

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
 Data File : BF085406.D
 Acq On : 12 Mar 2016 8:30
 Operator : UM/SJ
 Sample : H1730-08
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-19-COMP(0.5-3.0)

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-BF030316.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	4.630	203	205	208	rBV	126775	152091	3.19%	0.391%
2	5.144	247	250	256	rBV	225394	320566	6.71%	0.824%
3	5.544	282	285	287	rBV	3607665	3882340	81.31%	9.974%
4	6.573	371	375	377	rBV	3487431	4602832	96.40%	11.825%
5	6.710	384	387	389	rBV	3648861	4584955	96.03%	11.779%
6	6.939	404	407	409	rBV	844192	893587	18.71%	2.296%
7	7.099	418	421	423	rBV	2857878	3603142	75.46%	9.257%
8	7.499	453	456	459	rBV	2325070	2696935	56.48%	6.929%
9	8.219	517	519	521	rBV	1240323	1106158	23.17%	2.842%
10	9.305	611	614	616	rBV	4583390	4774733	100.00%	12.267%
11	9.693	646	648	650	rBV	820585	685432	14.36%	1.761%
12	9.910	665	667	669	rBV	104373	88249	1.85%	0.227%
13	9.979	671	673	675	rVB	1352504	1130714	23.68%	2.905%
14	10.413	708	711	712	rVB	98116	131159	2.75%	0.337%
15	10.631	727	730	731	rBV	52030	74533	1.56%	0.191%
16	10.768	739	742	745	rBV	2290934	2215210	46.39%	5.691%
17	10.882	749	752	759	rVV	165801	203008	4.25%	0.522%
18	11.328	789	791	793	rBV	67274	60498	1.27%	0.155%
19	11.465	801	803	805	rBV	1132017	944474	19.78%	2.426%
20	11.991	846	849	851	rBV	284963	277873	5.82%	0.714%
21	12.779	916	918	925	rBV	75660	138402	2.90%	0.356%
