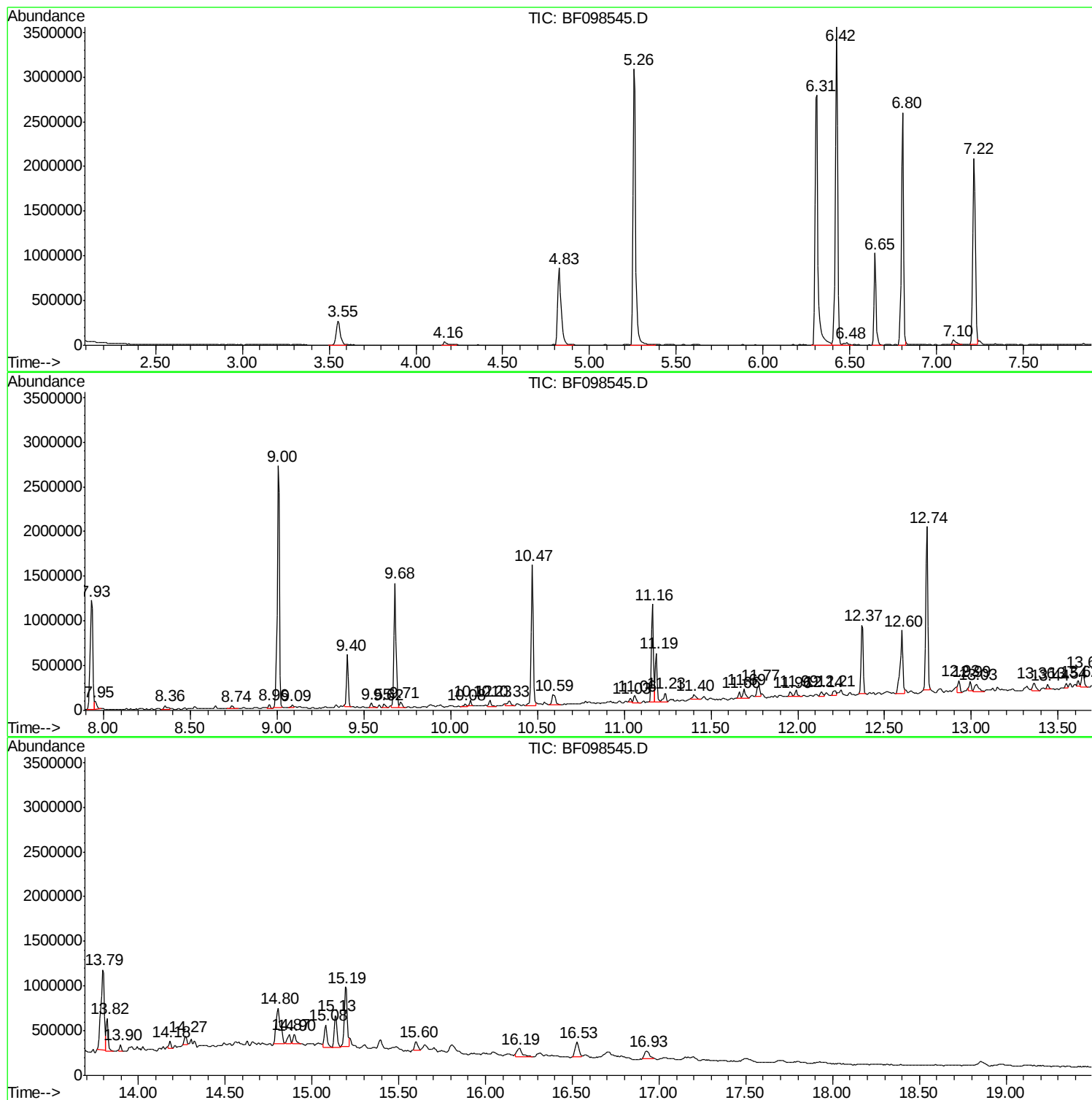
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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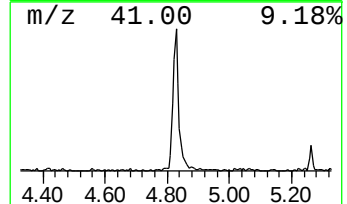
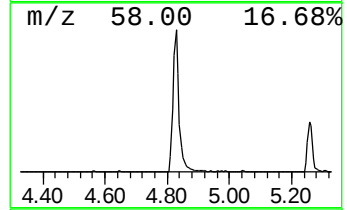
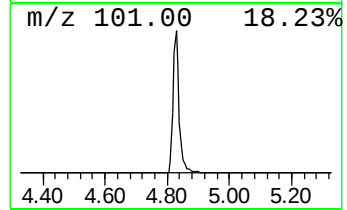
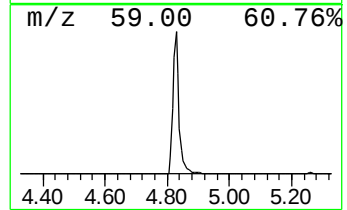
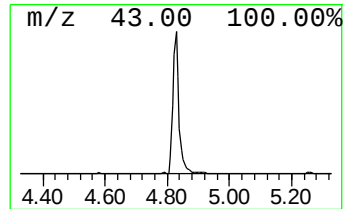
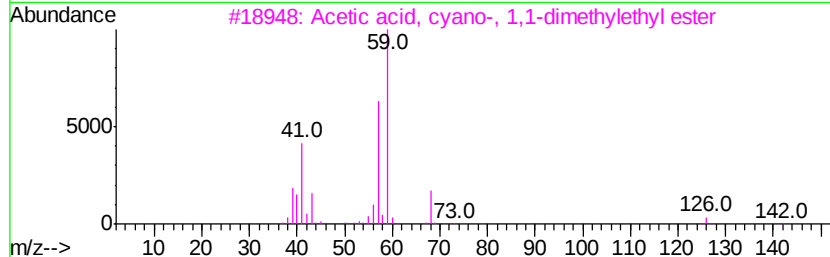
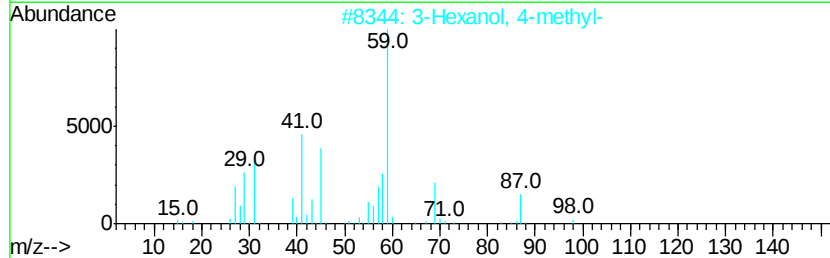
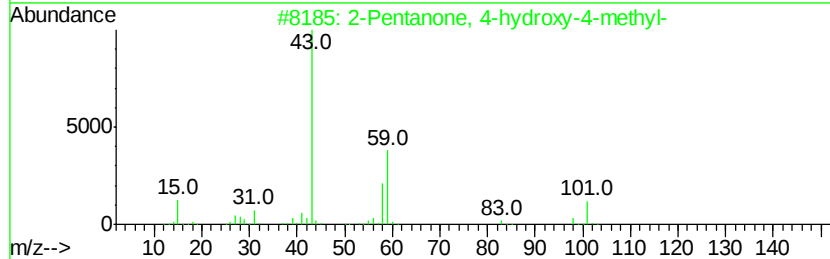
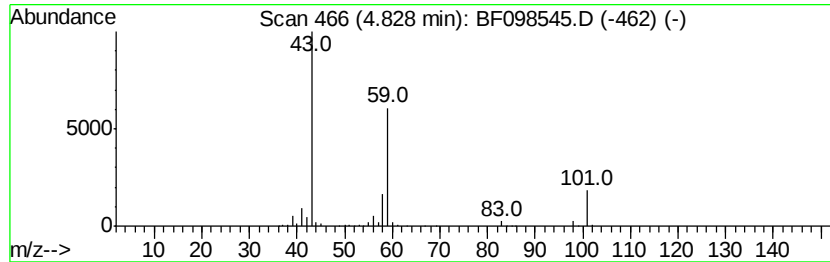
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	27.41 ng	1160090	1,4-Dichlorobenzene-d4	6.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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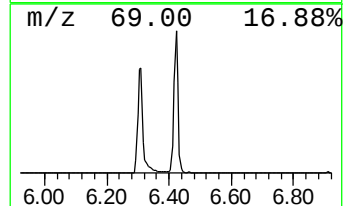
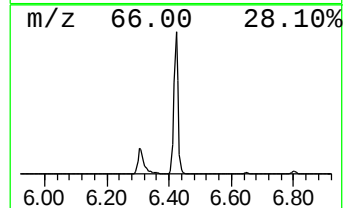
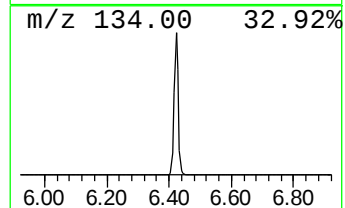
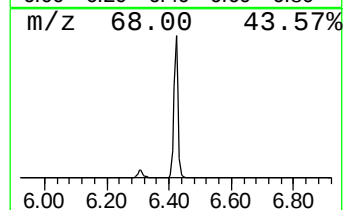
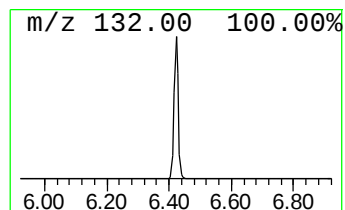
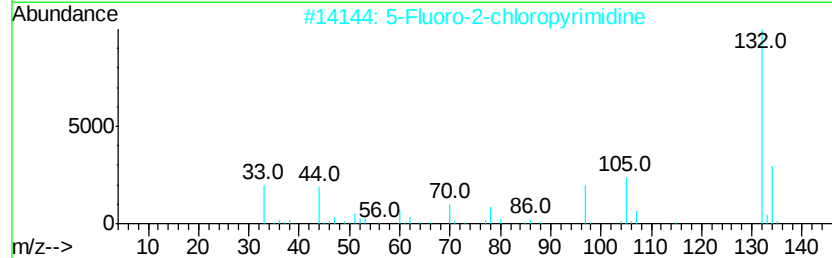
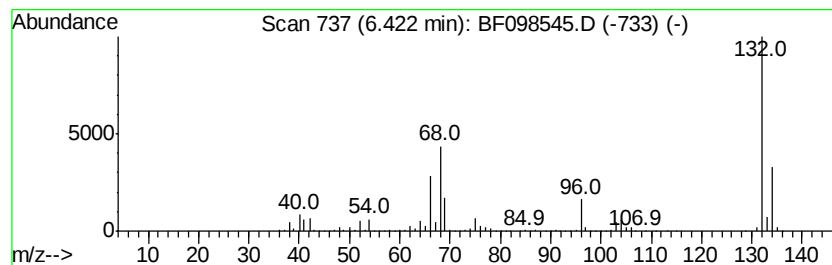
