

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
 Data File : BF087811.D
 Acq On : 8 Jun 2016 15:52
 Operator : UM/SJ
 Sample : H3378-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-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-BF060716.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	1.655	3	6	8	rVB	3160476	4928787	100.00%	16.076%
2	1.758	13	15	24	rVB	162497	340734	6.91%	1.111%
3	1.884	24	26	39	rVB	1785645	2718401	55.15%	8.867%
4	2.044	39	40	93	rVB4	91210	527536	10.70%	1.721%
5	4.993	296	298	305	rVB	104922	170567	3.46%	0.556%
6	5.416	332	335	338	rBV	1517786	1730824	35.12%	5.645%
7	6.456	423	426	429	rBV	1535754	1784590	36.21%	5.821%
8	6.593	435	438	440	rVB	2135997	2029158	41.17%	6.619%
9	6.822	456	458	461	rBV	668891	582561	11.82%	1.900%
10	6.982	469	472	474	rVB	1876714	1615008	32.77%	5.268%
11	7.393	505	508	510	rBV	1274454	1433103	29.08%	4.674%
12	8.113	568	571	573	rBV	894915	849445	17.23%	2.771%
13	9.199	663	666	668	rVB	2017597	2564227	52.03%	8.364%
14	9.588	698	700	702	rBV	246617	193133	3.92%	0.630%
15	9.873	722	725	727	rBV	791763	878002	17.81%	2.864%
16	10.662	791	794	796	rBV	1206502	1407124	28.55%	4.590%
17	11.348	852	854	858	rBV	591267	886259	17.98%	2.891%
18	11.896	899	902	904	rBV	87152	100287	2.03%	0.327%
19	11.965	906	908	913	rVB2	35392	53820	1.09%	0.176%
20	12.559	958	960	962	rBV	225934	216078	4.38%	0.705%
21	12.788	976	980	983	rBV	223331	261646	5.31%	0.853%
22	12.948	991	994	996	rVB	1904016	1922877	39.01%	6.272%
23	13.188	1011	1015	1016	rBV2	41293	51962	1.05%	0.169%
24	13.851	1071	1073	1077	rVB	105164	149095	3.02%	0.486%
25	13.988	1082	1085	1091	rVB2	905272	1034406	20.99%	3.374%
26	14.491	1126	1129	1135	rBV4	50309	113166	2.30%	0.369%
27	14.925	1165	1167	1169	rVB	46090	56747	1.15%	0.185%
