

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082515\
 Data File : BF081212.D
 Acq On : 25 Aug 2015 22:10
 Operator : UM/IZ
 Sample : G3407-08 5X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P004-BF001-01

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-BF081715.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	3.864	171	173	176	rBV	3801	6067	1.14%	0.084%
2	4.619	237	239	244	rBV	211349	264489	49.73%	3.642%
3	5.099	278	281	289	rVB	255622	368333	69.26%	5.072%
4	5.522	316	318	319	rBV	4614	5771	1.09%	0.079%
5	6.184	373	376	384	rBV	253617	390789	73.48%	5.381%
6	6.299	384	386	388	rBV	318327	363653	68.38%	5.008%
7	6.527	404	406	408	rBV	512302	424133	79.75%	5.840%
8	6.687	417	420	422	rVB	204695	274174	51.55%	3.775%
9	7.099	454	456	458	rBV	203833	225717	42.44%	3.108%
10	7.579	494	498	502	rBV2	3349	5697	1.07%	0.078%
11	7.819	516	519	521	rBV	476241	531820	100.00%	7.323%
12	8.539	580	582	585	rBV	12262	20806	3.91%	0.287%
13	8.596	585	587	594	rVB2	3885	10411	1.96%	0.143%
14	8.779	598	603	606	rBV2	2716	7434	1.40%	0.102%
15	8.893	611	613	615	rBV	501778	400527	75.31%	5.515%
16	9.293	646	648	651	rVB	93223	76847	14.45%	1.058%
17	9.419	658	659	662	rVB	11742	9550	1.80%	0.132%
18	9.522	662	668	669	rBV3	3985	8133	1.53%	0.112%
19	9.556	669	671	673	rBV2	465923	511070	96.10%	7.038%
20	10.013	710	711	713	rVB	6759	5487	1.03%	0.076%
21	10.105	717	719	722	rVB2	4234	6474	1.22%	0.089%
22	10.219	726	729	732	rBV3	2449	6283	1.18%	0.087%
23	10.345	737	740	742	rBV2	147029	186259	35.02%	2.565%
24	10.482	751	752	756	rBV	11144	15808	2.97%	0.218%
25	10.608	761	763	765	rVB	6323	6919	1.30%	0.095%
26	10.734	771	774	776	rBV2	5279	7177	1.35%	0.099%
