

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110515\
 Data File : BF082714.D
 Acq On : 4 Nov 2015 21:38
 Operator : UM/IZ
 Sample : G4241-09
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-13(10-12)

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-BF103015.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	5.059	256	260	267	rVB	1933091	2971774	42.31%	4.702%
2	5.470	293	296	299	rBV	4103797	6134023	87.33%	9.705%
3	6.499	383	386	388	rBV	5036694	5693287	81.06%	9.007%
4	6.636	395	398	400	rBV	6162024	6603090	94.01%	10.447%
5	6.864	415	418	420	rBV	1302598	1178331	16.78%	1.864%
6	7.024	429	432	434	rVB	4797545	4865564	69.27%	7.698%
7	7.425	464	467	469	rBV	3332879	3745703	53.33%	5.926%
8	8.145	528	530	533	rBV	1419870	1480920	21.09%	2.343%
9	9.105	611	614	616	rBV	90980	81295	1.16%	0.129%
10	9.230	622	625	627	rBV	7073662	7023569	100.00%	11.112%
11	9.619	656	659	661	rBV	1505175	1319874	18.79%	2.088%
12	9.848	677	679	681	rVB	90385	71241	1.01%	0.113%
13	9.905	681	684	686	rBV	1962281	1893428	26.96%	2.996%
14	10.316	717	720	721	rBV2	83930	114850	1.64%	0.182%
15	10.351	721	723	724	rVB	139204	144580	2.06%	0.229%
16	10.568	739	742	745	rBV	116113	157317	2.24%	0.249%
