

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
 Data File : BF091754.D
 Acq On : 18 Dec 2016 23:26
 Operator : UM/SJ
 Sample : H6099-13
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP10-3-4FT

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-BF121716.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	4.270	189	191	194	rBV	57501	82384	1.17%	0.115%
2	4.944	246	250	259	rBV	2582112	3761448	53.48%	5.229%
3	5.367	284	287	290	rBV	4448084	6286350	89.37%	8.739%
4	6.407	375	378	381	rBV	4956278	6204370	88.21%	8.626%
5	6.533	386	389	392	rBV	5383472	6007180	85.40%	8.351%
6	6.762	407	409	412	rBV	1822375	1772209	25.20%	2.464%
7	6.922	420	423	425	rBV	5203221	4788095	68.07%	6.657%
8	7.333	456	459	461	rBV	3860481	4305478	61.21%	5.986%
9	8.053	519	522	524	rBV	2428286	2545345	36.19%	3.539%
10	9.128	613	616	619	rBV	5968635	6970405	99.10%	9.690%
11	9.528	648	651	653	rBV	521308	569903	8.10%	0.792%
12	9.802	672	675	678	rBV	2993963	2825266	40.17%	3.928%
13	10.248	710	714	715	rBV2	152855	207165	2.95%	0.288%
14	10.465	730	733	736	rBV	70125	104312	1.48%	0.145%
15	10.591	741	744	747	rVV	3942500	4469670	63.55%	6.214%
16	10.682	750	752	753	rVV	67544	88950	1.26%	0.124%
17	10.716	753	755	760	rVB	276474	333449	4.74%	0.464%
18	11.162	792	794	796	rBV	224700	200410	2.85%	0.279%
19	11.288	802	805	807	rBV	2554681	2832779	40.27%	3.938%
20	11.585	829	831	834	rBV	73450	80177	1.14%	0.111%
21	11.825	850	852	856	rBV	306191	353588	5.03%	0.492%
22	11.996	863	867	871	rBV2	80958	123801	1.76%	0.172%
23	12.614	918	921	926	rBV2	71771	128270	1.82%	0.178%
24	12.705	926	929	931	rVV	679696	726998	10.34%	1.011%
