

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
 Data File : BF083770.D
 Acq On : 14 Dec 2015 10:41
 Operator : UM/IZ
 Sample : G4648-22
 Misc :
 ALS Vial : 60 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-06(0-0.16)

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-BF121315.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	2.212	9	11	21	rVB3	18349	50339	1.77%	0.139%
2	5.116	262	265	271	rBV	417342	577476	20.25%	1.590%
3	5.527	298	301	304	rVB	2313029	2466325	86.51%	6.792%
4	6.544	387	390	393	rBV	1924826	2508782	87.99%	6.909%
5	6.693	400	403	405	rBV	2283920	2851051	100.00%	7.852%
6	6.921	420	423	425	rBV	754354	676767	23.74%	1.864%
7	7.081	434	437	439	rVB	2076672	2272560	79.71%	6.259%
8	7.482	469	472	474	rBV	1759319	1860937	65.27%	5.125%
9	7.562	477	479	484	rVB	41963	40528	1.42%	0.112%
10	8.202	533	535	540	rBV	964275	849037	29.78%	2.338%
11	9.276	626	629	632	rBV	2619671	2573454	90.26%	7.087%
12	9.665	662	663	666	rVB	443565	467707	16.40%	1.288%
13	9.893	681	683	686	rVB	74506	56978	2.00%	0.157%
14	9.950	686	688	691	rBV	709026	815710	28.61%	2.246%
15	10.373	723	725	726	rBV	51661	73666	2.58%	0.203%
16	10.396	726	727	728	rVB	97464	67598	2.37%	0.186%
17	10.613	743	746	749	rBV	33607	57143	2.00%	0.157%
18	10.739	755	757	760	rBV	1589723	1480037	51.91%	4.076%
19	10.865	766	768	772	rVB	116902	136890	4.80%	0.377%
20	10.945	772	775	778	rBV4	17699	40095	1.41%	0.110%
21	11.059	783	785	787	rBV3	16809	29530	1.04%	0.081%
22	11.310	805	807	809	rBV	64964	58501	2.05%	0.161%
23	11.402	812	815	816	rBV	28249	47179	1.65%	0.130%
24	11.436	816	818	819	rBV	815140	742475	26.04%	2.045%
25	11.459	819	820	822	rVV	175397	149386	5.24%	0.411%
26	11.505	822	824	826	rVB2	108991	158192	5.55%	0.436%