17	10.693	750	753	755	rVV	4587663	4982490	70.94%	7.883%
18	10.819	762	764	768	rVB	262415	354533	5.05%	0.561%
19	11.265	801	803	805	rBV	239023	215432	3.07%	0.341%
20	11.299	805	806	809	rVB	106388	87725	1.25%	0.139%
21	11.379	811	813	816	rVV	1490302	1695770	24.14%	2.683%
22	11.448	816	819	821	rVB2	37193	70753	1.01%	0.112%
23	11.688	838	840	843	rVB	125584	158623	2.26%	0.251%
24	11.928	858	861	862	rBV	384354	435725	6.20%	0.689%
25	12.099	874	876	878	rVB	154605	125636	1.79%	0.199%
26	12.488	909	910	912	rVB	120987	90484	1.29%	0.143%
27	12.705	927	929	935	rVV	128871	147110	2.09%	0.233%
28	12.808	935	938	939	rVB	70004	82995	1.18%	0.131%
29	12.865	941	943	950	rBV	75896	76780	1.09%	0.121%
30	12.979	950	953	955	rVB	5831097	6773485	96.44%	10.716%
31	13.219	972	974	975	rVB	83420	85941	1.22%	0.136%
32	13.459	991	995	998	rVB	138595	230486	3.28%	0.365%
33	13.562	1002	1004	1005	rVB	71442	73327	1.04%	0.116%
34	13.871	1029	1031	1041	rBV2	377242	554755	7.90%	0.878%

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ClientSampleId :
SB-13(10-12)

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-BF103015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.019	1041	1044	1046	rBV	1911012	1776932	25.30%	2.811%