25	12.774	931	935	938	rVB2	218781	284969	4.05%	0.396%
26	12.876	941	944	946	rBV	6397297	7033830	100.00%	9.779%
27	13.105	961	964	966	rBV2	62539	100716	1.43%	0.140%
28	13.345	983	985	988	rVB2	81175	145669	2.07%	0.203%
29	13.402	988	990	992	rBV2	511143	532796	7.57%	0.741%
30	13.448	992	994	995	rVV2	57493	85566	1.22%	0.119%
31	13.768	1020	1022	1032	rBV	619908	859095	12.21%	1.194%
32	13.917	1032	1035	1037	rBV	2604664	2476139	35.20%	3.442%
33	14.099	1048	1051	1056	rVB	145429	160083	2.28%	0.223%
34	14.408	1076	1078	1084	rVB	278344	384625	5.47%	0.535%

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Integration Parameters: rteint.p
Integrator: RTE
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

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35	14.694	1099	1103	1106	rBV2	148293	282330	4.01%	0.393%
36	14.762	1107	1109	1112	rVB	164518	166261	2.36%	0.231%
37	15.014	1128	1131	1136	rBV	168347	285693	4.06%	0.397%
38	15.322	1154	1158	1160	rBV	1421105	1904897	27.08%	2.648%
39	15.357	1160	1161	1167	rVB	100698	151568	2.15%	0.211%
40	15.757	1193	1196	1199	rBV	127293	223156	3.17%	0.310%
41	15.802	1199	1200	1205	rVB	42413	78850	1.12%	0.110%
42	16.225	1232	1237	1242	rVB3	66800	176737	2.51%	0.246%
43	16.488	1257	1260	1265	rVB	62488	110761	1.57%	0.154%
44	16.763	1281	1284	1287	rBV	39271	74845	1.06%	0.104%
45	16.831	1287	1290	1296	rVB6	26060	73631	1.05%	0.102%
46	17.197	1318	1322	1327	rBV2	120962	286824	4.08%	0.399%
47	17.391	1336	1339	1343	rBV	77438	187511	2.67%	0.261%
48	18.146	1400	1405	1411	rBV6	26156	95950	1.36%	0.133%

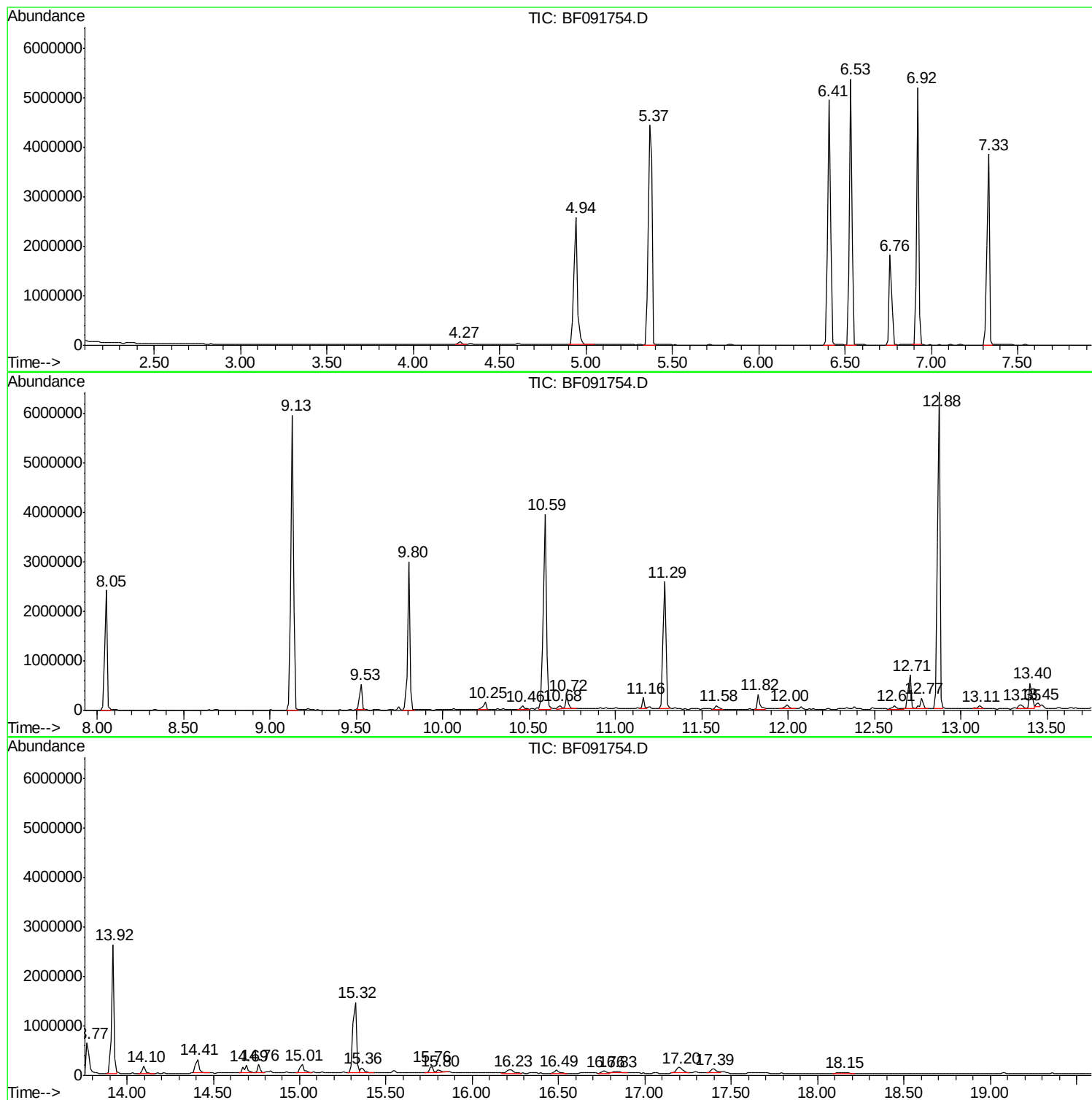