27	10.791	776	779	782	rVV2	3865	6357	1.20%	0.088%
28	10.928	789	791	793	rBV	11190	10249	1.93%	0.141%
29	11.031	797	800	801	rBV	568219	496901	93.43%	6.842%
30	11.054	801	802	804	rVV	49297	36097	6.79%	0.497%
31	11.099	804	806	811	rVB2	16515	30682	5.77%	0.422%
32	11.282	816	822	825	rBV3	9706	24421	4.59%	0.336%
33	11.351	827	828	833	rVB	9018	9849	1.85%	0.136%
34	11.454	833	837	840	rVB2	7955	14199	2.67%	0.196%

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35	11.534	840	844	845	rBV4	9309	22976	4.32%	0.316%
36	11.556	845	846	847	rVV	10152	7083	1.33%	0.098%
37	11.591	847	849	852	rVV2	58465	77933	14.65%	1.073%
38	11.636	852	853	854	rVV	15378	14774	2.78%	0.203%
39	11.671	854	856	858	rVB2	7631	11570	2.18%	0.159%
40	11.762	862	864	866	rVV	12425	14546	2.74%	0.200%
41	11.854	869	872	875	rVB4	6371	12493	2.35%	0.172%
42	12.071	890	891	893	rBV	4977	7732	1.45%	0.106%
43	12.151	896	898	899	rVV2	6077	7843	1.47%	0.108%
44	12.231	903	905	907	rBV	83970	77776	14.62%	1.071%
45	12.288	908	910	911	rBV2	12232	18475	3.47%	0.254%
46	12.368	915	917	919	rBV2	13990	21508	4.04%	0.296%
47	12.448	922	924	926	rVV	61628	71720	13.49%	0.988%
48	12.574	934	935	936	rBV	7357	7132	1.34%	0.098%
49	12.608	936	938	941	rVV	289942	276097	51.92%	3.802%
50	12.677	941	944	947	rBV4	8334	16929	3.18%	0.233%
51	12.779	949	953	956	rBV2	11137	22282	4.19%	0.307%
52	12.848	957	959	960	rBV	14879	15302	2.88%	0.211%
53	12.974	968	970	972	rBV3	8539	15537	2.92%	0.214%
54	13.328	999	1001	1002	rBV	10433	10992	2.07%	0.151%
55	13.534	1017	1019	1022	rBV2	56176	79005	14.86%	1.088%
56	13.648	1026	1029	1034	rVV	382089	529042	99.48%	7.285%
57	14.162	1071	1074	1077	rBV2	53865	99370	18.68%	1.368%