28	15.005	1171	1174	1179	rBV	118394	238315	4.84%	0.777%
29	15.108	1181	1183	1189	rBV2	86911	165684	3.36%	0.540%
30	15.291	1197	1199	1202	rVB	63138	96652	1.96%	0.315%
31	15.360	1202	1205	1207	rBV	78964	120438	2.44%	0.393%
32	15.417	1207	1210	1213	rBV	469717	602876	12.23%	1.966%
33	15.668	1230	1232	1235	rVB2	28943	51054	1.04%	0.167%
34	15.897	1249	1252	1255	rBV	82309	157709	3.20%	0.514%

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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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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35	15.954	1255	1257	1260	rVB2	29775	58113	1.18%	0.190%
36	16.663	1316	1319	1323	rVB4	30022	64130	1.30%	0.209%
37	16.800	1328	1331	1341	rVB2	40980	125608	2.55%	0.410%
38	16.971	1341	1346	1350	rBV3	28495	114724	2.33%	0.374%
39	17.211	1365	1367	1374	rVB	26316	57686	1.17%	0.188%
40	17.394	1380	1383	1390	rBV5	42370	144253	2.93%	0.471%
41	19.360	1551	1555	1561	rVB5	17490	61770	1.25%	0.201%

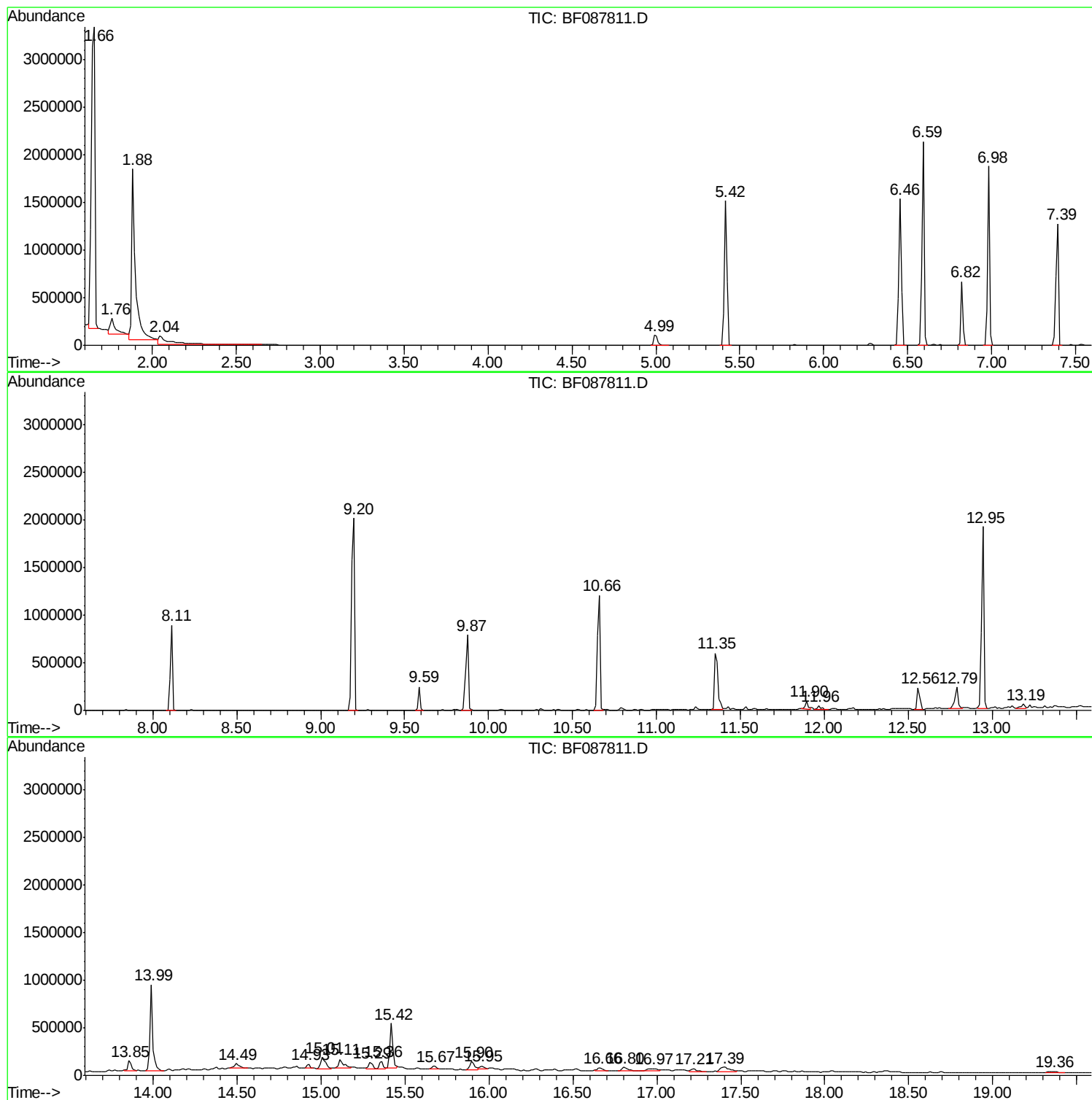
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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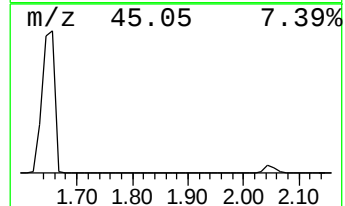
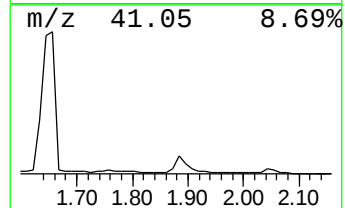
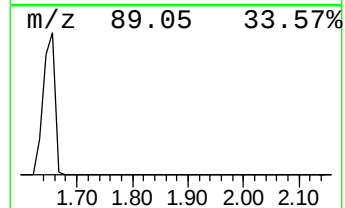
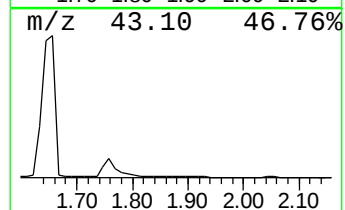
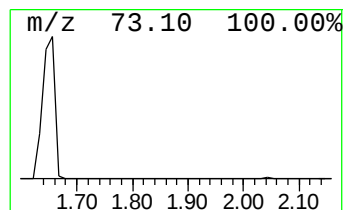
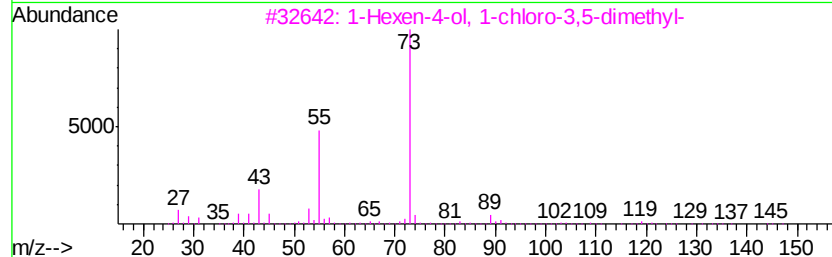
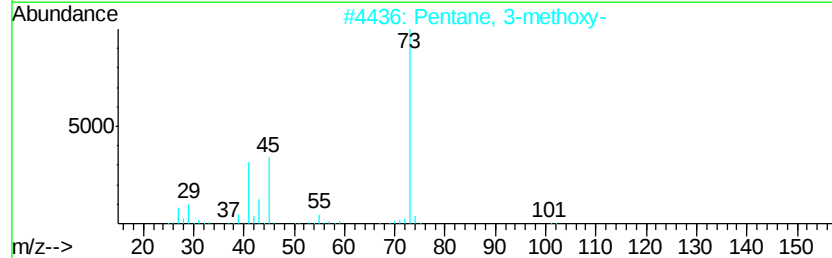
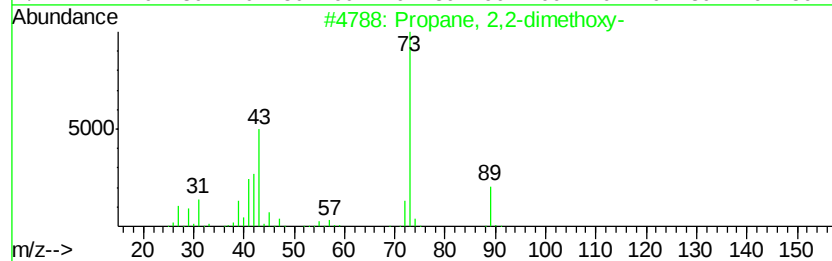
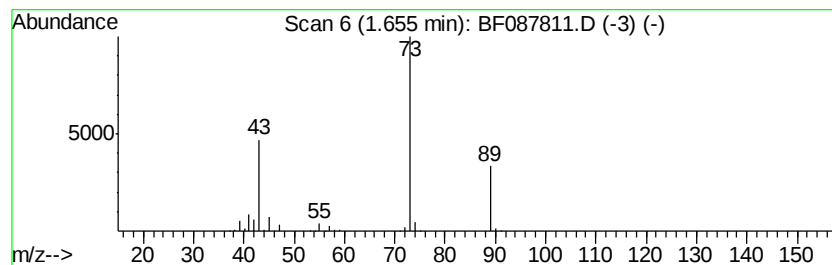
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	169.21 ng	4928790	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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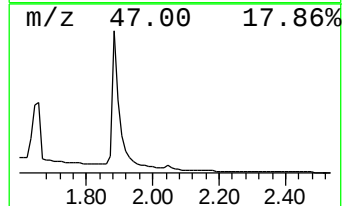
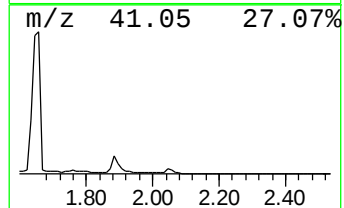
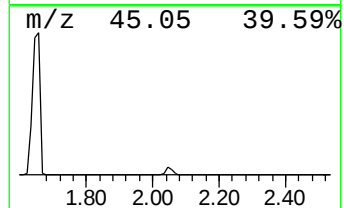
