

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
 Data File : BF086951.D
 Acq On : 13 May 2016 1:16
 Operator : UM/SJ
 Sample : H2977-04
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 90TH-AVE-SB-21-0.5-6.0

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-BF050916.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	1.632	3	4	12	rVB	454790	704661	10.82%	1.557%
2	1.747	12	14	56	rVB	2794079	6509859	100.00%	14.384%
3	4.764	275	278	285	rBV	244533	383078	5.88%	0.846%
4	5.221	315	318	320	rBV	3359426	4170139	64.06%	9.214%
5	6.296	409	412	414	rBV	3653588	4459610	68.51%	9.854%
6	6.399	418	421	423	rBV	4168986	4222429	64.86%	9.329%
7	6.616	438	440	443	rBV	883732	1120808	17.22%	2.476%
8	6.776	452	454	457	rBV	3019762	2849968	43.78%	6.297%
9	7.199	488	491	493	rBV	2841971	2893303	44.44%	6.393%
10	7.907	551	553	556	rBV	1574555	1423641	21.87%	3.146%
11	8.993	645	648	650	rBV	3659867	3974940	61.06%	8.783%
12	9.393	680	683	684	rBV	416140	489713	7.52%	1.082%
13	9.599	699	701	703	rBV	150959	138929	2.13%	0.307%
14	9.656	703	706	709	rBV	1607340	1421818	21.84%	3.142%
15	10.102	743	745	746	rBV	219692	170664	2.62%	0.377%
16	10.319	761	764	767	rBV	63726	97710	1.50%	0.216%
17	10.445	772	775	777	rBV	2079245	1958854	30.09%	4.328%
18	10.570	784	786	790	rBV	211232	222698	3.42%	0.492%
19	11.016	823	825	826	rBV	119626	97740	1.50%	0.216%