27	11.665	835	838	843	rBV3	45927	67167	2.36%	0.185%
28	11.733	843	844	849	rVB2	25292	38849	1.36%	0.107%
29	11.836	849	853	855	rBV3	18882	31579	1.11%	0.087%
30	11.893	856	858	860	rBV2	29008	44382	1.56%	0.122%
31	11.962	863	864	866	rVV	124984	175145	6.14%	0.482%
32	11.996	866	867	870	rVV	43406	53641	1.88%	0.148%
33	12.042	870	871	876	rVB3	30226	57976	2.03%	0.160%
34	12.145	876	880	882	rBV2	29690	56268	1.97%	0.155%

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35	12.248	885	889	890	rBV2	35810	60959	2.14%	0.168%
36	12.476	907	909	912	rVV	213762	261647	9.18%	0.721%
37	12.579	916	918	921	rVV	505627	505788	17.74%	1.393%
38	12.648	921	924	925	rVB	260697	331799	11.64%	0.914%
39	12.865	940	943	945	rBV3	238196	493915	17.32%	1.360%
40	12.922	945	948	949	rVB2	64690	64697	2.27%	0.178%
41	13.013	954	956	959	rVB	1755560	1924665	67.51%	5.301%
42	13.094	959	963	964	rBV2	15791	35140	1.23%	0.097%
43	13.196	968	972	973	rBV2	43230	71237	2.50%	0.196%
44	13.265	976	978	979	rVB2	31580	41457	1.45%	0.114%
45	13.299	979	981	983	rBV	28397	29314	1.03%	0.081%
46	13.379	985	988	990	rBV4	19202	46790	1.64%	0.129%
47	13.471	994	996	997	rBV	37009	35569	1.25%	0.098%
48	13.505	997	999	1001	rBV	26983	36963	1.30%	0.102%
49	13.551	1001	1003	1005	rBV	192878	176352	6.19%	0.486%
50	13.596	1005	1007	1010	rBV2	43701	51659	1.81%	0.142%
51	13.676	1012	1014	1015	rBV2	39258	29266	1.03%	0.081%
52	13.711	1015	1017	1019	rVB3	43033	74891	2.63%	0.206%
53	13.814	1023	1026	1027	rBV2	38754	49737	1.74%	0.137%
54	13.871	1029	1031	1032	rVB	33298	31901	1.12%	0.088%
55	13.916	1032	1035	1038	rVB3	202052	301636	10.58%	0.831%
56	13.985	1039	1041	1044	rBV	47785	57705	2.02%	0.159%
57	14.065	1044	1048	1049	rBV2	733605	933028	32.73%	2.570%
58	14.236	1061	1063	1065	rVB2	101177	122617	4.30%	0.338%