22	13.054	939	942	944	rBV	3431678	3152485	66.02%	8.099%
23	13.259	957	960	964	rBV3	24965	48464	1.02%	0.125%
24	13.945	1018	1020	1028	rBV	737851	826947	17.32%	2.124%
25	14.105	1031	1034	1037	rVB	896368	836735	17.52%	2.150%
26	14.265	1046	1048	1052	rBV	26343	51031	1.07%	0.131%
27	14.574	1074	1075	1079	rBV	69215	102492	2.15%	0.263%
28	14.859	1098	1100	1103	rBV	278744	321673	6.74%	0.826%
29	14.951	1106	1108	1113	rVB3	33162	55027	1.15%	0.141%
30	15.214	1129	1131	1137	rVB2	37847	74234	1.55%	0.191%
31	15.568	1159	1162	1165	rBV	477455	663887	13.90%	1.706%
32	16.082	1205	1207	1211	rBV	84981	156186	3.27%	0.401%
33	17.614	1339	1341	1347	rVB5	27128	68285	1.43%	0.175%

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W170TH-SB-19-COMP(0.5-3.0)

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

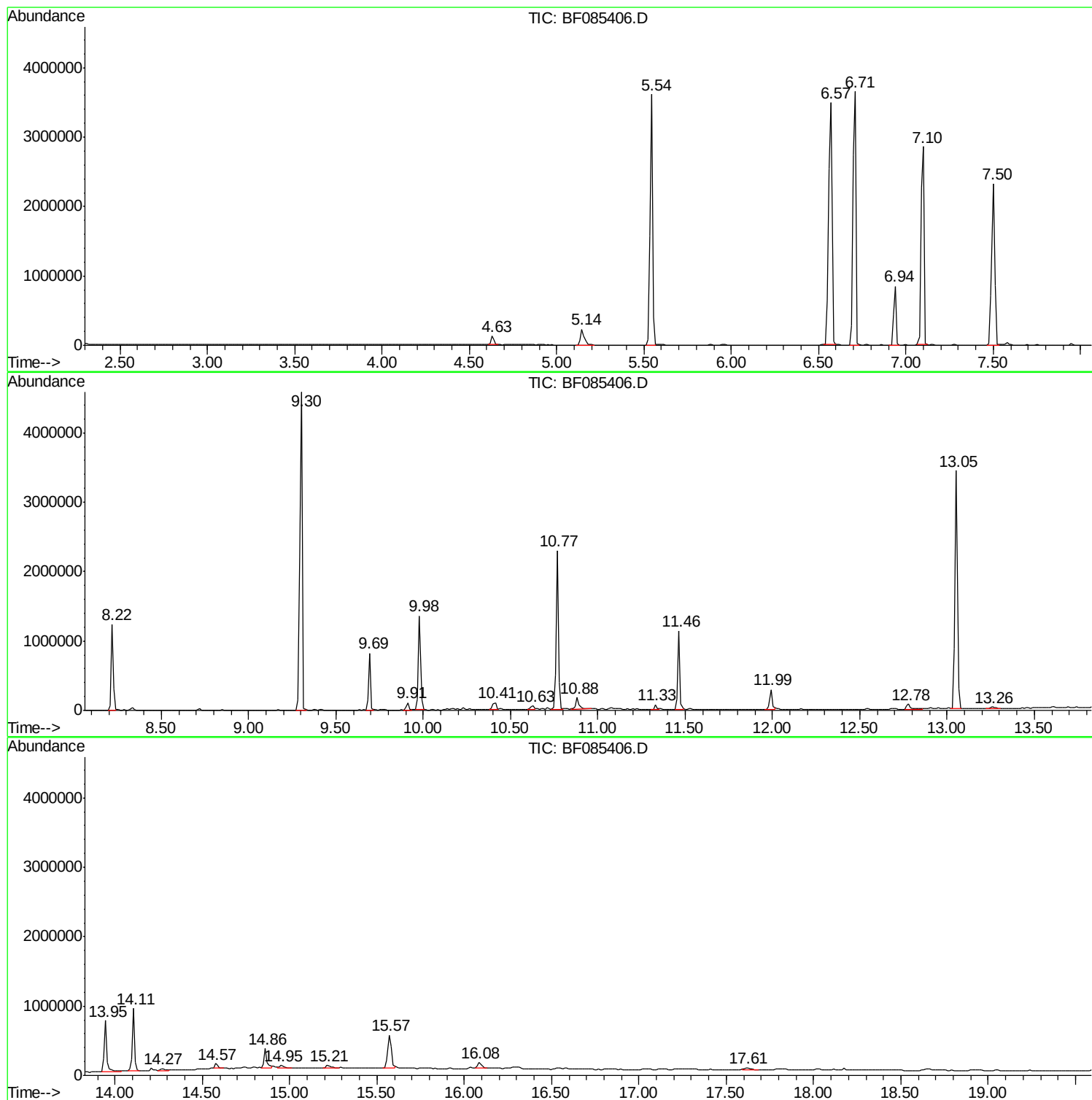
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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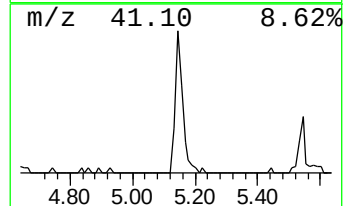
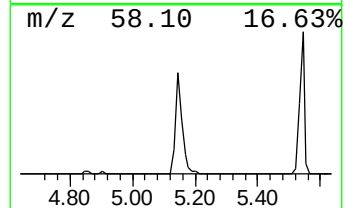
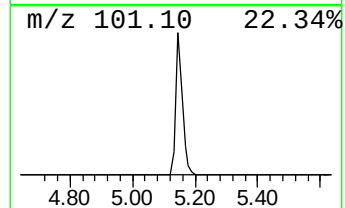
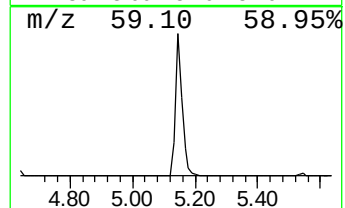
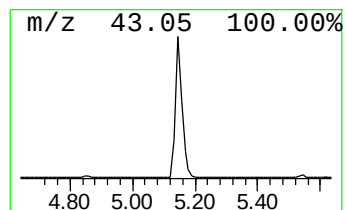
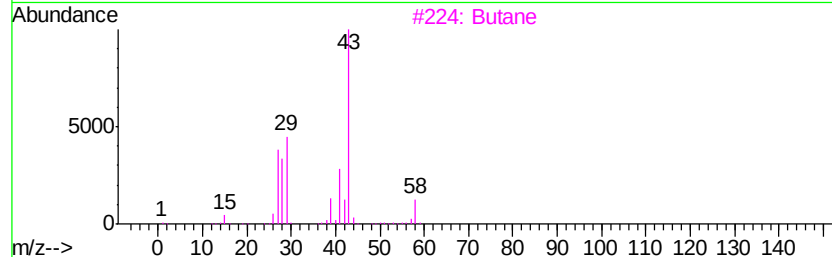
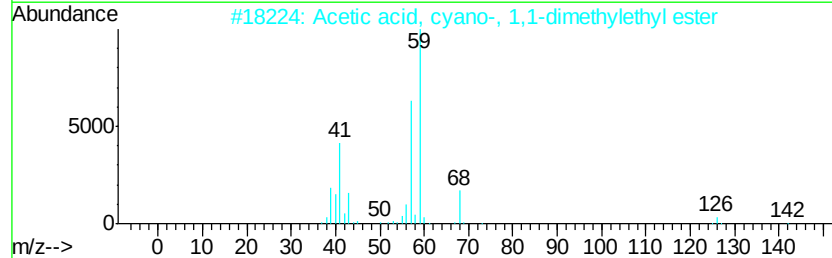
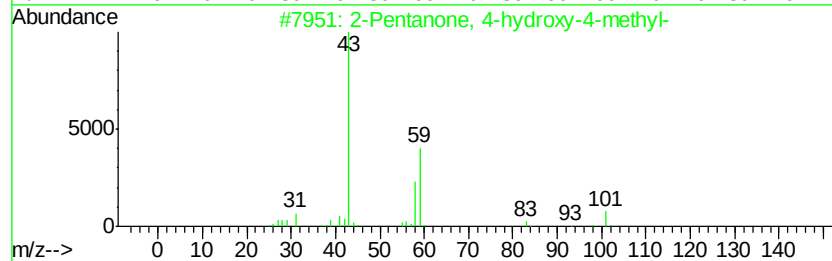
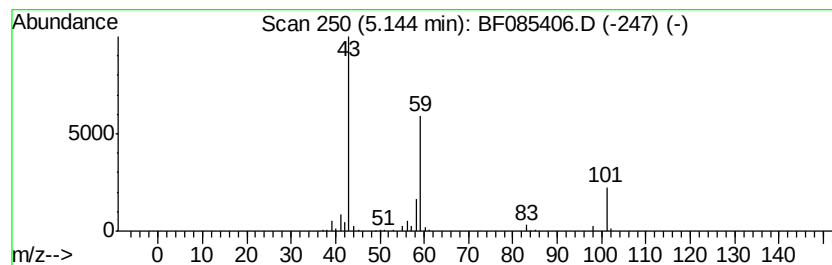
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	7.17 ng	320566	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Butane	58	C4H10	000106-97-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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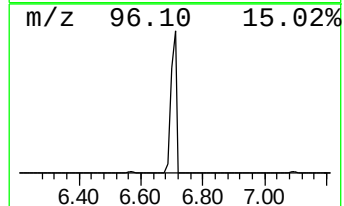