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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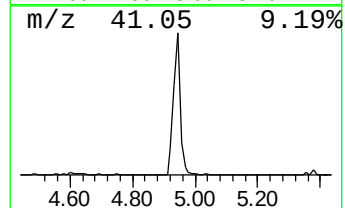
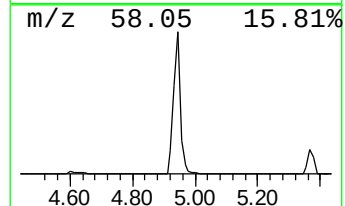
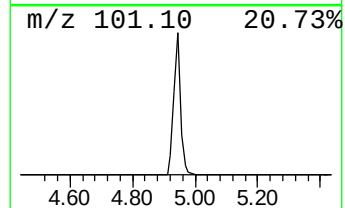
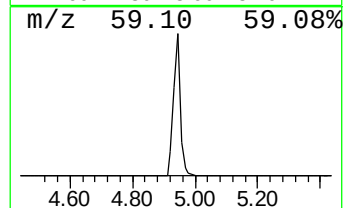
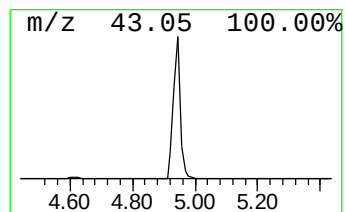
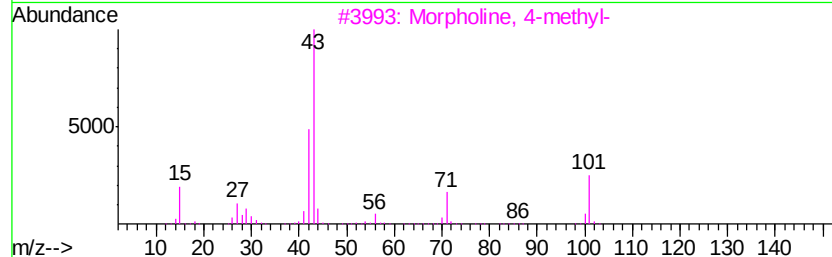
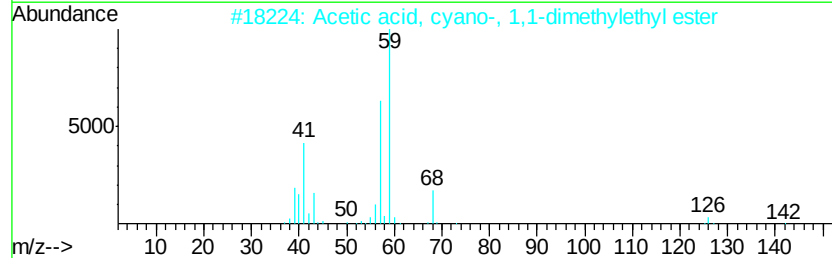
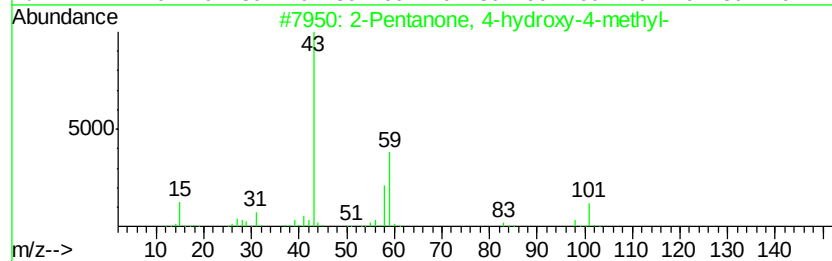
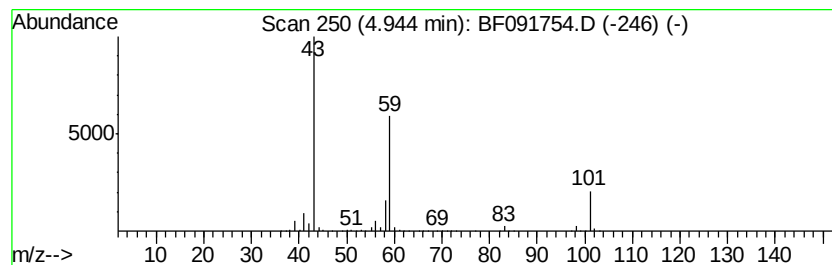
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	42.45 ng	3761450	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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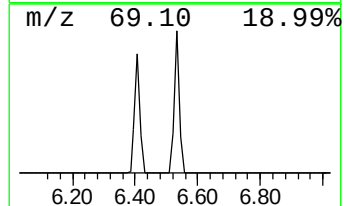
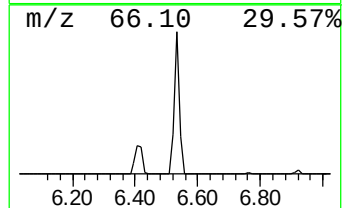
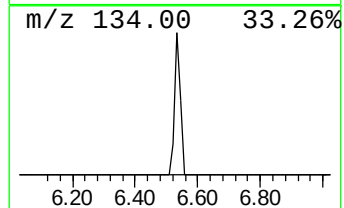
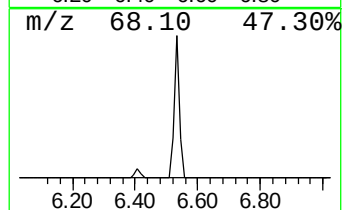
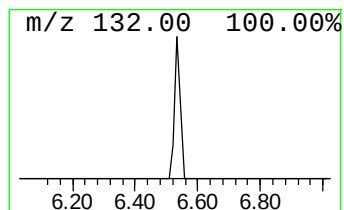
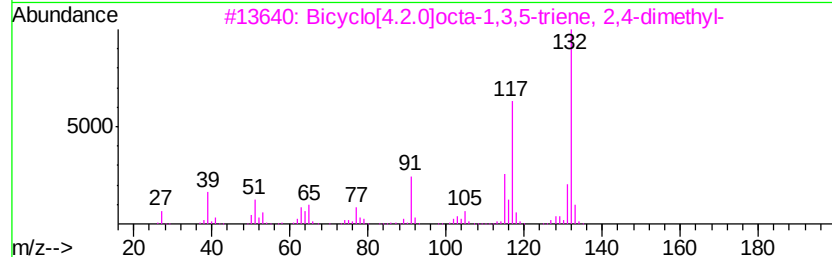
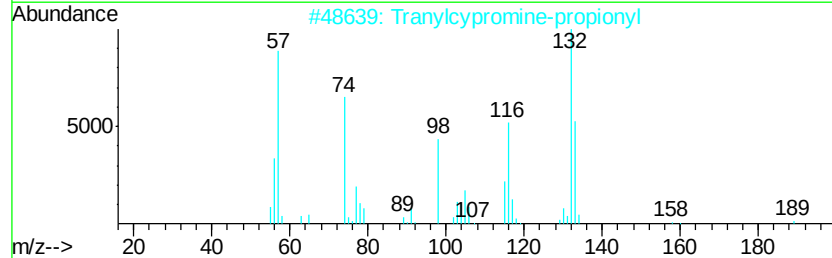
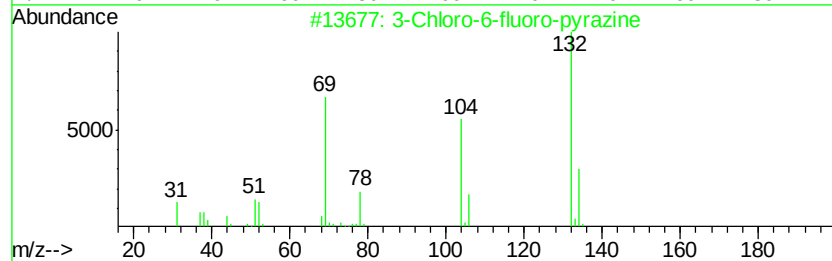
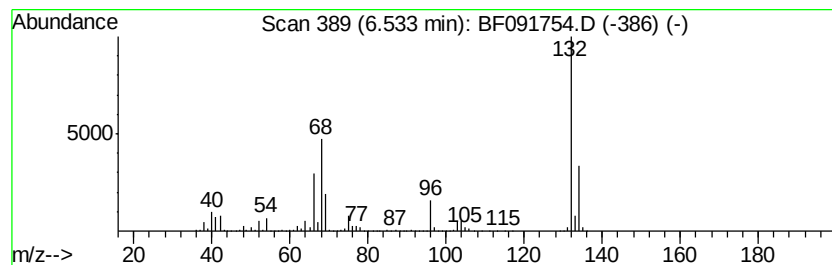
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	67.79 ng	6007180	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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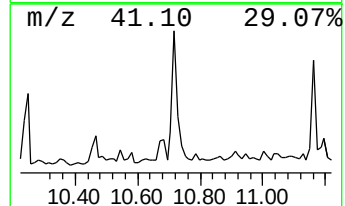
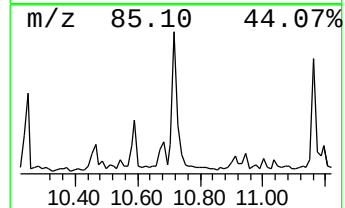
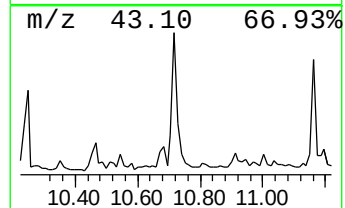
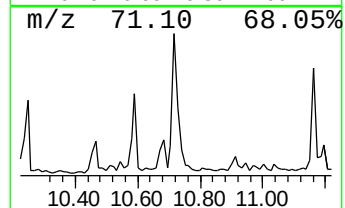
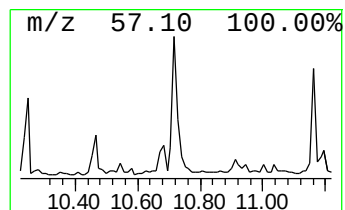
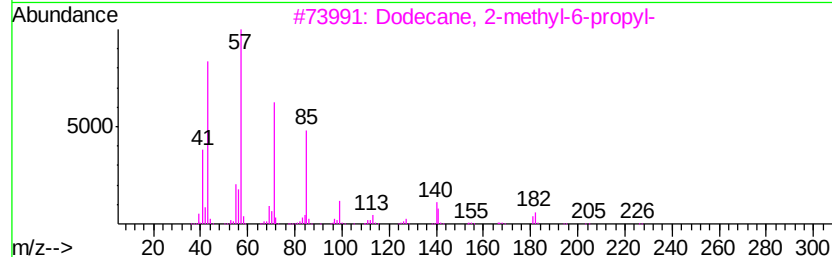
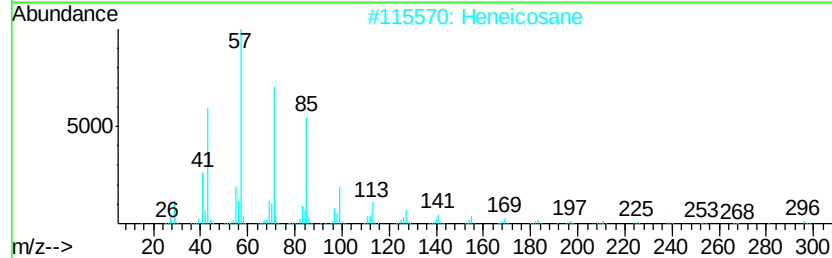
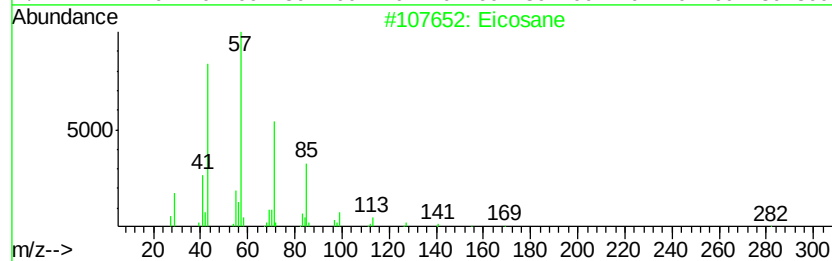
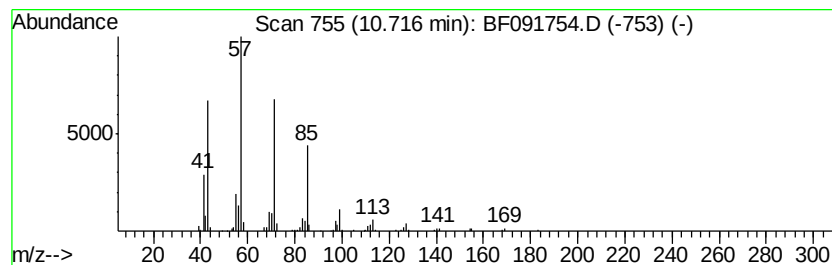
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.35 ng	333449	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Pentadecane		212	C15H32	000629-62-9	86



