

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
 Data File : BF091687.D
 Acq On : 16 Dec 2016 21:54
 Operator : UM/SJ
 Sample : H6099-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS03-0-2IN

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-BF120916.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	4.944	246	250	259	rBV	2042705	2889447	45.16%	3.341%
2	5.379	285	288	290	rBV	5716119	5646855	88.27%	6.529%
3	6.419	376	379	382	rBV	4104825	4481787	70.05%	5.182%
4	6.544	387	390	392	rBV	5272825	5015375	78.39%	5.799%
5	6.773	407	410	412	rBV	1941447	1655104	25.87%	1.914%
6	6.933	421	424	426	rBV	4900980	5139982	80.34%	5.943%
7	7.333	456	459	462	rBV	2919545	4273071	66.79%	4.941%
8	7.425	465	467	476	rVB2	31616	72453	1.13%	0.084%
9	7.779	496	498	503	rBV2	50501	102475	1.60%	0.118%
10	8.053	520	522	525	rBV	1715205	2133249	33.34%	2.467%
11	8.453	555	557	565	rBV	113813	219630	3.43%	0.254%
12	9.139	614	617	619	rBV	6719784	6397593	100.00%	7.398%
13	9.276	626	629	632	rVB2	46782	82496	1.29%	0.095%
14	9.470	642	646	649	rBV4	48362	86945	1.36%	0.101%
15	9.528	649	651	654	rVB	691830	704529	11.01%	0.815%
16	9.756	667	671	673	rVB2	62554	79335	1.24%	0.092%
17	9.813	673	676	678	rBV	2369192	2404099	37.58%	2.780%
18	10.019	692	694	696	rBV2	58329	84447	1.32%	0.098%
19	10.248	713	714	717	rVB	90535	95282	1.49%	0.110%
20	10.351	722	723	726	rVB	82044	100344	1.57%	0.116%
21	10.465	730	733	735	rBV	44167	82924	1.30%	0.096%
22	10.602	742	745	747	rVB	2836318	3342685	52.25%	3.865%
23	10.728	754	756	758	rBV	146700	199159	3.11%	0.230%
24	10.968	775	777	780	rVB4	62117	95656	1.50%	0.111%
25	11.173	790	795	800	rBV3	169105	319891	5.00%	0.370%
26	11.253	800	802	803	rBV	185075	196880	3.08%	0.228%
27	11.288	803	805	810	rVV2	2264220	3078905	48.13%	3.560%
28	11.356	810	811	813	rVB2	213189	260727	4.08%	0.301%
29	11.528	823	826	829	rBV2	191402	297595	4.65%	0.344%
30	11.596	829	832	833	rBV	144474	136087	2.13%	0.157%
31	11.688	837	840	843	rVB3	31167	72637	1.14%	0.084%
32	11.756	843	846	848	rBV	139544	245316	3.83%	0.284%
33	11.791	848	849	850	rVV	176627	173068	2.71%	0.200%
34	11.836	850	853	855	rVV	880244	1081475	16.90%	1.251%

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 SS03-0-2IN

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.905	857	859	863	rVV	151455	269640	4.21%	0.312%
36	11.996	863	867	872	rVV3	97462	241338	3.77%	0.279%
37	12.088	872	875	878	rVB2	73379	156468	2.45%	0.181%
38	12.339	895	897	900	rBV	820765	853800	13.35%	0.987%
39	12.431	903	905	908	rVB3	69259	106913	1.67%	0.124%
40	12.499	908	911	913	rBV	1150528	1036960	16.21%	1.199%
41	12.556	913	916	918	rVV4	35562	93553	1.46%	0.108%
42	12.614	920	921	923	rVV2	79725	93864	1.47%	0.109%
43	12.728	927	931	933	rBV	640219	905849	14.16%	1.047%
44	12.762	933	934	939	rVB2	74128	97609	1.53%	0.113%
45	12.876	942	944	946	rVB	4331185	4018383	62.81%	4.646%
46	13.048	958	959	961	rVB	94288	117660	1.84%	0.136%
47	13.094	961	963	964	rBV2	122519	164442	2.57%	0.190%
48	13.117	964	965	967	rVV	262402	229369	3.59%	0.265%
49	13.151	967	968	972	rVB2	72485	98047	1.53%	0.113%
50	13.334	982	984	986	rBV	92578	156682	2.45%	0.181%
51	13.425	991	992	993	rVV	71619	89985	1.41%	0.104%
52	13.459	993	995	998	rVB2	87445	138069	2.16%	0.160%
53	13.574	1003	1005	1007	rVB2	129625	134255	2.10%	0.155%
54	13.779	1020	1023	1026	rBV	1052224	1237037	19.34%	1.430%
55	13.917	1032	1035	1040	rVB2	1574690	2085366	32.60%	2.411%
56	14.019	1043	1044	1046	rVB	90084	115093	1.80%	0.133%
57	14.099	1049	1051	1054	rBV2	135429	246937	3.86%	0.286%
58	14.225	1059	1062	1064	rBV	135528	199721	3.12%	0.231%
59	14.339	1070	1072	1076	rVB5	54715	125895	1.97%	0.146%
60	14.408	1076	1078	1082	rBV	1073431	1306576	20.42%	1.511%
61	14.534	1087	1089	1090	rBV	78801	109109	1.71%	0.126%
62	14.682	1100	1102	1108	rBV2	136287	352820	5.51%	0.408%
63	14.774	1108	1110	1112	rVB2	72697	95235	1.49%	0.110%
64	14.831	1113	1115	1117	rBV	214845	232792	3.64%	0.269%
65	14.922	1121	1123	1128	rBV	256452	588544	9.20%	0.681%
66	15.014	1129	1131	1137	rVV	1624487	2703209	42.25%	3.126%
67	15.174	1143	1145	1146	rBV	88784	120110	1.88%	0.139%
68	15.208	1146	1148	1150	rVB	172402	221206	3.46%	0.256%
69	15.265	1150	1153	1156	rBV	263848	346484	5.42%	0.401%
70	15.322	1156	1158	1160	rBV	1099075	1348760	21.08%	1.560%
71	15.357	1160	1161	1164	rVB	205651	298558	4.67%	0.345%

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72	15.551	1175	1178	1181	rBV	510575	678889	10.61%	0.785%
73	15.665	1185	1188	1191	rBV	126533	180760	2.83%	0.209%
74	15.768	1194	1197	1199	rBV	1471616	2276374	35.58%	2.632%
75	15.814	1199	1201	1205	rVB2	434968	633856	9.91%	0.733%
76	15.883	1205	1207	1208	rBV	93880	156274	2.44%	0.181%
77	16.008	1214	1218	1225	rVB3	266934	694384	10.85%	0.803%
78	16.237	1235	1238	1240	rBV	102264	190559	2.98%	0.220%
79	16.500	1257	1261	1265	rBV	690166	1315469	20.56%	1.521%
80	16.660	1272	1275	1277	rBV	126585	273267	4.27%	0.316%
81	16.774	1282	1285	1288	rVV	187276	379504	5.93%	0.439%
82	16.854	1288	1292	1296	rVV3	227379	624865	9.77%	0.723%
83	16.945	1297	1300	1307	rVB	163693	445952	6.97%	0.516%
84	17.060	1308	1310	1317	rVB	108557	326257	5.10%	0.377%
85	17.208	1319	1323	1328	rBV2	579127	1469452	22.97%	1.699%
86	17.414	1337	1341	1347	rVB	180851	457177	7.15%	0.529%
87	17.563	1351	1354	1357	rBV2	137945	339749	5.31%	0.393%
88	17.723	1365	1368	1372	rBV4	206221	495028	7.74%	0.572%
89	17.803	1372	1375	1378	rVB2	123740	252616	3.95%	0.292%
90	17.940	1384	1387	1396	rVB5	196142	676351	10.57%	0.782%
91	18.088	1396	1400	1402	rBV3	135156	355100	5.55%	0.411%
92	18.157	1402	1406	1413	rVB3	265500	849018	13.27%	0.982%
93	18.408	1425	1428	1433	rBV2	83865	235321	3.68%	0.272%
94	19.106	1484	1489	1496	rVB3	367909	1192765	18.64%	1.379%