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	80.25 ng	3396650	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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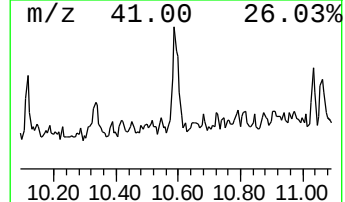
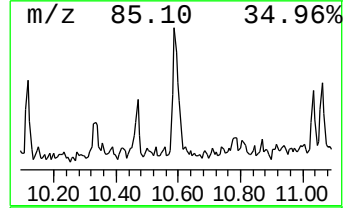
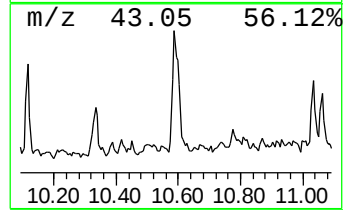
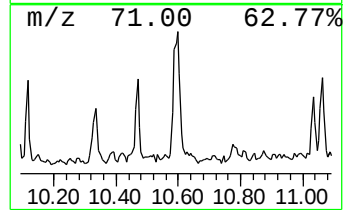
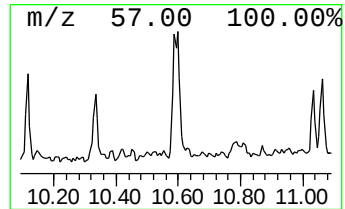
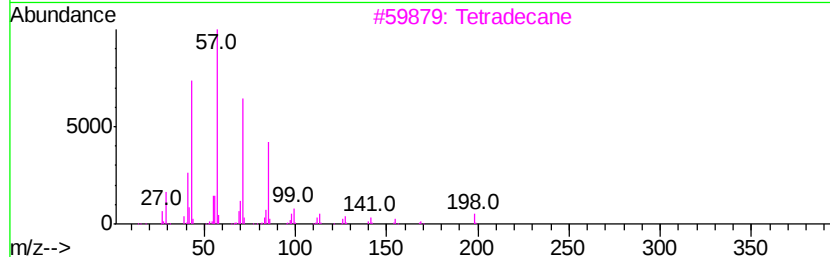
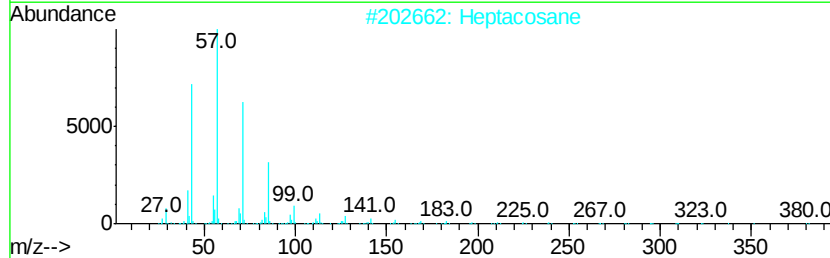
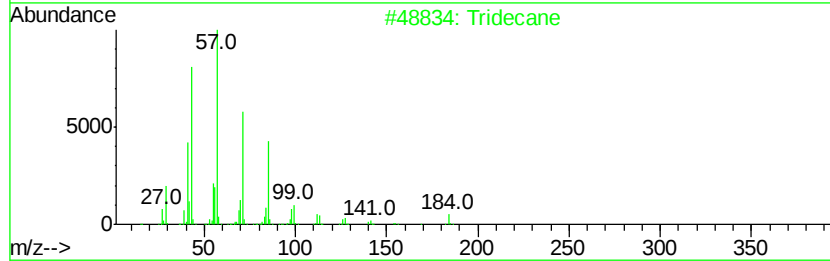
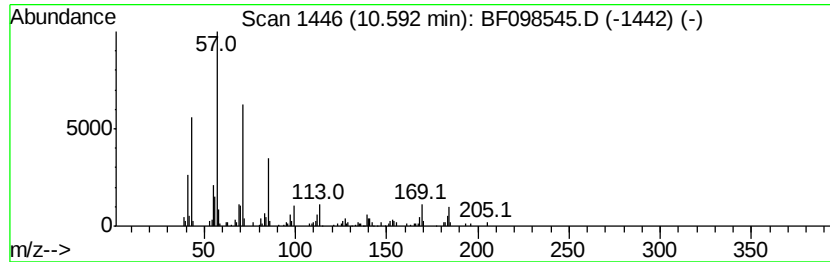
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	3.66 ng	178276	Phenanthrene-d10	11.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	90
2	Heptacosane		380	C27H56	000593-49-7	86
3	Tetradecane		198	C14H30	000629-59-4	86
4	Eicosane		282	C20H42	000112-95-8	80
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80



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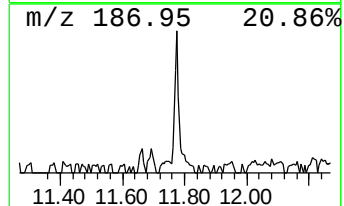
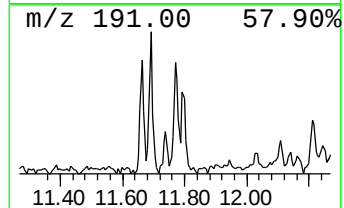