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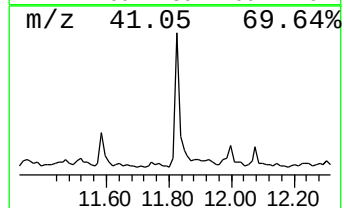
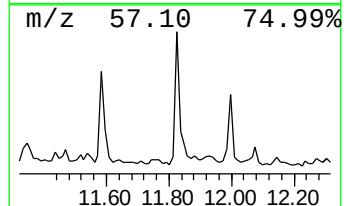
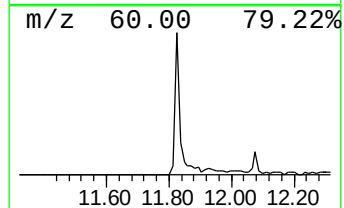
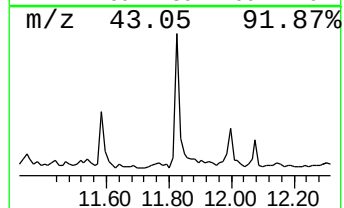
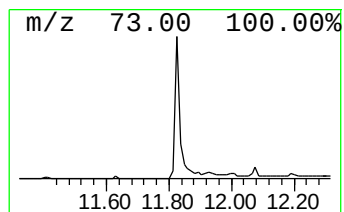
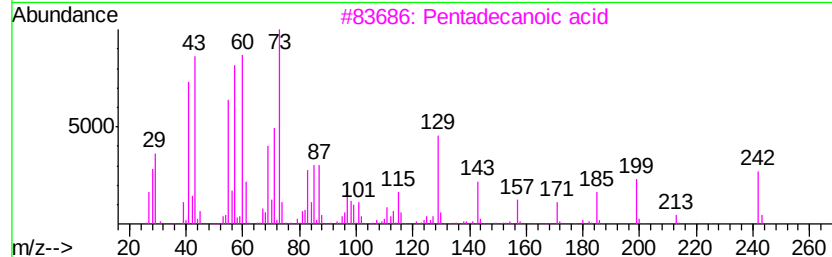
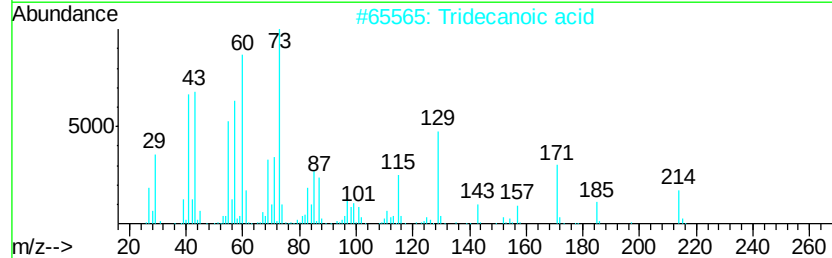
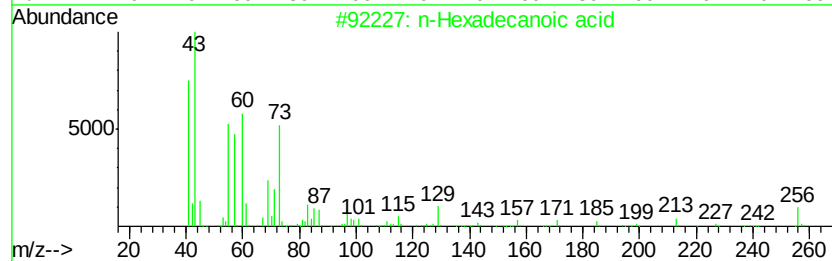
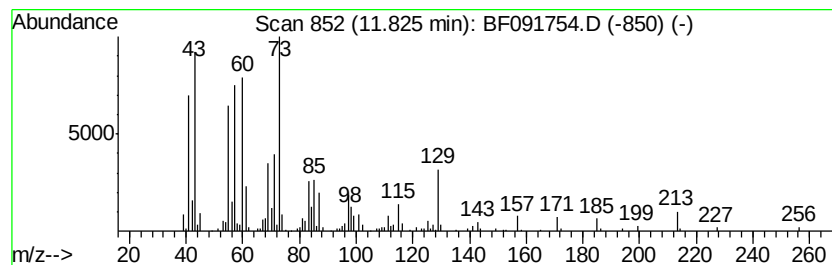
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.82	2.50 ng	353588	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	18
5	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	11



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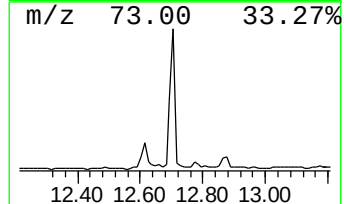
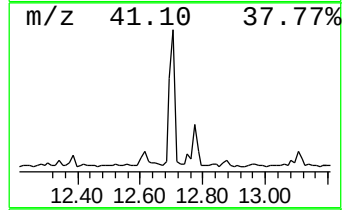
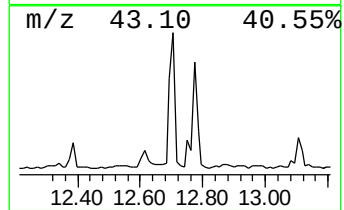
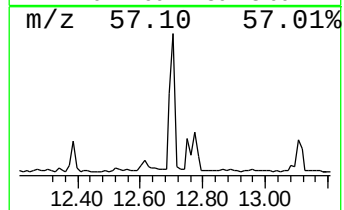
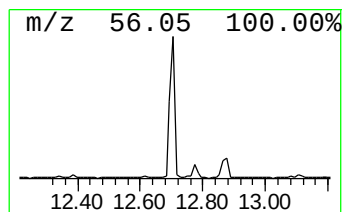
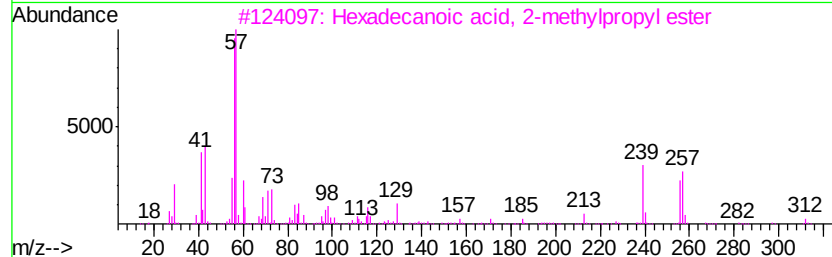
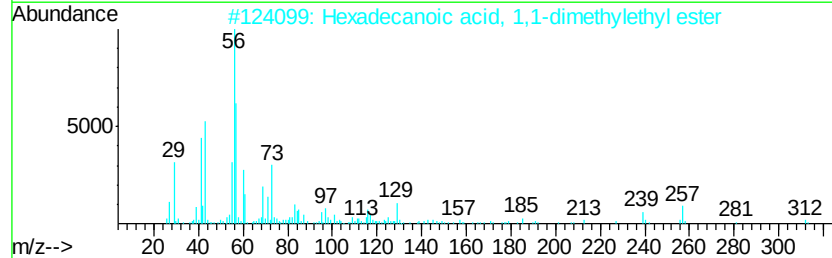
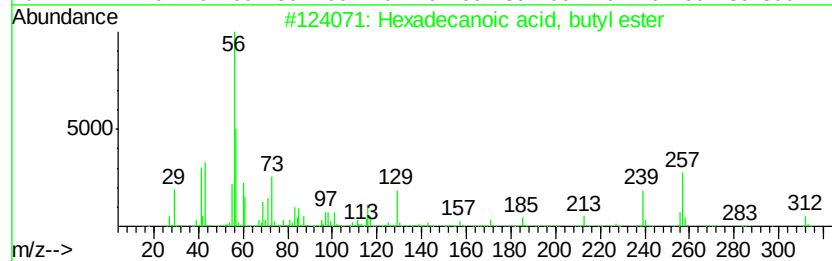
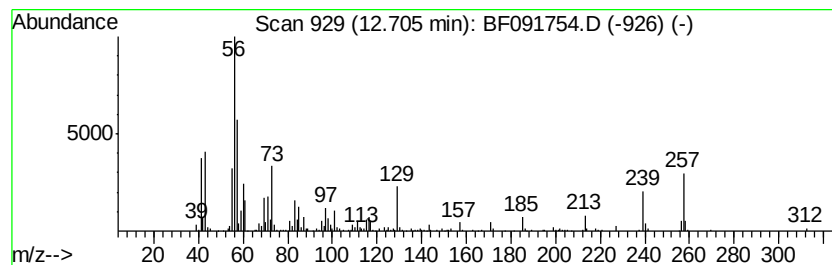
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	5.87 ng	726998	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	53
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091754.D
Acq On : 18 Dec 2016 23:26
Operator : UM/SJ
Sample : H6099-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP10-3-4FT

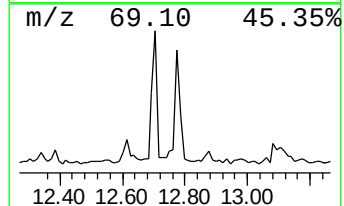
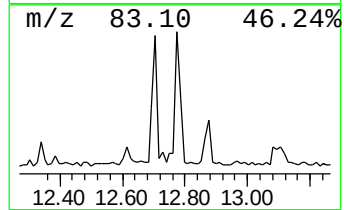
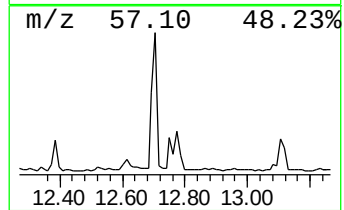
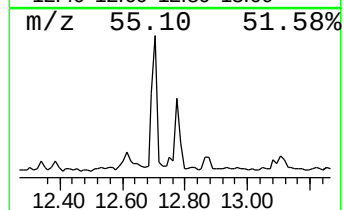
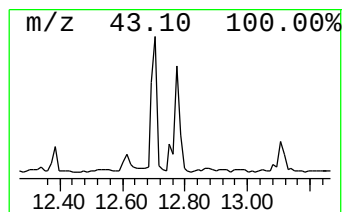