20	11.131	833	835	839	rVB	1183479	1090566	16.75%	2.410%
21	11.679	881	883	887	rBV	195160	230389	3.54%	0.509%
22	12.559	958	960	963	rBV	57423	74527	1.14%	0.165%
23	12.719	971	974	976	rBV	2633985	2532611	38.90%	5.596%
24	13.211	1014	1017	1022	rBV	108466	287673	4.42%	0.636%
25	13.622	1051	1053	1062	rBV	333593	496892	7.63%	1.098%
26	13.759	1062	1065	1067	rBV	1291337	1283223	19.71%	2.835%
27	13.885	1072	1076	1080	rBV2	43279	133924	2.06%	0.296%
28	14.262	1104	1109	1114	rBV3	106579	286413	4.40%	0.633%
29	14.662	1143	1144	1147	rVB	56244	72837	1.12%	0.161%
30	14.754	1150	1152	1156	rVB2	40268	79258	1.22%	0.175%
31	14.834	1157	1159	1161	rBV	111535	127442	1.96%	0.282%
32	15.119	1181	1184	1187	rBV	788875	907264	13.94%	2.005%
33	15.325	1200	1202	1205	rBV2	77968	108542	1.67%	0.240%
34	15.577	1221	1224	1228	rBV4	49945	153254	2.35%	0.339%

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
90TH-AVE-SB-21-0.5-6.0

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

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35	16.182	1275	1277	1281	rVB	45037	83675	1.29%	0.185%
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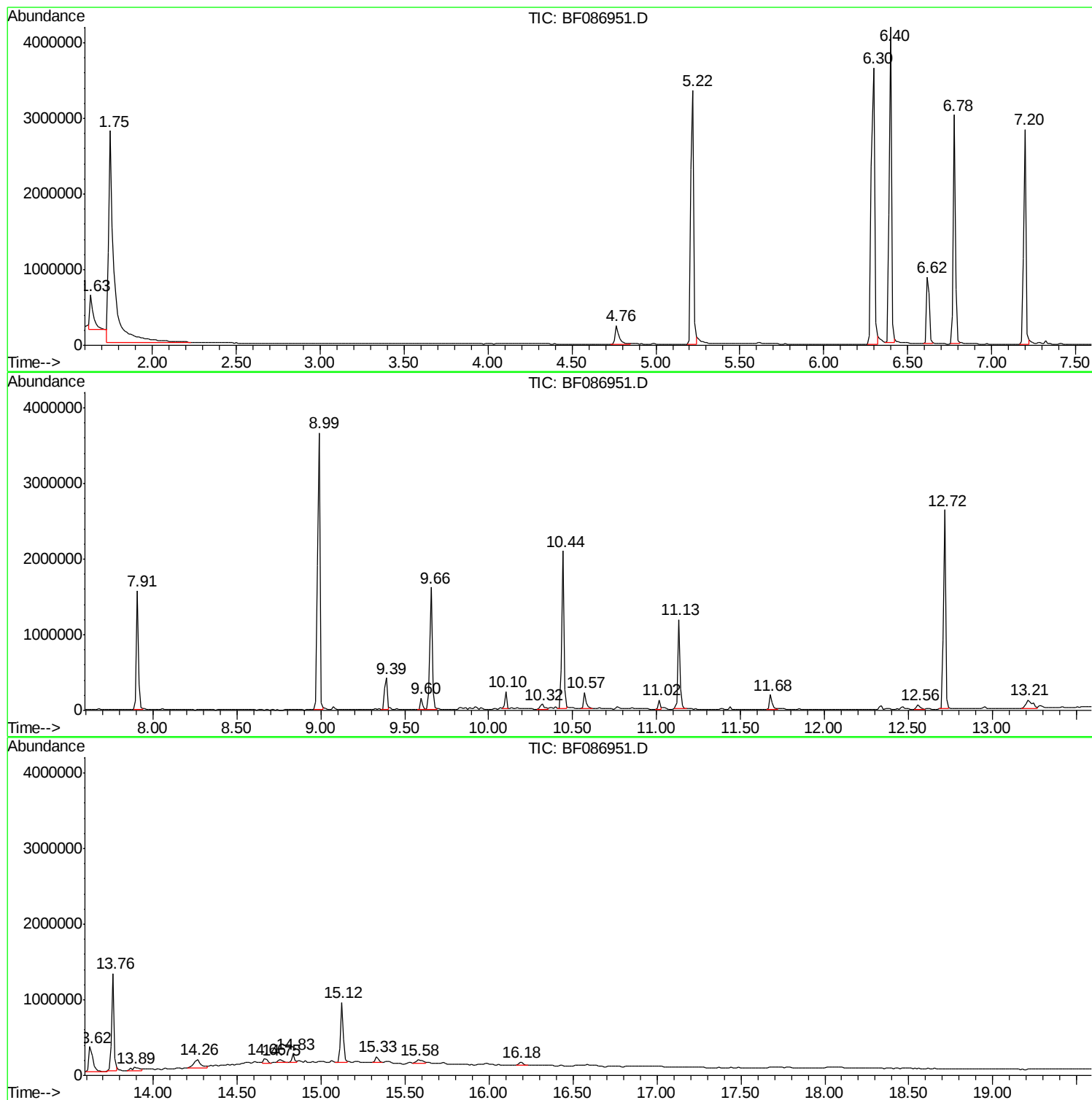
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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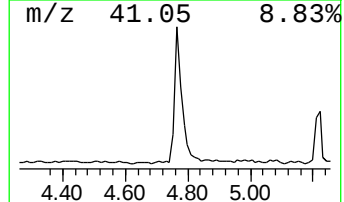
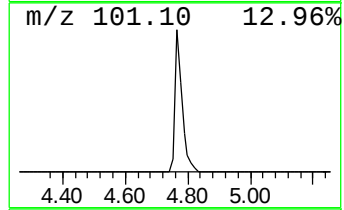
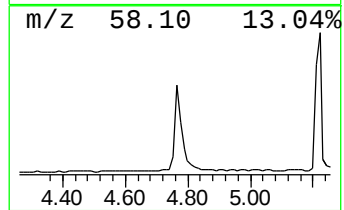