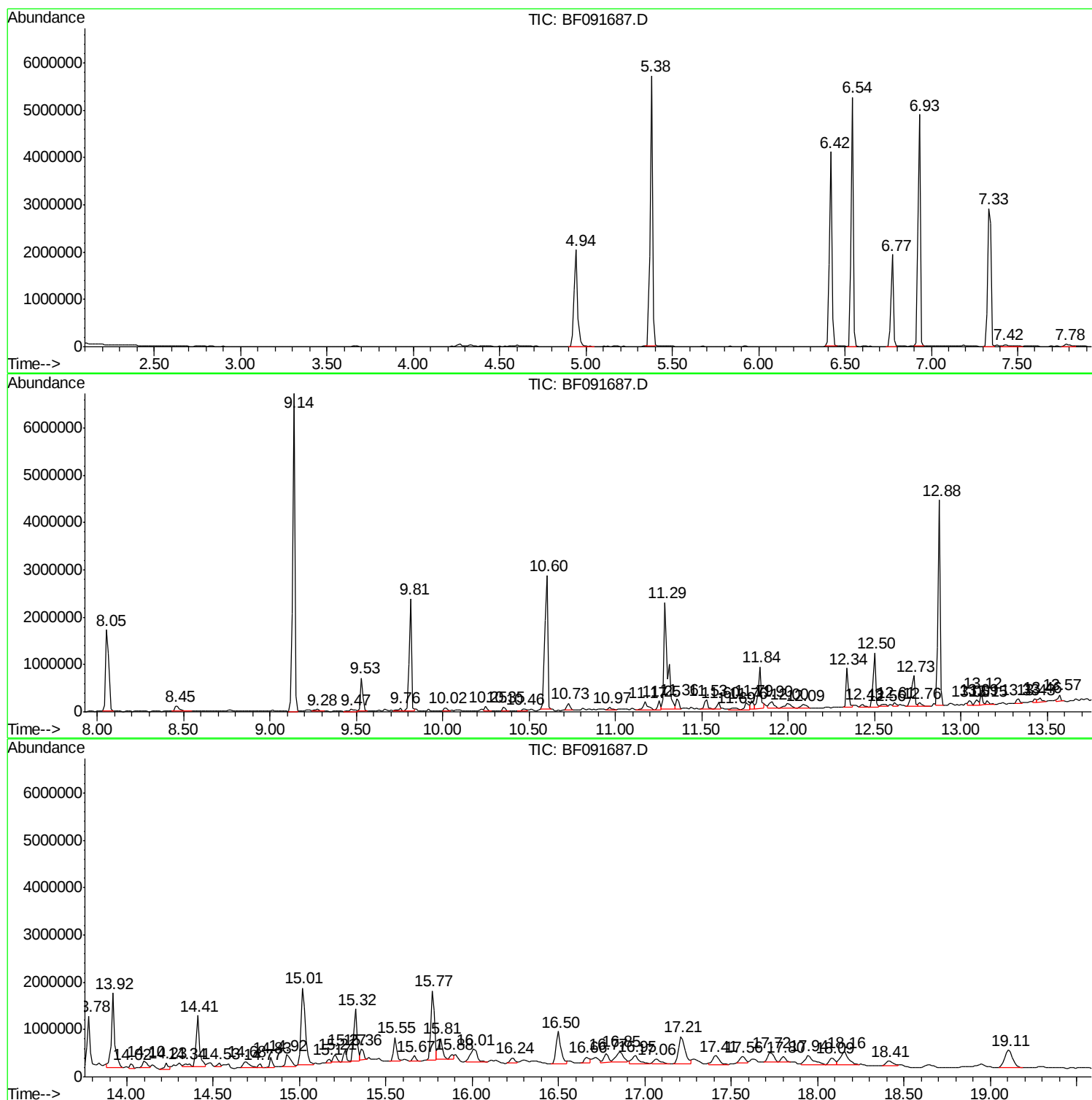
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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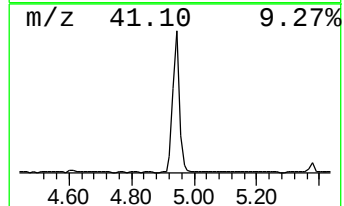
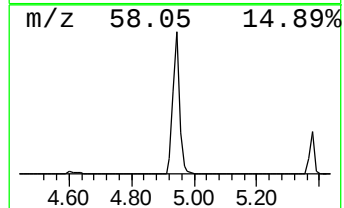
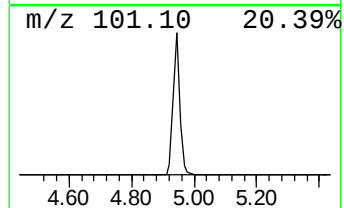
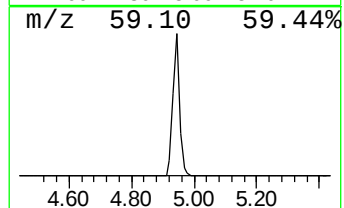
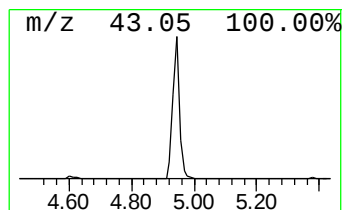
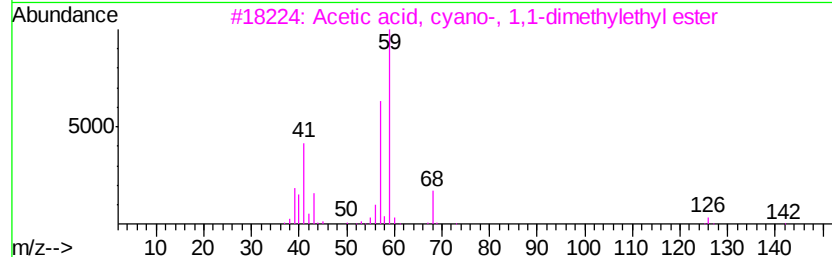
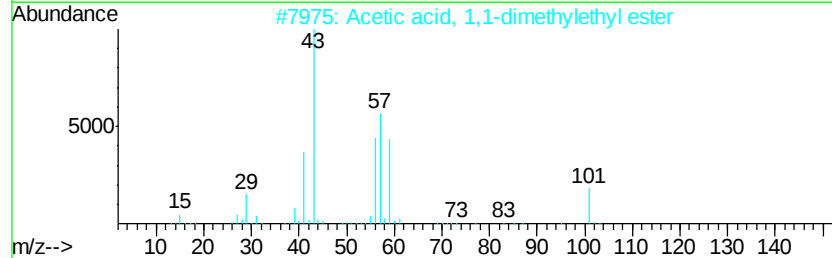
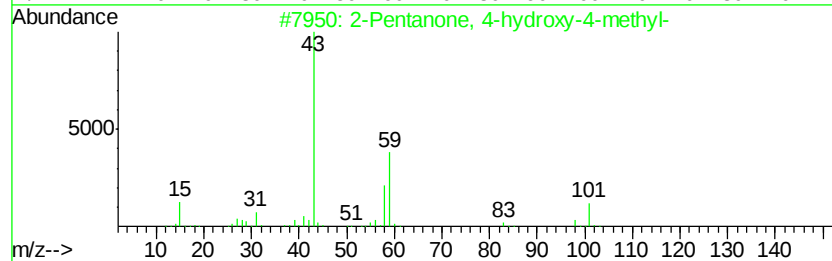
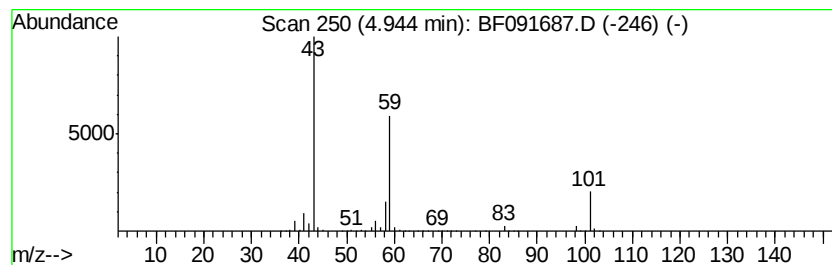
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	34.92 ng	2889450	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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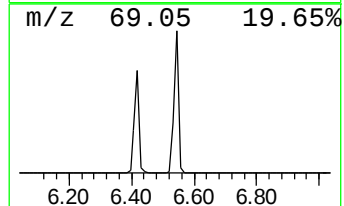
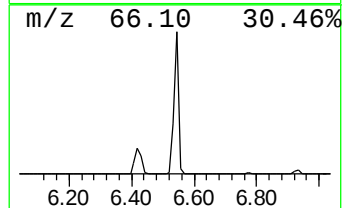
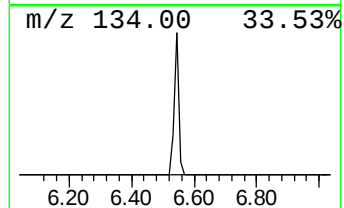
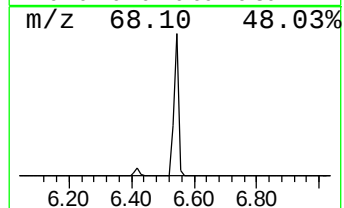
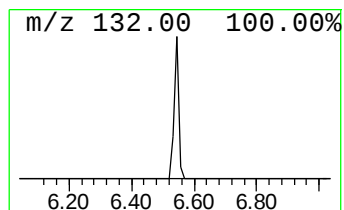
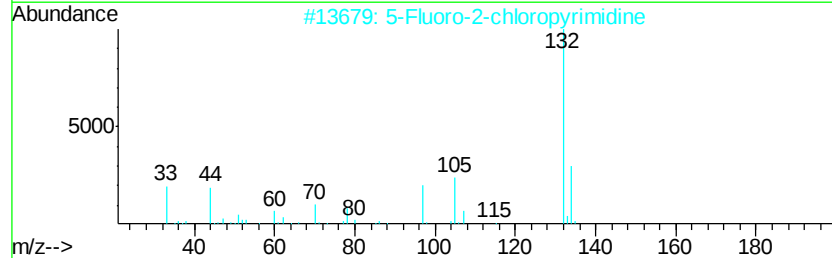
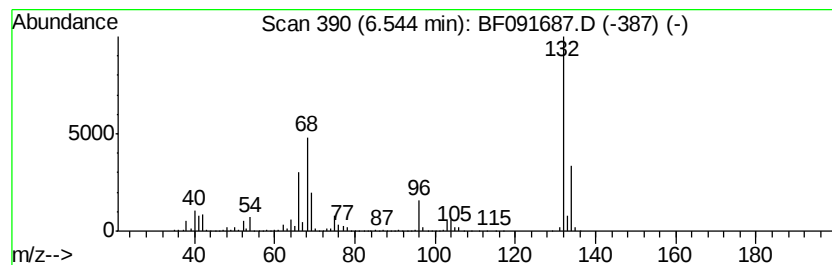
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	60.61 ng	5015380	1,4-Dichlorobenzene-d4	6.77

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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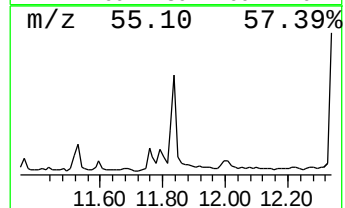
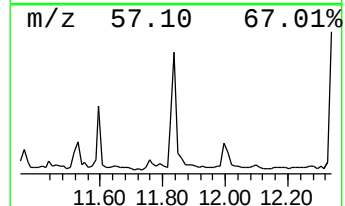
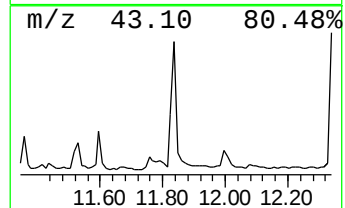
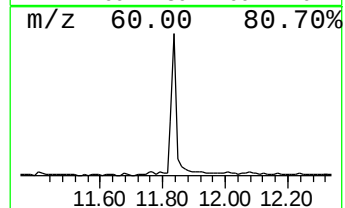
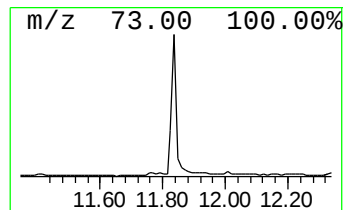
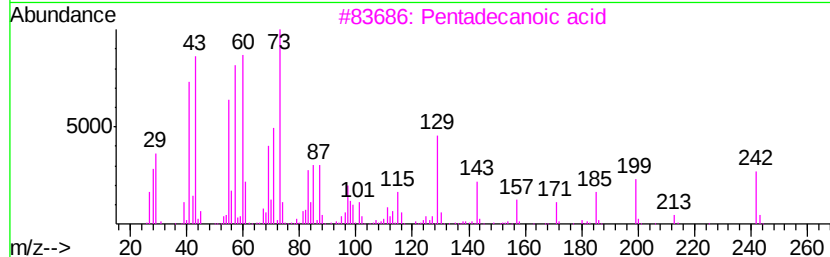
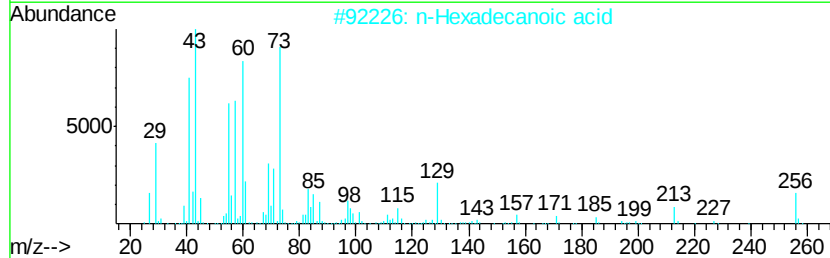
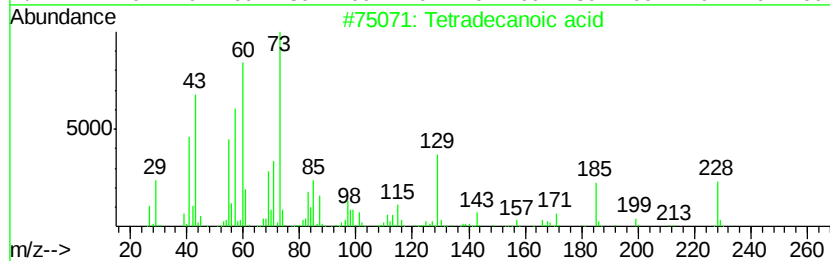
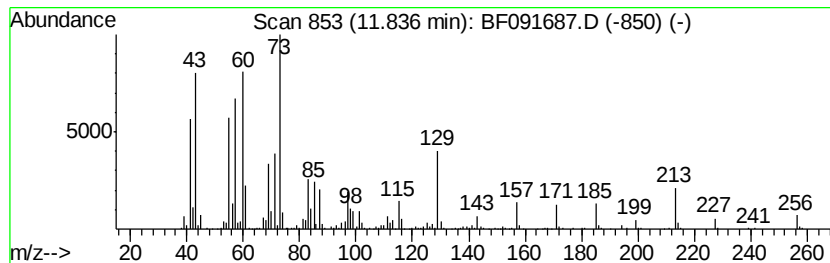
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	7.03 ng	1081480	Phenanthrene-d10	11.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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SS03-0-2IN