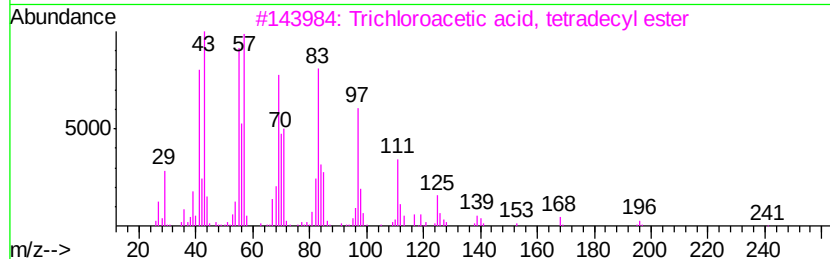
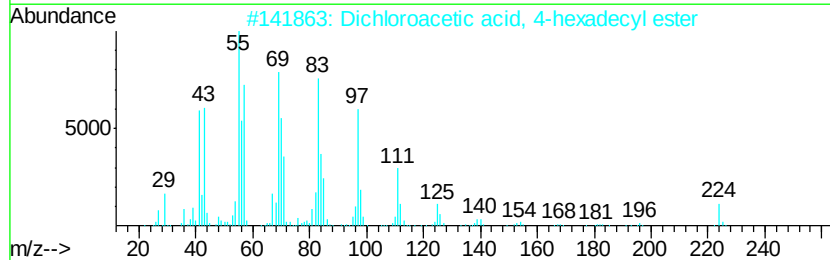
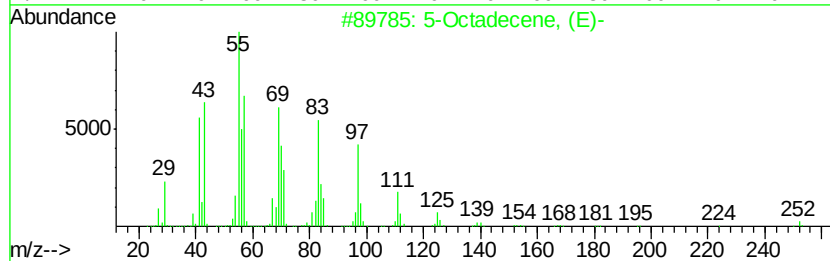
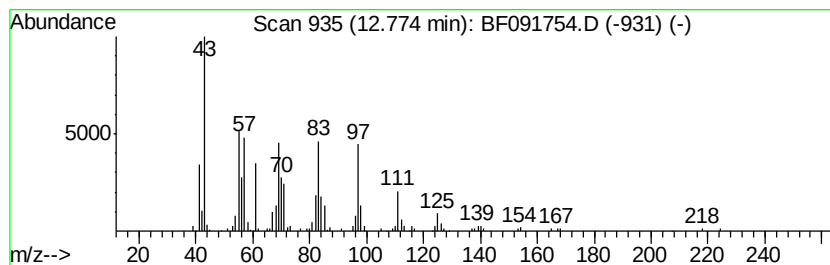
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Octadecene, (E)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.30 ng	284969	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Octadecene, (E)-	252	C18H36	007206-21-5	87
2		Dichloroacetic acid, 4-hexadecyl...	352	C18H34Cl2O2	1000282-98-1	81
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	81
4		5-Eicosene, (E)-	280	C20H40	074685-30-6	76
5		Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
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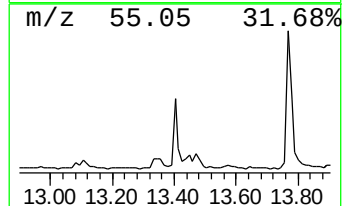
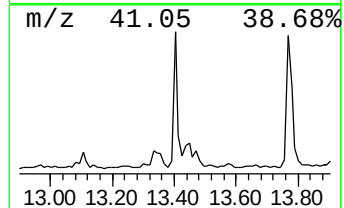
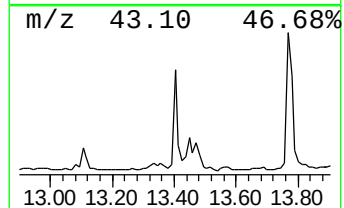
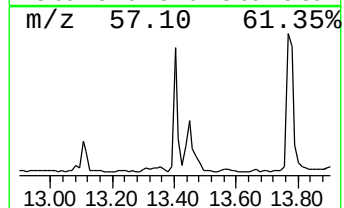
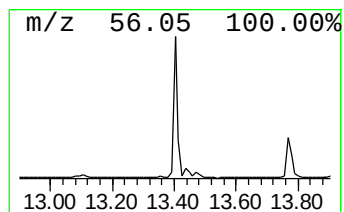
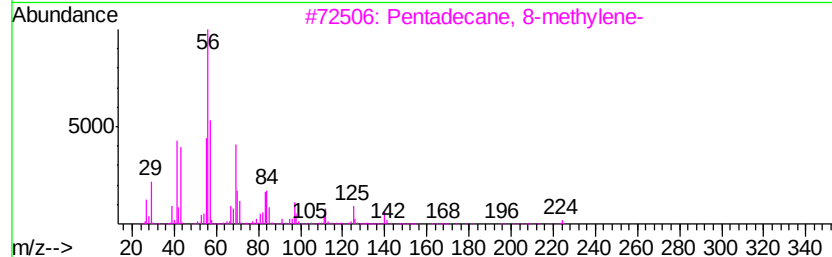
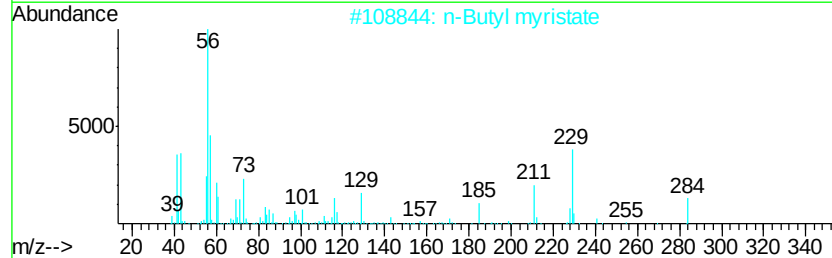
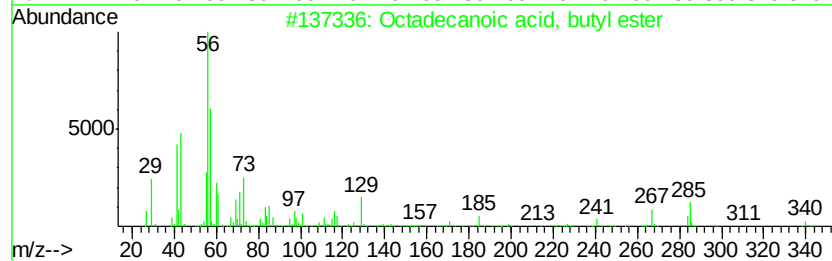
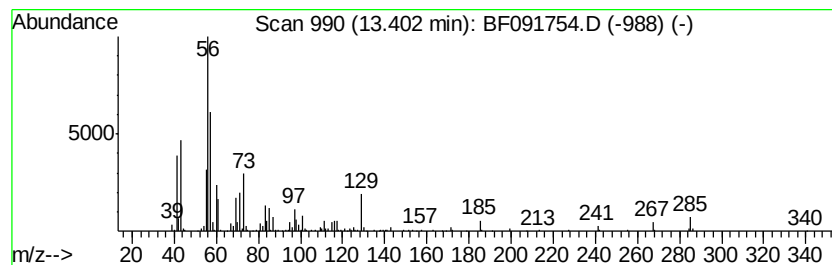
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.40	4.30 ng	532796	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2	n-Butyl myristate	284	C18H36O2	000110-36-1	80
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091754.D
Acq On : 18 Dec 2016 23:26
Operator : UM/SJ
Sample : H6099-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

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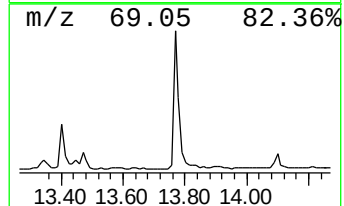
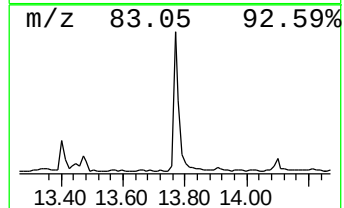
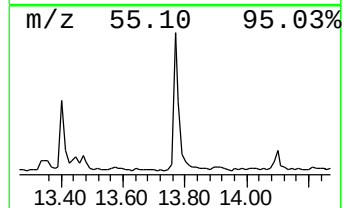
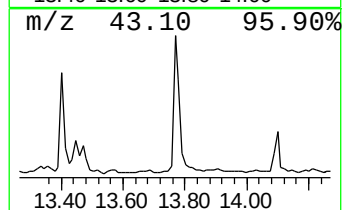
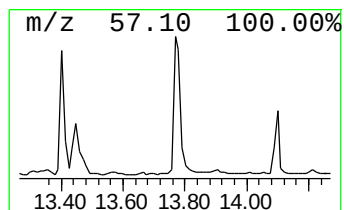
