

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
 Data File : BF104845.D
 Acq On : 26 Apr 2018 18:53
 Operator : JU/SJ
 Sample : J2156-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-05-042518-A

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-BF040618.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	5.004	490	496	505	rVB	59322	79376	4.21%	0.421%
2	5.263	536	540	544	rBV	48515	44282	2.35%	0.235%
3	5.375	555	559	560	rBV	25446	25979	1.38%	0.138%
4	5.416	562	566	581	rVB	1938901	1798640	95.50%	9.541%
5	6.440	736	740	753	rBV	1784484	1866230	99.09%	9.899%
6	6.569	758	762	766	rVV	2077762	1883416	100.00%	9.990%
7	6.622	768	771	774	rVB	29191	26009	1.38%	0.138%
8	6.798	797	801	807	rBV	748557	597206	31.71%	3.168%
9	6.951	823	827	831	rBV	1515288	1400480	74.36%	7.429%
10	7.363	893	897	900	rBV	1199818	1084214	57.57%	5.751%
11	8.057	1012	1015	1016	rBV	77822	59602	3.16%	0.316%
12	8.081	1016	1019	1025	rVV	836737	767882	40.77%	4.073%
13	8.134	1025	1028	1031	rVV2	50870	57399	3.05%	0.304%
14	8.163	1031	1033	1041	rVB6	18845	28780	1.53%	0.153%
15	8.281	1050	1053	1055	rVB3	22632	21766	1.16%	0.115%
16	8.369	1064	1068	1072	rVB5	41951	46523	2.47%	0.247%
17	8.451	1080	1082	1086	rVB4	24212	26898	1.43%	0.143%
18	8.492	1086	1089	1091	rBV	72353	55745	2.96%	0.296%
19	8.581	1102	1104	1107	rBV3	39120	38917	2.07%	0.206%
20	8.663	1116	1118	1122	rBV	154472	125514	6.66%	0.666%
21	8.739	1127	1131	1133	rBV4	17612	23053	1.22%	0.122%
22	8.851	1148	1150	1153	rBV3	14764	20095	1.07%	0.107%
23	8.898	1156	1158	1161	rVV	51126	45125	2.40%	0.239%
24	8.945	1164	1166	1170	rVV3	30583	37193	1.97%	0.197%