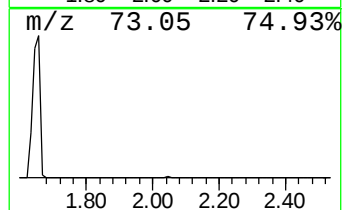
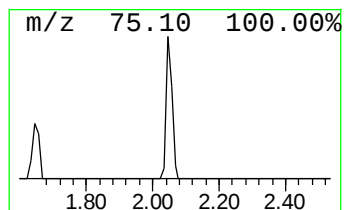
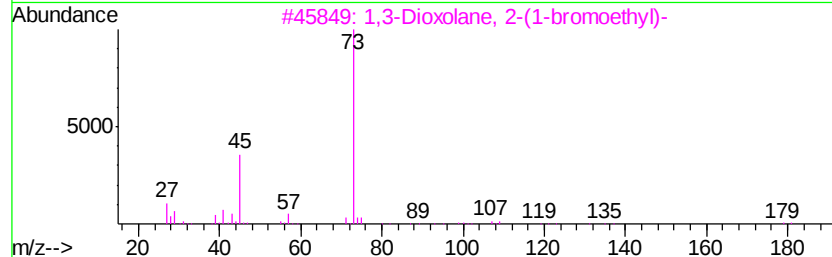
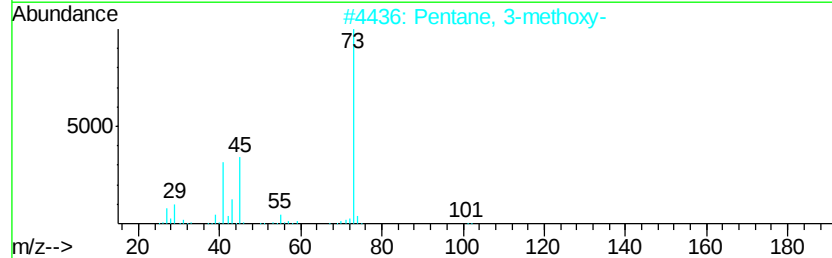
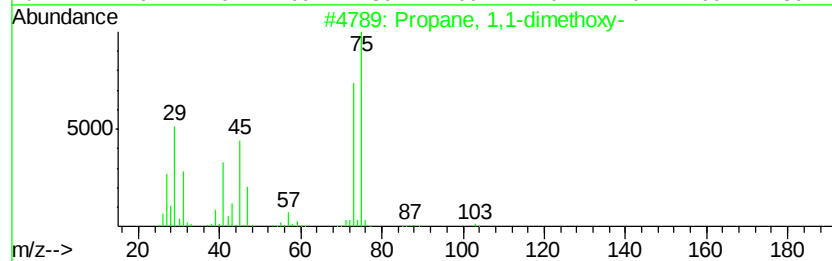
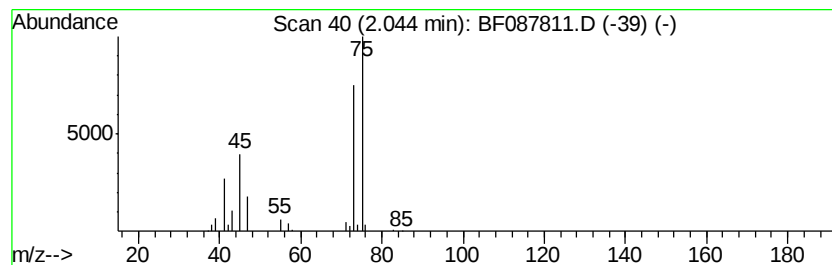
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Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	18.11 ng	527536	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4		1-Butanamine	73	C4H11N	000109-73-9	7
5		Glycine	75	C2H5NO2	000056-40-6	7



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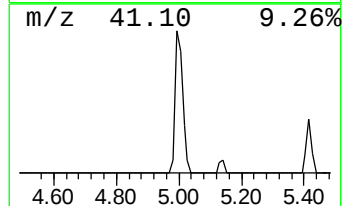
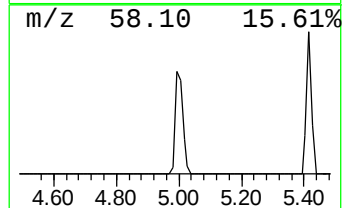
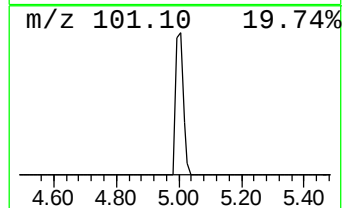
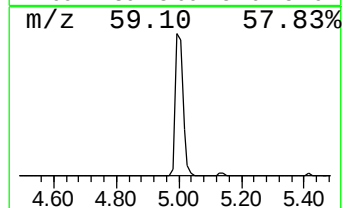
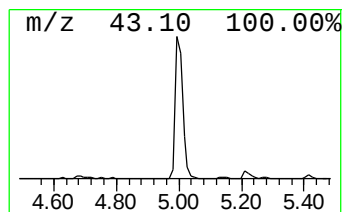
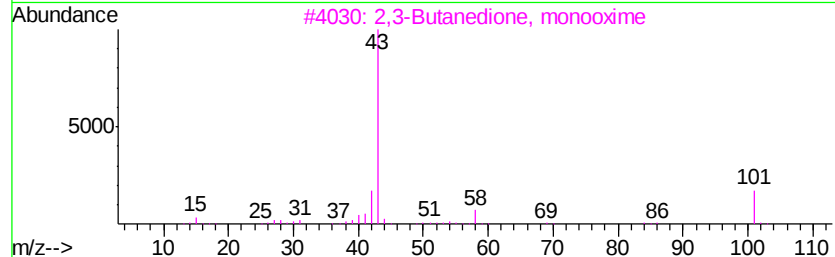
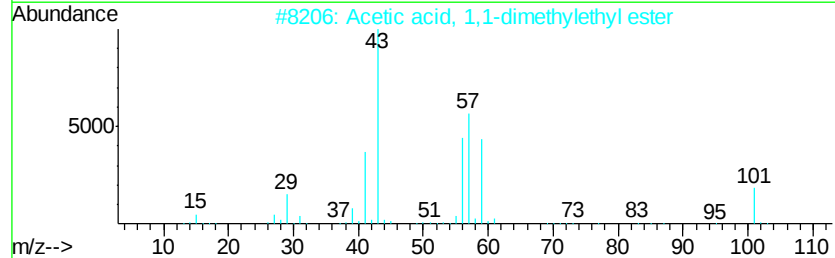
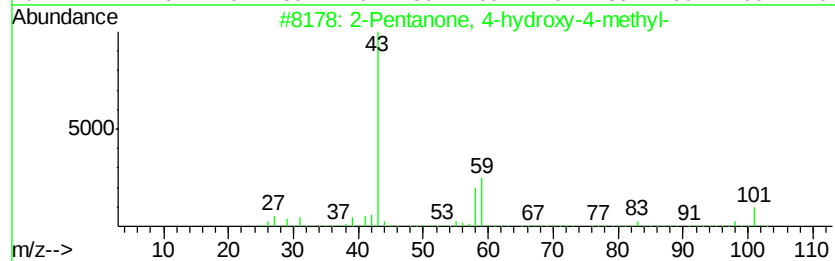
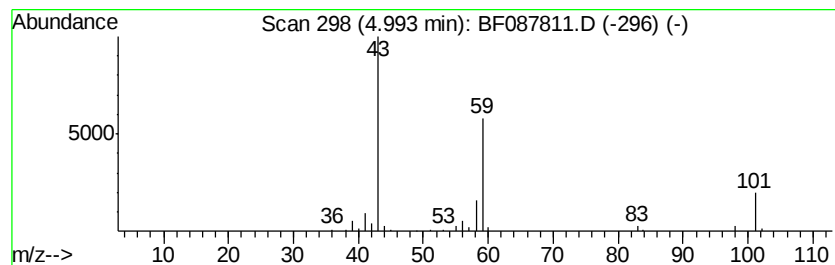
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	5.86 ng	170567	1,4-Dichlorobenzene-d4	6.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		3-Hexanol	102	C6H14O	000623-37-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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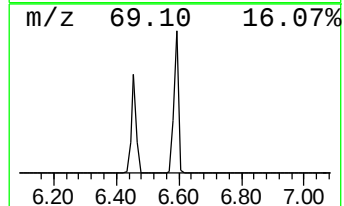
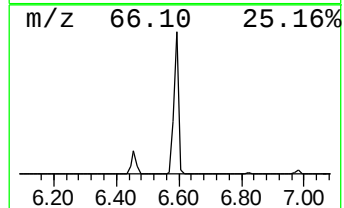
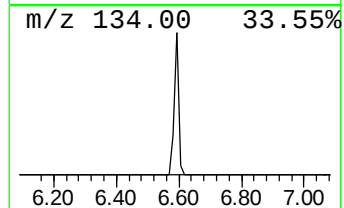
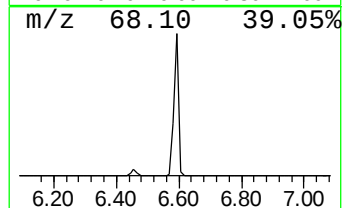
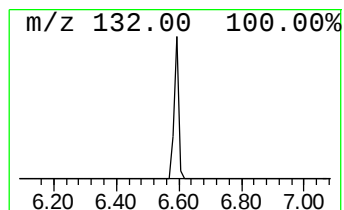
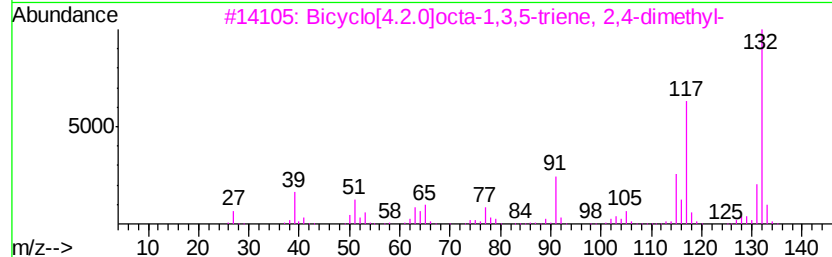
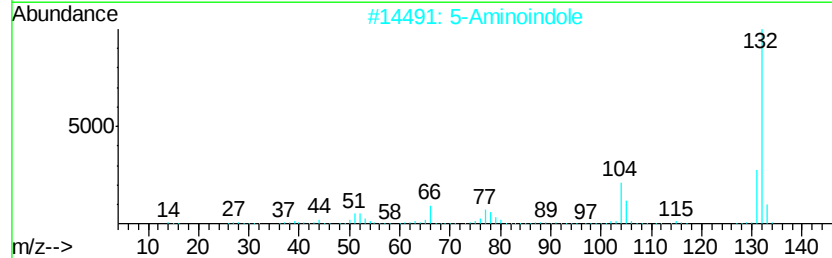
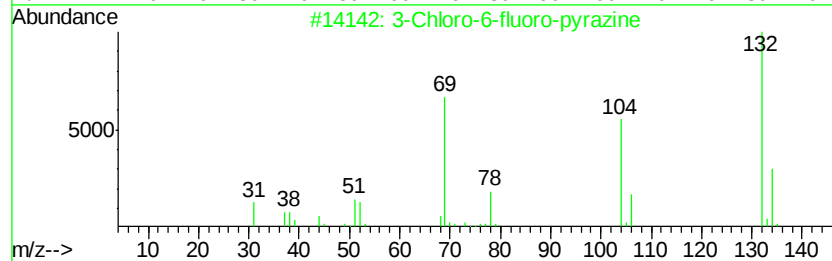
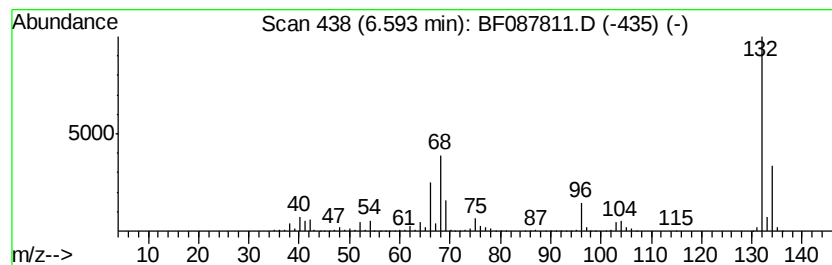
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown6.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	69.66 ng	2029160	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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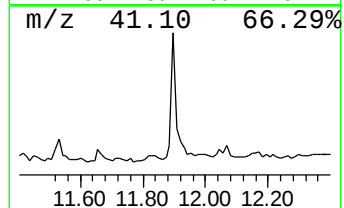