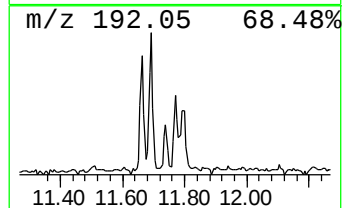
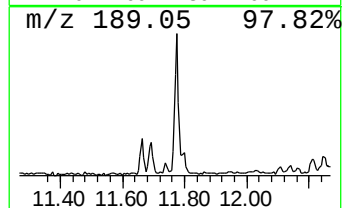
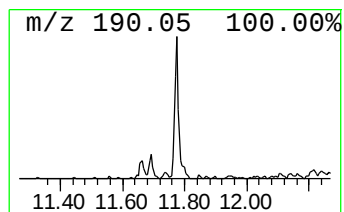
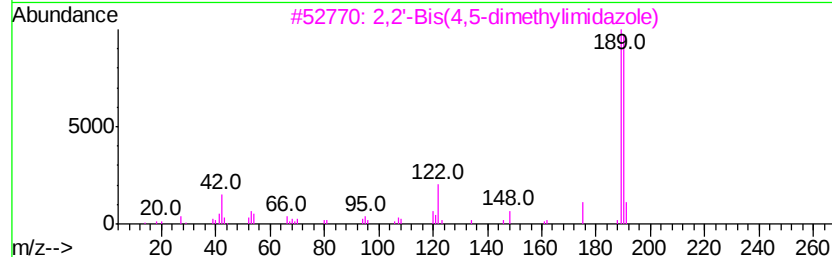
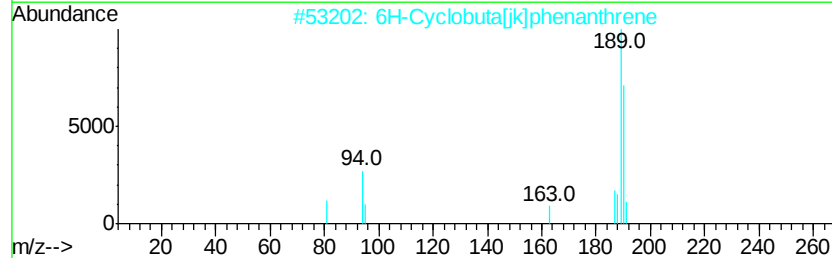
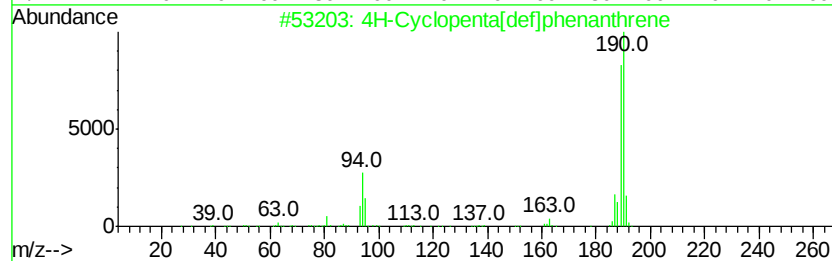
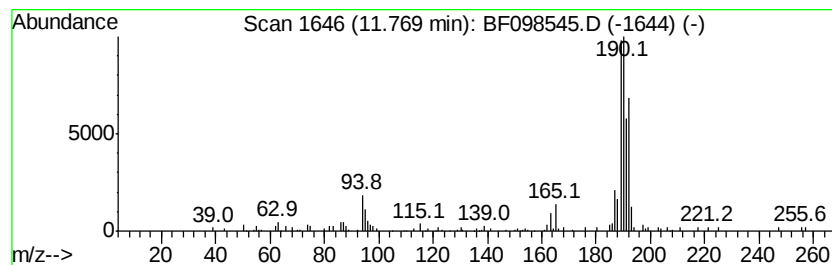
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	2.40 ng	116816	Phenanthrene-d10	11.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	74
2	6H-Cyclobuta[i]k]phenanthrene	190	C15H10	083469-43-6	64
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	49
4	Benzo[1,2-b:5,4-b']dithiophene	190	C10H6S2	000267-61-8	22
5	Benzo[1,2-b:3,4-b']dithiophene	190	C10H6S2	000211-02-9	22



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ClientSampleId :
RL-12-0-13

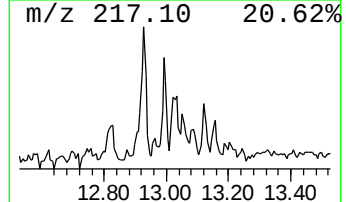
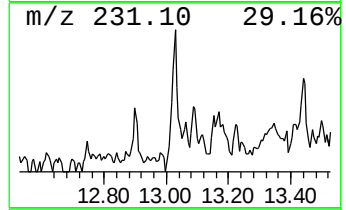
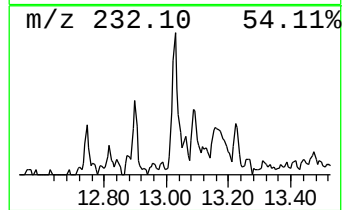
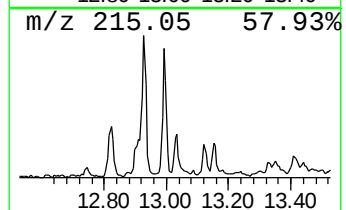
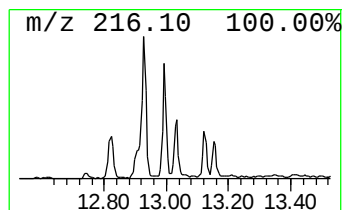
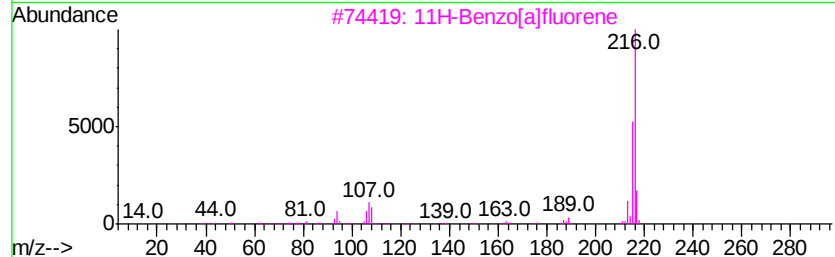
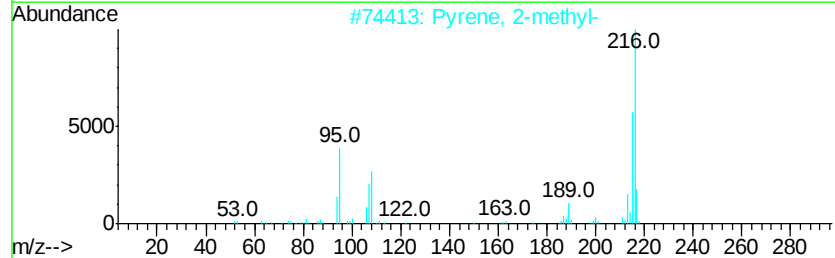