25	8.981	1170	1172	1176	rVB4	27576	39164	2.08%	0.208%
26	9.028	1176	1180	1185	rBV4	47610	63768	3.39%	0.338%
27	9.069	1185	1187	1189	rVB	40002	24778	1.32%	0.131%
28	9.092	1189	1191	1194	rBV	109584	87927	4.67%	0.466%
29	9.157	1198	1202	1206	rBV	2051061	1639460	87.05%	8.696%
30	9.228	1211	1214	1218	rVV	175518	169508	9.00%	0.899%
31	9.269	1218	1221	1223	rVV3	32850	34730	1.84%	0.184%
32	9.304	1225	1227	1230	rVB2	47273	39055	2.07%	0.207%
33	9.428	1245	1248	1252	rVB5	23253	25915	1.38%	0.137%
34	9.469	1252	1255	1256	rBV2	23826	24204	1.29%	0.128%

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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

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35	9.551	1265	1269	1272	rBV	278552	276011	14.65%	1.464%
36	9.610	1276	1279	1282	rVB4	33699	27373	1.45%	0.145%
37	9.698	1291	1294	1297	rBV4	33443	36290	1.93%	0.192%
38	9.763	1302	1305	1309	rVB	112786	103586	5.50%	0.549%
39	9.798	1309	1311	1313	rBV2	22340	25198	1.34%	0.134%
40	9.839	1314	1318	1321	rVB	809239	681883	36.20%	3.617%
41	9.939	1332	1335	1339	rVB4	23267	29367	1.56%	0.156%
42	9.992	1340	1344	1346	rBV4	28834	41332	2.19%	0.219%
43	10.045	1351	1353	1356	rVB3	29984	30885	1.64%	0.164%
44	10.081	1356	1359	1363	rBV3	54254	61535	3.27%	0.326%
45	10.116	1363	1365	1368	rVB3	24176	21821	1.16%	0.116%
46	10.151	1368	1371	1375	rBV4	33341	52024	2.76%	0.276%
47	10.239	1383	1386	1387	rBV2	27993	29371	1.56%	0.156%
48	10.257	1387	1389	1392	rVB2	104256	92134	4.89%	0.489%
49	10.316	1397	1399	1405	rVB5	21122	29478	1.57%	0.156%
50	10.480	1423	1427	1429	rBV	87362	92336	4.90%	0.490%
51	10.533	1433	1436	1438	rVB4	25072	22329	1.19%	0.118%