58	14.574	1108	1110	1112	rVB2	43690	54624	10.27%	0.752%
59	14.631	1112	1115	1119	rBV	56965	124198	23.35%	1.710%
60	14.757	1122	1126	1131	rVV3	67577	181985	34.22%	2.506%
61	14.871	1134	1136	1139	rVB	43250	56517	10.63%	0.778%
62	14.928	1139	1141	1143	rBV	45929	68945	12.96%	0.949%
63	14.974	1143	1145	1148	rBV	232792	333987	62.80%	4.599%
64	15.203	1163	1165	1168	rBV	44672	47874	9.00%	0.659%
65	15.385	1179	1181	1184	rBV	29847	49260	9.26%	0.678%
66	16.288	1257	1260	1263	rVB3	81562	137964	25.94%	1.900%

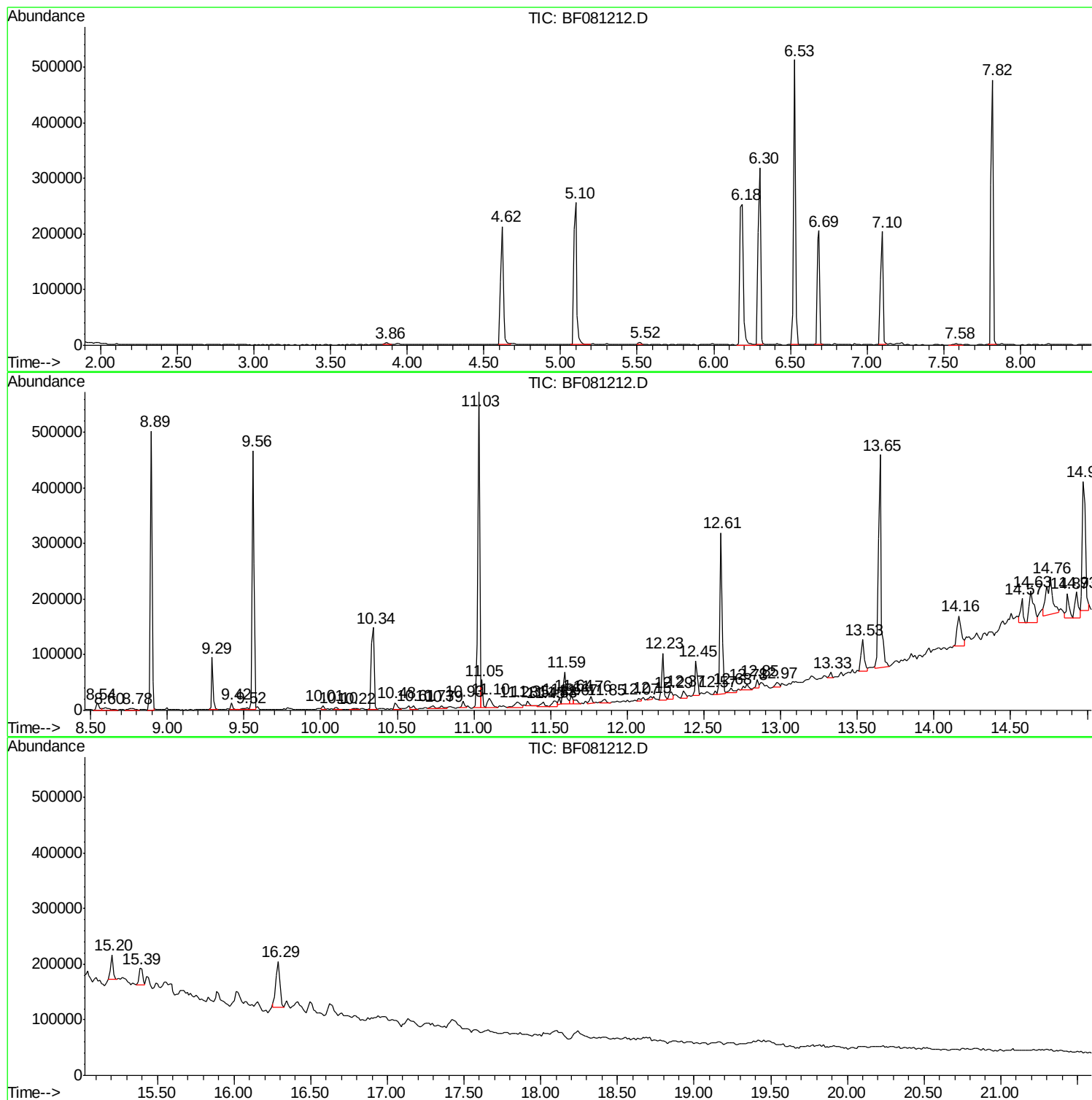
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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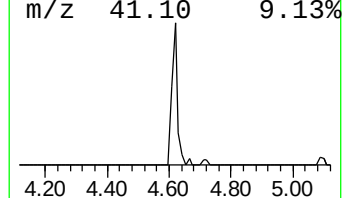
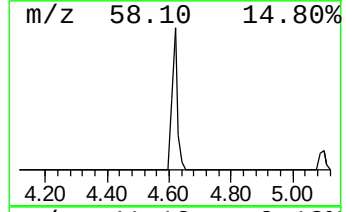
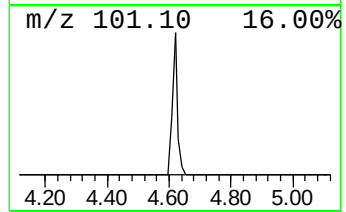
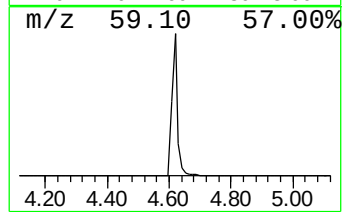
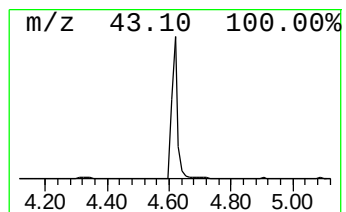
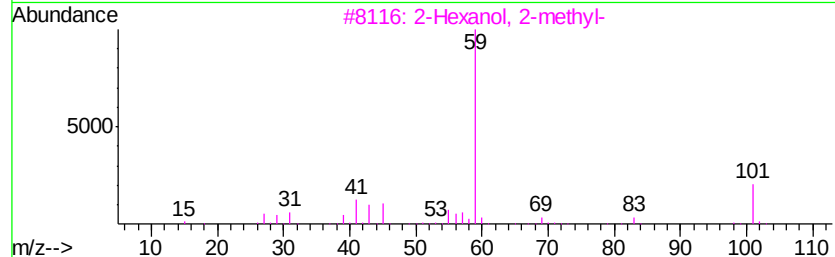
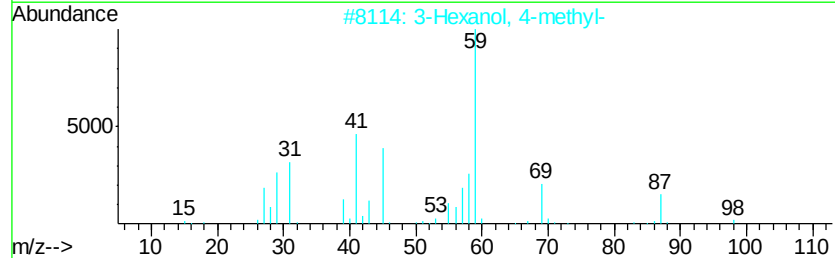
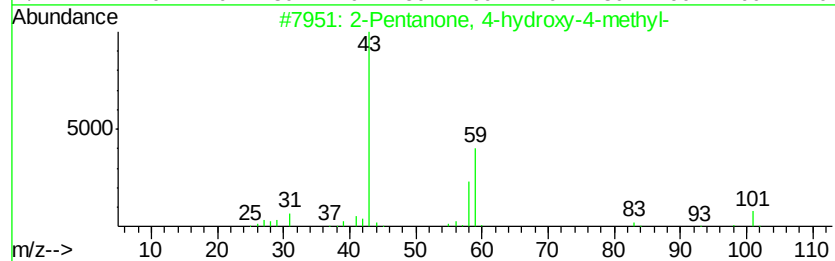
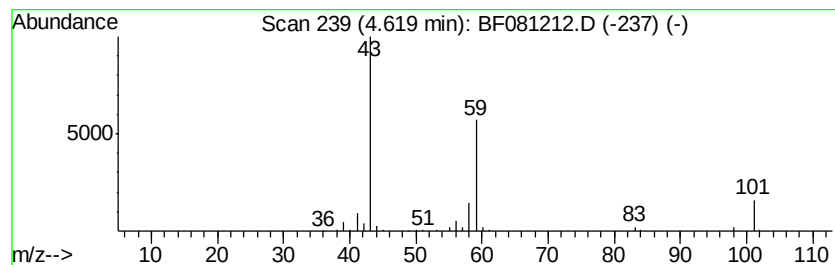
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.62	12.47 ng	264489	1,4-Dichlorobenzene-d4	6.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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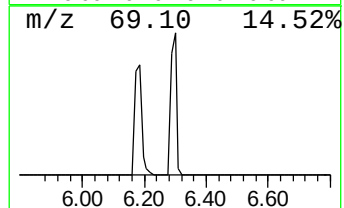
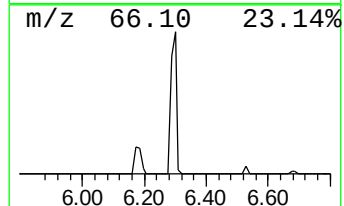
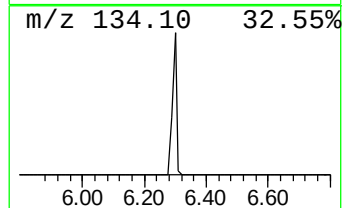
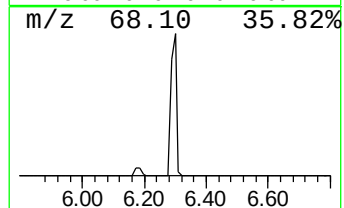
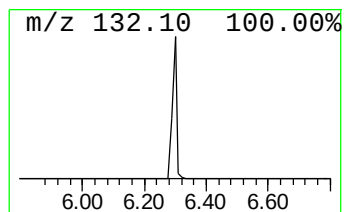
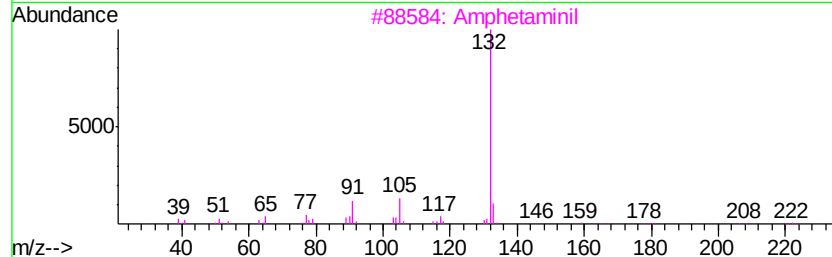
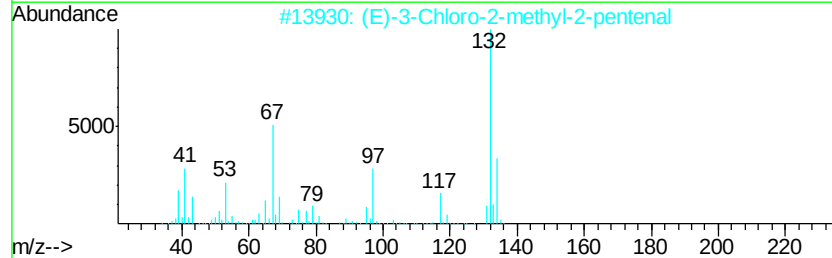
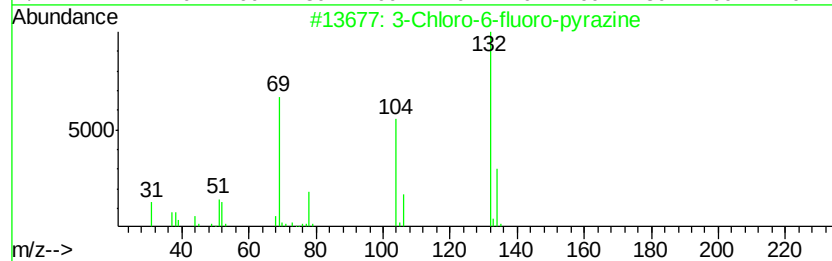
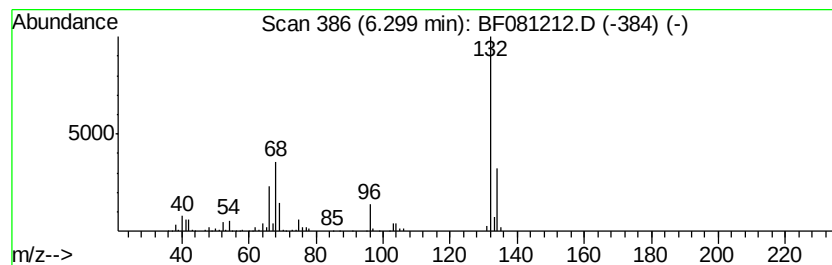