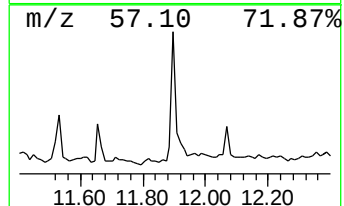
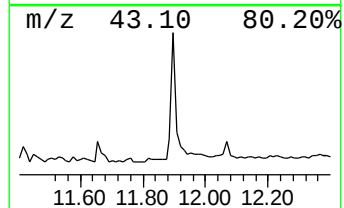
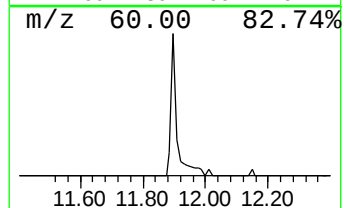
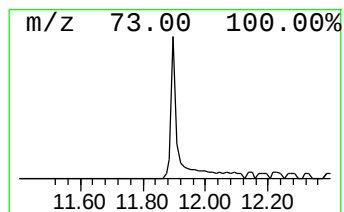
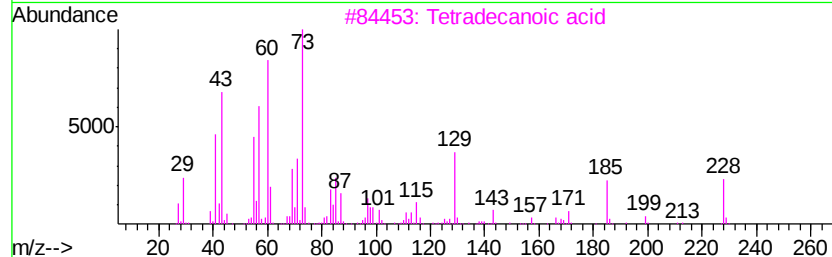
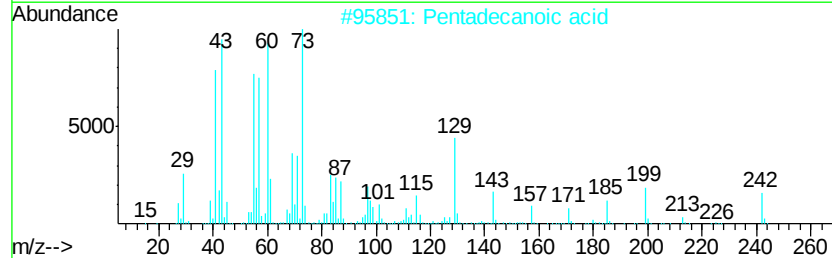
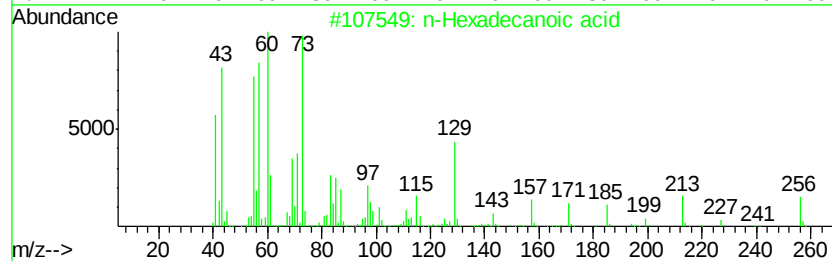
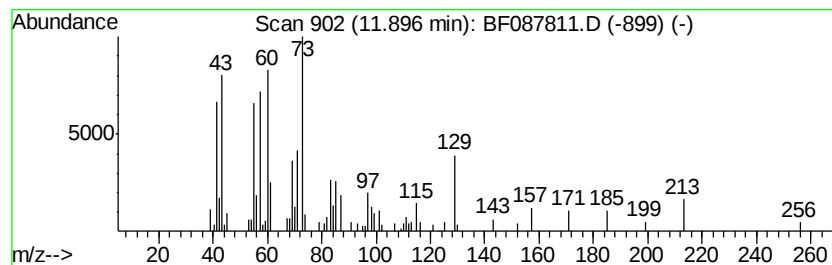
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.26 ng	100287	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087811.D
Acq On : 8 Jun 2016 15:52
Operator : UM/SJ
Sample : H3378-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-16

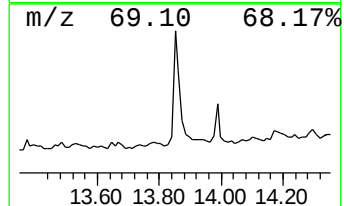
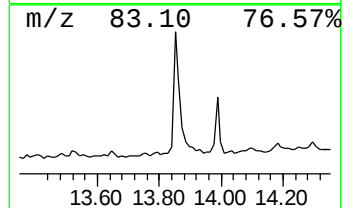
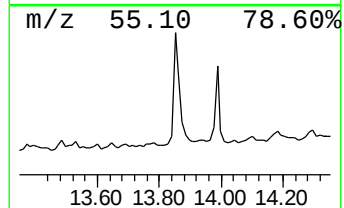
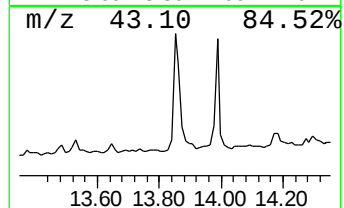
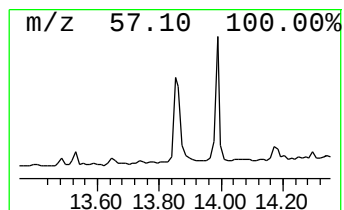
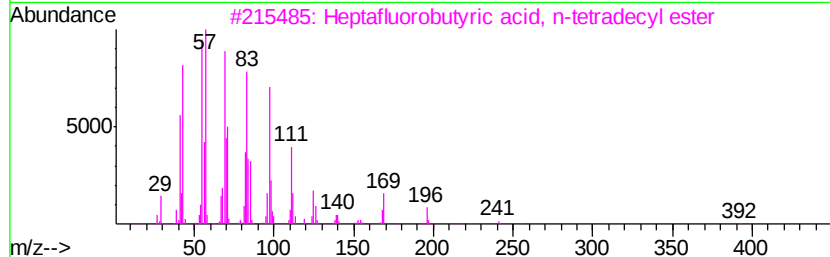
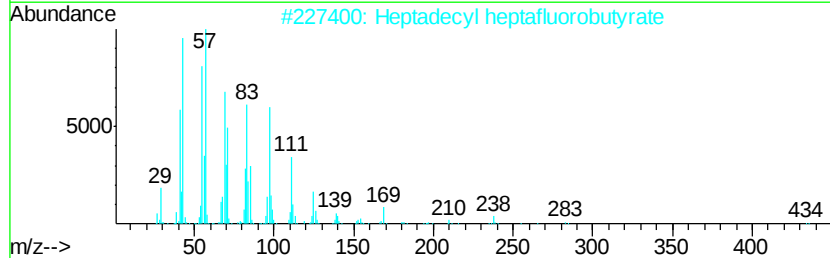
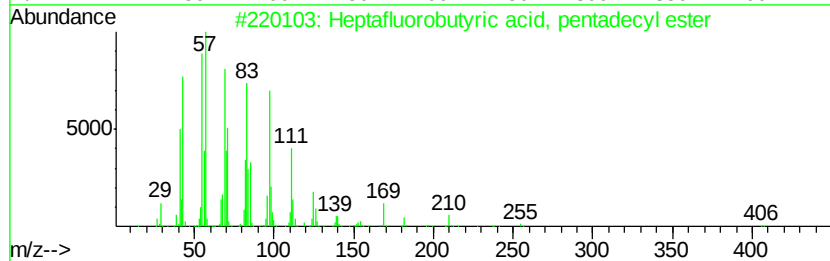
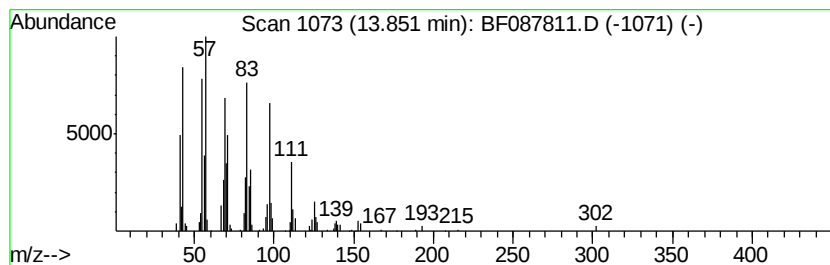
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptafluorobutyric acid, pe... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.88 ng	149095	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087811.D
Acq On : 8 Jun 2016 15:52
Operator : UM/SJ
Sample : H3378-04
Misc :
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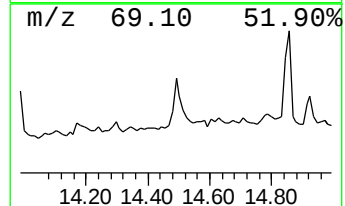
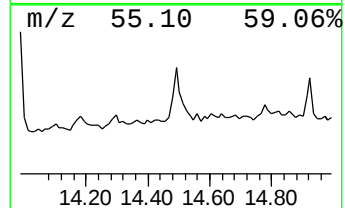
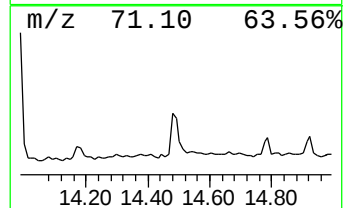
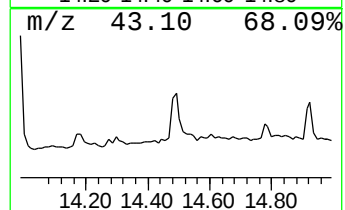
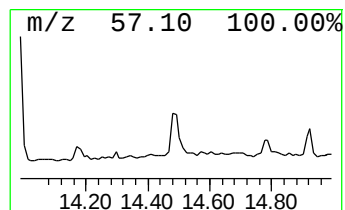
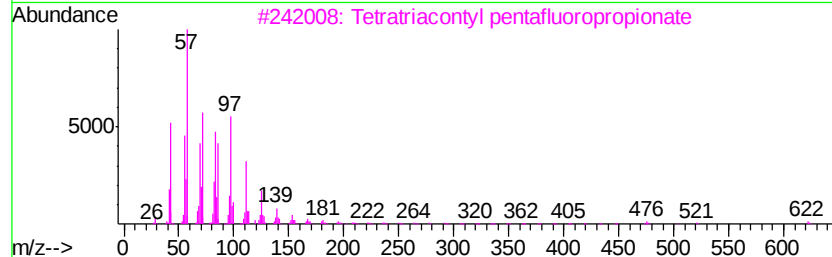
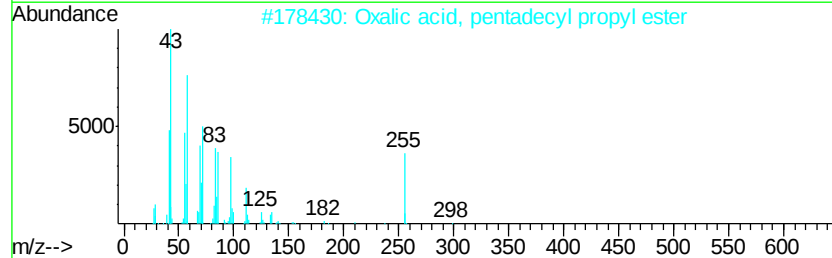
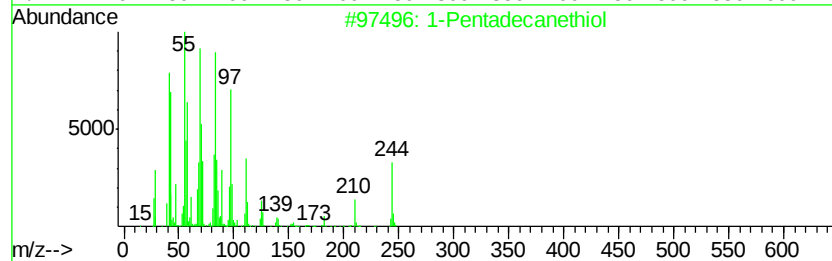
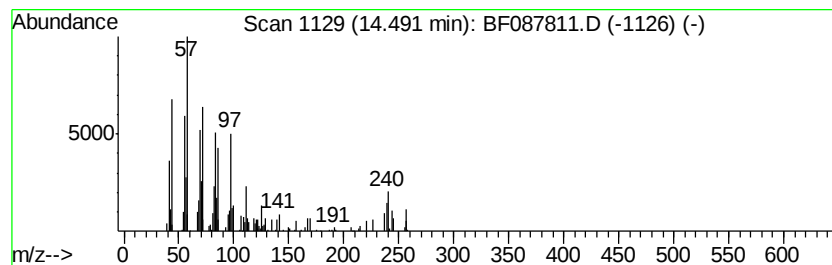