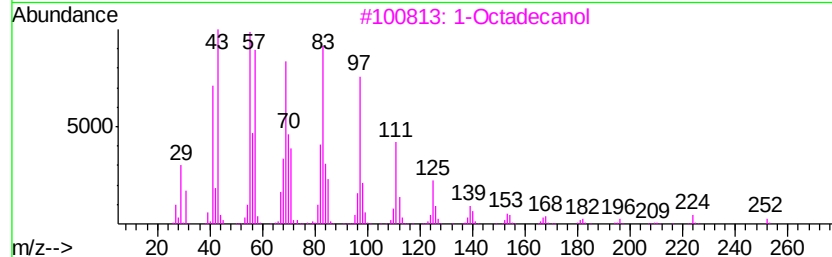
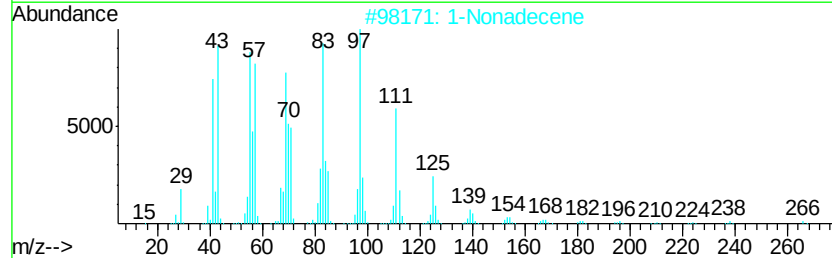
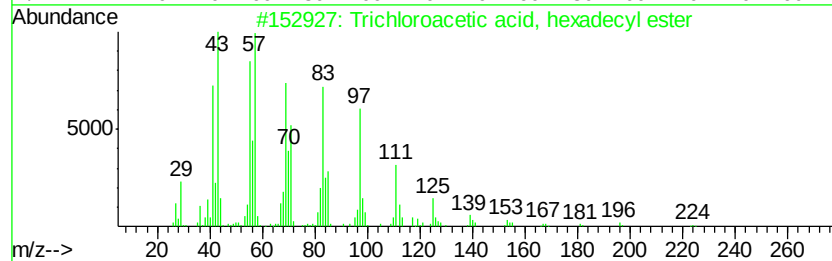
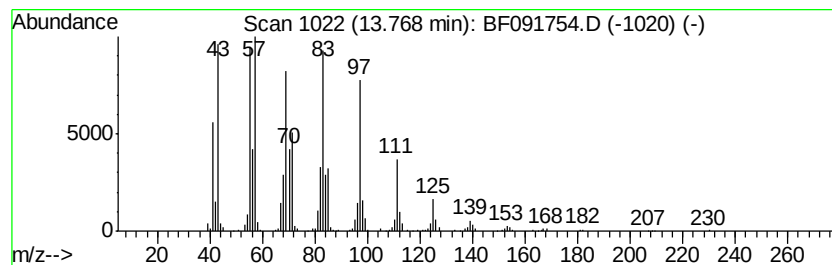
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	6.94 ng	859095	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	Cyclohexadecane	224	C16H32	000295-65-8	87
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
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Acq On : 18 Dec 2016 23:26
Operator : UM/SJ
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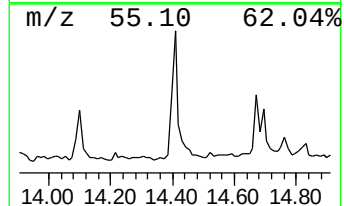
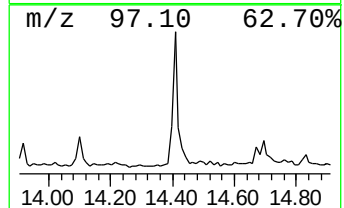
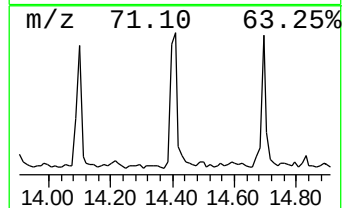
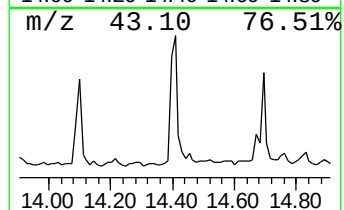
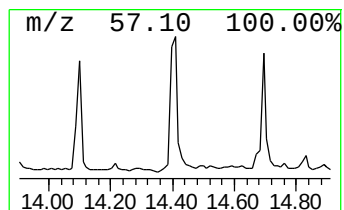
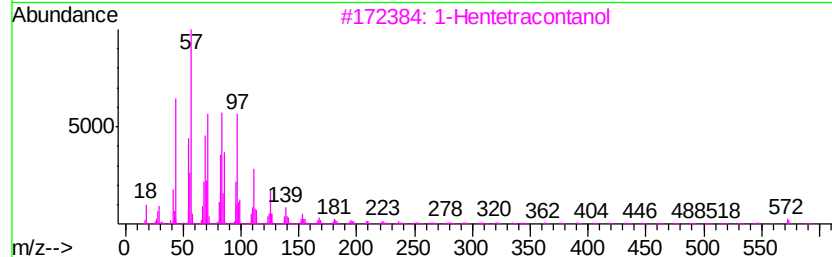
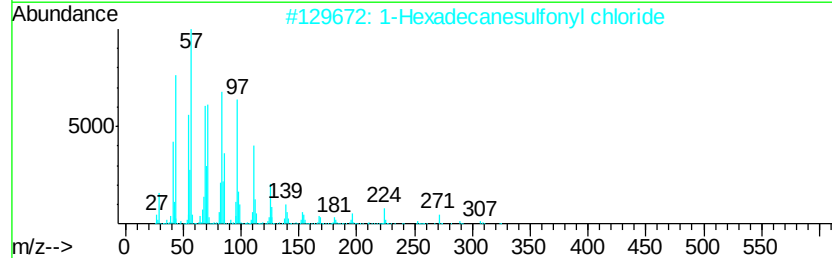
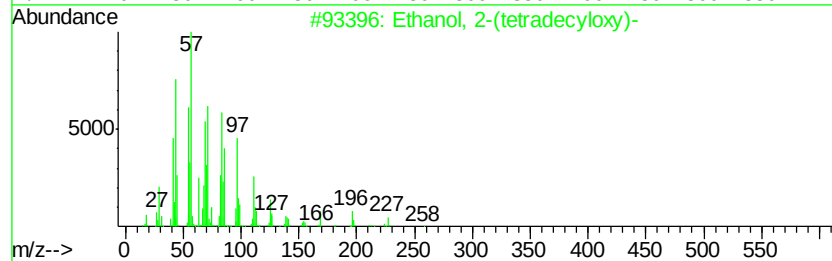
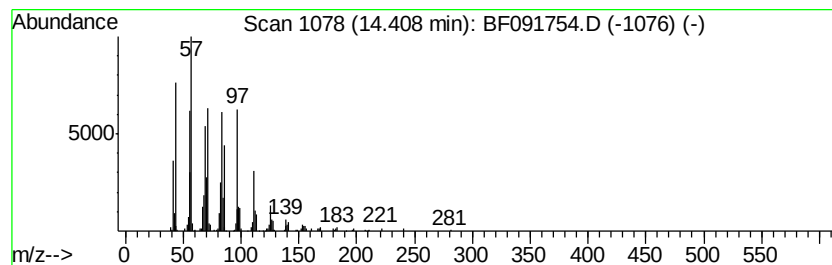
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Ethanol, 2-(tetradecyloxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.41	3.11 ng	384625	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
3	1-Hentetracontanol	593	C41H84O	040710-42-7	83
4	17-Pentatriacontene	491	C35H70	006971-40-0	83
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121816\
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Acq On : 18 Dec 2016 23:26
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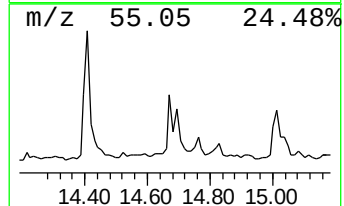
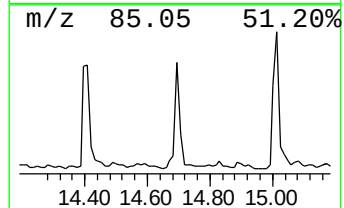
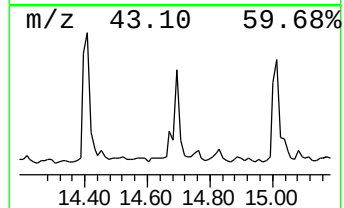
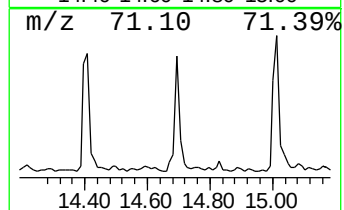
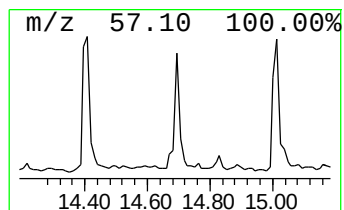