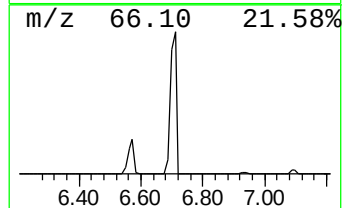
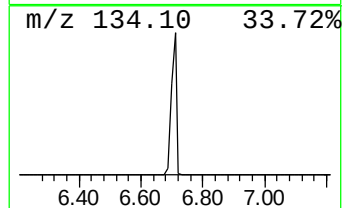
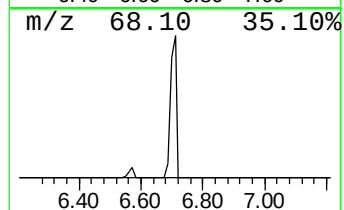
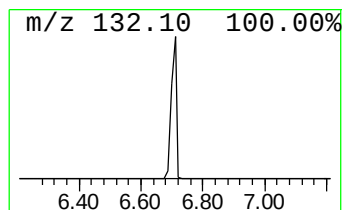
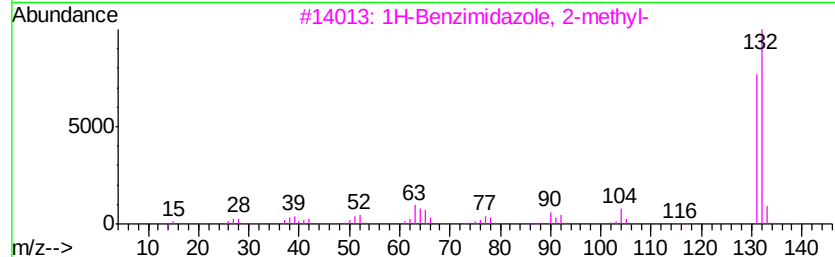
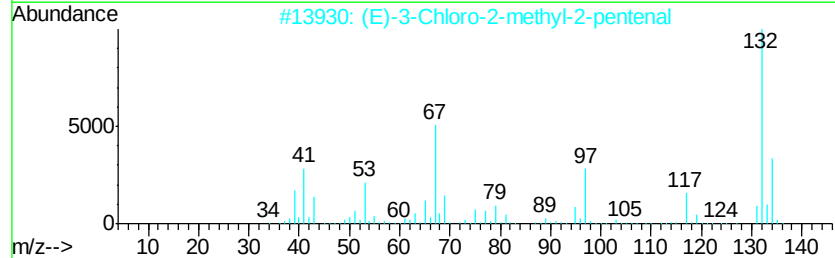
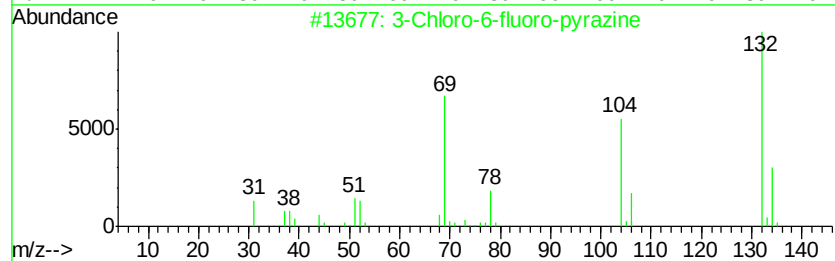
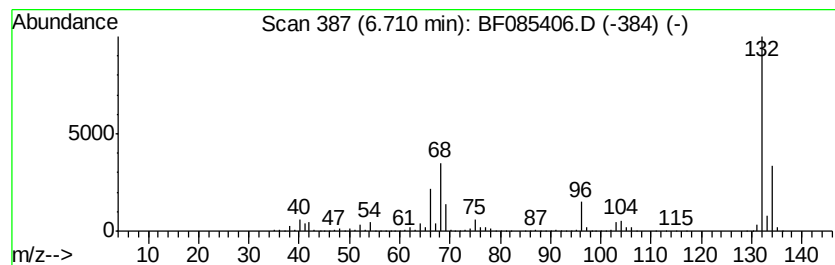
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	102.62 ng	4584960	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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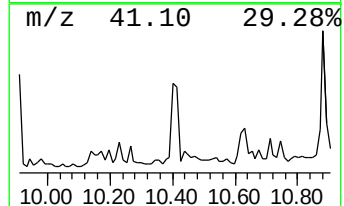
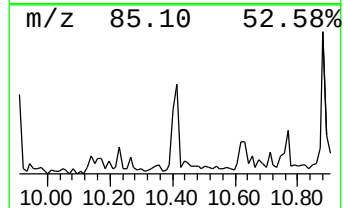
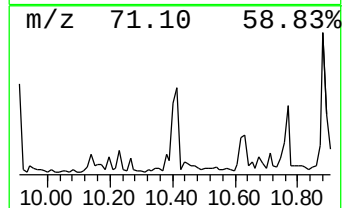
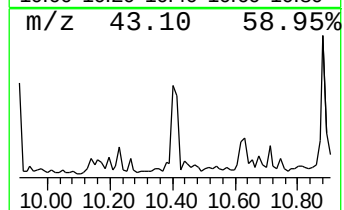
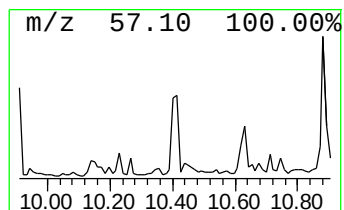
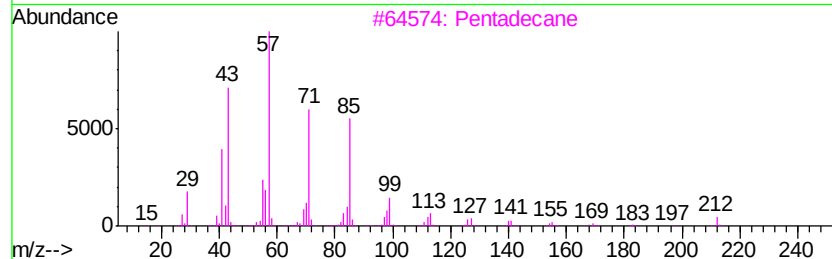
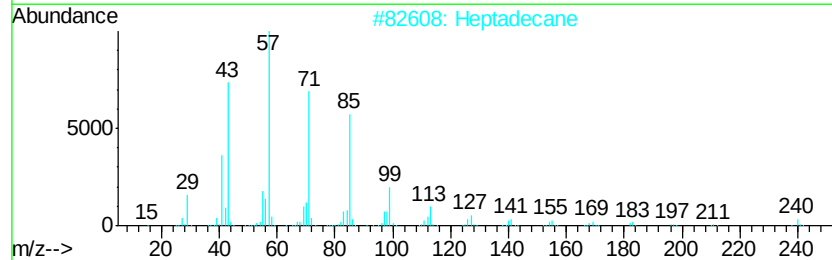
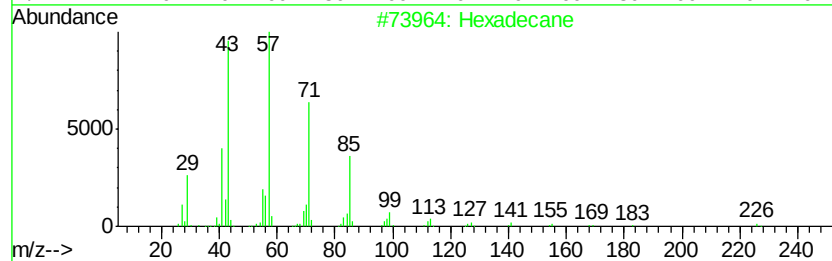
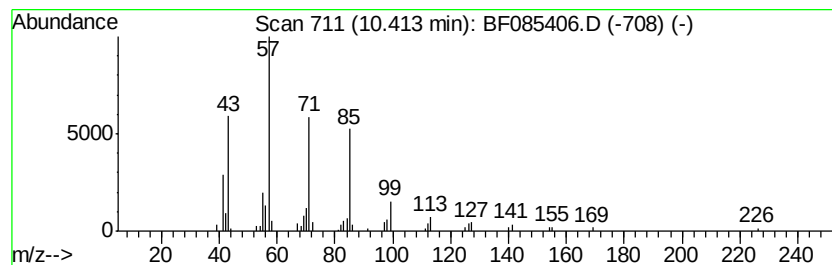
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.41	2.32 ng	131159	Acenaphthene-d10		9.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Heptadecane	240	C17H36	000629-78-7	91
3	Pentadecane	212	C15H32	000629-62-9	91
4	Tetradecane	198	C14H30	000629-59-4	91
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72



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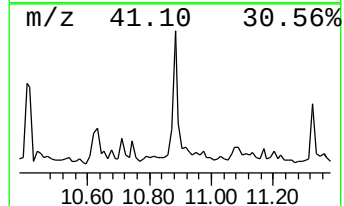
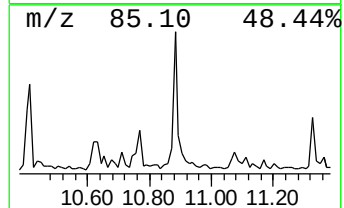