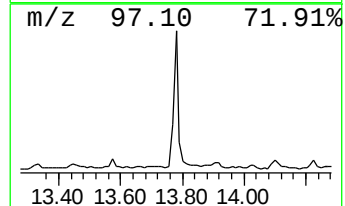
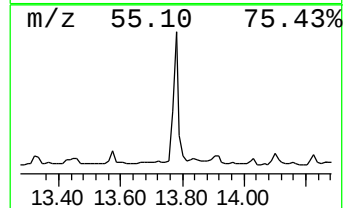
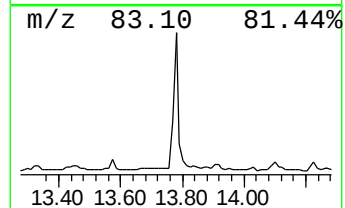
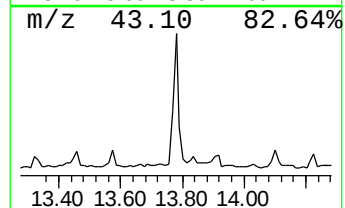
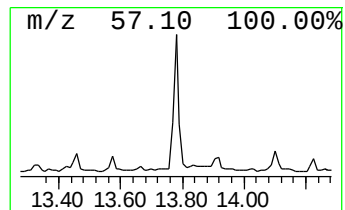
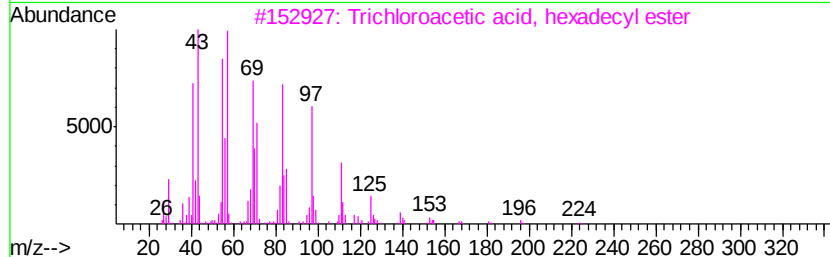
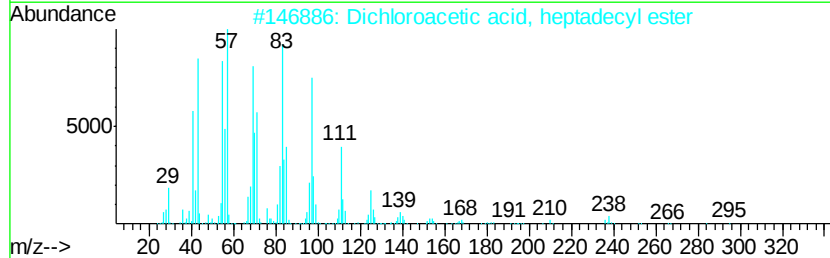
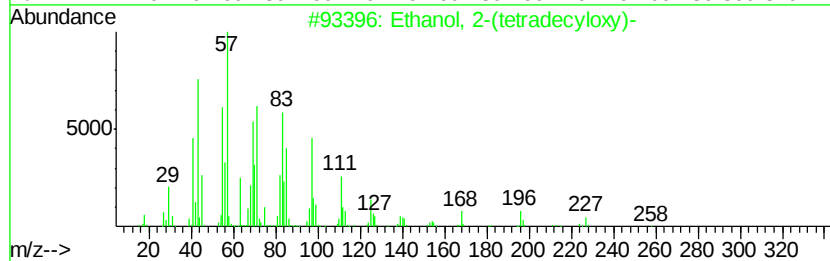
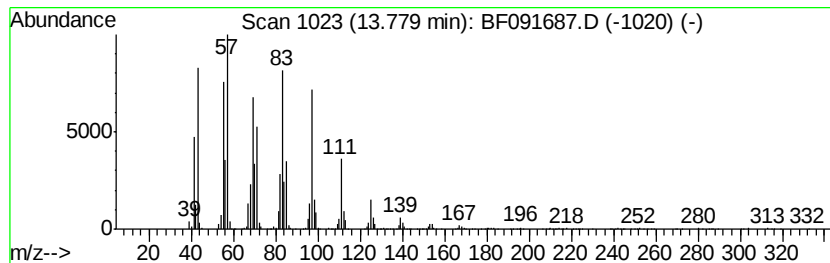
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	11.86 ng	1237040	Chrysene-d12	13.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	93
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		1-Tricosene	322	C23H46	018835-32-0	91
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS03-0-2IN