36	14.202	1058	1060	1062	rBV	102729	94016	1.34%	0.149%
37	14.511	1085	1087	1089	rBV	109940	120540	1.72%	0.191%
38	14.877	1117	1119	1122	rVB	146462	200810	2.86%	0.318%
39	15.140	1139	1142	1144	rBV	64214	80974	1.15%	0.128%
40	15.448	1166	1169	1172	rBV	1049648	1213631	17.28%	1.920%

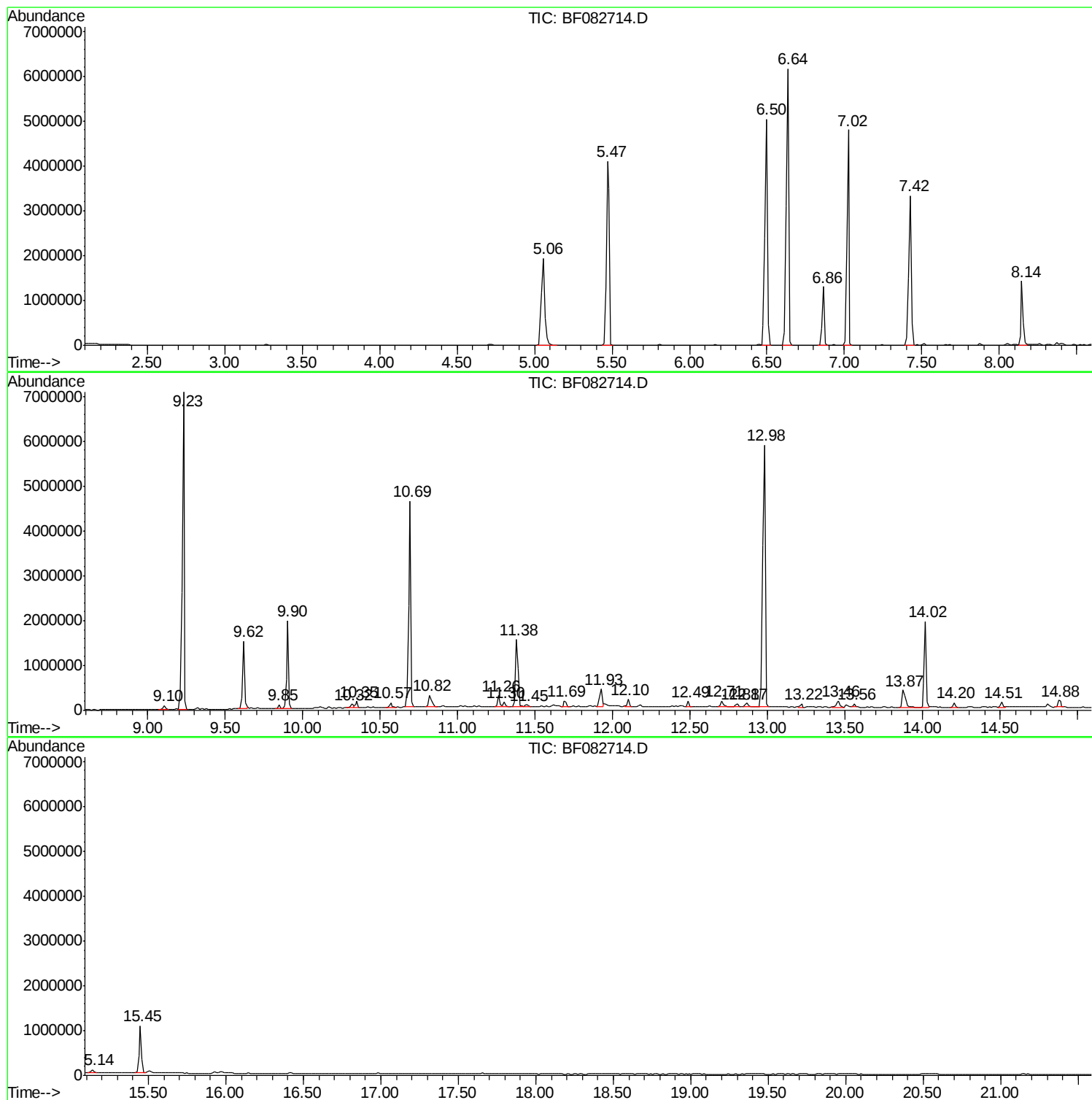
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : UM/IZ
Sample : G4241-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SB-13(10-12)

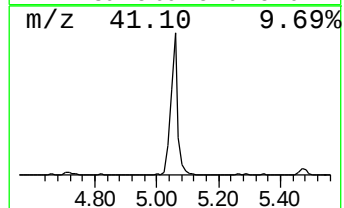
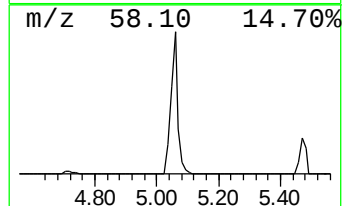
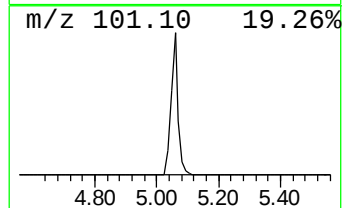
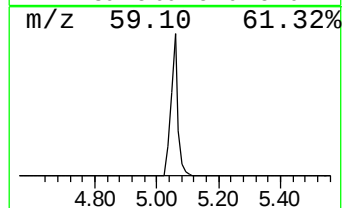
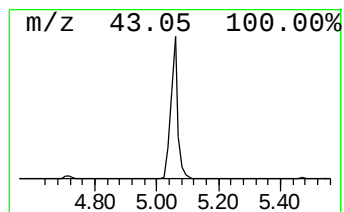
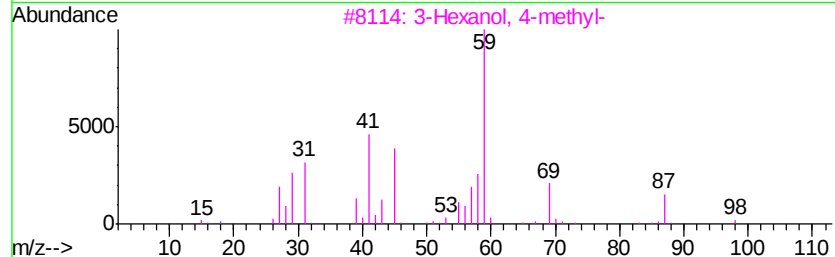
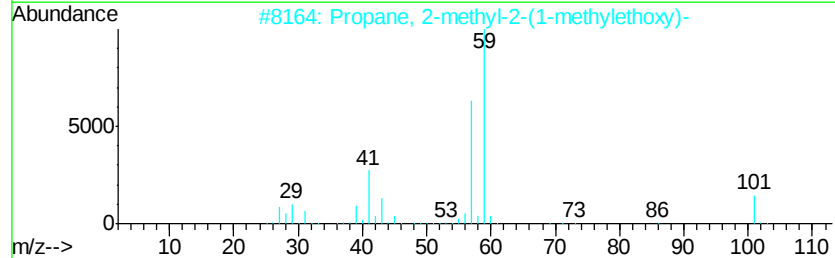
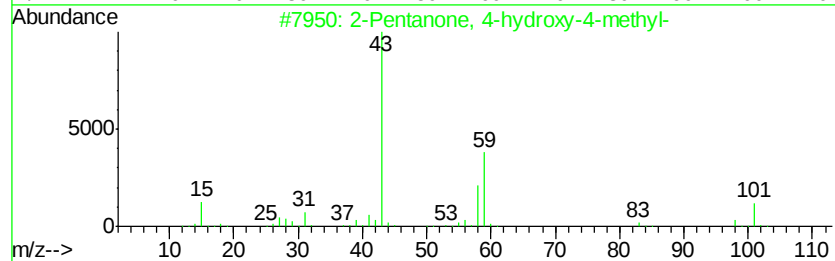
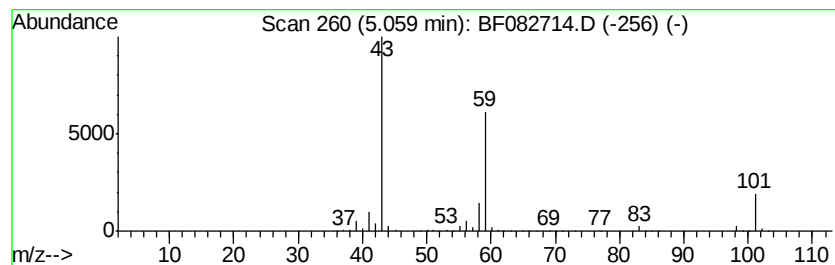
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.06	50.44 ng	2971770	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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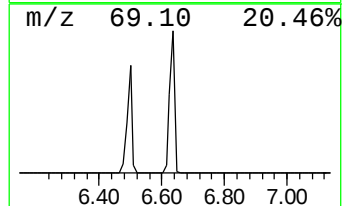
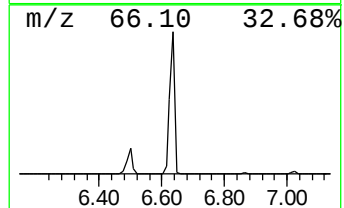
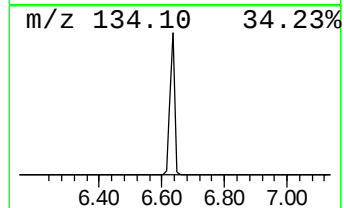
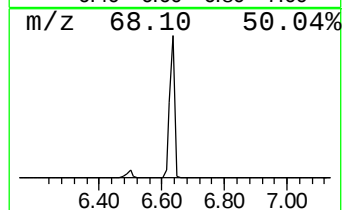