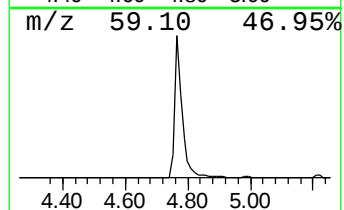
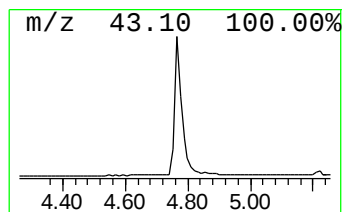
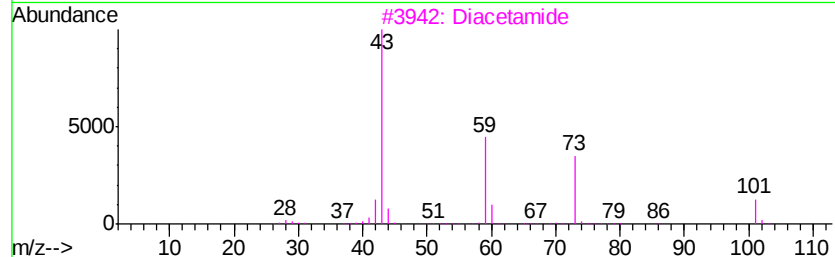
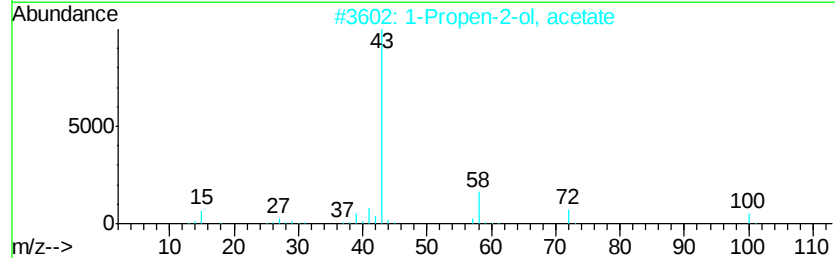
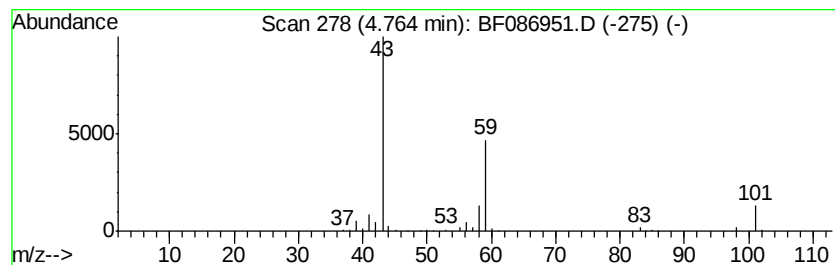
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	6.84 ng	383078	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Diacetamide	101	C4H7NO2	000625-77-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane	58	C4H10	000106-97-8	9



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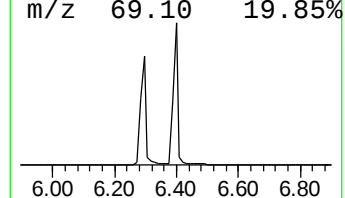
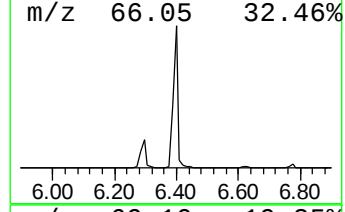
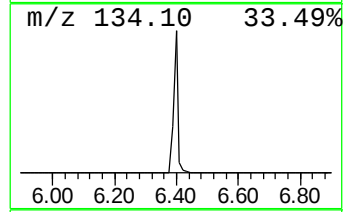
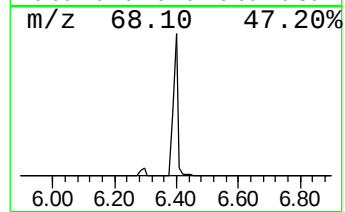
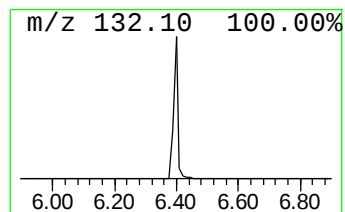
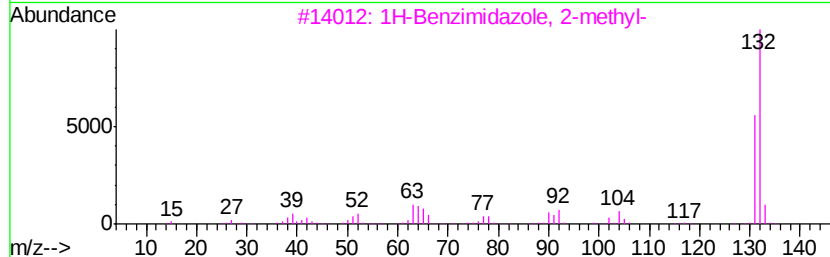
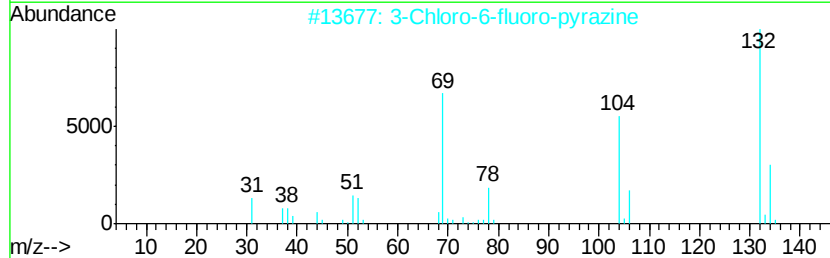
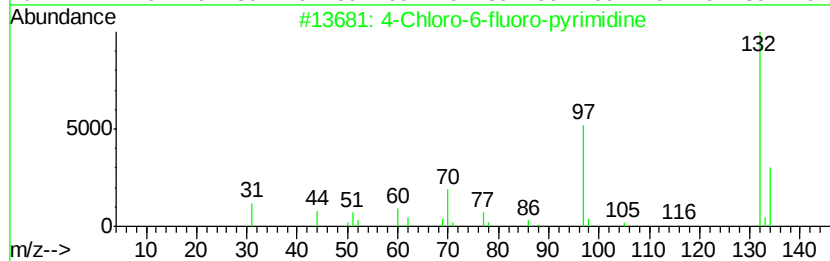
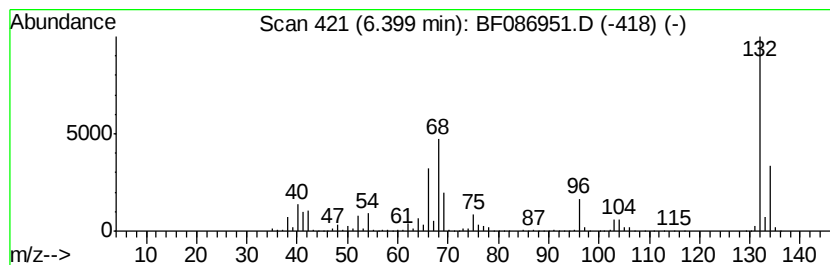
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	75.35 ng	4222430	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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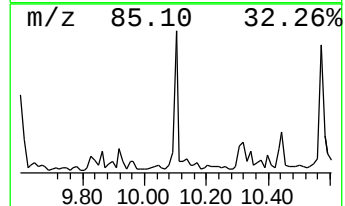
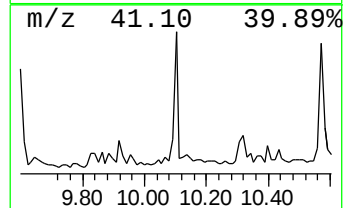
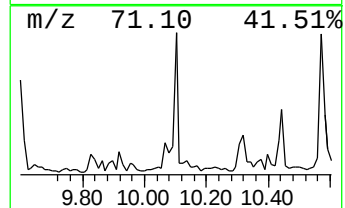
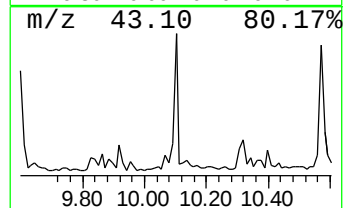
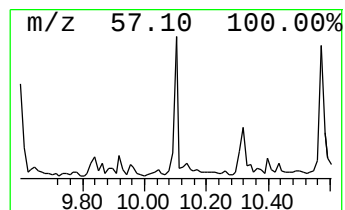
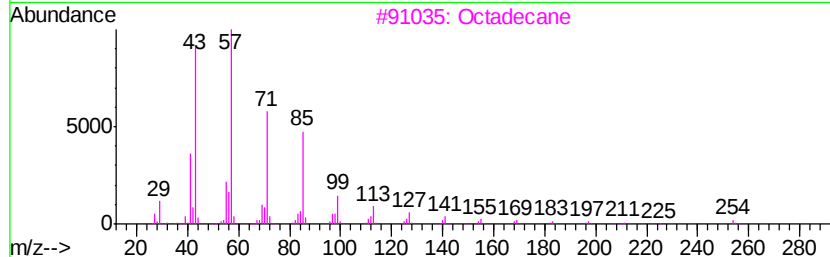
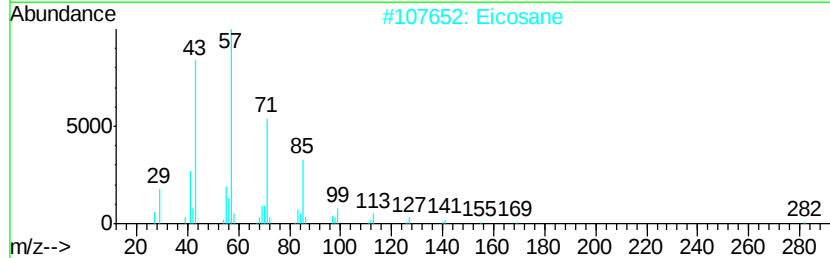
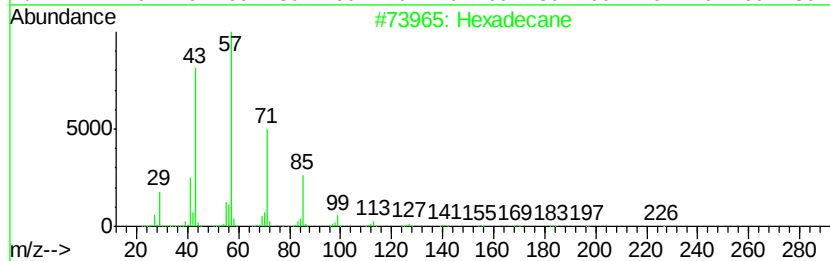