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.30	17.15 ng	363653	1,4-Dichlorobenzene-d4	6.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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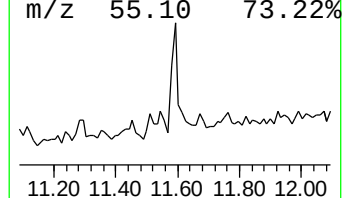
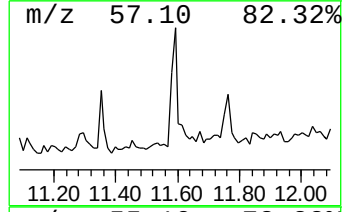
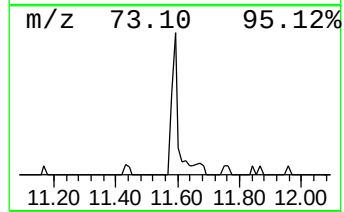
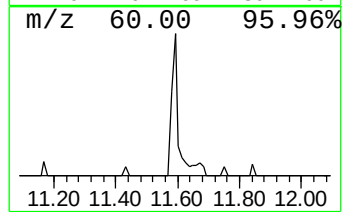
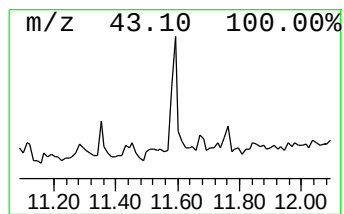
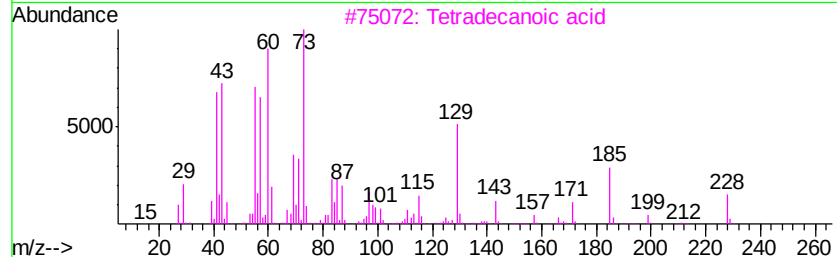
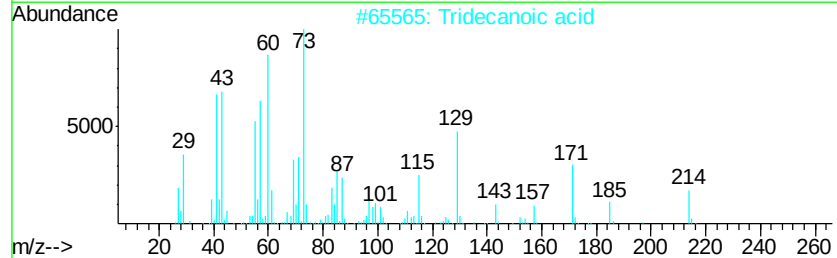
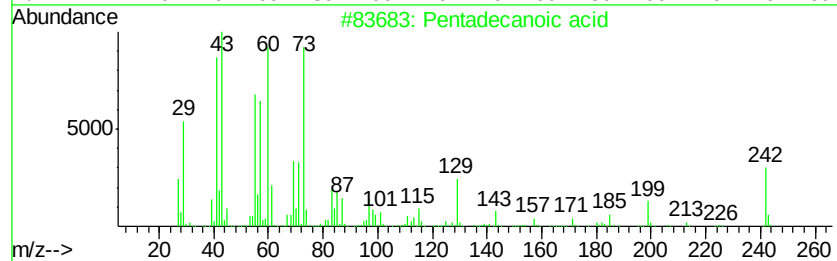
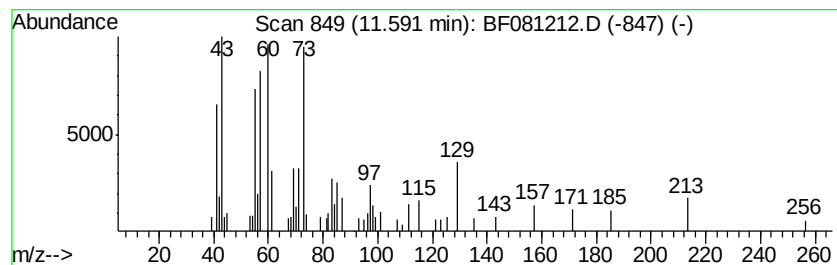
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	3.14 ng	77933	Phenanthrene-d10	11.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2		Tridecanoic acid	214	C13H26O2	000638-53-9	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Dodecanoic acid	200	C12H24O2	000143-07-7	64
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



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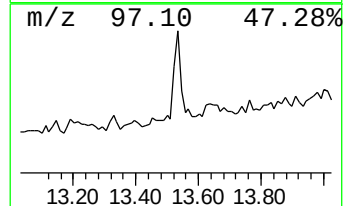
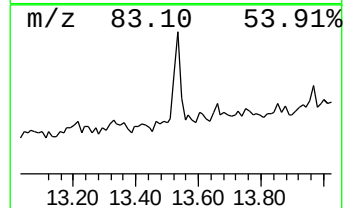
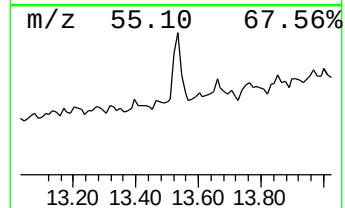
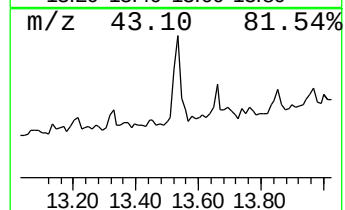
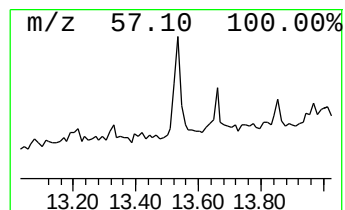
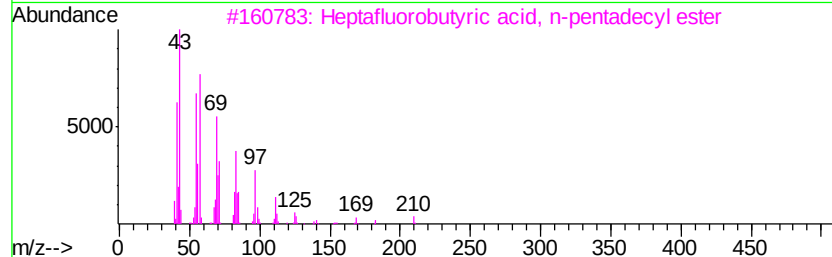
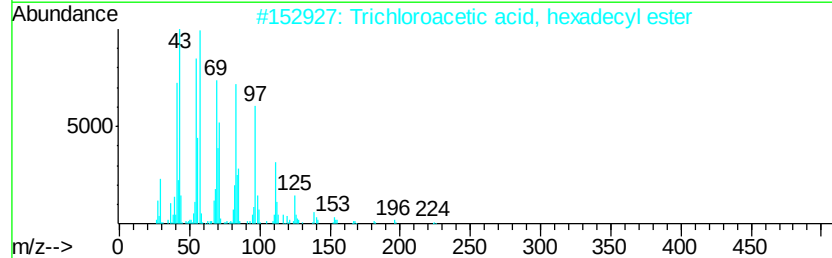
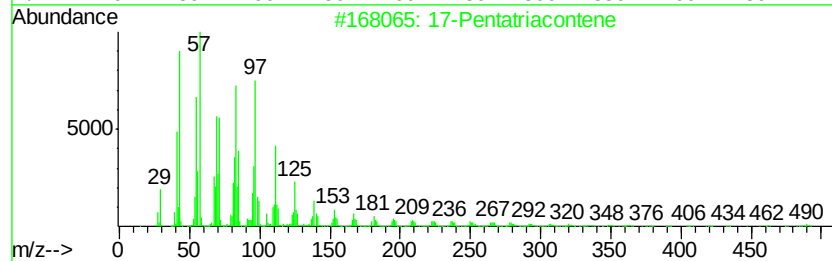
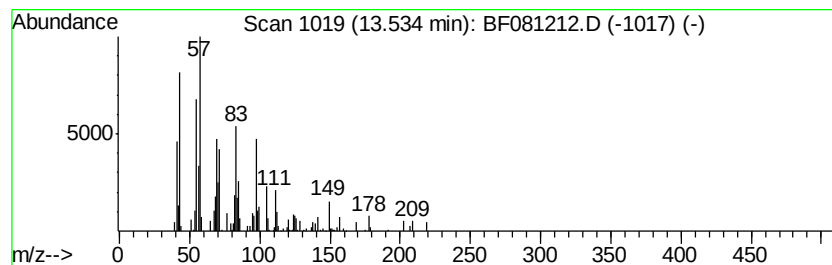
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 17-Pentatriacontene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.99 ng	79005	Chrysene-d12	13.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	83
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76
3		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	70
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	70
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	68