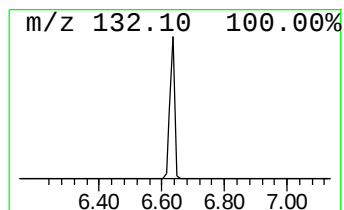
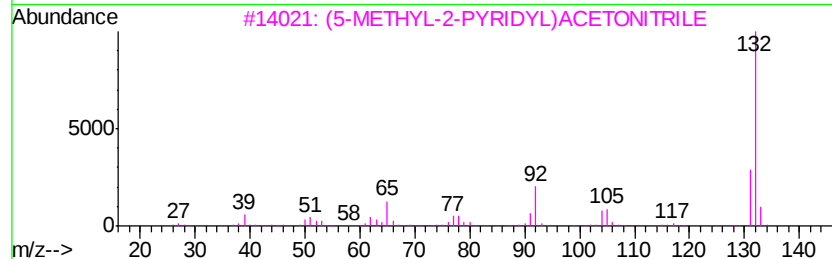
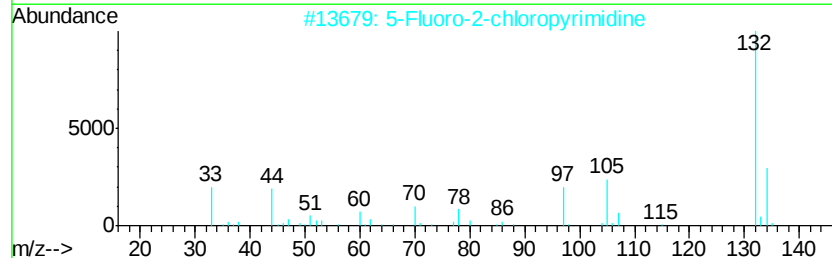
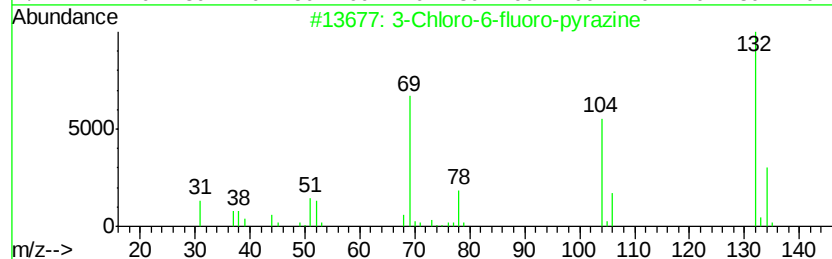
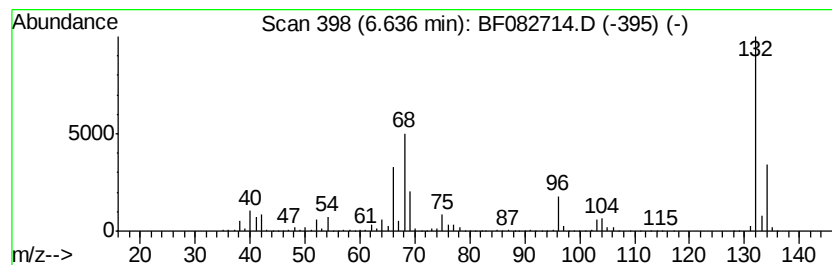
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	112.08 ng	6603090	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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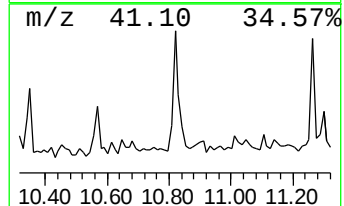
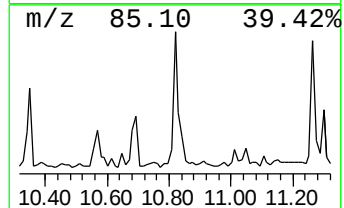
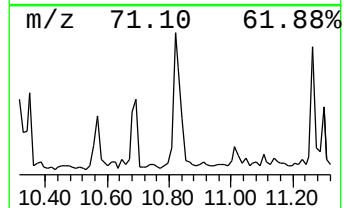
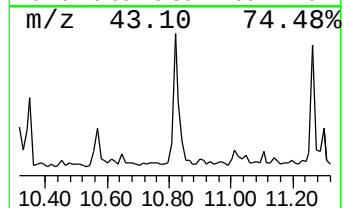
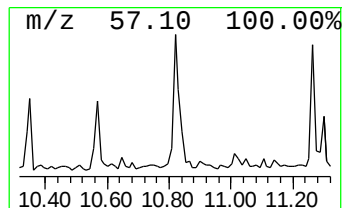
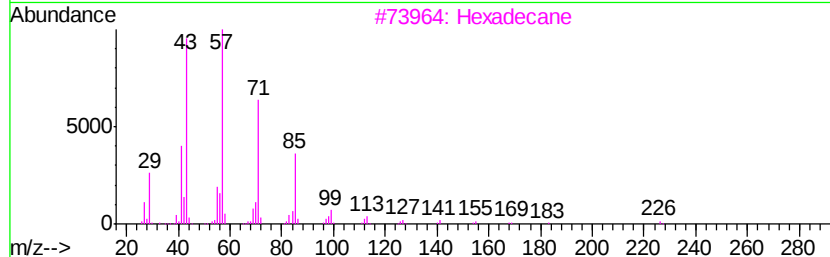
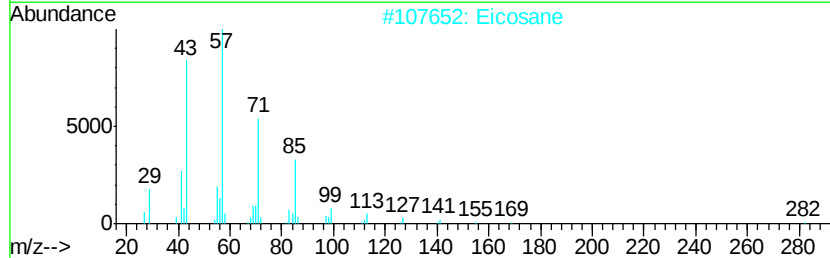
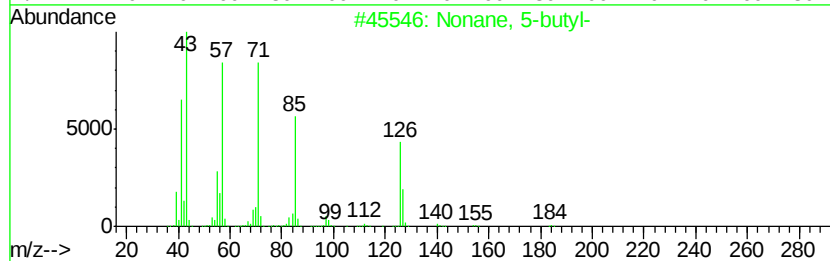
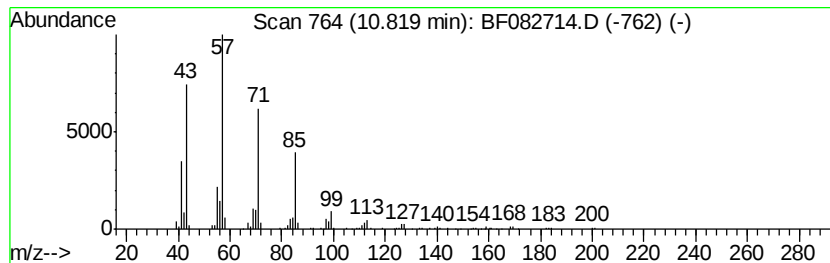
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nonane, 5-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	4.18 ng	354533	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 5-butyl-	184	C13H28	017312-63-9	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Hexadecane	226	C16H34	000544-76-3	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Tetradecane	198	C14H30	000629-59-4	86