59	14.294	1065	1068	1069	rBV2	34840	48957	1.72%	0.135%
60	14.545	1087	1090	1092	rBV	353290	350159	12.28%	0.964%
61	14.591	1092	1094	1096	rVB	53371	67593	2.37%	0.186%
62	14.797	1110	1112	1114	rVB	32701	35167	1.23%	0.097%
63	14.842	1114	1116	1120	rBV	160081	226412	7.94%	0.624%
64	14.922	1121	1123	1126	rVB	106580	114121	4.00%	0.314%
65	14.991	1126	1129	1134	rVB4	54958	79578	2.79%	0.219%
66	15.094	1135	1138	1143	rBV	112391	278565	9.77%	0.767%
67	15.185	1143	1146	1150	rBV	681592	1010960	35.46%	2.784%
68	15.288	1153	1155	1158	rVB3	30373	36963	1.30%	0.102%
69	15.345	1158	1160	1161	rBV	36812	40415	1.42%	0.111%
70	15.379	1161	1163	1166	rVB	74390	96591	3.39%	0.266%
71	15.437	1166	1168	1171	rBV	60849	88380	3.10%	0.243%

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72	15.505	1171	1174	1176	rBV	376688	468473	16.43%	1.290%
73	15.551	1176	1178	1181	rVB2	70004	106588	3.74%	0.294%
74	15.745	1193	1195	1200	rBV2	155808	294512	10.33%	0.811%
75	15.871	1204	1206	1208	rVV2	73508	116870	4.10%	0.322%
76	15.928	1208	1211	1213	rVV2	51801	113632	3.99%	0.313%
77	15.985	1213	1216	1218	rVV	380261	577774	20.27%	1.591%
78	16.031	1218	1220	1225	rVV4	85913	232194	8.14%	0.639%
79	16.145	1228	1230	1234	rVV4	59522	133912	4.70%	0.369%
80	16.225	1234	1237	1244	rVV2	89201	274651	9.63%	0.756%
81	16.374	1246	1250	1255	rVB3	38326	133079	4.67%	0.367%
82	16.774	1281	1285	1291	rVB	426913	953024	33.43%	2.625%
83	16.934	1296	1299	1302	rBV2	29844	59000	2.07%	0.162%
84	17.071	1308	1311	1314	rBV	64926	139879	4.91%	0.385%
85	17.151	1314	1318	1321	rVV	86342	209974	7.36%	0.578%
86	17.540	1348	1352	1356	rBV2	75093	175896	6.17%	0.484%
87	17.757	1367	1371	1376	rVB3	76201	193976	6.80%	0.534%
88	17.985	1388	1391	1398	rVB	143177	387453	13.59%	1.067%