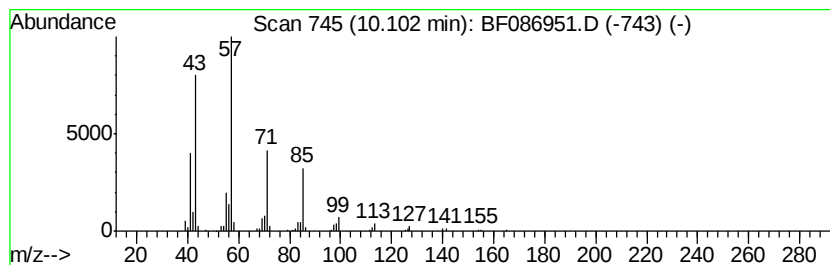
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	2.40 ng	170664	Acenaphthene-d10	9.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Eicosane	282 C20H42	000112-95-8	91
3	Octadecane	254 C18H38	000593-45-3	86
4	Undecane	156 C11H24	001120-21-4	86
5	Tridecane	184 C13H28	000629-50-5	86



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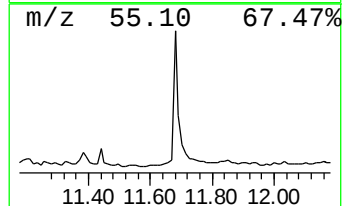
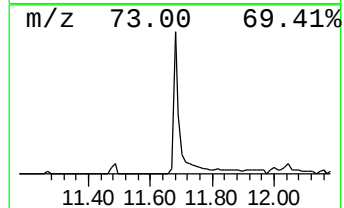
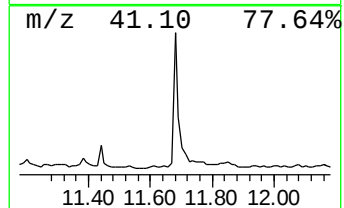
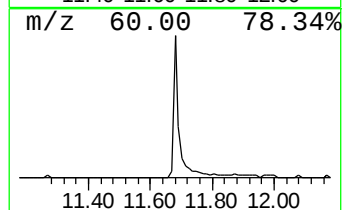
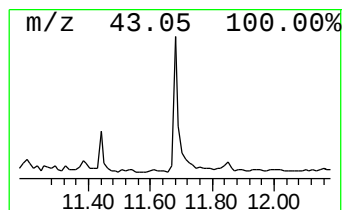
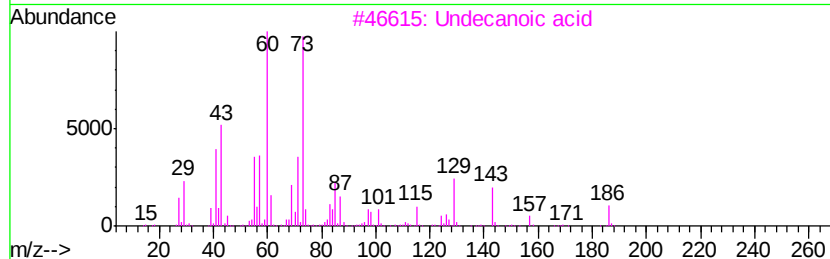
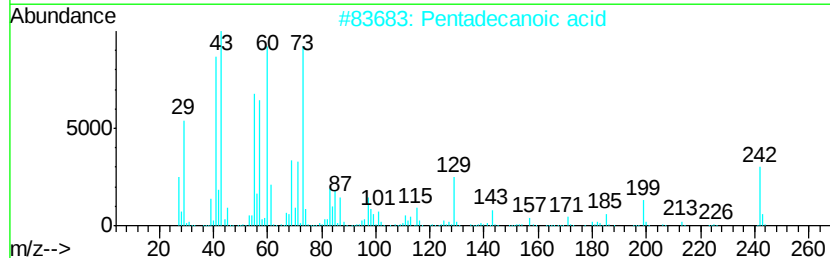
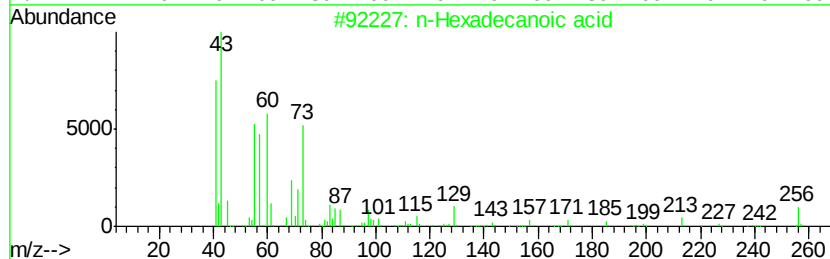
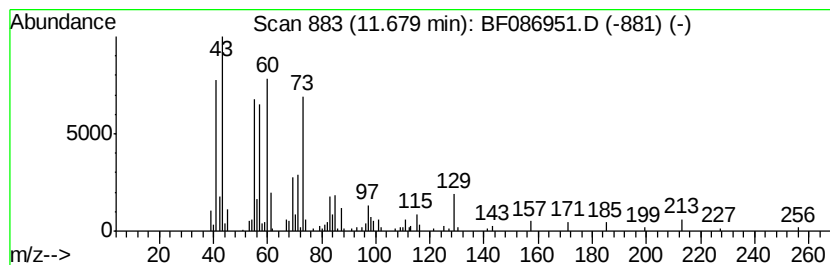
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	4.23 ng	230389	Phenanthrene-d10	11.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Undecanoic acid	186	C11H22O2	000112-37-8	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Tridecanoic acid	214	C13H26O2	000638-53-9	64



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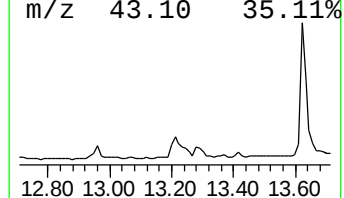
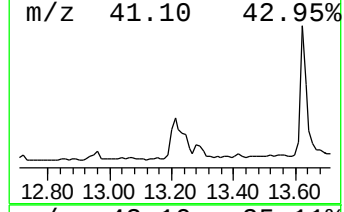
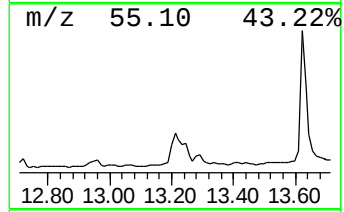
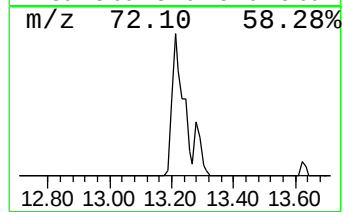
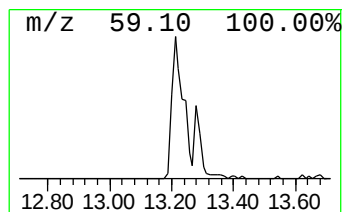
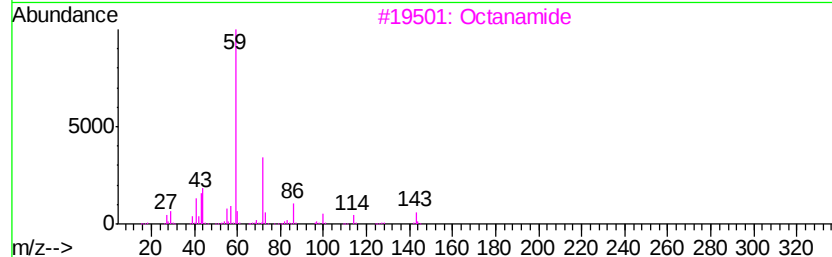
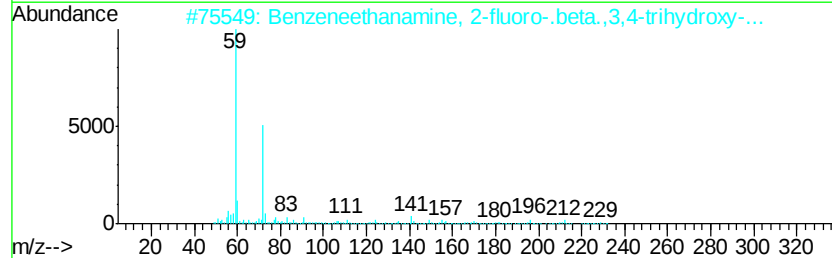