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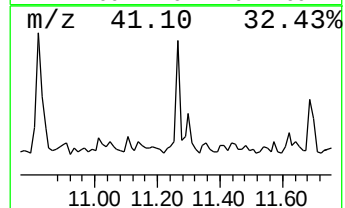
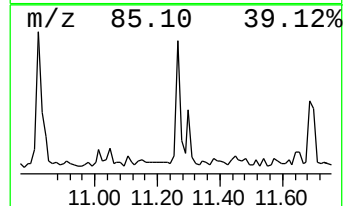
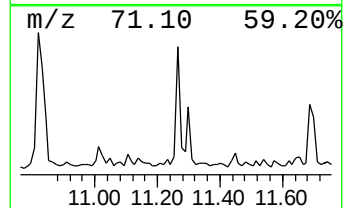
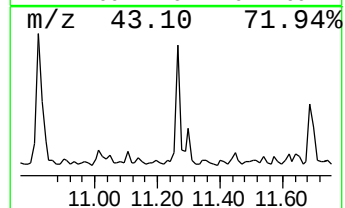
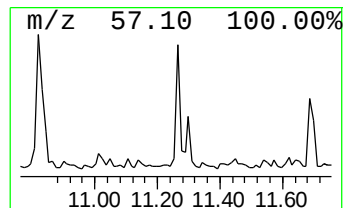
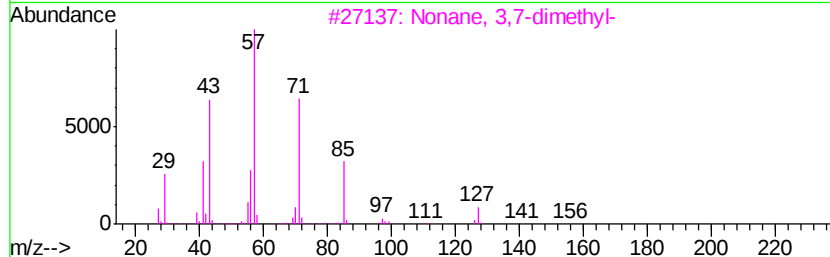
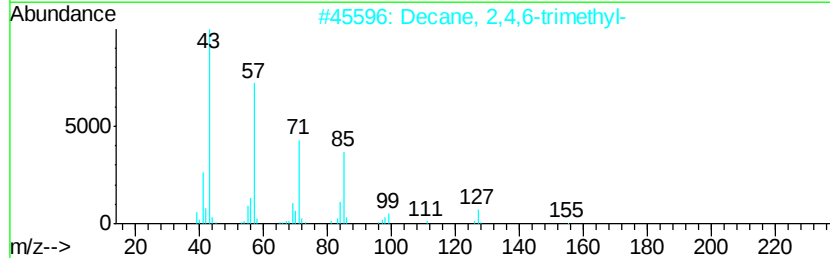
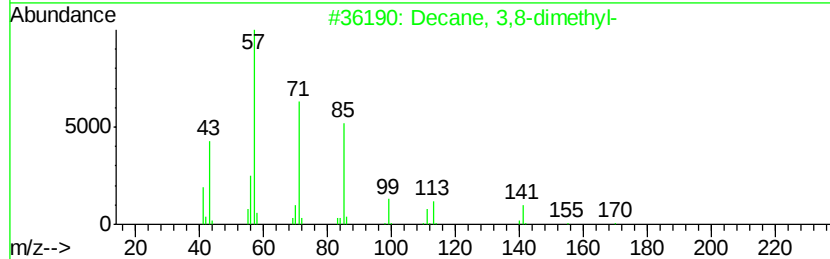
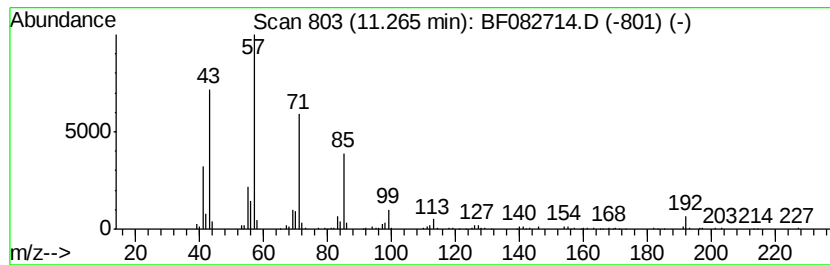
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Decane, 3,8-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.54 ng	215432	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	90
2	Decane, 2,4,6-trimethyl-		184	C13H28	062108-27-4	86
3	Nonane, 3,7-dimethyl-		156	C11H24	017302-32-8	74
4	Dodecane		170	C12H26	000112-40-3	72
5	Hexadecane		226	C16H34	000544-76-3	72



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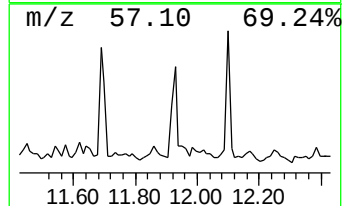
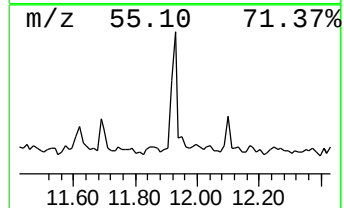
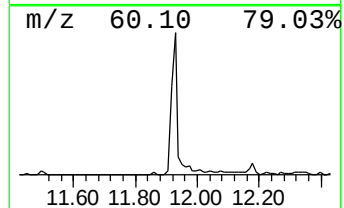
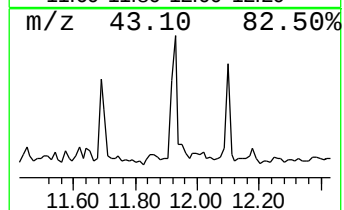
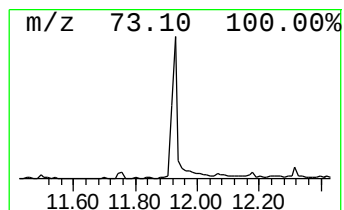
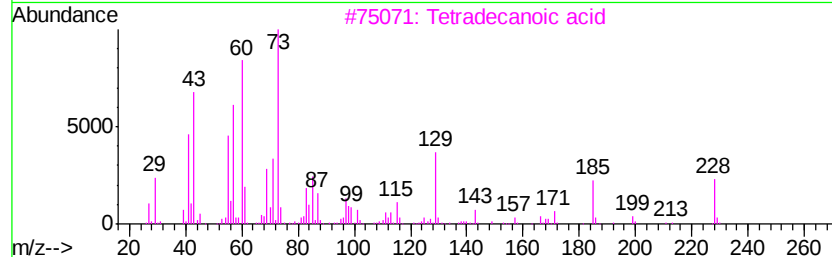
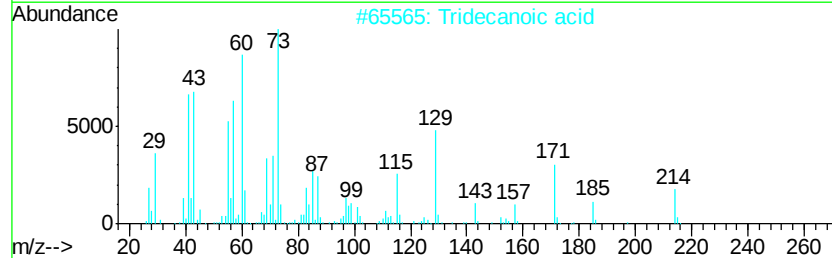
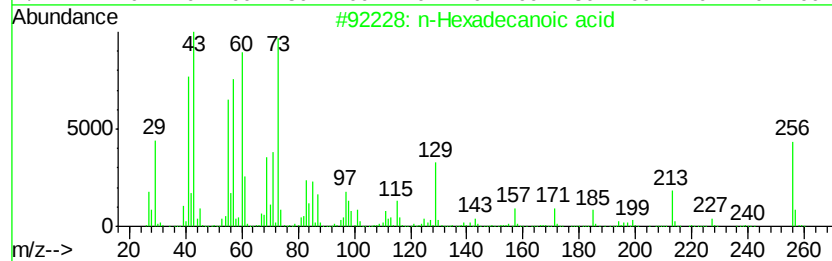
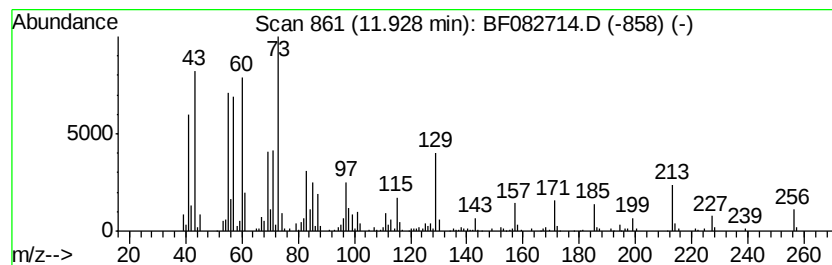