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Pentadecanethiol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.19 ng	113166	Chrysene-d12	13.99
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Pentadecanethiol	244 C15H32S	025276-70-4 90
2		Oxalic acid, pentadecyl propyl e...	342 C20H38O4	1000309-26-8 81
3		Tetratriacontyl pentafluoropropi...	641 C37H69F5O2	1000351-81-5 76
4		Tetratriacontyl heptafluorobutyrate	691 C38H69F7O2	1000351-84-1 76
5		Oxalic acid, cyclobutyl heptadec...	382 C23H42O4	1000309-70-7 68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087811.D
Acq On : 8 Jun 2016 15:52
Operator : UM/SJ
Sample : H3378-04
Misc :
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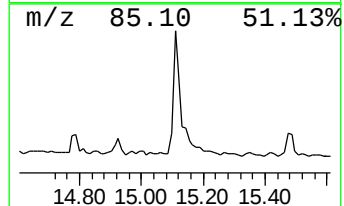
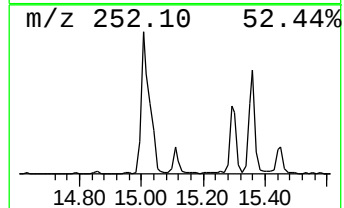
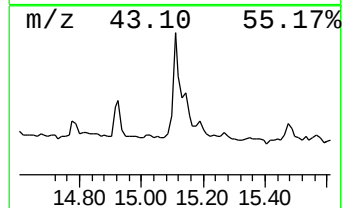
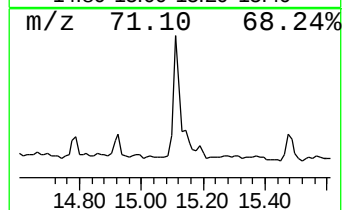
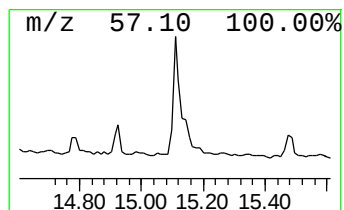
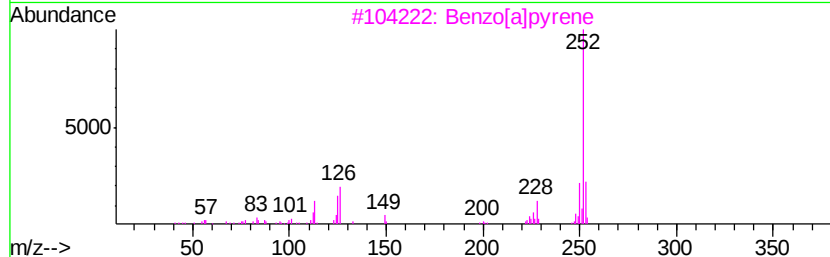
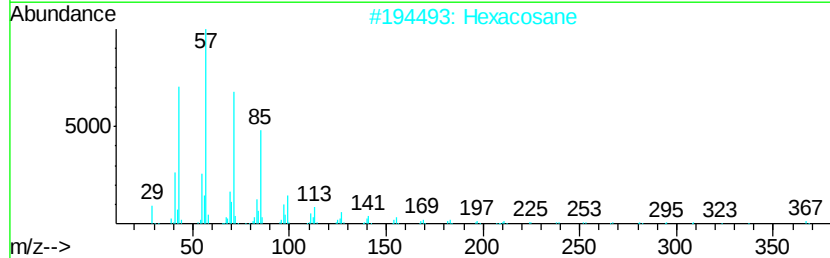
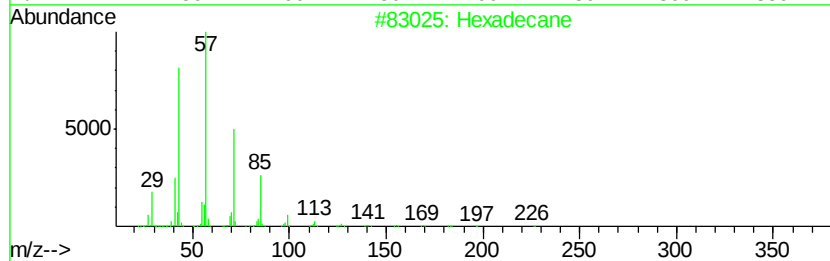
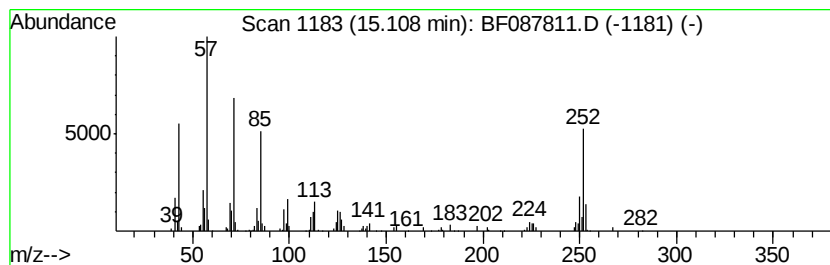
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.11	5.50 ng	165684	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	52
2	Hexacosane	366	C26H54	000630-01-3	46
3	Benzo[ap]vrene	252	C20H12	000050-32-8	46
4	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	41
5	Heneicosane	296	C21H44	000629-94-7	41



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087811.D
Acq On : 8 Jun 2016 15:52
Operator : UM/SJ
Sample : H3378-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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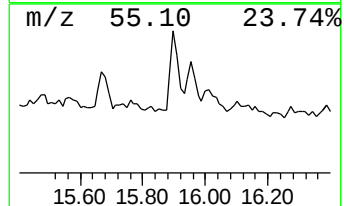
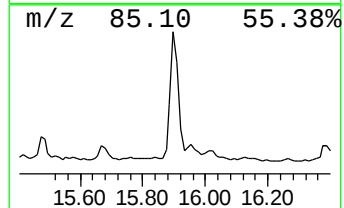
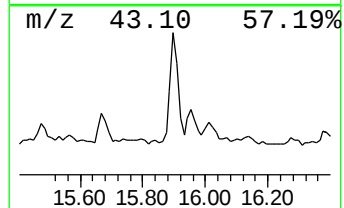
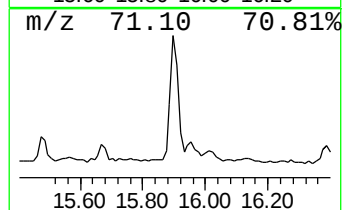
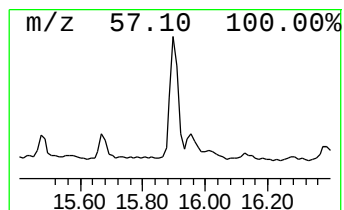