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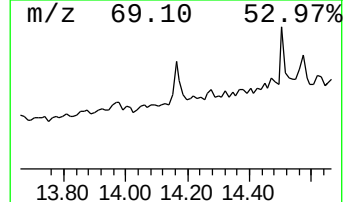
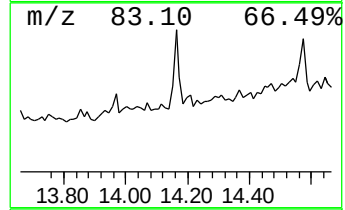
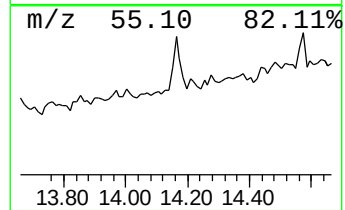
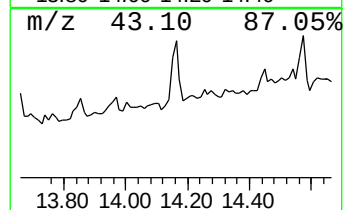
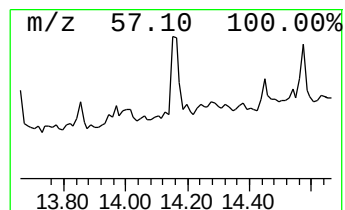
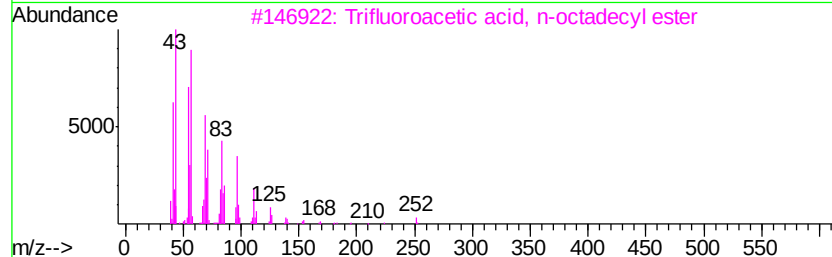
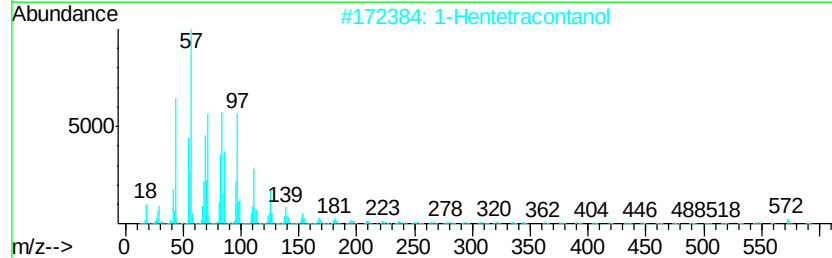
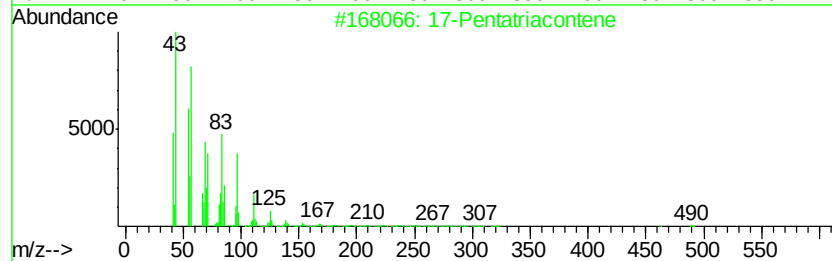
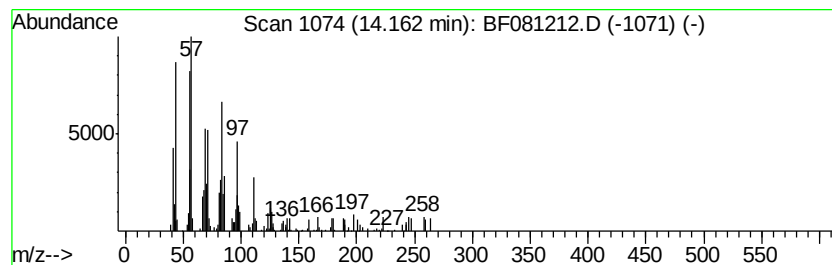
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BNA_F
ClientSampleId :
P004-BF001-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hentetracontanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	3.76 ng	99370	Chrysene-d12	13.65
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	17-Pentatriacontene	491 C35H70	006971-40-0	91
2	1-Hentetracontanol	593 C41H84O	040710-42-7	83
3	Trifluoroacetic acid, n-octadecy...	366 C20H37F3O2	079392-43-1	83
4	Cyclopentane, (4-octyldodecyl)-	350 C25H50	005638-09-5	83
5	Pentafluoropropionic acid, hepta...	402 C20H35F5O2	1000283-04-2	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082515\
Data File : BF081212.D
Acq On : 25 Aug 2015 22:10
Operator : UM/IZ
Sample : G3407-08 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

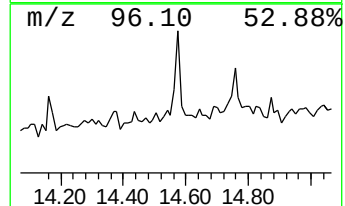
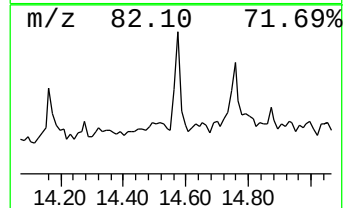
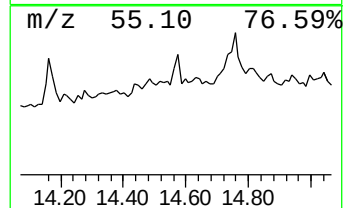
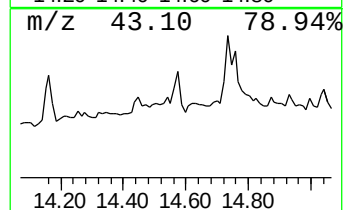
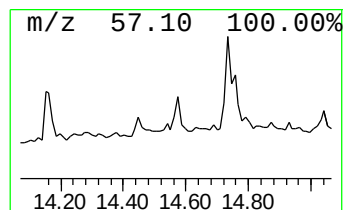
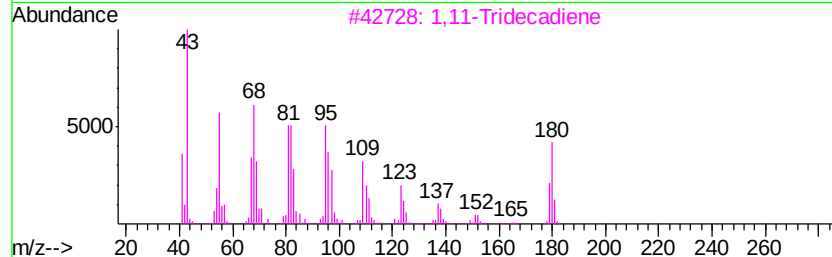
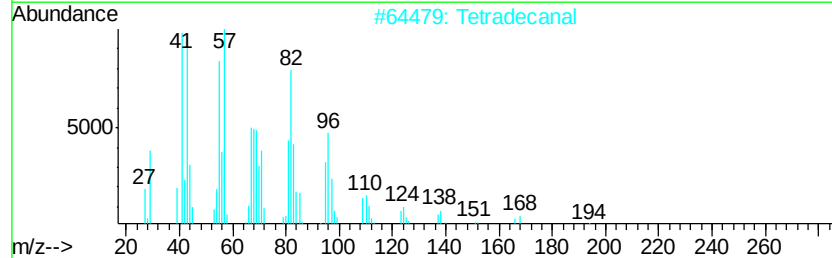
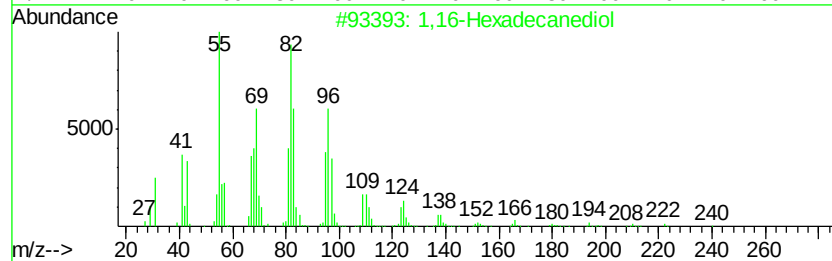
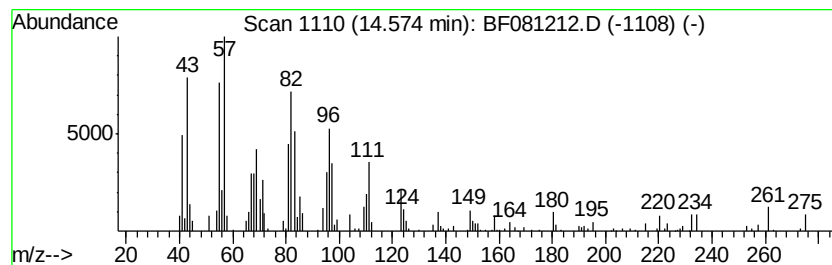