52	10.633	1449	1453	1462	rBV	998463	983117	52.20%	5.215%
53	10.745	1468	1472	1480	rVB	156871	210483	11.18%	1.116%
54	10.922	1500	1502	1507	rBV4	22496	37662	2.00%	0.200%
55	10.957	1507	1508	1512	rVB4	24895	22999	1.22%	0.122%
56	11.057	1522	1525	1527	rBV4	17994	22454	1.19%	0.119%
57	11.180	1544	1546	1548	rBV	45407	36200	1.92%	0.192%
58	11.210	1548	1551	1554	rVV	84312	71361	3.79%	0.379%
59	11.327	1567	1571	1574	rBV	714822	626867	33.28%	3.325%
60	11.563	1608	1611	1614	rVB3	29644	27132	1.44%	0.144%
61	11.610	1616	1619	1622	rVB	35461	31799	1.69%	0.169%
62	11.669	1622	1629	1633	rBV10	19262	45575	2.42%	0.242%
63	12.404	1752	1754	1758	rVB5	26293	35928	1.91%	0.191%
64	12.504	1769	1771	1775	rVB5	24468	22395	1.19%	0.119%
65	12.545	1775	1778	1781	rBV	41442	42359	2.25%	0.225%
66	12.774	1815	1817	1820	rBV2	47492	49234	2.61%	0.261%
67	12.916	1837	1841	1844	rBV	1553450	1277442	67.83%	6.776%
68	13.804	1989	1992	1998	rVB	129900	126356	6.71%	0.670%
69	13.980	2018	2022	2030	rBV	668206	693743	36.83%	3.680%
70	15.451	2268	2272	2276	rVB	437457	527754	28.02%	2.799%

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Integration Parameters: rteint.p
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Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

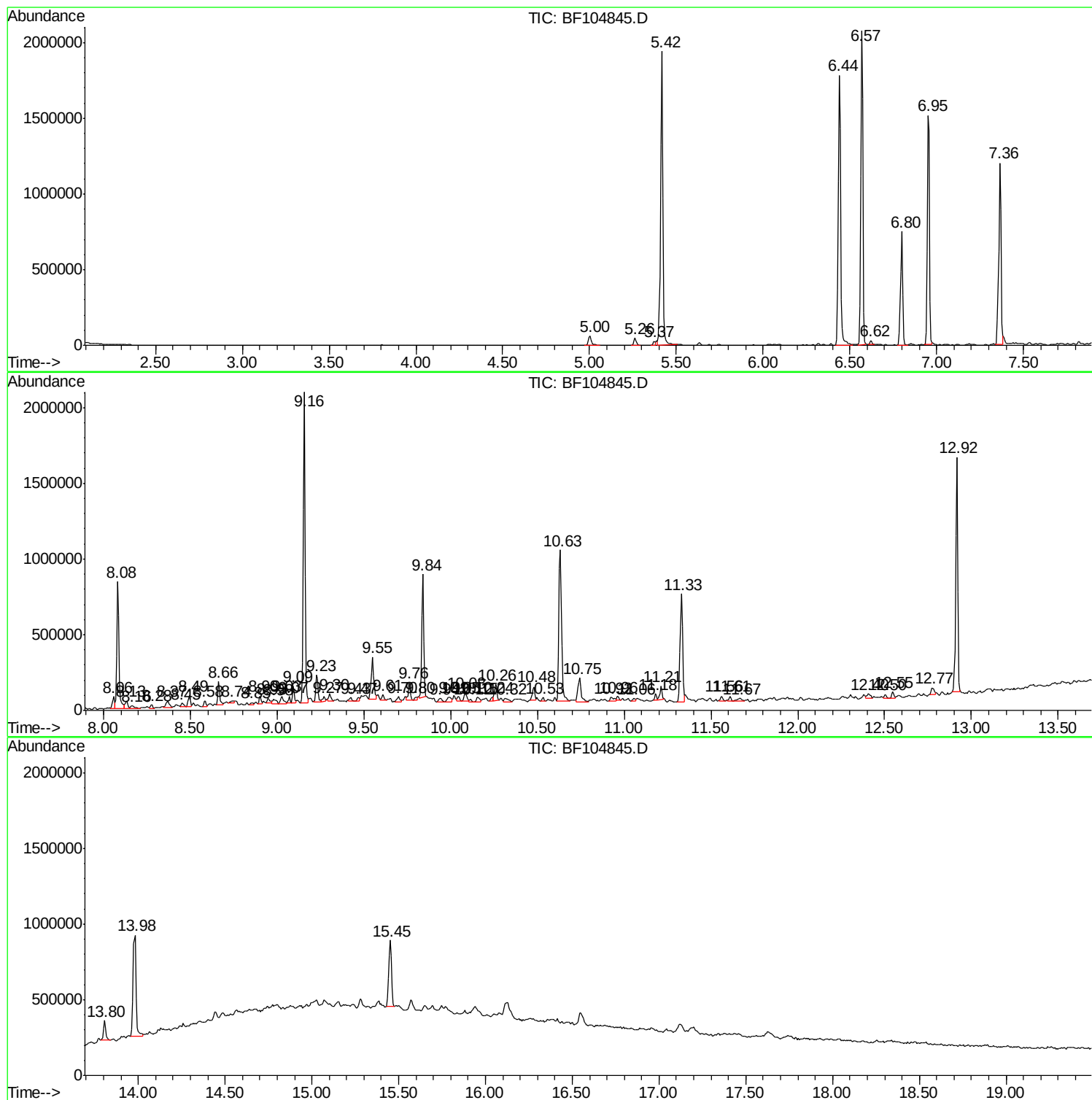
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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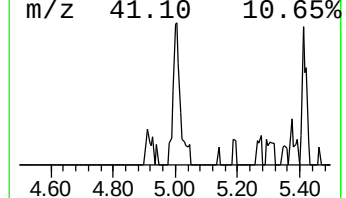
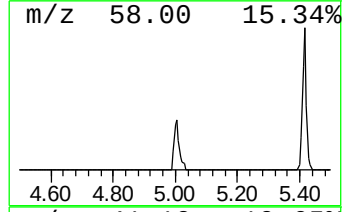
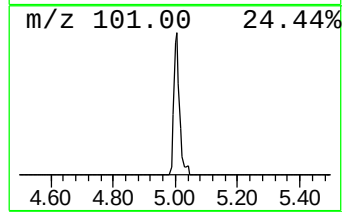
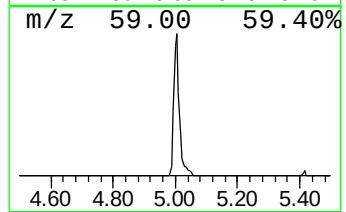
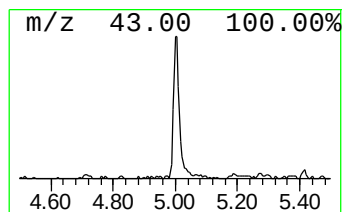