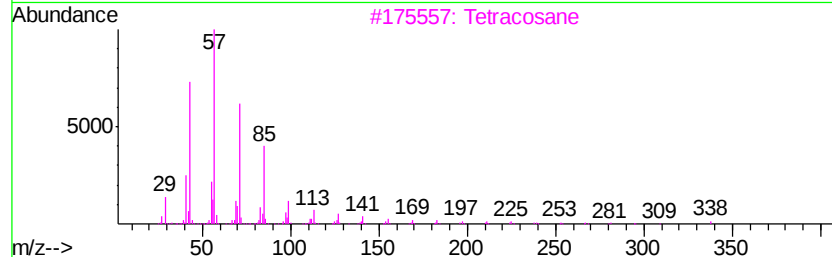
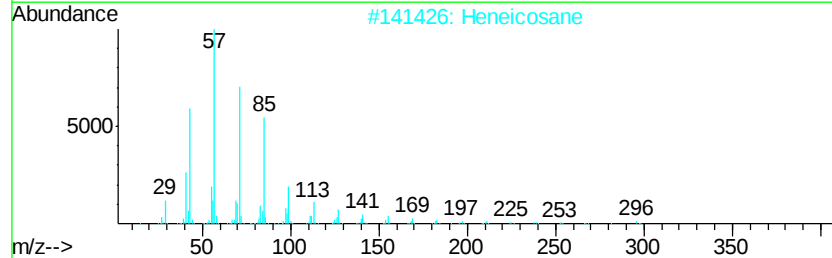
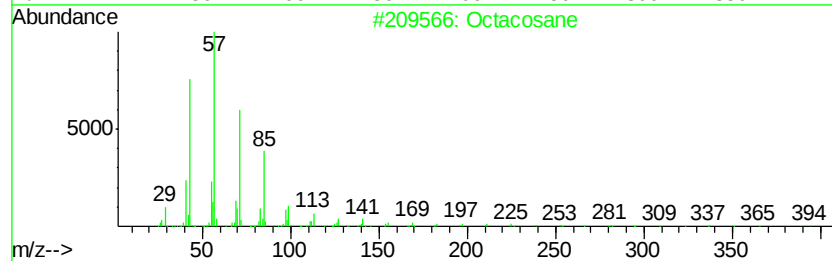
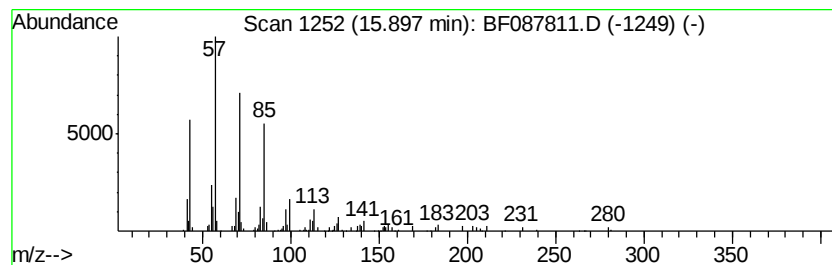
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	5.23 ng	157709	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heptadecane	240	C17H36	000629-78-7	90
5			Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
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Acq On : 8 Jun 2016 15:52
Operator : UM/SJ
Sample : H3378-04
Misc :
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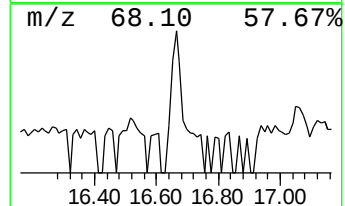
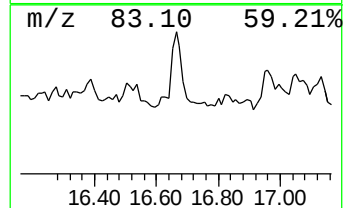
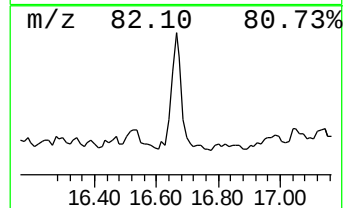
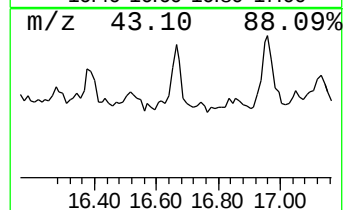
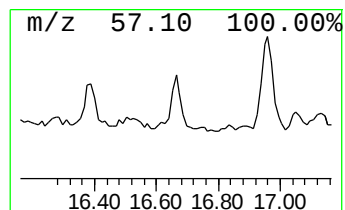
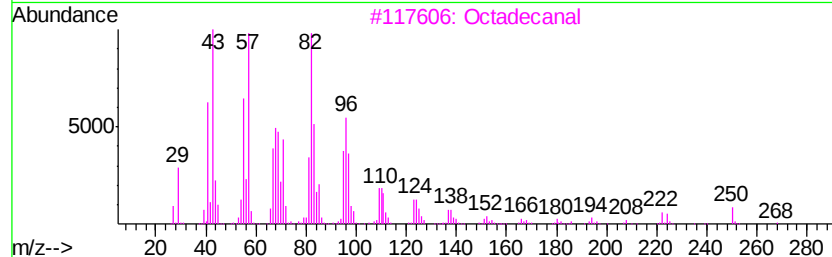
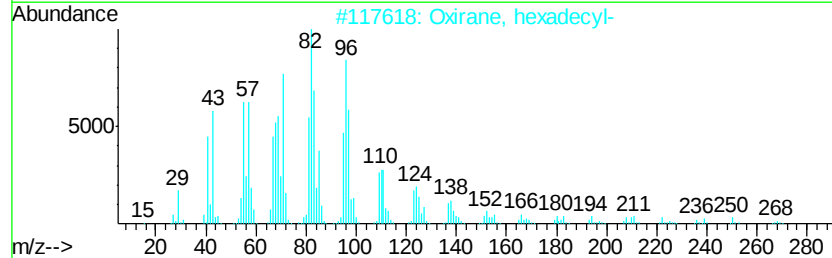
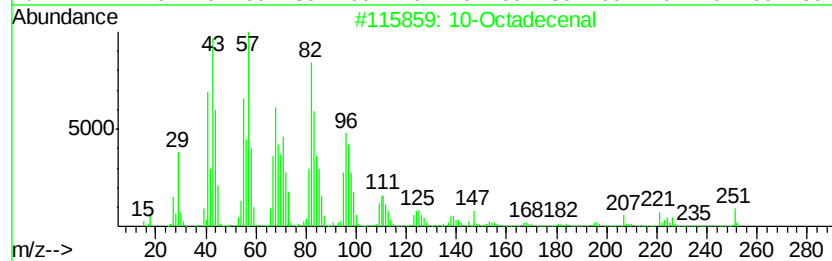
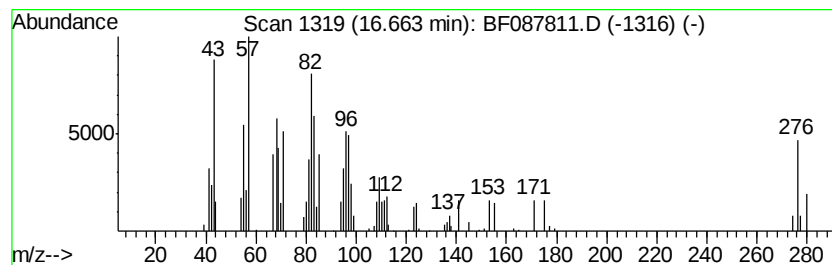
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 10-Octadecenal Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.66	2.13 ng	64130	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenal	266	C18H34O	056554-92-8	58
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	58
3	Octadecanal	268	C18H36O	000638-66-4	53
4	Heptadecanal	254	C17H34O	1000376-70-0	53
5	13-Octadecenal	266	C18H34O	056554-90-6	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087811.D
Acq On : 8 Jun 2016 15:52
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Sample : H3378-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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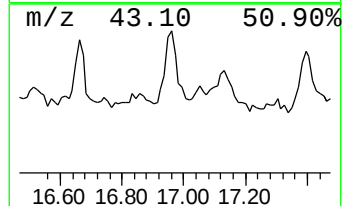
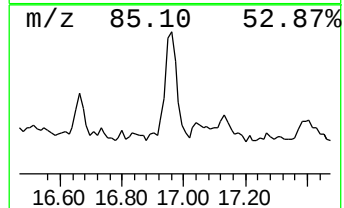
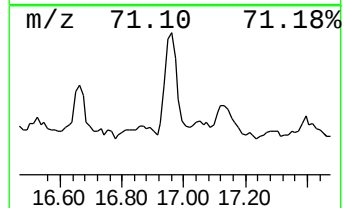
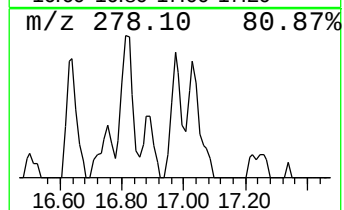