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,16-Hexadecanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.27 ng	54624	Perylene-d12	14.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,16-Hexadecanediol	258 C16H34O2	007735-42-4	68
2	Tetradecanal	212 C14H28O	000124-25-4	59
3	1,11-Tridecadiene	180 C13H24	1000130-76-4	50
4	8-Azabicyclo[3.2.1]octan-3-ol, 8...	141 C8H15NO	000120-29-6	47
5	Octadecanal	268 C18H36O	000638-66-4	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082515\
Data File : BF081212.D
Acq On : 25 Aug 2015 22:10
Operator : UM/IZ
Sample : G3407-08 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

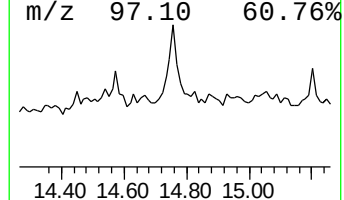
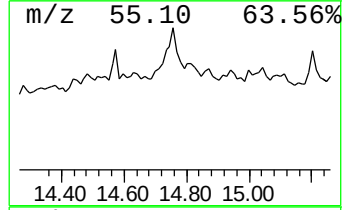
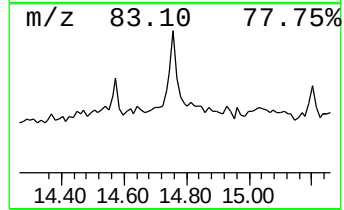
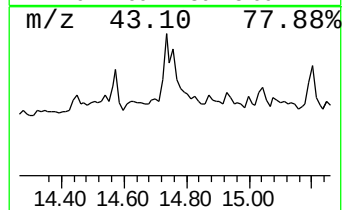
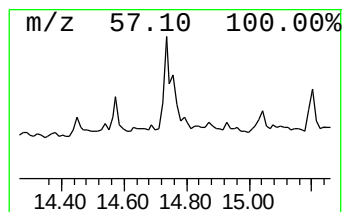
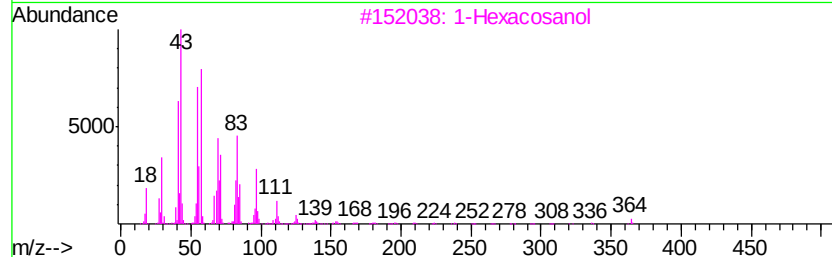
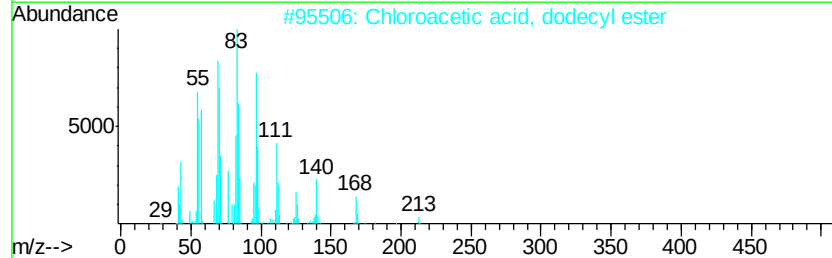
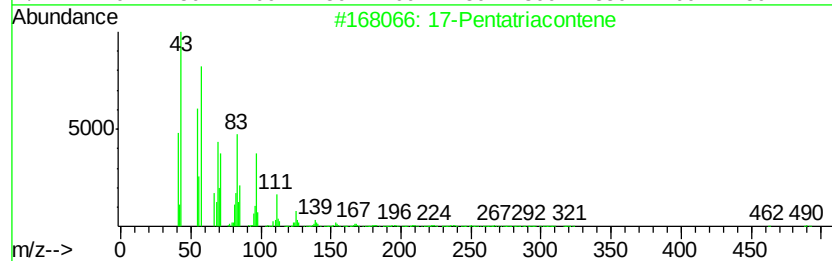
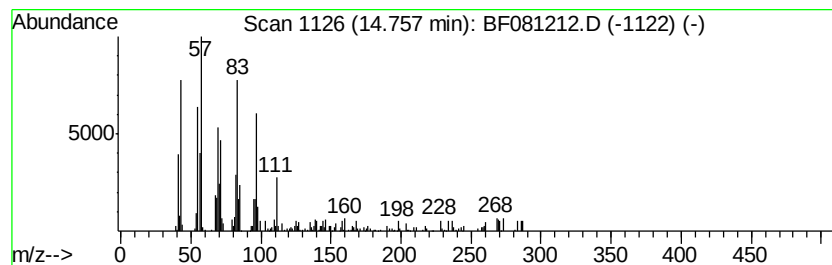
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Chloroacetic acid, dodecyl ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.76	10.90 ng	181985	Perylene-d12	14.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene		491	C35H70	006971-40-0	83
2	Chloroacetic acid, dodecyl ester		262	C14H27ClO2	006316-04-7	64
3	1-Hexacosanol		382	C26H54O	000506-52-5	52
4	Acetic acid, octadecyl ester		312	C20H40O2	000822-23-1	43
5	1-Octadecanol		270	C18H38O	000112-92-5	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082515\
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Acq On : 25 Aug 2015 22:10
Operator : UM/IZ
Sample : G3407-08 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

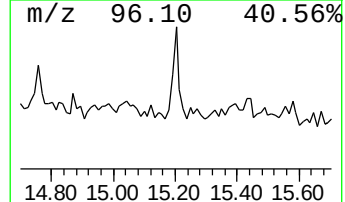