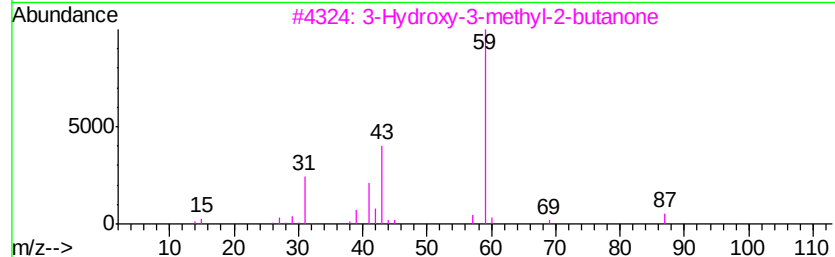
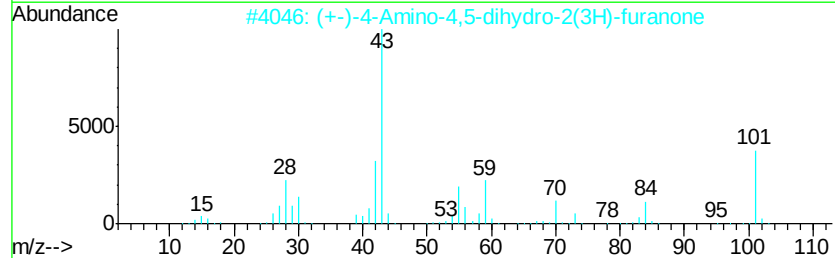
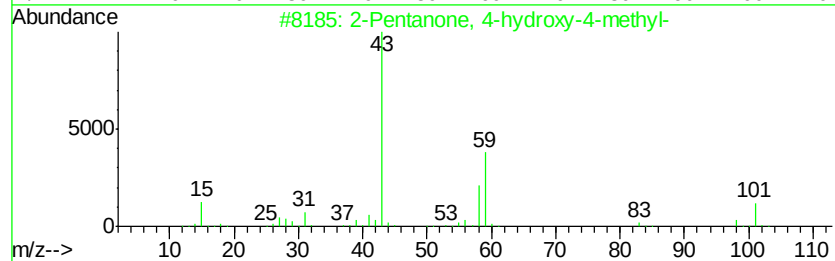
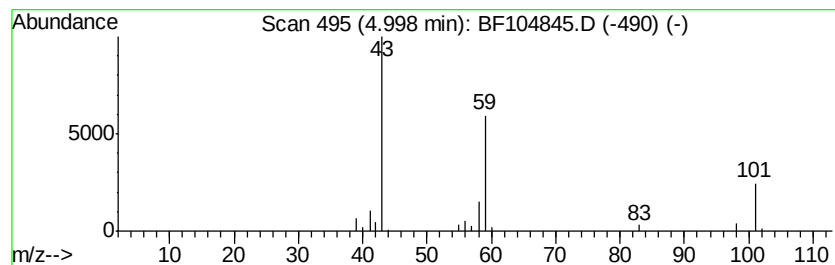
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.00	2.66 ng	79376	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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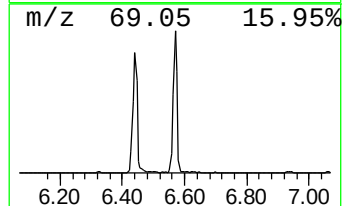
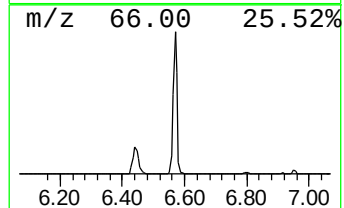
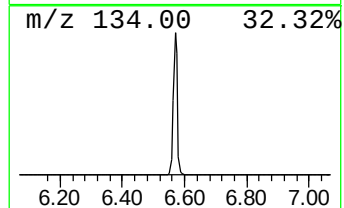
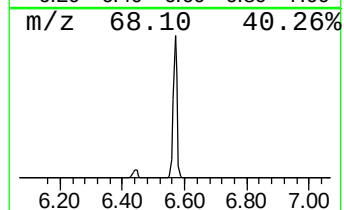
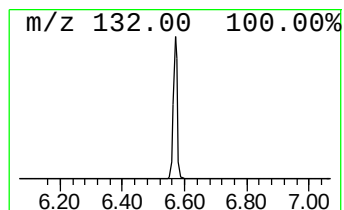
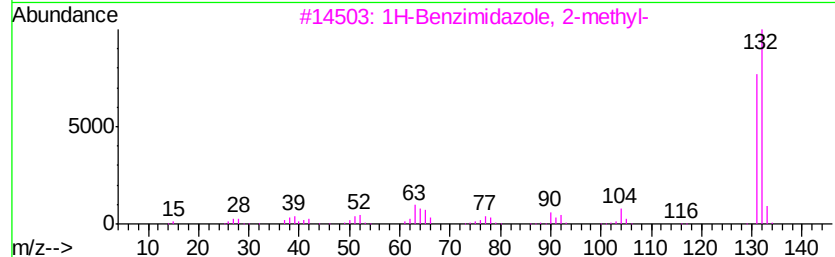
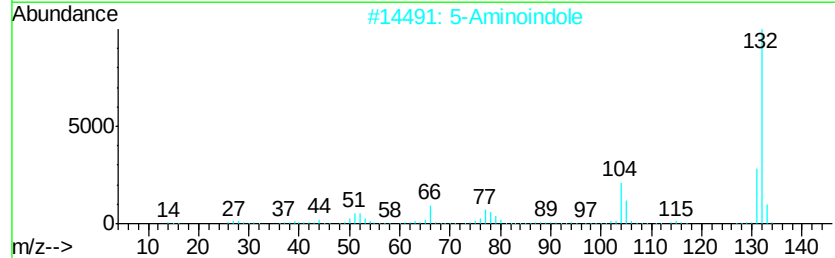
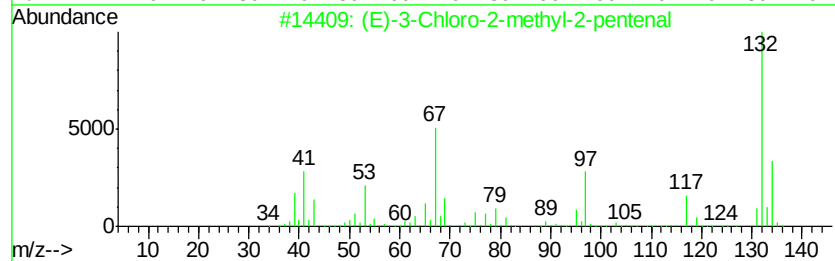
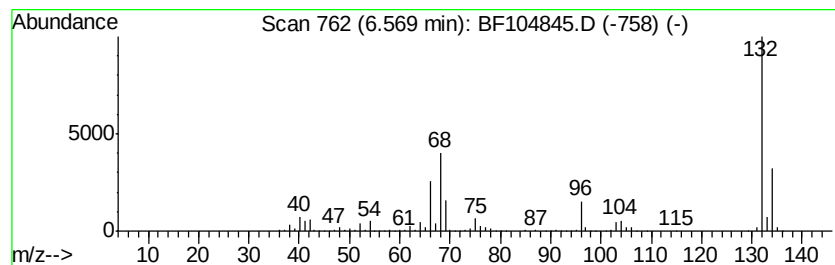
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	63.07 ng	1883420	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17		
2	5-Aminoindole	132	C8H8N2	005192-03-0	12		
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10		
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9		
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9		



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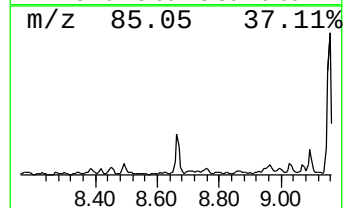
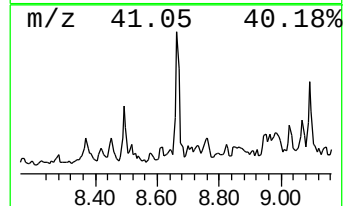
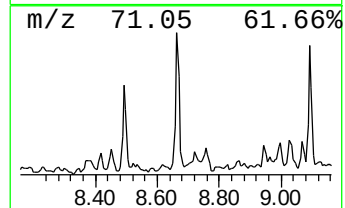
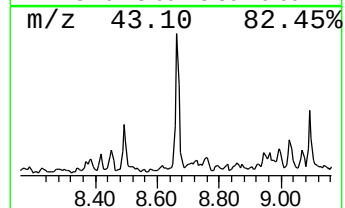
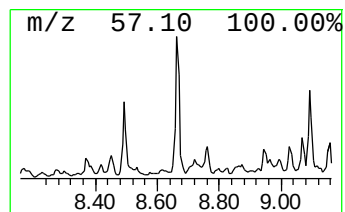
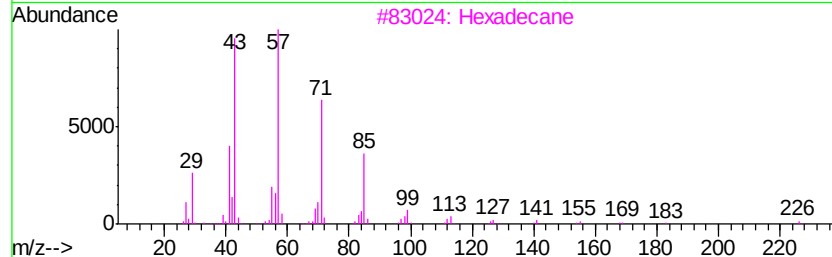
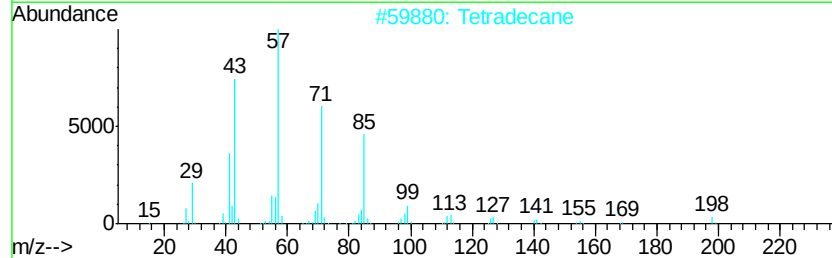
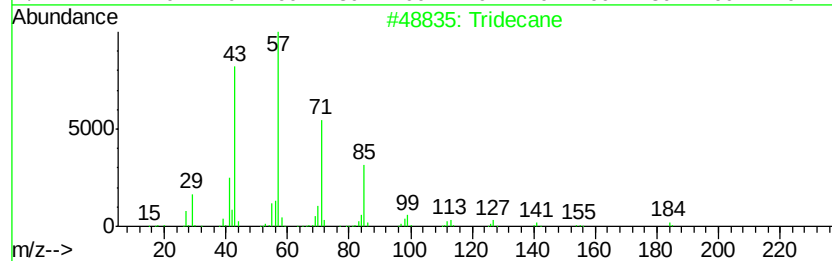
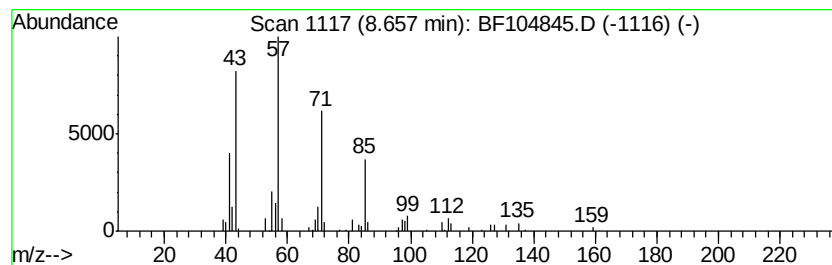
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
8.66	3.27 ng	125514	Naphthalene-d8		8.08