89	18.180	1405	1408	1417	rVB6	34520	118849	4.17%	0.327%
90	18.614	1437	1446	1457	rVB	461251	1525494	53.51%	4.201%
91	18.991	1475	1479	1484	rVB2	77688	219140	7.69%	0.604%

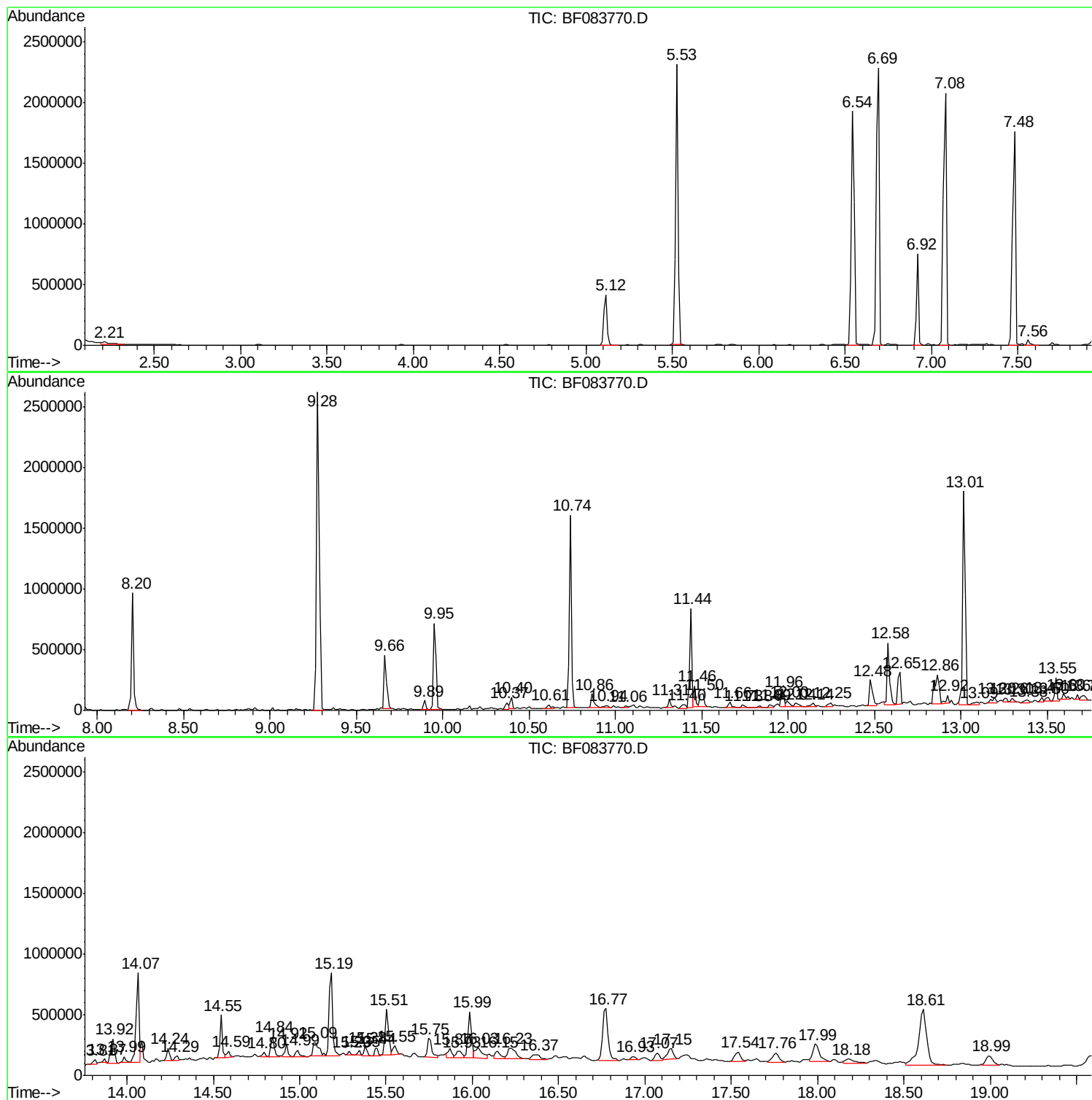
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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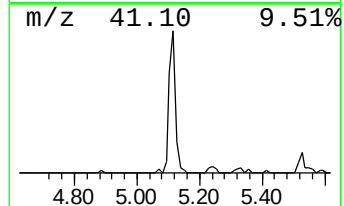
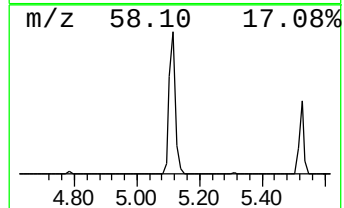
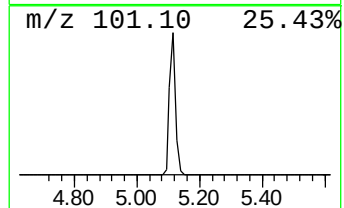
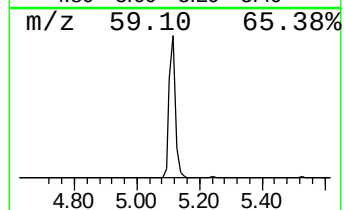
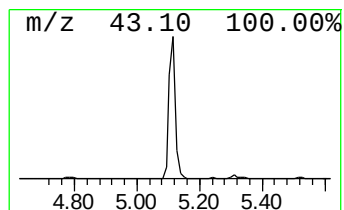
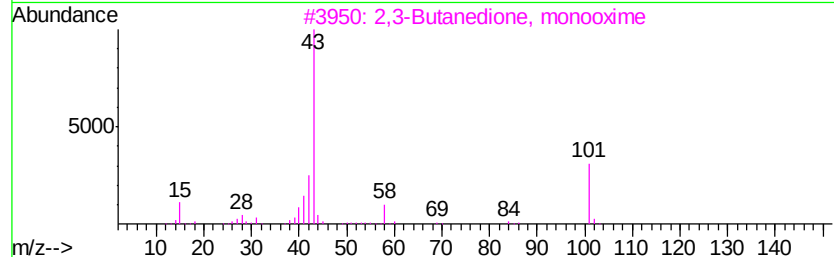
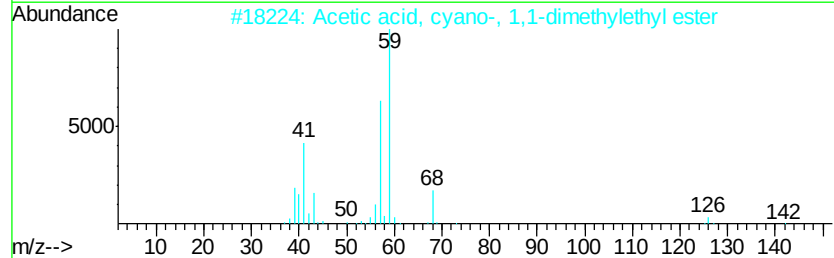
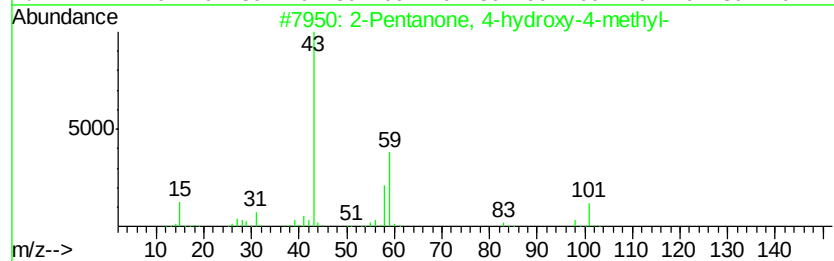
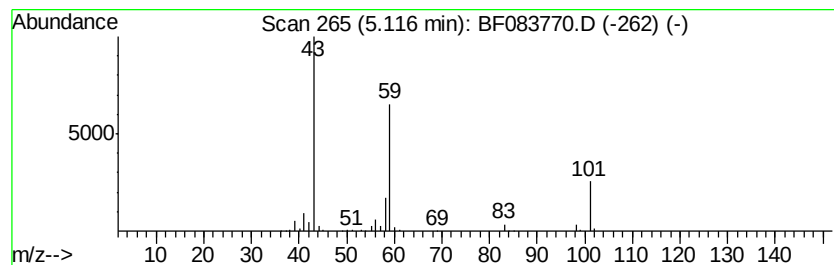
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	17.07 ng	577476	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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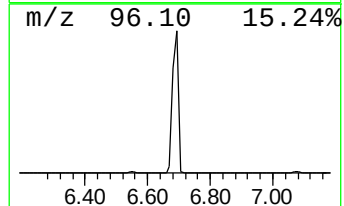
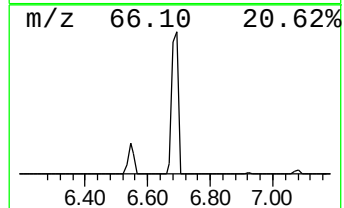
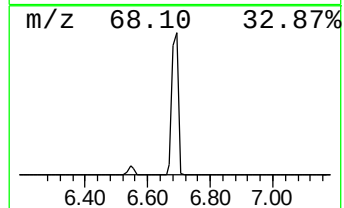
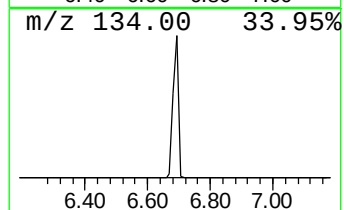
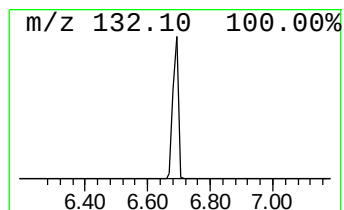
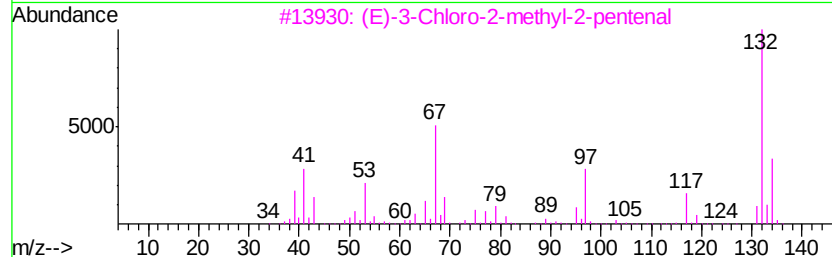
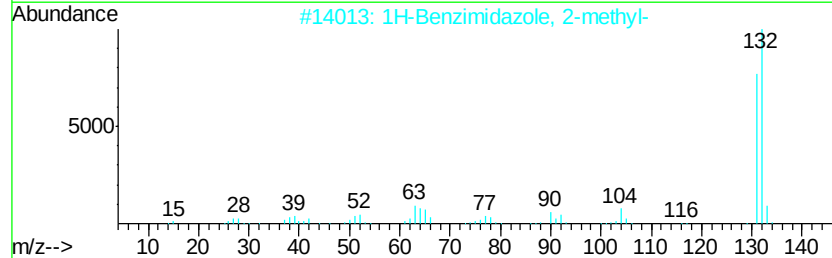
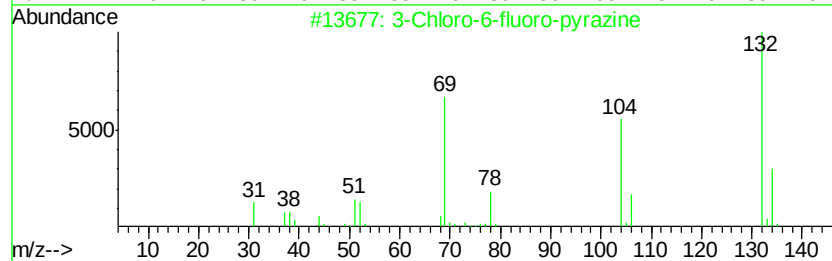
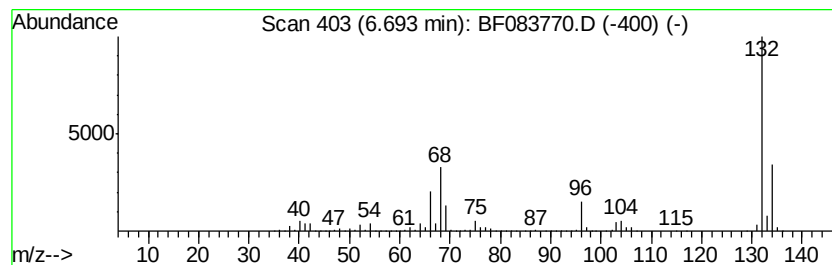
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	84.26 ng	2851050	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9



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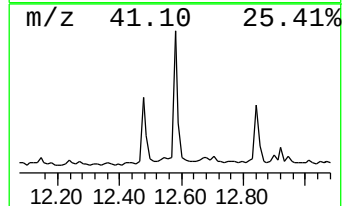
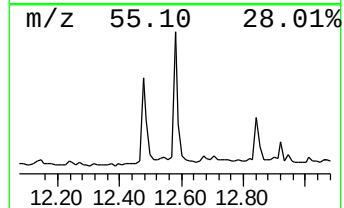
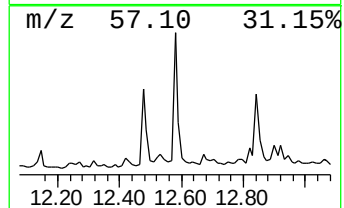
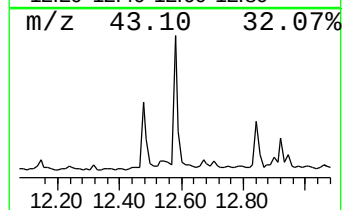
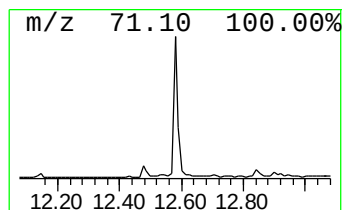
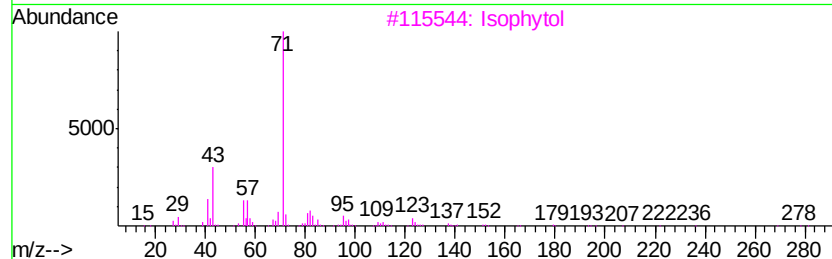
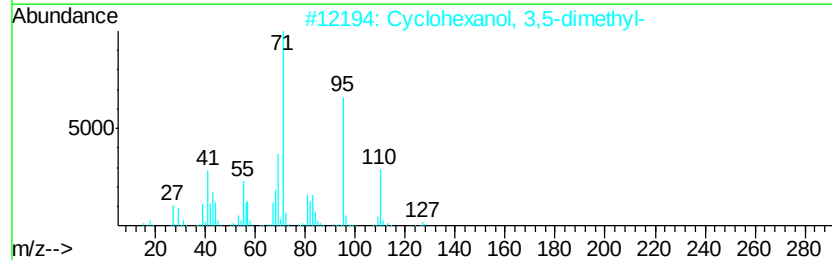
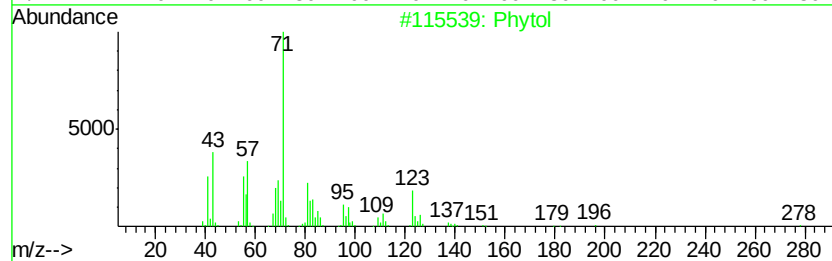