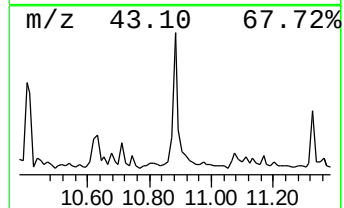
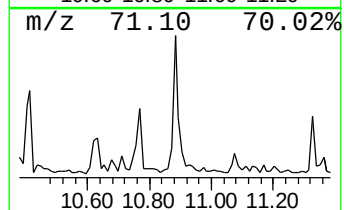
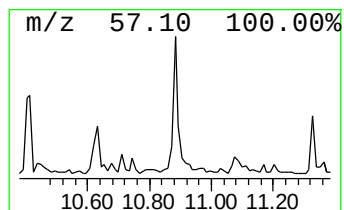
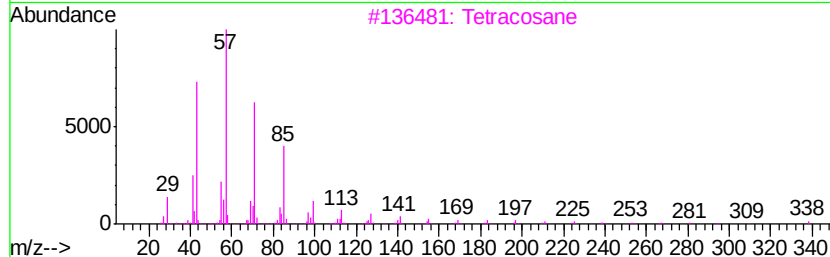
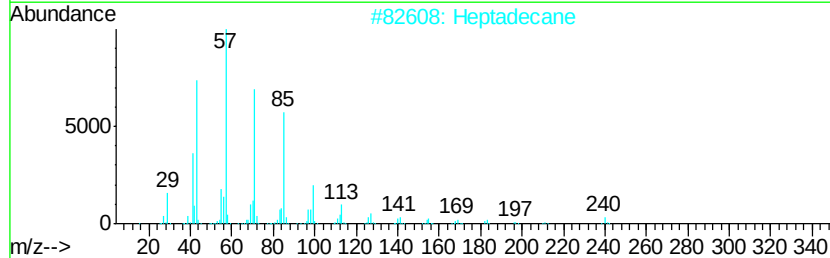
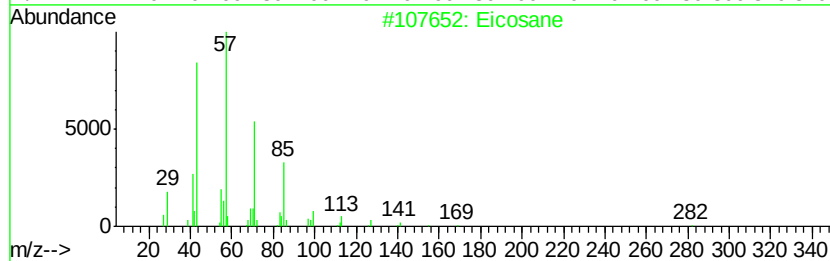
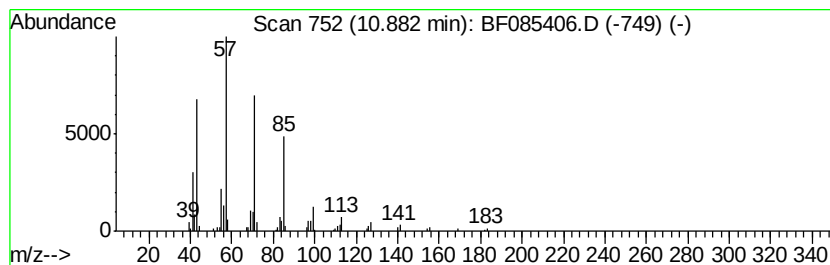
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.88	4.30 ng	203008	Phenanthrene-d10		11.46	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	Heneicosane		296	C21H44	000629-94-7	91
5	Hexadecane		226	C16H34	000544-76-3	90



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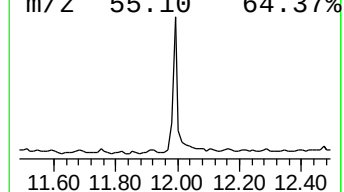
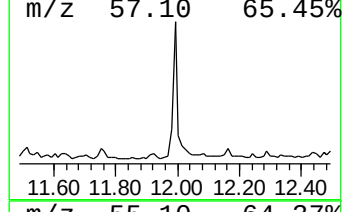
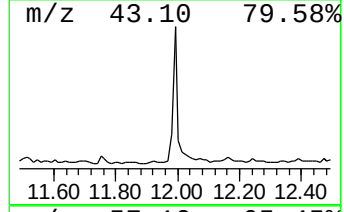
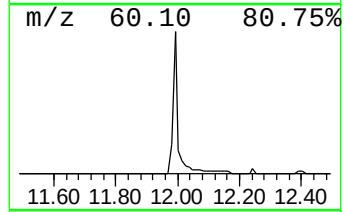
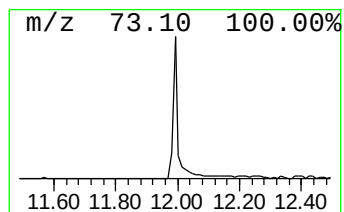
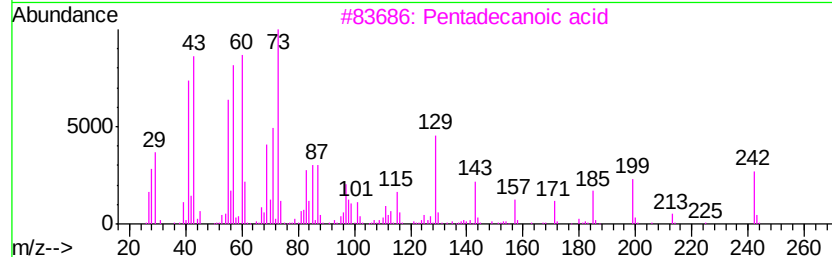
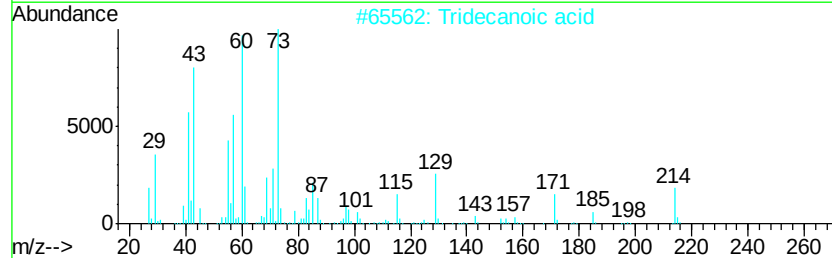
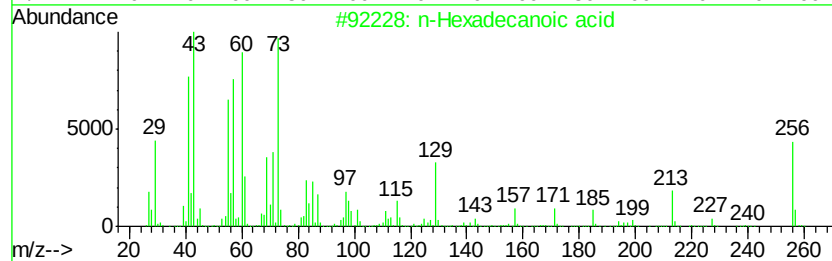
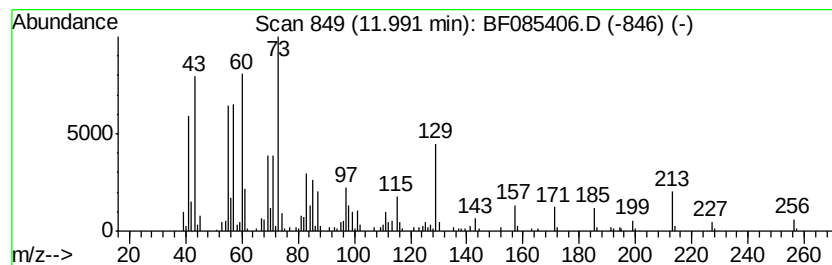
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.99	5.88 ng	277873	Phenanthrene-d10		11.46	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	n-Decanoic acid		172	C10H20O2	000334-48-5	76



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W170TH-SB-19-COMP(0.5-3.0)

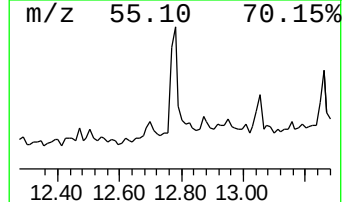
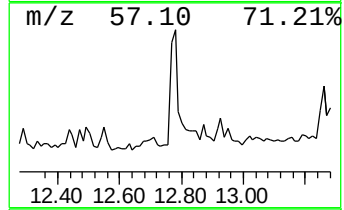
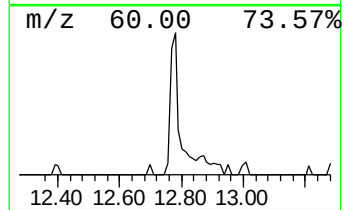
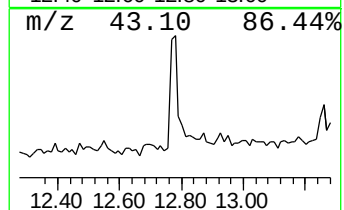
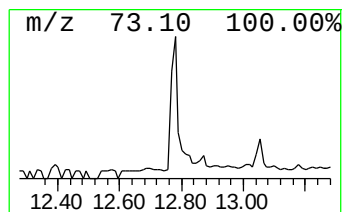