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	86
2	Tetradecane	198	C14H30	000629-59-4	80
3	Hexadecane	226	C16H34	000544-76-3	74
4	Pentadecane	212	C15H32	000629-62-9	72
5	Nonadecane	268	C19H40	000629-92-5	64



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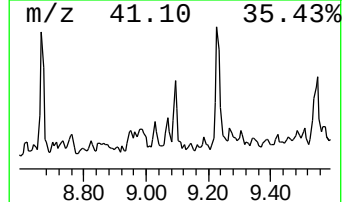
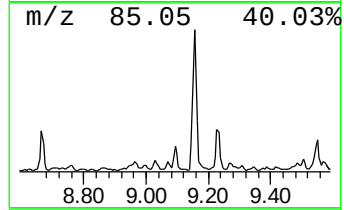
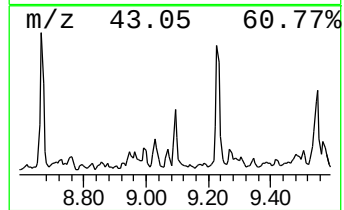
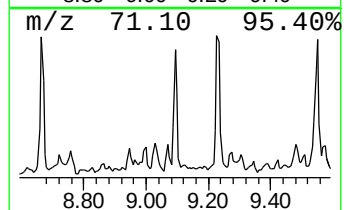
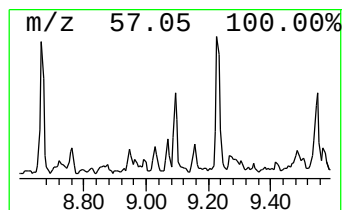
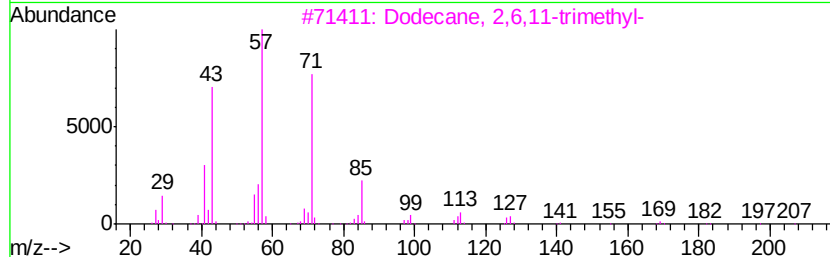
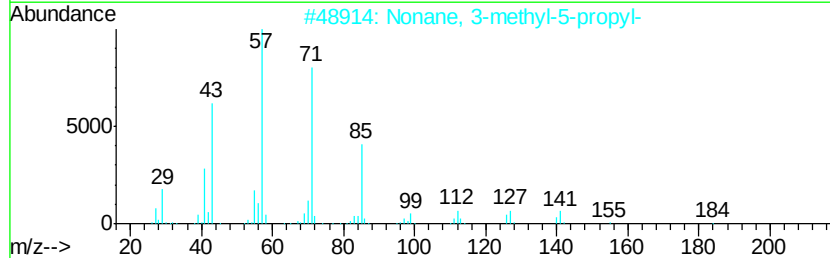
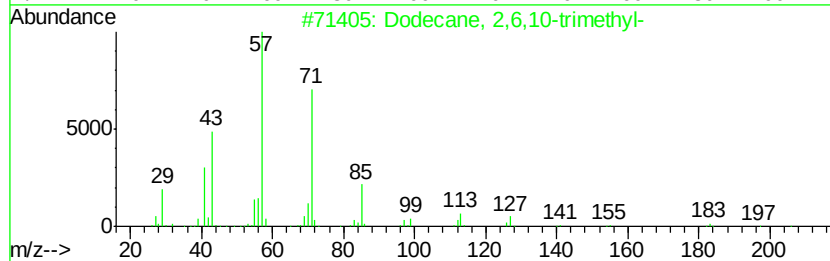
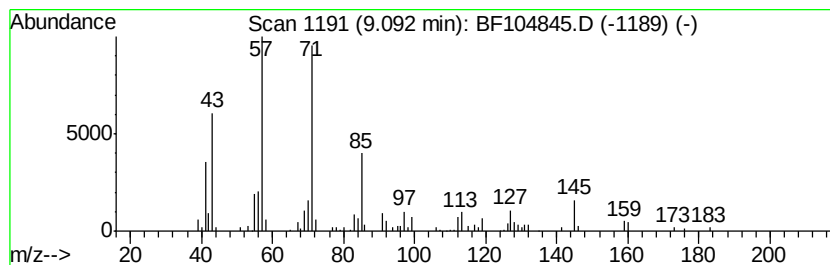
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 2,6,10-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	2.58 ng	87927	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
2		Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	59
3		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59
4		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	52
5		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
Data File : BF104845.D
Acq On : 26 Apr 2018 18:53
Operator : JU/SJ
Sample : J2156-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

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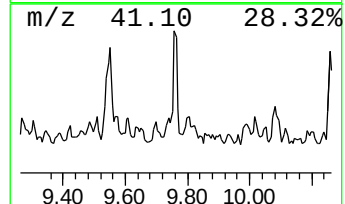
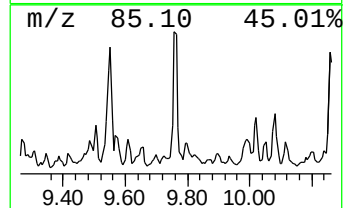
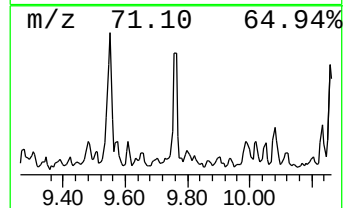
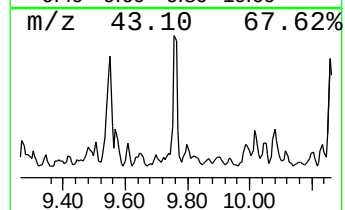
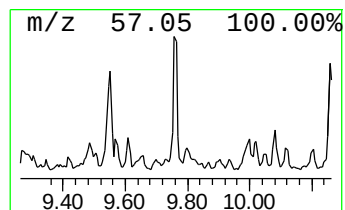
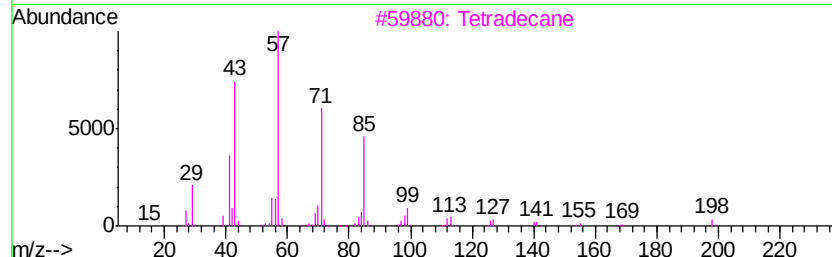
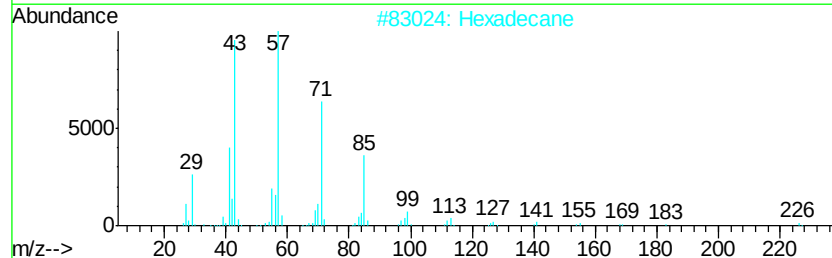
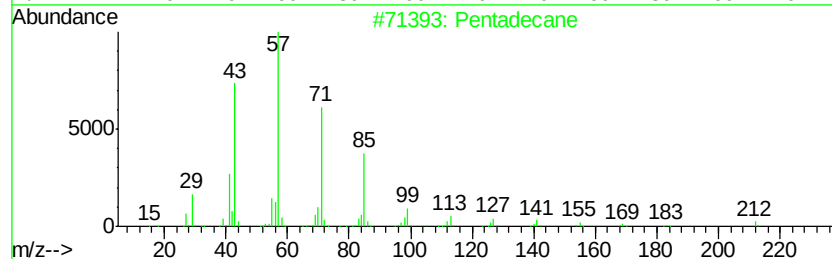
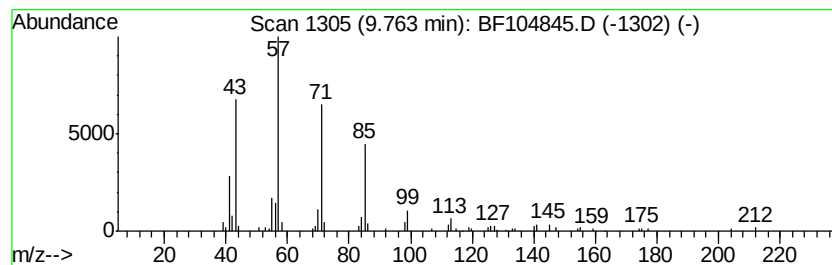