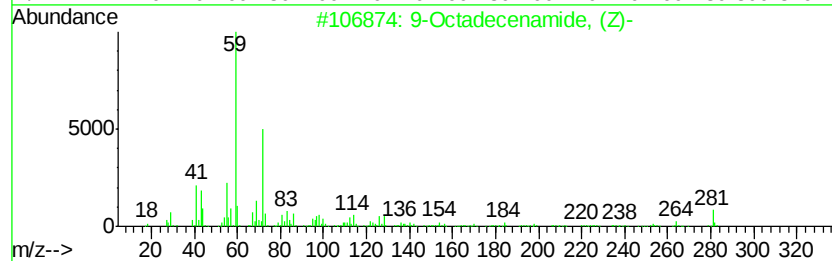
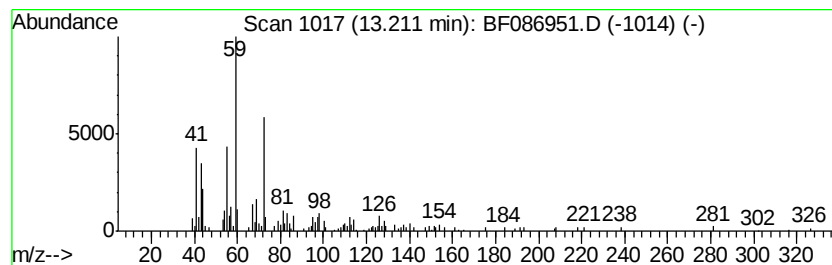
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	4.48 ng	287673	Chrysene-d12	13.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	72
3		Octanamide	143	C8H17NO	000629-01-6	56
4		Decanamide-	171	C10H21NO	002319-29-1	53
5		Octadecanamide	283	C18H37NO	000124-26-5	53



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ClientSampleId :
90TH-AVE-SB-21-0.5-6.0

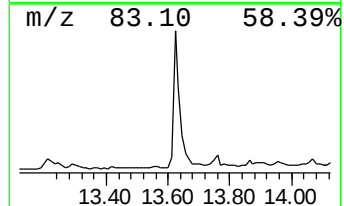
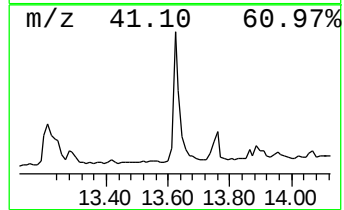
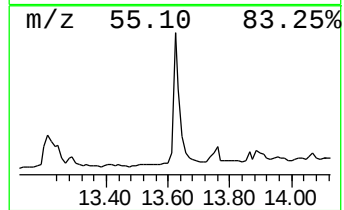
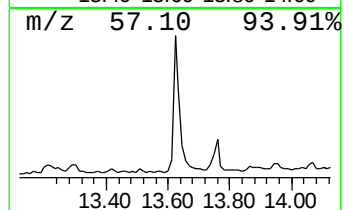
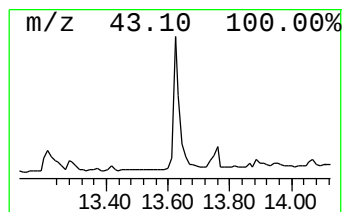
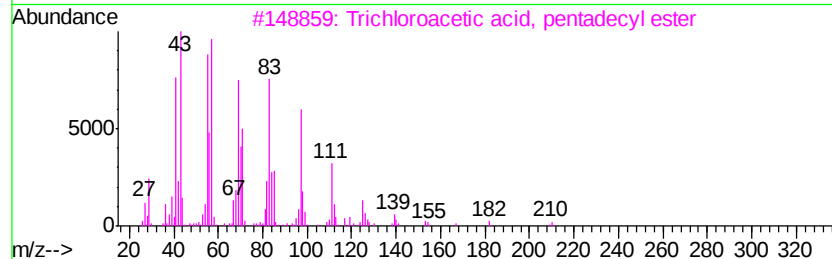
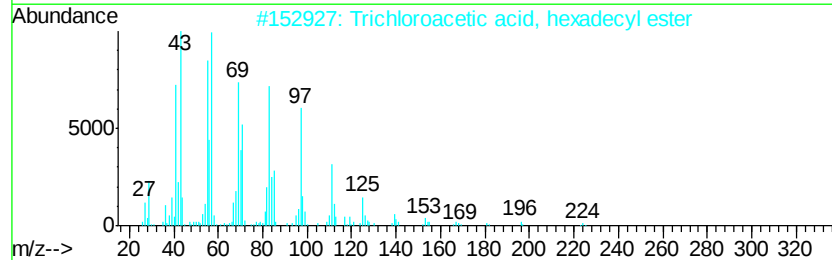
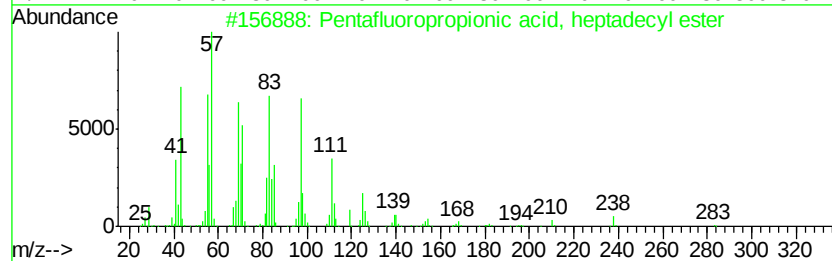
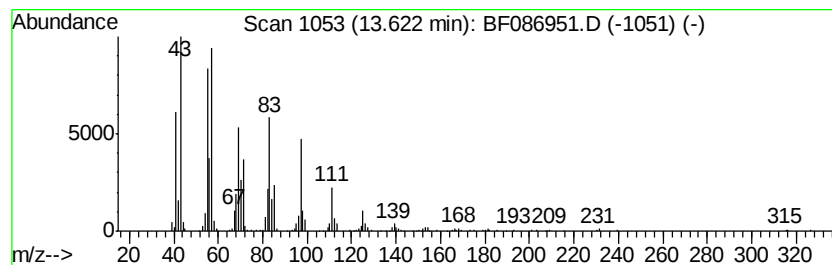
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	7.74 ng	496892	Chrysene-d12	13.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4			Cycloeicosane	280	C20H40	000296-56-0	91
5			1-Tricosene	322	C23H46	018835-32-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086951.D
Acq On : 13 May 2016 1:16
Operator : UM/SJ
Sample : H2977-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

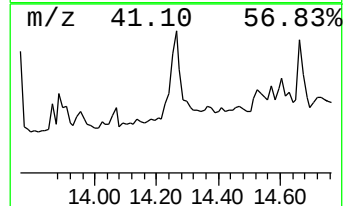
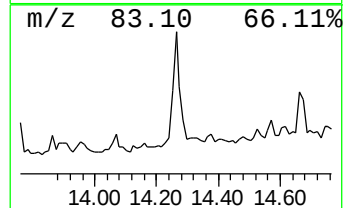
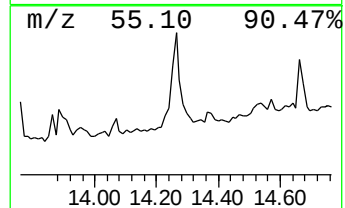