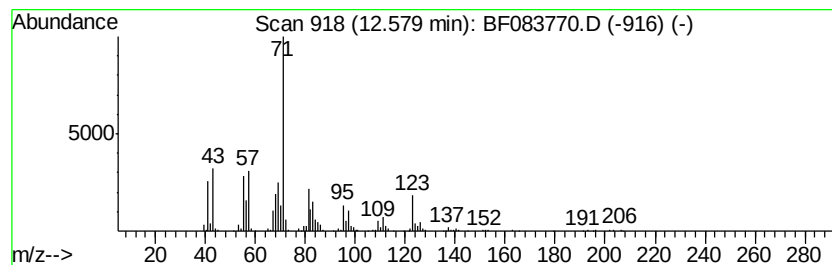
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phytol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	13.62 ng	505788	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phytol	296	C20H40O	000150-86-7	91
2		Cyclohexanol, 3,5-dimethyl-	128	C8H16O	005441-52-1	64
3		Isophytol	296	C20H40O	000505-32-8	50
4		Butyric acid, 3-tetradecyl ester	284	C18H36O2	1000280-57-1	50
5		2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	47



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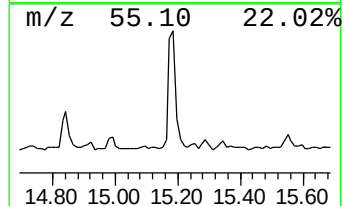
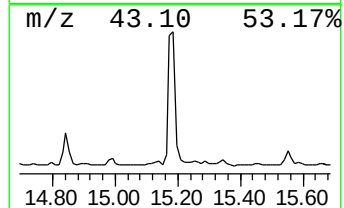
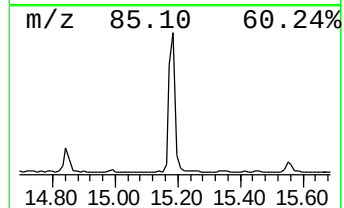
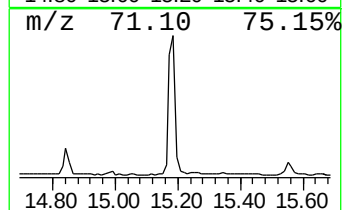
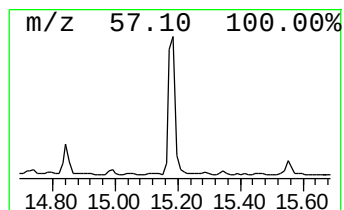
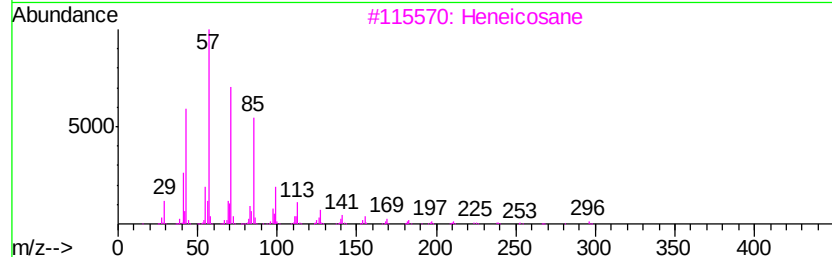
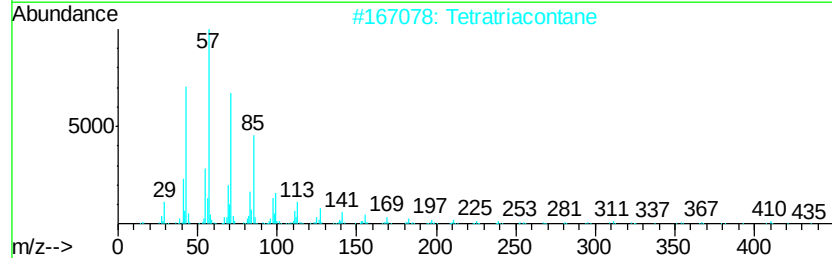
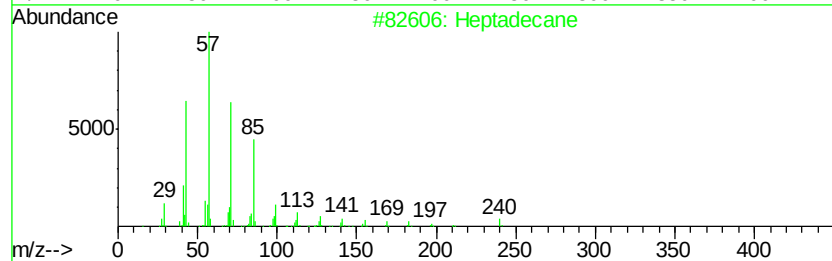
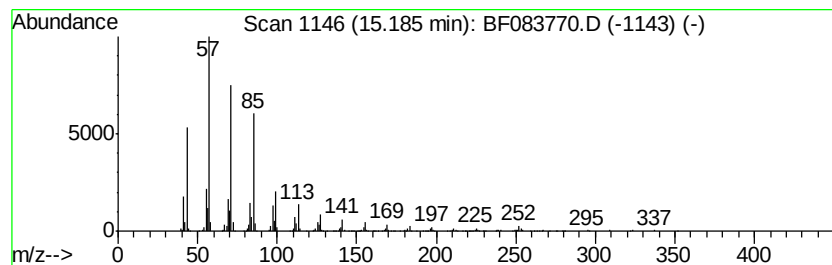
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	43.16 ng	1010960	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	94
2	Tetratriacontane		479	C34H70	014167-59-0	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Pentadecane, 8-hexyl-		296	C21H44	013475-75-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083770.D
Acq On : 14 Dec 2015 10:41
Operator : UM/IZ
Sample : G4648-22
Misc :
ALS Vial : 60 Sample Multiplier: 1

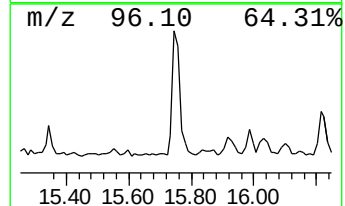
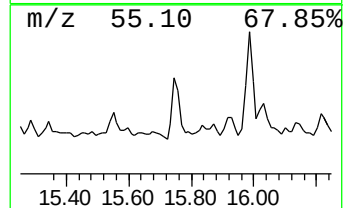
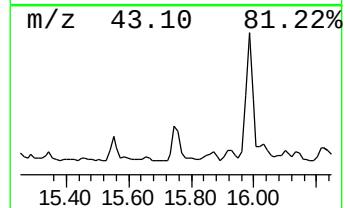
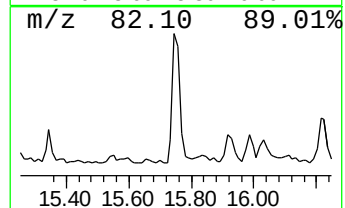
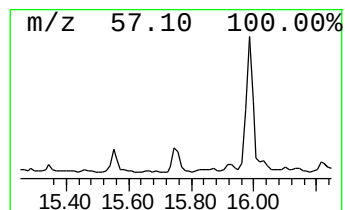
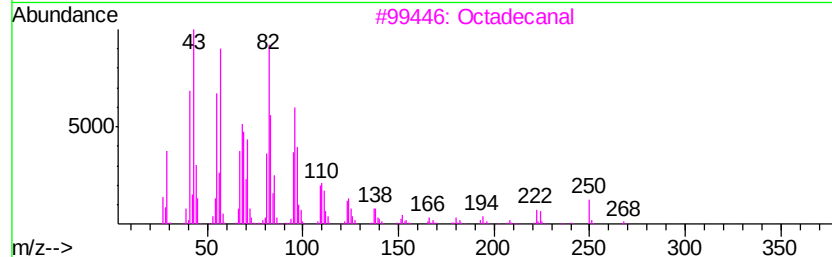
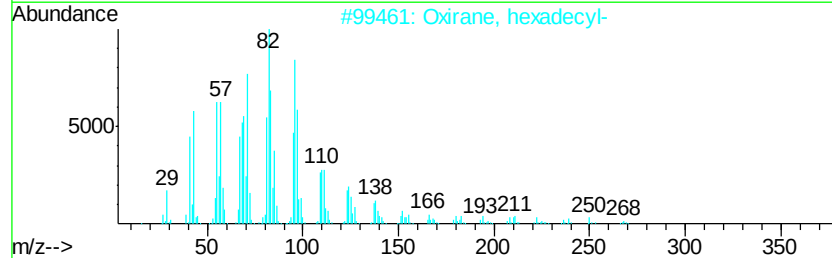
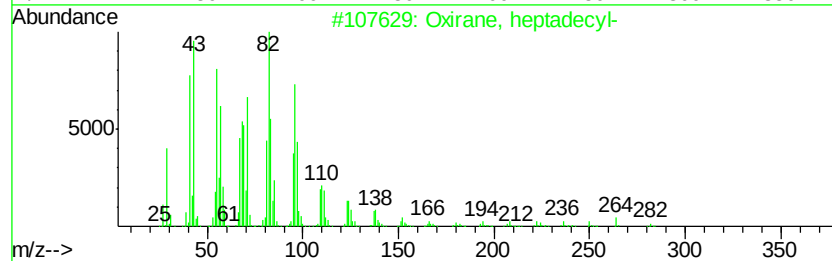
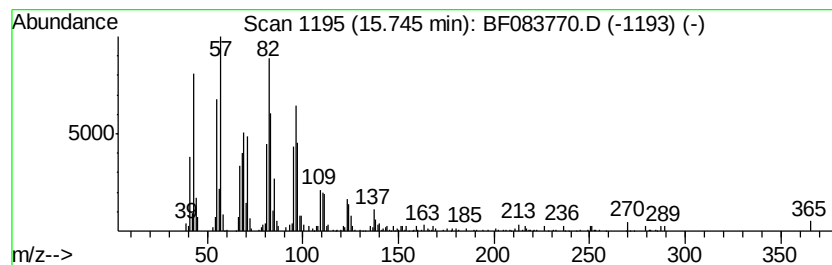