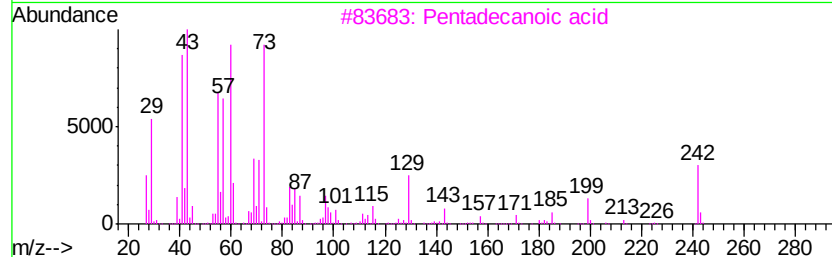
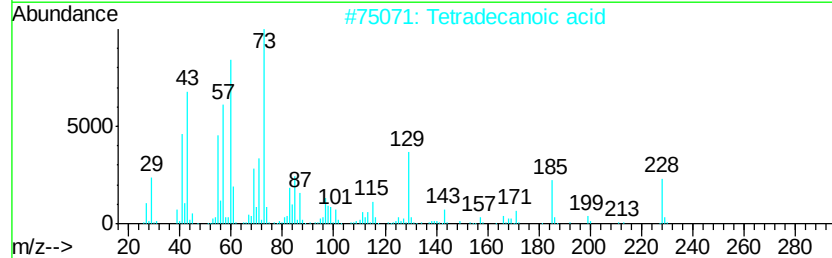
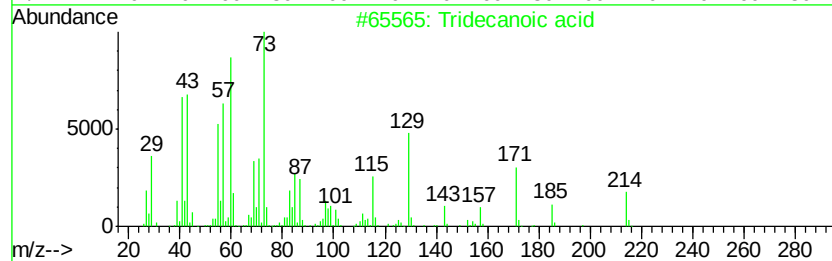
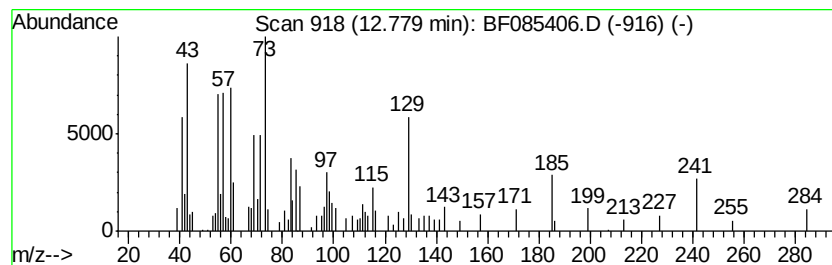
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.93 ng	138402	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanoic acid	214	C13H26O2	000638-53-9	64
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
5		Undecanoic acid	186	C11H22O2	000112-37-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085406.D
Acq On : 12 Mar 2016 8:30
Operator : UM/SJ
Sample : H1730-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-19-COMP(0.5-3.0)

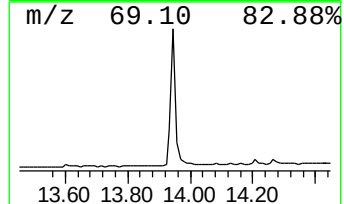
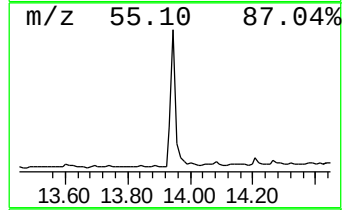
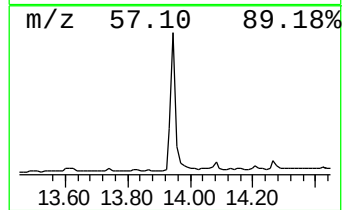
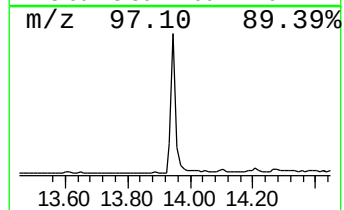
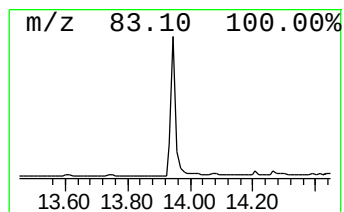
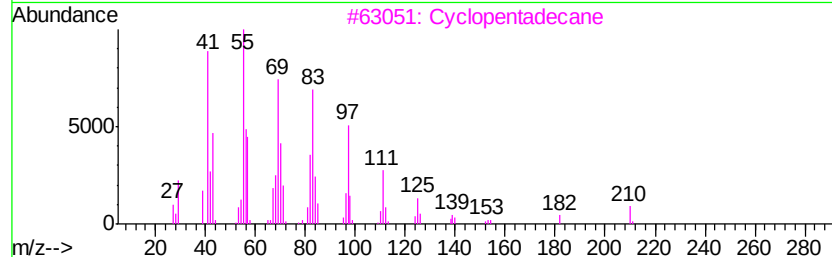
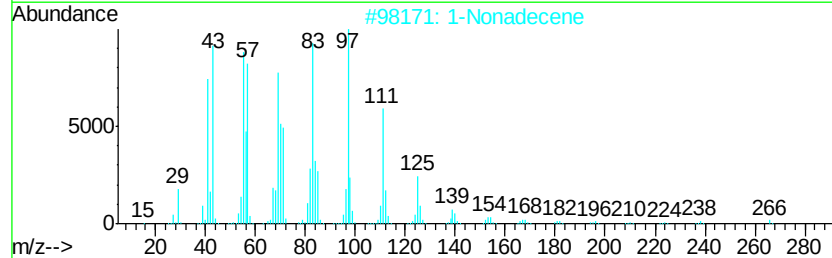
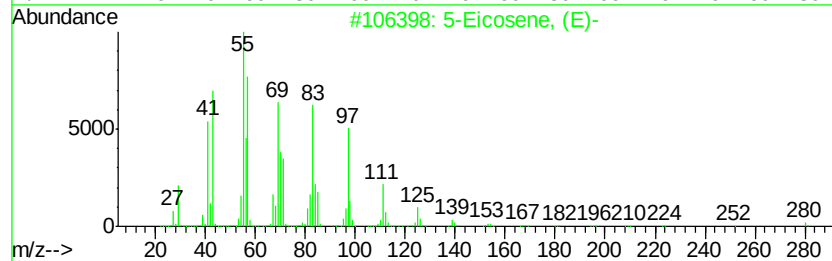
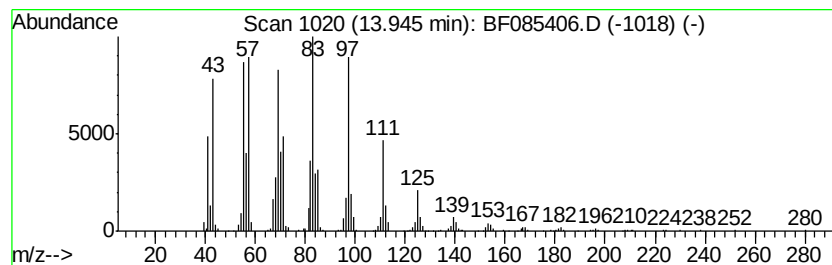
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	19.77 ng	826947	Chrysene-d12	14.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Nonadecene	266	C19H38	018435-45-5	94
3		Cyclopentadecane	210	C15H30	000295-48-7	93
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
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Sample : H1730-08
Misc :
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ClientSampleId :
W170TH-SB-19-COMP(0.5-3.0)

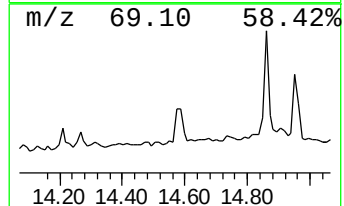