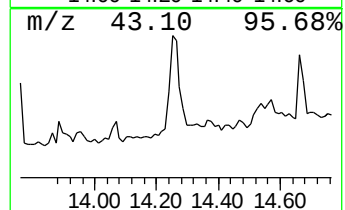
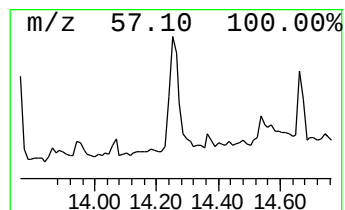
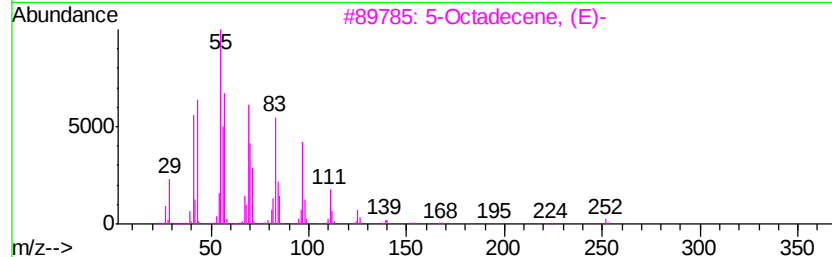
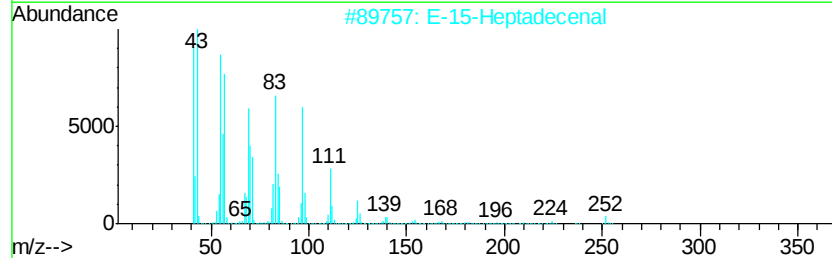
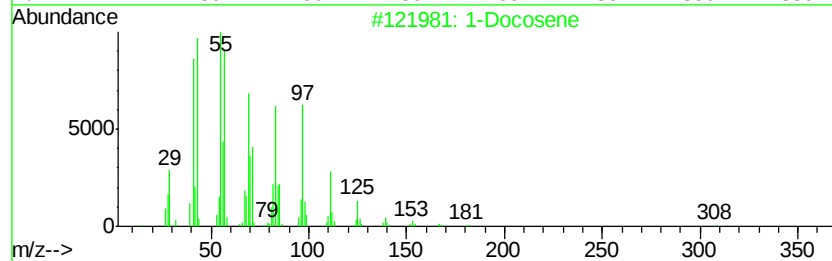
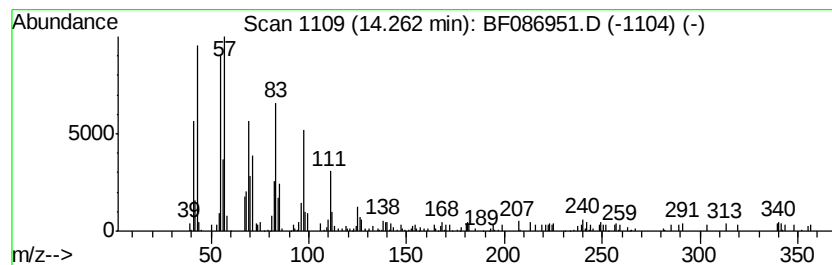
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	4.46 ng	286413	Chrysene-d12	13.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene	308 C22H44	001599-67-3	93
2	E-15-Heptadecenal	252 C17H32O	1000130-97-9	92
3	5-Octadecene, (E)-	252 C18H36	007206-21-5	91
4	9-Octadecene, (E)-	252 C18H36	007206-25-9	90
5	2-Heptadecenal	252 C17H32O	1000143-48-6	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086951.D
Acq On : 13 May 2016 1:16
Operator : UM/SJ
Sample : H2977-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
90TH-AVE-SB-21-0.5-6.0

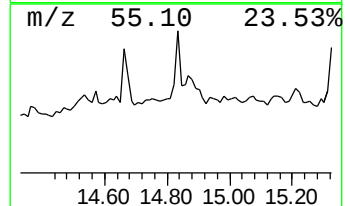
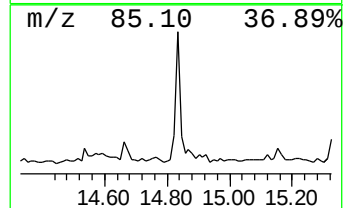
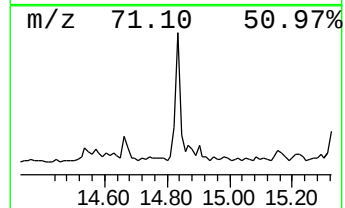
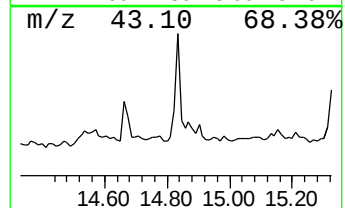
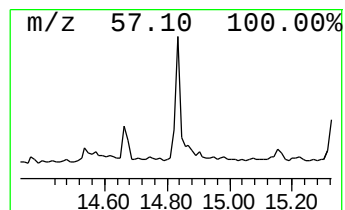
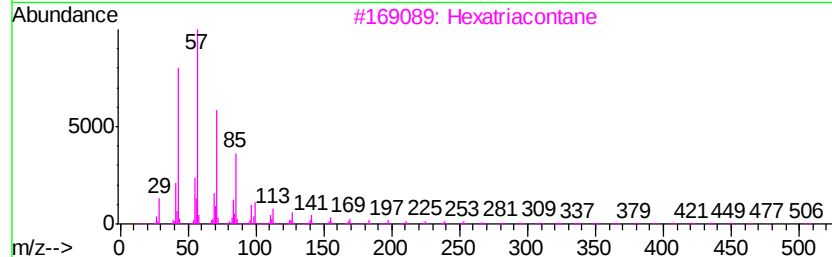
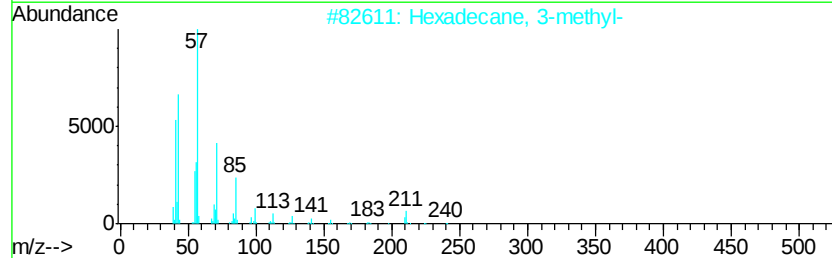
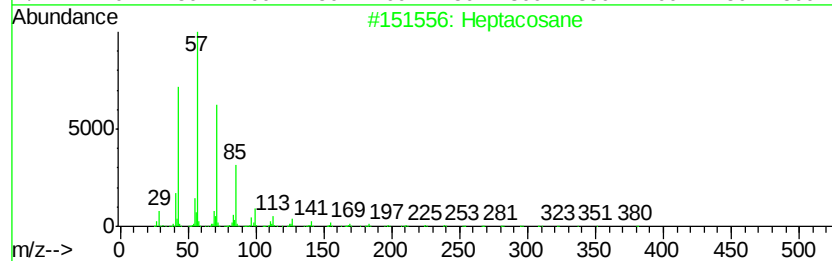
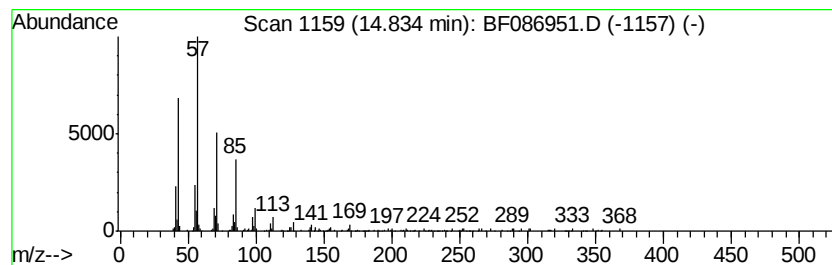
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.81 ng	127442	Perylene-d12	15.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	87
2		Hexadecane, 3-methyl-	240	C17H36	006418-43-5	87
3		Hexatriacontane	507	C36H74	000630-06-8	87