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxirane, heptadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.75	12.57 ng	294512	Perylene-d12		15.51	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	96	
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91	
3	Octadecanal	268	C18H36O	000638-66-4	91	
4	1,19-Eicosadiene	278	C20H38	014811-95-1	87	
5	Pentadecanal-	226	C15H30O	002765-11-9	86	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083770.D
Acq On : 14 Dec 2015 10:41
Operator : UM/IZ
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Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06(0-0.16)

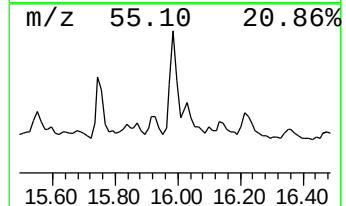
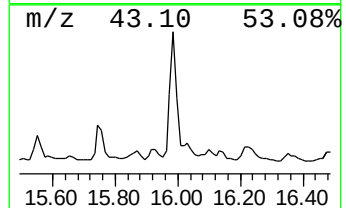
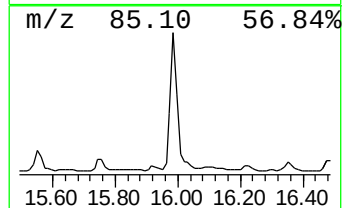
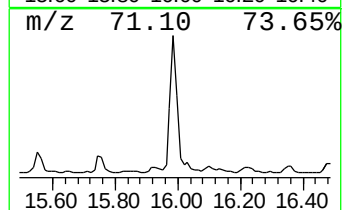
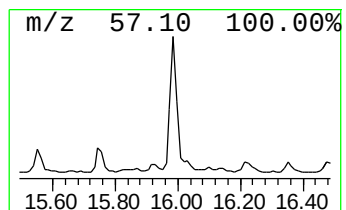
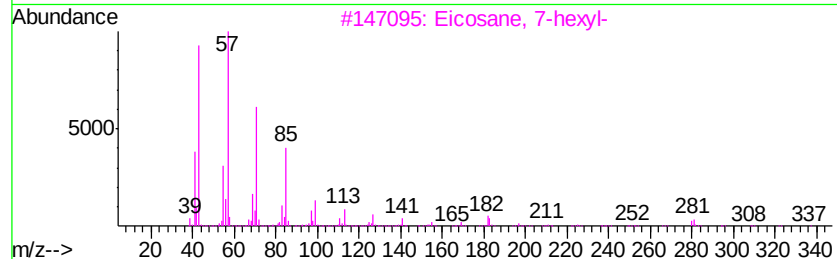
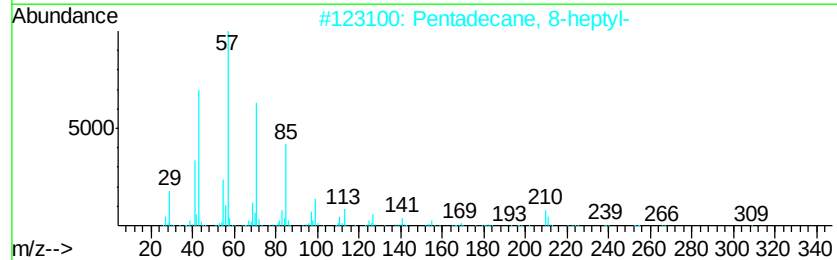
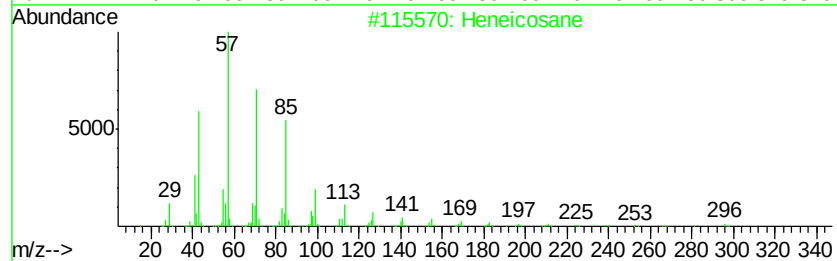
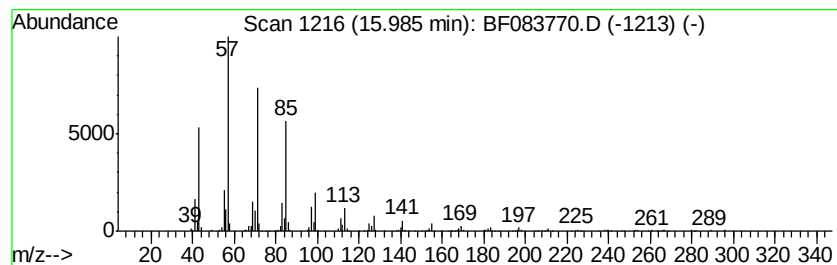
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	24.67 ng	577774	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	96
2	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	91
3	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90
4	Tetratriacontane		479	C34H70	014167-59-0	87
5	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083770.D
Acq On : 14 Dec 2015 10:41
Operator : UM/IZ
Sample : G4648-22
Misc :
ALS Vial : 60 Sample Multiplier: 1

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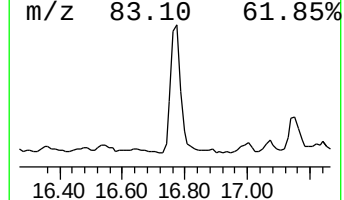
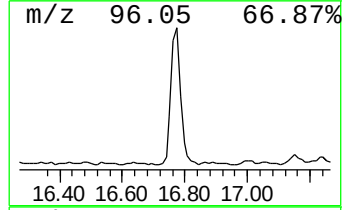
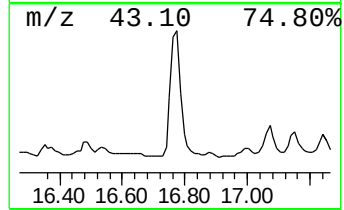
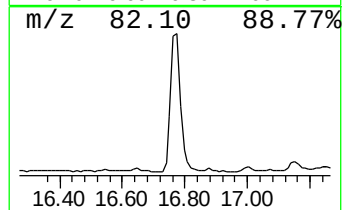
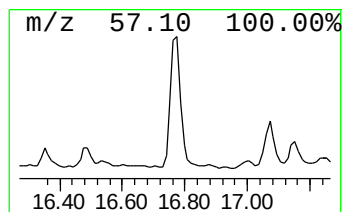
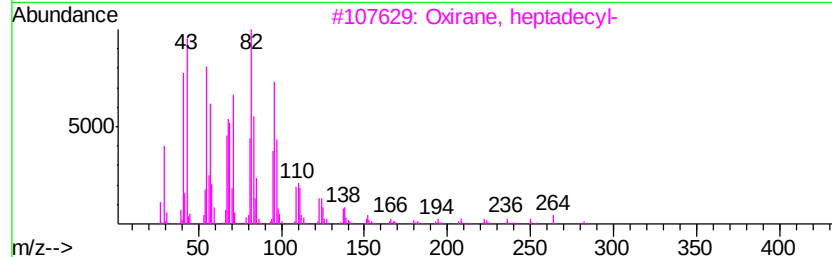