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.93	5.14 ng	435725	Phenanthrene-d10		11.38
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110515\
Data File : BF082714.D
Acq On : 4 Nov 2015 21:38
Operator : UM/IZ
Sample : G4241-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13(10-12)

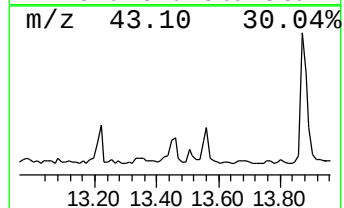
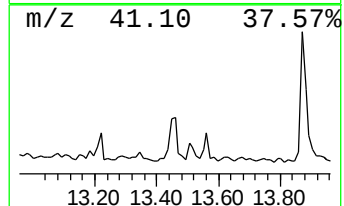
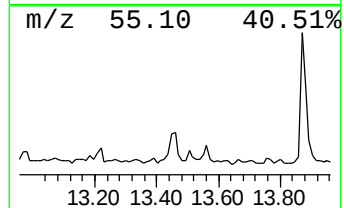
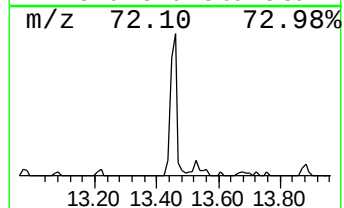
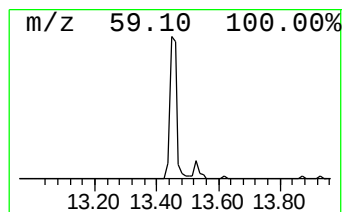
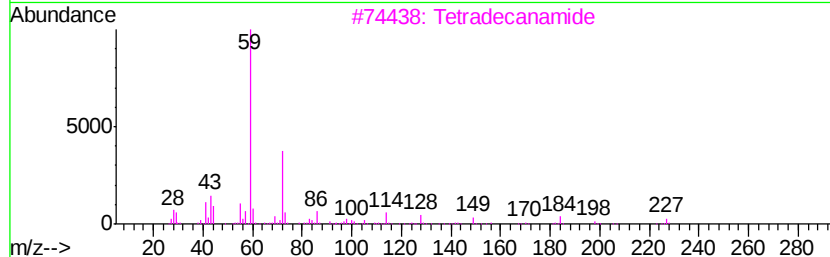
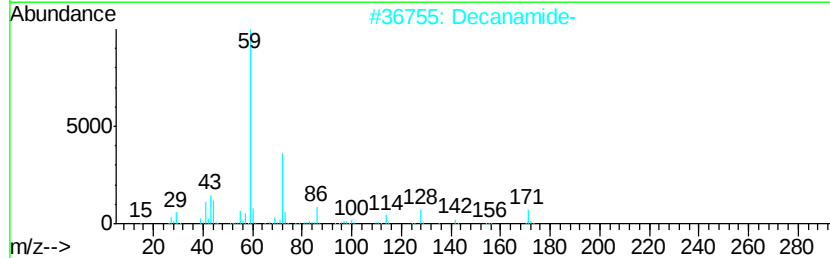
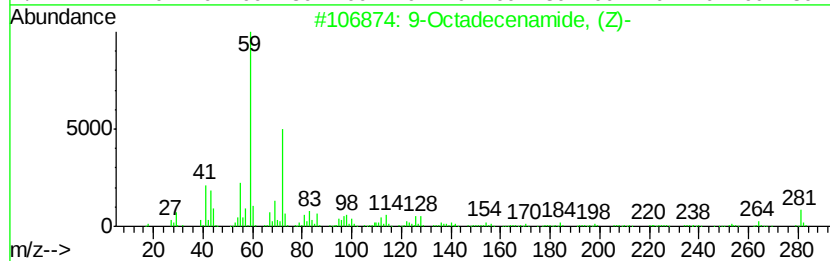
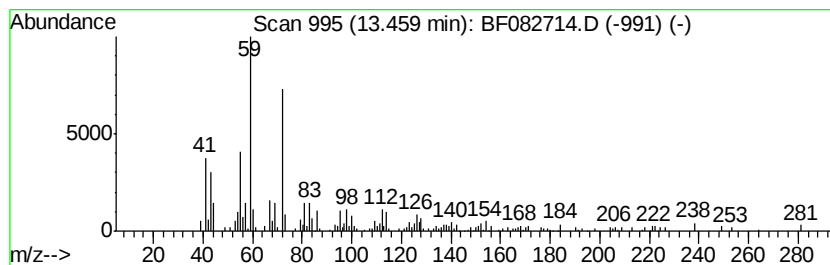
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.59 ng	230486	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Decanamide-	171	C10H21NO	002319-29-1	59
3		Tetradecanamide	227	C14H29NO	000638-58-4	53
4		Hexadecanamide	255	C16H33NO	000629-54-9	50
5		Dodecanamide	199	C12H25NO	001120-16-7	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110515\
Data File : BF082714.D
Acq On : 4 Nov 2015 21:38
Operator : UM/IZ
Sample : G4241-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