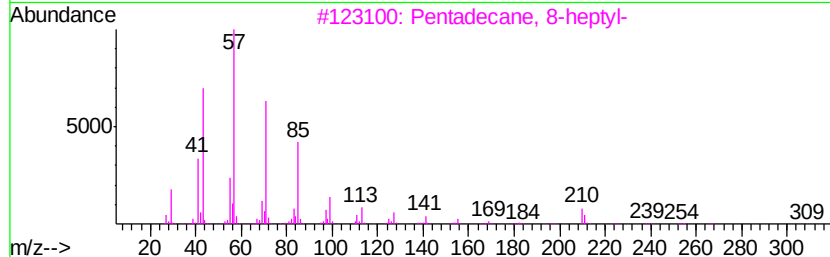
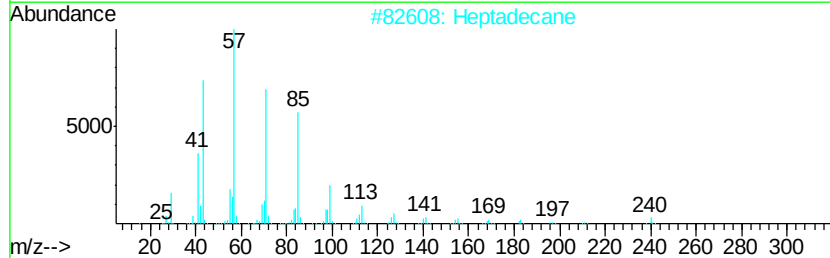
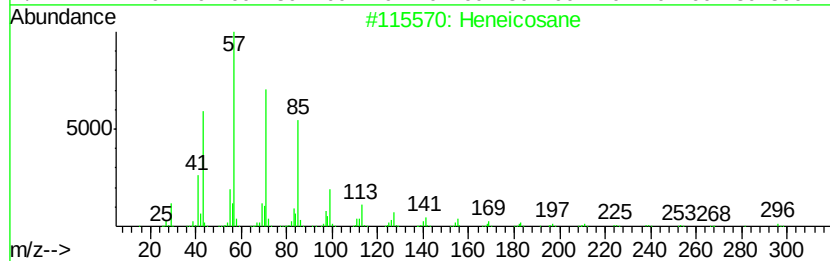
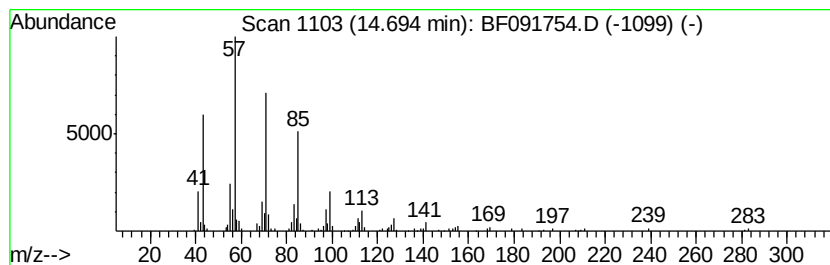
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.96 ng	282330	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Heptadecane	240 C17H36	000629-78-7	90
3	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	90
4	Octadecane	254 C18H38	000593-45-3	86
5	Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091754.D
Acq On : 18 Dec 2016 23:26
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Sample : H6099-13
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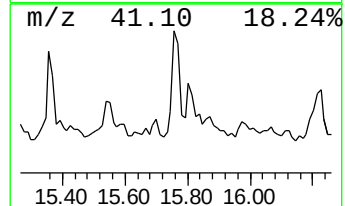
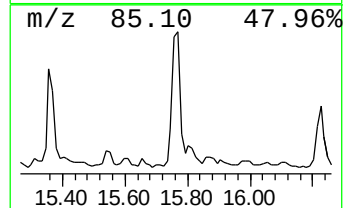
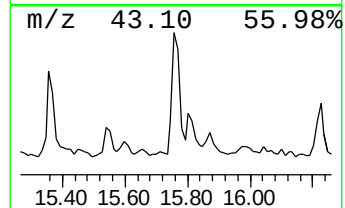
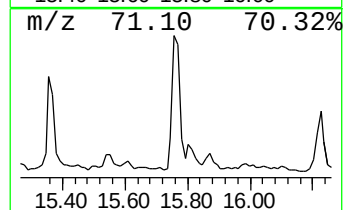
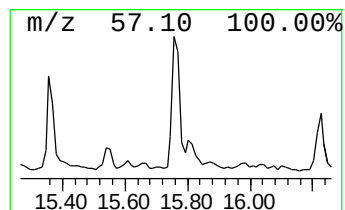
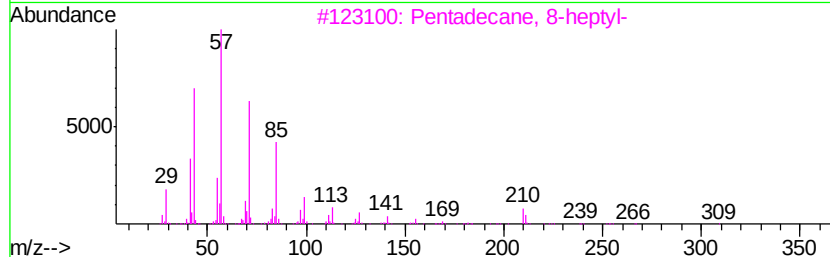
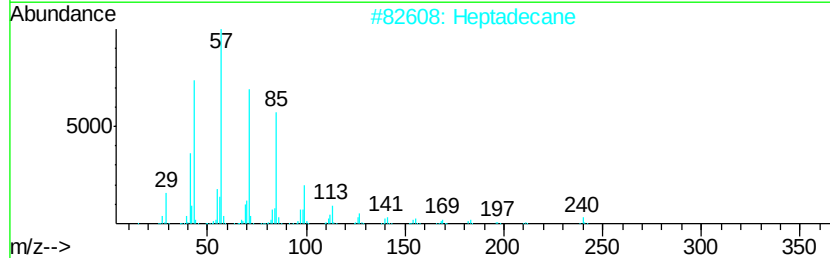
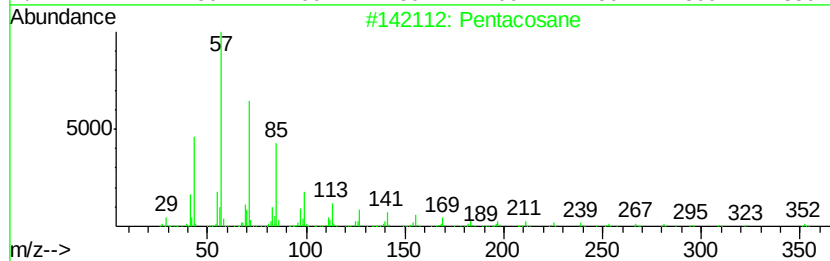
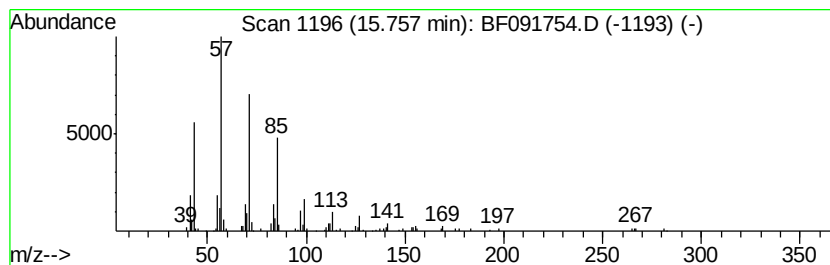
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	2.34 ng	223156	Perylene-d12	15.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	90
2	Heptadecane	240 C17H36	000629-78-7	87
3	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	87
4	Heneicosane	296 C21H44	000629-94-7	87
5	Octacosane	394 C28H58	000630-02-4	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
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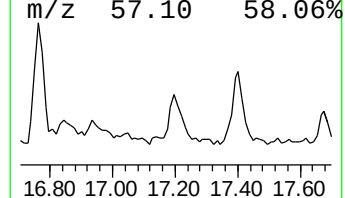
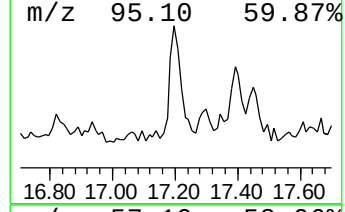
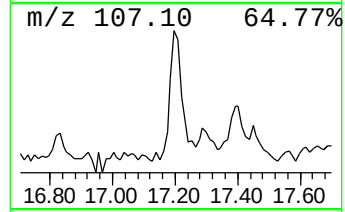
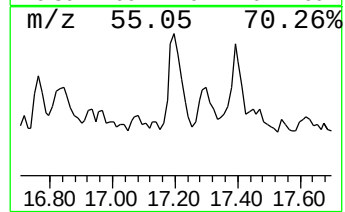
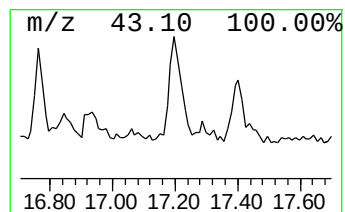