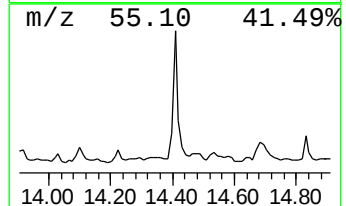
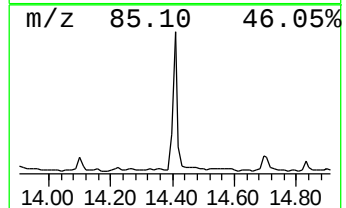
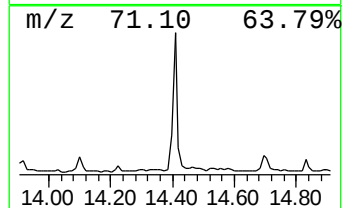
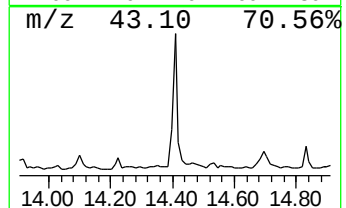
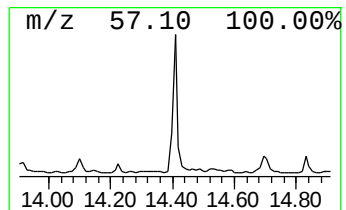
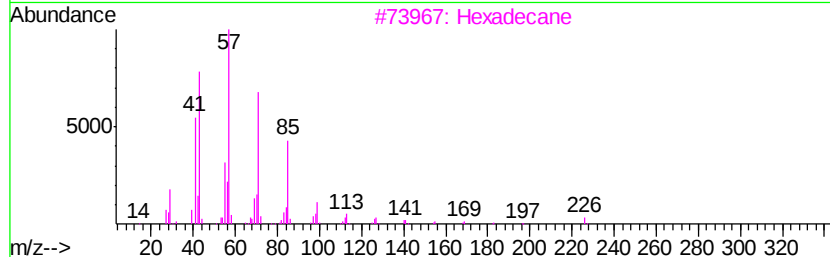
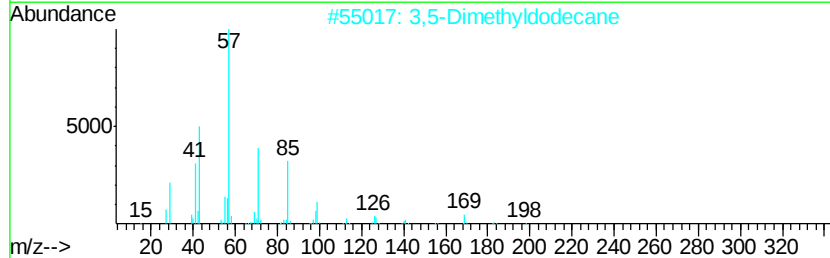
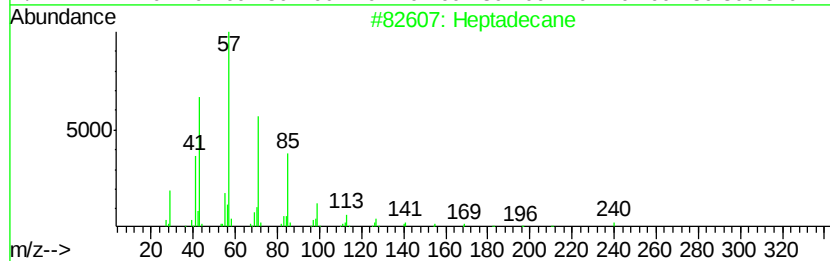
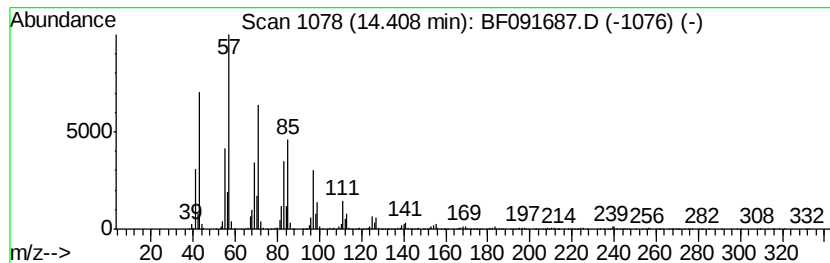
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	12.53 ng	1306580	Chrysene-d12	13.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	86
2	3,5-Dimethyldodecane		198	C14H30	107770-99-0	70
3	Hexadecane		226	C16H34	000544-76-3	68
4	Pentadecane		212	C15H32	000629-62-9	68
5	Tetradecane		198	C14H30	000629-59-4	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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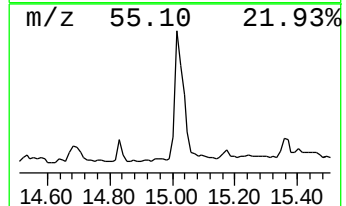
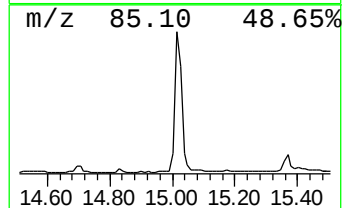
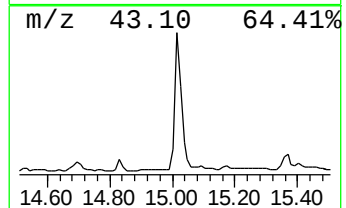
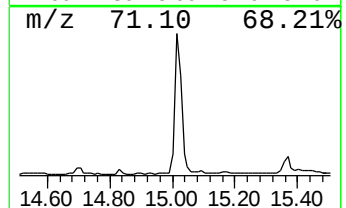
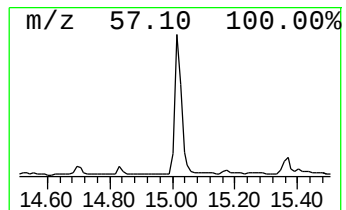
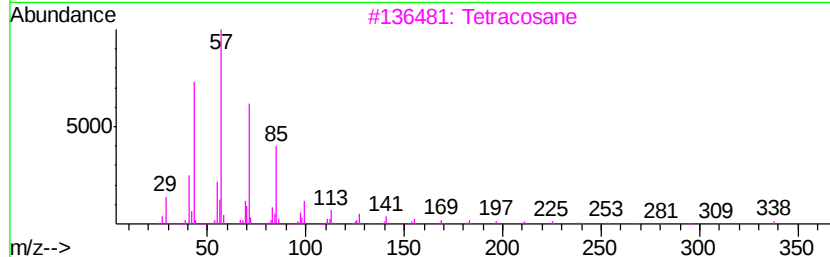
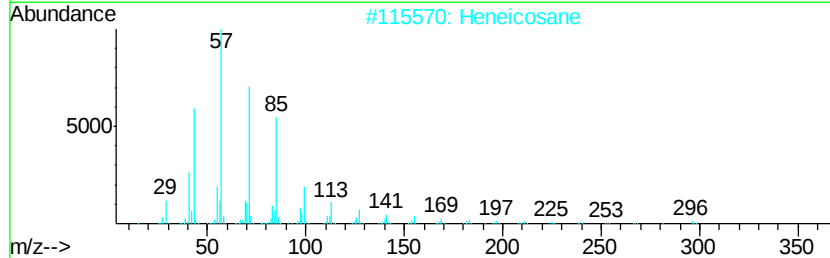
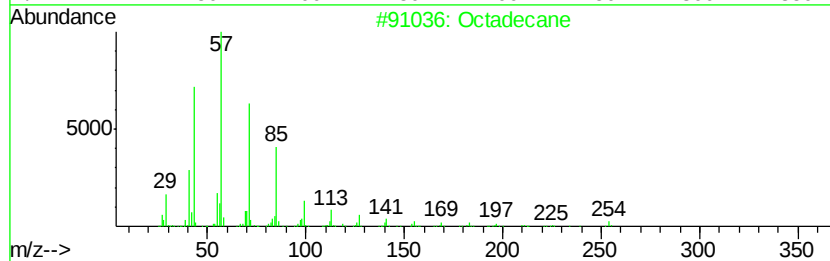
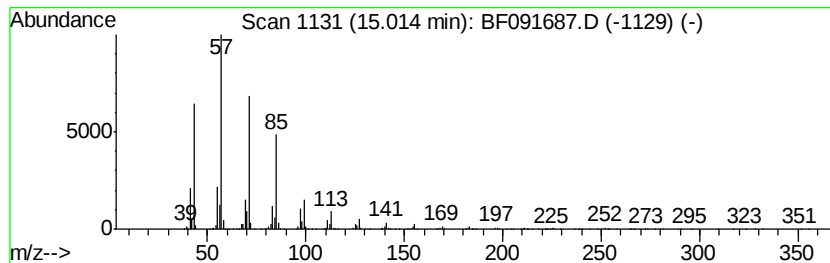
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	40.08 ng	2703210	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hexadecane	226	C16H34	000544-76-3	86
5		Hexatriacontane	507	C36H74	000630-06-8	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
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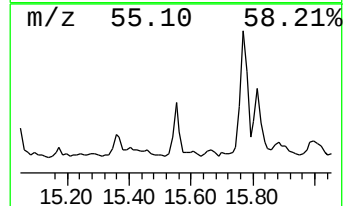
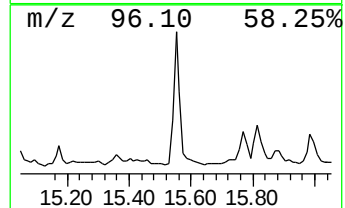
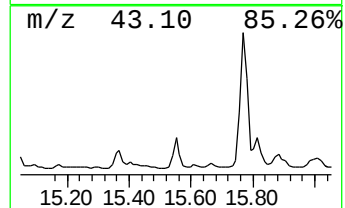
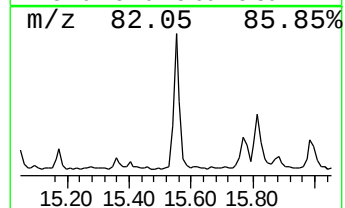
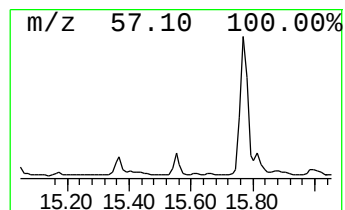
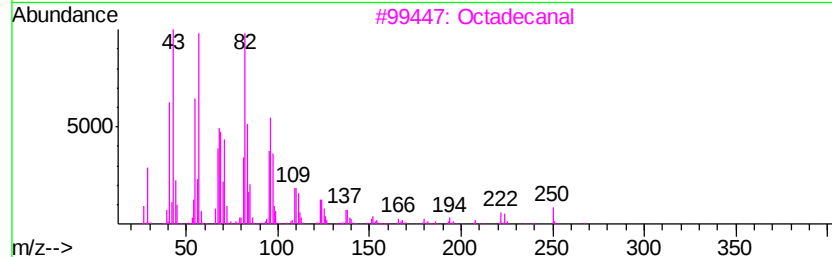
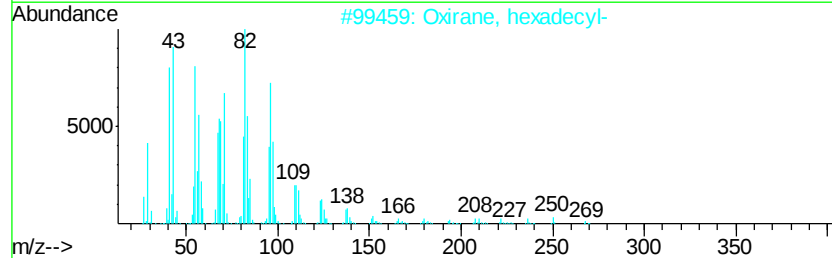
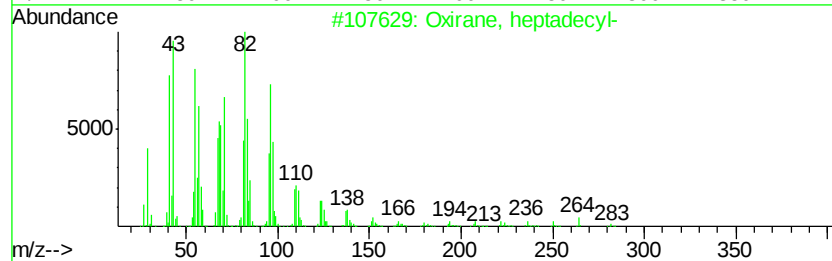
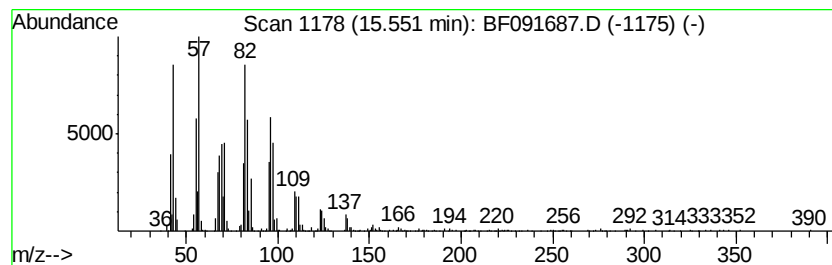
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.55	10.07 ng	678889	Perylene-d12	15.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91	
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91	
3	Octadecanal	268	C18H36O	000638-66-4	90	
4	17-Octadecenal	266	C18H34O	056554-86-0	90	
5	16-Octadecenal	266	C18H34O	056554-87-1	90	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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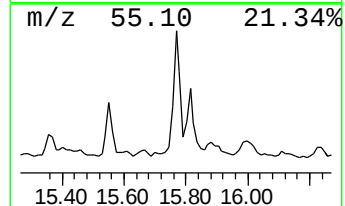
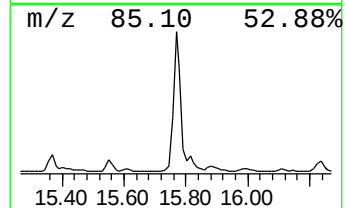
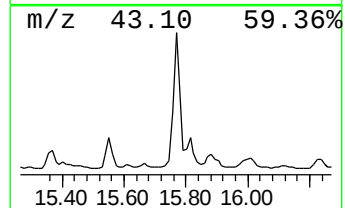
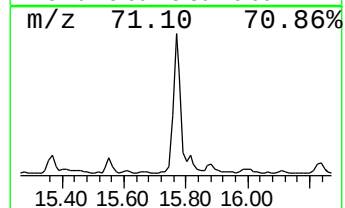
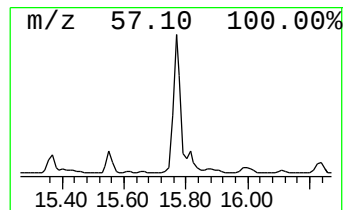
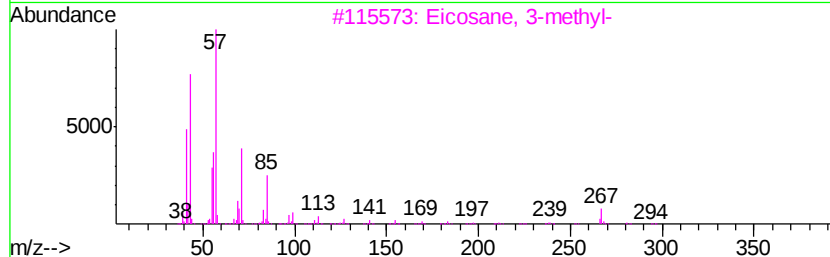
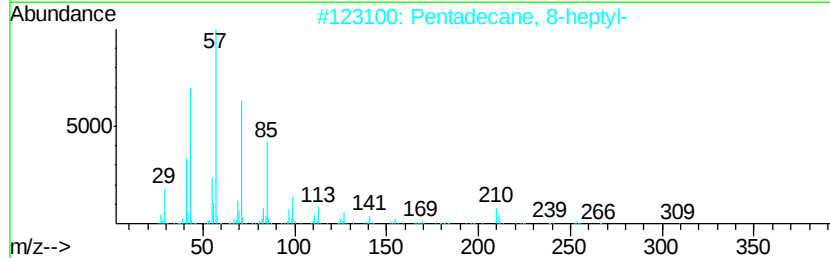
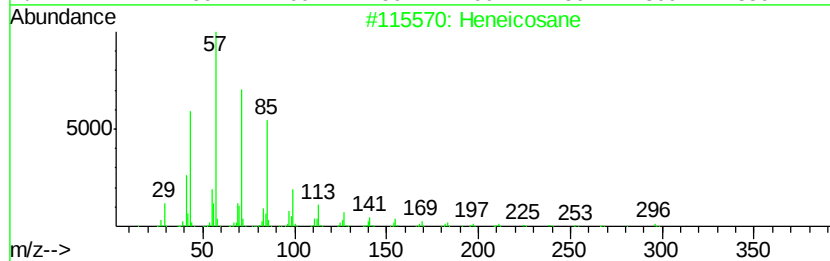
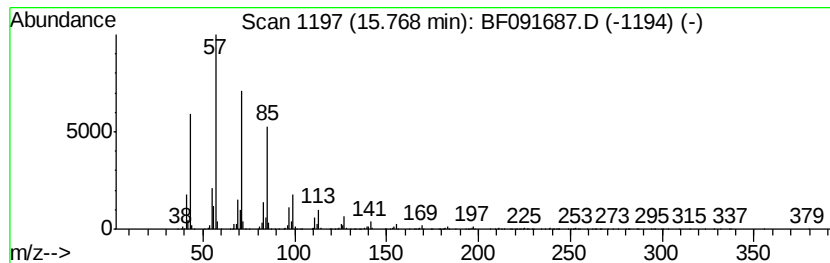
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	33.76 ng	2276370	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	91
3	Eicosane, 3-methyl-		296	C21H44	006418-46-8	91
4	Tetratetracontane		619	C44H90	007098-22-8	83
5	Hexatriacontane		507	C36H74	000630-06-8	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
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Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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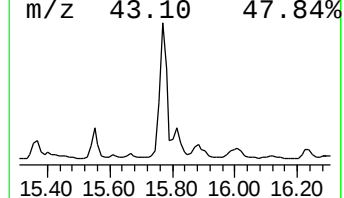
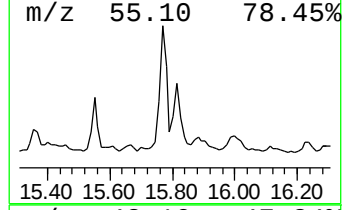
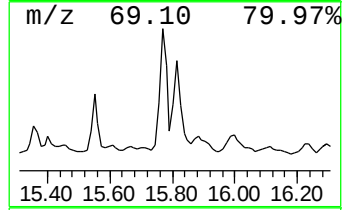
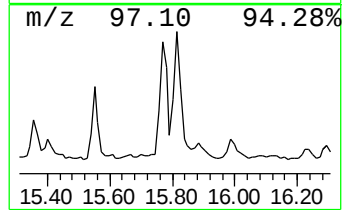
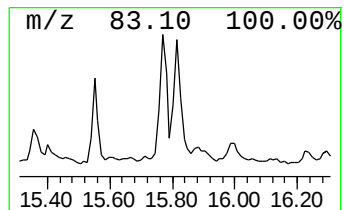
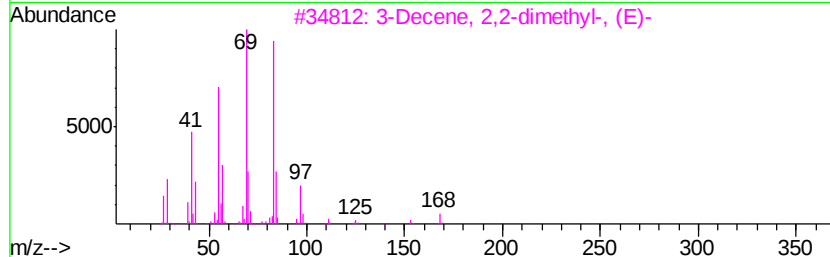
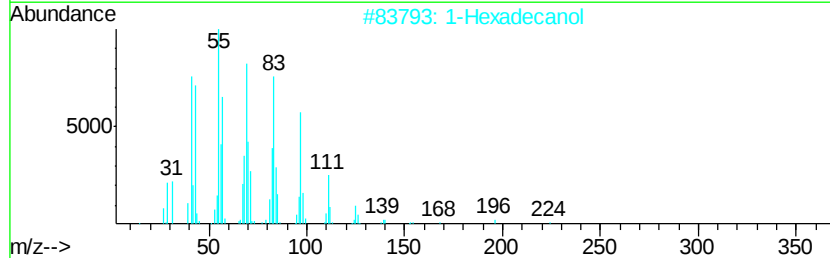
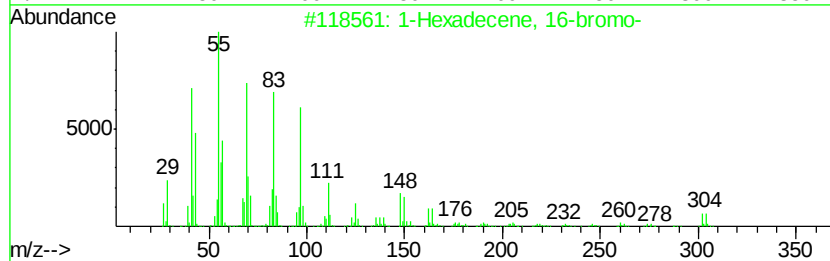
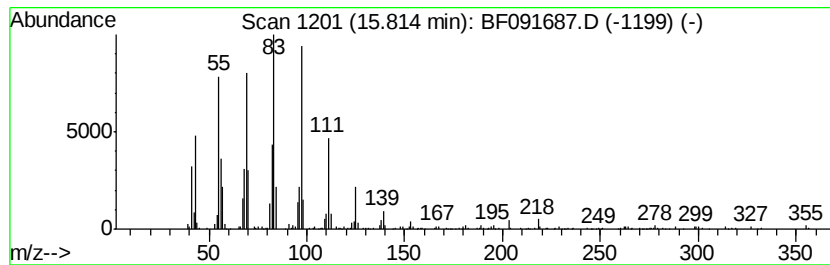
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Hexadecene, 16-bromo- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	9.40 ng	633856	Perylene-d12	15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	64
2			1-Hexadecanol	242	C16H34O	036653-82-4	43
3			3-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055499-02-0	38
4			Cycloheptane, methyl-	112	C8H16	004126-78-7	38
5			Cyclopentane, 1-butyl-2-propyl-	168	C12H24	062199-50-2	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
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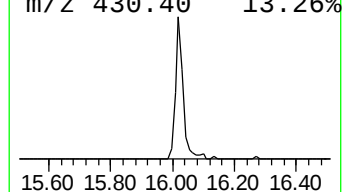
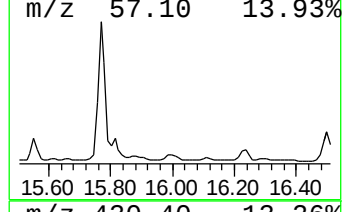
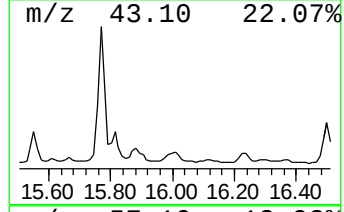
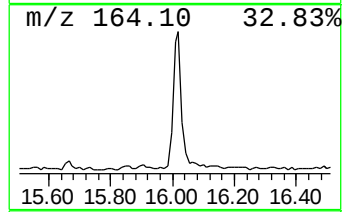
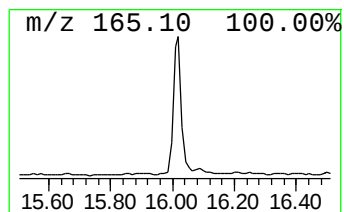
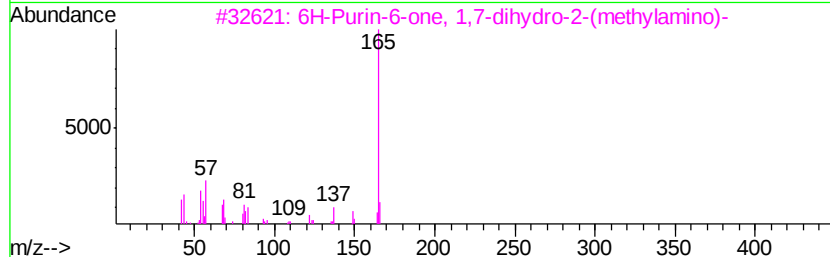
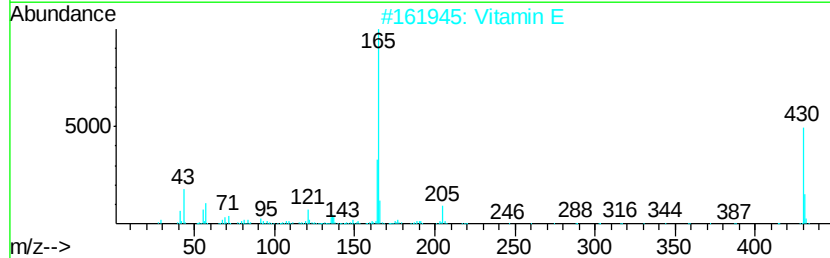
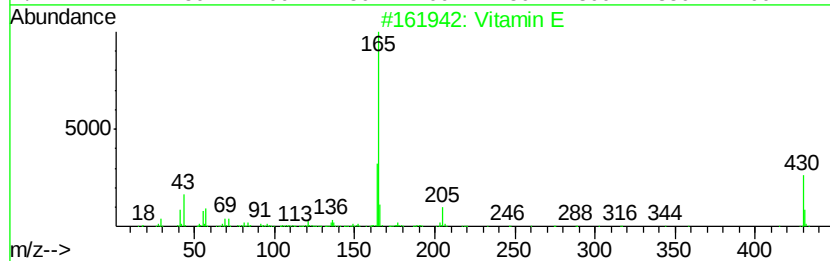
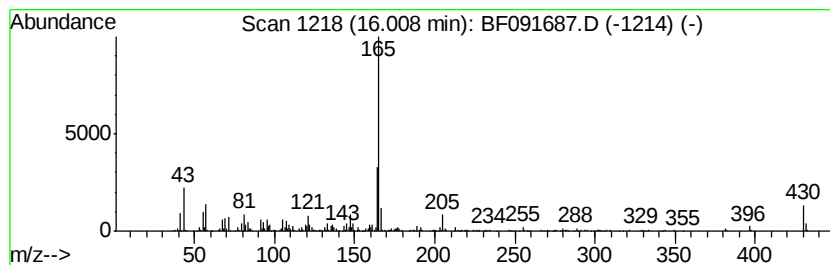
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Vitamin E Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	10.30 ng	694384	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vitamin E	430	C29H50O2	010191-41-0	96
2		Vitamin E	430	C29H50O2	000059-02-9	93
3		6H-Purin-6-one, 1,7-dihydro-2-(m...	165	C6H7N5O	010030-78-1	53
4		3-[5-Isobutyl-2-methyl-furan-3-...	301	C17H19NO4	1000295-19-6	52
5		2-Amino-6-hydroxy-9-methylpurine	165	C6H7N5O	005502-78-3	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