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.04 ng	103586	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	93
2		Hexadecane	226	C16H34	000544-76-3	90
3		Tetradecane	198	C14H30	000629-59-4	87
4		Tridecane	184	C13H28	000629-50-5	86
5		Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042618\
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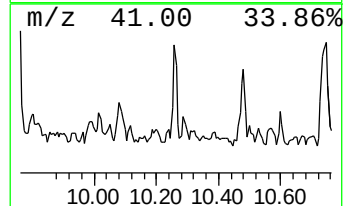
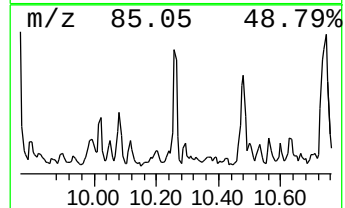
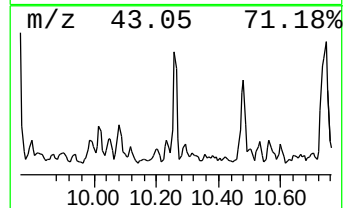
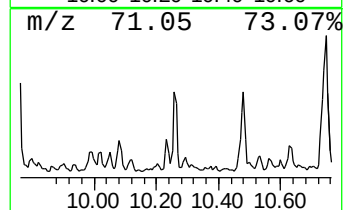
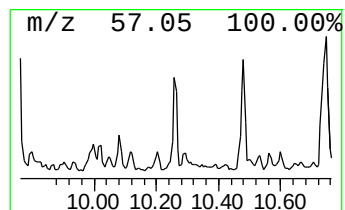
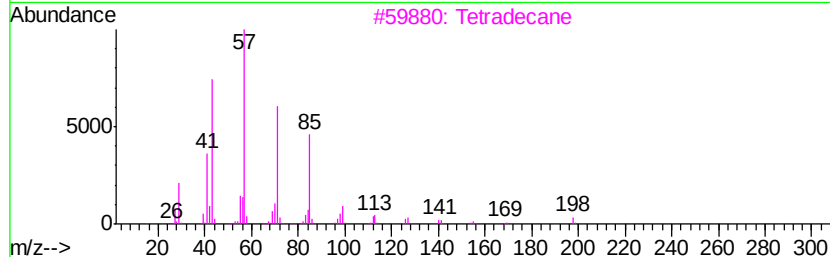
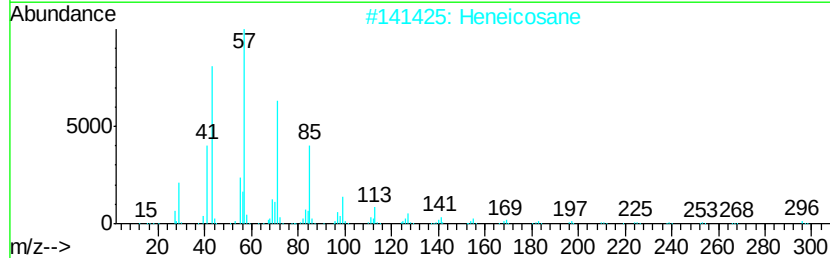
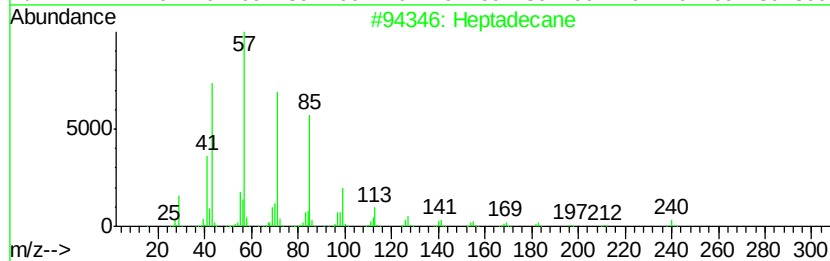
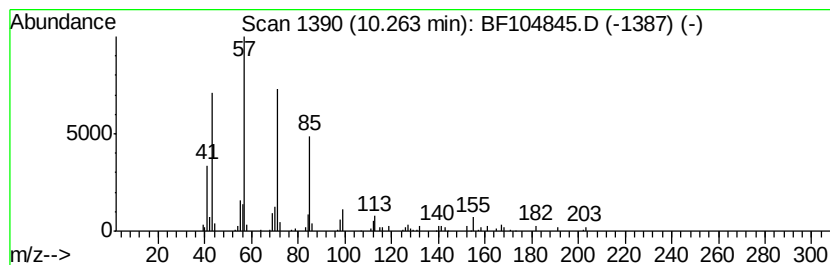
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.26	2.70 ng	92134	Acenaphthene-d10		9.84
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heneicosane	296	C21H44	000629-94-7	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
Data File : BF104845.D
Acq On : 26 Apr 2018 18:53
Operator : JU/SJ
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-05-042518-A

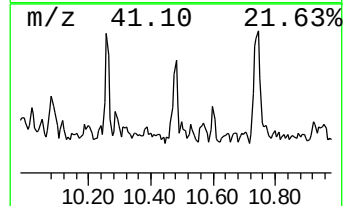
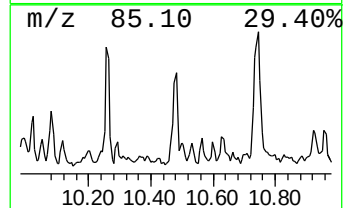
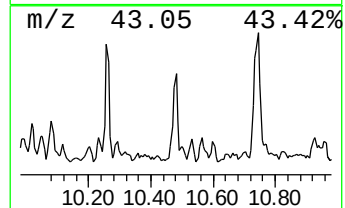
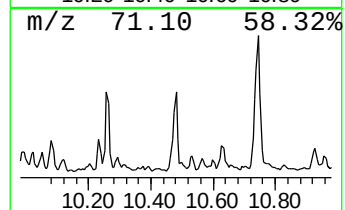
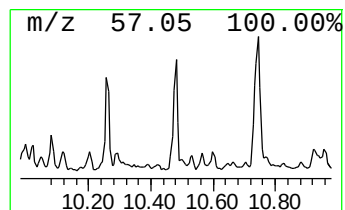
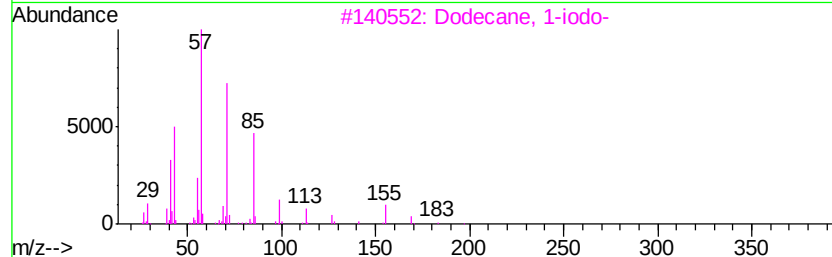
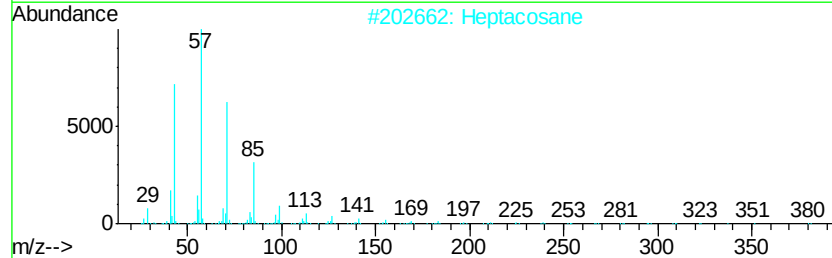
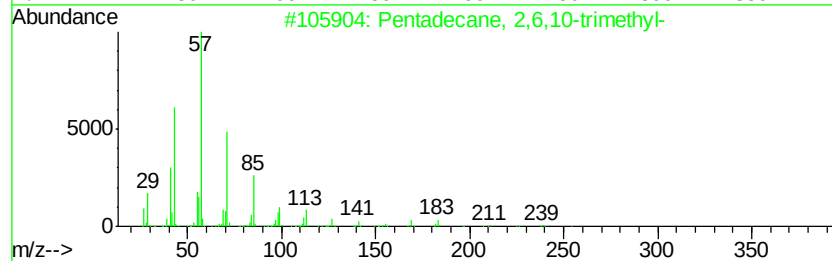
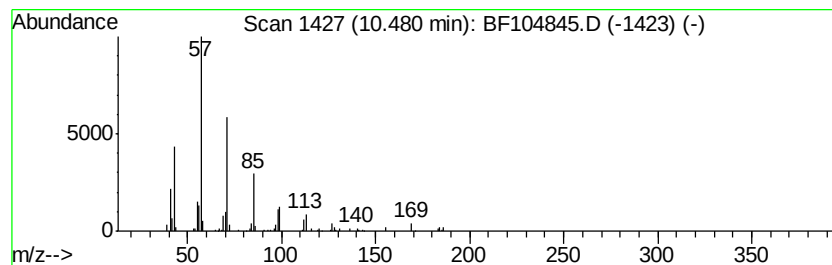
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.48	2.71 ng	92336	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	83
2		Heptacosane	380	C27H56	000593-49-7	72