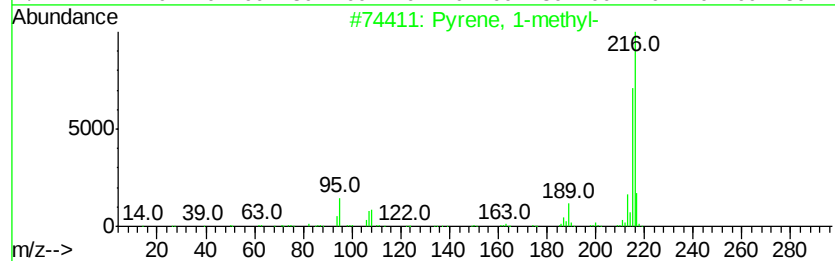
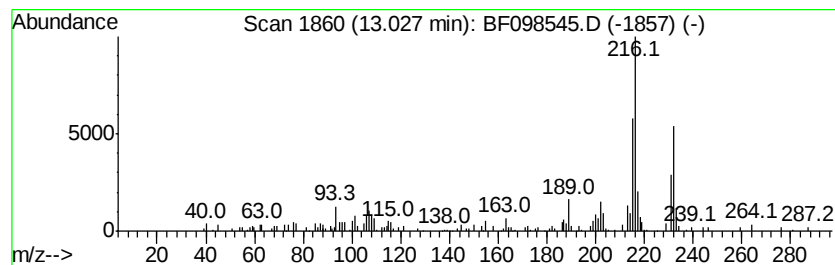
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	2.08 ng	124524	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
2		Pyrene, 2-methyl-	216	C17H12	003442-78-2	64
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	60
4		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	49
5		Pyrene, 4-methyl-	216	C17H12	003353-12-6	49



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091417\
Data File : BF098545.D
Acq On : 14 Sep 2017 23:18
Operator : SJ/JU
Sample : I5161-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

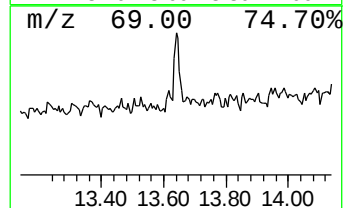
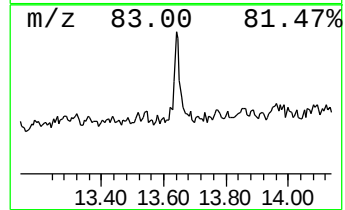
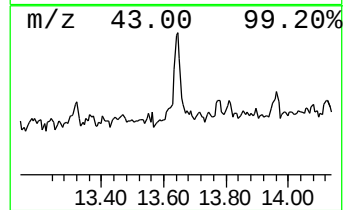
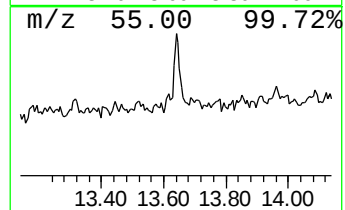
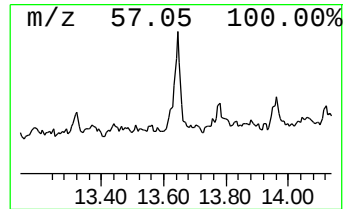
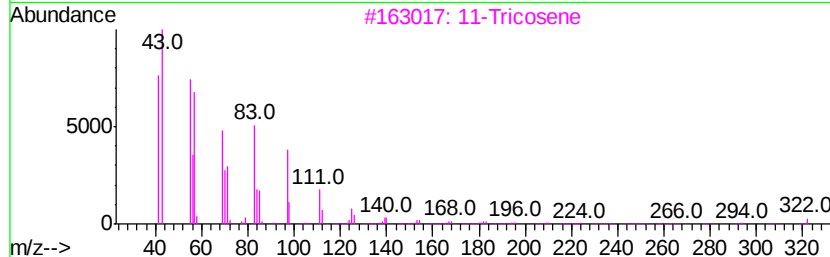
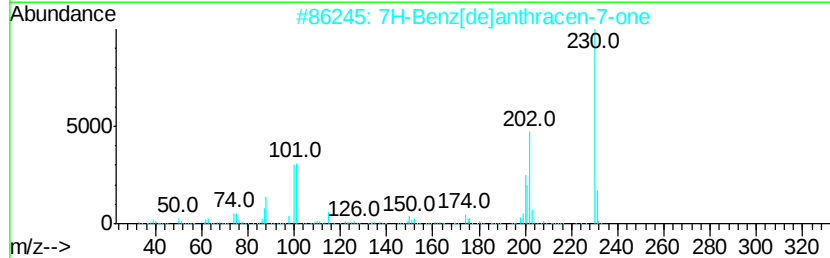
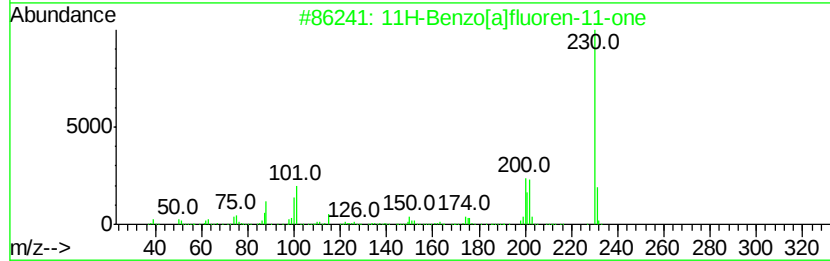
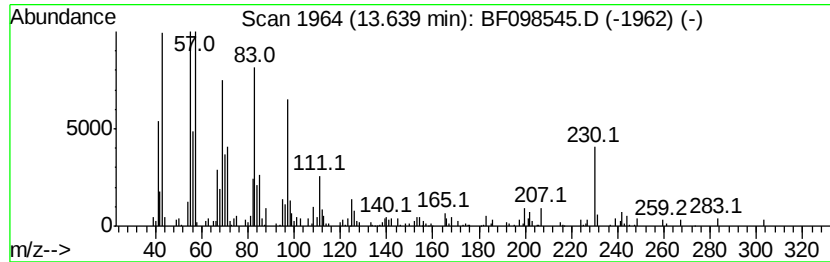