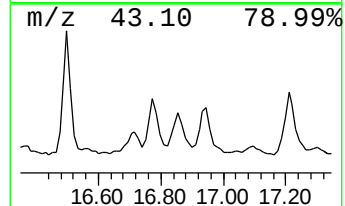
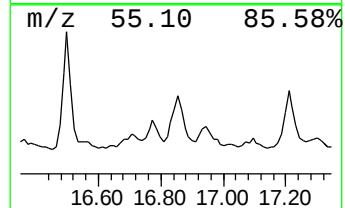
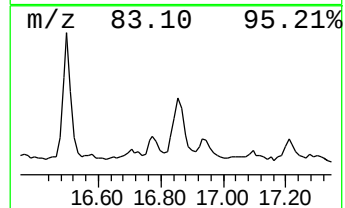
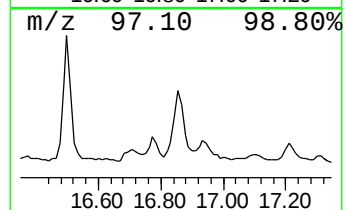
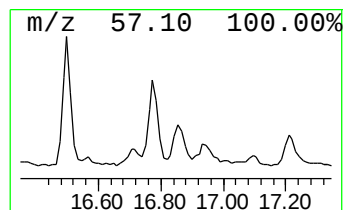
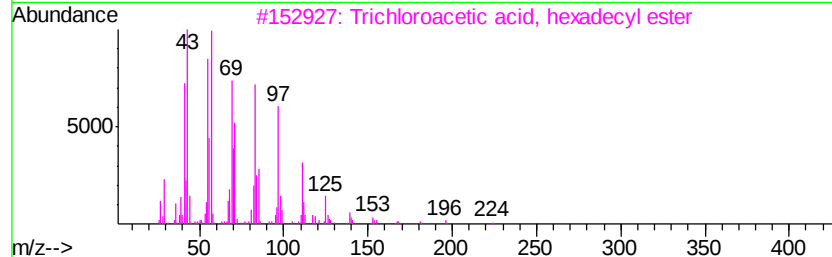
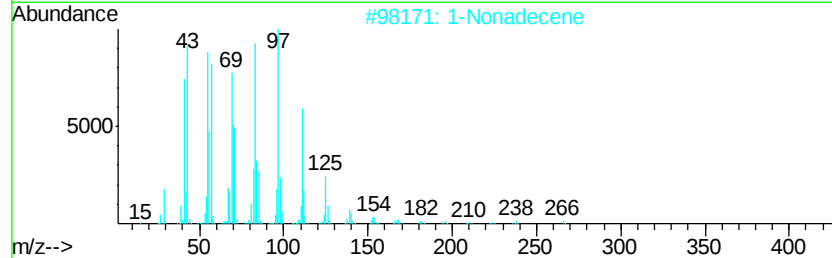
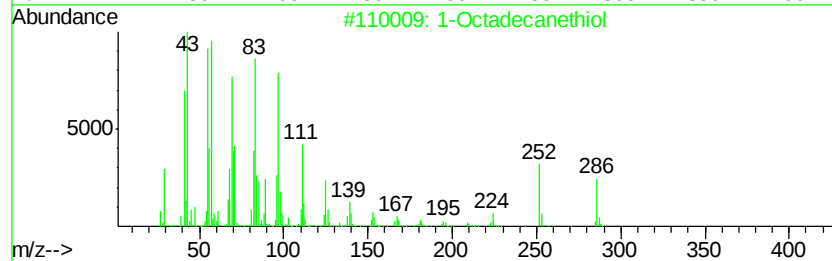
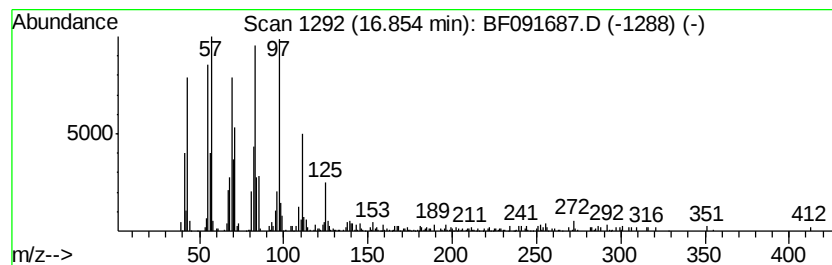
Instrument :
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ClientSampleId :
SS03-0-2IN