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086951.D
Acq On : 13 May 2016 1:16
Operator : UM/SJ
Sample : H2977-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

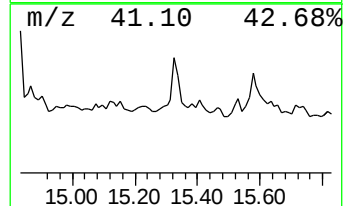
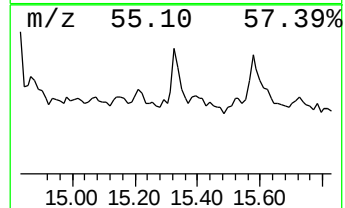
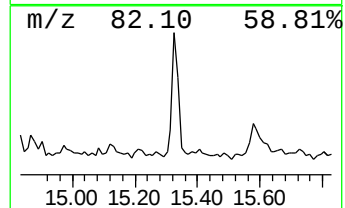
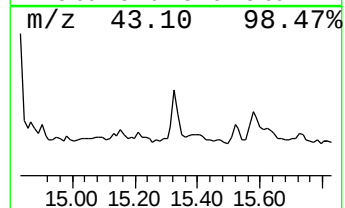
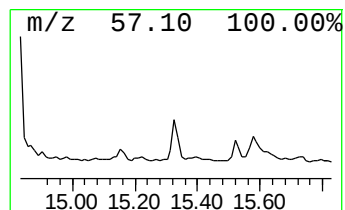
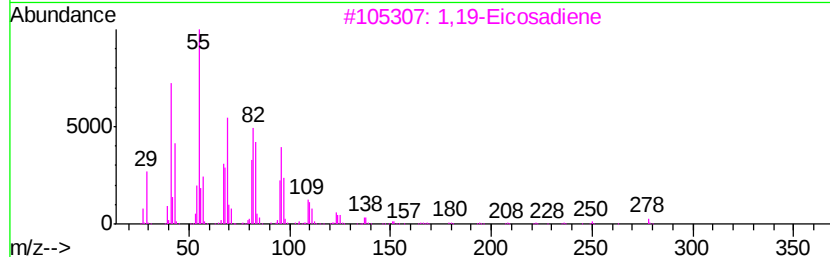
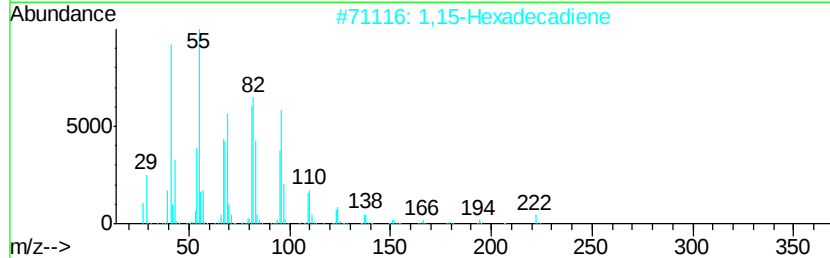
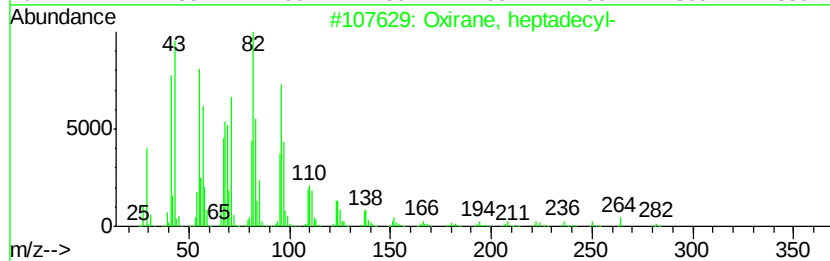
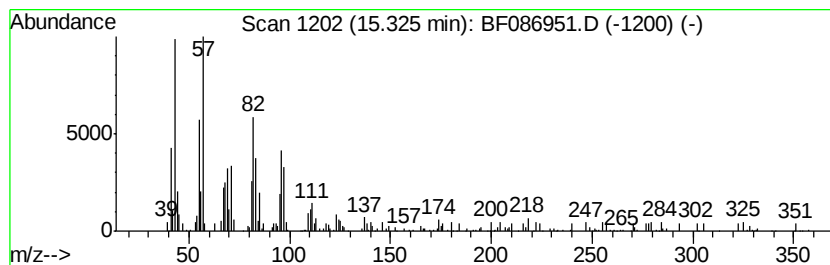
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Oxirane, heptadecyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	2.39 ng	108542	Perylene-d12	15.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Oxirane, heptadecyl-	282 C19H380	067860-04-2 86
2		1,15-Hexadecadiene	222 C16H30	021964-51-2 70
3		1,19-Eicosadiene	278 C20H38	014811-95-1 70
4		Oxirane, hexadecyl-	268 C18H360	007390-81-0 58
5		(Z)-14-Tricosenyl formate	366 C24H4602	077899-10-6 53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
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Acq On : 13 May 2016 1:16
Operator : UM/SJ
Sample : H2977-04
Misc :
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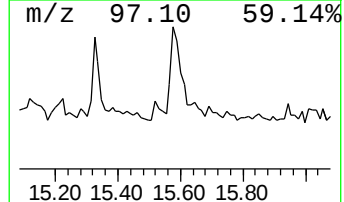
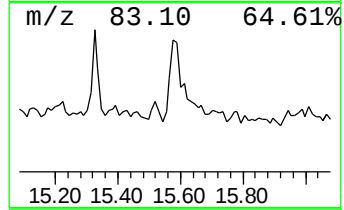
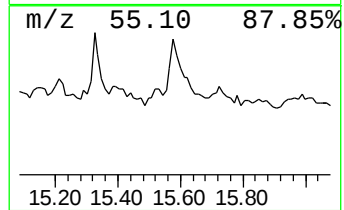