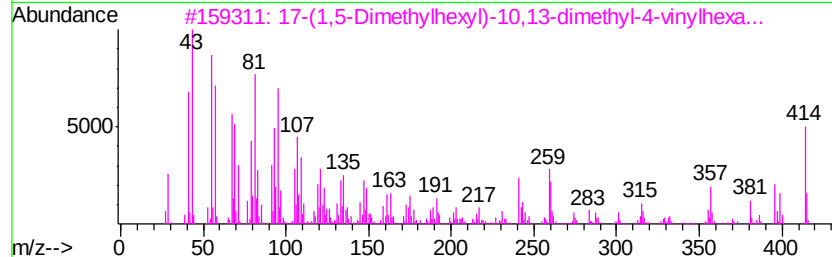
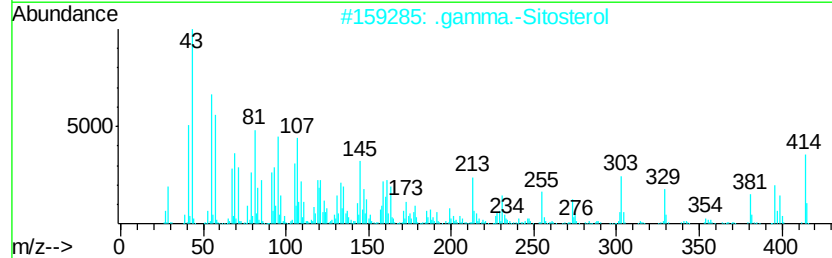
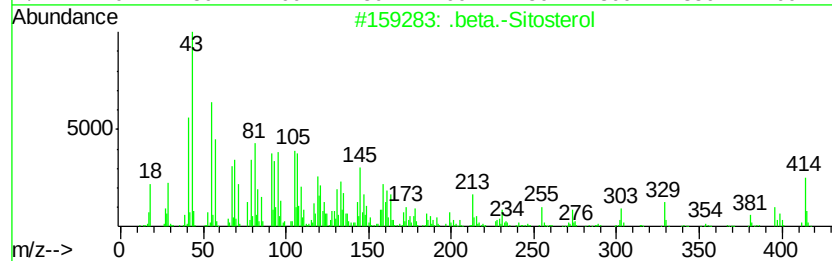
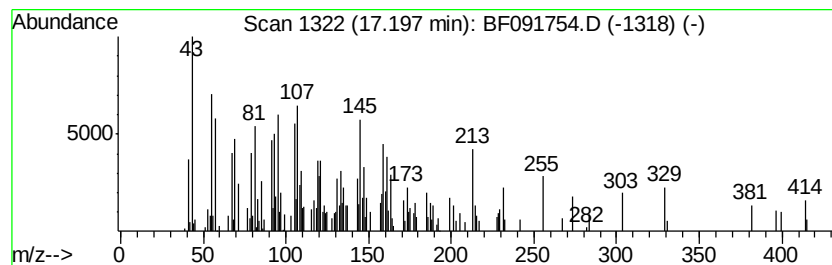
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BNA_F
ClientSampleId :
TP10-3-4FT

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 .beta.-Sitosterol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	3.01 ng	286824	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 91
3		17-(1,5-Dimethylhexyl)-10,13-dim...	414 C29H50O	1000210-86-9 40
4		.beta.-Sitosterol acetate	456 C31H52O2	000915-05-9 35
5		5-Cholene, 3,24-dihydroxy-	360 C24H40O2	1000251-69-2 22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121816\
 Data File : BF091754.D
 Acq On : 18 Dec 2016 23:26
 Operator : UM/SJ
 Sample : H6099-13
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP10-3-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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	42.5	ng	3761450	1	6.76	1772210	20.0
unknown6.53	6.53	67.8	ng	6007180	1	6.76	1772210	20.0
Eicosane	10.72	2.4	ng	333449	4	11.29	2832780	20.0
n-Hexadecanoic acid	11.82	2.5	ng	353588	4	11.29	2832780	20.0
Hexadecanoic acid...	12.71	5.9	ng	726998	5	13.92	2476140	20.0
5-Octadecene, (E)-	12.77	2.3	ng	284969	5	13.92	2476140	20.0
Octadecanoic acid...	13.40	4.3	ng	532796	5	13.92	2476140	20.0
Trichloroacetic a...	13.77	6.9	ng	859095	5	13.92	2476140	20.0
Ethanol, 2-(tetra...	14.41	3.1	ng	384625	5	13.92	2476140	20.0
Heneicosane	14.69	3.0	ng	282330	6	15.32	1904900	20.0
Pentacosane	15.76	2.3	ng	223156	6	15.32	1904900	20.0
.beta.-Sitosterol	17.20	3.0	ng	286824	6	15.32	1904900	20.0