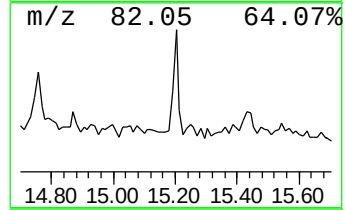
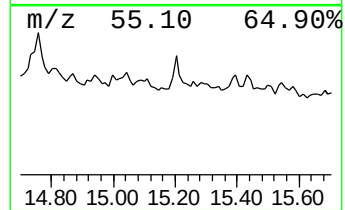
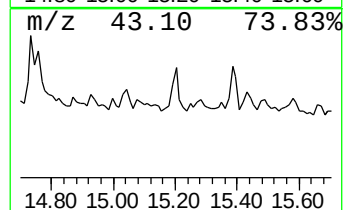
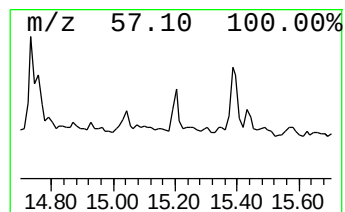
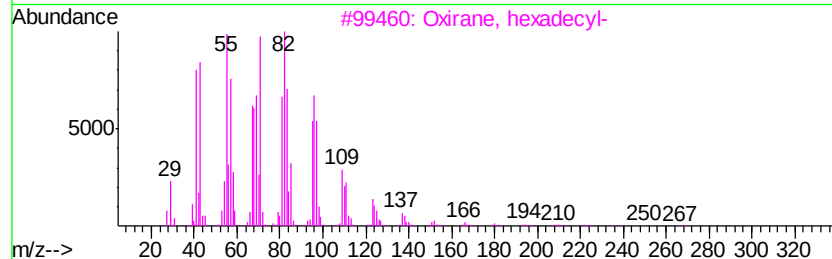
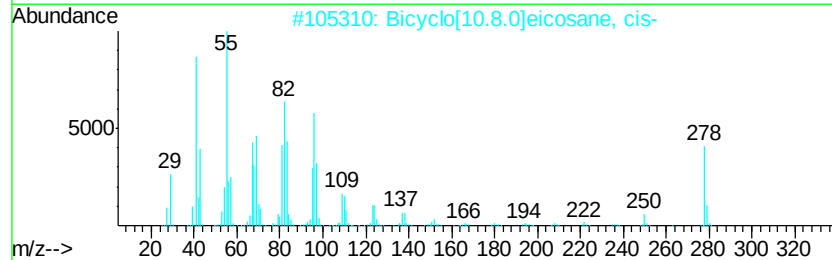
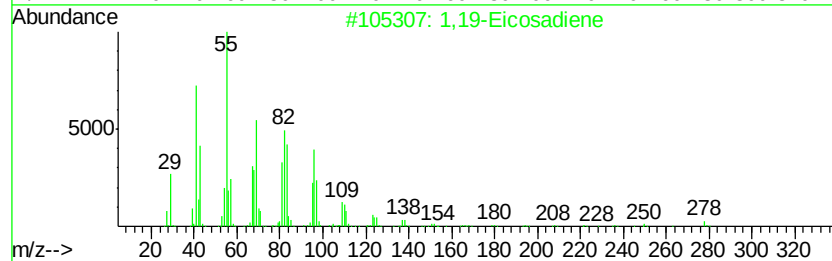
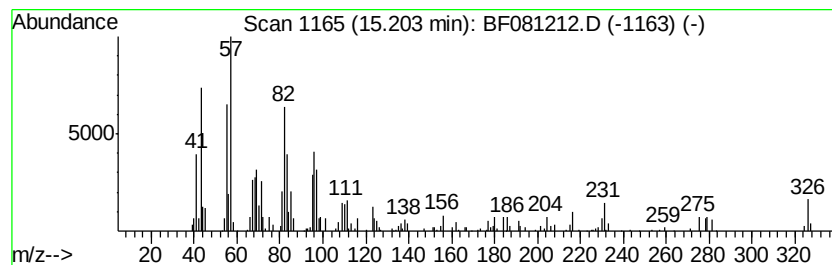
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,19-Eicosadiene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.20	2.87 ng	47874	Perylene-d12	14.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	89
2	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	89
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
4	Tetradecanal	212	C14H28O	000124-25-4	80
5	Octadecanal	268	C18H36O	000638-66-4	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082515\
Data File : BF081212.D
Acq On : 25 Aug 2015 22:10
Operator : UM/IZ
Sample : G3407-08 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-BF001-01

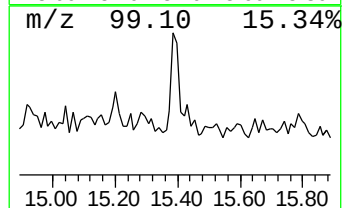
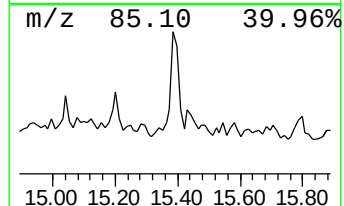
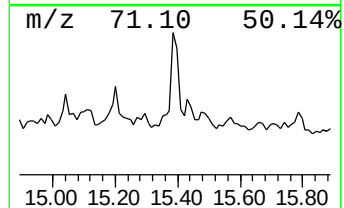
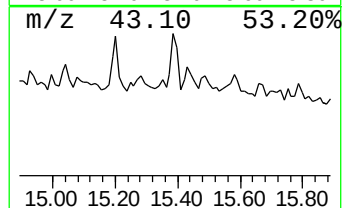
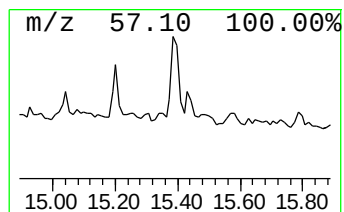
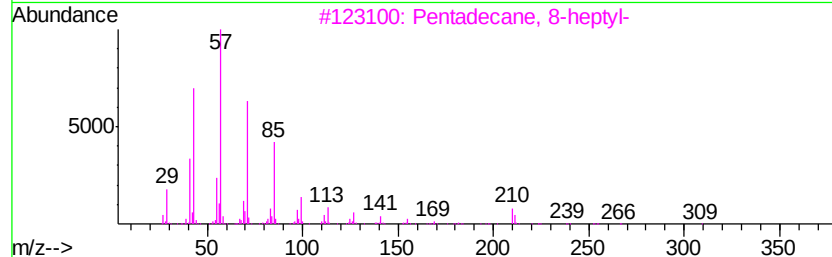
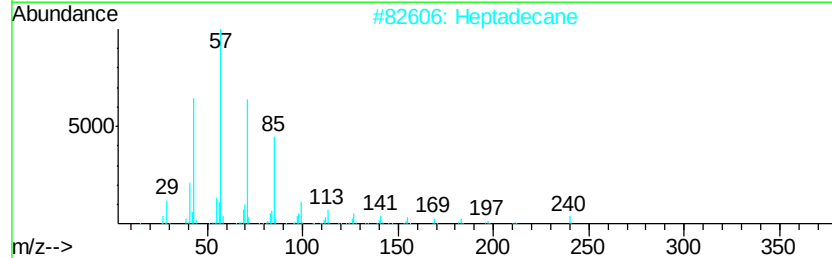
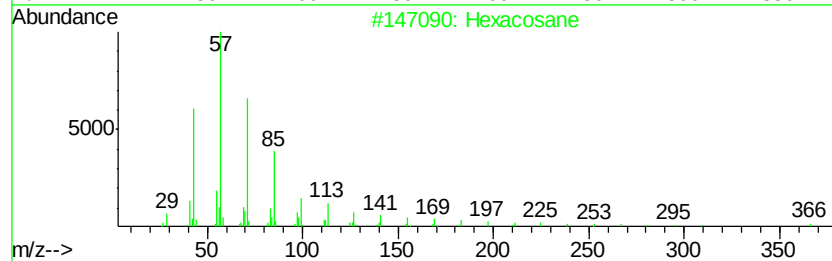
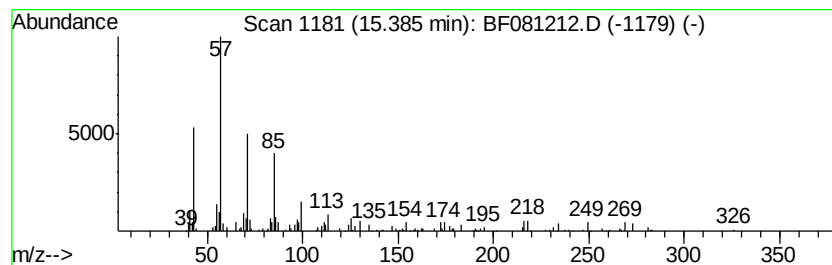
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	2.95 ng	49260	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	72
2		Heptadecane	240	C17H36	000629-78-7	72
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	64
4		Heneicosane	296	C21H44	000629-94-7	64
5		Octadecane	254	C18H38	000593-45-3	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082515\