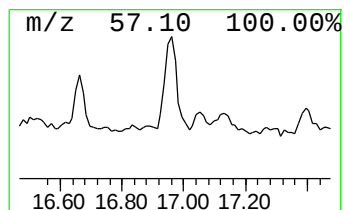
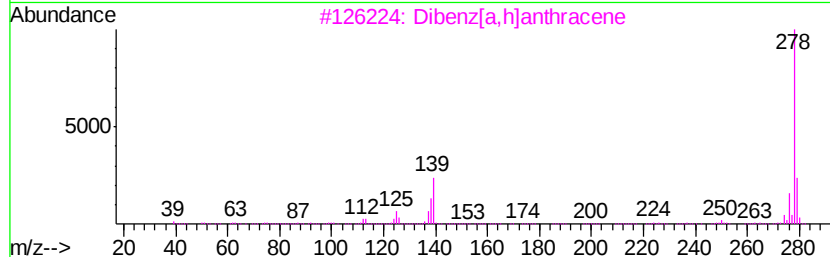
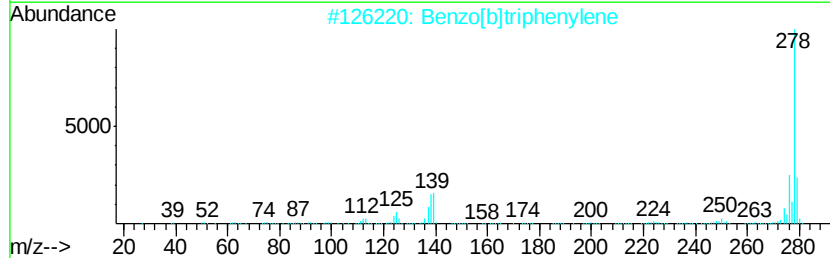
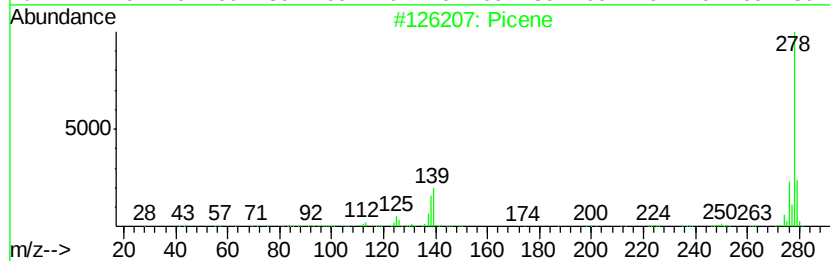
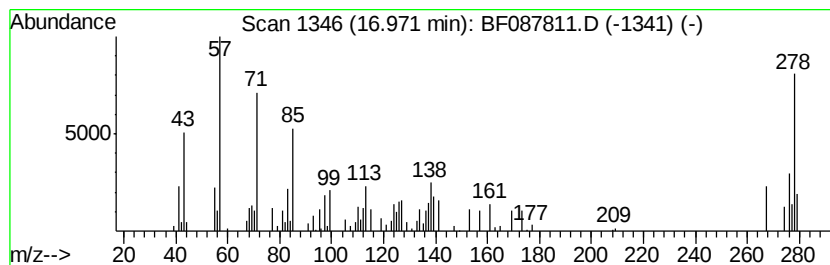
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown16.97 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	3.81 ng	114724	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Picene	278	C22H14	000213-46-7	49
2		Benzo[b]triphenylene	278	C22H14	000215-58-7	45
3		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	35
4		6-(Adamantyl-1)napthol-2	278	C20H22O	037436-35-4	27
5		[1,2,4]oxadiazole-5-carboxylic a...	278	C13H14N2O5	1000316-89-9	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087811.D
Acq On : 8 Jun 2016 15:52
Operator : UM/SJ
Sample : H3378-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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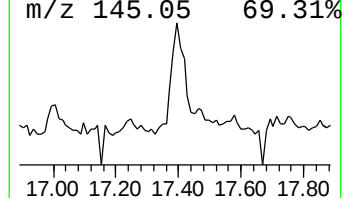
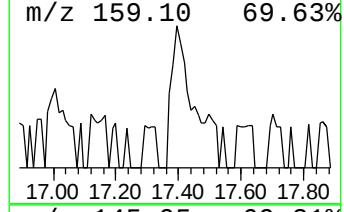
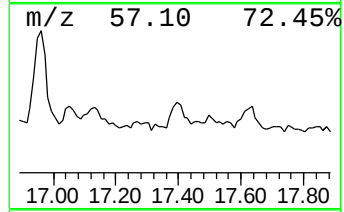
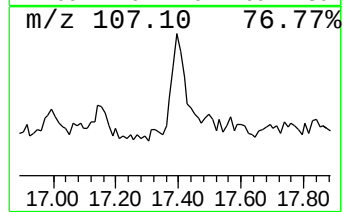
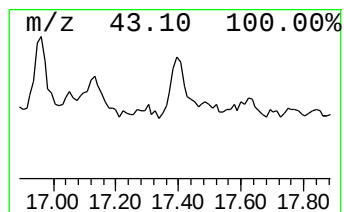
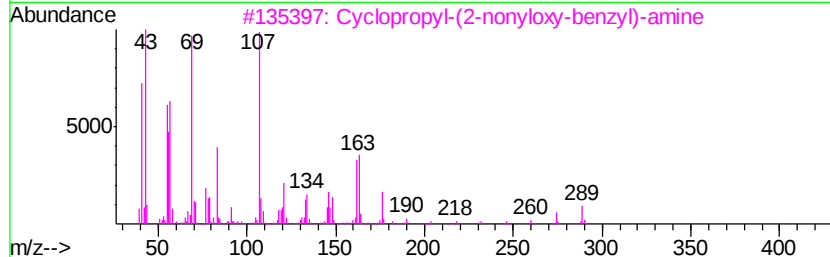
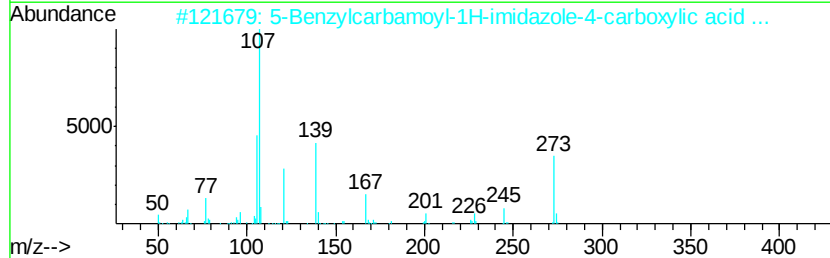
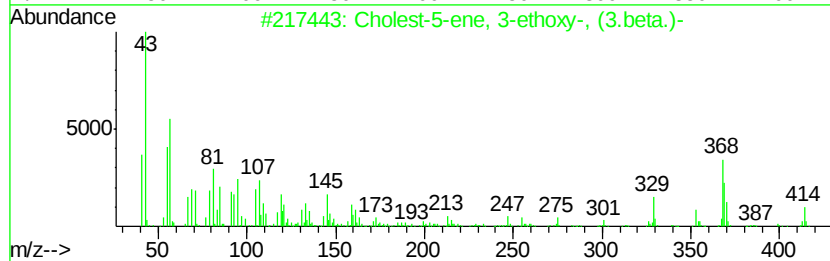
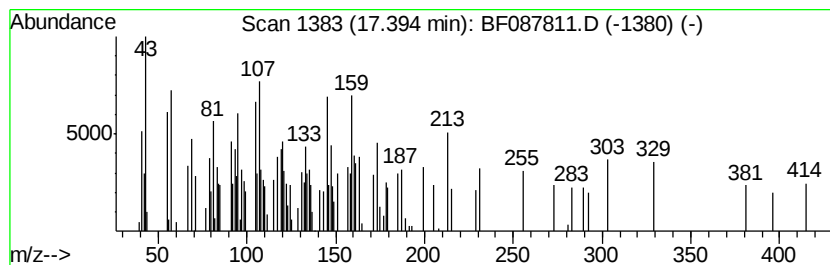
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown17.39 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	4.79 ng	144253	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	38
2		5-Benzylcarbamoyl-1H-imidazole-4...	273	C14H15N3O3	312758-83-1	22
3		Cyclopropyl-(2-nonyloxy-benzyl)-...	289	C19H31NO	1000297-00-6	12
4		5,16-Pregnenolone oxime	329	C21H31NO2	001045-71-2	10
5		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087811.D
Acq On : 8 Jun 2016 15:52
Operator : UM/SJ
Sample : H3378-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-16