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Octadecanethiol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.85	9.27 ng	624865	Perylene-d12	15.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanethiol	286	C18H38S	002885-00-9	91
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	53
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	53
5	1-Hexadecanol	242	C16H34O	036653-82-4	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

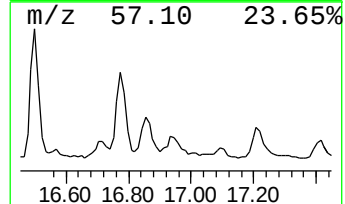
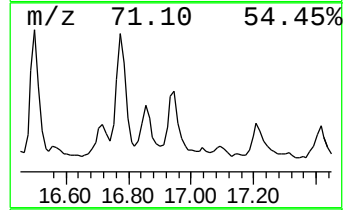
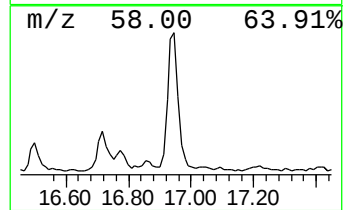
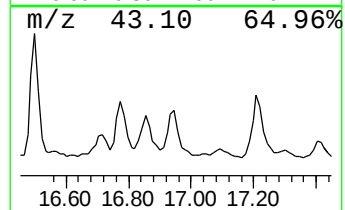
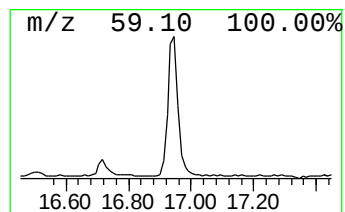
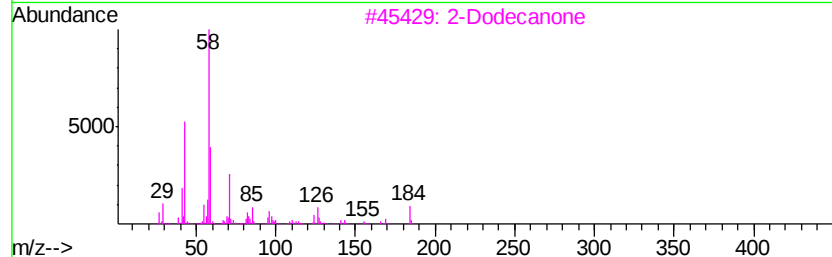
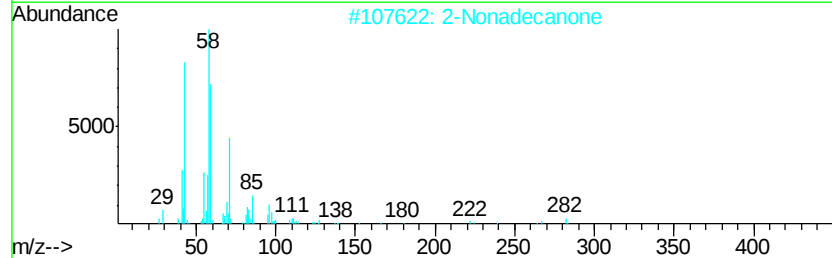
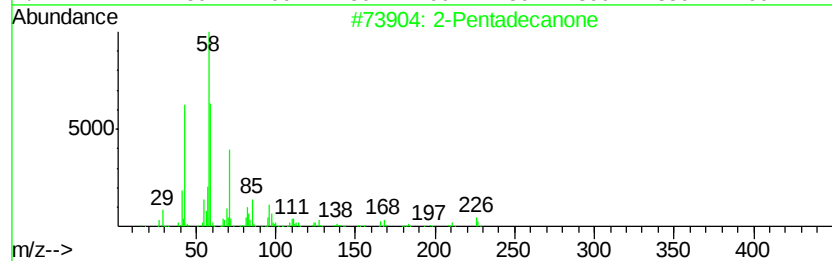
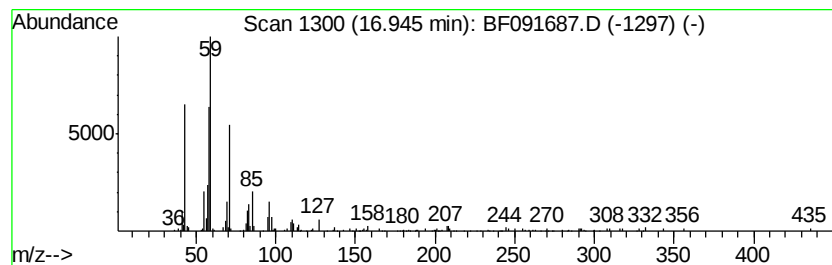
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2-Pentadecanone Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.95	6.61 ng	445952	Perylene-d12		15.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentadecanone	226	C15H30O	002345-28-0	59
2	2-Nonadecanone	282	C19H38O	000629-66-3	59
3	2-Dodecanone	184	C12H24O	006175-49-1	59
4	2-Pentacosanone	366	C25H50O	075207-54-4	50
5	2-Tridecanone	198	C13H26O	000593-08-8	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

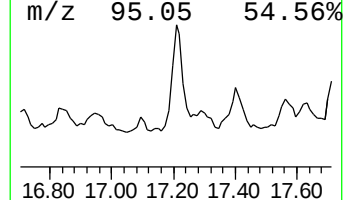
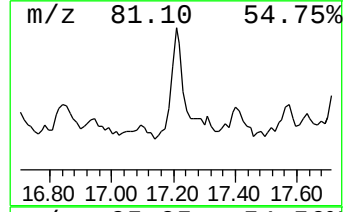
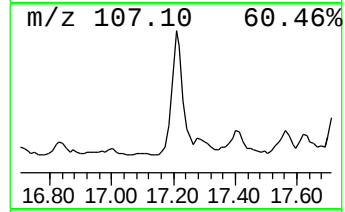
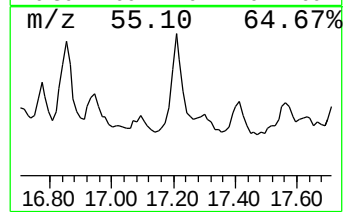
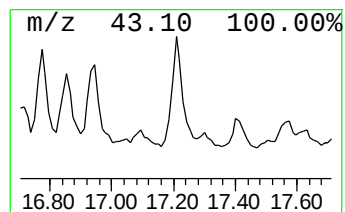
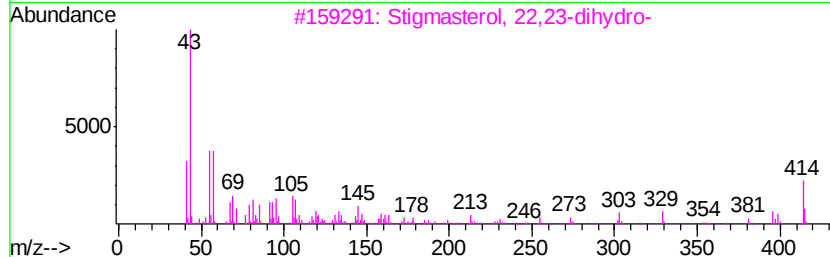
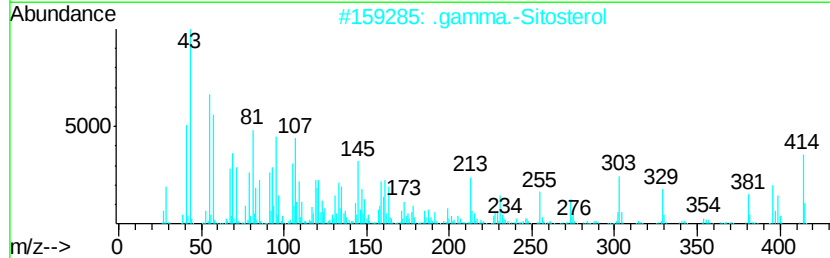
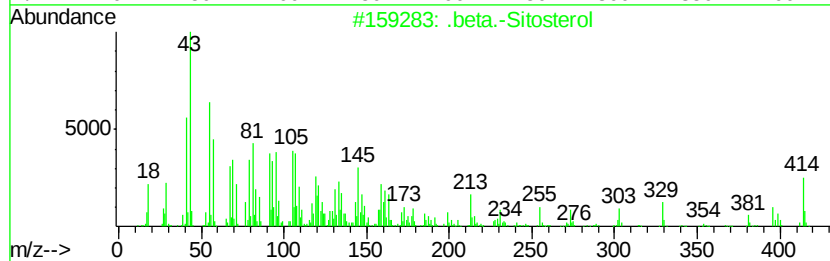
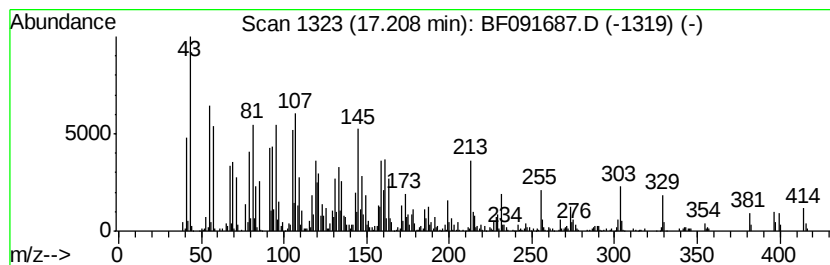
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	21.79 ng	1469450	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 99
2		.gamma.-Sitosterol	414 C29H50O	000083-47-6 99
3		Stigmasterol, 22,23-dihydro-	414 C29H50O	1000214-20-7 90
4		Stigmastan-3,5-diene	396 C29H48	1000214-16-4 45
5		Ergost-5-en-3-ol, (3.beta.)-	400 C28H48O	004651-51-8 43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS03-0-2IN