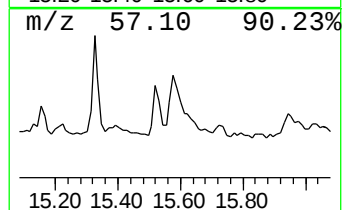
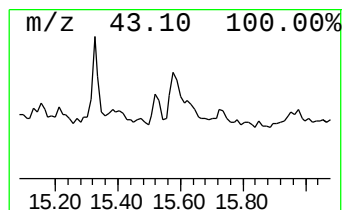
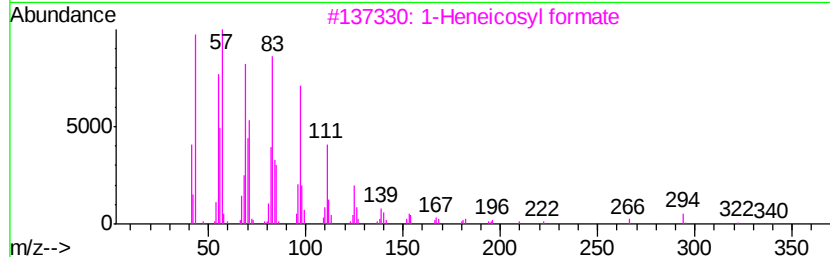
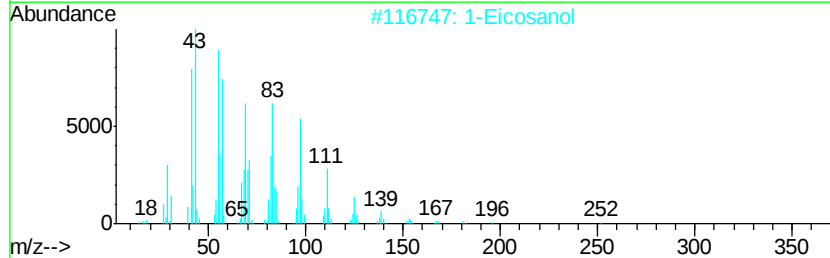
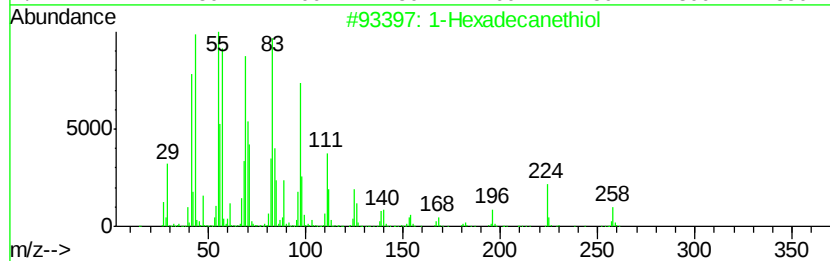
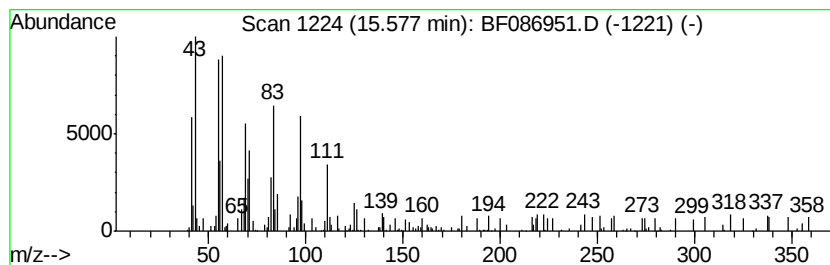
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Hexadecanethiol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.58	3.38 ng	153254	Perylene-d12	15.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanethiol	258	C16H34S	002917-26-2	89
2	1-Eicosanol	298	C20H42O	000629-96-9	87
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	83
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086951.D
Acq On : 13 May 2016 1:16
Operator : UM/SJ
Sample : H2977-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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...	4.76	6.8	ng	383078	1	6.63	1120810	20.0
unknown6.40	6.40	75.3	ng	4222430	1	6.63	1120810	20.0
Hexadecane	10.10	2.4	ng	170664	3	9.66	1421820	20.0
n-Hexadecanoic acid	11.68	4.2	ng	230389	4	11.13	1090570	20.0
9-Octadecenamide,...	13.21	4.5	ng	287673	5	13.76	1283220	20.0
Pentafluoropropio...	13.62	7.7	ng	496892	5	13.76	1283220	20.0
1-Docosene	14.26	4.5	ng	286413	5	13.76	1283220	20.0
Heptacosane	14.83	2.8	ng	127442	6	15.12	907264	20.0
Oxirane, heptadecyl-	15.33	2.4	ng	108542	6	15.12	907264	20.0
1-Hexadecanethiol	15.58	3.4	ng	153254	6	15.12	907264	20.0