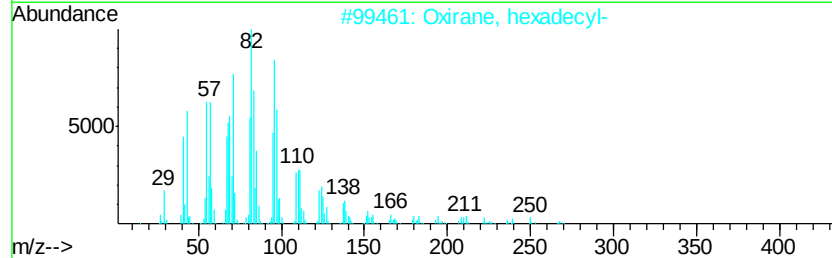
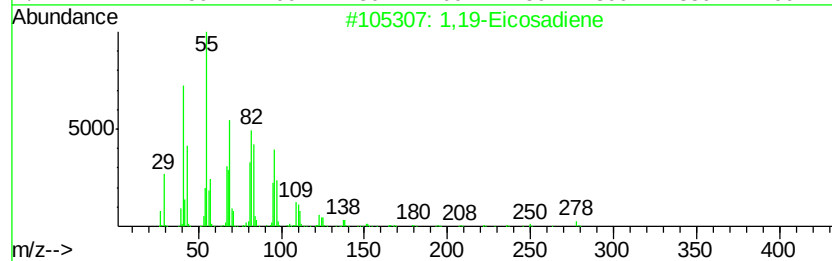
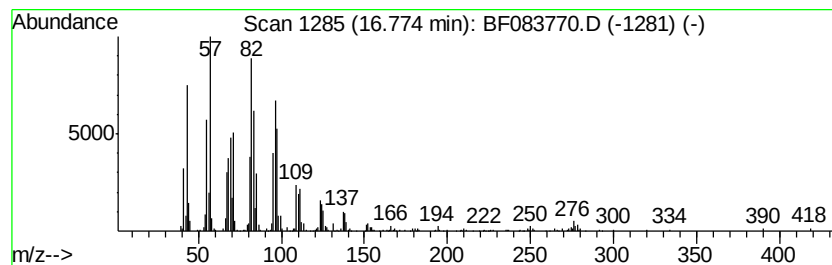
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1,19-Eicosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	40.69 ng	953024	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,19-Eicosadiene	278	C20H38	014811-95-1	95
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
3		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
4		Octadecanal	268	C18H36O	000638-66-4	90
5		Tetradecanal	212	C14H28O	000124-25-4	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083770.D
Acq On : 14 Dec 2015 10:41
Operator : UM/IZ
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Misc :
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Instrument :
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ClientSampleId :
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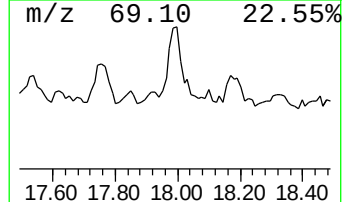
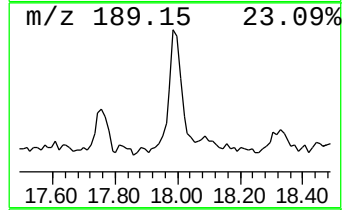
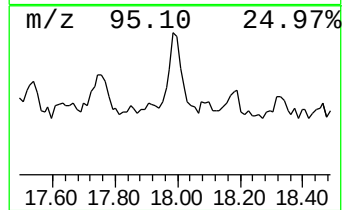
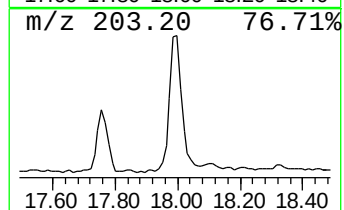
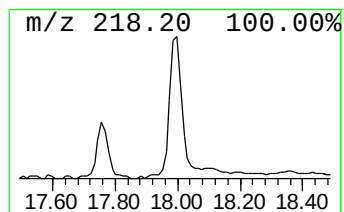
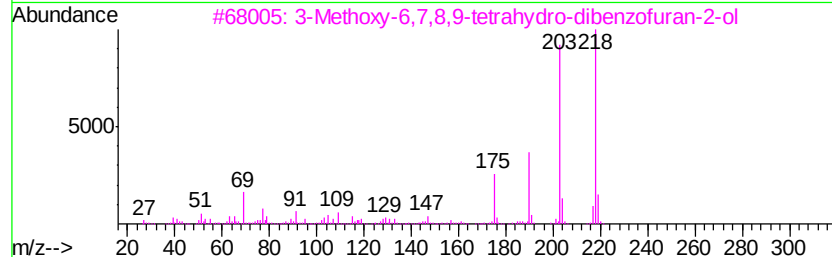
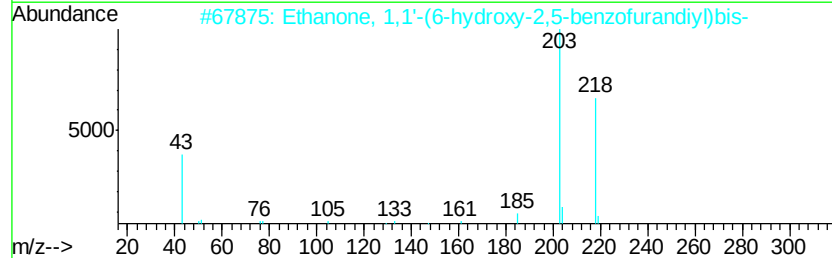
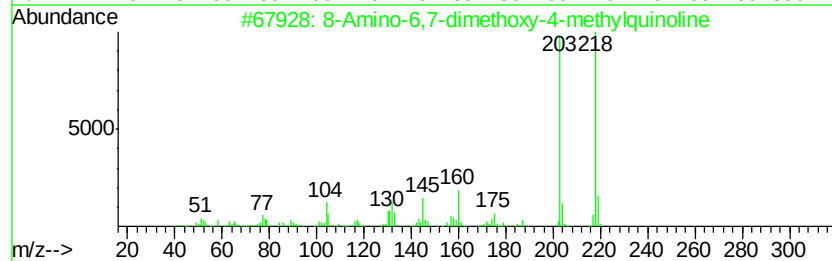
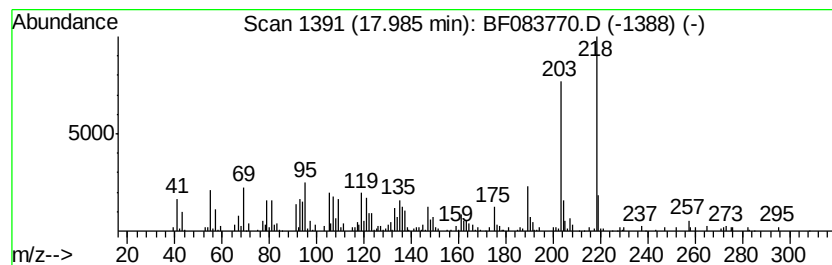
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 8-Amino-6,7-dimethoxy-4-met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	16.54 ng	387453	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	50
2		Ethanone, 1,1'-(6-hydroxy-2,5-be...	218	C12H10O4	053947-86-7	50
3		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	50
4		2H-[1,2]Dioxeto[3',4':4,5]furo[3...	260	C14H12O5	129833-00-7	46
5		2H-Cyclopropa[g]benzofuran, 4,5,...	218	C15H22O	102681-49-2	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083770.D