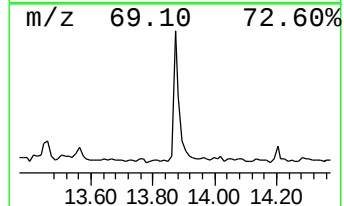
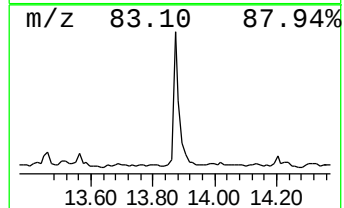
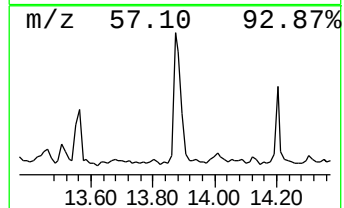
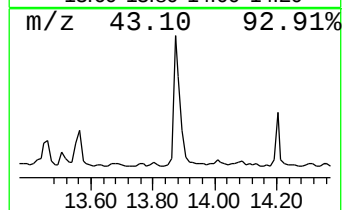
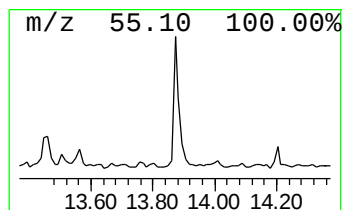
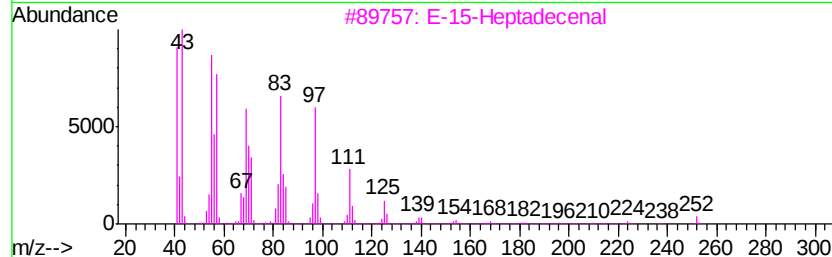
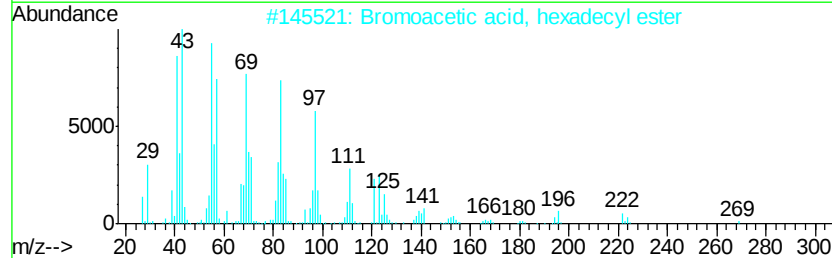
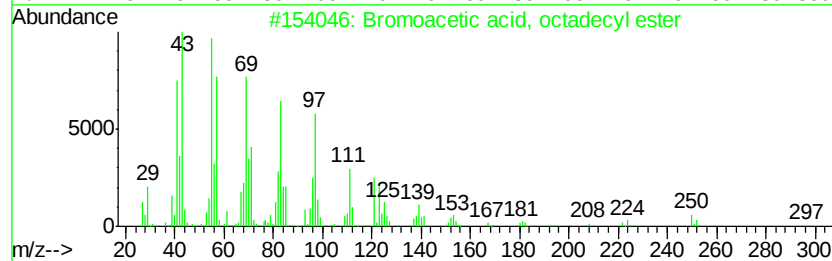
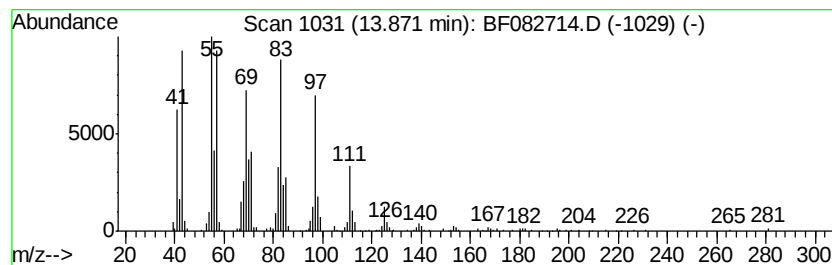
Instrument :
BNA_F
ClientSampleId :
SB-13(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.87	6.24 ng	554755	Chrysene-d12	14.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3		E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110515\
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Acq On : 4 Nov 2015 21:38
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Sample : G4241-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

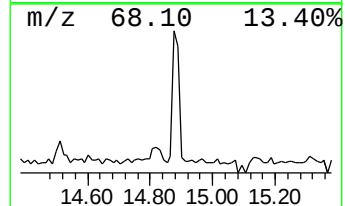
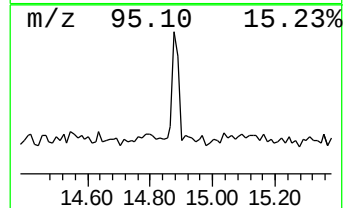
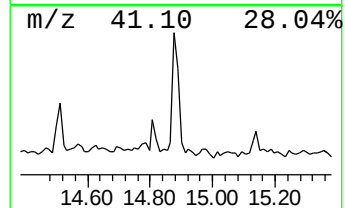
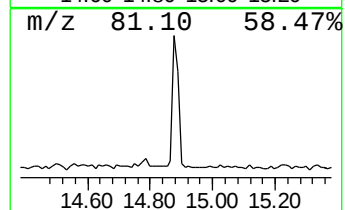
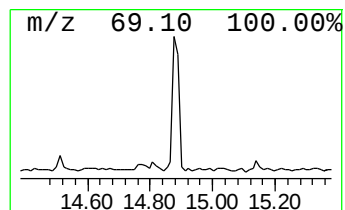
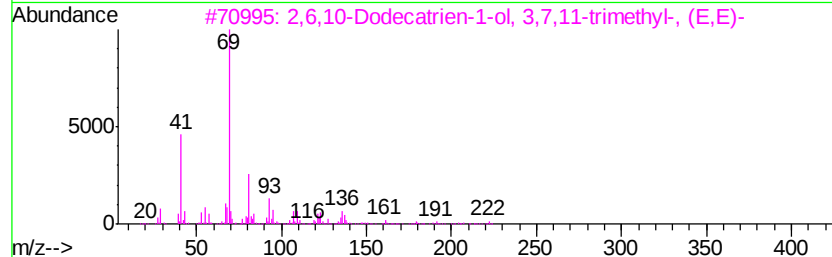
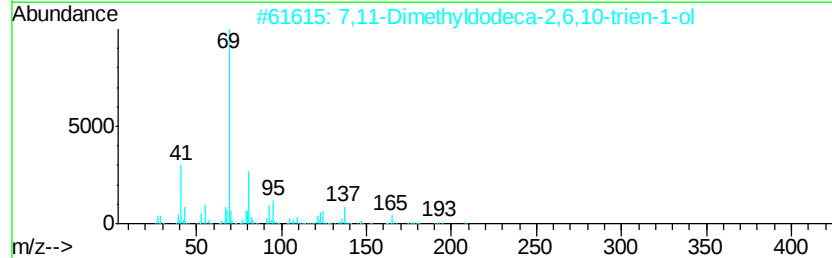
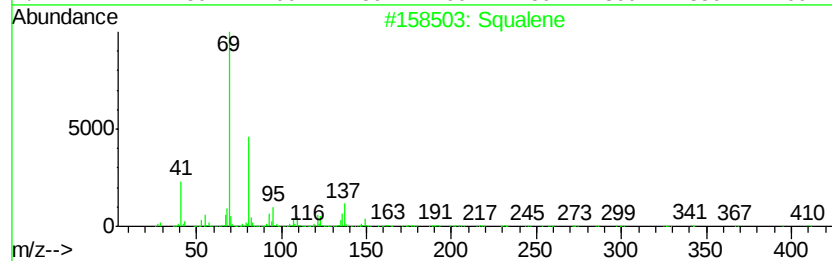
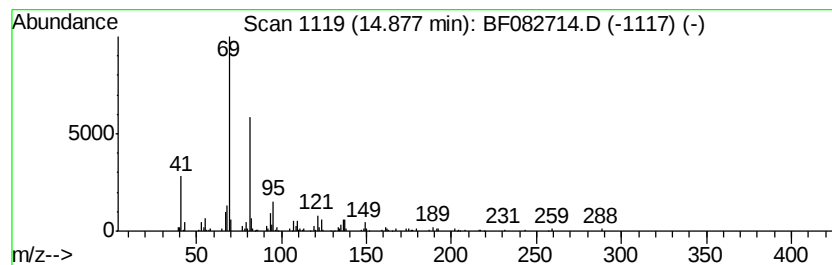
Instrument :
BNA_F
ClientSampleId :
SB-13(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	3.31 ng	200810	Perylene-d12	15.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	87
2	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	83
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	000106-28-5	80
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264 C17H28O2	004128-17-0	64
5	Propanoic acid, 2,2-dimethyl-, [...]	306 C20H34O2	1000164-38-8	64



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 Acq On : 4 Nov 2015 21:38
 Operator : UM/IZ
 Sample : G4241-09
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-13(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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...	5.06	50.4	ng	2971770	1	6.86	1178330	20.0
unknown6.64	6.64	112.1	ng	6603090	1	6.86	1178330	20.0
Nonane, 5-butyl-	10.82	4.2	ng	354533	4	11.38	1695770	20.0
Decane, 3,8-dimet...	11.26	2.5	ng	215432	4	11.38	1695770	20.0
n-Hexadecanoic acid	11.93	5.1	ng	435725	4	11.38	1695770	20.0
9-Octadecenamide,...	13.46	2.6	ng	230486	5	14.02	1776930	20.0
Bromoacetic acid,...	13.87	6.2	ng	554755	5	14.02	1776930	20.0
Squalene	14.88	3.3	ng	200810	6	15.45	1213630	20.0