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ClientSampleId :
RL-12-0-13

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.64	3.15 ng	188611	Chrysene-d12	13.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[alfluoren-11-one	230	C17H10O	000479-79-8	70
2	7H-Benz[delanthracen-7-one	230	C17H10O	000082-05-3	49
3	11-Tricosene	322	C23H46	052078-56-5	30
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	30
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	30



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091417\
Data File : BF098545.D
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Misc :
ALS Vial : 15 Sample Multiplier: 1

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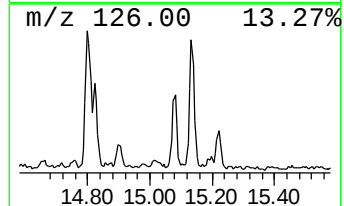
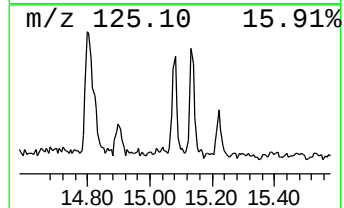
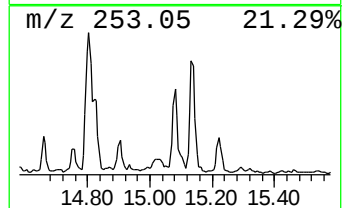
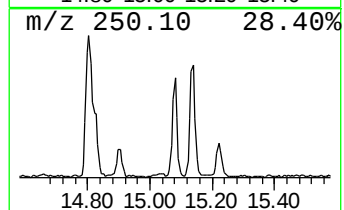
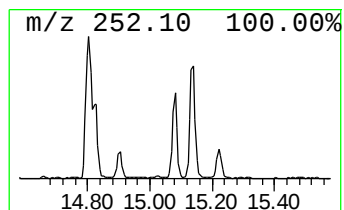
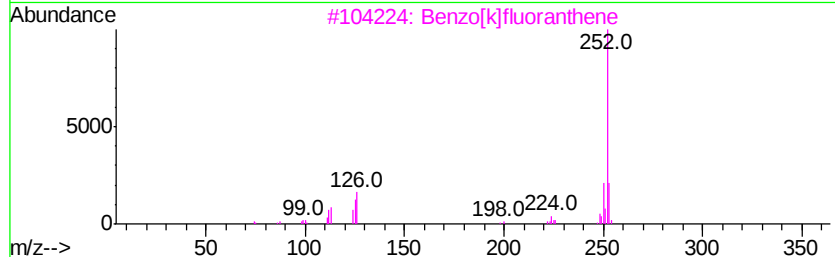
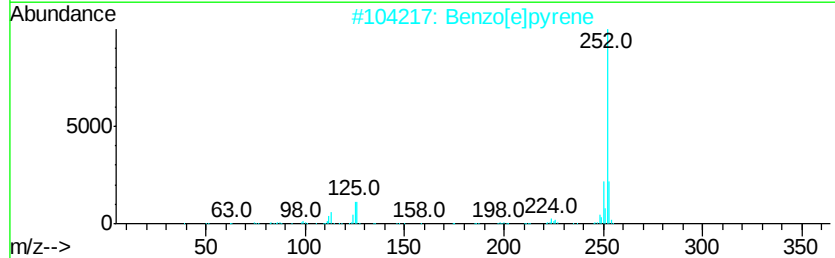
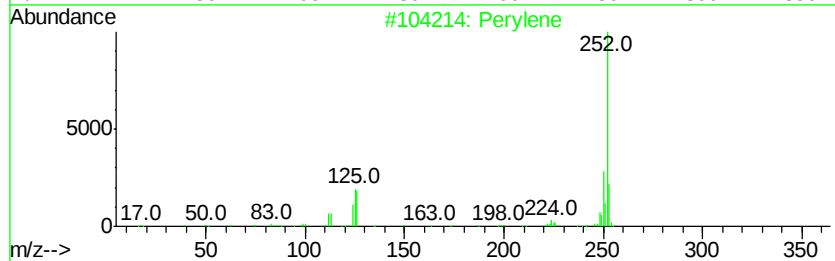