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
4		Dodecane, 6-methyl-	184	C13H28	006044-71-9	64
5		Octadecane	254	C18H38	000593-45-3	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
Data File : BF104845.D
Acq On : 26 Apr 2018 18:53
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ALS Vial : 16 Sample Multiplier: 1

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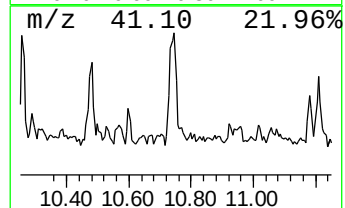
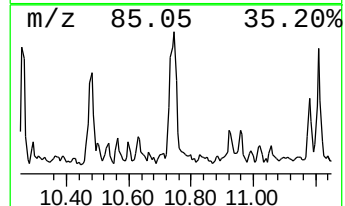
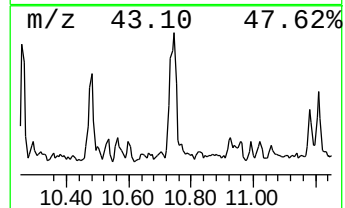
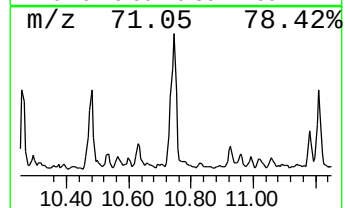
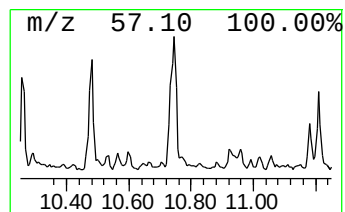
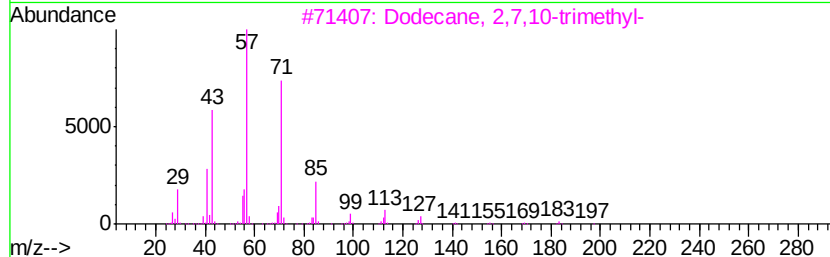
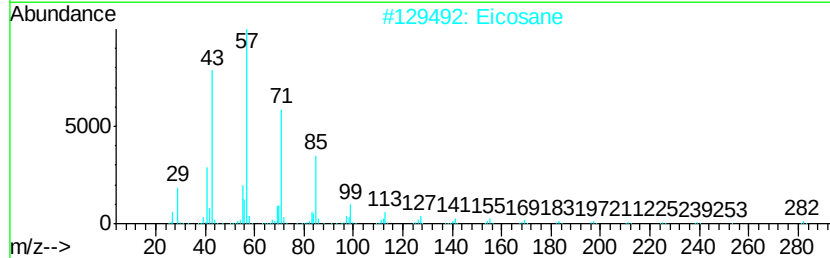
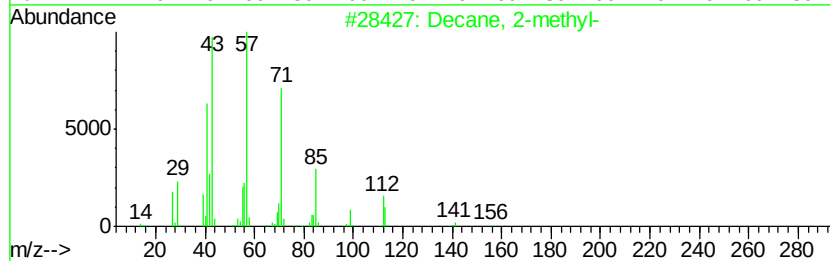
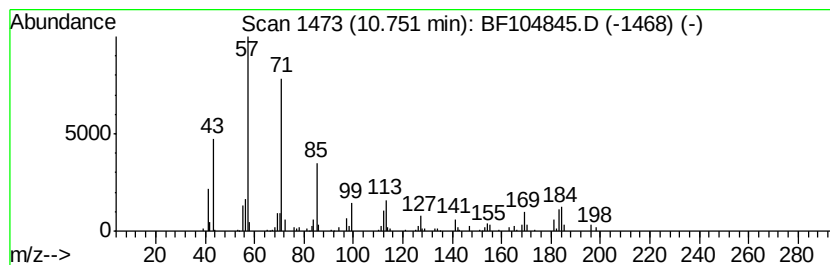
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Decane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	6.72 ng	210483	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2-methyl-	156	C11H24	006975-98-0	87
2		Eicosane	282	C20H42	000112-95-8	80
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
4		Tridecane, 7-methyl-	198	C14H30	026730-14-3	76
5		Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
Data File : BF104845.D
Acq On : 26 Apr 2018 18:53
Operator : JU/SJ
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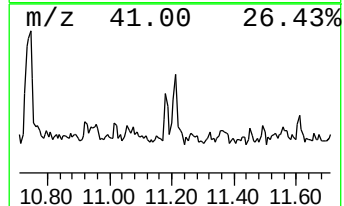
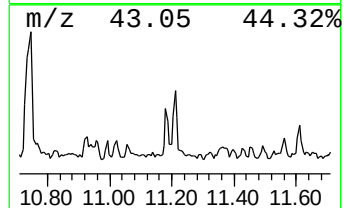
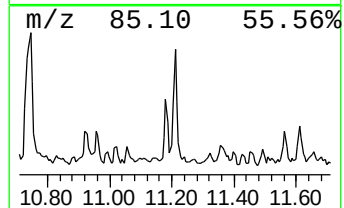
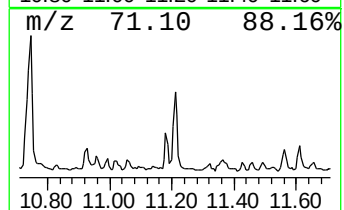
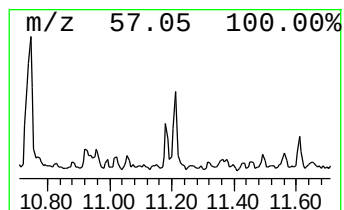
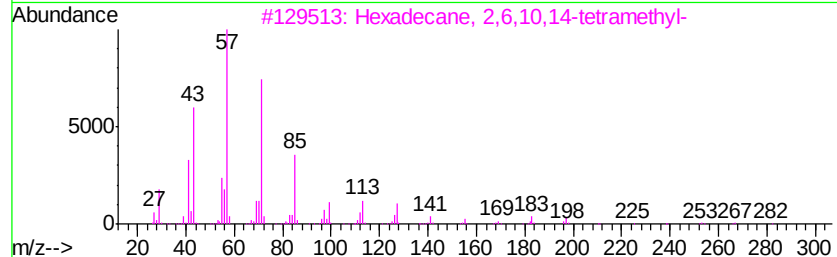
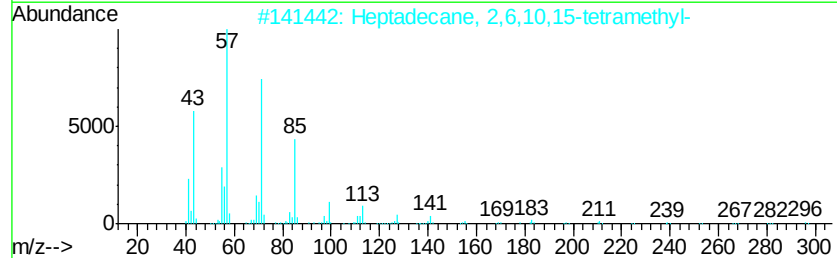