Data File : BF081212.D
Acq On : 25 Aug 2015 22:10
Operator : UM/IZ
Sample : G3407-08 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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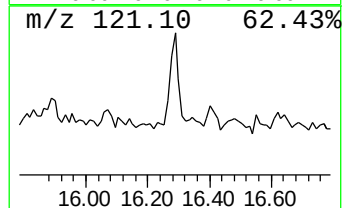
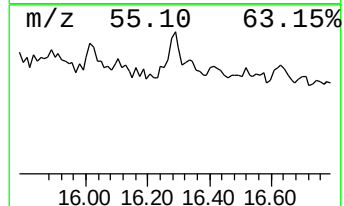
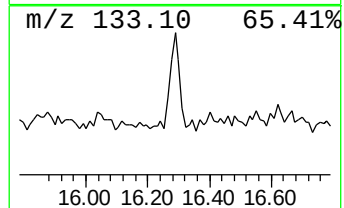
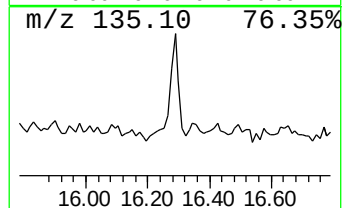
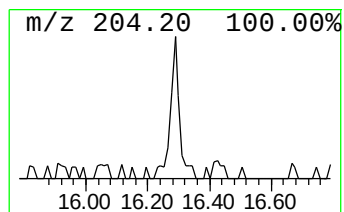
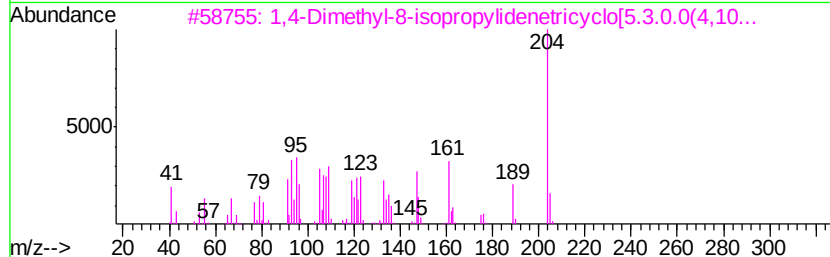
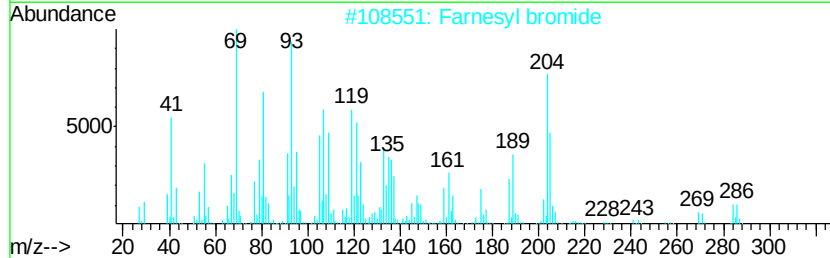
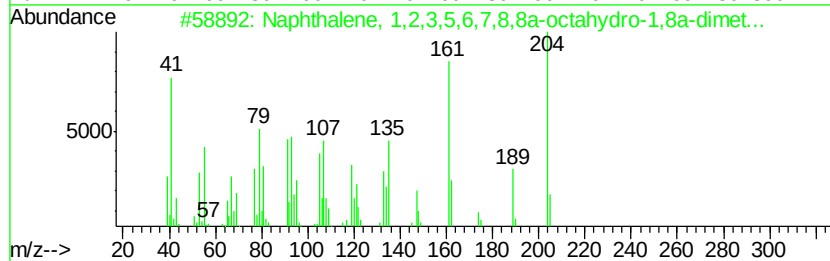
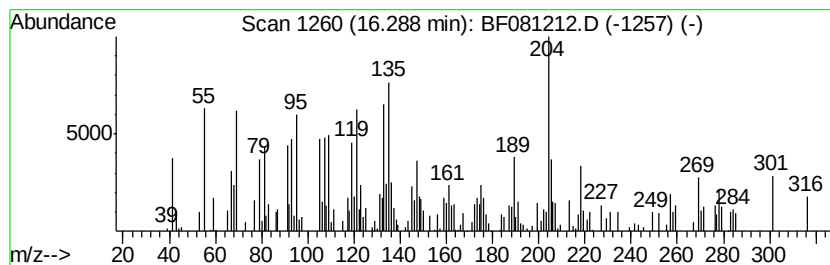
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	8.26 ng	137964	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	58
2		Farnesyl bromide	284	C15H25Br	006874-67-5	53
3		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	49
4		3-Cyclohexene-1-methanol, .alpha...	222	C15H26O	023178-88-3	46
5		1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082515\
Data File : BF081212.D
Acq On : 25 Aug 2015 22:10
Operator : UM/IZ
Sample : G3407-08 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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...	4.62	12.5	ng	264489	1	6.53	424133	20.0
unknown6.30	6.30	17.1	ng	363653	1	6.53	424133	20.0
Pentadecanoic acid	11.59	3.1	ng	77933	4	11.03	496901	20.0
17-Pentatriacontene	13.53	3.0	ng	79005	5	13.65	529042	20.0
1-Hentetracontanol	14.16	3.8	ng	99370	5	13.65	529042	20.0
1,16-Hexadecanediol	14.57	3.3	ng	54624	6	14.97	333987	20.0
Chloroacetic acid...	14.76	10.9	ng	181985	6	14.97	333987	20.0
1,19-Eicosadiene	15.20	2.9	ng	47874	6	14.97	333987	20.0
Hexacosane	15.39	3.0	ng	49260	6	14.97	333987	20.0
Naphthalene, 1,2,...	16.29	8.3	ng	137964	6	14.97	333987	20.0