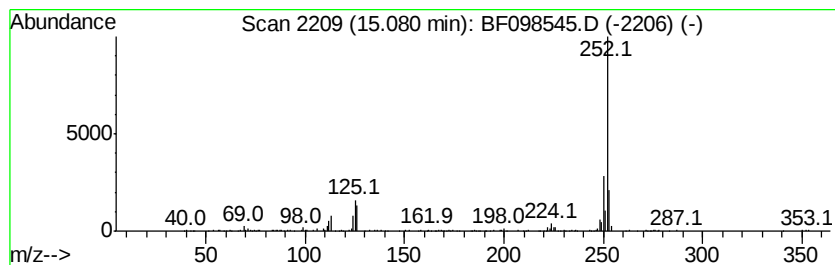
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	6.95 ng	289159	Perylene-d12	15.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Perylene	252	C20H12	000198-55-0	99
2		Benzo[e]pyrene	252	C20H12	000192-97-2	99
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4		Benzo[a]pyrene	252	C20H12	000050-32-8	95
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091417\
Data File : BF098545.D
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Operator : SJ/JU
Sample : I5161-13
Misc :
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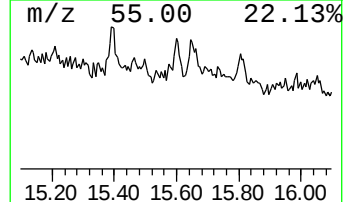
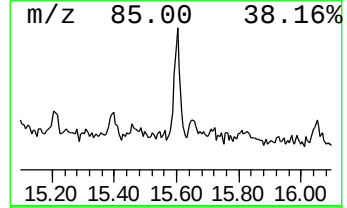
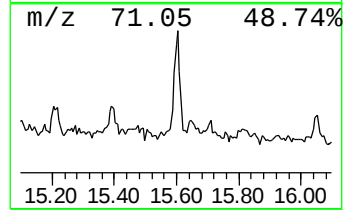
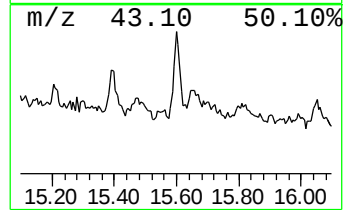
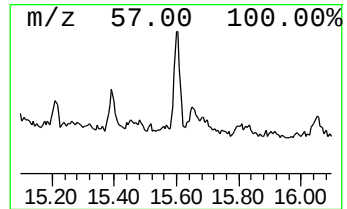
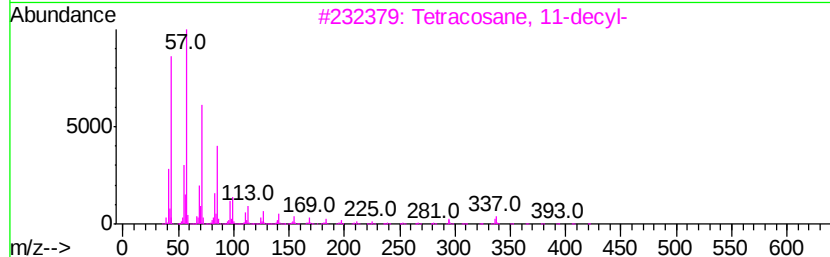
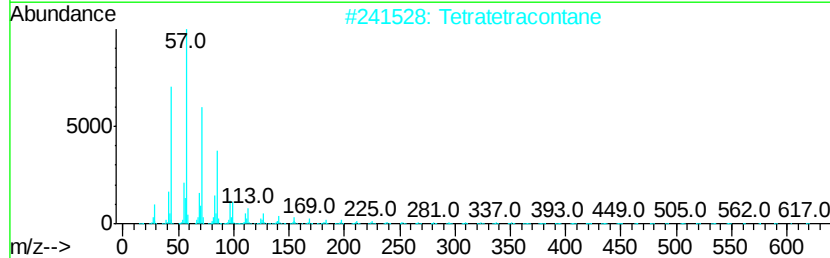
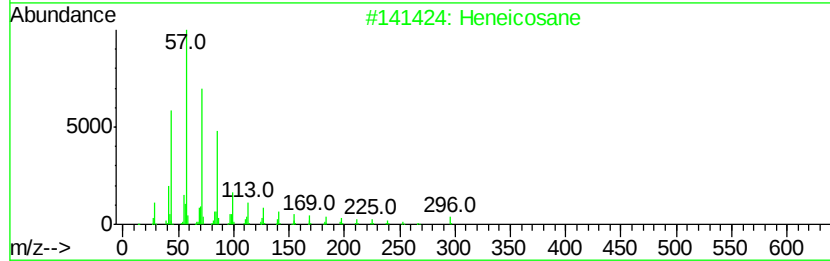
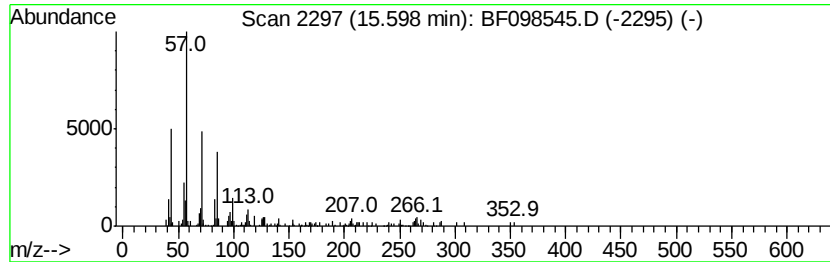
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.79 ng	115982	Perylene-d12	15.19