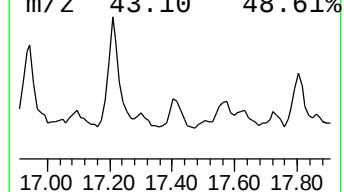
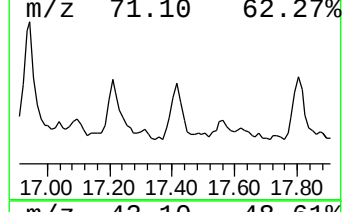
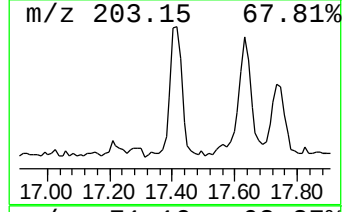
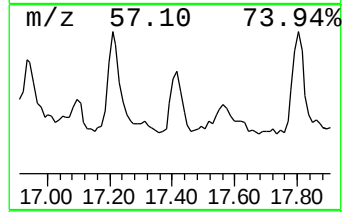
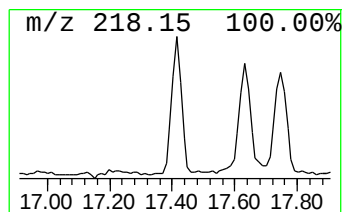
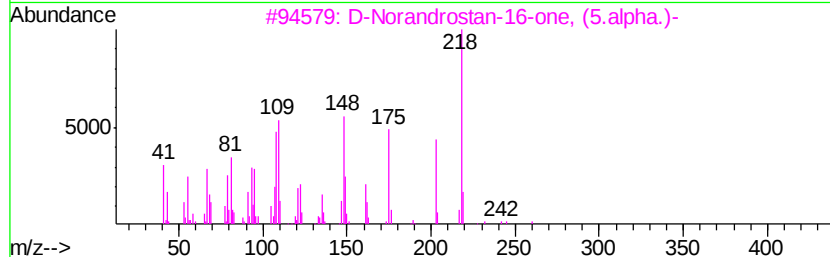
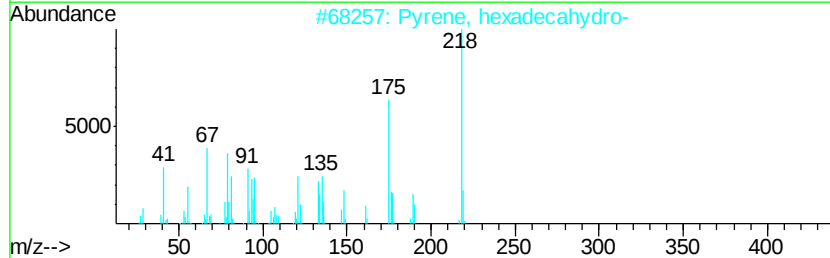
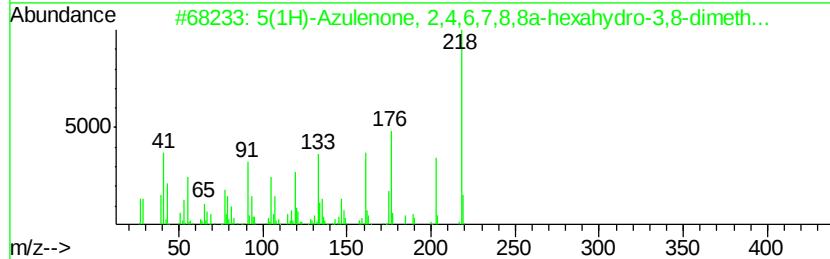
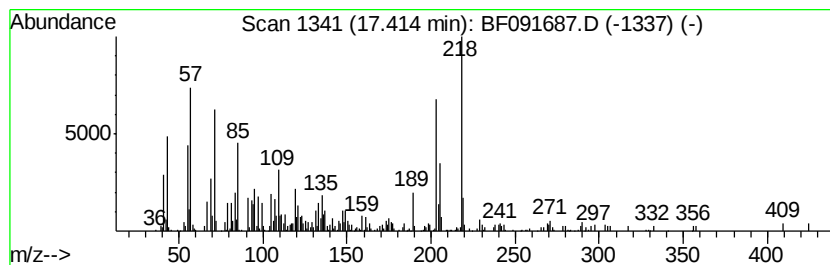
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.41 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.41	6.78 ng	457177	Perylene-d12	15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	41
2			Pyrene, hexadecahydro-	218	C16H26	002435-85-0	38
3			D-Norandrostane-16-one, (5.alpha.)-	260	C18H28O	032319-06-5	38
4			1-Pyrrolidin-2-amine, N-(1-adamant...	218	C14H22N2	300695-00-5	38
5			8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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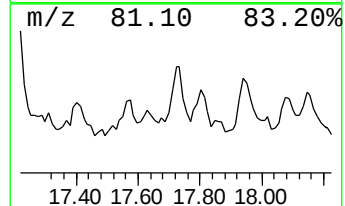
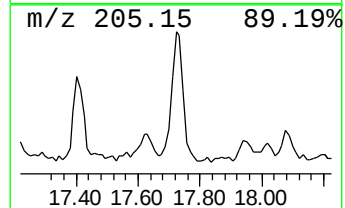
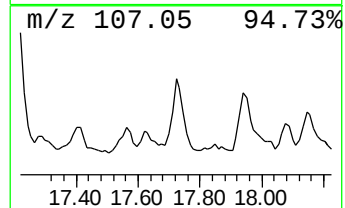
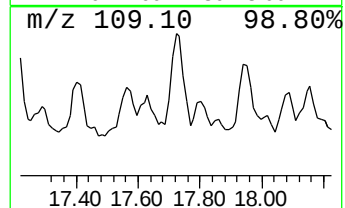
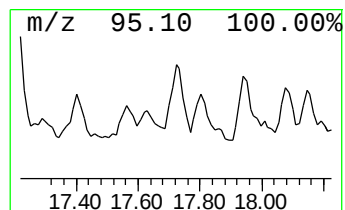
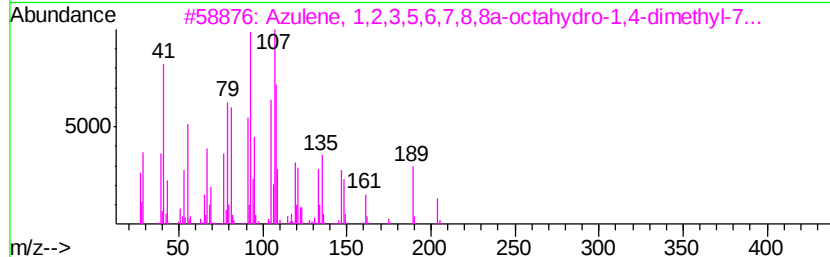
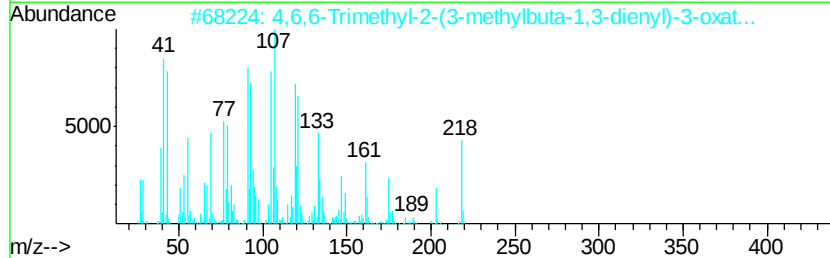
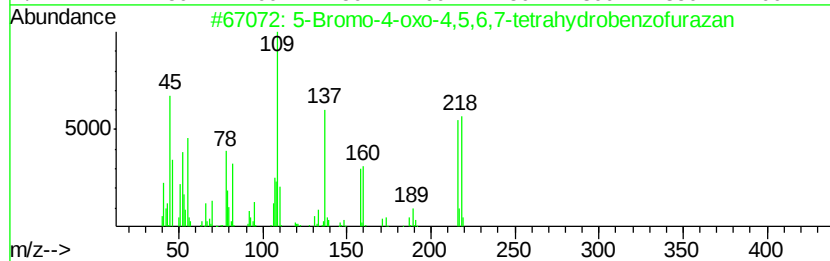
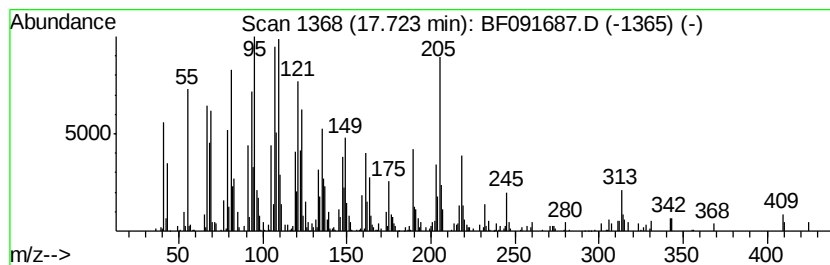
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown17.72 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.72	7.34 ng	495028	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	42
2		4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	35
3		Azulene, 1,2,3,5,6,7,8,8a-octahv...	204	C15H24	003691-11-0	35
4		Sesquirosefuran	218	C15H22O	039007-93-7	30
5		.gamma.-Elemene	204	C15H24	030824-67-0	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
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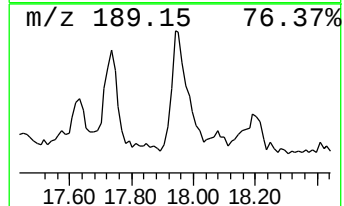
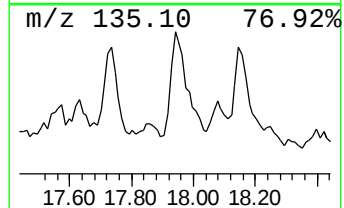
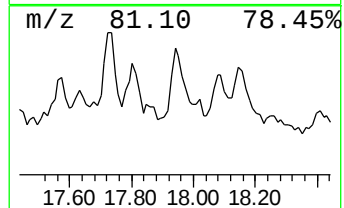
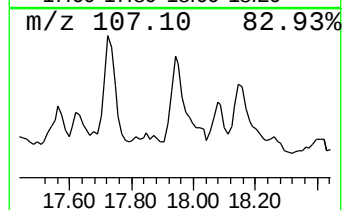
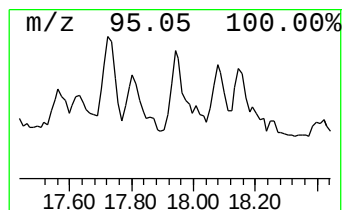
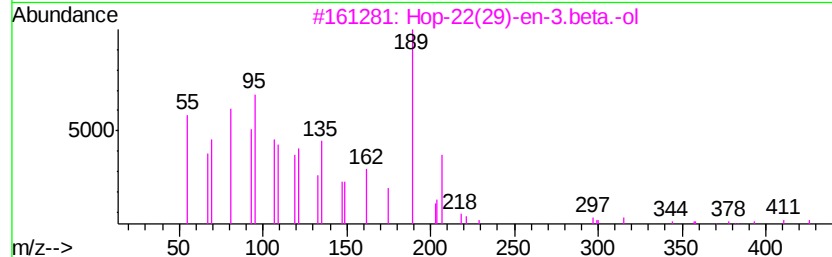
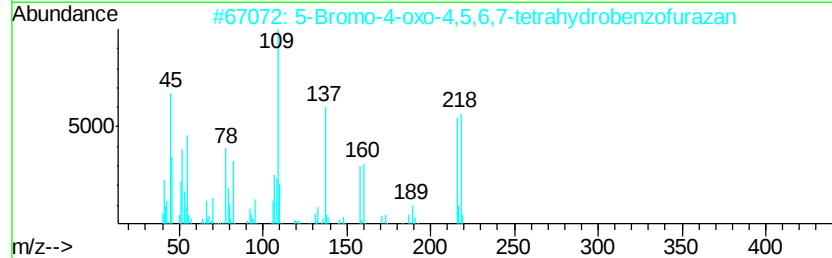
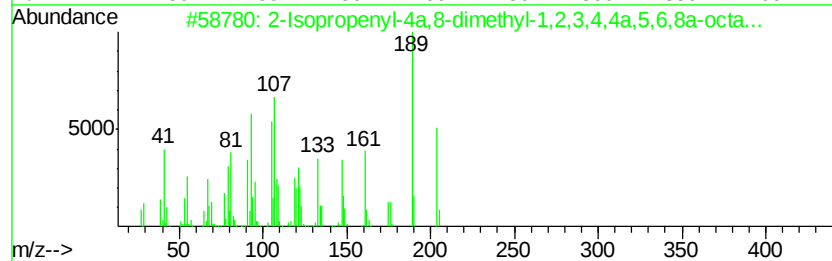
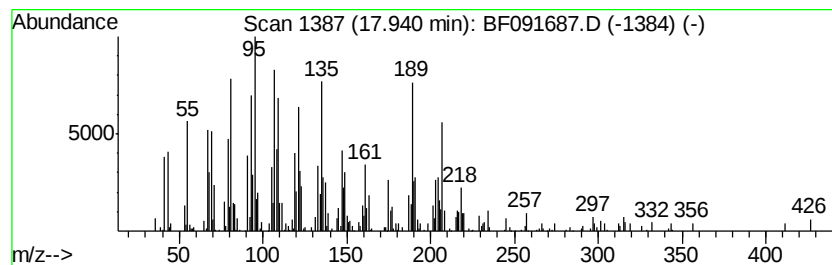
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 2-Isopropenyl-4a,8-dimethyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.94	10.03 ng	676351	Perylene-d12	15.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	87	
2	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	60	
3	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	50	
4	3-Isopropyltricyclo[4.3.1.1(2,5)...]	206	C14H22O	1000195-22-9	44	
5	Longifolenaldehyde	220	C15H24O	019890-84-7	43	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS03-0-2IN