Acq On : 14 Dec 2015 10:41
Operator : UM/IZ
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Instrument :
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ClientSampleId :
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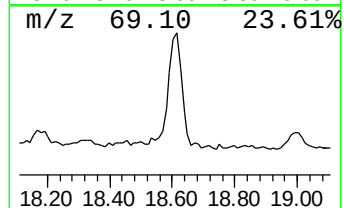
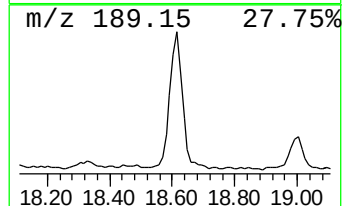
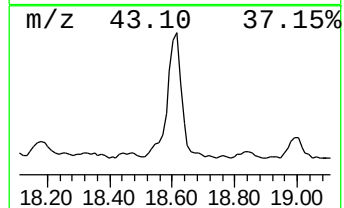
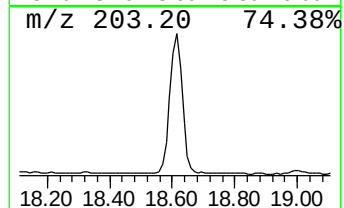
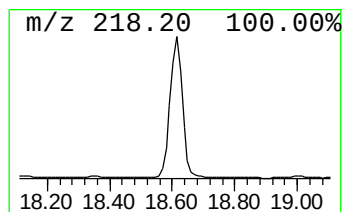
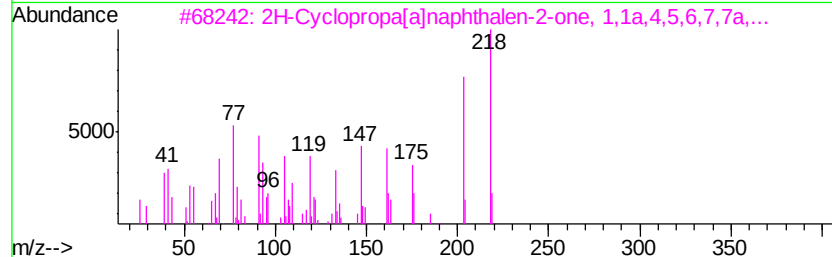
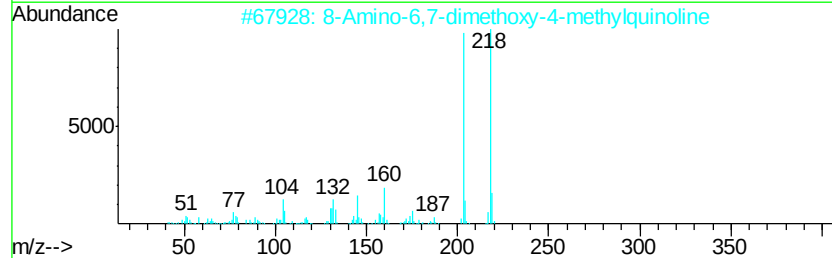
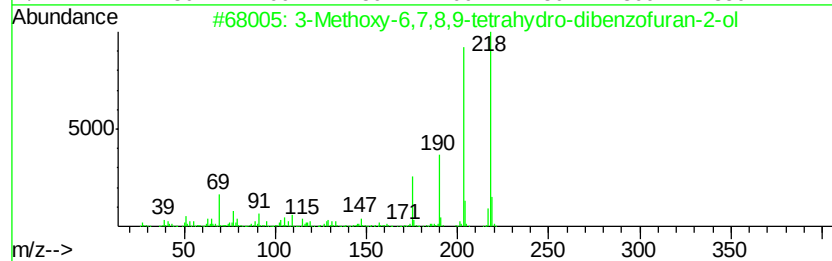
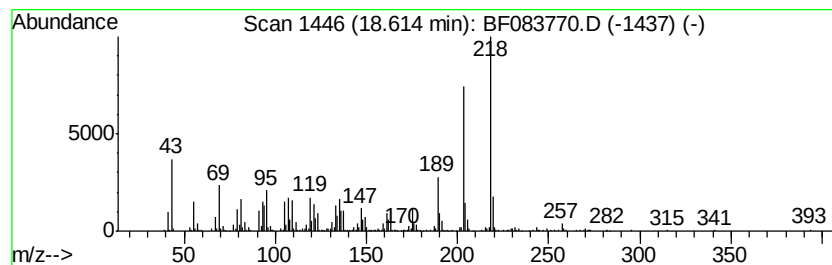
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 3-Methoxy-6,7,8,9-tetrahydr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.61	65.13 ng	1525490	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	64
2		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	53
3		2H-Cyclopropa[<i>a</i>]naphthalen-2-one...	218	C15H22O	006831-17-0	53
4		Pyrene, hexadecahydro-	218	C16H26	002435-85-0	50
5		Neoisolongifolene, 8-bromo-	282	C15H23Br	1000151-64-8	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083770.D
Acq On : 14 Dec 2015 10:41
Operator : UM/IZ
Sample : G4648-22
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.69	6.69	84.3	ng	2851050	1	6.92	676767	20.0
Phytol	12.58	13.6	ng	505788	4	11.44	742475	20.0
Heptadecane	15.19	43.2	ng	1010960	6	15.51	468473	20.0
Oxirane, heptadecyl-	15.75	12.6	ng	294512	6	15.51	468473	20.0
Heneicosane	15.99	24.7	ng	577774	6	15.51	468473	20.0
1,19-Eicosadiene	16.77	40.7	ng	953024	6	15.51	468473	20.0
8-Amino-6,7-dimet...	17.99	16.5	ng	387453	6	15.51	468473	20.0
3-Methoxy-6,7,8,9...	18.61	65.1	ng	1525490	6	15.51	468473	20.0