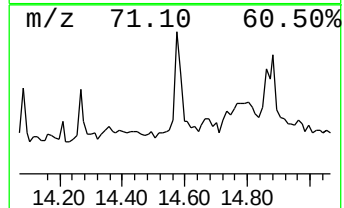
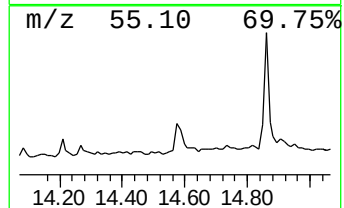
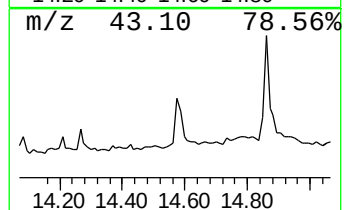
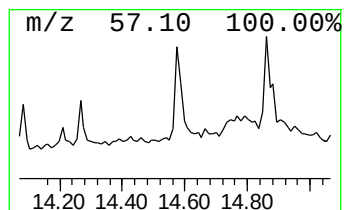
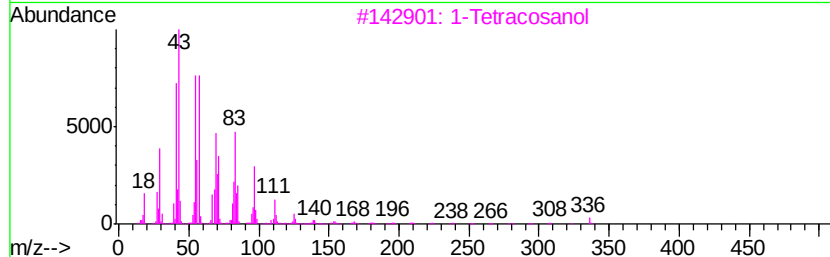
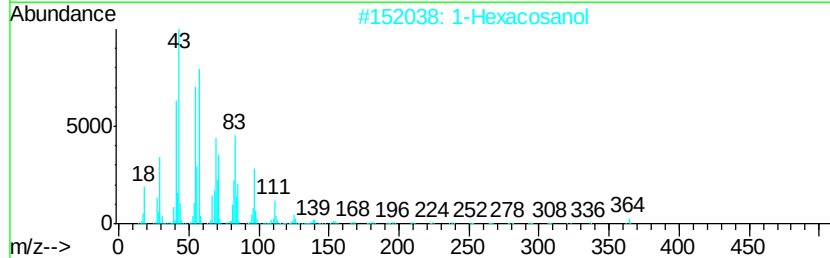
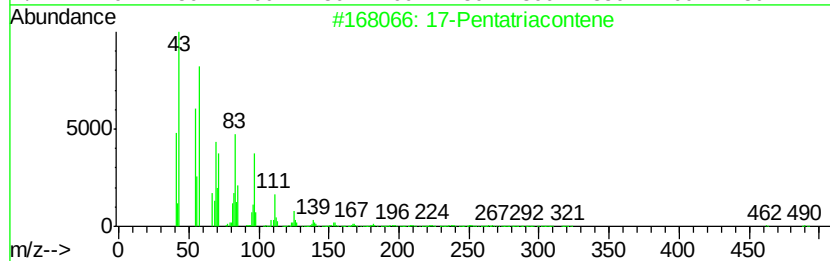
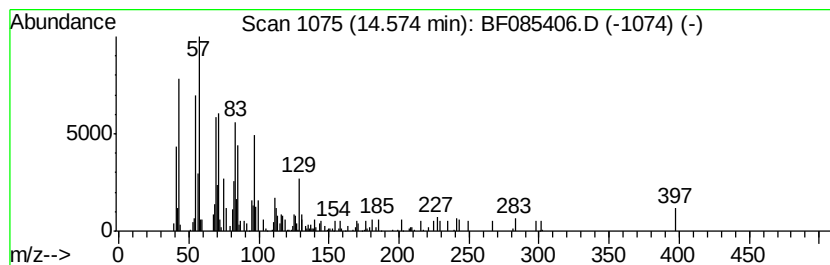
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.57 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.45 ng	102492	Chrysene-d12	14.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	49
2		1-Hexacosanol	382	C26H54O	000506-52-5	46
3		1-Tetracosanol	354	C24H50O	000506-51-4	46
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	46
5		Cyclotetracosane	336	C24H48	000297-03-0	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
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Sample : H1730-08
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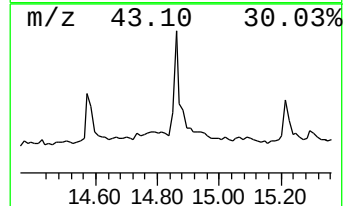
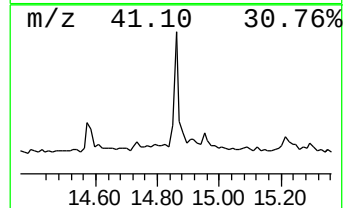
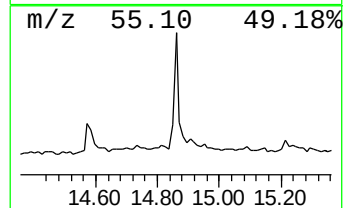
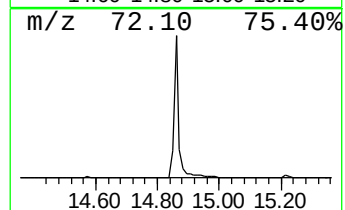
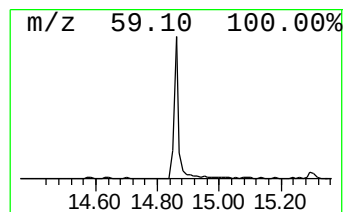
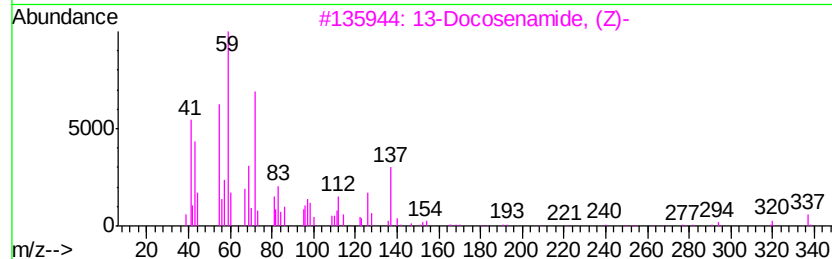
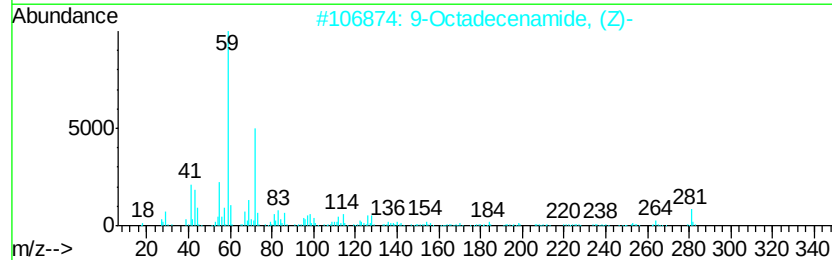
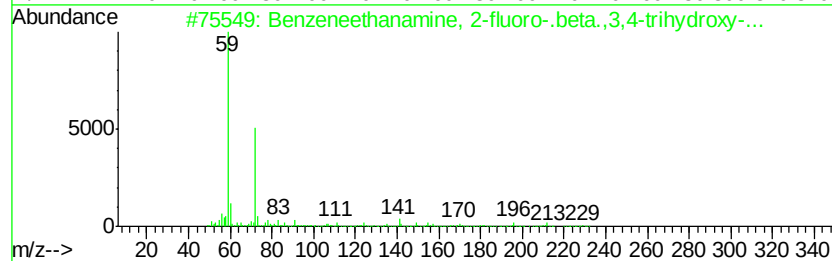
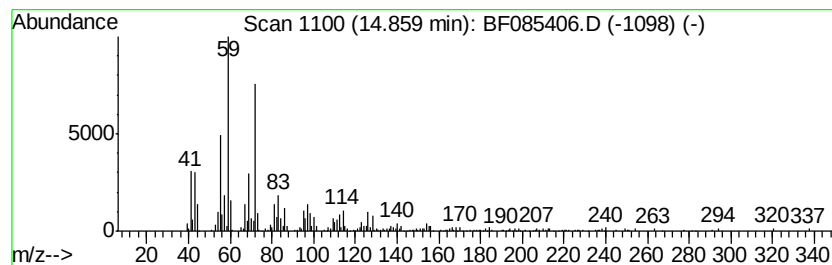
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzeneethanamine, 2-fluoro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.86	9.69 ng	321673	Perylene-d12	15.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	68