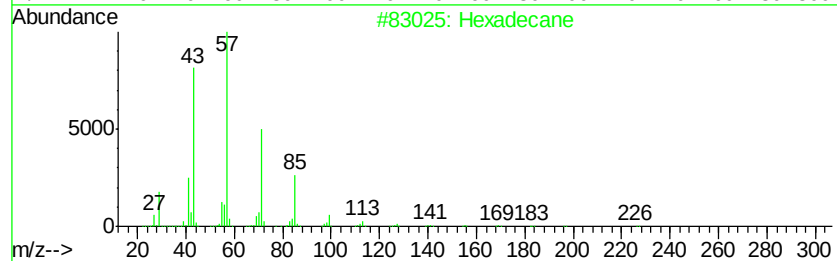
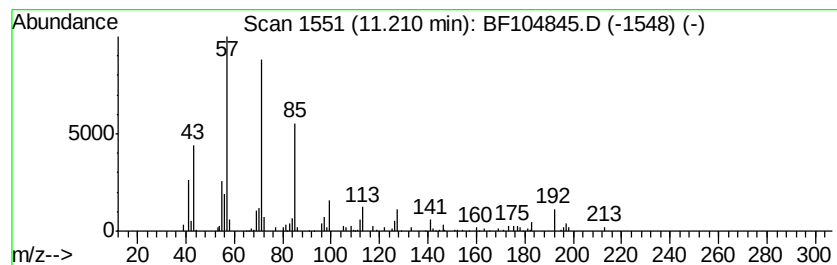
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	2.28 ng	71361	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	86
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4		Tetradecane	198	C14H30	000629-59-4	78
5		2-methyltetracosane	352	C25H52	1000376-72-6	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
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Acq On : 26 Apr 2018 18:53
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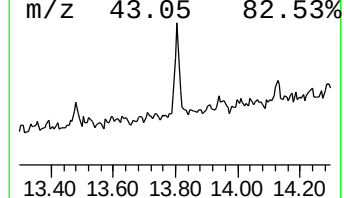
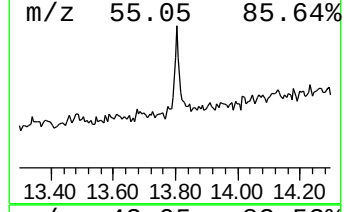
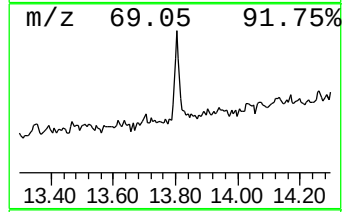
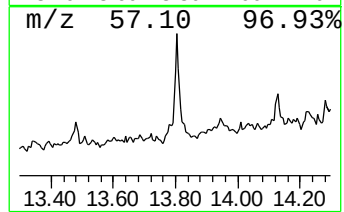
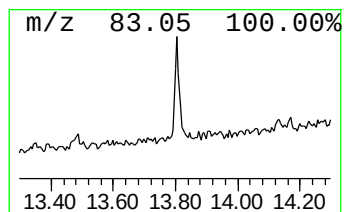
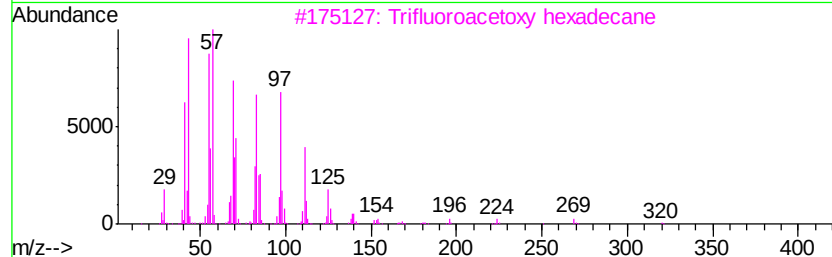
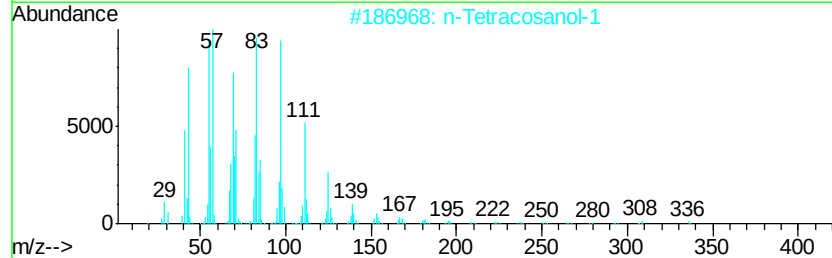
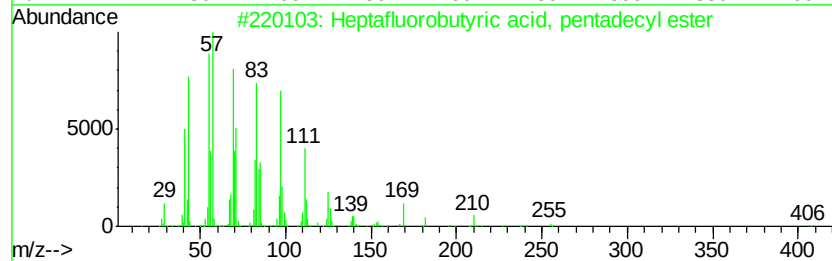
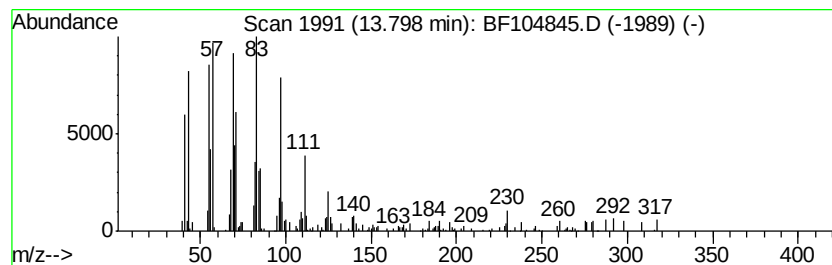
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.64 ng	126356	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042618\
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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unknown6.57	6.57	63.1	ng	1883420	1	6.80	597206	20.0
Tridecane	8.66	3.3	ng	125514	2	8.08	767882	20.0
Dodecane, 2,6,10-...	9.09	2.6	ng	87927	3	9.84	681883	20.0
Pentadecane	9.76	3.0	ng	103586	3	9.84	681883	20.0
Heptadecane	10.26	2.7	ng	92134	3	9.84	681883	20.0
Pentadecane, 2,6,...	10.48	2.7	ng	92336	3	9.84	681883	20.0
Decane, 2-methyl-	10.75	6.7	ng	210483	4	11.33	626867	20.0
Hexadecane	11.21	2.3	ng	71361	4	11.33	626867	20.0
Heptafluorobutyri...	13.80	3.6	ng	126356	5	13.98	693743	20.0