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Tetratetracontane	619 C44H90	007098-22-8	87
3	Tetracosane, 11-decyl-	479 C34H70	055429-84-0	87
4	2-methyloctacosane	408 C29H60	1000376-72-8	87
5	Tricosane	324 C23H48	000638-67-5	86



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091417\
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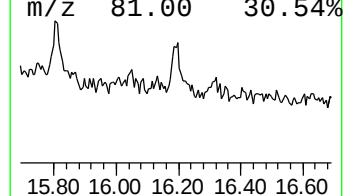
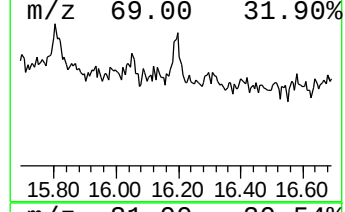
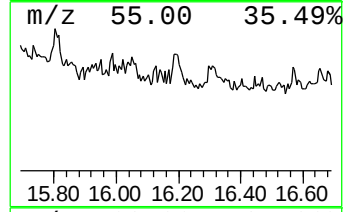
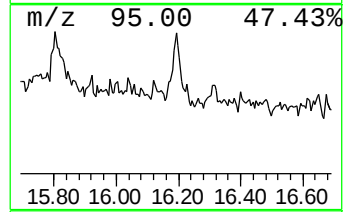
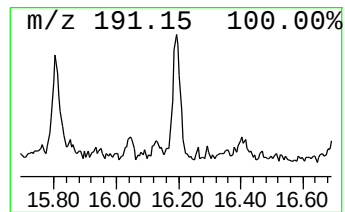
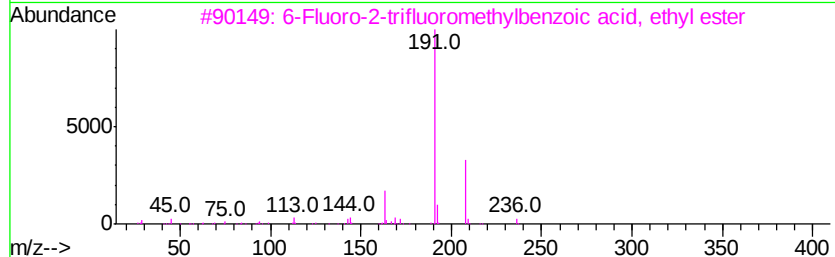
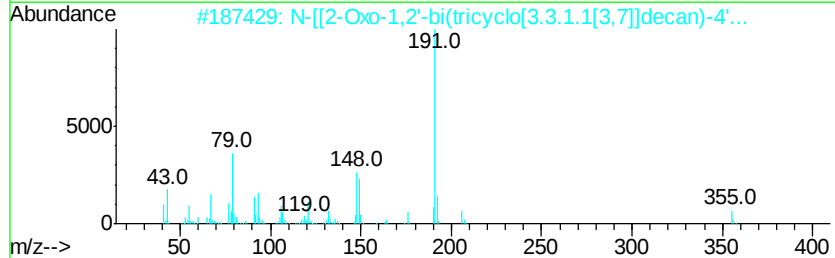
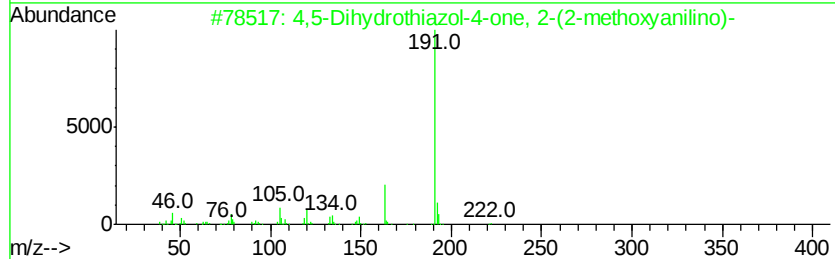
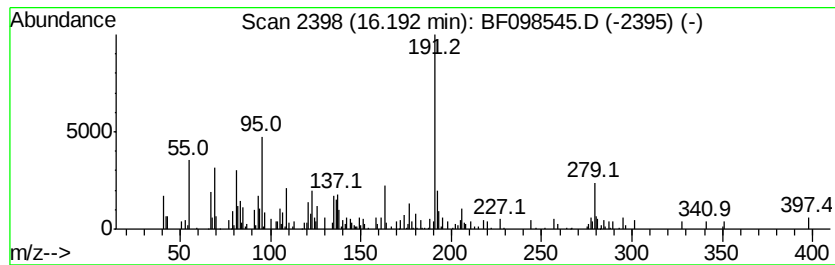
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.19 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	4.93 ng	205234	Perylene-d12	15.19
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	4,5-Dihydrothiazol-4-one, 2-(2-m...	222	C10H10N2O2S	022476-61-5 38
2	N-[[2-Oxo-1,2'-bi(tricyclo[3.3.1...	355	C23H33N02	1000305-39-6 35
3	6-Fluoro-2-trifluoromethylbenzoi...	236	C10H8F4O2	1000338-97-5 35
4	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6 35
5	2-Fluoro-5-(trifluoromethyl)prop...	220	C10H8F4O	207974-18-3 30



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091417\
Data File : BF098545.D
Acq On : 14 Sep 2017 23:18
Operator : SJ/JU
Sample : I5161-13
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-BF091117.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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unknown6.42	6.42	80.3	ng	3396650	1	6.65	846487	20.0
Tridecane	10.59	3.7	ng	178276	4	11.16	973279	20.0
4H-Cyclopenta[def...	11.77	2.4	ng	116816	4	11.16	973279	20.0
Pyrene, 1-methyl-	13.03	2.1	ng	124524	5	13.80	1197300	20.0
11H-Benzo[a]fluor...	13.64	3.1	ng	188611	5	13.80	1197300	20.0
Perylene	15.08	7.0	ng	289159	6	15.19	832036	20.0
Heneicosane	15.60	2.8	ng	115982	6	15.19	832036	20.0
unknown16.19	16.19	4.9	ng	205234	6	15.19	832036	20.0