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	56
4	Dodecanamide	199	C12H25NO	001120-16-7	32
5	Cyclopentylsilane	100	C5H12Si	080249-74-7	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085406.D
Acq On : 12 Mar 2016 8:30
Operator : UM/SJ
Sample : H1730-08
Misc :
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Instrument :
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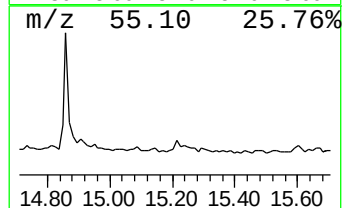
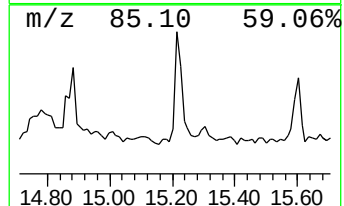
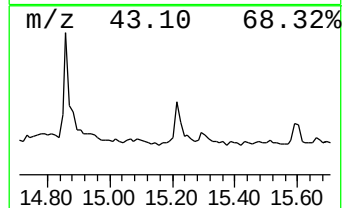
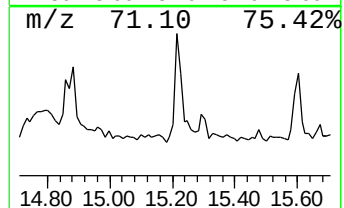
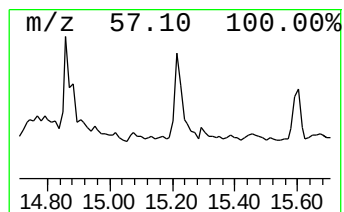
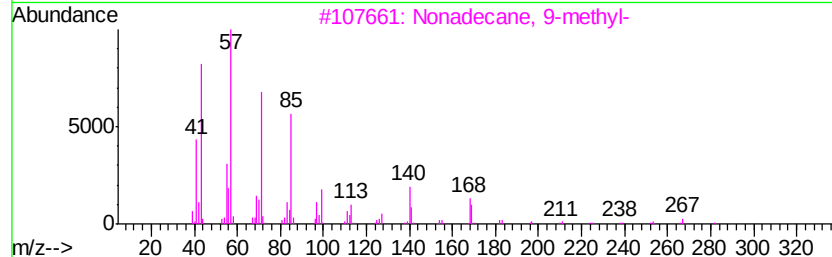
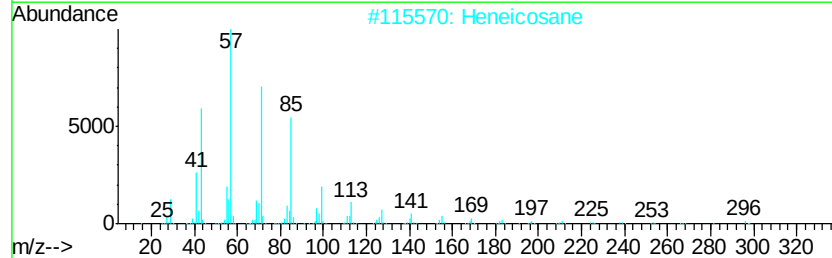
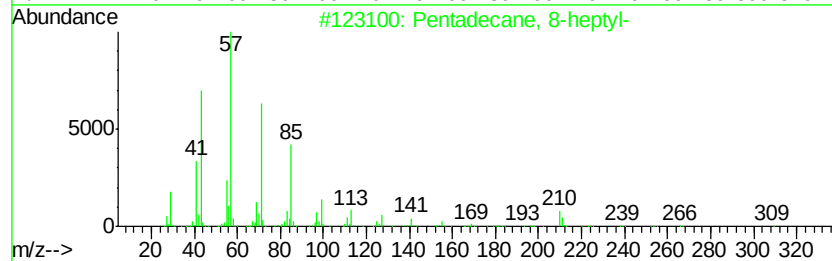
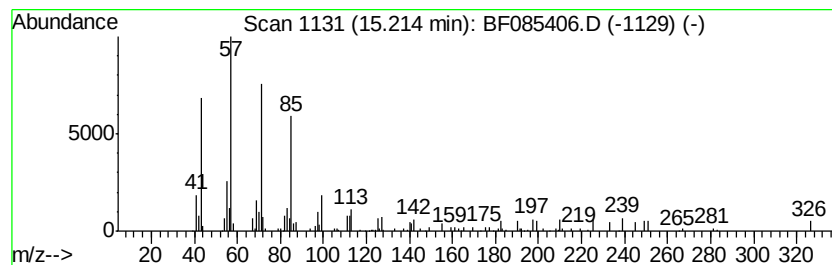
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentadecane, 8-heptyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.24 ng	74234	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	74
2		Heneicosane	296	C21H44	000629-94-7	74
3		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	72
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
5		Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085406.D
Acq On : 12 Mar 2016 8:30
Operator : UM/SJ
Sample : H1730-08
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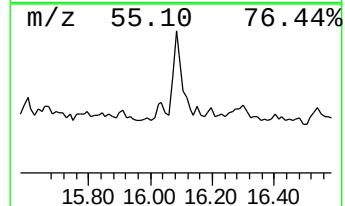
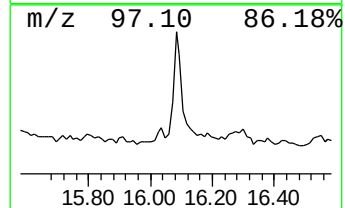
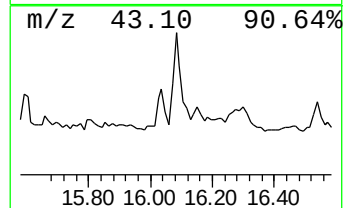
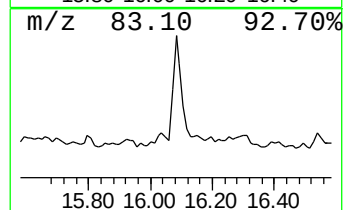