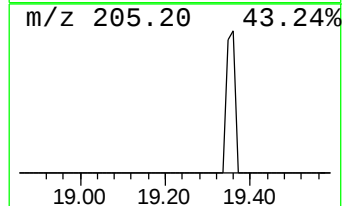
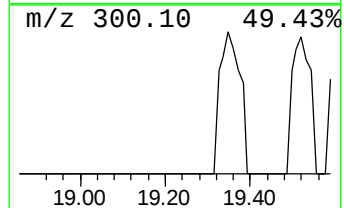
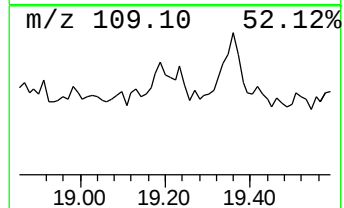
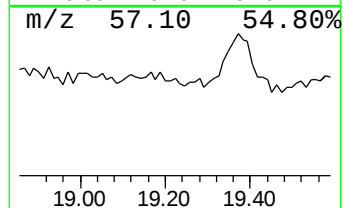
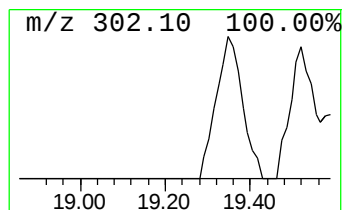
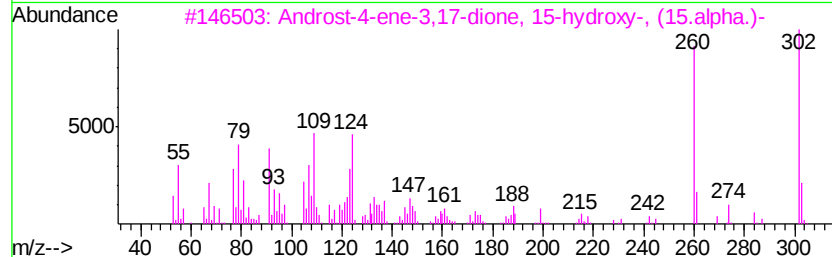
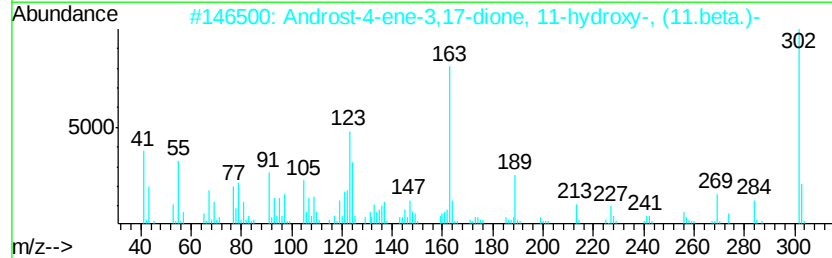
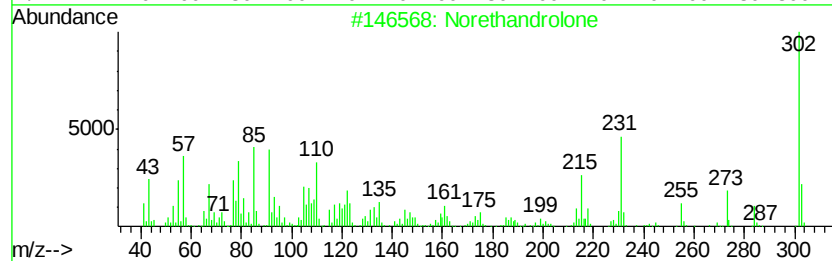
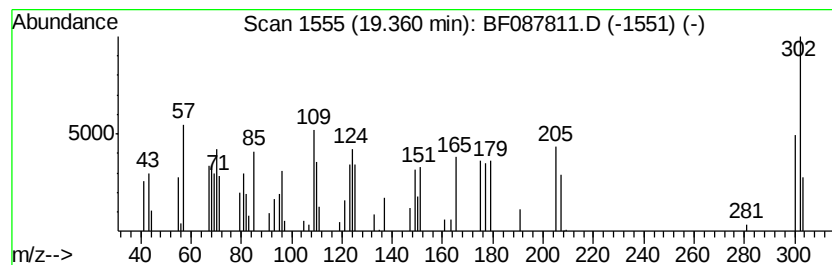
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown19.36 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.36	2.05 ng	61770	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Norethandrolone	302	C20H30O2	000052-78-8	22
2		Androst-4-ene-3,17-dione, 11-hyd...	302	C19H26O3	000382-44-5	18
3		Androst-4-ene-3,17-dione, 15-hyd...	302	C19H26O3	000566-08-5	16
4		1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	14
5		Androstane-3,11,17-trione, (5.alpha.)...	302	C19H26O3	001482-70-8	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
 Data File : BF087811.D
 Acq On : 8 Jun 2016 15:52
 Operator : UM/SJ
 Sample : H3378-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.66	169.2	ng	4928790	1	6.82	582561	20.0
Propane, 1,1-dime...	2.04	18.1	ng	527536	1	6.82	582561	20.0
2-Pentanone, 4-hy...	4.99	5.9	ng	170567	1	6.82	582561	20.0
unknown6.59	6.59	69.7	ng	2029160	1	6.82	582561	20.0
n-Hexadecanoic acid	11.90	2.3	ng	100287	4	11.35	886259	20.0
Heptafluorobutyri...	13.85	2.9	ng	149095	5	13.99	1034410	20.0
1-Pentadecanethiol	14.49	2.2	ng	113166	5	13.99	1034410	20.0
Hexadecane	15.11	5.5	ng	165684	6	15.42	602876	20.0
Octacosane	15.90	5.2	ng	157709	6	15.42	602876	20.0
10-Octadecenal	16.66	2.1	ng	64130	6	15.42	602876	20.0
unknown16.97	16.97	3.8	ng	114724	6	15.42	602876	20.0
unknown17.39	17.39	4.8	ng	144253	6	15.42	602876	20.0
unknown19.36	19.36	2.0	ng	61770	6	15.42	602876	20.0