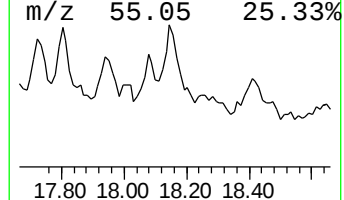
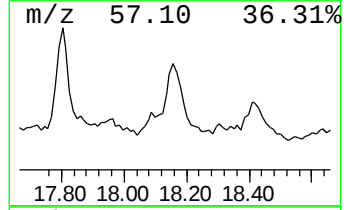
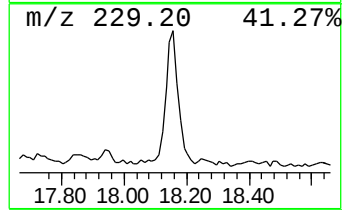
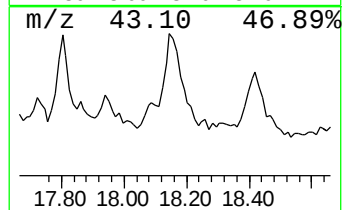
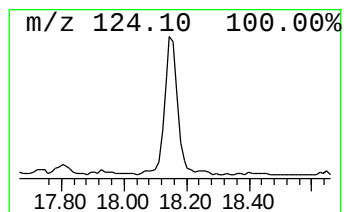
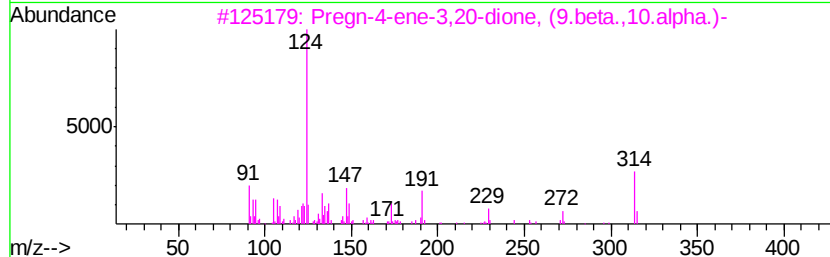
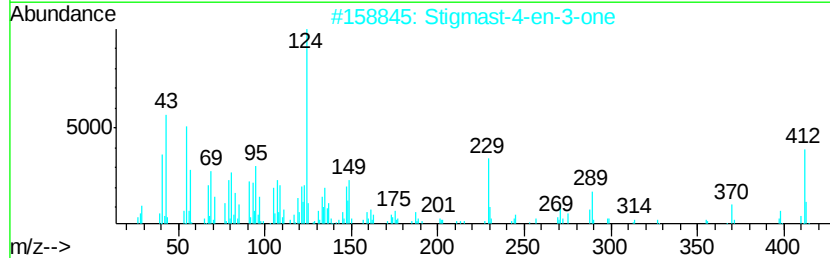
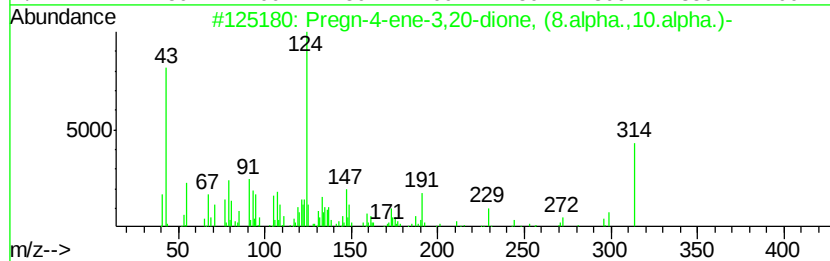
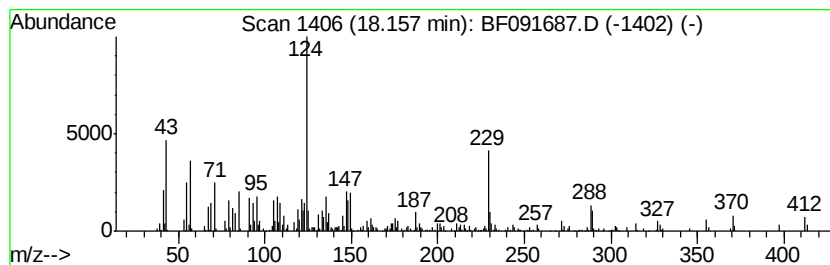
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Pregn-4-ene-3,20-dione, (8.... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	12.59 ng	849018	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pregn-4-ene-3,20-dione, (8.alpha...	314	C21H30O2	003795-19-5	55
2		Stigmast-4-en-3-one	412	C29H48O	001058-61-3	55
3		Pregn-4-ene-3,20-dione, (9.beta....	314	C21H30O2	002755-10-4	52
4		Pregn-4-ene-3,20-dione, (10.alph...	314	C21H30O2	003562-13-8	50
5		Testosterone	288	C19H28O2	000058-22-0	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121616\
Data File : BF091687.D
Acq On : 16 Dec 2016 21:54
Operator : UM/SJ
Sample : H6099-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS03-0-2IN

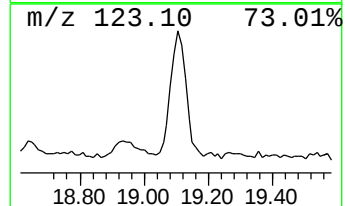
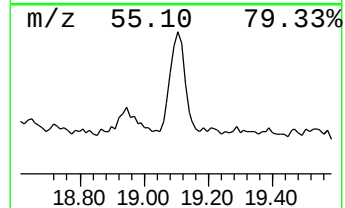
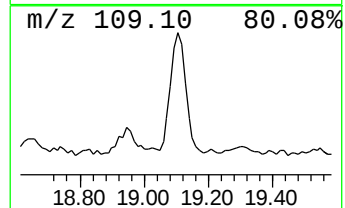
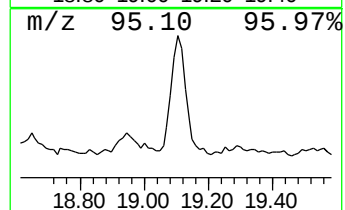
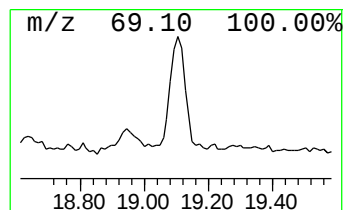
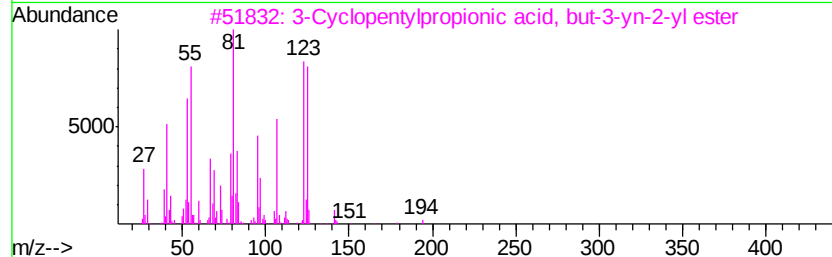
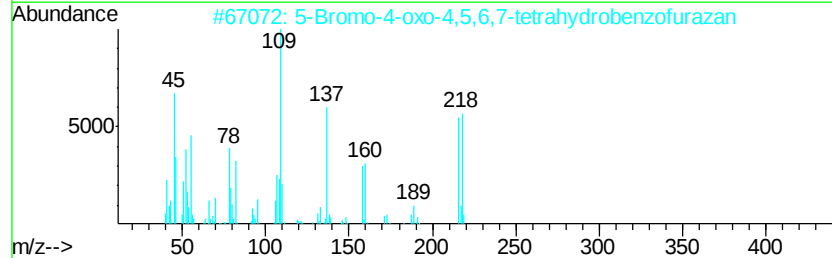
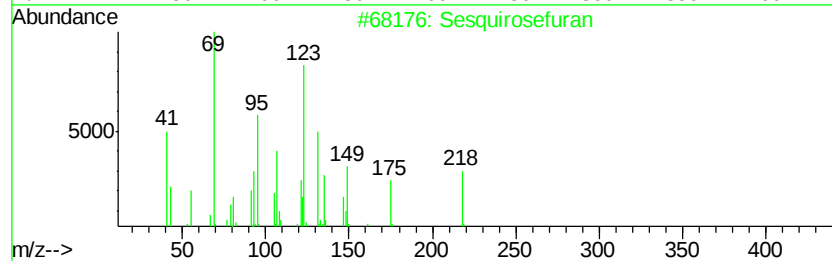
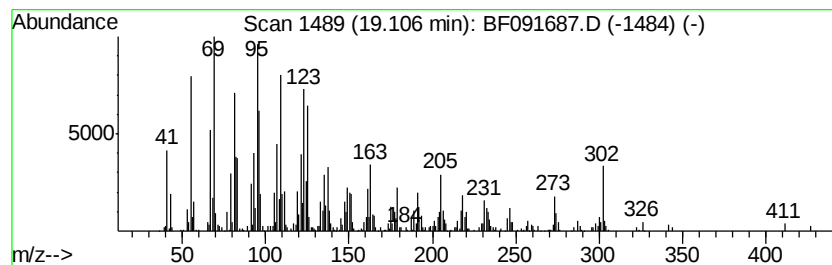
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Sesquirosefuran Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.11	17.69 ng	1192770	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sesquirosefuran	218	C15H22O	039007-93-7	83
2		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	68
3		3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	47
4		Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	42
5		2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121616\
 Data File : BF091687.D
 Acq On : 16 Dec 2016 21:54
 Operator : UM/SJ
 Sample : H6099-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS03-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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
2-Pentanone, 4-hy...	4.94	34.9	ng	2889450	1	6.77	1655100	20.0
unknown6.54	6.54	60.6	ng	5015380	1	6.77	1655100	20.0
Tetradecanoic acid	11.84	7.0	ng	1081480	4	11.29	3078910	20.0
Ethanol, 2-(tetra...	13.78	11.9	ng	1237040	5	13.92	2085370	20.0
Heptadecane	14.41	12.5	ng	1306580	5	13.92	2085370	20.0
Octadecane	15.01	40.1	ng	2703210	6	15.32	1348760	20.0
Oxirane, heptadecyl-	15.55	10.1	ng	678889	6	15.32	1348760	20.0
Heneicosane	15.77	33.8	ng	2276370	6	15.32	1348760	20.0
1-Hexadecene, 16-...	15.81	9.4	ng	633856	6	15.32	1348760	20.0
Vitamin E	16.01	10.3	ng	694384	6	15.32	1348760	20.0
1-Octadecanethiol	16.85	9.3	ng	624865	6	15.32	1348760	20.0
2-Pentadecanone	16.95	6.6	ng	445952	6	15.32	1348760	20.0
.beta.-Sitosterol	17.21	21.8	ng	1469450	6	15.32	1348760	20.0
unknown17.41	17.41	6.8	ng	457177	6	15.32	1348760	20.0
unknown17.72	17.72	7.3	ng	495028	6	15.32	1348760	20.0
2-Isopropenyl-4a,...	17.94	10.0	ng	676351	6	15.32	1348760	20.0
Pregn-4-ene-3,20-...	18.16	12.6	ng	849018	6	15.32	1348760	20.0
Sesquirosefuran	19.11	17.7	ng	1192770	6	15.32	1348760	20.0