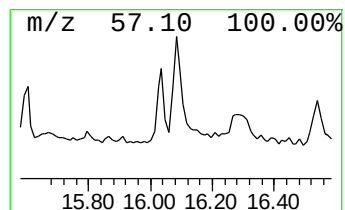
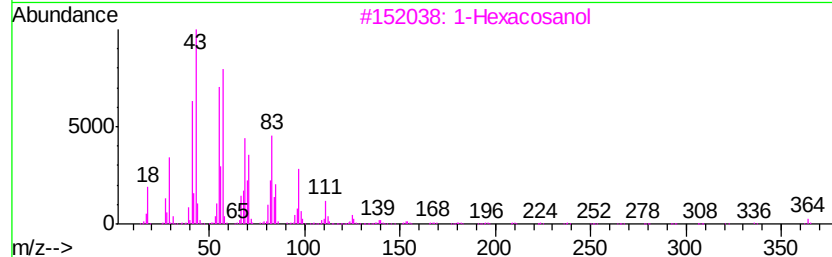
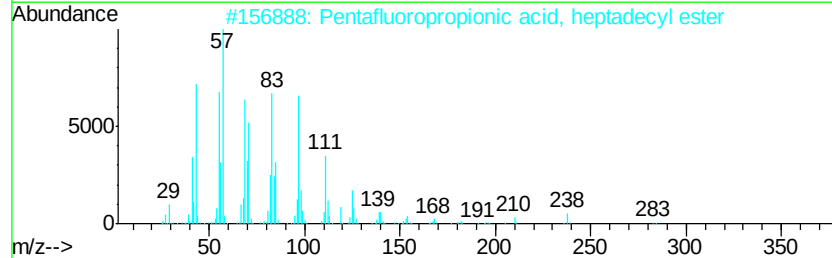
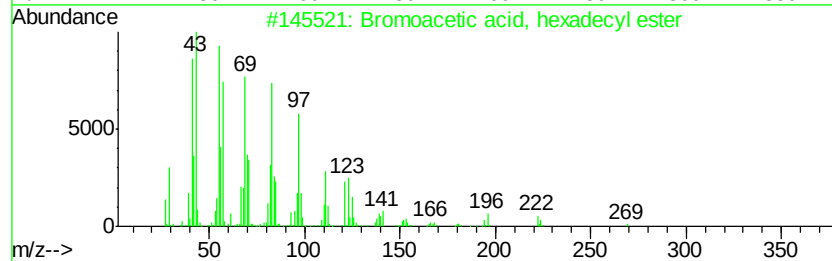
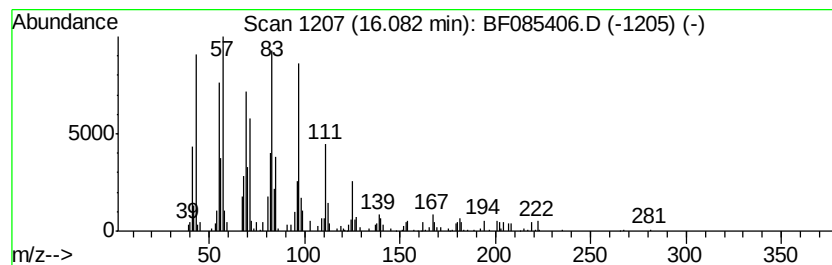
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Bromoacetic acid, hexadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	4.71 ng	156186	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	86
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	76
3		1-Hexacosanol	382	C26H54O	000506-52-5	68
4		1-Tetracosanol	354	C24H50O	000506-51-4	68
5		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
 Data File : BF085406.D
 Acq On : 12 Mar 2016 8:30
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 Sample : H1730-08
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 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...	5.14	7.2	ng	320566	1	6.94	893587	20.0
unknown6.71	6.71	102.6	ng	4584960	1	6.94	893587	20.0
Hexadecane	10.41	2.3	ng	131159	3	9.98	1130710	20.0
Eicosane	10.88	4.3	ng	203008	4	11.46	944474	20.0
n-Hexadecanoic acid	11.99	5.9	ng	277873	4	11.46	944474	20.0
Tridecanoic acid	12.78	2.9	ng	138402	4	11.46	944474	20.0
5-Eicosene, (E)-	13.95	19.8	ng	826947	5	14.11	836735	20.0
unknown14.57	14.57	2.5	ng	102492	5	14.11	836735	20.0
Benzeneethanamine...	14.86	9.7	ng	321673	6	15.57	663887	20.0
Pentadecane, 8-he...	15.21	2.2	ng	74234	6	15.57	663887	20.0
Bromoacetic acid,...	16.08	4.7	ng	156186	6	15.57	663887	20.0